



Full wwPDB EM Validation Report ⓘ

Dec 12, 2022 – 08:45 pm GMT

PDB ID : 6QVK
EMDB ID : EMD-4655
Title : The cryo-EM structure of bacteriophage phi29 prohead
Authors : Xu, J.; Gui, M.; Xiang, Y.
Deposited on : 2019-03-03
Resolution : 3.60 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:

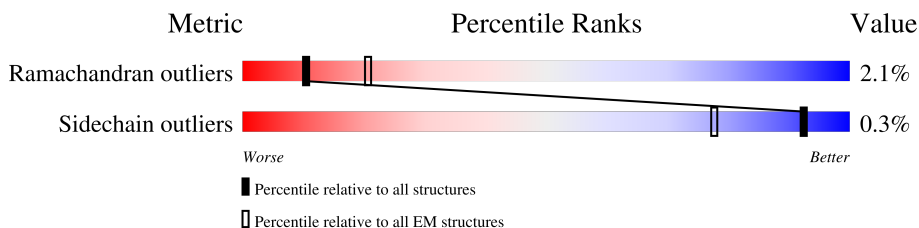
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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 3.60 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	24% (red), 94% (green), 2% (yellow), 2% (grey)
1	1B	448	12% (red), 96% (green), 2% (yellow), 2% (grey)
1	1C	448	12% (red), 96% (green), 2% (yellow), 2% (grey)
1	1D	448	10% (red), 96% (green), 2% (yellow), 2% (grey)
1	1E	448	12% (red), 94% (green), 2% (yellow), 2% (grey)
1	1F	448	23% (red), 96% (green), 2% (yellow), 2% (grey)
1	1G	448	24% (red), 94% (green), 2% (yellow), 2% (grey)
1	1H	448	12% (red), 96% (green), 2% (yellow), 2% (grey)
1	1I	448	11% (red), 96% (green), 2% (yellow), 2% (grey)

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Mol	Chain	Length	Quality of chain
1	1J	448	10% 97%
1	1K	448	12% 94%
1	1L	448	23% 96%
1	1M	448	24% 94%
1	1N	448	13% 96%
1	1O	448	13% 96%
1	1P	448	10% 97%
1	1Q	448	12% 94%
1	1R	448	24% 96%
1	1S	448	23% 94%
1	1T	448	12% 96%
1	1U	448	11% 96%
1	1V	448	10% 96%
1	1W	448	12% 94%
1	1X	448	24% 96%
1	1Y	448	24% 94%
1	1Z	448	12% 96%
1	1a	448	12% 96%
1	1b	448	9% 97%
1	1c	448	13% 94%
1	1d	448	24% 96%
1	2A	448	12% 96%
1	2B	448	12% 96%
1	2C	448	14% 97%
1	2D	448	14% 97%

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Mol	Chain	Length	Quality of chain
1	2E	448	13% 96%
1	2F	448	12% 96%
1	2G	448	12% 96%
1	2H	448	12% 97%
1	2I	448	15% 97%
1	2J	448	14% 96%
1	2K	448	12% 96%
1	2L	448	11% 96%
1	2M	448	14% 97%
1	2N	448	14% 97%
1	2O	448	13% 96%
1	2P	448	12% 96%
1	2Q	448	10% 96%
1	2R	448	13% 97%
1	2S	448	14% 97%
1	2T	448	13% 96%
1	2U	448	11% 96%
1	2V	448	12% 96%
1	2W	448	14% 97%
1	2X	448	15% 97%
1	2Y	448	13% 96%
1	3A	448	7% 93%
1	3B	448	6% 94%
1	3C	448	7% 96%
1	3D	448	8% 94% 5%

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Mol	Chain	Length	Quality of chain
1	3E	448	8% 97%
1	3F	448	8% 96%
1	3G	448	7% 93%
1	3H	448	7% 94%
1	3I	448	7% 96%
1	3J	448	9% 94%
1	3K	448	8% 97%
1	3L	448	9% 96%
1	3M	448	7% 93%
1	3N	448	6% 94%
1	3O	448	7% 96%
1	3P	448	9% 94%
1	3Q	448	8% 97%
1	3R	448	9% 96%
1	3S	448	7% 93%
1	3T	448	6% 94%
1	3U	448	7% 96%
1	3V	448	8% 94%
1	3W	448	8% 97%
1	3X	448	9% 96%
1	3Y	448	8% 93%
1	3Z	448	7% 94%
1	3a	448	6% 96%
1	3b	448	8% 94%
1	3c	448	8% 97%

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Mol	Chain	Length	Quality of chain
1	3d	448	8% 96%
1	4A	448	7% 96%
1	4B	448	6% 92% 5%
1	4C	448	6% 94%
1	4D	448	96%
1	4E	448	8% 96%
1	4F	448	8% 96%
1	4G	448	7% 96%
1	4H	448	8% 92% 5%
1	4I	448	5% 94%
1	4J	448	96%
1	4K	448	7% 96%
1	4L	448	8% 96%
1	4M	448	6% 96%
1	4N	448	6% 92% 5%
1	4O	448	5% 94%
1	4P	448	96%
1	4Q	448	7% 96%
1	4R	448	8% 96%
1	4S	448	6% 96%
1	4T	448	6% 92% 5%
1	4U	448	5% 94%
1	4V	448	96%
1	4W	448	7% 96%
1	4X	448	8% 96%

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Mol	Chain	Length	Quality of chain
1	4Y	448	7% 96%
1	4Z	448	6% 92% 5%
1	4a	448	5% 94%
1	4b	448	• 95%
1	4c	448	6% 96%
1	4d	448	7% 96%
1	5A	448	10% 94%
1	5B	448	6% 93%
1	5C	448	5% 92% 5%
1	5D	448	• 95%
1	5E	448	10% 95%
1	5F	448	13% 96%
1	5G	448	10% 94%
1	5H	448	6% 93%
1	5I	448	5% 92% 5%
1	5J	448	• 95%
1	5K	448	10% 95%
1	5L	448	12% 95%
1	5M	448	9% 94%
1	5N	448	6% 93%
1	5O	448	5% 92% 5%
1	5P	448	• 95%
1	5Q	448	10% 95%
1	5R	448	13% 96%
1	5S	448	9% 94%

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Mol	Chain	Length	Quality of chain
1	5T	448	6% 93%
1	5U	448	5% 92% 5%
1	5V	448	95%
1	5W	448	10% 95%
1	5X	448	14% 96%
1	5Y	448	10% 94%
1	5Z	448	6% 93%
1	5a	448	5% 92% 5%
1	5b	448	95%
1	5c	448	10% 95%
1	5d	448	13% 96%
1	6A	448	17% 98%
1	6B	448	12% 96%
1	6C	448	11% 95%
1	6D	448	9% 94%
1	6E	448	8% 96%
1	6F	448	12% 95%
1	6G	448	16% 98%
1	6H	448	12% 96%
1	6I	448	11% 95%
1	6J	448	9% 94%
1	6K	448	8% 96%
1	6L	448	12% 95%
1	6M	448	16% 98%
1	6N	448	13% 96%

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Mol	Chain	Length	Quality of chain
1	6O	448	11% 95%
1	6P	448	9% 94%
1	6Q	448	8% 96%
1	6R	448	12% 95%
1	6S	448	16% 98%
1	6T	448	13% 96%
1	6U	448	11% 95%
1	6V	448	9% 94%
1	6W	448	8% 96%
1	6X	448	12% 95%
1	6Y	448	16% 98%
1	6Z	448	12% 96%
1	6a	448	11% 95%
1	6b	448	9% 94%
1	6c	448	8% 96%
1	6d	448	12% 95%
1	7A	448	29% 97%
1	7B	448	26% 98%
1	7C	448	27% 96%
1	7D	448	25% 95%
1	7E	448	28% 98%
1	7F	448	31% 97%
1	7G	448	27% 98%
1	7H	448	26% 96%
1	7I	448	25% 95%

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Mol	Chain	Length	Quality of chain
1	7J	448	27% 98%
1	7K	448	30% 97%
1	7L	448	29% 98%
1	7M	448	26% 96%
1	7N	448	25% 95%
1	7O	448	28% 98%
1	7P	448	33% 97%
1	7Q	448	29% 98%
1	7R	448	27% 96%
1	7S	448	25% 95%
1	7T	448	29% 98%
1	7U	448	31% 97%
1	7V	448	27% 98%
1	7W	448	27% 96%
1	7X	448	25% 95%
1	7Y	448	27% 98%
1	8A	448	21% 96%
1	8B	448	22% 96%
1	8C	448	19% 97%
1	8D	448	20% 98%
1	8E	448	20% 96%
1	8F	448	22% 98%
1	8G	448	20% 96%
1	8H	448	23% 96%
1	8I	448	19% 97%

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Mol	Chain	Length	Quality of chain
1	8J	448	20% 98%
1	8K	448	20% 96%
1	8L	448	22% 98%
1	8M	448	20% 96%
1	8N	448	25% 96%
1	8O	448	19% 97%
1	8P	448	20% 98%
1	8Q	448	21% 96%
1	8R	448	22% 98%
1	8S	448	20% 96%
1	8T	448	24% 96%
1	8U	448	20% 97%
1	8V	448	19% 98%
1	8W	448	20% 96%
1	8X	448	22% 98%
1	8Y	448	21% 96%
1	8Z	448	23% 96%
1	8a	448	20% 97%
1	8b	448	19% 98%
1	8c	448	20% 96%
1	8d	448	22% 98%
1	9A	448	37% 98%
1	9B	448	37% 97%
1	9C	448	36% 98%
1	9D	448	36% 97%

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Mol	Chain	Length	Quality of chain
1	9E	448	37% 98% ..
2	1e	281	85% 97% .
2	1f	281	93% 96% ..
2	1g	281	82% 97% .
2	1h	281	78% 96% ..
2	1i	281	86% 97% .
2	1j	281	93% 96% ..
2	1k	281	81% 97% .
2	1l	281	78% 96% ..
2	1m	281	88% 97% .
2	1n	281	94% 96% ..
2	1o	281	84% 97% .
2	1p	281	79% 96% ..
2	1q	281	87% 97% .
2	1r	281	95% 96% ..
2	1s	281	83% 97% .
2	1t	281	79% 96% ..
2	1u	281	86% 97% .
2	1v	281	93% 96% ..
2	1w	281	83% 97% .
2	1x	281	79% 96% ..
2	2Z	281	78% 98% .
2	2a	281	91% 98% .
2	2b	281	79% 98% .
2	2c	281	97% 98% .

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Mol	Chain	Length	Quality of chain
2	2d	281	81% 98%
2	2e	281	78% 98%
2	2f	281	90% 98%
2	2g	281	78% 98%
2	2h	281	95% 98%
2	2i	281	80% 98%
2	2j	281	79% 98%
2	2k	281	90% 98%
2	2l	281	81% 98%
2	2m	281	96% 98%
2	2n	281	79% 98%
2	2o	281	78% 98%
2	2p	281	89% 98%
2	2q	281	80% 98%
2	2r	281	95% 98%
2	2s	281	81% 98%
2	2t	281	77% 98%
2	2u	281	86% 98%
2	2v	281	82% 98%
2	2w	281	96% 98%
2	2x	281	81% 98%
2	3e	281	84% 96%
2	3f	281	95% 97%
2	3g	281	81% 96%
2	3h	281	96% 97%

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Mol	Chain	Length	Quality of chain
2	3i	281	84% 96% ..
2	3j	281	94% 97% .
2	3k	281	81% 96% ..
2	3l	281	96% 97% .
2	3m	281	83% 96% ..
2	3n	281	94% 97% .
2	3o	281	80% 96% ..
2	3p	281	94% 97% .
2	3q	281	85% 96% ..
2	3r	281	95% 97% .
2	3s	281	77% 96% ..
2	3t	281	95% 97% .
2	3u	281	84% 96% ..
2	3v	281	95% 97% .
2	3w	281	78% 96% ..
2	3x	281	95% 97% .
2	4e	281	84% 97% .
2	4f	281	94% 96% ..
2	4g	281	84% 97% .
2	4h	281	93% 96% ..
2	4i	281	84% 97% .
2	4j	281	95% 96% ..
2	4k	281	84% 97% .
2	4l	281	94% 96% ..
2	4m	281	84% 97% .

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Mol	Chain	Length	Quality of chain
2	4n	281	95%
2	5e	281	96%
2	5f	281	95%
2	5g	281	97%
2	5h	281	99%
2	5i	281	96%
2	5j	281	97%
2	5k	281	97%
2	5l	281	98%
2	5m	281	96%
2	5n	281	97%
2	6e	281	96%
2	6f	281	100%
2	6g	281	97%
2	6h	281	96%
2	6i	281	99%
2	6j	281	97%
2	6k	281	97%
2	6l	281	96%
2	6m	281	99%
2	6n	281	97%
2	6o	281	97%
2	6p	281	96%
2	6q	281	96%
2	6r	281	99%

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Mol	Chain	Length	Quality of chain
2	6s	281	95%
2	6t	281	99%
2	6u	281	96%
2	6v	281	100%
2	6w	281	97%
2	6x	281	99%
2	7Z	281	94%
2	7a	281	99%
2	7b	281	97%
2	7c	281	99%
2	7d	281	97%
2	7e	281	92%
2	7f	281	98%
2	7g	281	96%
2	7h	281	99%
2	7i	281	96%
2	7j	281	92%
2	7k	281	98%
2	7l	281	95%
2	7m	281	99%
2	7n	281	96%
2	7o	281	94%
2	7p	281	98%
2	7q	281	97%
2	7r	281	100%

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Mol	Chain	Length	Quality of chain
2	7s	281	97% 98% .
2	7t	281	94% 98% .
2	7u	281	98% 98% .
2	7v	281	98% 98% .
2	7w	281	99% 98% .
2	7x	281	98% 98% .
2	8e	281	97% 96% ..
2	8f	281	99% 97% .
2	8g	281	98% 97% .
2	8h	281	98% 96% ..
2	8i	281	98% 97% .
2	8j	281	99% 96% ..
2	8k	281	98% 96% ..
2	8l	281	100% 97% .
2	8m	281	98% 97% .
2	8n	281	98% 96% ..
2	8o	281	97% 97% .
2	8p	281	98% 96% ..
2	8q	281	98% 96% ..
2	8r	281	99% 97% .
2	8s	281	98% 97% .
2	8t	281	99% 96% ..
2	8u	281	98% 97% .
2	8v	281	98% 96% ..
2	8w	281	98% 96% ..

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Mol	Chain	Length	Quality of chain
2	8x	281	99% 97% .
2	8y	281	99% 97% .
2	8z	281	98% 96% ..
2	9F	281	98% 98% .
2	9G	281	99% 98% .
2	9H	281	98% 98% .
2	9I	281	98% 98% .
2	9J	281	98% 98% .
2	9K	281	98% 97% .
2	9L	281	99% 96% ..
2	9M	281	99% 96% ..
2	9N	281	99% 97% .
2	9O	281	98% 97% .
2	9P	281	99% 96% ..
2	9Q	281	98% 97% .
2	9R	281	99% 96% ..

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 1161605 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Major capsid protein.

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 2 is a protein called Capsid fiber protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1e	280	Total 2106	C 1317	N 349	O 436	S 4	8	0
2	1f	279	Total 2098	C 1312	N 348	O 435	S 3	8	0
2	1g	280	Total 2106	C 1317	N 349	O 436	S 4	8	0
2	1h	279	Total 2098	C 1312	N 348	O 435	S 3	8	0
2	2Z	280	Total 2106	C 1317	N 349	O 436	S 4	8	0
2	2a	280	Total 2106	C 1317	N 349	O 436	S 4	8	0
2	2b	280	Total 2106	C 1317	N 349	O 436	S 4	8	0
2	2c	280	Total 2106	C 1317	N 349	O 436	S 4	8	0
2	2d	280	Total 2106	C 1317	N 349	O 436	S 4	8	0
2	3e	279	Total 2098	C 1312	N 348	O 435	S 3	8	0
2	3f	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	3g	279	Total 2098	C 1312	N 348	O 435	S 3	8	0
2	3h	280	Total 2106	C 1317	N 349	O 436	S 4	8	0
2	4e	280	Total 2106	C 1317	N 349	O 436	S 4	8	0
2	4f	279	Total 2098	C 1312	N 348	O 435	S 3	8	0
2	5e	280	Total 2106	C 1317	N 349	O 436	S 4	8	0
2	5f	279	Total 2098	C 1312	N 348	O 435	S 3	8	0
2	6e	279	Total 2098	C 1312	N 348	O 435	S 3	8	0
2	6f	280	Total 2106	C 1317	N 349	O 436	S 4	8	0
2	6g	279	Total 2098	C 1312	N 348	O 435	S 3	8	0
2	6h	280	Total 2106	C 1317	N 349	O 436	S 4	8	0
2	7Z	280	Total 2106	C 1317	N 349	O 436	S 4	8	0
2	7a	280	Total 2106	C 1317	N 349	O 436	S 4	8	0
2	7b	280	Total 2106	C 1317	N 349	O 436	S 4	8	0
2	7c	280	Total 2106	C 1317	N 349	O 436	S 4	8	0
2	7d	280	Total 2106	C 1317	N 349	O 436	S 4	8	0
2	8e	279	Total 2098	C 1312	N 348	O 435	S 3	8	0
2	8f	280	Total 2106	C 1317	N 349	O 436	S 4	8	0
2	8g	280	Total 2106	C 1317	N 349	O 436	S 4	8	0
2	8h	279	Total 2098	C 1312	N 348	O 435	S 3	8	0
2	8i	280	Total 2106	C 1317	N 349	O 436	S 4	8	0
2	8j	279	Total 2098	C 1312	N 348	O 435	S 3	8	0

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

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

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

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

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

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

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

There are 330 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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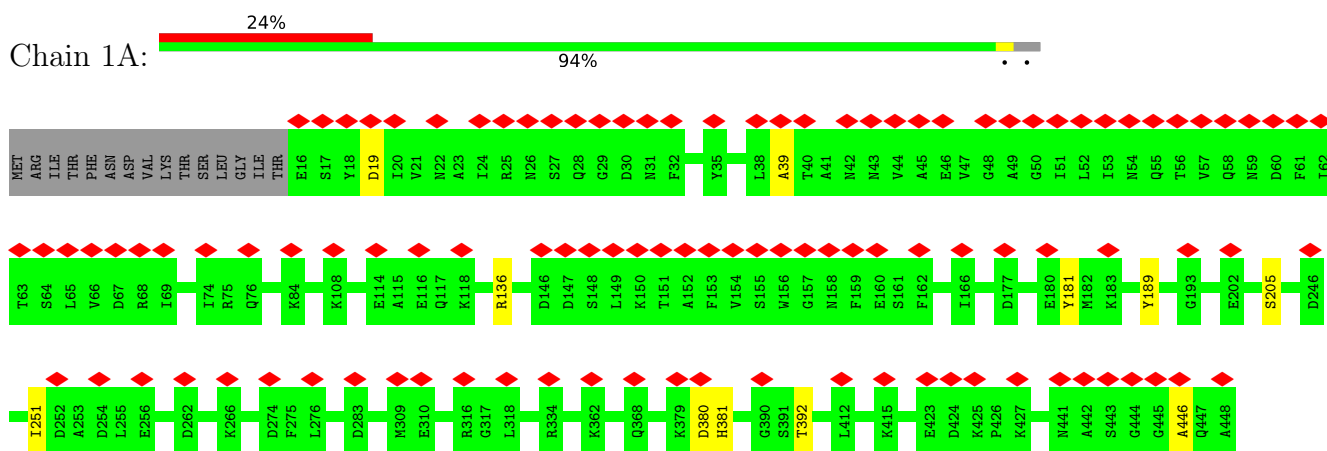
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Chain	Residue	Modelled	Actual	Comment	Reference
9N	281	LEU	-	insertion	UNP B3VMP4
9O	123	GLU	ASP	conflict	UNP B3VMP4
9O	281	LEU	-	insertion	UNP B3VMP4
9P	123	GLU	ASP	conflict	UNP B3VMP4
9P	281	LEU	-	insertion	UNP B3VMP4
9Q	123	GLU	ASP	conflict	UNP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

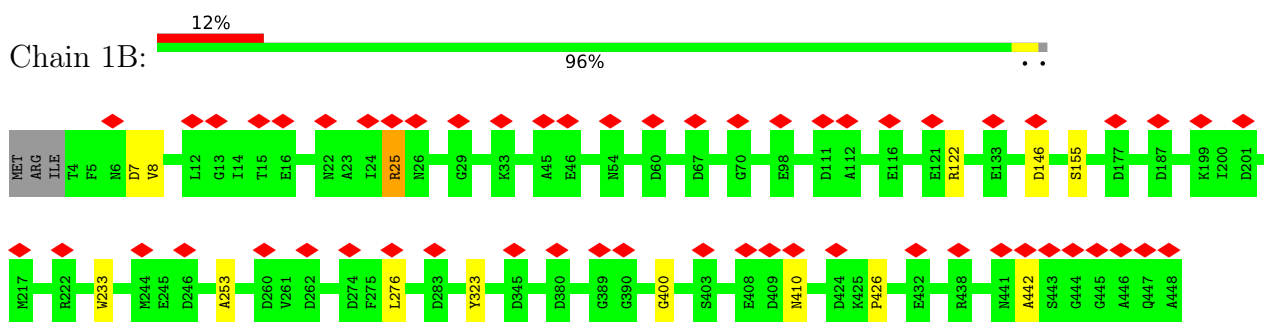
3 Residue-property plots

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

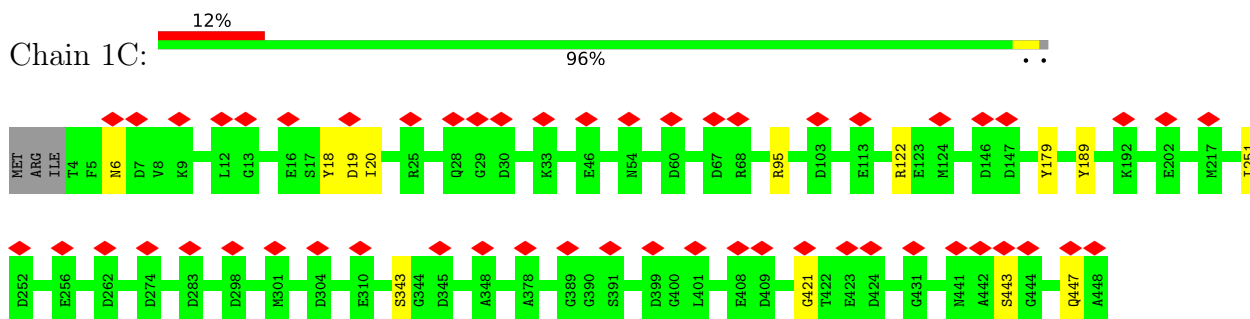
- Molecule 1: Major capsid protein



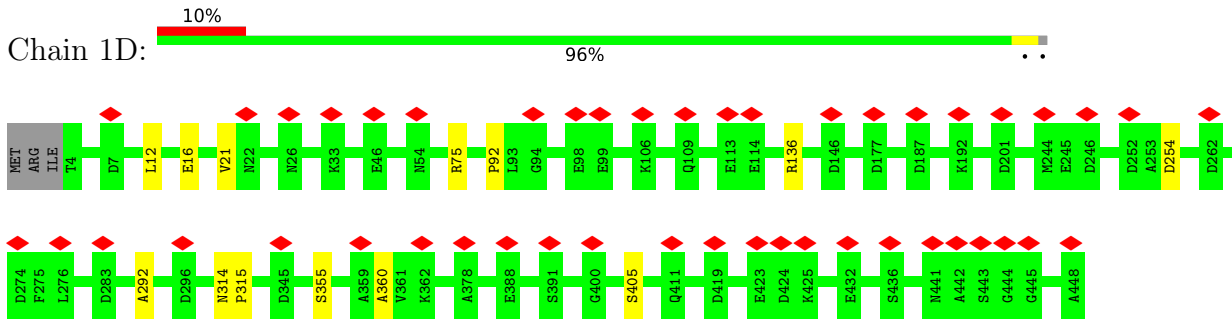
- Molecule 1: Major capsid protein



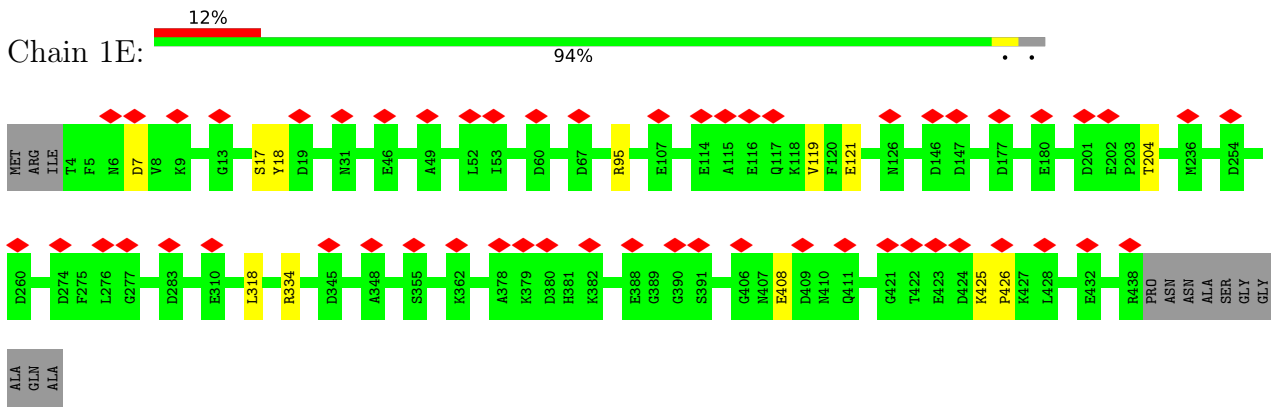
- Molecule 1: Major capsid protein



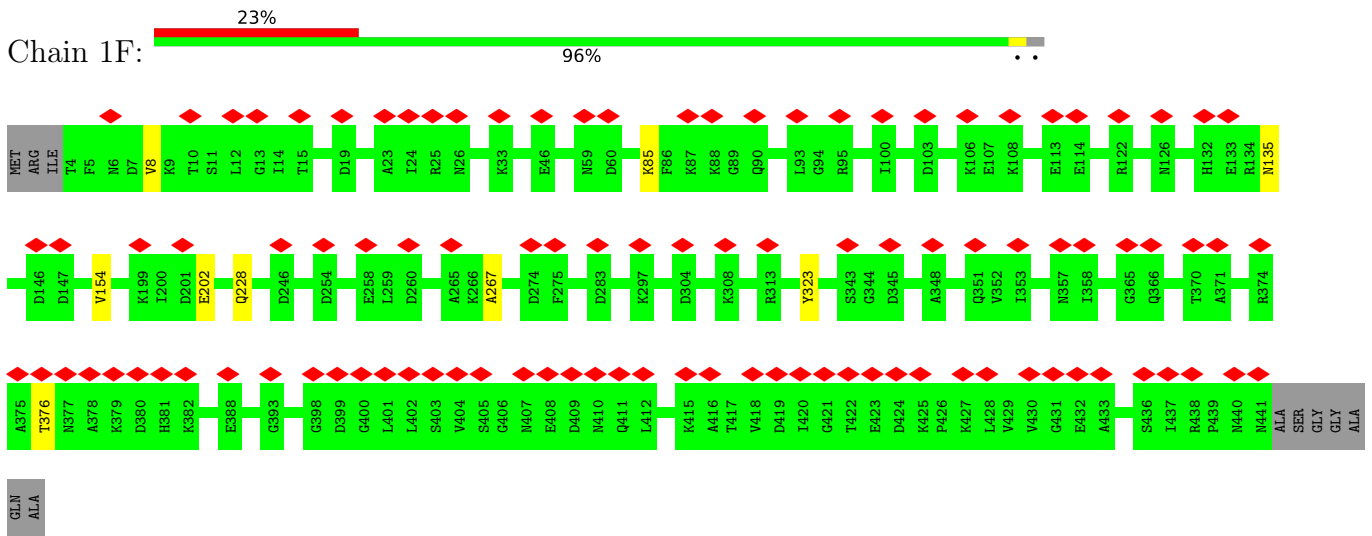
• Molecule 1: Major capsid protein



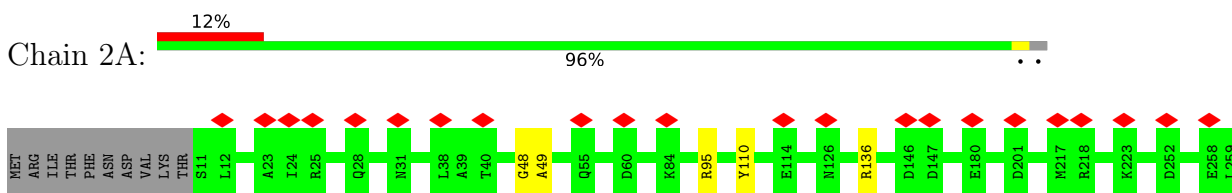
• Molecule 1: Major capsid protein



• Molecule 1: Major capsid protein

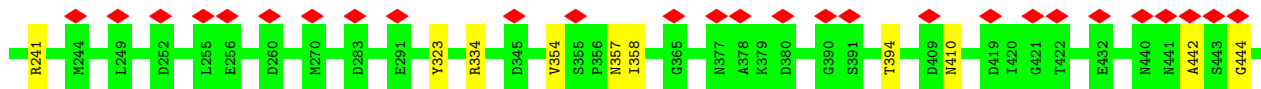
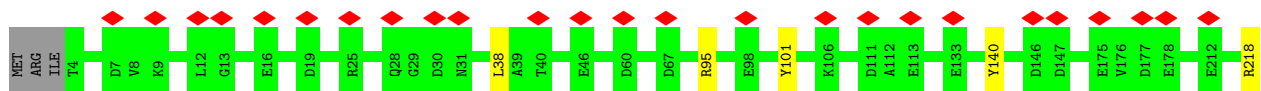


• Molecule 1: Major capsid protein

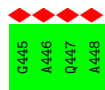
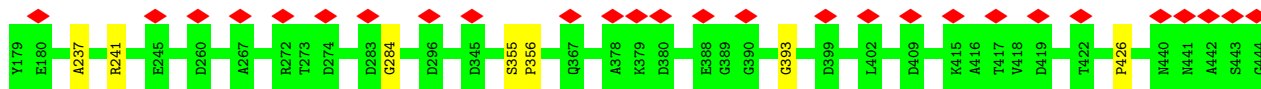
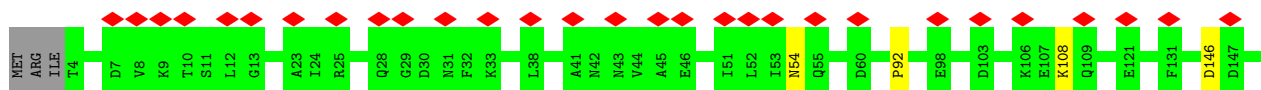




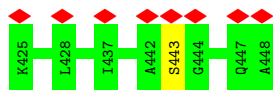
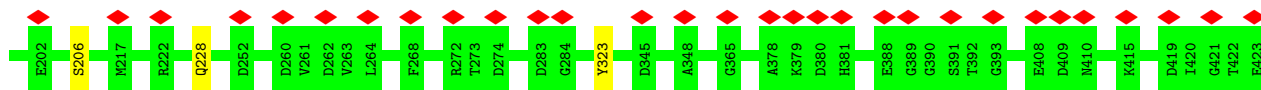
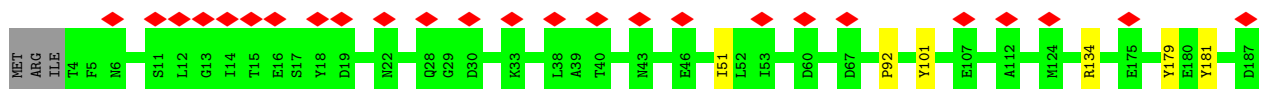
• Molecule 1: Major capsid protein



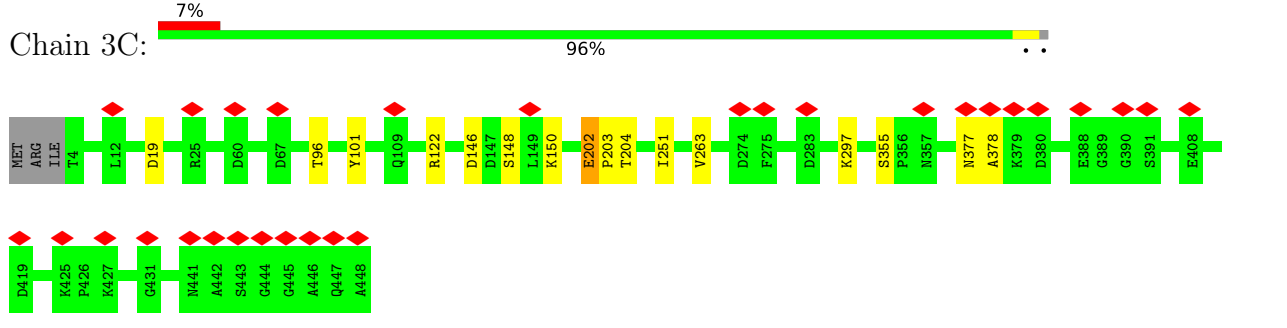
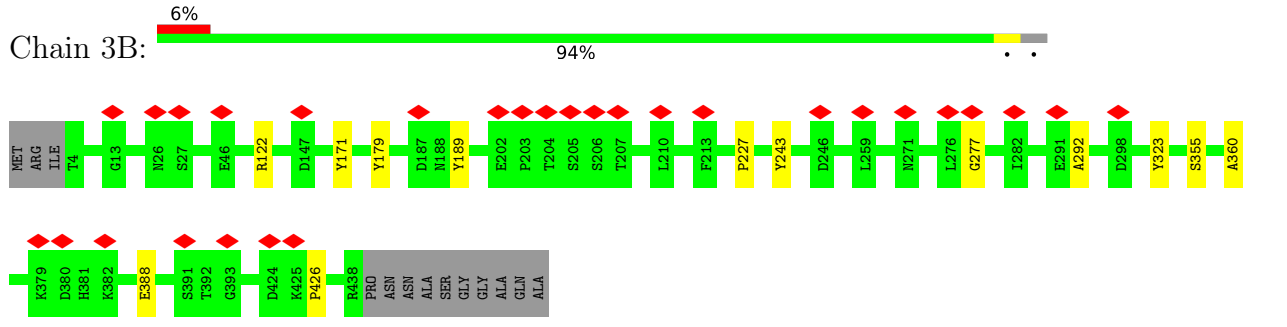
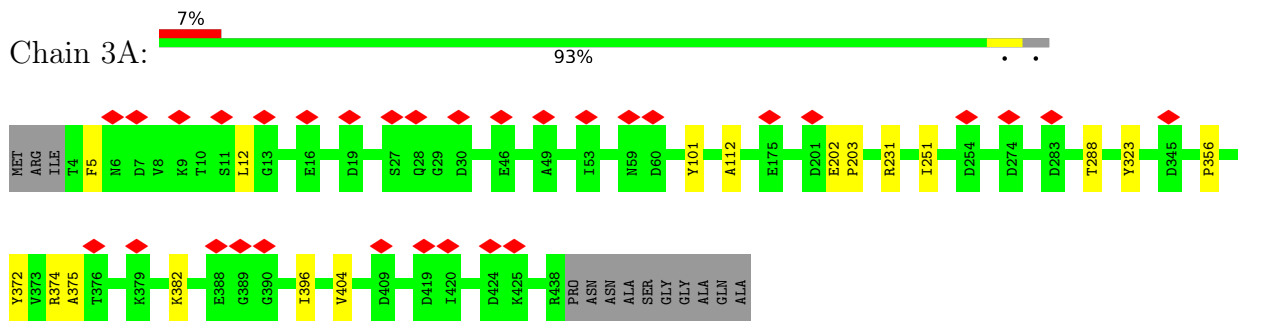
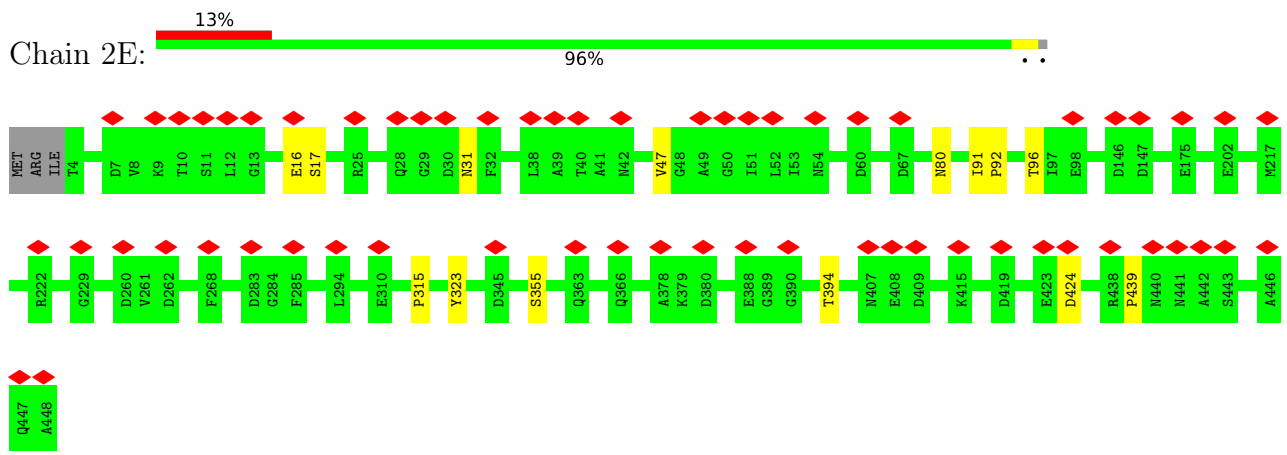
• Molecule 1: Major capsid protein

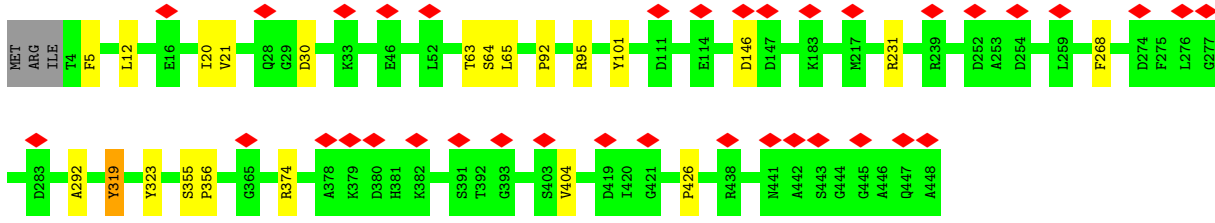


• Molecule 1: Major capsid protein

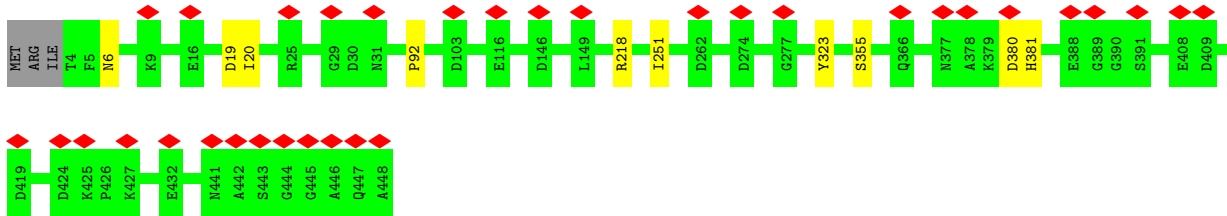


• Molecule 1: Major capsid protein

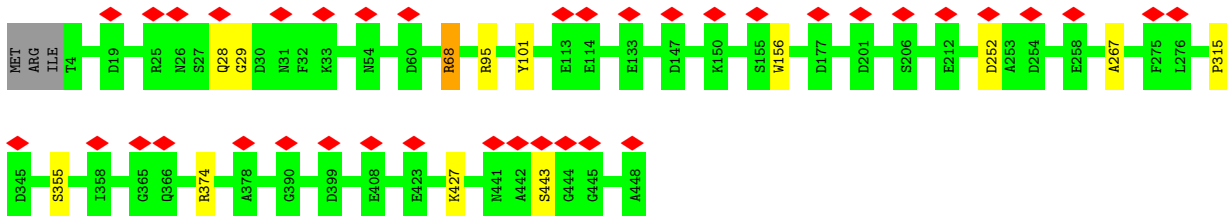




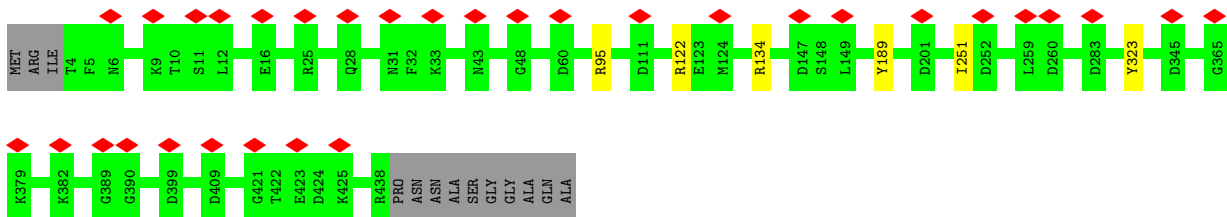
• Molecule 1: Major capsid protein



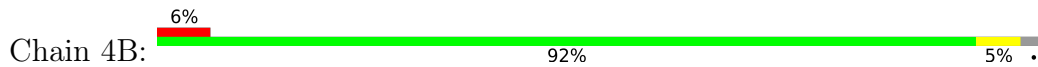
• Molecule 1: Major capsid protein

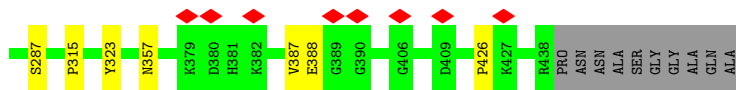


• Molecule 1: Major capsid protein

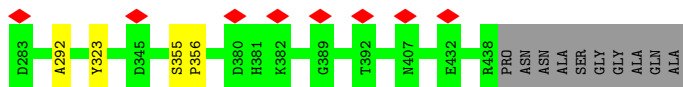
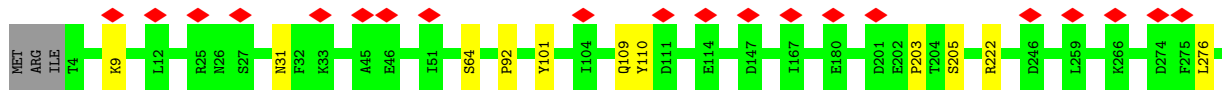


• Molecule 1: Major capsid protein





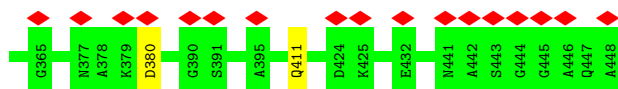
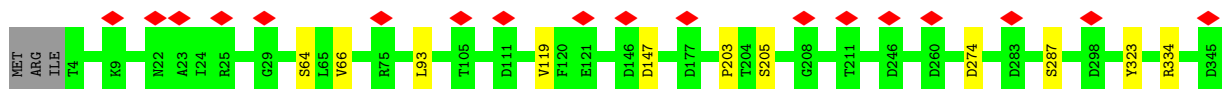
• Molecule 1: Major capsid protein



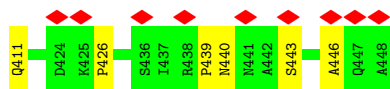
• Molecule 1: Major capsid protein



• Molecule 1: Major capsid protein

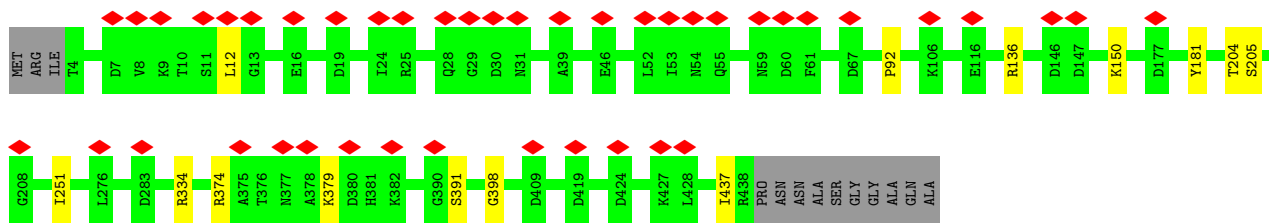


• Molecule 1: Major capsid protein

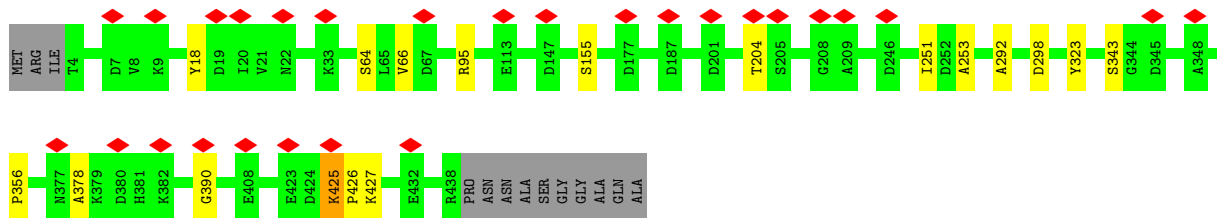


• Molecule 1: Major capsid protein

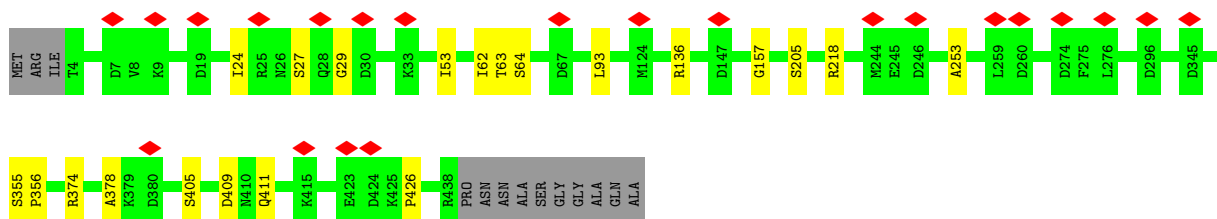




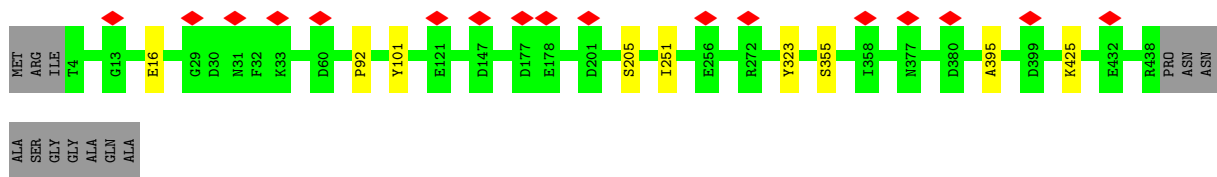
• Molecule 1: Major capsid protein



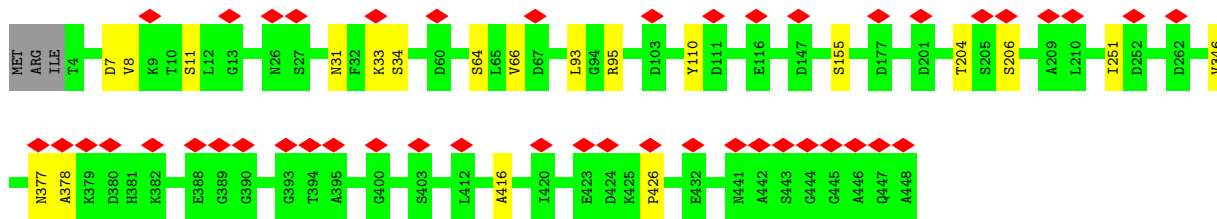
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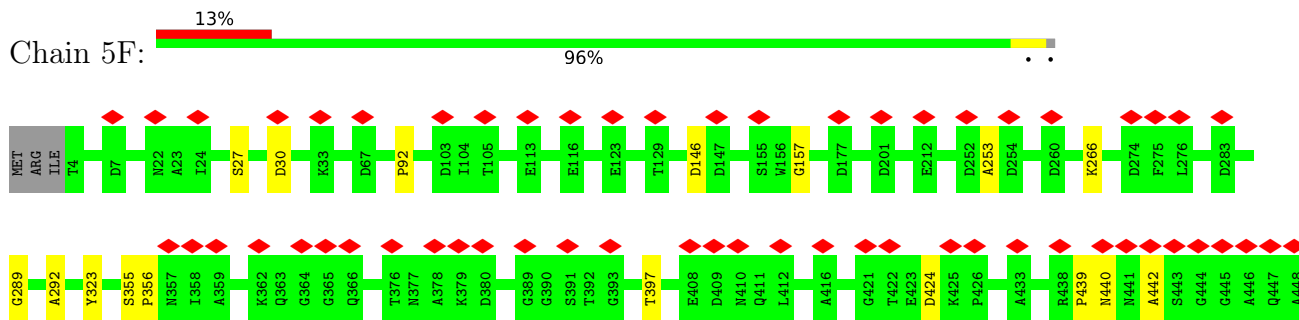
• Molecule 1: Major capsid protein



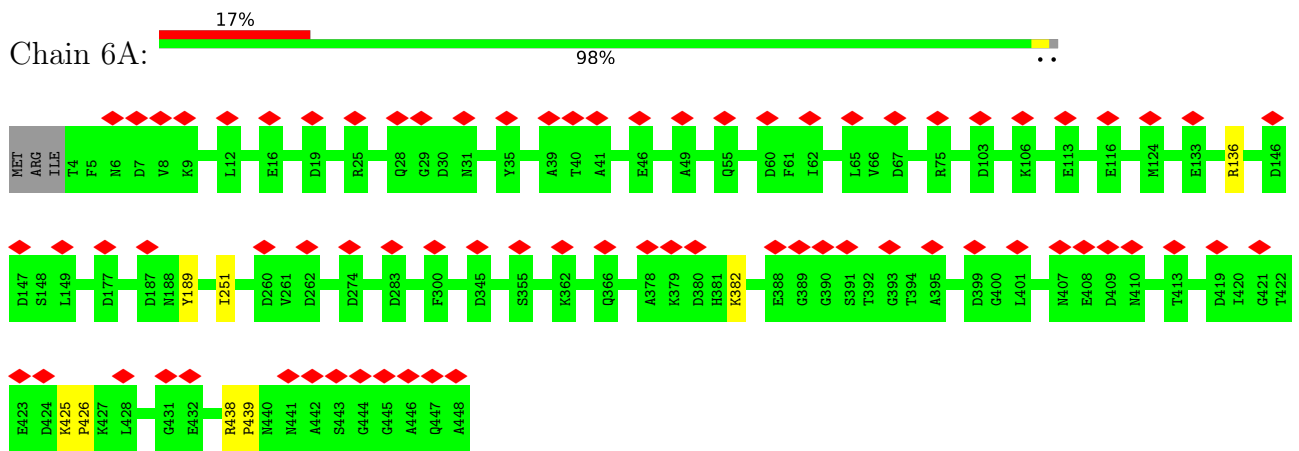
• Molecule 1: Major capsid protein



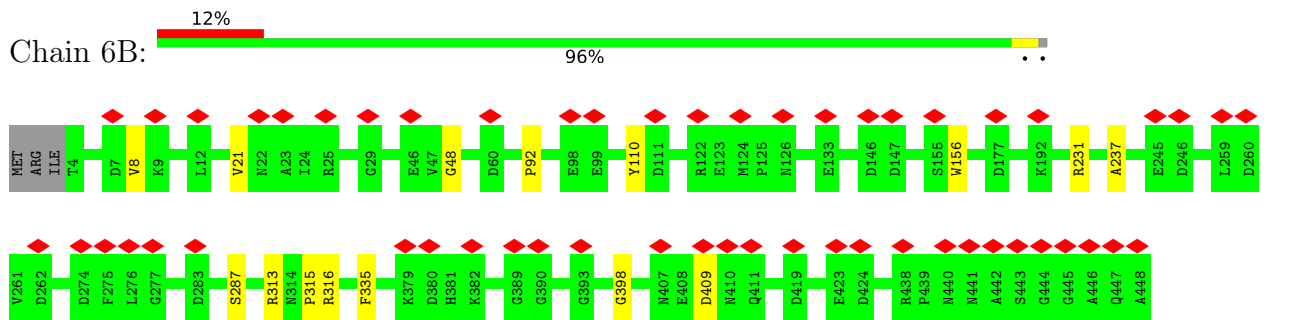
• Molecule 1: Major capsid protein



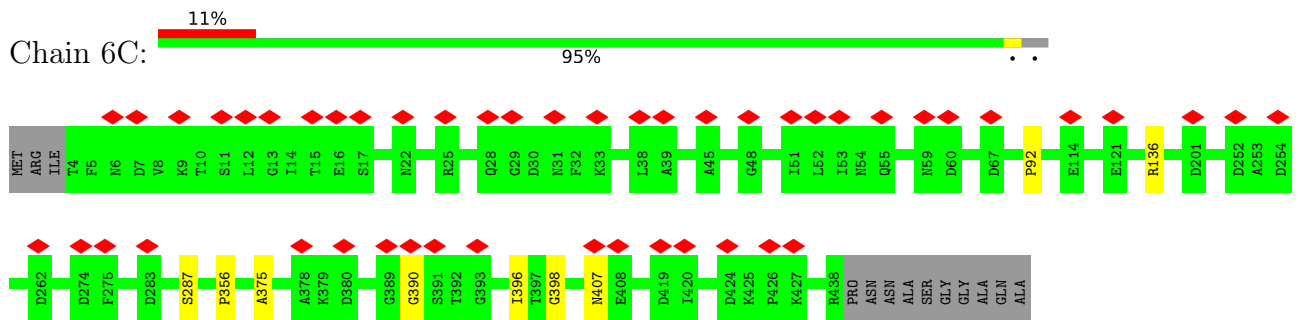
• Molecule 1: Major capsid protein



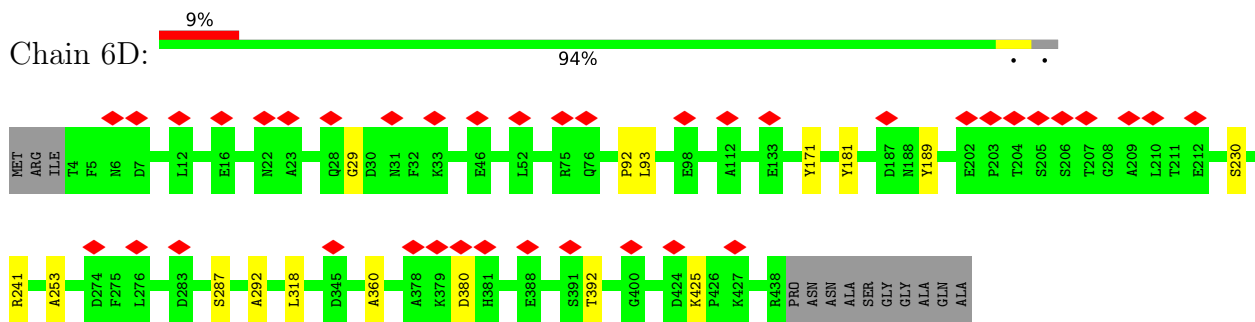
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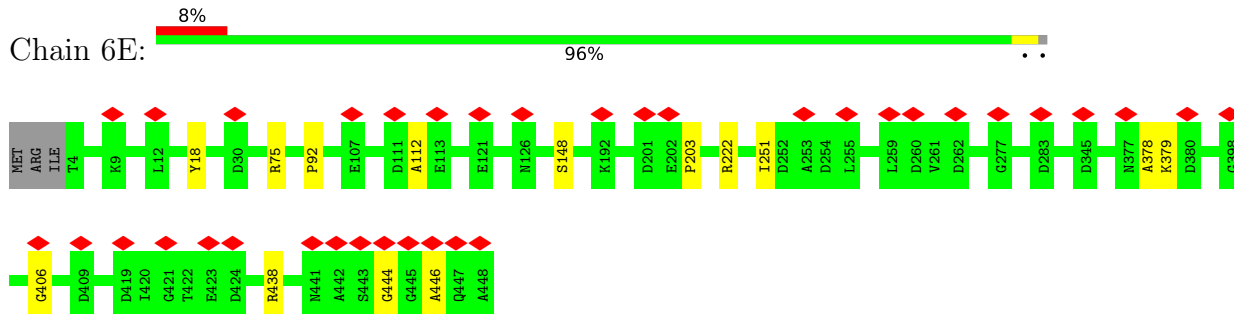
• Molecule 1: Major capsid protein



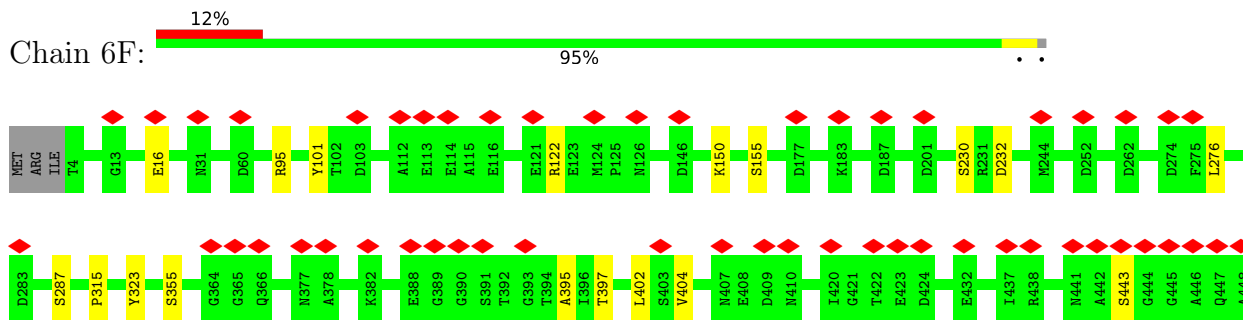
• Molecule 1: Major capsid protein



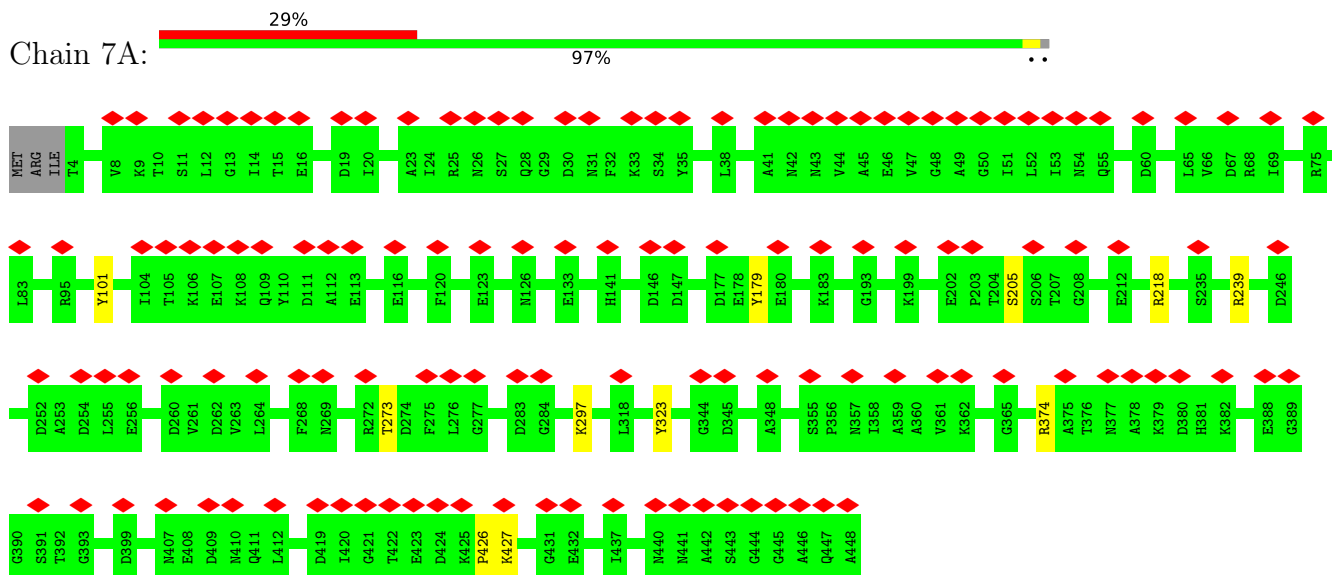
• Molecule 1: Major capsid protein



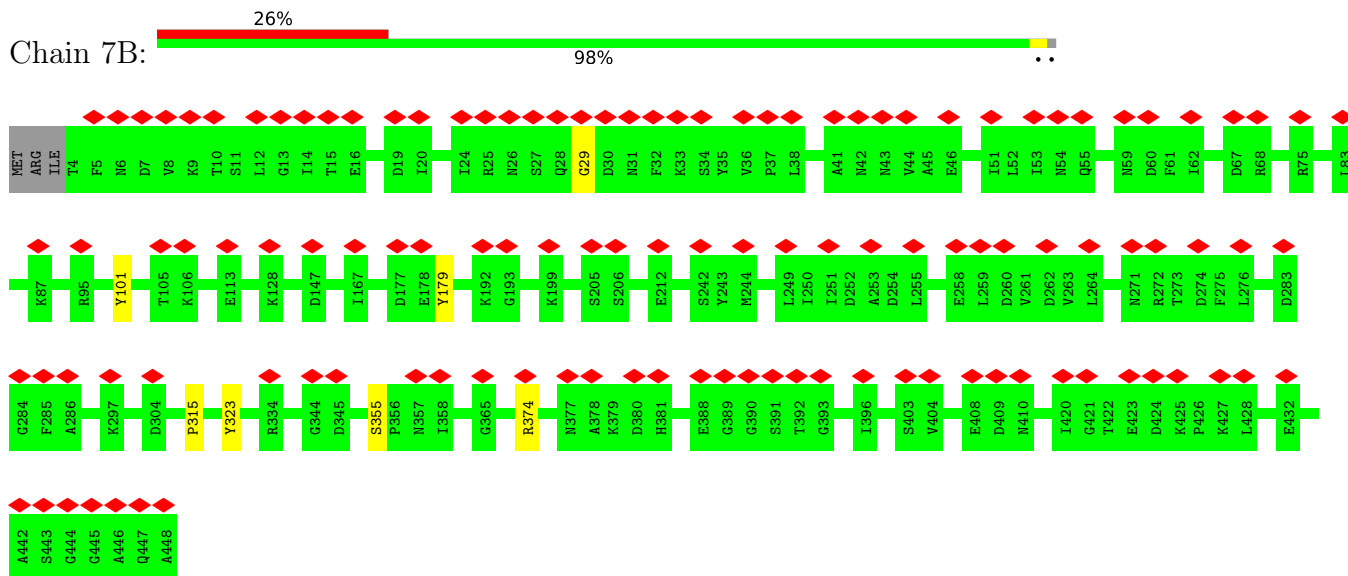
• Molecule 1: Major capsid protein



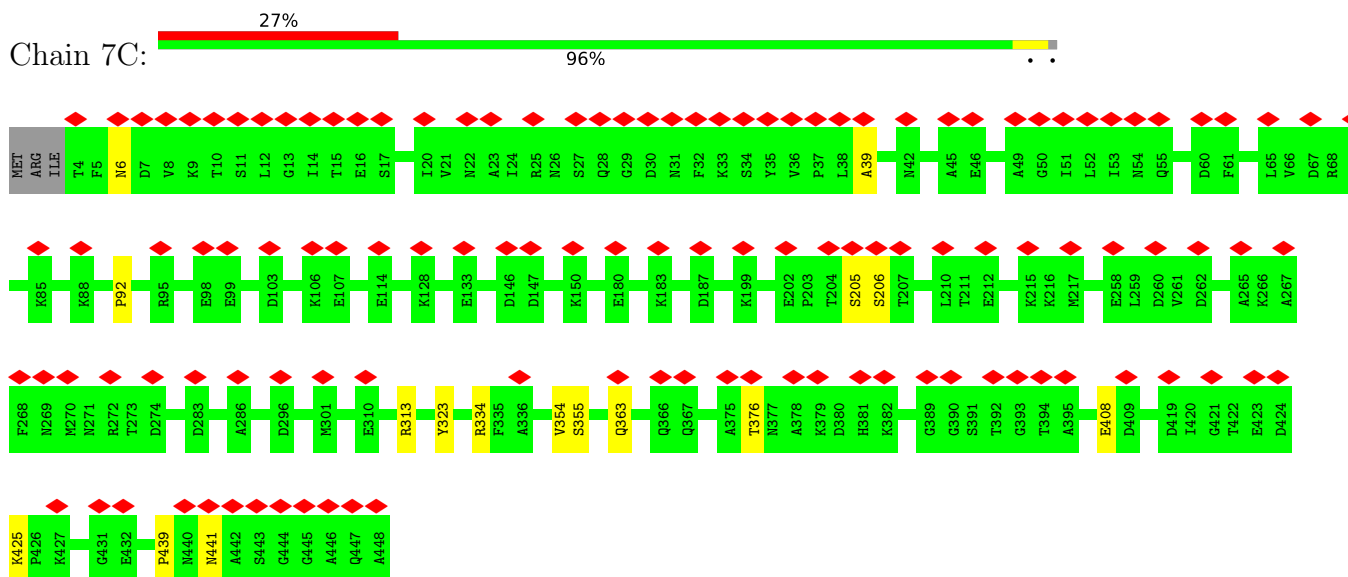
• Molecule 1: Major capsid protein



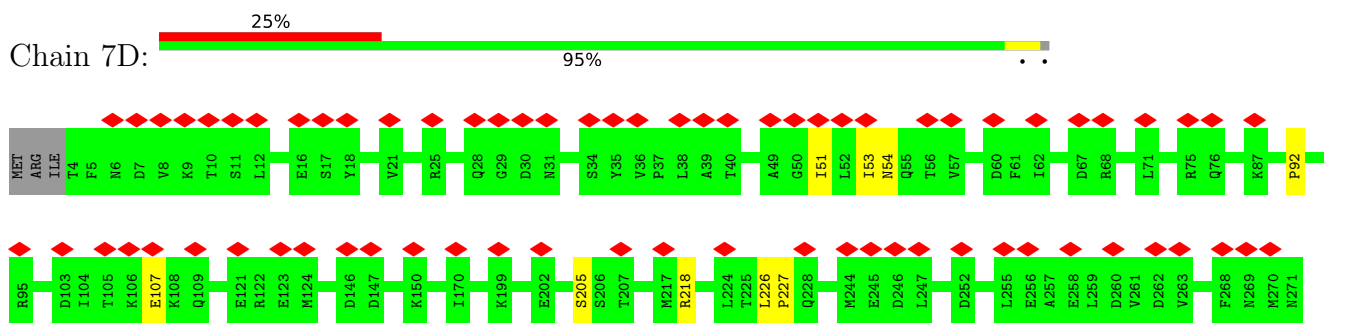
• Molecule 1: Major capsid protein

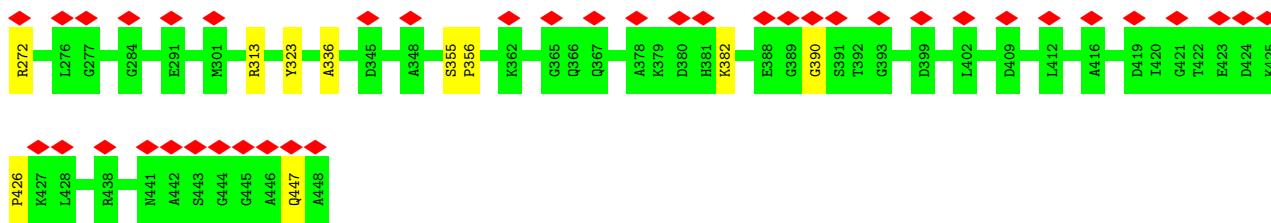


• Molecule 1: Major capsid protein

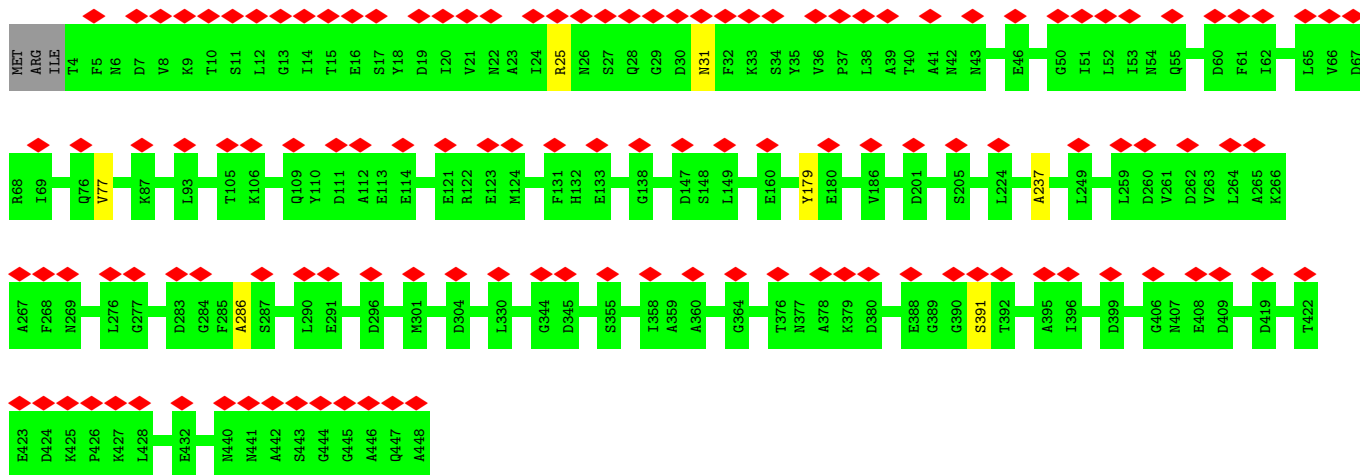


• Molecule 1: Major capsid protein

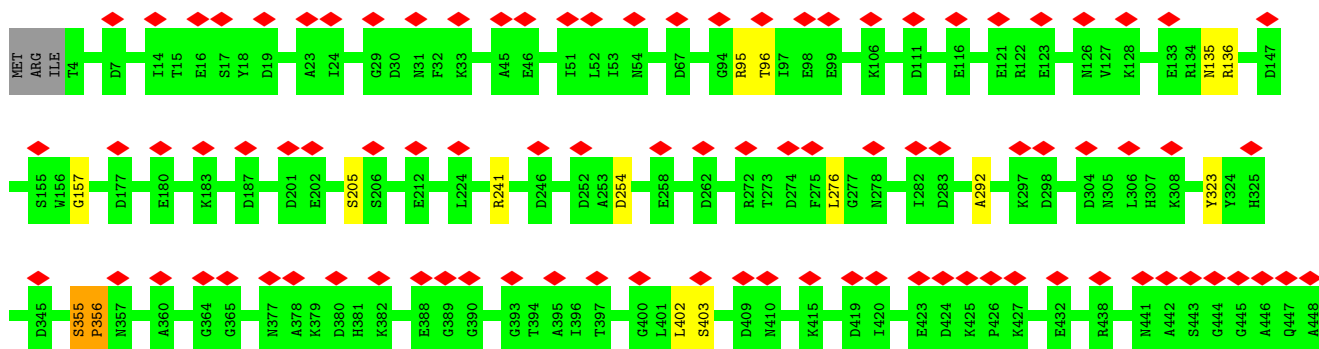




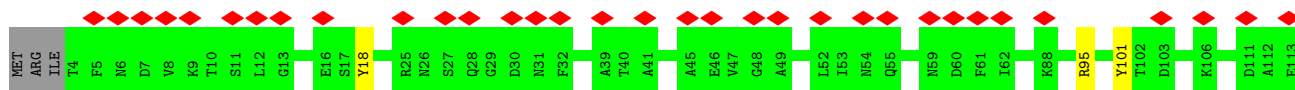
• Molecule 1: Major capsid protein

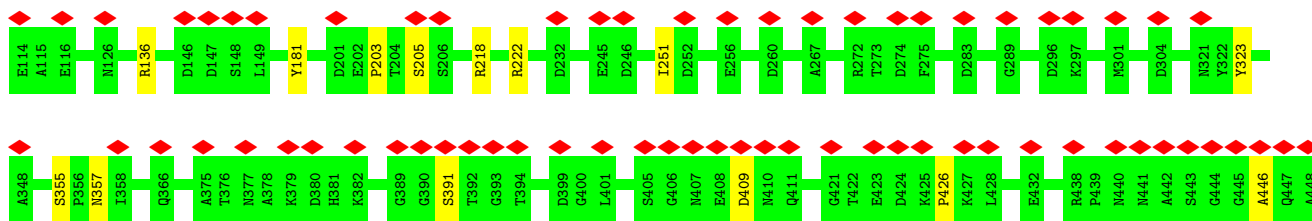


• Molecule 1: Major capsid protein

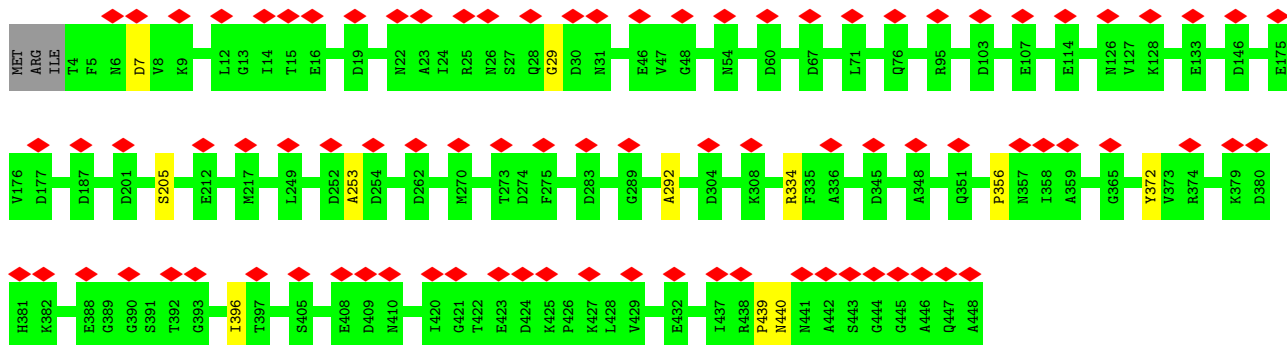


• Molecule 1: Major capsid protein

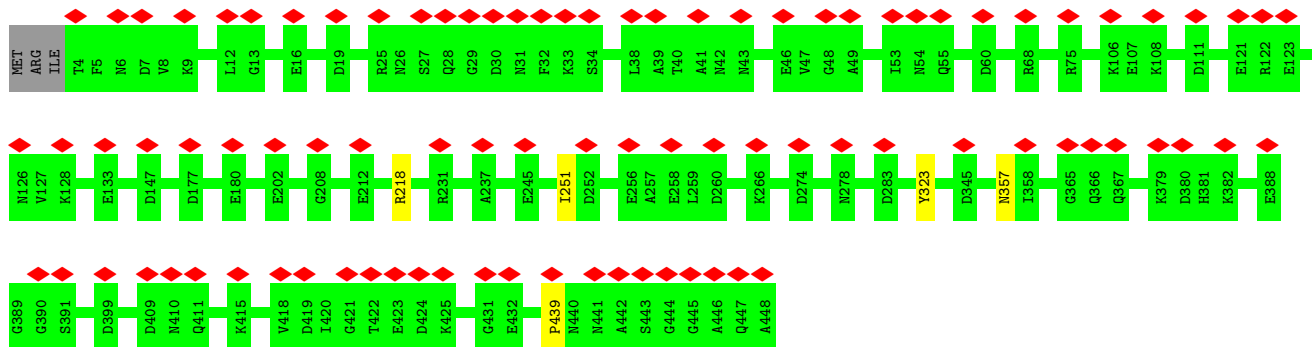




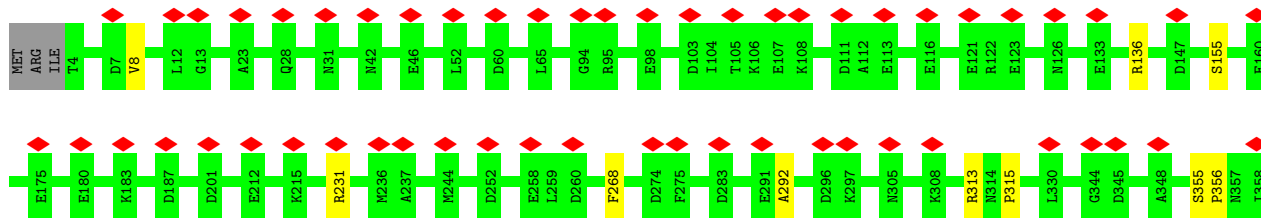
• Molecule 1: Major capsid protein



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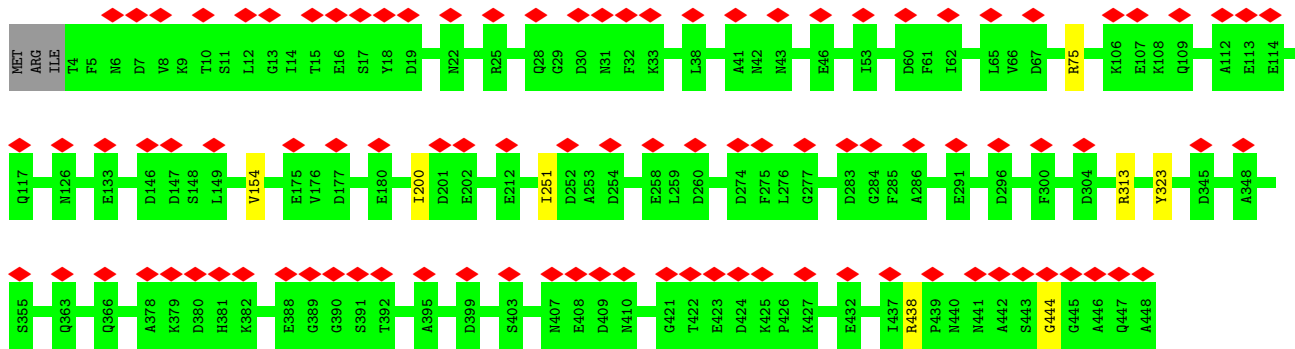


• Molecule 1: Major capsid protein

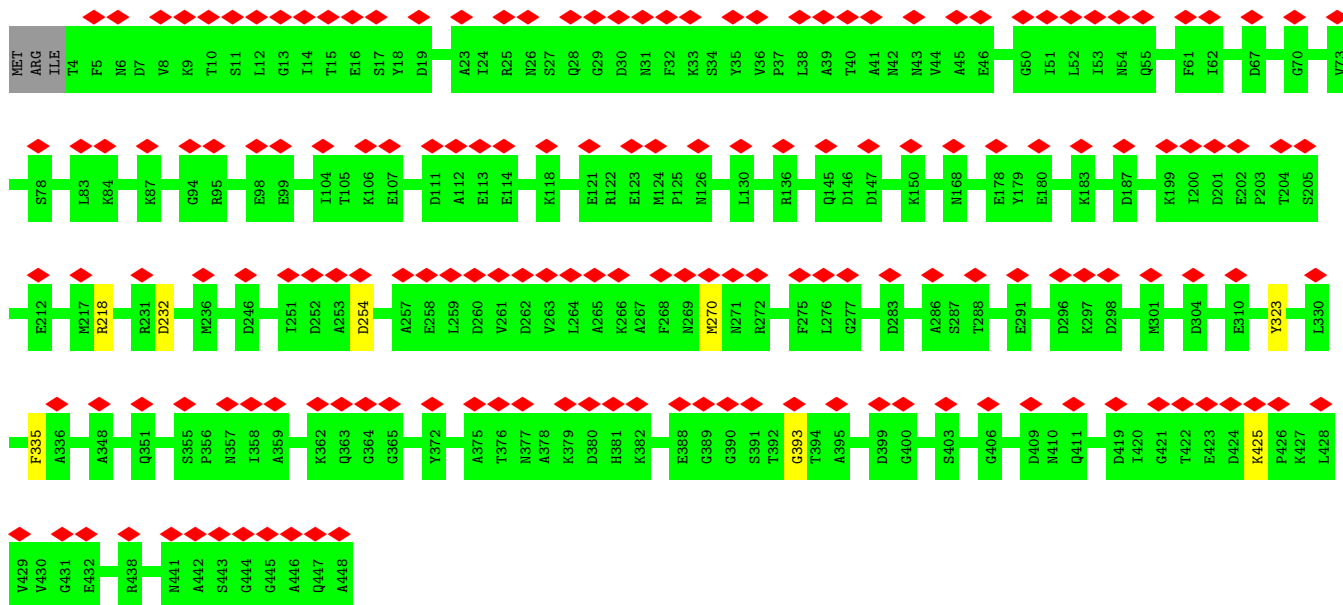




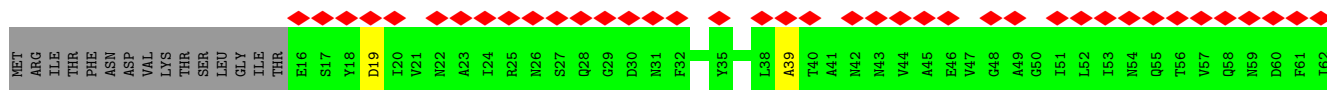
• Molecule 1: Major capsid protein

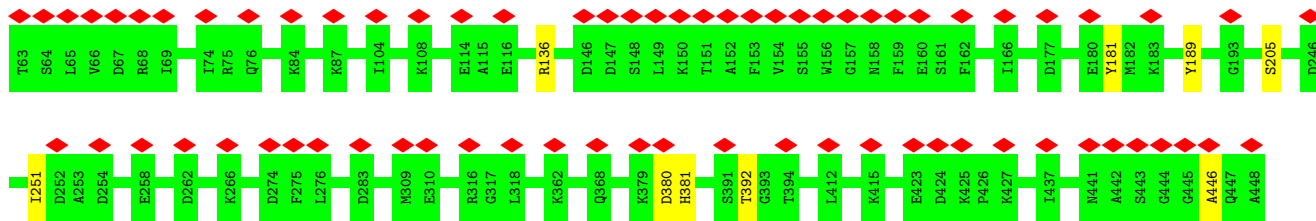


• Molecule 1: Major capsid protein

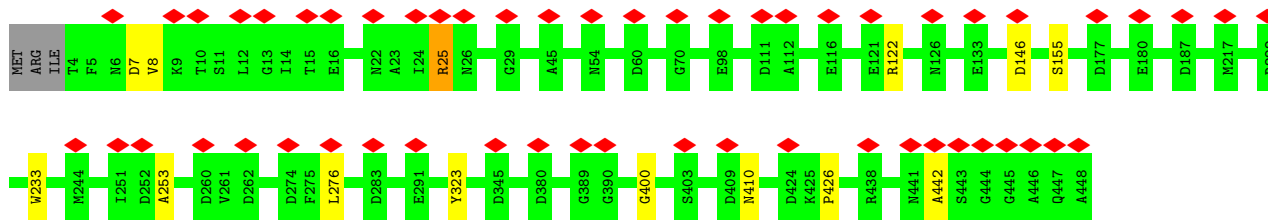


• Molecule 1: Major capsid protein

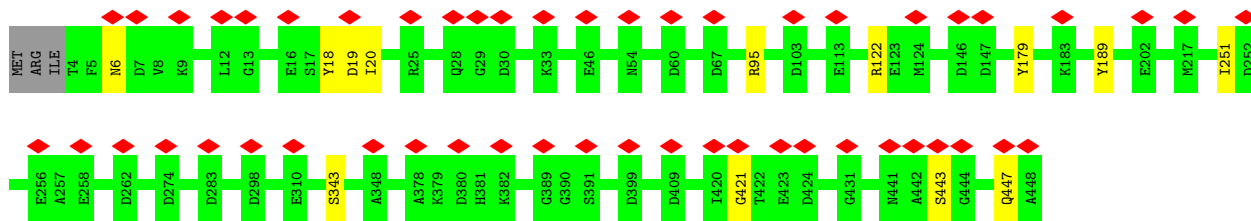




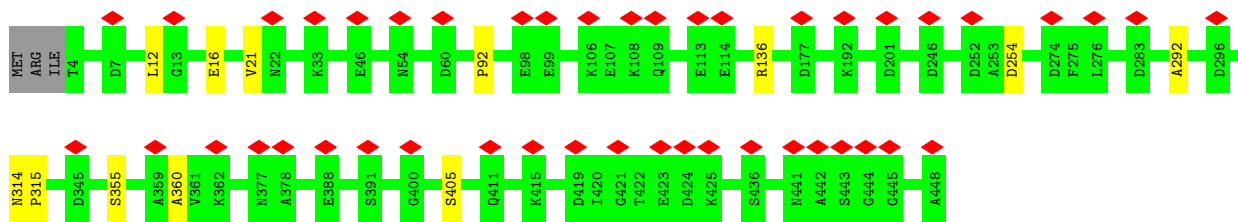
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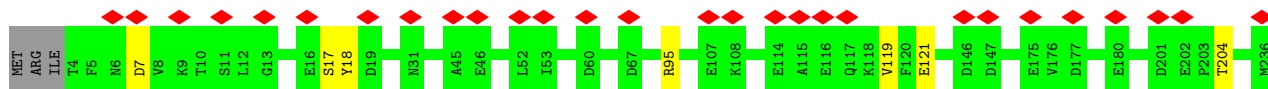
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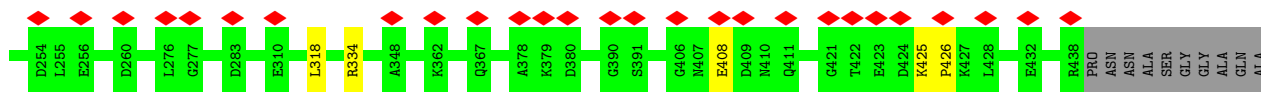


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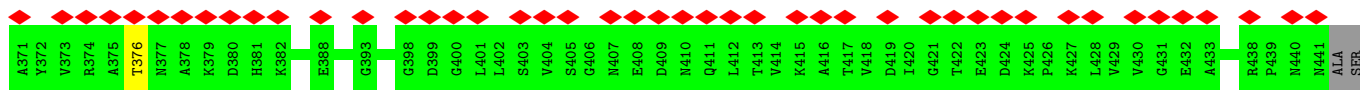
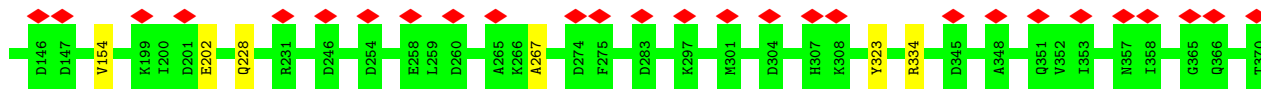
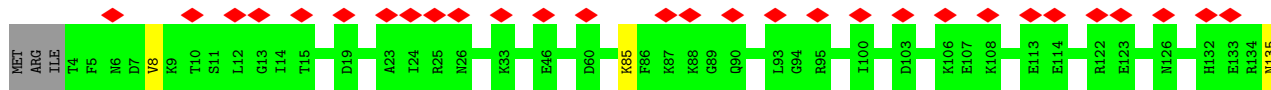


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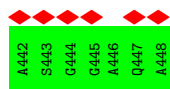
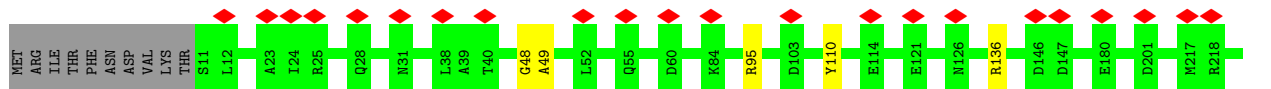


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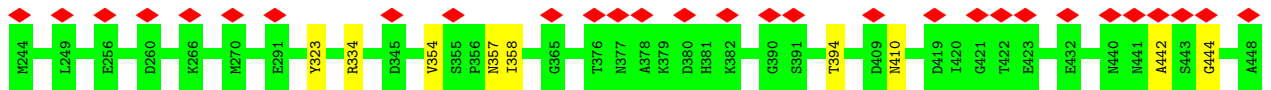
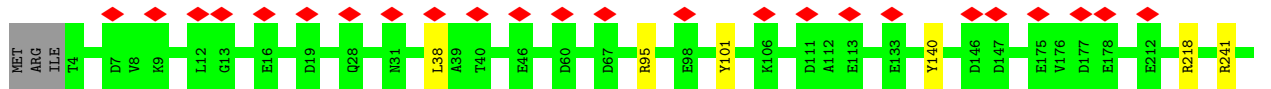


GLY
GLY
ALA
GLN
ALA

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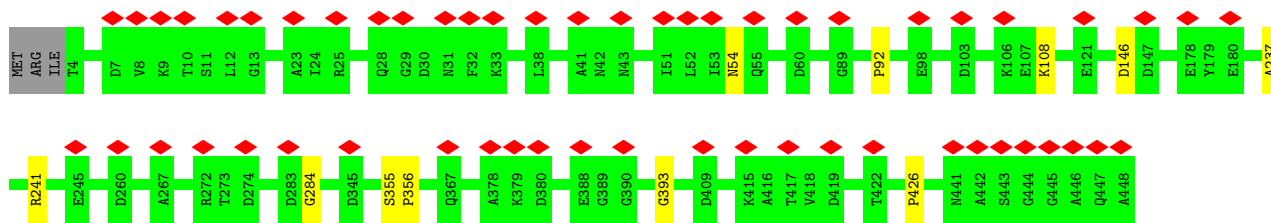


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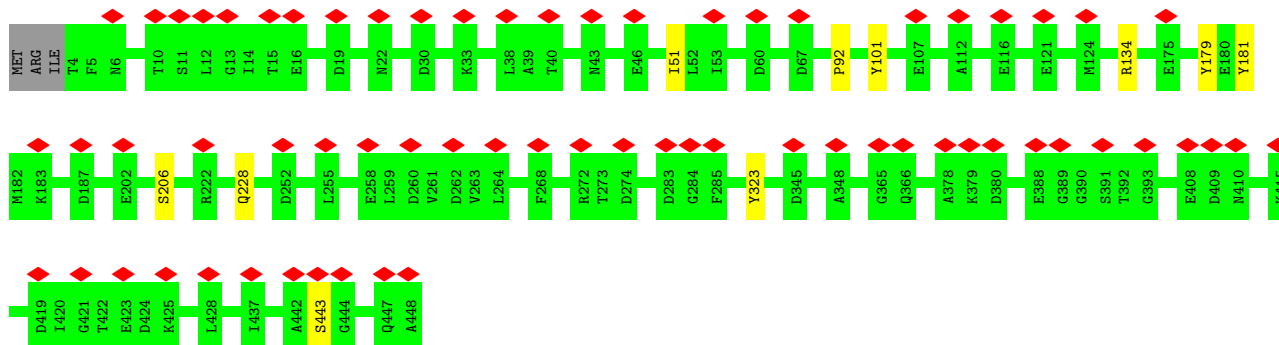


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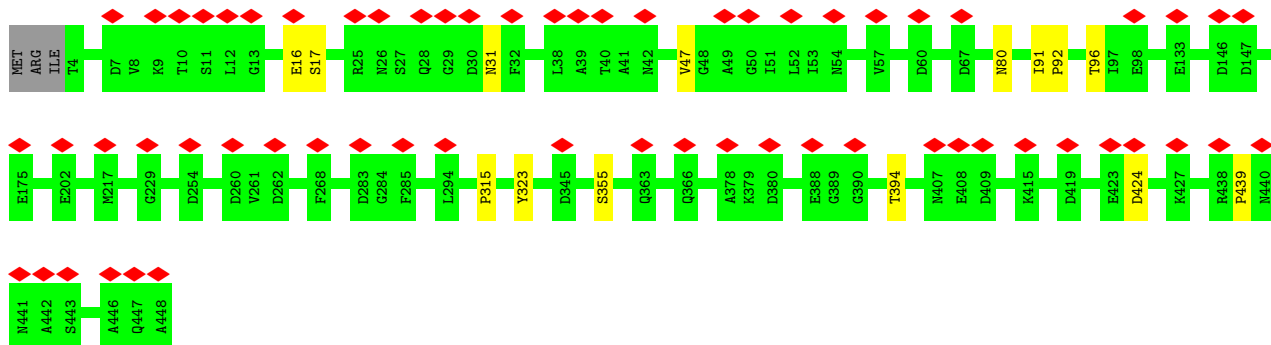




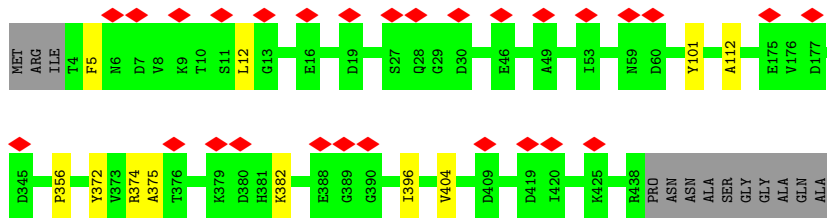
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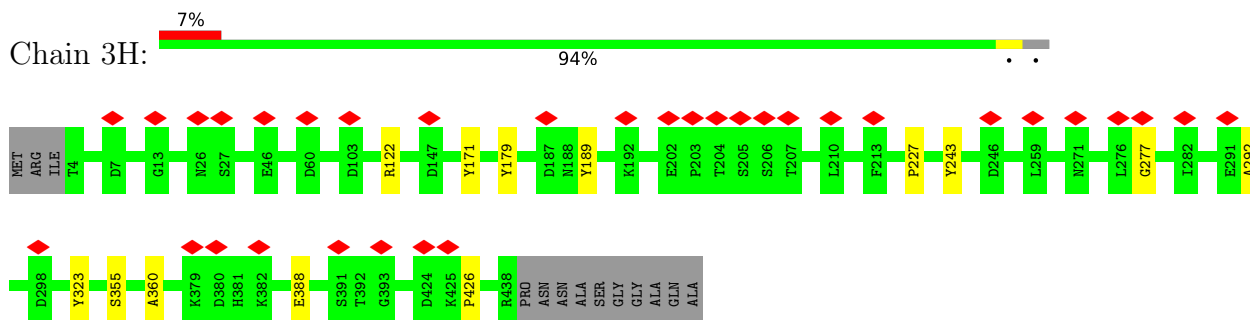
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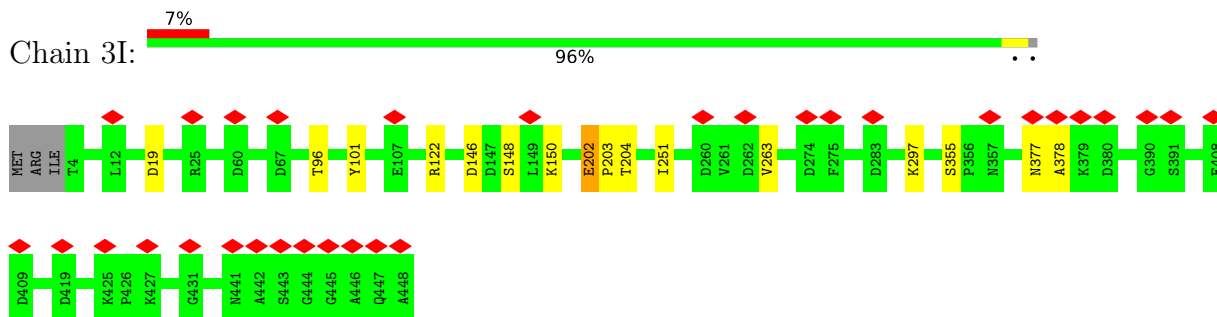
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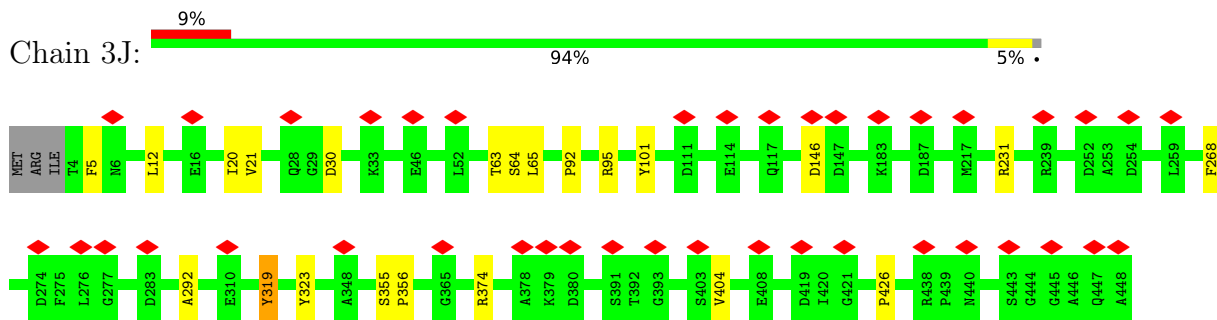
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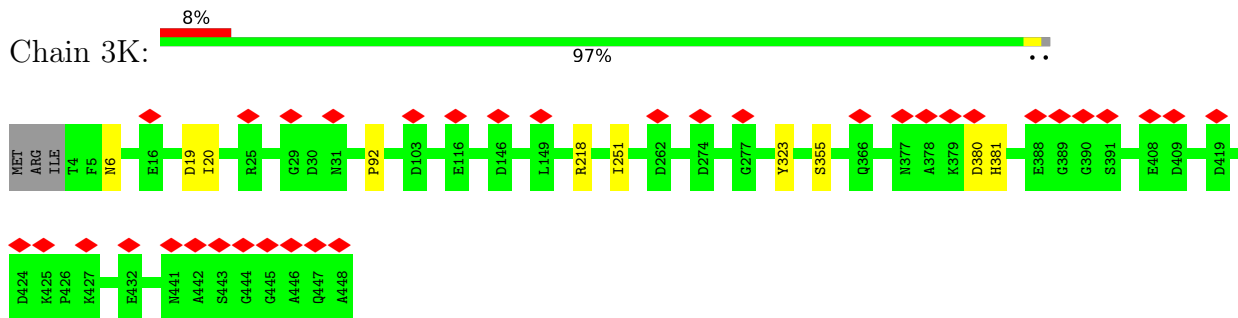
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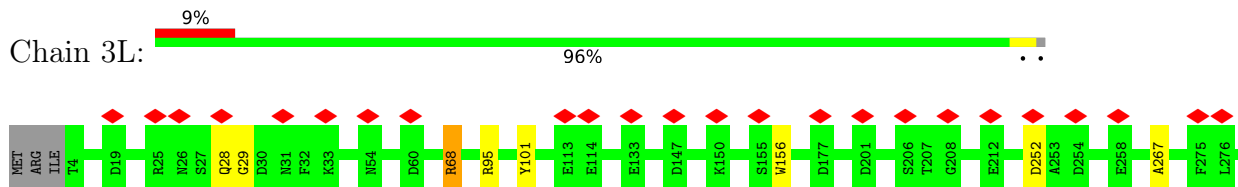
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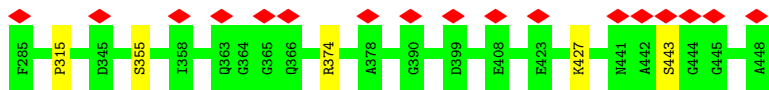


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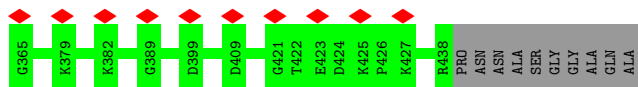
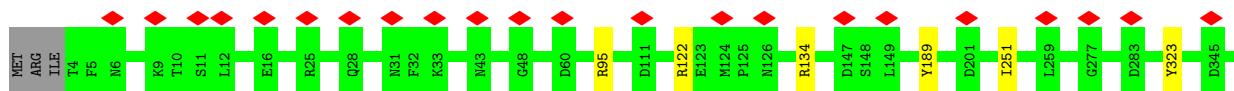


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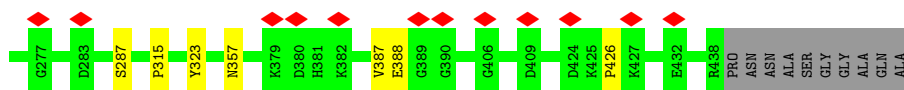
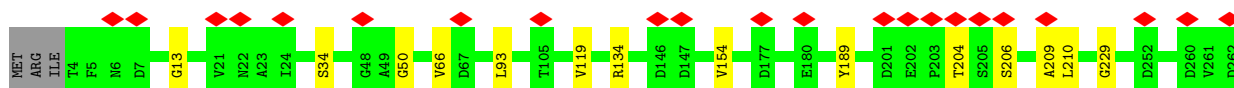




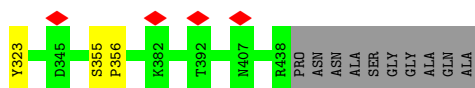
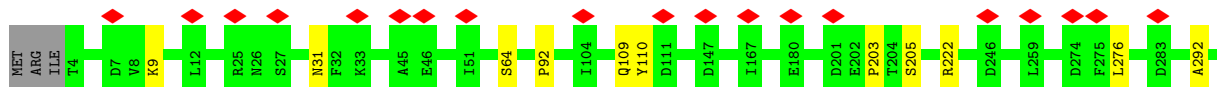
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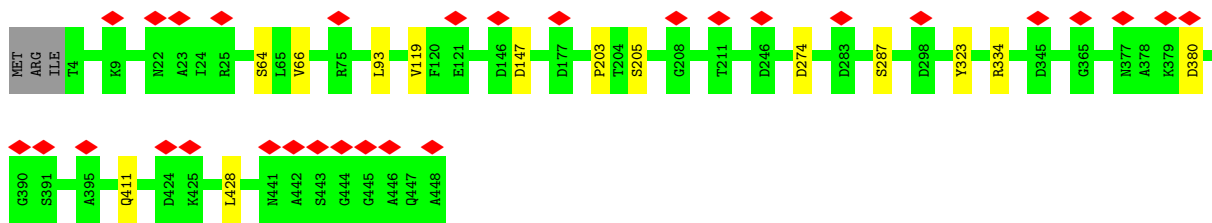


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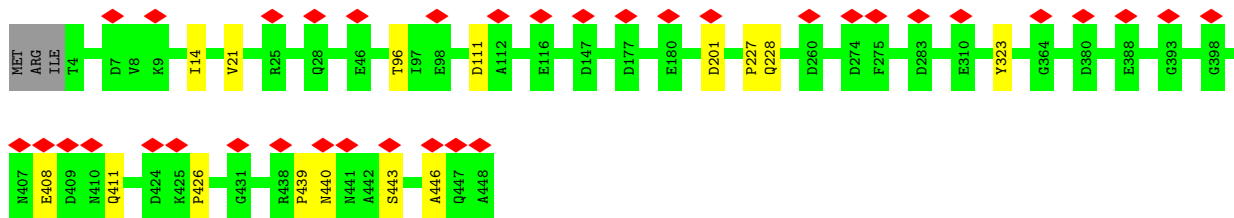


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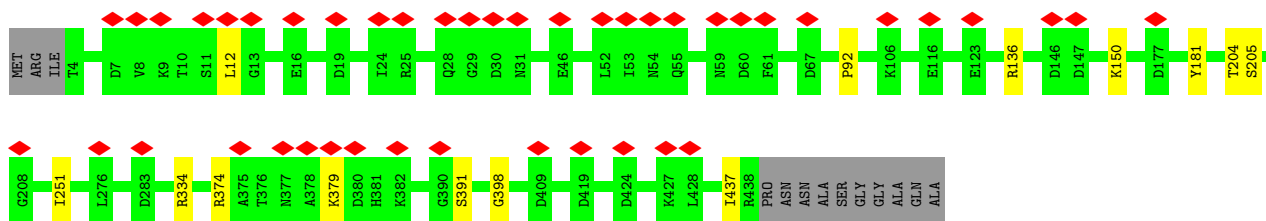




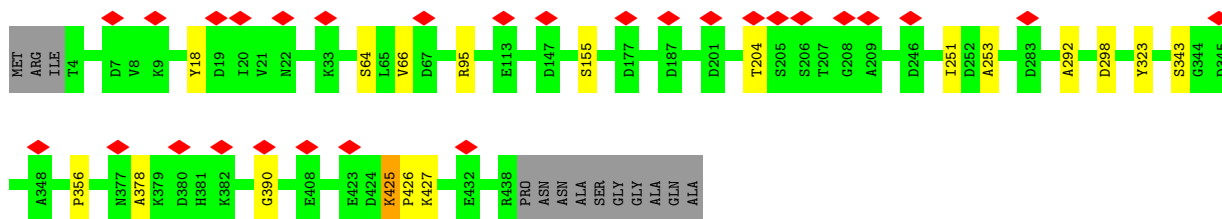
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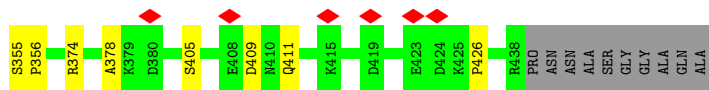


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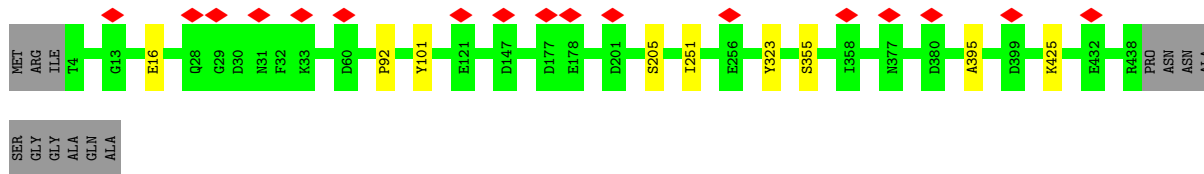


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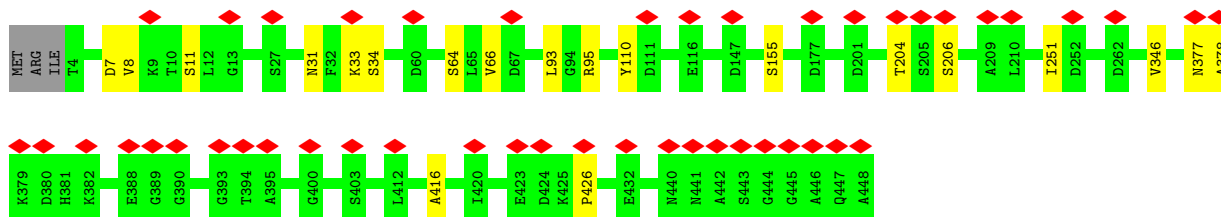




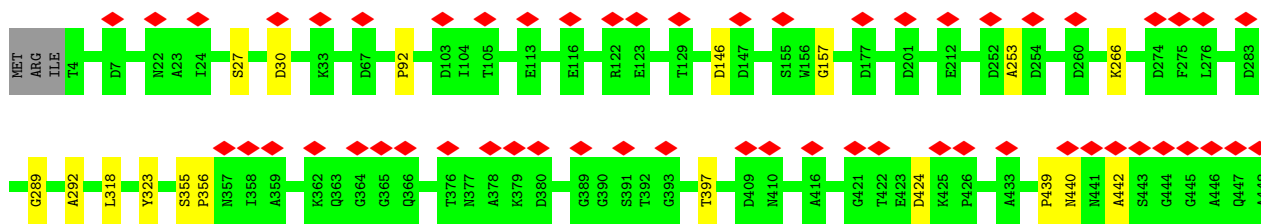
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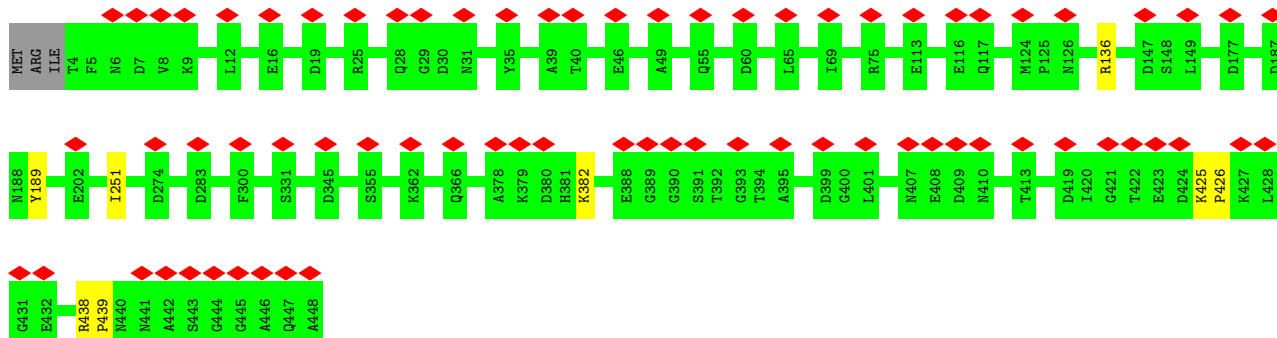
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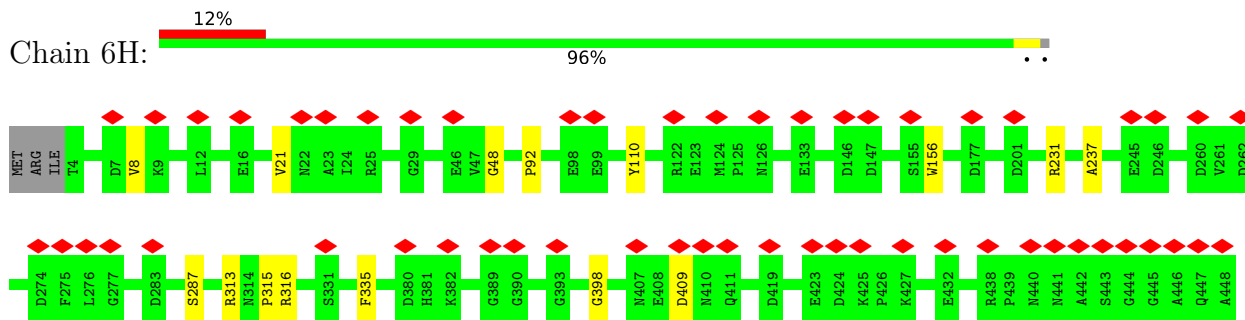
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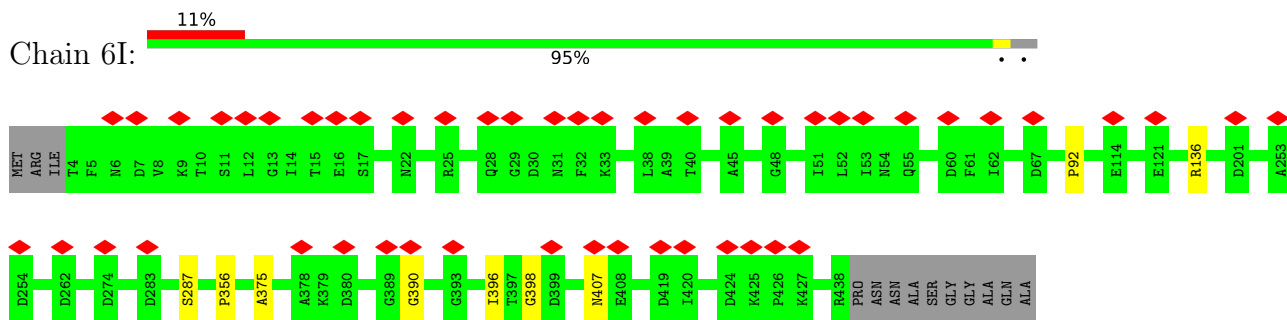
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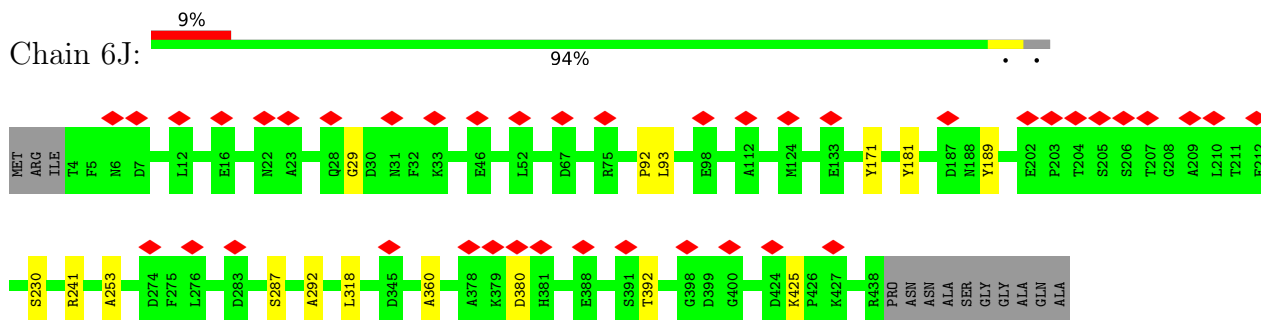
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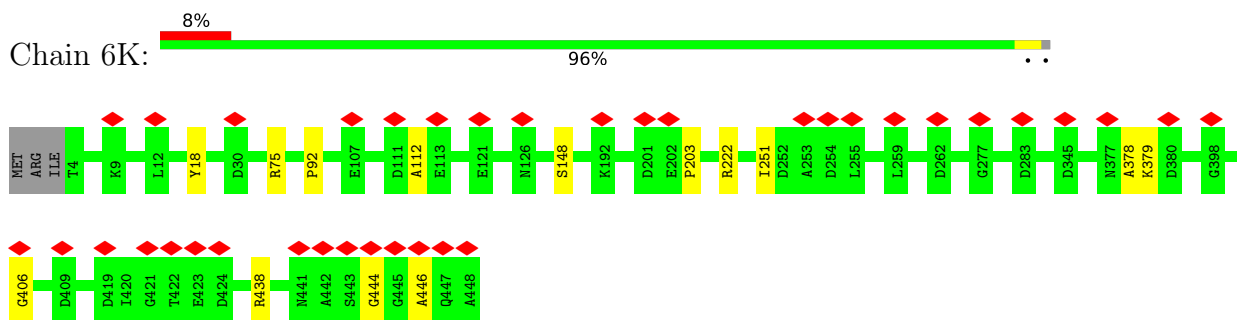
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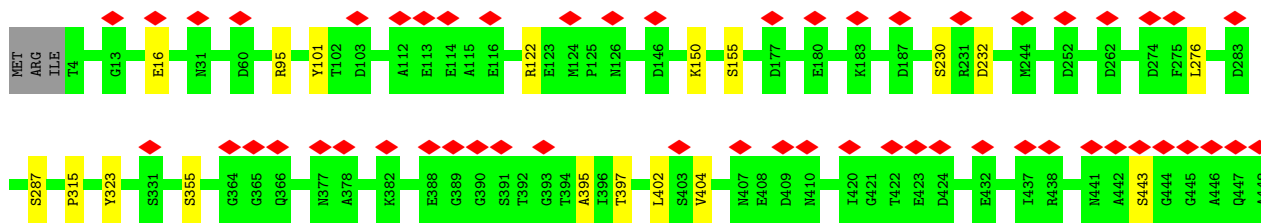


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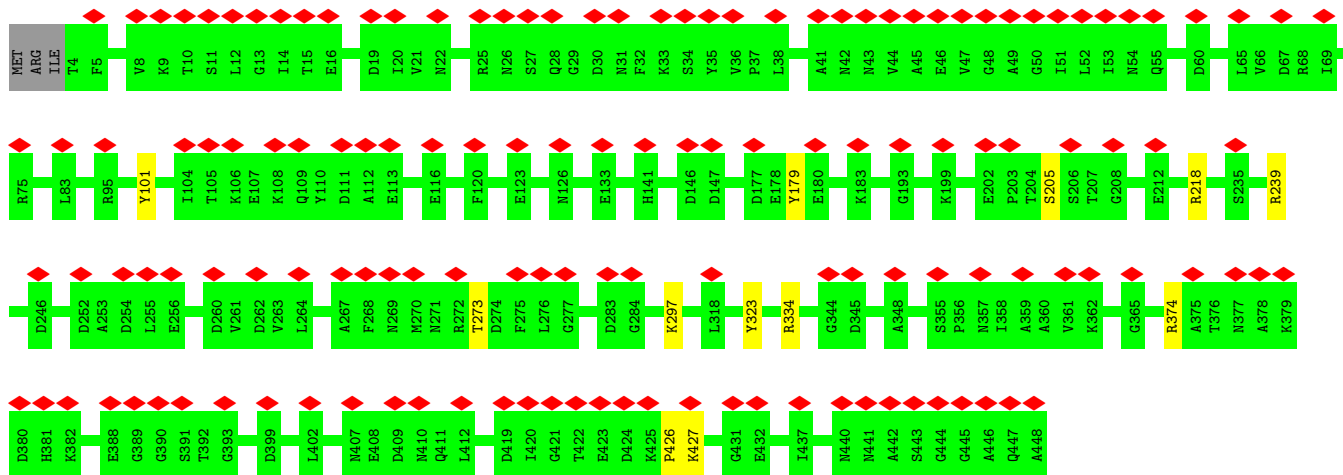


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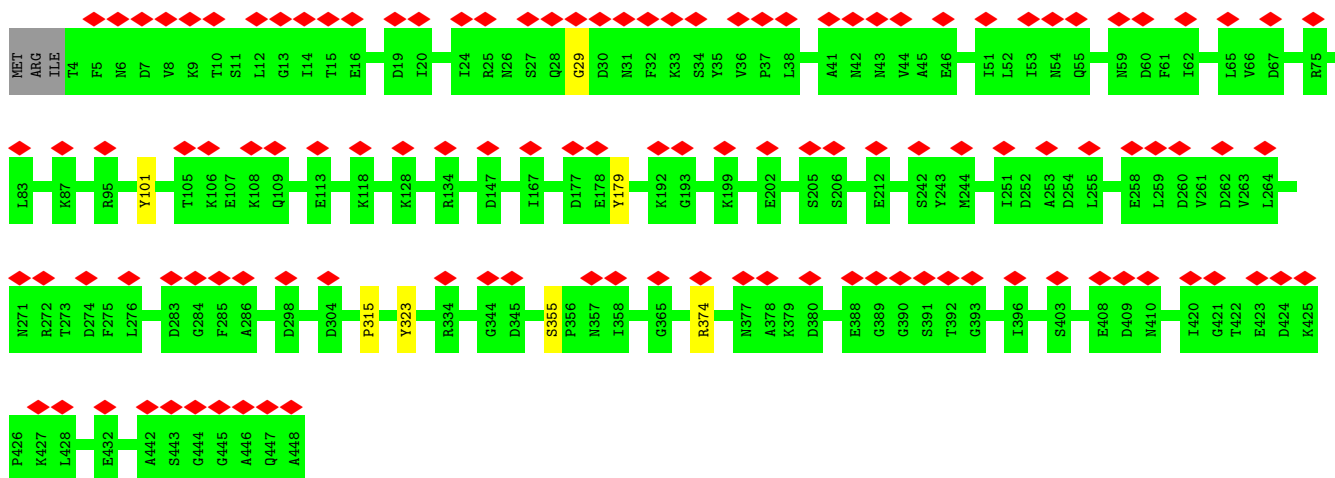




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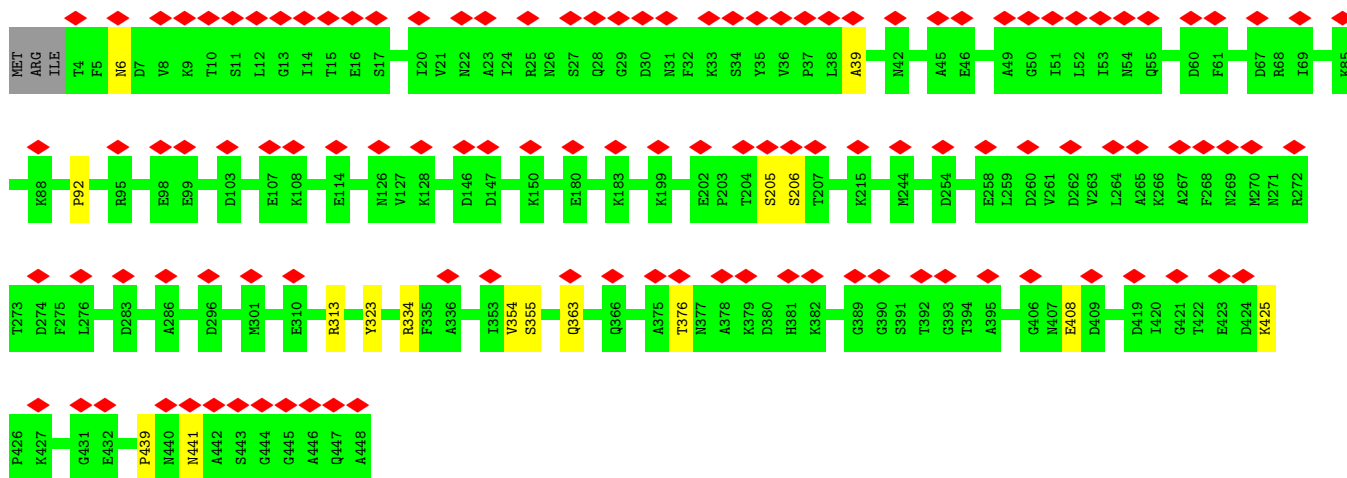


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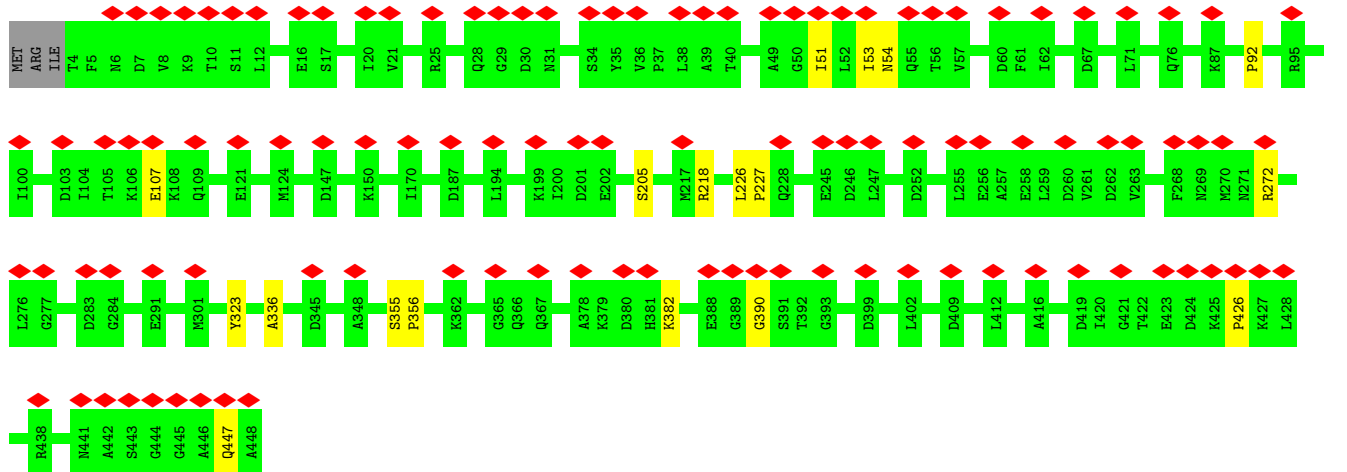


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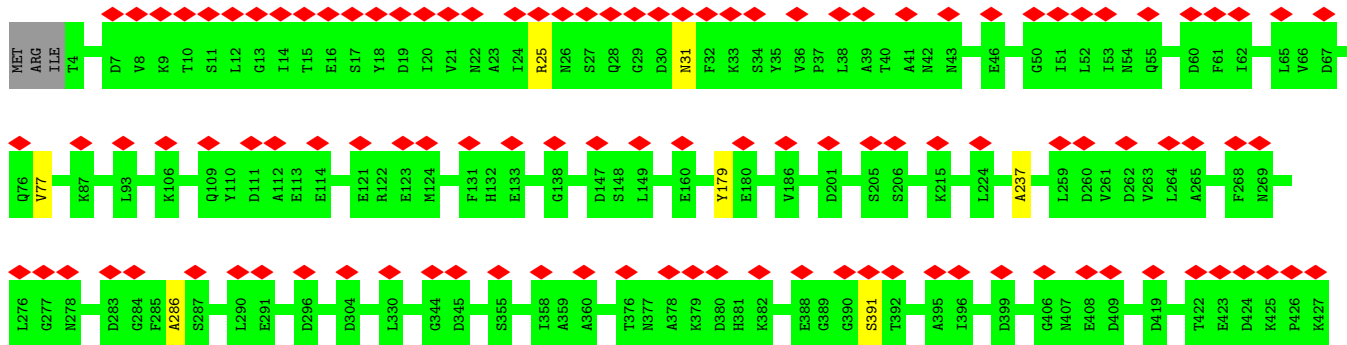


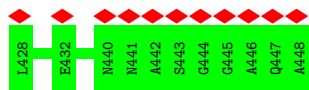


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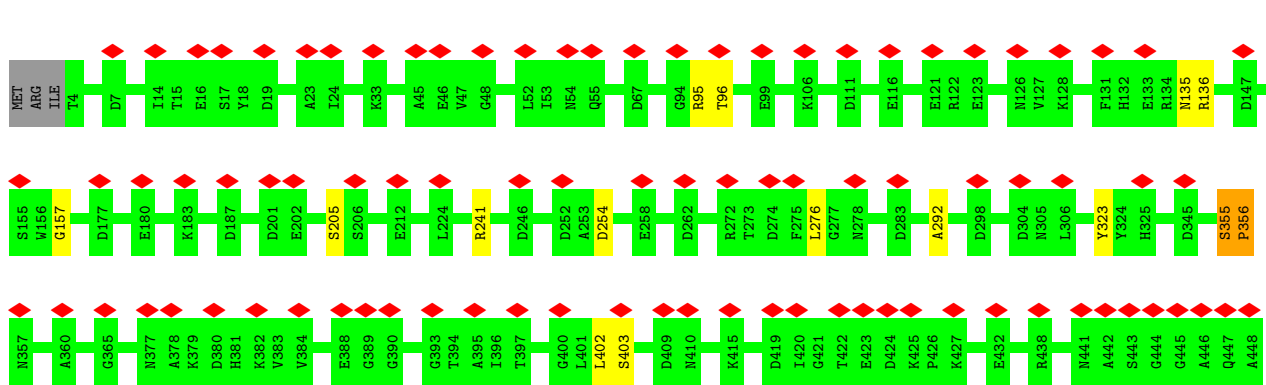


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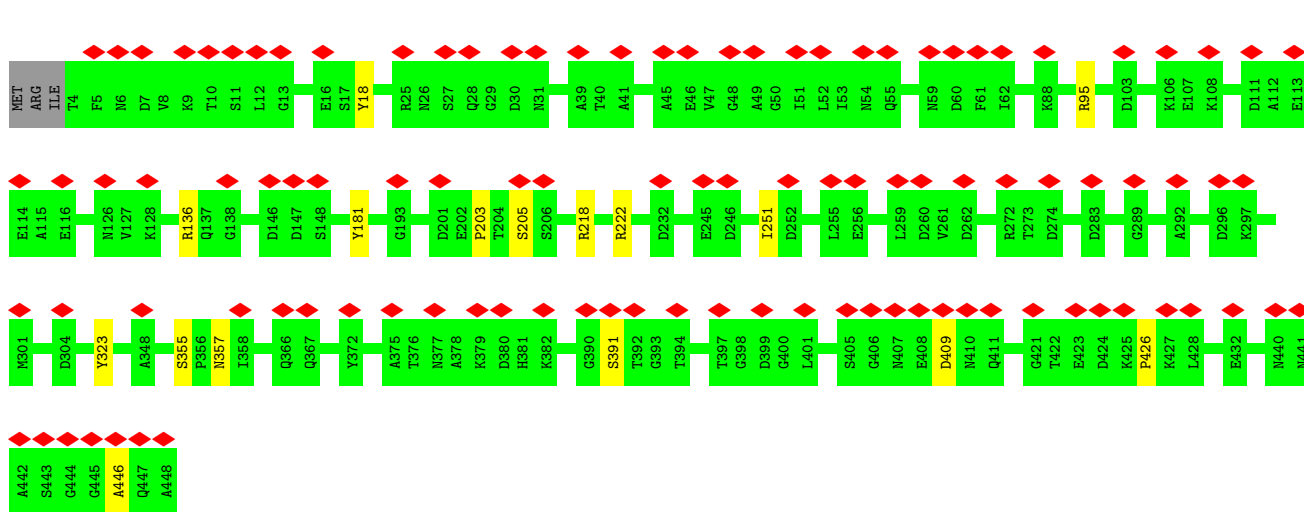




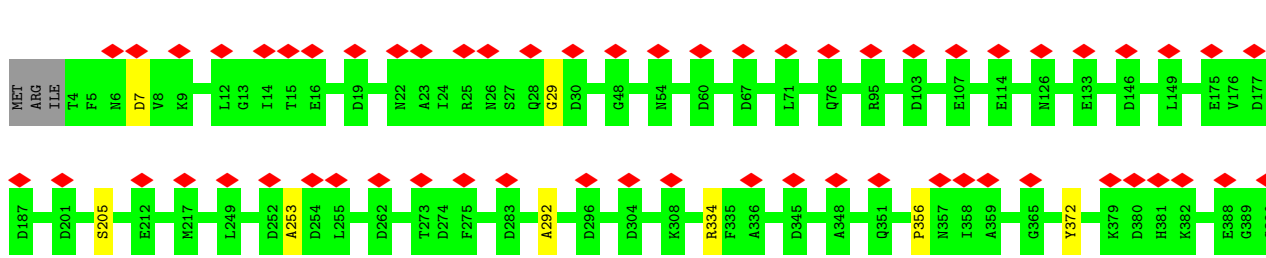
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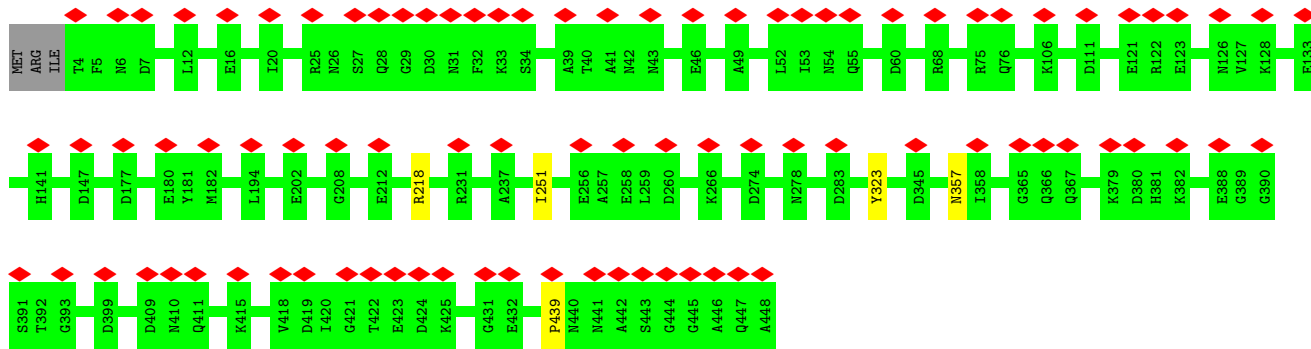


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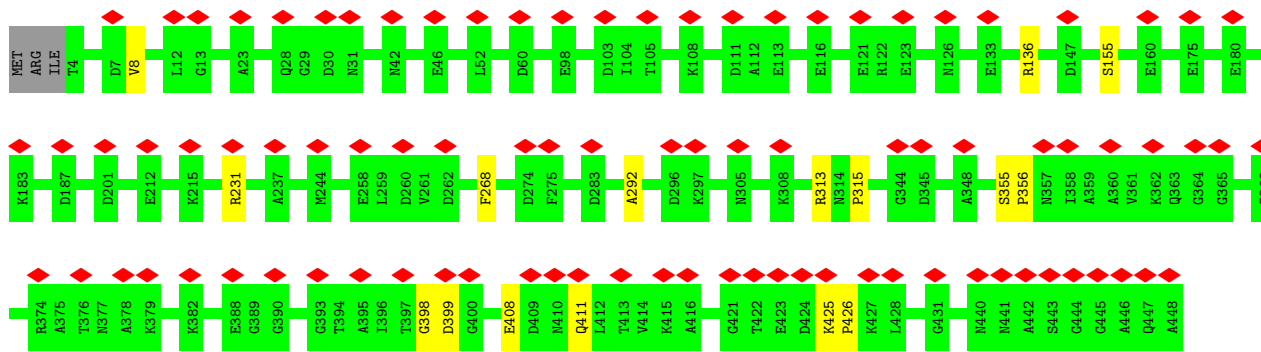




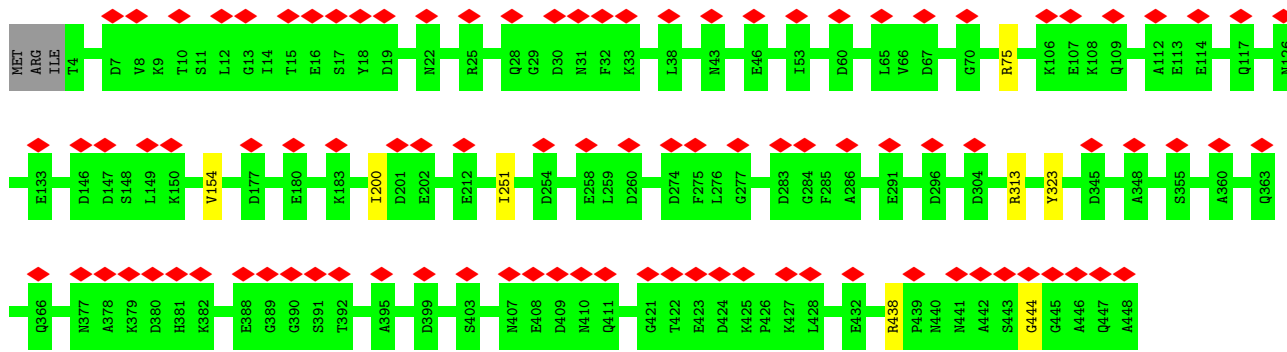
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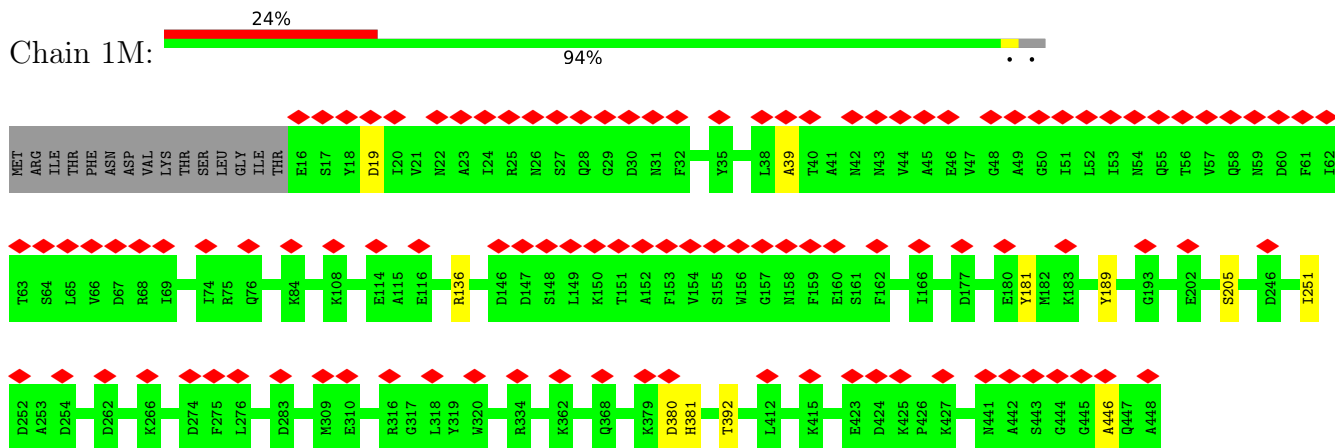
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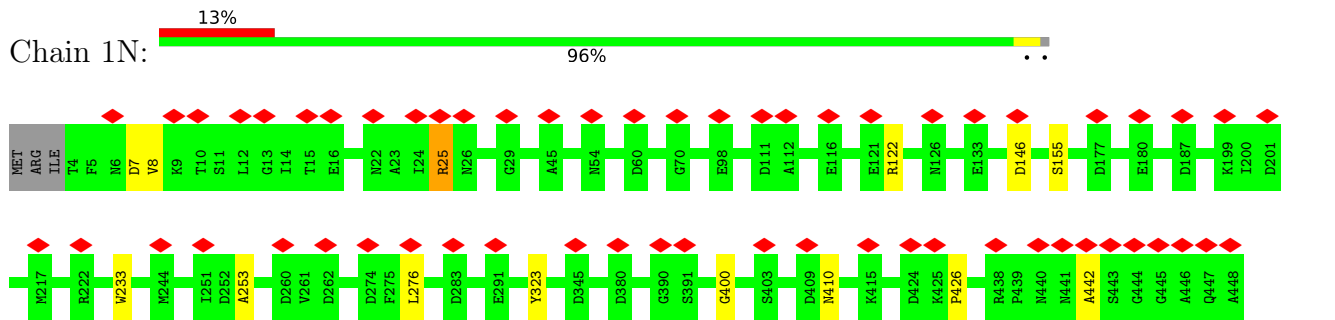
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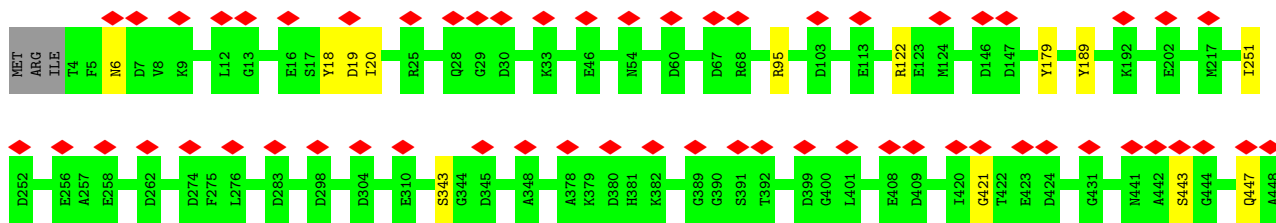


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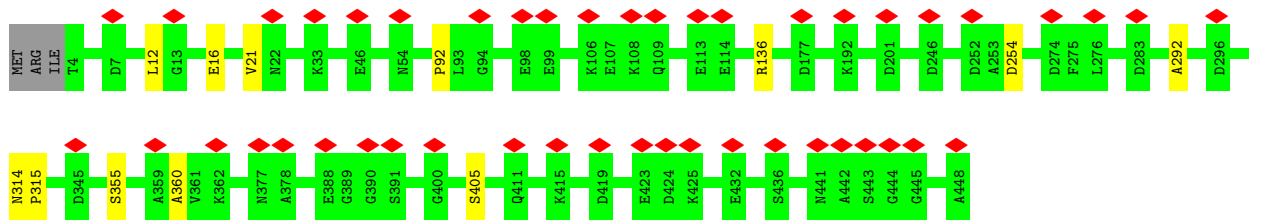


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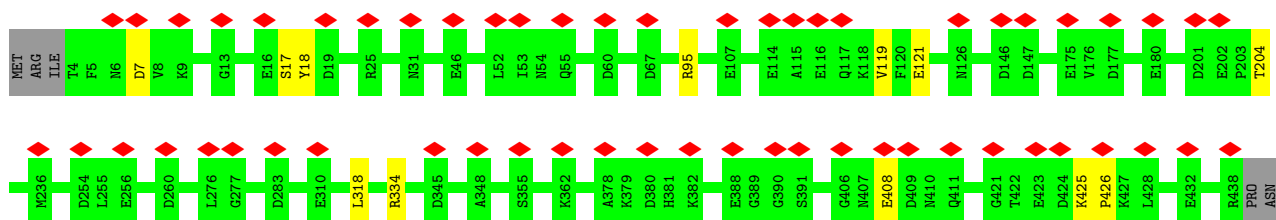




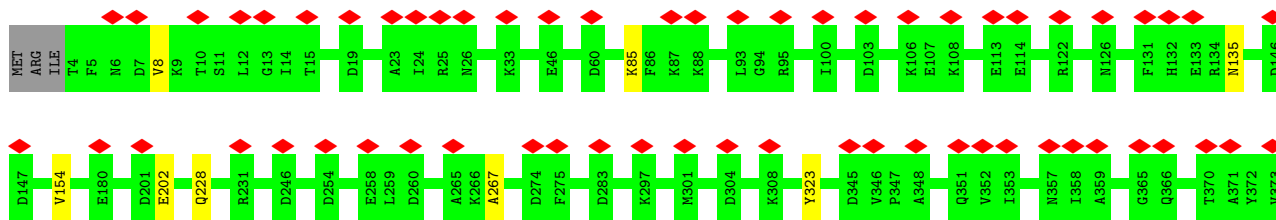
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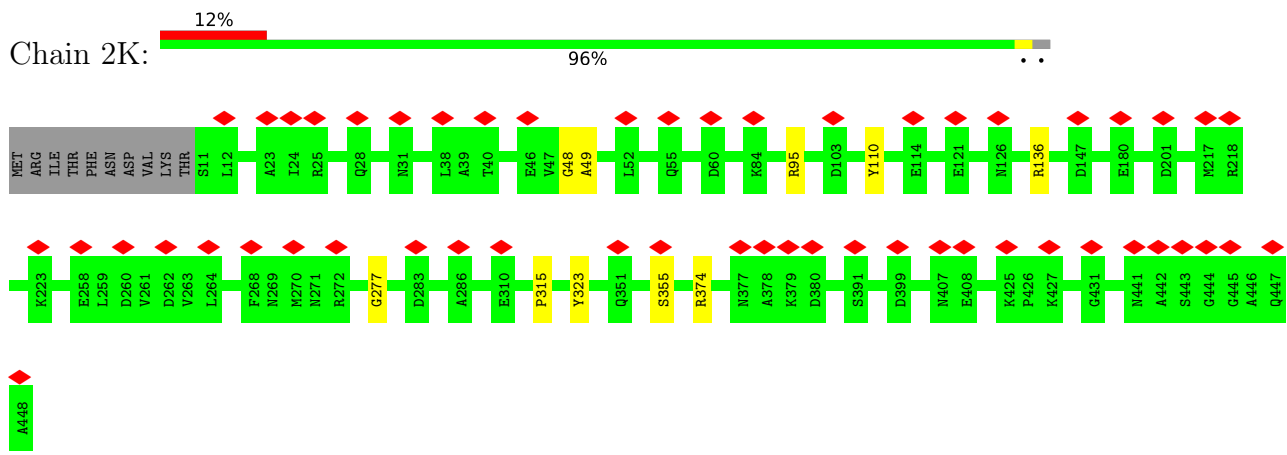
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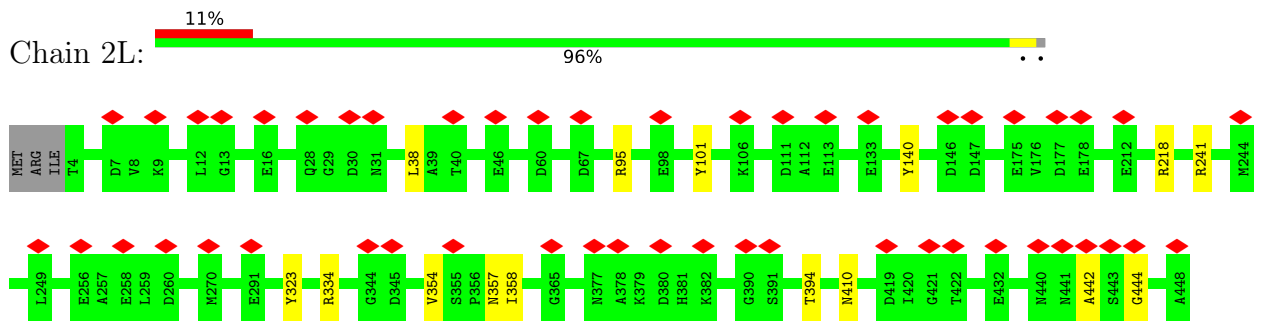
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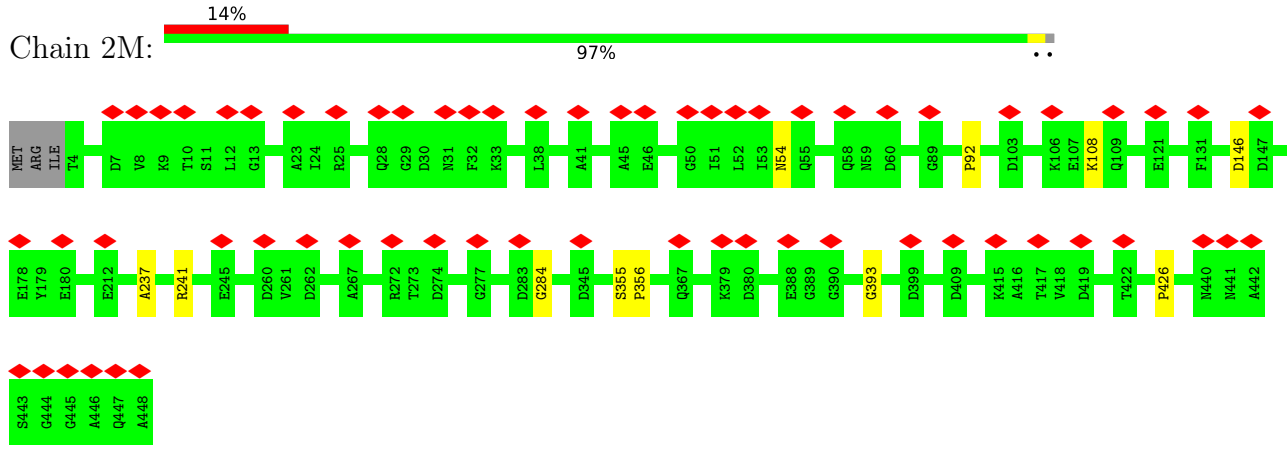
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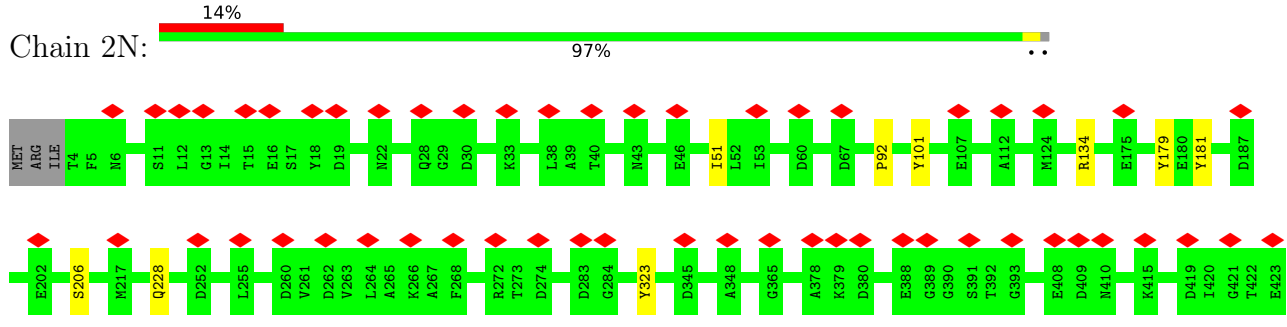
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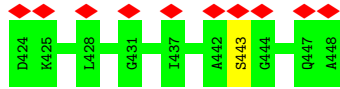


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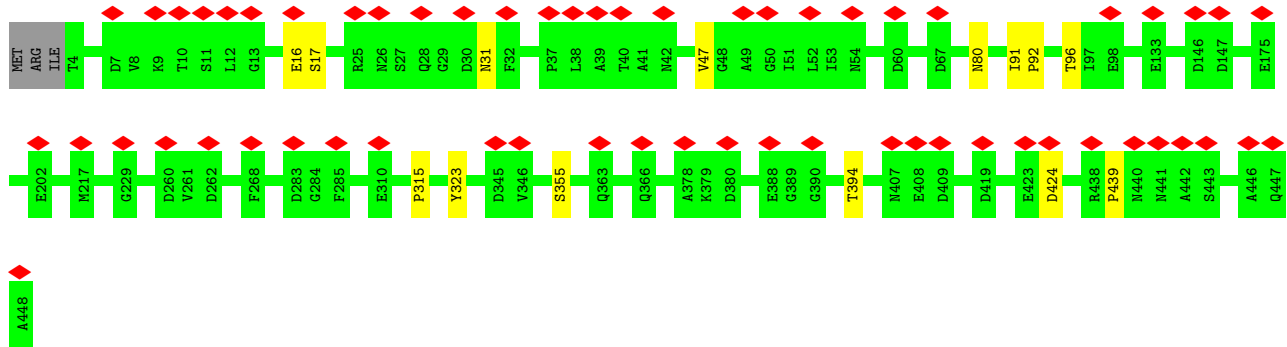


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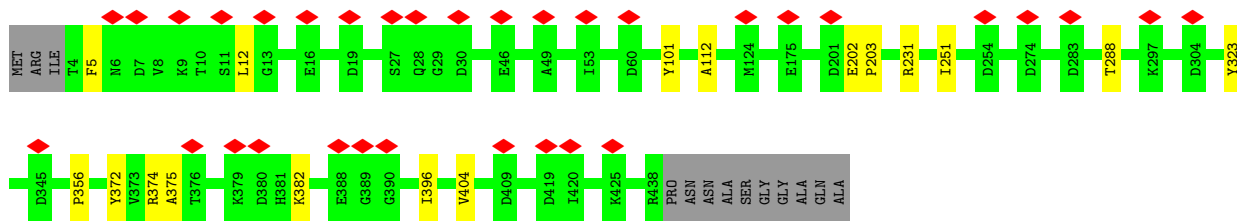




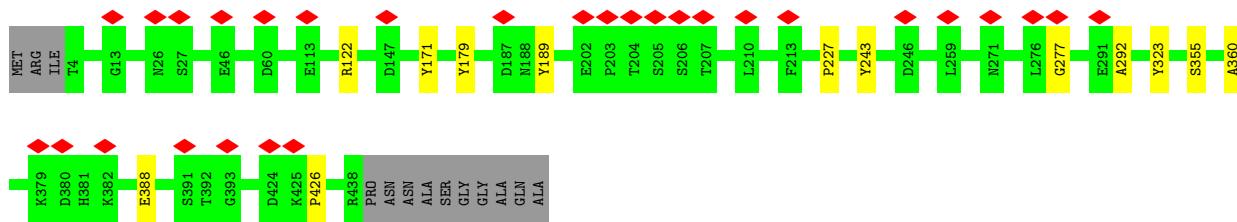
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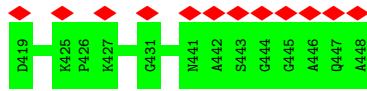


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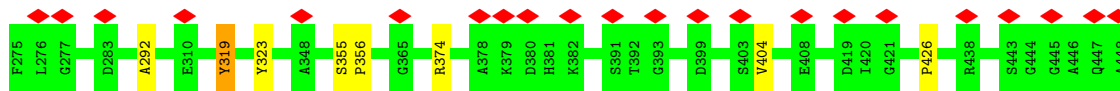


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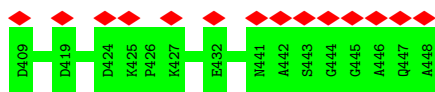




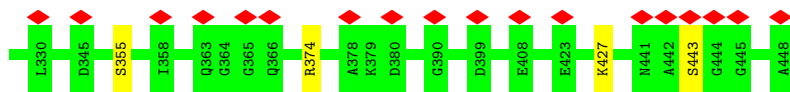
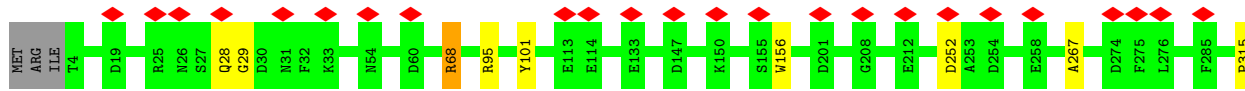
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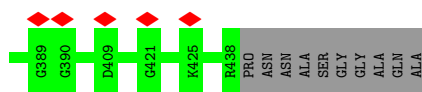
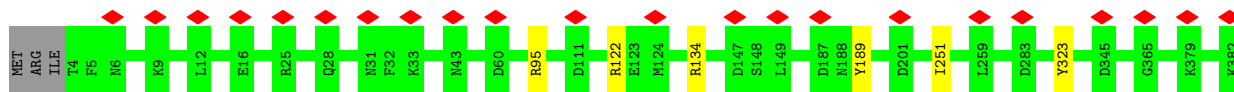
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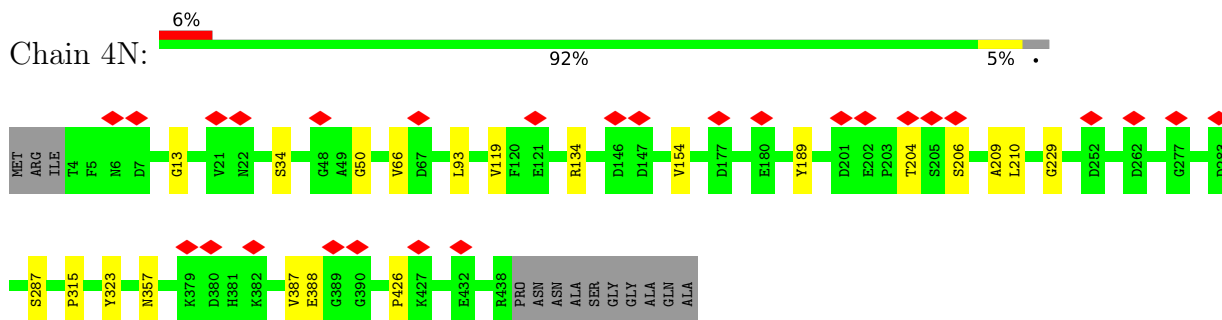
• Molecule 1: Major capsid protein



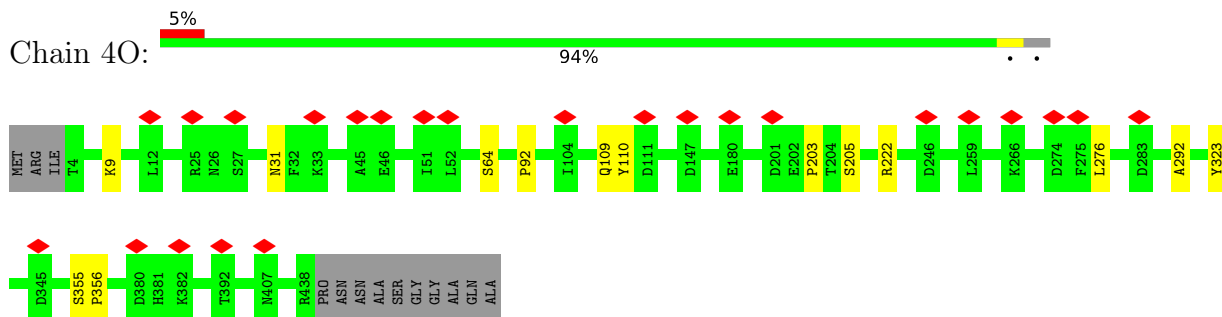
• Molecule 1: Major capsid protein



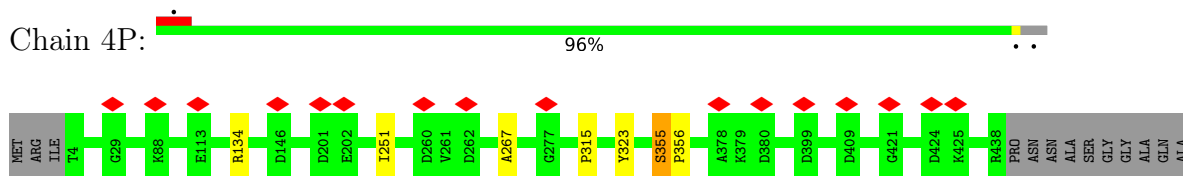
• Molecule 1: Major capsid protein



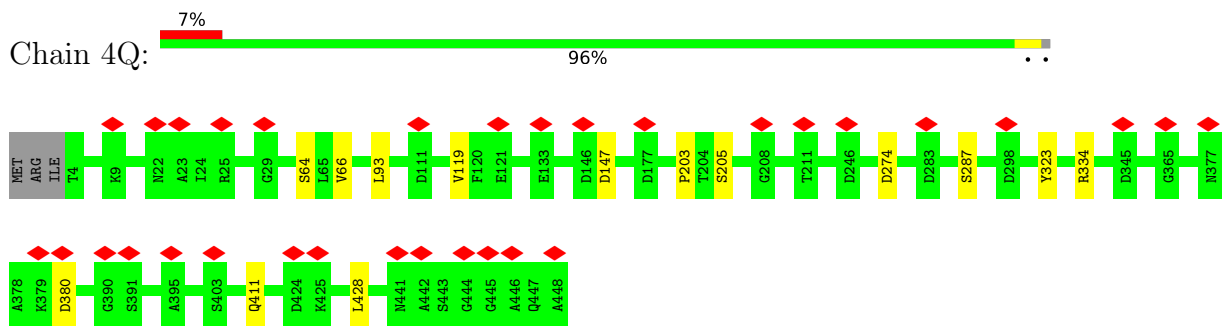
• Molecule 1: Major capsid protein



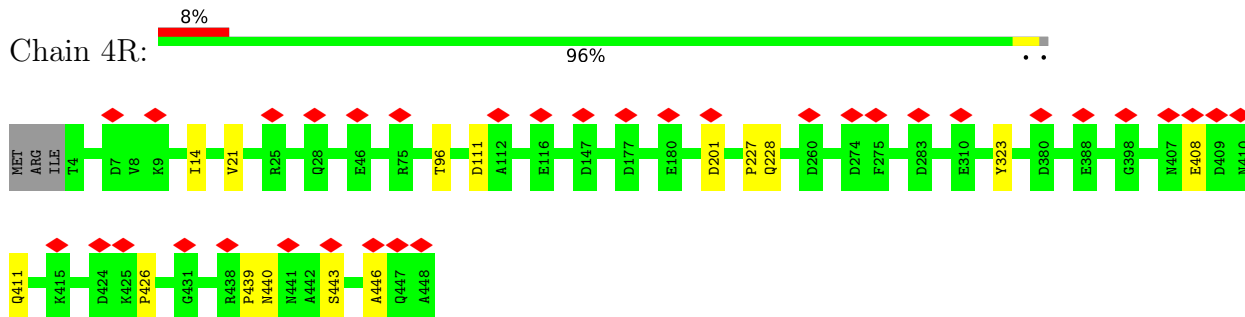
• Molecule 1: Major capsid protein



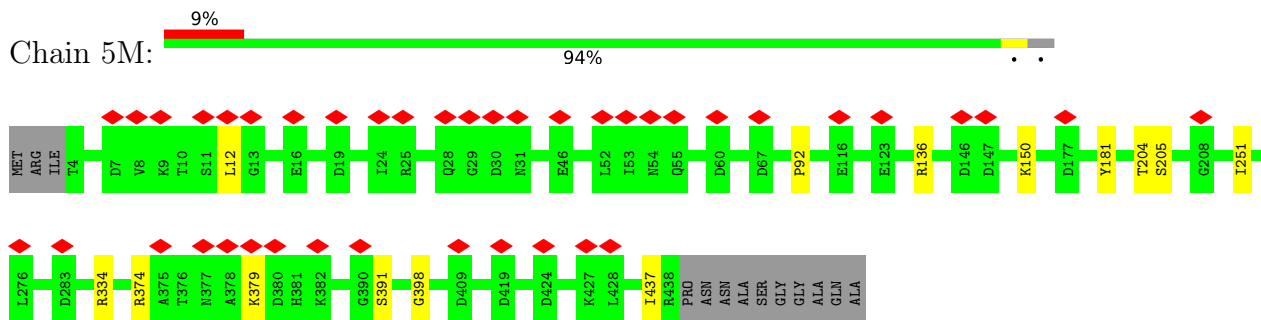
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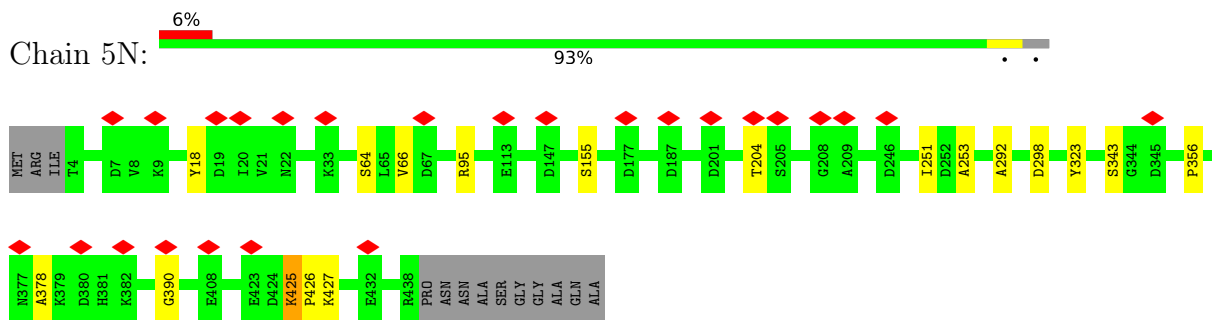
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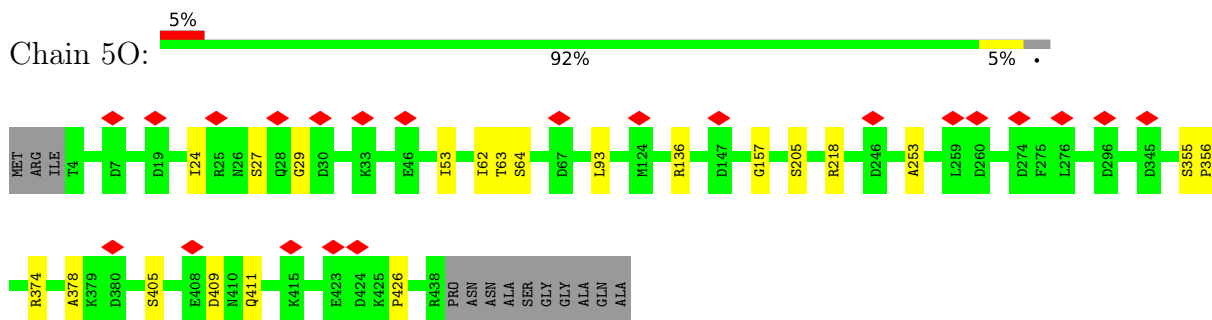
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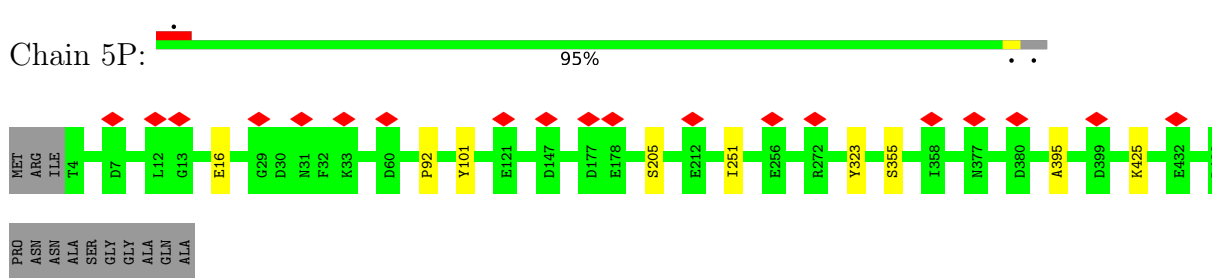
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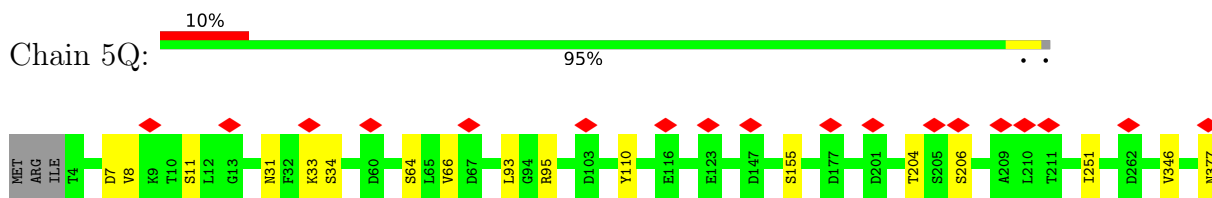
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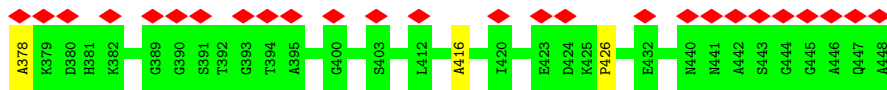


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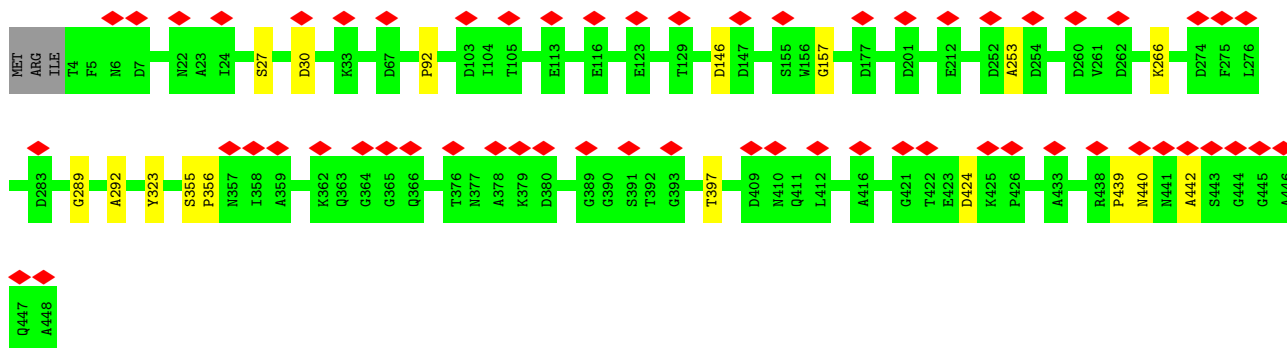


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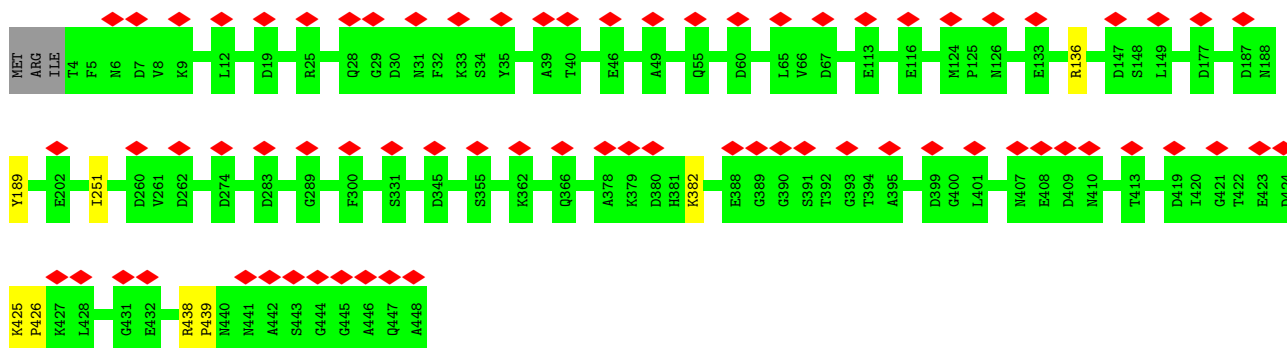




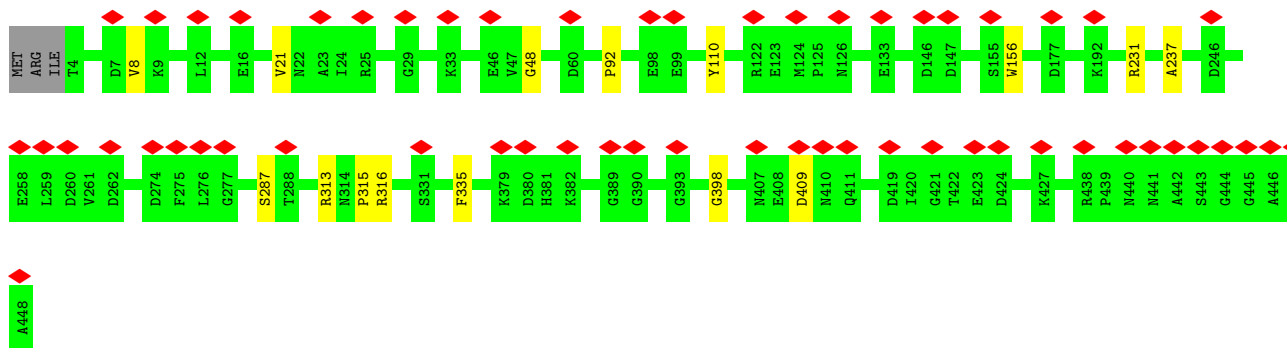
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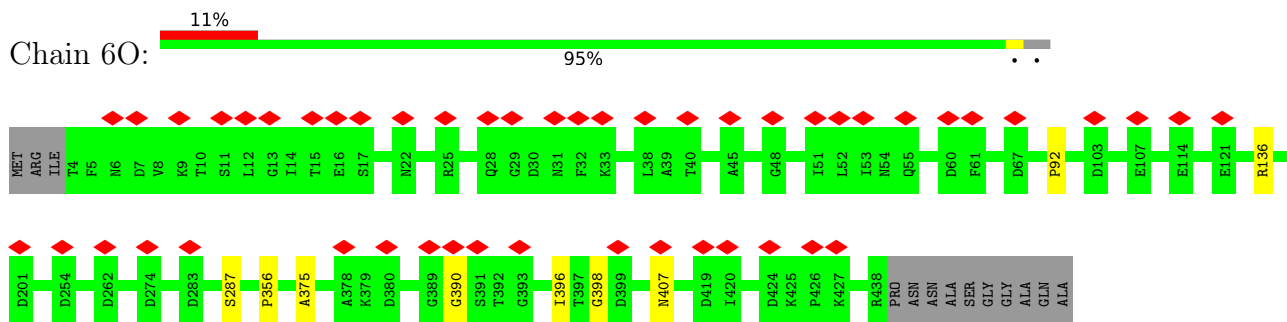
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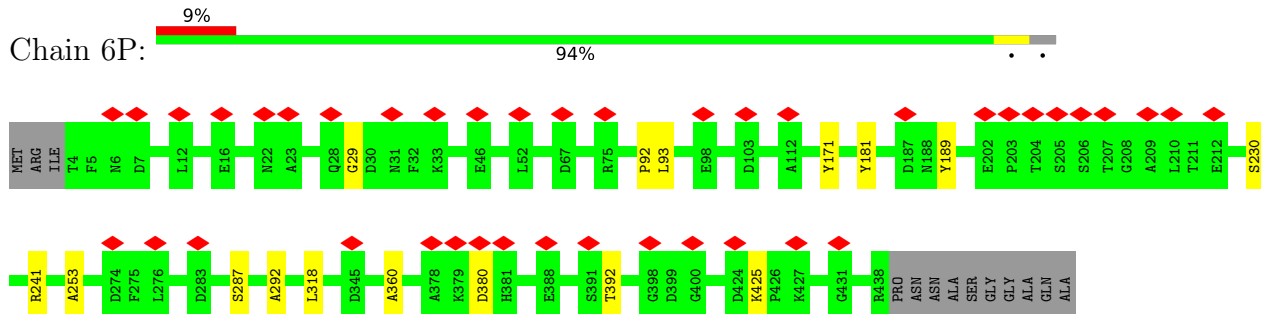
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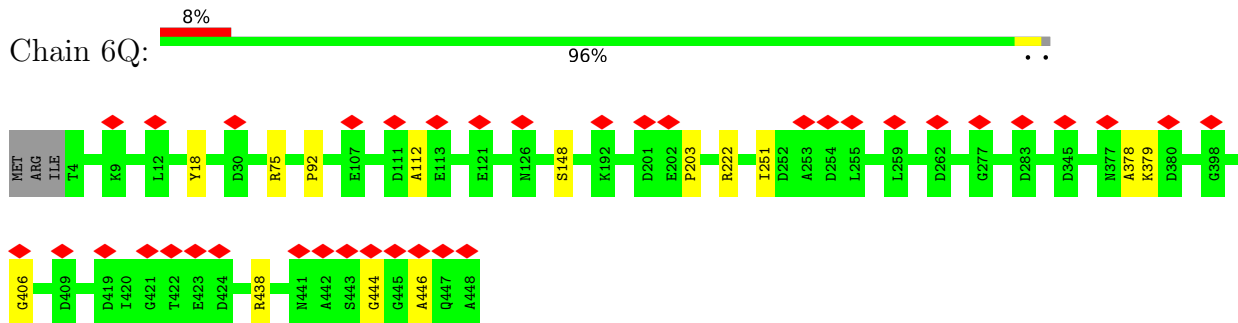
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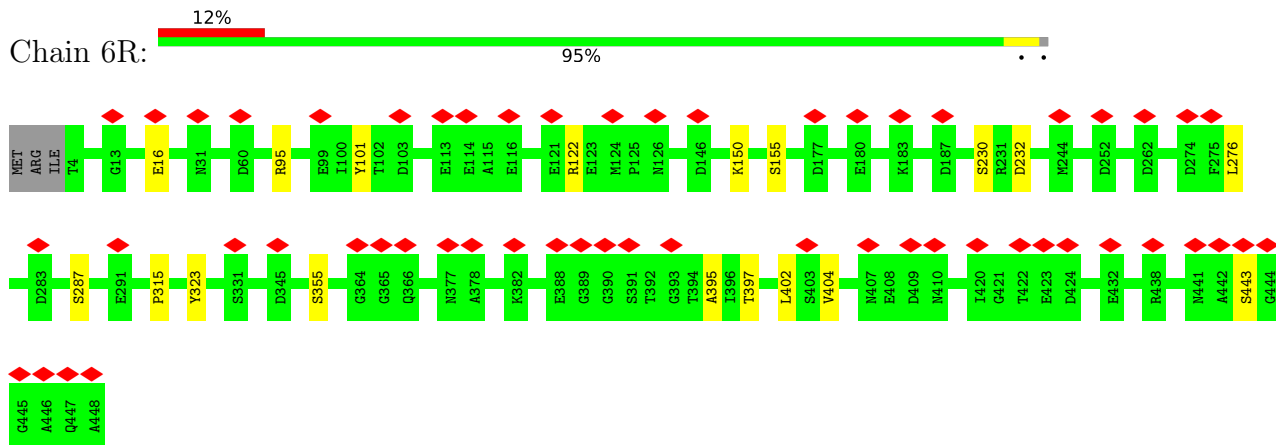
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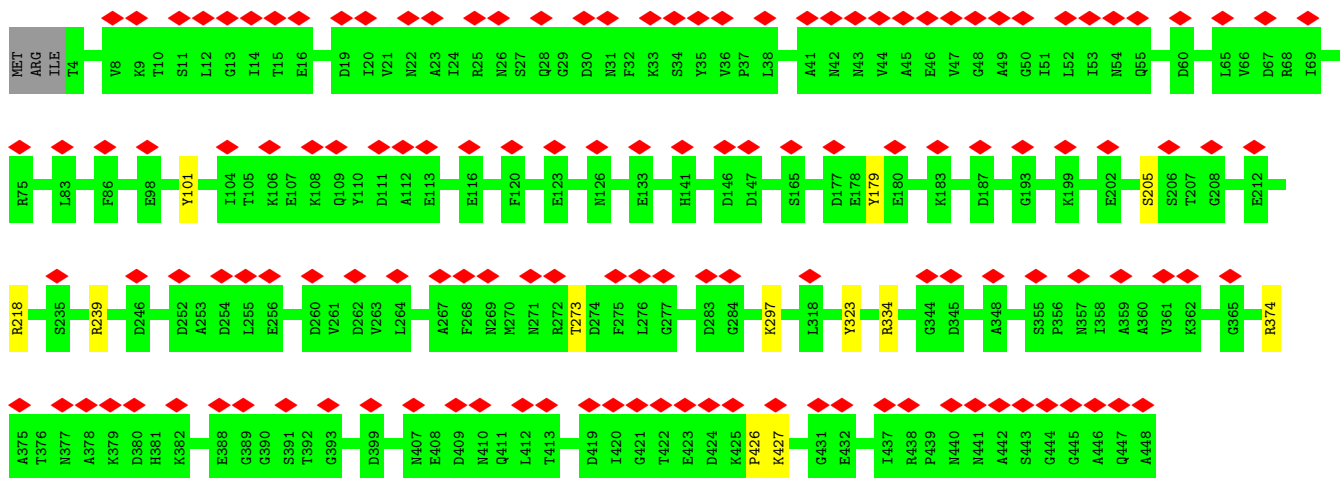


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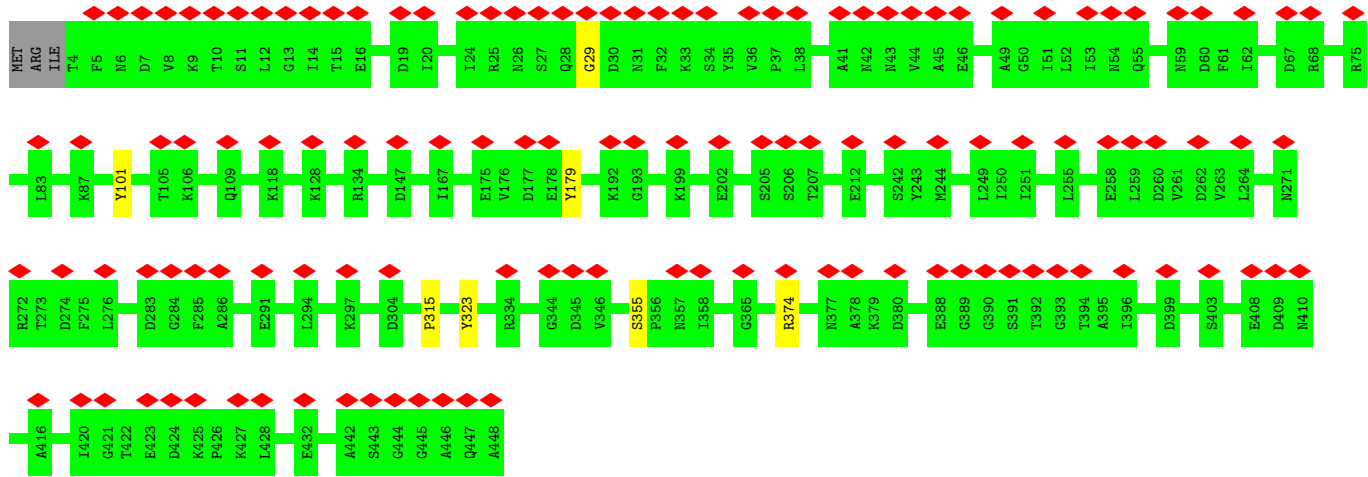


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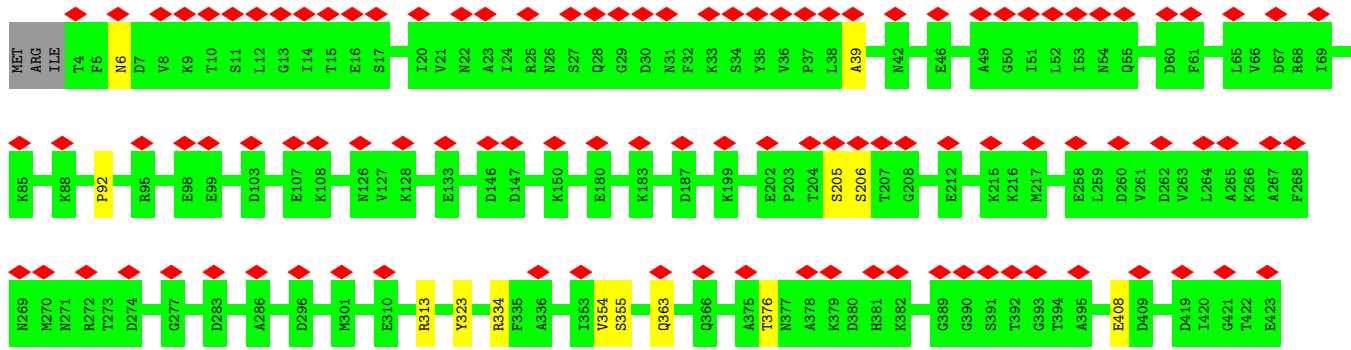


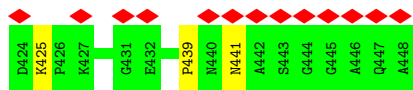


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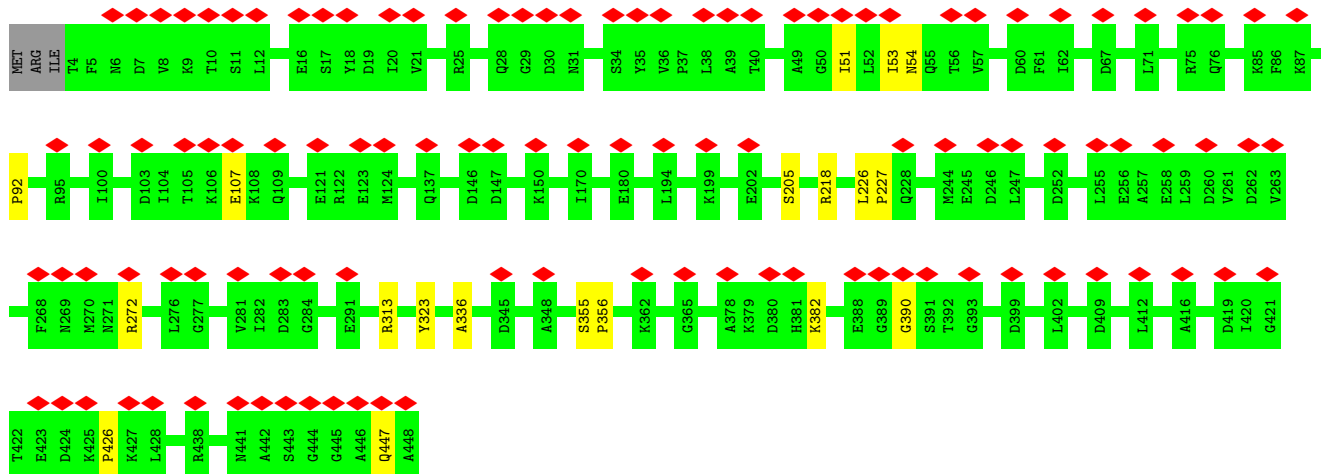


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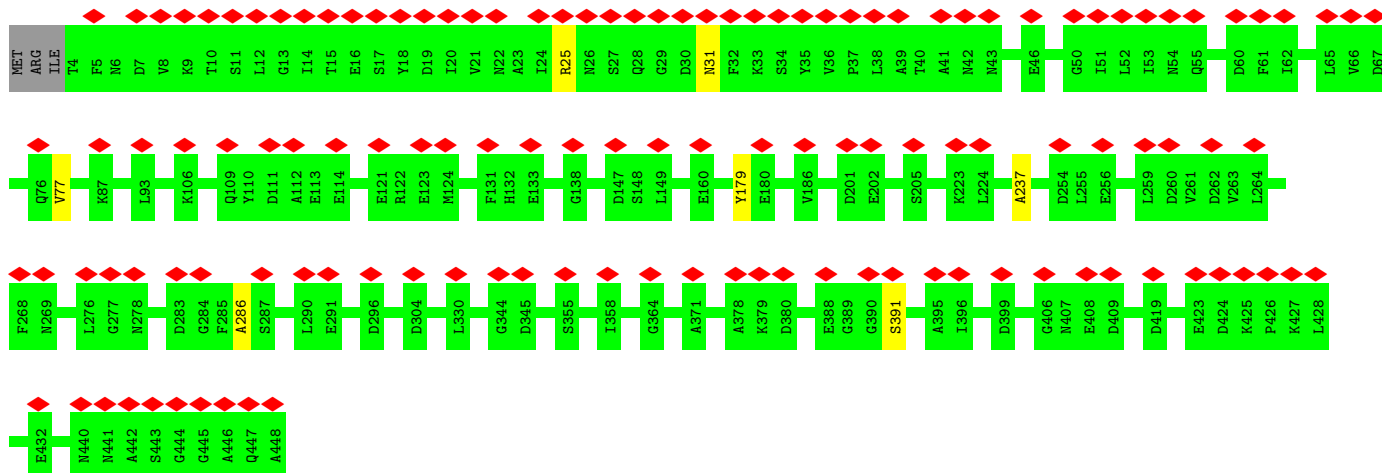




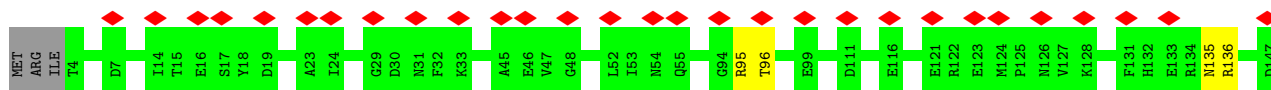
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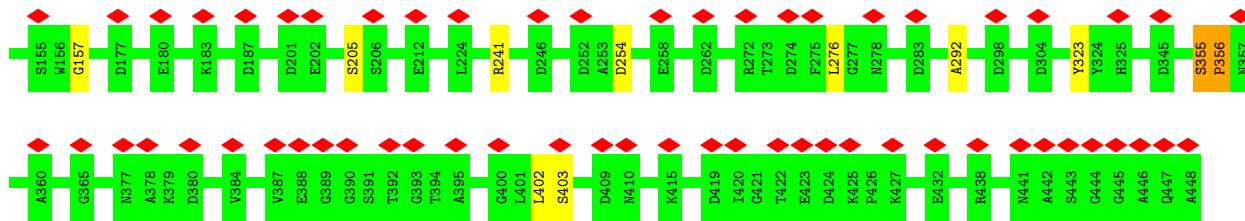


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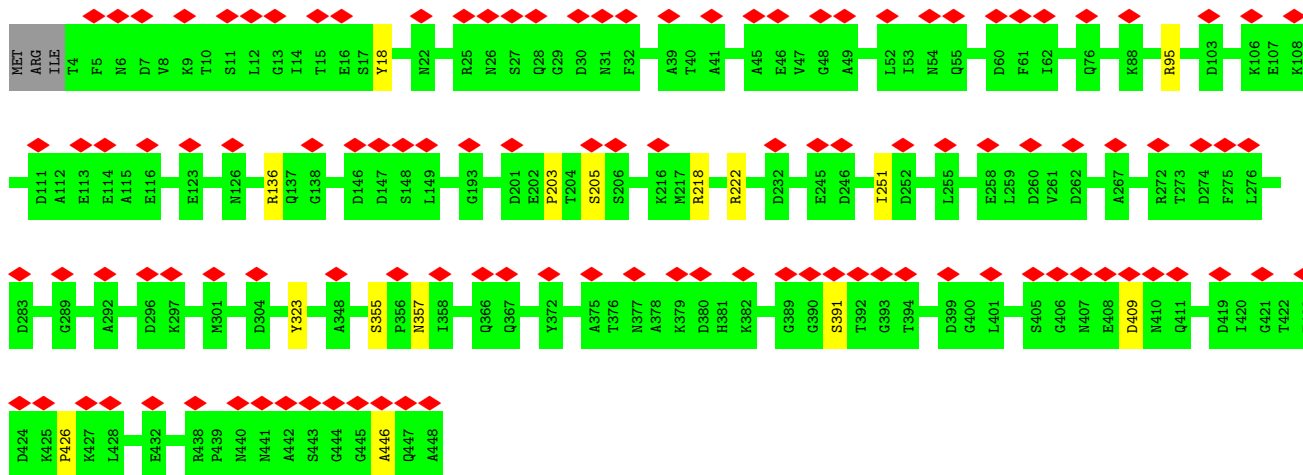


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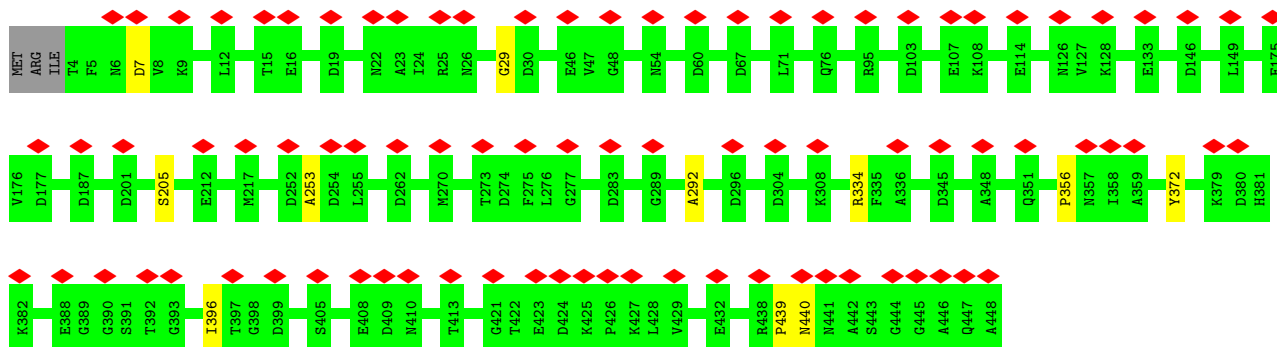




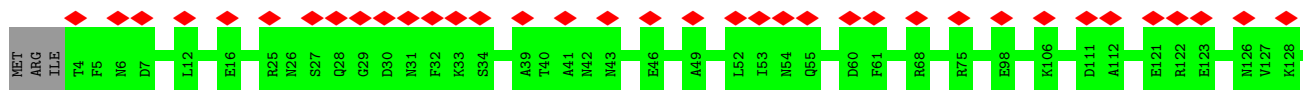
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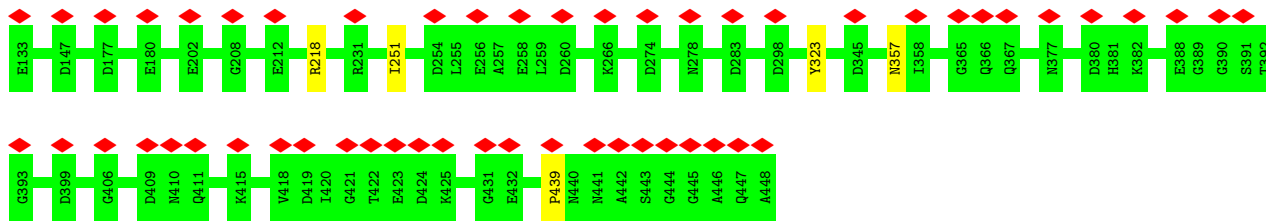


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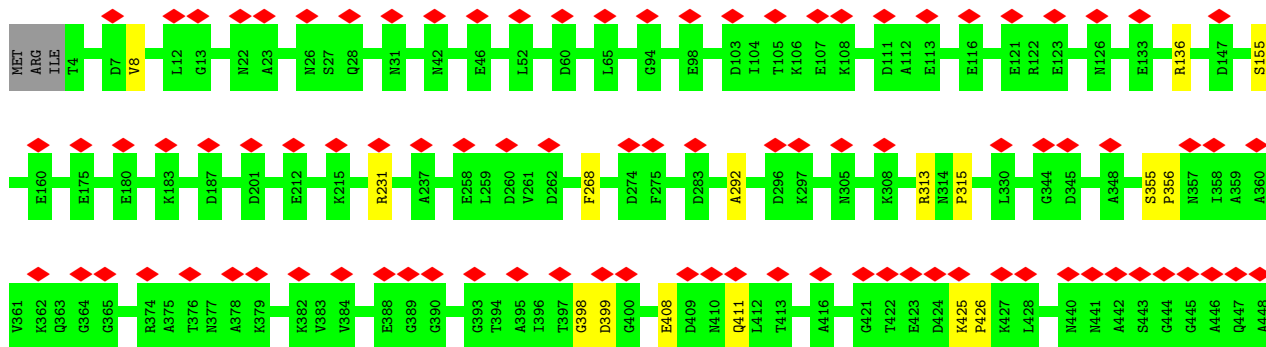


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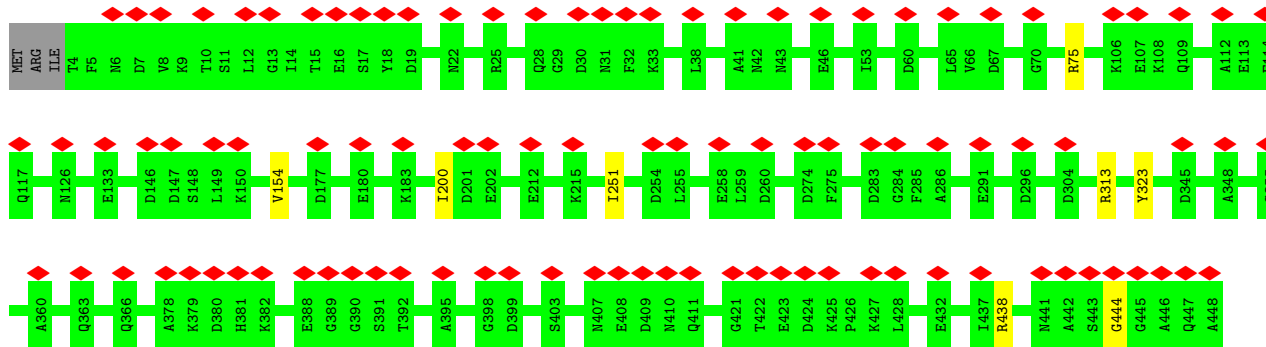




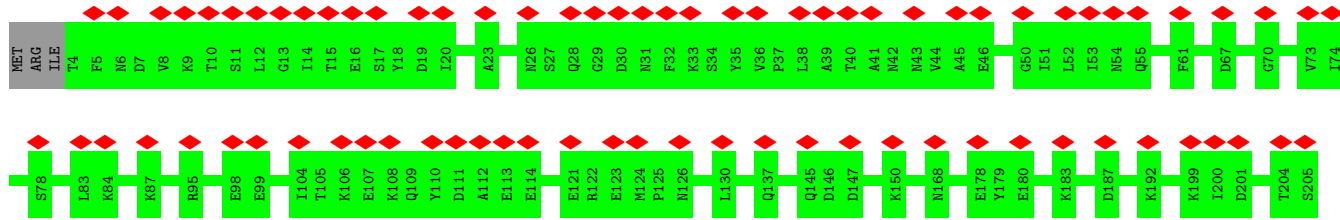
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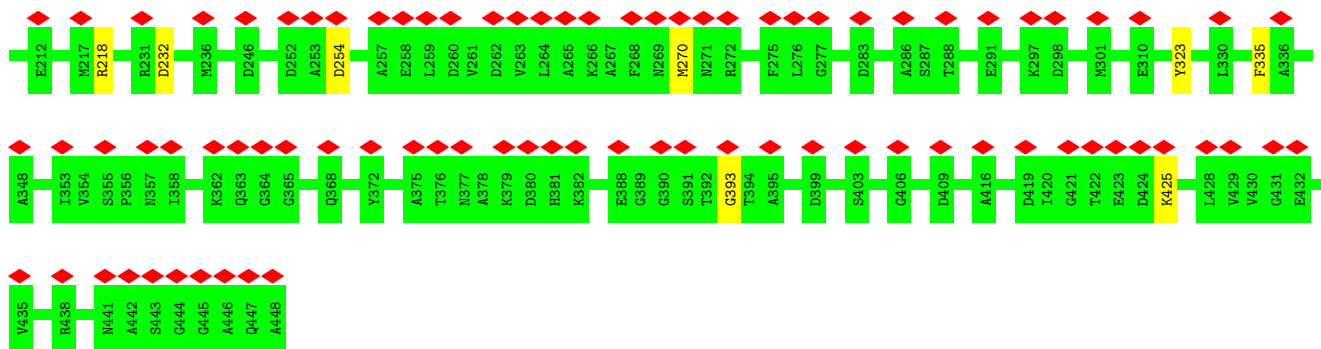


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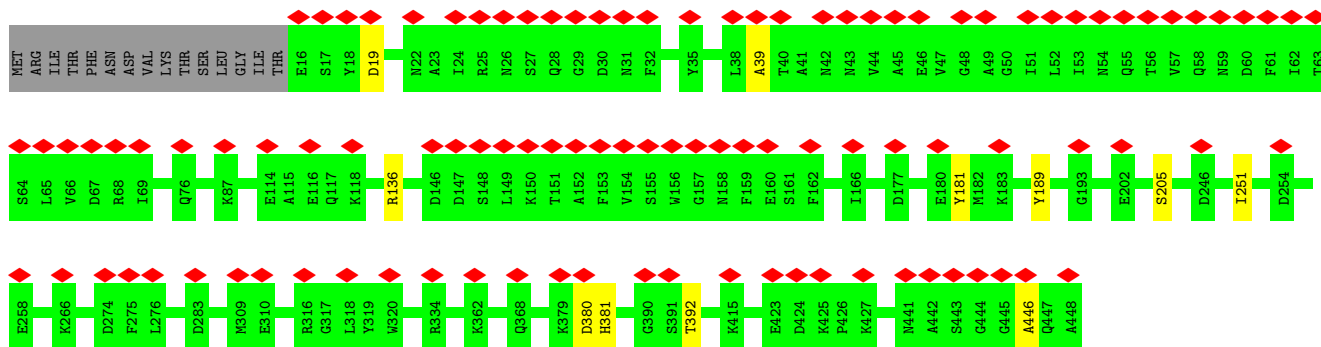


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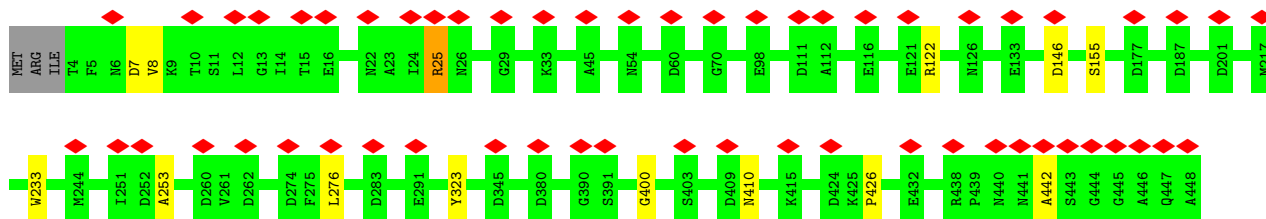




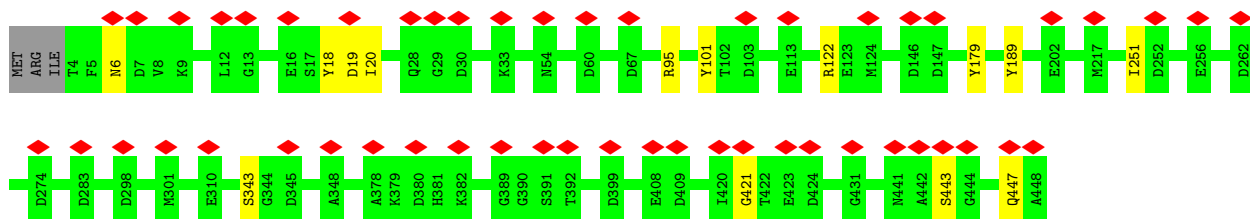
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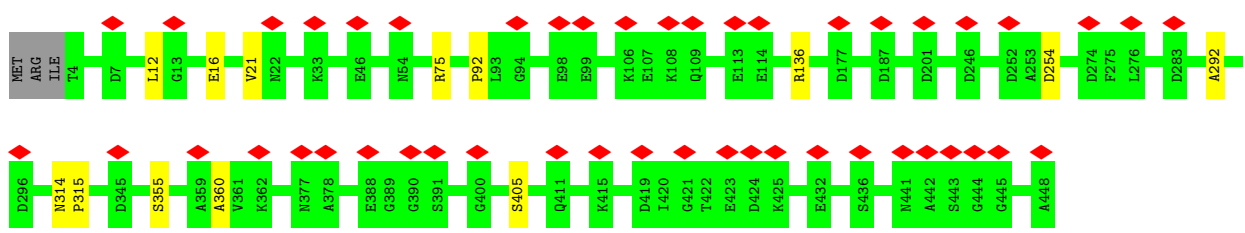
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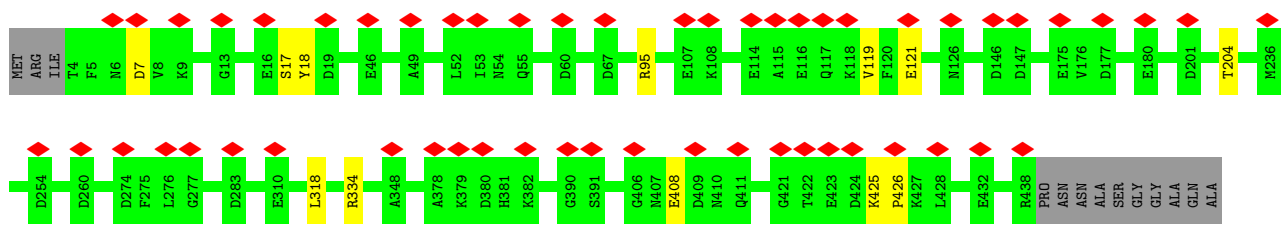
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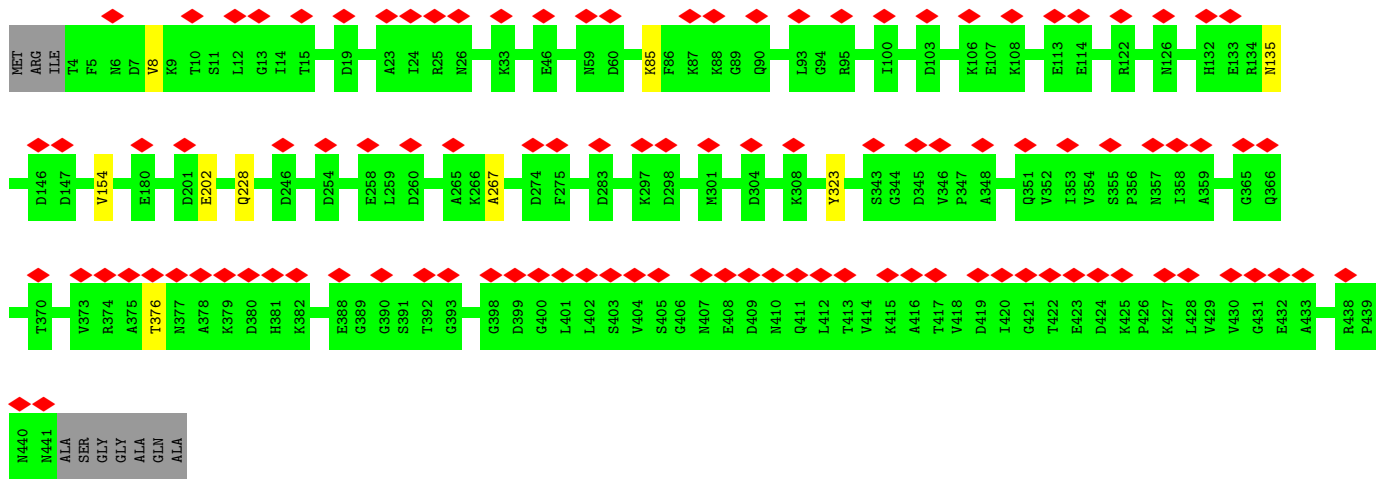
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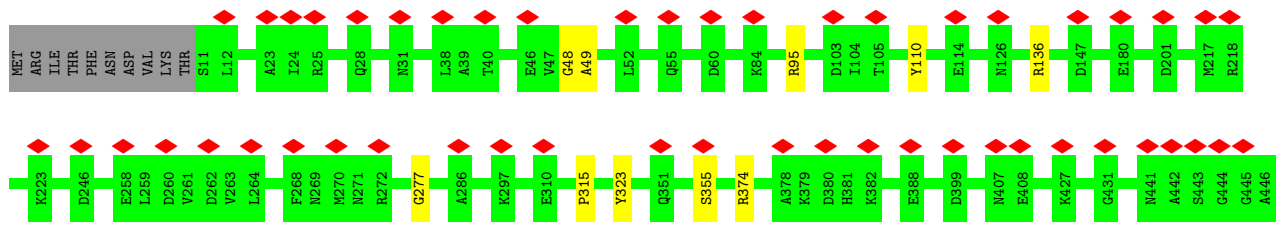
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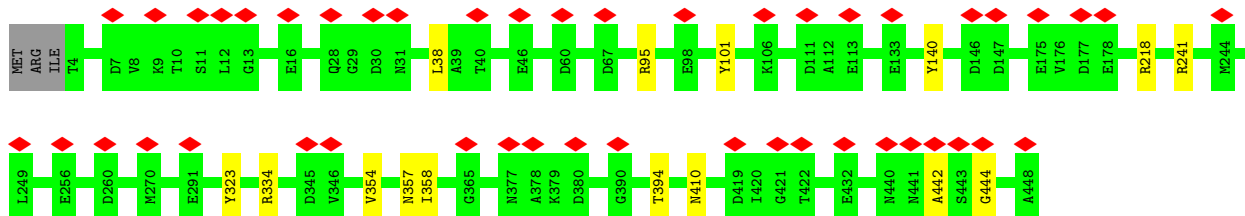


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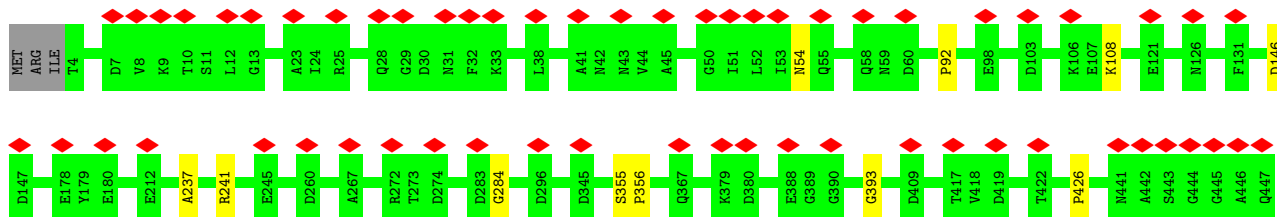




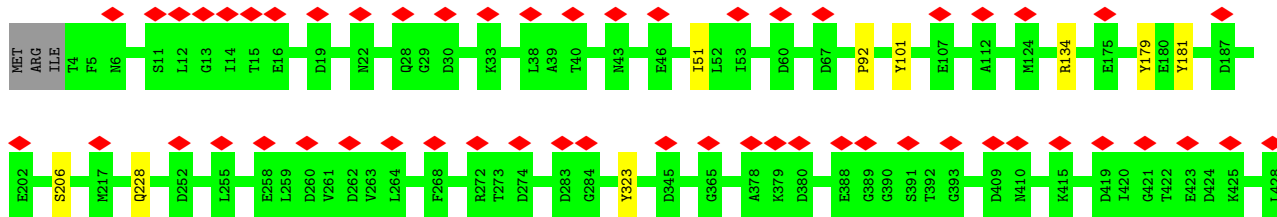
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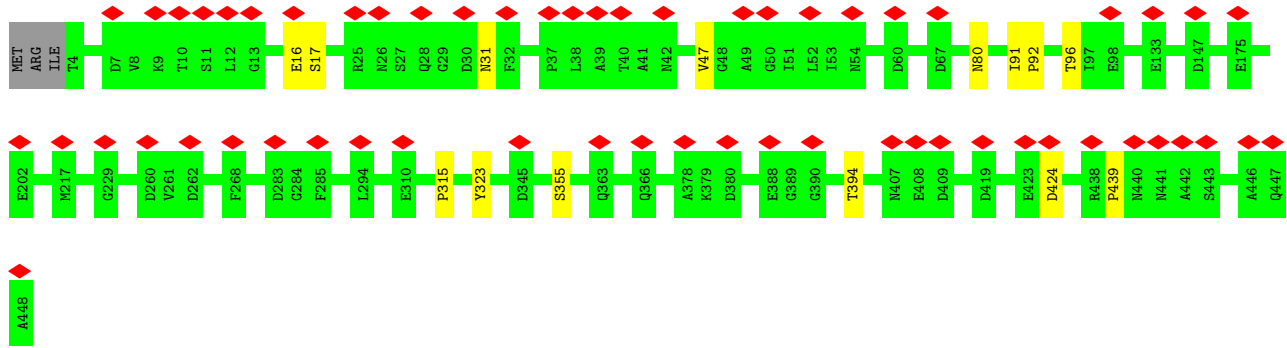


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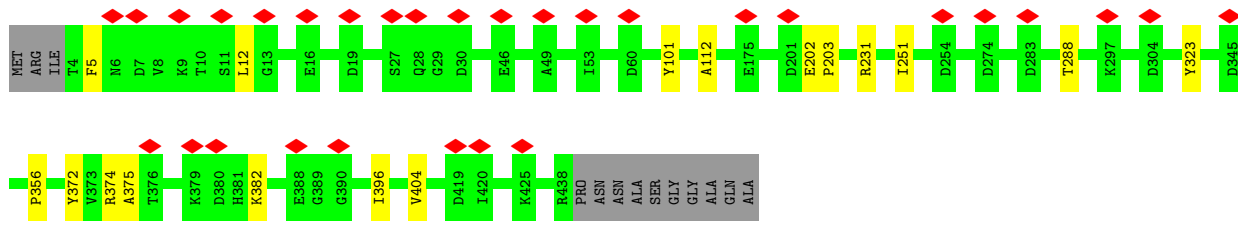
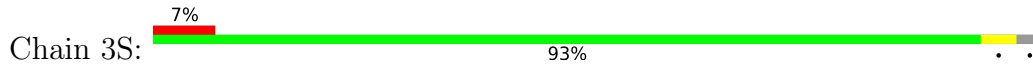


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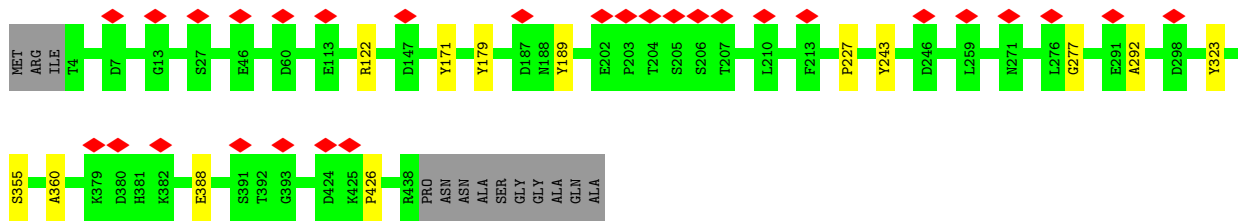




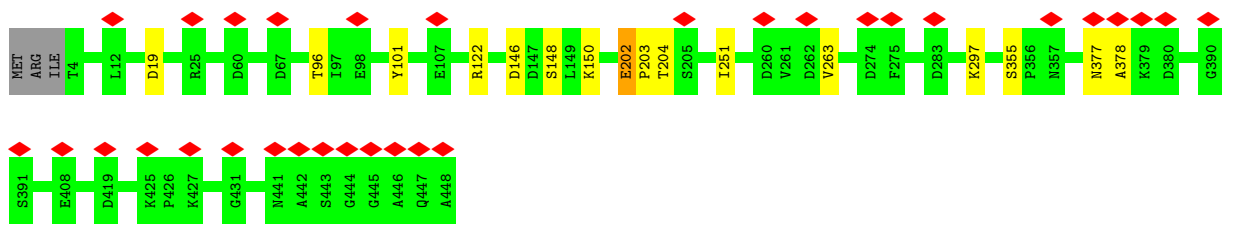
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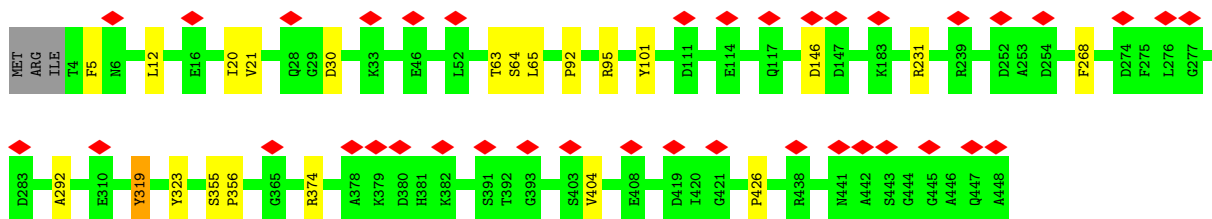


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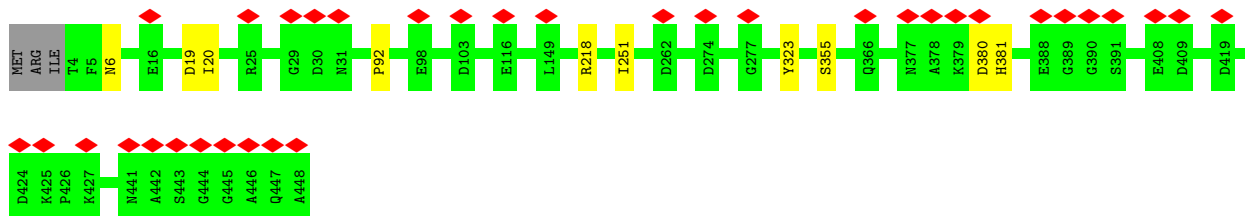


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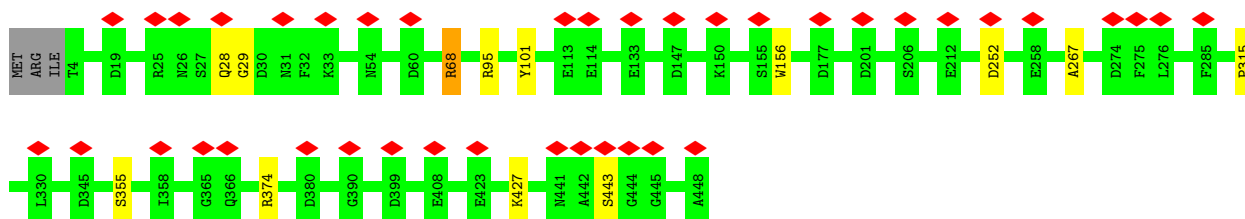




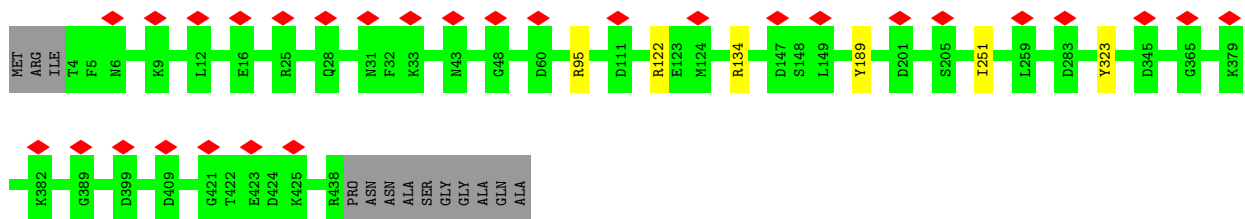
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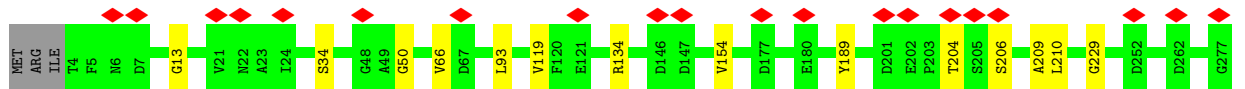
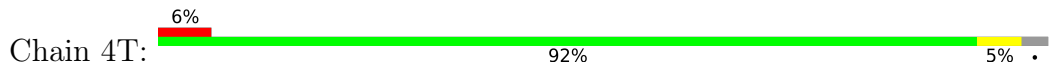
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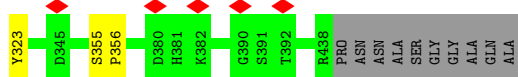
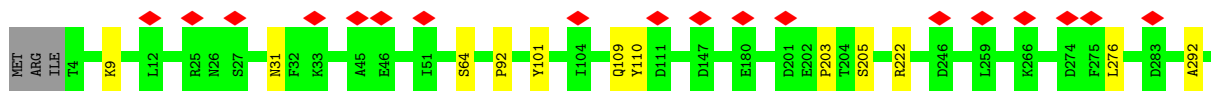


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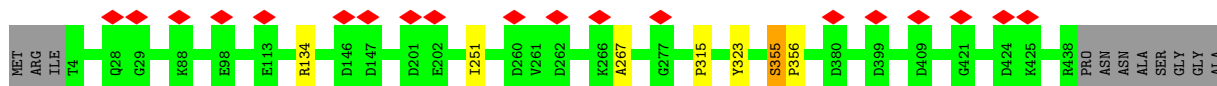




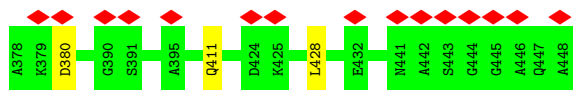
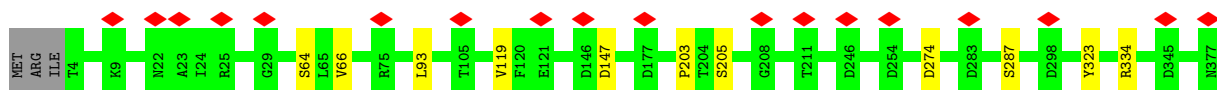
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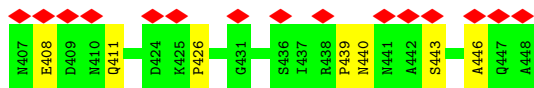
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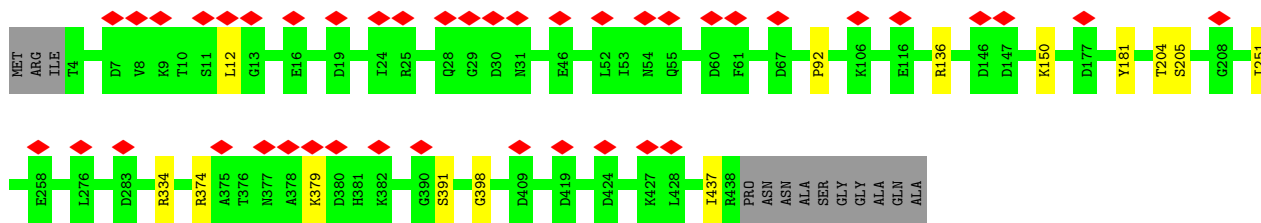


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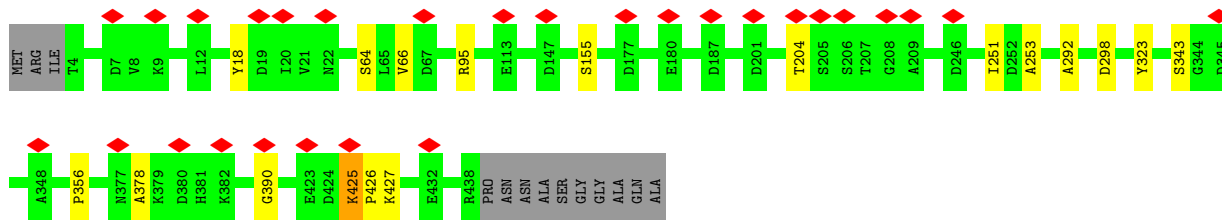


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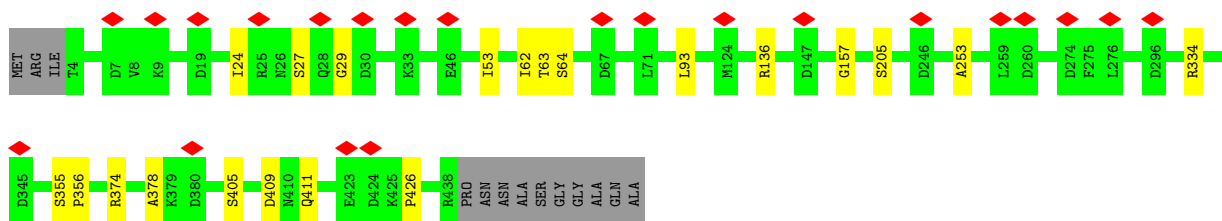




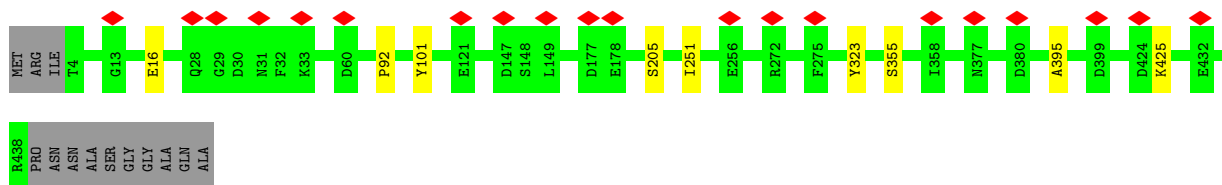
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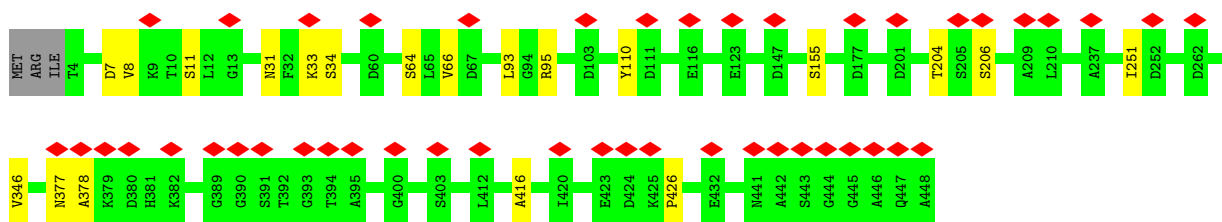
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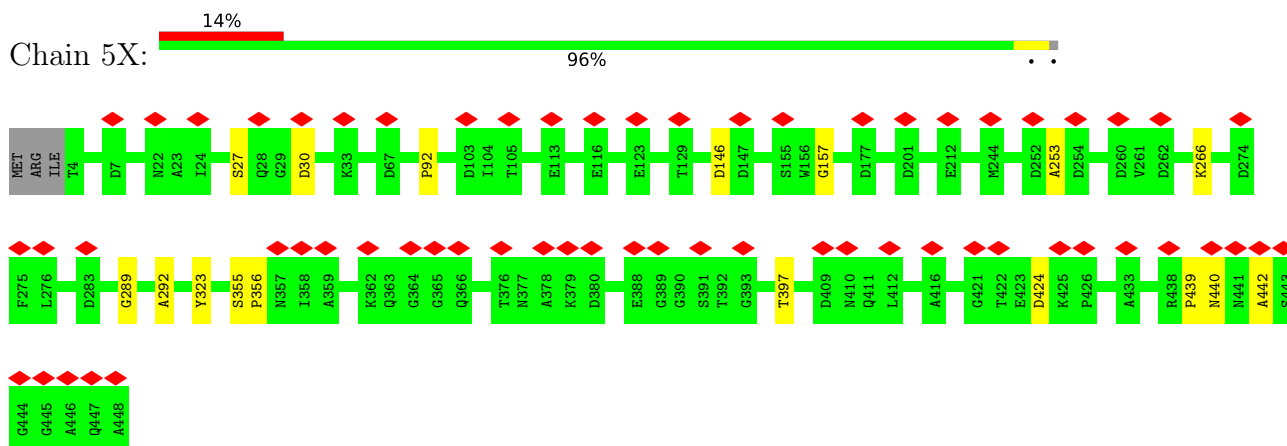
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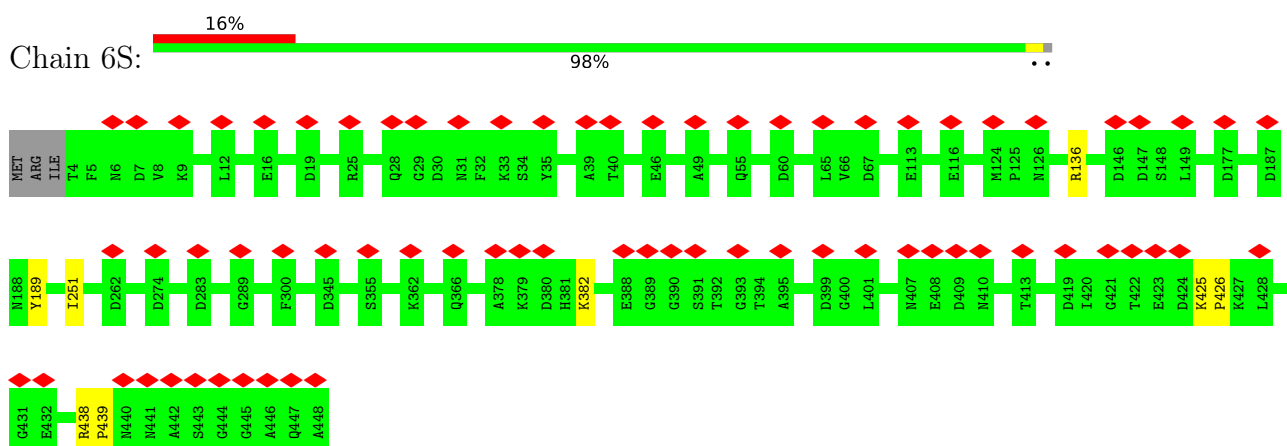
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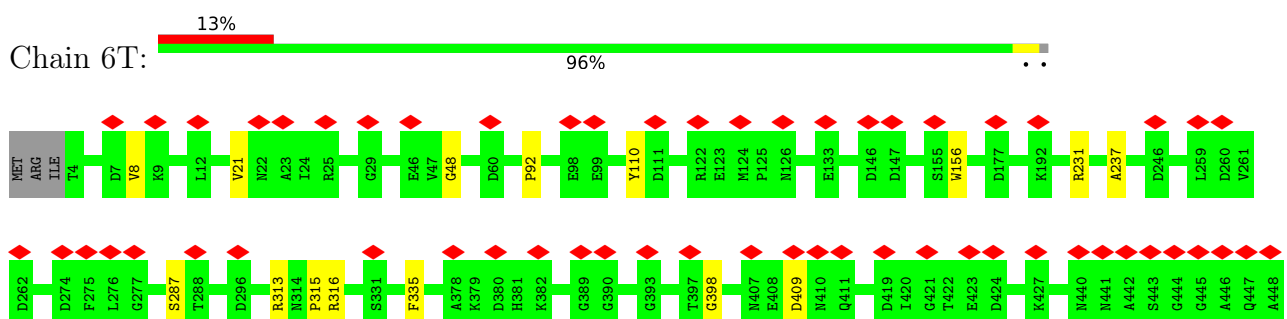
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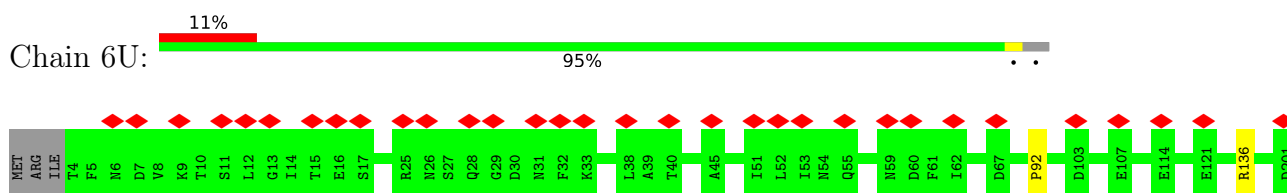
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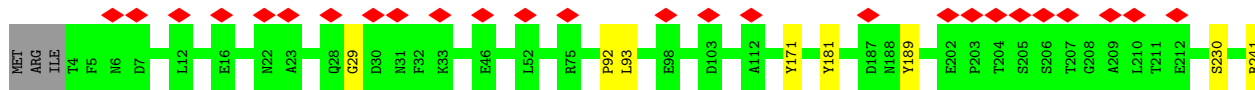


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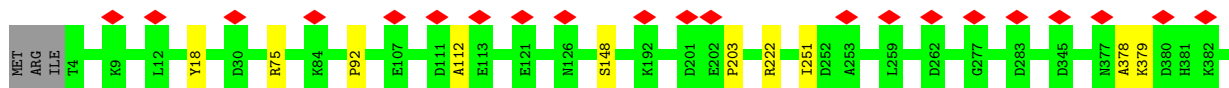




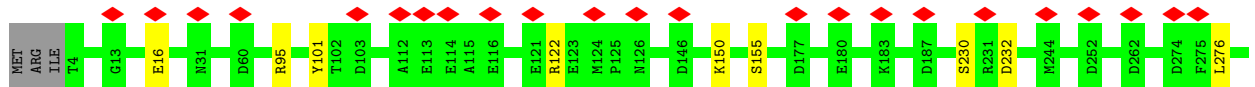
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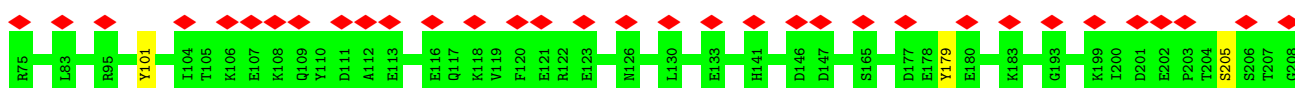
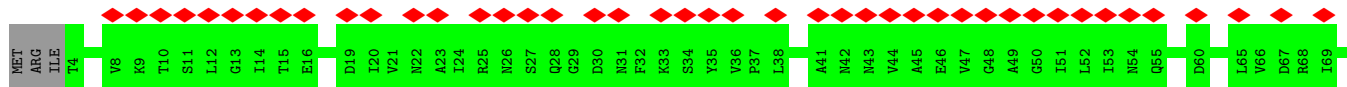
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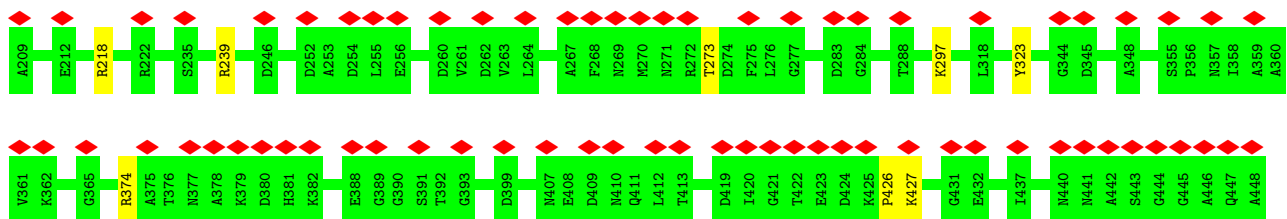


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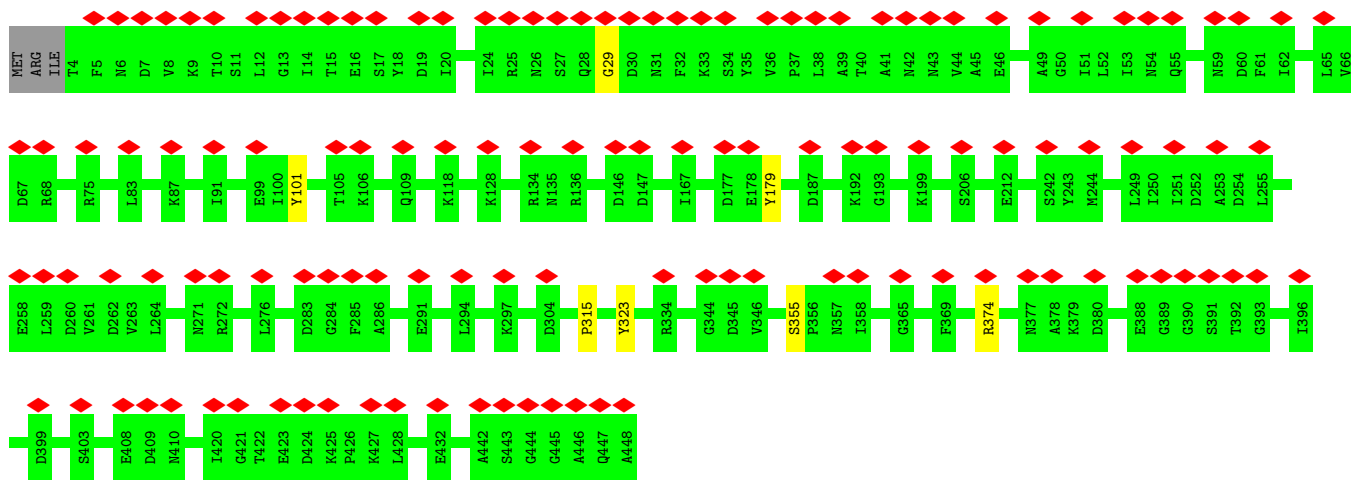


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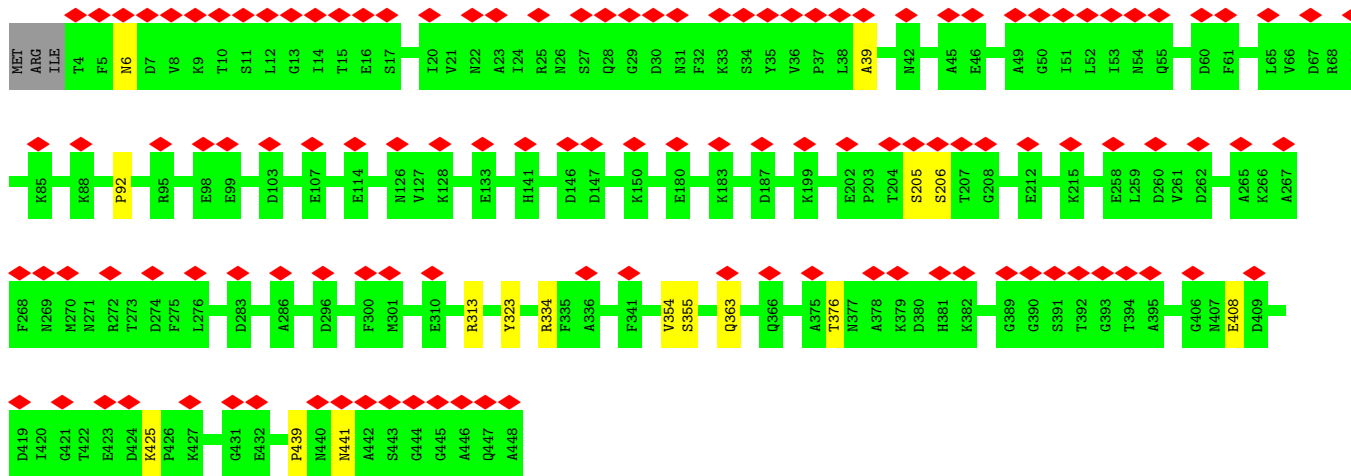




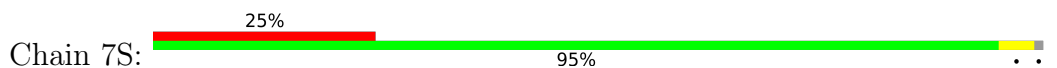
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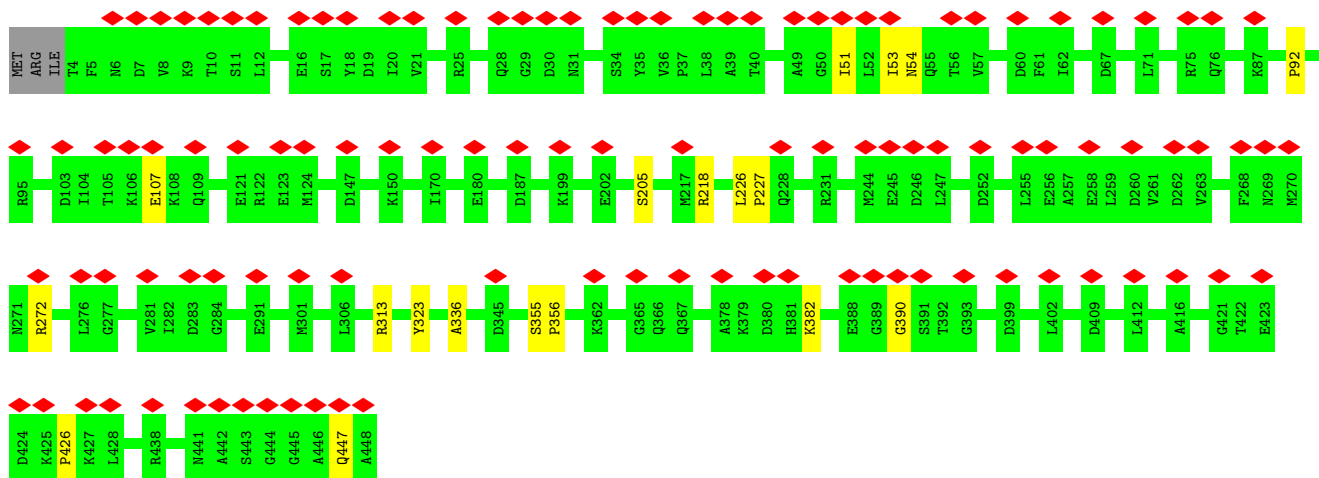


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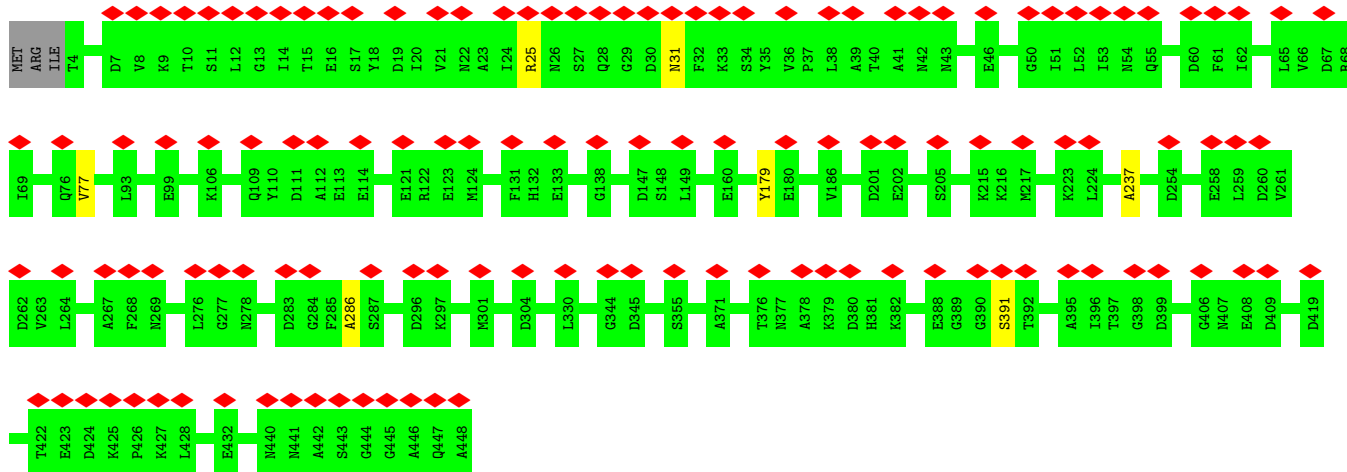


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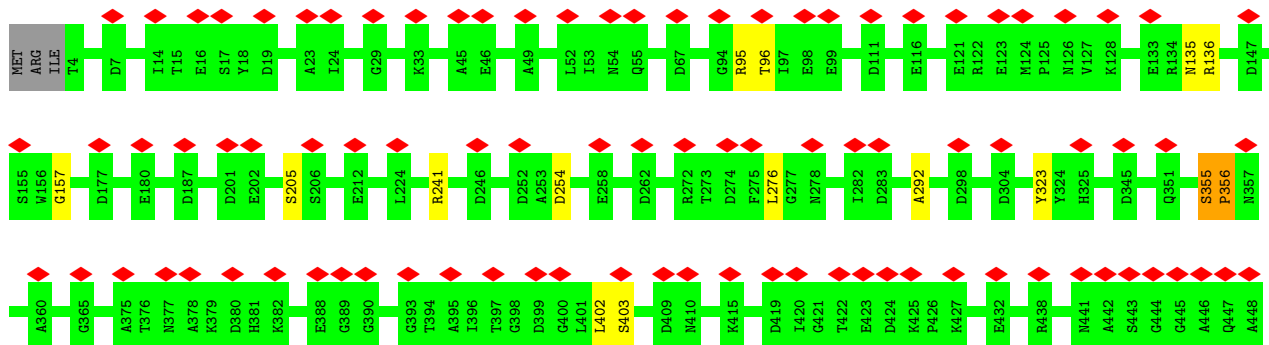




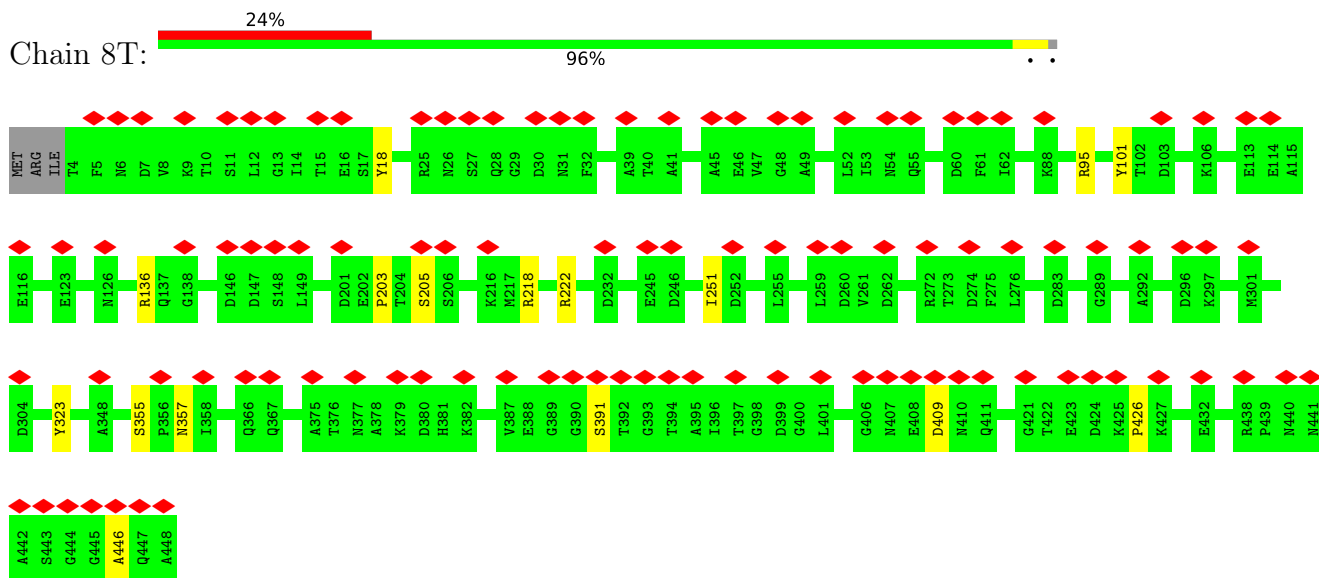
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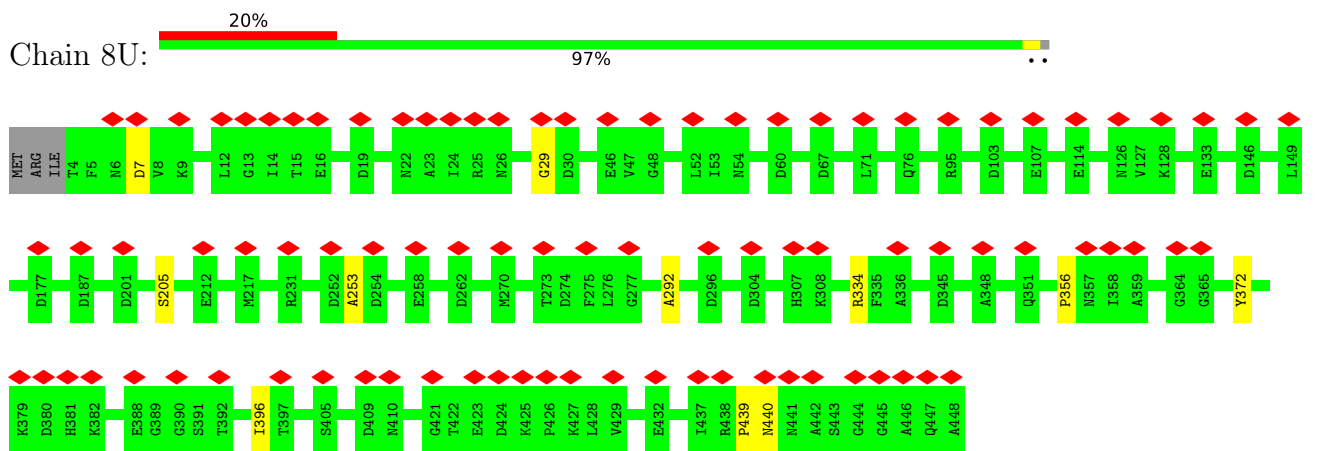
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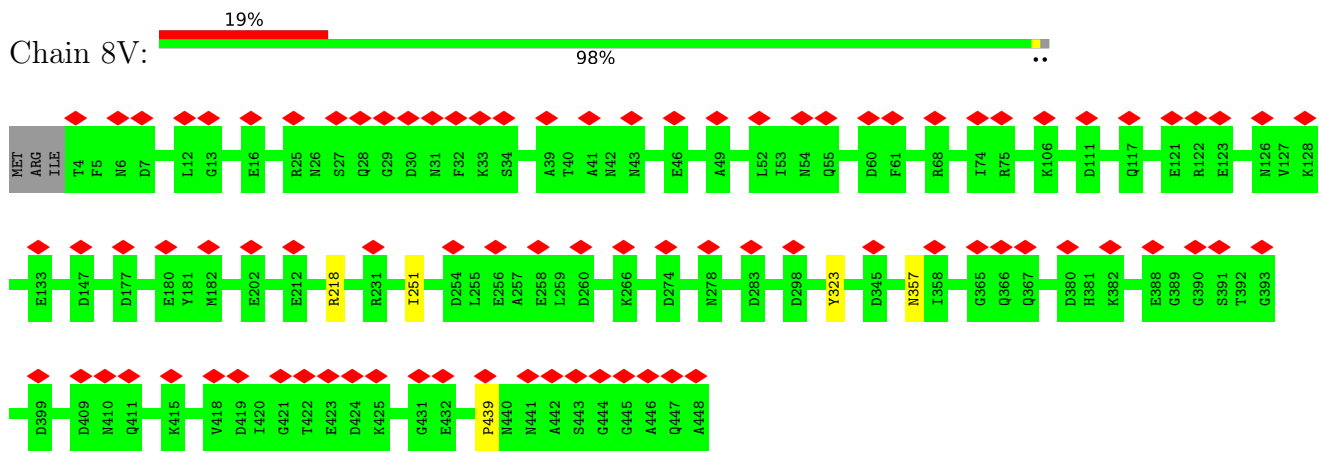
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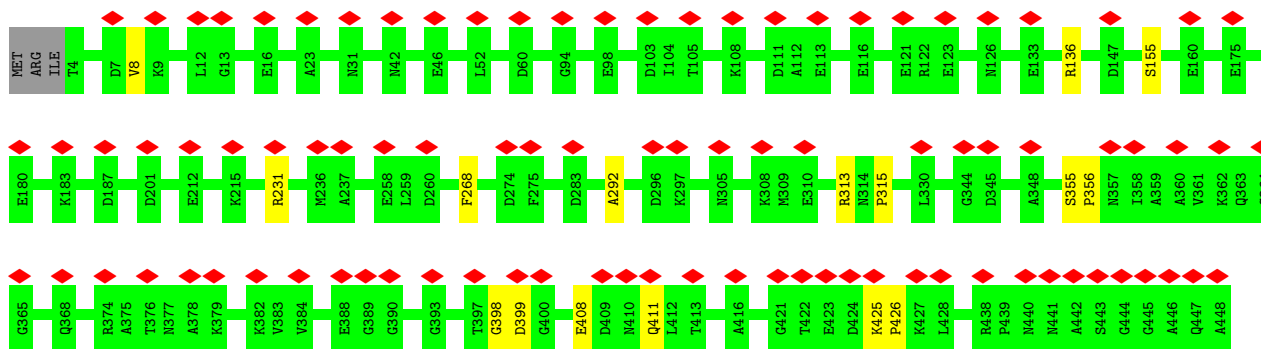


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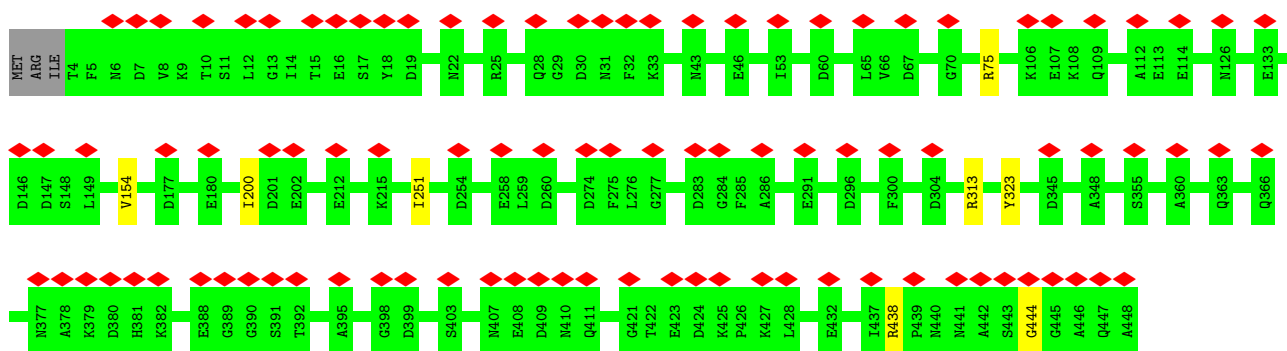


• Molecule 1: Major capsid protein

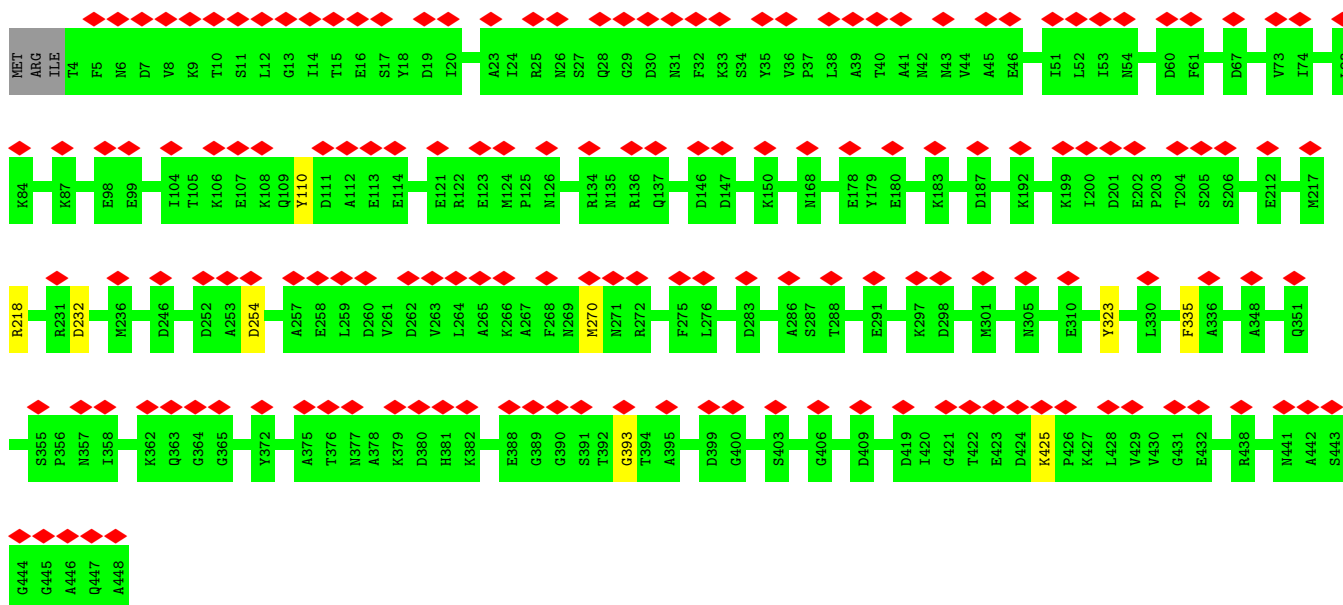




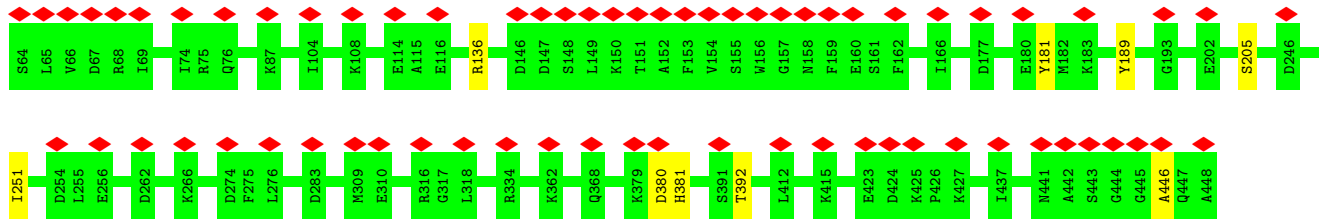
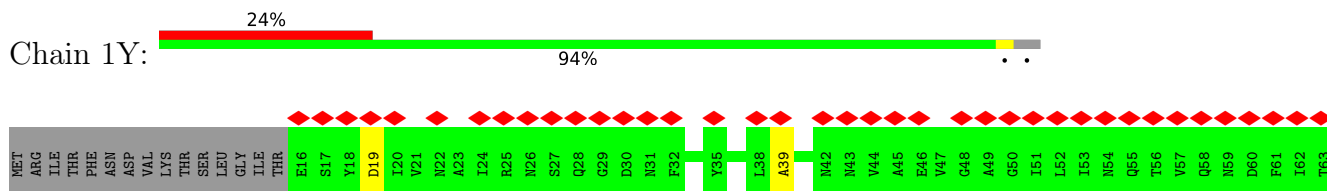
• Molecule 1: Major capsid protein



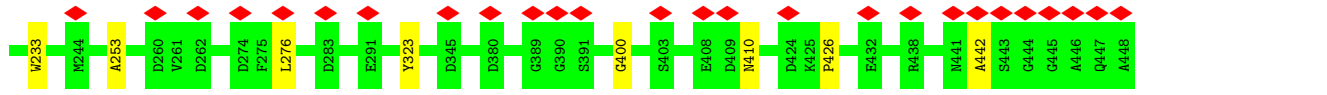
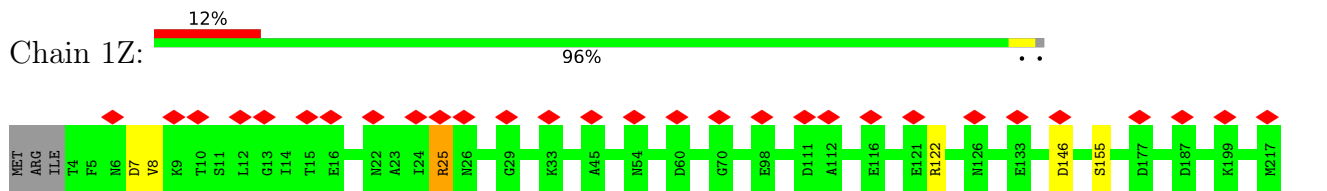
• Molecule 1: Major capsid protein



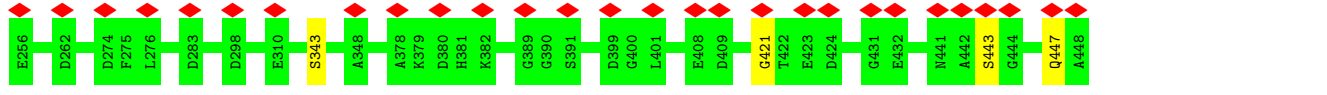
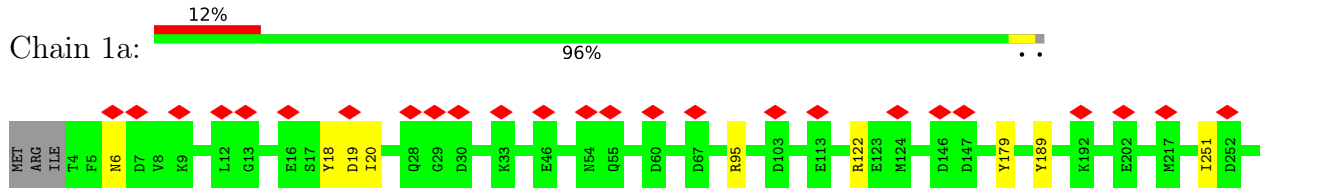
• Molecule 1: Major capsid protein



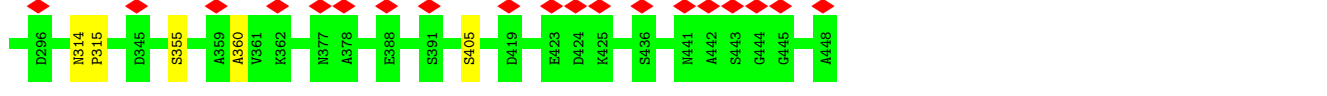
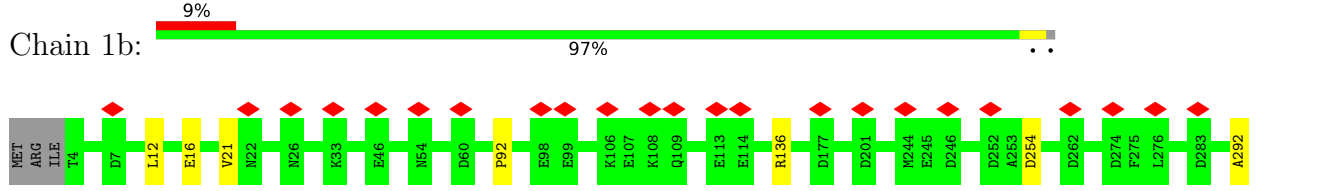
• Molecule 1: Major capsid protein



• Molecule 1: Major capsid protein

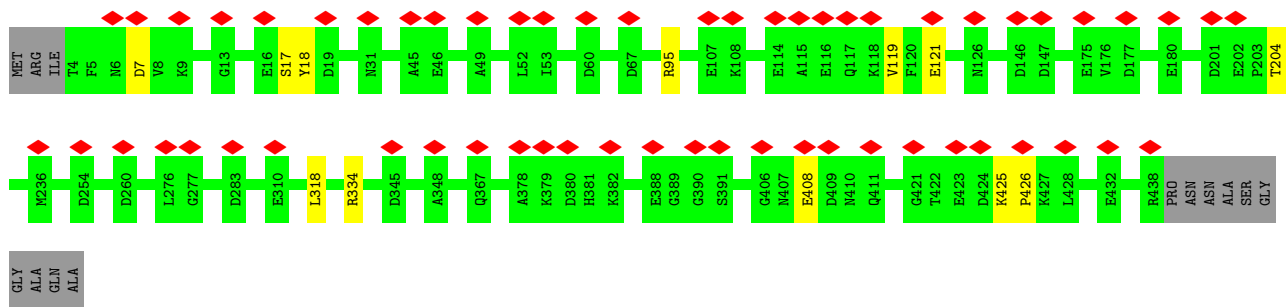


• Molecule 1: Major capsid protein

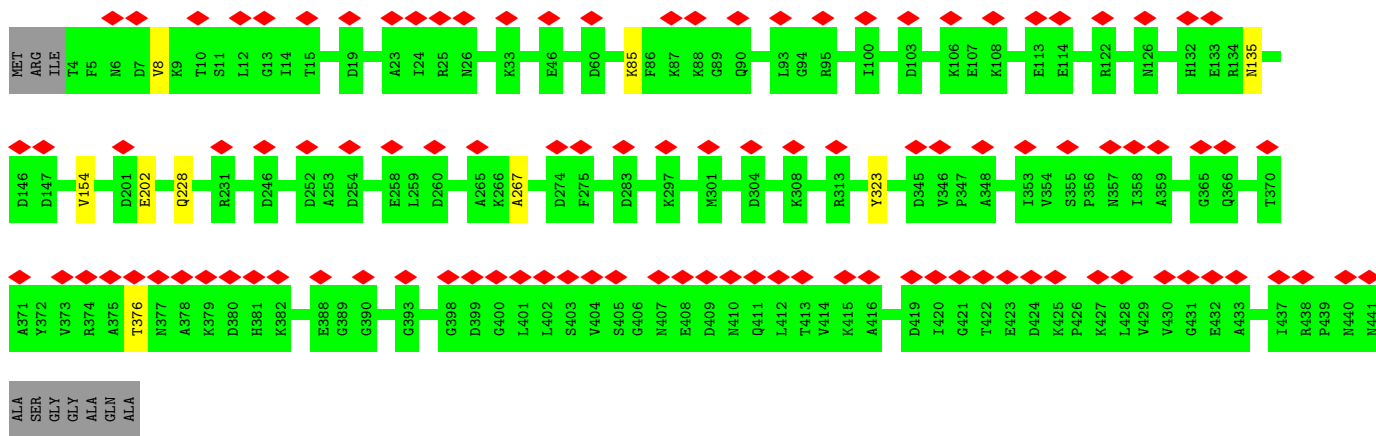


• Molecule 1: Major capsid protein

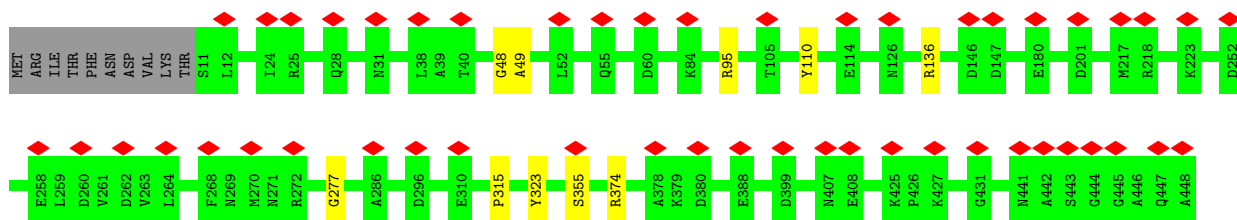




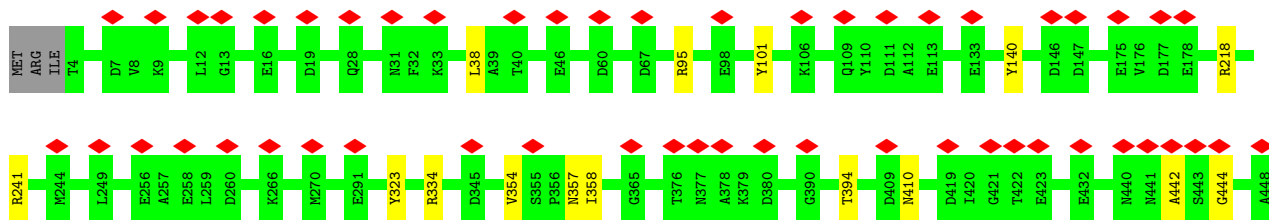
• Molecule 1: Major capsid protein



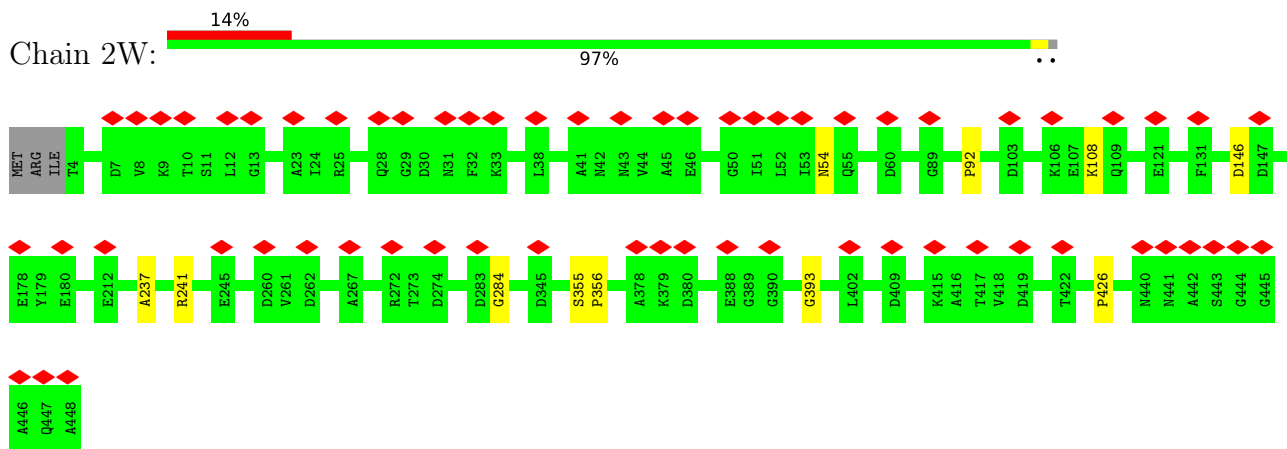
• Molecule 1: Major capsid protein



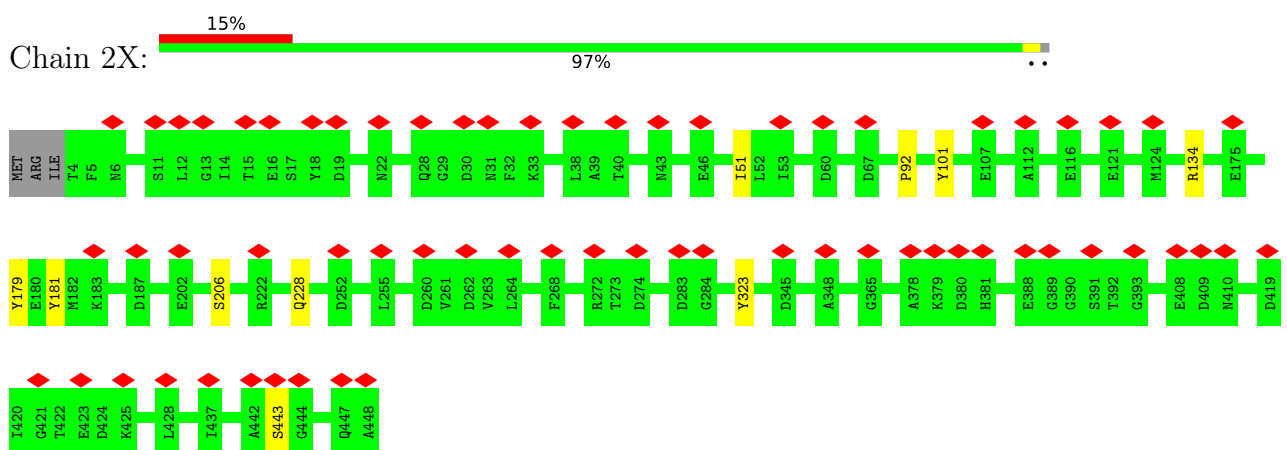
• Molecule 1: Major capsid protein



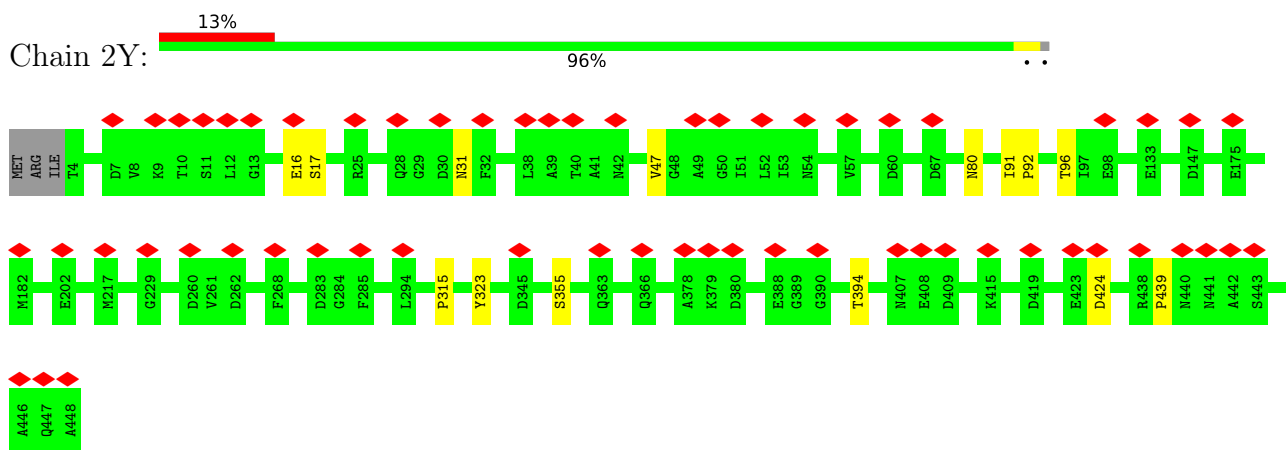
• Molecule 1: Major capsid protein



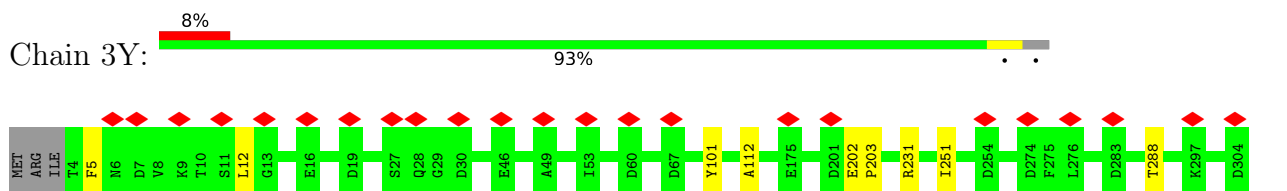
• Molecule 1: Major capsid protein

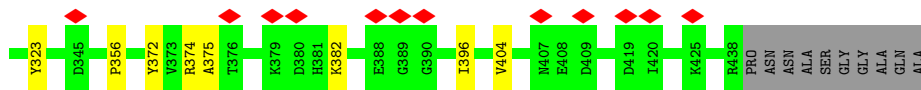


• Molecule 1: Major capsid protein

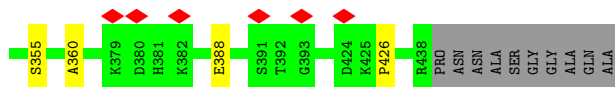
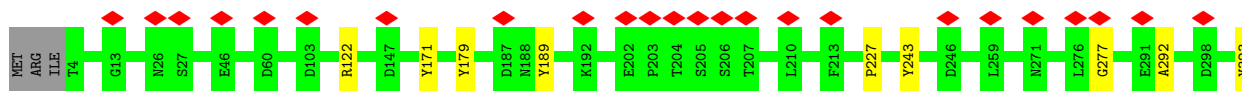


• Molecule 1: Major capsid protein

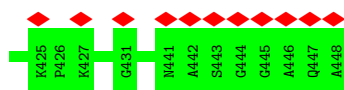
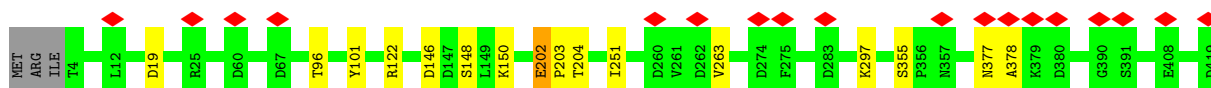




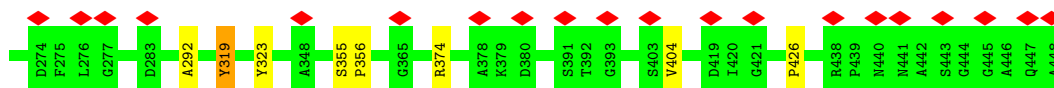
• Molecule 1: Major capsid protein



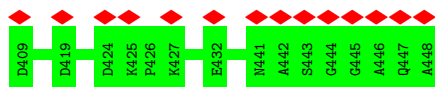
• Molecule 1: Major capsid protein



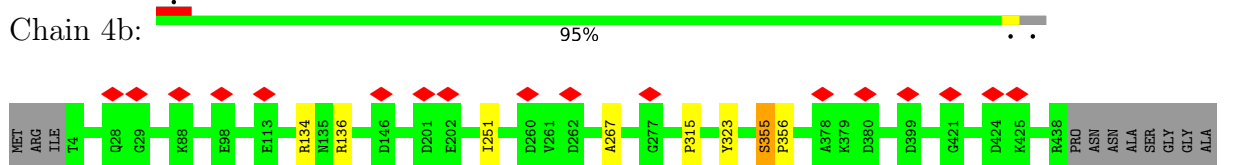
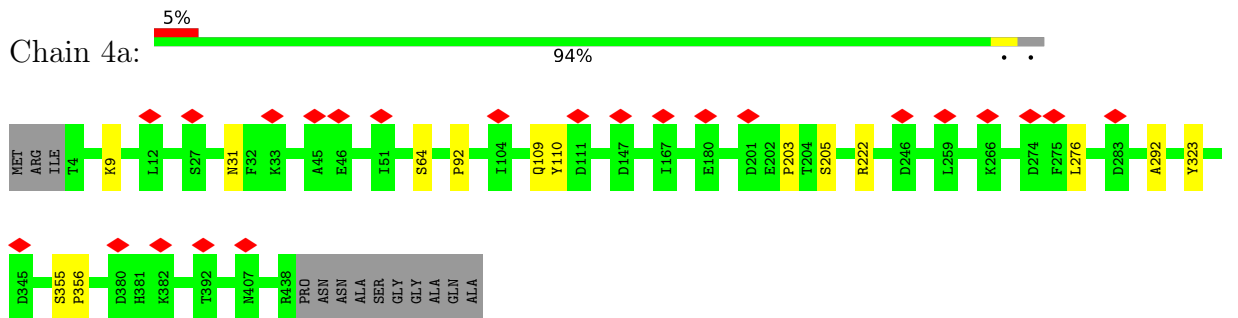
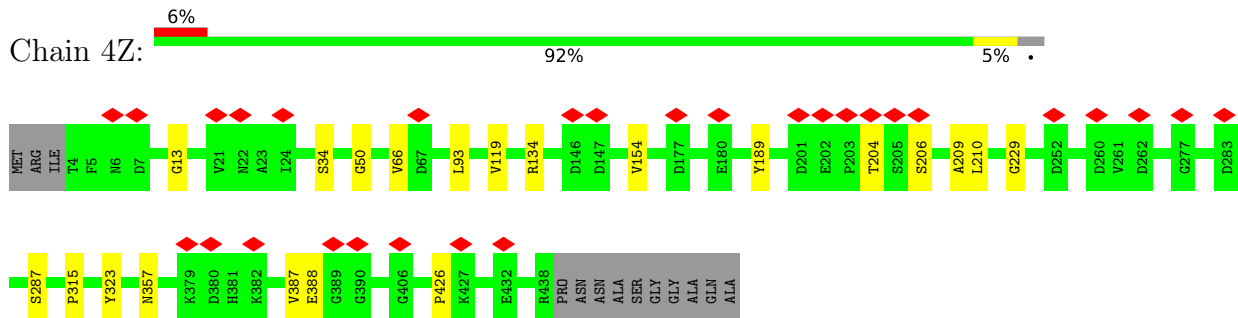
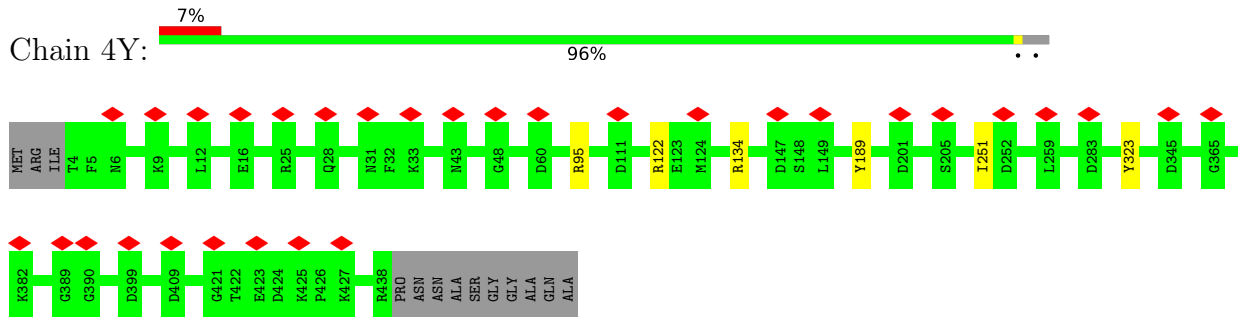
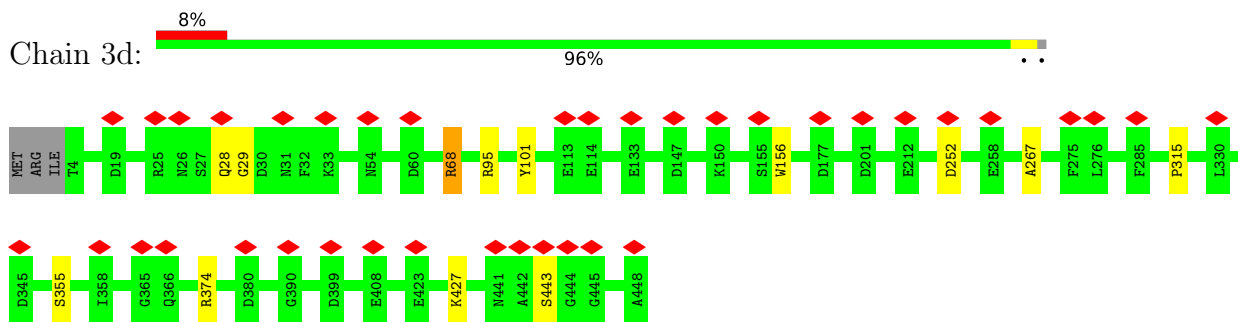
• Molecule 1: Major capsid protein



• Molecule 1: Major capsid protein

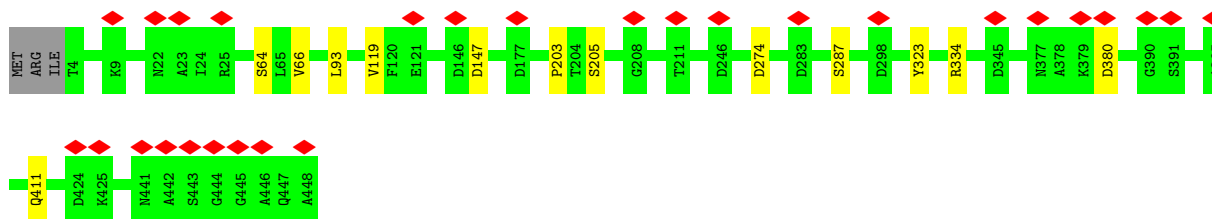


• Molecule 1: Major capsid protein

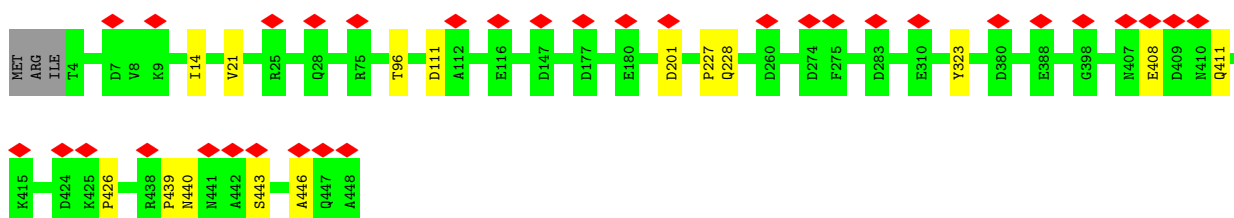


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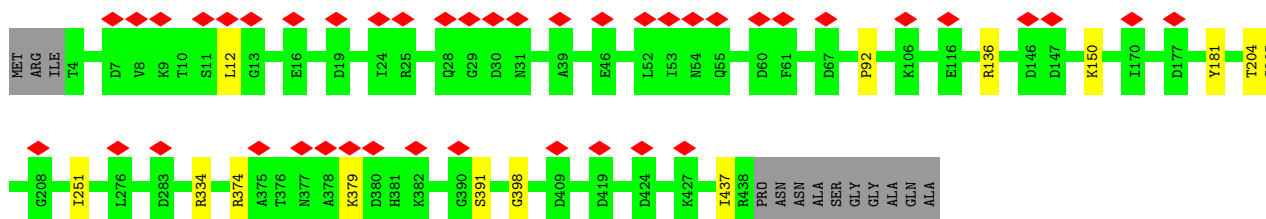
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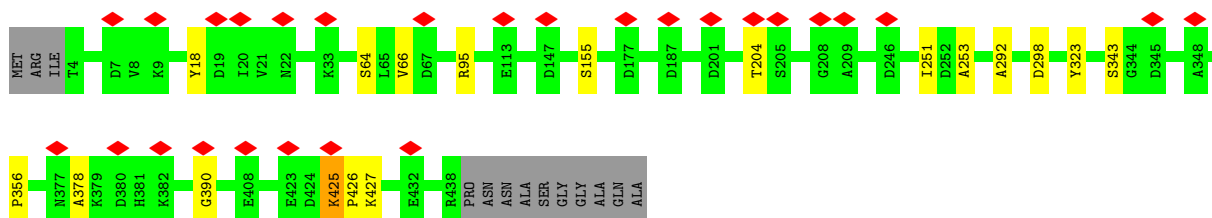
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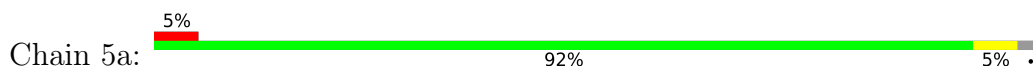
• Molecule 1: Major capsid protein

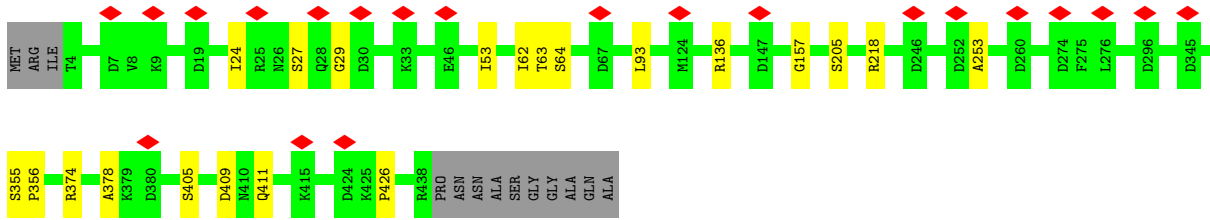


• Molecule 1: Major capsid protein

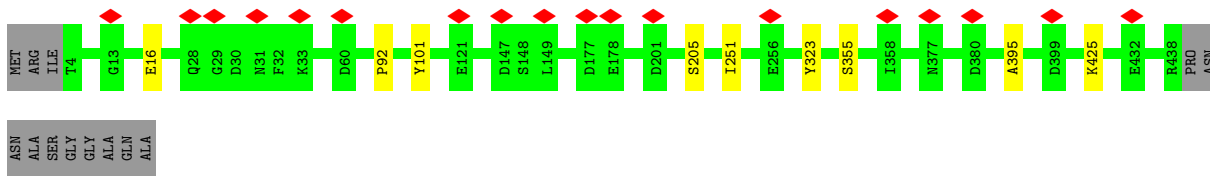


• Molecule 1: Major capsid protein

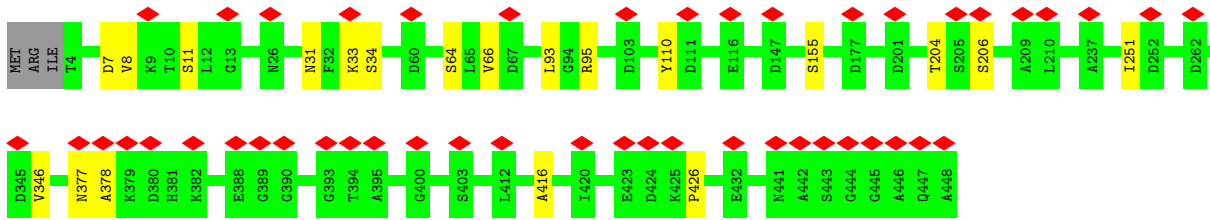




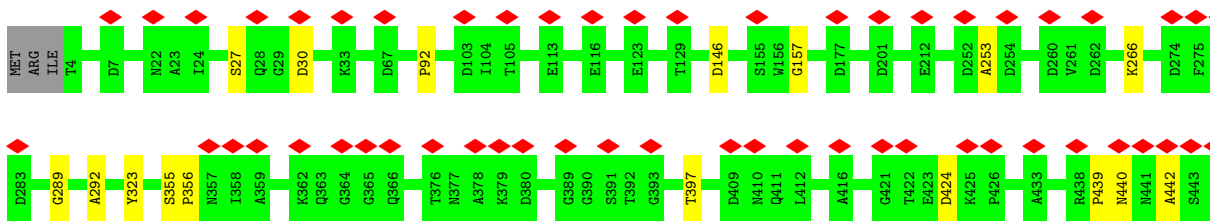
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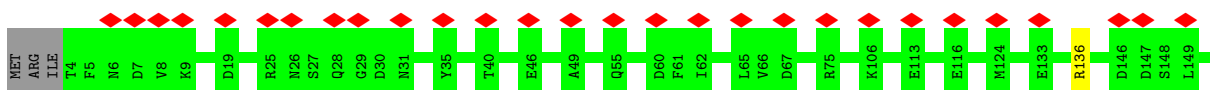
• Molecule 1: Major capsid protein

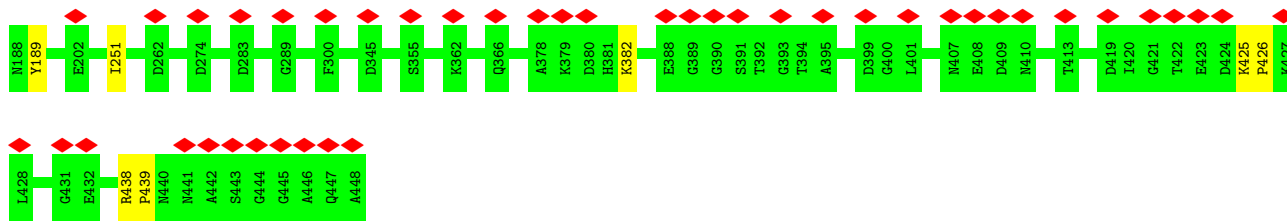


• Molecule 1: Major capsid protein

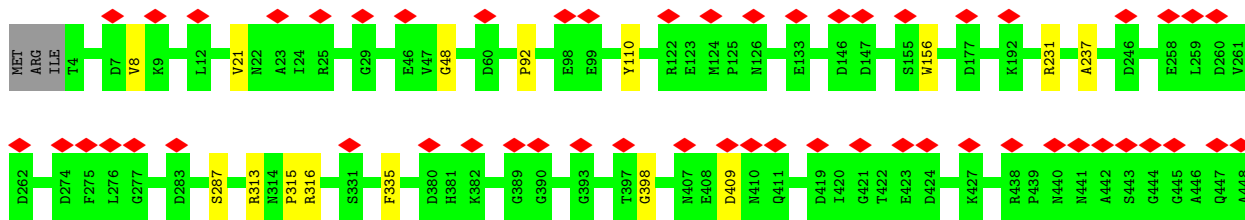


• Molecule 1: Major capsid protein

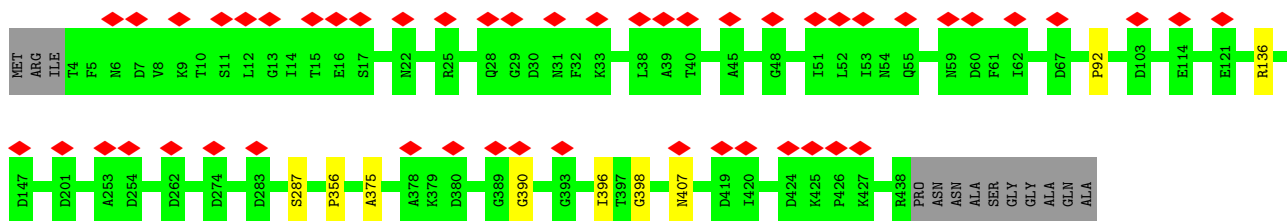




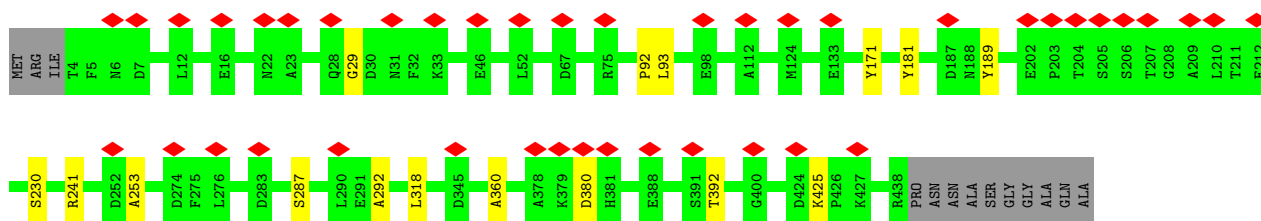
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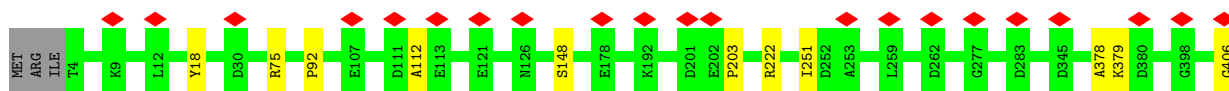
• Molecule 1: Major capsid protein



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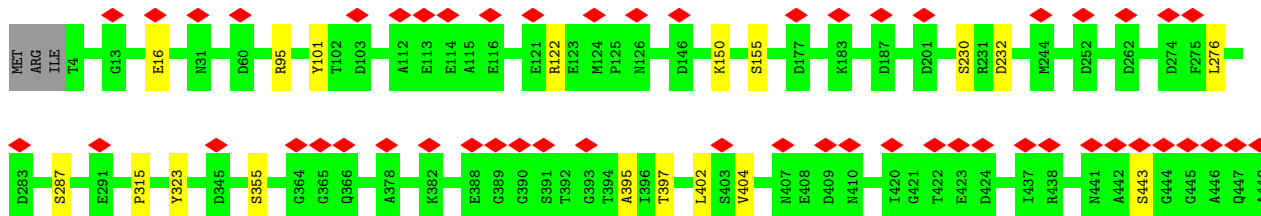


• Molecule 1: Major capsid protein

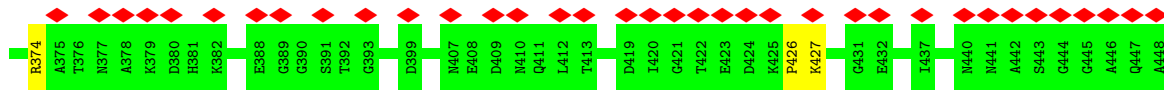
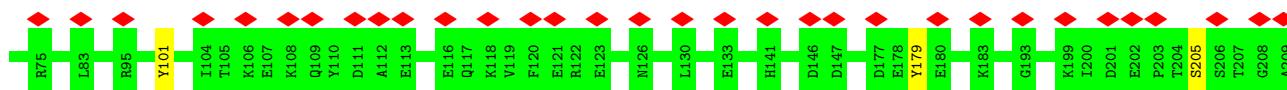
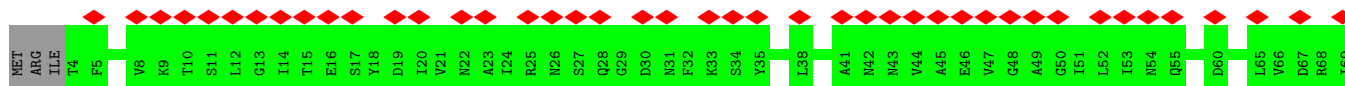




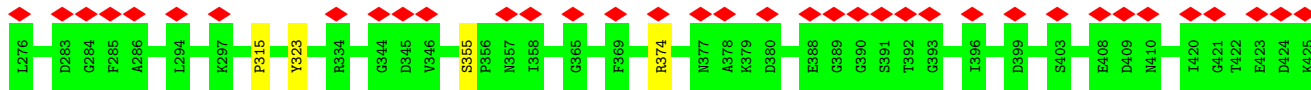
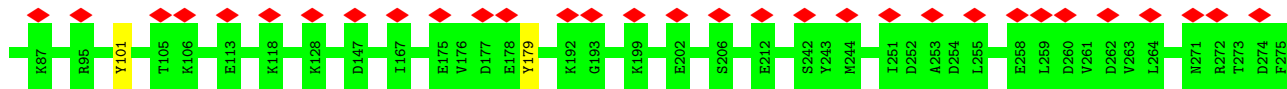
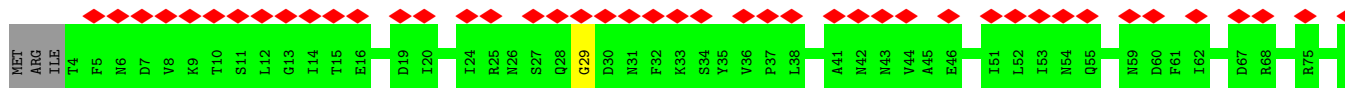
• Molecule 1: Major capsid protein

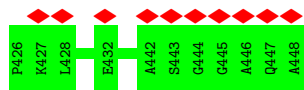


• Molecule 1: Major capsid protein

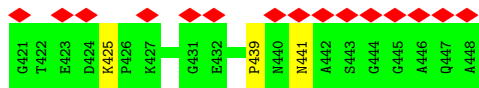
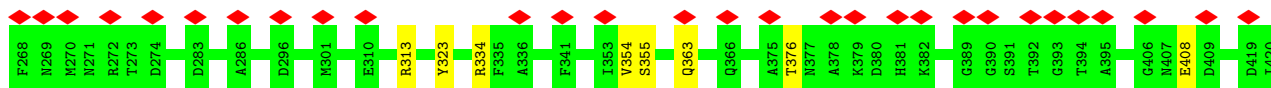
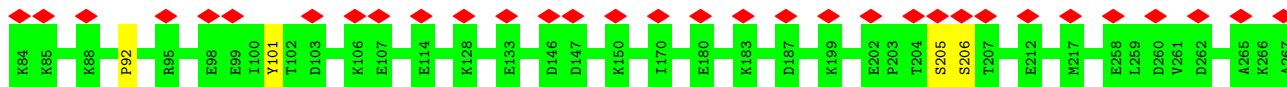
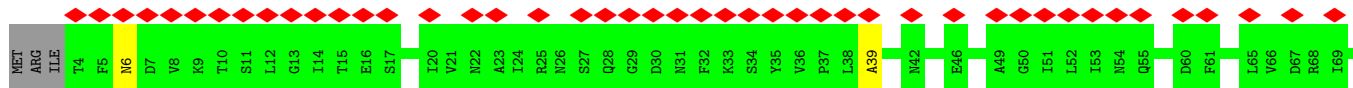


• Molecule 1: Major capsid protein

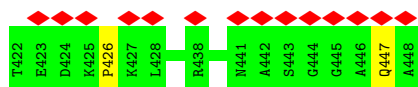
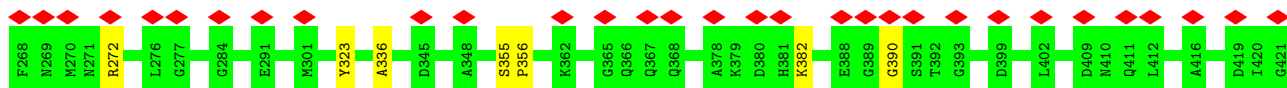
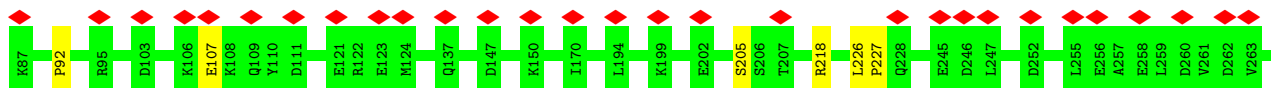
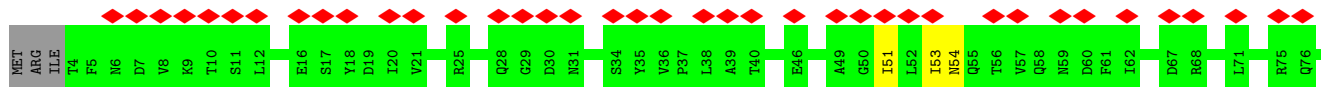




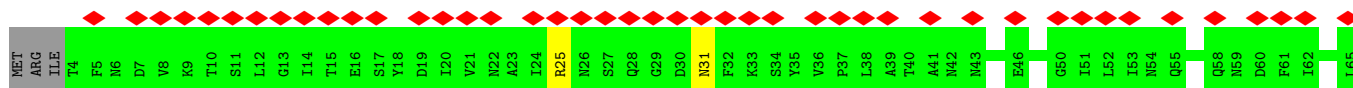
• Molecule 1: Major capsid protein

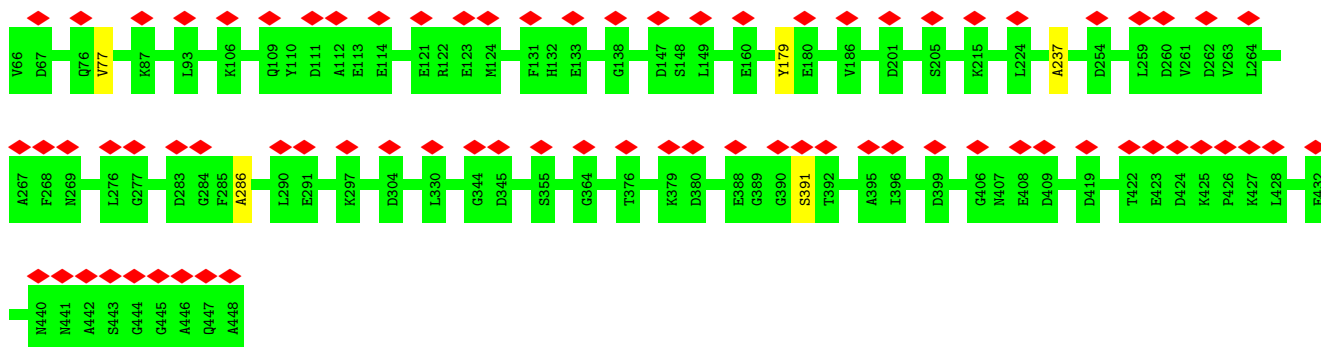


• Molecule 1: Major capsid protein

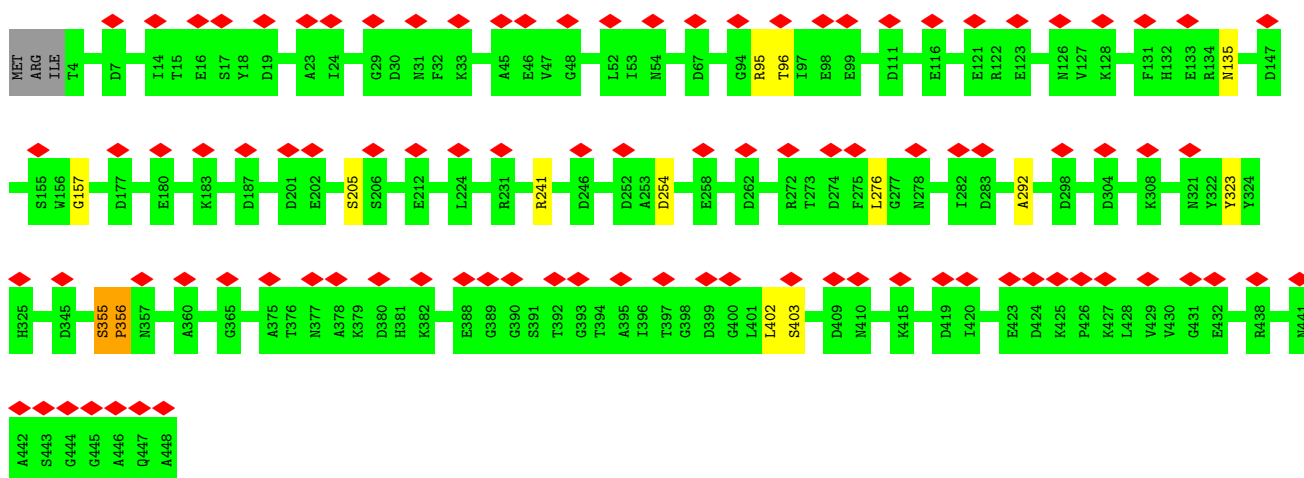


• Molecule 1: Major capsid protein

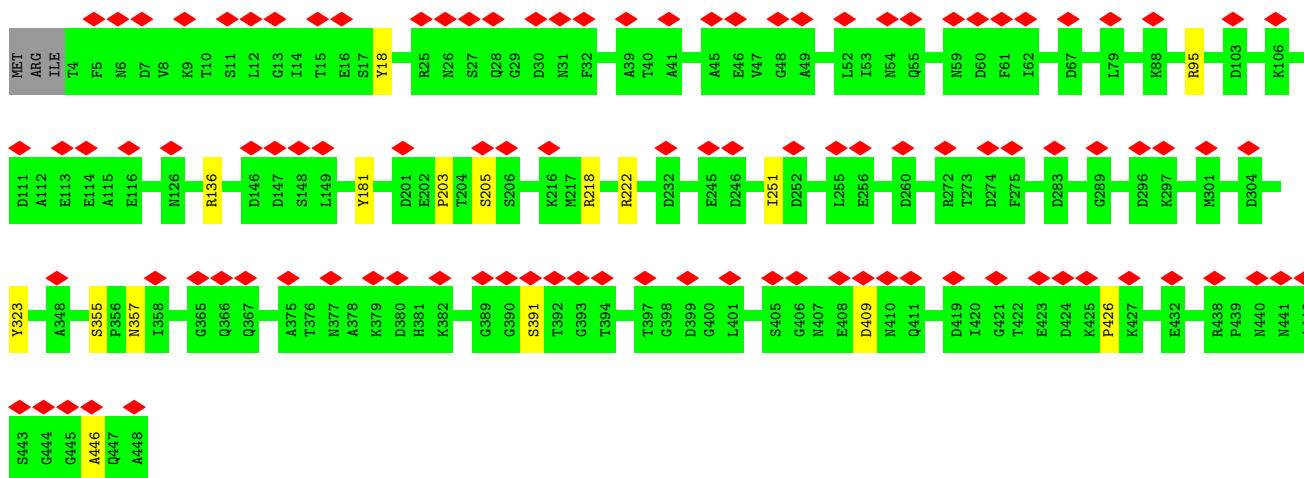




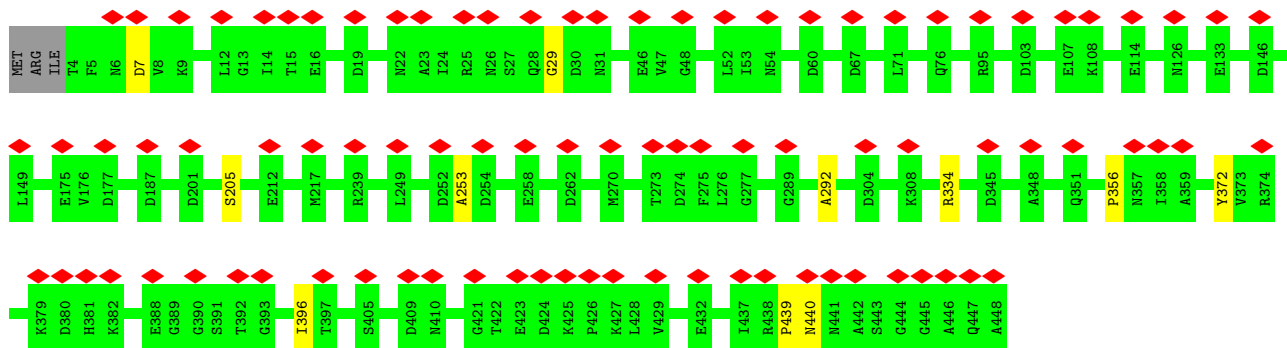
• Molecule 1: Major capsid protein



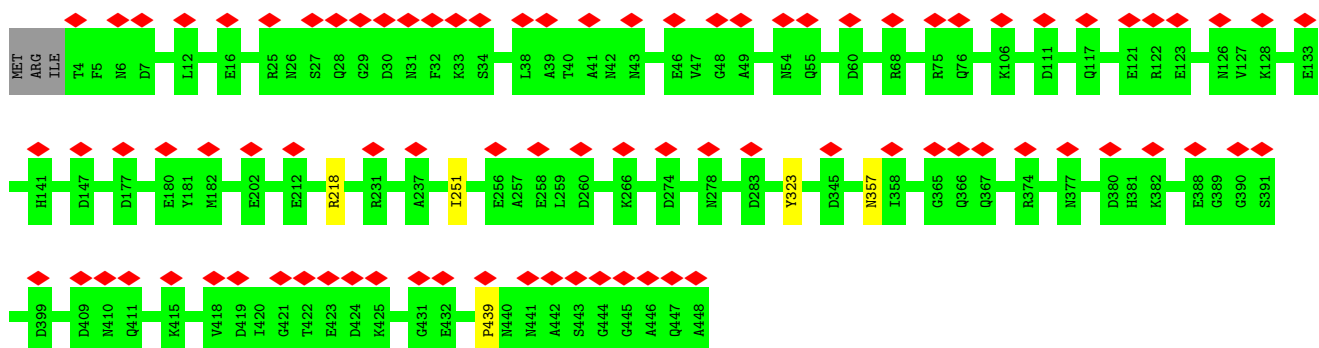
• Molecule 1: Major capsid protein



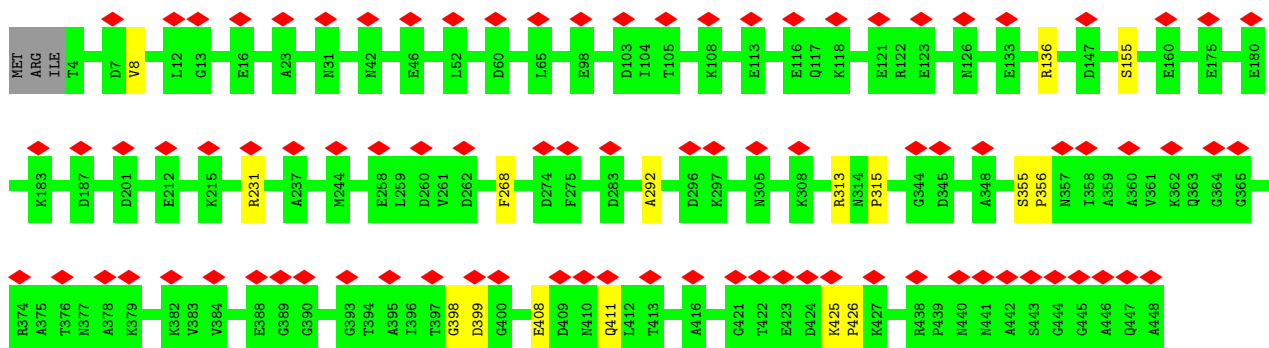
• Molecule 1: Major capsid protein



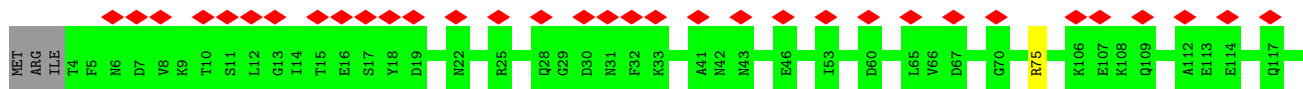
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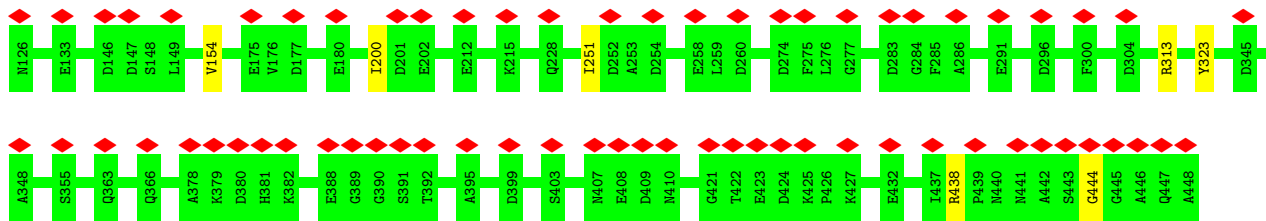


• Molecule 1: Major capsid protein

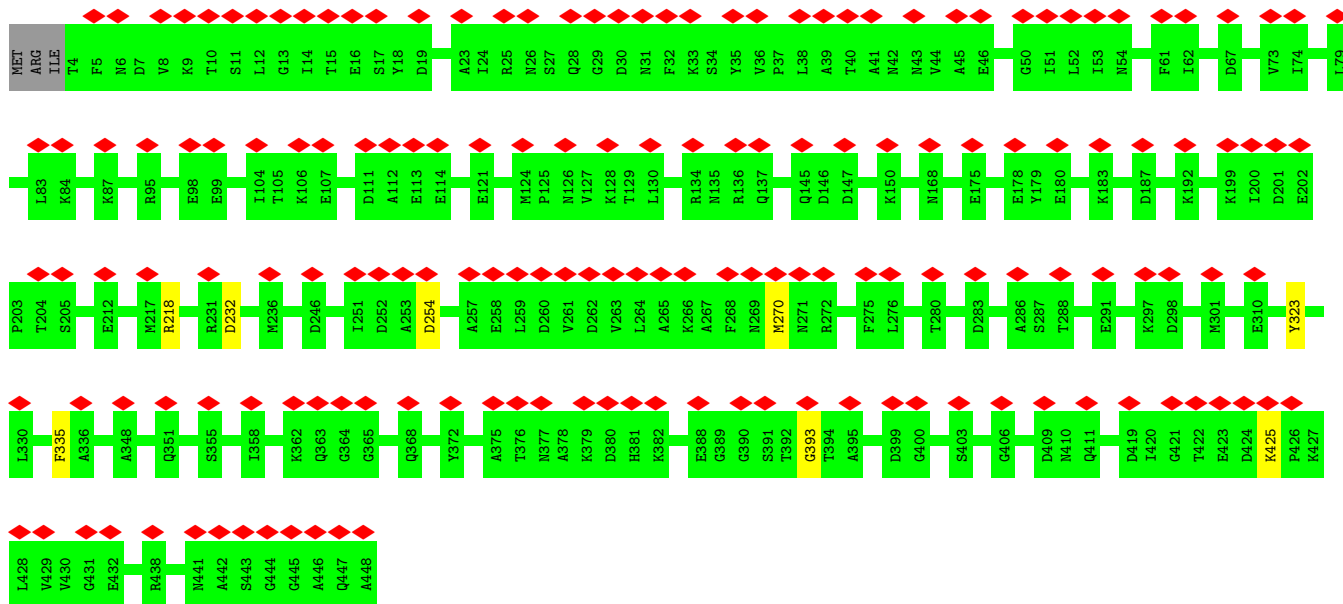


• Molecule 1: Major capsid protein

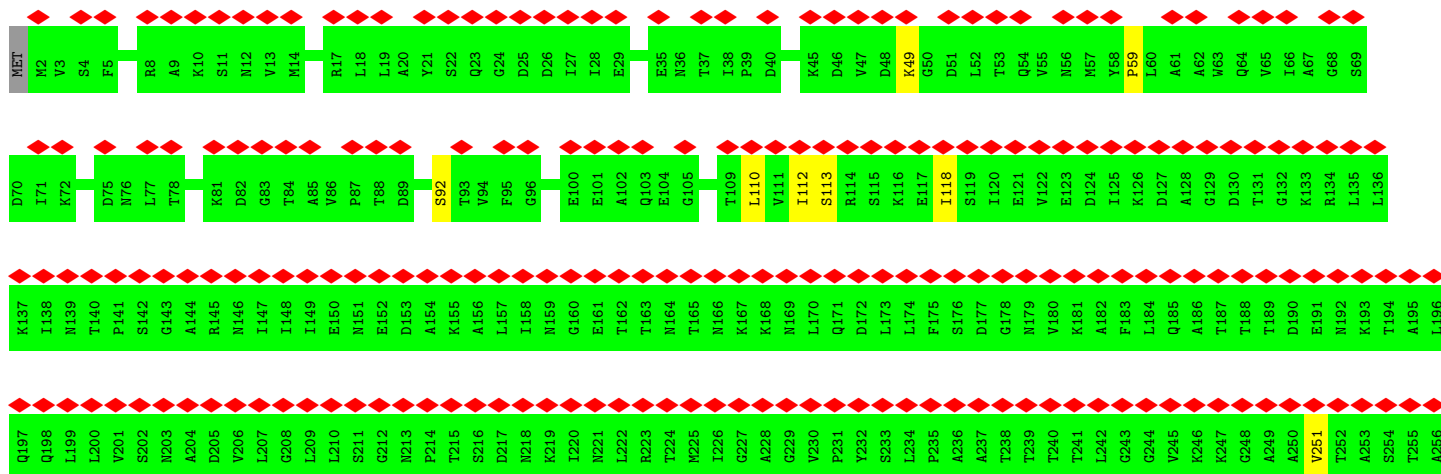
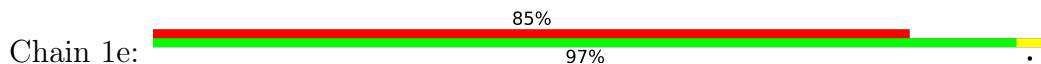


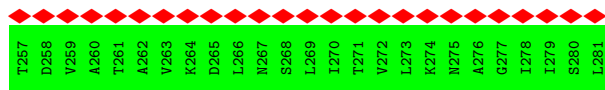


• Molecule 1: Major capsid protein

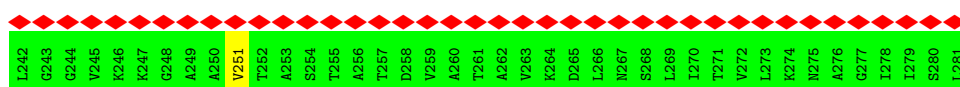
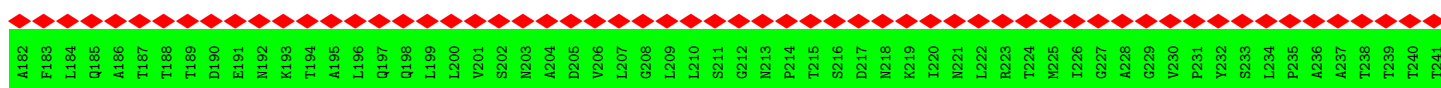
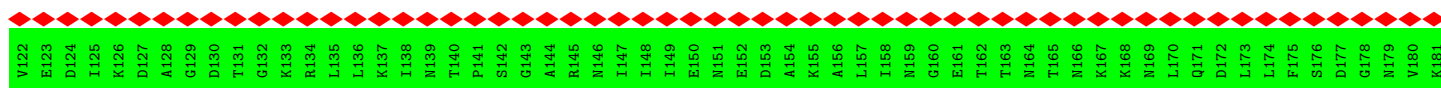
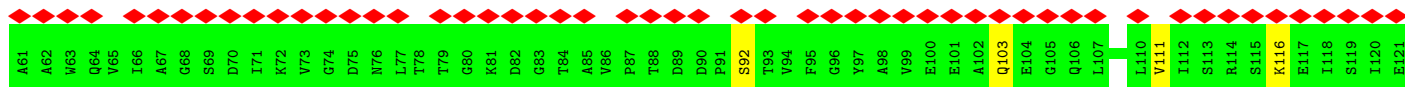
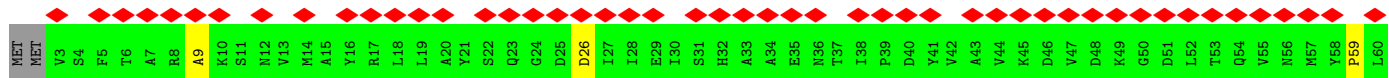


• Molecule 2: Capsid fiber protein

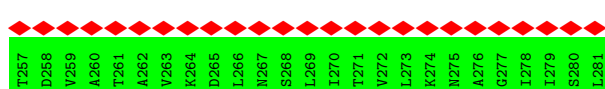
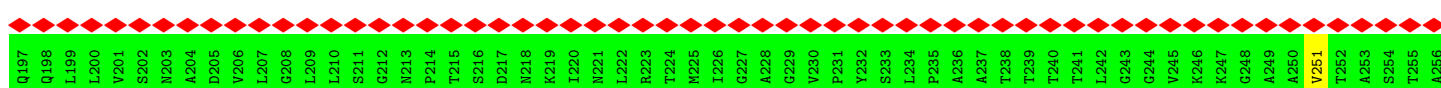
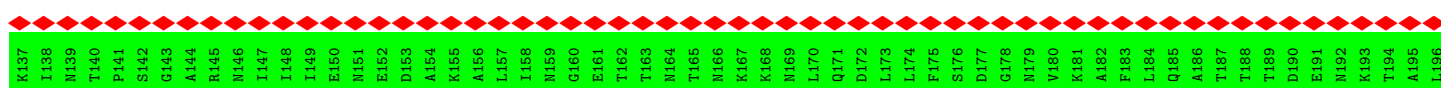
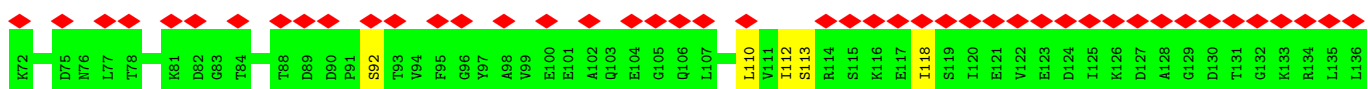
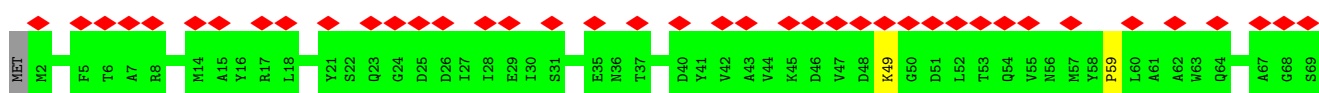
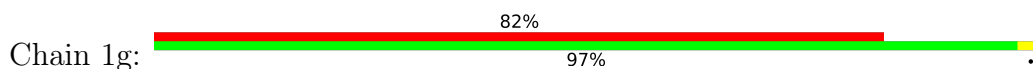




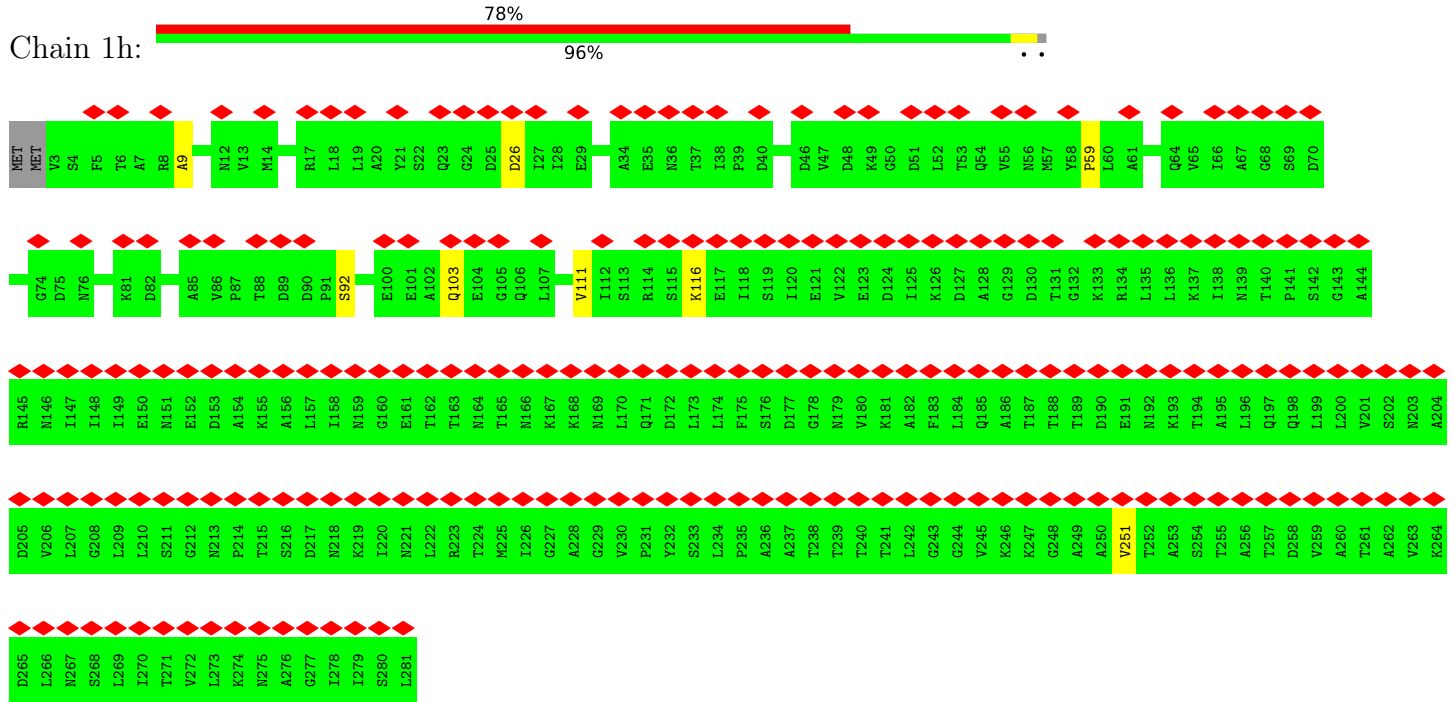
• Molecule 2: Capsid fiber protein



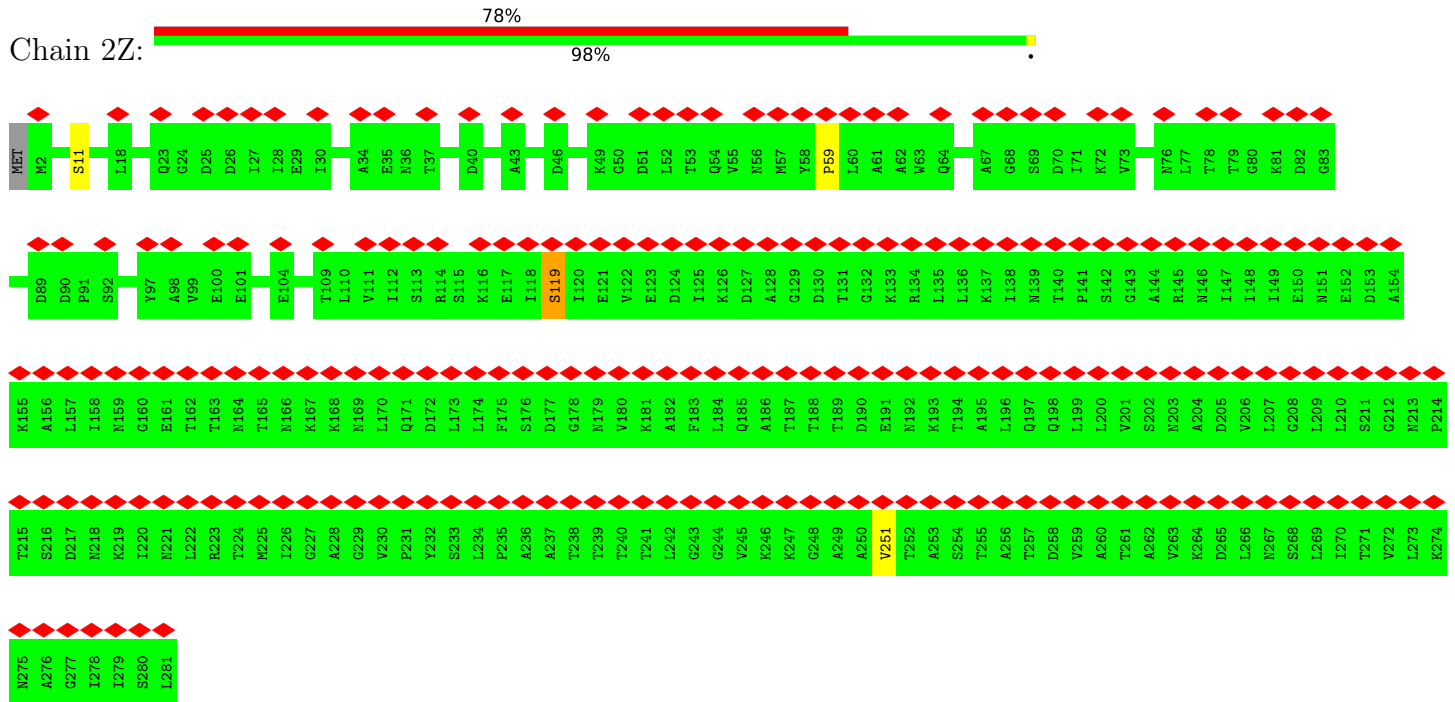
• Molecule 2: Capsid fiber protein



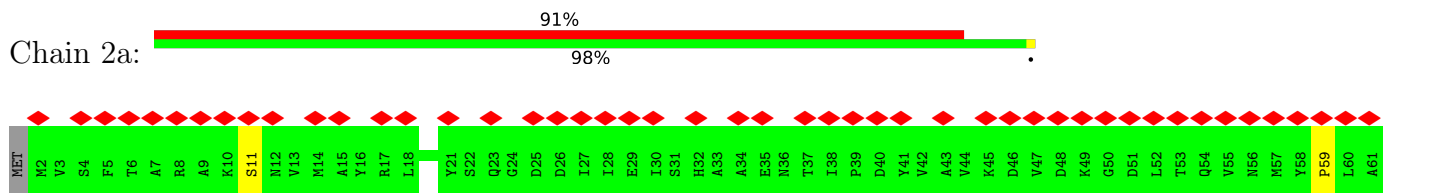
• Molecule 2: Capsid fiber protein

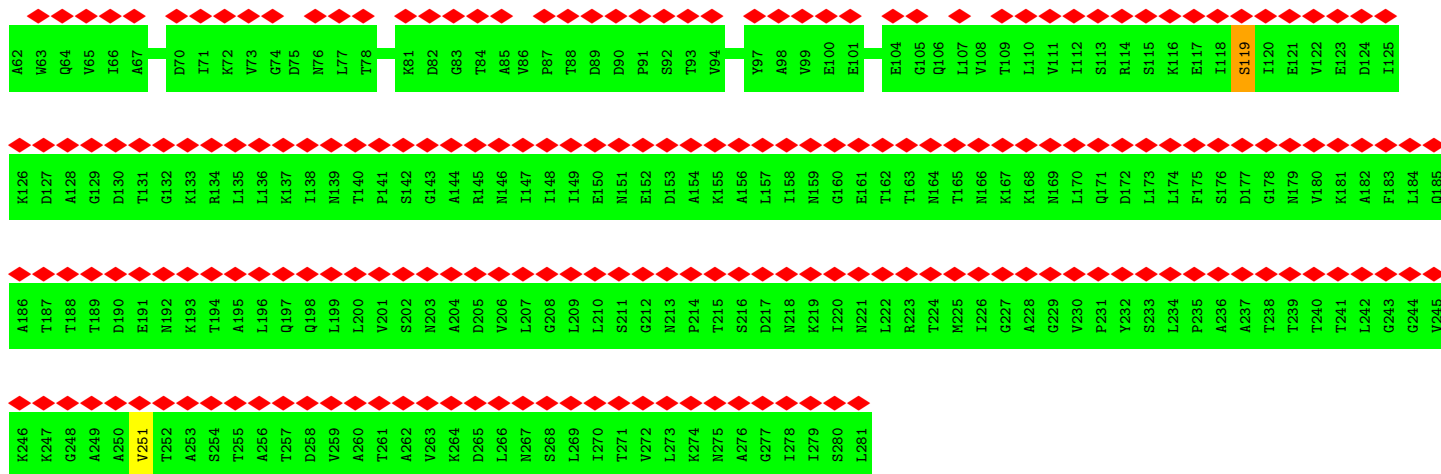


• Molecule 2: Capsid fiber protein

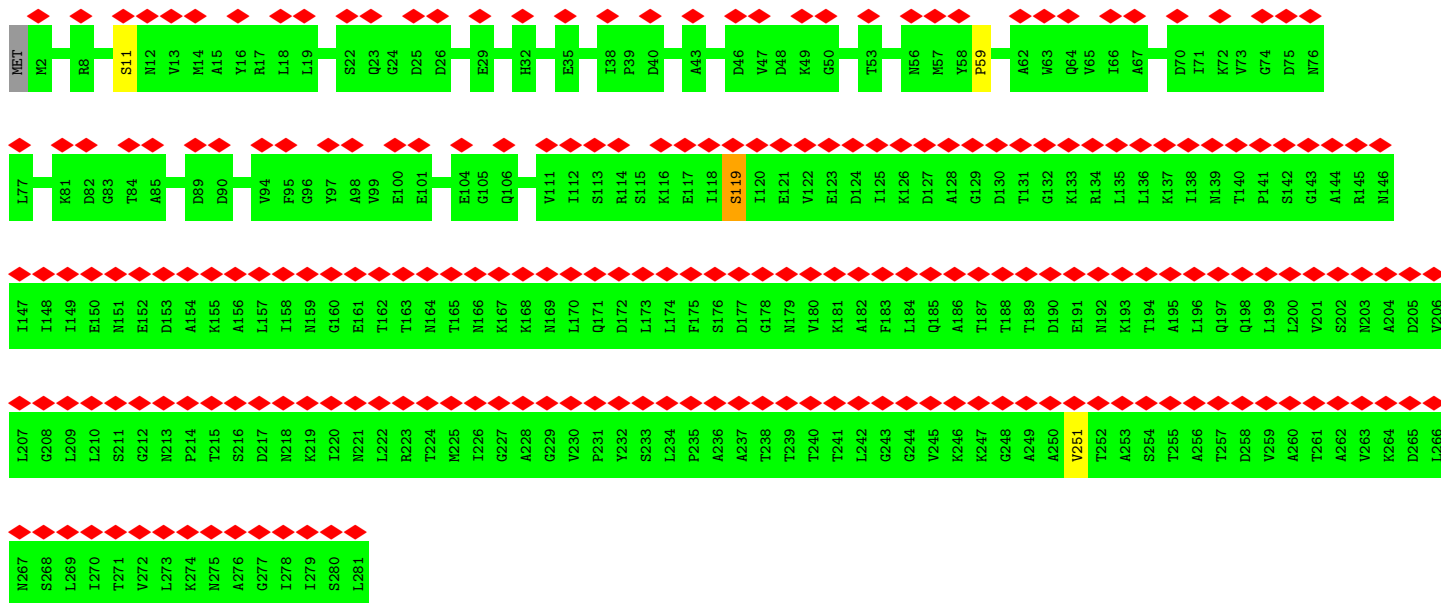
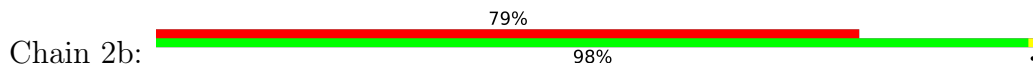


• Molecule 2: Capsid fiber protein

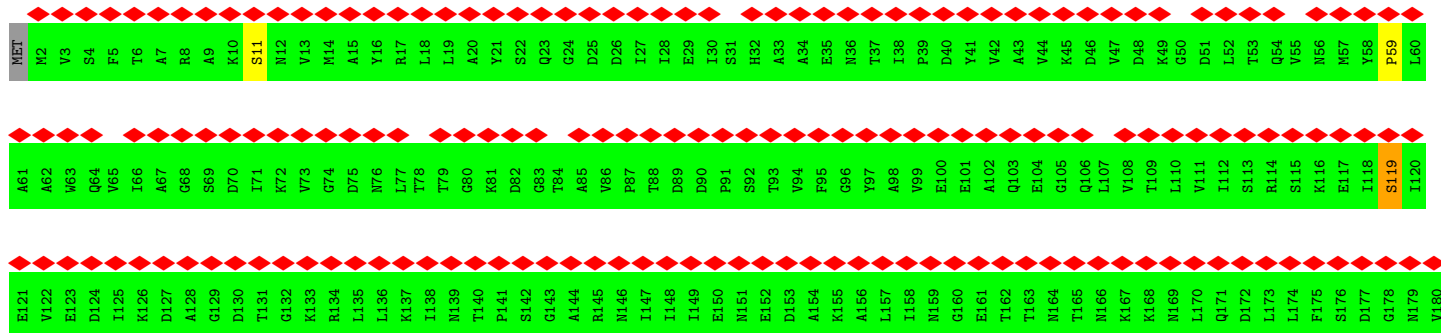


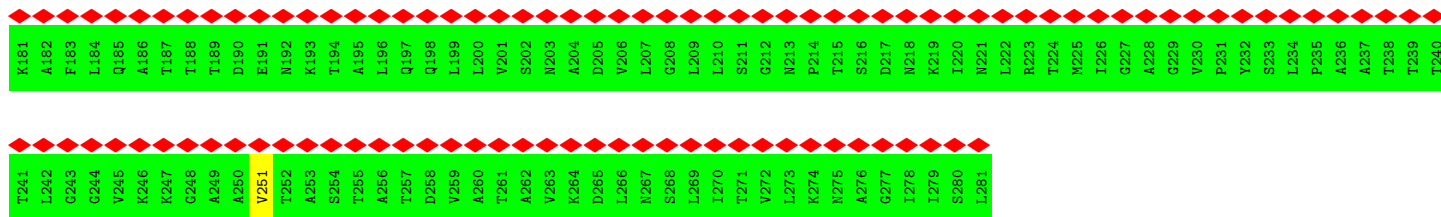


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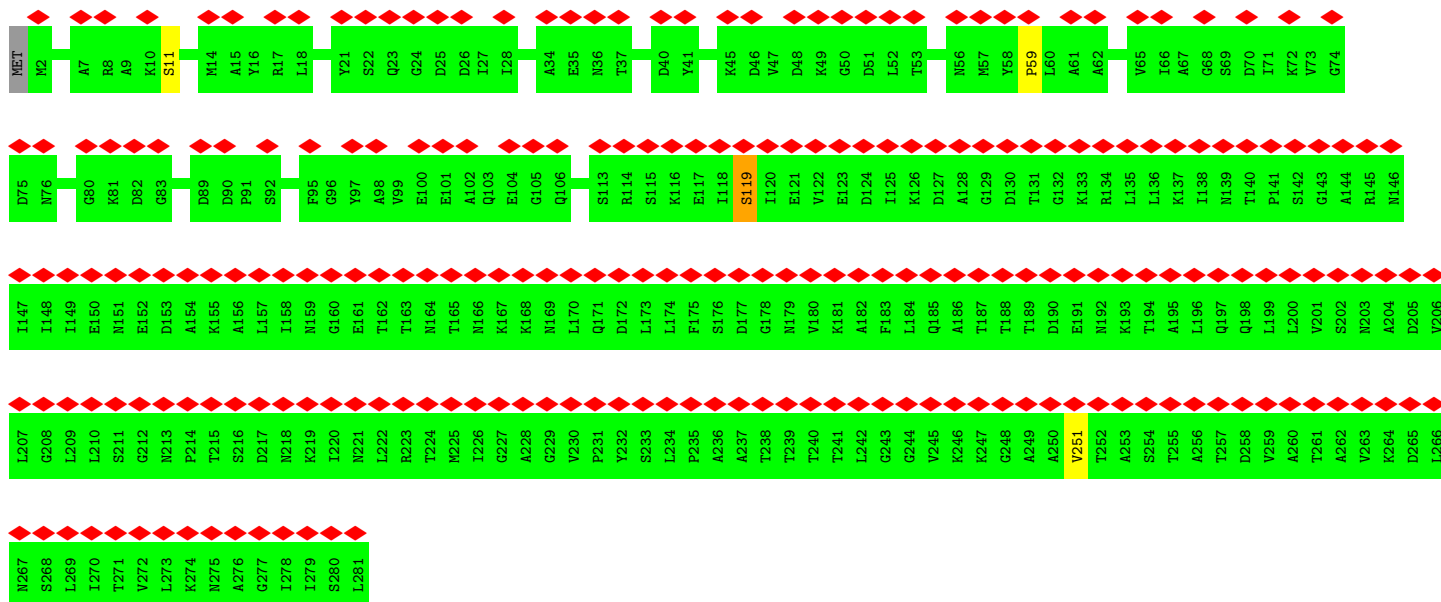
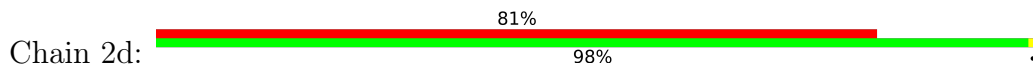


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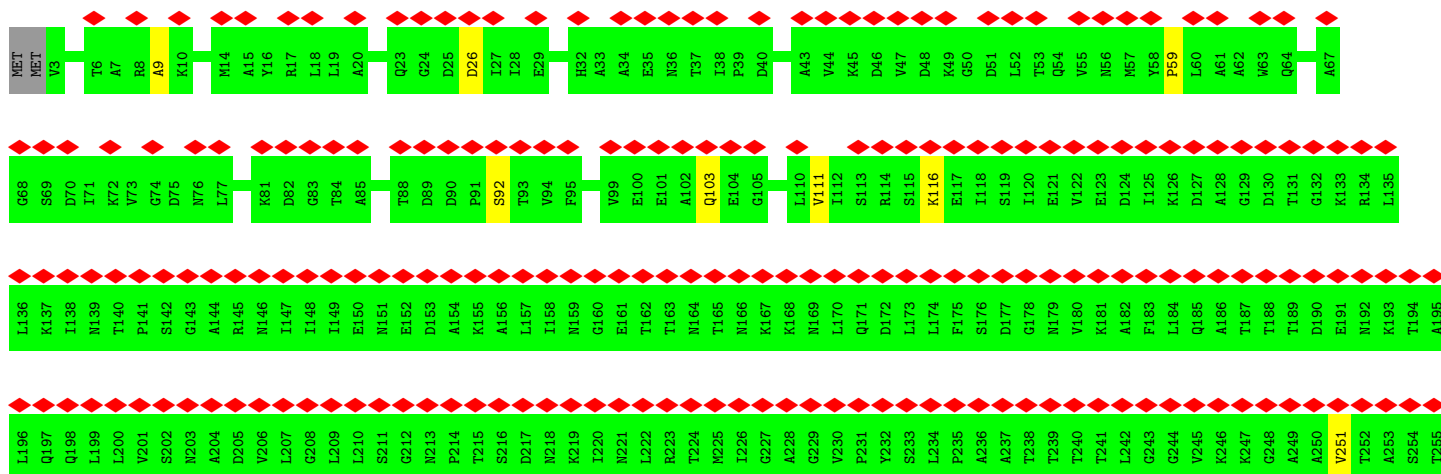
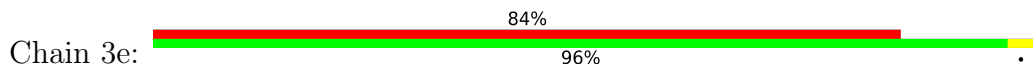


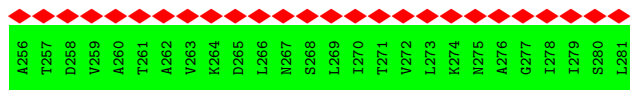


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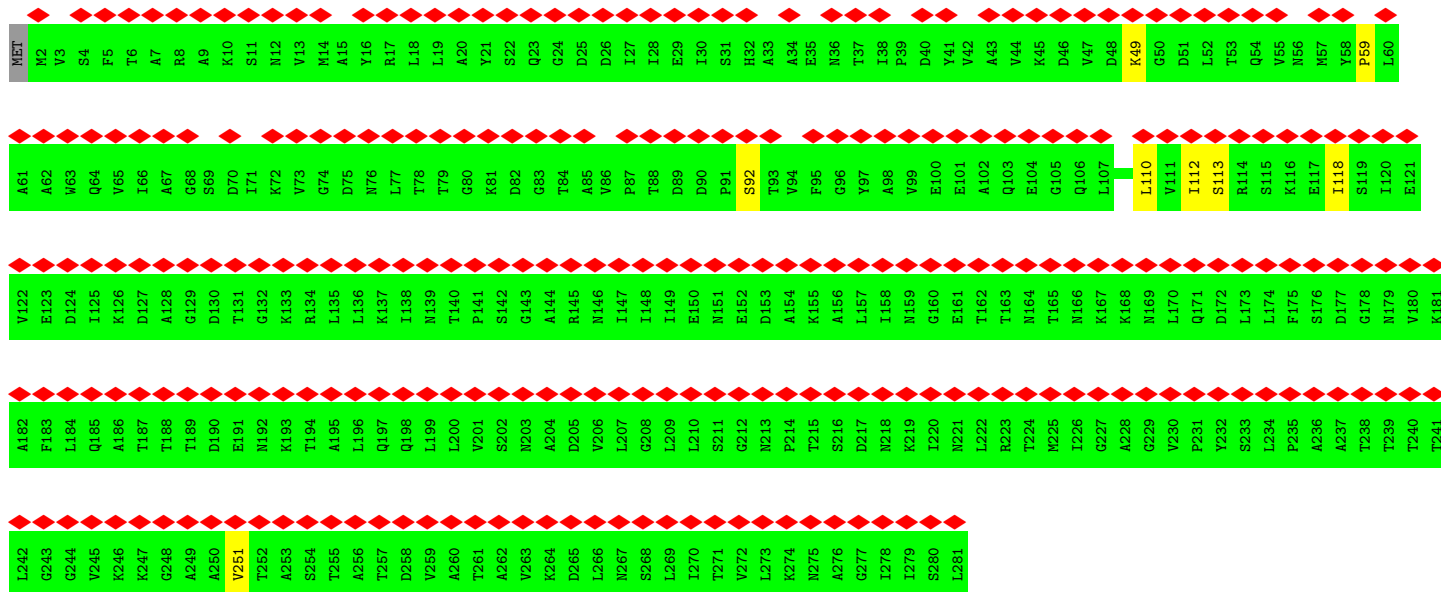


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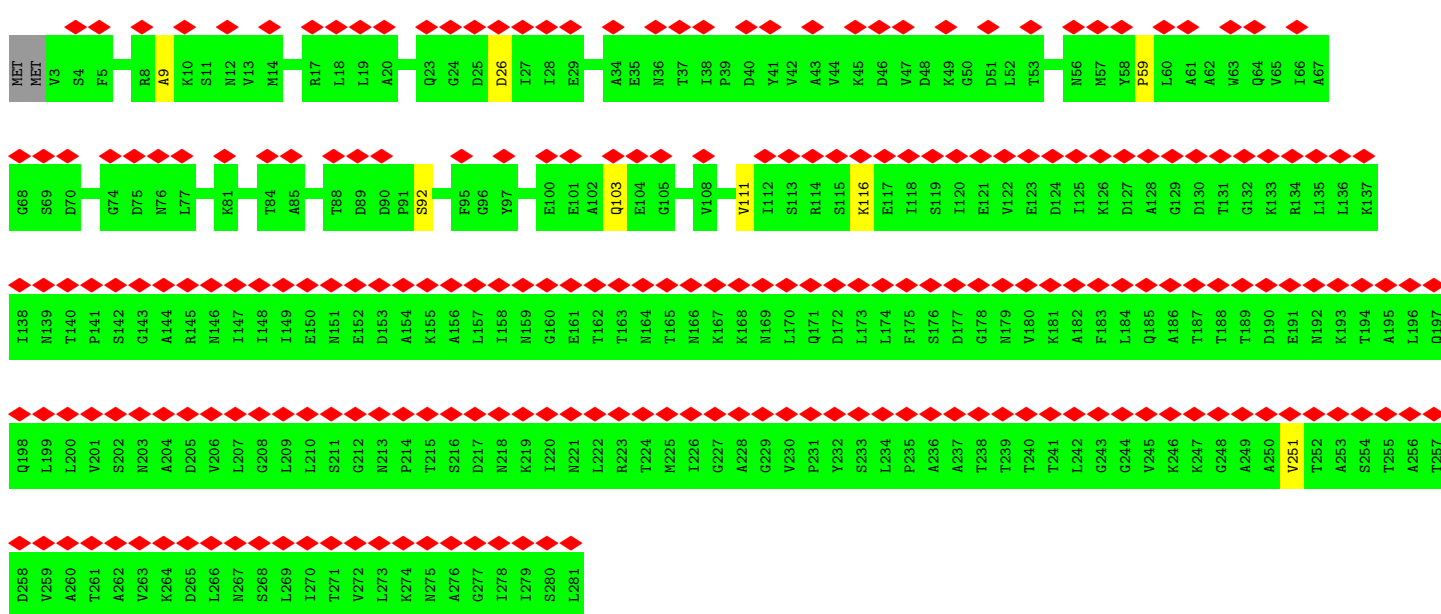
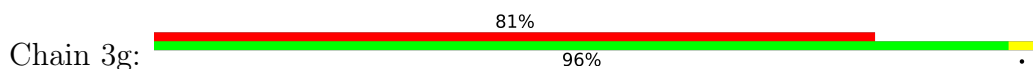




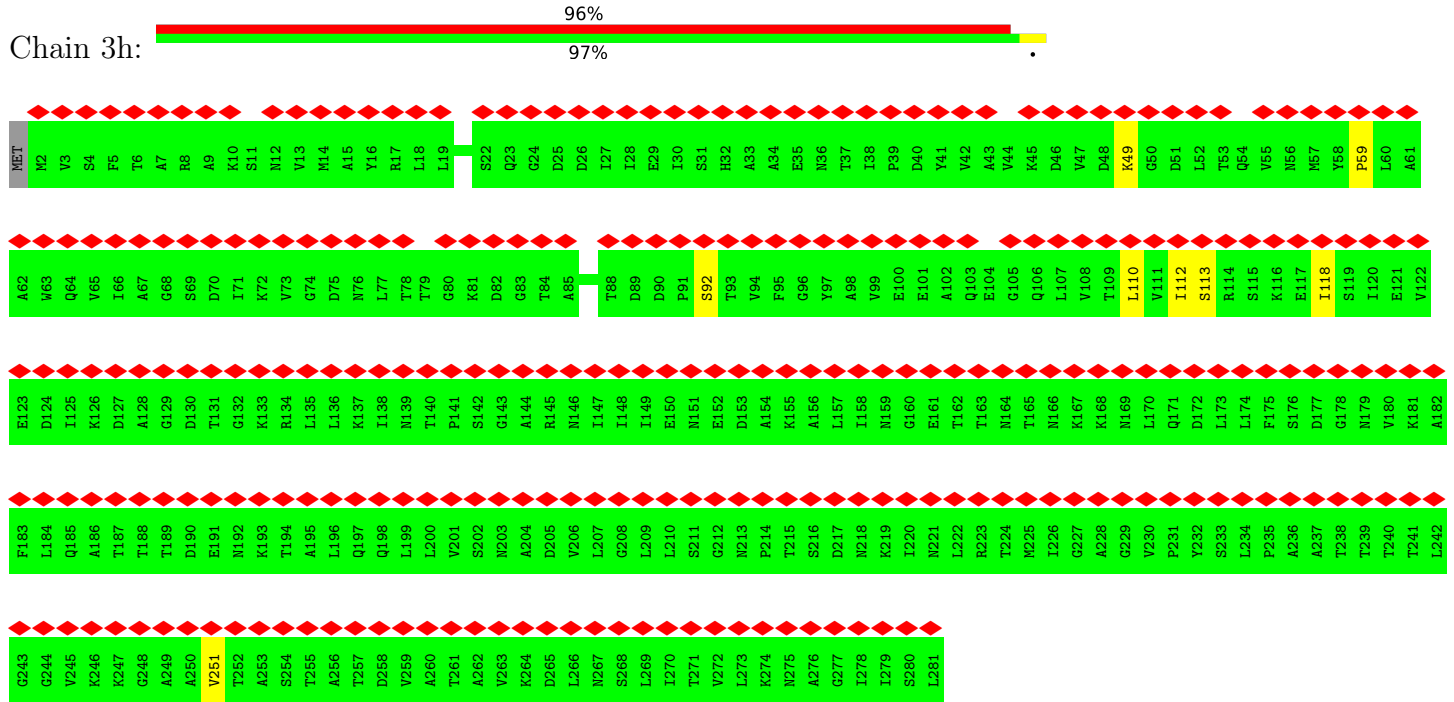
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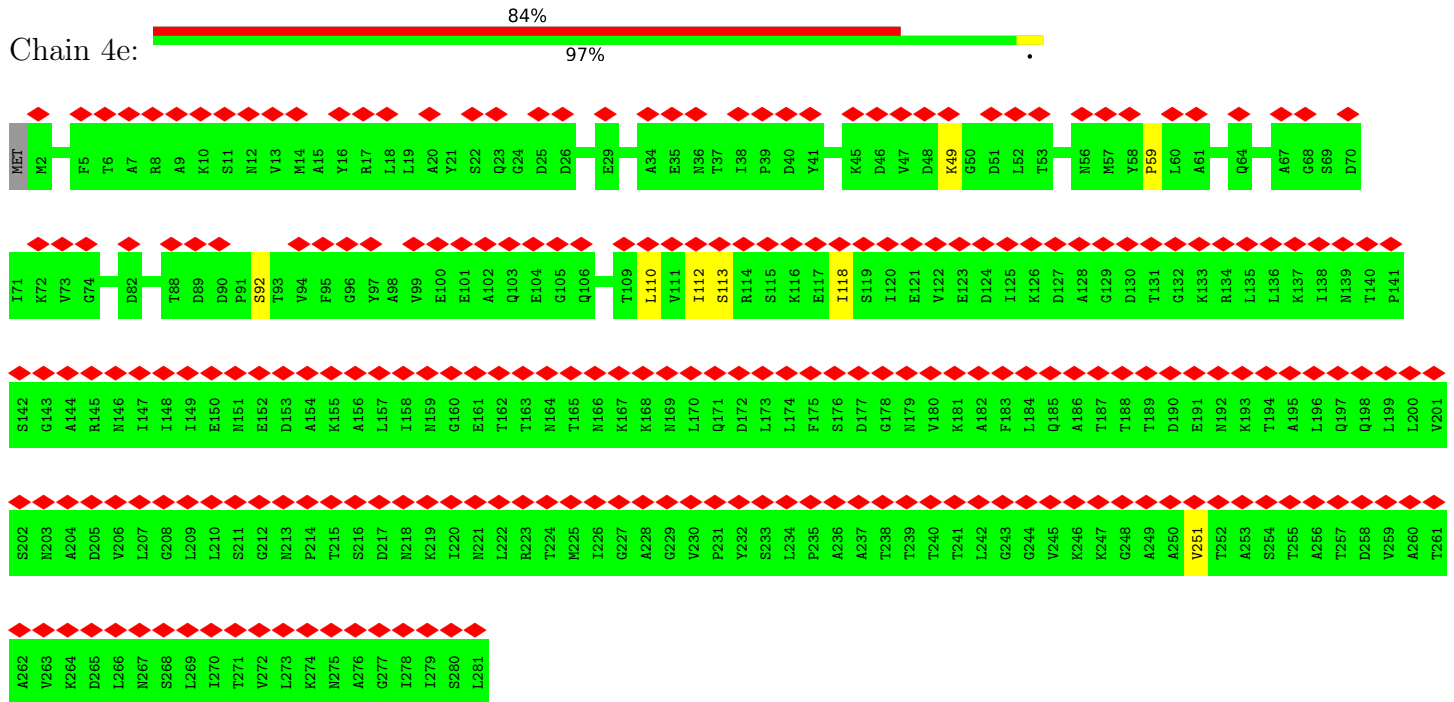
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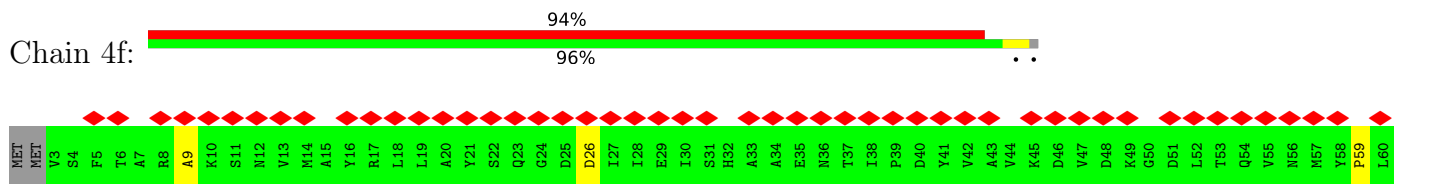
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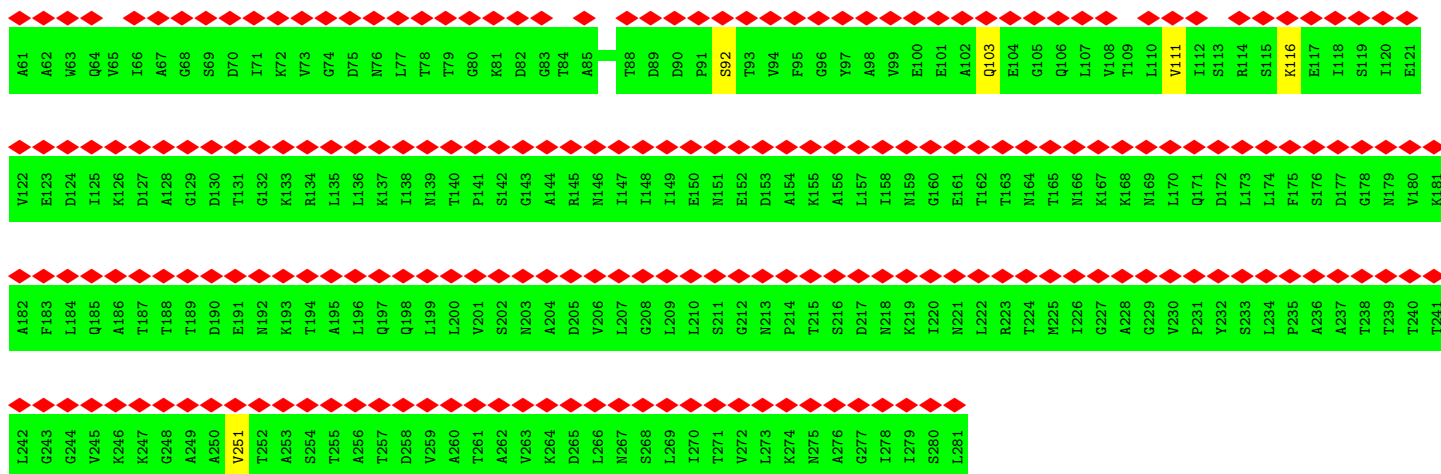


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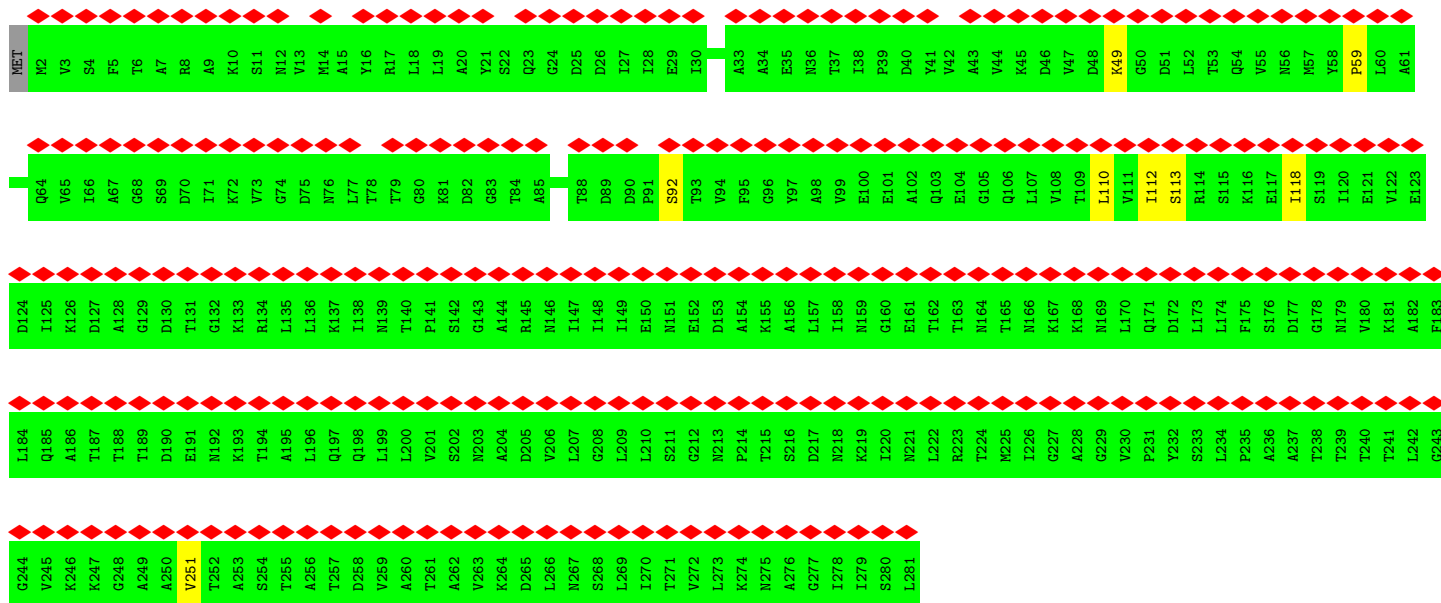


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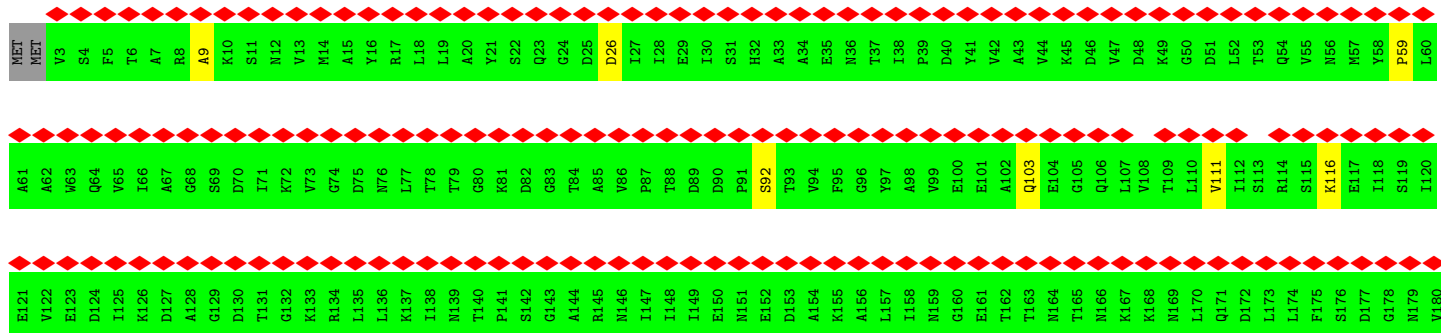


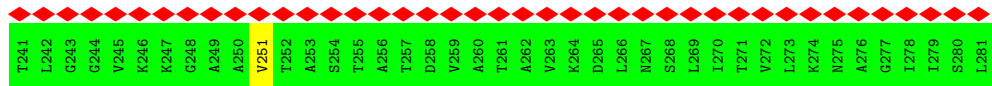
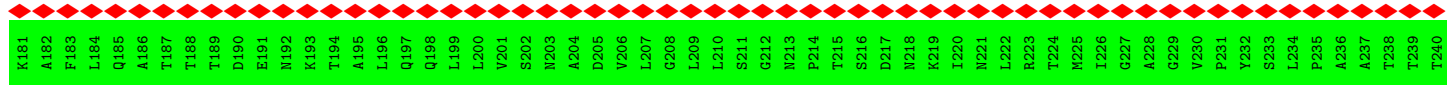


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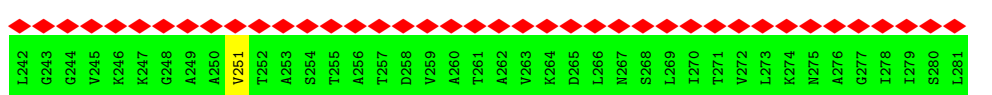
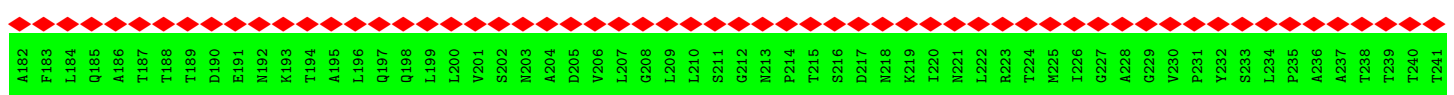
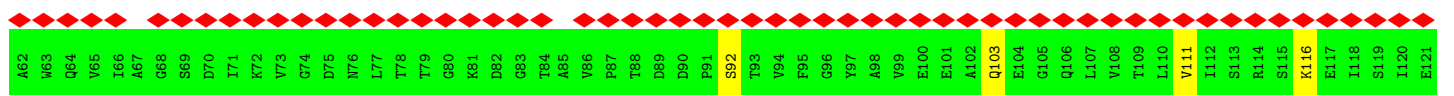
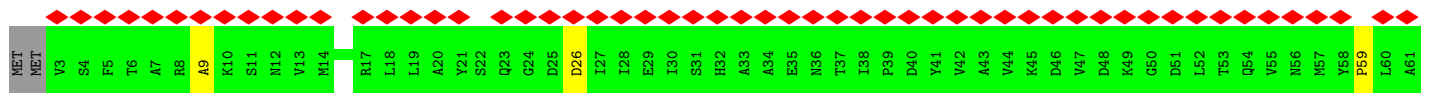


• Molecule 2: Capsid fiber protein

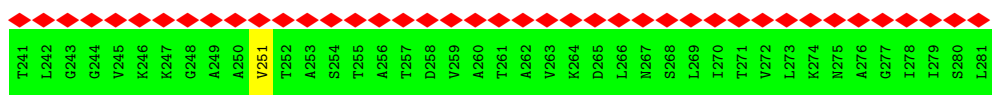
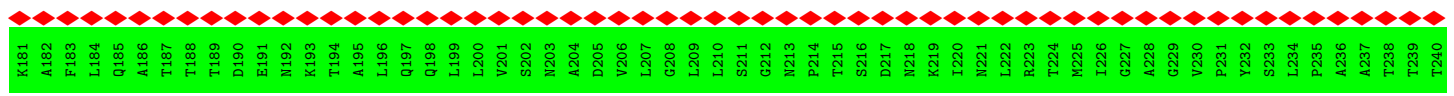
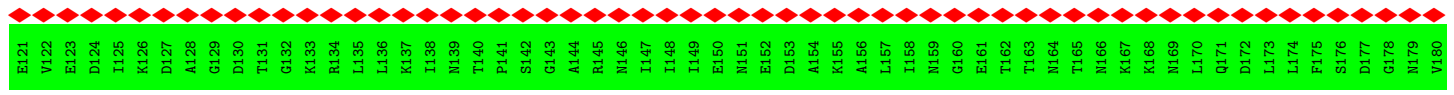
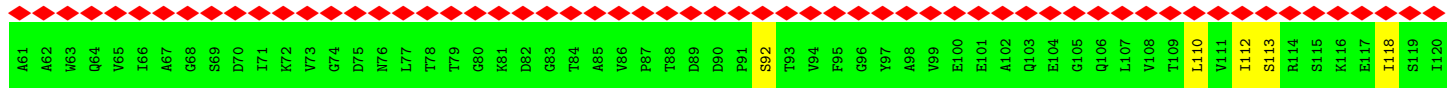
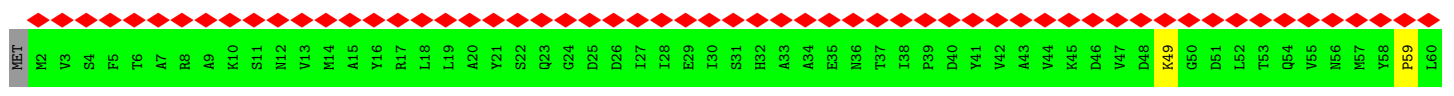




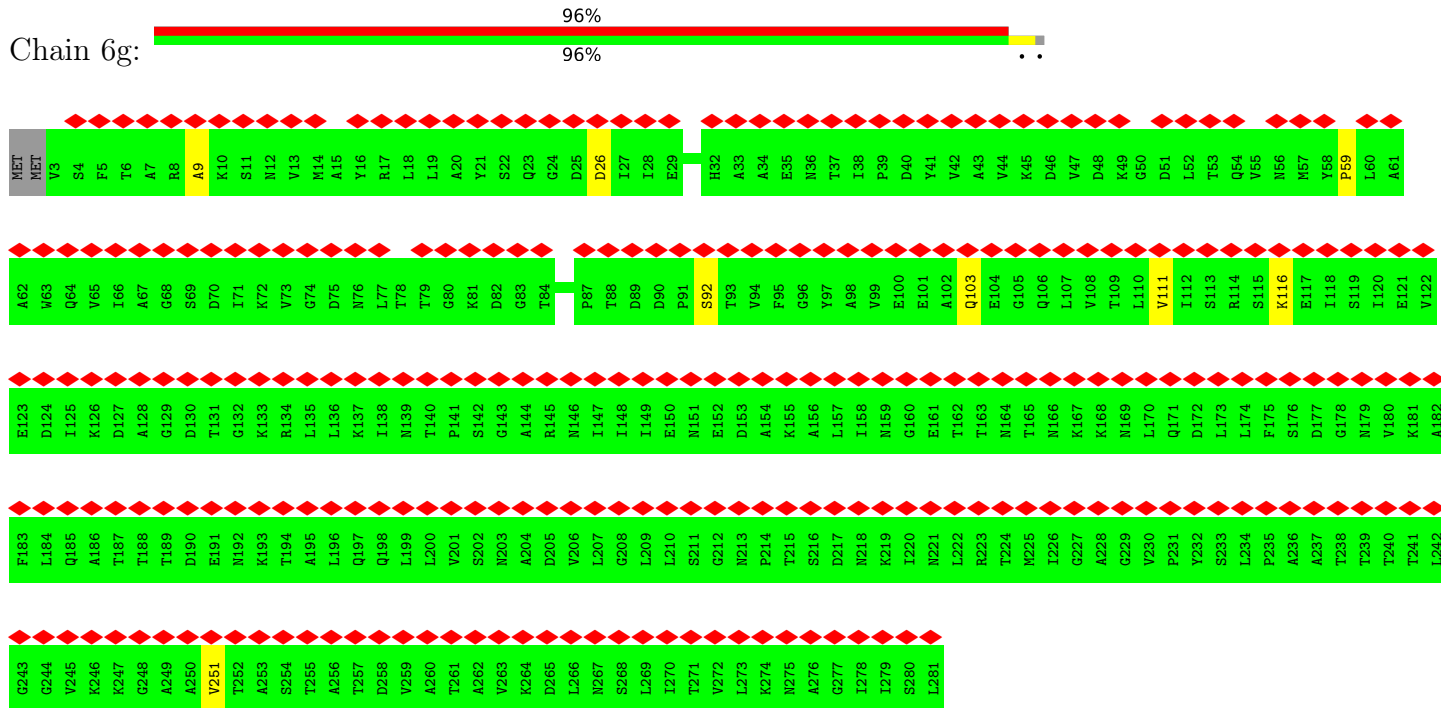
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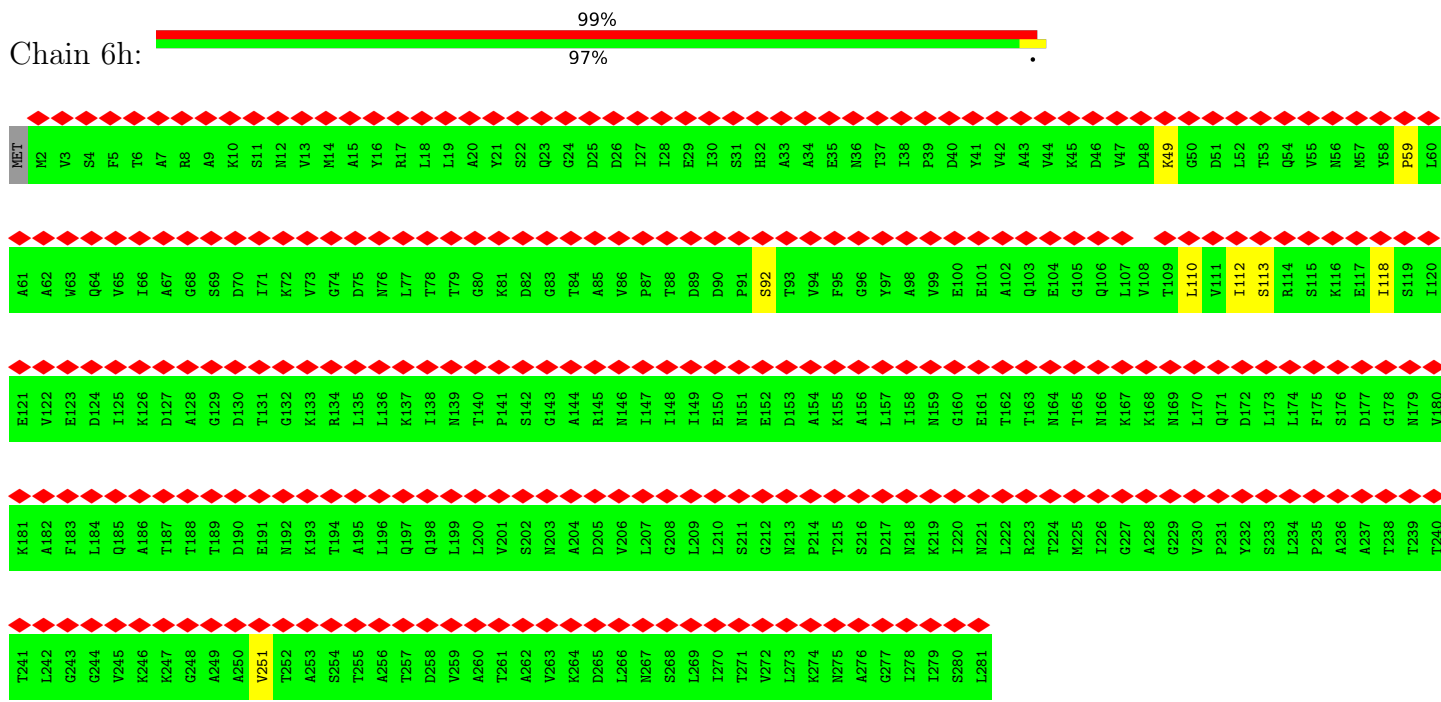
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• Molecule 2: Capsid fiber protein

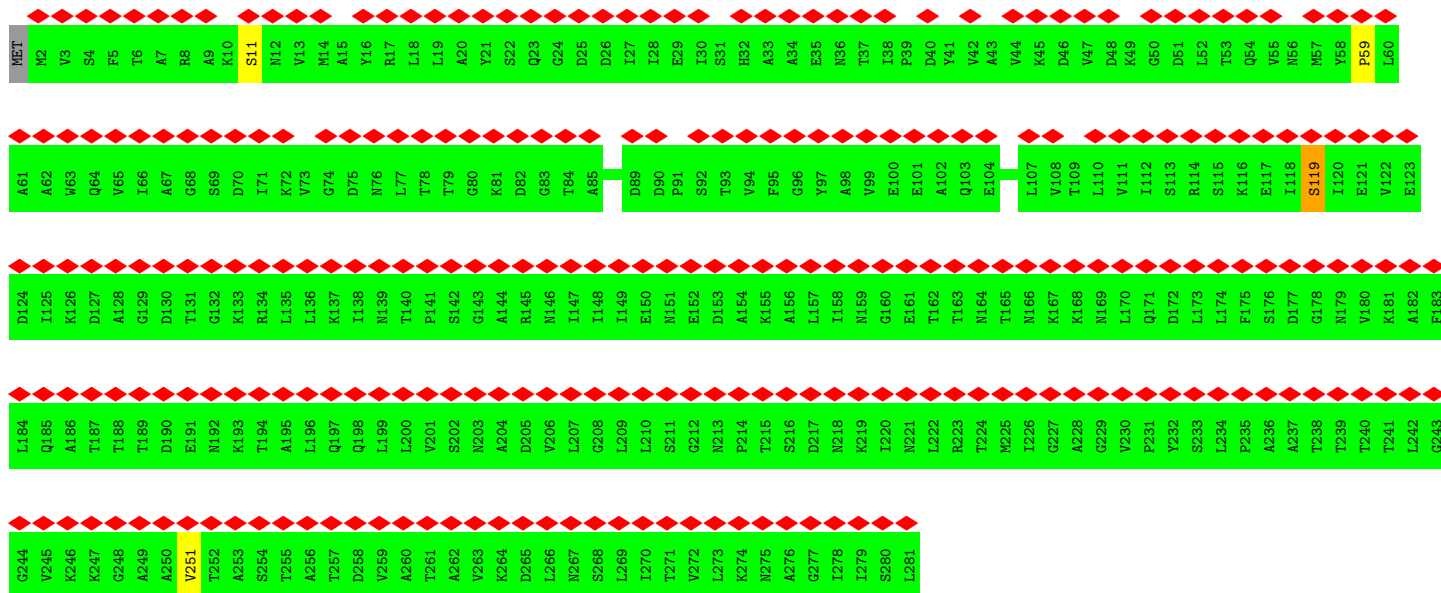


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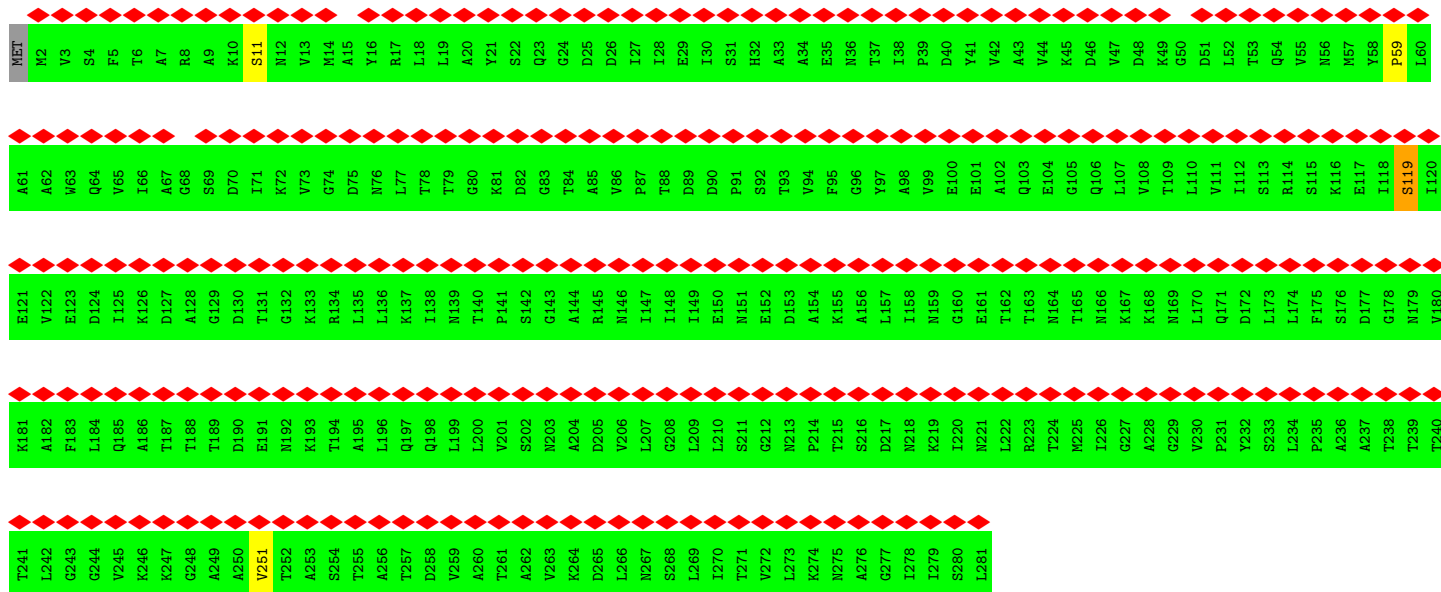


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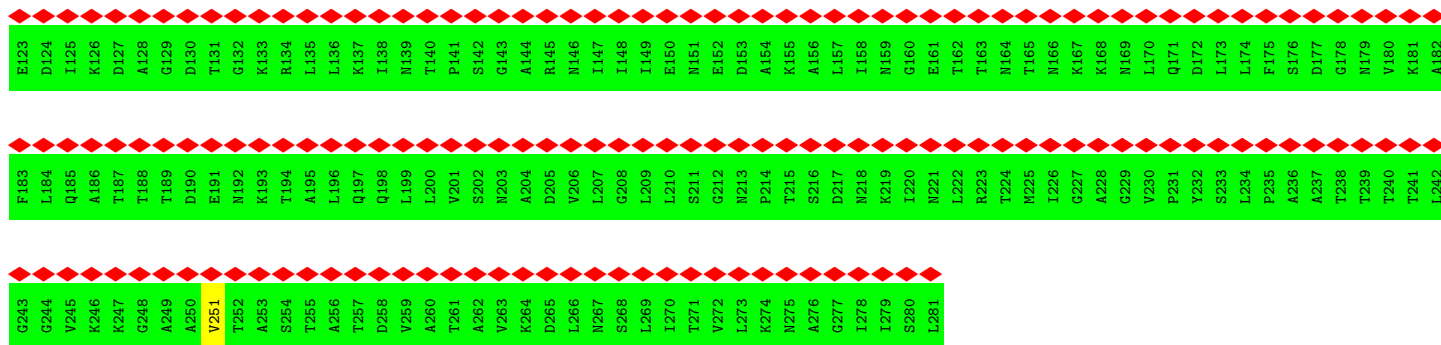


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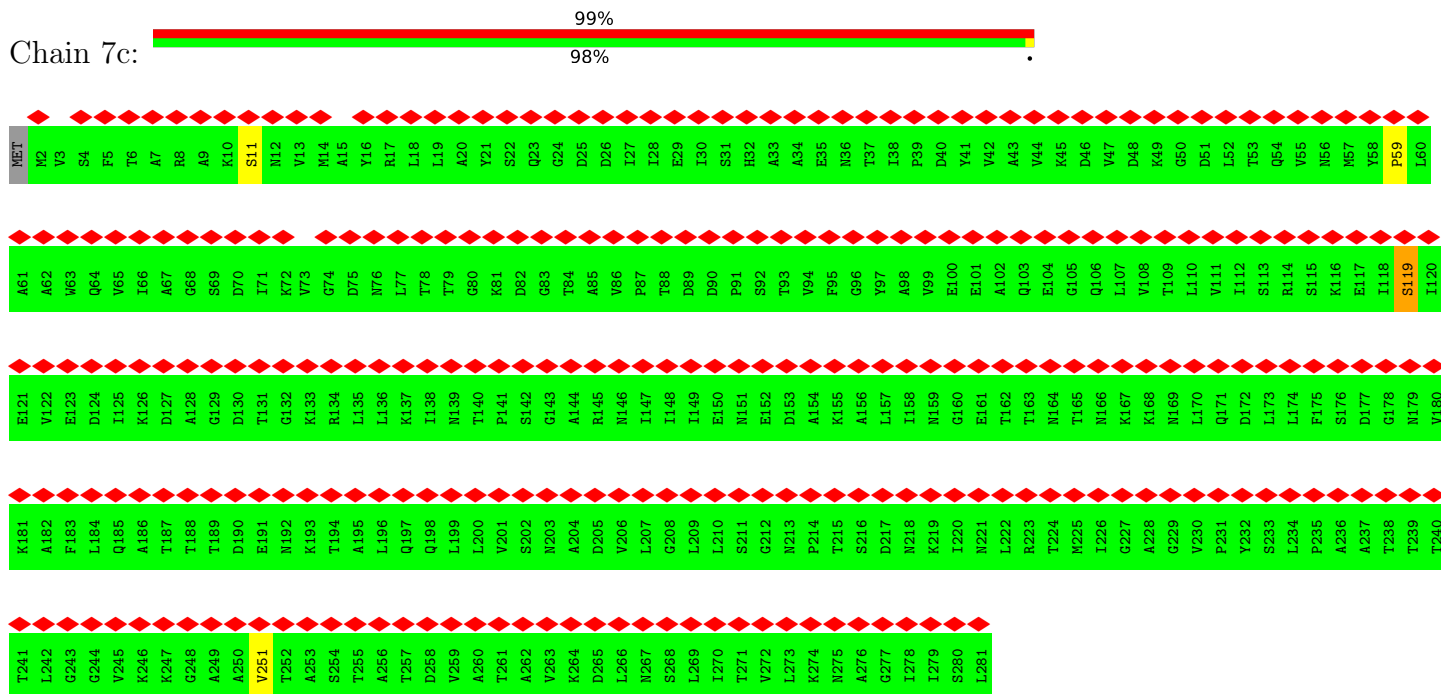


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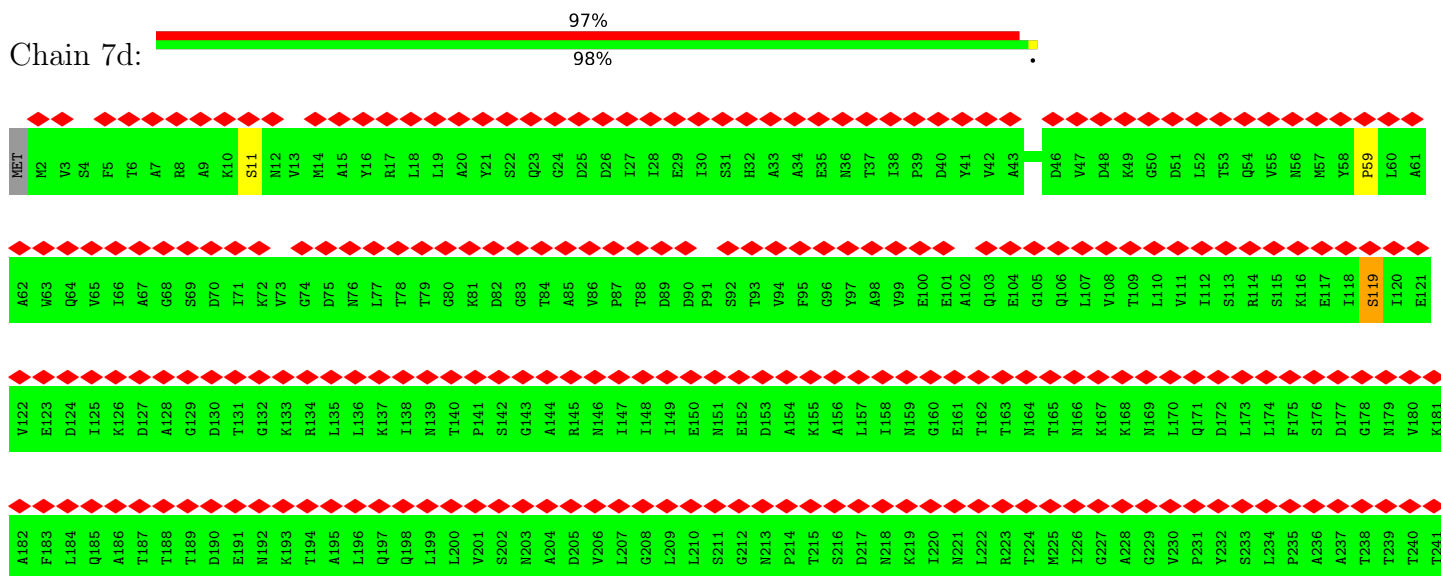


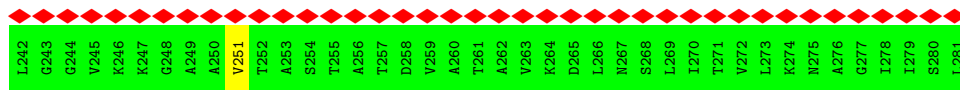


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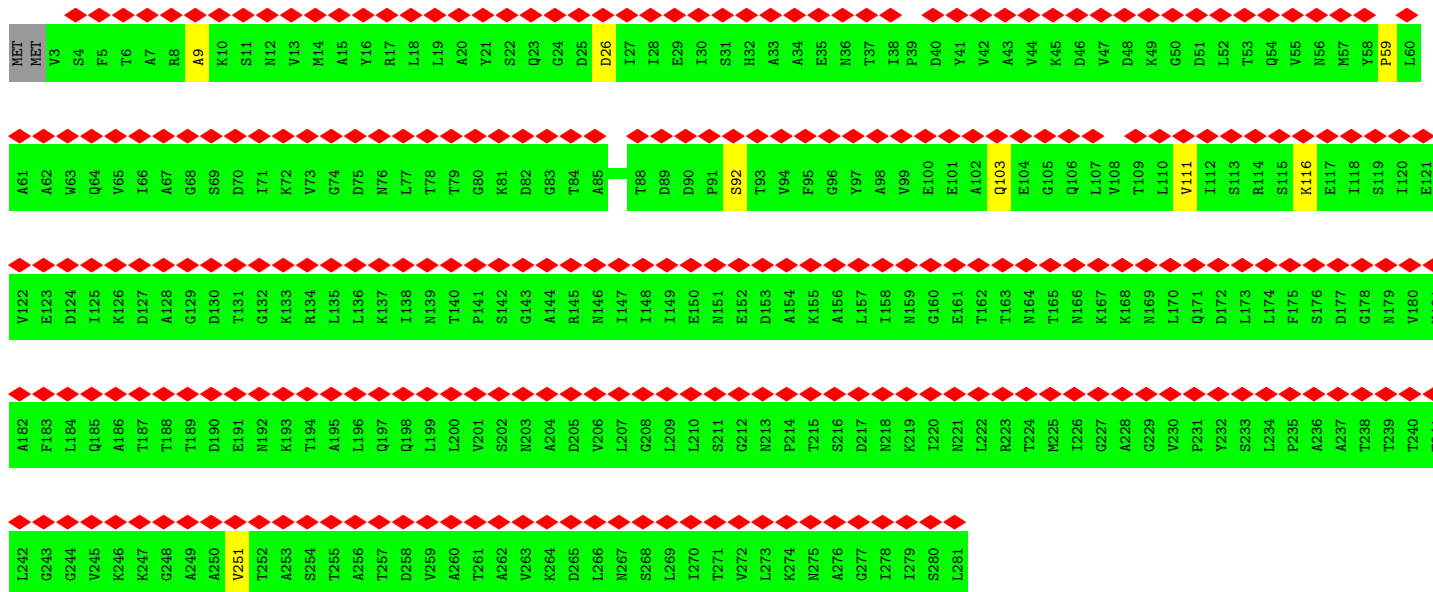


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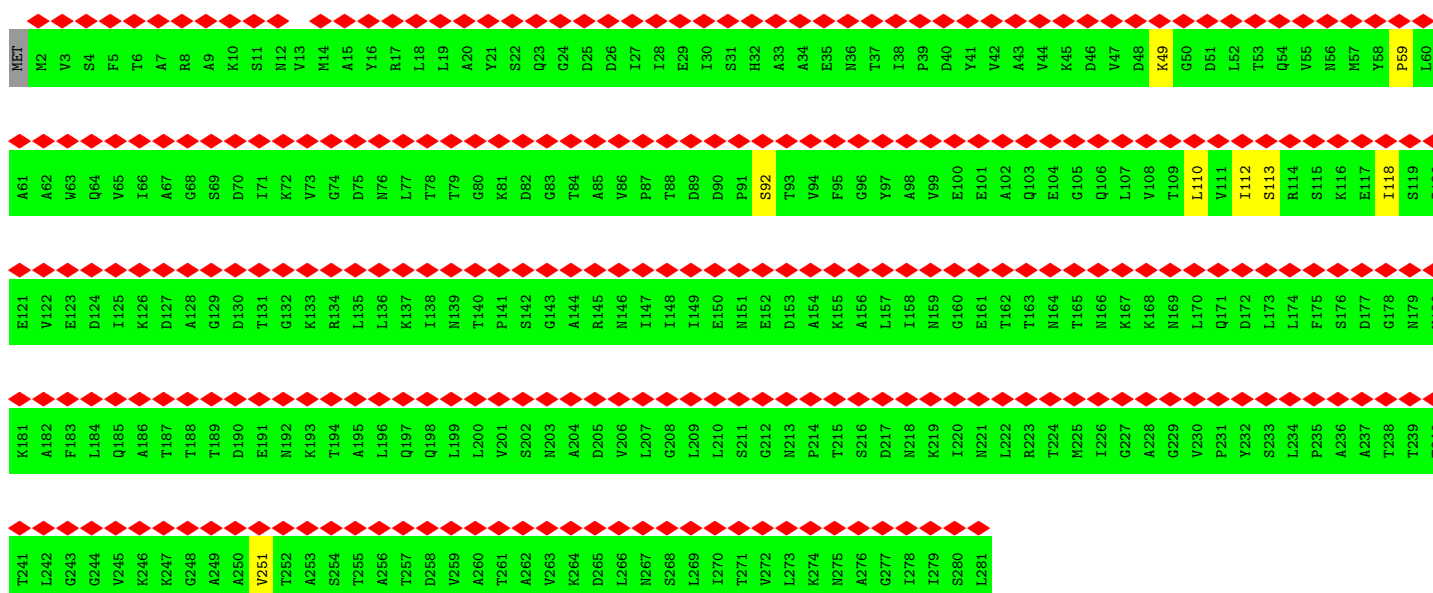




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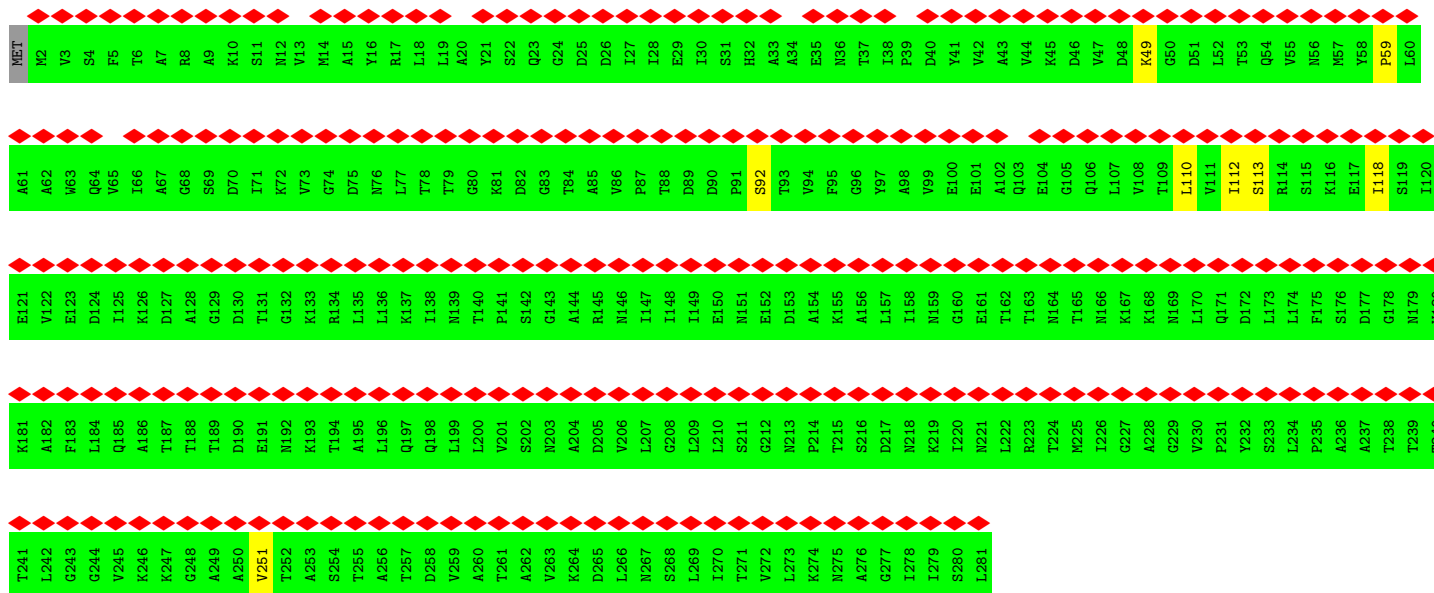


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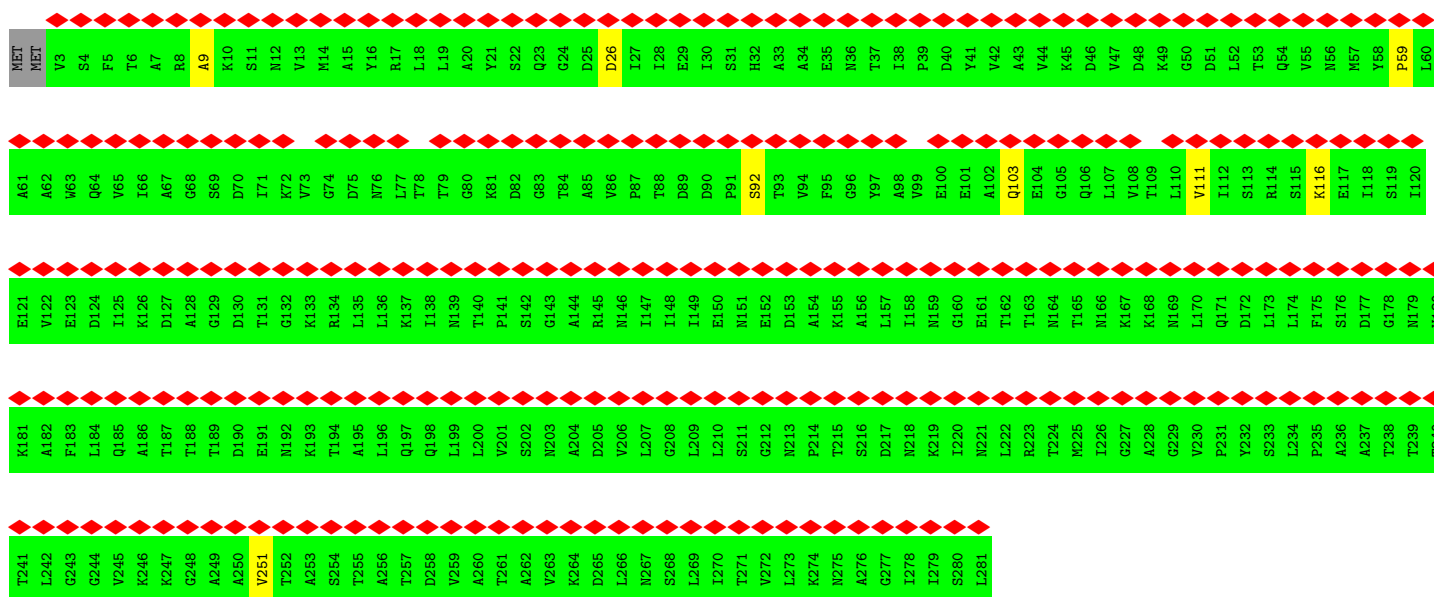


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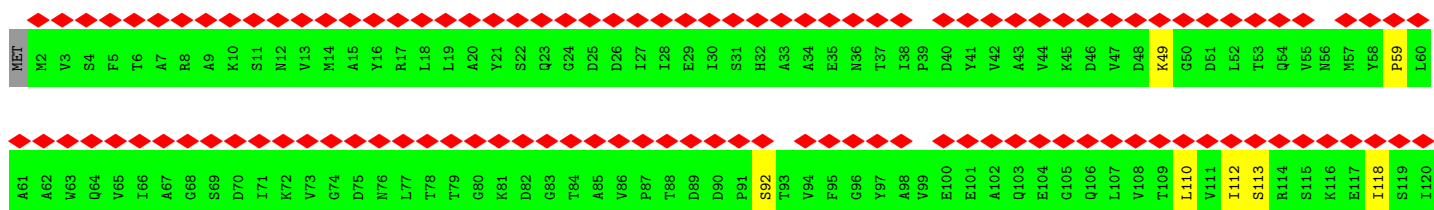


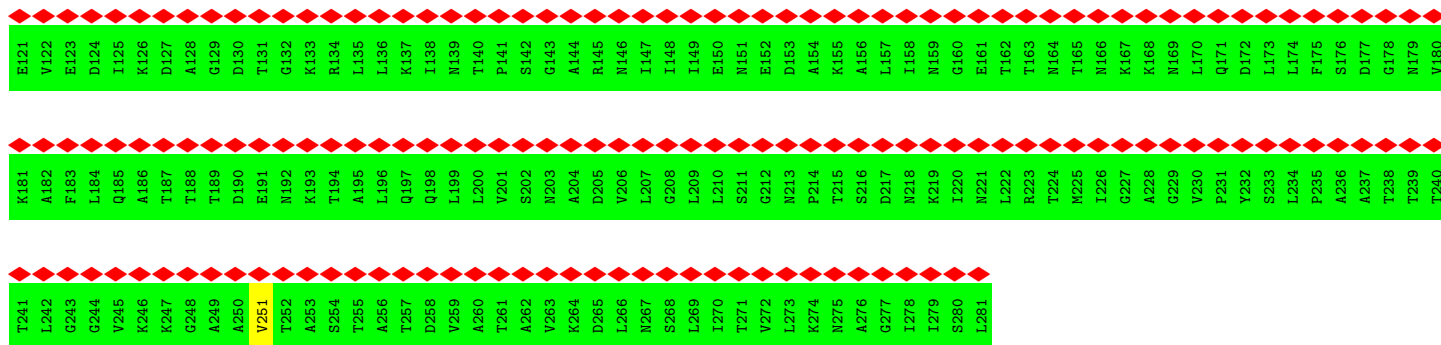


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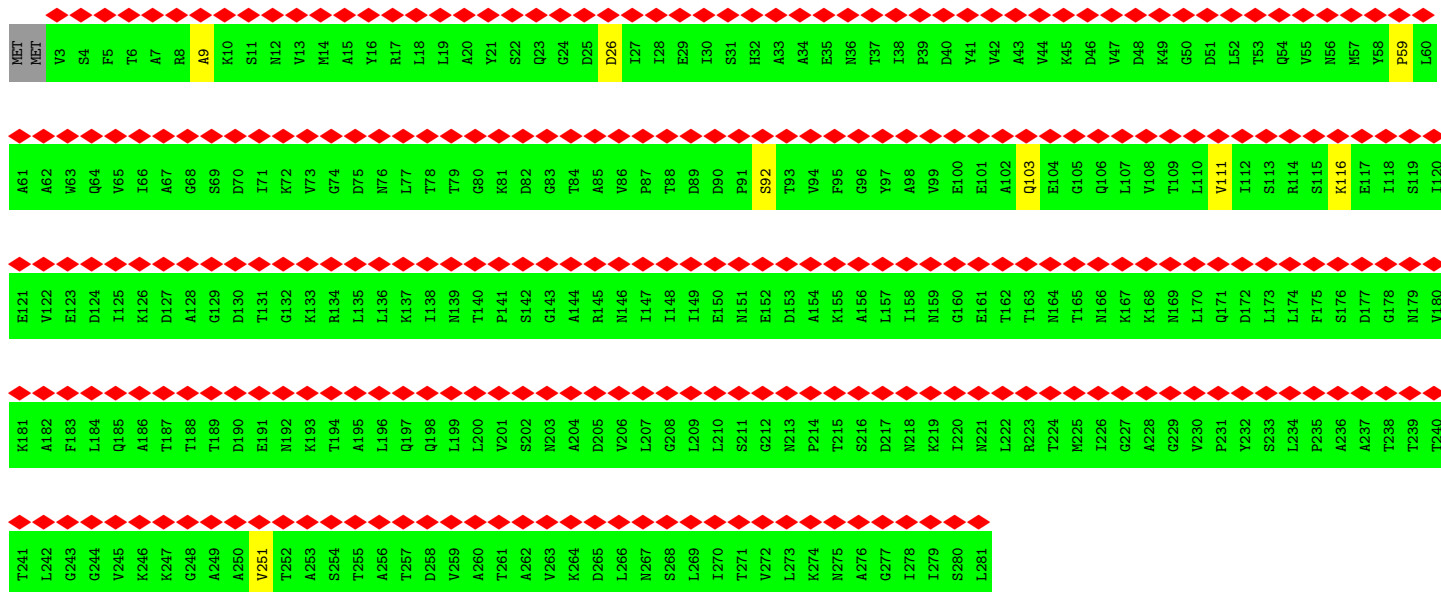


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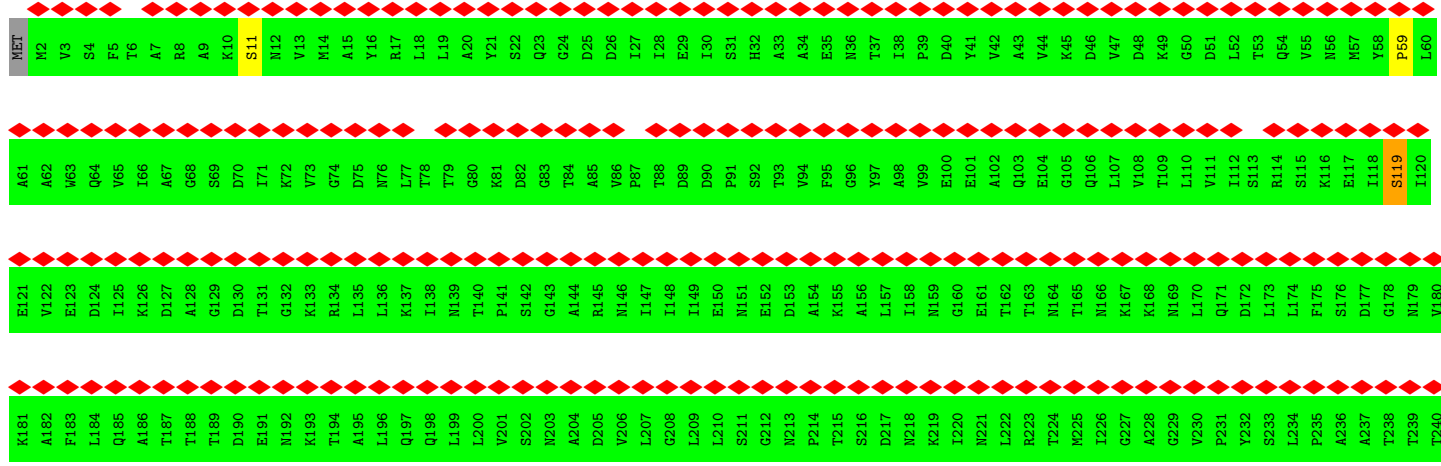


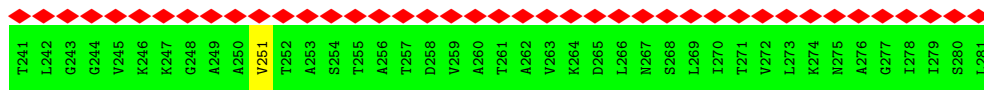


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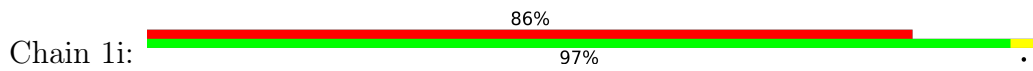


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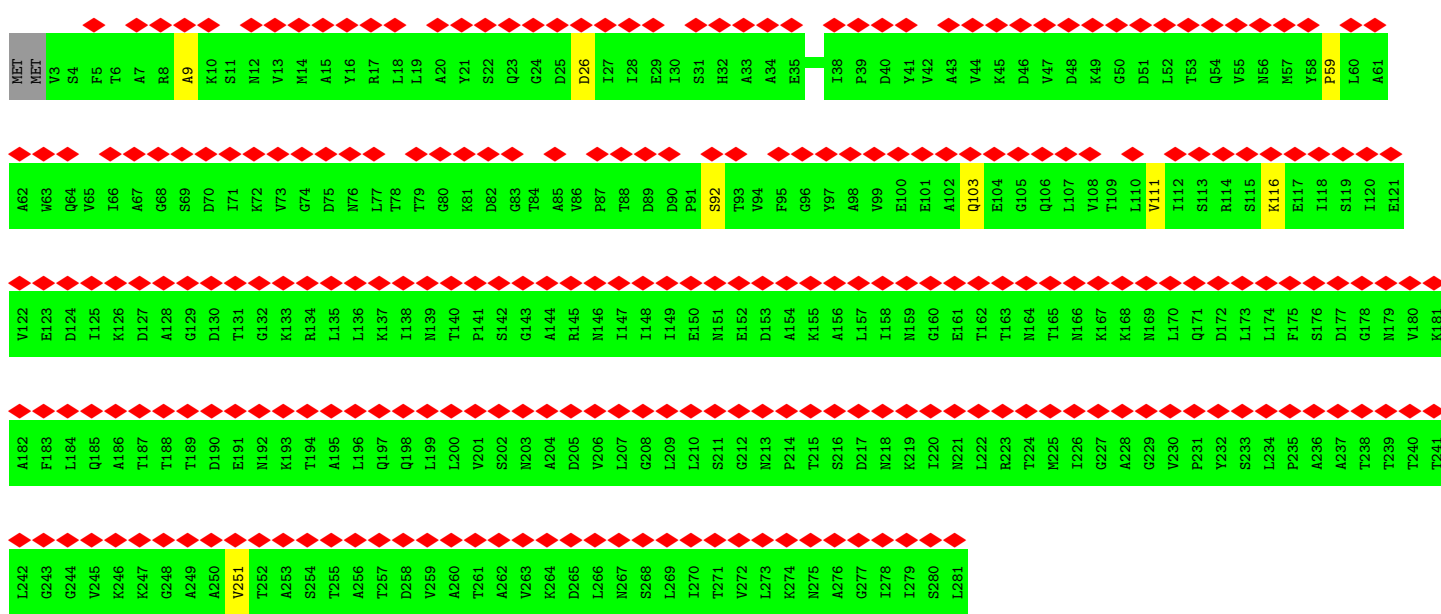
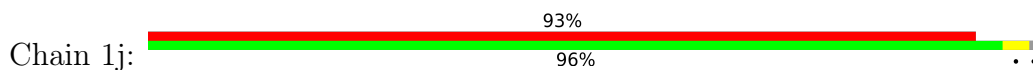




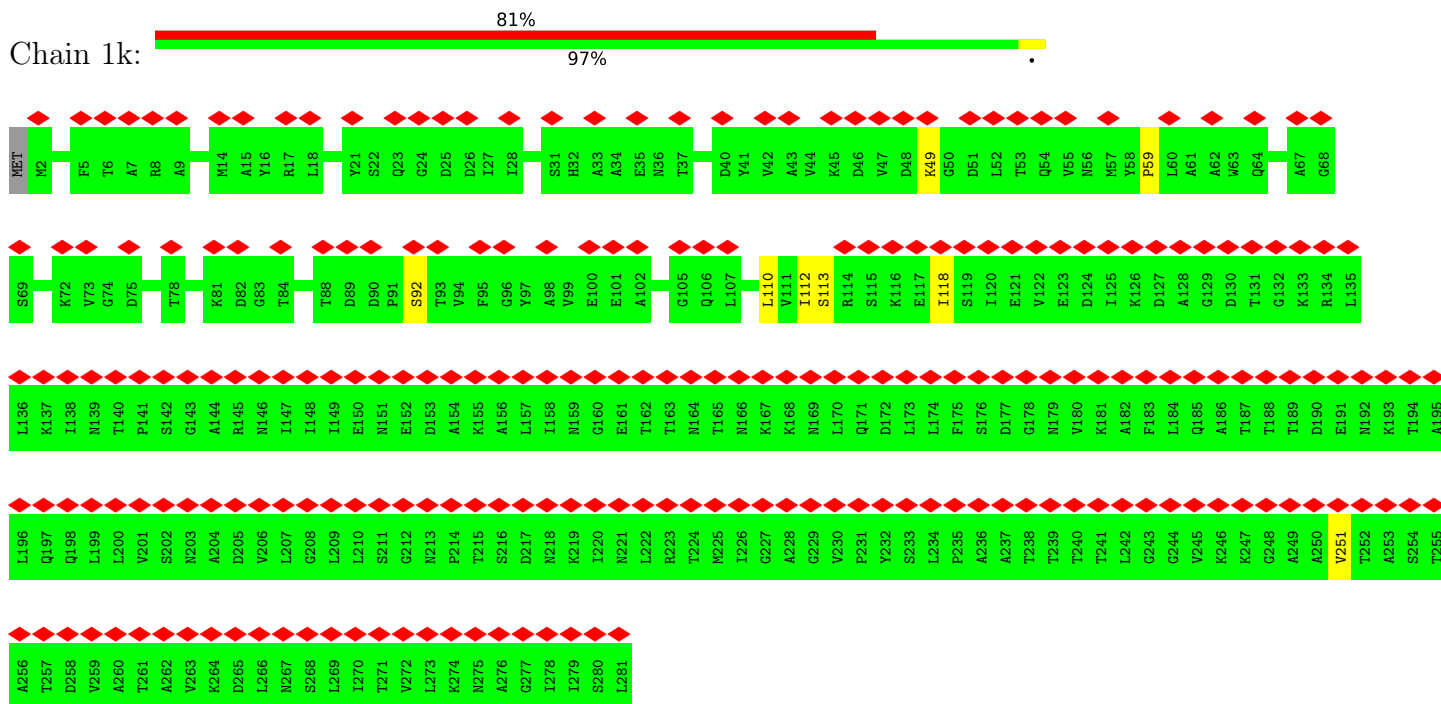
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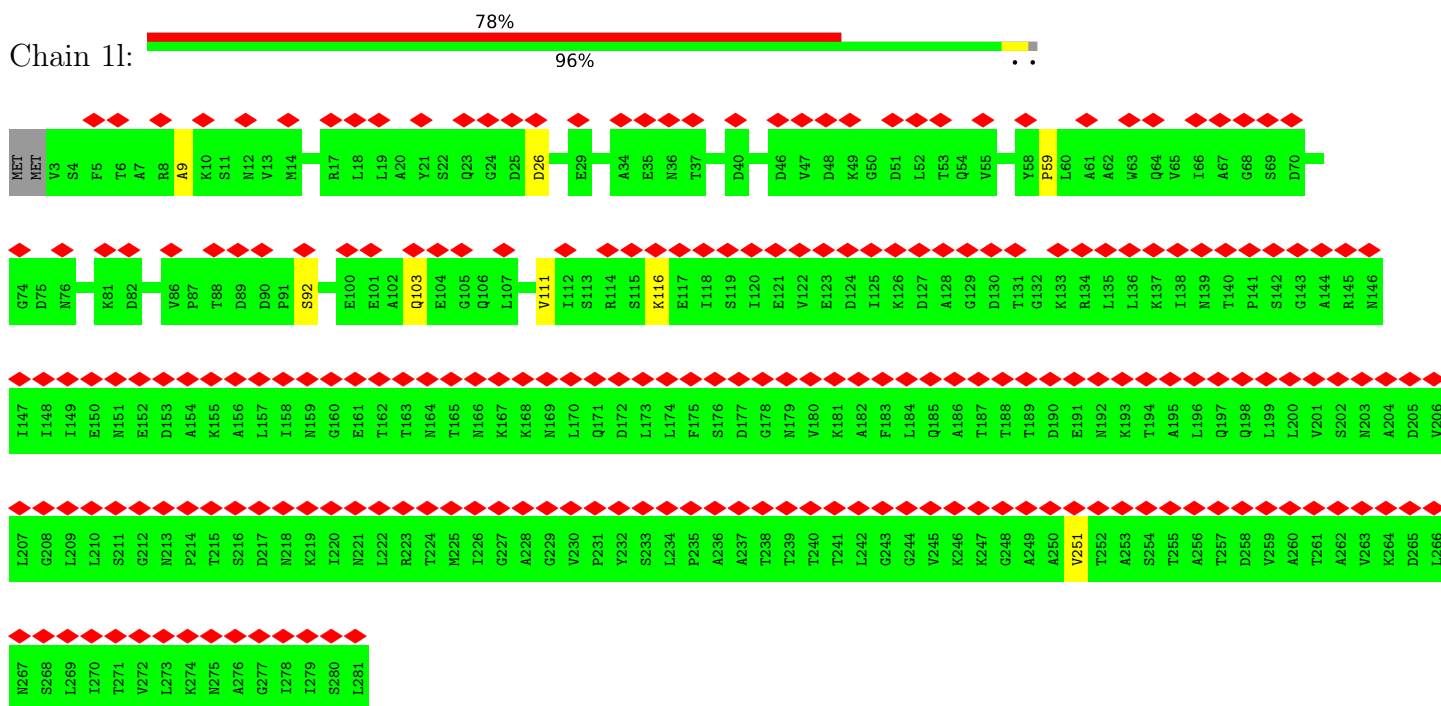
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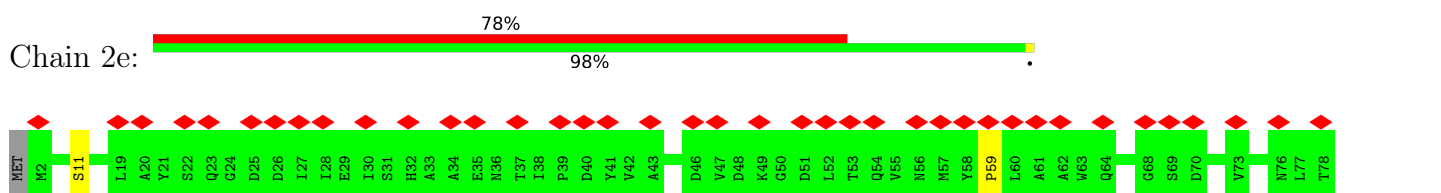
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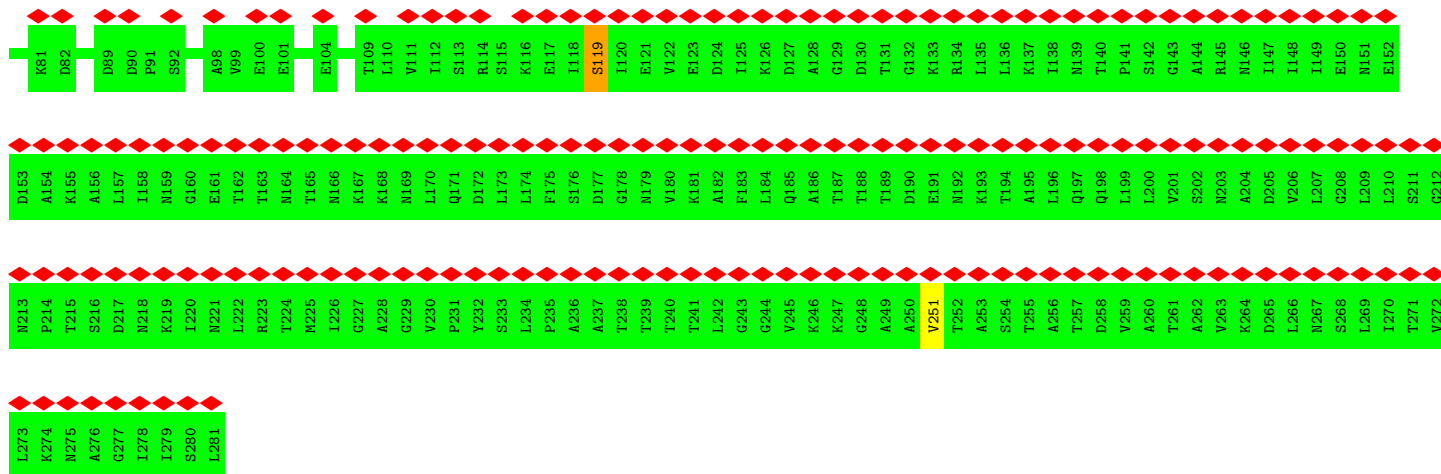


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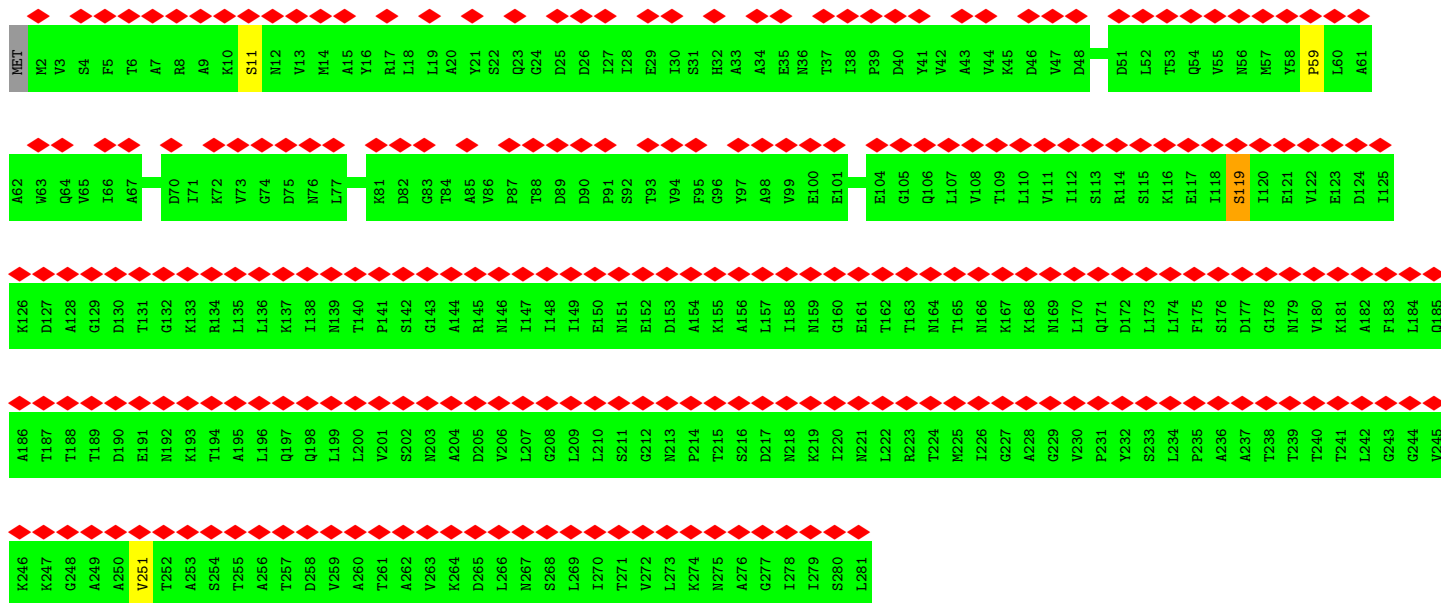


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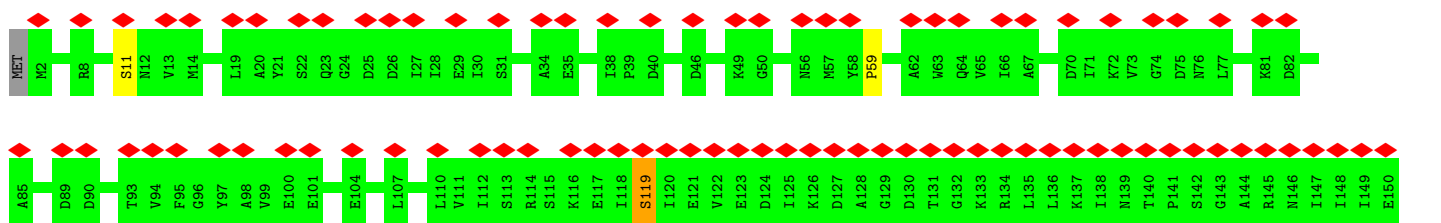
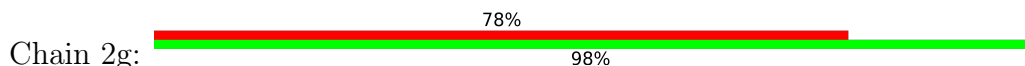


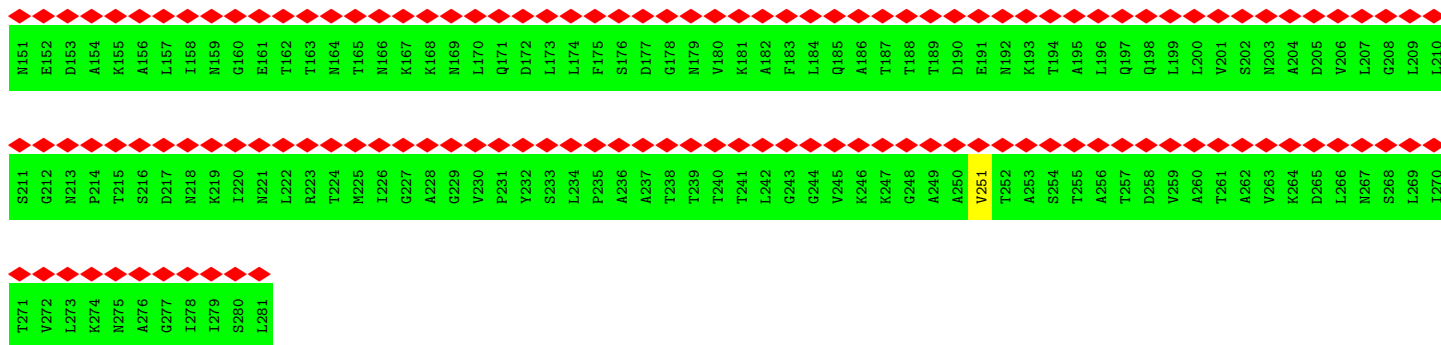


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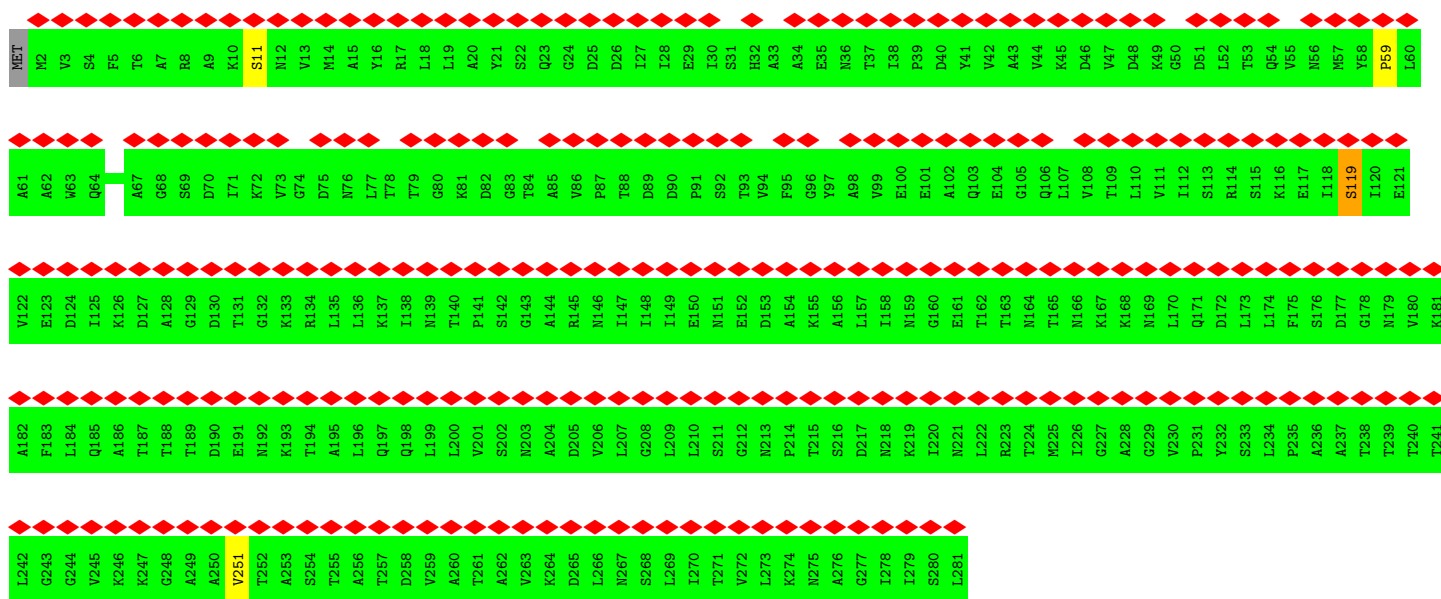


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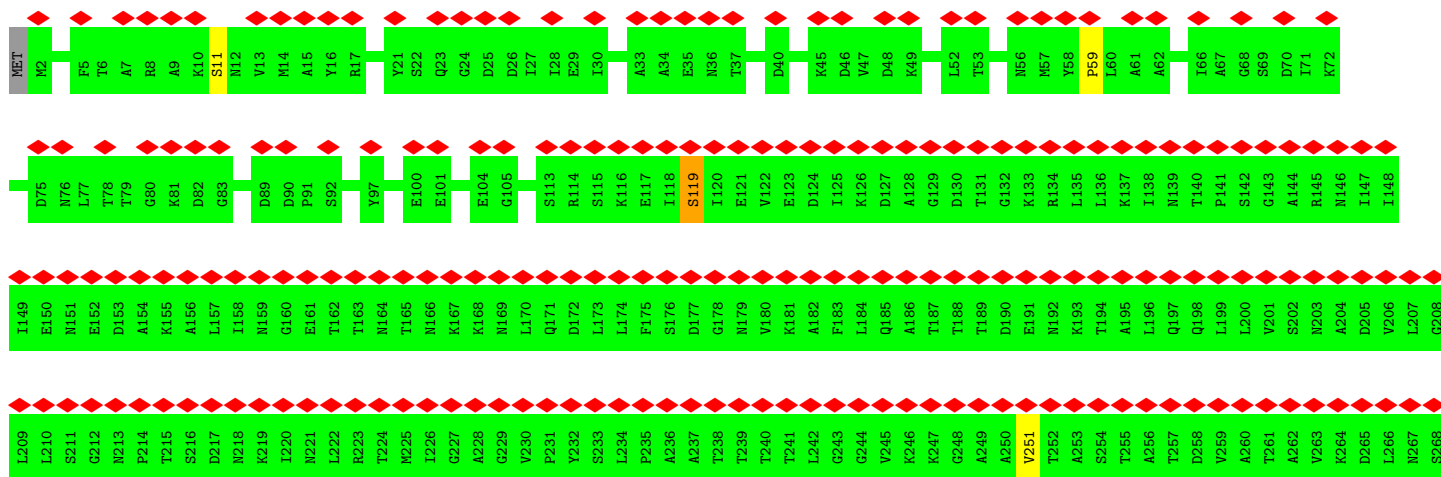
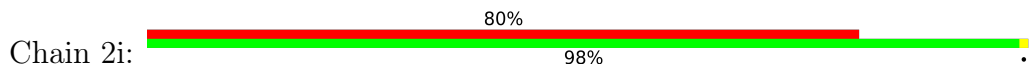


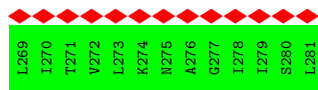


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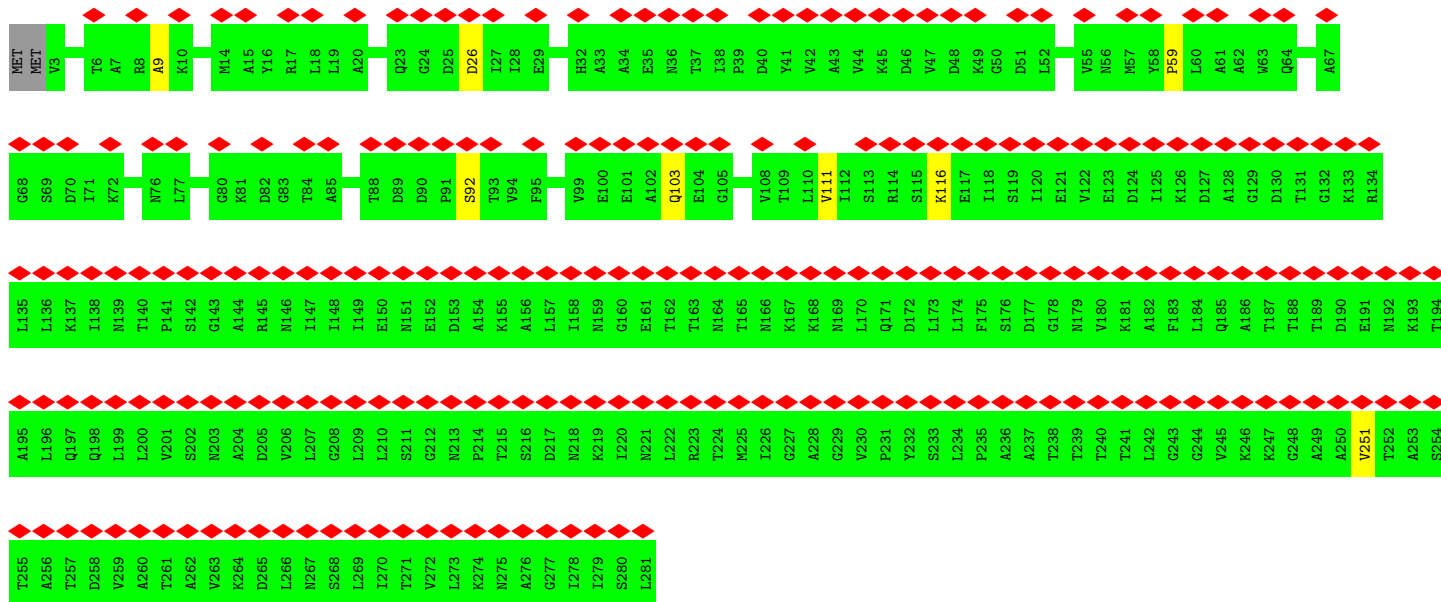
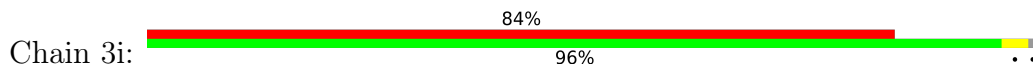


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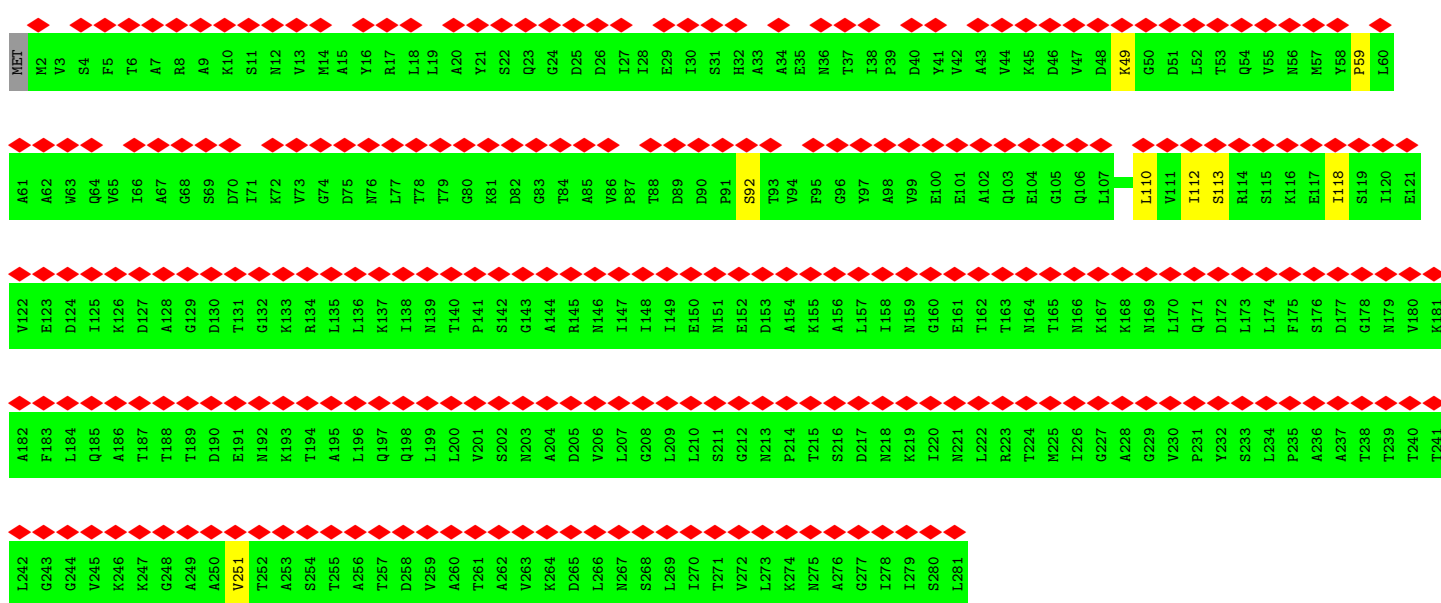




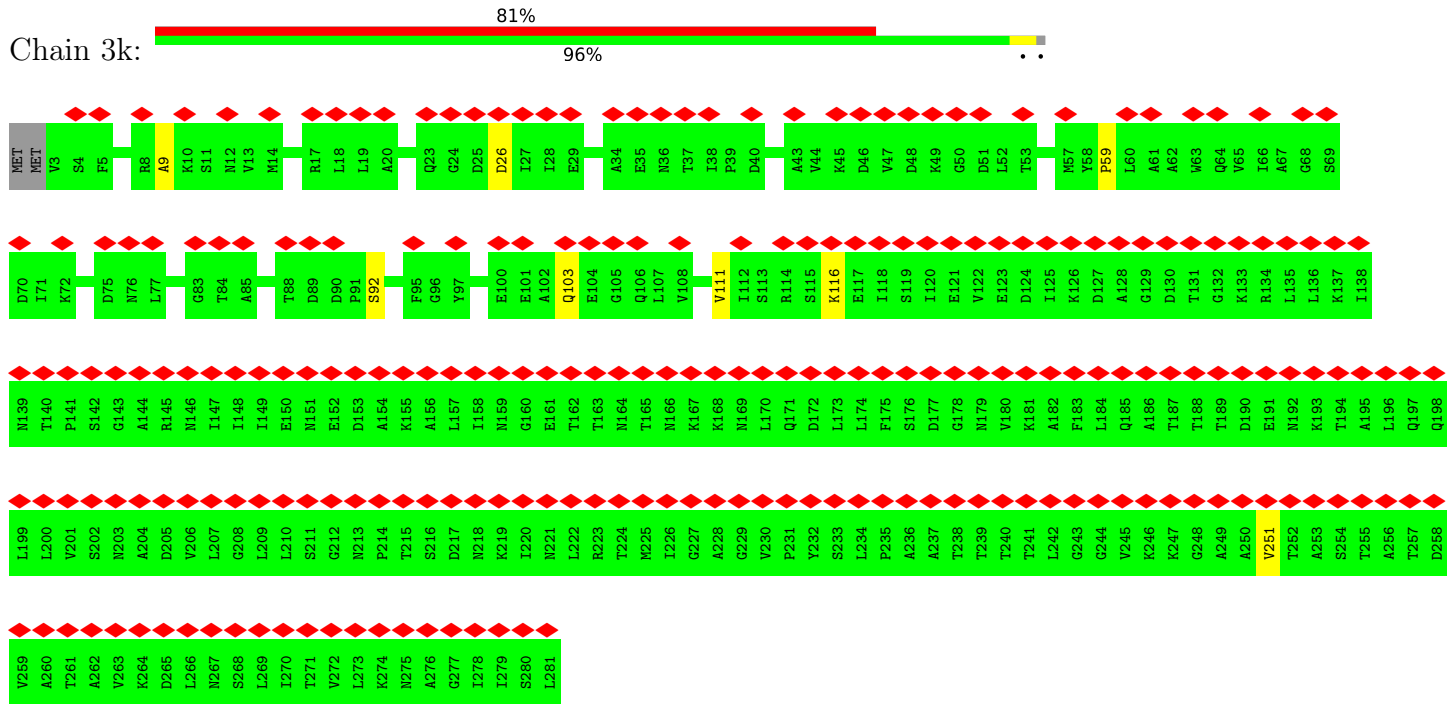
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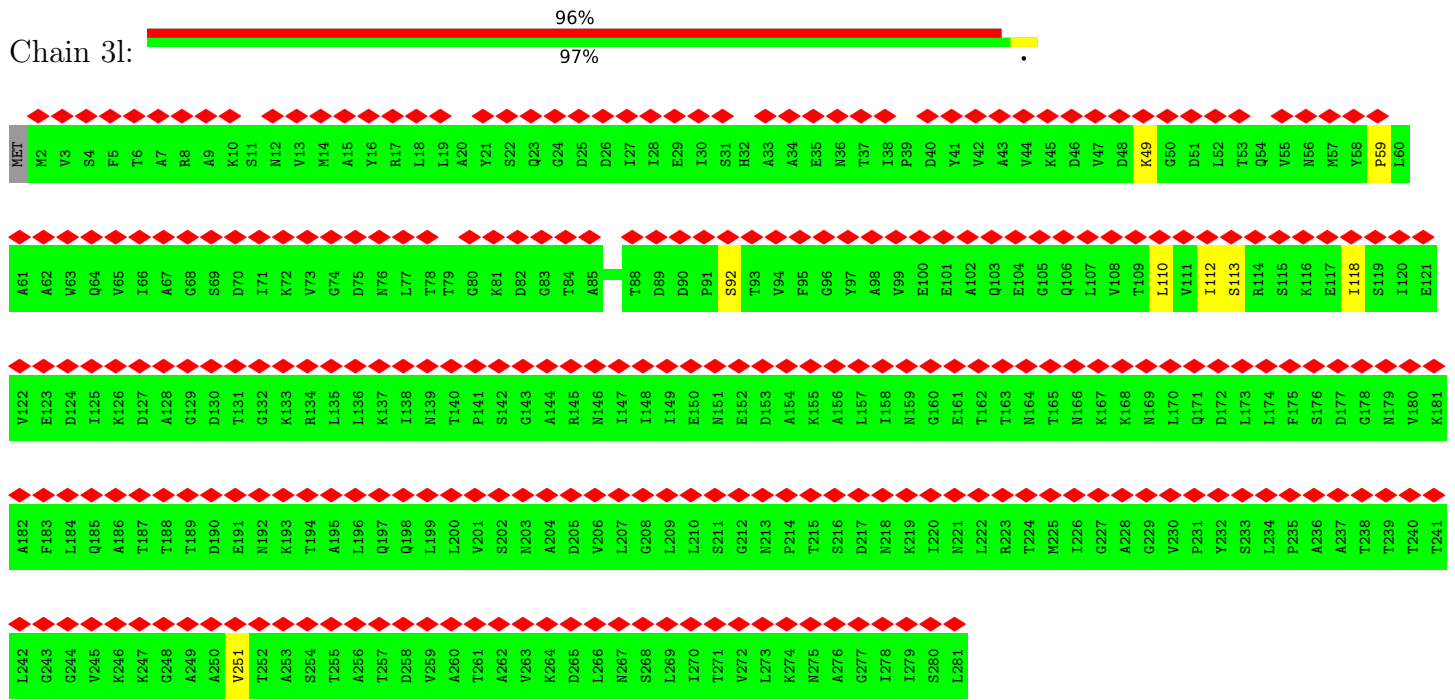
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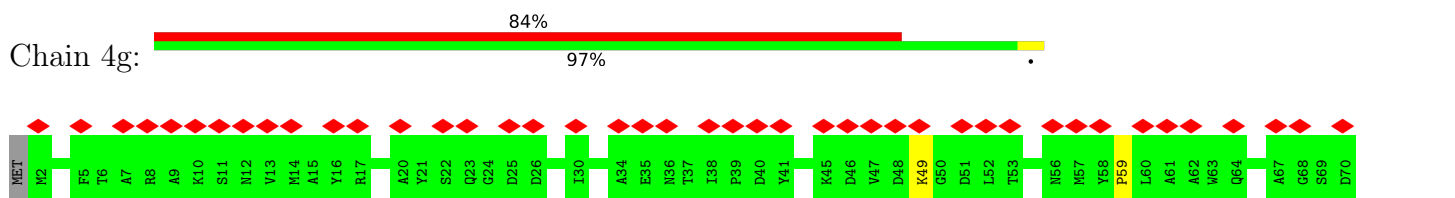
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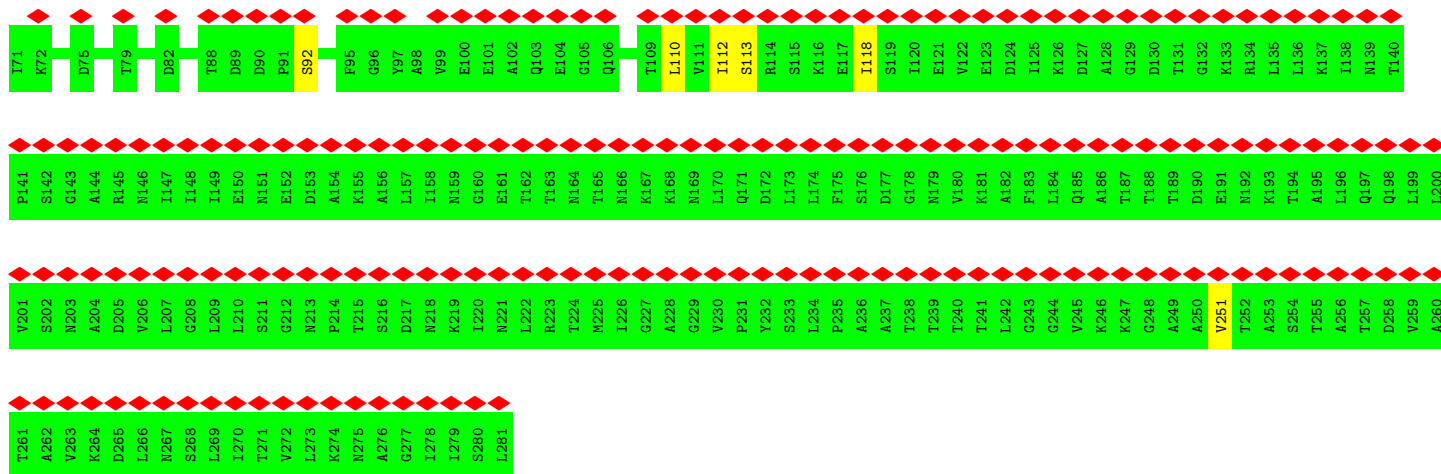


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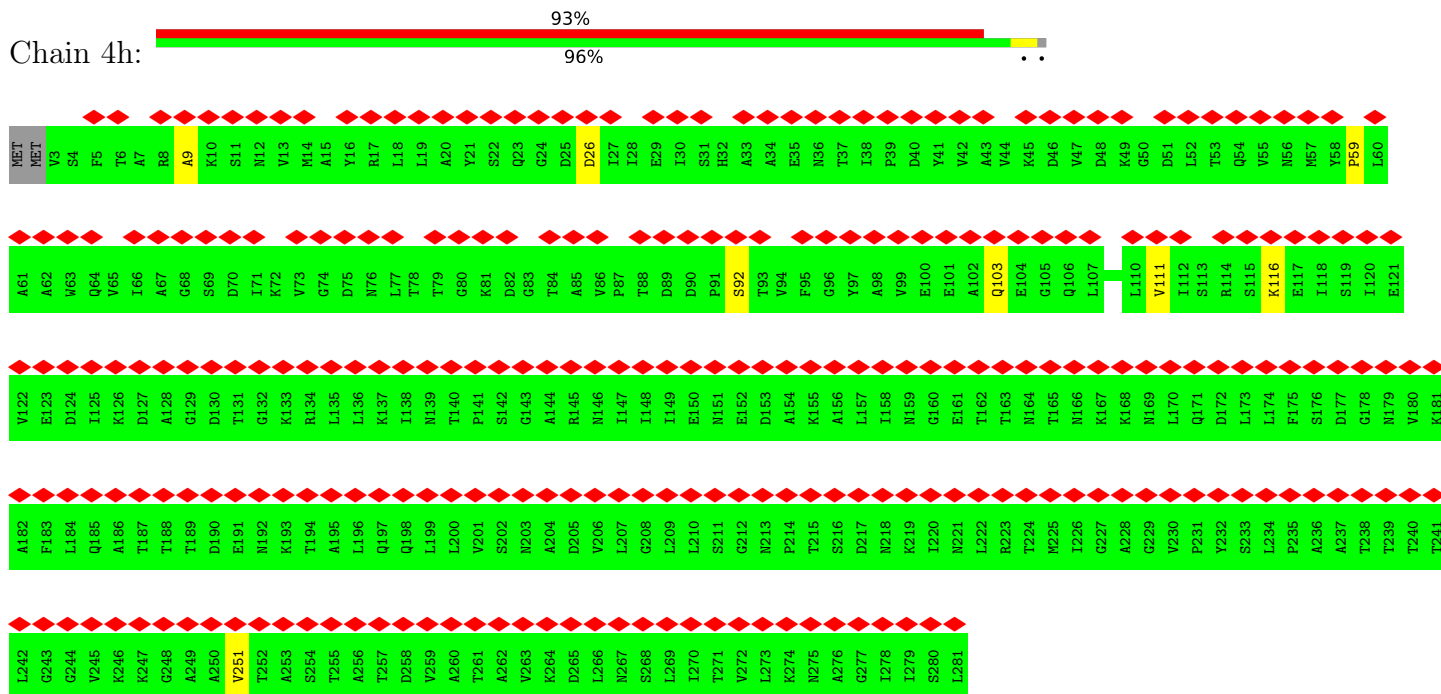


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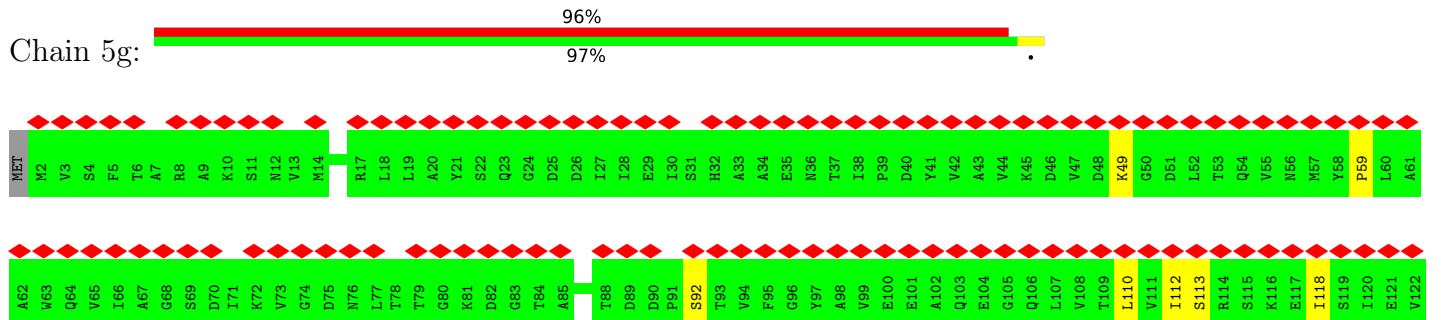


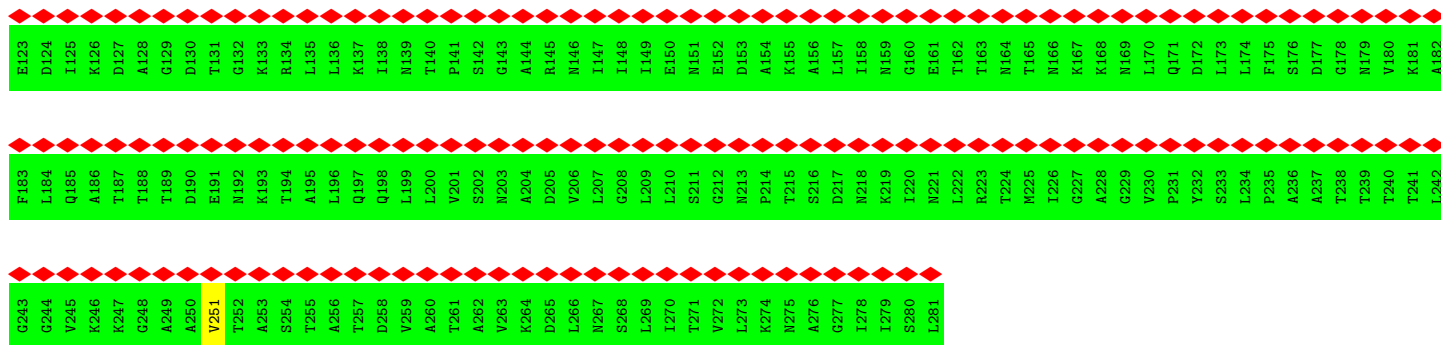


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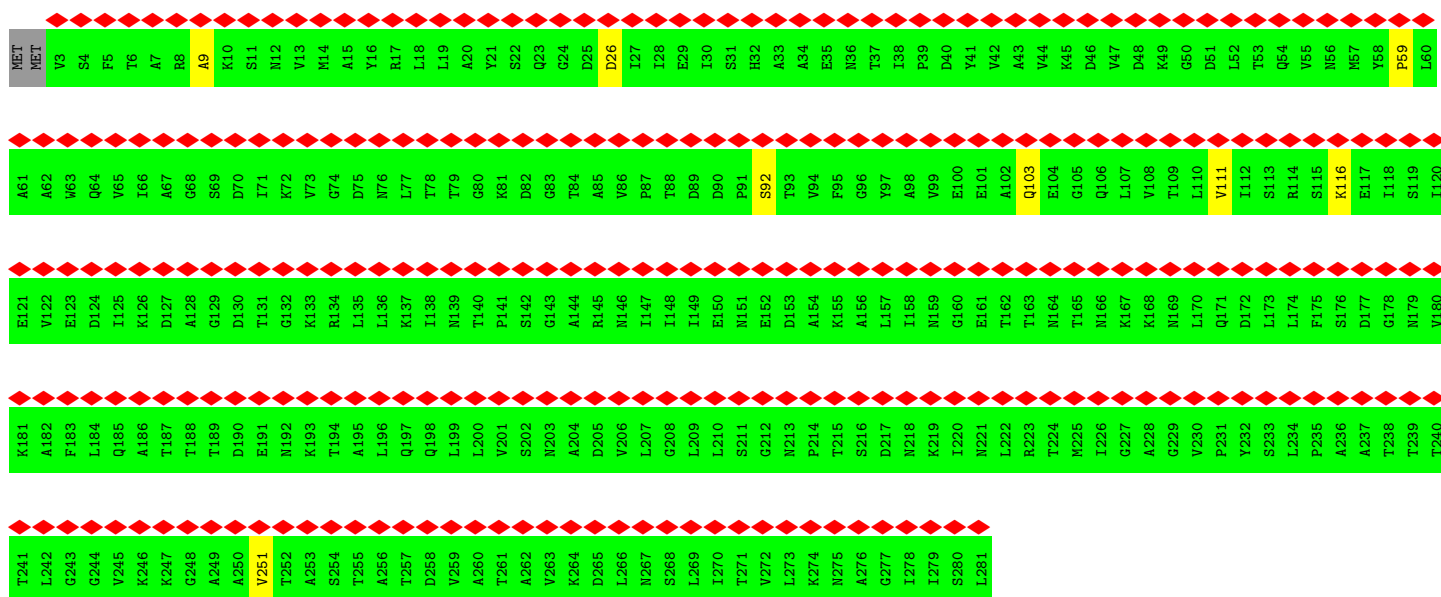


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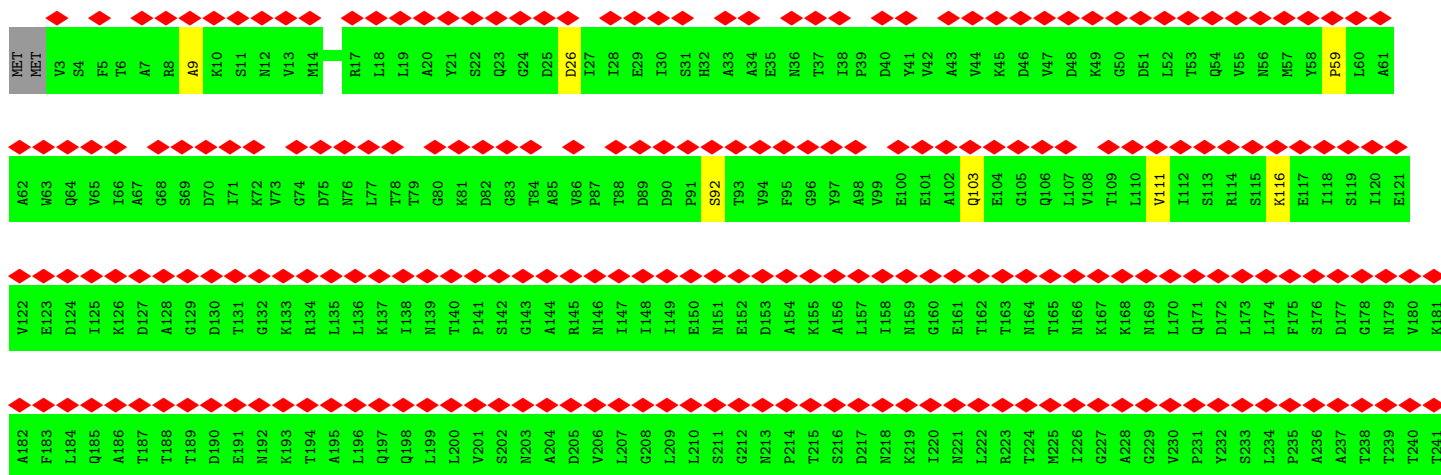


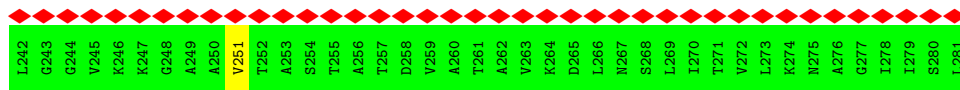


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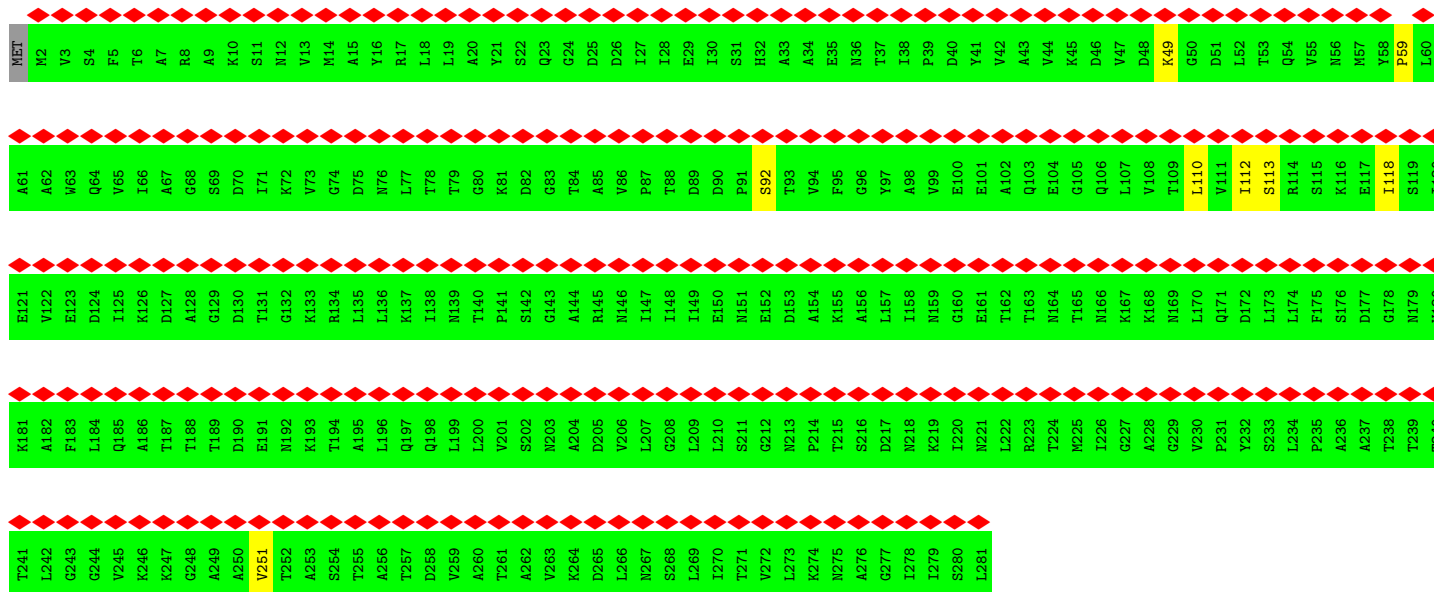


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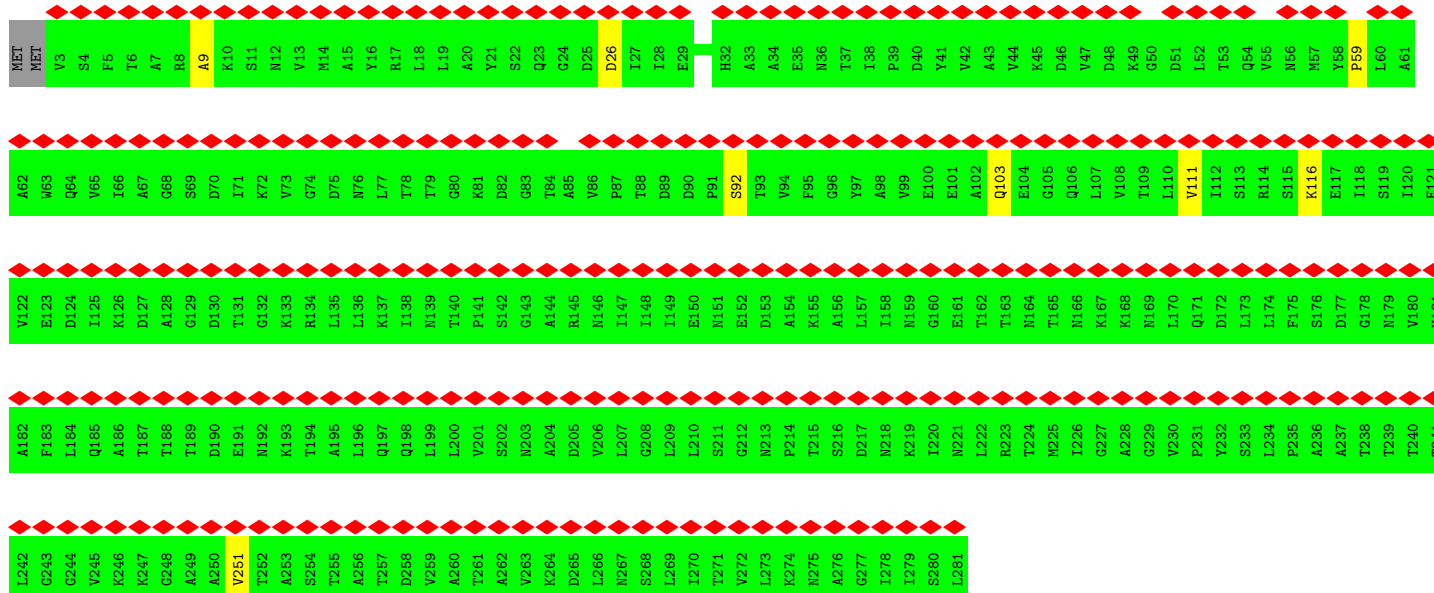




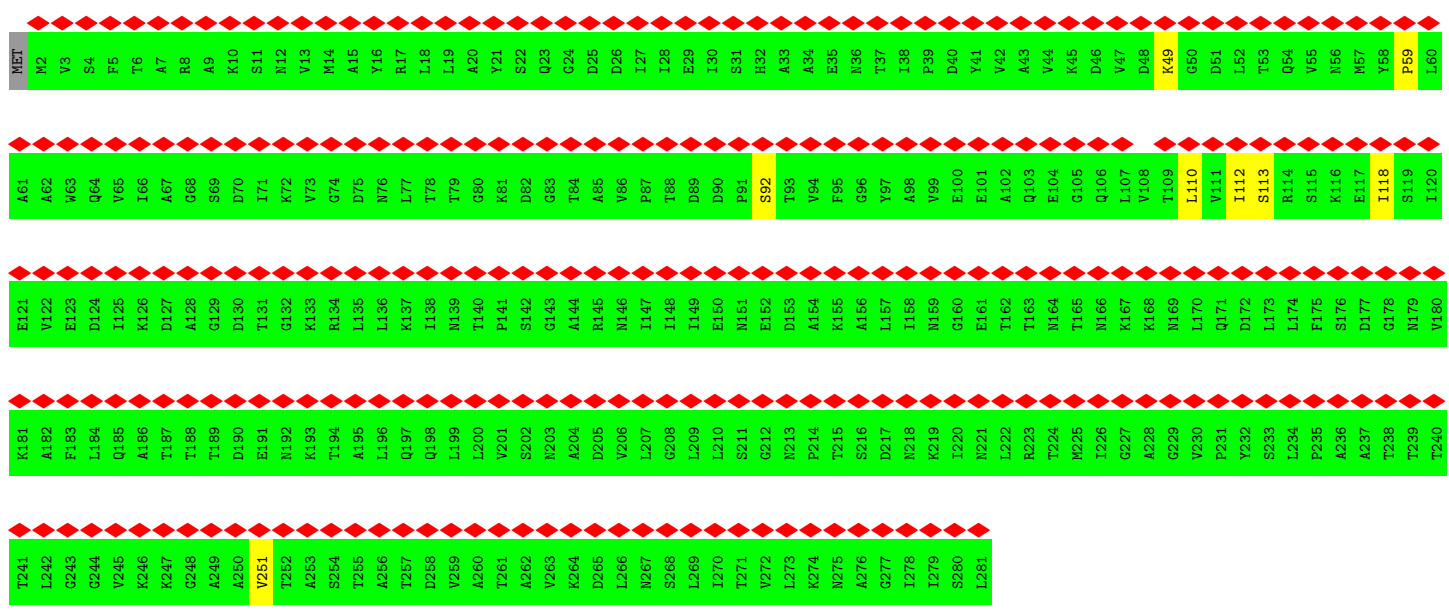
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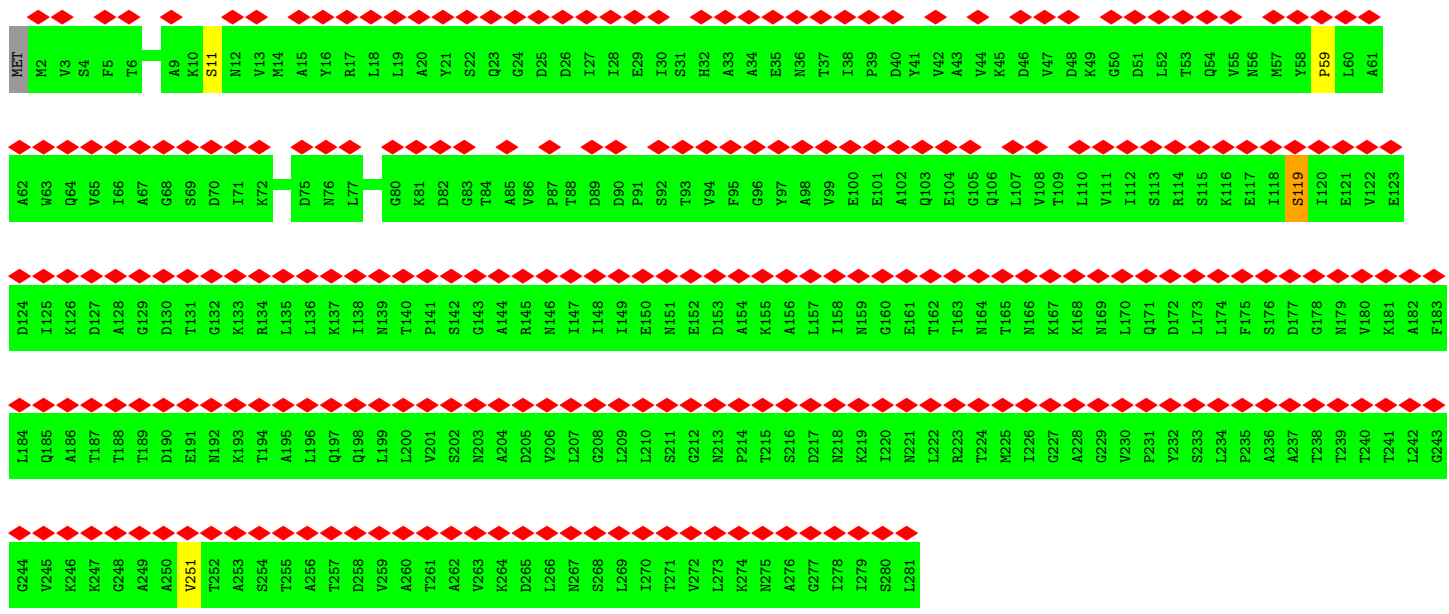
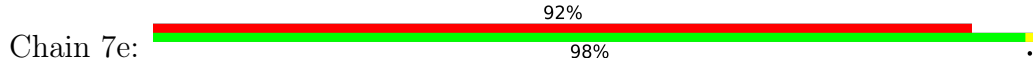
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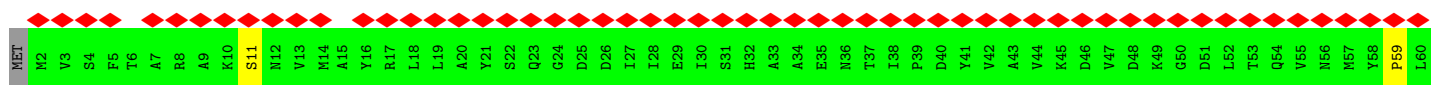
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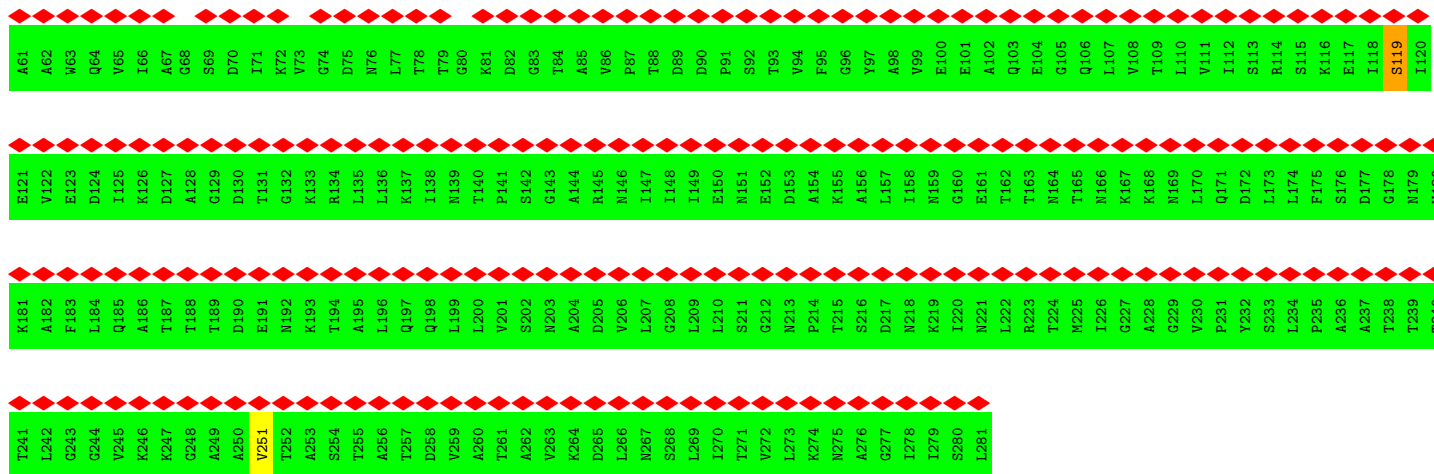


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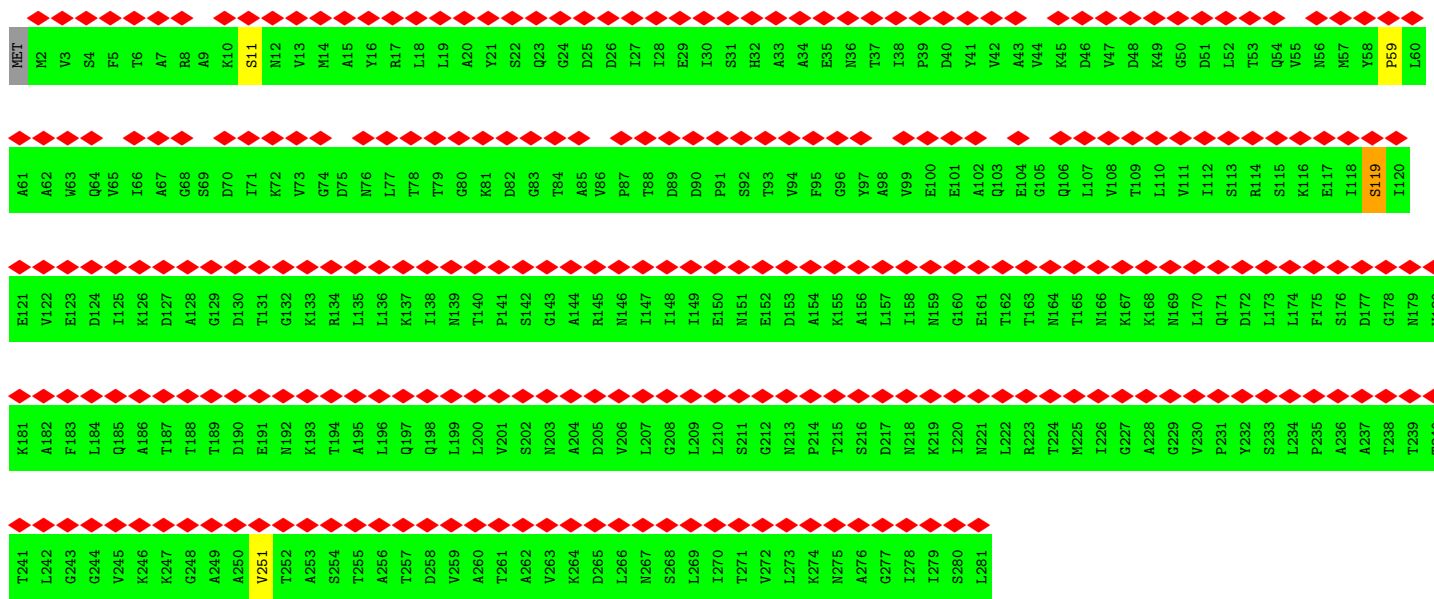


• Molecule 2: Capsid fiber protein

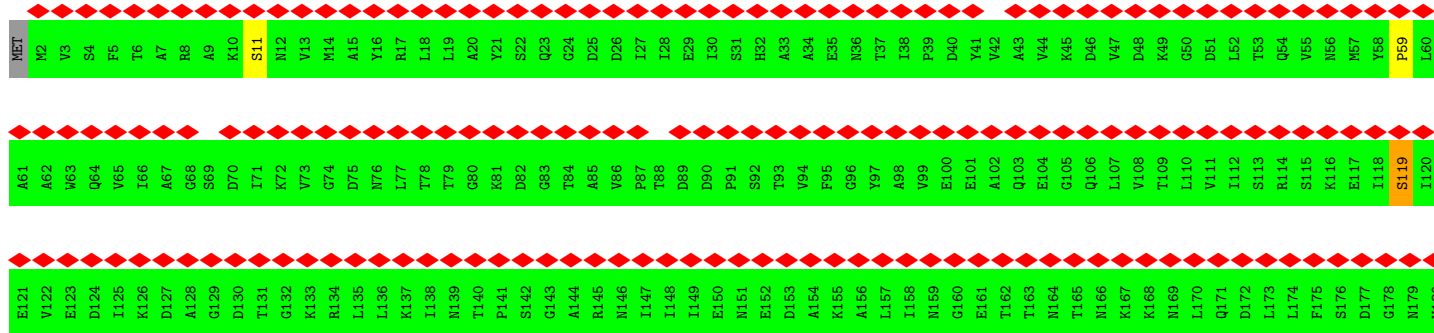


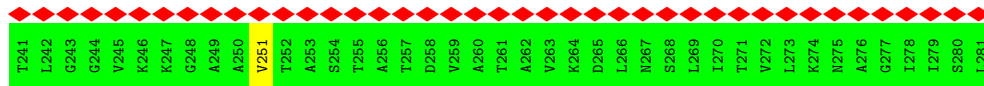
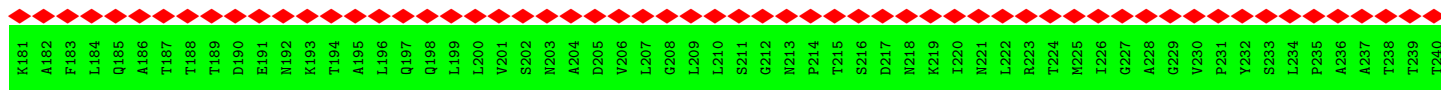


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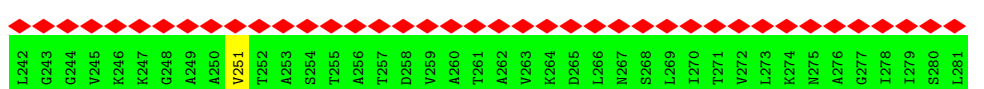
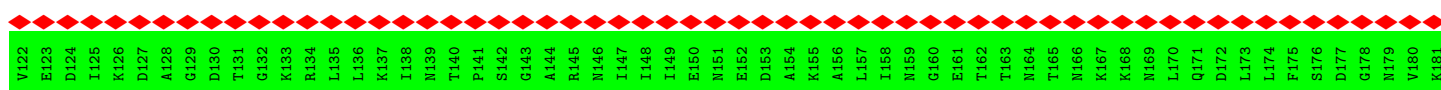
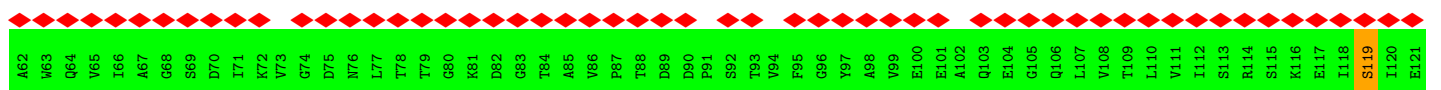


• Molecule 2: Capsid fiber protein

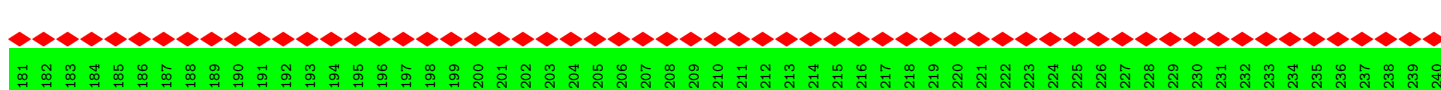
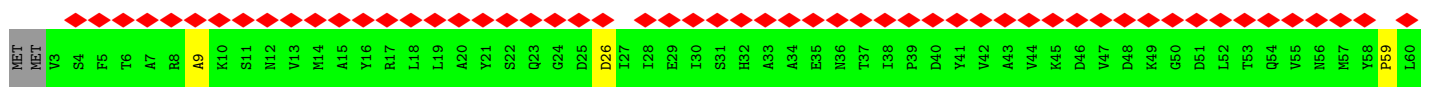




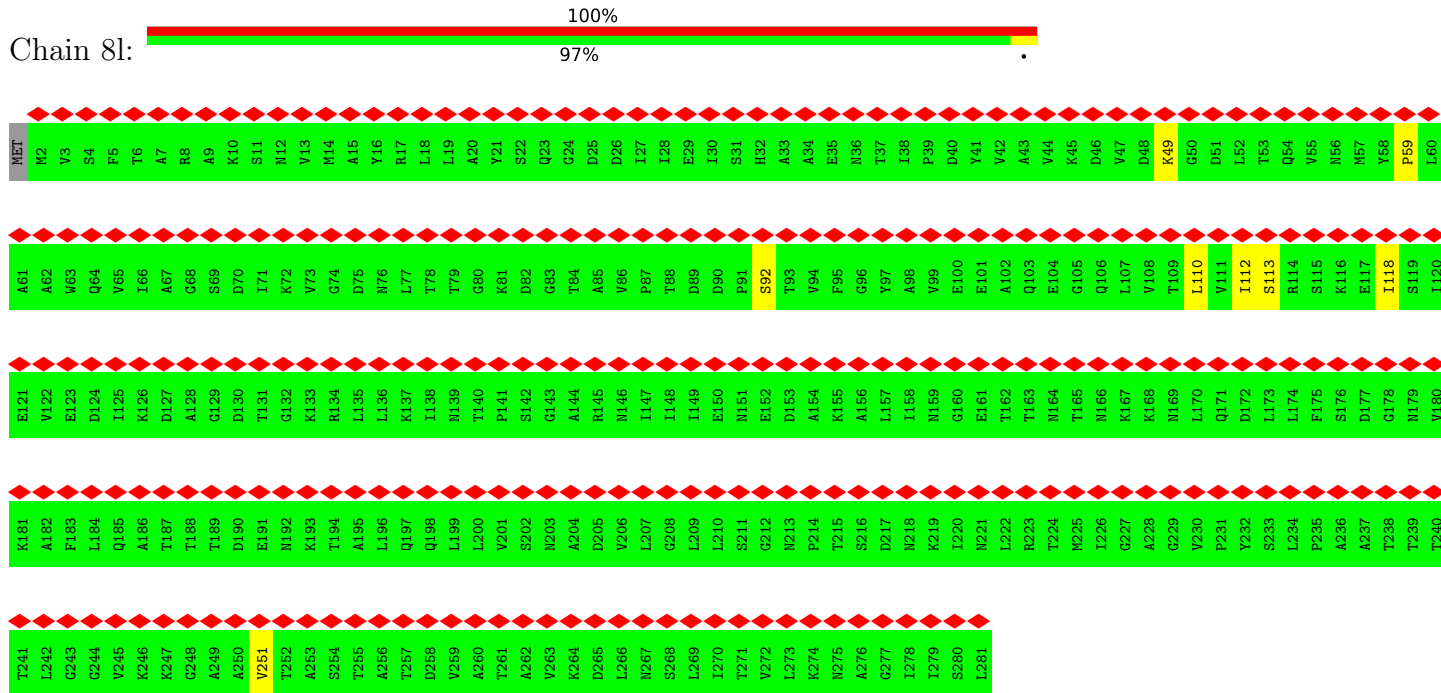
• Molecule 2: Capsid fiber protein



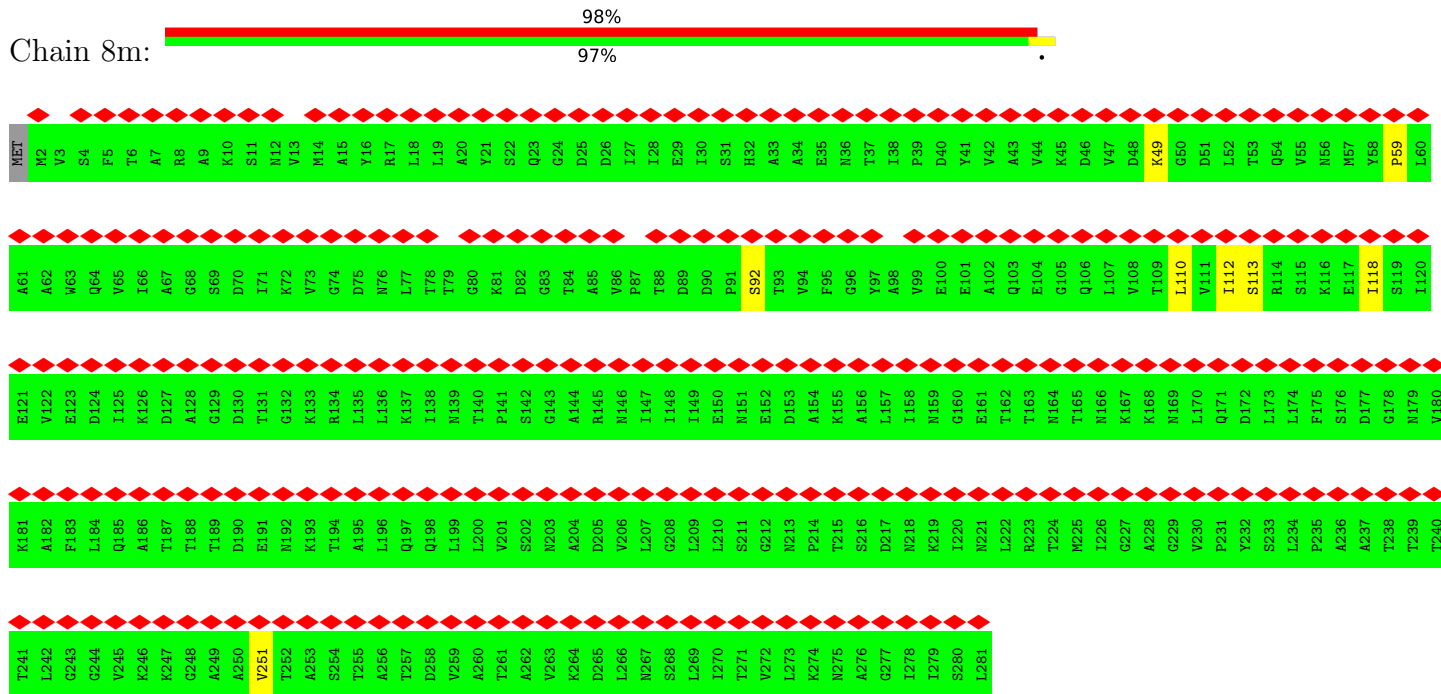
• Molecule 2: Capsid fiber protein



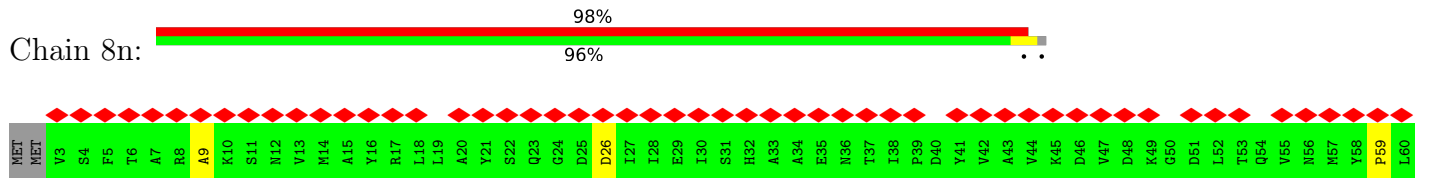
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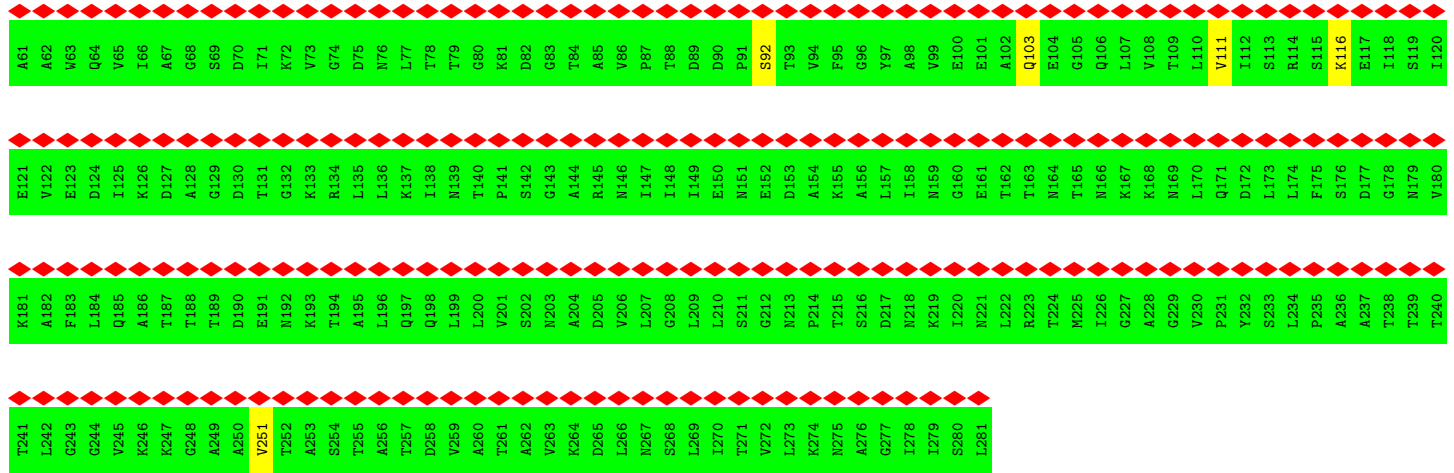


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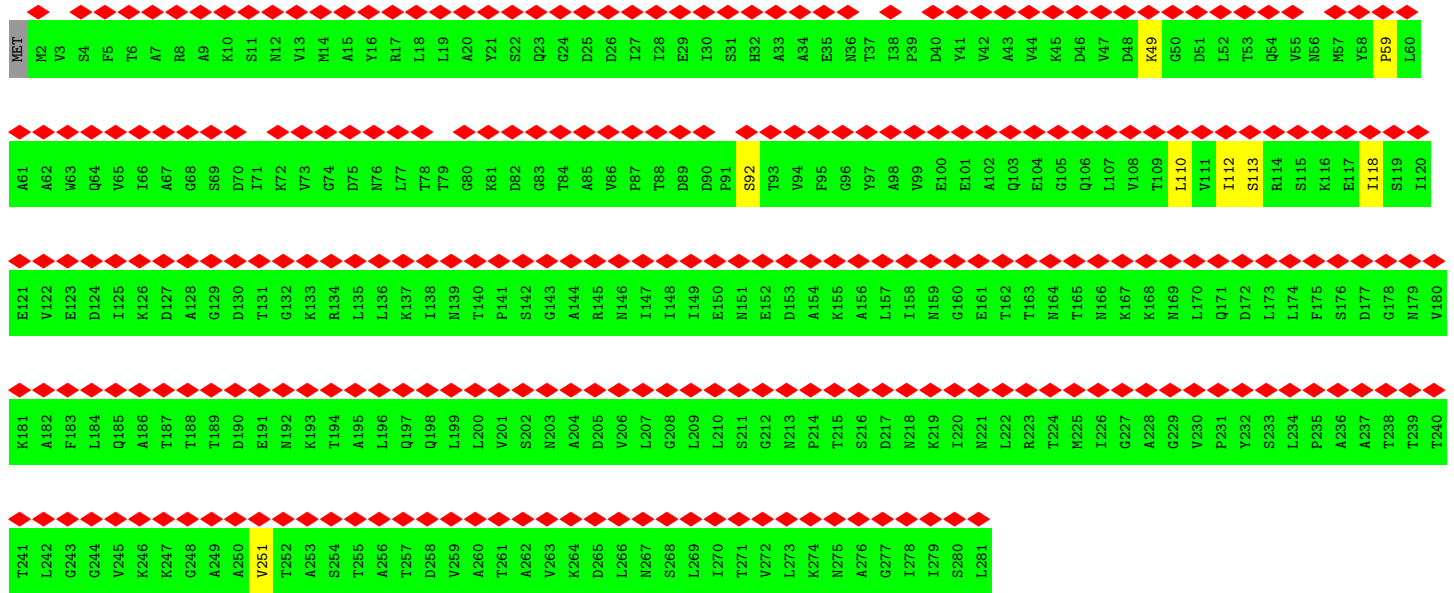


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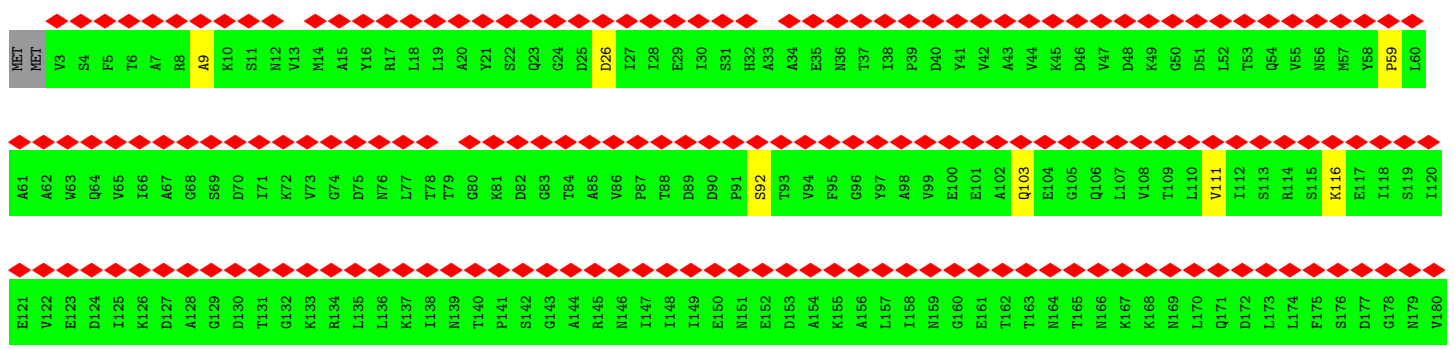


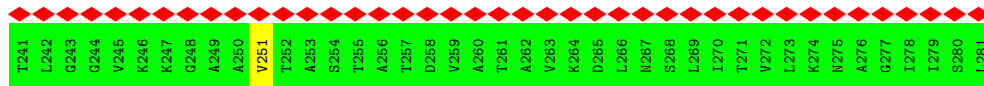
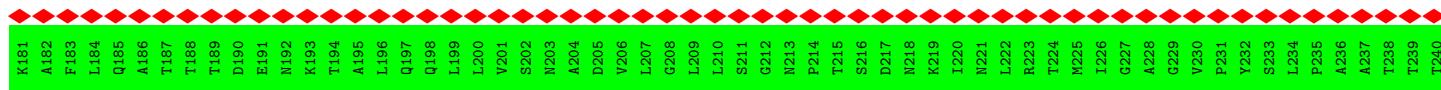


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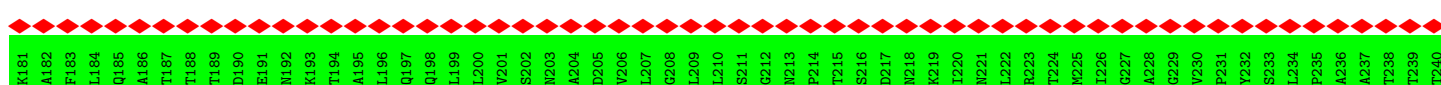
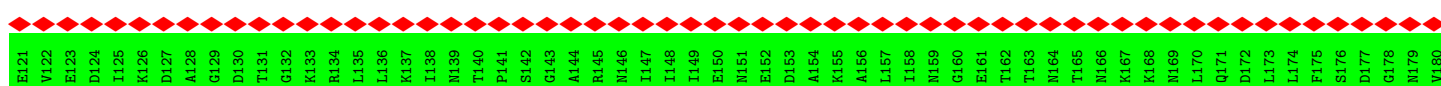
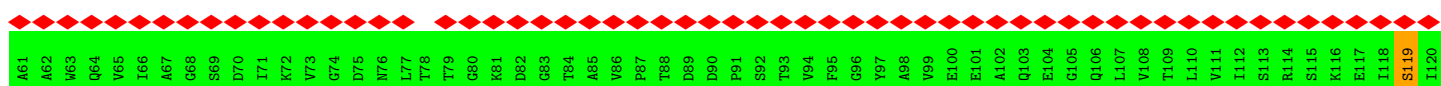
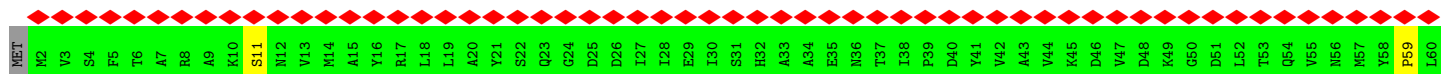


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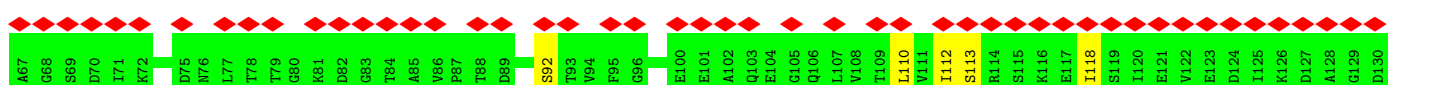
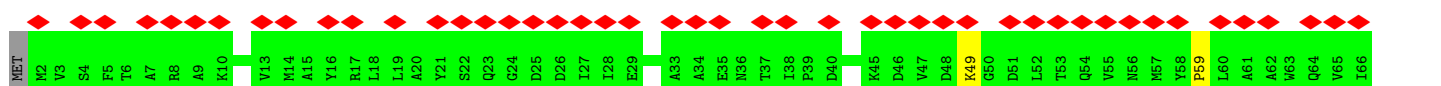
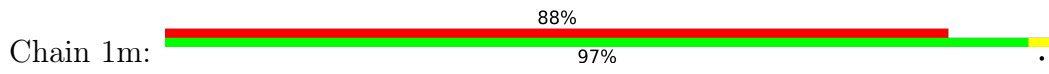




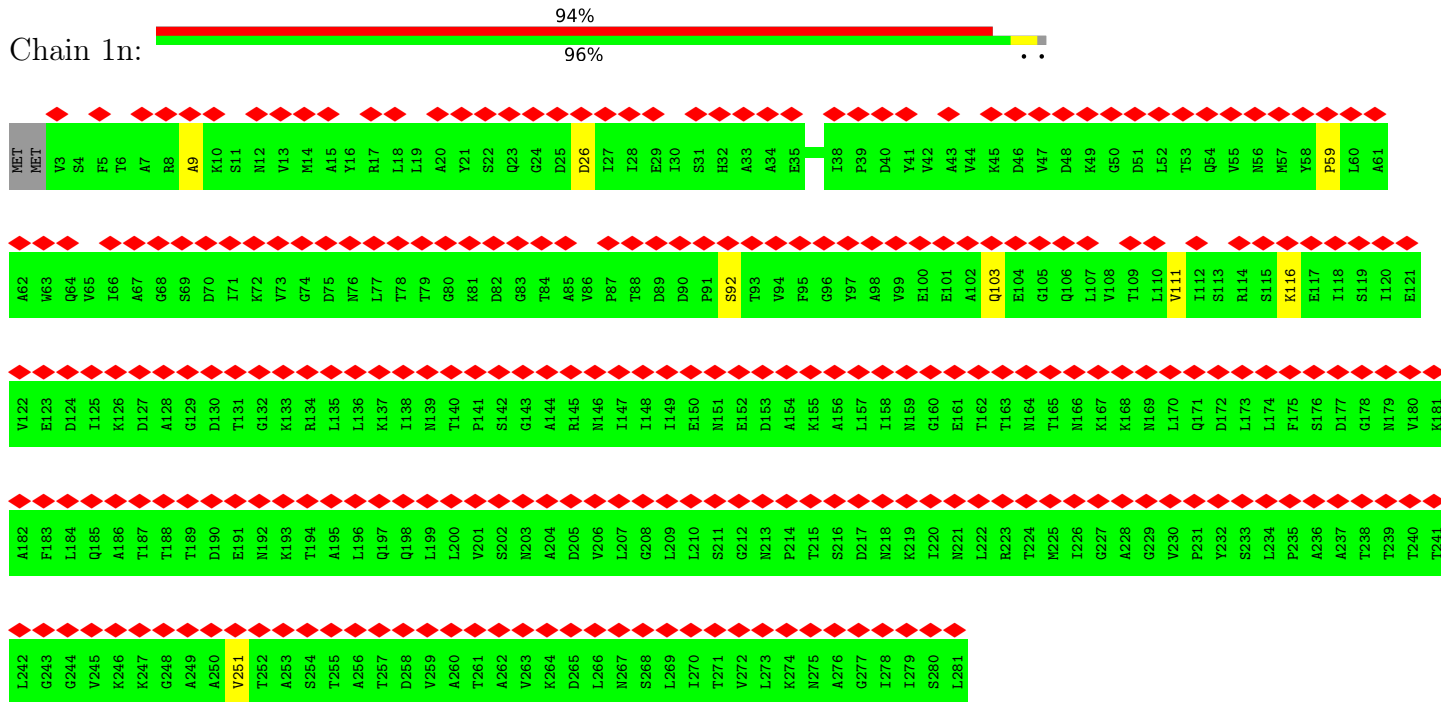
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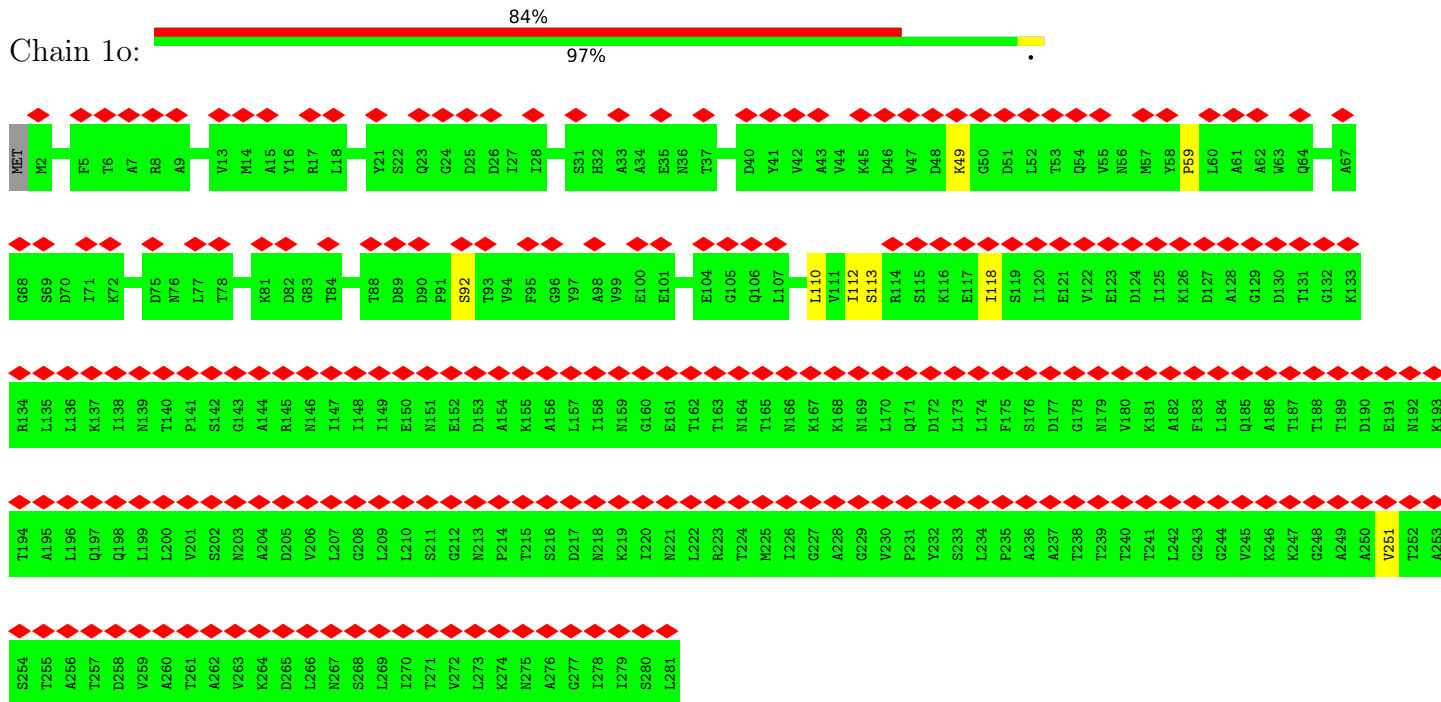
• Molecule 2: Capsid fiber protein



• Molecule 2: Capsid fiber protein

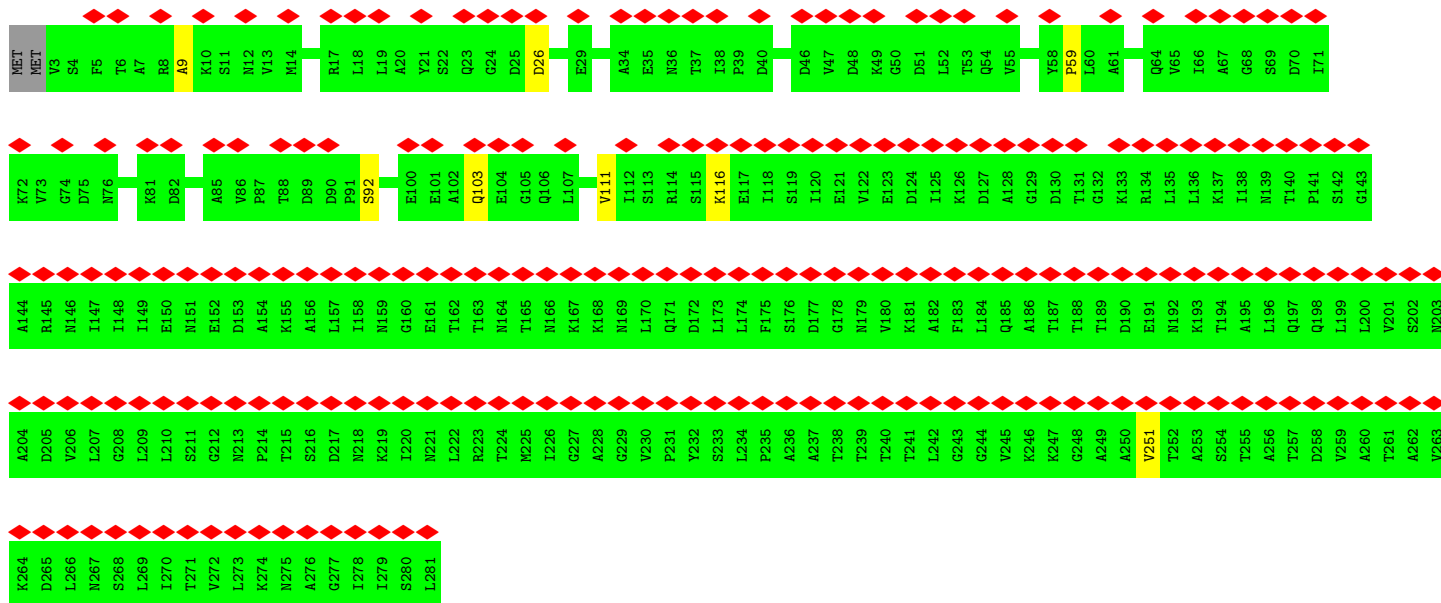


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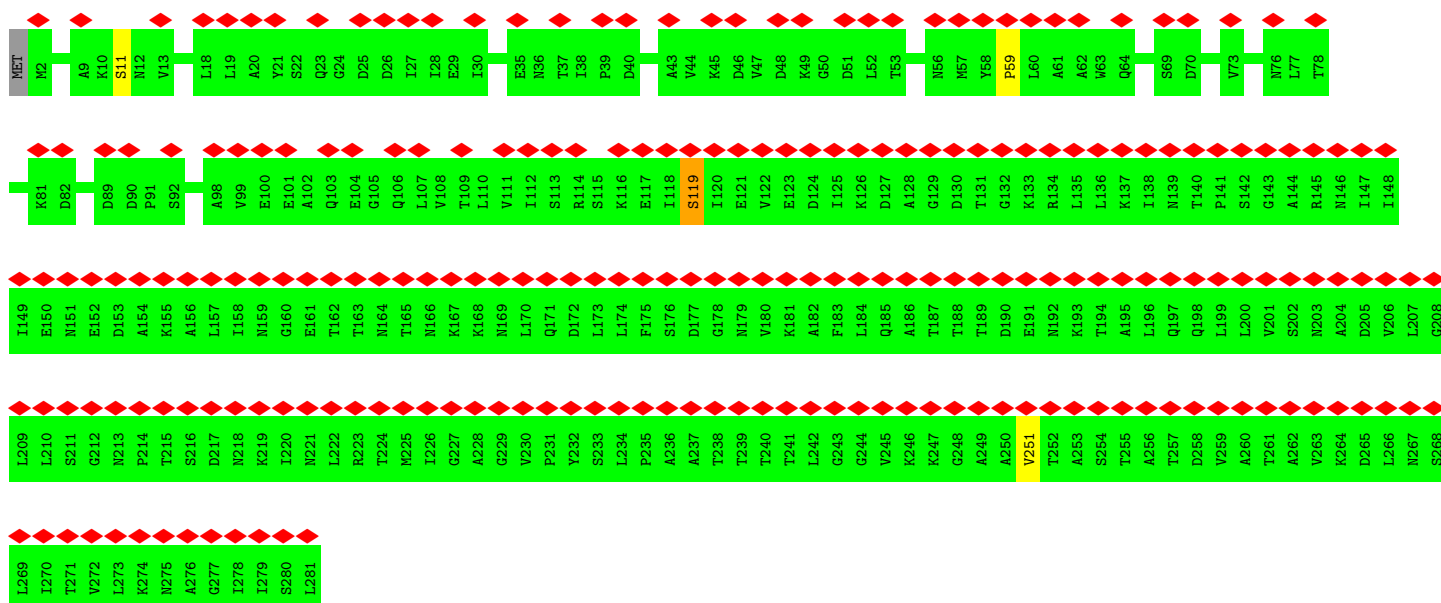
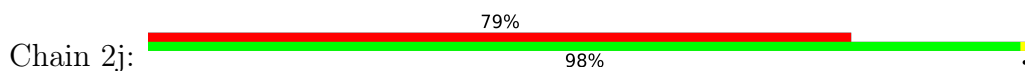


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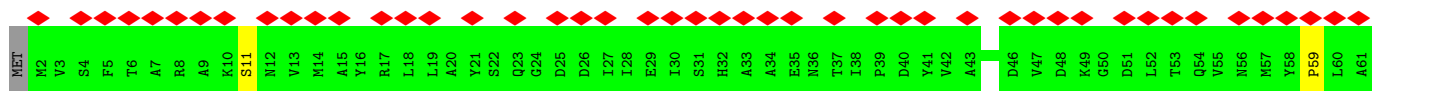


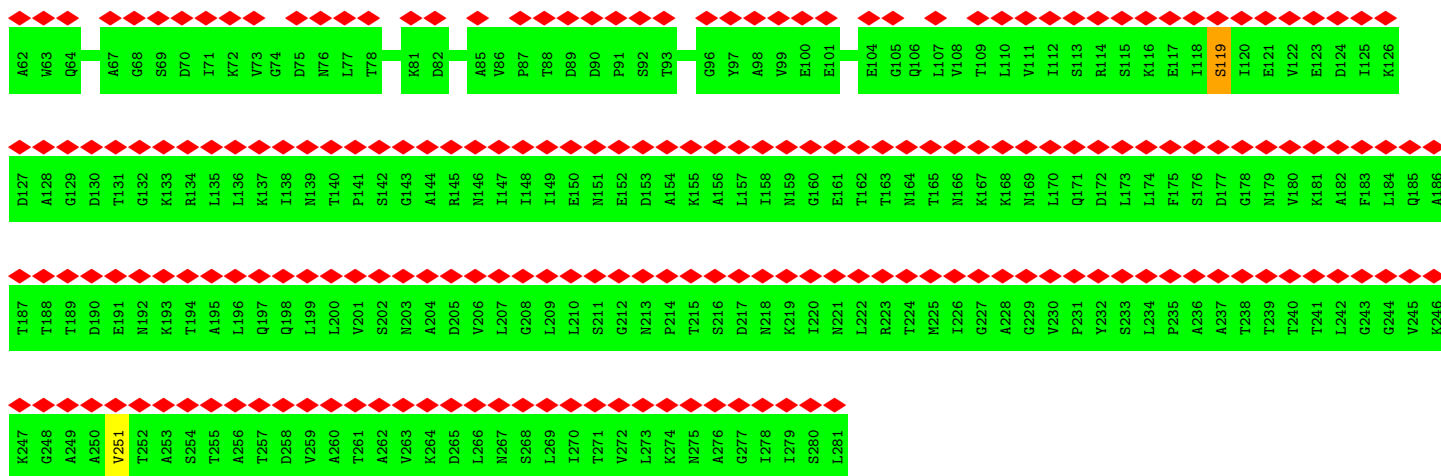


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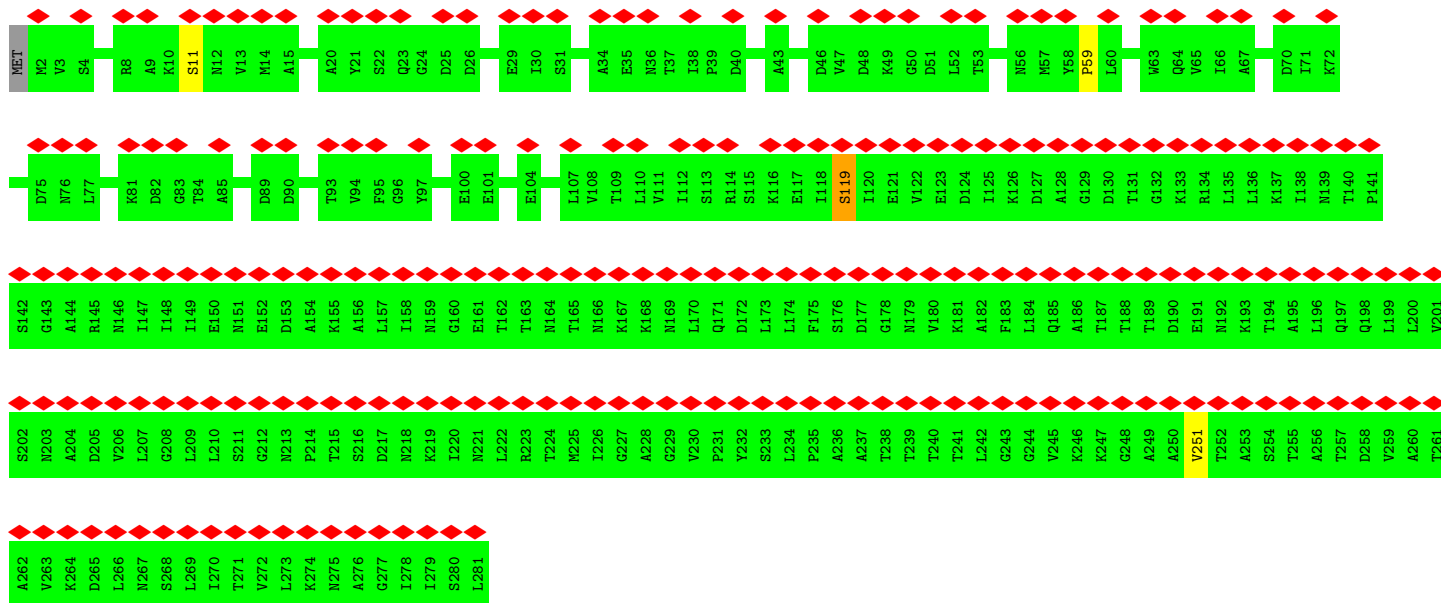
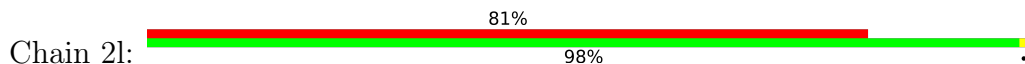


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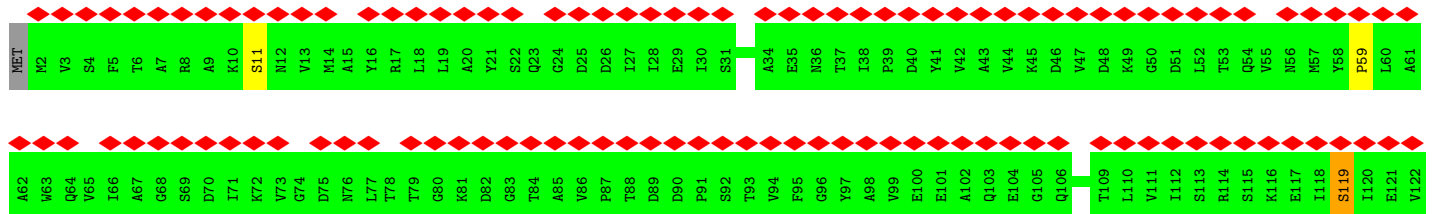


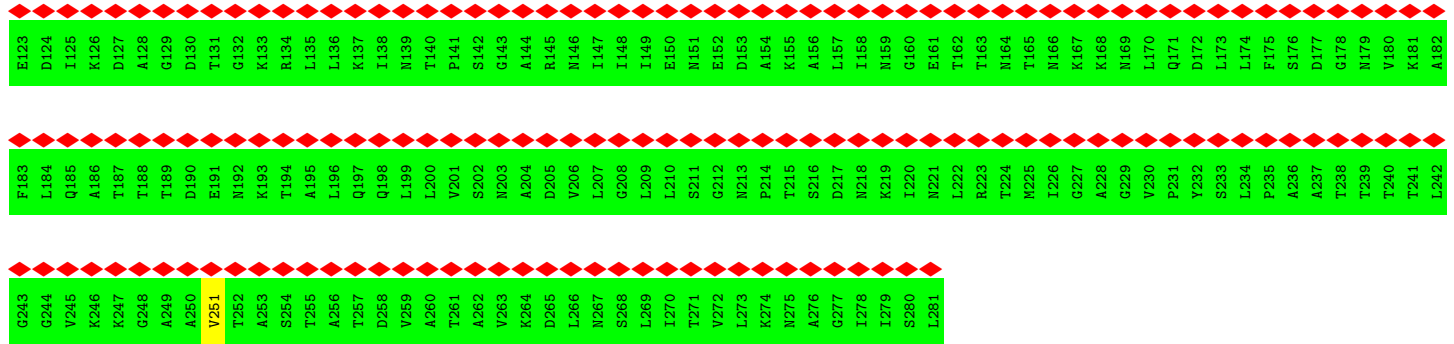


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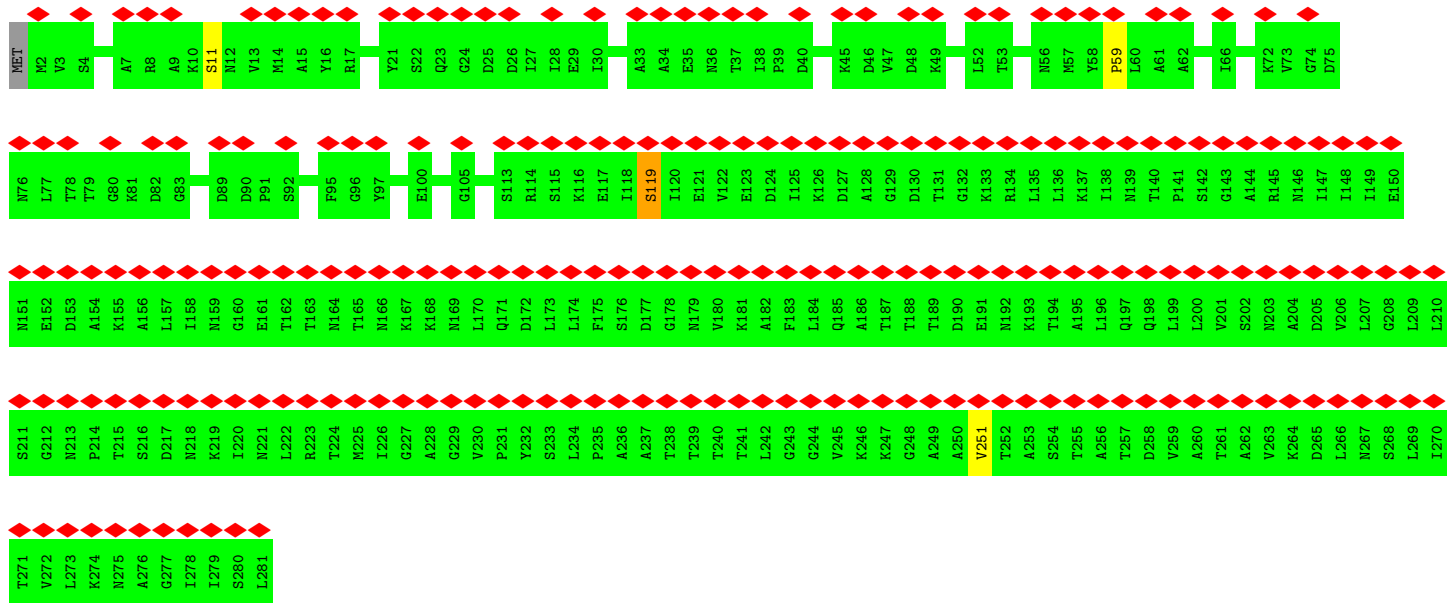
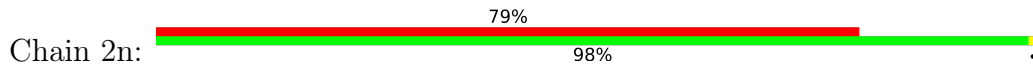


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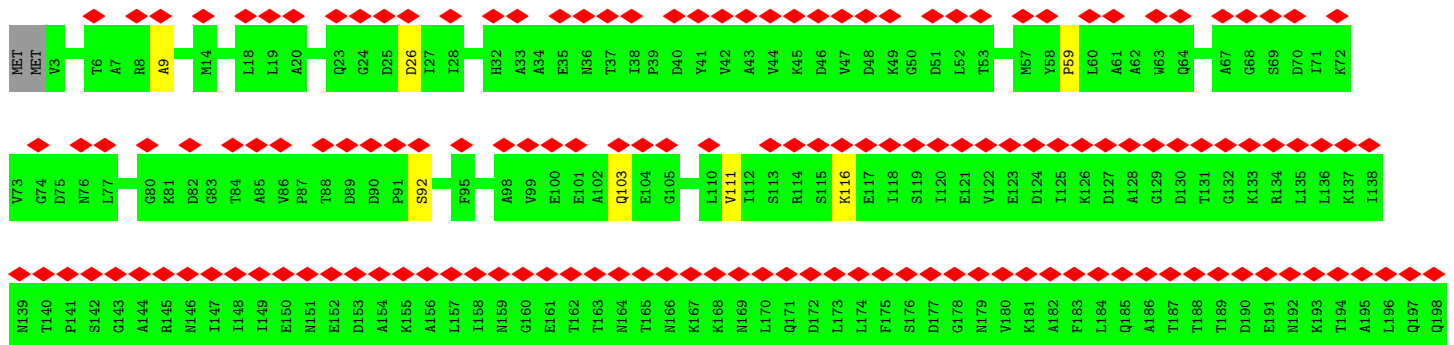
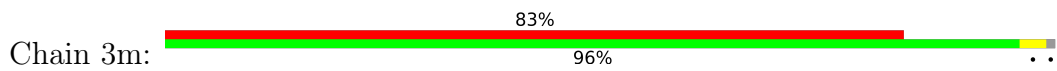


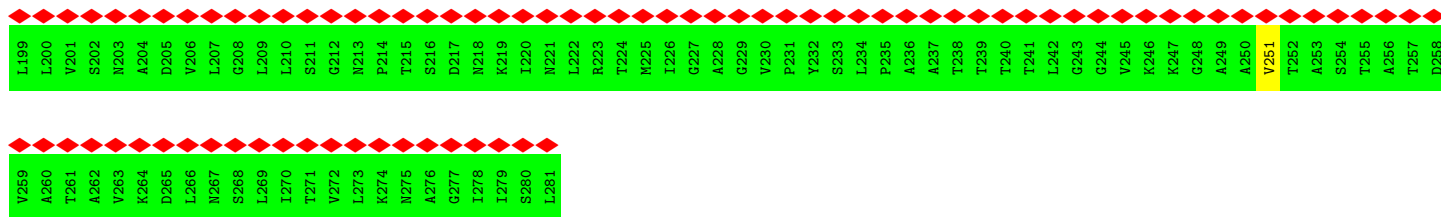


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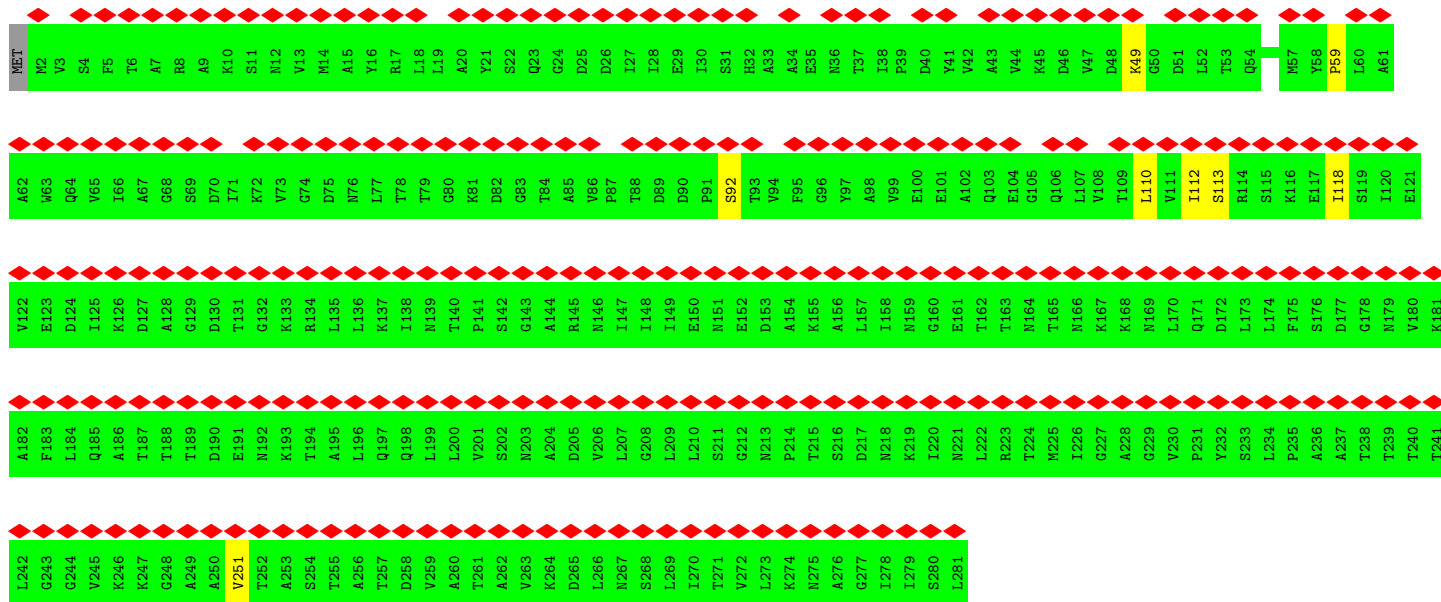


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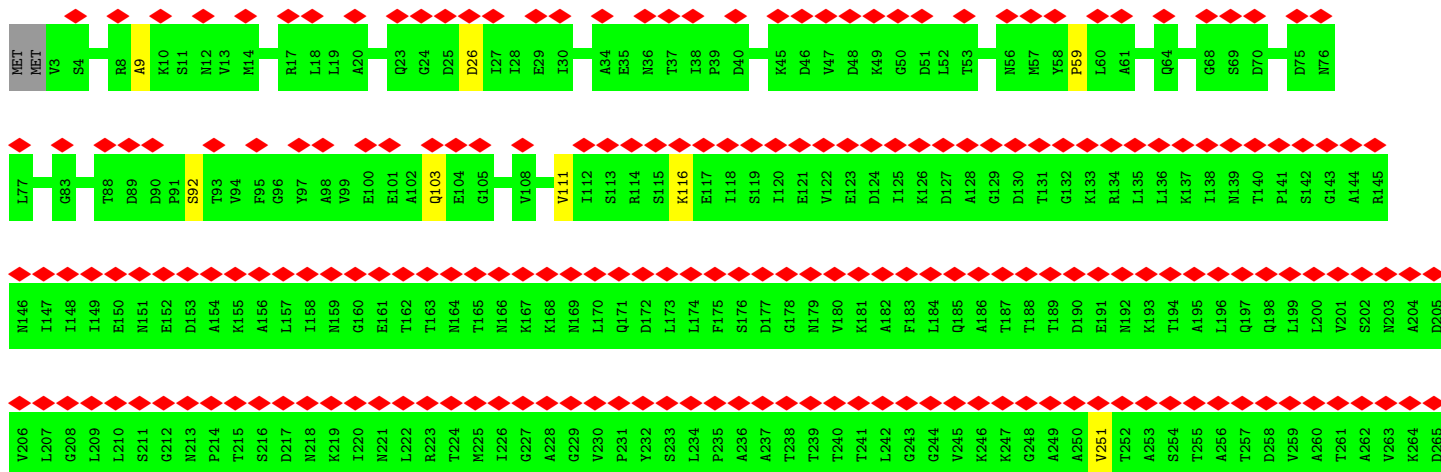
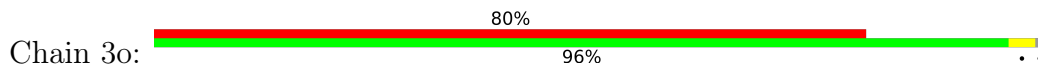


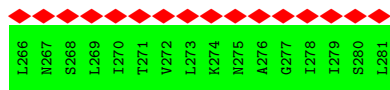


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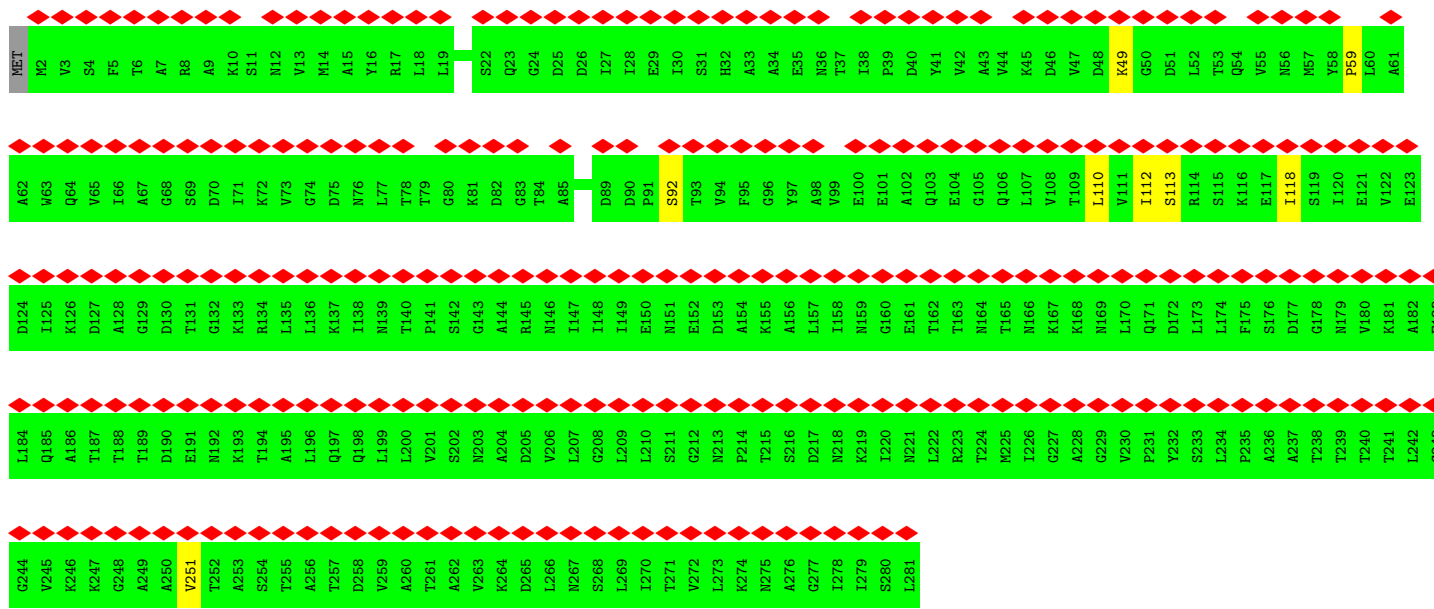


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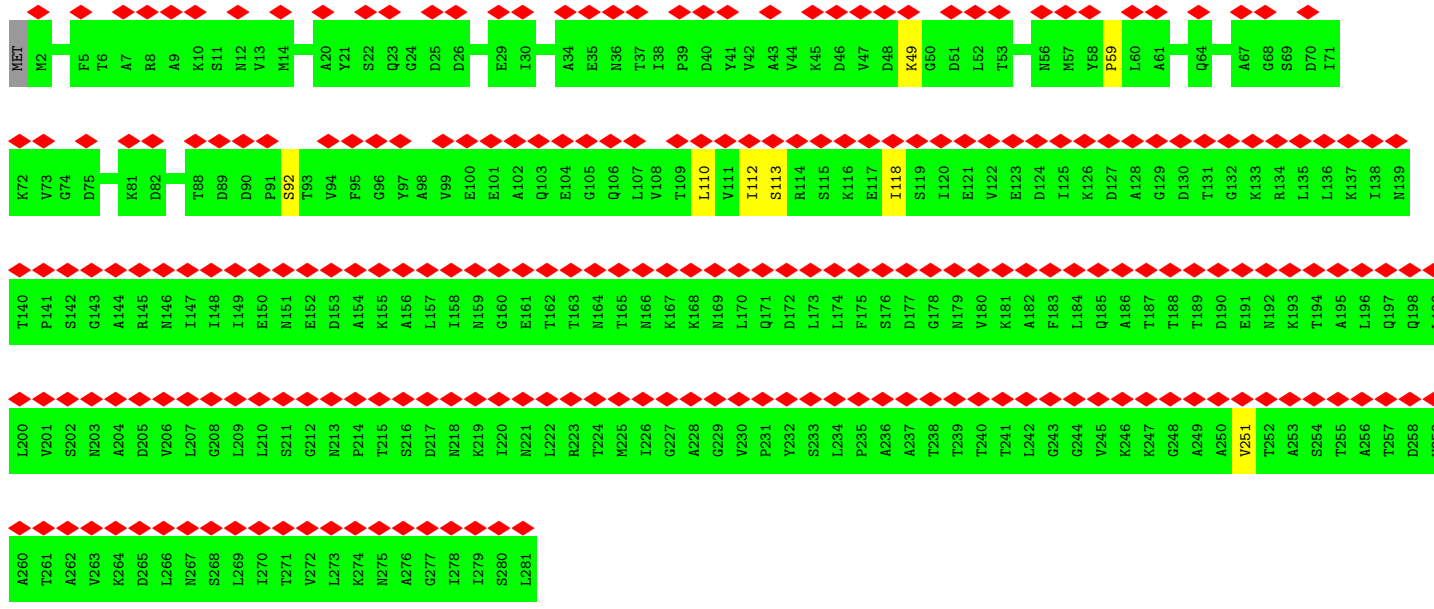
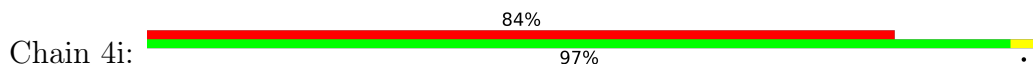




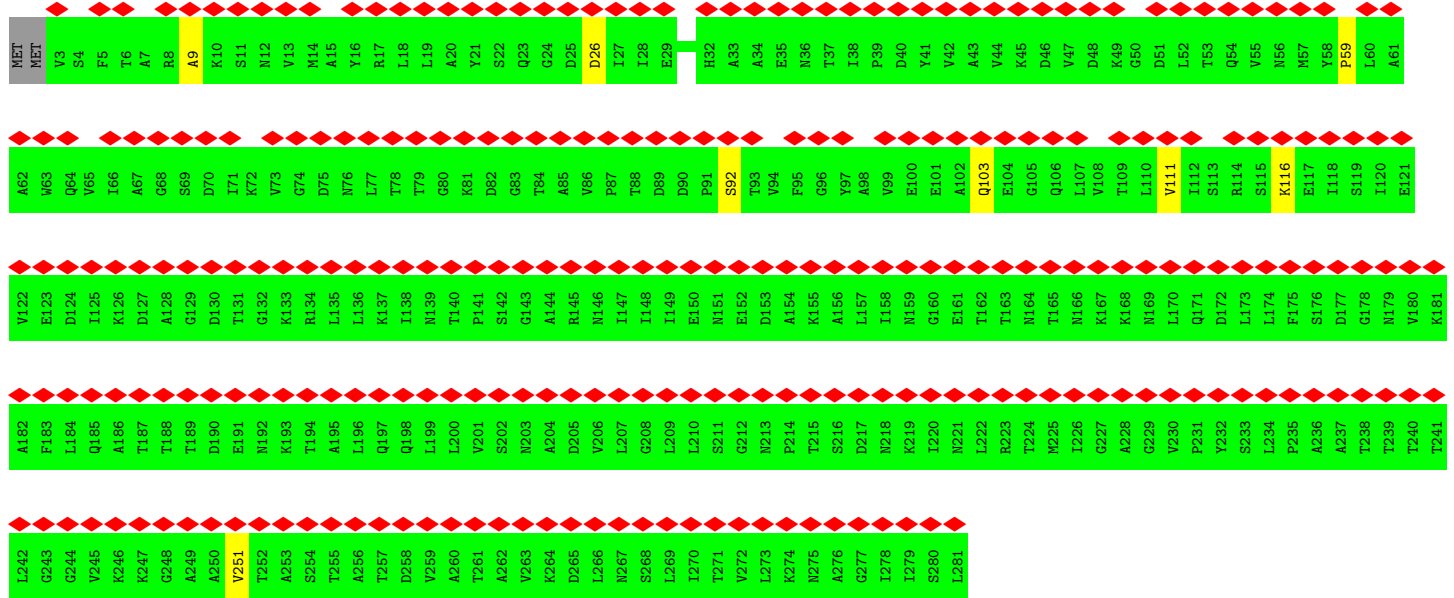
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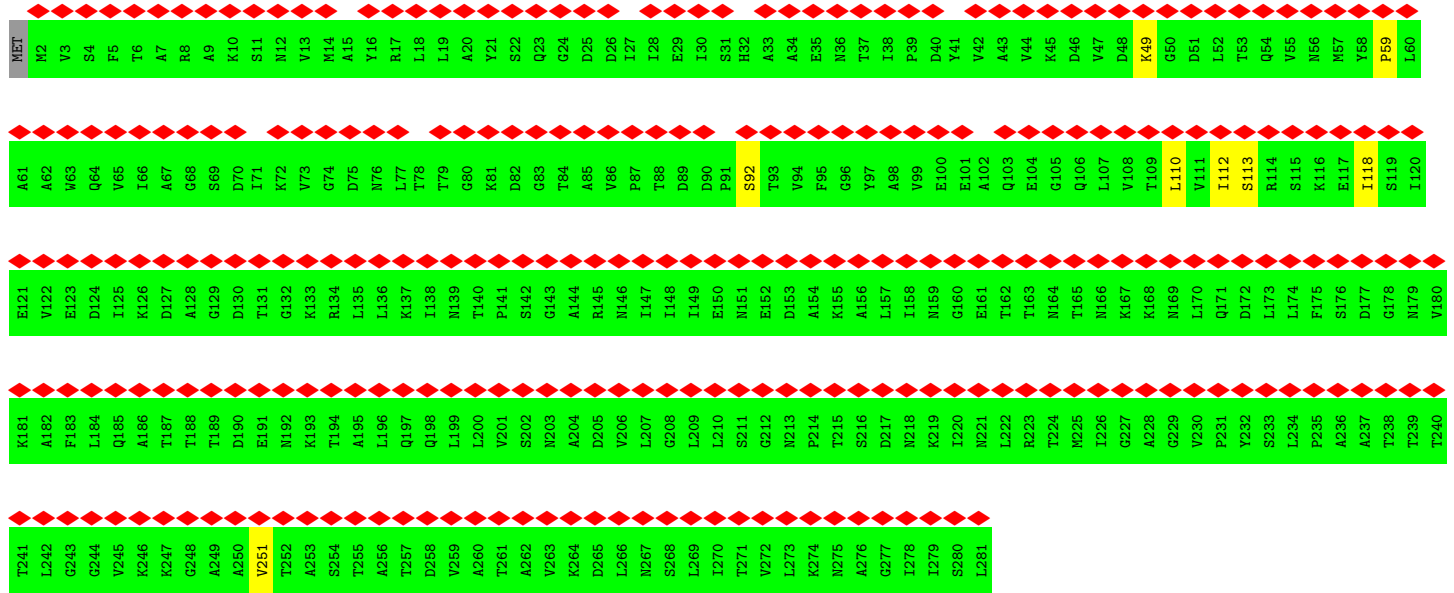
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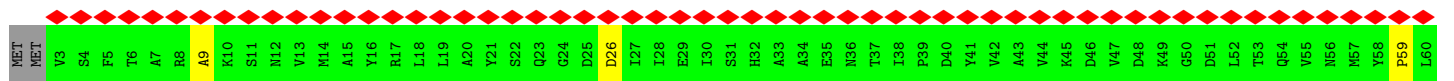
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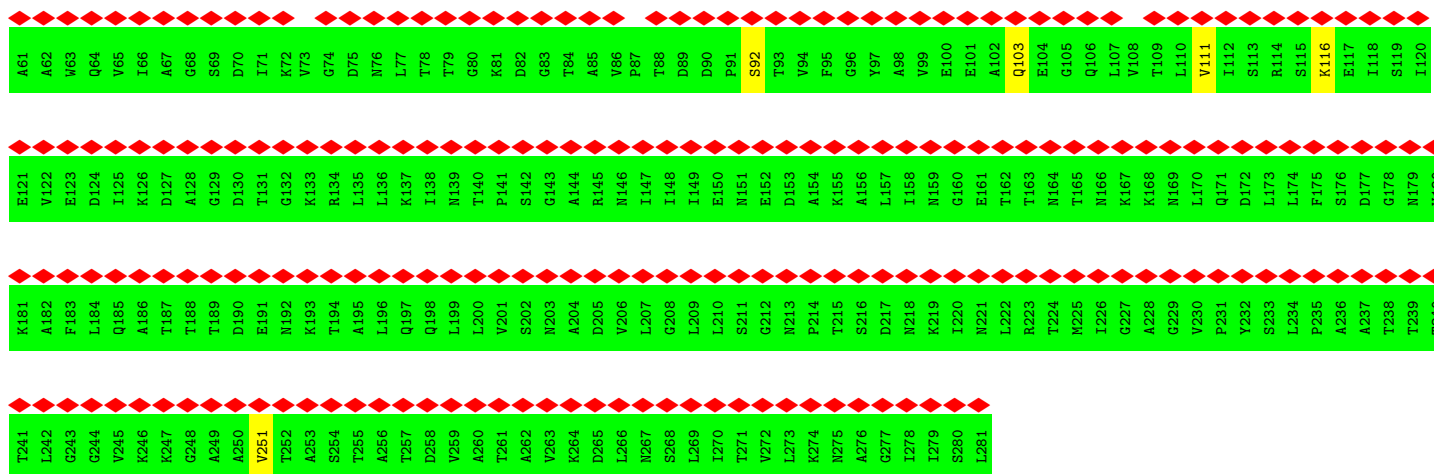


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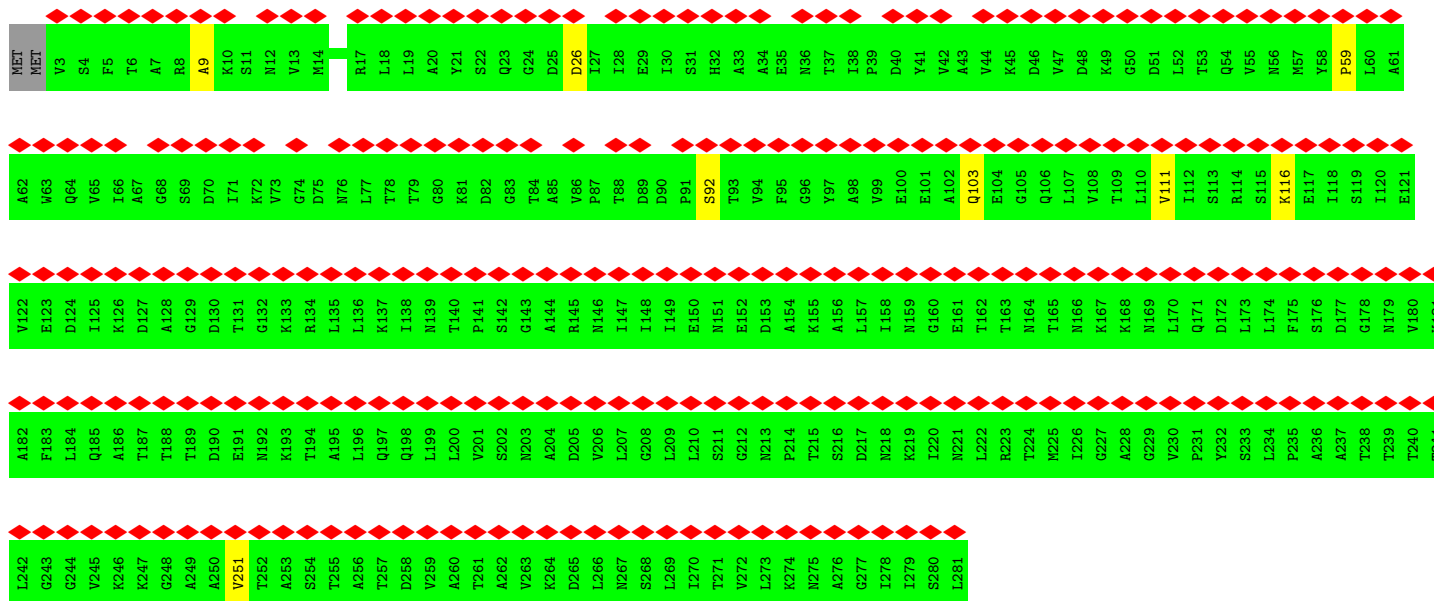


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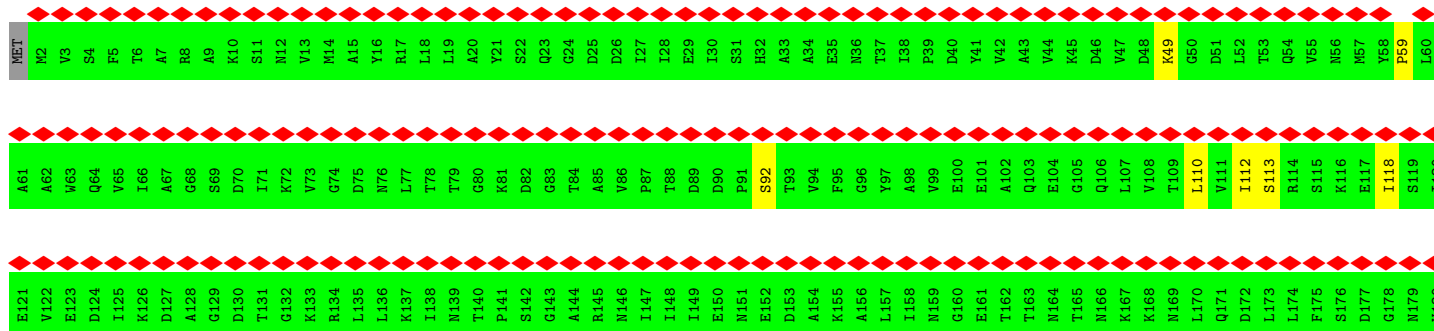


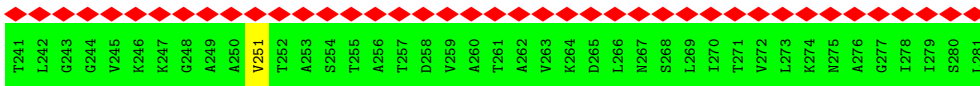
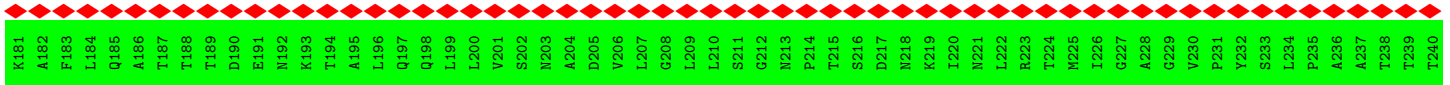


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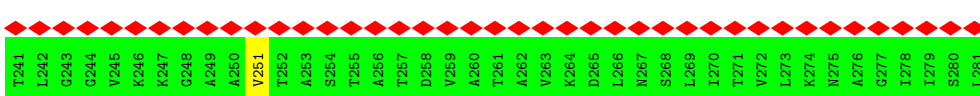
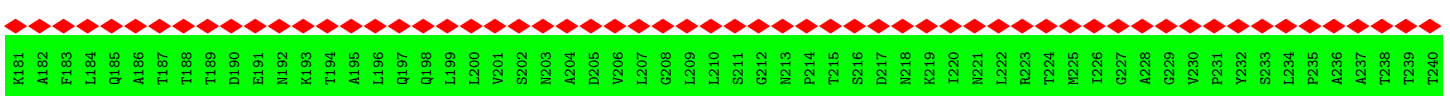
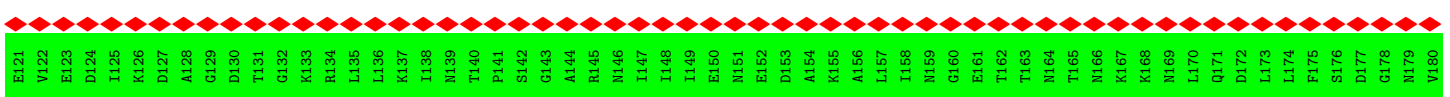
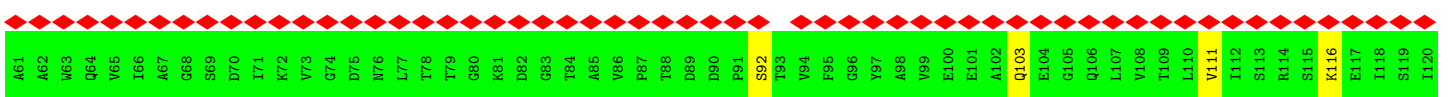
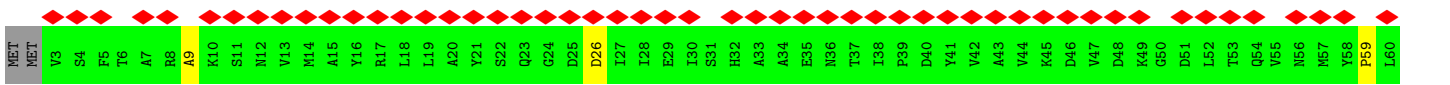


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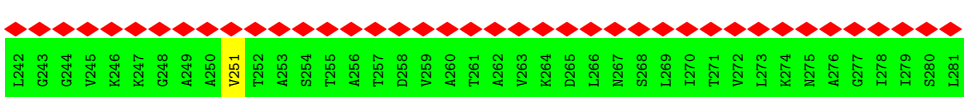
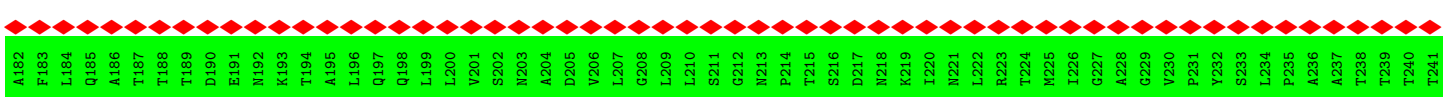
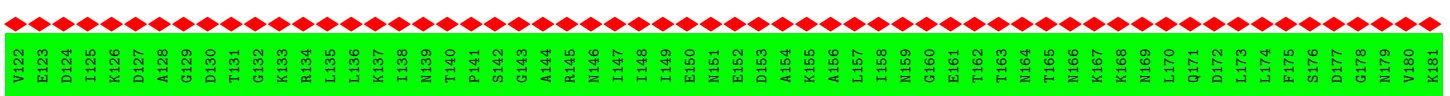
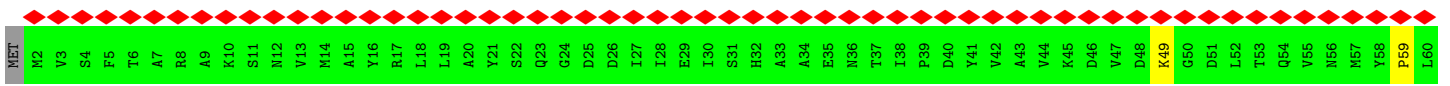


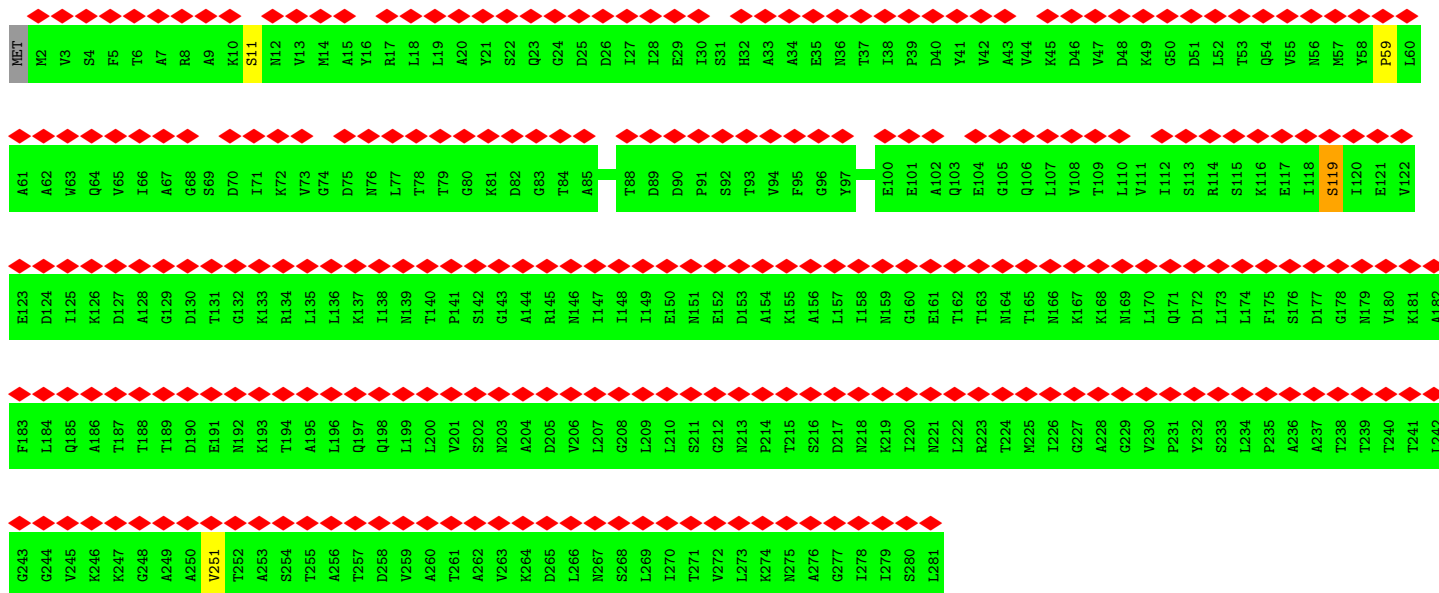


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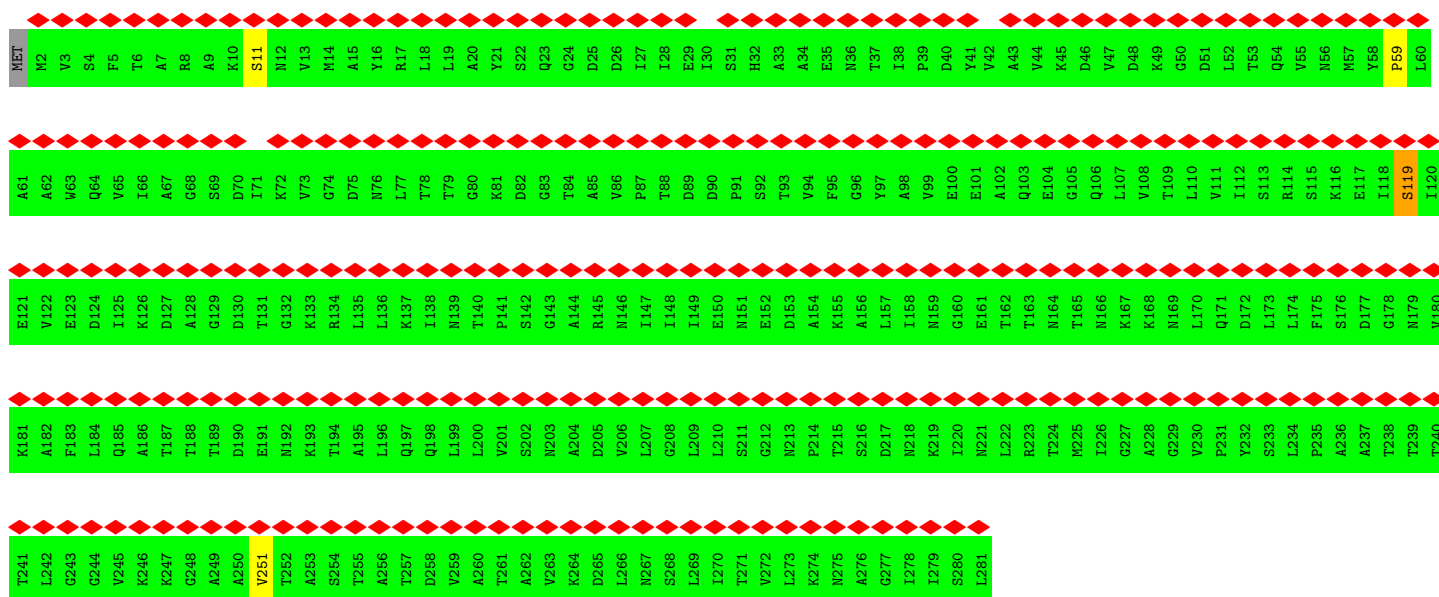


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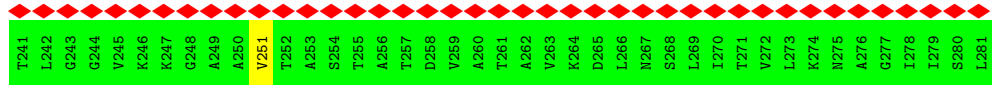


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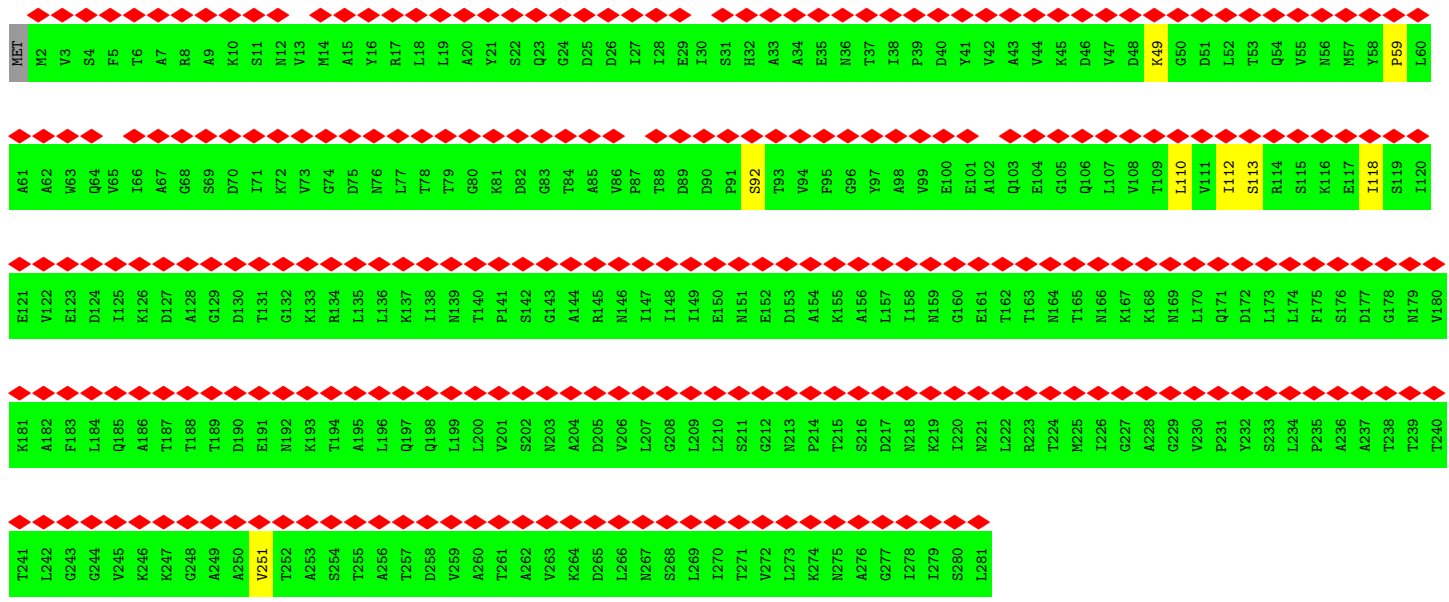


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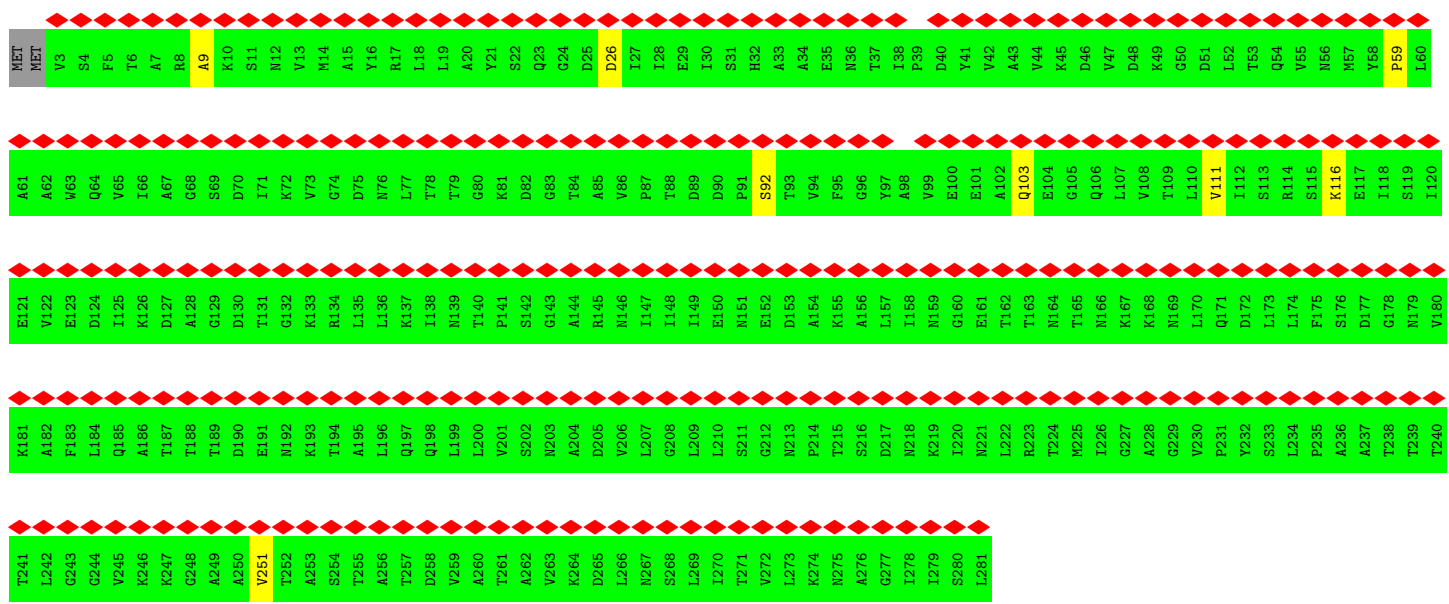




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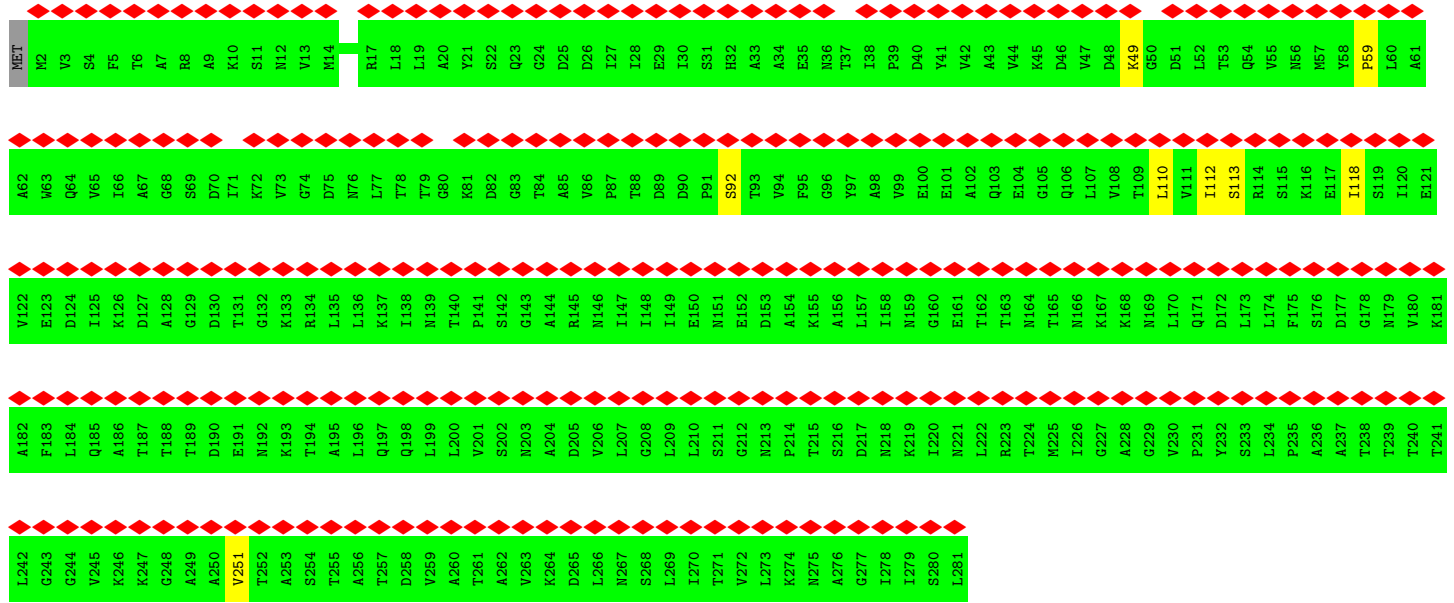


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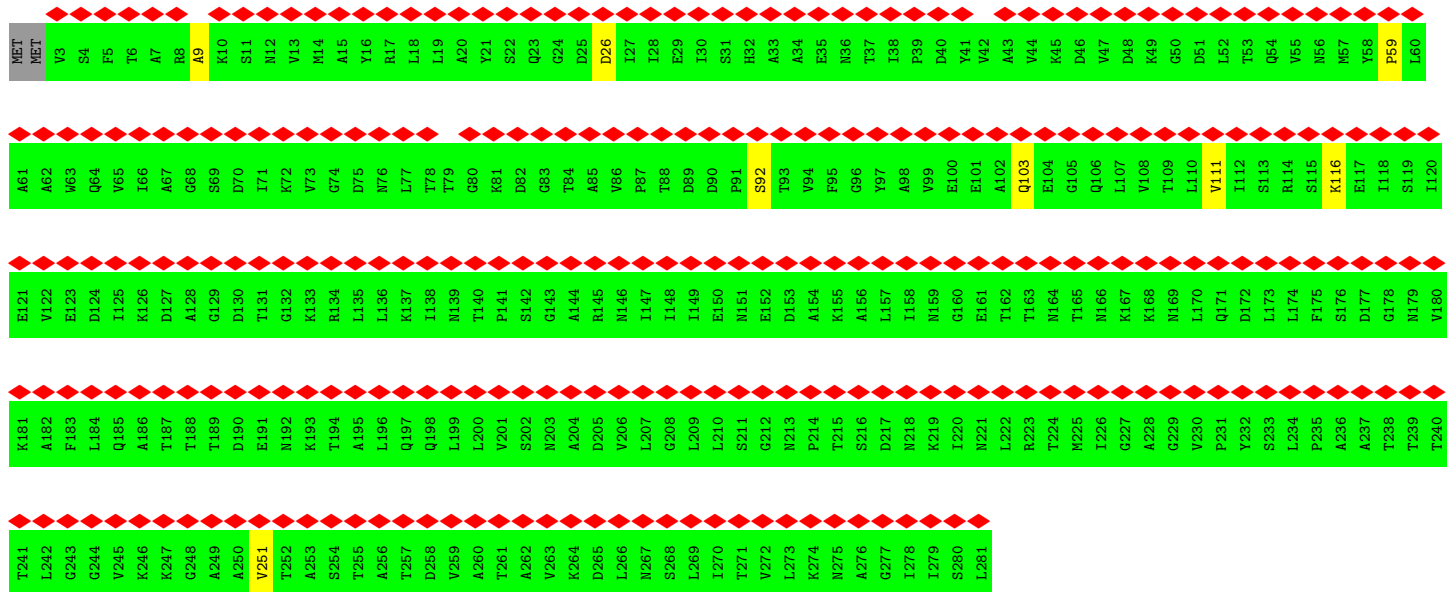


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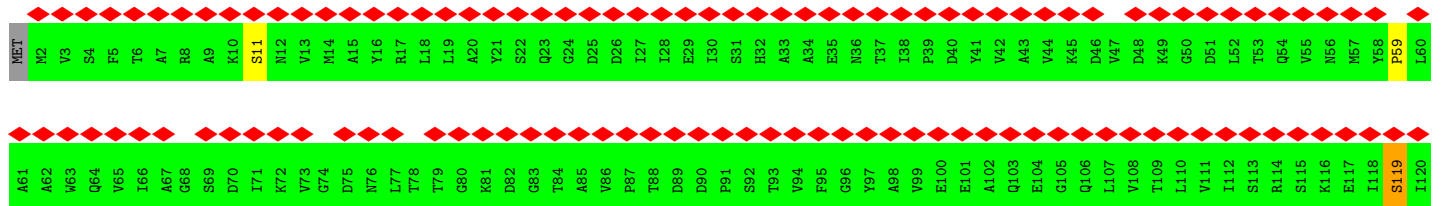


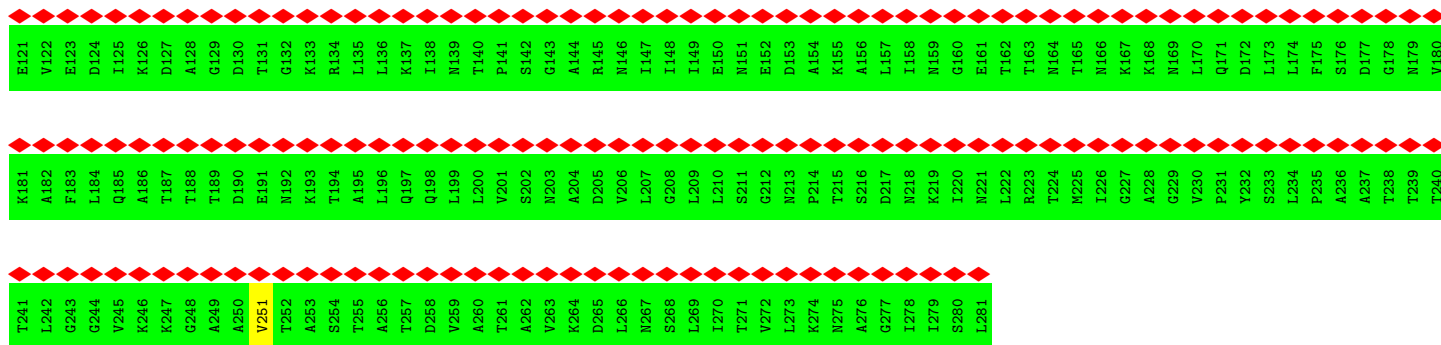


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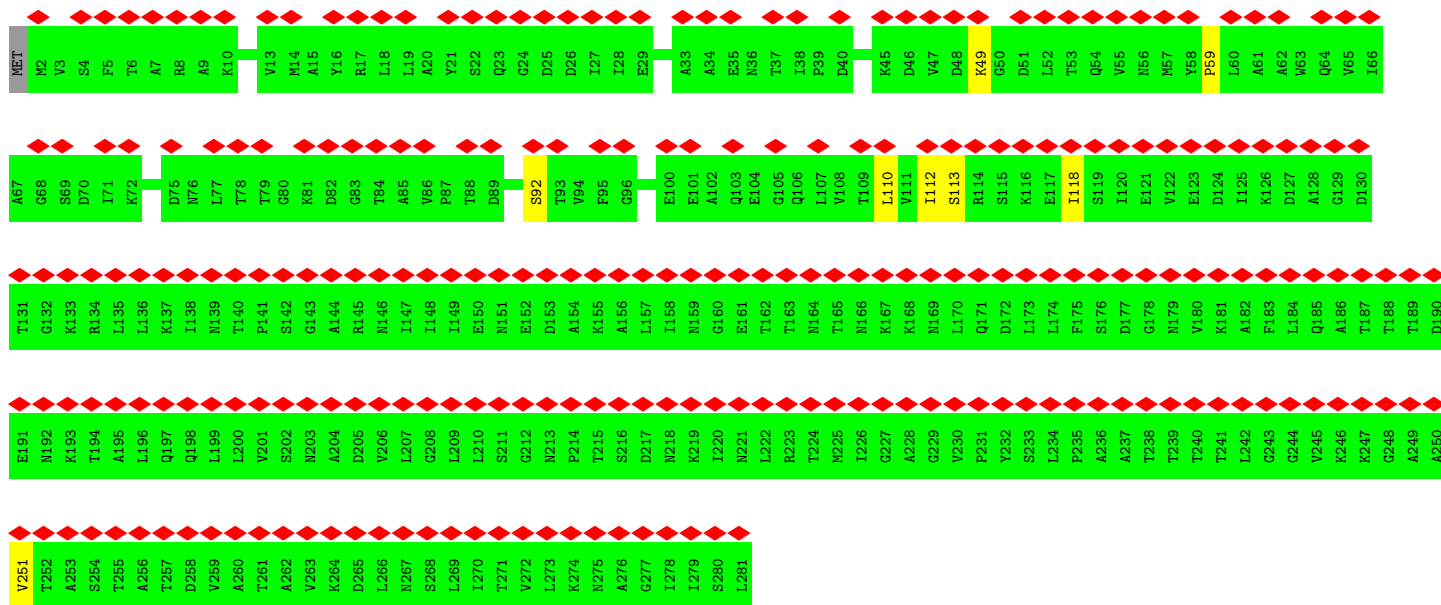
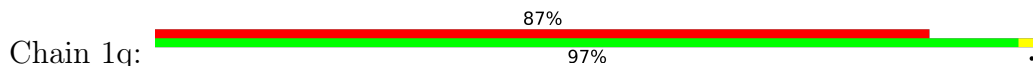


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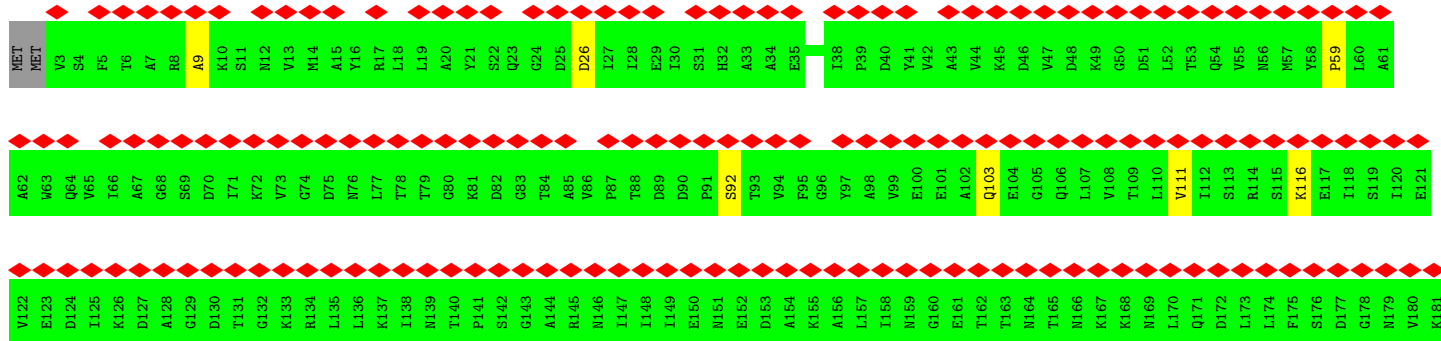


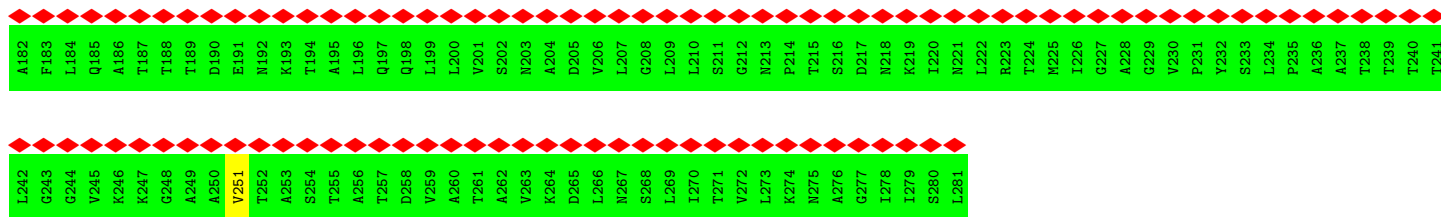


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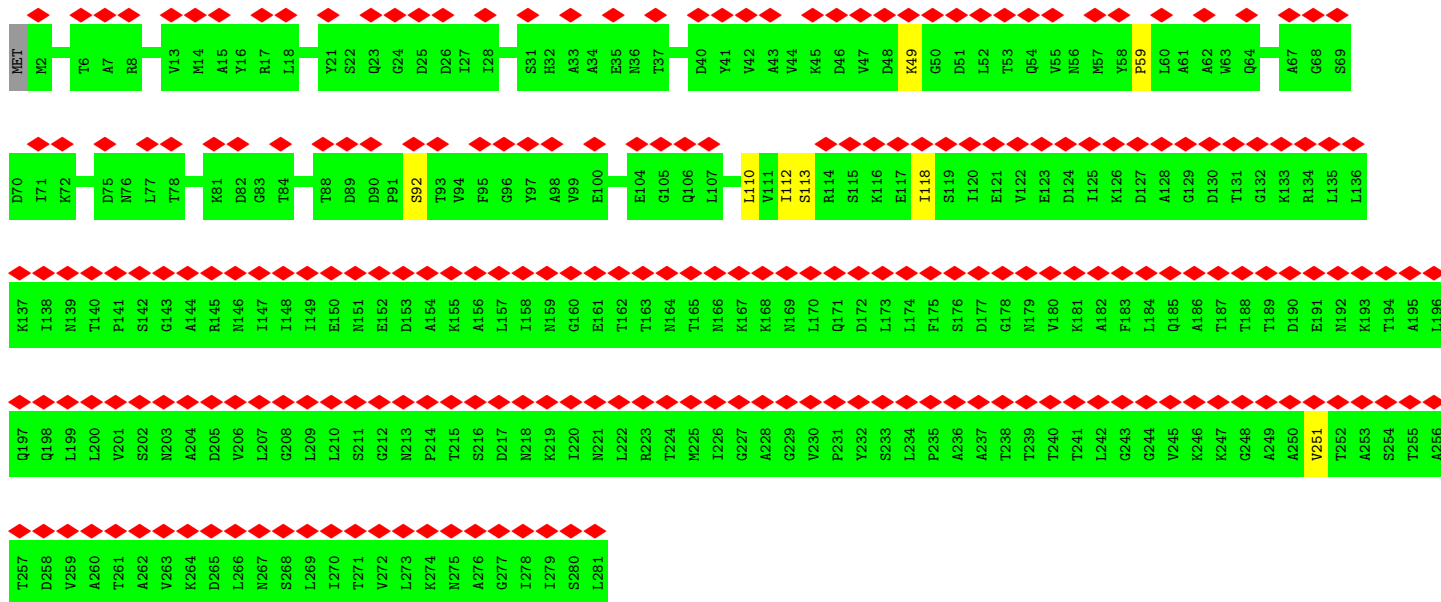
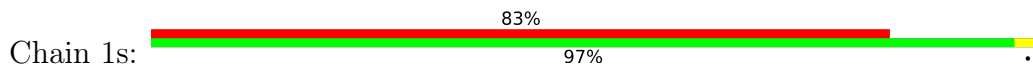


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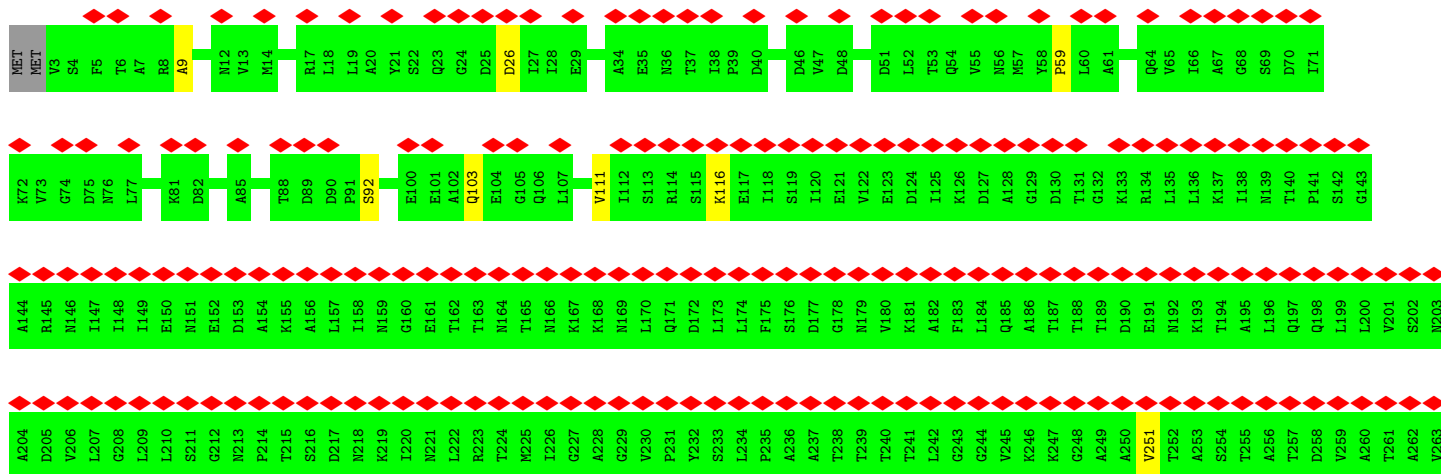
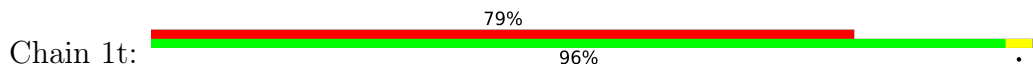




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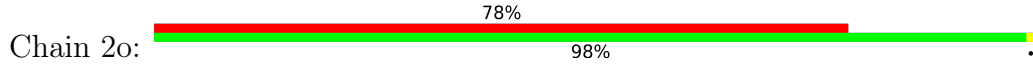


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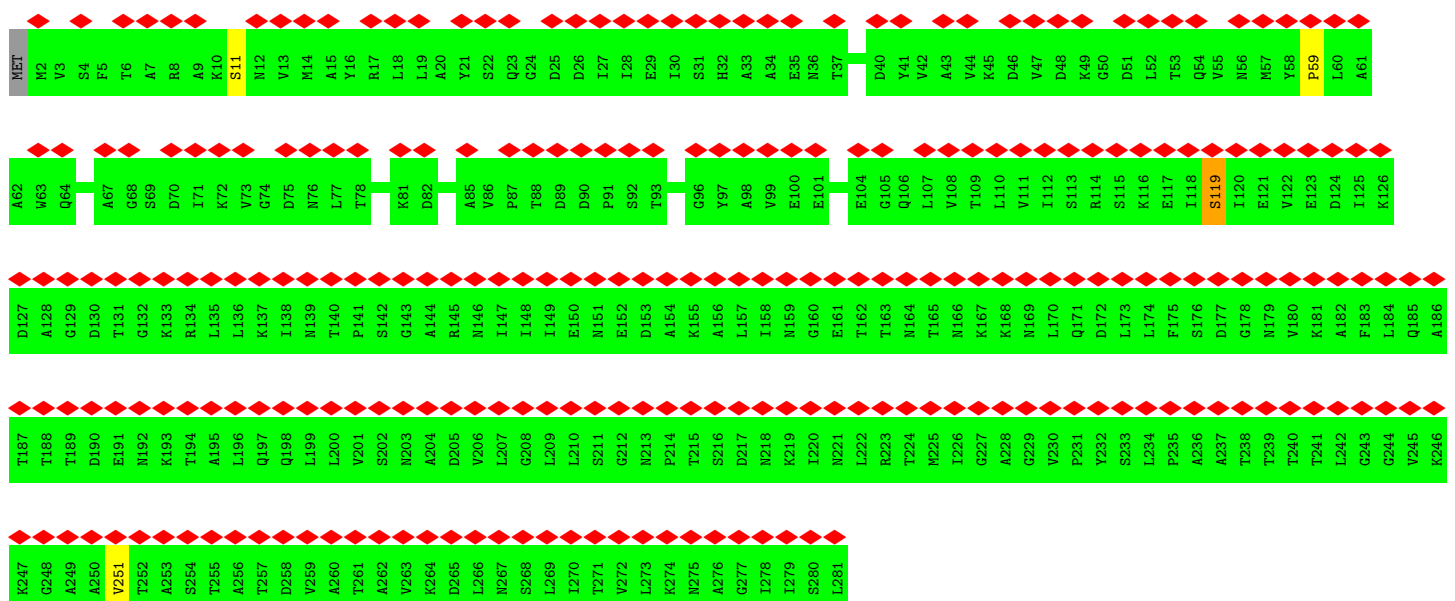
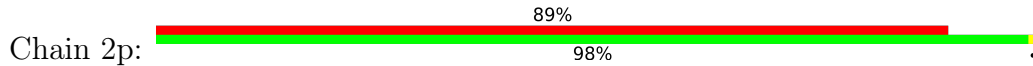




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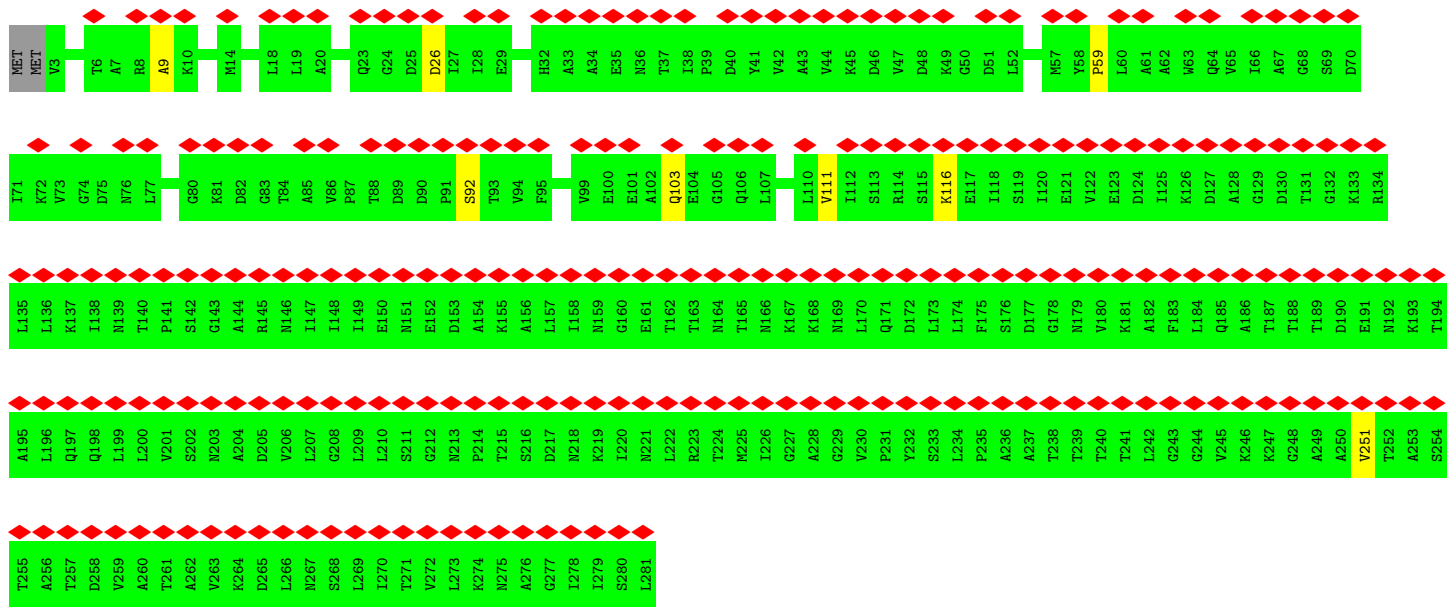
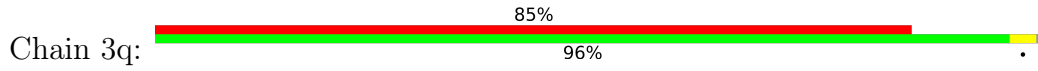
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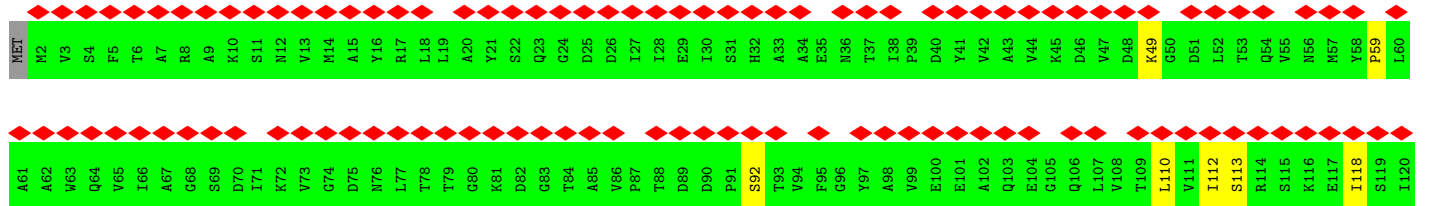
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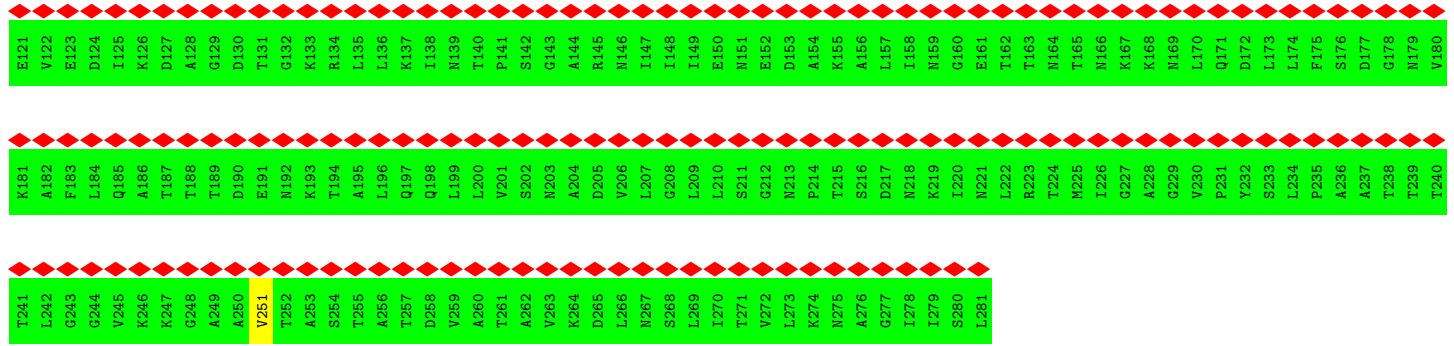


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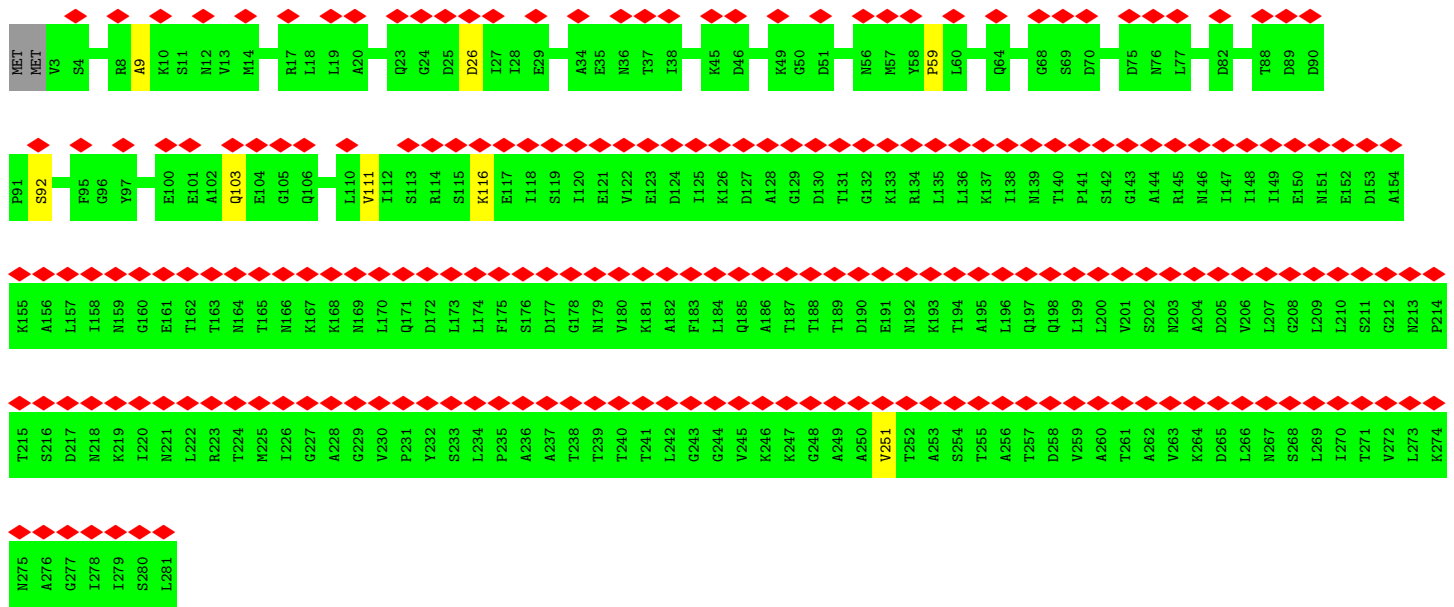
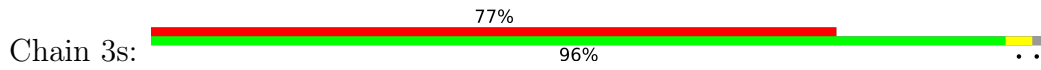


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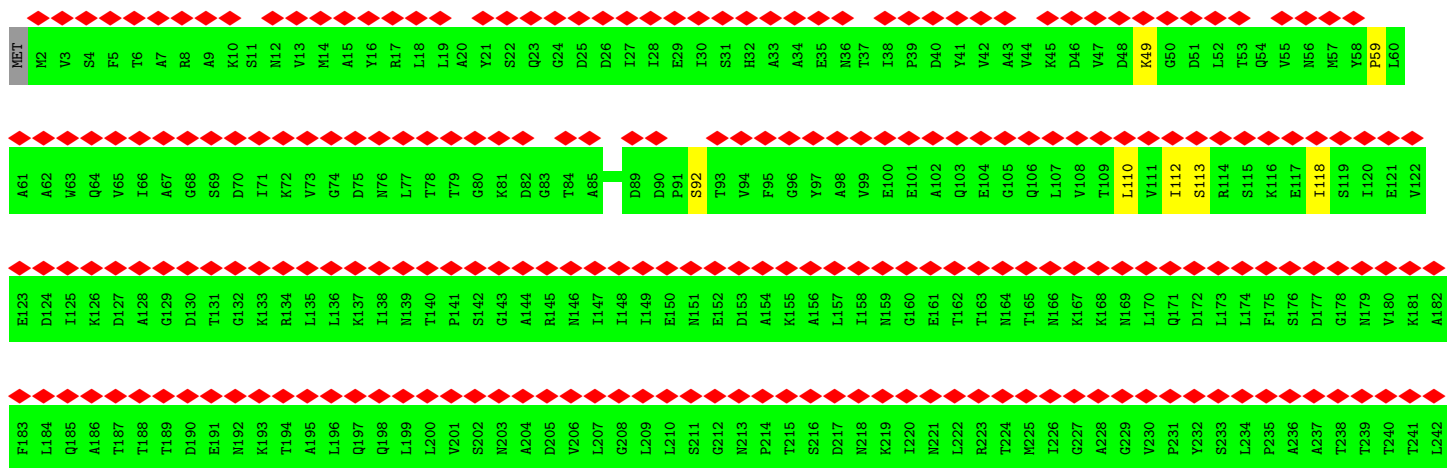


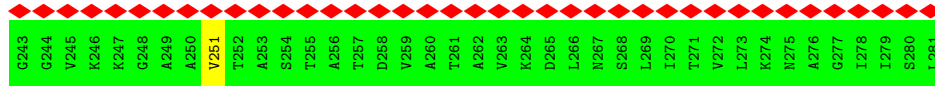


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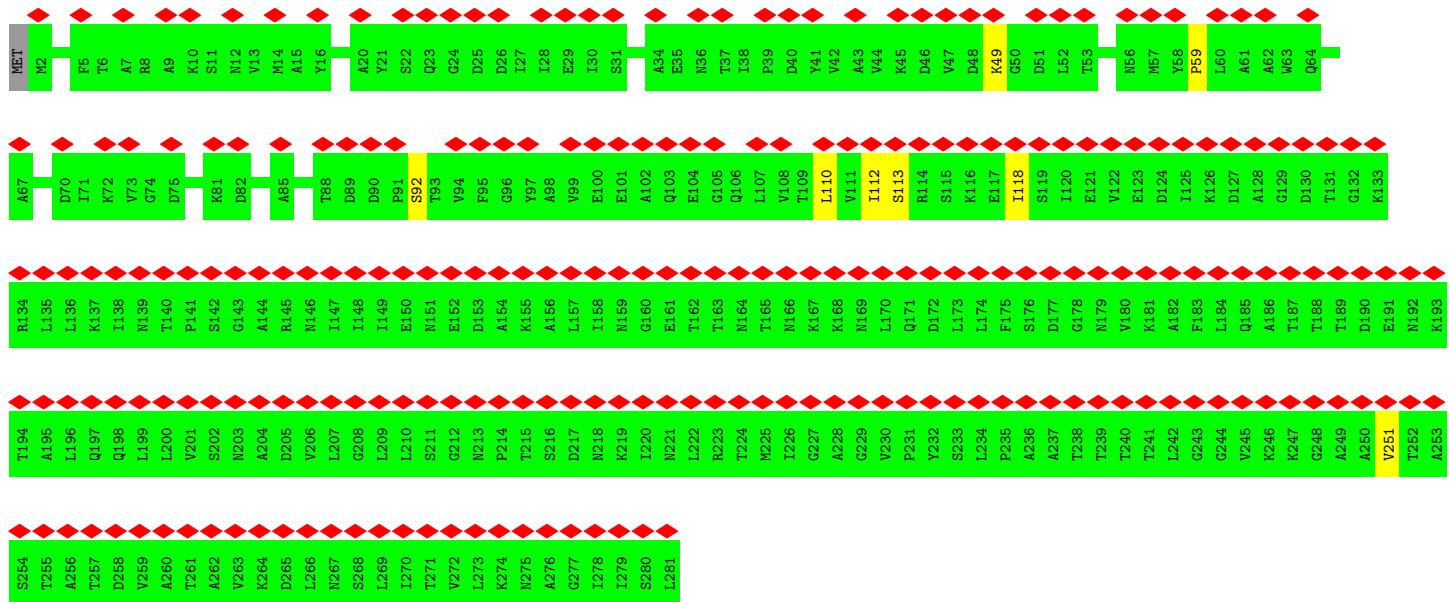
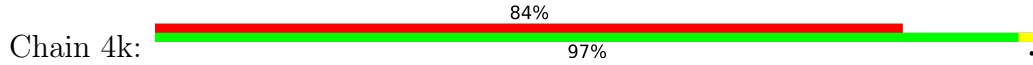


• Molecule 2: Capsid fiber protein

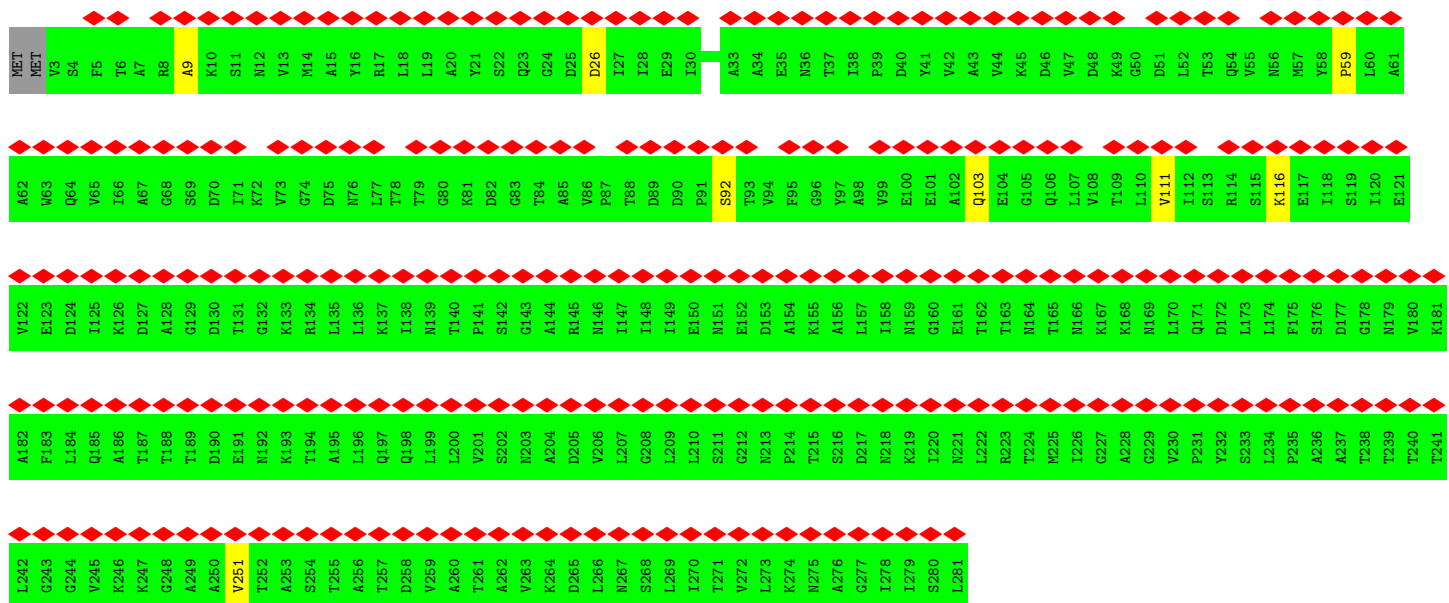




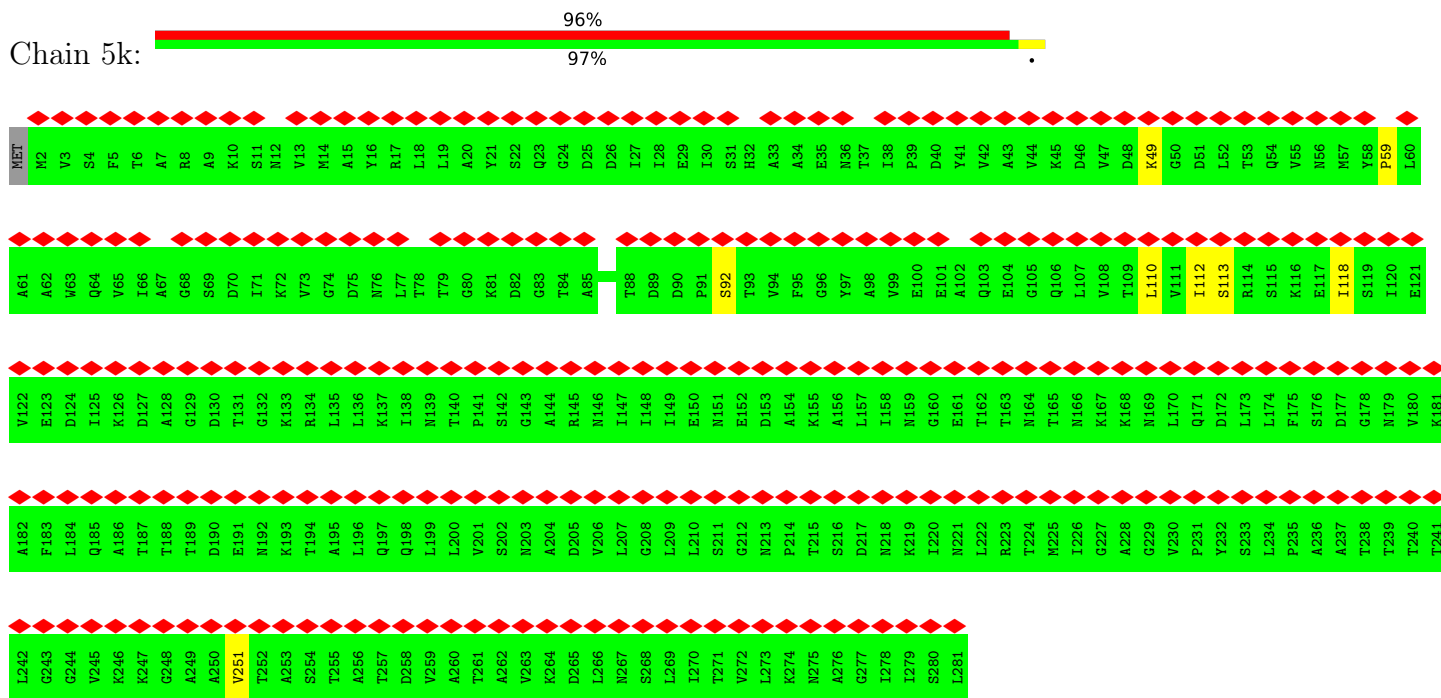
• Molecule 2: Capsid fiber protein



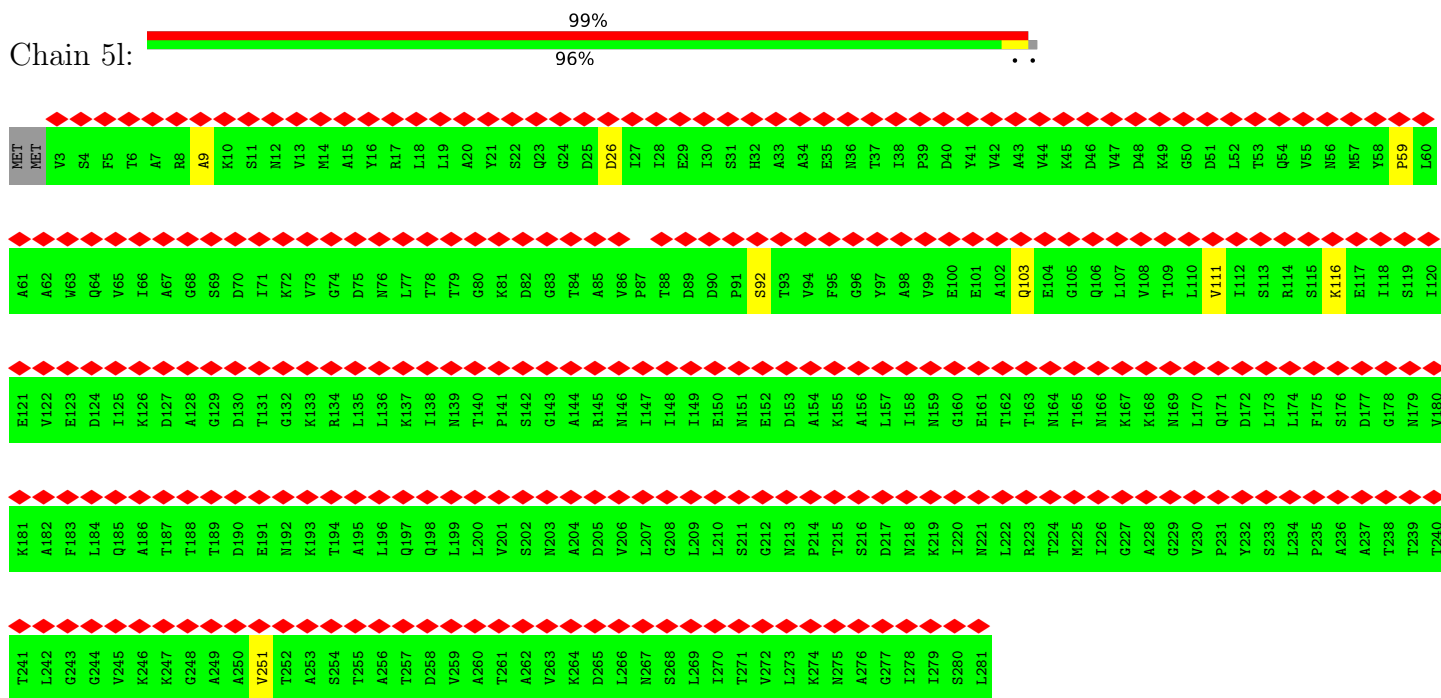
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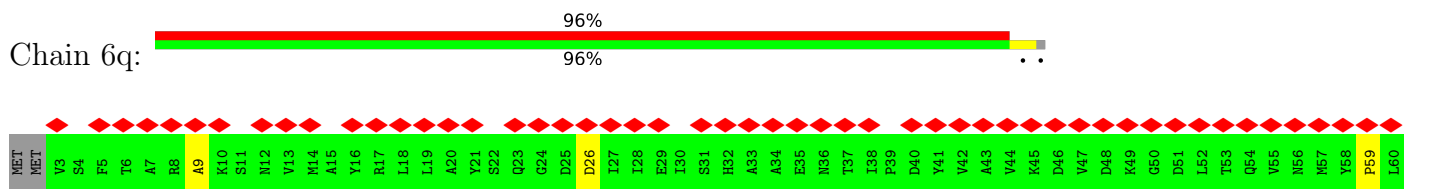
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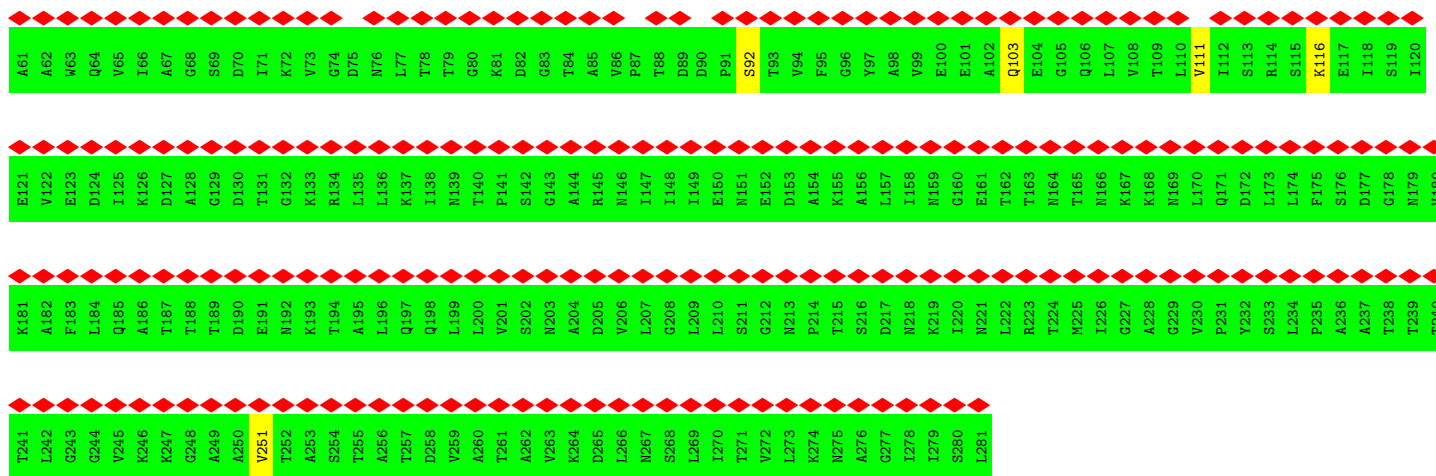


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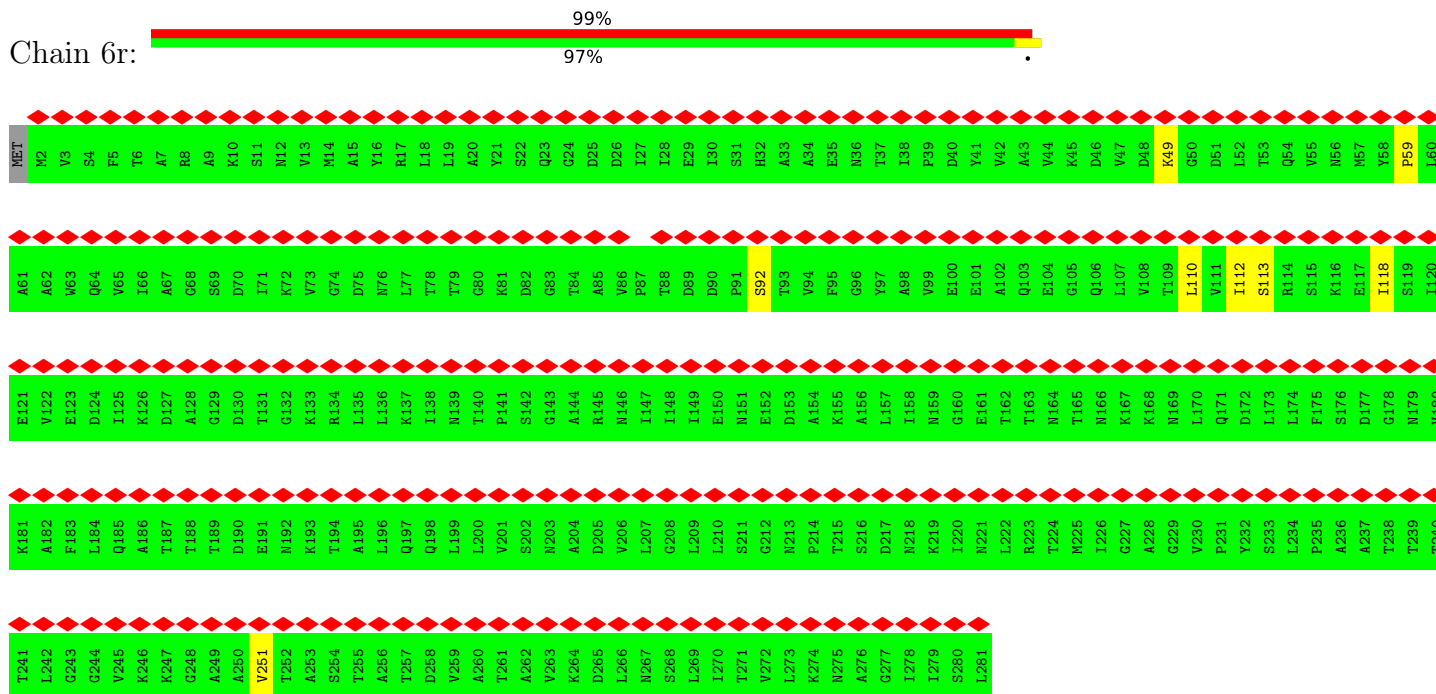


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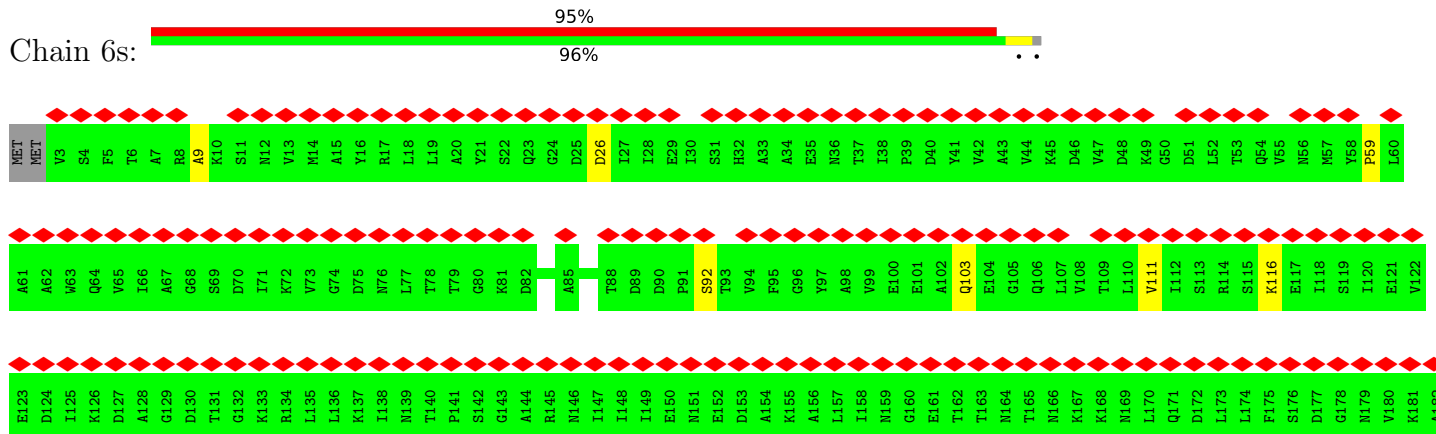


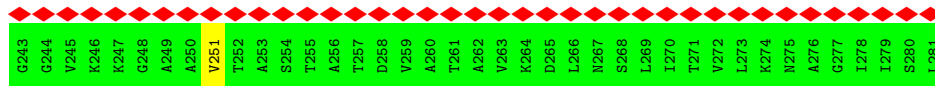
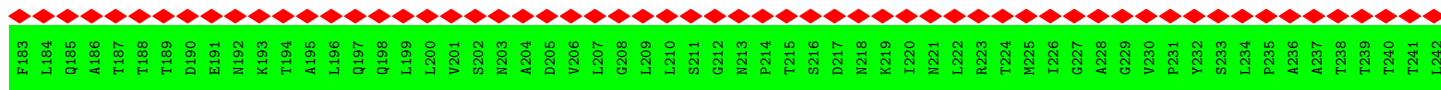


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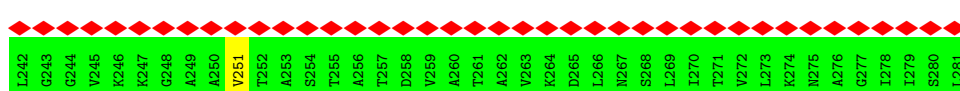
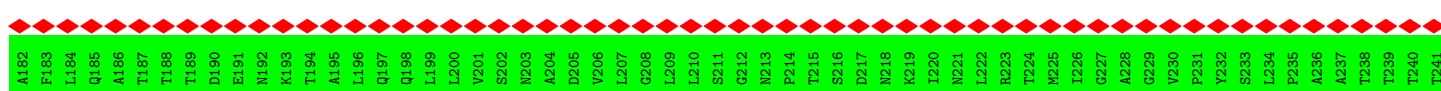
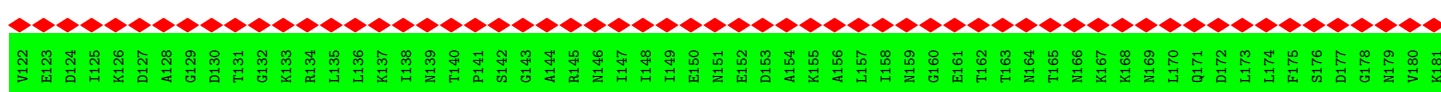
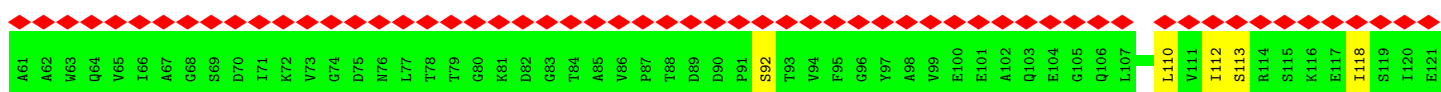
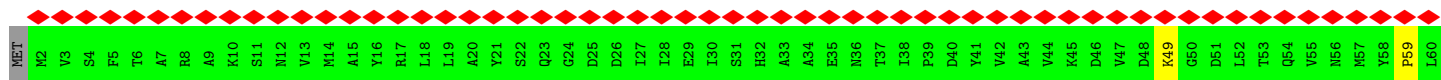


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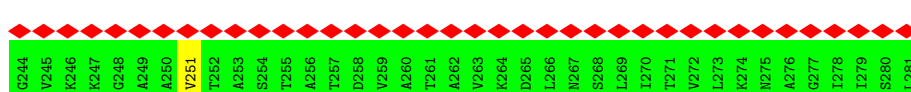
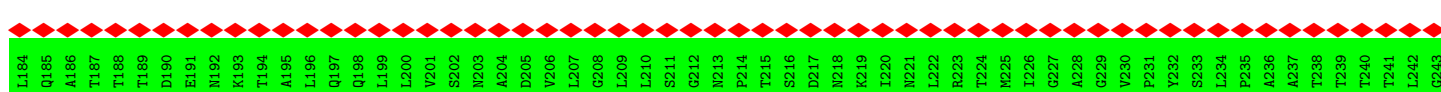
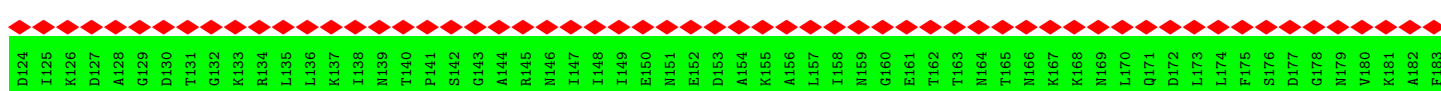
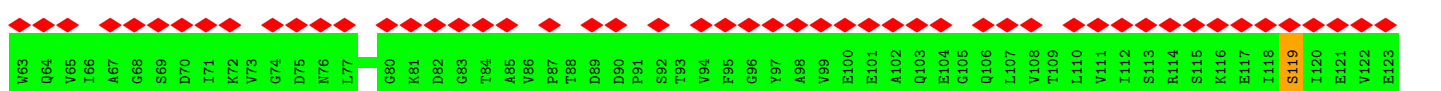
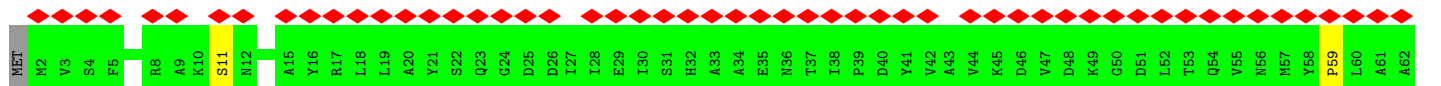




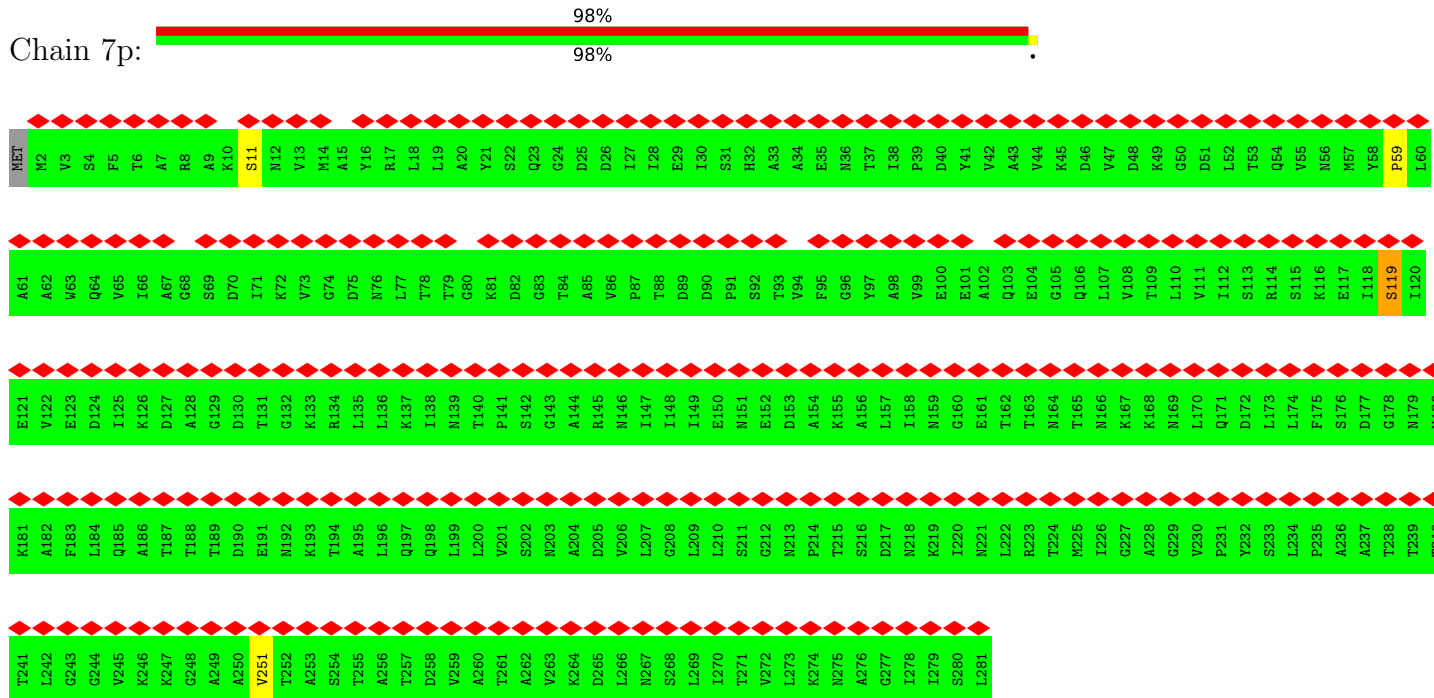
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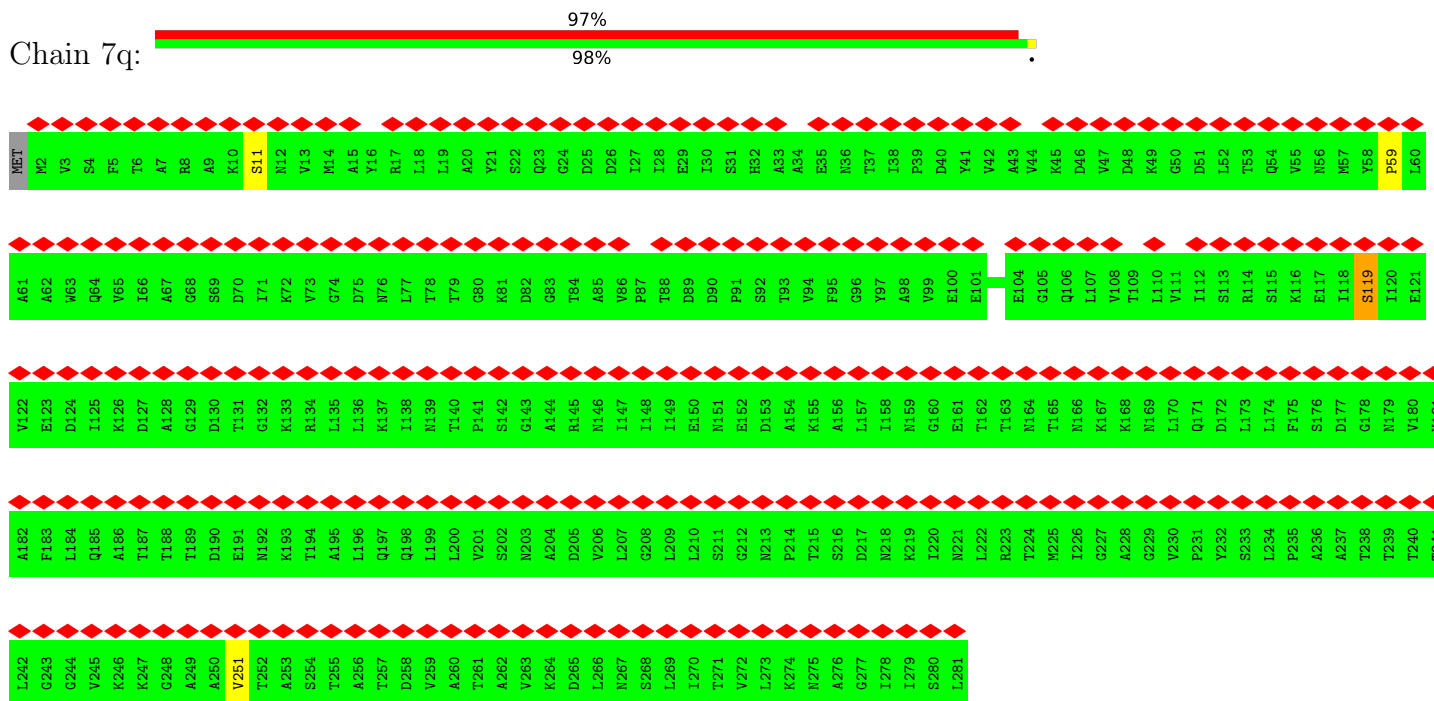
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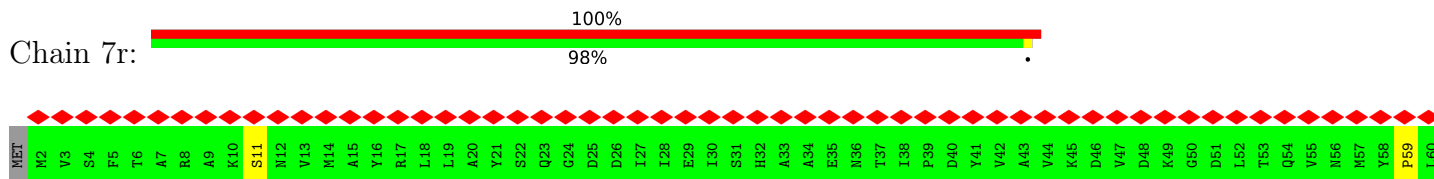
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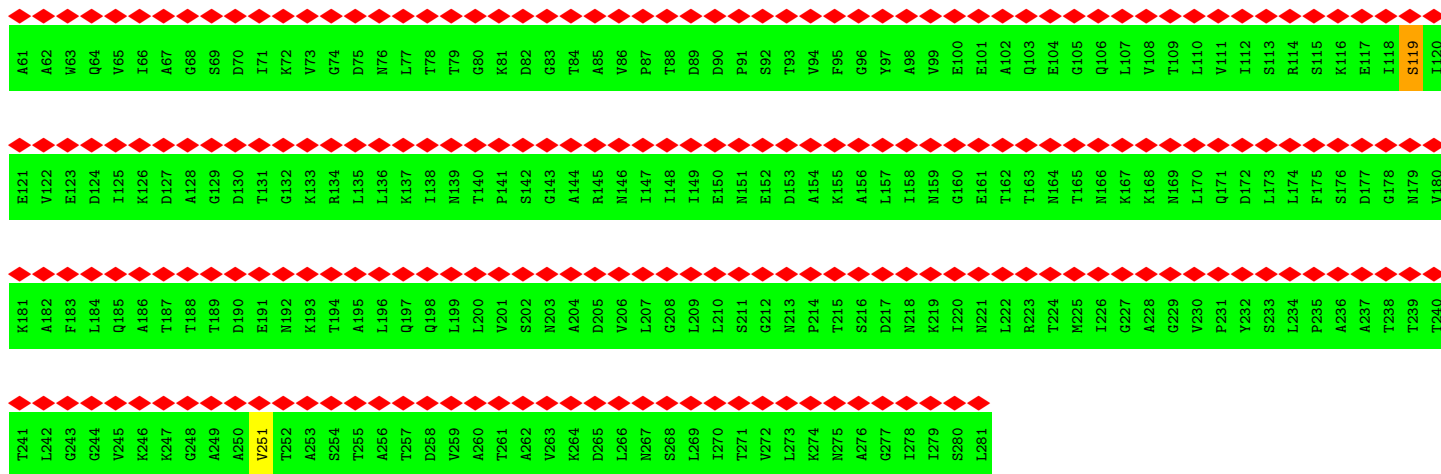


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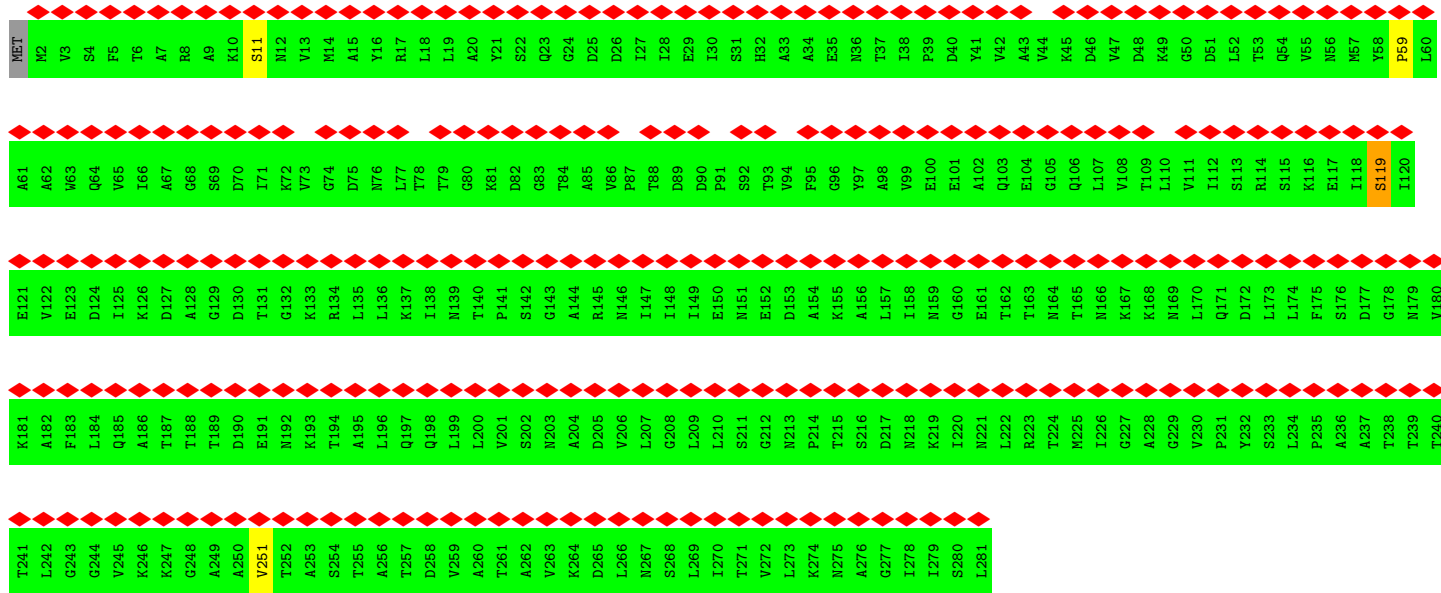


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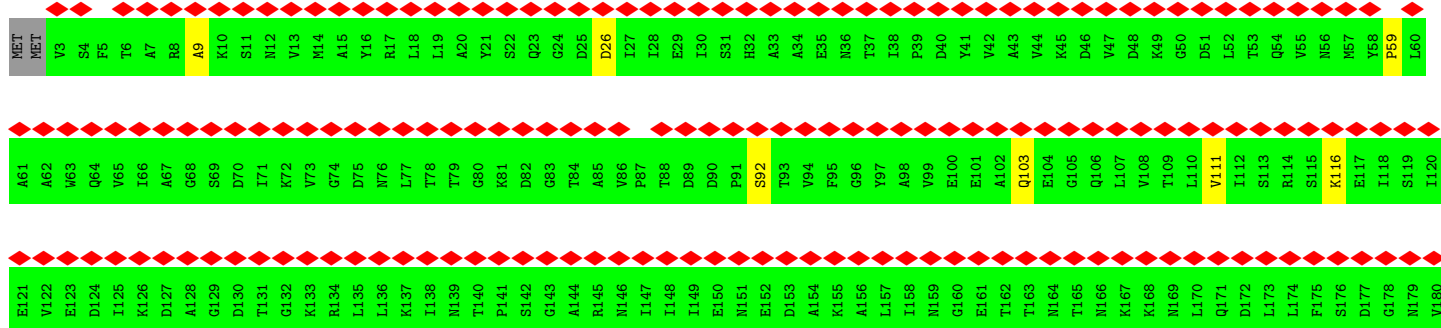


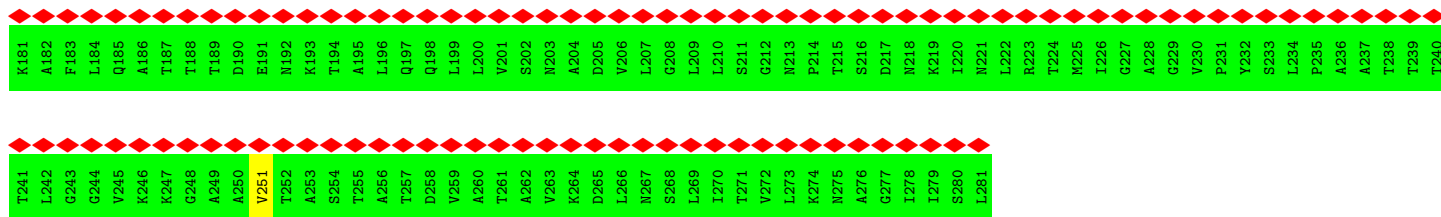


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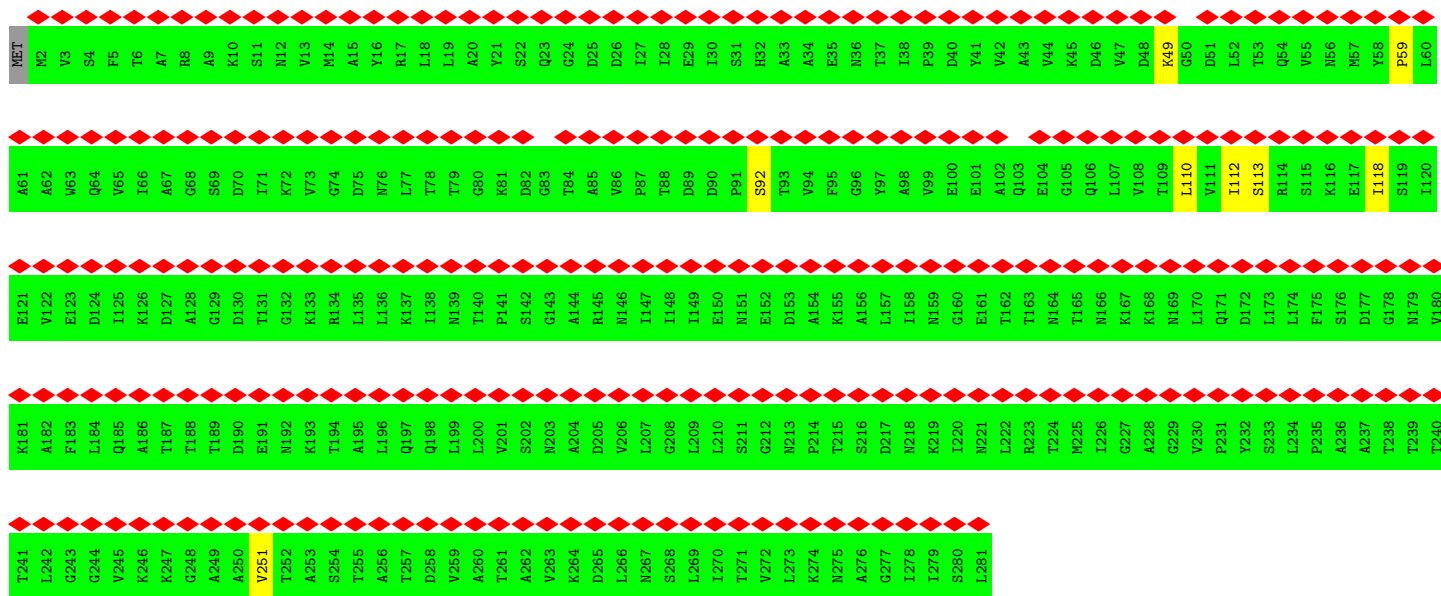


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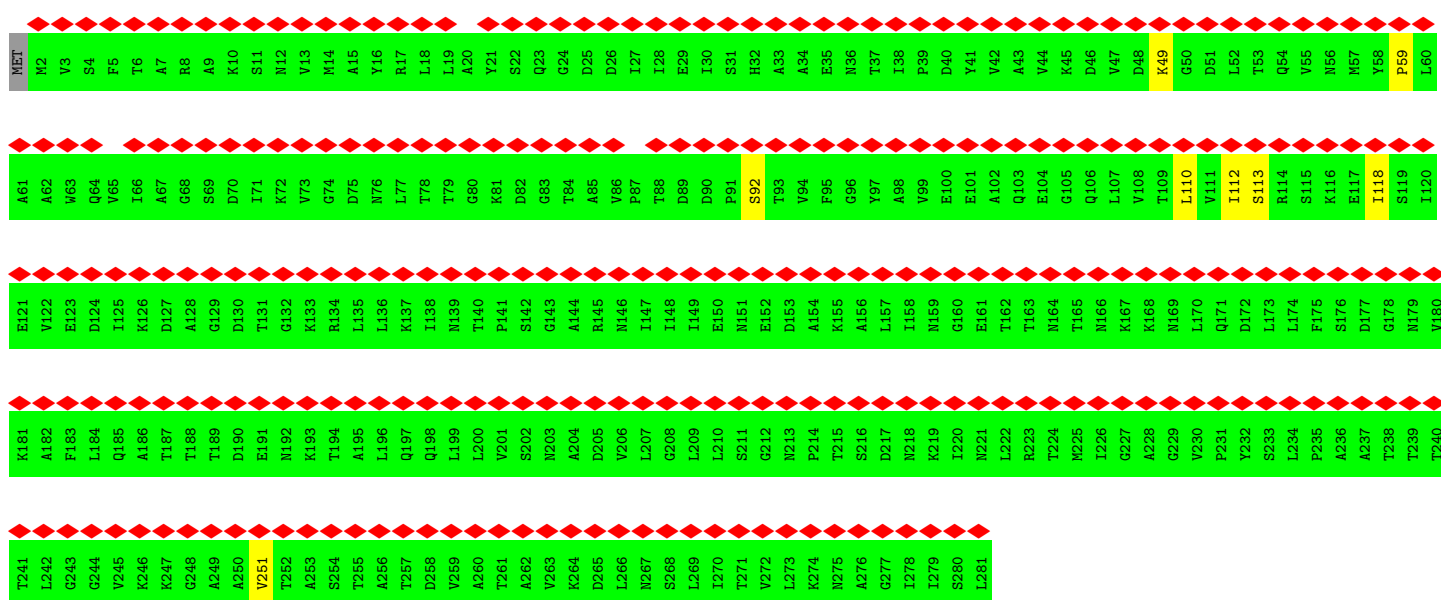




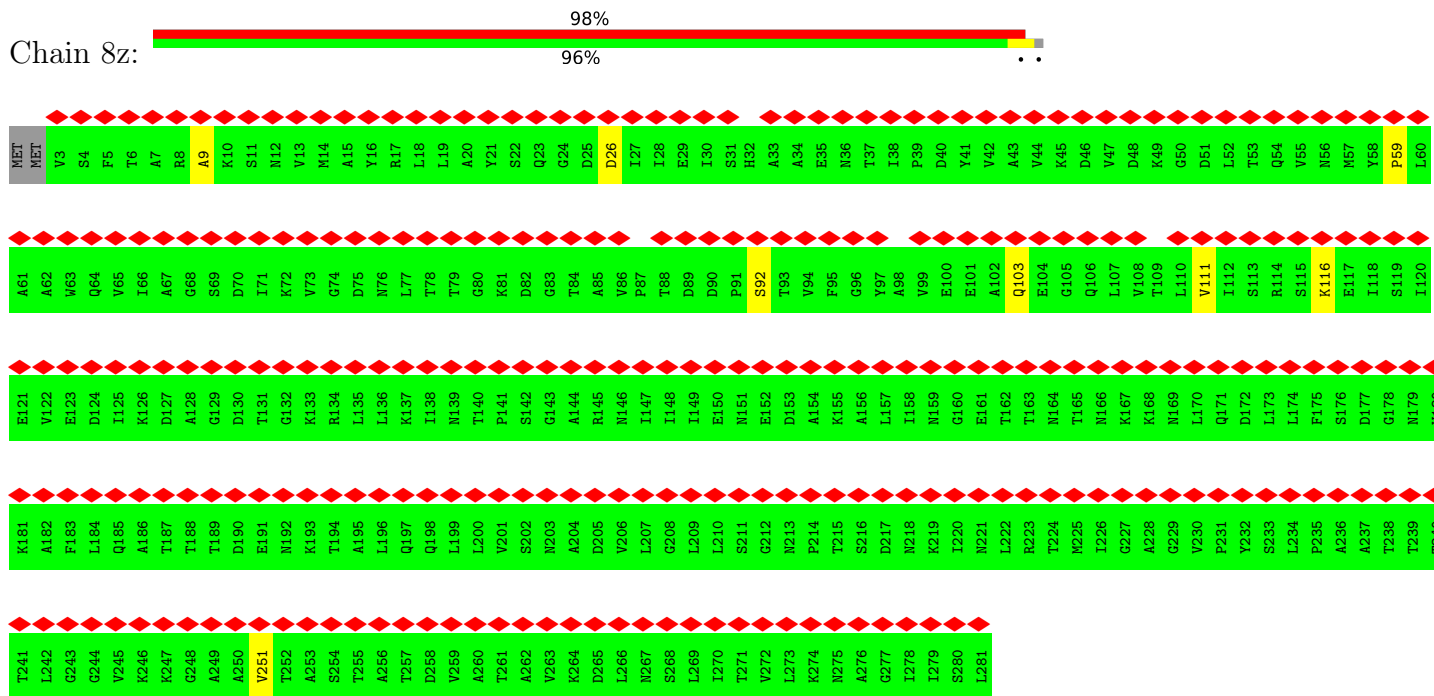
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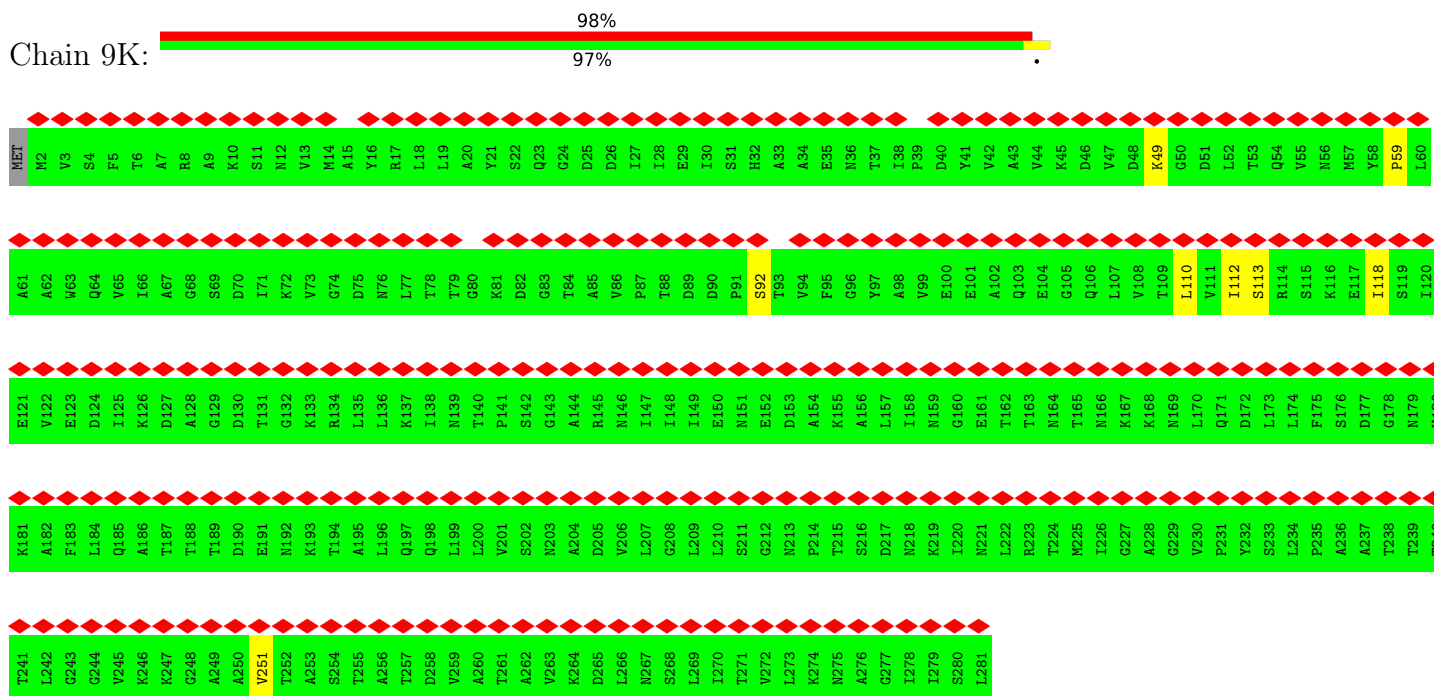
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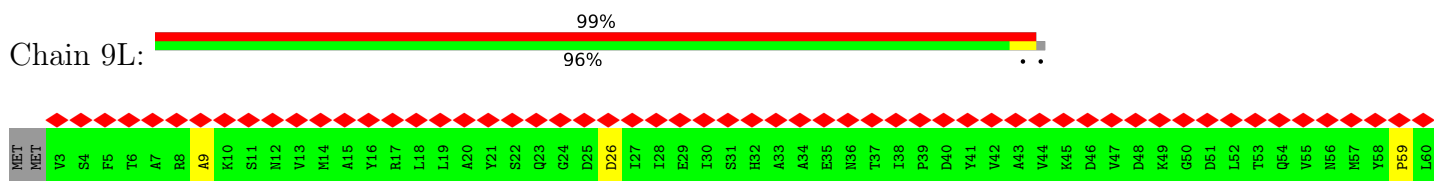
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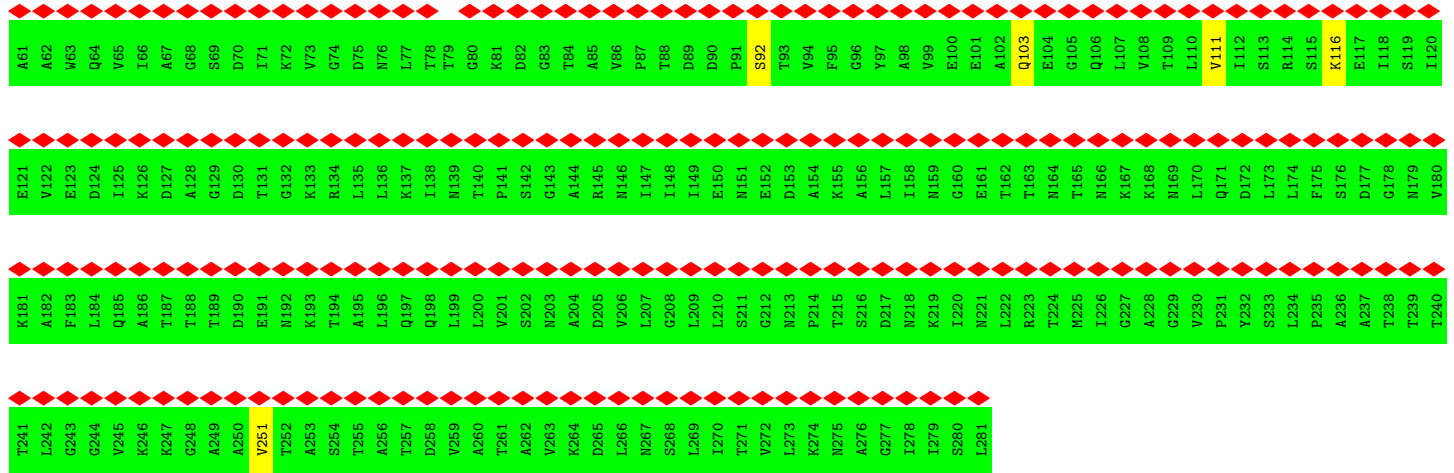


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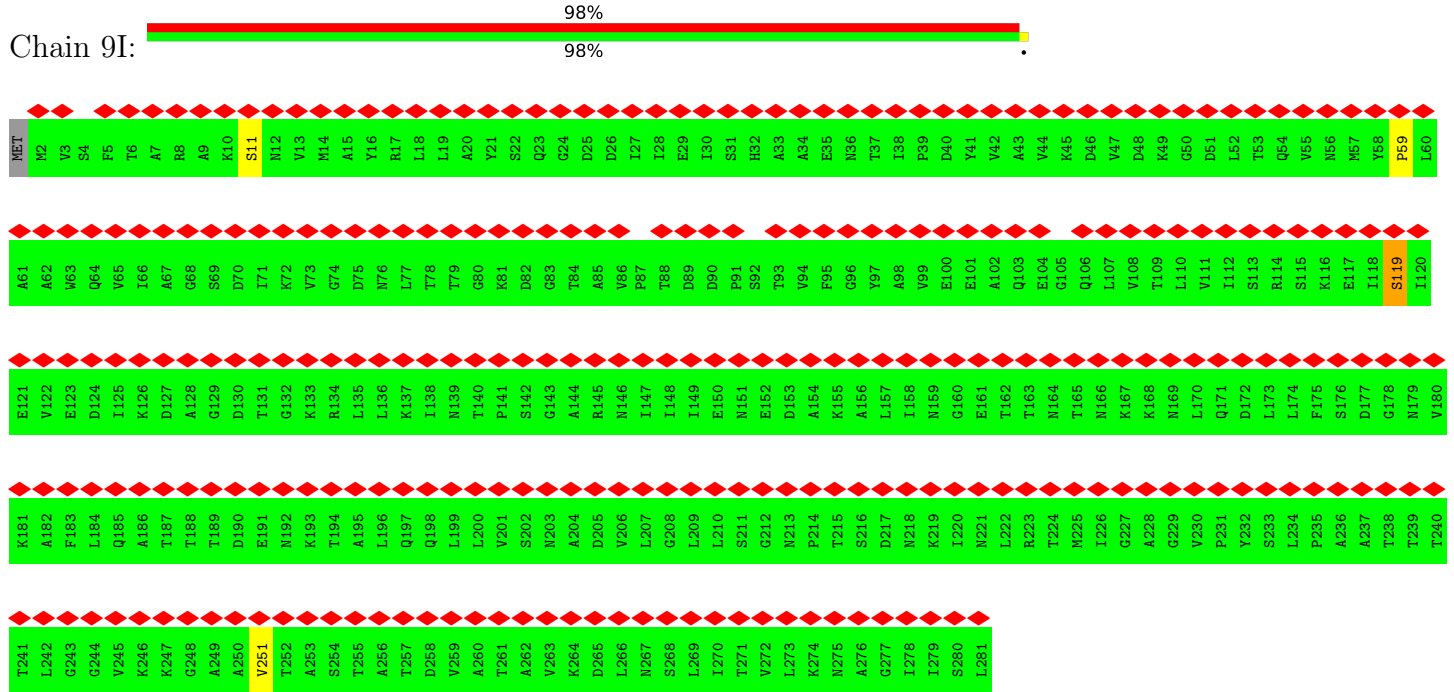


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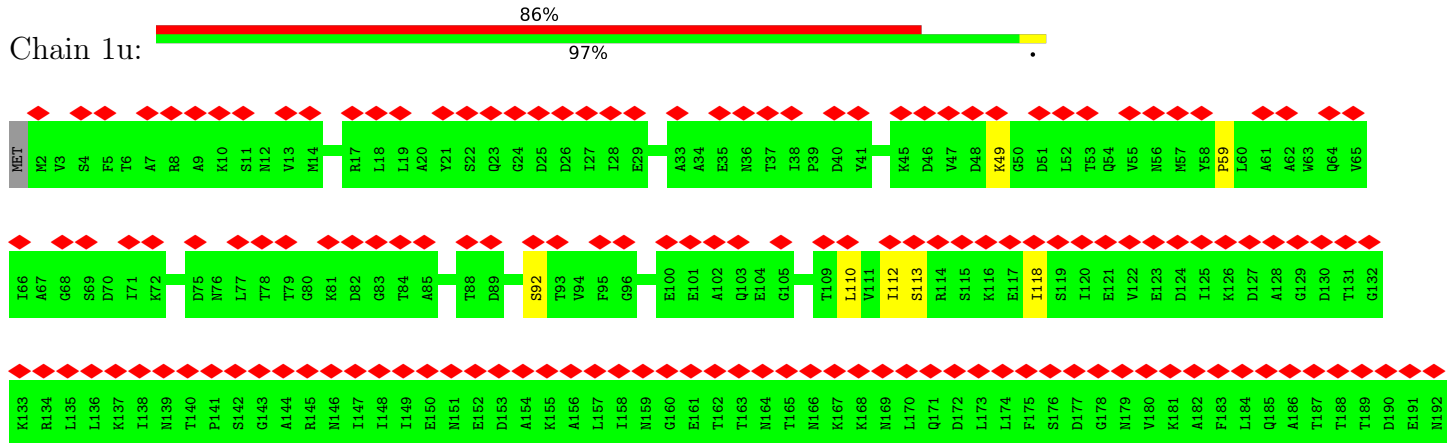


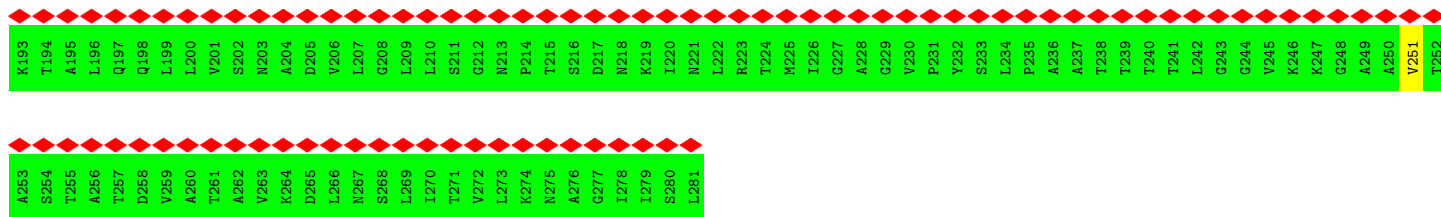


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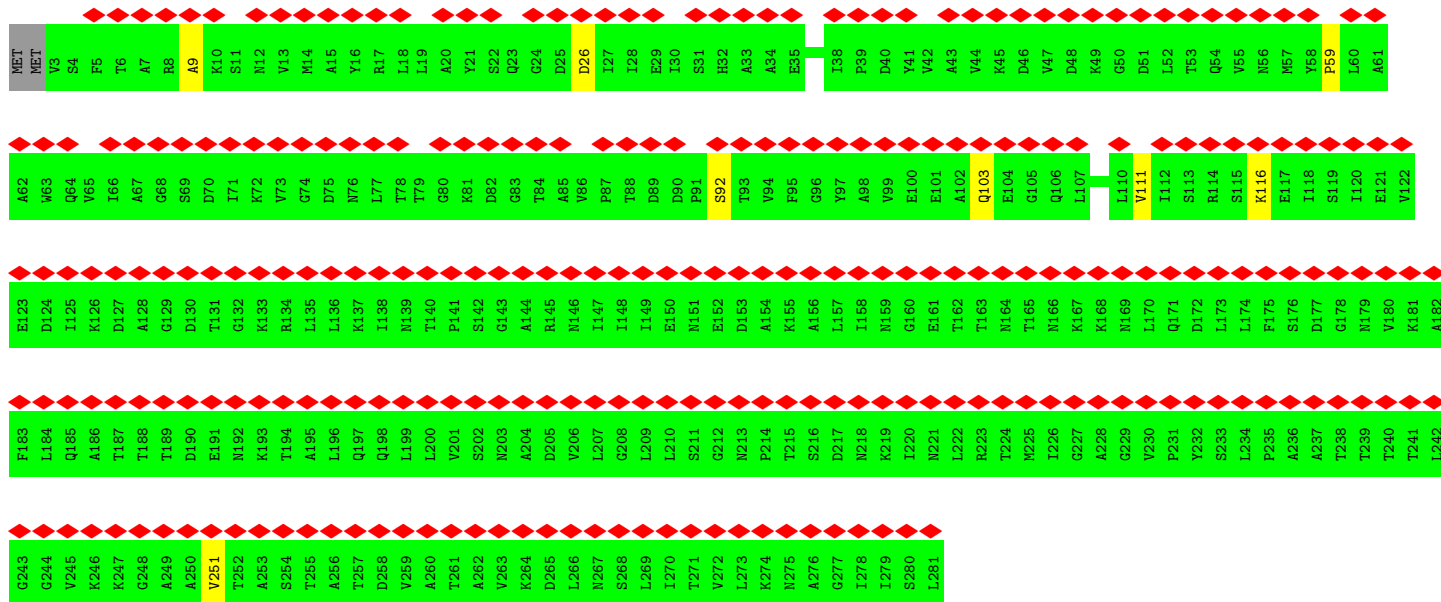


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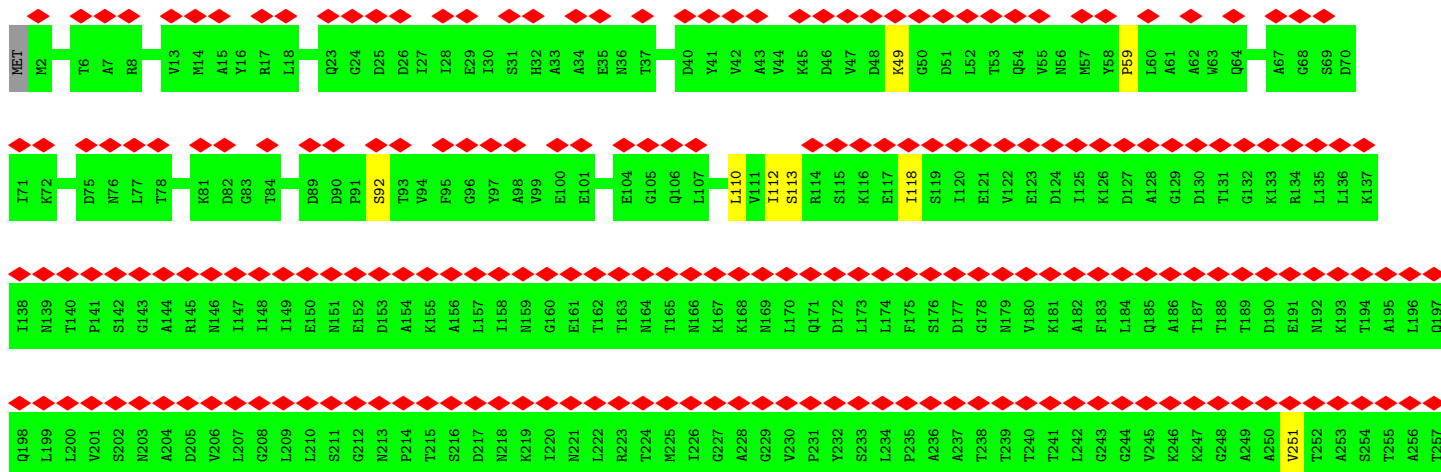
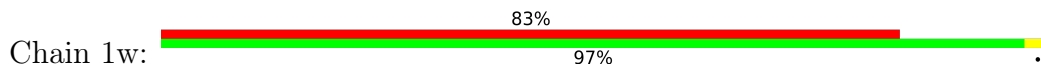


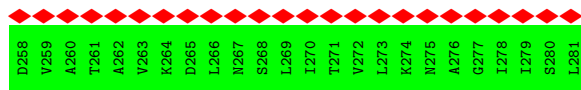


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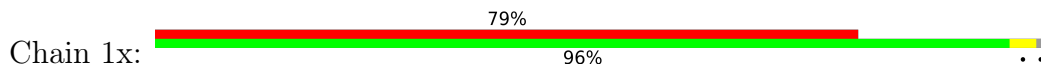


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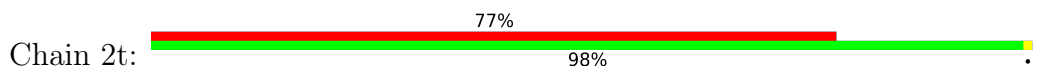




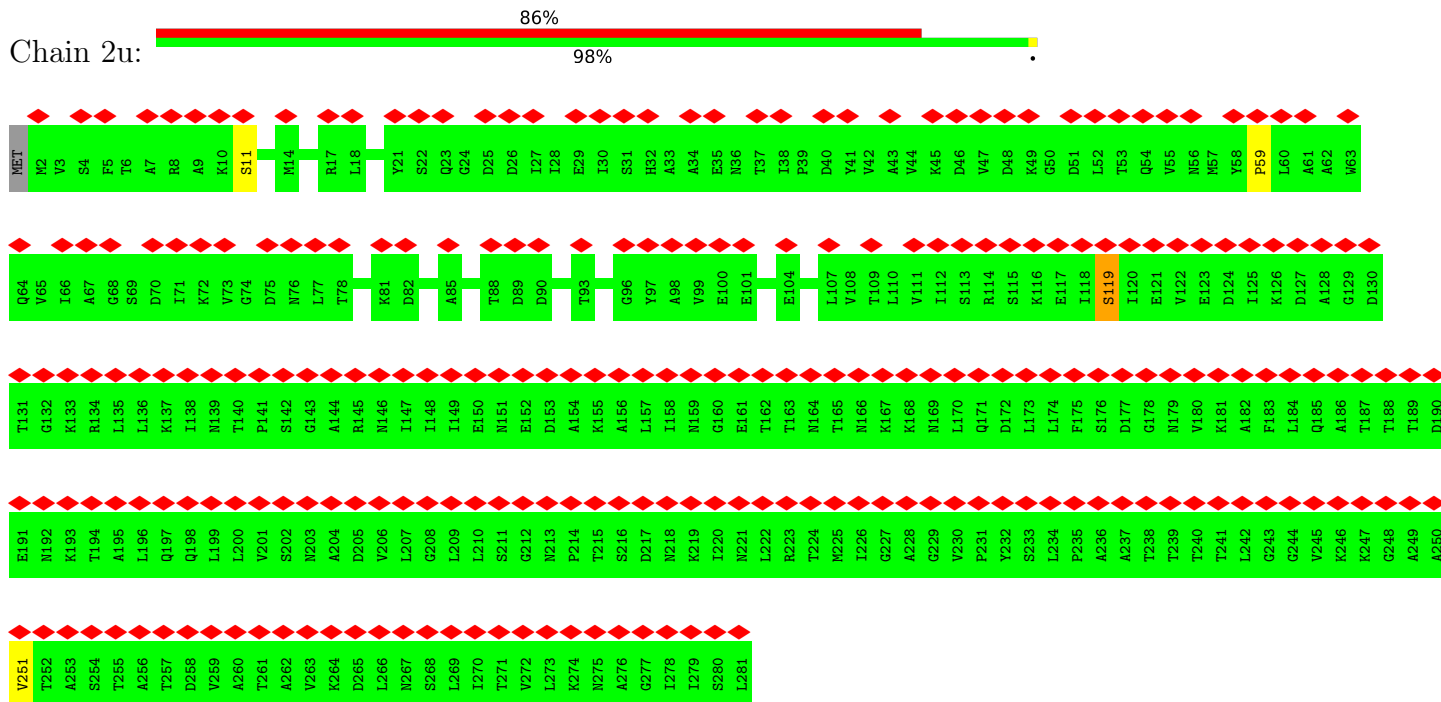
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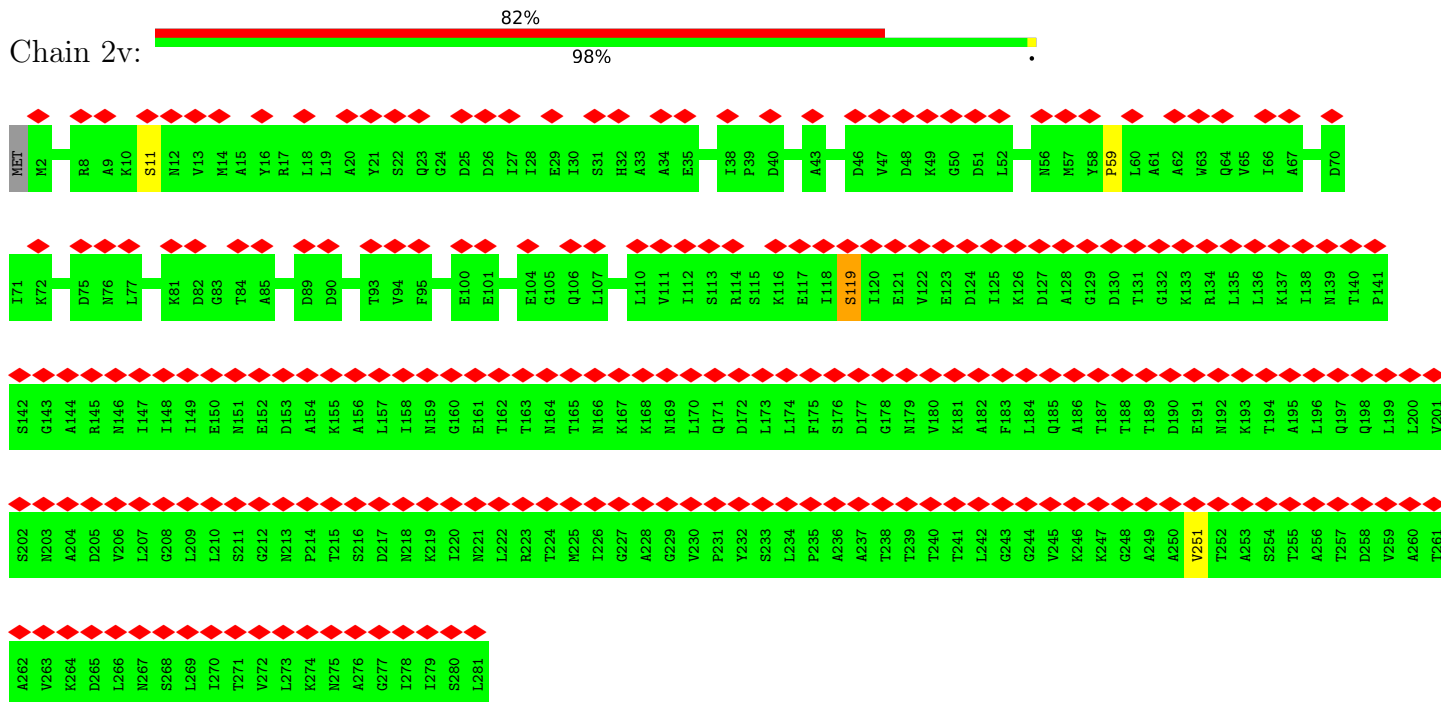
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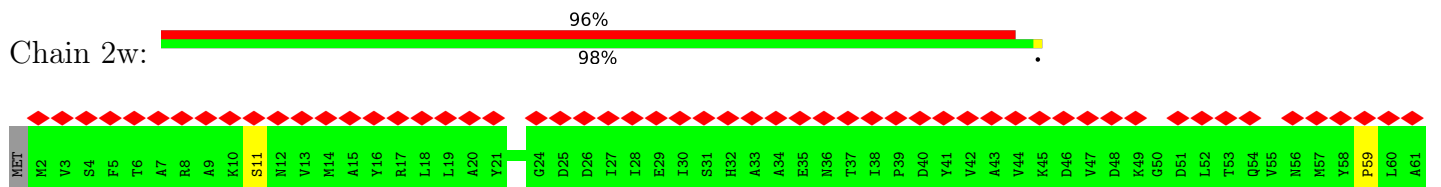
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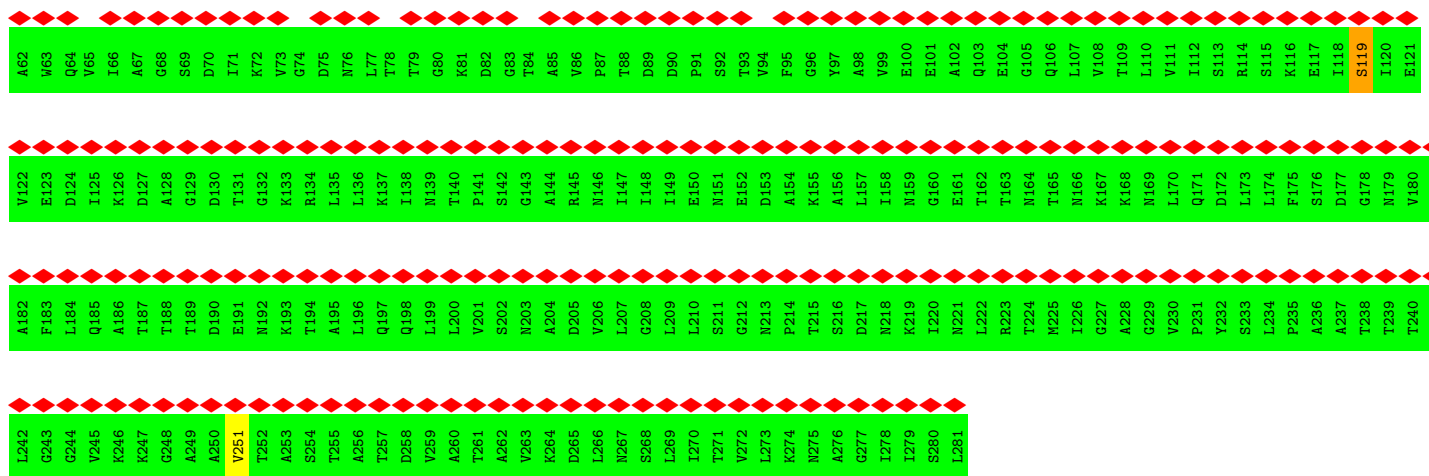


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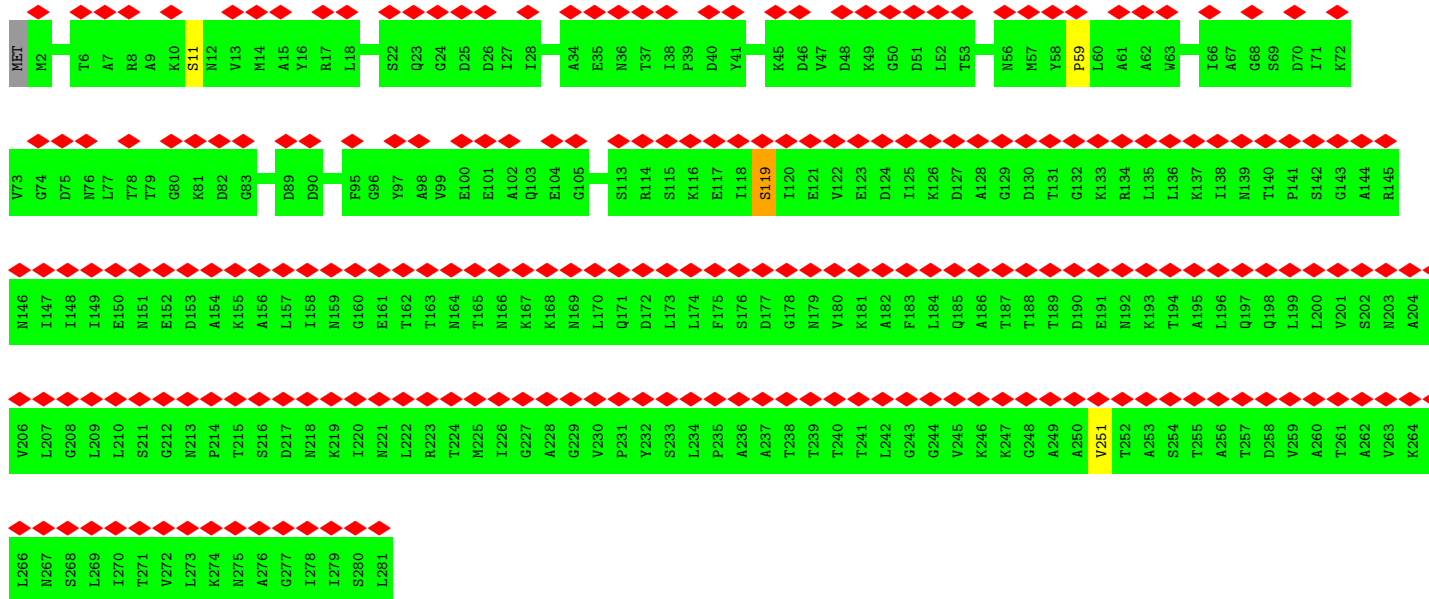
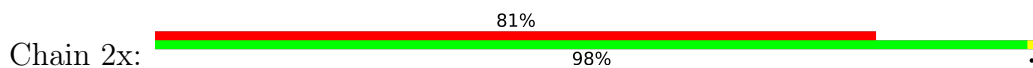


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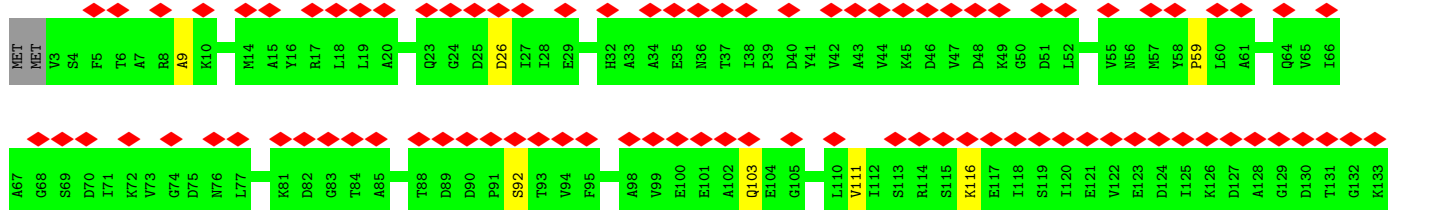
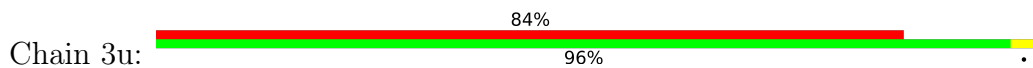


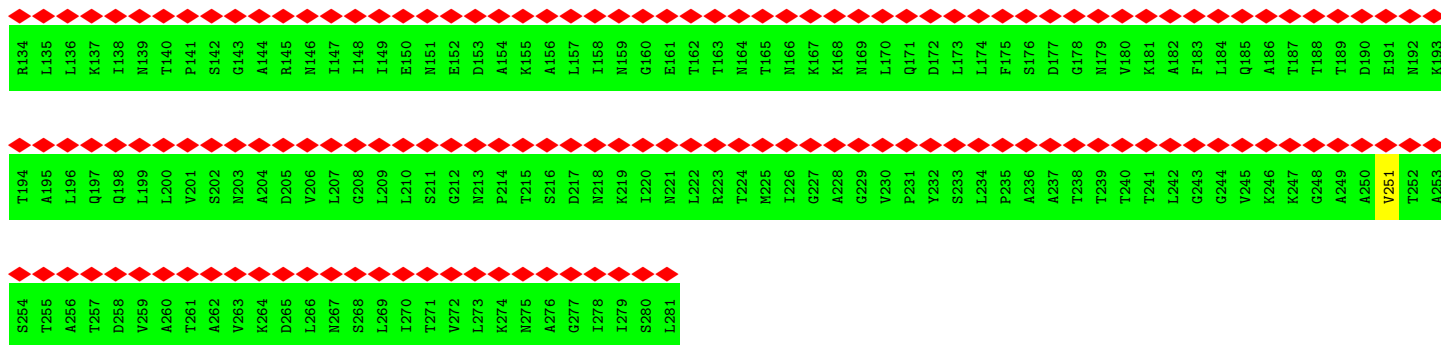


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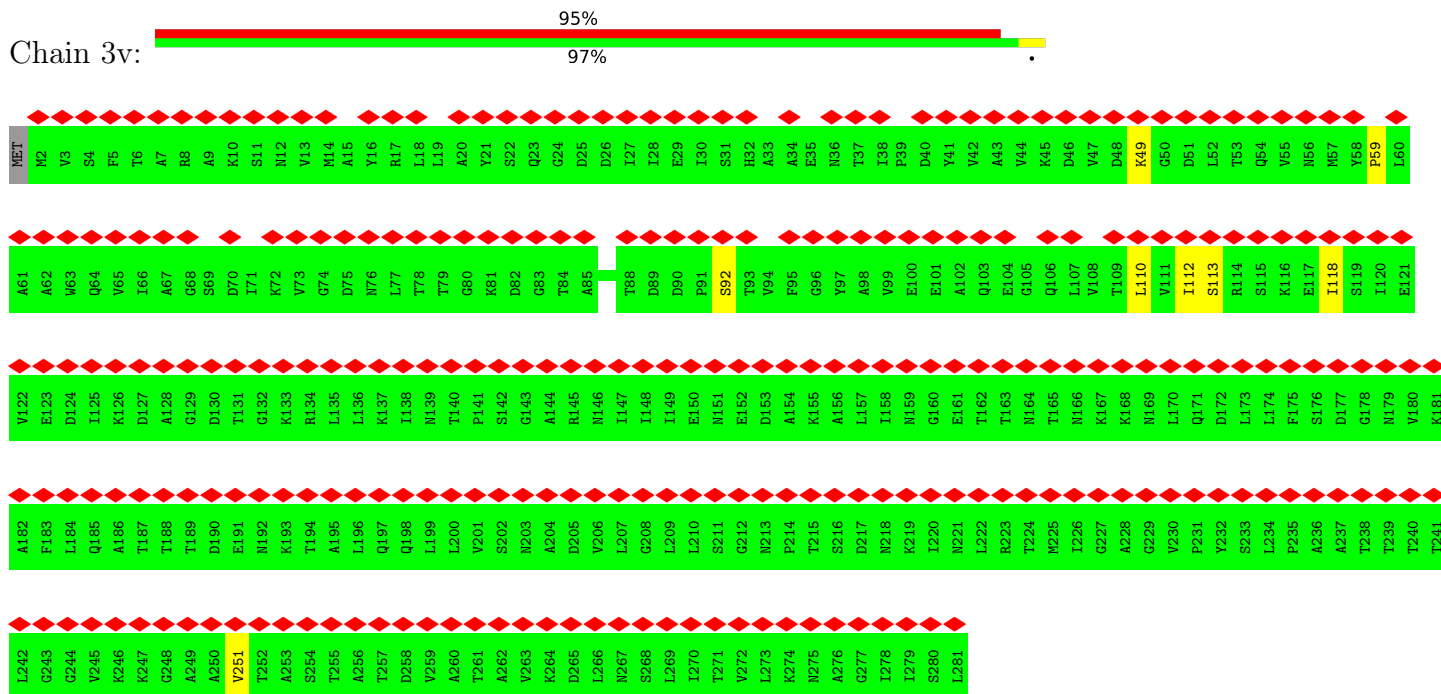


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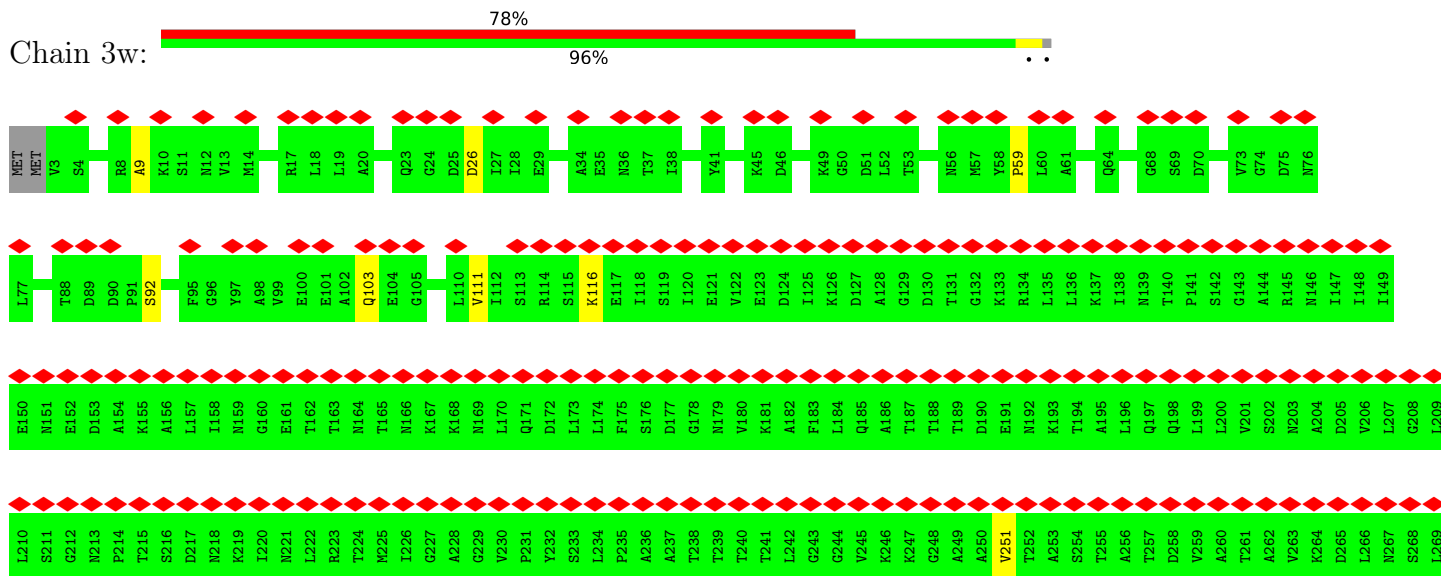


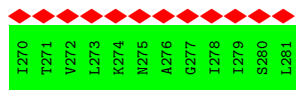


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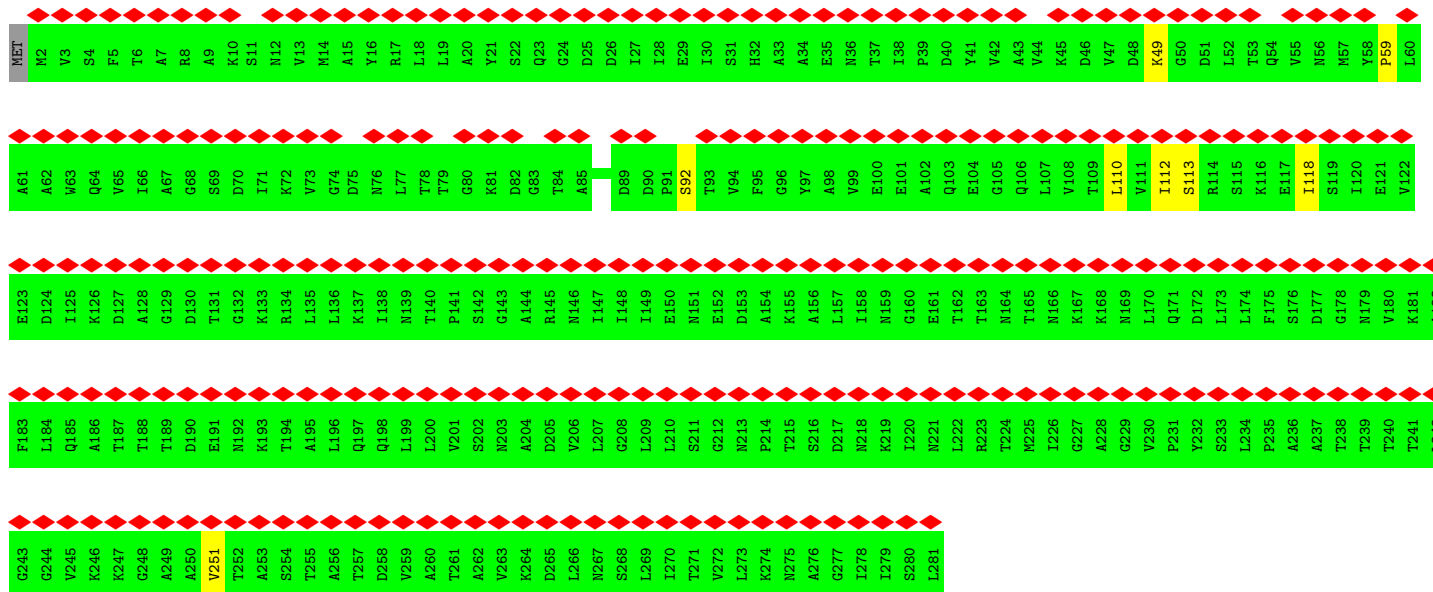


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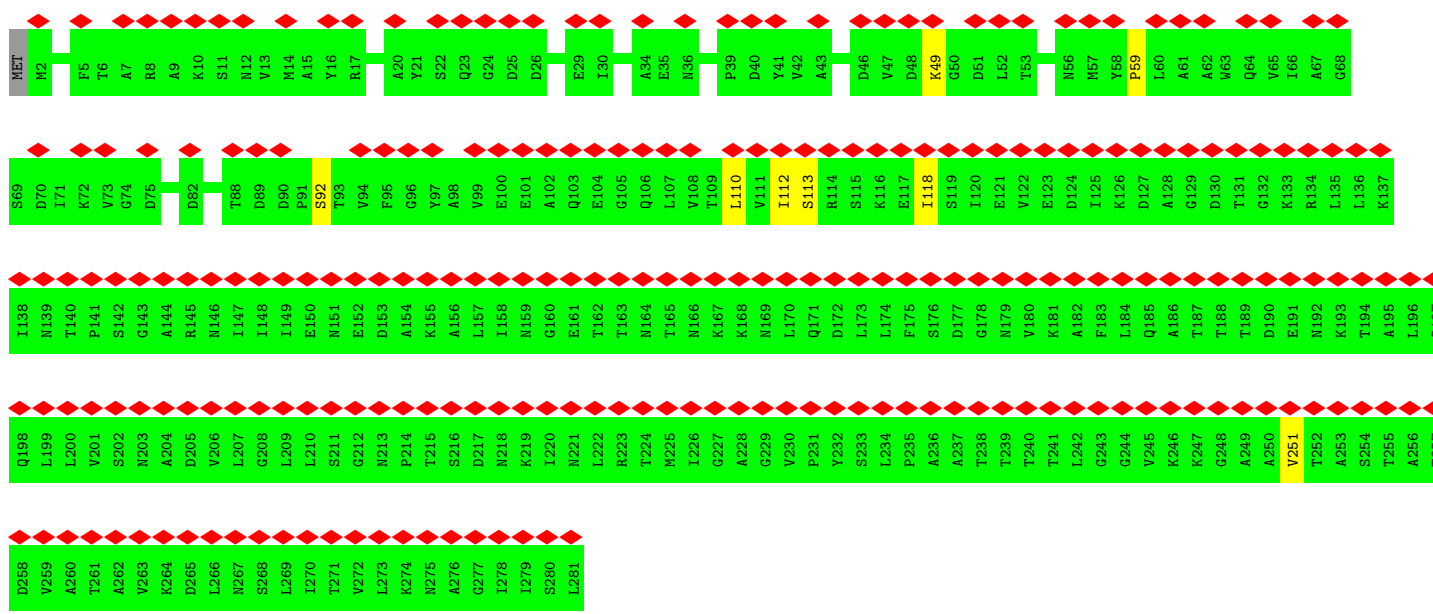
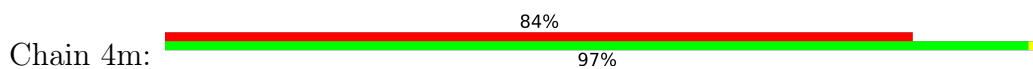




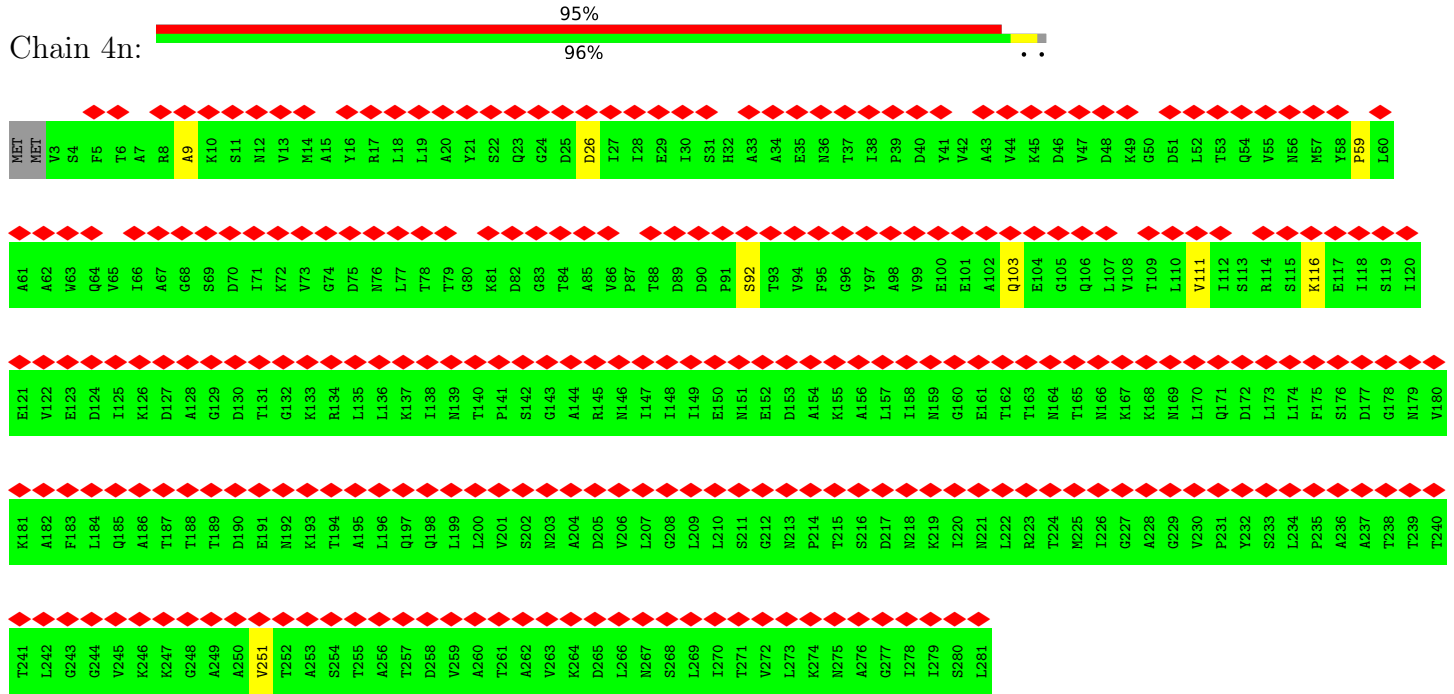
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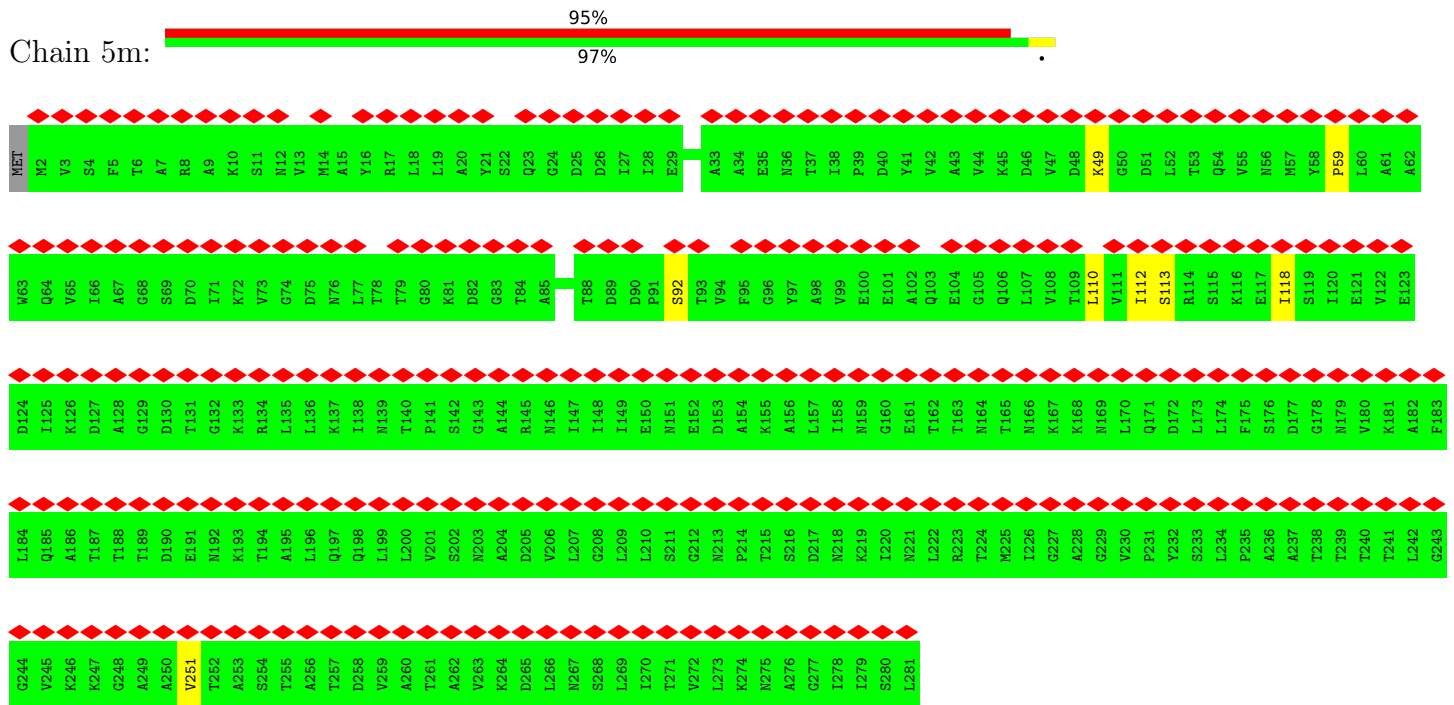
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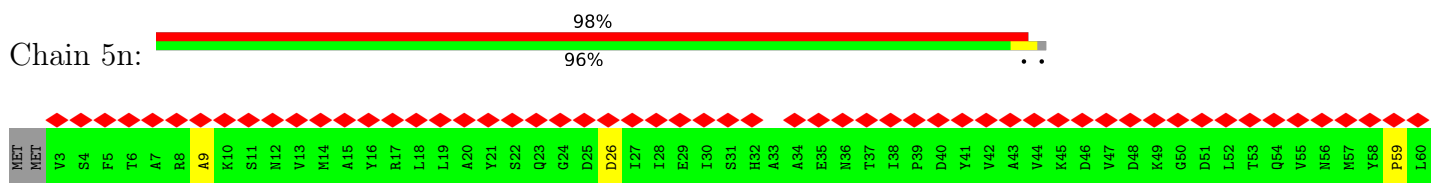
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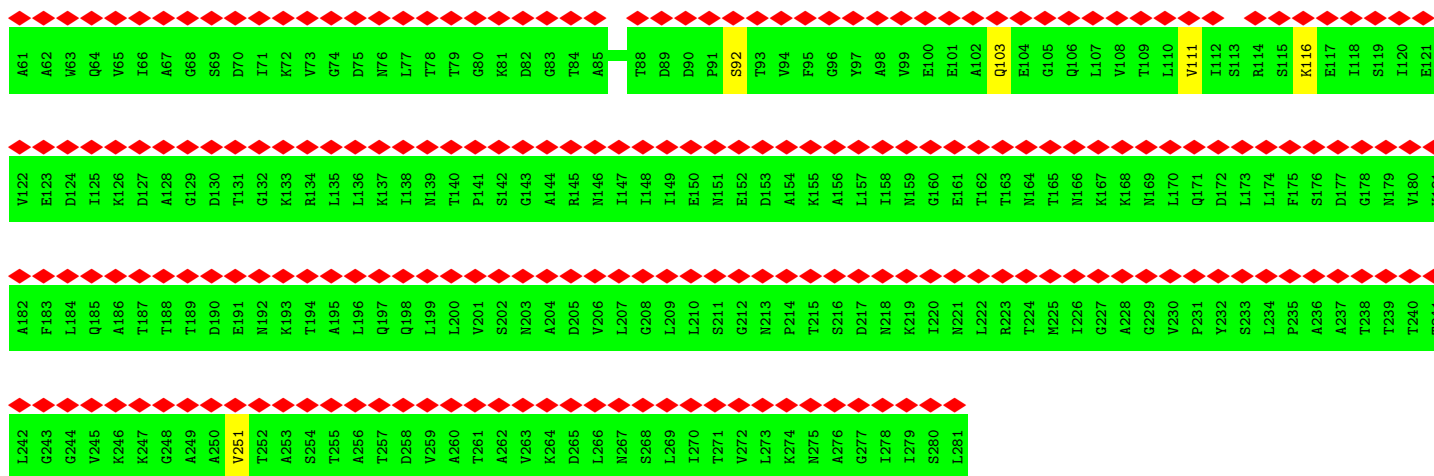


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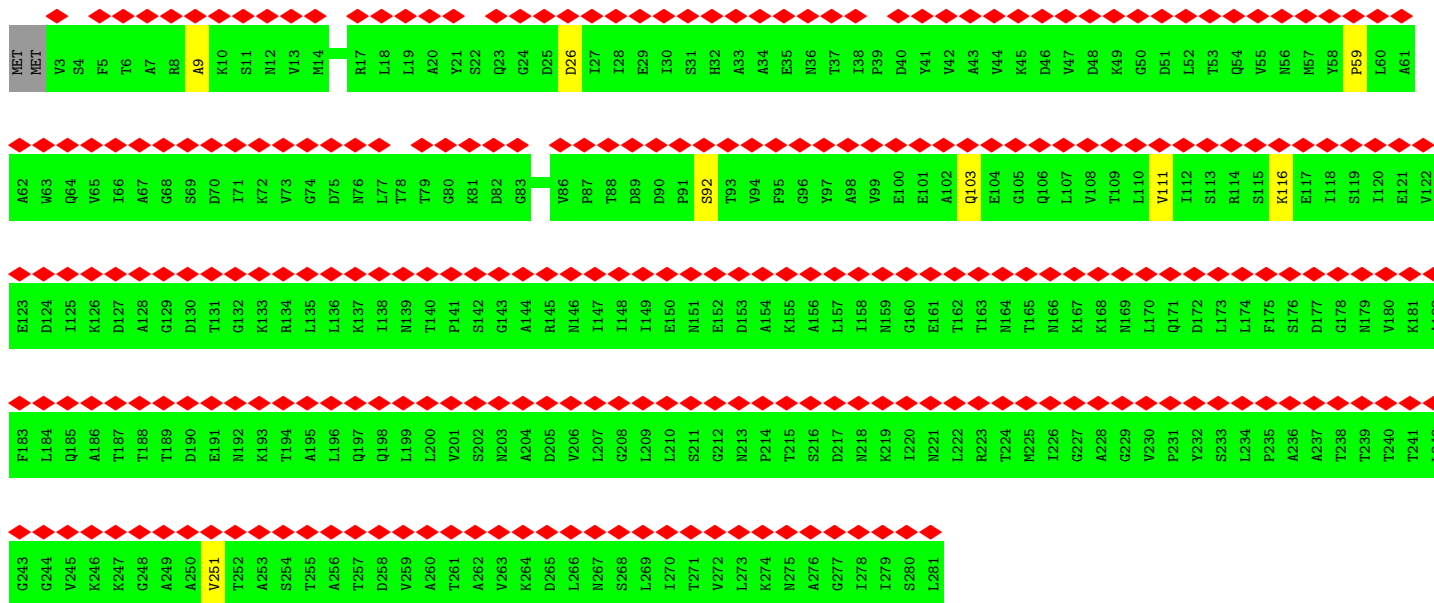


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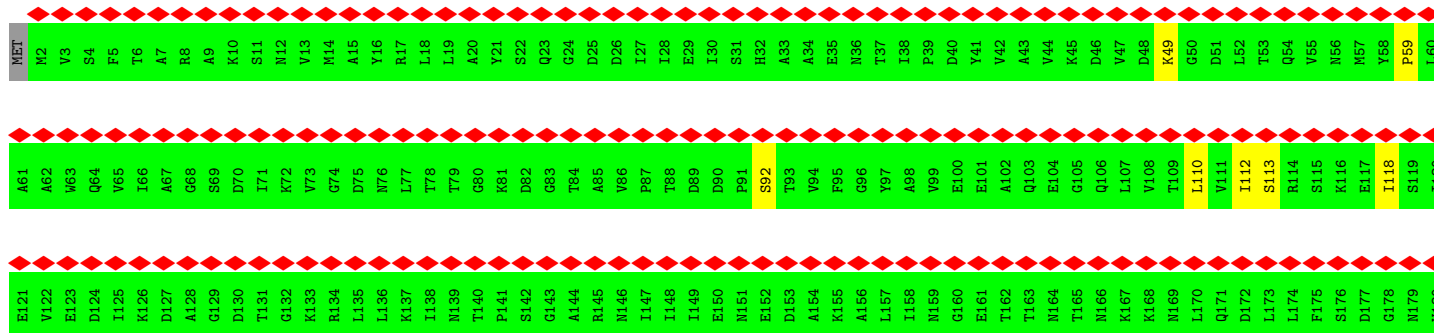


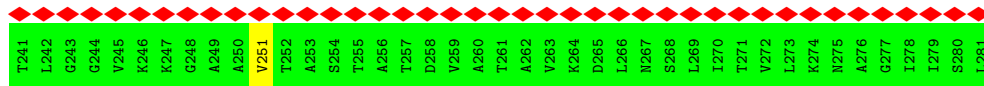
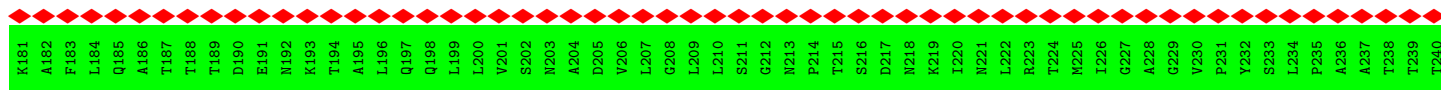


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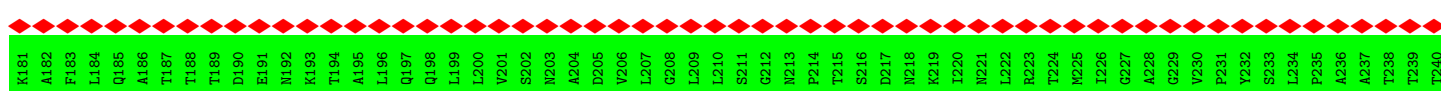
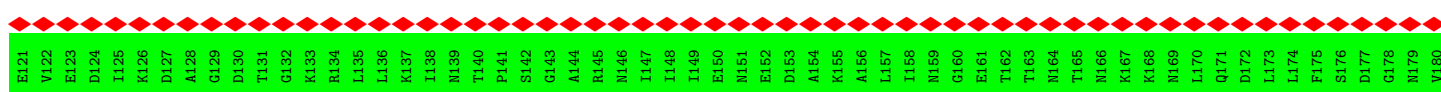
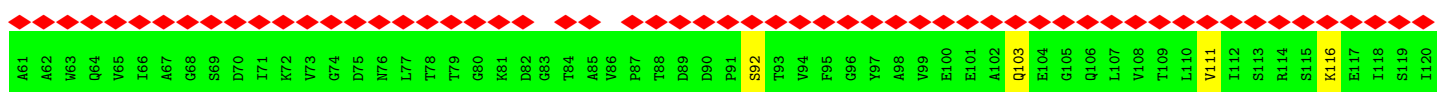
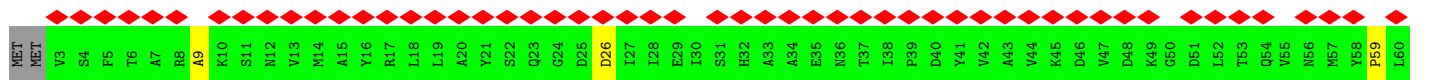


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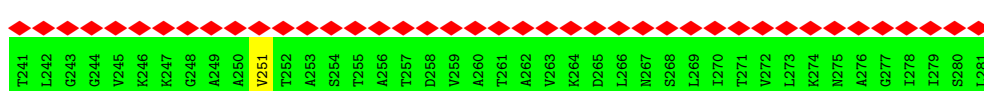
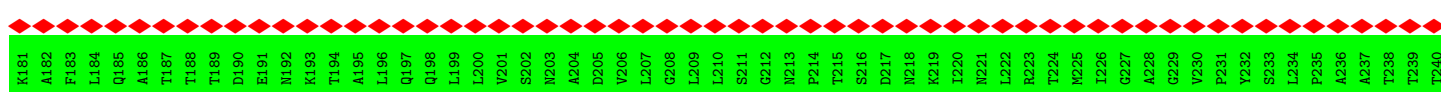
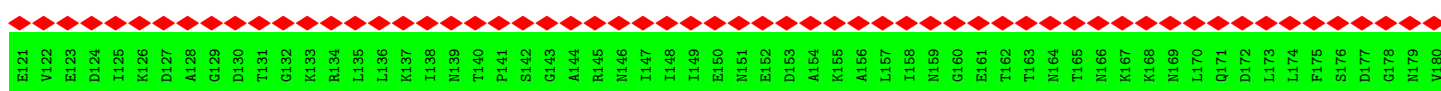
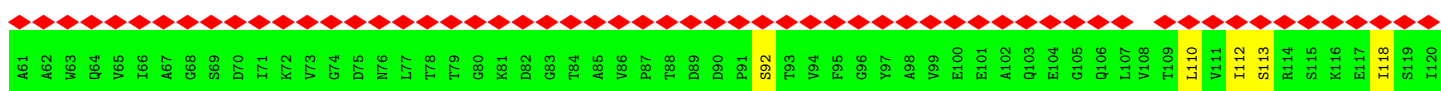
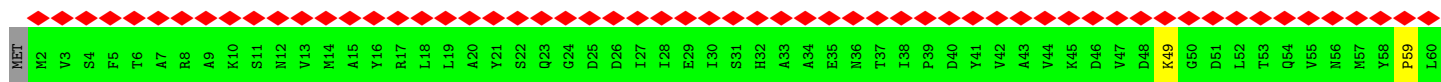




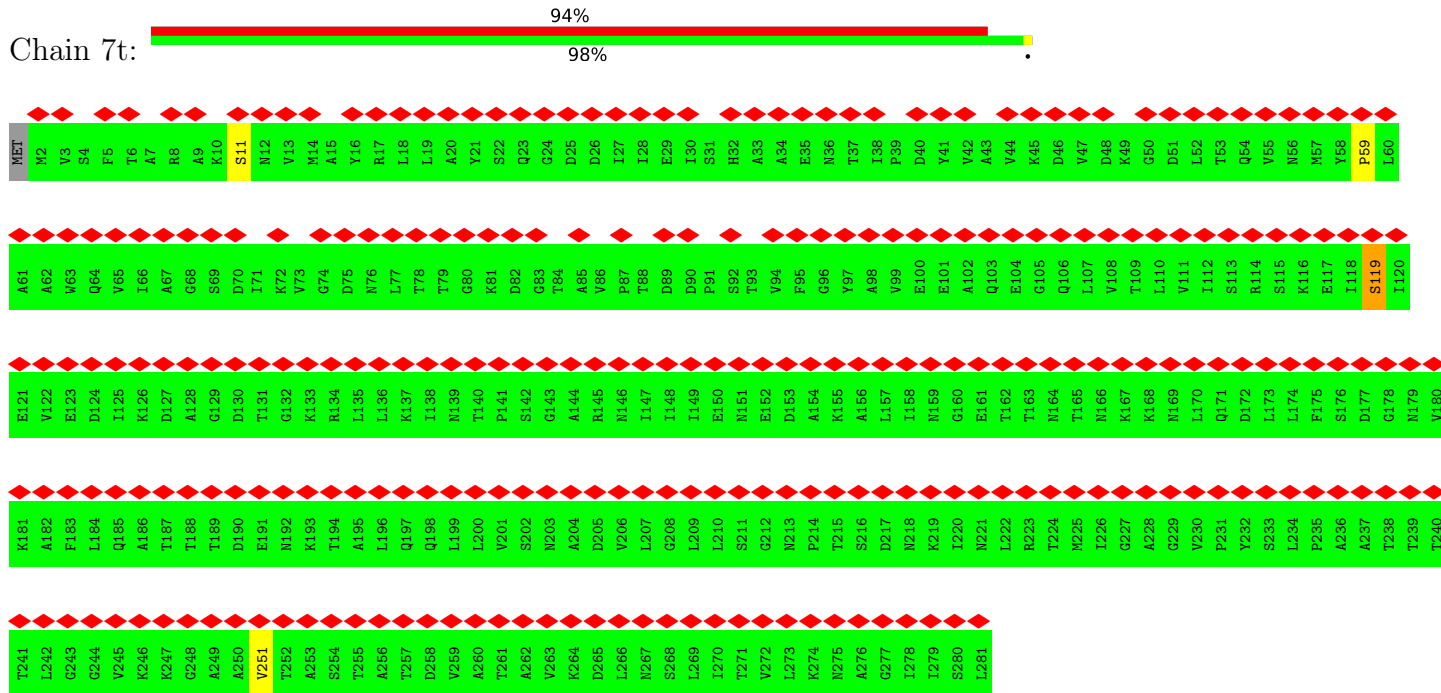
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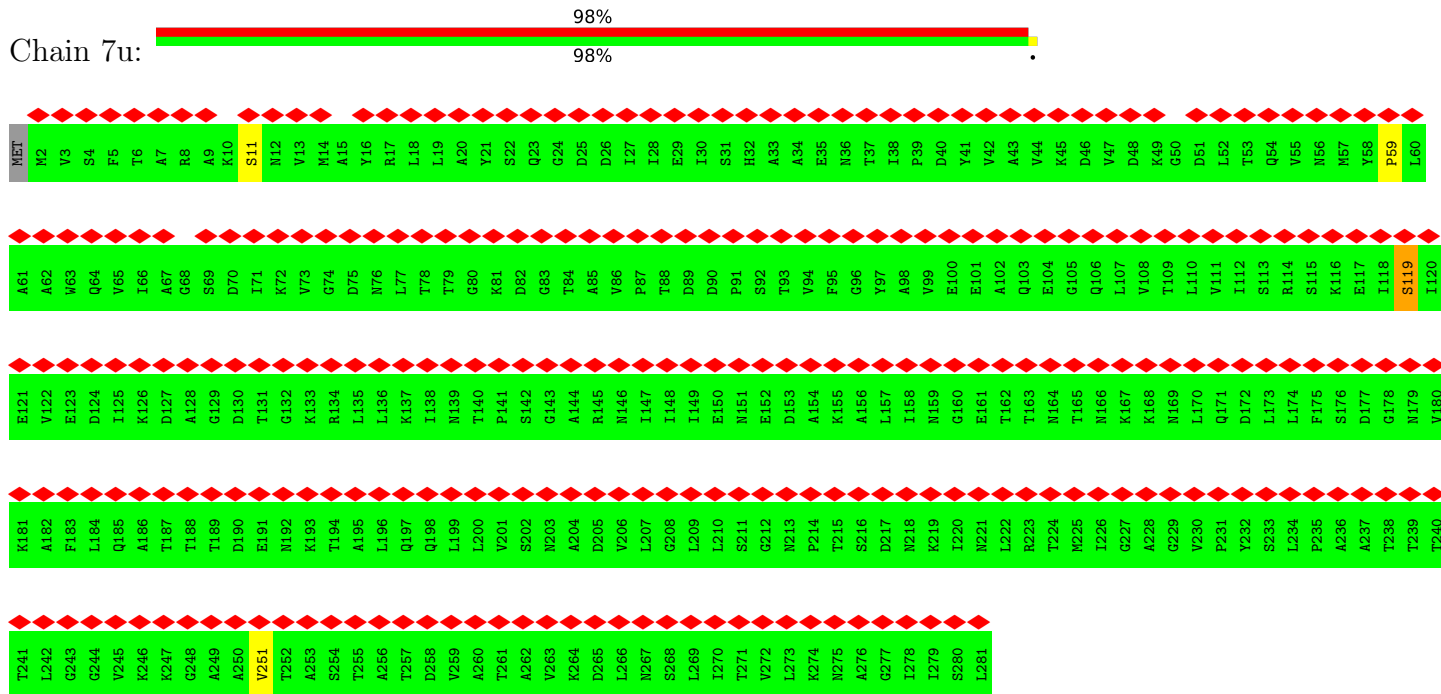
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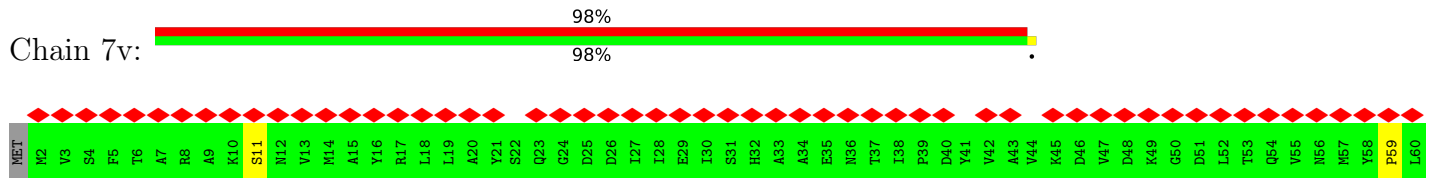
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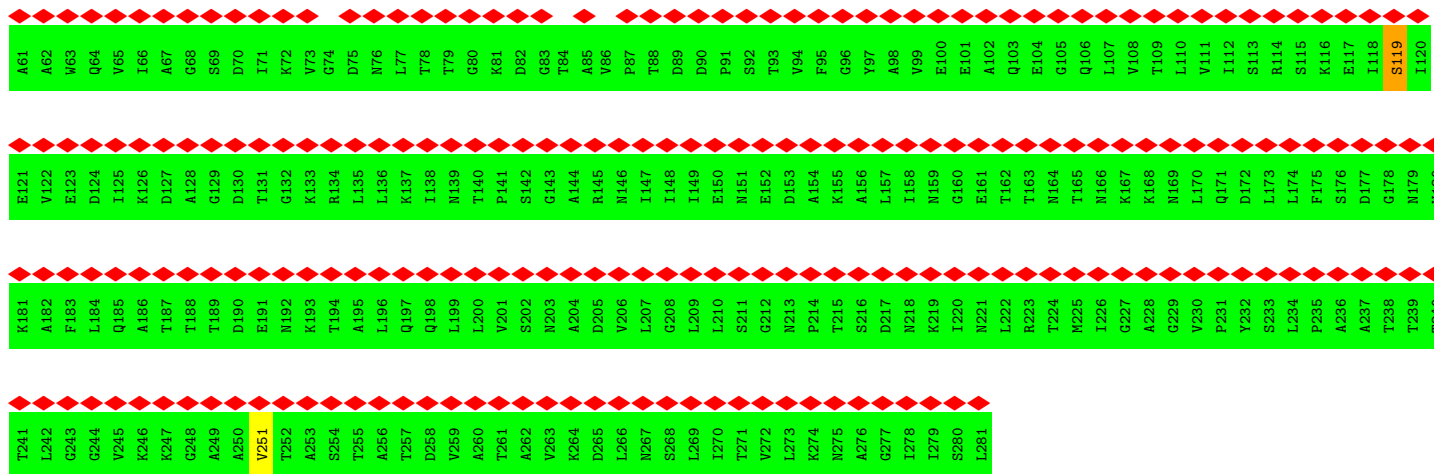


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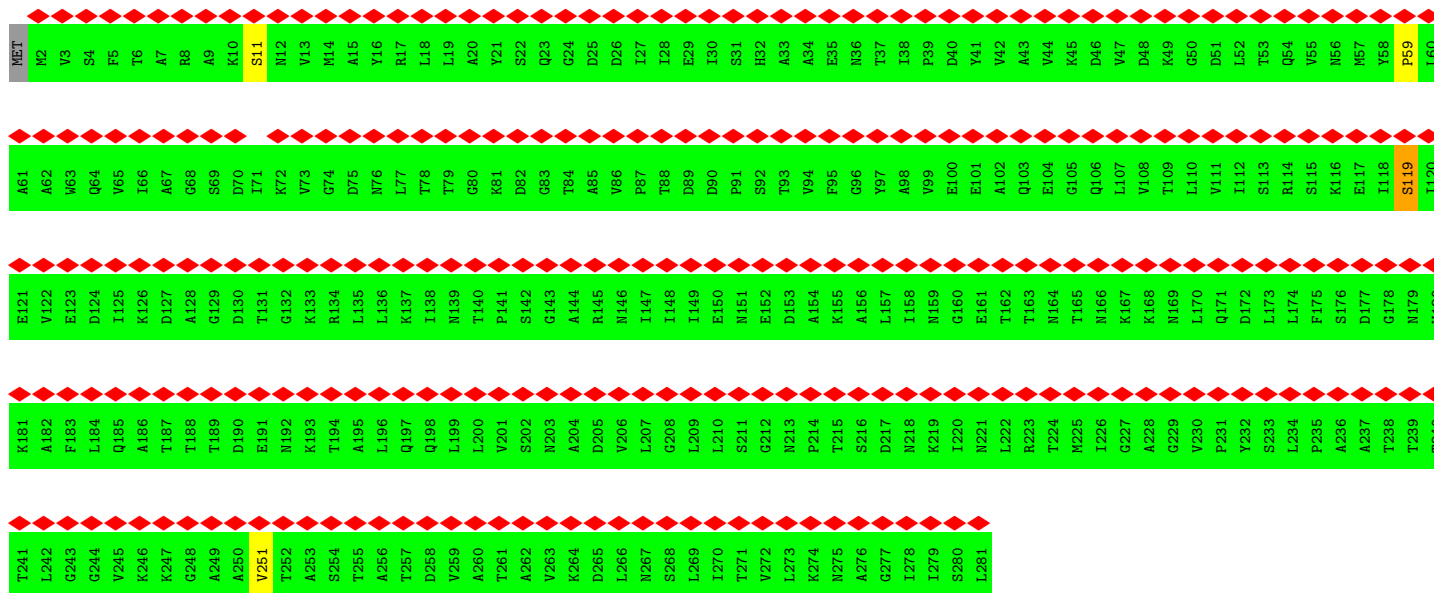


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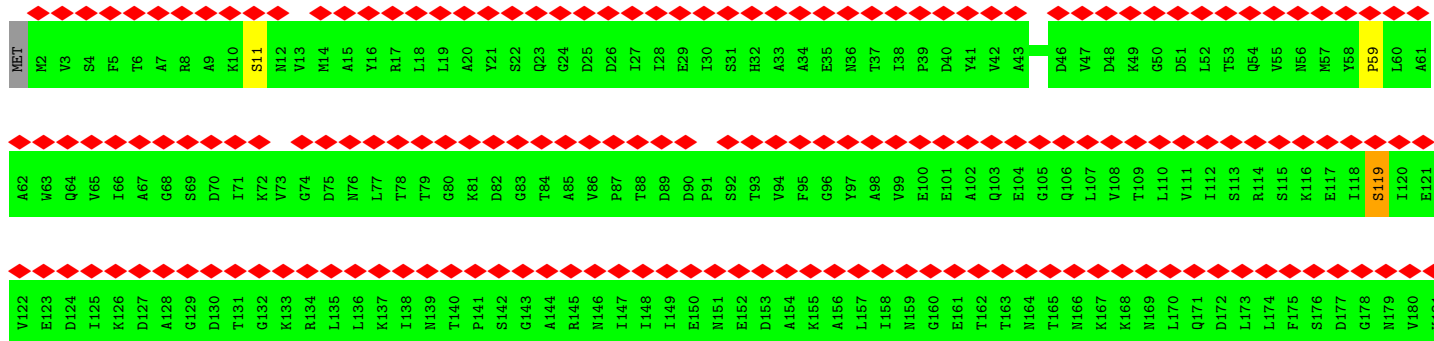




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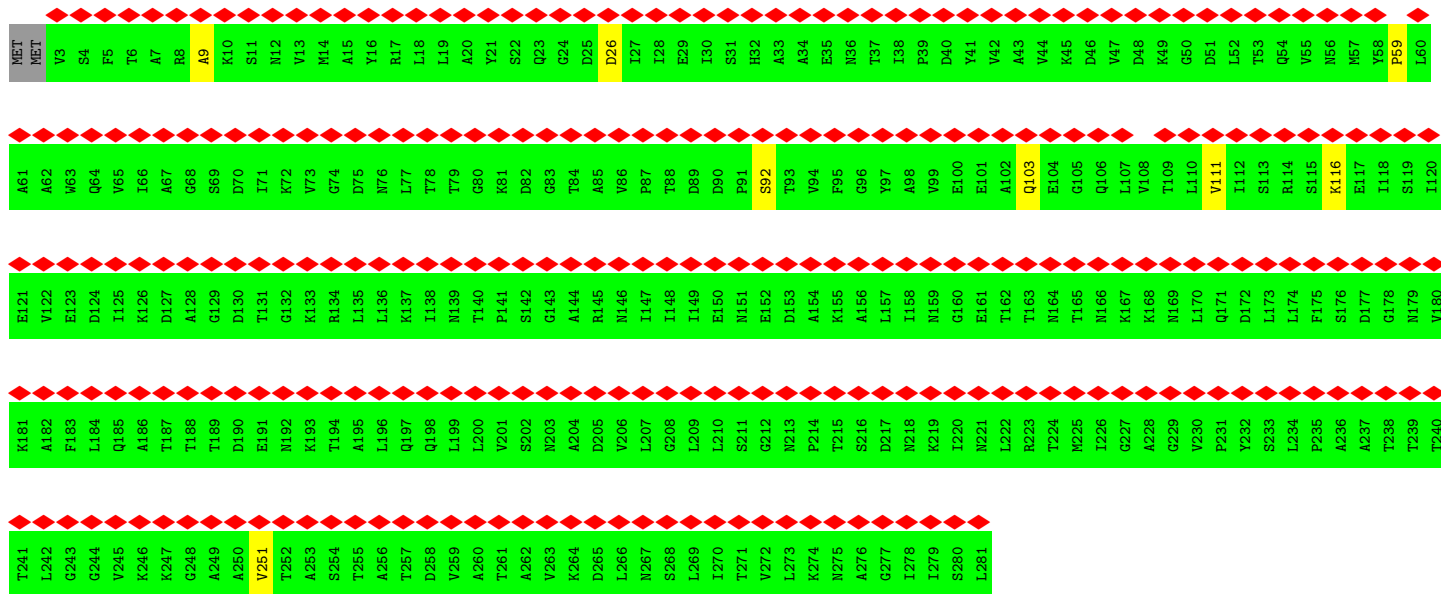


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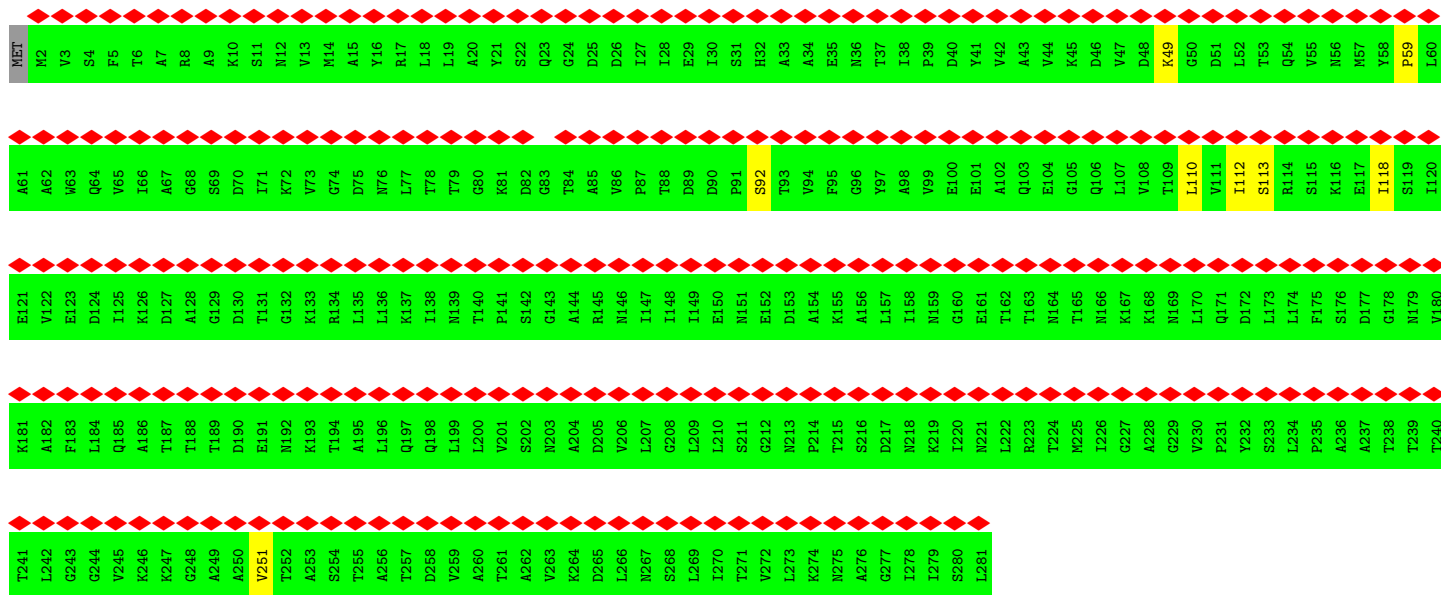




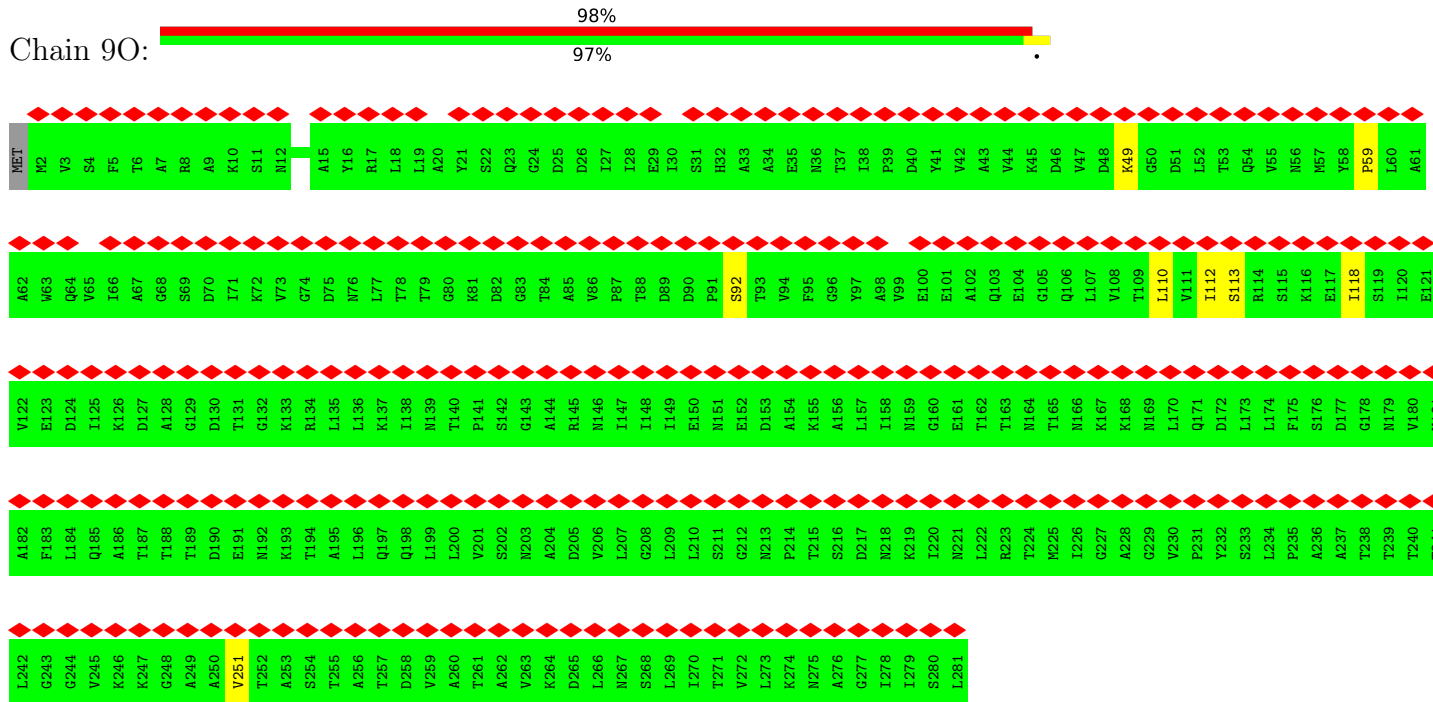
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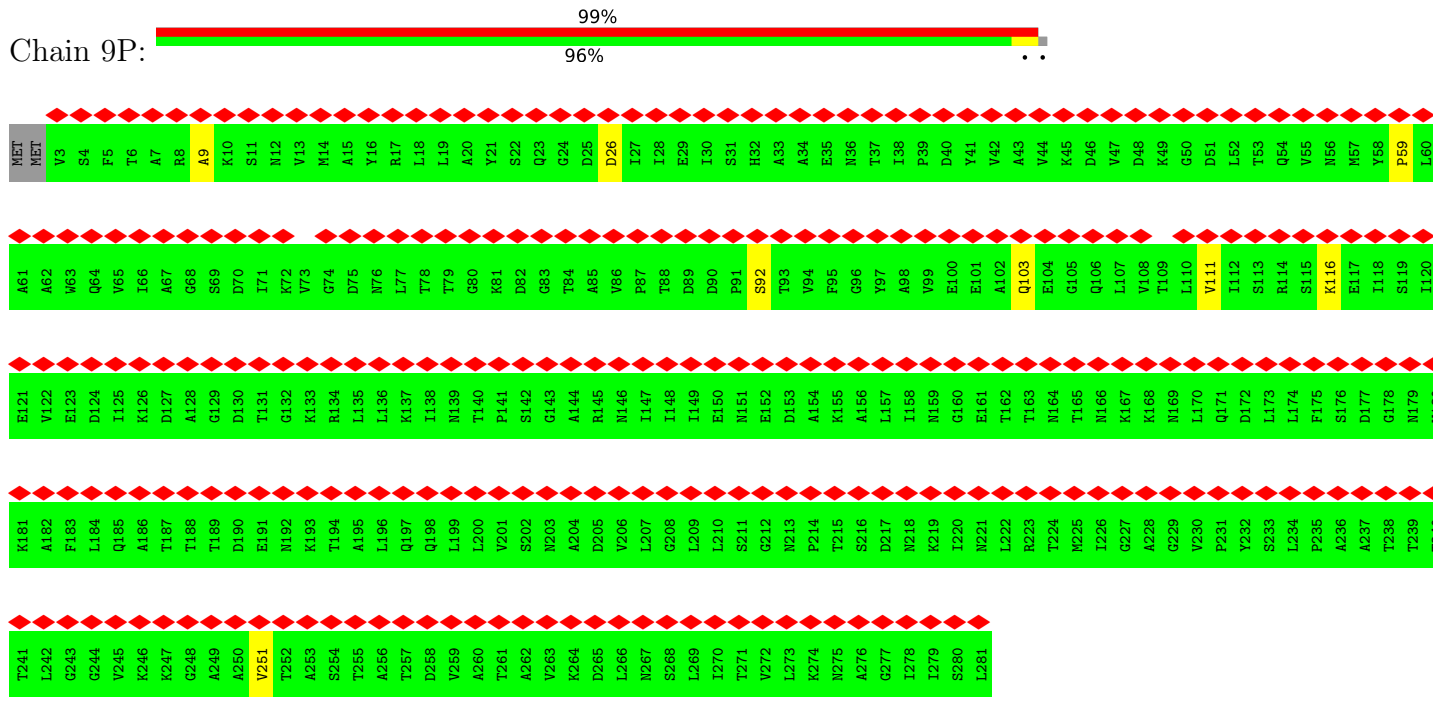
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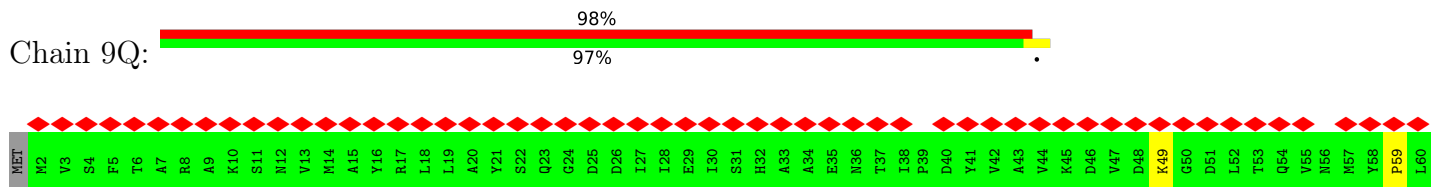
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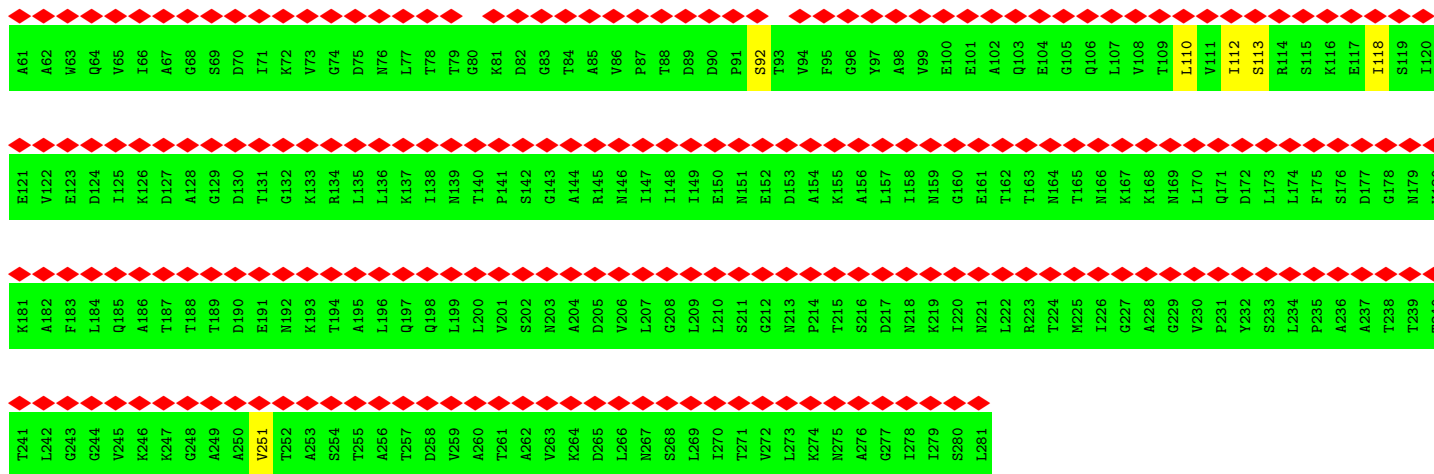


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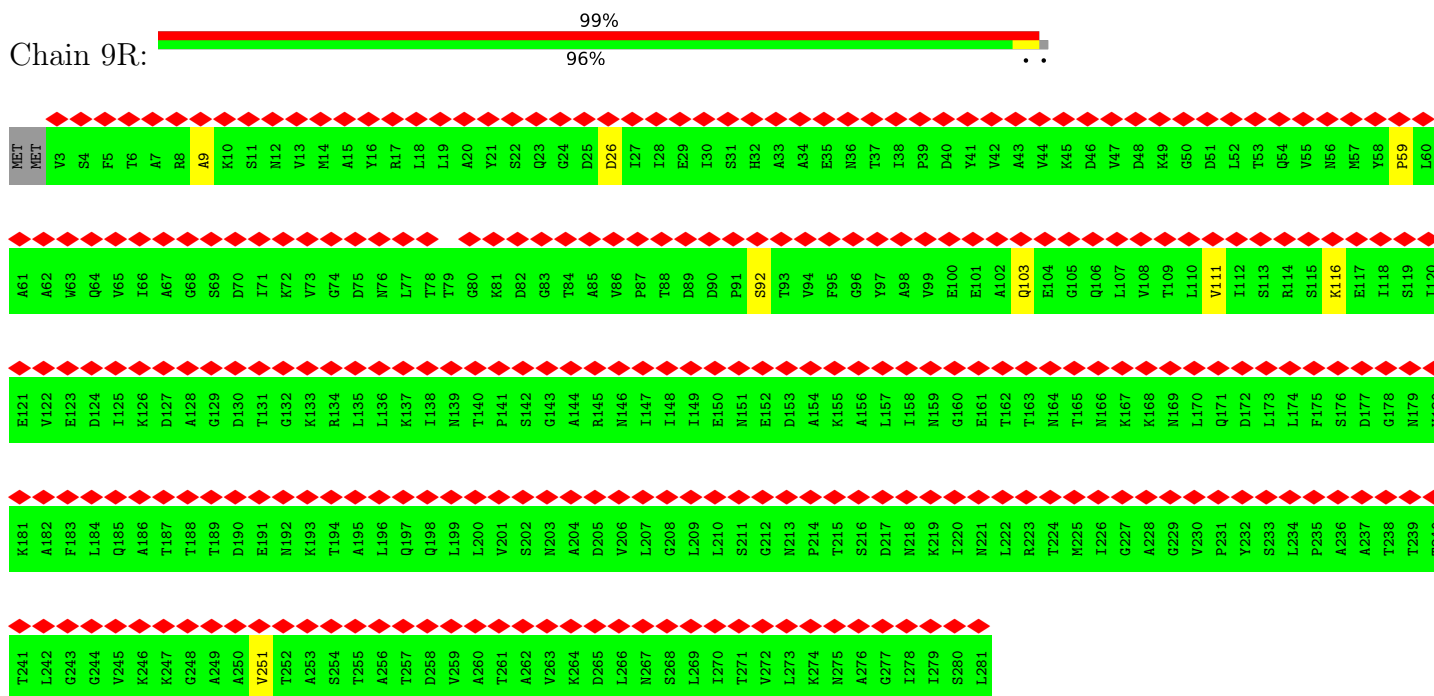


• Molecule 2: Capsid fiber protein

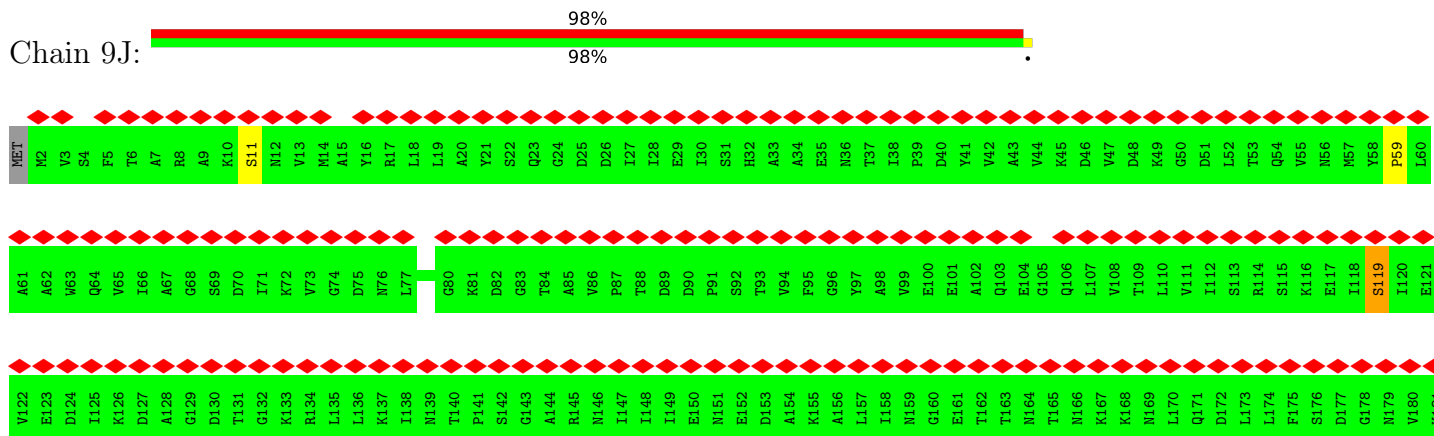




• Molecule 2: Capsid fiber protein



• Molecule 2: Capsid fiber protein



A182 F183 L184 Q185 A186 T187 T188 T189 D190 E191 N192 K193 T194 A195 L196 Q197 Q198 L199 L200 V201 S202 N203 A204 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 T240 T241

L242 G243 G244 V245 K246 G248 A249 A250 V251 T252 A253 S254 T255 A256 T257 D258 V259 A260 T261 A262 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	18230	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 ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	22.243	Depositor
Minimum map value	-0.425	Depositor
Average map value	0.118	Depositor
Map value standard deviation	0.805	Depositor
Recommended contour level	4.5	Depositor
Map size (\AA)	754.688, 754.688, 754.688	wwPDB
Map dimensions	704, 704, 704	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.072, 1.072, 1.072	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	0.82	0/3460	0.78	3/4698 (0.1%)
1	1B	0.89	0/3551	0.77	2/4822 (0.0%)
1	1C	0.89	0/3551	0.78	3/4822 (0.1%)
1	1D	0.90	0/3551	0.78	2/4822 (0.0%)
1	1E	0.89	0/3489	0.77	1/4737 (0.0%)
1	1F	0.89	0/3513	0.76	1/4771 (0.0%)
1	1G	0.82	0/3460	0.78	3/4698 (0.1%)
1	1H	0.89	0/3551	0.78	2/4822 (0.0%)
1	1I	0.89	0/3551	0.77	3/4822 (0.1%)
1	1J	0.90	0/3551	0.78	1/4822 (0.0%)
1	1K	0.89	0/3489	0.77	1/4737 (0.0%)
1	1L	0.89	0/3513	0.76	2/4771 (0.0%)
1	1M	0.82	0/3460	0.78	3/4698 (0.1%)
1	1N	0.89	0/3551	0.78	2/4822 (0.0%)
1	1O	0.90	0/3551	0.78	3/4822 (0.1%)
1	1P	0.90	0/3551	0.78	1/4822 (0.0%)
1	1Q	0.89	0/3489	0.77	1/4737 (0.0%)
1	1R	0.89	0/3513	0.76	1/4771 (0.0%)
1	1S	0.82	0/3460	0.78	3/4698 (0.1%)
1	1T	0.89	0/3551	0.78	2/4822 (0.0%)
1	1U	0.90	0/3551	0.78	4/4822 (0.1%)
1	1V	0.90	0/3551	0.78	2/4822 (0.0%)
1	1W	0.89	0/3489	0.77	1/4737 (0.0%)
1	1X	0.89	0/3513	0.76	1/4771 (0.0%)
1	1Y	0.82	0/3460	0.78	3/4698 (0.1%)
1	1Z	0.89	0/3551	0.77	2/4822 (0.0%)
1	1a	0.90	0/3551	0.78	3/4822 (0.1%)
1	1b	0.90	0/3551	0.78	1/4822 (0.0%)
1	1c	0.89	0/3489	0.77	1/4737 (0.0%)
1	1d	0.89	0/3513	0.76	1/4771 (0.0%)
1	2A	0.91	0/3493	0.78	4/4743 (0.1%)
1	2B	0.92	0/3551	0.81	7/4822 (0.1%)
1	2C	0.90	0/3551	0.79	2/4822 (0.0%)
1	2D	0.92	0/3551	0.79	5/4822 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	2E	0.91	0/3551	0.80	2/4822 (0.0%)
1	2F	0.91	0/3493	0.78	4/4743 (0.1%)
1	2G	0.92	0/3551	0.81	7/4822 (0.1%)
1	2H	0.90	0/3551	0.79	2/4822 (0.0%)
1	2I	0.92	0/3551	0.79	5/4822 (0.1%)
1	2J	0.91	0/3551	0.80	2/4822 (0.0%)
1	2K	0.91	0/3493	0.78	4/4743 (0.1%)
1	2L	0.92	0/3551	0.81	7/4822 (0.1%)
1	2M	0.90	0/3551	0.79	2/4822 (0.0%)
1	2N	0.92	0/3551	0.79	5/4822 (0.1%)
1	2O	0.91	0/3551	0.80	2/4822 (0.0%)
1	2P	0.91	0/3493	0.78	4/4743 (0.1%)
1	2Q	0.92	0/3551	0.81	7/4822 (0.1%)
1	2R	0.90	0/3551	0.79	2/4822 (0.0%)
1	2S	0.92	0/3551	0.79	5/4822 (0.1%)
1	2T	0.91	0/3551	0.80	2/4822 (0.0%)
1	2U	0.91	0/3493	0.78	4/4743 (0.1%)
1	2V	0.92	0/3551	0.81	7/4822 (0.1%)
1	2W	0.90	0/3551	0.79	2/4822 (0.0%)
1	2X	0.92	0/3551	0.80	5/4822 (0.1%)
1	2Y	0.91	0/3551	0.80	2/4822 (0.0%)
1	3A	0.91	0/3489	0.79	6/4737 (0.1%)
1	3B	0.93	0/3489	0.80	5/4737 (0.1%)
1	3C	0.91	0/3551	0.78	3/4822 (0.1%)
1	3D	0.94	0/3551	0.83	7/4822 (0.1%)
1	3E	0.91	0/3551	0.77	2/4822 (0.0%)
1	3F	0.92	0/3551	0.80	3/4822 (0.1%)
1	3G	0.91	0/3489	0.79	6/4737 (0.1%)
1	3H	0.92	0/3489	0.80	5/4737 (0.1%)
1	3I	0.91	0/3551	0.78	3/4822 (0.1%)
1	3J	0.94	0/3551	0.83	7/4822 (0.1%)
1	3K	0.91	0/3551	0.77	2/4822 (0.0%)
1	3L	0.92	0/3551	0.80	3/4822 (0.1%)
1	3M	0.91	0/3489	0.79	6/4737 (0.1%)
1	3N	0.93	0/3489	0.80	5/4737 (0.1%)
1	3O	0.91	0/3551	0.78	3/4822 (0.1%)
1	3P	0.94	0/3551	0.83	7/4822 (0.1%)
1	3Q	0.91	0/3551	0.76	2/4822 (0.0%)
1	3R	0.92	0/3551	0.80	3/4822 (0.1%)
1	3S	0.91	0/3489	0.79	6/4737 (0.1%)
1	3T	0.93	0/3489	0.80	5/4737 (0.1%)
1	3U	0.91	0/3551	0.78	3/4822 (0.1%)
1	3V	0.94	0/3551	0.83	7/4822 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	3W	0.91	0/3551	0.77	2/4822 (0.0%)
1	3X	0.92	0/3551	0.80	3/4822 (0.1%)
1	3Y	0.91	0/3489	0.79	6/4737 (0.1%)
1	3Z	0.93	0/3489	0.80	5/4737 (0.1%)
1	3a	0.91	0/3551	0.78	3/4822 (0.1%)
1	3b	0.94	0/3551	0.83	7/4822 (0.1%)
1	3c	0.91	0/3551	0.77	2/4822 (0.0%)
1	3d	0.92	0/3551	0.80	3/4822 (0.1%)
1	4A	0.93	0/3489	0.78	4/4737 (0.1%)
1	4B	0.92	0/3489	0.80	3/4737 (0.1%)
1	4C	0.94	0/3489	0.81	4/4737 (0.1%)
1	4D	0.93	0/3489	0.78	3/4737 (0.1%)
1	4E	0.93	0/3551	0.78	2/4822 (0.0%)
1	4F	0.92	0/3551	0.79	2/4822 (0.0%)
1	4G	0.93	0/3489	0.78	4/4737 (0.1%)
1	4H	0.92	0/3489	0.80	3/4737 (0.1%)
1	4I	0.94	0/3489	0.81	3/4737 (0.1%)
1	4J	0.93	0/3489	0.78	3/4737 (0.1%)
1	4K	0.93	0/3551	0.78	2/4822 (0.0%)
1	4L	0.92	0/3551	0.79	2/4822 (0.0%)
1	4M	0.93	0/3489	0.78	4/4737 (0.1%)
1	4N	0.92	0/3489	0.80	3/4737 (0.1%)
1	4O	0.94	0/3489	0.81	3/4737 (0.1%)
1	4P	0.93	0/3489	0.78	3/4737 (0.1%)
1	4Q	0.93	0/3551	0.78	2/4822 (0.0%)
1	4R	0.92	0/3551	0.79	2/4822 (0.0%)
1	4S	0.93	0/3489	0.78	4/4737 (0.1%)
1	4T	0.92	0/3489	0.79	3/4737 (0.1%)
1	4U	0.94	0/3489	0.81	4/4737 (0.1%)
1	4V	0.93	0/3489	0.78	3/4737 (0.1%)
1	4W	0.93	0/3551	0.78	2/4822 (0.0%)
1	4X	0.92	0/3551	0.79	2/4822 (0.0%)
1	4Y	0.93	0/3489	0.78	4/4737 (0.1%)
1	4Z	0.92	0/3489	0.80	3/4737 (0.1%)
1	4a	0.94	0/3489	0.81	3/4737 (0.1%)
1	4b	0.93	0/3489	0.78	4/4737 (0.1%)
1	4c	0.93	0/3551	0.78	2/4822 (0.0%)
1	4d	0.92	0/3551	0.79	2/4822 (0.0%)
1	5A	0.92	0/3489	0.82	4/4737 (0.1%)
1	5B	0.91	0/3489	0.82	3/4737 (0.1%)
1	5C	0.93	0/3489	0.82	4/4737 (0.1%)
1	5D	0.91	0/3489	0.77	2/4737 (0.0%)
1	5E	0.92	0/3551	0.79	2/4822 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	5F	0.90	0/3551	0.81	3/4822 (0.1%)
1	5G	0.92	0/3489	0.82	4/4737 (0.1%)
1	5H	0.91	0/3489	0.82	3/4737 (0.1%)
1	5I	0.93	0/3489	0.82	4/4737 (0.1%)
1	5J	0.91	0/3489	0.77	2/4737 (0.0%)
1	5K	0.92	0/3551	0.79	2/4822 (0.0%)
1	5L	0.90	0/3551	0.81	3/4822 (0.1%)
1	5M	0.92	0/3489	0.82	4/4737 (0.1%)
1	5N	0.91	0/3489	0.82	3/4737 (0.1%)
1	5O	0.93	0/3489	0.82	4/4737 (0.1%)
1	5P	0.91	0/3489	0.77	2/4737 (0.0%)
1	5Q	0.92	0/3551	0.79	2/4822 (0.0%)
1	5R	0.90	0/3551	0.81	3/4822 (0.1%)
1	5S	0.92	0/3489	0.82	4/4737 (0.1%)
1	5T	0.91	0/3489	0.82	3/4737 (0.1%)
1	5U	0.93	0/3489	0.82	4/4737 (0.1%)
1	5V	0.91	0/3489	0.77	2/4737 (0.0%)
1	5W	0.92	0/3551	0.79	2/4822 (0.0%)
1	5X	0.90	0/3551	0.81	3/4822 (0.1%)
1	5Y	0.92	0/3489	0.82	4/4737 (0.1%)
1	5Z	0.91	0/3489	0.82	3/4737 (0.1%)
1	5a	0.93	0/3489	0.82	4/4737 (0.1%)
1	5b	0.91	0/3489	0.77	2/4737 (0.0%)
1	5c	0.92	0/3551	0.79	2/4822 (0.0%)
1	5d	0.90	0/3551	0.81	3/4822 (0.1%)
1	6A	0.88	0/3551	0.77	2/4822 (0.0%)
1	6B	0.89	0/3551	0.77	4/4822 (0.1%)
1	6C	0.89	0/3489	0.78	1/4737 (0.0%)
1	6D	0.91	0/3489	0.80	3/4737 (0.1%)
1	6E	0.90	0/3551	0.77	2/4822 (0.0%)
1	6F	0.89	0/3551	0.79	4/4822 (0.1%)
1	6G	0.88	0/3551	0.77	2/4822 (0.0%)
1	6H	0.89	0/3551	0.77	4/4822 (0.1%)
1	6I	0.89	0/3489	0.78	1/4737 (0.0%)
1	6J	0.91	0/3489	0.80	3/4737 (0.1%)
1	6K	0.90	0/3551	0.77	2/4822 (0.0%)
1	6L	0.89	0/3551	0.79	4/4822 (0.1%)
1	6M	0.88	0/3551	0.77	2/4822 (0.0%)
1	6N	0.89	0/3551	0.77	4/4822 (0.1%)
1	6O	0.89	0/3489	0.78	1/4737 (0.0%)
1	6P	0.91	0/3489	0.80	3/4737 (0.1%)
1	6Q	0.90	0/3551	0.77	2/4822 (0.0%)
1	6R	0.89	0/3551	0.79	4/4822 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	6S	0.88	0/3551	0.77	2/4822 (0.0%)
1	6T	0.89	0/3551	0.77	4/4822 (0.1%)
1	6U	0.89	0/3489	0.78	1/4737 (0.0%)
1	6V	0.91	0/3489	0.80	3/4737 (0.1%)
1	6W	0.90	0/3551	0.77	2/4822 (0.0%)
1	6X	0.89	0/3551	0.79	4/4822 (0.1%)
1	6Y	0.88	0/3551	0.77	2/4822 (0.0%)
1	6Z	0.89	0/3551	0.77	4/4822 (0.1%)
1	6a	0.89	0/3489	0.77	1/4737 (0.0%)
1	6b	0.91	0/3489	0.80	3/4737 (0.1%)
1	6c	0.90	0/3551	0.77	2/4822 (0.0%)
1	6d	0.89	0/3551	0.79	4/4822 (0.1%)
1	7A	0.87	0/3551	0.80	6/4822 (0.1%)
1	7B	0.86	0/3551	0.79	3/4822 (0.1%)
1	7C	0.86	0/3551	0.80	4/4822 (0.1%)
1	7D	0.87	0/3551	0.79	5/4822 (0.1%)
1	7E	0.87	0/3551	0.79	2/4822 (0.0%)
1	7F	0.87	0/3551	0.80	7/4822 (0.1%)
1	7G	0.86	0/3551	0.79	3/4822 (0.1%)
1	7H	0.86	0/3551	0.80	4/4822 (0.1%)
1	7I	0.87	0/3551	0.79	4/4822 (0.1%)
1	7J	0.87	0/3551	0.79	2/4822 (0.0%)
1	7K	0.87	0/3551	0.80	7/4822 (0.1%)
1	7L	0.86	0/3551	0.79	3/4822 (0.1%)
1	7M	0.86	0/3551	0.80	4/4822 (0.1%)
1	7N	0.87	0/3551	0.79	5/4822 (0.1%)
1	7O	0.87	0/3551	0.79	2/4822 (0.0%)
1	7P	0.87	0/3551	0.80	6/4822 (0.1%)
1	7Q	0.86	0/3551	0.79	3/4822 (0.1%)
1	7R	0.86	0/3551	0.80	4/4822 (0.1%)
1	7S	0.87	0/3551	0.79	5/4822 (0.1%)
1	7T	0.87	0/3551	0.79	2/4822 (0.0%)
1	7U	0.87	0/3551	0.80	6/4822 (0.1%)
1	7V	0.86	0/3551	0.79	3/4822 (0.1%)
1	7W	0.86	0/3551	0.80	5/4822 (0.1%)
1	7X	0.87	0/3551	0.79	4/4822 (0.1%)
1	7Y	0.87	0/3551	0.79	2/4822 (0.0%)
1	8A	0.86	0/3551	0.80	8/4822 (0.2%)
1	8B	0.85	0/3551	0.78	6/4822 (0.1%)
1	8C	0.87	0/3551	0.79	2/4822 (0.0%)
1	8D	0.85	0/3551	0.75	2/4822 (0.0%)
1	8E	0.87	0/3551	0.79	3/4822 (0.1%)
1	8F	0.86	0/3551	0.77	3/4822 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	8G	0.87	0/3551	0.80	8/4822 (0.2%)
1	8H	0.85	0/3551	0.78	5/4822 (0.1%)
1	8I	0.87	0/3551	0.79	2/4822 (0.0%)
1	8J	0.85	0/3551	0.75	2/4822 (0.0%)
1	8K	0.87	0/3551	0.79	3/4822 (0.1%)
1	8L	0.86	0/3551	0.77	3/4822 (0.1%)
1	8M	0.87	0/3551	0.80	8/4822 (0.2%)
1	8N	0.85	0/3551	0.78	4/4822 (0.1%)
1	8O	0.87	0/3551	0.79	2/4822 (0.0%)
1	8P	0.85	0/3551	0.75	2/4822 (0.0%)
1	8Q	0.87	0/3551	0.79	3/4822 (0.1%)
1	8R	0.86	0/3551	0.77	3/4822 (0.1%)
1	8S	0.87	0/3551	0.80	8/4822 (0.2%)
1	8T	0.85	0/3551	0.78	5/4822 (0.1%)
1	8U	0.87	0/3551	0.79	2/4822 (0.0%)
1	8V	0.85	0/3551	0.75	2/4822 (0.0%)
1	8W	0.87	0/3551	0.79	3/4822 (0.1%)
1	8X	0.86	0/3551	0.77	3/4822 (0.1%)
1	8Y	0.86	0/3551	0.80	7/4822 (0.1%)
1	8Z	0.85	0/3551	0.78	5/4822 (0.1%)
1	8a	0.87	0/3551	0.79	2/4822 (0.0%)
1	8b	0.85	0/3551	0.75	2/4822 (0.0%)
1	8c	0.87	0/3551	0.79	3/4822 (0.1%)
1	8d	0.86	0/3551	0.77	3/4822 (0.1%)
1	9A	0.86	0/3551	0.79	3/4822 (0.1%)
1	9B	0.86	0/3551	0.79	4/4822 (0.1%)
1	9C	0.86	0/3551	0.79	3/4822 (0.1%)
1	9D	0.86	0/3551	0.79	4/4822 (0.1%)
1	9E	0.86	0/3551	0.79	3/4822 (0.1%)
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	0.83	55/1183830 (0.0%)	0.76	779/1608450 (0.0%)

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	6i	111	VAL	C-N	-5.69	1.21	1.34
2	1j	111	VAL	C-N	-5.68	1.21	1.34
2	6u	111	VAL	C-N	-5.68	1.21	1.34
2	1f	111	VAL	C-N	-5.67	1.21	1.34
2	6m	111	VAL	C-N	-5.67	1.21	1.34
2	9R	111	VAL	C-N	-5.67	1.21	1.34
2	1n	111	VAL	C-N	-5.67	1.21	1.34
2	6q	111	VAL	C-N	-5.67	1.21	1.34
2	4n	111	VAL	C-N	-5.67	1.21	1.34
2	5l	111	VAL	C-N	-5.66	1.21	1.34
2	4f	111	VAL	C-N	-5.66	1.21	1.34
2	6e	111	VAL	C-N	-5.66	1.21	1.34
2	1r	111	VAL	C-N	-5.66	1.21	1.34
2	9L	111	VAL	C-N	-5.66	1.21	1.34
2	8h	111	VAL	C-N	-5.66	1.21	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	8k	111	VAL	C-N	-5.66	1.21	1.34
2	8n	111	VAL	C-N	-5.66	1.21	1.34
2	4l	111	VAL	C-N	-5.66	1.21	1.34
2	8z	111	VAL	C-N	-5.66	1.21	1.34
2	9P	111	VAL	C-N	-5.66	1.21	1.34
2	8j	111	VAL	C-N	-5.66	1.21	1.34
2	1v	111	VAL	C-N	-5.66	1.21	1.34
2	8q	111	VAL	C-N	-5.66	1.21	1.34
2	8v	111	VAL	C-N	-5.65	1.21	1.34
2	8p	111	VAL	C-N	-5.64	1.21	1.34
2	8t	111	VAL	C-N	-5.64	1.21	1.34
2	8e	111	VAL	C-N	-5.64	1.21	1.34
2	3o	111	VAL	C-N	-5.64	1.21	1.34
2	3i	111	VAL	C-N	-5.64	1.21	1.34
2	5h	111	VAL	C-N	-5.64	1.21	1.34
2	4j	111	VAL	C-N	-5.64	1.21	1.34
2	5j	111	VAL	C-N	-5.64	1.21	1.34
2	9M	111	VAL	C-N	-5.64	1.21	1.34
2	5f	111	VAL	C-N	-5.63	1.21	1.34
2	4h	111	VAL	C-N	-5.63	1.21	1.34
2	3w	111	VAL	C-N	-5.63	1.21	1.34
2	5n	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	3g	111	VAL	C-N	-5.63	1.21	1.34
2	3q	111	VAL	C-N	-5.63	1.21	1.34
2	3s	111	VAL	C-N	-5.63	1.21	1.34
2	3m	111	VAL	C-N	-5.62	1.21	1.34
2	1x	111	VAL	C-N	-5.62	1.21	1.34
2	3k	111	VAL	C-N	-5.62	1.21	1.34
2	1l	111	VAL	C-N	-5.62	1.21	1.34
2	1h	111	VAL	C-N	-5.61	1.21	1.34
2	1p	111	VAL	C-N	-5.61	1.21	1.34
2	3u	111	VAL	C-N	-5.60	1.21	1.34
2	6g	111	VAL	C-N	-5.59	1.21	1.34
2	1t	111	VAL	C-N	-5.59	1.21	1.34
2	6k	111	VAL	C-N	-5.59	1.21	1.34
2	6o	111	VAL	C-N	-5.58	1.21	1.34
2	6s	111	VAL	C-N	-5.58	1.21	1.34
2	6w	111	VAL	C-N	-5.57	1.21	1.34

All (779) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5a	374	ARG	NE-CZ-NH1	-8.52	116.04	120.30
1	5U	374	ARG	NE-CZ-NH1	-8.45	116.08	120.30
1	5O	374	ARG	NE-CZ-NH1	-8.44	116.08	120.30
1	5C	374	ARG	NE-CZ-NH1	-8.43	116.08	120.30
1	5I	374	ARG	NE-CZ-NH1	-8.38	116.11	120.30
1	3b	319	TYR	CB-CG-CD2	-8.19	116.09	121.00
1	3J	319	TYR	CB-CG-CD2	-8.16	116.10	121.00
1	3P	319	TYR	CB-CG-CD2	-8.16	116.10	121.00
1	3D	319	TYR	CB-CG-CD2	-8.15	116.11	121.00
1	3V	319	TYR	CB-CG-CD2	-8.10	116.14	121.00
1	8Z	136	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	1Y	181	TYR	CB-CG-CD1	-8.03	116.18	121.00
1	8B	136	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	1M	181	TYR	CB-CG-CD1	-8.02	116.19	121.00
1	1G	181	TYR	CB-CG-CD1	-8.02	116.19	121.00
1	8T	136	ARG	NE-CZ-NH2	-8.01	116.30	120.30
1	1A	181	TYR	CB-CG-CD1	-7.99	116.21	121.00
1	8H	136	ARG	NE-CZ-NH2	-7.98	116.31	120.30
1	8N	136	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	1S	181	TYR	CB-CG-CD1	-7.95	116.23	121.00
1	8Y	355	SER	C-N-CD	-7.90	103.22	120.60
1	8G	355	SER	C-N-CD	-7.89	103.23	120.60
1	8S	355	SER	C-N-CD	-7.89	103.25	120.60
1	8A	355	SER	C-N-CD	-7.88	103.25	120.60
1	8M	355	SER	C-N-CD	-7.88	103.26	120.60
1	2L	140	TYR	CB-CG-CD2	-7.77	116.34	121.00
1	2B	140	TYR	CB-CG-CD2	-7.73	116.36	121.00
1	2V	140	TYR	CB-CG-CD2	-7.73	116.36	121.00
1	2Q	140	TYR	CB-CG-CD2	-7.71	116.37	121.00
1	2G	140	TYR	CB-CG-CD2	-7.71	116.38	121.00
1	5Y	181	TYR	CB-CG-CD1	-7.48	116.51	121.00
1	3P	374	ARG	NE-CZ-NH1	-7.46	116.57	120.30
1	5M	181	TYR	CB-CG-CD1	-7.45	116.53	121.00
1	8S	95	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	6J	181	TYR	CB-CG-CD2	-7.44	116.53	121.00
1	5S	181	TYR	CB-CG-CD1	-7.43	116.54	121.00
1	5G	181	TYR	CB-CG-CD1	-7.42	116.55	121.00
1	3D	374	ARG	NE-CZ-NH1	-7.41	116.59	120.30
1	8G	95	ARG	NE-CZ-NH2	-7.41	116.60	120.30
1	6P	181	TYR	CB-CG-CD2	-7.41	116.56	121.00
1	3b	374	ARG	NE-CZ-NH1	-7.41	116.60	120.30
1	5A	181	TYR	CB-CG-CD1	-7.41	116.56	121.00
1	7K	374	ARG	NE-CZ-NH1	-7.40	116.60	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6D	181	TYR	CB-CG-CD2	-7.40	116.56	121.00
1	8A	95	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	8M	95	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	3V	374	ARG	NE-CZ-NH1	-7.38	116.61	120.30
1	6V	181	TYR	CB-CG-CD2	-7.38	116.57	121.00
1	2Y	323	TYR	CB-CG-CD1	-7.37	116.58	121.00
1	7U	374	ARG	NE-CZ-NH1	-7.36	116.62	120.30
1	6b	181	TYR	CB-CG-CD2	-7.34	116.60	121.00
1	3J	374	ARG	NE-CZ-NH1	-7.34	116.63	120.30
1	8Y	95	ARG	NE-CZ-NH2	-7.33	116.63	120.30
1	7F	374	ARG	NE-CZ-NH1	-7.33	116.63	120.30
1	2T	323	TYR	CB-CG-CD1	-7.32	116.61	121.00
1	2O	323	TYR	CB-CG-CD1	-7.32	116.61	121.00
1	2E	323	TYR	CB-CG-CD1	-7.30	116.62	121.00
1	3J	323	TYR	CB-CG-CD2	-7.30	116.62	121.00
1	7A	374	ARG	NE-CZ-NH1	-7.29	116.66	120.30
1	7P	374	ARG	NE-CZ-NH1	-7.28	116.66	120.30
1	2J	323	TYR	CB-CG-CD1	-7.27	116.64	121.00
1	3V	323	TYR	CB-CG-CD2	-7.24	116.65	121.00
1	3D	323	TYR	CB-CG-CD2	-7.20	116.68	121.00
1	3b	323	TYR	CB-CG-CD2	-7.20	116.68	121.00
1	1T	122	ARG	NE-CZ-NH2	-7.19	116.71	120.30
1	3P	323	TYR	CB-CG-CD2	-7.18	116.69	121.00
1	1B	122	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	1H	122	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	1Z	122	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	1N	122	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	7L	323	TYR	CB-CG-CD1	-7.07	116.76	121.00
1	7G	323	TYR	CB-CG-CD1	-7.05	116.77	121.00
1	7V	323	TYR	CB-CG-CD1	-7.05	116.77	121.00
1	7B	323	TYR	CB-CG-CD1	-7.04	116.78	121.00
1	6H	313	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	6N	313	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	6B	313	ARG	NE-CZ-NH2	-6.99	116.80	120.30
1	7Y	25	ARG	NE-CZ-NH2	-6.97	116.82	120.30
1	7T	25	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	7Q	323	TYR	CB-CG-CD1	-6.96	116.83	121.00
1	6T	313	ARG	NE-CZ-NH2	-6.95	116.82	120.30
1	7E	25	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	9C	323	TYR	CB-CG-CD2	-6.91	116.85	121.00
1	1U	122	ARG	NE-CZ-NH2	-6.91	116.84	120.30
1	6Z	313	ARG	NE-CZ-NH2	-6.91	116.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	7J	25	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	9E	323	TYR	CB-CG-CD2	-6.90	116.86	121.00
1	7O	25	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	9D	323	TYR	CB-CG-CD2	-6.87	116.88	121.00
1	5d	424	ASP	N-CA-C	-6.87	92.46	111.00
1	9A	323	TYR	CB-CG-CD2	-6.86	116.88	121.00
1	5X	424	ASP	N-CA-C	-6.86	92.48	111.00
1	5F	424	ASP	N-CA-C	-6.86	92.48	111.00
1	5R	424	ASP	N-CA-C	-6.86	92.48	111.00
1	5L	424	ASP	N-CA-C	-6.86	92.49	111.00
1	8J	323	TYR	CB-CG-CD2	-6.84	116.90	121.00
1	8b	323	TYR	CB-CG-CD2	-6.84	116.89	121.00
1	9B	323	TYR	CB-CG-CD2	-6.83	116.90	121.00
1	8P	323	TYR	CB-CG-CD2	-6.82	116.91	121.00
1	8V	323	TYR	CB-CG-CD2	-6.82	116.91	121.00
1	8D	323	TYR	CB-CG-CD2	-6.82	116.91	121.00
1	1I	122	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	1C	122	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	7Q	179	TYR	CB-CG-CD2	-6.80	116.92	121.00
1	1a	122	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	4d	323	TYR	CB-CG-CD1	-6.79	116.92	121.00
1	4R	323	TYR	CB-CG-CD1	-6.79	116.93	121.00
1	4F	323	TYR	CB-CG-CD1	-6.79	116.93	121.00
1	7B	179	TYR	CB-CG-CD2	-6.79	116.93	121.00
1	1O	122	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	4L	323	TYR	CB-CG-CD1	-6.76	116.94	121.00
1	7G	179	TYR	CB-CG-CD2	-6.75	116.95	121.00
1	3S	323	TYR	CB-CG-CD1	-6.75	116.95	121.00
1	7V	179	TYR	CB-CG-CD2	-6.74	116.95	121.00
1	4X	323	TYR	CB-CG-CD1	-6.73	116.96	121.00
1	4U	222	ARG	NE-CZ-NH2	-6.71	116.95	120.30
1	7L	179	TYR	CB-CG-CD2	-6.70	116.98	121.00
1	7N	218	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	7I	218	ARG	NE-CZ-NH2	-6.69	116.95	120.30
1	6X	323	TYR	CB-CG-CD1	-6.69	116.98	121.00
1	3O	101	TYR	CB-CG-CD1	-6.68	116.99	121.00
1	4a	222	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	3M	323	TYR	CB-CG-CD1	-6.67	117.00	121.00
1	6R	323	TYR	CB-CG-CD1	-6.67	117.00	121.00
1	5N	425	LYS	C-N-CD	-6.67	105.94	120.60
1	5Z	425	LYS	C-N-CD	-6.66	105.94	120.60
1	5H	425	LYS	C-N-CD	-6.66	105.94	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3a	101	TYR	CB-CG-CD1	-6.66	117.00	121.00
1	5B	425	LYS	C-N-CD	-6.66	105.95	120.60
1	4C	222	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	3C	101	TYR	CB-CG-CD1	-6.66	117.01	121.00
1	4I	222	ARG	NE-CZ-NH2	-6.65	116.98	120.30
1	5T	425	LYS	C-N-CD	-6.65	105.97	120.60
1	3U	101	TYR	CB-CG-CD1	-6.65	117.01	121.00
1	7X	218	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	7D	218	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	1L	323	TYR	CB-CG-CD2	-6.64	117.02	121.00
1	3Y	323	TYR	CB-CG-CD1	-6.64	117.02	121.00
1	3I	101	TYR	CB-CG-CD1	-6.63	117.02	121.00
1	4O	323	TYR	CB-CG-CD2	-6.63	117.03	121.00
1	4a	323	TYR	CB-CG-CD2	-6.62	117.03	121.00
1	3A	323	TYR	CB-CG-CD1	-6.62	117.03	121.00
1	1F	323	TYR	CB-CG-CD2	-6.61	117.03	121.00
1	8Q	136	ARG	NE-CZ-NH2	-6.61	116.99	120.30
1	1R	323	TYR	CB-CG-CD2	-6.61	117.04	121.00
1	6G	136	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	6F	323	TYR	CB-CG-CD1	-6.60	117.04	121.00
1	1K	334	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	6d	323	TYR	CB-CG-CD1	-6.60	117.04	121.00
1	6L	323	TYR	CB-CG-CD1	-6.60	117.04	121.00
1	6M	136	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	1X	323	TYR	CB-CG-CD2	-6.59	117.05	121.00
1	7S	218	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	4O	222	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	8W	136	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	8c	136	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	4I	323	TYR	CB-CG-CD2	-6.58	117.06	121.00
1	1W	334	ARG	NE-CZ-NH2	-6.57	117.01	120.30
1	1Q	334	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	4C	323	TYR	CB-CG-CD2	-6.57	117.06	121.00
1	1E	334	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	1O	179	TYR	CB-CG-CD2	-6.56	117.06	121.00
1	1d	323	TYR	CB-CG-CD2	-6.56	117.06	121.00
1	3G	323	TYR	CB-CG-CD1	-6.55	117.07	121.00
1	1C	179	TYR	CB-CG-CD2	-6.55	117.07	121.00
1	6S	136	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	6A	136	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	8K	136	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	8E	136	ARG	NE-CZ-NH2	-6.54	117.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1I	179	TYR	CB-CG-CD2	-6.53	117.08	121.00
1	1a	179	TYR	CB-CG-CD2	-6.52	117.08	121.00
1	1U	179	TYR	CB-CG-CD2	-6.52	117.09	121.00
1	4M	134	ARG	NE-CZ-NH2	6.52	123.56	120.30
1	1c	334	ARG	NE-CZ-NH2	-6.51	117.04	120.30
1	6Y	136	ARG	NE-CZ-NH2	-6.51	117.05	120.30
1	6R	101	TYR	CB-CG-CD1	-6.50	117.10	121.00
1	4Y	134	ARG	NE-CZ-NH2	6.50	123.55	120.30
1	4U	323	TYR	CB-CG-CD2	-6.49	117.10	121.00
1	5M	136	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	5Y	136	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	5A	136	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	5S	136	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	4A	134	ARG	NE-CZ-NH2	6.46	123.53	120.30
1	4G	134	ARG	NE-CZ-NH2	6.46	123.53	120.30
1	5G	136	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	6X	101	TYR	CB-CG-CD1	-6.46	117.13	121.00
1	5R	323	TYR	CB-CG-CD1	-6.42	117.15	121.00
1	6F	101	TYR	CB-CG-CD1	-6.42	117.15	121.00
1	8O	372	TYR	CB-CG-CD2	-6.41	117.16	121.00
1	8a	372	TYR	CB-CG-CD2	-6.40	117.16	121.00
1	8C	372	TYR	CB-CG-CD2	-6.38	117.17	121.00
1	6d	101	TYR	CB-CG-CD1	-6.38	117.17	121.00
1	5L	323	TYR	CB-CG-CD1	-6.37	117.18	121.00
1	2C	355	SER	C-N-CD	-6.37	106.59	120.60
1	5X	323	TYR	CB-CG-CD1	-6.37	117.18	121.00
1	2H	355	SER	C-N-CD	-6.37	106.59	120.60
1	2W	355	SER	C-N-CD	-6.37	106.59	120.60
1	2R	355	SER	C-N-CD	-6.36	106.60	120.60
1	8U	334	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	6L	101	TYR	CB-CG-CD1	-6.36	117.18	121.00
1	2M	355	SER	C-N-CD	-6.36	106.61	120.60
1	5Q	110	TYR	CB-CG-CD2	-6.36	117.19	121.00
1	6b	241	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	2X	101	TYR	CB-CG-CD1	-6.35	117.19	121.00
1	5F	323	TYR	CB-CG-CD1	-6.35	117.19	121.00
1	8I	372	TYR	CB-CG-CD2	-6.34	117.19	121.00
1	4S	134	ARG	NE-CZ-NH2	6.33	123.46	120.30
1	2S	101	TYR	CB-CG-CD1	-6.32	117.21	121.00
1	2I	101	TYR	CB-CG-CD1	-6.32	117.21	121.00
1	2D	101	TYR	CB-CG-CD1	-6.31	117.22	121.00
1	6D	241	ARG	NE-CZ-NH2	-6.31	117.15	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2N	101	TYR	CB-CG-CD1	-6.31	117.22	121.00
1	5K	110	TYR	CB-CG-CD2	-6.30	117.22	121.00
1	6P	241	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	8H	323	TYR	CB-CG-CD2	-6.29	117.23	121.00
1	5d	323	TYR	CB-CG-CD1	-6.29	117.23	121.00
1	8U	372	TYR	CB-CG-CD2	-6.27	117.24	121.00
1	5E	110	TYR	CB-CG-CD2	-6.27	117.24	121.00
1	8O	334	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	6V	241	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	8d	313	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	8B	323	TYR	CB-CG-CD2	-6.26	117.25	121.00
1	4Q	334	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	8Z	323	TYR	CB-CG-CD2	-6.25	117.25	121.00
1	6J	241	ARG	NE-CZ-NH2	-6.25	117.18	120.30
1	8K	313	ARG	NE-CZ-NH2	-6.25	117.18	120.30
1	8L	313	ARG	NE-CZ-NH2	-6.25	117.18	120.30
1	5W	110	TYR	CB-CG-CD2	-6.24	117.25	121.00
1	5c	110	TYR	CB-CG-CD2	-6.23	117.26	121.00
1	8I	334	ARG	NE-CZ-NH2	-6.23	117.19	120.30
1	8S	241	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	4c	334	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	8F	313	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	8N	323	TYR	CB-CG-CD2	-6.22	117.27	121.00
1	8T	323	TYR	CB-CG-CD2	-6.22	117.27	121.00
1	8X	313	ARG	NE-CZ-NH2	-6.21	117.20	120.30
1	8c	313	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	8C	334	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	4E	334	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	8M	241	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	8G	241	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	8W	313	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	8R	313	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	8E	313	ARG	NE-CZ-NH2	-6.19	117.21	120.30
1	1H	323	TYR	CB-CG-CD2	-6.18	117.29	121.00
1	8a	334	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	1N	323	TYR	CB-CG-CD2	-6.17	117.30	121.00
1	4K	334	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	8Q	313	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	2I	323	TYR	CB-CG-CD2	-6.14	117.31	121.00
1	8Y	241	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	1B	323	TYR	CB-CG-CD2	-6.13	117.32	121.00
1	1T	323	TYR	CB-CG-CD2	-6.12	117.33	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3B	323	TYR	CB-CG-CD2	-6.11	117.33	121.00
1	1Z	323	TYR	CB-CG-CD2	-6.11	117.34	121.00
1	3H	323	TYR	CB-CG-CD2	-6.10	117.34	121.00
1	8A	241	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	2X	323	TYR	CB-CG-CD2	-6.10	117.34	121.00
1	4W	334	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	3Z	323	TYR	CB-CG-CD2	-6.09	117.35	121.00
1	3N	323	TYR	CB-CG-CD2	-6.08	117.35	121.00
1	2G	334	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	7W	323	TYR	CB-CG-CD2	-6.07	117.36	121.00
1	4b	355	SER	C-N-CD	-6.07	107.24	120.60
1	4J	355	SER	C-N-CD	-6.07	107.25	120.60
1	4D	355	SER	C-N-CD	-6.07	107.25	120.60
1	3M	372	TYR	CB-CG-CD1	-6.06	117.36	121.00
1	4P	355	SER	C-N-CD	-6.06	107.26	120.60
1	2S	323	TYR	CB-CG-CD2	-6.06	117.36	121.00
1	7M	323	TYR	CB-CG-CD2	-6.06	117.36	121.00
1	4V	355	SER	C-N-CD	-6.06	107.27	120.60
1	3A	372	TYR	CB-CG-CD1	-6.05	117.37	121.00
1	2Q	334	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	8X	75	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	6Y	189	TYR	CB-CG-CD2	-6.04	117.38	121.00
1	2D	323	TYR	CB-CG-CD2	-6.04	117.38	121.00
1	6G	189	TYR	CB-CG-CD2	-6.04	117.38	121.00
1	2B	334	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	8d	75	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	3T	323	TYR	CB-CG-CD2	-6.03	117.38	121.00
1	2L	334	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	7C	323	TYR	CB-CG-CD2	-6.03	117.38	121.00
1	6R	95	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	2N	323	TYR	CB-CG-CD2	-6.03	117.39	121.00
1	3Y	372	TYR	CB-CG-CD1	-6.03	117.39	121.00
1	3S	372	TYR	CB-CG-CD1	-6.01	117.40	121.00
1	7H	323	TYR	CB-CG-CD2	-6.00	117.40	121.00
1	7R	323	TYR	CB-CG-CD2	-6.00	117.40	121.00
1	6S	189	TYR	CB-CG-CD2	-6.00	117.40	121.00
1	6L	95	ARG	NE-CZ-NH2	-5.99	117.30	120.30
1	6A	189	TYR	CB-CG-CD2	-5.99	117.41	121.00
1	3G	372	TYR	CB-CG-CD1	-5.99	117.41	121.00
1	6M	189	TYR	CB-CG-CD2	-5.99	117.41	121.00
1	2V	334	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	2T	355	SER	N-CA-C	5.99	127.17	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	8R	75	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	8F	75	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	8L	75	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	2O	355	SER	N-CA-C	5.99	127.16	111.00
1	2E	355	SER	N-CA-C	5.97	127.13	111.00
1	2J	355	SER	N-CA-C	5.97	127.13	111.00
1	3U	202	GLU	C-N-CD	-5.97	107.46	120.60
1	2Y	355	SER	N-CA-C	5.97	127.13	111.00
1	3O	202	GLU	C-N-CD	-5.97	107.47	120.60
1	1Y	189	TYR	CB-CG-CD2	-5.97	117.42	121.00
1	6F	95	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	3C	202	GLU	C-N-CD	-5.96	107.49	120.60
1	3a	202	GLU	C-N-CD	-5.96	107.50	120.60
1	3I	202	GLU	C-N-CD	-5.95	107.51	120.60
1	7Y	179	TYR	CB-CG-CD2	-5.95	117.43	121.00
1	3H	122	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	3c	218	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	1A	189	TYR	CB-CG-CD2	-5.90	117.46	121.00
1	6X	95	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	6d	95	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	7J	179	TYR	CB-CG-CD2	-5.89	117.46	121.00
1	7E	179	TYR	CB-CG-CD2	-5.89	117.47	121.00
1	3Y	202	GLU	C-N-CD	-5.89	107.65	120.60
1	3T	122	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	3A	202	GLU	C-N-CD	-5.88	107.66	120.60
1	3M	202	GLU	C-N-CD	-5.88	107.66	120.60
1	3Z	122	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	3B	122	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	7T	179	TYR	CB-CG-CD2	-5.88	117.47	121.00
1	1G	189	TYR	CB-CG-CD2	-5.88	117.47	121.00
1	3S	202	GLU	C-N-CD	-5.87	107.68	120.60
1	3E	218	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	3G	202	GLU	C-N-CD	-5.86	107.70	120.60
1	7O	179	TYR	CB-CG-CD2	-5.86	117.48	121.00
1	2K	136	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	7P	101	TYR	CB-CG-CD1	-5.85	117.49	121.00
1	2U	136	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	5O	355	SER	C-N-CD	-5.84	107.74	120.60
1	5a	355	SER	C-N-CD	-5.84	107.74	120.60
1	5C	355	SER	C-N-CD	-5.84	107.75	120.60
1	5I	355	SER	C-N-CD	-5.84	107.75	120.60
1	5U	355	SER	C-N-CD	-5.84	107.75	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1S	189	TYR	CB-CG-CD2	-5.83	117.50	121.00
1	3N	122	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	3W	218	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	2A	136	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	1M	189	TYR	CB-CG-CD2	-5.82	117.51	121.00
1	3K	218	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	7U	101	TYR	CB-CG-CD1	-5.82	117.51	121.00
1	2F	136	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	2P	136	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	7A	101	TYR	CB-CG-CD1	-5.80	117.52	121.00
1	3Q	218	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	7K	101	TYR	CB-CG-CD1	-5.79	117.53	121.00
1	7R	313	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	4B	323	TYR	CB-CG-CD1	-5.79	117.53	121.00
1	3V	101	TYR	CB-CG-CD1	-5.79	117.53	121.00
1	7F	101	TYR	CB-CG-CD1	-5.78	117.53	121.00
1	7H	313	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	4N	323	TYR	CB-CG-CD1	-5.78	117.53	121.00
1	3J	101	TYR	CB-CG-CD1	-5.78	117.53	121.00
1	2K	110	TYR	CB-CG-CD2	-5.78	117.53	121.00
1	4Z	323	TYR	CB-CG-CD1	-5.77	117.54	121.00
1	7W	313	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	4H	323	TYR	CB-CG-CD1	-5.77	117.54	121.00
1	7K	323	TYR	CB-CG-CD2	-5.77	117.54	121.00
1	5X	355	SER	C-N-CD	-5.76	107.92	120.60
1	7F	323	TYR	CB-CG-CD2	-5.76	117.54	121.00
1	2K	323	TYR	CB-CG-CD2	-5.75	117.55	121.00
1	5d	355	SER	C-N-CD	-5.75	107.95	120.60
1	2A	323	TYR	CB-CG-CD2	-5.75	117.55	121.00
1	7P	323	TYR	CB-CG-CD2	-5.75	117.55	121.00
1	7A	323	TYR	CB-CG-CD2	-5.74	117.55	121.00
1	3P	319	TYR	N-CA-CB	-5.74	100.26	110.60
1	5F	355	SER	C-N-CD	-5.74	107.97	120.60
1	3D	319	TYR	N-CA-CB	-5.74	100.27	110.60
1	4T	323	TYR	CB-CG-CD1	-5.74	117.56	121.00
1	3b	101	TYR	CB-CG-CD1	-5.74	117.56	121.00
1	7M	313	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	7C	313	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	5R	355	SER	C-N-CD	-5.73	108.00	120.60
1	3b	319	TYR	N-CA-CB	-5.73	100.29	110.60
1	3J	319	TYR	N-CA-CB	-5.73	100.29	110.60
1	3V	63	THR	CA-CB-CG2	-5.72	104.39	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3V	319	TYR	N-CA-CB	-5.72	100.30	110.60
1	2A	110	TYR	CB-CG-CD2	-5.72	117.57	121.00
1	3D	101	TYR	CB-CG-CD1	-5.72	117.57	121.00
1	5L	355	SER	C-N-CD	-5.72	108.01	120.60
1	1J	136	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	3P	101	TYR	CB-CG-CD1	-5.71	117.57	121.00
1	3d	68	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	2U	110	TYR	CB-CG-CD2	-5.71	117.58	121.00
1	3D	63	THR	CA-CB-CG2	-5.70	104.42	112.40
1	3P	63	THR	CA-CB-CG2	-5.70	104.42	112.40
1	3b	63	THR	CA-CB-CG2	-5.70	104.42	112.40
1	2F	110	TYR	CB-CG-CD2	-5.69	117.58	121.00
1	3J	63	THR	CA-CB-CG2	-5.69	104.43	112.40
1	2P	323	TYR	CB-CG-CD2	-5.69	117.59	121.00
1	2F	323	TYR	CB-CG-CD2	-5.68	117.59	121.00
1	3L	68	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	7U	323	TYR	CB-CG-CD2	-5.68	117.59	121.00
1	3X	68	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	2S	181	TYR	CB-CG-CD2	-5.67	117.60	121.00
1	2U	323	TYR	CB-CG-CD2	-5.67	117.60	121.00
1	2F	374	ARG	NE-CZ-NH1	-5.67	117.47	120.30
1	2P	110	TYR	CB-CG-CD2	-5.67	117.60	121.00
1	5D	323	TYR	CB-CG-CD2	-5.66	117.60	121.00
1	5P	323	TYR	CB-CG-CD2	-5.66	117.60	121.00
1	5J	323	TYR	CB-CG-CD2	-5.66	117.60	121.00
1	8Z	218	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	2X	181	TYR	CB-CG-CD2	-5.64	117.62	121.00
1	2N	181	TYR	CB-CG-CD2	-5.63	117.62	121.00
1	8H	218	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	5b	323	TYR	CB-CG-CD2	-5.63	117.62	121.00
1	2D	181	TYR	CB-CG-CD2	-5.62	117.63	121.00
1	8B	218	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	4b	323	TYR	CB-CG-CD2	-5.62	117.63	121.00
1	2X	179	TYR	CB-CG-CD2	-5.62	117.63	121.00
1	3F	68	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	2A	374	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	3M	231	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	4P	134	ARG	NE-CZ-NH2	5.61	123.10	120.30
1	8N	218	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	2I	181	TYR	CB-CG-CD2	-5.61	117.64	121.00
1	4G	122	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	2U	374	ARG	NE-CZ-NH1	-5.60	117.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2I	179	TYR	CB-CG-CD2	-5.60	117.64	121.00
1	5V	323	TYR	CB-CG-CD2	-5.60	117.64	121.00
1	1V	136	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	4C	355	SER	C-N-CD	-5.59	108.29	120.60
1	4U	355	SER	C-N-CD	-5.59	108.30	120.60
1	3S	231	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	4a	355	SER	C-N-CD	-5.58	108.32	120.60
1	4O	355	SER	C-N-CD	-5.58	108.32	120.60
1	4S	122	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	5V	101	TYR	CB-CG-CD1	-5.58	117.65	121.00
1	6c	75	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	1b	136	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	4M	122	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	1D	136	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	6N	110	TYR	CB-CG-CD2	-5.57	117.66	121.00
1	2P	374	ARG	NE-CZ-NH1	-5.57	117.51	120.30
1	4A	122	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	8W	355	SER	C-N-CD	-5.57	108.35	120.60
1	6Z	110	TYR	CB-CG-CD2	-5.57	117.66	121.00
1	4I	355	SER	C-N-CD	-5.57	108.36	120.60
1	3R	101	TYR	CB-CG-CD1	-5.57	117.66	121.00
1	2D	179	TYR	CB-CG-CD2	-5.56	117.66	121.00
1	2Q	323	TYR	CB-CG-CD1	-5.56	117.66	121.00
1	5b	101	TYR	CB-CG-CD1	-5.56	117.66	121.00
1	3R	68	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	2L	323	TYR	CB-CG-CD1	-5.56	117.67	121.00
1	3F	101	TYR	CB-CG-CD1	-5.56	117.67	121.00
1	8K	355	SER	C-N-CD	-5.56	108.37	120.60
1	4R	227	PRO	N-CA-C	-5.55	97.66	112.10
1	6Q	75	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	8Q	355	SER	C-N-CD	-5.55	108.38	120.60
1	3X	101	TYR	CB-CG-CD1	-5.55	117.67	121.00
1	8c	355	SER	C-N-CD	-5.55	108.39	120.60
1	8E	355	SER	C-N-CD	-5.55	108.39	120.60
1	3M	374	ARG	NE-CZ-NH1	-5.55	117.53	120.30
1	2S	179	TYR	CB-CG-CD2	-5.55	117.67	121.00
1	1P	136	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	4X	227	PRO	N-CA-C	-5.55	97.68	112.10
1	8T	218	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	4J	323	TYR	CB-CG-CD2	-5.54	117.67	121.00
1	6T	110	TYR	CB-CG-CD2	-5.54	117.67	121.00
1	3d	101	TYR	CB-CG-CD1	-5.54	117.67	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4D	323	TYR	CB-CG-CD2	-5.54	117.67	121.00
1	4L	227	PRO	N-CA-C	-5.54	97.69	112.10
1	3L	101	TYR	CB-CG-CD1	-5.54	117.67	121.00
1	2B	323	TYR	CB-CG-CD1	-5.54	117.68	121.00
1	4F	227	PRO	N-CA-C	-5.54	97.69	112.10
1	3A	231	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	7R	334	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	4Y	122	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	3Y	374	ARG	NE-CZ-NH1	-5.54	117.53	120.30
1	6E	75	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	2Q	101	TYR	CB-CG-CD1	-5.53	117.68	121.00
1	3M	101	TYR	CB-CG-CD1	-5.53	117.68	121.00
1	4d	227	PRO	N-CA-C	-5.53	97.72	112.10
1	2K	374	ARG	NE-CZ-NH1	-5.53	117.53	120.30
1	3I	122	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	6W	75	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	5D	101	TYR	CB-CG-CD1	-5.53	117.69	121.00
1	3Y	231	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	3U	122	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	6B	110	TYR	CB-CG-CD2	-5.52	117.69	121.00
1	5J	101	TYR	CB-CG-CD1	-5.52	117.69	121.00
1	2G	241	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	6H	110	TYR	CB-CG-CD2	-5.51	117.69	121.00
1	4V	323	TYR	CB-CG-CD2	-5.51	117.69	121.00
1	4J	134	ARG	NE-CZ-NH2	5.51	123.05	120.30
1	5P	101	TYR	CB-CG-CD1	-5.51	117.70	121.00
1	2B	101	TYR	CB-CG-CD1	-5.50	117.70	121.00
1	3G	374	ARG	NE-CZ-NH1	-5.50	117.55	120.30
1	3J	355	SER	C-N-CD	-5.50	108.49	120.60
1	3S	101	TYR	CB-CG-CD1	-5.50	117.70	121.00
1	3P	355	SER	C-N-CD	-5.50	108.50	120.60
1	3K	323	TYR	CB-CG-CD2	-5.50	117.70	121.00
1	2V	323	TYR	CB-CG-CD1	-5.50	117.70	121.00
1	4D	134	ARG	NE-CZ-NH2	5.49	123.05	120.30
1	2N	179	TYR	CB-CG-CD2	-5.49	117.70	121.00
1	4P	323	TYR	CB-CG-CD2	-5.49	117.70	121.00
1	2G	323	TYR	CB-CG-CD1	-5.49	117.71	121.00
1	3G	101	TYR	CB-CG-CD1	-5.49	117.71	121.00
1	6K	75	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	2L	101	TYR	CB-CG-CD1	-5.49	117.71	121.00
1	2L	241	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	3b	355	SER	C-N-CD	-5.49	108.52	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3D	355	SER	C-N-CD	-5.48	108.54	120.60
1	3A	374	ARG	NE-CZ-NH1	-5.48	117.56	120.30
1	7X	355	SER	C-N-CD	-5.48	108.54	120.60
1	7M	334	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	8S	356	PRO	CA-N-CD	-5.48	103.83	111.50
1	6Q	222	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	7C	334	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	7S	355	SER	C-N-CD	-5.47	108.56	120.60
1	3G	231	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	7I	355	SER	C-N-CD	-5.47	108.57	120.60
1	7W	334	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	7D	355	SER	C-N-CD	-5.46	108.58	120.60
1	7N	355	SER	C-N-CD	-5.46	108.58	120.60
1	3V	355	SER	C-N-CD	-5.46	108.58	120.60
1	3C	122	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	2V	101	TYR	CB-CG-CD1	-5.46	117.72	121.00
1	6X	122	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	3E	323	TYR	CB-CG-CD2	-5.46	117.72	121.00
1	2G	101	TYR	CB-CG-CD1	-5.46	117.72	121.00
1	3S	374	ARG	NE-CZ-NH1	-5.46	117.57	120.30
1	7F	218	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	2X	134	ARG	NE-CZ-NH1	-5.45	117.57	120.30
1	3a	122	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	2B	241	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	3A	101	TYR	CB-CG-CD1	-5.45	117.73	121.00
1	8A	356	PRO	CA-N-CD	-5.45	103.87	111.50
1	3Q	323	TYR	CB-CG-CD2	-5.45	117.73	121.00
1	8M	356	PRO	CA-N-CD	-5.45	103.87	111.50
1	3W	323	TYR	CB-CG-CD2	-5.44	117.73	121.00
1	6E	222	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	6K	222	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	8G	356	PRO	CA-N-CD	-5.43	103.89	111.50
1	3c	323	TYR	CB-CG-CD2	-5.43	117.74	121.00
1	2R	241	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	7P	218	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	6W	222	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	7H	334	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	2N	134	ARG	NE-CZ-NH1	-5.43	117.59	120.30
1	8Y	356	PRO	CA-N-CD	-5.42	103.91	111.50
1	1U	189	TYR	CB-CG-CD1	-5.42	117.75	121.00
1	4b	134	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	7A	218	ARG	NE-CZ-NH2	-5.42	117.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	7K	218	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	2V	241	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	6L	122	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	3O	122	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	6d	122	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	2W	241	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	6c	222	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	6H	231	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	2Q	218	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	8d	323	TYR	CB-CG-CD2	-5.41	117.75	121.00
1	6F	122	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	5H	323	TYR	CB-CG-CD2	-5.41	117.76	121.00
1	7F	179	TYR	CB-CG-CD2	-5.40	117.76	121.00
1	3Y	101	TYR	CB-CG-CD1	-5.40	117.76	121.00
1	2V	218	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	1C	189	TYR	CB-CG-CD1	-5.40	117.76	121.00
1	1O	189	TYR	CB-CG-CD1	-5.39	117.76	121.00
1	6N	231	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	2Q	241	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	1I	189	TYR	CB-CG-CD1	-5.39	117.77	121.00
1	6R	122	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	6T	316	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	7S	323	TYR	CB-CG-CD2	-5.39	117.77	121.00
1	5Z	323	TYR	CB-CG-CD2	-5.39	117.77	121.00
1	2C	241	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	4V	134	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	5A	374	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	7D	323	TYR	CB-CG-CD2	-5.38	117.77	121.00
1	2B	218	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	5G	334	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	7U	218	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	8F	323	TYR	CB-CG-CD2	-5.37	117.78	121.00
1	5B	323	TYR	CB-CG-CD2	-5.37	117.78	121.00
1	6B	231	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	6N	316	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	1a	189	TYR	CB-CG-CD1	-5.37	117.78	121.00
1	8L	323	TYR	CB-CG-CD2	-5.37	117.78	121.00
1	2D	134	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	8X	323	TYR	CB-CG-CD2	-5.36	117.78	121.00
1	4A	323	TYR	CB-CG-CD1	-5.36	117.78	121.00
1	5T	323	TYR	CB-CG-CD2	-5.36	117.79	121.00
1	7I	323	TYR	CB-CG-CD2	-5.36	117.79	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5N	18	TYR	CB-CG-CD1	-5.36	117.79	121.00
1	6Z	231	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	4G	323	TYR	CB-CG-CD1	-5.35	117.79	121.00
1	7X	323	TYR	CB-CG-CD2	-5.35	117.79	121.00
1	6I	136	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	4M	323	TYR	CB-CG-CD1	-5.35	117.79	121.00
1	5Y	374	ARG	NE-CZ-NH1	-5.35	117.62	120.30
1	7N	323	TYR	CB-CG-CD2	-5.35	117.79	121.00
1	6H	316	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	5N	323	TYR	CB-CG-CD2	-5.35	117.79	121.00
1	7U	179	TYR	CB-CG-CD2	-5.35	117.79	121.00
1	4N	134	ARG	NE-CZ-NH2	5.35	122.97	120.30
1	2S	134	ARG	NE-CZ-NH1	-5.35	117.63	120.30
1	8R	323	TYR	CB-CG-CD2	-5.34	117.79	121.00
1	6O	136	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	3H	189	TYR	CB-CG-CD2	-5.34	117.80	121.00
1	5T	18	TYR	CB-CG-CD1	-5.34	117.80	121.00
1	5M	374	ARG	NE-CZ-NH1	-5.33	117.63	120.30
1	7A	179	TYR	CB-CG-CD2	-5.33	117.80	121.00
1	5S	334	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	8M	323	TYR	CB-CG-CD2	-5.33	117.80	121.00
1	6B	316	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	2M	241	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	5A	334	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	2G	218	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	8Y	323	TYR	CB-CG-CD2	-5.32	117.81	121.00
1	6Z	316	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	6C	136	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	4Y	323	TYR	CB-CG-CD1	-5.31	117.81	121.00
1	5B	18	TYR	CB-CG-CD1	-5.31	117.81	121.00
1	2L	218	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	7K	179	TYR	CB-CG-CD2	-5.31	117.81	121.00
1	3T	189	TYR	CB-CG-CD2	-5.31	117.81	121.00
1	5W	95	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	5H	18	TYR	CB-CG-CD1	-5.31	117.82	121.00
1	8P	218	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	3Z	189	TYR	CB-CG-CD2	-5.30	117.82	121.00
1	4Z	134	ARG	NE-CZ-NH2	5.30	122.95	120.30
1	2H	241	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	7P	179	TYR	CB-CG-CD2	-5.30	117.82	121.00
1	4S	323	TYR	CB-CG-CD1	-5.30	117.82	121.00
1	2I	134	ARG	NE-CZ-NH1	-5.30	117.65	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5S	374	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	8G	241	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	5G	374	ARG	NE-CZ-NH1	-5.29	117.66	120.30
1	7X	272	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	8A	323	TYR	CB-CG-CD2	-5.29	117.83	121.00
1	7I	272	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	6a	136	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	4B	134	ARG	NE-CZ-NH2	5.28	122.94	120.30
1	8M	241	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	6T	231	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	6U	136	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	8G	323	TYR	CB-CG-CD2	-5.27	117.84	121.00
1	5M	334	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	8V	218	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	3B	189	TYR	CB-CG-CD2	-5.26	117.84	121.00
1	4Z	189	TYR	CB-CG-CD2	-5.26	117.84	121.00
1	3d	374	ARG	NE-CZ-NH1	-5.26	117.67	120.30
1	5Y	334	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	7D	272	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	4T	134	ARG	NE-CZ-NH2	5.26	122.93	120.30
1	8S	241	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	8Z	222	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	3N	189	TYR	CB-CG-CD2	-5.24	117.86	121.00
1	5Z	18	TYR	CB-CG-CD1	-5.24	117.86	121.00
1	2L	95	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	7N	272	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	8S	323	TYR	CB-CG-CD2	-5.23	117.86	121.00
1	8N	222	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	4c	323	TYR	CB-CG-CD1	-5.23	117.86	121.00
1	3N	243	TYR	CB-CG-CD1	-5.23	117.86	121.00
1	5K	95	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	8D	218	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	7V	101	TYR	CB-CG-CD1	-5.22	117.87	121.00
1	5E	95	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	4Q	323	TYR	CB-CG-CD1	-5.22	117.87	121.00
1	4H	134	ARG	NE-CZ-NH2	5.22	122.91	120.30
1	7L	101	TYR	CB-CG-CD1	-5.21	117.87	121.00
1	7F	239	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	1S	136	ARG	NE-CZ-NH2	5.21	122.90	120.30
1	3R	374	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	3L	374	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	4H	189	TYR	CB-CG-CD2	-5.20	117.88	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	8J	218	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	7B	101	TYR	CB-CG-CD1	-5.20	117.88	121.00
1	8Y	241	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	3F	374	ARG	NE-CZ-NH1	-5.19	117.70	120.30
1	7M	354	VAL	O-C-N	5.19	131.01	122.70
1	7W	354	VAL	O-C-N	5.19	131.00	122.70
1	3H	243	TYR	CB-CG-CD1	-5.19	117.89	121.00
1	7K	239	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	8B	222	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	5I	218	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	7A	239	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	7C	354	VAL	O-C-N	5.18	130.99	122.70
1	8A	241	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	4N	189	TYR	CB-CG-CD2	-5.18	117.89	121.00
1	5c	95	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	3B	243	TYR	CB-CG-CD1	-5.18	117.89	121.00
1	4B	189	TYR	CB-CG-CD2	-5.17	117.90	121.00
1	2V	95	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	7H	354	VAL	O-C-N	5.17	130.97	122.70
1	8H	222	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	5Q	95	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	7S	272	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	4T	189	TYR	CB-CG-CD2	-5.16	117.91	121.00
1	4E	323	TYR	CB-CG-CD1	-5.16	117.91	121.00
1	7G	101	TYR	CB-CG-CD1	-5.16	117.91	121.00
1	7R	354	VAL	O-C-N	5.16	130.95	122.70
1	5O	218	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	2B	95	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	7Q	101	TYR	CB-CG-CD1	-5.15	117.91	121.00
1	4K	323	TYR	CB-CG-CD1	-5.14	117.91	121.00
1	4W	323	TYR	CB-CG-CD1	-5.14	117.92	121.00
1	6V	189	TYR	CB-CG-CD2	-5.14	117.92	121.00
1	8T	222	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	8b	218	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	9D	218	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	6D	189	TYR	CB-CG-CD2	-5.13	117.92	121.00
1	9C	218	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	1A	136	ARG	NE-CZ-NH2	5.12	122.86	120.30
1	5C	218	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	6P	189	TYR	CB-CG-CD2	-5.11	117.93	121.00
1	2Q	95	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	5a	136	ARG	NE-CZ-NH2	-5.11	117.74	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	8G	136	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	6J	189	TYR	CB-CG-CD2	-5.11	117.94	121.00
1	3Z	243	TYR	CB-CG-CD1	-5.11	117.94	121.00
1	6b	189	TYR	CB-CG-CD2	-5.11	117.94	121.00
1	2G	95	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	3T	243	TYR	CB-CG-CD1	-5.10	117.94	121.00
1	8Y	402	LEU	CB-CA-C	-5.10	100.51	110.20
1	9B	218	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	1G	136	ARG	NE-CZ-NH2	5.09	122.85	120.30
1	9E	218	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	8G	402	LEU	CB-CA-C	-5.09	100.53	110.20
1	3X	374	ARG	NE-CZ-NH1	-5.09	117.75	120.30
1	7U	239	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	8S	136	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	1Y	136	ARG	NE-CZ-NH2	5.09	122.84	120.30
1	7P	239	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	8S	402	LEU	CB-CA-C	-5.09	100.54	110.20
1	8A	402	LEU	CB-CA-C	-5.08	100.54	110.20
1	8M	402	LEU	CB-CA-C	-5.08	100.54	110.20
1	5a	218	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	8H	181	TYR	CB-CG-CD1	-5.08	117.95	121.00
1	3N	179	TYR	CB-CG-CD2	-5.08	117.95	121.00
1	8Z	181	TYR	CB-CG-CD1	-5.08	117.95	121.00
1	9A	218	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	5C	136	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	4S	189	TYR	CB-CG-CD2	-5.07	117.96	121.00
1	3B	179	TYR	CB-CG-CD2	-5.06	117.96	121.00
1	5O	136	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	5U	136	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	8M	136	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	4A	189	TYR	CB-CG-CD2	-5.05	117.97	121.00
1	4G	189	TYR	CB-CG-CD2	-5.05	117.97	121.00
1	1M	136	ARG	NE-CZ-NH2	5.05	122.82	120.30
1	8T	101	TYR	CB-CG-CD1	-5.04	117.97	121.00
1	3H	179	TYR	CB-CG-CD2	-5.04	117.97	121.00
1	1V	75	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	3T	179	TYR	CB-CG-CD2	-5.04	117.97	121.00
1	7K	334	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	5U	334	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	5I	136	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	4Y	189	TYR	CB-CG-CD2	-5.04	117.98	121.00
1	8A	136	ARG	NE-CZ-NH2	-5.03	117.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	7S	313	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	9C	254	ASP	CB-CG-OD2	5.03	122.83	118.30
1	4C	101	TYR	CB-CG-CD1	-5.03	117.98	121.00
1	7N	313	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	3Z	179	TYR	CB-CG-CD2	-5.03	117.98	121.00
1	7D	313	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	1D	75	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	4b	136	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	9A	254	ASP	CB-CG-OD2	5.02	122.82	118.30
1	1L	334	ARG	NE-CZ-NH2	5.02	122.81	120.30
1	4M	189	TYR	CB-CG-CD2	-5.02	117.99	121.00
1	9D	254	ASP	CB-CG-OD2	5.02	122.82	118.30
1	8B	101	TYR	CB-CG-CD1	-5.02	117.99	121.00
1	1U	101	TYR	CB-CG-CD1	-5.01	117.99	121.00
1	9D	110	TYR	CB-CG-CD2	-5.01	117.99	121.00
1	7F	334	ARG	NE-CZ-NH2	-5.01	117.79	120.30
1	4U	101	TYR	CB-CG-CD1	-5.01	117.99	121.00
1	9E	254	ASP	CB-CG-OD2	5.01	122.81	118.30
1	8B	181	TYR	CB-CG-CD1	-5.01	117.99	121.00
1	9B	254	ASP	CB-CG-OD2	5.00	122.80	118.30
1	7W	101	TYR	CB-CG-CD1	-5.00	118.00	121.00
1	9B	110	TYR	CB-CG-CD2	-5.00	118.00	121.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	390 (90%)	33 (8%)	8 (2%)	8	42
1	1B	443/448 (99%)	389 (88%)	42 (10%)	12 (3%)	5	35
1	1C	443/448 (99%)	391 (88%)	42 (10%)	10 (2%)	6	38
1	1D	443/448 (99%)	391 (88%)	41 (9%)	11 (2%)	5	36
1	1E	433/448 (97%)	395 (91%)	27 (6%)	11 (2%)	5	36
1	1F	436/448 (97%)	397 (91%)	31 (7%)	8 (2%)	8	43
1	1G	431/448 (96%)	390 (90%)	33 (8%)	8 (2%)	8	42
1	1H	443/448 (99%)	389 (88%)	42 (10%)	12 (3%)	5	35
1	1I	443/448 (99%)	391 (88%)	42 (10%)	10 (2%)	6	38
1	1J	443/448 (99%)	391 (88%)	41 (9%)	11 (2%)	5	36
1	1K	433/448 (97%)	395 (91%)	27 (6%)	11 (2%)	5	36
1	1L	436/448 (97%)	397 (91%)	31 (7%)	8 (2%)	8	43
1	1M	431/448 (96%)	390 (90%)	33 (8%)	8 (2%)	8	42
1	1N	443/448 (99%)	389 (88%)	42 (10%)	12 (3%)	5	35
1	1O	443/448 (99%)	391 (88%)	42 (10%)	10 (2%)	6	38
1	1P	443/448 (99%)	391 (88%)	41 (9%)	11 (2%)	5	36
1	1Q	433/448 (97%)	395 (91%)	27 (6%)	11 (2%)	5	36
1	1R	436/448 (97%)	397 (91%)	31 (7%)	8 (2%)	8	43
1	1S	431/448 (96%)	390 (90%)	33 (8%)	8 (2%)	8	42
1	1T	443/448 (99%)	389 (88%)	42 (10%)	12 (3%)	5	35
1	1U	443/448 (99%)	391 (88%)	42 (10%)	10 (2%)	6	38
1	1V	443/448 (99%)	391 (88%)	41 (9%)	11 (2%)	5	36
1	1W	433/448 (97%)	395 (91%)	27 (6%)	11 (2%)	5	36
1	1X	436/448 (97%)	397 (91%)	31 (7%)	8 (2%)	8	43
1	1Y	431/448 (96%)	390 (90%)	33 (8%)	8 (2%)	8	42
1	1Z	443/448 (99%)	389 (88%)	42 (10%)	12 (3%)	5	35
1	1a	443/448 (99%)	391 (88%)	42 (10%)	10 (2%)	6	38
1	1b	443/448 (99%)	391 (88%)	41 (9%)	11 (2%)	5	36
1	1c	433/448 (97%)	395 (91%)	27 (6%)	11 (2%)	5	36
1	1d	436/448 (97%)	397 (91%)	31 (7%)	8 (2%)	8	43
1	2A	436/448 (97%)	399 (92%)	31 (7%)	6 (1%)	11	48
1	2B	443/448 (99%)	402 (91%)	37 (8%)	4 (1%)	17	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2C	443/448 (99%)	390 (88%)	44 (10%)	9 (2%)	7	41
1	2D	443/448 (99%)	402 (91%)	36 (8%)	5 (1%)	14	53
1	2E	443/448 (99%)	396 (89%)	36 (8%)	11 (2%)	5	36
1	2F	436/448 (97%)	399 (92%)	31 (7%)	6 (1%)	11	48
1	2G	443/448 (99%)	402 (91%)	37 (8%)	4 (1%)	17	57
1	2H	443/448 (99%)	390 (88%)	44 (10%)	9 (2%)	7	41
1	2I	443/448 (99%)	402 (91%)	36 (8%)	5 (1%)	14	53
1	2J	443/448 (99%)	396 (89%)	36 (8%)	11 (2%)	5	36
1	2K	436/448 (97%)	399 (92%)	31 (7%)	6 (1%)	11	48
1	2L	443/448 (99%)	402 (91%)	37 (8%)	4 (1%)	17	57
1	2M	443/448 (99%)	390 (88%)	44 (10%)	9 (2%)	7	41
1	2N	443/448 (99%)	402 (91%)	36 (8%)	5 (1%)	14	53
1	2O	443/448 (99%)	396 (89%)	36 (8%)	11 (2%)	5	36
1	2P	436/448 (97%)	399 (92%)	31 (7%)	6 (1%)	11	48
1	2Q	443/448 (99%)	402 (91%)	37 (8%)	4 (1%)	17	57
1	2R	443/448 (99%)	390 (88%)	44 (10%)	9 (2%)	7	41
1	2S	443/448 (99%)	402 (91%)	36 (8%)	5 (1%)	14	53
1	2T	443/448 (99%)	396 (89%)	36 (8%)	11 (2%)	5	36
1	2U	436/448 (97%)	399 (92%)	31 (7%)	6 (1%)	11	48
1	2V	443/448 (99%)	402 (91%)	37 (8%)	4 (1%)	17	57
1	2W	443/448 (99%)	390 (88%)	44 (10%)	9 (2%)	7	41
1	2X	443/448 (99%)	402 (91%)	36 (8%)	5 (1%)	14	53
1	2Y	443/448 (99%)	396 (89%)	36 (8%)	11 (2%)	5	36
1	3A	433/448 (97%)	391 (90%)	31 (7%)	11 (2%)	5	36
1	3B	433/448 (97%)	370 (86%)	55 (13%)	8 (2%)	8	43
1	3C	443/448 (99%)	399 (90%)	30 (7%)	14 (3%)	4	31
1	3D	443/448 (99%)	393 (89%)	34 (8%)	16 (4%)	3	29
1	3E	443/448 (99%)	406 (92%)	29 (6%)	8 (2%)	8	43
1	3F	443/448 (99%)	386 (87%)	47 (11%)	10 (2%)	6	38
1	3G	433/448 (97%)	391 (90%)	31 (7%)	11 (2%)	5	36
1	3H	433/448 (97%)	369 (85%)	56 (13%)	8 (2%)	8	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	3I	443/448 (99%)	399 (90%)	30 (7%)	14 (3%)	4	31
1	3J	443/448 (99%)	393 (89%)	34 (8%)	16 (4%)	3	29
1	3K	443/448 (99%)	406 (92%)	29 (6%)	8 (2%)	8	43
1	3L	443/448 (99%)	386 (87%)	47 (11%)	10 (2%)	6	38
1	3M	433/448 (97%)	391 (90%)	31 (7%)	11 (2%)	5	36
1	3N	433/448 (97%)	370 (86%)	55 (13%)	8 (2%)	8	43
1	3O	443/448 (99%)	399 (90%)	30 (7%)	14 (3%)	4	31
1	3P	443/448 (99%)	393 (89%)	34 (8%)	16 (4%)	3	29
1	3Q	443/448 (99%)	406 (92%)	29 (6%)	8 (2%)	8	43
1	3R	443/448 (99%)	386 (87%)	47 (11%)	10 (2%)	6	38
1	3S	433/448 (97%)	391 (90%)	31 (7%)	11 (2%)	5	36
1	3T	433/448 (97%)	370 (86%)	55 (13%)	8 (2%)	8	43
1	3U	443/448 (99%)	399 (90%)	30 (7%)	14 (3%)	4	31
1	3V	443/448 (99%)	393 (89%)	34 (8%)	16 (4%)	3	29
1	3W	443/448 (99%)	406 (92%)	29 (6%)	8 (2%)	8	43
1	3X	443/448 (99%)	386 (87%)	47 (11%)	10 (2%)	6	38
1	3Y	433/448 (97%)	391 (90%)	31 (7%)	11 (2%)	5	36
1	3Z	433/448 (97%)	370 (86%)	55 (13%)	8 (2%)	8	43
1	3a	443/448 (99%)	399 (90%)	30 (7%)	14 (3%)	4	31
1	3b	443/448 (99%)	393 (89%)	34 (8%)	16 (4%)	3	29
1	3c	443/448 (99%)	406 (92%)	29 (6%)	8 (2%)	8	43
1	3d	443/448 (99%)	386 (87%)	47 (11%)	10 (2%)	6	38
1	4A	433/448 (97%)	402 (93%)	29 (7%)	2 (0%)	29	68
1	4B	433/448 (97%)	365 (84%)	50 (12%)	18 (4%)	3	25
1	4C	433/448 (97%)	385 (89%)	37 (8%)	11 (2%)	5	36
1	4D	433/448 (97%)	402 (93%)	26 (6%)	5 (1%)	13	51
1	4E	443/448 (99%)	393 (89%)	39 (9%)	11 (2%)	5	36
1	4F	443/448 (99%)	395 (89%)	35 (8%)	13 (3%)	4	33
1	4G	433/448 (97%)	402 (93%)	29 (7%)	2 (0%)	29	68
1	4H	433/448 (97%)	365 (84%)	50 (12%)	18 (4%)	3	25
1	4I	433/448 (97%)	385 (89%)	37 (8%)	11 (2%)	5	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	4J	433/448 (97%)	402 (93%)	26 (6%)	5 (1%)	13	51
1	4K	443/448 (99%)	393 (89%)	38 (9%)	12 (3%)	5	35
1	4L	443/448 (99%)	395 (89%)	35 (8%)	13 (3%)	4	33
1	4M	433/448 (97%)	401 (93%)	30 (7%)	2 (0%)	29	68
1	4N	433/448 (97%)	365 (84%)	50 (12%)	18 (4%)	3	25
1	4O	433/448 (97%)	385 (89%)	37 (8%)	11 (2%)	5	36
1	4P	433/448 (97%)	402 (93%)	26 (6%)	5 (1%)	13	51
1	4Q	443/448 (99%)	393 (89%)	38 (9%)	12 (3%)	5	35
1	4R	443/448 (99%)	395 (89%)	35 (8%)	13 (3%)	4	33
1	4S	433/448 (97%)	401 (93%)	30 (7%)	2 (0%)	29	68
1	4T	433/448 (97%)	365 (84%)	50 (12%)	18 (4%)	3	25
1	4U	433/448 (97%)	385 (89%)	37 (8%)	11 (2%)	5	36
1	4V	433/448 (97%)	402 (93%)	26 (6%)	5 (1%)	13	51
1	4W	443/448 (99%)	393 (89%)	38 (9%)	12 (3%)	5	35
1	4X	443/448 (99%)	395 (89%)	35 (8%)	13 (3%)	4	33
1	4Y	433/448 (97%)	401 (93%)	30 (7%)	2 (0%)	29	68
1	4Z	433/448 (97%)	365 (84%)	50 (12%)	18 (4%)	3	25
1	4a	433/448 (97%)	385 (89%)	37 (8%)	11 (2%)	5	36
1	4b	433/448 (97%)	402 (93%)	26 (6%)	5 (1%)	13	51
1	4c	443/448 (99%)	393 (89%)	39 (9%)	11 (2%)	5	36
1	4d	443/448 (99%)	395 (89%)	35 (8%)	13 (3%)	4	33
1	5A	433/448 (97%)	396 (92%)	27 (6%)	10 (2%)	6	38
1	5B	433/448 (97%)	367 (85%)	50 (12%)	16 (4%)	3	28
1	5C	433/448 (97%)	381 (88%)	35 (8%)	17 (4%)	3	27
1	5D	433/448 (97%)	392 (90%)	34 (8%)	7 (2%)	9	46
1	5E	443/448 (99%)	390 (88%)	35 (8%)	18 (4%)	3	26
1	5F	443/448 (99%)	383 (86%)	46 (10%)	14 (3%)	4	31
1	5G	433/448 (97%)	396 (92%)	27 (6%)	10 (2%)	6	38
1	5H	433/448 (97%)	367 (85%)	50 (12%)	16 (4%)	3	28
1	5I	433/448 (97%)	380 (88%)	36 (8%)	17 (4%)	3	27
1	5J	433/448 (97%)	392 (90%)	34 (8%)	7 (2%)	9	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	5K	443/448 (99%)	390 (88%)	35 (8%)	18 (4%)	3	26
1	5L	443/448 (99%)	383 (86%)	45 (10%)	15 (3%)	3	31
1	5M	433/448 (97%)	396 (92%)	27 (6%)	10 (2%)	6	38
1	5N	433/448 (97%)	367 (85%)	50 (12%)	16 (4%)	3	28
1	5O	433/448 (97%)	380 (88%)	36 (8%)	17 (4%)	3	27
1	5P	433/448 (97%)	391 (90%)	35 (8%)	7 (2%)	9	46
1	5Q	443/448 (99%)	390 (88%)	35 (8%)	18 (4%)	3	26
1	5R	443/448 (99%)	383 (86%)	46 (10%)	14 (3%)	4	31
1	5S	433/448 (97%)	396 (92%)	27 (6%)	10 (2%)	6	38
1	5T	433/448 (97%)	367 (85%)	50 (12%)	16 (4%)	3	28
1	5U	433/448 (97%)	381 (88%)	35 (8%)	17 (4%)	3	27
1	5V	433/448 (97%)	392 (90%)	34 (8%)	7 (2%)	9	46
1	5W	443/448 (99%)	390 (88%)	35 (8%)	18 (4%)	3	26
1	5X	443/448 (99%)	383 (86%)	46 (10%)	14 (3%)	4	31
1	5Y	433/448 (97%)	396 (92%)	27 (6%)	10 (2%)	6	38
1	5Z	433/448 (97%)	367 (85%)	50 (12%)	16 (4%)	3	28
1	5a	433/448 (97%)	380 (88%)	36 (8%)	17 (4%)	3	27
1	5b	433/448 (97%)	392 (90%)	34 (8%)	7 (2%)	9	46
1	5c	443/448 (99%)	390 (88%)	35 (8%)	18 (4%)	3	26
1	5d	443/448 (99%)	383 (86%)	46 (10%)	14 (3%)	4	31
1	6A	443/448 (99%)	415 (94%)	22 (5%)	6 (1%)	11	48
1	6B	443/448 (99%)	394 (89%)	38 (9%)	11 (2%)	5	36
1	6C	433/448 (97%)	382 (88%)	43 (10%)	8 (2%)	8	43
1	6D	433/448 (97%)	384 (89%)	36 (8%)	13 (3%)	4	33
1	6E	443/448 (99%)	393 (89%)	38 (9%)	12 (3%)	5	35
1	6F	443/448 (99%)	395 (89%)	34 (8%)	14 (3%)	4	31
1	6G	443/448 (99%)	415 (94%)	22 (5%)	6 (1%)	11	48
1	6H	443/448 (99%)	394 (89%)	38 (9%)	11 (2%)	5	36
1	6I	433/448 (97%)	382 (88%)	43 (10%)	8 (2%)	8	43
1	6J	433/448 (97%)	384 (89%)	36 (8%)	13 (3%)	4	33
1	6K	443/448 (99%)	393 (89%)	38 (9%)	12 (3%)	5	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	6L	443/448 (99%)	395 (89%)	34 (8%)	14 (3%)	4	31
1	6M	443/448 (99%)	415 (94%)	22 (5%)	6 (1%)	11	48
1	6N	443/448 (99%)	394 (89%)	38 (9%)	11 (2%)	5	36
1	6O	433/448 (97%)	382 (88%)	43 (10%)	8 (2%)	8	43
1	6P	433/448 (97%)	384 (89%)	36 (8%)	13 (3%)	4	33
1	6Q	443/448 (99%)	393 (89%)	38 (9%)	12 (3%)	5	35
1	6R	443/448 (99%)	395 (89%)	34 (8%)	14 (3%)	4	31
1	6S	443/448 (99%)	415 (94%)	22 (5%)	6 (1%)	11	48
1	6T	443/448 (99%)	394 (89%)	38 (9%)	11 (2%)	5	36
1	6U	433/448 (97%)	382 (88%)	43 (10%)	8 (2%)	8	43
1	6V	433/448 (97%)	384 (89%)	36 (8%)	13 (3%)	4	33
1	6W	443/448 (99%)	393 (89%)	38 (9%)	12 (3%)	5	35
1	6X	443/448 (99%)	395 (89%)	34 (8%)	14 (3%)	4	31
1	6Y	443/448 (99%)	415 (94%)	22 (5%)	6 (1%)	11	48
1	6Z	443/448 (99%)	394 (89%)	38 (9%)	11 (2%)	5	36
1	6a	433/448 (97%)	382 (88%)	43 (10%)	8 (2%)	8	43
1	6b	433/448 (97%)	384 (89%)	36 (8%)	13 (3%)	4	33
1	6c	443/448 (99%)	393 (89%)	38 (9%)	12 (3%)	5	35
1	6d	443/448 (99%)	395 (89%)	34 (8%)	14 (3%)	4	31
1	7A	443/448 (99%)	406 (92%)	32 (7%)	5 (1%)	14	53
1	7B	443/448 (99%)	400 (90%)	39 (9%)	4 (1%)	17	57
1	7C	443/448 (99%)	396 (89%)	35 (8%)	12 (3%)	5	35
1	7D	443/448 (99%)	396 (89%)	33 (7%)	14 (3%)	4	31
1	7E	443/448 (99%)	401 (90%)	37 (8%)	5 (1%)	14	53
1	7F	443/448 (99%)	406 (92%)	32 (7%)	5 (1%)	14	53
1	7G	443/448 (99%)	400 (90%)	39 (9%)	4 (1%)	17	57
1	7H	443/448 (99%)	396 (89%)	35 (8%)	12 (3%)	5	35
1	7I	443/448 (99%)	396 (89%)	33 (7%)	14 (3%)	4	31
1	7J	443/448 (99%)	401 (90%)	37 (8%)	5 (1%)	14	53
1	7K	443/448 (99%)	406 (92%)	32 (7%)	5 (1%)	14	53
1	7L	443/448 (99%)	400 (90%)	39 (9%)	4 (1%)	17	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	7M	443/448 (99%)	396 (89%)	35 (8%)	12 (3%)	5	35
1	7N	443/448 (99%)	397 (90%)	32 (7%)	14 (3%)	4	31
1	7O	443/448 (99%)	401 (90%)	37 (8%)	5 (1%)	14	53
1	7P	443/448 (99%)	406 (92%)	32 (7%)	5 (1%)	14	53
1	7Q	443/448 (99%)	400 (90%)	39 (9%)	4 (1%)	17	57
1	7R	443/448 (99%)	396 (89%)	35 (8%)	12 (3%)	5	35
1	7S	443/448 (99%)	396 (89%)	33 (7%)	14 (3%)	4	31
1	7T	443/448 (99%)	401 (90%)	37 (8%)	5 (1%)	14	53
1	7U	443/448 (99%)	406 (92%)	32 (7%)	5 (1%)	14	53
1	7V	443/448 (99%)	401 (90%)	38 (9%)	4 (1%)	17	57
1	7W	443/448 (99%)	396 (89%)	35 (8%)	12 (3%)	5	35
1	7X	443/448 (99%)	396 (89%)	33 (7%)	14 (3%)	4	31
1	7Y	443/448 (99%)	401 (90%)	37 (8%)	5 (1%)	14	53
1	8A	443/448 (99%)	398 (90%)	35 (8%)	10 (2%)	6	38
1	8B	443/448 (99%)	399 (90%)	33 (7%)	11 (2%)	5	36
1	8C	443/448 (99%)	384 (87%)	50 (11%)	9 (2%)	7	41
1	8D	443/448 (99%)	406 (92%)	34 (8%)	3 (1%)	22	61
1	8E	443/448 (99%)	392 (88%)	38 (9%)	13 (3%)	4	33
1	8F	443/448 (99%)	398 (90%)	40 (9%)	5 (1%)	14	53
1	8G	443/448 (99%)	398 (90%)	35 (8%)	10 (2%)	6	38
1	8H	443/448 (99%)	399 (90%)	33 (7%)	11 (2%)	5	36
1	8I	443/448 (99%)	384 (87%)	50 (11%)	9 (2%)	7	41
1	8J	443/448 (99%)	406 (92%)	34 (8%)	3 (1%)	22	61
1	8K	443/448 (99%)	392 (88%)	38 (9%)	13 (3%)	4	33
1	8L	443/448 (99%)	398 (90%)	40 (9%)	5 (1%)	14	53
1	8M	443/448 (99%)	398 (90%)	35 (8%)	10 (2%)	6	38
1	8N	443/448 (99%)	399 (90%)	33 (7%)	11 (2%)	5	36
1	8O	443/448 (99%)	384 (87%)	50 (11%)	9 (2%)	7	41
1	8P	443/448 (99%)	407 (92%)	33 (7%)	3 (1%)	22	61
1	8Q	443/448 (99%)	392 (88%)	38 (9%)	13 (3%)	4	33
1	8R	443/448 (99%)	398 (90%)	40 (9%)	5 (1%)	14	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	8S	443/448 (99%)	399 (90%)	34 (8%)	10 (2%)	6	38
1	8T	443/448 (99%)	399 (90%)	33 (7%)	11 (2%)	5	36
1	8U	443/448 (99%)	384 (87%)	50 (11%)	9 (2%)	7	41
1	8V	443/448 (99%)	406 (92%)	34 (8%)	3 (1%)	22	61
1	8W	443/448 (99%)	392 (88%)	38 (9%)	13 (3%)	4	33
1	8X	443/448 (99%)	398 (90%)	40 (9%)	5 (1%)	14	53
1	8Y	443/448 (99%)	398 (90%)	35 (8%)	10 (2%)	6	38
1	8Z	443/448 (99%)	399 (90%)	33 (7%)	11 (2%)	5	36
1	8a	443/448 (99%)	384 (87%)	50 (11%)	9 (2%)	7	41
1	8b	443/448 (99%)	406 (92%)	34 (8%)	3 (1%)	22	61
1	8c	443/448 (99%)	392 (88%)	38 (9%)	13 (3%)	4	33
1	8d	443/448 (99%)	398 (90%)	40 (9%)	5 (1%)	14	53
1	9A	443/448 (99%)	399 (90%)	40 (9%)	4 (1%)	17	57
1	9B	443/448 (99%)	399 (90%)	40 (9%)	4 (1%)	17	57
1	9C	443/448 (99%)	399 (90%)	40 (9%)	4 (1%)	17	57
1	9D	443/448 (99%)	398 (90%)	41 (9%)	4 (1%)	17	57
1	9E	443/448 (99%)	398 (90%)	41 (9%)	4 (1%)	17	57
2	1e	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	1f	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	1g	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	1h	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	1i	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	1j	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	1k	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	1l	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	1m	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	1n	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	1o	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	1p	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	1q	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	1r	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	1s	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	1t	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	1u	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	1v	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	1w	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	1x	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	2Z	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	2a	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	2b	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	2c	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	2d	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	2e	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	2f	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	2g	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	2h	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	2i	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	2j	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	2k	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	2l	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	2m	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	2n	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	2o	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	2p	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	2q	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	2r	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	2s	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	2t	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	2u	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	2v	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	2w	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	2x	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	3e	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	3f	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	3g	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	3h	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	3i	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	3j	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	3k	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	3l	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	3m	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	3n	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	3o	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	3p	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	3q	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	3r	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	3s	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	3t	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	3u	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	3v	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	3w	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	3x	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	4e	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	4f	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	4g	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	4h	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	4i	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	4j	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	4k	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	4l	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	4m	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	4n	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	5e	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	5f	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	5g	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	5h	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	5i	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	5j	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	5k	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	5l	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	5m	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	5n	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	6e	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	6f	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	6g	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	6h	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	6i	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	6j	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	6k	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	6l	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	6m	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	6n	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	6o	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	6p	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	6q	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	6r	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	6s	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	6t	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	6u	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	6v	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	6w	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	6x	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	7Z	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	7a	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	7b	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	7c	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	7d	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	7e	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	7f	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	7g	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	7h	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	7i	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	7j	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	7k	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	7l	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	7m	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	7n	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	7o	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	7p	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	7q	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	7r	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	7s	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	7t	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	7u	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	7v	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	7w	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	7x	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	8e	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	8f	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	8g	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	8h	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	8i	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	8j	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	8k	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	8l	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	8m	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	8n	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	8o	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	8p	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	8q	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	8r	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	8s	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	8t	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	8u	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	8v	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	8w	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	8x	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	8y	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	8z	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	9F	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	9G	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	9H	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	9I	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	9J	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	55
2	9K	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	9L	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	9M	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	9N	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	9O	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	9P	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
2	9Q	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	40
2	9R	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	43
All	All	150460/151645 (99%)	136704 (91%)	10667 (7%)	3089 (2%)	10	40

All (3089) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1A	251	ILE

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Mol	Chain	Res	Type
1	1B	7	ASP
1	1B	253	ALA
1	1C	19	ASP
1	1C	20	ILE
1	1C	95	ARG
1	1D	21	VAL
1	1D	355	SER
1	1E	119	VAL
1	1E	408	GLU
1	1F	228	GLN
1	2A	95	ARG
1	2B	38	LEU
1	2C	54	ASN
1	2C	356	PRO
1	2D	51	ILE
1	2D	228	GLN
1	2D	443	SER
1	2E	31	ASN
1	2E	439	PRO
1	3A	112	ALA
1	3A	251	ILE
1	3A	288	THR
1	3A	382	LYS
1	3A	396	ILE
1	3B	171	TYR
1	3B	277	GLY
1	3B	355	SER
1	3C	202	GLU
1	3C	203	PRO
1	3C	204	THR
1	3C	251	ILE
1	3C	378	ALA
1	3D	20	ILE
1	3D	146	ASP
1	3D	231	ARG
1	3D	356	PRO
1	3D	404	VAL
1	3D	426	PRO
1	3E	20	ILE
1	3E	92	PRO
1	4B	66	VAL
1	4B	119	VAL

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Mol	Chain	Res	Type
1	4B	204	THR
1	4B	206	SER
1	4B	209	ALA
1	4B	387	VAL
1	4B	426	PRO
1	4C	92	PRO
1	4C	356	PRO
1	4D	355	SER
1	4D	356	PRO
1	4E	119	VAL
1	4E	147	ASP
1	4E	203	PRO
1	4E	380	ASP
1	4F	21	VAL
1	4F	96	THR
1	4F	111	ASP
1	4F	439	PRO
1	4F	443	SER
1	4F	446	ALA
1	5A	205	SER
1	5A	391	SER
1	5B	253	ALA
1	5B	378	ALA
1	5B	426	PRO
1	5B	427	LYS
1	5C	253	ALA
1	5C	356	PRO
1	5D	251	ILE
1	5D	355	SER
1	5D	425	LYS
1	5E	8	VAL
1	5E	155	SER
1	5F	253	ALA
1	5F	356	PRO
1	6B	92	PRO
1	6B	335	PHE
1	6B	409	ASP
1	6C	287	SER
1	6C	356	PRO
1	6C	396	ILE
1	6C	407	ASN
1	6D	171	TYR

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Mol	Chain	Res	Type
1	6D	253	ALA
1	6D	318	LEU
1	6E	92	PRO
1	6E	112	ALA
1	6E	251	ILE
1	6F	355	SER
1	6F	404	VAL
1	7A	426	PRO
1	7C	39	ALA
1	7C	92	PRO
1	7C	355	SER
1	7C	363	GLN
1	7C	376	THR
1	7C	439	PRO
1	7C	441	ASN
1	7D	51	ILE
1	7D	54	ASN
1	7D	356	PRO
1	7E	31	ASN
1	7E	286	ALA
1	8A	356	PRO
1	8B	409	ASP
1	8C	253	ALA
1	8E	356	PRO
1	1G	251	ILE
1	1H	7	ASP
1	1H	253	ALA
1	1I	19	ASP
1	1I	20	ILE
1	1I	95	ARG
1	1J	21	VAL
1	1J	355	SER
1	1K	119	VAL
1	1K	408	GLU
1	1L	228	GLN
1	2F	95	ARG
1	2G	38	LEU
1	2H	54	ASN
1	2H	356	PRO
1	2I	51	ILE
1	2I	228	GLN
1	2I	443	SER

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Mol	Chain	Res	Type
1	2J	31	ASN
1	2J	439	PRO
1	3G	112	ALA
1	3G	251	ILE
1	3G	288	THR
1	3G	382	LYS
1	3G	396	ILE
1	3H	171	TYR
1	3H	277	GLY
1	3H	355	SER
1	3I	202	GLU
1	3I	203	PRO
1	3I	204	THR
1	3I	251	ILE
1	3I	378	ALA
1	3J	20	ILE
1	3J	146	ASP
1	3J	231	ARG
1	3J	356	PRO
1	3J	404	VAL
1	3J	426	PRO
1	3K	20	ILE
1	3K	92	PRO
1	4H	66	VAL
1	4H	119	VAL
1	4H	204	THR
1	4H	206	SER
1	4H	209	ALA
1	4H	387	VAL
1	4H	426	PRO
1	4I	92	PRO
1	4I	356	PRO
1	4J	355	SER
1	4J	356	PRO
1	4K	119	VAL
1	4K	147	ASP
1	4K	203	PRO
1	4K	380	ASP
1	4L	21	VAL
1	4L	96	THR
1	4L	111	ASP
1	4L	439	PRO

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Mol	Chain	Res	Type
1	4L	443	SER
1	4L	446	ALA
1	5G	205	SER
1	5G	391	SER
1	5H	253	ALA
1	5H	378	ALA
1	5H	426	PRO
1	5H	427	LYS
1	5I	253	ALA
1	5I	356	PRO
1	5J	251	ILE
1	5J	355	SER
1	5J	425	LYS
1	5K	8	VAL
1	5K	155	SER
1	5L	253	ALA
1	5L	356	PRO
1	6H	92	PRO
1	6H	335	PHE
1	6H	409	ASP
1	6I	287	SER
1	6I	356	PRO
1	6I	396	ILE
1	6I	407	ASN
1	6J	171	TYR
1	6J	253	ALA
1	6J	318	LEU
1	6K	92	PRO
1	6K	112	ALA
1	6K	251	ILE
1	6L	355	SER
1	6L	404	VAL
1	7F	426	PRO
1	7H	39	ALA
1	7H	92	PRO
1	7H	355	SER
1	7H	363	GLN
1	7H	376	THR
1	7H	439	PRO
1	7H	441	ASN
1	7I	51	ILE
1	7I	54	ASN

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Mol	Chain	Res	Type
1	7I	356	PRO
1	7J	31	ASN
1	7J	286	ALA
1	8G	356	PRO
1	8H	409	ASP
1	8I	253	ALA
1	8K	356	PRO
1	1M	251	ILE
1	1N	7	ASP
1	1N	253	ALA
1	1O	19	ASP
1	1O	20	ILE
1	1O	95	ARG
1	1P	21	VAL
1	1P	355	SER
1	1Q	119	VAL
1	1Q	408	GLU
1	1R	228	GLN
1	2K	95	ARG
1	2L	38	LEU
1	2M	54	ASN
1	2M	356	PRO
1	2N	51	ILE
1	2N	228	GLN
1	2N	443	SER
1	2O	31	ASN
1	2O	439	PRO
1	3M	112	ALA
1	3M	251	ILE
1	3M	288	THR
1	3M	382	LYS
1	3M	396	ILE
1	3N	171	TYR
1	3N	277	GLY
1	3N	355	SER
1	3O	202	GLU
1	3O	203	PRO
1	3O	204	THR
1	3O	251	ILE
1	3O	378	ALA
1	3P	20	ILE
1	3P	146	ASP

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Mol	Chain	Res	Type
1	3P	231	ARG
1	3P	356	PRO
1	3P	404	VAL
1	3P	426	PRO
1	3Q	20	ILE
1	3Q	92	PRO
1	4N	66	VAL
1	4N	119	VAL
1	4N	204	THR
1	4N	206	SER
1	4N	209	ALA
1	4N	387	VAL
1	4N	426	PRO
1	4O	92	PRO
1	4O	356	PRO
1	4P	355	SER
1	4P	356	PRO
1	4Q	119	VAL
1	4Q	147	ASP
1	4Q	203	PRO
1	4Q	380	ASP
1	4R	21	VAL
1	4R	96	THR
1	4R	111	ASP
1	4R	439	PRO
1	4R	443	SER
1	4R	446	ALA
1	5M	205	SER
1	5M	391	SER
1	5N	253	ALA
1	5N	378	ALA
1	5N	426	PRO
1	5N	427	LYS
1	5O	253	ALA
1	5O	356	PRO
1	5P	251	ILE
1	5P	355	SER
1	5P	425	LYS
1	5Q	8	VAL
1	5Q	155	SER
1	5R	253	ALA
1	5R	356	PRO

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Mol	Chain	Res	Type
1	6N	92	PRO
1	6N	335	PHE
1	6N	409	ASP
1	6O	287	SER
1	6O	356	PRO
1	6O	396	ILE
1	6O	407	ASN
1	6P	171	TYR
1	6P	253	ALA
1	6P	318	LEU
1	6Q	92	PRO
1	6Q	112	ALA
1	6Q	251	ILE
1	6R	355	SER
1	6R	404	VAL
1	7K	426	PRO
1	7M	39	ALA
1	7M	92	PRO
1	7M	355	SER
1	7M	363	GLN
1	7M	376	THR
1	7M	439	PRO
1	7M	441	ASN
1	7N	51	ILE
1	7N	54	ASN
1	7N	356	PRO
1	7O	31	ASN
1	7O	286	ALA
1	8M	356	PRO
1	8N	409	ASP
1	8O	253	ALA
1	8Q	356	PRO
1	1S	251	ILE
1	1T	7	ASP
1	1T	253	ALA
1	1U	19	ASP
1	1U	20	ILE
1	1U	95	ARG
1	1V	21	VAL
1	1V	355	SER
1	1W	119	VAL
1	1W	408	GLU

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Mol	Chain	Res	Type
1	1X	228	GLN
1	2P	95	ARG
1	2Q	38	LEU
1	2R	54	ASN
1	2R	356	PRO
1	2S	51	ILE
1	2S	228	GLN
1	2S	443	SER
1	2T	31	ASN
1	2T	439	PRO
1	3S	112	ALA
1	3S	251	ILE
1	3S	288	THR
1	3S	382	LYS
1	3S	396	ILE
1	3T	171	TYR
1	3T	277	GLY
1	3T	355	SER
1	3U	202	GLU
1	3U	203	PRO
1	3U	204	THR
1	3U	251	ILE
1	3U	378	ALA
1	3V	20	ILE
1	3V	146	ASP
1	3V	231	ARG
1	3V	356	PRO
1	3V	404	VAL
1	3V	426	PRO
1	3W	20	ILE
1	3W	92	PRO
1	4T	66	VAL
1	4T	119	VAL
1	4T	204	THR
1	4T	206	SER
1	4T	209	ALA
1	4T	387	VAL
1	4T	426	PRO
1	4U	92	PRO
1	4U	356	PRO
1	4V	355	SER
1	4V	356	PRO

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Mol	Chain	Res	Type
1	4W	119	VAL
1	4W	147	ASP
1	4W	203	PRO
1	4W	380	ASP
1	4X	21	VAL
1	4X	96	THR
1	4X	111	ASP
1	4X	439	PRO
1	4X	443	SER
1	4X	446	ALA
1	5S	205	SER
1	5S	391	SER
1	5T	253	ALA
1	5T	378	ALA
1	5T	426	PRO
1	5T	427	LYS
1	5U	253	ALA
1	5U	356	PRO
1	5V	251	ILE
1	5V	355	SER
1	5V	425	LYS
1	5W	8	VAL
1	5W	155	SER
1	5X	253	ALA
1	5X	356	PRO
1	6T	92	PRO
1	6T	335	PHE
1	6T	409	ASP
1	6U	287	SER
1	6U	356	PRO
1	6U	396	ILE
1	6U	407	ASN
1	6V	171	TYR
1	6V	253	ALA
1	6V	318	LEU
1	6W	92	PRO
1	6W	112	ALA
1	6W	251	ILE
1	6X	355	SER
1	6X	404	VAL
1	7P	426	PRO
1	7R	39	ALA

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Mol	Chain	Res	Type
1	7R	92	PRO
1	7R	355	SER
1	7R	363	GLN
1	7R	376	THR
1	7R	439	PRO
1	7R	441	ASN
1	7S	51	ILE
1	7S	54	ASN
1	7S	356	PRO
1	7T	31	ASN
1	7T	286	ALA
1	8S	356	PRO
1	8T	409	ASP
1	8U	253	ALA
1	8W	356	PRO
1	1Y	251	ILE
1	1Z	7	ASP
1	1Z	253	ALA
1	1a	19	ASP
1	1a	20	ILE
1	1a	95	ARG
1	1b	21	VAL
1	1b	355	SER
1	1c	119	VAL
1	1c	408	GLU
1	1d	228	GLN
1	2U	95	ARG
1	2V	38	LEU
1	2W	54	ASN
1	2W	356	PRO
1	2X	51	ILE
1	2X	228	GLN
1	2X	443	SER
1	2Y	31	ASN
1	2Y	439	PRO
1	3Y	112	ALA
1	3Y	251	ILE
1	3Y	288	THR
1	3Y	382	LYS
1	3Y	396	ILE
1	3Z	171	TYR
1	3Z	277	GLY

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Mol	Chain	Res	Type
1	3Z	355	SER
1	3a	202	GLU
1	3a	203	PRO
1	3a	204	THR
1	3a	251	ILE
1	3a	378	ALA
1	3b	20	ILE
1	3b	146	ASP
1	3b	231	ARG
1	3b	356	PRO
1	3b	404	VAL
1	3b	426	PRO
1	3c	20	ILE
1	3c	92	PRO
1	4Z	66	VAL
1	4Z	119	VAL
1	4Z	204	THR
1	4Z	206	SER
1	4Z	209	ALA
1	4Z	387	VAL
1	4Z	426	PRO
1	4a	92	PRO
1	4a	356	PRO
1	4b	355	SER
1	4b	356	PRO
1	4c	119	VAL
1	4c	147	ASP
1	4c	203	PRO
1	4c	380	ASP
1	4d	21	VAL
1	4d	96	THR
1	4d	111	ASP
1	4d	439	PRO
1	4d	443	SER
1	4d	446	ALA
1	5Y	205	SER
1	5Y	391	SER
1	5Z	253	ALA
1	5Z	378	ALA
1	5Z	426	PRO
1	5Z	427	LYS
1	5a	253	ALA

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Mol	Chain	Res	Type
1	5a	356	PRO
1	5b	251	ILE
1	5b	355	SER
1	5b	425	LYS
1	5c	8	VAL
1	5c	155	SER
1	5d	253	ALA
1	5d	356	PRO
1	6Z	92	PRO
1	6Z	335	PHE
1	6Z	409	ASP
1	6a	287	SER
1	6a	356	PRO
1	6a	396	ILE
1	6a	407	ASN
1	6b	171	TYR
1	6b	253	ALA
1	6b	318	LEU
1	6c	92	PRO
1	6c	112	ALA
1	6c	251	ILE
1	6d	355	SER
1	6d	404	VAL
1	7U	426	PRO
1	7W	39	ALA
1	7W	92	PRO
1	7W	355	SER
1	7W	363	GLN
1	7W	376	THR
1	7W	439	PRO
1	7W	441	ASN
1	7X	51	ILE
1	7X	54	ASN
1	7X	356	PRO
1	7Y	31	ASN
1	7Y	286	ALA
1	8Y	356	PRO
1	8Z	409	ASP
1	8a	253	ALA
1	8c	356	PRO
2	1e	112	ILE
2	1g	112	ILE

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Mol	Chain	Res	Type
2	3f	112	ILE
2	3h	112	ILE
2	4e	112	ILE
2	5e	112	ILE
2	6f	112	ILE
2	6h	112	ILE
2	8f	112	ILE
2	8g	112	ILE
2	8i	112	ILE
2	1i	112	ILE
2	1k	112	ILE
2	3j	112	ILE
2	3l	112	ILE
2	4g	112	ILE
2	5g	112	ILE
2	6j	112	ILE
2	6l	112	ILE
2	8l	112	ILE
2	8m	112	ILE
2	8o	112	ILE
2	1m	112	ILE
2	1o	112	ILE
2	3n	112	ILE
2	3p	112	ILE
2	4i	112	ILE
2	5i	112	ILE
2	6n	112	ILE
2	6p	112	ILE
2	8r	112	ILE
2	8s	112	ILE
2	8u	112	ILE
2	1q	112	ILE
2	1s	112	ILE
2	3r	112	ILE
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

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Mol	Chain	Res	Type
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	1A	205	SER
1	1A	380	ASP
1	1B	8	VAL
1	1B	25	ARG
1	1B	400	GLY
1	1B	410	ASN
1	1B	426	PRO
1	1C	18	TYR
1	1C	251	ILE
1	1D	12	LEU
1	1D	405	SER
1	1E	17	SER
1	1E	18	TYR
1	1E	204	THR
1	1F	8	VAL
1	1F	85	LYS
1	1F	376	THR
1	2A	48	GLY
1	2A	355	SER
1	2C	284	GLY
1	3A	12	LEU
1	3C	355	SER
1	3D	12	LEU
1	3D	21	VAL
1	3E	19	ASP
1	3E	251	ILE
1	3E	355	SER
1	3E	380	ASP
1	4A	251	ILE
1	4B	13	GLY
1	4B	50	GLY

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Mol	Chain	Res	Type
1	4B	154	VAL
1	4C	31	ASN
1	4C	109	GLN
1	4C	110	TYR
1	4D	251	ILE
1	4E	64	SER
1	4E	66	VAL
1	4E	287	SER
1	4E	411	GLN
1	5A	12	LEU
1	5A	150	LYS
1	5A	251	ILE
1	5A	379	LYS
1	5A	398	GLY
1	5B	66	VAL
1	5B	95	ARG
1	5B	155	SER
1	5B	204	THR
1	5B	298	ASP
1	5B	390	GLY
1	5C	62	ILE
1	5C	63	THR
1	5C	64	SER
1	5C	157	GLY
1	5C	405	SER
1	5C	409	ASP
1	5E	7	ASP
1	5E	33	LYS
1	5E	66	VAL
1	5F	30	ASP
1	5F	157	GLY
1	5F	266	LYS
1	5F	292	ALA
1	5F	439	PRO
1	6A	251	ILE
1	6B	8	VAL
1	6C	375	ALA
1	6C	390	GLY
1	6C	398	GLY
1	6D	93	LEU
1	6D	287	SER
1	6D	292	ALA

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Mol	Chain	Res	Type
1	6D	392	THR
1	6E	148	SER
1	6E	406	GLY
1	6F	287	SER
1	6F	395	ALA
1	7B	355	SER
1	7D	390	GLY
1	7E	237	ALA
1	8A	96	THR
1	8A	135	ASN
1	8A	157	GLY
1	8A	403	SER
1	8B	205	SER
1	8B	251	ILE
1	8B	355	SER
1	8B	357	ASN
1	8B	446	ALA
1	8C	356	PRO
1	8C	440	ASN
1	8D	251	ILE
1	8E	8	VAL
1	8E	231	ARG
1	8E	292	ALA
1	8E	399	ASP
1	8F	251	ILE
1	9A	335	PHE
1	9A	393	GLY
1	1G	205	SER
1	1G	380	ASP
1	1H	8	VAL
1	1H	25	ARG
1	1H	400	GLY
1	1H	410	ASN
1	1H	426	PRO
1	1I	18	TYR
1	1I	251	ILE
1	1J	12	LEU
1	1J	405	SER
1	1K	17	SER
1	1K	18	TYR
1	1K	204	THR
1	1L	8	VAL

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Mol	Chain	Res	Type
1	1L	85	LYS
1	1L	376	THR
1	2F	48	GLY
1	2F	355	SER
1	2H	284	GLY
1	3G	12	LEU
1	3I	355	SER
1	3J	12	LEU
1	3J	21	VAL
1	3K	19	ASP
1	3K	251	ILE
1	3K	355	SER
1	3K	380	ASP
1	4G	251	ILE
1	4H	13	GLY
1	4H	50	GLY
1	4H	154	VAL
1	4I	31	ASN
1	4I	109	GLN
1	4I	110	TYR
1	4J	251	ILE
1	4K	64	SER
1	4K	66	VAL
1	4K	287	SER
1	4K	411	GLN
1	5G	12	LEU
1	5G	150	LYS
1	5G	251	ILE
1	5G	379	LYS
1	5G	398	GLY
1	5H	66	VAL
1	5H	95	ARG
1	5H	155	SER
1	5H	204	THR
1	5H	298	ASP
1	5H	390	GLY
1	5I	62	ILE
1	5I	63	THR
1	5I	64	SER
1	5I	157	GLY
1	5I	405	SER
1	5I	409	ASP

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Mol	Chain	Res	Type
1	5K	7	ASP
1	5K	33	LYS
1	5K	66	VAL
1	5L	30	ASP
1	5L	157	GLY
1	5L	266	LYS
1	5L	292	ALA
1	5L	439	PRO
1	6G	251	ILE
1	6H	8	VAL
1	6I	375	ALA
1	6I	390	GLY
1	6I	398	GLY
1	6J	93	LEU
1	6J	287	SER
1	6J	292	ALA
1	6J	392	THR
1	6K	148	SER
1	6K	406	GLY
1	6L	287	SER
1	6L	395	ALA
1	7G	355	SER
1	7I	390	GLY
1	7J	237	ALA
1	8G	96	THR
1	8G	135	ASN
1	8G	157	GLY
1	8G	403	SER
1	8H	205	SER
1	8H	251	ILE
1	8H	355	SER
1	8H	357	ASN
1	8H	446	ALA
1	8I	356	PRO
1	8I	440	ASN
1	8J	251	ILE
1	8K	8	VAL
1	8K	231	ARG
1	8K	292	ALA
1	8K	399	ASP
1	8L	251	ILE
1	9B	335	PHE

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Mol	Chain	Res	Type
1	9B	393	GLY
1	1M	205	SER
1	1M	380	ASP
1	1N	8	VAL
1	1N	25	ARG
1	1N	400	GLY
1	1N	410	ASN
1	1N	426	PRO
1	1O	18	TYR
1	1O	251	ILE
1	1P	12	LEU
1	1P	405	SER
1	1Q	17	SER
1	1Q	18	TYR
1	1Q	204	THR
1	1R	8	VAL
1	1R	85	LYS
1	1R	376	THR
1	2K	48	GLY
1	2K	355	SER
1	2M	284	GLY
1	3M	12	LEU
1	3O	355	SER
1	3P	12	LEU
1	3P	21	VAL
1	3Q	19	ASP
1	3Q	251	ILE
1	3Q	355	SER
1	3Q	380	ASP
1	4M	251	ILE
1	4N	13	GLY
1	4N	50	GLY
1	4N	154	VAL
1	4O	31	ASN
1	4O	109	GLN
1	4O	110	TYR
1	4P	251	ILE
1	4Q	64	SER
1	4Q	66	VAL
1	4Q	287	SER
1	4Q	411	GLN
1	5M	12	LEU

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Mol	Chain	Res	Type
1	5M	150	LYS
1	5M	251	ILE
1	5M	379	LYS
1	5M	398	GLY
1	5N	66	VAL
1	5N	95	ARG
1	5N	155	SER
1	5N	204	THR
1	5N	298	ASP
1	5N	390	GLY
1	5O	62	ILE
1	5O	63	THR
1	5O	64	SER
1	5O	157	GLY
1	5O	405	SER
1	5O	409	ASP
1	5Q	7	ASP
1	5Q	33	LYS
1	5Q	66	VAL
1	5R	30	ASP
1	5R	157	GLY
1	5R	266	LYS
1	5R	292	ALA
1	5R	439	PRO
1	6M	251	ILE
1	6N	8	VAL
1	6O	375	ALA
1	6O	390	GLY
1	6O	398	GLY
1	6P	93	LEU
1	6P	287	SER
1	6P	292	ALA
1	6P	392	THR
1	6Q	148	SER
1	6Q	406	GLY
1	6R	287	SER
1	6R	395	ALA
1	7L	355	SER
1	7N	390	GLY
1	7O	237	ALA
1	8M	96	THR
1	8M	135	ASN

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Mol	Chain	Res	Type
1	8M	157	GLY
1	8M	403	SER
1	8N	205	SER
1	8N	251	ILE
1	8N	355	SER
1	8N	357	ASN
1	8N	446	ALA
1	8O	356	PRO
1	8O	440	ASN
1	8P	251	ILE
1	8Q	8	VAL
1	8Q	231	ARG
1	8Q	292	ALA
1	8Q	399	ASP
1	8R	251	ILE
1	9C	335	PHE
1	9C	393	GLY
1	1S	205	SER
1	1S	380	ASP
1	1T	8	VAL
1	1T	25	ARG
1	1T	400	GLY
1	1T	410	ASN
1	1T	426	PRO
1	1U	18	TYR
1	1U	251	ILE
1	1V	12	LEU
1	1V	254	ASP
1	1V	405	SER
1	1W	17	SER
1	1W	18	TYR
1	1W	204	THR
1	1X	8	VAL
1	1X	85	LYS
1	1X	376	THR
1	2P	48	GLY
1	2P	355	SER
1	2R	284	GLY
1	3S	12	LEU
1	3U	355	SER
1	3V	12	LEU
1	3V	21	VAL

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Mol	Chain	Res	Type
1	3W	19	ASP
1	3W	251	ILE
1	3W	355	SER
1	3W	380	ASP
1	4S	251	ILE
1	4T	13	GLY
1	4T	50	GLY
1	4T	154	VAL
1	4U	31	ASN
1	4U	109	GLN
1	4U	110	TYR
1	4V	251	ILE
1	4W	64	SER
1	4W	66	VAL
1	4W	287	SER
1	4W	411	GLN
1	5S	12	LEU
1	5S	150	LYS
1	5S	251	ILE
1	5S	379	LYS
1	5S	398	GLY
1	5T	66	VAL
1	5T	95	ARG
1	5T	155	SER
1	5T	204	THR
1	5T	298	ASP
1	5T	390	GLY
1	5U	62	ILE
1	5U	63	THR
1	5U	64	SER
1	5U	157	GLY
1	5U	405	SER
1	5U	409	ASP
1	5W	7	ASP
1	5W	33	LYS
1	5W	66	VAL
1	5X	30	ASP
1	5X	157	GLY
1	5X	266	LYS
1	5X	292	ALA
1	5X	439	PRO
1	6S	251	ILE

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Mol	Chain	Res	Type
1	6T	8	VAL
1	6U	375	ALA
1	6U	390	GLY
1	6U	398	GLY
1	6V	93	LEU
1	6V	287	SER
1	6V	292	ALA
1	6V	392	THR
1	6W	148	SER
1	6W	406	GLY
1	6X	287	SER
1	6X	395	ALA
1	7Q	355	SER
1	7S	390	GLY
1	7T	237	ALA
1	8S	96	THR
1	8S	135	ASN
1	8S	157	GLY
1	8S	403	SER
1	8T	205	SER
1	8T	251	ILE
1	8T	355	SER
1	8T	357	ASN
1	8T	446	ALA
1	8U	356	PRO
1	8U	440	ASN
1	8V	251	ILE
1	8W	8	VAL
1	8W	231	ARG
1	8W	292	ALA
1	8W	399	ASP
1	8X	251	ILE
1	9D	335	PHE
1	9D	393	GLY
1	1Y	205	SER
1	1Y	380	ASP
1	1Z	8	VAL
1	1Z	25	ARG
1	1Z	400	GLY
1	1Z	410	ASN
1	1Z	426	PRO
1	1a	18	TYR

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Mol	Chain	Res	Type
1	1a	251	ILE
1	1b	12	LEU
1	1b	254	ASP
1	1b	405	SER
1	1c	17	SER
1	1c	18	TYR
1	1c	204	THR
1	1d	8	VAL
1	1d	85	LYS
1	1d	376	THR
1	2U	48	GLY
1	2U	355	SER
1	2W	284	GLY
1	3Y	12	LEU
1	3a	355	SER
1	3b	12	LEU
1	3b	21	VAL
1	3c	19	ASP
1	3c	251	ILE
1	3c	355	SER
1	3c	380	ASP
1	4Y	251	ILE
1	4Z	13	GLY
1	4Z	50	GLY
1	4Z	154	VAL
1	4a	31	ASN
1	4a	109	GLN
1	4a	110	TYR
1	4b	251	ILE
1	4c	64	SER
1	4c	66	VAL
1	4c	287	SER
1	4c	411	GLN
1	5Y	12	LEU
1	5Y	150	LYS
1	5Y	251	ILE
1	5Y	379	LYS
1	5Y	398	GLY
1	5Z	66	VAL
1	5Z	95	ARG
1	5Z	155	SER
1	5Z	204	THR

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Mol	Chain	Res	Type
1	5Z	298	ASP
1	5Z	390	GLY
1	5a	62	ILE
1	5a	63	THR
1	5a	64	SER
1	5a	157	GLY
1	5a	405	SER
1	5a	409	ASP
1	5c	7	ASP
1	5c	33	LYS
1	5c	66	VAL
1	5d	30	ASP
1	5d	157	GLY
1	5d	266	LYS
1	5d	292	ALA
1	5d	439	PRO
1	6Y	251	ILE
1	6Z	8	VAL
1	6a	375	ALA
1	6a	390	GLY
1	6a	398	GLY
1	6b	93	LEU
1	6b	287	SER
1	6b	292	ALA
1	6b	392	THR
1	6c	148	SER
1	6c	406	GLY
1	6d	287	SER
1	6d	395	ALA
1	7V	355	SER
1	7X	390	GLY
1	7Y	237	ALA
1	8Y	96	THR
1	8Y	135	ASN
1	8Y	157	GLY
1	8Y	403	SER
1	8Z	205	SER
1	8Z	251	ILE
1	8Z	355	SER
1	8Z	357	ASN
1	8Z	446	ALA
1	8a	356	PRO

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Mol	Chain	Res	Type
1	8a	440	ASN
1	8b	251	ILE
1	8c	8	VAL
1	8c	231	ARG
1	8c	292	ALA
1	8c	399	ASP
1	8d	251	ILE
1	9E	335	PHE
1	9E	393	GLY
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
2	5g	92	SER

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Mol	Chain	Res	Type
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
2	4k	92	SER

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Mol	Chain	Res	Type
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	1A	39	ALA
1	1A	446	ALA
1	1C	343	SER
1	1C	447	GLN
1	1D	92	PRO
1	1D	254	ASP
1	1D	292	ALA

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Mol	Chain	Res	Type
1	1E	95	ARG
1	1F	154	VAL
1	2C	92	PRO
1	2C	108	LYS
1	2C	146	ASP
1	2C	237	ALA
1	2E	16	GLU
1	2E	17	SER
1	2E	92	PRO
1	3A	5	PHE
1	3A	203	PRO
1	3A	375	ALA
1	3A	404	VAL
1	3C	96	THR
1	3C	148	SER
1	3C	150	LYS
1	3C	377	ASN
1	3D	5	PHE
1	3D	92	PRO
1	3D	292	ALA
1	3F	28	GLN
1	3F	95	ARG
1	3F	156	TRP
1	3F	267	ALA
1	3F	355	SER
1	3F	427	LYS
1	3F	443	SER
1	4B	34	SER
1	4B	315	PRO
1	4C	64	SER
1	4C	205	SER
1	4C	292	ALA
1	4D	267	ALA
1	4E	93	LEU
1	4E	205	SER
1	4F	201	ASP
1	4F	411	GLN
1	4F	426	PRO
1	4F	440	ASN
1	5B	251	ILE
1	5B	356	PRO
1	5B	425	LYS

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Mol	Chain	Res	Type
1	5C	27	SER
1	5C	29	GLY
1	5C	93	LEU
1	5C	378	ALA
1	5C	426	PRO
1	5D	16	GLU
1	5D	92	PRO
1	5E	11	SER
1	5E	64	SER
1	5E	204	THR
1	5E	251	ILE
1	5E	426	PRO
1	5F	92	PRO
1	5F	440	ASN
1	6A	425	LYS
1	6B	156	TRP
1	6B	237	ALA
1	6B	398	GLY
1	6D	92	PRO
1	6D	380	ASP
1	6F	16	GLU
1	6F	155	SER
1	6F	232	ASP
1	6F	276	LEU
1	6F	443	SER
1	7A	273	THR
1	7A	297	LYS
1	7A	427	LYS
1	7C	408	GLU
1	7D	53	ILE
1	7D	107	GLU
1	7D	382	LYS
1	7D	447	GLN
1	7E	391	SER
1	8A	355	SER
1	8B	95	ARG
1	8B	426	PRO
1	8C	7	ASP
1	8C	292	ALA
1	8C	439	PRO
1	8E	268	PHE
1	8E	411	GLN

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Mol	Chain	Res	Type
1	1G	39	ALA
1	1G	446	ALA
1	1I	343	SER
1	1I	447	GLN
1	1J	92	PRO
1	1J	254	ASP
1	1J	292	ALA
1	1K	95	ARG
1	1L	154	VAL
1	2H	92	PRO
1	2H	108	LYS
1	2H	146	ASP
1	2H	237	ALA
1	2J	16	GLU
1	2J	17	SER
1	2J	92	PRO
1	3G	5	PHE
1	3G	375	ALA
1	3G	404	VAL
1	3I	96	THR
1	3I	148	SER
1	3I	150	LYS
1	3I	377	ASN
1	3J	5	PHE
1	3J	92	PRO
1	3J	292	ALA
1	3L	28	GLN
1	3L	95	ARG
1	3L	156	TRP
1	3L	267	ALA
1	3L	355	SER
1	3L	427	LYS
1	3L	443	SER
1	4H	34	SER
1	4H	315	PRO
1	4I	64	SER
1	4I	205	SER
1	4I	292	ALA
1	4J	267	ALA
1	4K	93	LEU
1	4K	205	SER
1	4L	201	ASP

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Mol	Chain	Res	Type
1	4L	411	GLN
1	4L	426	PRO
1	4L	440	ASN
1	5H	251	ILE
1	5H	356	PRO
1	5H	425	LYS
1	5I	27	SER
1	5I	29	GLY
1	5I	93	LEU
1	5I	378	ALA
1	5I	426	PRO
1	5J	16	GLU
1	5J	92	PRO
1	5K	11	SER
1	5K	64	SER
1	5K	204	THR
1	5K	251	ILE
1	5K	426	PRO
1	5L	92	PRO
1	5L	440	ASN
1	6G	425	LYS
1	6H	156	TRP
1	6H	237	ALA
1	6H	398	GLY
1	6J	92	PRO
1	6J	380	ASP
1	6L	16	GLU
1	6L	155	SER
1	6L	232	ASP
1	6L	276	LEU
1	6L	443	SER
1	7F	273	THR
1	7F	297	LYS
1	7F	427	LYS
1	7H	408	GLU
1	7I	53	ILE
1	7I	107	GLU
1	7I	382	LYS
1	7I	447	GLN
1	7J	391	SER
1	8G	355	SER
1	8H	95	ARG

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Mol	Chain	Res	Type
1	8H	426	PRO
1	8I	7	ASP
1	8I	292	ALA
1	8I	439	PRO
1	8K	268	PHE
1	8K	411	GLN
1	1M	39	ALA
1	1M	446	ALA
1	1O	343	SER
1	1O	447	GLN
1	1P	92	PRO
1	1P	254	ASP
1	1P	292	ALA
1	1Q	95	ARG
1	1R	154	VAL
1	2M	92	PRO
1	2M	108	LYS
1	2M	146	ASP
1	2M	237	ALA
1	2O	16	GLU
1	2O	17	SER
1	2O	92	PRO
1	3M	5	PHE
1	3M	375	ALA
1	3M	404	VAL
1	3O	96	THR
1	3O	148	SER
1	3O	150	LYS
1	3O	377	ASN
1	3P	5	PHE
1	3P	92	PRO
1	3P	292	ALA
1	3R	28	GLN
1	3R	95	ARG
1	3R	156	TRP
1	3R	267	ALA
1	3R	355	SER
1	3R	427	LYS
1	3R	443	SER
1	4N	34	SER
1	4N	315	PRO
1	4O	64	SER

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Mol	Chain	Res	Type
1	4O	205	SER
1	4O	292	ALA
1	4P	267	ALA
1	4Q	93	LEU
1	4Q	205	SER
1	4R	201	ASP
1	4R	411	GLN
1	4R	426	PRO
1	4R	440	ASN
1	5N	251	ILE
1	5N	356	PRO
1	5N	425	LYS
1	5O	27	SER
1	5O	29	GLY
1	5O	93	LEU
1	5O	378	ALA
1	5O	426	PRO
1	5P	16	GLU
1	5P	92	PRO
1	5Q	11	SER
1	5Q	64	SER
1	5Q	204	THR
1	5Q	251	ILE
1	5Q	426	PRO
1	5R	92	PRO
1	5R	440	ASN
1	6M	425	LYS
1	6N	156	TRP
1	6N	237	ALA
1	6N	398	GLY
1	6P	92	PRO
1	6P	380	ASP
1	6R	16	GLU
1	6R	155	SER
1	6R	232	ASP
1	6R	276	LEU
1	6R	443	SER
1	7K	273	THR
1	7K	297	LYS
1	7K	427	LYS
1	7M	408	GLU
1	7N	53	ILE

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Mol	Chain	Res	Type
1	7N	107	GLU
1	7N	382	LYS
1	7N	447	GLN
1	7O	391	SER
1	8M	355	SER
1	8N	95	ARG
1	8N	426	PRO
1	8O	7	ASP
1	8O	292	ALA
1	8O	439	PRO
1	8Q	268	PHE
1	8Q	411	GLN
1	1S	39	ALA
1	1S	446	ALA
1	1U	343	SER
1	1U	447	GLN
1	1V	92	PRO
1	1V	292	ALA
1	1W	95	ARG
1	1X	154	VAL
1	2R	92	PRO
1	2R	108	LYS
1	2R	146	ASP
1	2R	237	ALA
1	2T	16	GLU
1	2T	17	SER
1	2T	92	PRO
1	3S	5	PHE
1	3S	375	ALA
1	3S	404	VAL
1	3U	96	THR
1	3U	148	SER
1	3U	150	LYS
1	3U	377	ASN
1	3V	5	PHE
1	3V	92	PRO
1	3V	292	ALA
1	3X	28	GLN
1	3X	95	ARG
1	3X	156	TRP
1	3X	267	ALA
1	3X	355	SER

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Mol	Chain	Res	Type
1	3X	427	LYS
1	3X	443	SER
1	4T	34	SER
1	4T	315	PRO
1	4U	64	SER
1	4U	205	SER
1	4U	292	ALA
1	4V	267	ALA
1	4W	93	LEU
1	4W	205	SER
1	4X	201	ASP
1	4X	411	GLN
1	4X	426	PRO
1	4X	440	ASN
1	5T	251	ILE
1	5T	356	PRO
1	5T	425	LYS
1	5U	27	SER
1	5U	29	GLY
1	5U	93	LEU
1	5U	378	ALA
1	5U	426	PRO
1	5V	16	GLU
1	5V	92	PRO
1	5W	11	SER
1	5W	64	SER
1	5W	204	THR
1	5W	251	ILE
1	5W	426	PRO
1	5X	92	PRO
1	5X	440	ASN
1	6S	425	LYS
1	6T	156	TRP
1	6T	237	ALA
1	6T	398	GLY
1	6V	92	PRO
1	6V	380	ASP
1	6X	16	GLU
1	6X	155	SER
1	6X	232	ASP
1	6X	276	LEU
1	6X	443	SER

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Mol	Chain	Res	Type
1	7P	273	THR
1	7P	297	LYS
1	7P	427	LYS
1	7R	408	GLU
1	7S	53	ILE
1	7S	107	GLU
1	7S	382	LYS
1	7S	447	GLN
1	7T	391	SER
1	8S	355	SER
1	8T	95	ARG
1	8T	426	PRO
1	8U	7	ASP
1	8U	292	ALA
1	8U	439	PRO
1	8W	268	PHE
1	8W	411	GLN
1	1Y	39	ALA
1	1Y	446	ALA
1	1a	343	SER
1	1a	447	GLN
1	1b	92	PRO
1	1b	292	ALA
1	1c	95	ARG
1	1d	154	VAL
1	1d	267	ALA
1	2W	92	PRO
1	2W	108	LYS
1	2W	146	ASP
1	2W	237	ALA
1	2Y	16	GLU
1	2Y	17	SER
1	2Y	92	PRO
1	3Y	5	PHE
1	3Y	203	PRO
1	3Y	375	ALA
1	3Y	404	VAL
1	3a	96	THR
1	3a	148	SER
1	3a	150	LYS
1	3a	377	ASN
1	3b	5	PHE

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Mol	Chain	Res	Type
1	3b	92	PRO
1	3b	292	ALA
1	3d	28	GLN
1	3d	95	ARG
1	3d	156	TRP
1	3d	267	ALA
1	3d	355	SER
1	3d	427	LYS
1	3d	443	SER
1	4Z	34	SER
1	4Z	315	PRO
1	4a	64	SER
1	4a	205	SER
1	4a	292	ALA
1	4c	93	LEU
1	4c	205	SER
1	4d	201	ASP
1	4d	411	GLN
1	4d	426	PRO
1	4d	440	ASN
1	5Z	251	ILE
1	5Z	356	PRO
1	5Z	425	LYS
1	5a	27	SER
1	5a	29	GLY
1	5a	93	LEU
1	5a	378	ALA
1	5a	426	PRO
1	5b	16	GLU
1	5b	92	PRO
1	5c	11	SER
1	5c	64	SER
1	5c	204	THR
1	5c	251	ILE
1	5c	426	PRO
1	5d	92	PRO
1	5d	440	ASN
1	6Y	425	LYS
1	6Z	156	TRP
1	6Z	237	ALA
1	6Z	398	GLY
1	6b	92	PRO

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Mol	Chain	Res	Type
1	6b	380	ASP
1	6d	16	GLU
1	6d	155	SER
1	6d	232	ASP
1	6d	276	LEU
1	6d	443	SER
1	7U	273	THR
1	7U	297	LYS
1	7U	427	LYS
1	7W	408	GLU
1	7X	53	ILE
1	7X	107	GLU
1	7X	382	LYS
1	7X	447	GLN
1	7Y	391	SER
1	8Y	355	SER
1	8Z	95	ARG
1	8Z	426	PRO
1	8a	7	ASP
1	8a	292	ALA
1	8a	439	PRO
1	8c	268	PHE
1	8c	411	GLN
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
2	9R	9	ALA
2	9R	59	PRO
2	9R	92	SER
2	9R	103	GLN
1	1A	19	ASP
1	1A	381	HIS
1	1B	146	ASP
1	1B	155	SER
1	1C	6	ASN
1	1C	421	GLY
1	1C	443	SER
1	1D	16	GLU
1	1D	315	PRO
1	1D	360	ALA
1	1E	7	ASP
1	1E	121	GLU
1	1E	426	PRO
1	1F	135	ASN
1	1F	267	ALA
1	2A	49	ALA
1	2B	394	THR
1	2B	442	ALA
1	2C	426	PRO
1	2D	206	SER
1	2E	96	THR
1	2E	394	THR
1	2E	424	ASP
1	3A	356	PRO
1	3B	292	ALA
1	3B	360	ALA
1	3B	388	GLU
1	3C	146	ASP
1	3C	263	VAL
1	3D	64	SER
1	3D	95	ARG
1	3D	268	PHE
1	3E	6	ASN
1	3F	252	ASP
1	4A	95	ARG
1	4B	287	SER
1	4B	357	ASN
1	4C	9	LYS

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Mol	Chain	Res	Type
1	4E	274	ASP
1	4F	228	GLN
1	5A	204	THR
1	5B	64	SER
1	5B	292	ALA
1	5C	205	SER
1	5C	411	GLN
1	5D	205	SER
1	5D	395	ALA
1	5E	31	ASN
1	5E	34	SER
1	5E	93	LEU
1	5E	206	SER
1	5E	377	ASN
1	5E	378	ALA
1	5E	416	ALA
1	5F	27	SER
1	5F	146	ASP
1	5F	442	ALA
1	6A	382	LYS
1	6A	426	PRO
1	6A	438	ARG
1	6B	287	SER
1	6D	230	SER
1	6D	360	ALA
1	6E	438	ARG
1	6E	446	ALA
1	6F	315	PRO
1	7C	6	ASN
1	7D	92	PRO
1	7D	205	SER
1	7D	426	PRO
1	8A	205	SER
1	8A	254	ASP
1	8A	292	ALA
1	8B	18	TYR
1	8B	391	SER
1	8C	205	SER
1	8D	357	ASN
1	8E	155	SER
1	8E	426	PRO
1	8F	200	ILE

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Mol	Chain	Res	Type
1	9A	232	ASP
1	1G	19	ASP
1	1G	381	HIS
1	1H	146	ASP
1	1H	155	SER
1	1I	6	ASN
1	1I	421	GLY
1	1I	443	SER
1	1J	16	GLU
1	1J	315	PRO
1	1J	360	ALA
1	1K	7	ASP
1	1K	121	GLU
1	1K	426	PRO
1	1L	135	ASN
1	1L	267	ALA
1	2F	49	ALA
1	2G	394	THR
1	2G	442	ALA
1	2H	426	PRO
1	2I	206	SER
1	2J	96	THR
1	2J	394	THR
1	2J	424	ASP
1	3G	203	PRO
1	3G	356	PRO
1	3H	292	ALA
1	3H	360	ALA
1	3H	388	GLU
1	3I	146	ASP
1	3I	263	VAL
1	3J	64	SER
1	3J	95	ARG
1	3J	268	PHE
1	3K	6	ASN
1	3L	252	ASP
1	4G	95	ARG
1	4H	287	SER
1	4H	357	ASN
1	4I	9	LYS
1	4K	274	ASP
1	4L	228	GLN

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Mol	Chain	Res	Type
1	5G	204	THR
1	5H	64	SER
1	5H	292	ALA
1	5I	205	SER
1	5I	411	GLN
1	5J	205	SER
1	5J	395	ALA
1	5K	31	ASN
1	5K	34	SER
1	5K	93	LEU
1	5K	206	SER
1	5K	377	ASN
1	5K	378	ALA
1	5K	416	ALA
1	5L	27	SER
1	5L	146	ASP
1	5L	442	ALA
1	6G	382	LYS
1	6G	426	PRO
1	6G	438	ARG
1	6H	287	SER
1	6J	230	SER
1	6J	360	ALA
1	6K	438	ARG
1	6K	446	ALA
1	6L	315	PRO
1	7H	6	ASN
1	7I	92	PRO
1	7I	205	SER
1	7I	426	PRO
1	8G	205	SER
1	8G	254	ASP
1	8G	292	ALA
1	8H	18	TYR
1	8H	391	SER
1	8I	205	SER
1	8J	357	ASN
1	8K	155	SER
1	8K	426	PRO
1	8L	200	ILE
1	9B	232	ASP
1	1M	19	ASP

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Mol	Chain	Res	Type
1	1M	381	HIS
1	1N	146	ASP
1	1N	155	SER
1	1O	6	ASN
1	1O	421	GLY
1	1O	443	SER
1	1P	16	GLU
1	1P	315	PRO
1	1P	360	ALA
1	1Q	7	ASP
1	1Q	121	GLU
1	1Q	426	PRO
1	1R	135	ASN
1	1R	267	ALA
1	2K	49	ALA
1	2L	394	THR
1	2L	442	ALA
1	2M	426	PRO
1	2N	206	SER
1	2O	96	THR
1	2O	394	THR
1	2O	424	ASP
1	3M	203	PRO
1	3M	356	PRO
1	3N	292	ALA
1	3N	360	ALA
1	3N	388	GLU
1	3O	146	ASP
1	3O	263	VAL
1	3P	64	SER
1	3P	95	ARG
1	3P	268	PHE
1	3Q	6	ASN
1	3R	252	ASP
1	4M	95	ARG
1	4N	287	SER
1	4N	357	ASN
1	4O	9	LYS
1	4Q	274	ASP
1	4R	228	GLN
1	5M	204	THR
1	5N	64	SER

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Mol	Chain	Res	Type
1	5N	292	ALA
1	5O	205	SER
1	5O	411	GLN
1	5P	205	SER
1	5P	395	ALA
1	5Q	31	ASN
1	5Q	34	SER
1	5Q	93	LEU
1	5Q	206	SER
1	5Q	377	ASN
1	5Q	378	ALA
1	5Q	416	ALA
1	5R	27	SER
1	5R	146	ASP
1	5R	442	ALA
1	6M	382	LYS
1	6M	426	PRO
1	6M	438	ARG
1	6N	287	SER
1	6P	230	SER
1	6P	360	ALA
1	6Q	438	ARG
1	6Q	446	ALA
1	6R	315	PRO
1	7M	6	ASN
1	7N	92	PRO
1	7N	205	SER
1	7N	426	PRO
1	8M	205	SER
1	8M	254	ASP
1	8M	292	ALA
1	8N	18	TYR
1	8N	391	SER
1	8O	205	SER
1	8P	357	ASN
1	8Q	155	SER
1	8Q	426	PRO
1	8R	200	ILE
1	9C	232	ASP
1	1S	19	ASP
1	1S	381	HIS
1	1T	146	ASP

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Mol	Chain	Res	Type
1	1T	155	SER
1	1U	6	ASN
1	1U	421	GLY
1	1U	443	SER
1	1V	16	GLU
1	1V	315	PRO
1	1V	360	ALA
1	1W	7	ASP
1	1W	121	GLU
1	1W	426	PRO
1	1X	135	ASN
1	1X	267	ALA
1	2P	49	ALA
1	2Q	394	THR
1	2Q	442	ALA
1	2R	426	PRO
1	2S	206	SER
1	2T	96	THR
1	2T	394	THR
1	2T	424	ASP
1	3S	203	PRO
1	3S	356	PRO
1	3T	292	ALA
1	3T	360	ALA
1	3T	388	GLU
1	3U	146	ASP
1	3V	64	SER
1	3V	95	ARG
1	3V	268	PHE
1	3W	6	ASN
1	3X	252	ASP
1	4S	95	ARG
1	4T	287	SER
1	4T	357	ASN
1	4U	9	LYS
1	4W	274	ASP
1	4X	228	GLN
1	5S	204	THR
1	5T	64	SER
1	5T	292	ALA
1	5U	205	SER
1	5U	411	GLN

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Mol	Chain	Res	Type
1	5V	205	SER
1	5V	395	ALA
1	5W	31	ASN
1	5W	34	SER
1	5W	93	LEU
1	5W	206	SER
1	5W	377	ASN
1	5W	378	ALA
1	5W	416	ALA
1	5X	27	SER
1	5X	146	ASP
1	5X	442	ALA
1	6S	382	LYS
1	6S	426	PRO
1	6S	438	ARG
1	6T	287	SER
1	6V	230	SER
1	6V	360	ALA
1	6W	438	ARG
1	6W	446	ALA
1	6X	315	PRO
1	7R	6	ASN
1	7S	92	PRO
1	7S	205	SER
1	7S	426	PRO
1	8S	205	SER
1	8S	254	ASP
1	8S	292	ALA
1	8T	18	TYR
1	8T	391	SER
1	8U	205	SER
1	8V	357	ASN
1	8W	155	SER
1	8W	426	PRO
1	8X	200	ILE
1	9D	232	ASP
1	1Y	19	ASP
1	1Y	381	HIS
1	1Z	146	ASP
1	1Z	155	SER
1	1a	6	ASN
1	1a	421	GLY

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Mol	Chain	Res	Type
1	1a	443	SER
1	1b	16	GLU
1	1b	315	PRO
1	1b	360	ALA
1	1c	7	ASP
1	1c	121	GLU
1	1c	426	PRO
1	1d	135	ASN
1	2U	49	ALA
1	2V	394	THR
1	2V	442	ALA
1	2W	426	PRO
1	2X	206	SER
1	2Y	96	THR
1	2Y	394	THR
1	2Y	424	ASP
1	3Y	356	PRO
1	3Z	292	ALA
1	3Z	360	ALA
1	3Z	388	GLU
1	3a	146	ASP
1	3b	64	SER
1	3b	95	ARG
1	3b	268	PHE
1	3c	6	ASN
1	3d	252	ASP
1	4Y	95	ARG
1	4Z	287	SER
1	4Z	357	ASN
1	4a	9	LYS
1	4b	267	ALA
1	4c	274	ASP
1	4d	228	GLN
1	5Y	204	THR
1	5Z	64	SER
1	5Z	292	ALA
1	5a	205	SER
1	5a	411	GLN
1	5b	205	SER
1	5b	395	ALA
1	5c	31	ASN
1	5c	34	SER

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Mol	Chain	Res	Type
1	5c	93	LEU
1	5c	206	SER
1	5c	377	ASN
1	5c	378	ALA
1	5c	416	ALA
1	5d	27	SER
1	5d	146	ASP
1	5d	442	ALA
1	6Y	382	LYS
1	6Y	426	PRO
1	6Y	438	ARG
1	6Z	287	SER
1	6b	230	SER
1	6b	360	ALA
1	6c	438	ARG
1	6c	446	ALA
1	6d	315	PRO
1	7W	6	ASN
1	7X	92	PRO
1	7X	205	SER
1	7X	426	PRO
1	8Y	205	SER
1	8Y	254	ASP
1	8Y	292	ALA
1	8Z	18	TYR
1	8Z	391	SER
1	8a	205	SER
1	8b	357	ASN
1	8c	155	SER
1	8c	426	PRO
1	8d	200	ILE
1	9E	232	ASP
2	1e	49	LYS
2	1e	59	PRO
2	1g	49	LYS
2	1g	59	PRO
2	2Z	11	SER
2	2a	11	SER
2	2b	11	SER
2	2c	11	SER
2	2d	11	SER
2	3f	49	LYS

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

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

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

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Mol	Chain	Res	Type
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	1A	392	THR
1	1B	233	TRP
1	1B	442	ALA
1	1E	318	LEU
1	1F	202	GLU
1	3C	19	ASP
1	3D	30	ASP
1	3D	65	LEU
1	4B	93	LEU
1	4B	210	LEU
1	4B	388	GLU
1	4C	276	LEU
1	4F	408	GLU

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Mol	Chain	Res	Type
1	5A	437	ILE
1	5B	343	SER
1	5E	346	VAL
1	5F	397	THR
1	6A	439	PRO
1	6E	18	TYR
1	6E	203	PRO
1	6E	378	ALA
1	6E	379	LYS
1	6F	230	SER
1	6F	397	THR
1	6F	402	LEU
1	7A	205	SER
1	7B	374	ARG
1	7C	205	SER
1	7D	227	PRO
1	8C	29	GLY
1	8D	439	PRO
1	8E	408	GLU
1	8F	154	VAL
1	1G	392	THR
1	1H	233	TRP
1	1H	442	ALA
1	1K	318	LEU
1	1L	202	GLU
1	3I	19	ASP
1	3J	30	ASP
1	3J	65	LEU
1	4H	93	LEU
1	4H	210	LEU
1	4H	388	GLU
1	4I	276	LEU
1	4L	408	GLU
1	5G	437	ILE
1	5H	343	SER
1	5K	346	VAL
1	5L	397	THR
1	6G	439	PRO
1	6K	18	TYR
1	6K	203	PRO
1	6K	378	ALA
1	6K	379	LYS

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Mol	Chain	Res	Type
1	6L	150	LYS
1	6L	230	SER
1	6L	397	THR
1	6L	402	LEU
1	7F	205	SER
1	7G	374	ARG
1	7H	205	SER
1	7I	227	PRO
1	8I	29	GLY
1	8J	439	PRO
1	8K	408	GLU
1	8L	154	VAL
1	1M	392	THR
1	1N	233	TRP
1	1N	442	ALA
1	1Q	318	LEU
1	1R	202	GLU
1	3O	19	ASP
1	3P	30	ASP
1	3P	65	LEU
1	4N	93	LEU
1	4N	210	LEU
1	4N	388	GLU
1	4O	276	LEU
1	4R	408	GLU
1	5M	437	ILE
1	5N	343	SER
1	5Q	346	VAL
1	5R	397	THR
1	6M	439	PRO
1	6Q	18	TYR
1	6Q	203	PRO
1	6Q	378	ALA
1	6Q	379	LYS
1	6R	150	LYS
1	6R	230	SER
1	6R	397	THR
1	6R	402	LEU
1	7K	205	SER
1	7L	374	ARG
1	7M	205	SER
1	7N	227	PRO

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Mol	Chain	Res	Type
1	8O	29	GLY
1	8P	439	PRO
1	8Q	408	GLU
1	8R	154	VAL
1	1S	392	THR
1	1T	233	TRP
1	1T	442	ALA
1	1W	318	LEU
1	1X	202	GLU
1	3U	19	ASP
1	3U	263	VAL
1	3V	30	ASP
1	3V	65	LEU
1	4T	93	LEU
1	4T	210	LEU
1	4T	388	GLU
1	4U	276	LEU
1	4X	408	GLU
1	5S	437	ILE
1	5T	343	SER
1	5W	346	VAL
1	5X	397	THR
1	6S	439	PRO
1	6W	18	TYR
1	6W	203	PRO
1	6W	378	ALA
1	6W	379	LYS
1	6X	150	LYS
1	6X	230	SER
1	6X	397	THR
1	6X	402	LEU
1	7P	205	SER
1	7Q	374	ARG
1	7R	205	SER
1	7S	227	PRO
1	8U	29	GLY
1	8V	439	PRO
1	8W	408	GLU
1	8X	154	VAL
1	1Y	392	THR
1	1Z	233	TRP
1	1Z	442	ALA

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Mol	Chain	Res	Type
1	1c	318	LEU
1	1d	202	GLU
1	3a	19	ASP
1	3a	263	VAL
1	3b	30	ASP
1	3b	65	LEU
1	4Z	93	LEU
1	4Z	210	LEU
1	4Z	388	GLU
1	4a	276	LEU
1	4d	408	GLU
1	5Y	437	ILE
1	5Z	343	SER
1	5c	346	VAL
1	5d	397	THR
1	6Y	439	PRO
1	6c	18	TYR
1	6c	203	PRO
1	6c	378	ALA
1	6c	379	LYS
1	6d	230	SER
1	6d	397	THR
1	6d	402	LEU
1	7U	205	SER
1	7V	374	ARG
1	7W	205	SER
1	7X	227	PRO
1	8a	29	GLY
1	8b	439	PRO
1	8c	408	GLU
1	8d	154	VAL
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

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Mol	Chain	Res	Type
2	6f	113	SER
2	6h	113	SER
2	7Z	119	SER
2	7a	119	SER
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

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Mol	Chain	Res	Type
2	4i	113	SER
2	5i	113	SER
2	6n	113	SER
2	6p	113	SER
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

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Mol	Chain	Res	Type
2	3v	113	SER
2	3x	113	SER
2	4m	113	SER
2	5m	113	SER
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	1B	276	LEU
1	2B	444	GLY
1	2E	91	ILE
1	3C	297	LYS
1	3E	381	HIS
1	3F	315	PRO
1	5C	24	ILE
1	6B	315	PRO
1	6D	29	GLY
1	6E	444	GLY
1	6F	150	LYS
1	7C	206	SER
1	7D	336	ALA
1	8A	276	LEU
1	1H	276	LEU
1	2G	444	GLY
1	2J	91	ILE
1	3I	297	LYS
1	3K	381	HIS
1	3L	315	PRO
1	4K	428	LEU
1	5I	24	ILE
1	5L	318	LEU
1	6H	315	PRO
1	6J	29	GLY
1	6K	444	GLY
1	7H	206	SER

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Mol	Chain	Res	Type
1	7I	336	ALA
1	8G	276	LEU
1	1N	276	LEU
1	2L	444	GLY
1	2O	91	ILE
1	3O	297	LYS
1	3Q	381	HIS
1	3R	315	PRO
1	4Q	428	LEU
1	5O	24	ILE
1	6N	315	PRO
1	6P	29	GLY
1	6Q	444	GLY
1	7M	206	SER
1	7N	336	ALA
1	8M	276	LEU
1	1T	276	LEU
1	2Q	444	GLY
1	2T	91	ILE
1	3U	297	LYS
1	3W	381	HIS
1	3X	315	PRO
1	4W	428	LEU
1	5U	24	ILE
1	6T	315	PRO
1	6V	29	GLY
1	6W	444	GLY
1	7R	206	SER
1	7S	336	ALA
1	7T	77	VAL
1	8S	276	LEU
1	1Z	276	LEU
1	2V	444	GLY
1	2Y	91	ILE
1	3a	297	LYS
1	3c	381	HIS
1	3d	315	PRO
1	5a	24	ILE
1	6Z	315	PRO
1	6b	29	GLY
1	6c	444	GLY
1	6d	150	LYS

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Mol	Chain	Res	Type
1	7W	206	SER
1	7X	336	ALA
1	7Y	77	VAL
1	8Y	276	LEU
1	2A	315	PRO
1	4B	229	GLY
1	4D	315	PRO
1	5C	53	ILE
1	6C	92	PRO
1	7D	226	LEU
1	7E	77	VAL
1	8B	203	PRO
1	8F	438	ARG
1	2F	315	PRO
1	4H	229	GLY
1	4J	315	PRO
1	5I	53	ILE
1	6I	92	PRO
1	7I	226	LEU
1	7J	77	VAL
1	8H	203	PRO
1	8L	438	ARG
1	2K	315	PRO
1	4N	229	GLY
1	4P	315	PRO
1	5O	53	ILE
1	6O	92	PRO
1	7N	226	LEU
1	7O	77	VAL
1	8N	203	PRO
1	8R	438	ARG
1	2P	315	PRO
1	4T	229	GLY
1	4V	315	PRO
1	5U	53	ILE
1	6U	92	PRO
1	7S	226	LEU
1	8T	203	PRO
1	8X	438	ARG
1	2U	315	PRO
1	4Z	229	GLY
1	4b	315	PRO

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Mol	Chain	Res	Type
1	5a	53	ILE
1	6Z	48	GLY
1	6a	92	PRO
1	8Z	203	PRO
1	8d	438	ARG
2	2Z	59	PRO
2	2b	59	PRO
2	2d	59	PRO
2	7Z	59	PRO
2	7a	59	PRO
2	7b	59	PRO
2	7d	59	PRO
2	2e	59	PRO
2	2g	59	PRO
2	2i	59	PRO
2	7e	59	PRO
2	7f	59	PRO
2	7g	59	PRO
2	7i	59	PRO
2	9G	59	PRO
2	2j	59	PRO
2	2k	59	PRO
2	7j	59	PRO
2	7k	59	PRO
2	7l	59	PRO
2	2o	59	PRO
2	7p	59	PRO
2	7s	59	PRO
2	2t	59	PRO
2	2u	59	PRO
2	2v	59	PRO
2	2x	59	PRO
2	7t	59	PRO
2	7u	59	PRO
2	7v	59	PRO
2	7x	59	PRO
1	2D	92	PRO
1	4C	203	PRO
1	5A	92	PRO
1	6B	48	GLY
1	6D	425	LYS
1	7B	315	PRO

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Mol	Chain	Res	Type
1	2I	92	PRO
1	4I	203	PRO
1	5G	92	PRO
1	6H	48	GLY
1	6J	425	LYS
1	7G	315	PRO
1	2N	92	PRO
1	4O	203	PRO
1	5M	92	PRO
1	6N	48	GLY
1	6P	425	LYS
1	7L	315	PRO
1	2S	92	PRO
1	4U	203	PRO
1	5S	92	PRO
1	6T	48	GLY
1	6V	425	LYS
1	7Q	315	PRO
1	2X	92	PRO
1	4a	203	PRO
1	5Y	92	PRO
1	6b	425	LYS
1	7V	315	PRO
1	7X	226	LEU
2	2a	59	PRO
2	2c	59	PRO
2	7c	59	PRO
2	9F	59	PRO
2	2f	59	PRO
2	2h	59	PRO
2	7h	59	PRO
2	2l	59	PRO
2	2m	59	PRO
2	2n	59	PRO
2	7m	59	PRO
2	7n	59	PRO
2	9H	59	PRO
2	2p	59	PRO
2	2q	59	PRO
2	2r	59	PRO
2	2s	59	PRO
2	7o	59	PRO

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Mol	Chain	Res	Type
2	7q	59	PRO
2	7r	59	PRO
2	9I	59	PRO
2	2w	59	PRO
2	7w	59	PRO
2	9J	59	PRO
1	2A	277	GLY
1	2C	393	GLY
1	2E	47	VAL
1	2E	315	PRO
1	3B	227	PRO
1	8E	315	PRO
1	8E	398	GLY
1	8F	444	GLY
1	2F	277	GLY
1	2H	393	GLY
1	2J	47	VAL
1	2J	315	PRO
1	3H	227	PRO
1	8K	315	PRO
1	8K	398	GLY
1	8L	444	GLY
1	2K	277	GLY
1	2M	393	GLY
1	2O	47	VAL
1	2O	315	PRO
1	3N	227	PRO
1	8Q	315	PRO
1	8R	444	GLY
1	2P	277	GLY
1	2R	393	GLY
1	2T	47	VAL
1	2T	315	PRO
1	3T	227	PRO
1	8W	315	PRO
1	8W	398	GLY
1	8X	444	GLY
1	2W	393	GLY
1	2Y	47	VAL
1	2Y	315	PRO
1	8c	315	PRO
1	8c	398	GLY

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Mol	Chain	Res	Type
1	8d	444	GLY
1	1D	314	ASN
1	3B	426	PRO
1	3F	29	GLY
1	4F	14	ILE
1	6B	21	VAL
1	7B	29	GLY
1	7C	425	LYS
1	8C	396	ILE
1	9A	425	LYS
1	1J	314	ASN
1	3H	426	PRO
1	3L	29	GLY
1	4L	14	ILE
1	6H	21	VAL
1	7G	29	GLY
1	7H	425	LYS
1	8I	396	ILE
1	9B	425	LYS
1	1P	314	ASN
1	3N	426	PRO
1	3R	29	GLY
1	4R	14	ILE
1	6N	21	VAL
1	7L	29	GLY
1	7M	425	LYS
1	8O	396	ILE
1	8Q	398	GLY
1	9C	425	LYS
1	1V	314	ASN
1	3T	426	PRO
1	3X	29	GLY
1	4X	14	ILE
1	6T	21	VAL
1	7Q	29	GLY
1	7R	425	LYS
1	8U	396	ILE
1	9D	425	LYS
1	1b	314	ASN
1	2U	277	GLY
1	3Z	227	PRO
1	3Z	426	PRO

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Mol	Chain	Res	Type
1	3d	29	GLY
1	4d	14	ILE
1	6Z	21	VAL
1	7V	29	GLY
1	7W	425	LYS
1	8a	396	ILE
1	9E	425	LYS
1	1E	425	LYS
1	5F	289	GLY
1	8E	425	LYS
1	1K	425	LYS
1	5L	289	GLY
1	8K	425	LYS
1	1Q	425	LYS
1	5R	289	GLY
1	8Q	425	LYS
1	1W	425	LYS
1	5X	289	GLY
1	8W	425	LYS
1	1c	425	LYS
1	5d	289	GLY
1	8c	425	LYS

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1A	370/384 (96%)	370 (100%)	0	100	100
1	1B	381/384 (99%)	380 (100%)	1 (0%)	92	97
1	1C	381/384 (99%)	381 (100%)	0	100	100
1	1D	381/384 (99%)	381 (100%)	0	100	100
1	1E	376/384 (98%)	376 (100%)	0	100	100
1	1F	379/384 (99%)	379 (100%)	0	100	100
1	1G	370/384 (96%)	370 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1H	381/384 (99%)	380 (100%)	1 (0%)	92	97
1	1I	381/384 (99%)	381 (100%)	0	100	100
1	1J	381/384 (99%)	381 (100%)	0	100	100
1	1K	376/384 (98%)	376 (100%)	0	100	100
1	1L	379/384 (99%)	379 (100%)	0	100	100
1	1M	370/384 (96%)	370 (100%)	0	100	100
1	1N	381/384 (99%)	380 (100%)	1 (0%)	92	97
1	1O	381/384 (99%)	381 (100%)	0	100	100
1	1P	381/384 (99%)	381 (100%)	0	100	100
1	1Q	376/384 (98%)	376 (100%)	0	100	100
1	1R	379/384 (99%)	379 (100%)	0	100	100
1	1S	370/384 (96%)	370 (100%)	0	100	100
1	1T	381/384 (99%)	380 (100%)	1 (0%)	92	97
1	1U	381/384 (99%)	381 (100%)	0	100	100
1	1V	381/384 (99%)	381 (100%)	0	100	100
1	1W	376/384 (98%)	376 (100%)	0	100	100
1	1X	379/384 (99%)	379 (100%)	0	100	100
1	1Y	370/384 (96%)	370 (100%)	0	100	100
1	1Z	381/384 (99%)	380 (100%)	1 (0%)	92	97
1	1a	381/384 (99%)	381 (100%)	0	100	100
1	1b	381/384 (99%)	381 (100%)	0	100	100
1	1c	376/384 (98%)	376 (100%)	0	100	100
1	1d	379/384 (99%)	379 (100%)	0	100	100
1	2A	374/384 (97%)	374 (100%)	0	100	100
1	2B	381/384 (99%)	377 (99%)	4 (1%)	76	88
1	2C	381/384 (99%)	381 (100%)	0	100	100
1	2D	381/384 (99%)	381 (100%)	0	100	100
1	2E	381/384 (99%)	380 (100%)	1 (0%)	92	97
1	2F	374/384 (97%)	374 (100%)	0	100	100
1	2G	381/384 (99%)	377 (99%)	4 (1%)	76	88
1	2H	381/384 (99%)	381 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2I	381/384 (99%)	381 (100%)	0	100	100
1	2J	381/384 (99%)	380 (100%)	1 (0%)	92	97
1	2K	374/384 (97%)	374 (100%)	0	100	100
1	2L	381/384 (99%)	377 (99%)	4 (1%)	76	88
1	2M	381/384 (99%)	381 (100%)	0	100	100
1	2N	381/384 (99%)	381 (100%)	0	100	100
1	2O	381/384 (99%)	380 (100%)	1 (0%)	92	97
1	2P	374/384 (97%)	374 (100%)	0	100	100
1	2Q	381/384 (99%)	377 (99%)	4 (1%)	76	88
1	2R	381/384 (99%)	381 (100%)	0	100	100
1	2S	381/384 (99%)	381 (100%)	0	100	100
1	2T	381/384 (99%)	380 (100%)	1 (0%)	92	97
1	2U	374/384 (97%)	374 (100%)	0	100	100
1	2V	381/384 (99%)	377 (99%)	4 (1%)	76	88
1	2W	381/384 (99%)	381 (100%)	0	100	100
1	2X	381/384 (99%)	381 (100%)	0	100	100
1	2Y	381/384 (99%)	380 (100%)	1 (0%)	92	97
1	3A	376/384 (98%)	376 (100%)	0	100	100
1	3B	376/384 (98%)	376 (100%)	0	100	100
1	3C	381/384 (99%)	381 (100%)	0	100	100
1	3D	381/384 (99%)	380 (100%)	1 (0%)	92	97
1	3E	381/384 (99%)	381 (100%)	0	100	100
1	3F	381/384 (99%)	380 (100%)	1 (0%)	92	97
1	3G	376/384 (98%)	376 (100%)	0	100	100
1	3H	376/384 (98%)	376 (100%)	0	100	100
1	3I	381/384 (99%)	381 (100%)	0	100	100
1	3J	381/384 (99%)	380 (100%)	1 (0%)	92	97
1	3K	381/384 (99%)	381 (100%)	0	100	100
1	3L	381/384 (99%)	380 (100%)	1 (0%)	92	97
1	3M	376/384 (98%)	376 (100%)	0	100	100
1	3N	376/384 (98%)	376 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	3O	381/384 (99%)	381 (100%)	0	100	100
1	3P	381/384 (99%)	380 (100%)	1 (0%)	92	97
1	3Q	381/384 (99%)	381 (100%)	0	100	100
1	3R	381/384 (99%)	380 (100%)	1 (0%)	92	97
1	3S	376/384 (98%)	376 (100%)	0	100	100
1	3T	376/384 (98%)	376 (100%)	0	100	100
1	3U	381/384 (99%)	381 (100%)	0	100	100
1	3V	381/384 (99%)	380 (100%)	1 (0%)	92	97
1	3W	381/384 (99%)	381 (100%)	0	100	100
1	3X	381/384 (99%)	380 (100%)	1 (0%)	92	97
1	3Y	376/384 (98%)	376 (100%)	0	100	100
1	3Z	376/384 (98%)	376 (100%)	0	100	100
1	3a	381/384 (99%)	381 (100%)	0	100	100
1	3b	381/384 (99%)	380 (100%)	1 (0%)	92	97
1	3c	381/384 (99%)	381 (100%)	0	100	100
1	3d	381/384 (99%)	380 (100%)	1 (0%)	92	97
1	4A	376/384 (98%)	376 (100%)	0	100	100
1	4B	376/384 (98%)	376 (100%)	0	100	100
1	4C	376/384 (98%)	376 (100%)	0	100	100
1	4D	376/384 (98%)	376 (100%)	0	100	100
1	4E	381/384 (99%)	381 (100%)	0	100	100
1	4F	381/384 (99%)	381 (100%)	0	100	100
1	4G	376/384 (98%)	376 (100%)	0	100	100
1	4H	376/384 (98%)	376 (100%)	0	100	100
1	4I	376/384 (98%)	376 (100%)	0	100	100
1	4J	376/384 (98%)	376 (100%)	0	100	100
1	4K	381/384 (99%)	381 (100%)	0	100	100
1	4L	381/384 (99%)	381 (100%)	0	100	100
1	4M	376/384 (98%)	376 (100%)	0	100	100
1	4N	376/384 (98%)	376 (100%)	0	100	100
1	4O	376/384 (98%)	376 (100%)	0	100	100

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	6R	381/384 (99%)	381 (100%)	0	100	100
1	6S	381/384 (99%)	381 (100%)	0	100	100
1	6T	381/384 (99%)	381 (100%)	0	100	100
1	6U	376/384 (98%)	376 (100%)	0	100	100
1	6V	376/384 (98%)	376 (100%)	0	100	100
1	6W	381/384 (99%)	381 (100%)	0	100	100
1	6X	381/384 (99%)	381 (100%)	0	100	100
1	6Y	381/384 (99%)	381 (100%)	0	100	100
1	6Z	381/384 (99%)	381 (100%)	0	100	100
1	6a	376/384 (98%)	376 (100%)	0	100	100
1	6b	376/384 (98%)	376 (100%)	0	100	100
1	6c	381/384 (99%)	381 (100%)	0	100	100
1	6d	381/384 (99%)	381 (100%)	0	100	100
1	7A	381/384 (99%)	381 (100%)	0	100	100
1	7B	381/384 (99%)	381 (100%)	0	100	100
1	7C	381/384 (99%)	381 (100%)	0	100	100
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%)	381 (100%)	0	100	100
1	7G	381/384 (99%)	381 (100%)	0	100	100
1	7H	381/384 (99%)	381 (100%)	0	100	100
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%)	381 (100%)	0	100	100
1	7L	381/384 (99%)	381 (100%)	0	100	100
1	7M	381/384 (99%)	381 (100%)	0	100	100
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%)	381 (100%)	0	100	100
1	7Q	381/384 (99%)	381 (100%)	0	100	100
1	7R	381/384 (99%)	381 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	7S	381/384 (99%)	381 (100%)	0	100	100
1	7T	381/384 (99%)	381 (100%)	0	100	100
1	7U	381/384 (99%)	381 (100%)	0	100	100
1	7V	381/384 (99%)	381 (100%)	0	100	100
1	7W	381/384 (99%)	381 (100%)	0	100	100
1	7X	381/384 (99%)	381 (100%)	0	100	100
1	7Y	381/384 (99%)	381 (100%)	0	100	100
1	8A	381/384 (99%)	381 (100%)	0	100	100
1	8B	381/384 (99%)	381 (100%)	0	100	100
1	8C	381/384 (99%)	381 (100%)	0	100	100
1	8D	381/384 (99%)	381 (100%)	0	100	100
1	8E	381/384 (99%)	381 (100%)	0	100	100
1	8F	381/384 (99%)	381 (100%)	0	100	100
1	8G	381/384 (99%)	381 (100%)	0	100	100
1	8H	381/384 (99%)	381 (100%)	0	100	100
1	8I	381/384 (99%)	381 (100%)	0	100	100
1	8J	381/384 (99%)	381 (100%)	0	100	100
1	8K	381/384 (99%)	381 (100%)	0	100	100
1	8L	381/384 (99%)	381 (100%)	0	100	100
1	8M	381/384 (99%)	381 (100%)	0	100	100
1	8N	381/384 (99%)	381 (100%)	0	100	100
1	8O	381/384 (99%)	381 (100%)	0	100	100
1	8P	381/384 (99%)	381 (100%)	0	100	100
1	8Q	381/384 (99%)	381 (100%)	0	100	100
1	8R	381/384 (99%)	381 (100%)	0	100	100
1	8S	381/384 (99%)	381 (100%)	0	100	100
1	8T	381/384 (99%)	381 (100%)	0	100	100
1	8U	381/384 (99%)	381 (100%)	0	100	100
1	8V	381/384 (99%)	381 (100%)	0	100	100
1	8W	381/384 (99%)	381 (100%)	0	100	100
1	8X	381/384 (99%)	381 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	8Y	381/384 (99%)	381 (100%)	0	100	100
1	8Z	381/384 (99%)	381 (100%)	0	100	100
1	8a	381/384 (99%)	381 (100%)	0	100	100
1	8b	381/384 (99%)	381 (100%)	0	100	100
1	8c	381/384 (99%)	381 (100%)	0	100	100
1	8d	381/384 (99%)	381 (100%)	0	100	100
1	9A	381/384 (99%)	380 (100%)	1 (0%)	92	97
1	9B	381/384 (99%)	380 (100%)	1 (0%)	92	97
1	9C	381/384 (99%)	380 (100%)	1 (0%)	92	97
1	9D	381/384 (99%)	380 (100%)	1 (0%)	92	97
1	9E	381/384 (99%)	380 (100%)	1 (0%)	92	97
2	1e	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	1f	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	1g	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	1h	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	1i	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	1j	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	1k	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	1l	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	1m	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	1n	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	1o	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	1p	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	1q	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	1r	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	1s	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	1t	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	1u	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	1v	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	1w	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	1x	235/229 (103%)	233 (99%)	2 (1%)	78	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	2Z	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	2a	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	2b	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	2c	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	2d	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	2e	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	2f	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	2g	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	2h	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	2i	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	2j	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	2k	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	2l	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	2m	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	2n	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	2o	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	2p	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	2q	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	2r	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	2s	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	2t	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	2u	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	2v	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	2w	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	2x	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	3e	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	3f	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	3g	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	3h	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	3i	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	3j	236/229 (103%)	234 (99%)	2 (1%)	81	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	3k	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	3l	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	3m	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	3n	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	3o	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	3p	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	3q	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	3r	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	3s	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	3t	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	3u	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	3v	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	3w	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	3x	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	4e	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	4f	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	4g	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	4h	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	4i	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	4j	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	4k	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	4l	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	4m	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	4n	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	5e	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	5f	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	5g	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	5h	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	5i	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	5j	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	5k	236/229 (103%)	234 (99%)	2 (1%)	81	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	5l	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	5m	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	5n	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	6e	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	6f	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	6g	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	6h	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	6i	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	6j	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	6k	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	6l	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	6m	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	6n	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	6o	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	6p	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	6q	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	6r	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	6s	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	6t	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	6u	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	6v	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	6w	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	6x	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	7Z	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	7a	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	7b	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	7c	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	7d	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	7e	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	7f	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	7g	236/229 (103%)	234 (99%)	2 (1%)	81	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	7h	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	7i	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	7j	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	7k	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	7l	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	7m	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	7n	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	7o	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	7p	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	7q	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	7r	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	7s	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	7t	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	7u	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	7v	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	7w	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	7x	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	8e	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	8f	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	8g	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	8h	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	8i	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	8j	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	8k	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	8l	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	8m	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	8n	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	8o	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	8p	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	8q	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	8r	236/229 (103%)	234 (99%)	2 (1%)	81	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	8s	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	8t	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	8u	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	8v	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	8w	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	8x	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	8y	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	8z	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	9F	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	9G	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	9H	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	9I	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	9J	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	9K	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	9L	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	9M	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	9N	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	9O	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	9P	235/229 (103%)	233 (99%)	2 (1%)	78	90
2	9Q	236/229 (103%)	234 (99%)	2 (1%)	81	91
2	9R	235/229 (103%)	233 (99%)	2 (1%)	78	90
All	All	127995/128025 (100%)	127620 (100%)	375 (0%)	92	97

All (375) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1B	25	ARG
1	2B	354	VAL
1	2B	357	ASN
1	2B	358	ILE
1	2B	410	ASN
1	2E	80	ASN
1	3D	319	TYR
1	3F	68	ARG
1	9A	270	MET

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Mol	Chain	Res	Type
1	1H	25	ARG
1	2G	354	VAL
1	2G	357	ASN
1	2G	358	ILE
1	2G	410	ASN
1	2J	80	ASN
1	3J	319	TYR
1	3L	68	ARG
1	9B	270	MET
1	1N	25	ARG
1	2L	354	VAL
1	2L	357	ASN
1	2L	358	ILE
1	2L	410	ASN
1	2O	80	ASN
1	3P	319	TYR
1	3R	68	ARG
1	9C	270	MET
1	1T	25	ARG
1	2Q	354	VAL
1	2Q	357	ASN
1	2Q	358	ILE
1	2Q	410	ASN
1	2T	80	ASN
1	3V	319	TYR
1	3X	68	ARG
1	9D	270	MET
1	1Z	25	ARG
1	2V	354	VAL
1	2V	357	ASN
1	2V	358	ILE
1	2V	410	ASN
1	2Y	80	ASN
1	3b	319	TYR
1	3d	68	ARG
1	9E	270	MET
2	1e	110	LEU
2	1e	251	VAL
2	1f	116	LYS
2	1f	251	VAL
2	1g	110	LEU
2	1g	251	VAL

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 (966) such sidechains are listed below:

Mol	Chain	Res	Type
1	1A	337	ASN
1	1F	90	GLN
1	2A	28	GLN
1	2B	28	GLN
1	2C	28	GLN
1	2C	58	GLN
1	3A	58	GLN
1	3A	305	ASN

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Mol	Chain	Res	Type
1	3C	447	GLN
1	3E	447	GLN
1	3F	447	GLN
1	4E	278	ASN
1	5A	58	GLN
1	5E	145	GLN
1	5F	447	GLN
1	6B	145	GLN
1	6F	58	GLN
1	7B	142	GLN
1	7C	28	GLN
1	7C	410	ASN
1	7E	407	ASN
1	8A	447	GLN
1	8F	407	ASN
1	9A	28	GLN
1	1G	337	ASN
1	1L	90	GLN
1	2F	28	GLN
1	2G	28	GLN
1	2H	28	GLN
1	2H	58	GLN
1	3G	58	GLN
1	3I	447	GLN
1	3K	447	GLN
1	3L	447	GLN
1	4K	278	ASN
1	5G	58	GLN
1	5K	145	GLN
1	5L	447	GLN
1	6L	58	GLN
1	7G	142	GLN
1	7H	28	GLN
1	7H	142	GLN
1	7H	410	ASN
1	7J	407	ASN
1	8L	407	ASN
1	9B	28	GLN
1	1M	337	ASN
1	1R	90	GLN
1	2K	28	GLN
1	2L	28	GLN

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Mol	Chain	Res	Type
1	2M	28	GLN
1	2M	58	GLN
1	2O	447	GLN
1	3M	58	GLN
1	3M	305	ASN
1	3O	447	GLN
1	3Q	447	GLN
1	4Q	278	ASN
1	5M	58	GLN
1	5Q	145	GLN
1	5R	447	GLN
1	6R	58	GLN
1	7L	142	GLN
1	7L	447	GLN
1	7M	410	ASN
1	7O	26	ASN
1	8M	447	GLN
1	9C	28	GLN
1	1S	337	ASN
1	1W	141	HIS
1	1X	90	GLN
1	2P	28	GLN
1	2Q	366	GLN
1	2R	28	GLN
1	2R	58	GLN
1	2T	447	GLN
1	3S	58	GLN
1	3S	305	ASN
1	3U	447	GLN
1	3W	447	GLN
1	4W	278	ASN
1	5S	58	GLN
1	5W	145	GLN
1	5X	447	GLN
1	6T	145	GLN
1	6X	58	GLN
1	7P	407	ASN
1	7Q	142	GLN
1	7Q	366	GLN
1	7Q	447	GLN
1	7R	142	GLN
1	7R	410	ASN

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Mol	Chain	Res	Type
1	7S	26	ASN
1	9D	28	GLN
1	1Y	337	ASN
1	1a	447	GLN
1	1d	90	GLN
1	2U	28	GLN
1	2V	28	GLN
1	2W	28	GLN
1	2W	58	GLN
1	3Y	58	GLN
1	3Y	305	ASN
1	3a	447	GLN
1	3c	447	GLN
1	4c	278	ASN
1	5Y	58	GLN
1	5c	145	GLN
1	6d	58	GLN
1	7V	142	GLN
1	7V	366	GLN
1	7W	142	GLN
1	7W	410	ASN
1	7X	26	ASN
1	8Y	447	GLN
1	9E	28	GLN
2	1e	56	ASN
2	1e	159	ASN
2	1e	166	ASN
2	1e	179	ASN
2	1e	197	GLN
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	159	ASN
2	1g	166	ASN
2	1g	179	ASN
2	1g	218	ASN
2	1g	267	ASN
2	1h	56	ASN
2	1h	76	ASN

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Mol	Chain	Res	Type
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	197	GLN
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	159	ASN
2	2b	166	ASN
2	2b	179	ASN
2	2b	197	GLN
2	2b	218	ASN
2	2c	159	ASN
2	2c	166	ASN
2	2c	179	ASN
2	2c	218	ASN
2	2d	159	ASN
2	2d	166	ASN
2	2d	179	ASN
2	2d	197	GLN
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	56	ASN
2	3f	159	ASN
2	3f	166	ASN
2	3f	179	ASN
2	3f	197	GLN
2	3f	218	ASN
2	3g	56	ASN
2	3g	76	ASN

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Mol	Chain	Res	Type
2	3g	159	ASN
2	3g	166	ASN
2	3g	179	ASN
2	3g	218	ASN
2	3h	56	ASN
2	3h	159	ASN
2	3h	166	ASN
2	3h	179	ASN
2	3h	197	GLN
2	3h	218	ASN
2	4e	159	ASN
2	4e	166	ASN
2	4e	179	ASN
2	4e	218	ASN
2	4f	56	ASN
2	4f	76	ASN
2	4f	159	ASN
2	4f	166	ASN
2	4f	179	ASN
2	4f	218	ASN
2	5e	56	ASN
2	5e	159	ASN
2	5e	166	ASN
2	5e	179	ASN
2	5e	218	ASN
2	5f	76	ASN
2	5f	159	ASN
2	5f	166	ASN
2	5f	179	ASN
2	5f	218	ASN
2	6e	23	GLN
2	6e	76	ASN
2	6e	159	ASN
2	6e	166	ASN
2	6e	179	ASN
2	6e	218	ASN
2	6f	159	ASN
2	6f	166	ASN
2	6f	179	ASN
2	6f	218	ASN
2	6g	56	ASN
2	6g	76	ASN

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Mol	Chain	Res	Type
2	6g	159	ASN
2	6g	166	ASN
2	6g	179	ASN
2	6g	218	ASN
2	6h	23	GLN
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	197	GLN
2	7Z	218	ASN
2	7a	159	ASN
2	7a	166	ASN
2	7a	179	ASN
2	7a	218	ASN
2	7b	23	GLN
2	7b	159	ASN
2	7b	166	ASN
2	7b	179	ASN
2	7b	218	ASN
2	7c	56	ASN
2	7c	159	ASN
2	7c	166	ASN
2	7c	179	ASN
2	7c	218	ASN
2	7d	159	ASN
2	7d	166	ASN
2	7d	179	ASN
2	7d	218	ASN
2	8e	76	ASN
2	8e	159	ASN
2	8e	166	ASN
2	8e	179	ASN
2	8e	218	ASN
2	8e	267	ASN
2	8f	159	ASN
2	8f	166	ASN
2	8f	179	ASN

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Mol	Chain	Res	Type
2	8f	218	ASN
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	218	ASN
2	8j	76	ASN
2	8j	159	ASN
2	8j	166	ASN
2	8j	179	ASN
2	8j	218	ASN
2	9F	159	ASN
2	9F	166	ASN
2	9F	179	ASN
2	9F	197	GLN
2	9F	218	ASN
2	1i	56	ASN
2	1i	159	ASN
2	1i	166	ASN
2	1i	179	ASN
2	1i	197	GLN
2	1i	218	ASN
2	1j	76	ASN
2	1j	159	ASN
2	1j	166	ASN
2	1j	179	ASN
2	1j	218	ASN
2	1k	56	ASN
2	1k	159	ASN
2	1k	166	ASN
2	1k	179	ASN
2	1k	218	ASN

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Mol	Chain	Res	Type
2	1k	267	ASN
2	1l	56	ASN
2	1l	76	ASN
2	1l	159	ASN
2	1l	166	ASN
2	1l	179	ASN
2	1l	218	ASN
2	2e	159	ASN
2	2e	166	ASN
2	2e	179	ASN
2	2e	197	GLN
2	2e	218	ASN
2	2f	103	GLN
2	2f	159	ASN
2	2f	166	ASN
2	2f	179	ASN
2	2f	218	ASN
2	2g	159	ASN
2	2g	166	ASN
2	2g	179	ASN
2	2g	197	GLN
2	2g	218	ASN
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	197	GLN
2	2i	218	ASN
2	3i	56	ASN
2	3i	76	ASN
2	3i	159	ASN
2	3i	166	ASN
2	3i	179	ASN
2	3i	218	ASN
2	3j	56	ASN
2	3j	159	ASN
2	3j	166	ASN
2	3j	179	ASN
2	3j	197	GLN

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Mol	Chain	Res	Type
2	3j	218	ASN
2	3k	56	ASN
2	3k	76	ASN
2	3k	159	ASN
2	3k	166	ASN
2	3k	179	ASN
2	3k	218	ASN
2	3l	56	ASN
2	3l	159	ASN
2	3l	166	ASN
2	3l	179	ASN
2	3l	197	GLN
2	3l	218	ASN
2	4g	159	ASN
2	4g	166	ASN
2	4g	179	ASN
2	4g	218	ASN
2	4h	56	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	218	ASN
2	6i	23	GLN
2	6i	76	ASN
2	6i	159	ASN
2	6i	166	ASN
2	6i	179	ASN
2	6i	218	ASN
2	6j	159	ASN
2	6j	166	ASN
2	6j	179	ASN

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Mol	Chain	Res	Type
2	6j	218	ASN
2	6k	56	ASN
2	6k	76	ASN
2	6k	159	ASN
2	6k	166	ASN
2	6k	179	ASN
2	6k	218	ASN
2	6l	23	GLN
2	6l	159	ASN
2	6l	166	ASN
2	6l	179	ASN
2	6l	218	ASN
2	7e	159	ASN
2	7e	166	ASN
2	7e	179	ASN
2	7e	197	GLN
2	7e	218	ASN
2	7f	159	ASN
2	7f	166	ASN
2	7f	179	ASN
2	7f	218	ASN
2	7g	23	GLN
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
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	8k	267	ASN
2	8l	159	ASN

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Mol	Chain	Res	Type
2	8l	166	ASN
2	8l	179	ASN
2	8l	218	ASN
2	8m	159	ASN
2	8m	166	ASN
2	8m	179	ASN
2	8m	197	GLN
2	8m	218	ASN
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	159	ASN
2	9G	166	ASN
2	9G	171	GLN
2	9G	179	ASN
2	9G	185	GLN
2	9G	197	GLN
2	9G	218	ASN
2	1m	56	ASN
2	1m	159	ASN
2	1m	166	ASN
2	1m	179	ASN
2	1m	197	GLN
2	1m	218	ASN
2	1n	76	ASN
2	1n	159	ASN
2	1n	166	ASN
2	1n	179	ASN
2	1n	218	ASN
2	1o	159	ASN
2	1o	166	ASN

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Mol	Chain	Res	Type
2	1o	179	ASN
2	1o	218	ASN
2	1o	267	ASN
2	1p	56	ASN
2	1p	76	ASN
2	1p	159	ASN
2	1p	166	ASN
2	1p	179	ASN
2	1p	218	ASN
2	2j	159	ASN
2	2j	166	ASN
2	2j	179	ASN
2	2j	197	GLN
2	2j	218	ASN
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	197	GLN
2	2l	218	ASN
2	2m	159	ASN
2	2m	166	ASN
2	2m	179	ASN
2	2m	203	ASN
2	2m	218	ASN
2	2n	103	GLN
2	2n	159	ASN
2	2n	166	ASN
2	2n	179	ASN
2	2n	218	ASN
2	3m	56	ASN
2	3m	76	ASN
2	3m	159	ASN
2	3m	166	ASN
2	3m	179	ASN
2	3m	218	ASN
2	3n	56	ASN
2	3n	159	ASN

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Mol	Chain	Res	Type
2	3n	166	ASN
2	3n	179	ASN
2	3n	197	GLN
2	3n	218	ASN
2	3o	56	ASN
2	3o	76	ASN
2	3o	159	ASN
2	3o	166	ASN
2	3o	179	ASN
2	3o	218	ASN
2	3p	159	ASN
2	3p	166	ASN
2	3p	179	ASN
2	3p	197	GLN
2	3p	218	ASN
2	4i	159	ASN
2	4i	166	ASN
2	4i	179	ASN
2	4i	218	ASN
2	4j	56	ASN
2	4j	76	ASN
2	4j	159	ASN
2	4j	166	ASN
2	4j	179	ASN
2	4j	218	ASN
2	5i	159	ASN
2	5i	166	ASN
2	5i	179	ASN
2	5i	218	ASN
2	5j	76	ASN
2	5j	159	ASN
2	5j	166	ASN
2	5j	179	ASN
2	5j	218	ASN
2	6m	23	GLN
2	6m	56	ASN
2	6m	76	ASN
2	6m	159	ASN
2	6m	166	ASN
2	6m	179	ASN
2	6m	218	ASN
2	6n	159	ASN

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Mol	Chain	Res	Type
2	6n	166	ASN
2	6n	179	ASN
2	6n	218	ASN
2	6o	56	ASN
2	6o	76	ASN
2	6o	159	ASN
2	6o	166	ASN
2	6o	179	ASN
2	6o	218	ASN
2	6p	23	GLN
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	197	GLN
2	7j	218	ASN
2	7k	159	ASN
2	7k	166	ASN
2	7k	179	ASN
2	7k	218	ASN
2	7l	23	GLN
2	7l	159	ASN
2	7l	166	ASN
2	7l	179	ASN
2	7l	218	ASN
2	7m	56	ASN
2	7m	159	ASN
2	7m	166	ASN
2	7m	179	ASN
2	7m	218	ASN
2	7n	159	ASN
2	7n	166	ASN
2	7n	179	ASN
2	7n	218	ASN
2	8q	76	ASN
2	8q	159	ASN
2	8q	166	ASN
2	8q	179	ASN
2	8q	218	ASN

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Mol	Chain	Res	Type
2	8q	267	ASN
2	8r	159	ASN
2	8r	166	ASN
2	8r	179	ASN
2	8r	218	ASN
2	8s	159	ASN
2	8s	166	ASN
2	8s	179	ASN
2	8s	197	GLN
2	8s	218	ASN
2	8t	76	ASN
2	8t	159	ASN
2	8t	166	ASN
2	8t	179	ASN
2	8t	218	ASN
2	8u	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	159	ASN
2	9H	166	ASN
2	9H	171	GLN
2	9H	179	ASN
2	9H	185	GLN
2	9H	197	GLN
2	9H	218	ASN
2	1q	56	ASN
2	1q	159	ASN
2	1q	166	ASN
2	1q	179	ASN
2	1q	197	GLN
2	1q	218	ASN
2	1r	76	ASN
2	1r	159	ASN
2	1r	166	ASN
2	1r	179	ASN
2	1r	218	ASN

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Mol	Chain	Res	Type
2	1s	159	ASN
2	1s	166	ASN
2	1s	179	ASN
2	1s	218	ASN
2	1s	267	ASN
2	1t	56	ASN
2	1t	76	ASN
2	1t	159	ASN
2	1t	166	ASN
2	1t	179	ASN
2	1t	218	ASN
2	2o	159	ASN
2	2o	166	ASN
2	2o	179	ASN
2	2o	197	GLN
2	2o	218	ASN
2	2p	103	GLN
2	2p	159	ASN
2	2p	166	ASN
2	2p	179	ASN
2	2p	218	ASN
2	2q	64	GLN
2	2q	159	ASN
2	2q	166	ASN
2	2q	179	ASN
2	2q	197	GLN
2	2q	218	ASN
2	2r	159	ASN
2	2r	166	ASN
2	2r	179	ASN
2	2r	203	ASN
2	2r	218	ASN
2	2s	159	ASN
2	2s	166	ASN
2	2s	179	ASN
2	2s	197	GLN
2	2s	218	ASN
2	3q	76	ASN
2	3q	159	ASN
2	3q	166	ASN
2	3q	179	ASN
2	3q	218	ASN

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Mol	Chain	Res	Type
2	3r	56	ASN
2	3r	159	ASN
2	3r	166	ASN
2	3r	179	ASN
2	3r	197	GLN
2	3r	218	ASN
2	3s	56	ASN
2	3s	76	ASN
2	3s	159	ASN
2	3s	166	ASN
2	3s	179	ASN
2	3s	218	ASN
2	3t	159	ASN
2	3t	166	ASN
2	3t	179	ASN
2	3t	197	GLN
2	3t	218	ASN
2	4k	159	ASN
2	4k	166	ASN
2	4k	179	ASN
2	4k	218	ASN
2	4l	56	ASN
2	4l	76	ASN
2	4l	159	ASN
2	4l	166	ASN
2	4l	179	ASN
2	4l	218	ASN
2	5k	159	ASN
2	5k	166	ASN
2	5k	179	ASN
2	5k	218	ASN
2	5l	76	ASN
2	5l	159	ASN
2	5l	166	ASN
2	5l	179	ASN
2	5l	218	ASN
2	6q	23	GLN
2	6q	56	ASN
2	6q	76	ASN
2	6q	159	ASN
2	6q	166	ASN
2	6q	179	ASN

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Mol	Chain	Res	Type
2	6q	218	ASN
2	6r	159	ASN
2	6r	166	ASN
2	6r	179	ASN
2	6r	218	ASN
2	6s	56	ASN
2	6s	76	ASN
2	6s	159	ASN
2	6s	166	ASN
2	6s	179	ASN
2	6s	218	ASN
2	6t	23	GLN
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	197	GLN
2	7o	218	ASN
2	7p	159	ASN
2	7p	166	ASN
2	7p	179	ASN
2	7p	218	ASN
2	7q	23	GLN
2	7q	64	GLN
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	218	ASN
2	7s	159	ASN
2	7s	166	ASN
2	7s	179	ASN
2	7s	218	ASN
2	8w	76	ASN
2	8w	159	ASN

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Mol	Chain	Res	Type
2	8w	166	ASN
2	8w	179	ASN
2	8w	218	ASN
2	8w	267	ASN
2	8x	159	ASN
2	8x	166	ASN
2	8x	179	ASN
2	8x	218	ASN
2	8y	159	ASN
2	8y	166	ASN
2	8y	179	ASN
2	8y	197	GLN
2	8y	218	ASN
2	8z	76	ASN
2	8z	159	ASN
2	8z	166	ASN
2	8z	179	ASN
2	8z	218	ASN
2	9K	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	159	ASN
2	9I	166	ASN
2	9I	171	GLN
2	9I	179	ASN
2	9I	185	GLN
2	9I	197	GLN
2	9I	218	ASN
2	1u	56	ASN
2	1u	159	ASN
2	1u	166	ASN
2	1u	179	ASN
2	1u	218	ASN
2	1v	76	ASN
2	1v	159	ASN
2	1v	166	ASN

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Mol	Chain	Res	Type
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	1w	267	ASN
2	1x	56	ASN
2	1x	76	ASN
2	1x	159	ASN
2	1x	166	ASN
2	1x	179	ASN
2	1x	218	ASN
2	2t	159	ASN
2	2t	166	ASN
2	2t	179	ASN
2	2t	197	GLN
2	2t	218	ASN
2	2u	103	GLN
2	2u	159	ASN
2	2u	166	ASN
2	2u	179	ASN
2	2u	218	ASN
2	2v	159	ASN
2	2v	166	ASN
2	2v	179	ASN
2	2v	197	GLN
2	2v	218	ASN
2	2w	159	ASN
2	2w	166	ASN
2	2w	179	ASN
2	2w	218	ASN
2	2x	159	ASN
2	2x	166	ASN
2	2x	179	ASN
2	2x	197	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

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Mol	Chain	Res	Type
2	3u	218	ASN
2	3v	56	ASN
2	3v	159	ASN
2	3v	166	ASN
2	3v	179	ASN
2	3v	197	GLN
2	3v	218	ASN
2	3w	56	ASN
2	3w	76	ASN
2	3w	159	ASN
2	3w	166	ASN
2	3w	179	ASN
2	3w	218	ASN
2	3x	159	ASN
2	3x	166	ASN
2	3x	179	ASN
2	3x	197	GLN
2	3x	218	ASN
2	4m	159	ASN
2	4m	166	ASN
2	4m	179	ASN
2	4m	218	ASN
2	4n	56	ASN
2	4n	76	ASN
2	4n	159	ASN
2	4n	166	ASN
2	4n	179	ASN
2	4n	218	ASN
2	5m	159	ASN
2	5m	166	ASN
2	5m	179	ASN
2	5m	218	ASN
2	5n	76	ASN
2	5n	159	ASN
2	5n	166	ASN
2	5n	179	ASN
2	5n	218	ASN
2	6u	23	GLN
2	6u	76	ASN
2	6u	159	ASN
2	6u	166	ASN
2	6u	179	ASN

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

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Mol	Chain	Res	Type
2	9M	166	ASN
2	9M	179	ASN
2	9M	218	ASN
2	9M	267	ASN
2	9N	159	ASN
2	9N	166	ASN
2	9N	179	ASN
2	9N	218	ASN
2	9O	159	ASN
2	9O	166	ASN
2	9O	179	ASN
2	9O	197	GLN
2	9O	218	ASN
2	9P	76	ASN
2	9P	159	ASN
2	9P	166	ASN
2	9P	179	ASN
2	9P	218	ASN
2	9Q	159	ASN
2	9Q	166	ASN
2	9Q	179	ASN
2	9Q	218	ASN
2	9R	76	ASN
2	9R	159	ASN
2	9R	166	ASN
2	9R	179	ASN
2	9R	218	ASN
2	9J	159	ASN
2	9J	166	ASN
2	9J	171	GLN
2	9J	179	ASN
2	9J	185	GLN
2	9J	197	GLN
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.

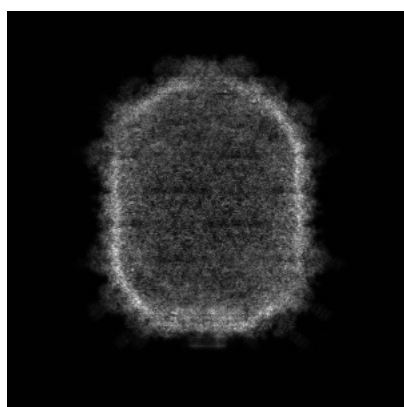
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4655. These allow visual inspection of the internal detail of the map and identification of artifacts.

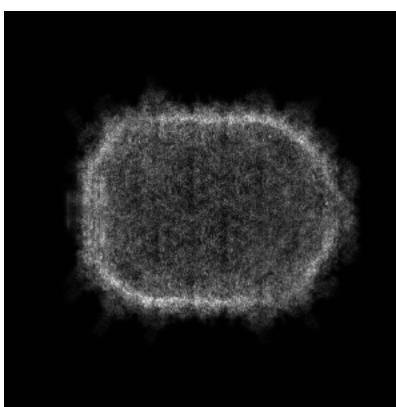
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

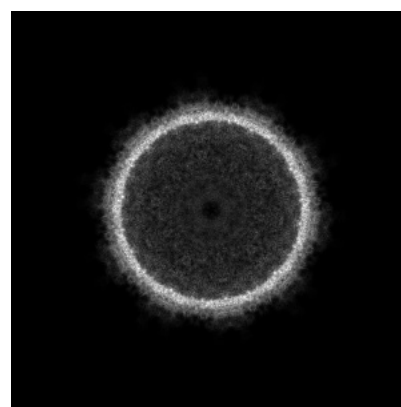
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

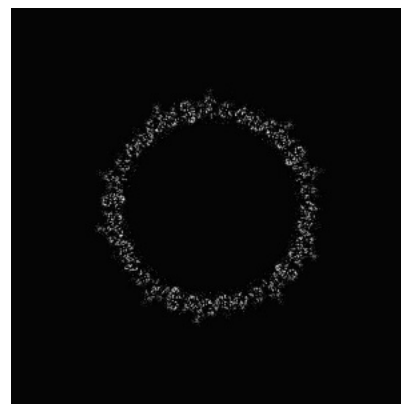
6.2.1 Primary map



X Index: 352



Y Index: 352

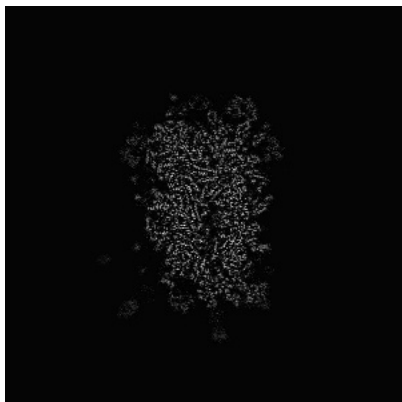


Z Index: 352

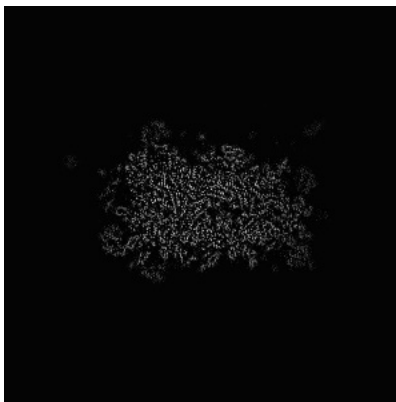
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 511



Y Index: 192



Z Index: 280

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

6.4 Orthogonal surface views [i](#)

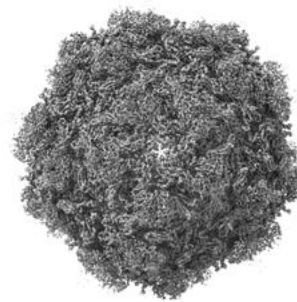
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

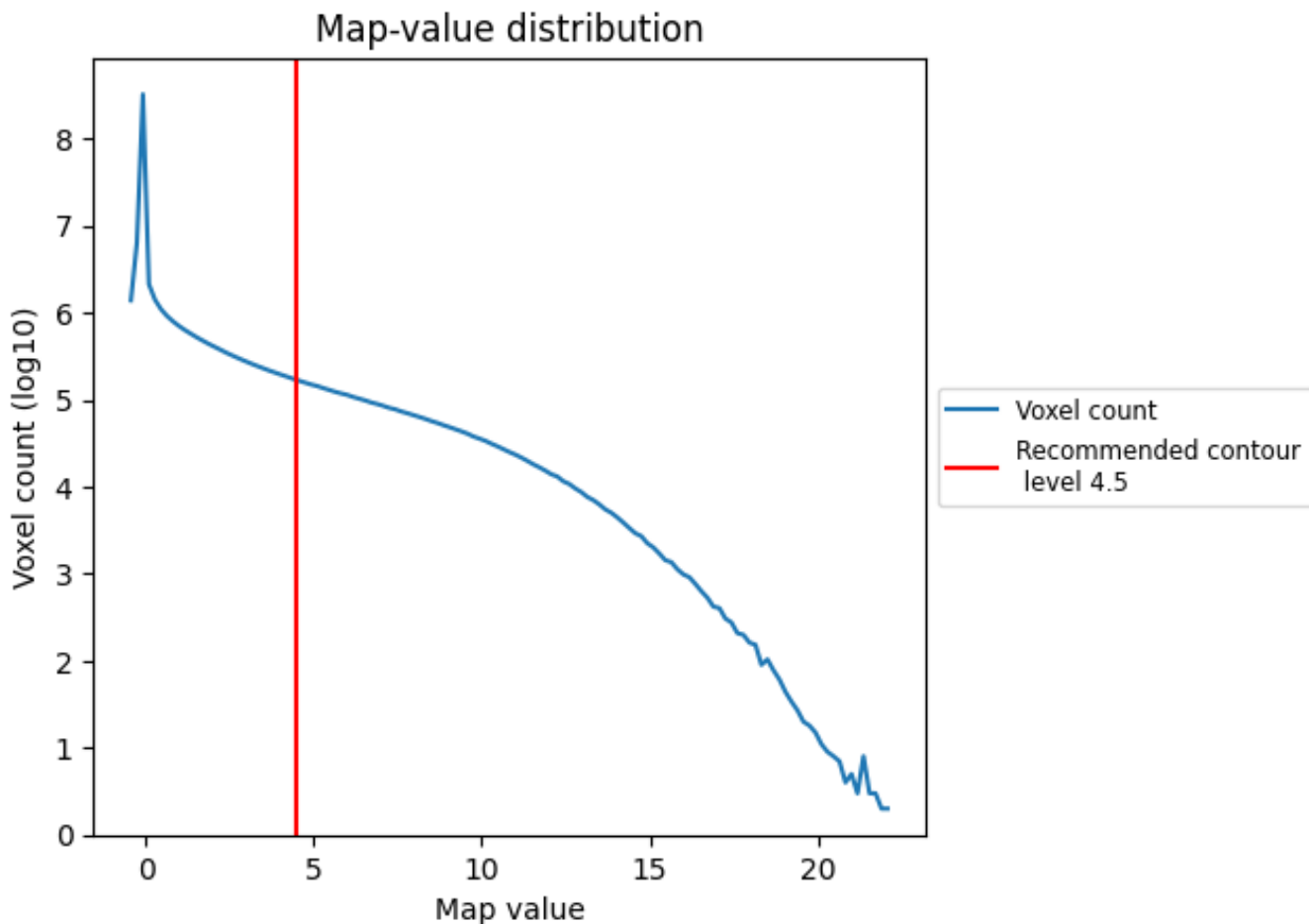
6.5 Mask visualisation

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

7 Map analysis [i](#)

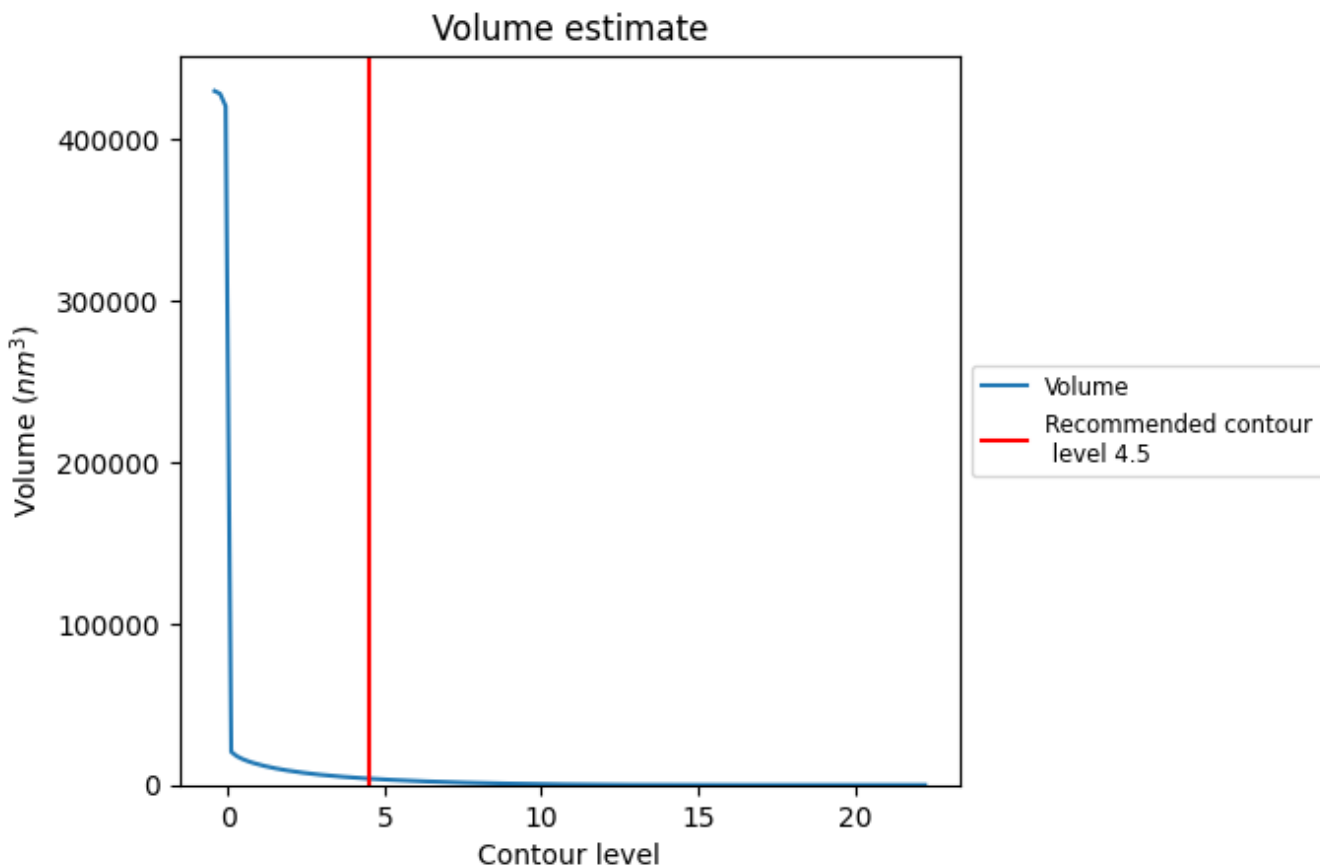
This section contains the results of statistical analysis of the map.

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.

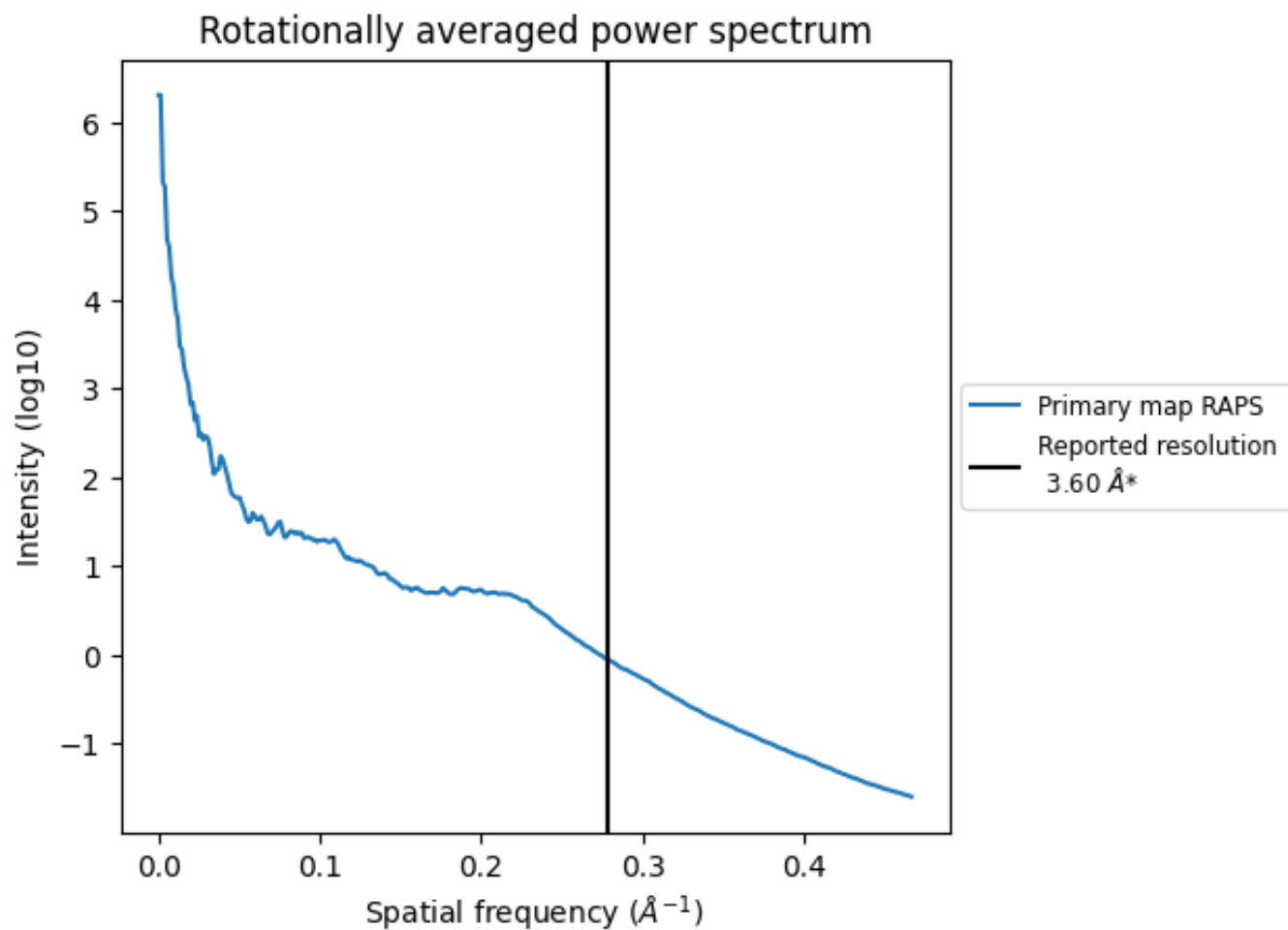
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 3930 nm^3 ; this corresponds to an approximate mass of 3550 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 0.278 Å⁻¹

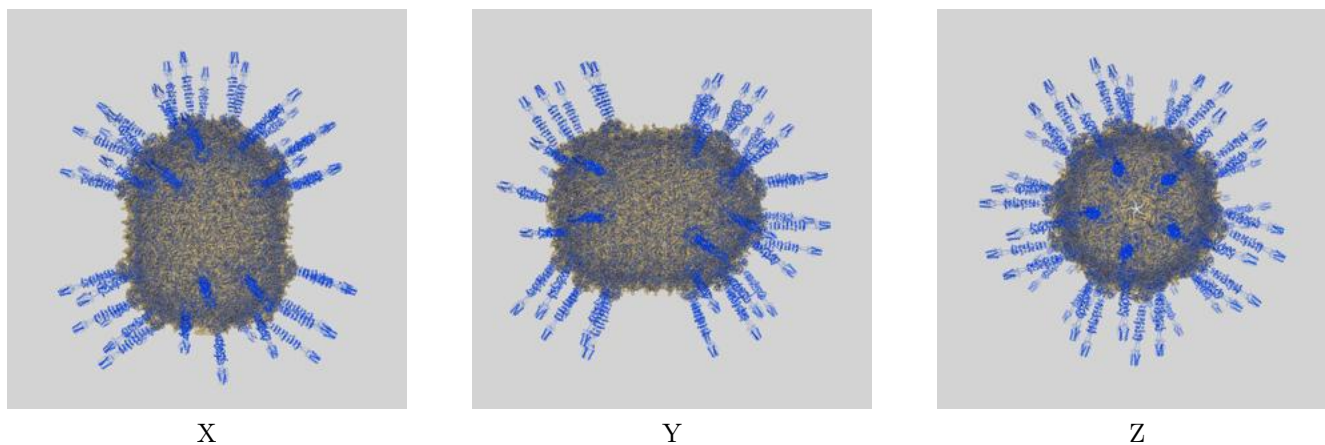
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

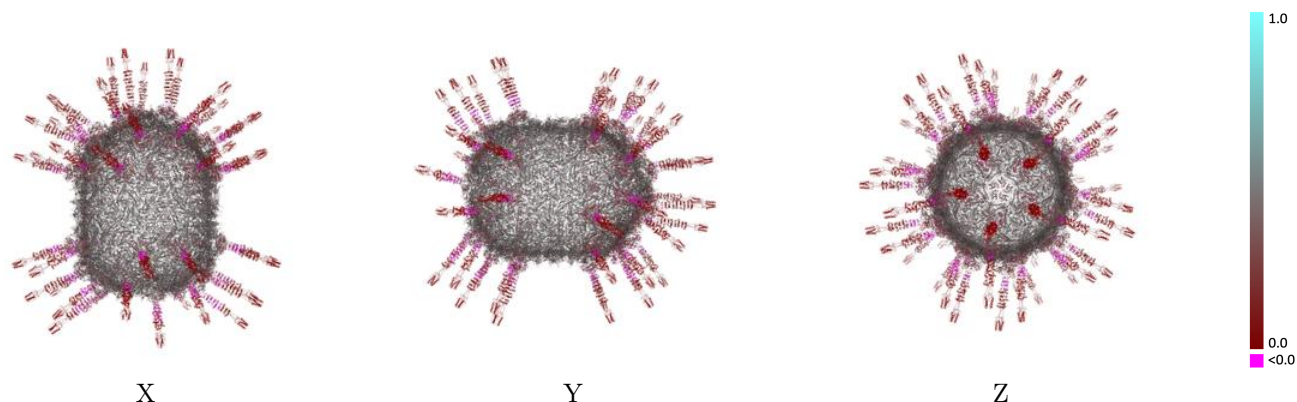
This section contains information regarding the fit between EMDB map EMD-4655 and PDB model 6QVK. Per-residue inclusion information can be found in section 3 on page 47.

9.1 Map-model overlay [i](#)



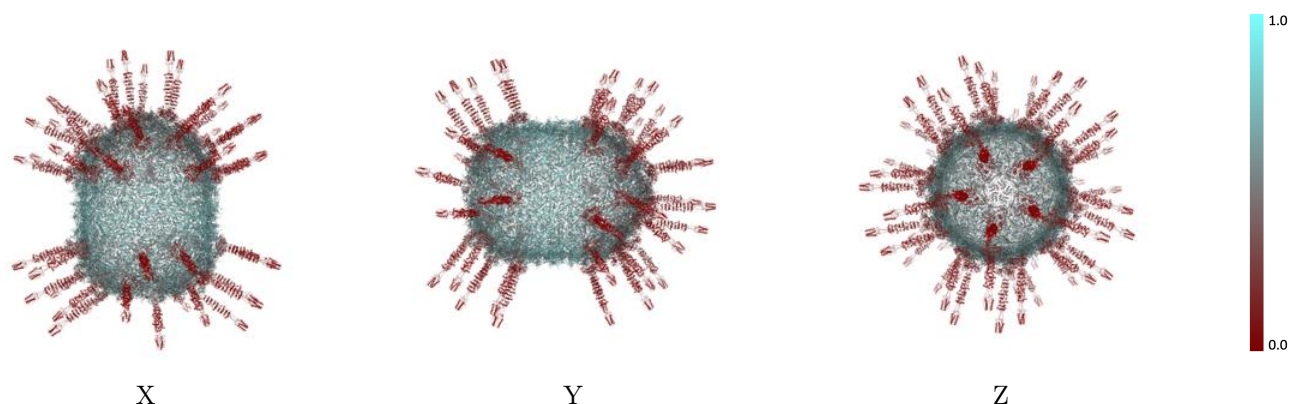
The images above show the 3D surface view of the map at the recommended contour level 4.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



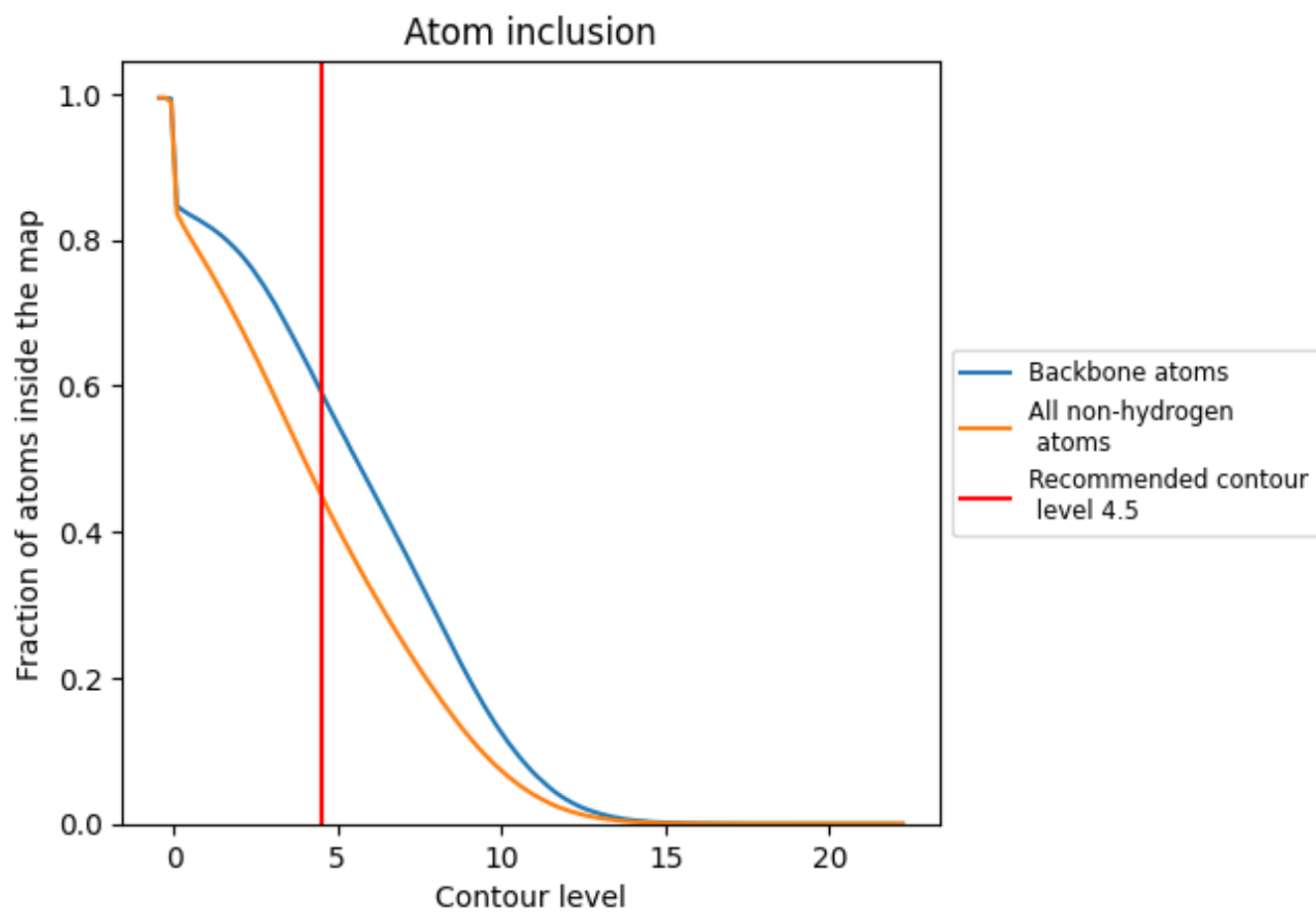
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.5).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 45% 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 (4.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4508	 0.3280
1A	 0.5294	 0.4160
1B	 0.6152	 0.4310
1C	 0.6068	 0.4240
1D	 0.6257	 0.4330
1E	 0.6047	 0.4310
1F	 0.5265	 0.4070
1G	 0.5255	 0.4130
1H	 0.6179	 0.4320
1I	 0.6068	 0.4240
1J	 0.6272	 0.4330
1K	 0.6035	 0.4320
1L	 0.5283	 0.4080
1M	 0.5297	 0.4130
1N	 0.6158	 0.4330
1O	 0.6082	 0.4240
1P	 0.6257	 0.4320
1Q	 0.6017	 0.4320
1R	 0.5236	 0.4090
1S	 0.5291	 0.4130
1T	 0.6173	 0.4310
1U	 0.6076	 0.4230
1V	 0.6225	 0.4320
1W	 0.6041	 0.4320
1X	 0.5245	 0.4100
1Y	 0.5300	 0.4130
1Z	 0.6181	 0.4310
1a	 0.6103	 0.4230
1b	 0.6263	 0.4330
1c	 0.6011	 0.4320
1d	 0.5254	 0.4070
1e	 0.1459	 0.1390
1f	 0.0926	 0.1260
1g	 0.1576	 0.1300
1h	 0.1675	 0.1580























































































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Chain	Atom inclusion	Q-score
1i	0.1429	0.1360
1j	0.0940	0.1270
1k	0.1532	0.1290
1l	0.1685	0.1560
1m	0.1356	0.1260
1n	0.0901	0.1230
1o	0.1527	0.1310
1p	0.1685	0.1570
1q	0.1351	0.1260
1r	0.0881	0.1200
1s	0.1541	0.1260
1t	0.1694	0.1550
1u	0.1395	0.1330
1v	0.0945	0.1260
1w	0.1522	0.1300
1x	0.1680	0.1560
2A	0.6058	0.4300
2B	0.6176	0.4310
2C	0.5954	0.4240
2D	0.5966	0.4290
2E	0.5907	0.4250
2F	0.6016	0.4300
2G	0.6164	0.4290
2H	0.5977	0.4230
2I	0.5971	0.4280
2J	0.5863	0.4240
2K	0.6058	0.4310
2L	0.6170	0.4310
2M	0.5963	0.4240
2N	0.5995	0.4280
2O	0.5901	0.4240
2P	0.6075	0.4290
2Q	0.6187	0.4310
2R	0.5963	0.4230
2S	0.5998	0.4280
2T	0.5907	0.4230
2U	0.6078	0.4300
2V	0.6164	0.4290
2W	0.5980	0.4230
2X	0.5974	0.4290
2Y	0.5907	0.4230
2Z	0.1668	0.1470





















































































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Chain	Atom inclusion	Q-score
2a	 0.1107	 0.1400
2b	 0.1615	 0.1410
2c	 0.0737	 0.1110
2d	 0.1654	 0.1450
2e	 0.1717	 0.1480
2f	 0.1132	 0.1420
2g	 0.1663	 0.1450
2h	 0.0800	 0.1160
2i	 0.1668	 0.1520
2j	 0.1683	 0.1380
2k	 0.1112	 0.1350
2l	 0.1566	 0.1370
2m	 0.0795	 0.1130
2n	 0.1659	 0.1480
2o	 0.1693	 0.1340
2p	 0.1112	 0.1320
2q	 0.1551	 0.1310
2r	 0.0776	 0.1090
2s	 0.1639	 0.1460
2t	 0.1698	 0.1400
2u	 0.1127	 0.1360
2v	 0.1556	 0.1390
2w	 0.0751	 0.1100
2x	 0.1654	 0.1450
3A	 0.6593	 0.4270
3B	 0.6644	 0.4230
3C	 0.6707	 0.4240
3D	 0.6450	 0.4320
3E	 0.6415	 0.4350
3F	 0.6450	 0.4310
3G	 0.6590	 0.4270
3H	 0.6626	 0.4220
3I	 0.6704	 0.4260
3J	 0.6438	 0.4320
3K	 0.6453	 0.4350
3L	 0.6426	 0.4300
3M	 0.6567	 0.4260
3N	 0.6650	 0.4220
3O	 0.6733	 0.4260
3P	 0.6441	 0.4330
3Q	 0.6432	 0.4370
3R	 0.6429	 0.4300





















































































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Chain	Atom inclusion	Q-score
3S	 0.6593	 0.4240
3T	 0.6632	 0.4230
3U	 0.6677	 0.4270
3V	 0.6453	 0.4300
3W	 0.6435	 0.4350
3X	 0.6461	 0.4300
3Y	 0.6608	 0.4260
3Z	 0.6605	 0.4220
3a	 0.6674	 0.4240
3b	 0.6453	 0.4310
3c	 0.6435	 0.4360
3d	 0.6429	 0.4300
3e	 0.1396	 0.1230
3f	 0.0893	 0.1100
3g	 0.1641	 0.1300
3h	 0.0702	 0.1020
3i	 0.1459	 0.1250
3j	 0.0859	 0.1080
3k	 0.1592	 0.1290
3l	 0.0741	 0.1000
3m	 0.1420	 0.1190
3n	 0.0883	 0.1090
3o	 0.1709	 0.1410
3p	 0.0790	 0.1080
3q	 0.1381	 0.1150
3r	 0.0810	 0.1030
3s	 0.1778	 0.1420
3t	 0.0771	 0.1070
3u	 0.1405	 0.1180
3v	 0.0844	 0.1050
3w	 0.1753	 0.1390
3x	 0.0756	 0.1060
4A	 0.6629	 0.4350
4B	 0.6718	 0.4210
4C	 0.6795	 0.4260
4D	 0.6843	 0.4380
4E	 0.6599	 0.4230
4F	 0.6602	 0.4370
4G	 0.6623	 0.4360
4H	 0.6721	 0.4200
4I	 0.6807	 0.4250
4J	 0.6798	 0.4370





















































































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Chain	Atom inclusion	Q-score
4K	 0.6575	 0.4230
4L	 0.6569	 0.4370
4M	 0.6653	 0.4360
4N	 0.6769	 0.4200
4O	 0.6843	 0.4270
4P	 0.6810	 0.4370
4Q	 0.6587	 0.4240
4R	 0.6561	 0.4360
4S	 0.6650	 0.4350
4T	 0.6748	 0.4200
4U	 0.6825	 0.4270
4V	 0.6792	 0.4370
4W	 0.6590	 0.4210
4X	 0.6575	 0.4340
4Y	 0.6644	 0.4350
4Z	 0.6703	 0.4200
4a	 0.6792	 0.4250
4b	 0.6834	 0.4380
4c	 0.6610	 0.4220
4d	 0.6575	 0.4360
4e	 0.1429	 0.1200
4f	 0.0793	 0.1110
4g	 0.1434	 0.1230
4h	 0.0857	 0.1220
4i	 0.1449	 0.1150
4j	 0.0808	 0.1190
4k	 0.1420	 0.1060
4l	 0.0808	 0.1110
4m	 0.1429	 0.1120
4n	 0.0793	 0.1100
5A	 0.6350	 0.4180
5B	 0.6709	 0.4220
5C	 0.6828	 0.4340
5D	 0.6763	 0.4330
5E	 0.6368	 0.4160
5F	 0.6214	 0.4110
5G	 0.6353	 0.4200
5H	 0.6712	 0.4220
5I	 0.6819	 0.4340
5J	 0.6763	 0.4320
5K	 0.6383	 0.4170
5L	 0.6181	 0.4100





















































































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Chain	Atom inclusion	Q-score
5M	 0.6359	 0.4180
5N	 0.6665	 0.4210
5O	 0.6834	 0.4340
5P	 0.6754	 0.4340
5Q	 0.6386	 0.4160
5R	 0.6202	 0.4100
5S	 0.6335	 0.4180
5T	 0.6703	 0.4220
5U	 0.6789	 0.4310
5V	 0.6801	 0.4300
5W	 0.6386	 0.4160
5X	 0.6187	 0.4100
5Y	 0.6359	 0.4170
5Z	 0.6677	 0.4210
5a	 0.6828	 0.4330
5b	 0.6766	 0.4310
5c	 0.6421	 0.4150
5d	 0.6193	 0.4100
5e	 0.0756	 0.1000
5f	 0.0299	 0.0910
5g	 0.0751	 0.1060
5h	 0.0362	 0.0970
5i	 0.0751	 0.0990
5j	 0.0411	 0.1100
5k	 0.0654	 0.0890
5l	 0.0348	 0.1030
5m	 0.0688	 0.0950
5n	 0.0353	 0.0960
6A	 0.5764	 0.4080
6B	 0.5977	 0.4150
6C	 0.6178	 0.4130
6D	 0.6469	 0.4140
6E	 0.6377	 0.4190
6F	 0.6199	 0.4190
6G	 0.5802	 0.4090
6H	 0.5974	 0.4150
6I	 0.6228	 0.4130
6J	 0.6481	 0.4150
6K	 0.6368	 0.4180
6L	 0.6240	 0.4190
6M	 0.5802	 0.4090
6N	 0.6001	 0.4140

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Chain	Atom inclusion	Q-score
6O	 0.6234	 0.4130
6P	 0.6489	 0.4130
6Q	 0.6362	 0.4180
6R	 0.6240	 0.4200
6S	 0.5817	 0.4090
6T	 0.5989	 0.4130
6U	 0.6222	 0.4140
6V	 0.6501	 0.4130
6W	 0.6377	 0.4180
6X	 0.6208	 0.4180
6Y	 0.5799	 0.4080
6Z	 0.5998	 0.4130
6a	 0.6198	 0.4130
6b	 0.6492	 0.4120
6c	 0.6418	 0.4180
6d	 0.6263	 0.4180
6e	 0.0705	 0.0780
6f	 0.0337	 0.0910
6g	 0.0700	 0.0930
6h	 0.0283	 0.0840
6i	 0.0872	 0.0910
6j	 0.0356	 0.1010
6k	 0.0744	 0.1030
6l	 0.0278	 0.0900
6m	 0.0779	 0.0830
6n	 0.0332	 0.0920
6o	 0.0784	 0.1070
6p	 0.0302	 0.0910
6q	 0.0671	 0.0670
6r	 0.0341	 0.0880
6s	 0.0725	 0.0970
6t	 0.0327	 0.0900
6u	 0.0700	 0.0690
6v	 0.0341	 0.0880
6w	 0.0695	 0.0920
6x	 0.0249	 0.0860
7A	 0.5053	 0.3990
7B	 0.5044	 0.4010
7C	 0.5137	 0.4040
7D	 0.5280	 0.4040
7E	 0.5125	 0.3930
7F	 0.5015	 0.4010





















































































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Chain	Atom inclusion	Q-score
7G	█ 0.5076	█ 0.4010
7H	█ 0.5096	█ 0.4050
7I	█ 0.5300	█ 0.4040
7J	█ 0.5114	█ 0.3940
7K	█ 0.5061	█ 0.4010
7L	█ 0.5047	█ 0.4030
7M	█ 0.5114	█ 0.4030
7N	█ 0.5295	█ 0.4030
7O	█ 0.5128	█ 0.3930
7P	█ 0.5020	█ 0.3990
7Q	█ 0.5026	█ 0.4030
7R	█ 0.5117	█ 0.4020
7S	█ 0.5306	█ 0.4000
7T	█ 0.5105	█ 0.3920
7U	█ 0.5032	█ 0.3990
7V	█ 0.5070	█ 0.4020
7W	█ 0.5149	█ 0.4030
7X	█ 0.5265	█ 0.4020
7Y	█ 0.5166	█ 0.3930
7Z	█ 0.0902	█ 0.1180
7a	█ 0.0380	█ 0.0960
7b	█ 0.0693	█ 0.0990
7c	█ 0.0346	█ 0.0780
7d	█ 0.0600	█ 0.0990
7e	█ 0.0980	█ 0.1230
7f	█ 0.0410	█ 0.0970
7g	█ 0.0712	█ 0.1010
7h	█ 0.0385	█ 0.0890
7i	█ 0.0639	█ 0.1050
7j	█ 0.0961	█ 0.1190
7k	█ 0.0390	█ 0.1030
7l	█ 0.0761	█ 0.1130
7m	█ 0.0483	█ 0.1060
7n	█ 0.0668	█ 0.1120
7o	█ 0.0844	█ 0.1070
7p	█ 0.0410	█ 0.1000
7q	█ 0.0702	█ 0.1100
7r	█ 0.0390	█ 0.0960
7s	█ 0.0610	█ 0.1080
7t	█ 0.0873	█ 0.1130
7u	█ 0.0356	█ 0.0970
7v	█ 0.0712	█ 0.1030

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Chain	Atom inclusion	Q-score
7w	 0.0351	 0.0850
7x	 0.0585	 0.1020
8A	 0.5420	 0.4110
8B	 0.5338	 0.4050
8C	 0.5534	 0.4110
8D	 0.5548	 0.4120
8E	 0.5616	 0.4090
8F	 0.5385	 0.4150
8G	 0.5432	 0.4110
8H	 0.5335	 0.4060
8I	 0.5551	 0.4120
8J	 0.5534	 0.4120
8K	 0.5604	 0.4100
8L	 0.5376	 0.4150
8M	 0.5435	 0.4100
8N	 0.5277	 0.4040
8O	 0.5551	 0.4110
8P	 0.5551	 0.4100
8Q	 0.5613	 0.4080
8R	 0.5344	 0.4150
8S	 0.5423	 0.4090
8T	 0.5303	 0.4040
8U	 0.5505	 0.4110
8V	 0.5557	 0.4090
8W	 0.5601	 0.4060
8X	 0.5376	 0.4140
8Y	 0.5411	 0.4090
8Z	 0.5315	 0.4040
8a	 0.5481	 0.4110
8b	 0.5543	 0.4100
8c	 0.5639	 0.4090
8d	 0.5356	 0.4130
8e	 0.0524	 0.1020
8f	 0.0366	 0.0830
8g	 0.0551	 0.1200
8h	 0.0411	 0.0740
8i	 0.0556	 0.0840
8j	 0.0289	 0.0720
8k	 0.0548	 0.0990
8l	 0.0434	 0.0890
8m	 0.0512	 0.1100
8n	 0.0573	 0.0960

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Chain	Atom inclusion	Q-score
8o	■ 0.0678	■ 0.1000
8p	■ 0.0377	■ 0.0870
8q	■ 0.0583	■ 0.0890
8r	■ 0.0444	■ 0.1030
8s	■ 0.0493	■ 0.0980
8t	■ 0.0495	■ 0.0930
8u	■ 0.0649	■ 0.0960
8v	■ 0.0416	■ 0.1080
8w	■ 0.0480	■ 0.0870
8x	■ 0.0488	■ 0.1070
8y	■ 0.0502	■ 0.0970
8z	■ 0.0421	■ 0.0770
9A	■ 0.4630	■ 0.4000
9B	■ 0.4653	■ 0.3990
9C	■ 0.4682	■ 0.4020
9D	■ 0.4667	■ 0.4010
9E	■ 0.4667	■ 0.3980
9F	■ 0.0595	■ 0.1160
9G	■ 0.0605	■ 0.1210
9H	■ 0.0571	■ 0.1070
9I	■ 0.0566	■ 0.0970
9J	■ 0.0580	■ 0.1040
9K	■ 0.0537	■ 0.0840
9L	■ 0.0387	■ 0.1040
9M	■ 0.0539	■ 0.0910
9N	■ 0.0400	■ 0.0930
9O	■ 0.0566	■ 0.1120
9P	■ 0.0333	■ 0.0630
9Q	■ 0.0488	■ 0.0740
9R	■ 0.0328	■ 0.0880