wwPDB EM Validation Summary Report ⓘ

Dec 12, 2022 – 10:47 pm GMT

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

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

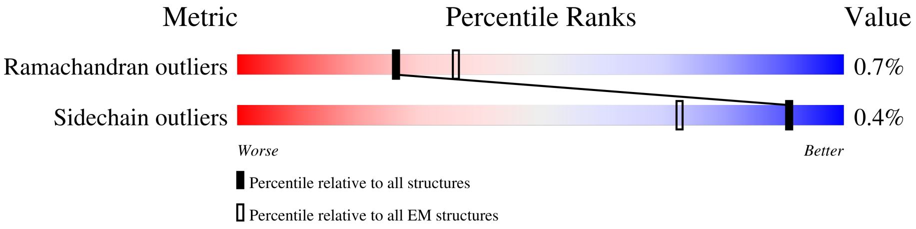
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance ⓘ

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

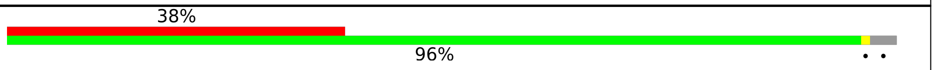
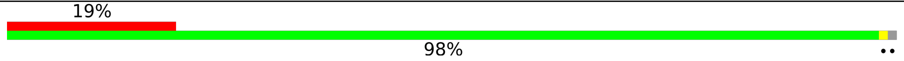
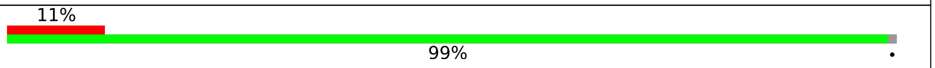
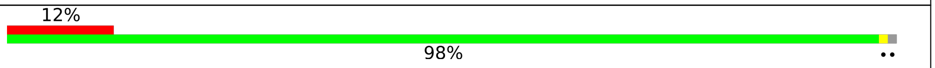
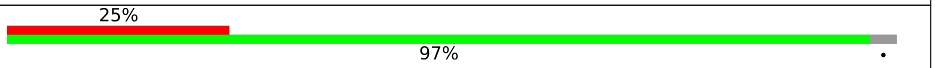
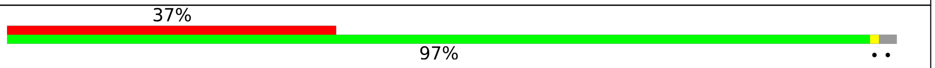
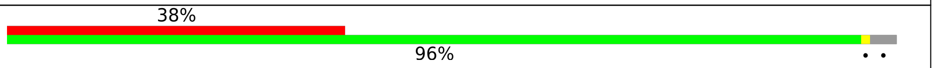
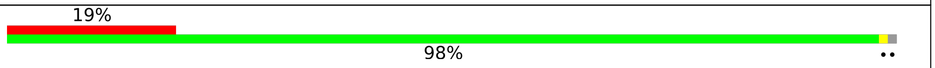
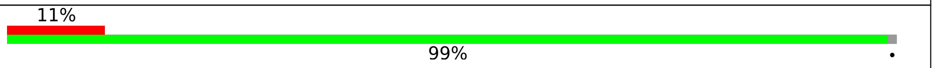
The reported resolution of this entry is 3.20 Å.

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



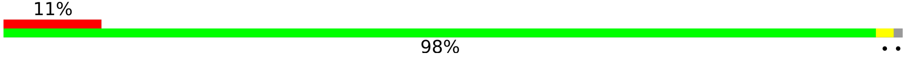
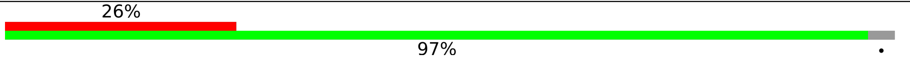
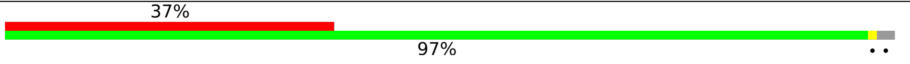
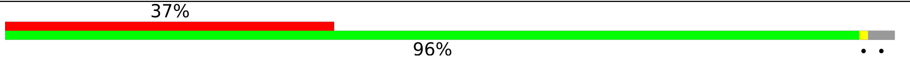
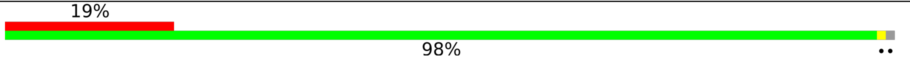
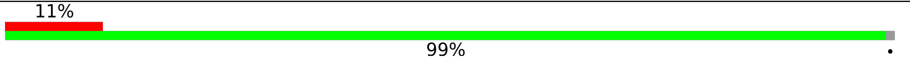
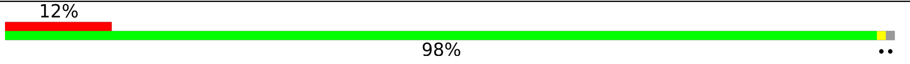
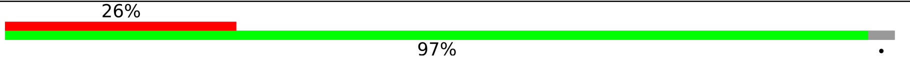
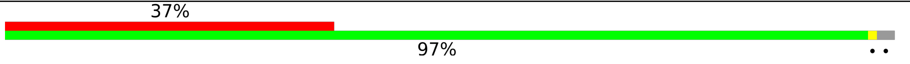
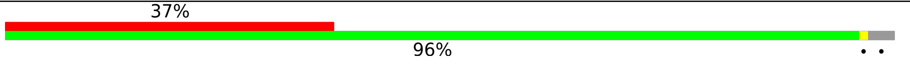
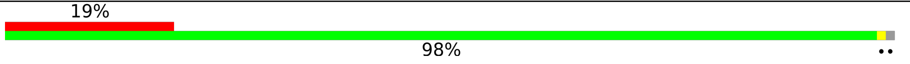
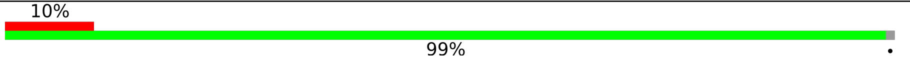
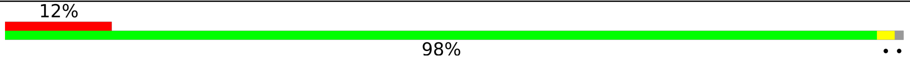
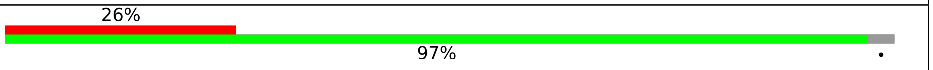
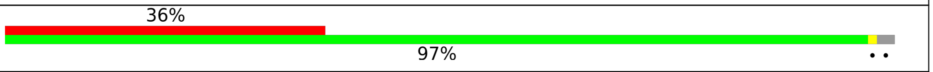
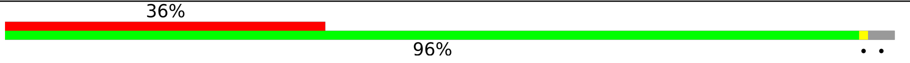
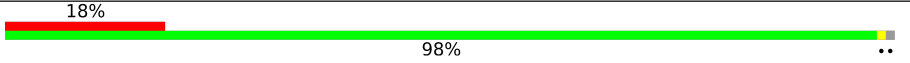
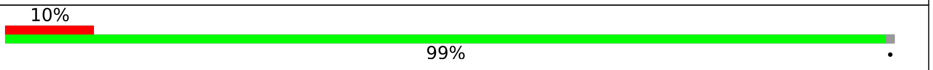
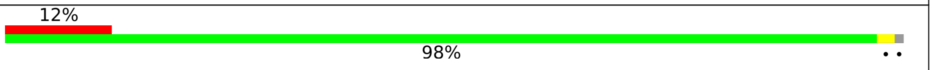
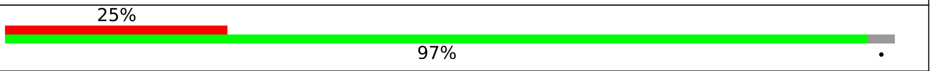
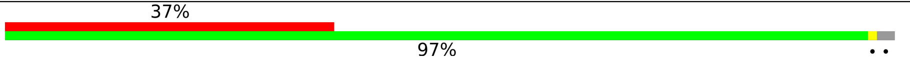
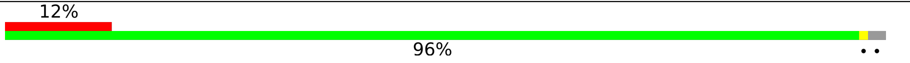
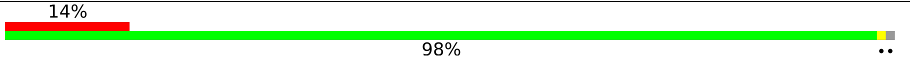
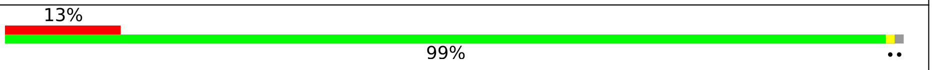
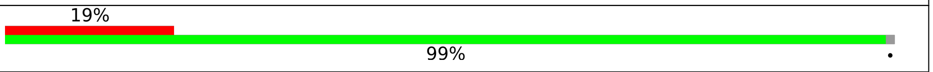
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	
1	1B	448	
1	1C	448	
1	1D	448	
1	1E	448	
1	1F	448	
1	1G	448	
1	1H	448	
1	1I	448	

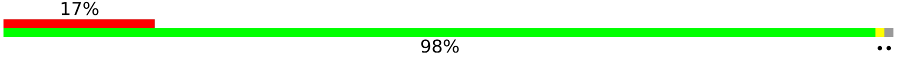
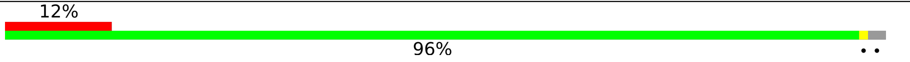
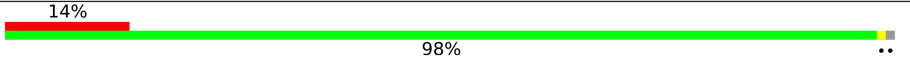
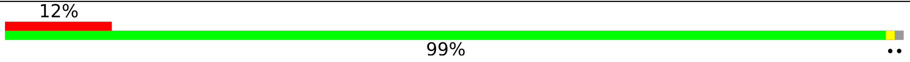
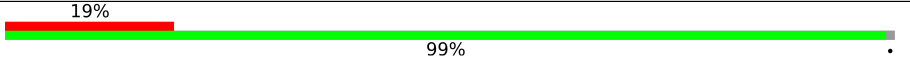
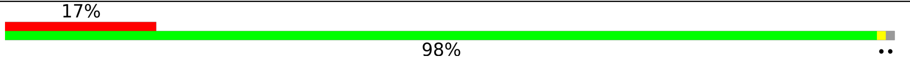
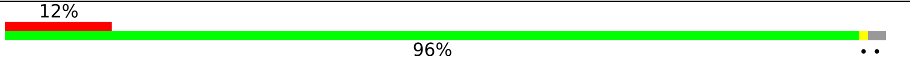
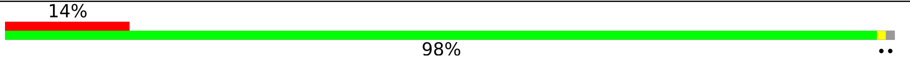
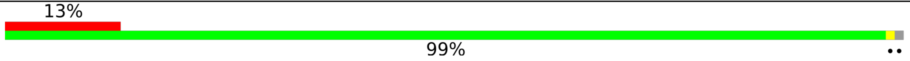
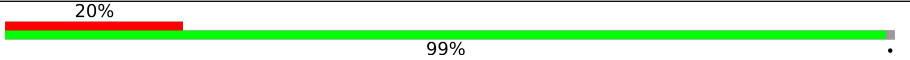
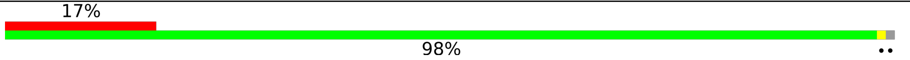
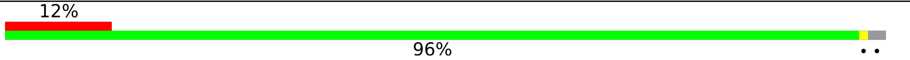
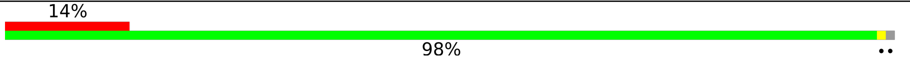
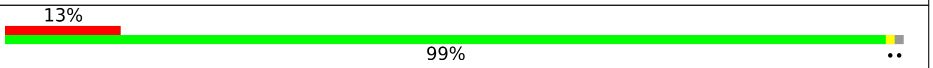
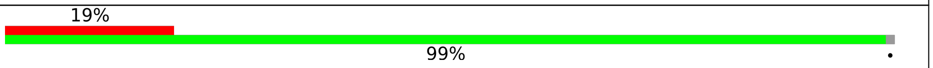
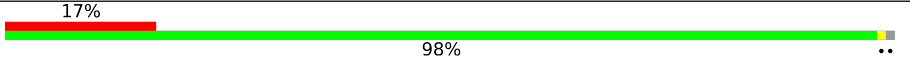
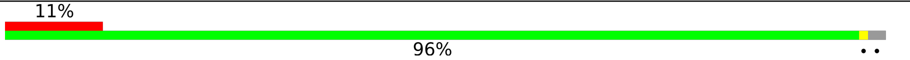
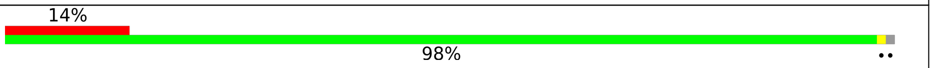
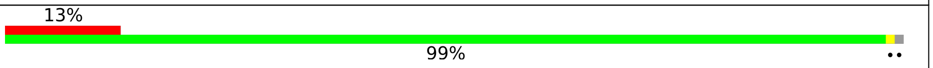
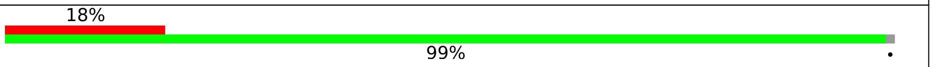
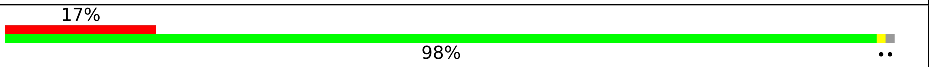
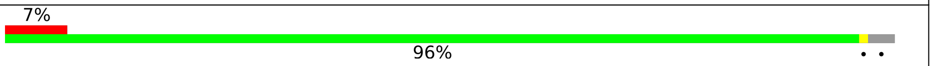
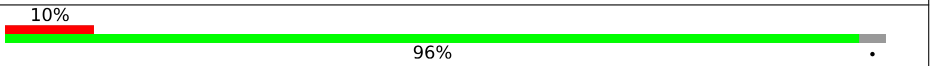
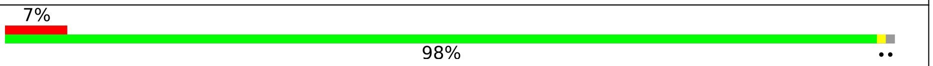
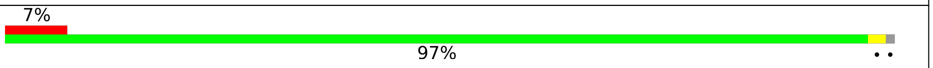
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	1J	448	
1	1K	448	
1	1L	448	
1	1M	448	
1	1N	448	
1	1O	448	
1	1P	448	
1	1Q	448	
1	1R	448	
1	1S	448	
1	1T	448	
1	1U	448	
1	1V	448	
1	1W	448	
1	1X	448	
1	1Y	448	
1	1Z	448	
1	1a	448	
1	1b	448	
1	1c	448	
1	1d	448	
1	2A	448	
1	2B	448	
1	2C	448	
1	2D	448	

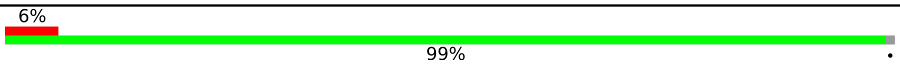
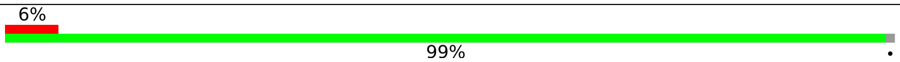
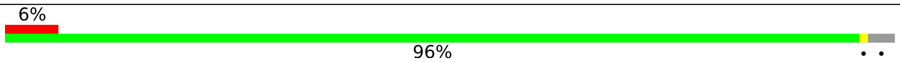
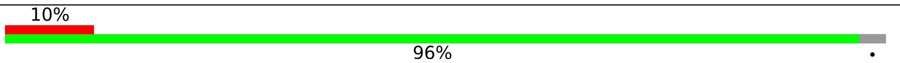
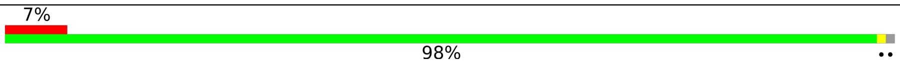
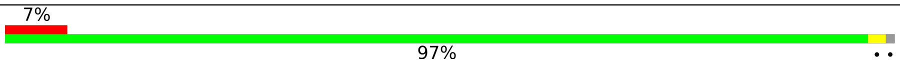
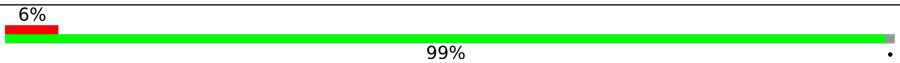
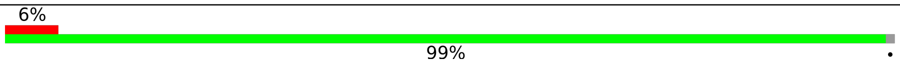
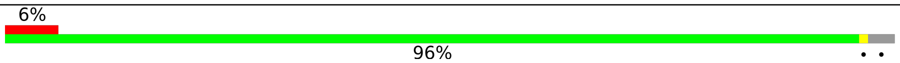
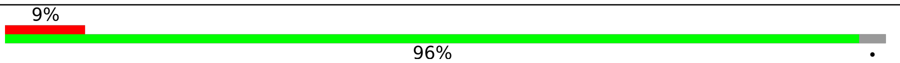
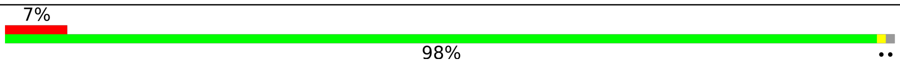
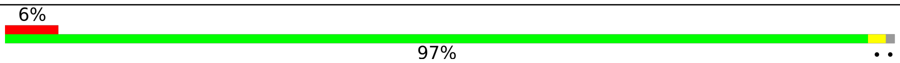
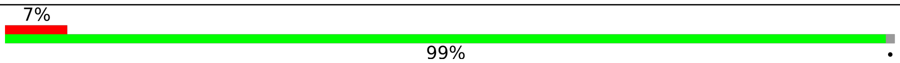
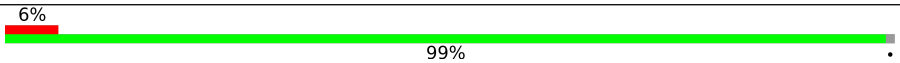
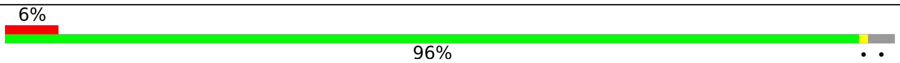
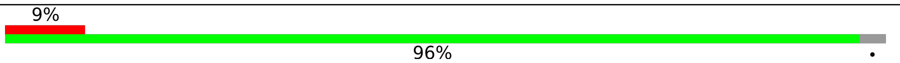
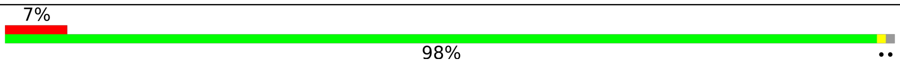
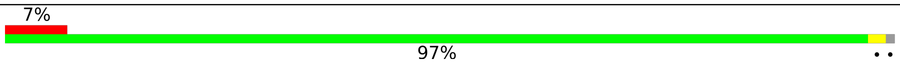
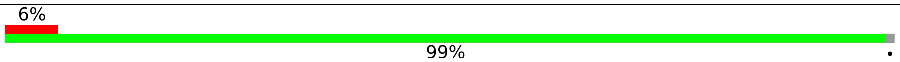
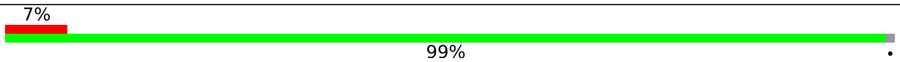
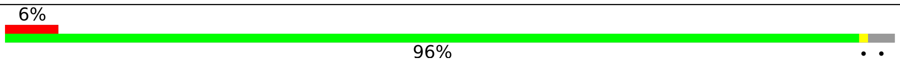
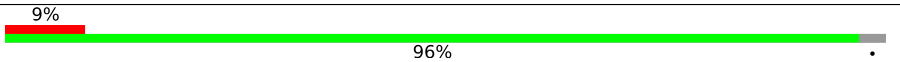
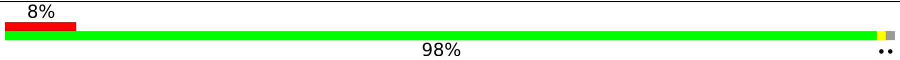
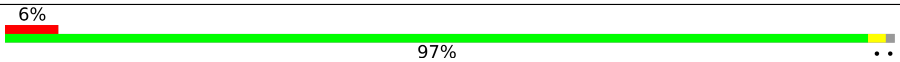
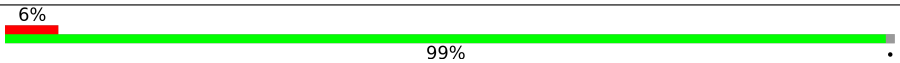
Continued on next page...

Continued from previous page...

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

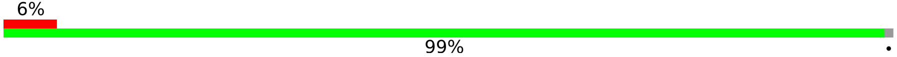
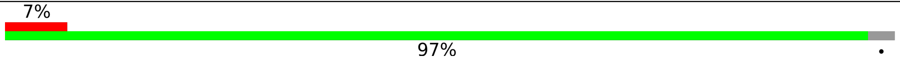
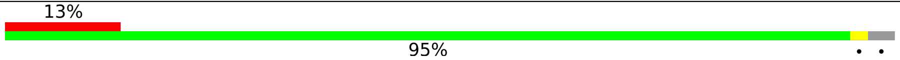
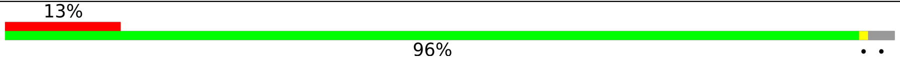
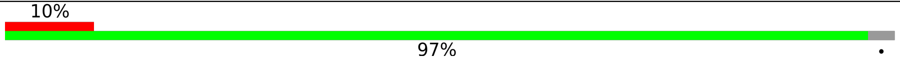
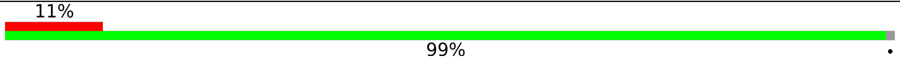
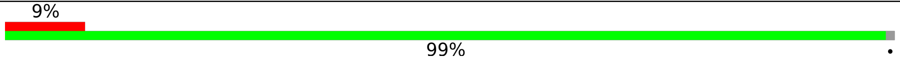
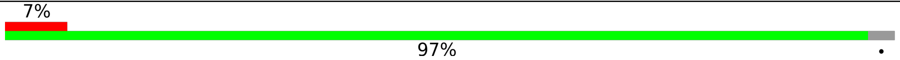
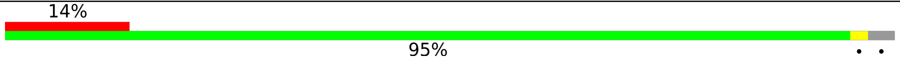
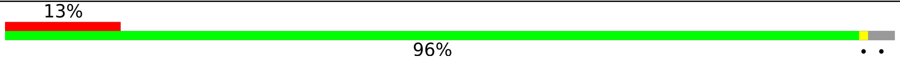
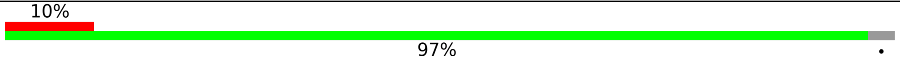
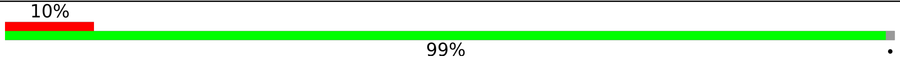
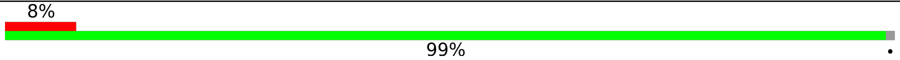
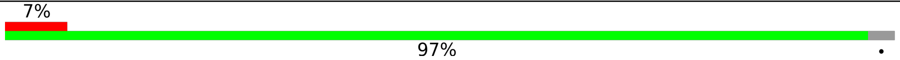
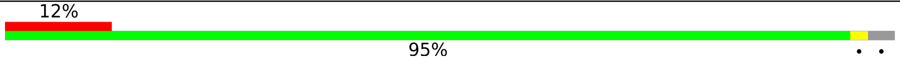
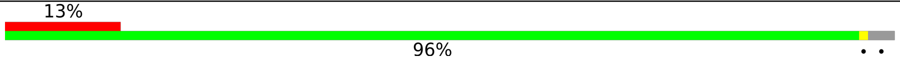
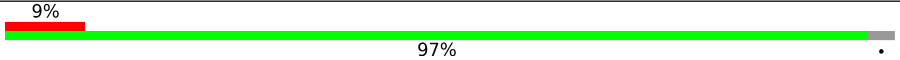
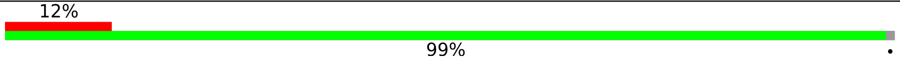
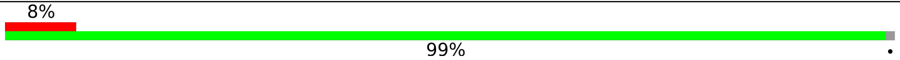
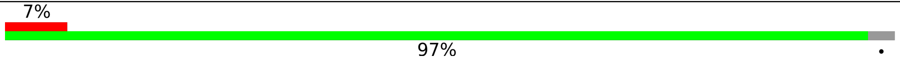
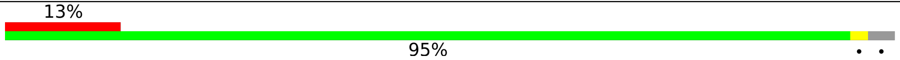
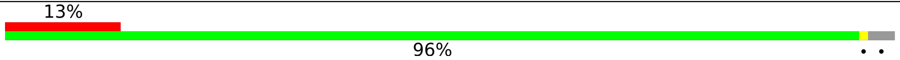
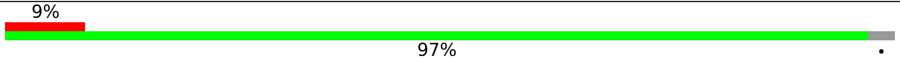
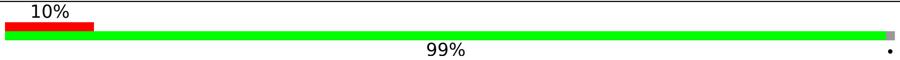
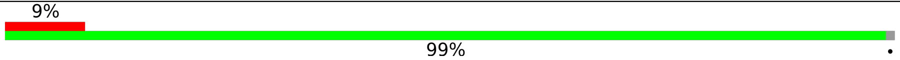
Continued on next page...

Continued from previous page...

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

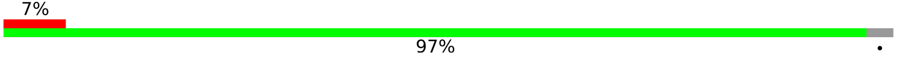
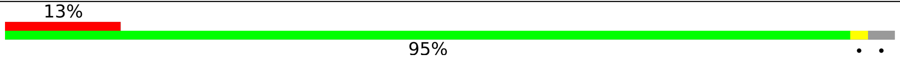
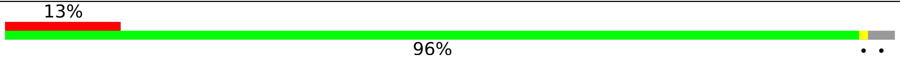
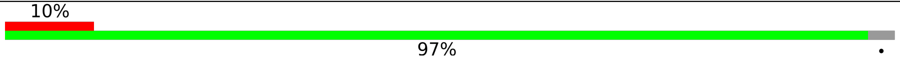
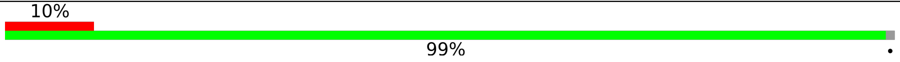
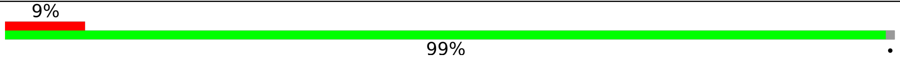
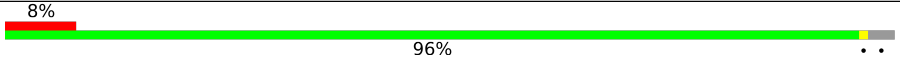
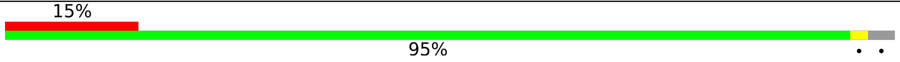
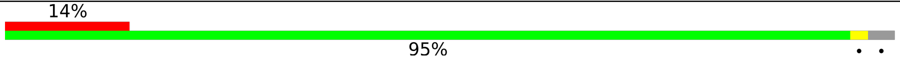
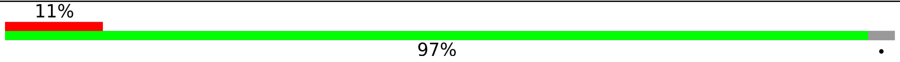
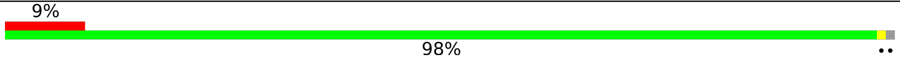
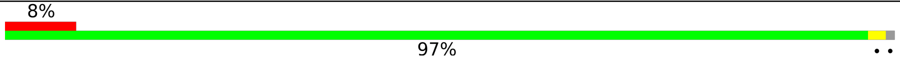
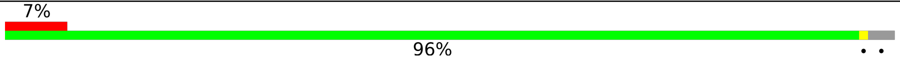
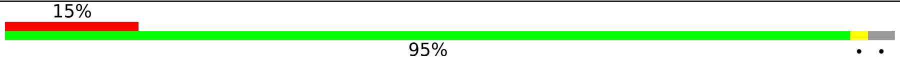
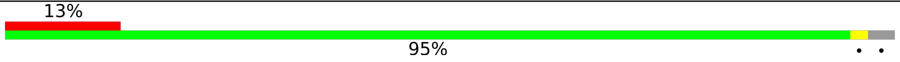
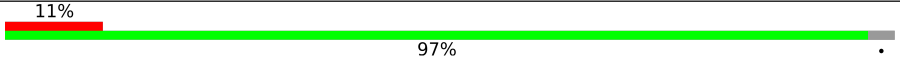
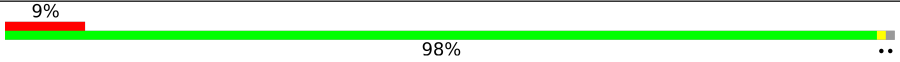
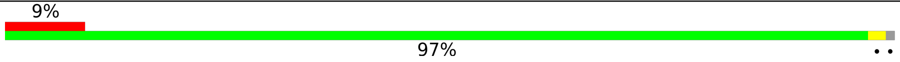
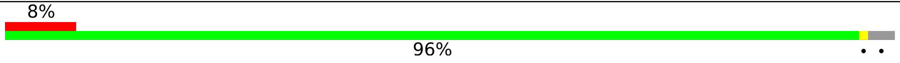
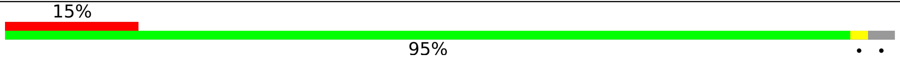
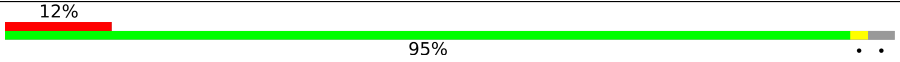
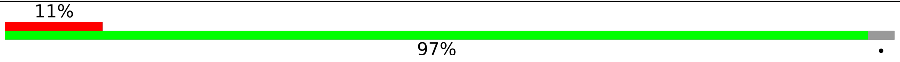
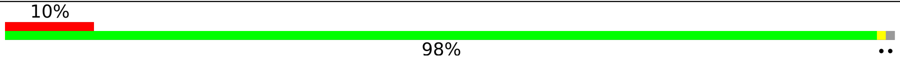
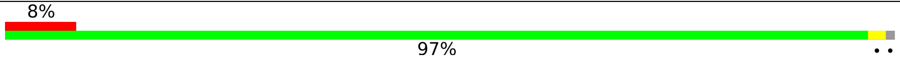
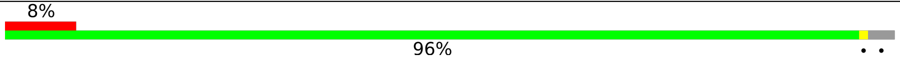
Continued on next page...

Continued from previous page...

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

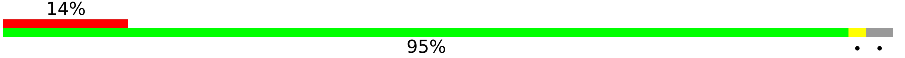
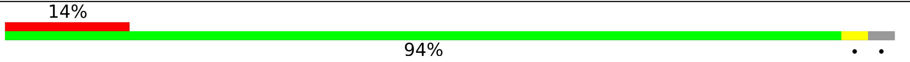
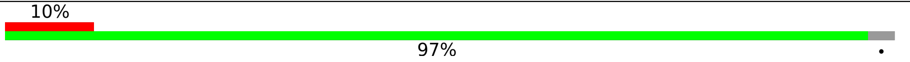
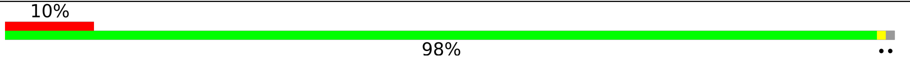
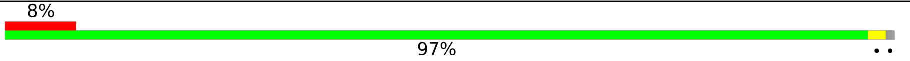
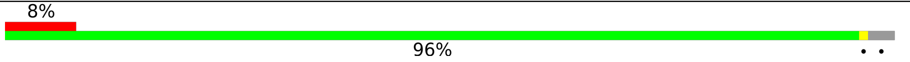
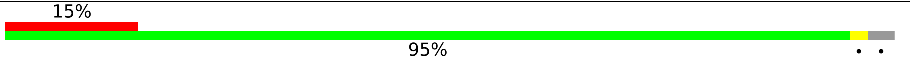
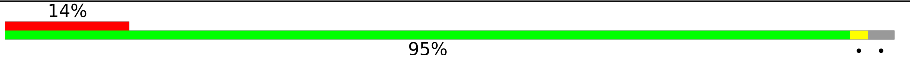
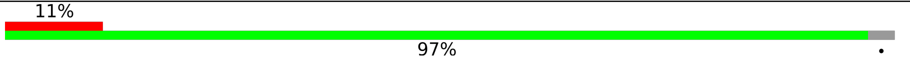
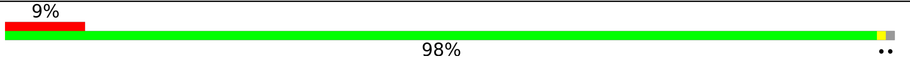
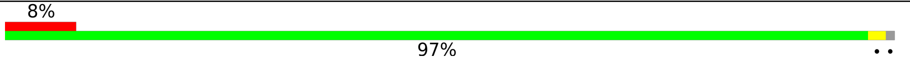
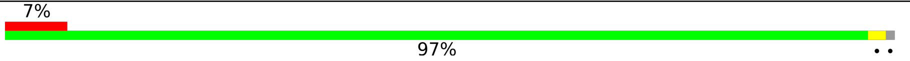
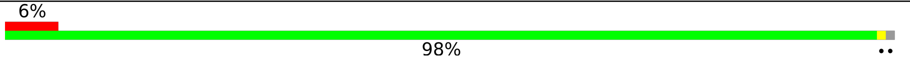
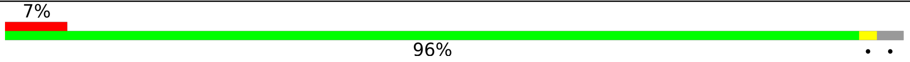
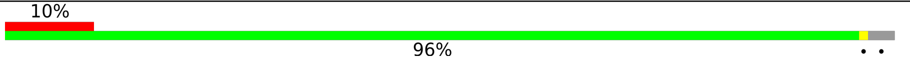
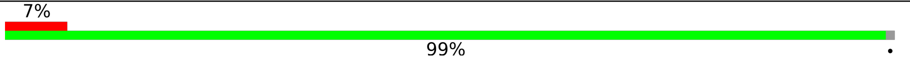
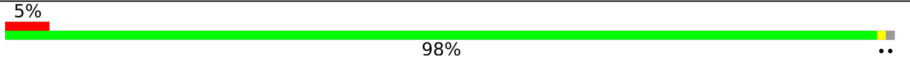
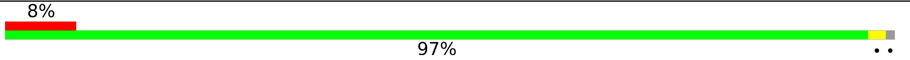
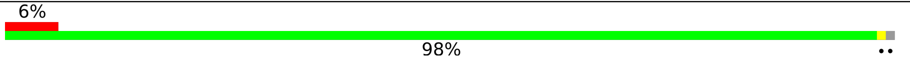
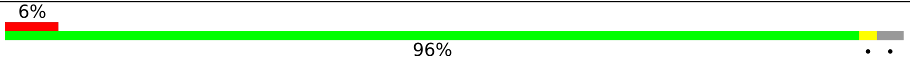
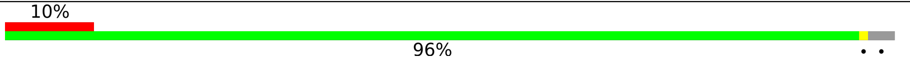
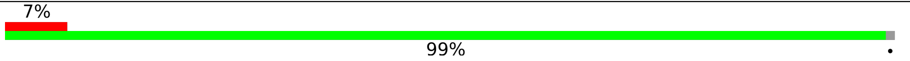
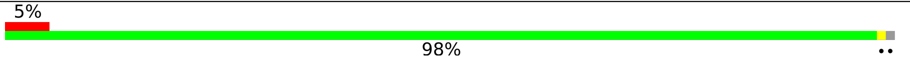
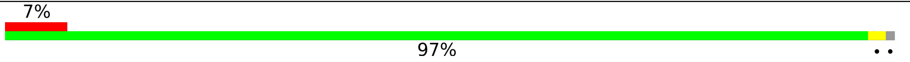
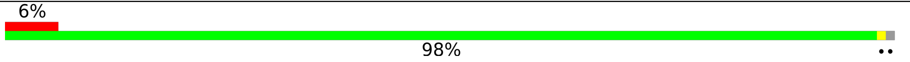
Continued on next page...

Continued from previous page...

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

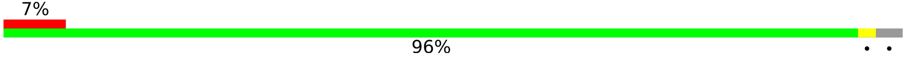
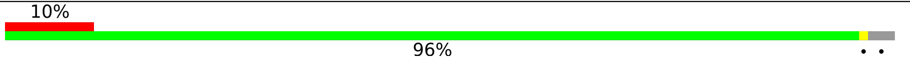
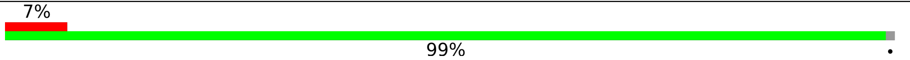
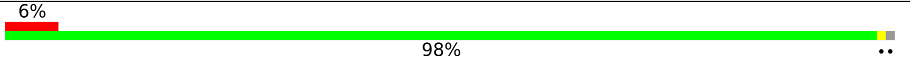
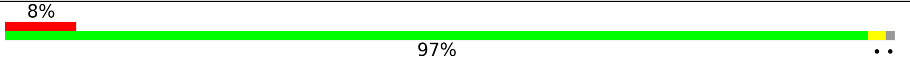
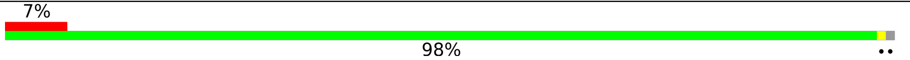
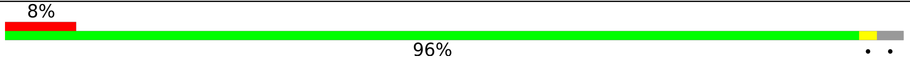
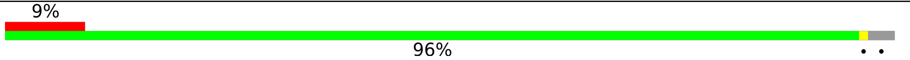
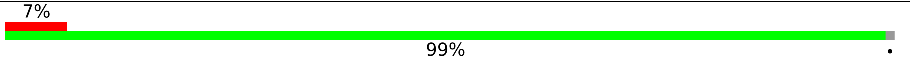
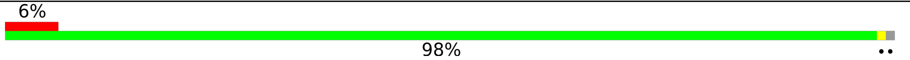
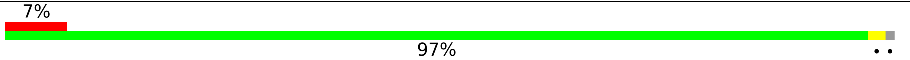
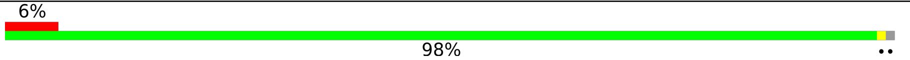
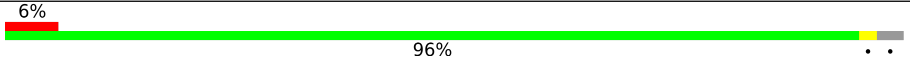
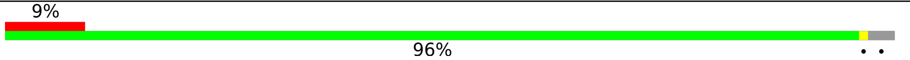
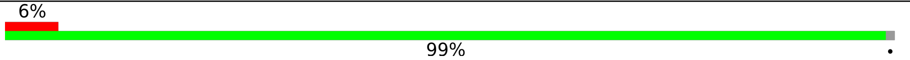
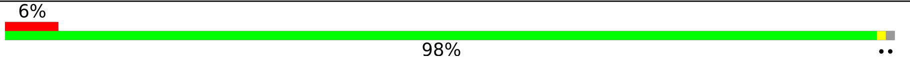
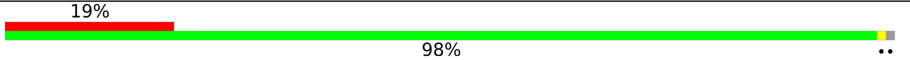
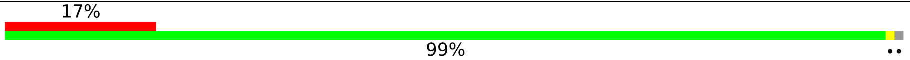
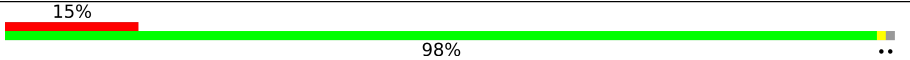
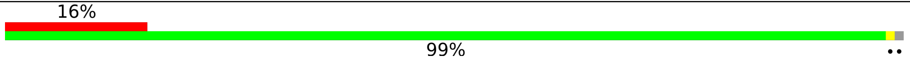
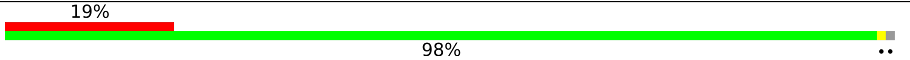
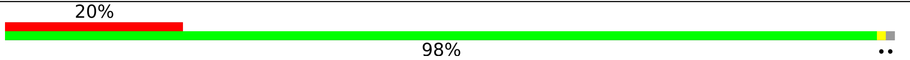
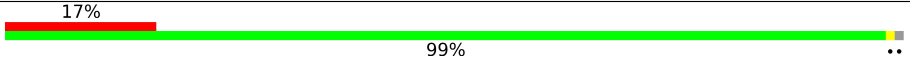
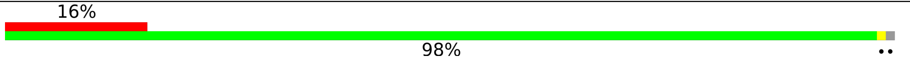
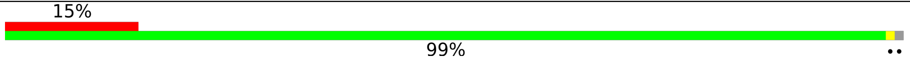
Continued on next page...

Continued from previous page...

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

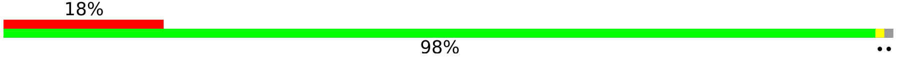
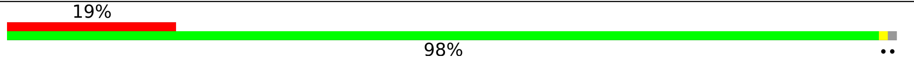
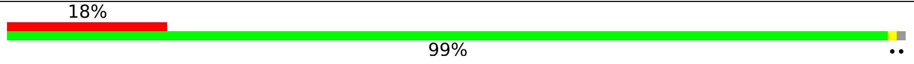
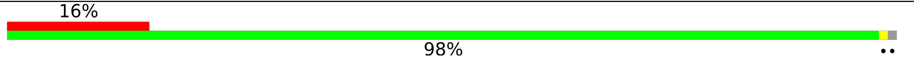
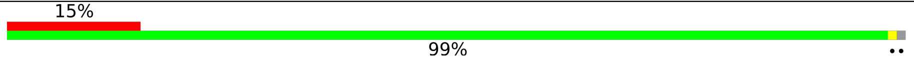
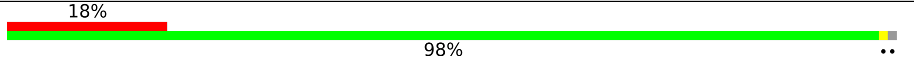
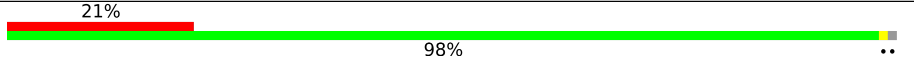
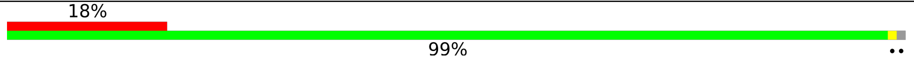
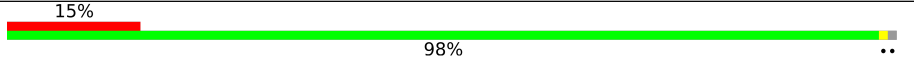
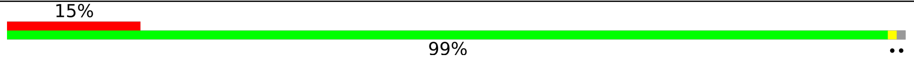
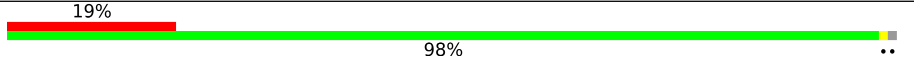
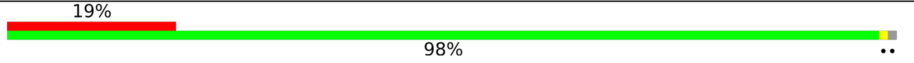
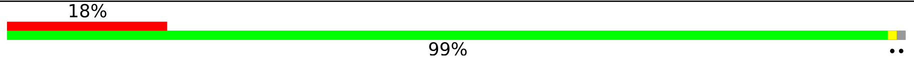
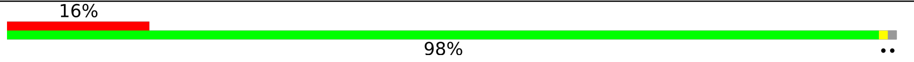
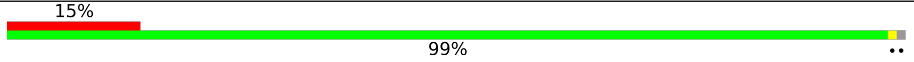
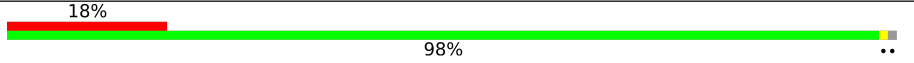
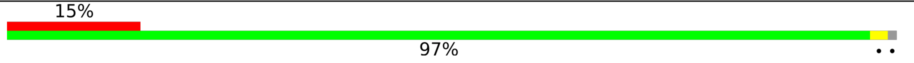
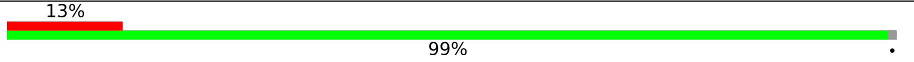
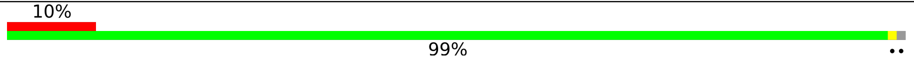
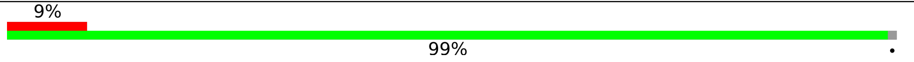
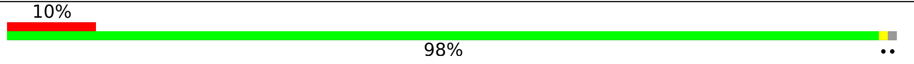
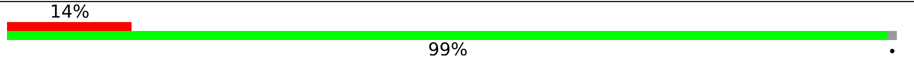
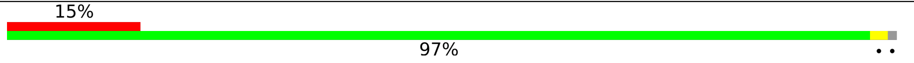
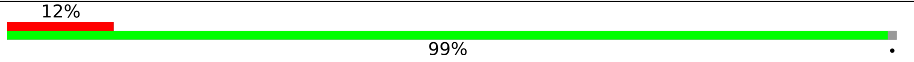
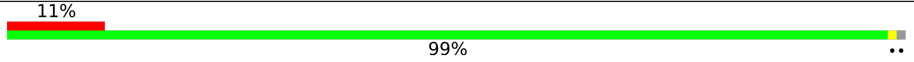
Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

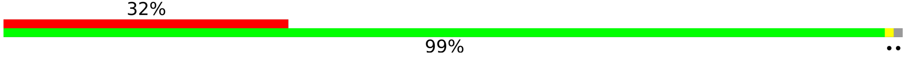
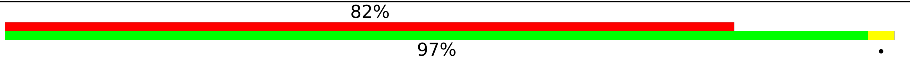
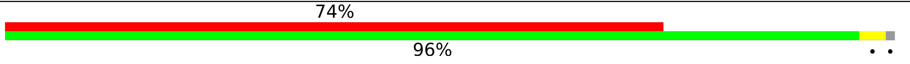
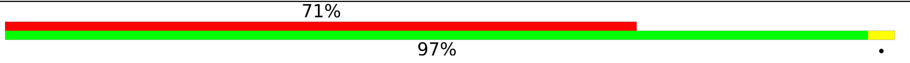
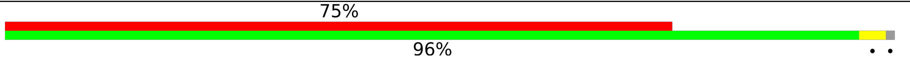
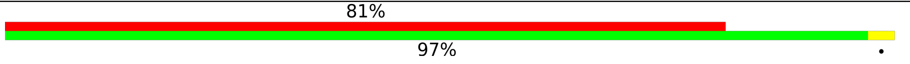
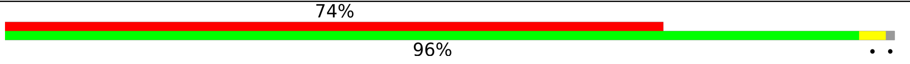
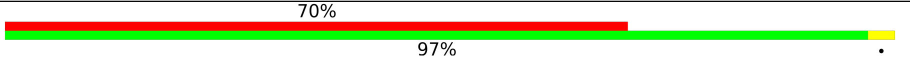
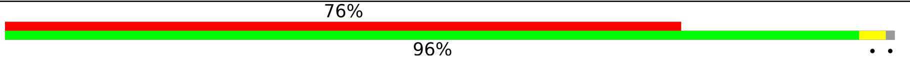
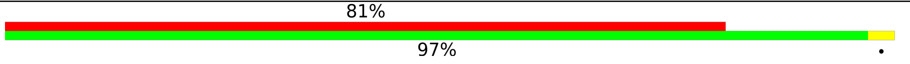
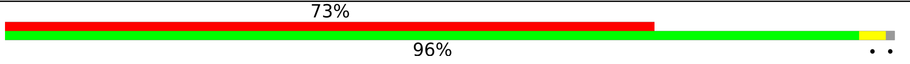
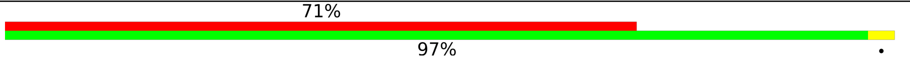
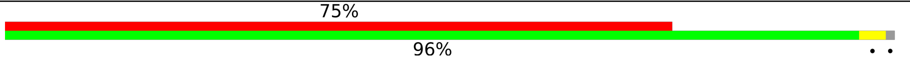
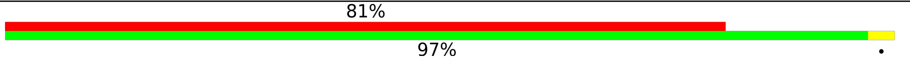
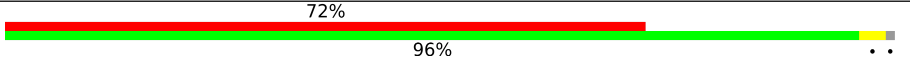
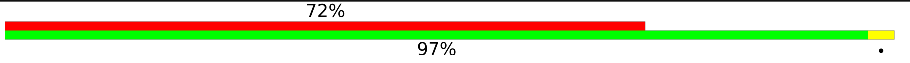
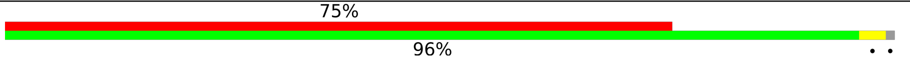
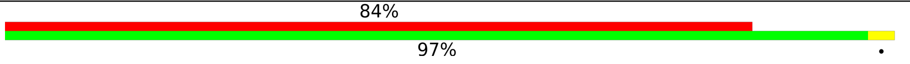
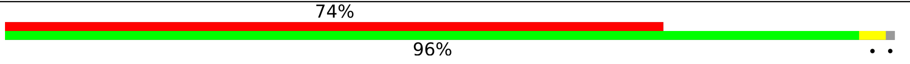
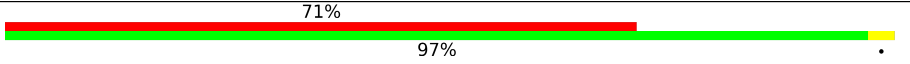
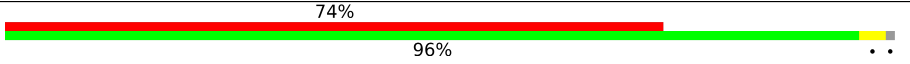
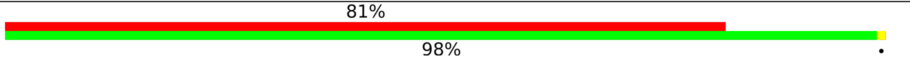
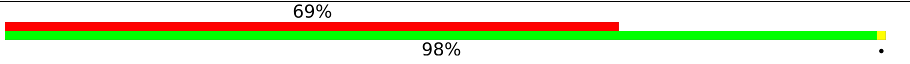
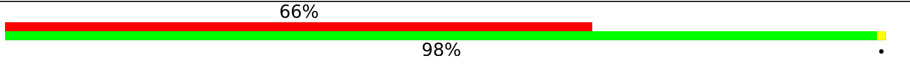
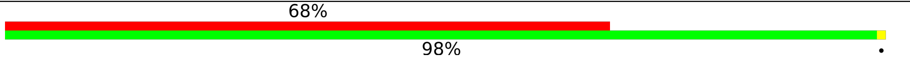
Continued on next page...

Continued from previous page...

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

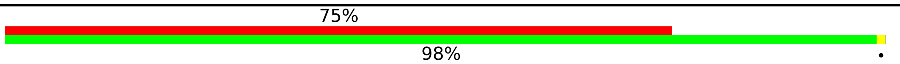
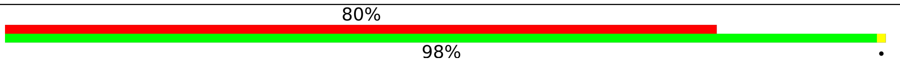
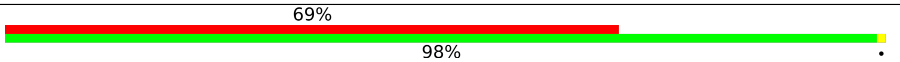
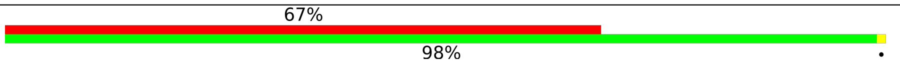
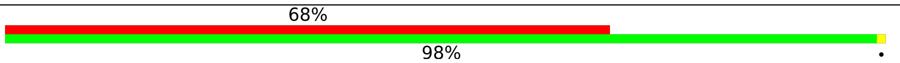
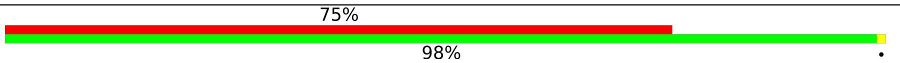
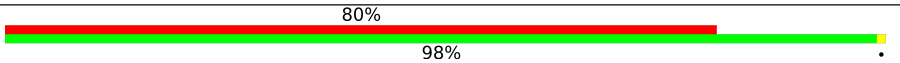
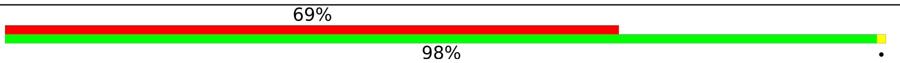
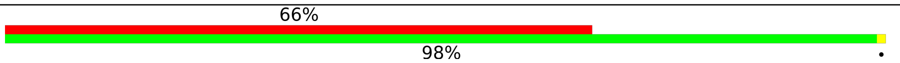
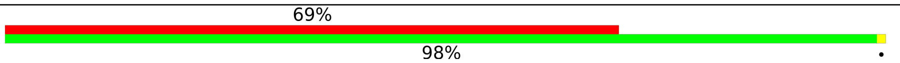
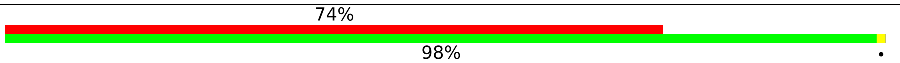
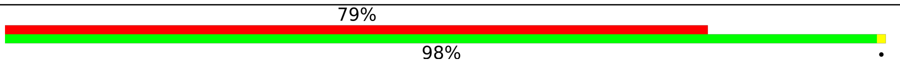
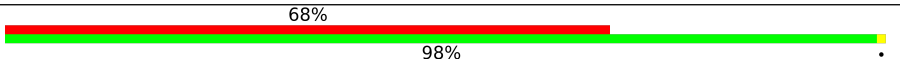
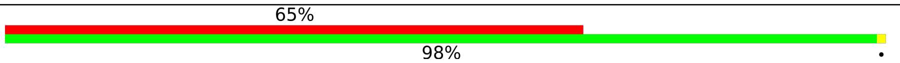
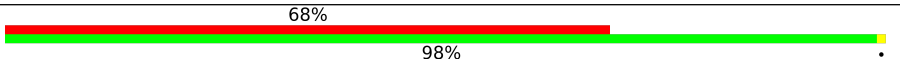
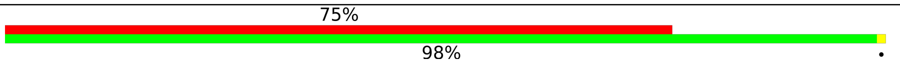
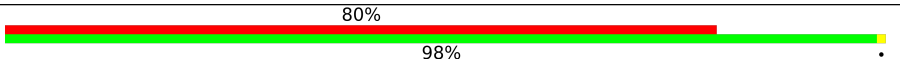
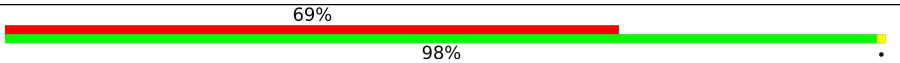
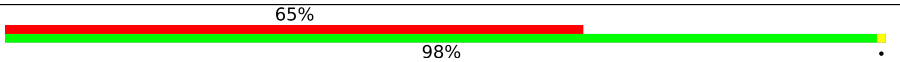
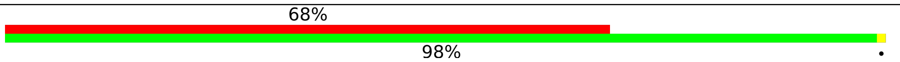
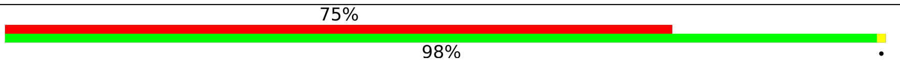
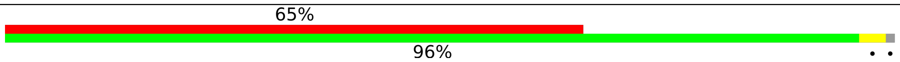
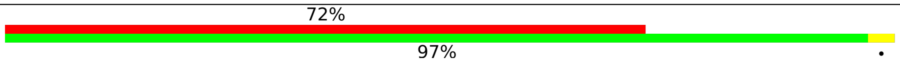
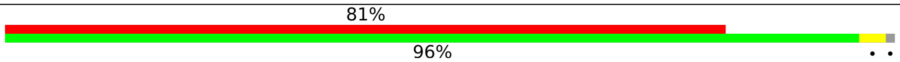
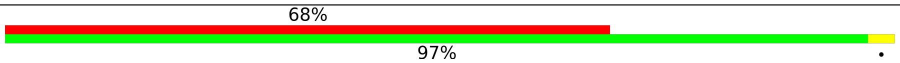
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	9E	448	
2	1e	281	
2	1f	281	
2	1g	281	
2	1h	281	
2	1i	281	
2	1j	281	
2	1k	281	
2	1l	281	
2	1m	281	
2	1n	281	
2	1o	281	
2	1p	281	
2	1q	281	
2	1r	281	
2	1s	281	
2	1t	281	
2	1u	281	
2	1v	281	
2	1w	281	
2	1x	281	
2	2Z	281	
2	2a	281	
2	2b	281	
2	2c	281	

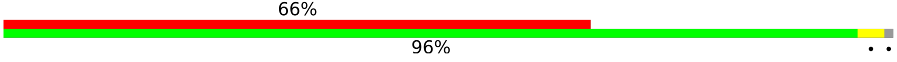
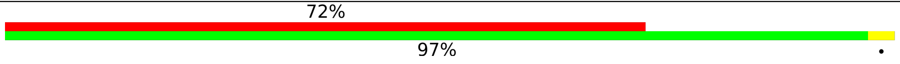
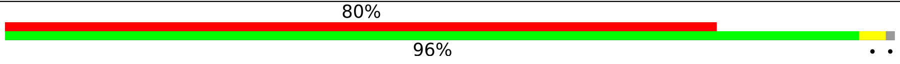
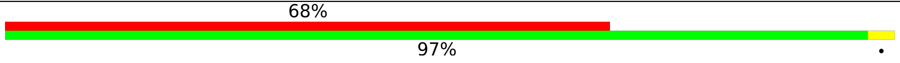
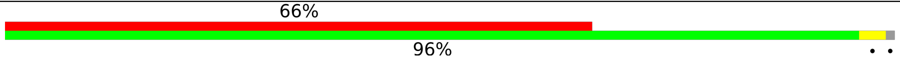
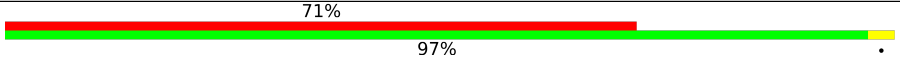
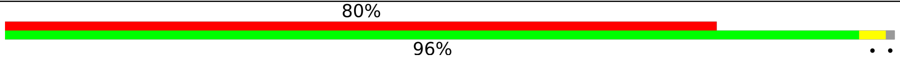
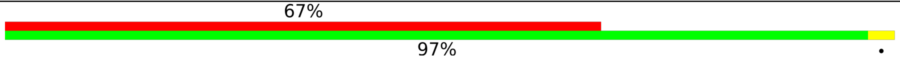
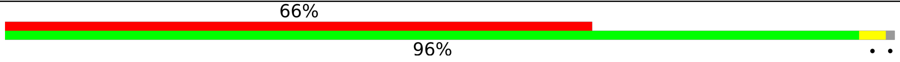
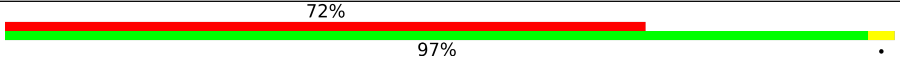
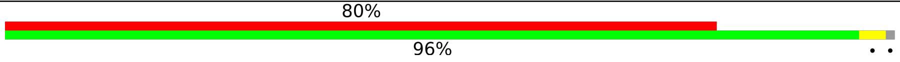
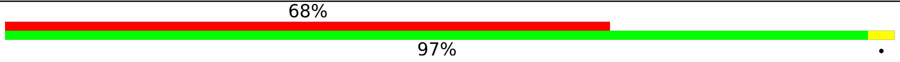
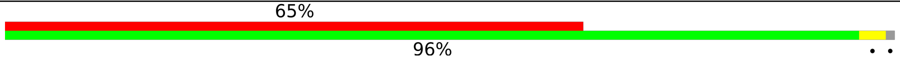
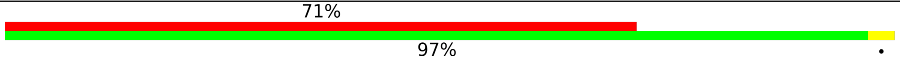
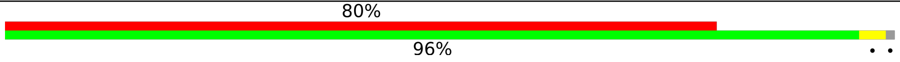
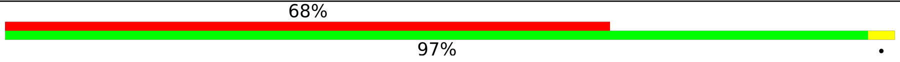
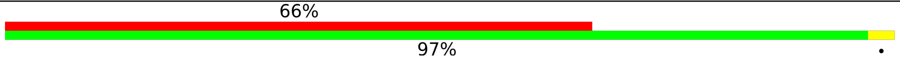
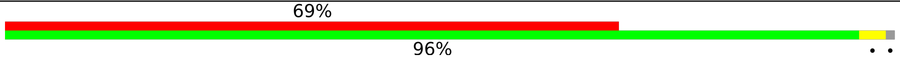
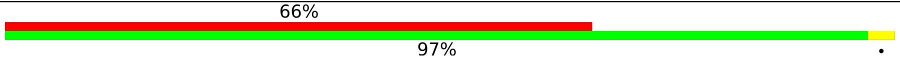
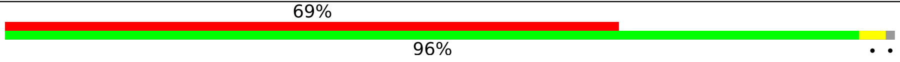
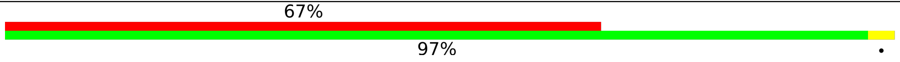
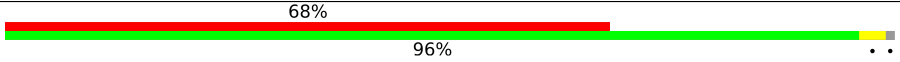
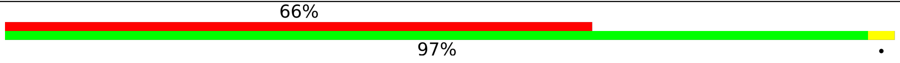
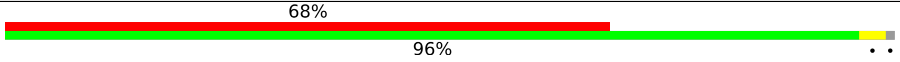
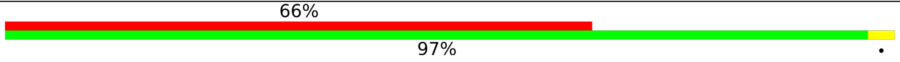
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	2d	281	
2	2e	281	
2	2f	281	
2	2g	281	
2	2h	281	
2	2i	281	
2	2j	281	
2	2k	281	
2	2l	281	
2	2m	281	
2	2n	281	
2	2o	281	
2	2p	281	
2	2q	281	
2	2r	281	
2	2s	281	
2	2t	281	
2	2u	281	
2	2v	281	
2	2w	281	
2	2x	281	
2	3e	281	
2	3f	281	
2	3g	281	
2	3h	281	

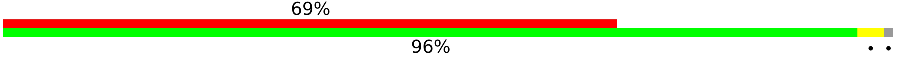
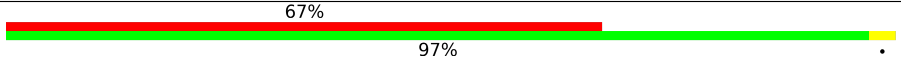
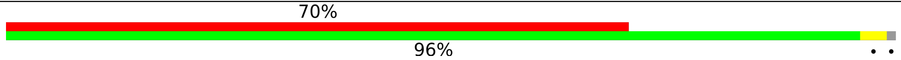
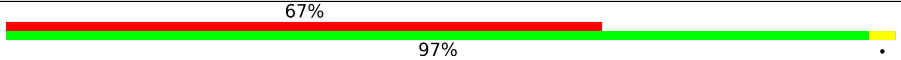
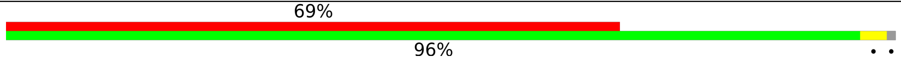
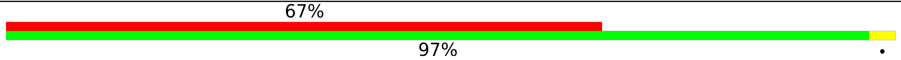
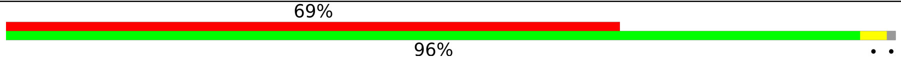
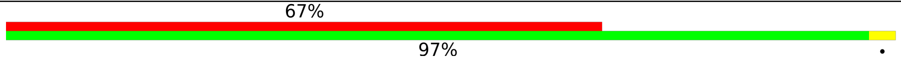
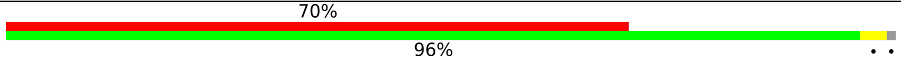
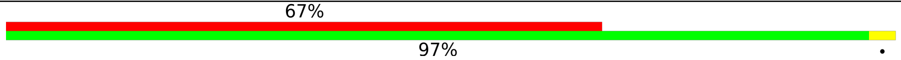
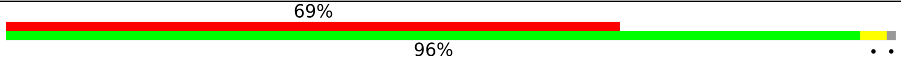
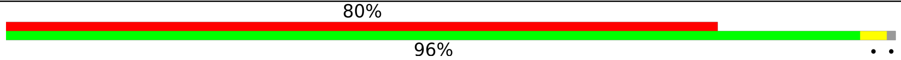
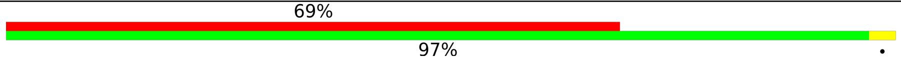
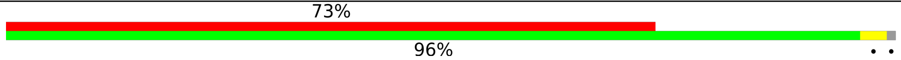
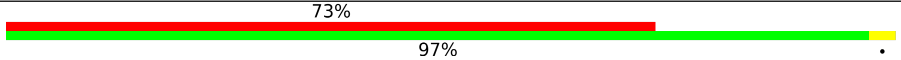
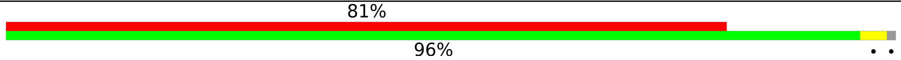
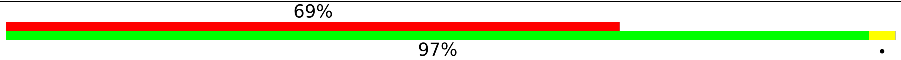
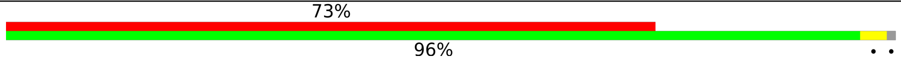
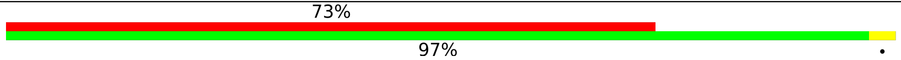
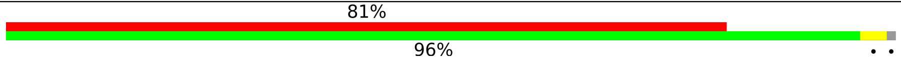
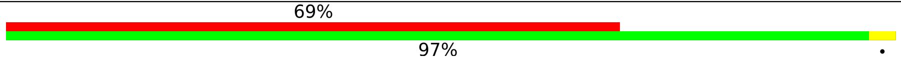
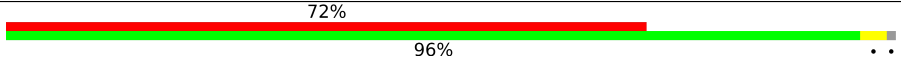
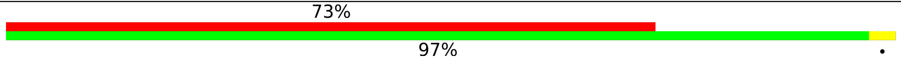
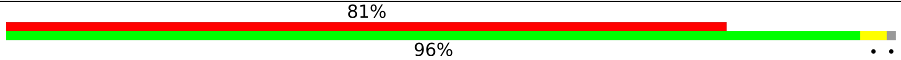
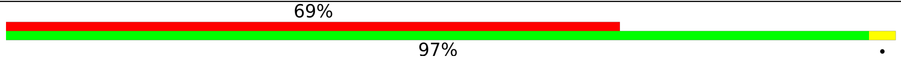
Continued on next page...

Continued from previous page...

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

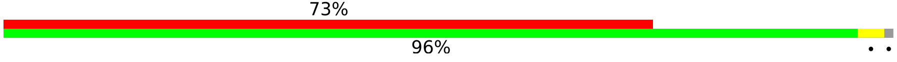
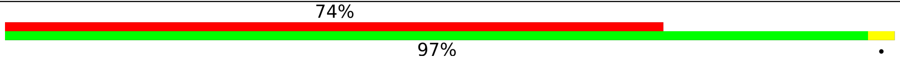
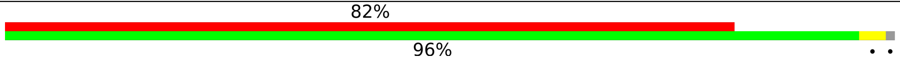
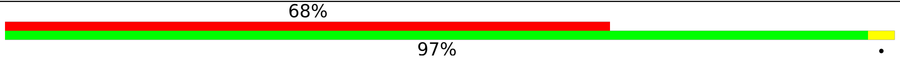
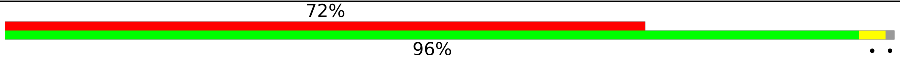
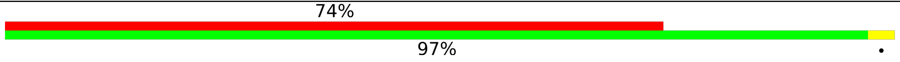
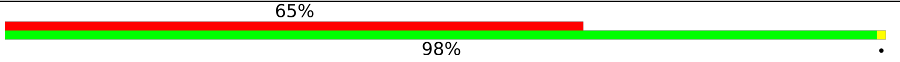
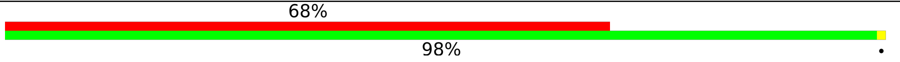
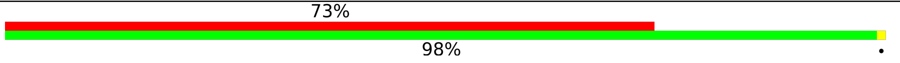
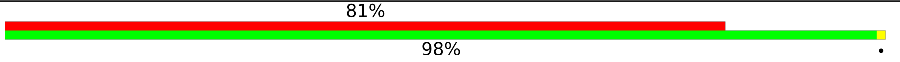
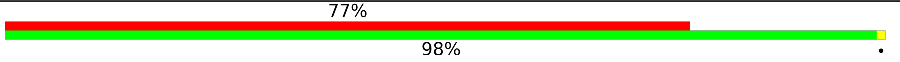
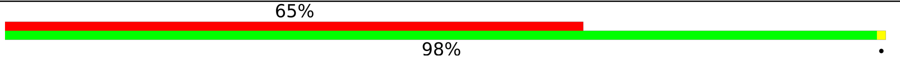
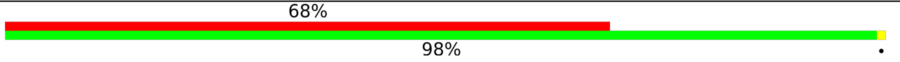
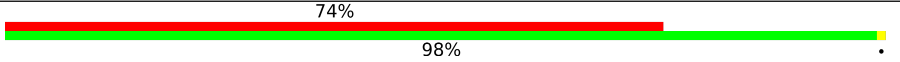
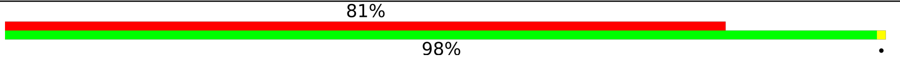
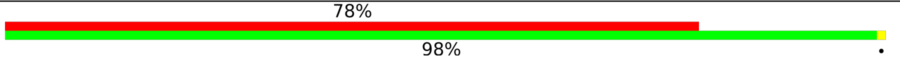
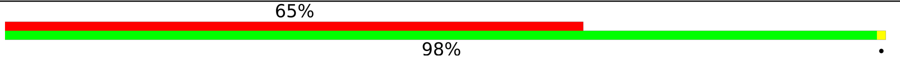
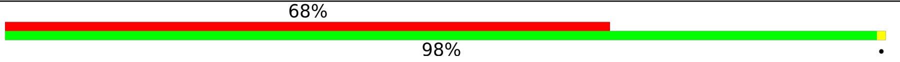
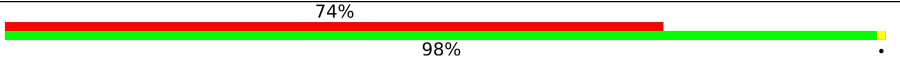
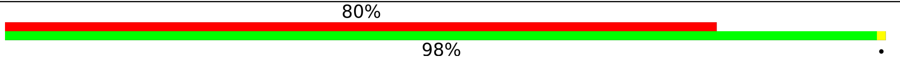
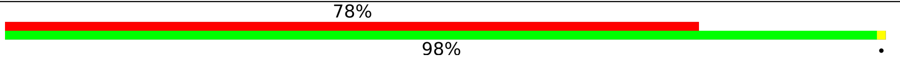
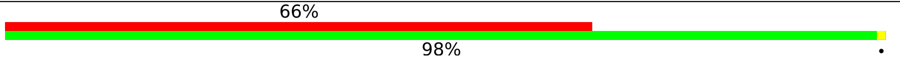
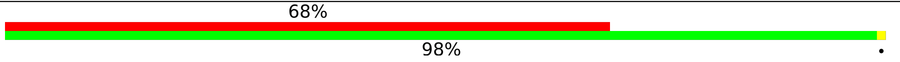
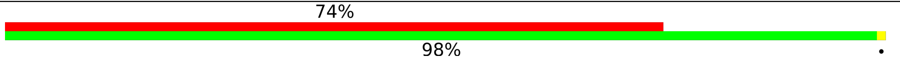
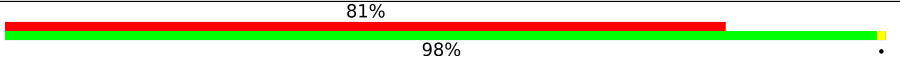
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	4n	281	
2	5e	281	
2	5f	281	
2	5g	281	
2	5h	281	
2	5i	281	
2	5j	281	
2	5k	281	
2	5l	281	
2	5m	281	
2	5n	281	
2	6e	281	
2	6f	281	
2	6g	281	
2	6h	281	
2	6i	281	
2	6j	281	
2	6k	281	
2	6l	281	
2	6m	281	
2	6n	281	
2	6o	281	
2	6p	281	
2	6q	281	
2	6r	281	

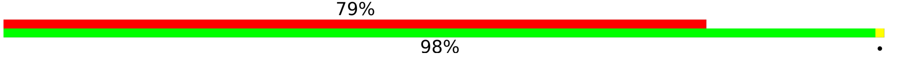
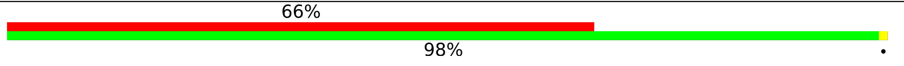
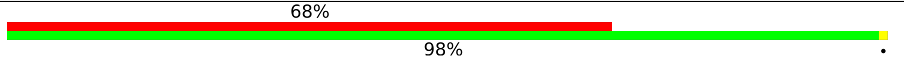
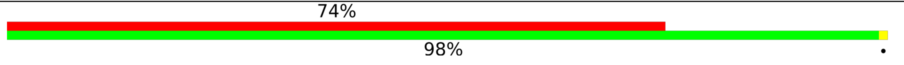
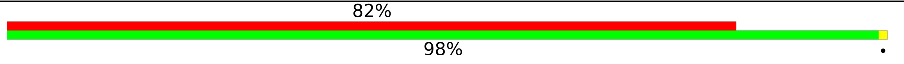
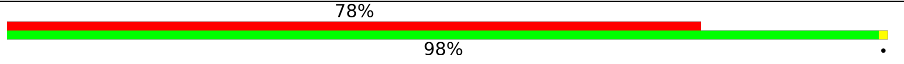
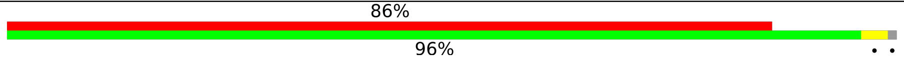
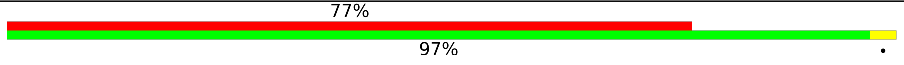
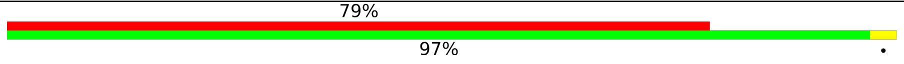
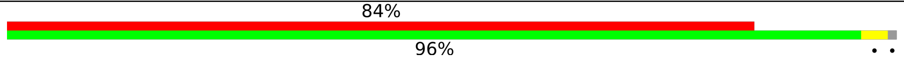
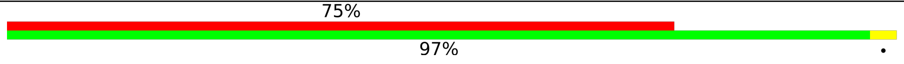
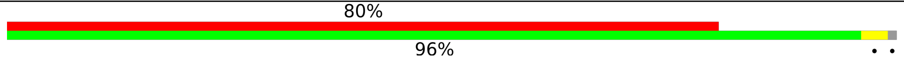
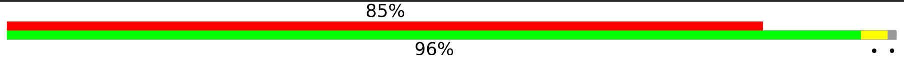
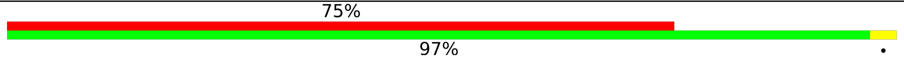
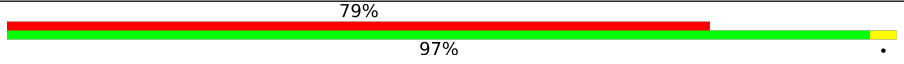
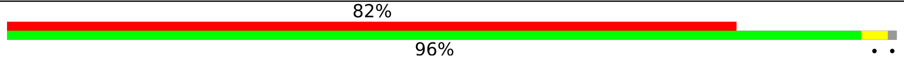
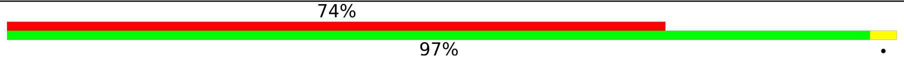
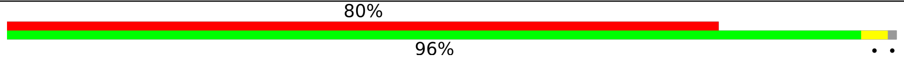
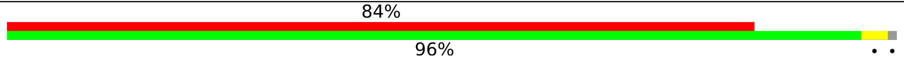
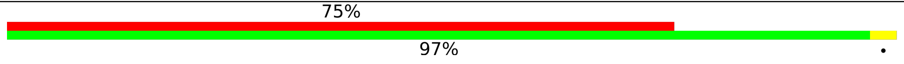
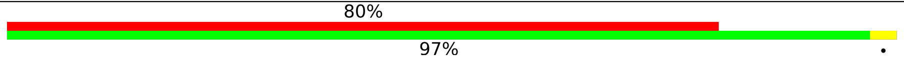
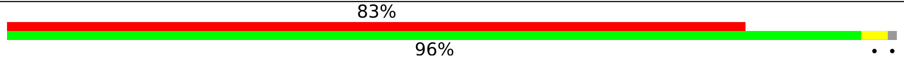
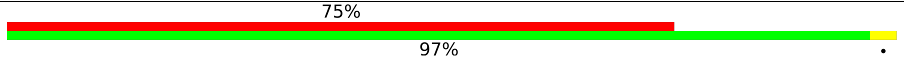
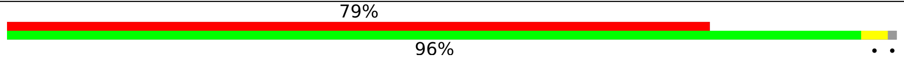
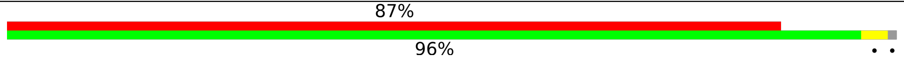
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	6s	281	
2	6t	281	
2	6u	281	
2	6v	281	
2	6w	281	
2	6x	281	
2	7Z	281	
2	7a	281	
2	7b	281	
2	7c	281	
2	7d	281	
2	7e	281	
2	7f	281	
2	7g	281	
2	7h	281	
2	7i	281	
2	7j	281	
2	7k	281	
2	7l	281	
2	7m	281	
2	7n	281	
2	7o	281	
2	7p	281	
2	7q	281	
2	7r	281	

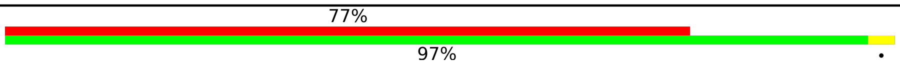
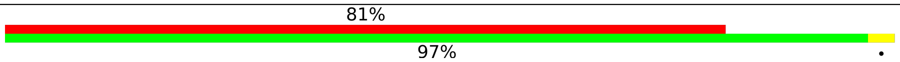
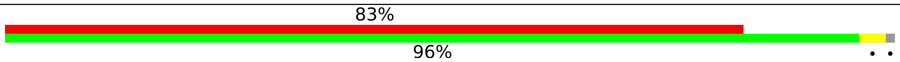
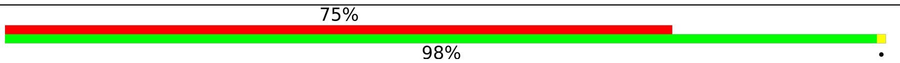
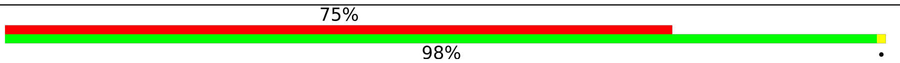
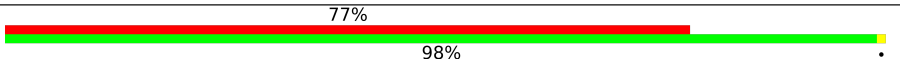
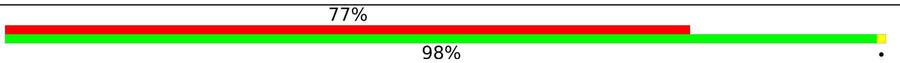
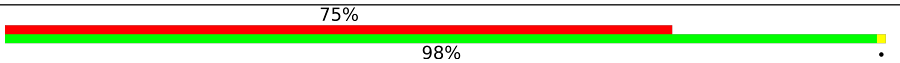
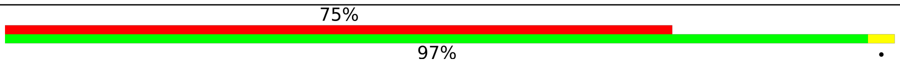
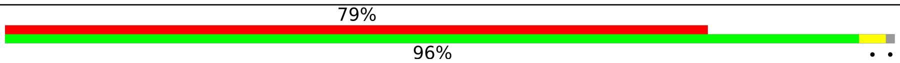
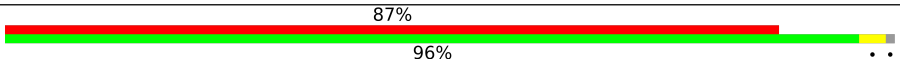
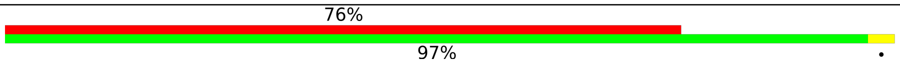
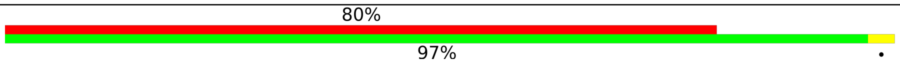
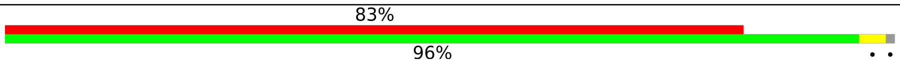
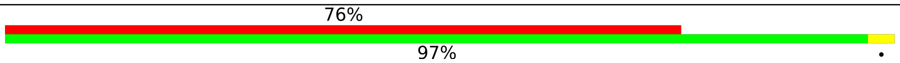
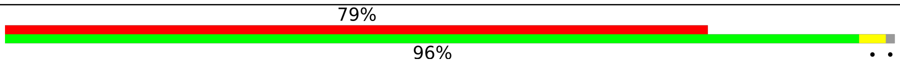
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	7s	281	
2	7t	281	
2	7u	281	
2	7v	281	
2	7w	281	
2	7x	281	
2	8e	281	
2	8f	281	
2	8g	281	
2	8h	281	
2	8i	281	
2	8j	281	
2	8k	281	
2	8l	281	
2	8m	281	
2	8n	281	
2	8o	281	
2	8p	281	
2	8q	281	
2	8r	281	
2	8s	281	
2	8t	281	
2	8u	281	
2	8v	281	
2	8w	281	

Continued on next page...

Continued from previous page...

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

2 Entry composition

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

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

- Molecule 1 is a protein called Major capsid protein.

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

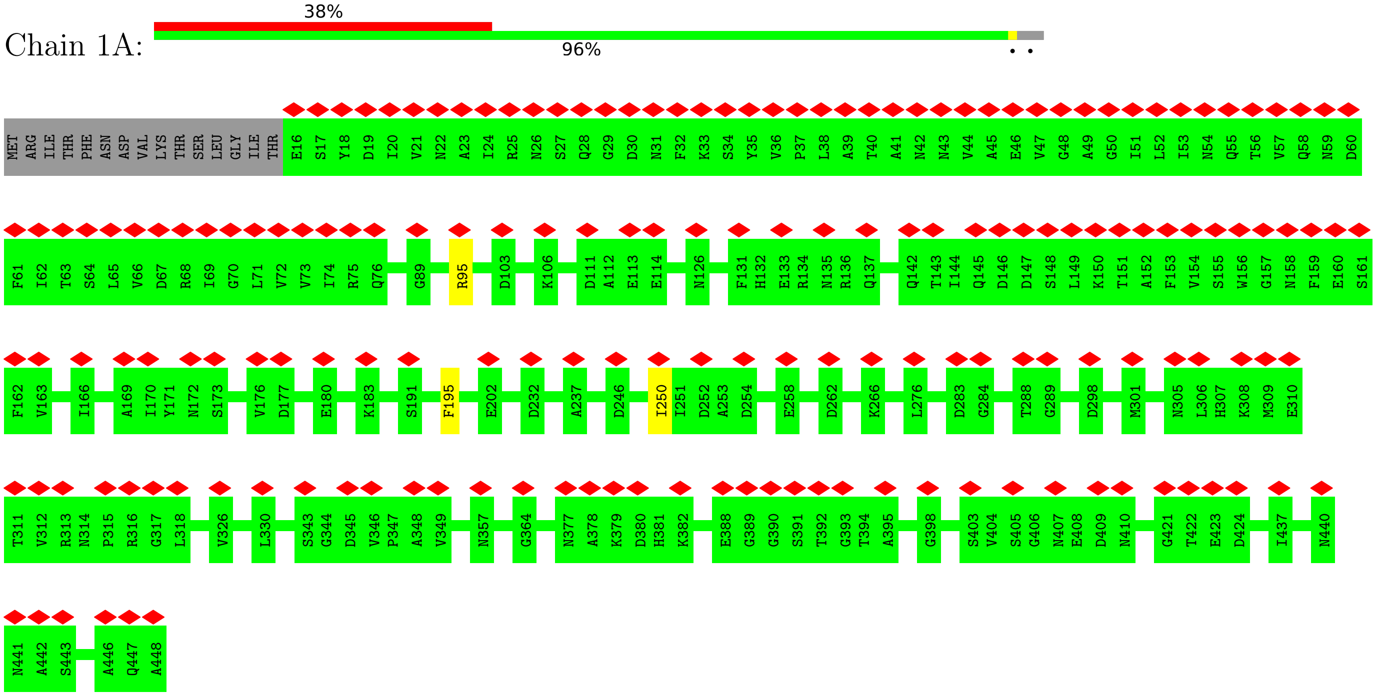
Chain	Residue	Modelled	Actual	Comment	Reference
9N	281	LEU	-	insertion	UNP B3VMP4
9O	123	GLU	ASP	conflict	UNP B3VMP4
9O	281	LEU	-	insertion	UNP B3VMP4
9P	123	GLU	ASP	conflict	UNP B3VMP4
9P	281	LEU	-	insertion	UNP B3VMP4
9Q	123	GLU	ASP	conflict	UNP B3VMP4
9Q	281	LEU	-	insertion	UNP B3VMP4
9R	123	GLU	ASP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

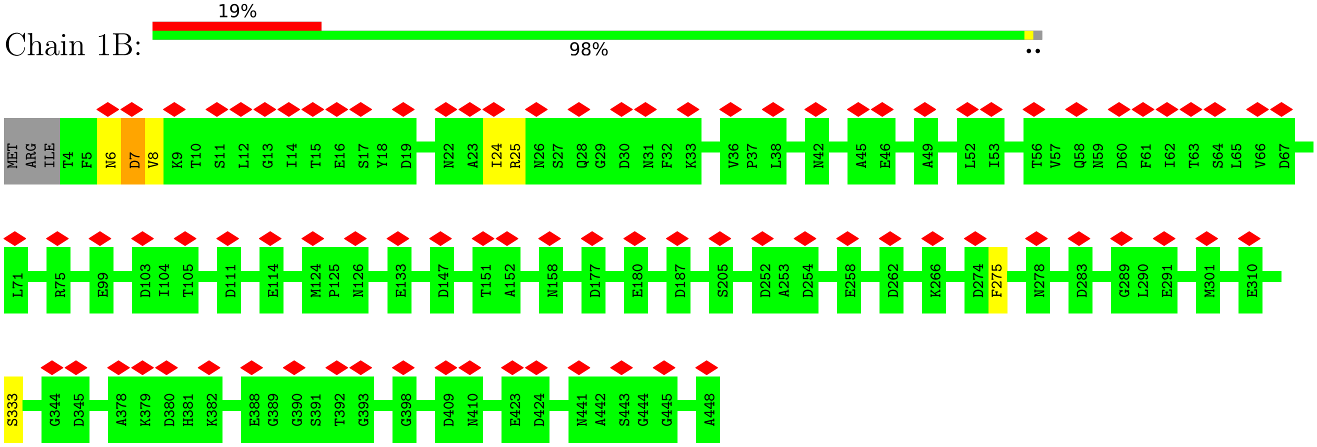
- Molecule 1: Major capsid protein

Chain 1A:



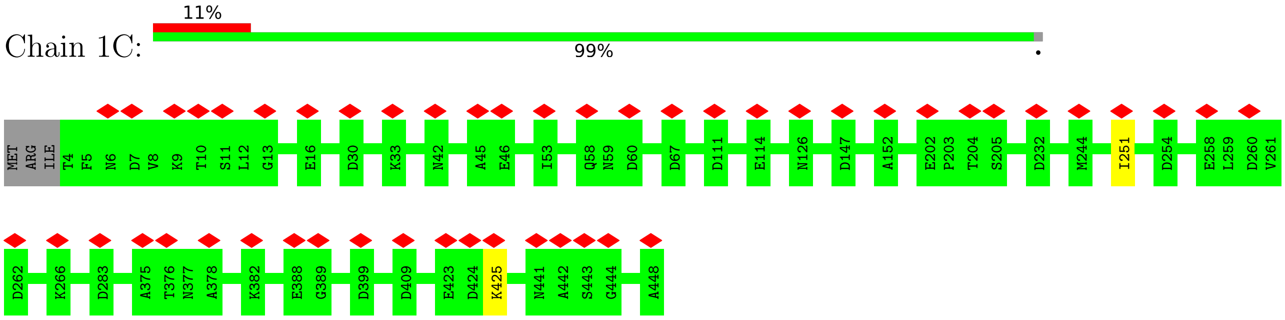
- Molecule 1: Major capsid protein

Chain 1B:



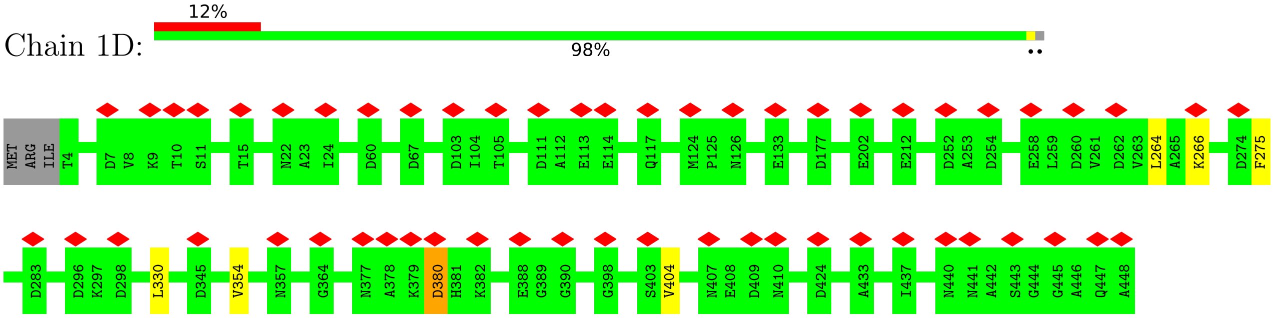
- Molecule 1: Major capsid protein

Chain 1C:



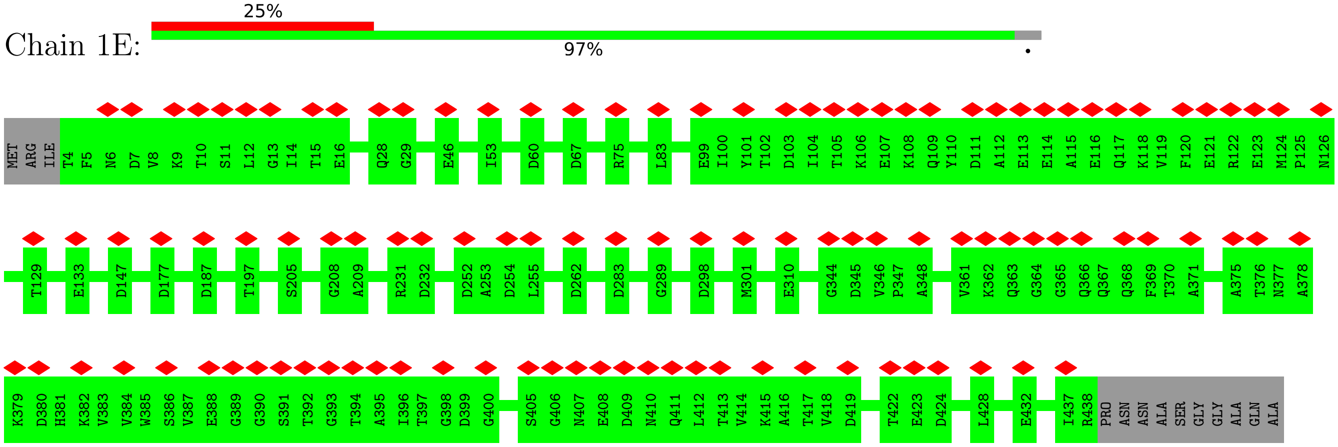
- Molecule 1: Major capsid protein

Chain 1D:



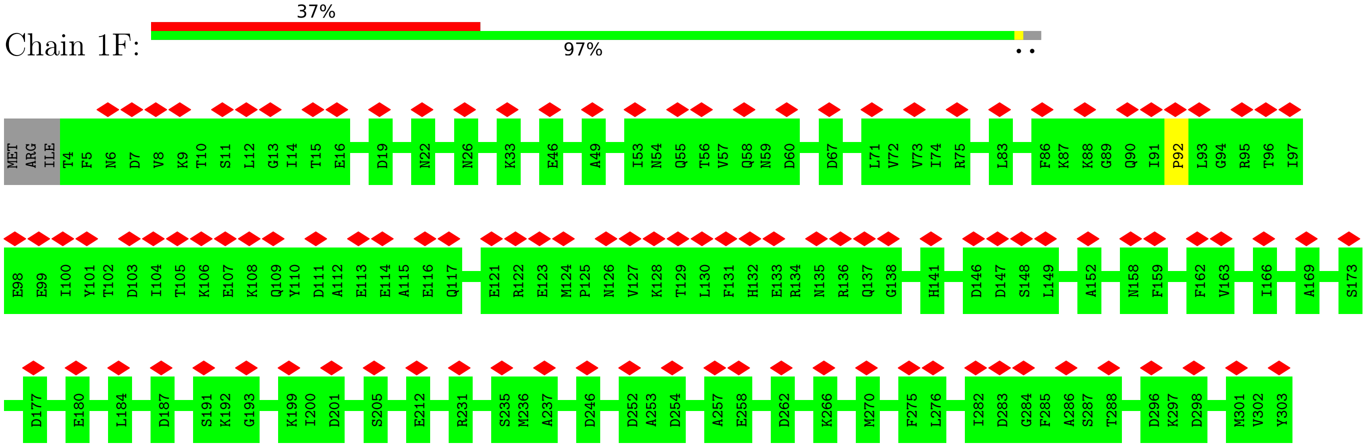
- Molecule 1: Major capsid protein

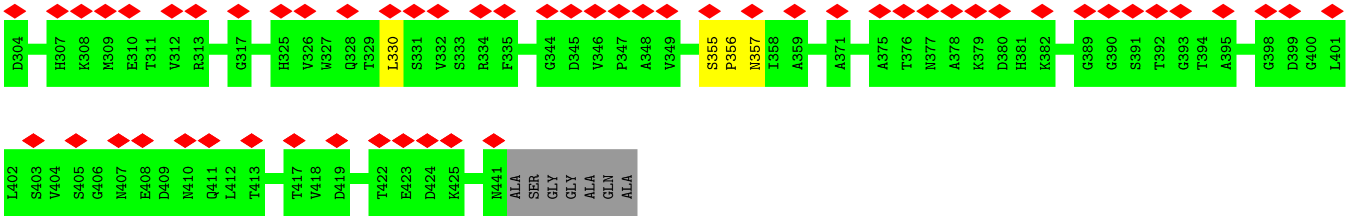
Chain 1E:



- Molecule 1: Major capsid protein

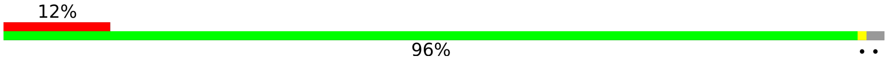
Chain 1F:

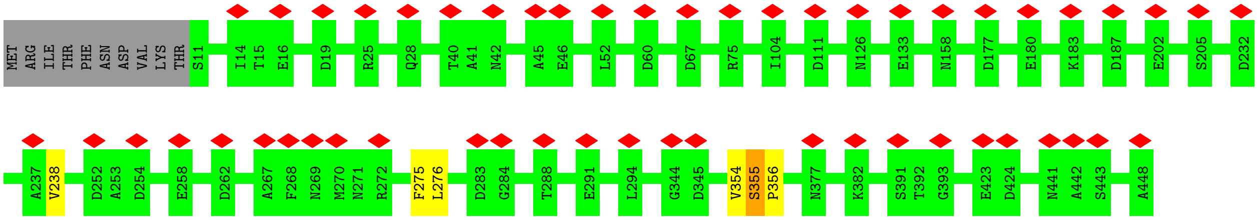




- Molecule 1: Major capsid protein

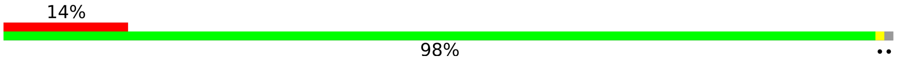
Chain 2A:

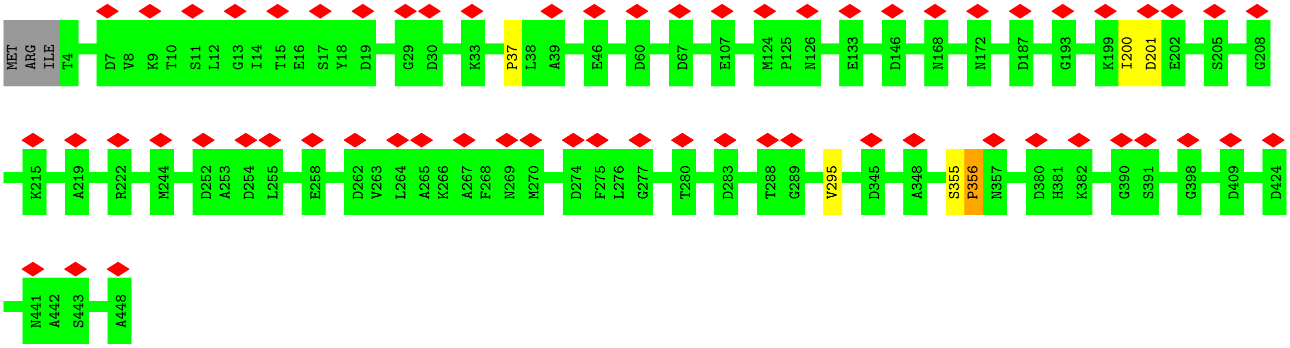




- Molecule 1: Major capsid protein

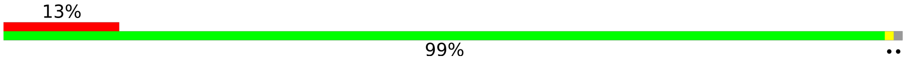
Chain 2B:

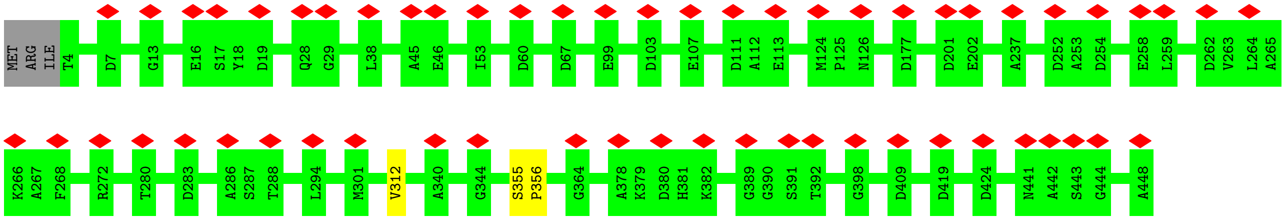




- Molecule 1: Major capsid protein

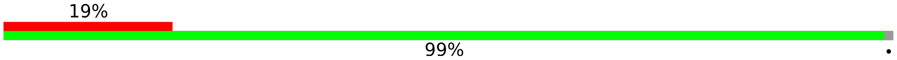
Chain 2C:

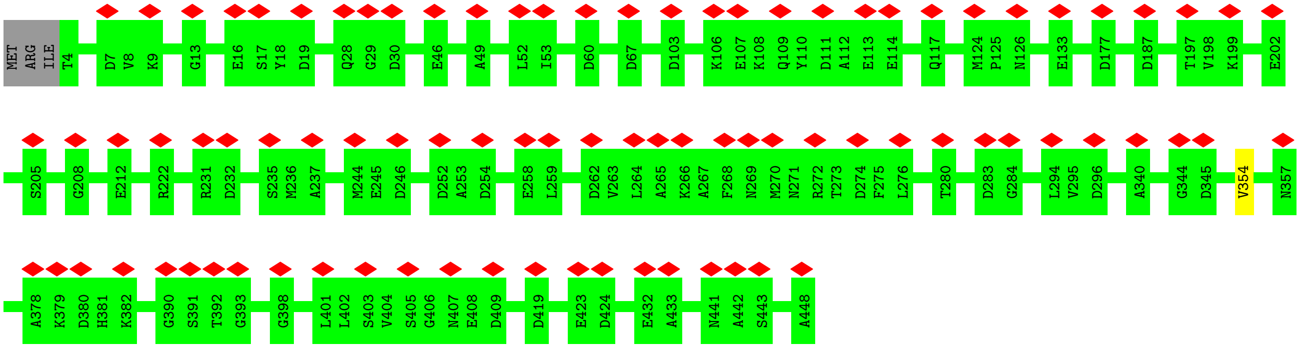




- Molecule 1: Major capsid protein

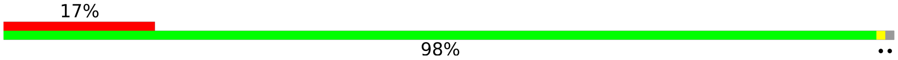
Chain 2D:

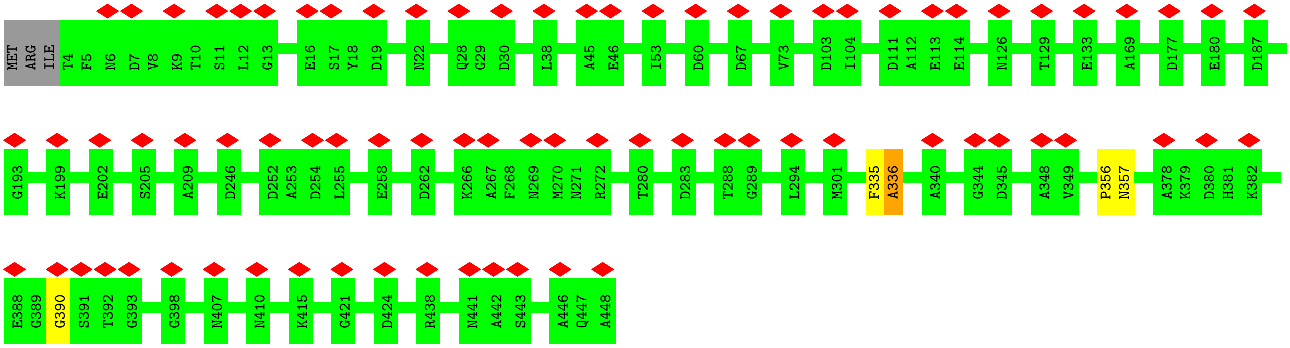




• Molecule 1: Major capsid protein

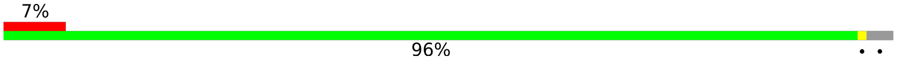
Chain 2E:

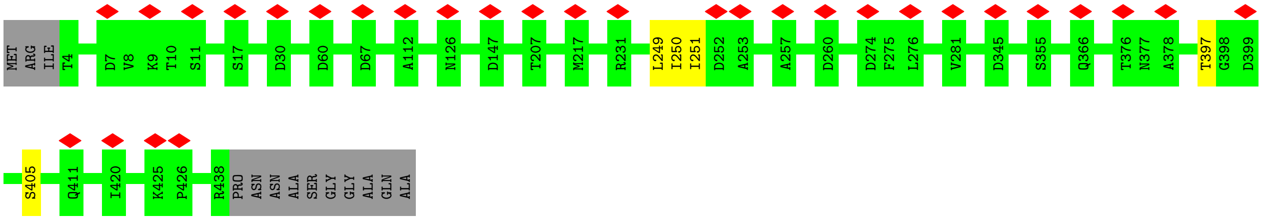




• Molecule 1: Major capsid protein

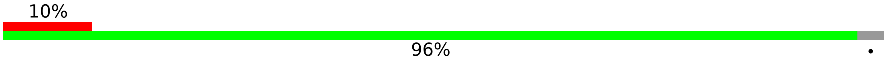
Chain 3A:

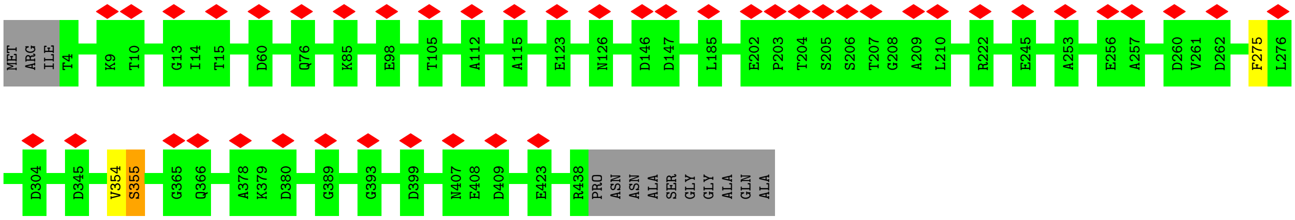




• Molecule 1: Major capsid protein

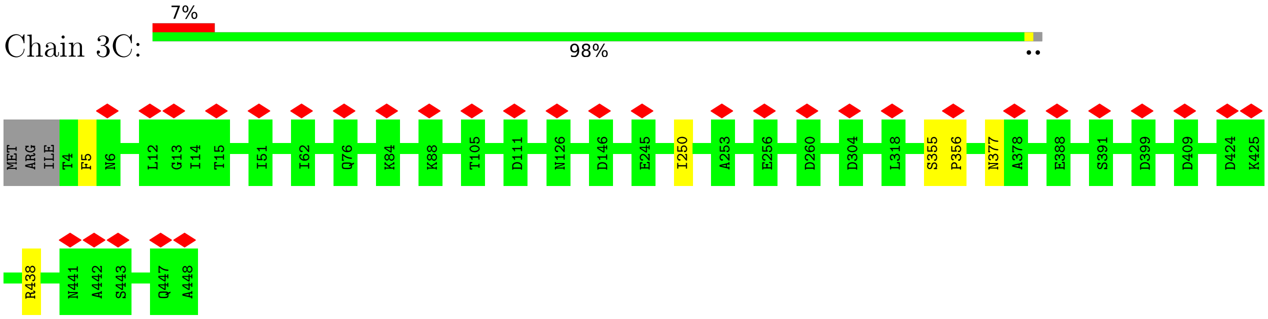
Chain 3B:





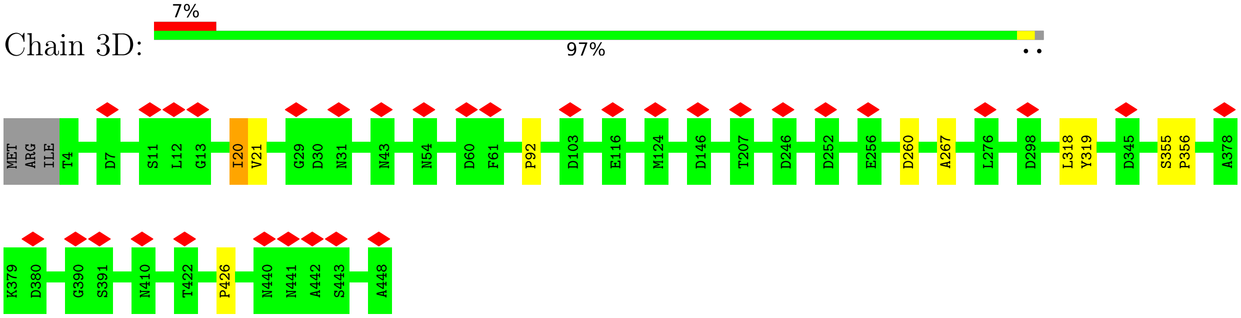
• Molecule 1: Major capsid protein

Chain 3C:



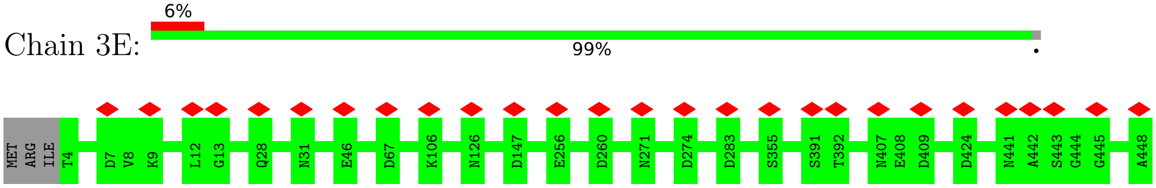
- Molecule 1: Major capsid protein

Chain 3D:



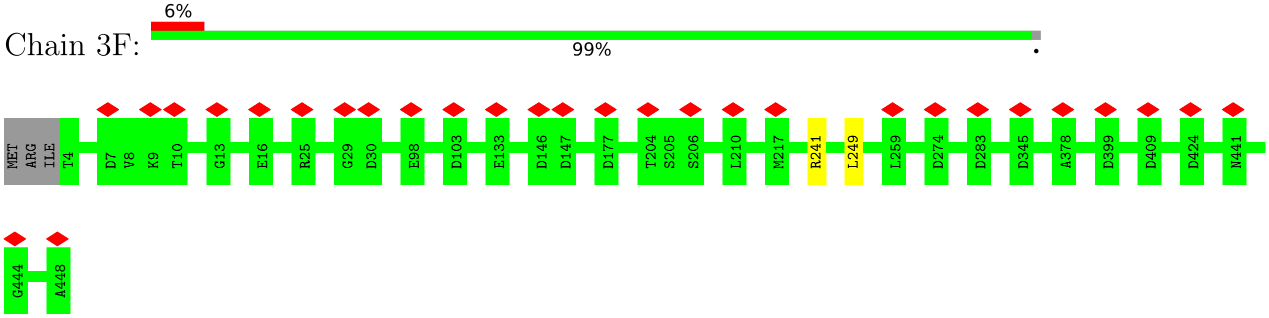
- Molecule 1: Major capsid protein

Chain 3E:



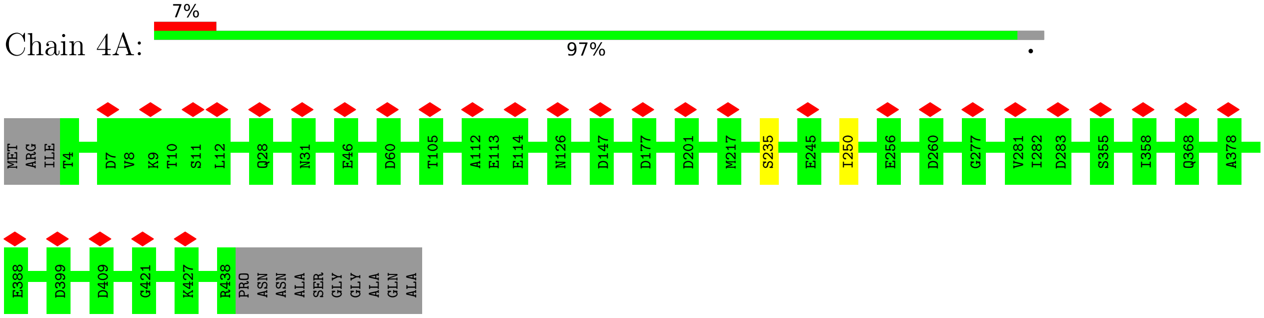
- Molecule 1: Major capsid protein

Chain 3F:

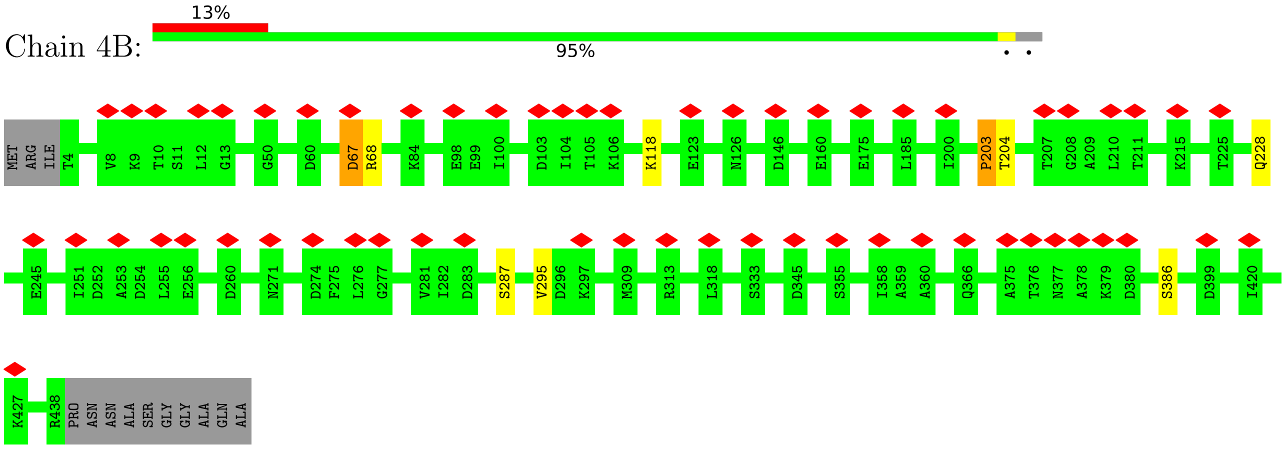


- Molecule 1: Major capsid protein

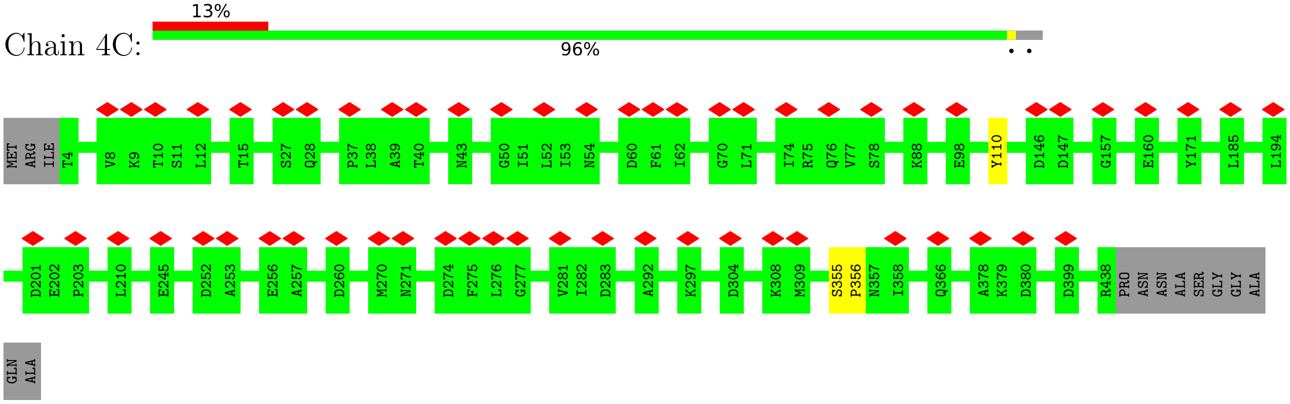
Chain 4A:



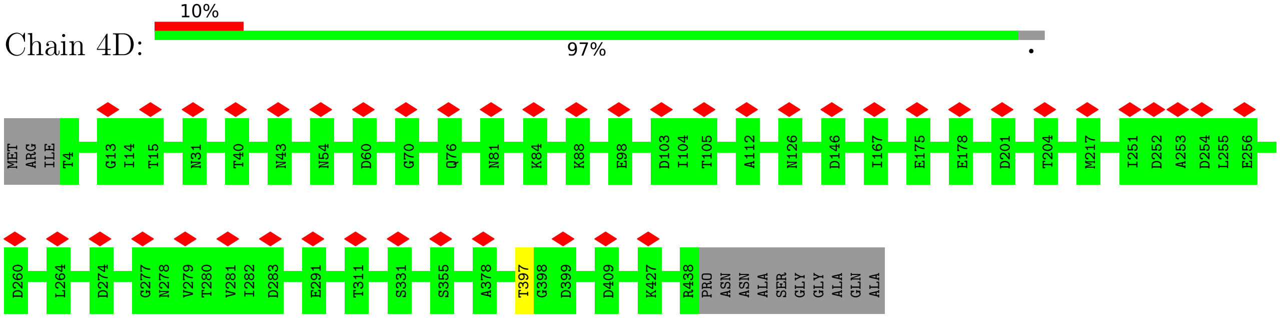
- Molecule 1: Major capsid protein



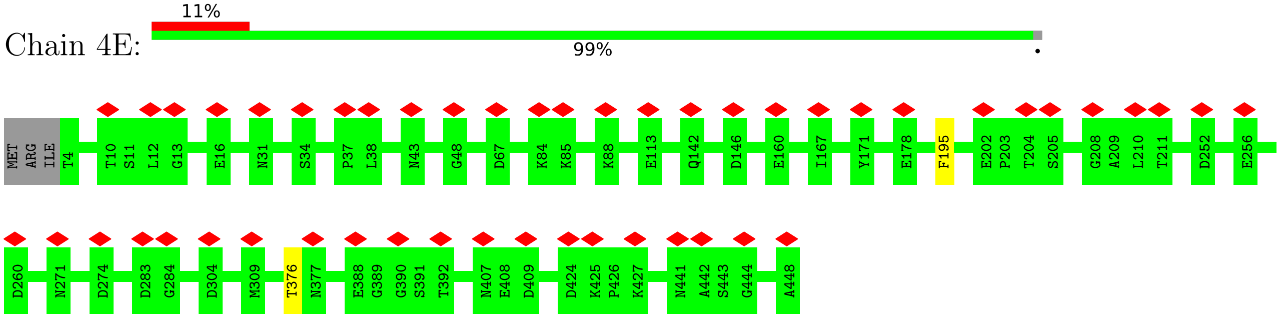
- Molecule 1: Major capsid protein



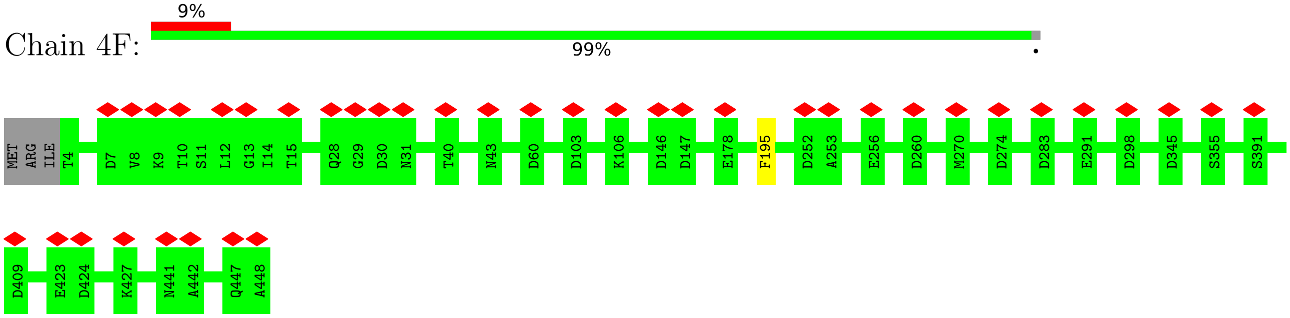
- Molecule 1: Major capsid protein



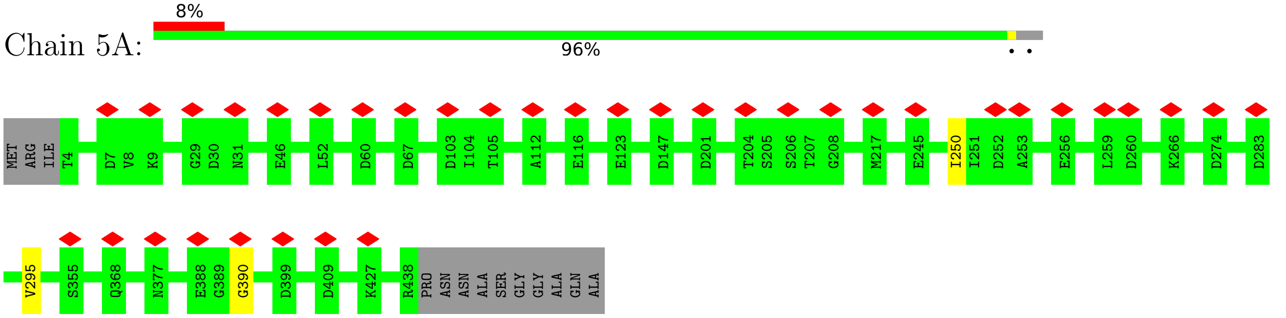
- Molecule 1: Major capsid protein



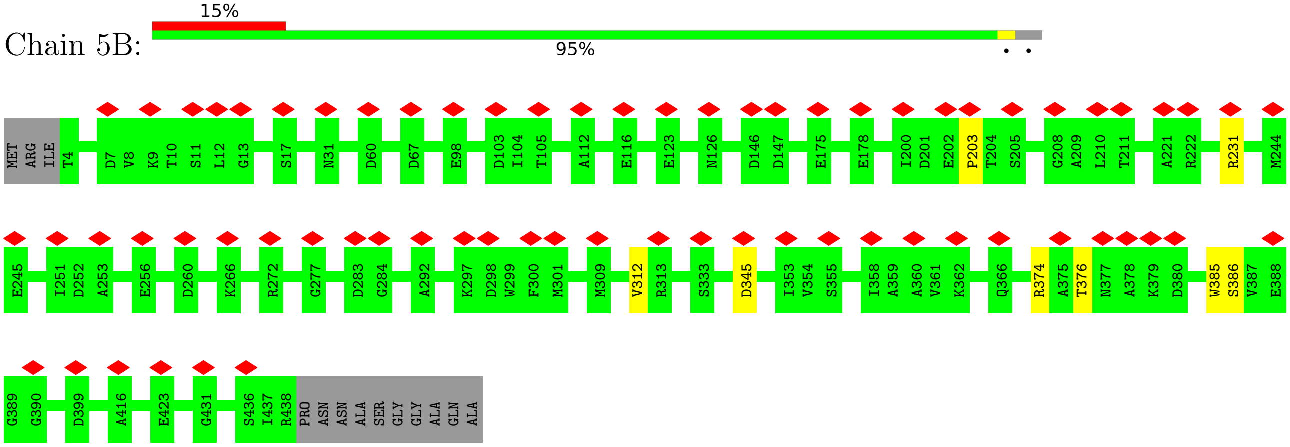
- Molecule 1: Major capsid protein



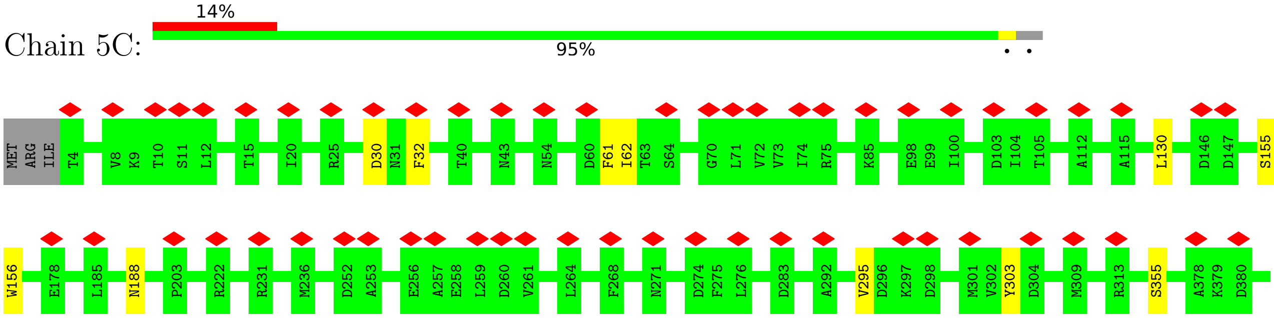
- Molecule 1: Major capsid protein

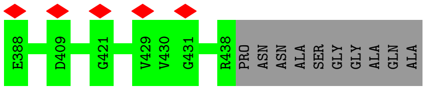


- Molecule 1: Major capsid protein



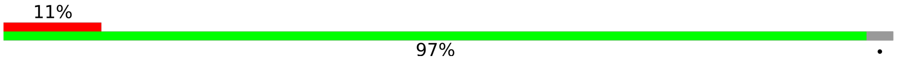
- Molecule 1: Major capsid protein

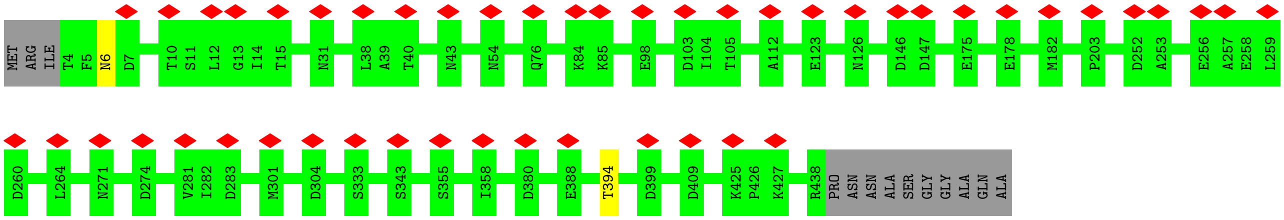




- Molecule 1: Major capsid protein

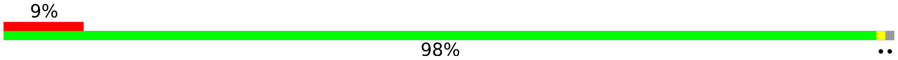
Chain 5D:

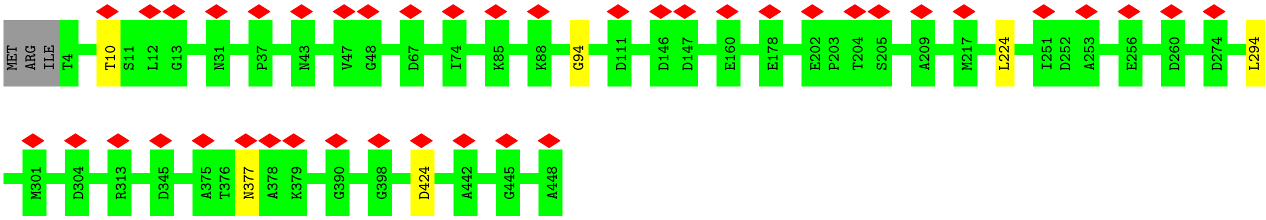




- Molecule 1: Major capsid protein

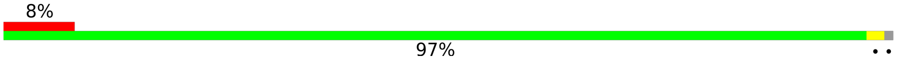
Chain 5E:

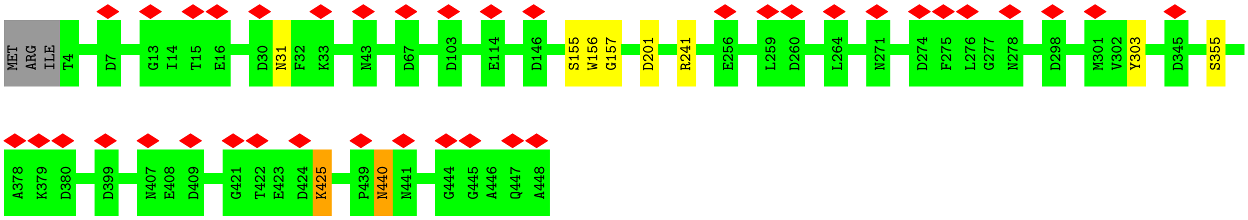




- Molecule 1: Major capsid protein

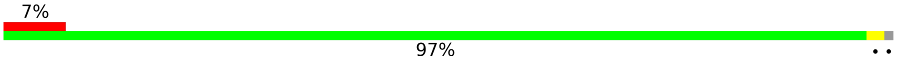
Chain 5F:

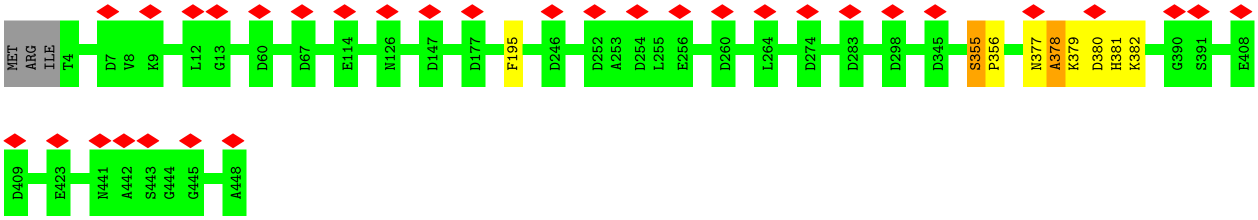




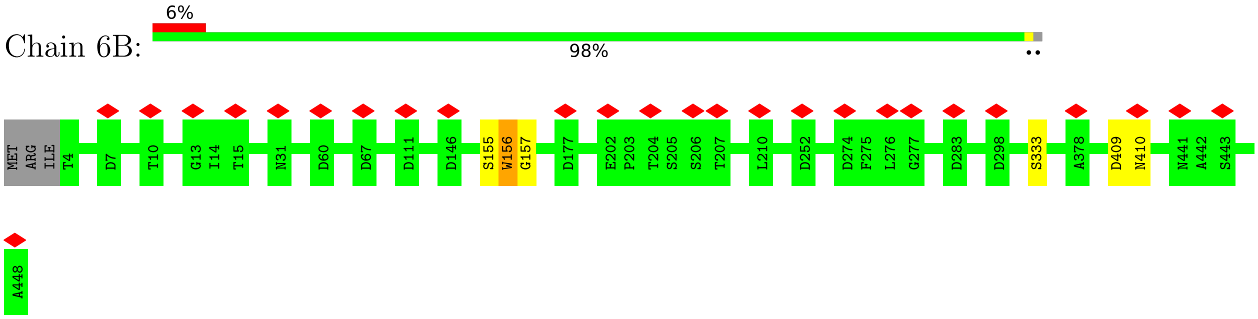
- Molecule 1: Major capsid protein

Chain 6A:

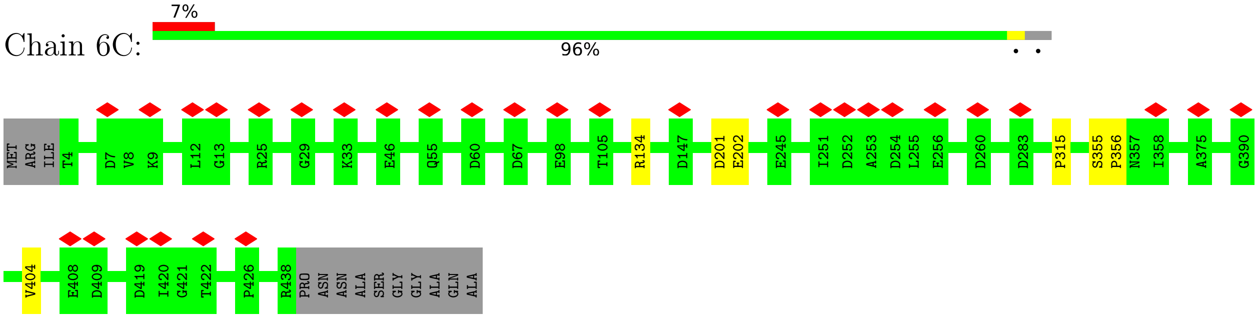




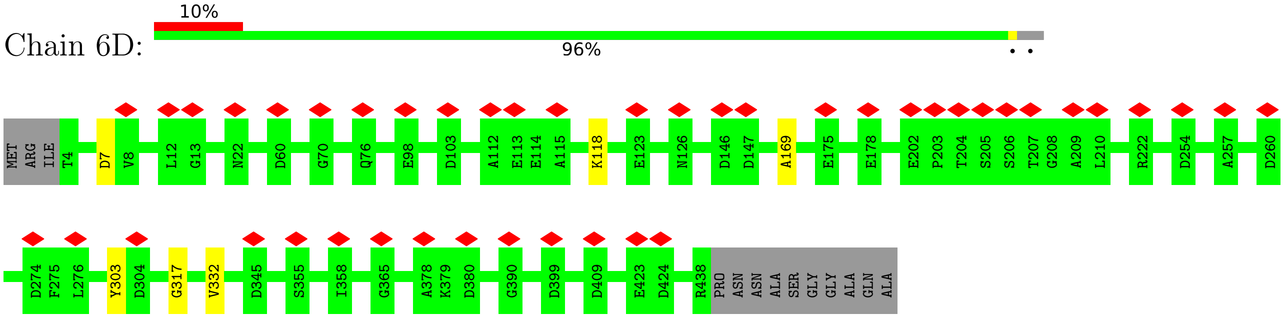
- Molecule 1: Major capsid protein



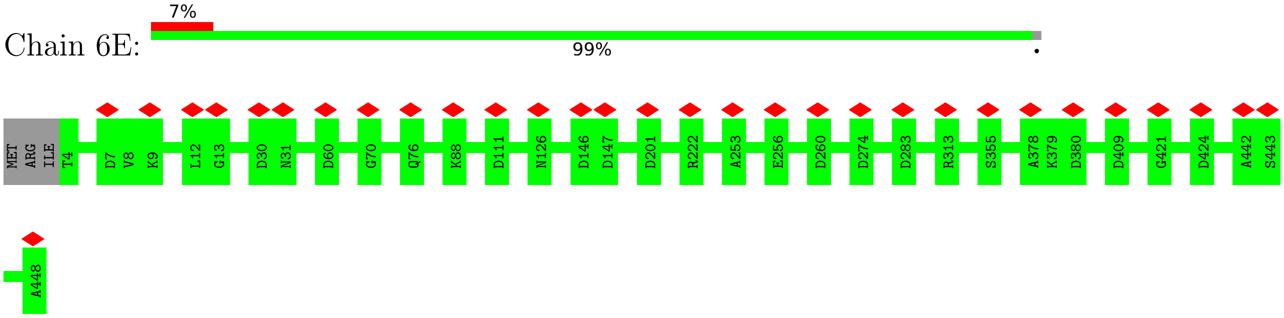
- Molecule 1: Major capsid protein



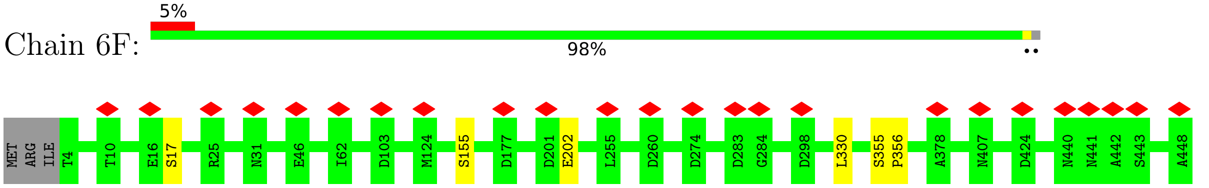
- Molecule 1: Major capsid protein



- Molecule 1: Major capsid protein

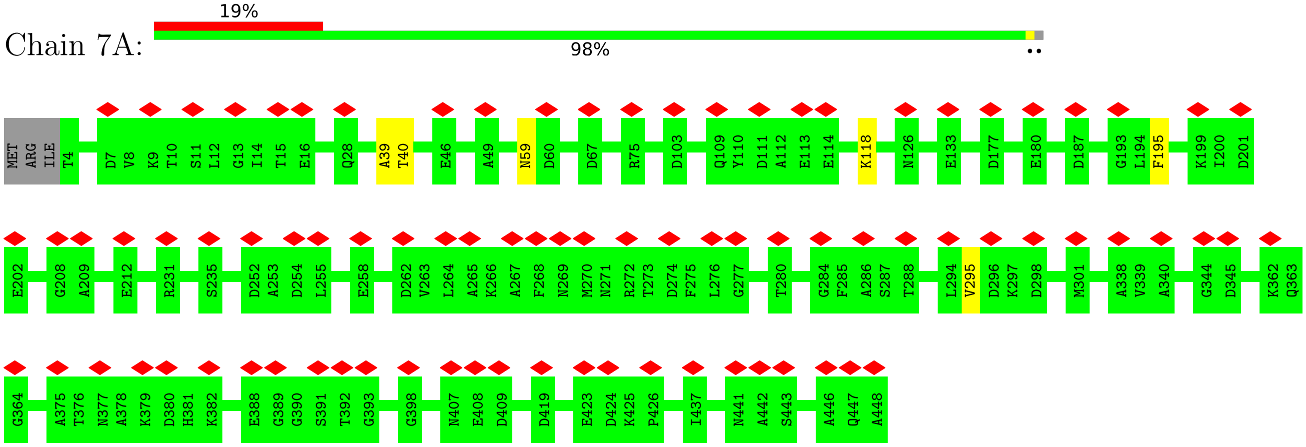


- Molecule 1: Major capsid protein



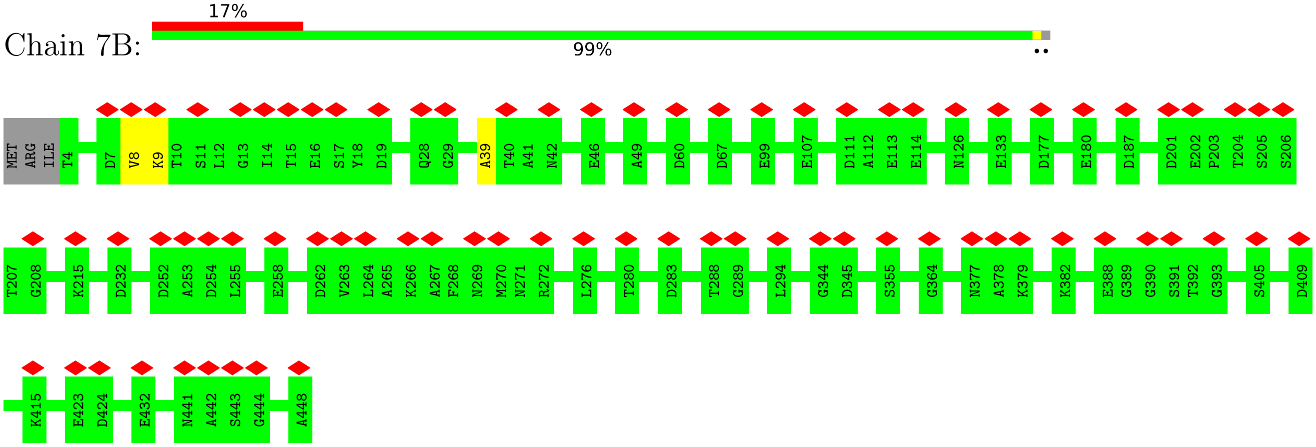
- Molecule 1: Major capsid protein

Chain 7A:



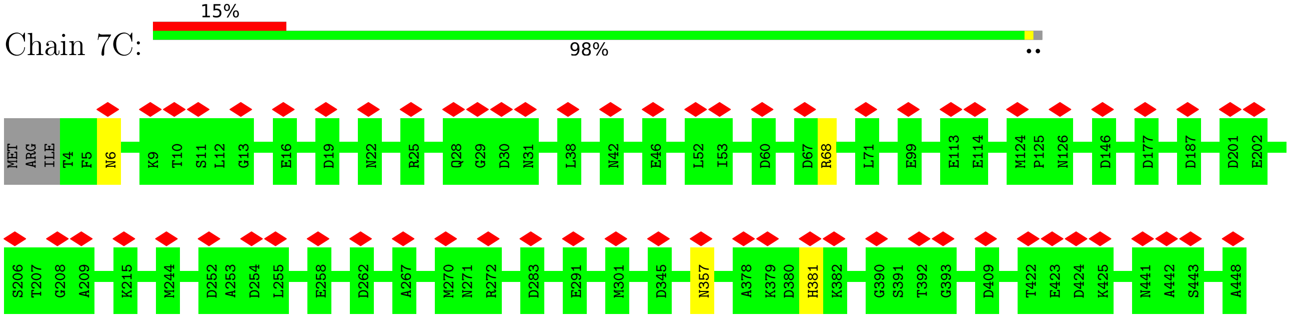
- Molecule 1: Major capsid protein

Chain 7B:



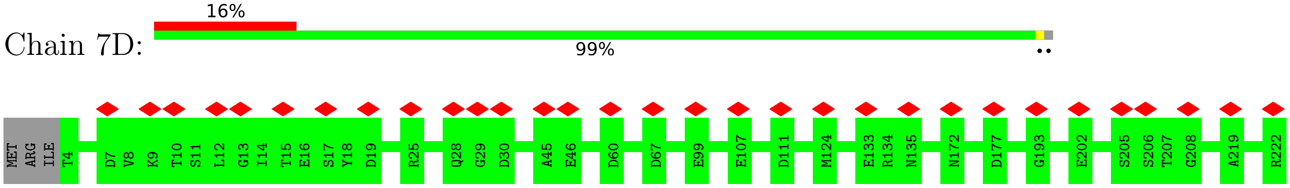
- Molecule 1: Major capsid protein

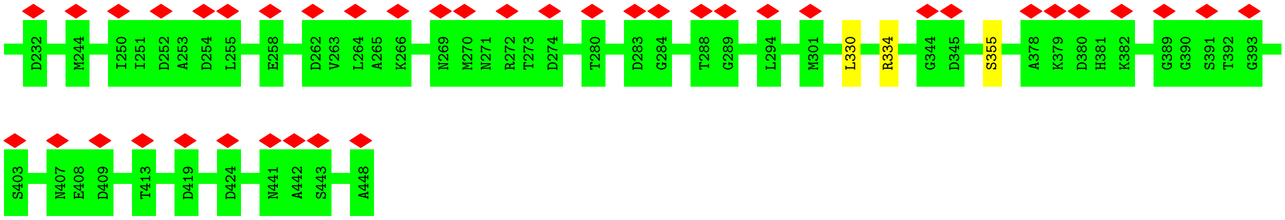
Chain 7C:



- Molecule 1: Major capsid protein

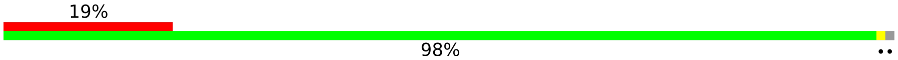
Chain 7D:

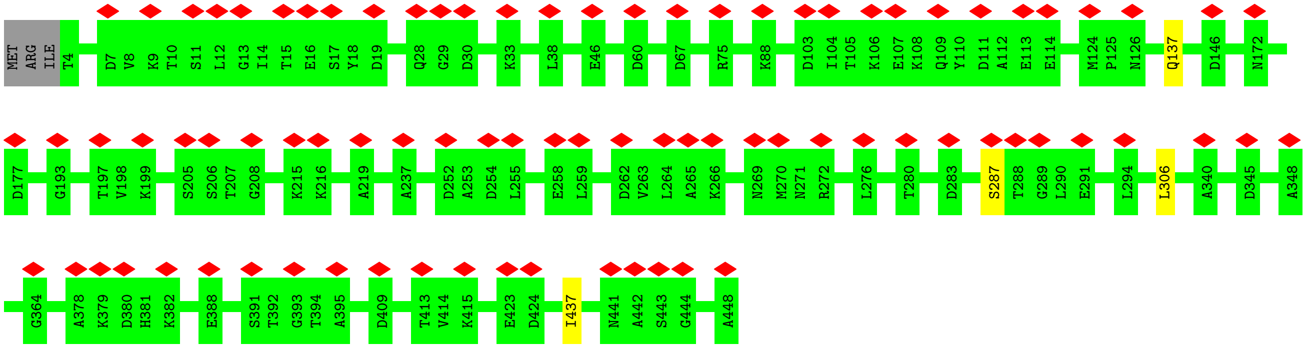




- Molecule 1: Major capsid protein

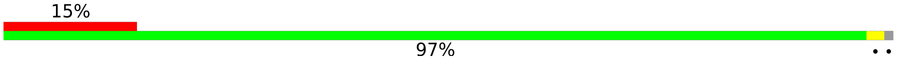
Chain 7E:

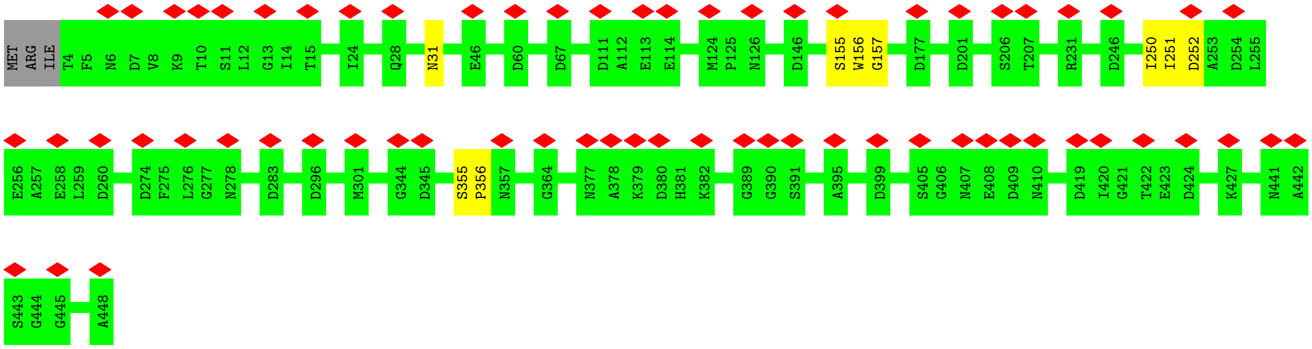




- Molecule 1: Major capsid protein

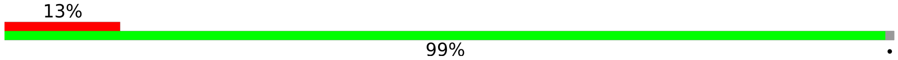
Chain 8A:

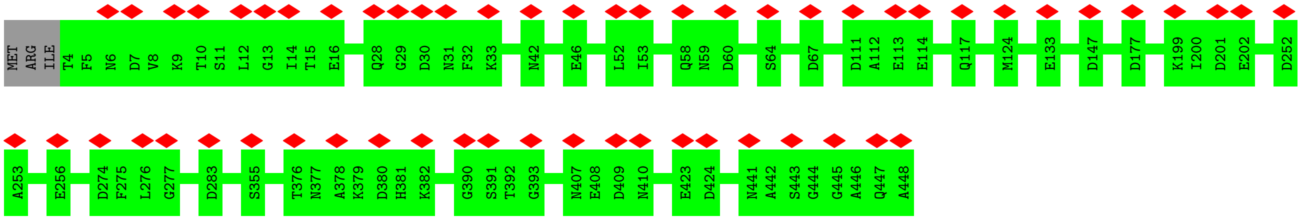




- Molecule 1: Major capsid protein

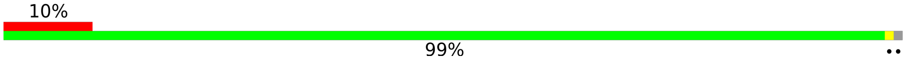
Chain 8B:

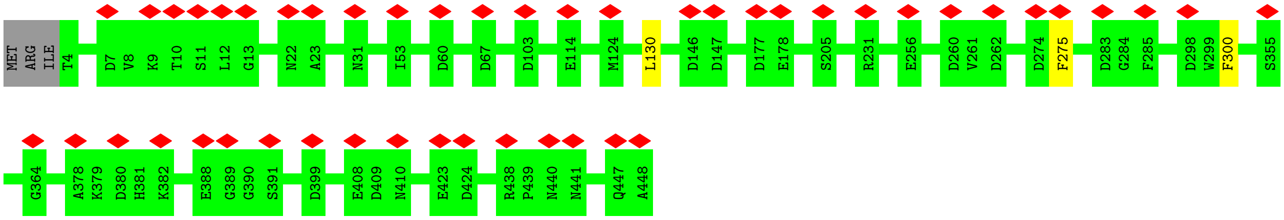




- Molecule 1: Major capsid protein

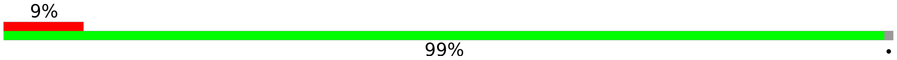
Chain 8C:

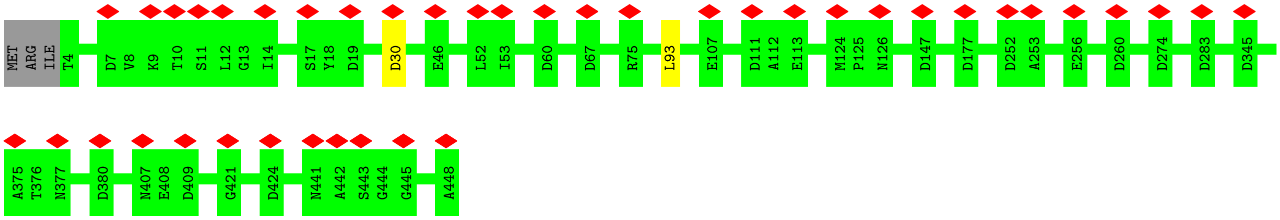




- Molecule 1: Major capsid protein

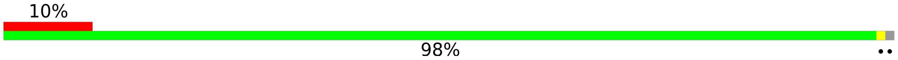
Chain 8D:

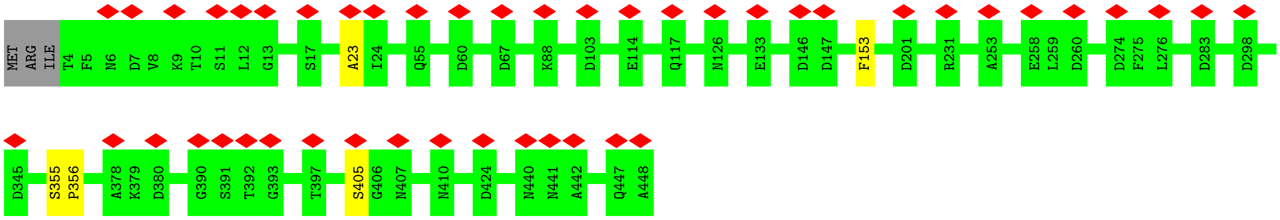




- Molecule 1: Major capsid protein

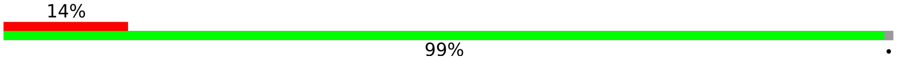
Chain 8E:

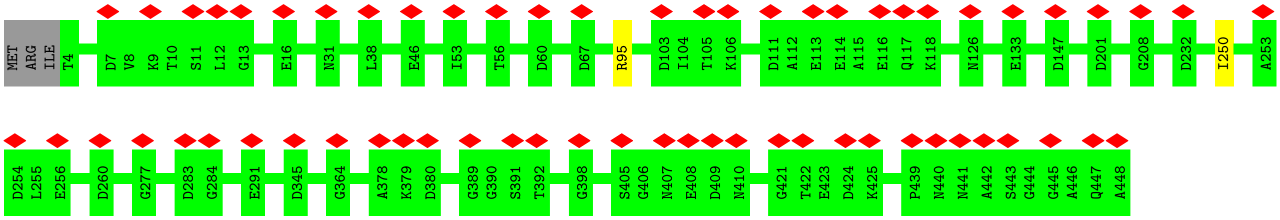




- Molecule 1: Major capsid protein

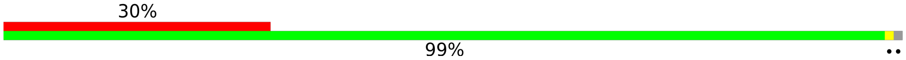
Chain 8F:

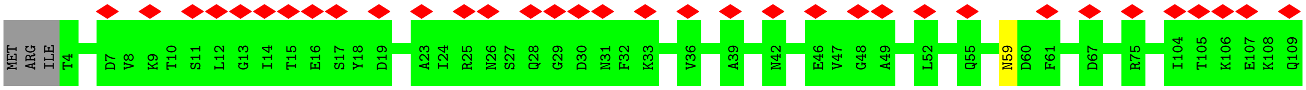


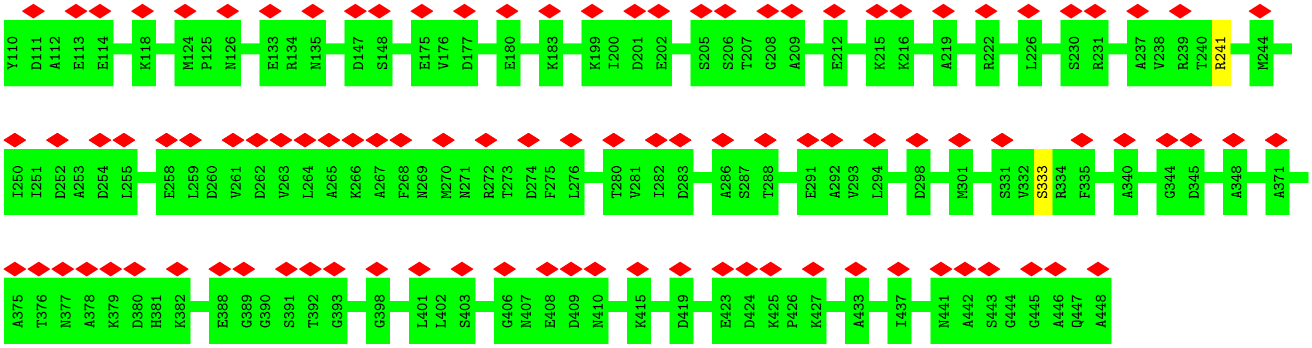


- Molecule 1: Major capsid protein

Chain 9A:

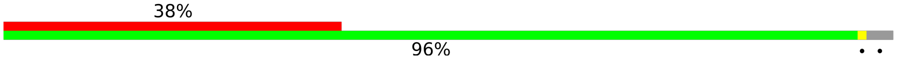


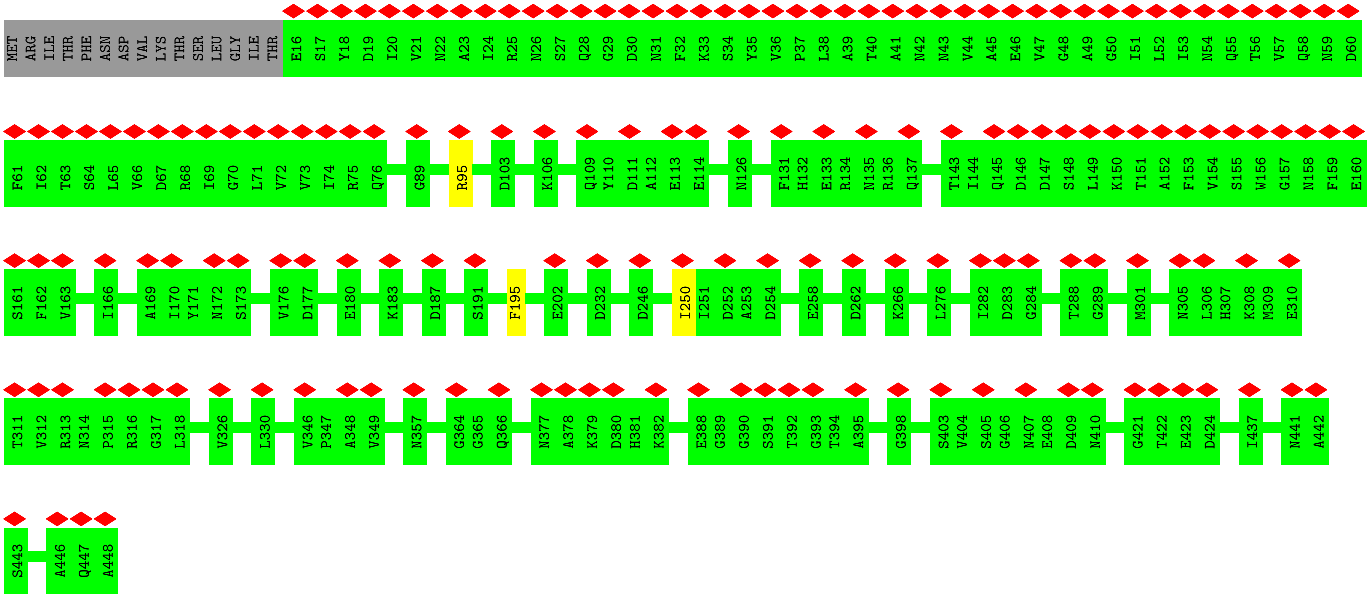




- Molecule 1: Major capsid protein

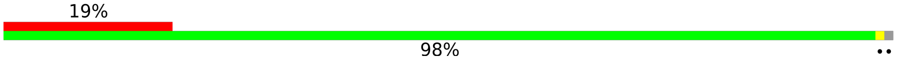
Chain 1G:

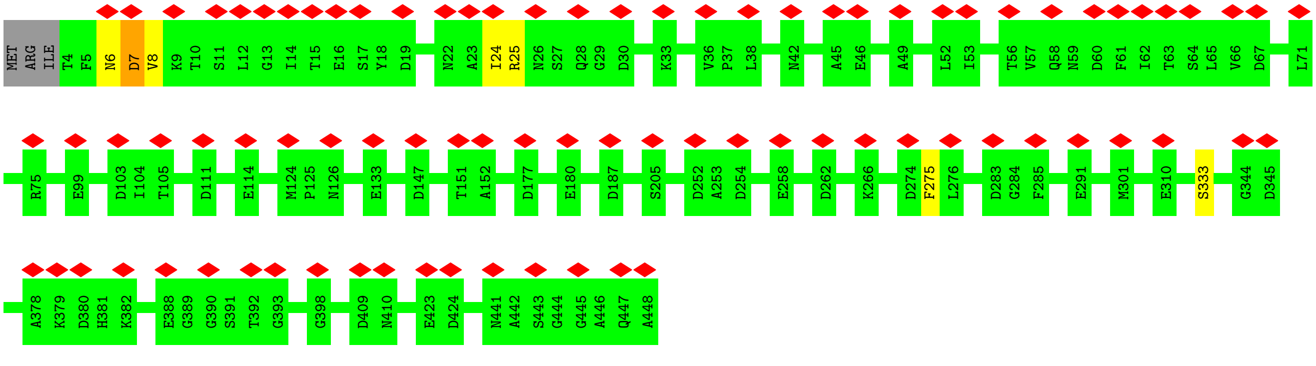




- Molecule 1: Major capsid protein

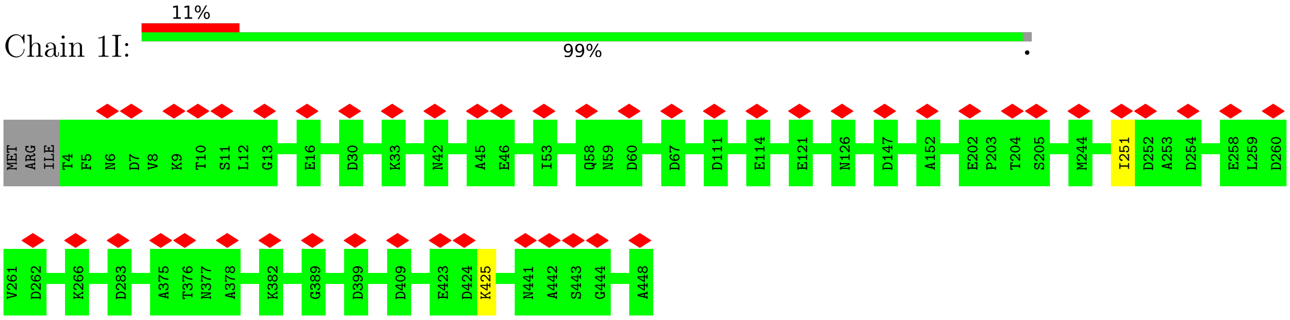
Chain 1H:





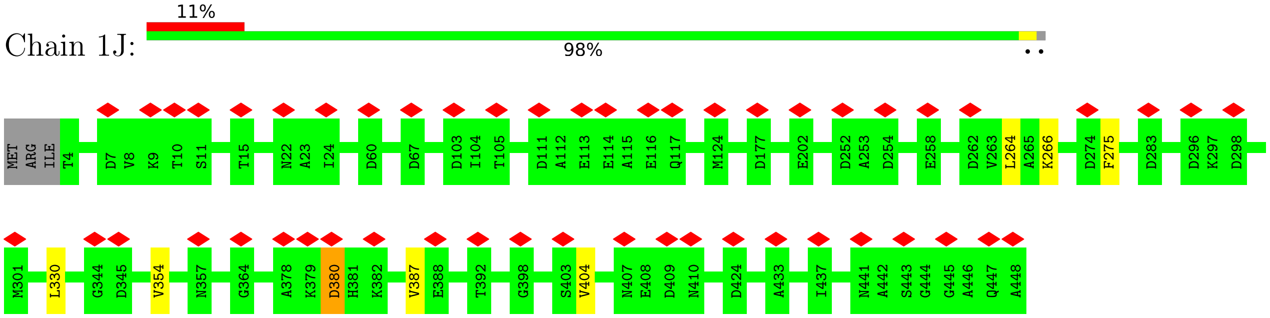
- Molecule 1: Major capsid protein

Chain 1I:



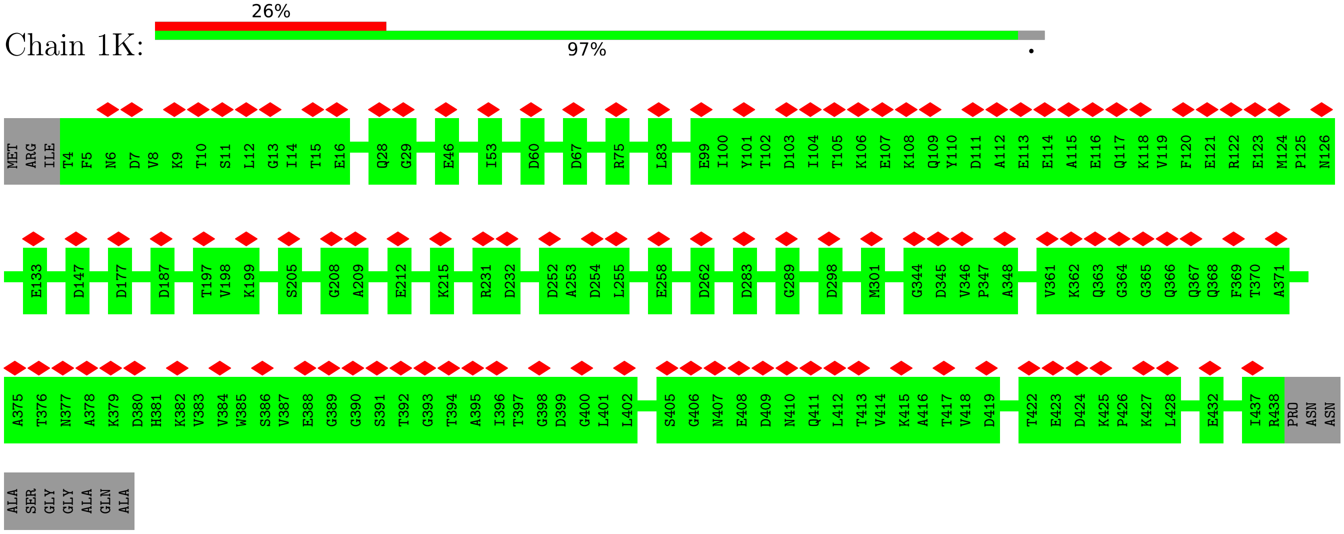
• Molecule 1: Major capsid protein

Chain 1J:



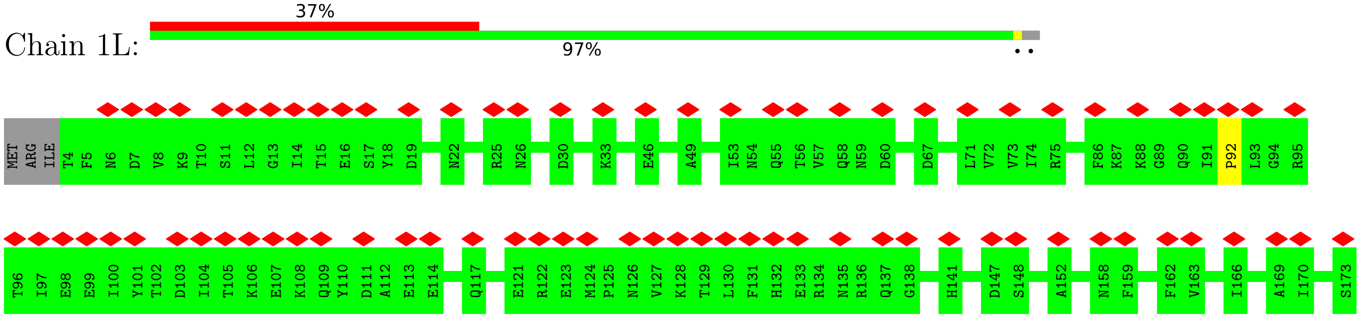
• Molecule 1: Major capsid protein

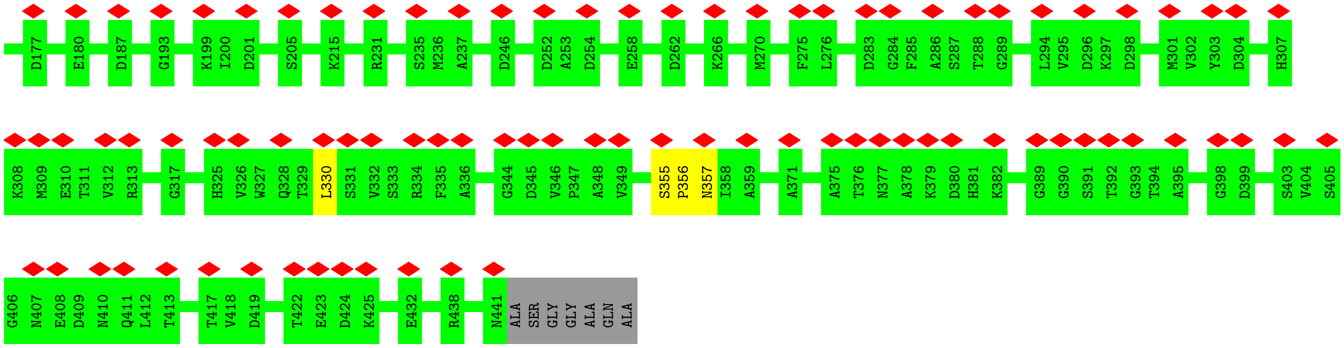
Chain 1K:



• Molecule 1: Major capsid protein

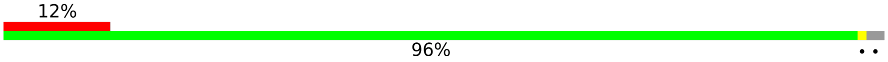
Chain 1L:

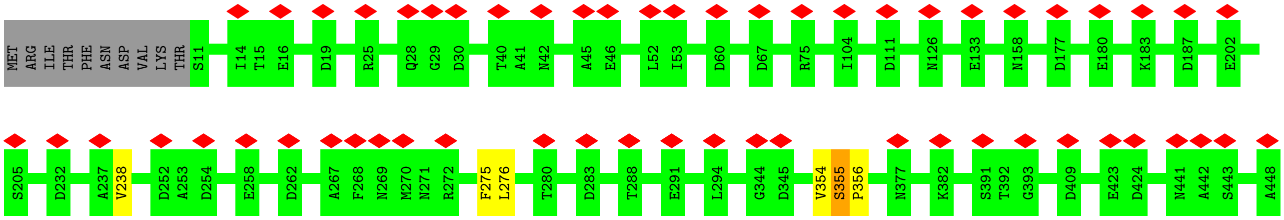




- Molecule 1: Major capsid protein

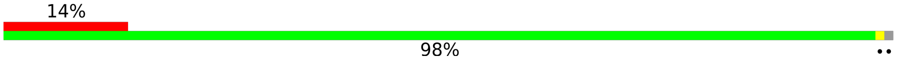
Chain 2F:

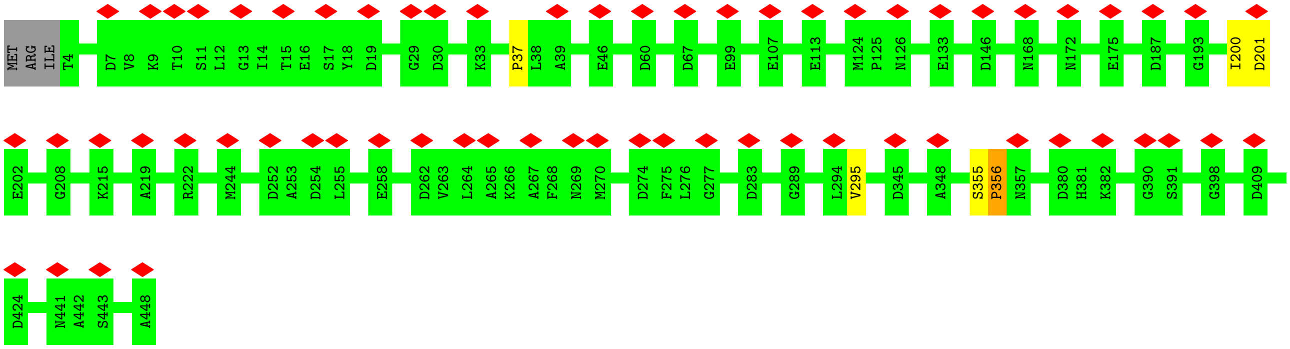




- Molecule 1: Major capsid protein

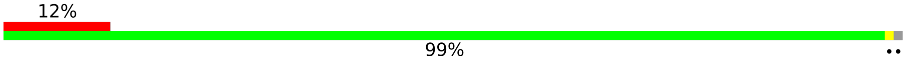
Chain 2G:

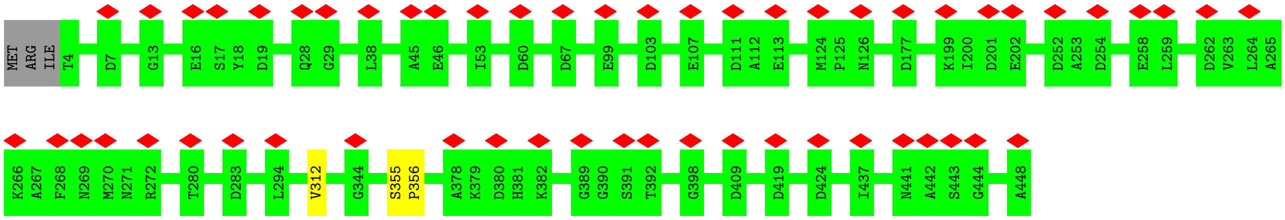




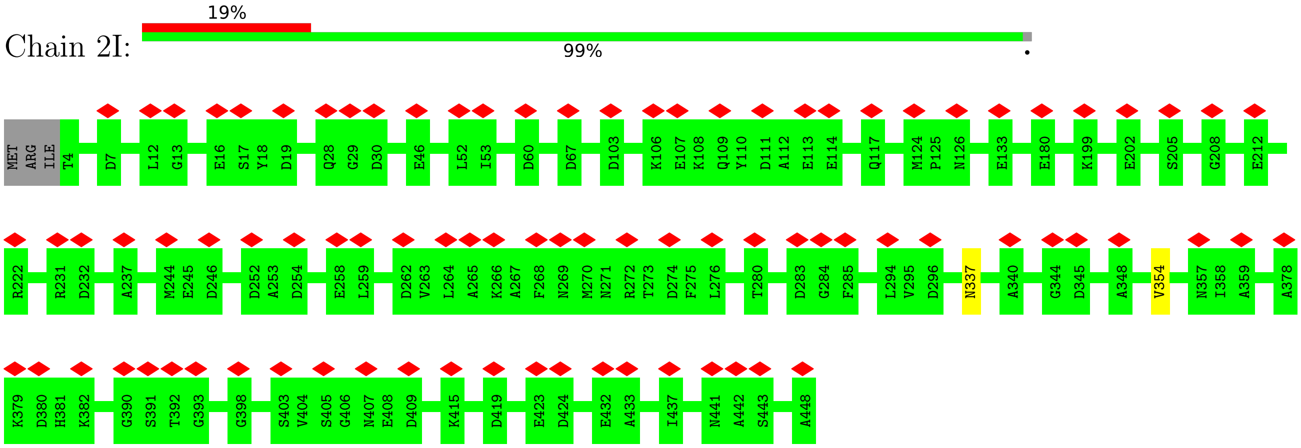
- Molecule 1: Major capsid protein

Chain 2H:

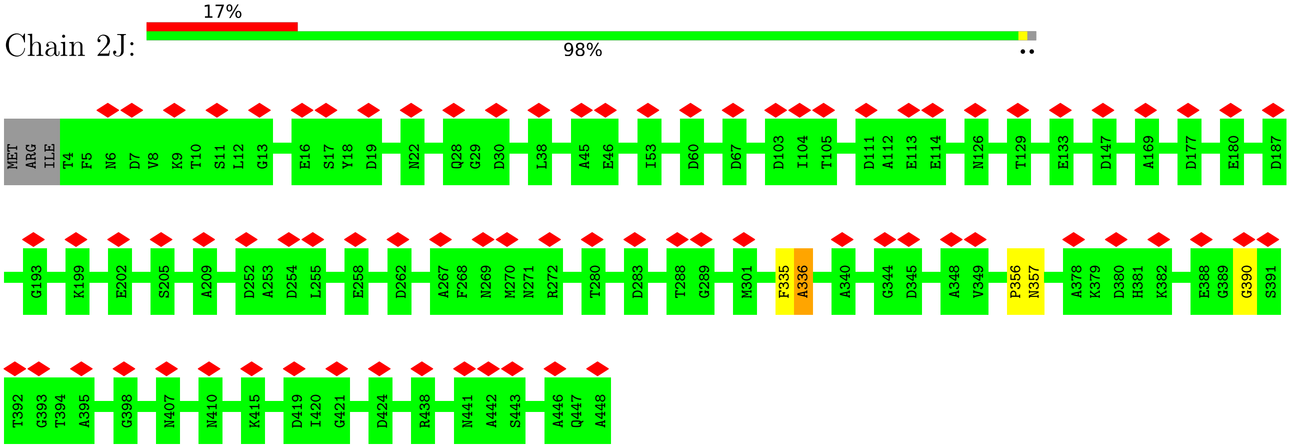




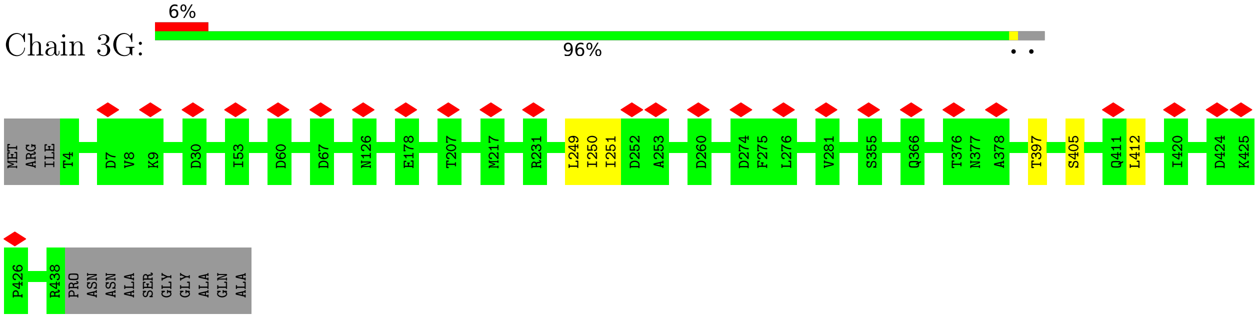
- Molecule 1: Major capsid protein



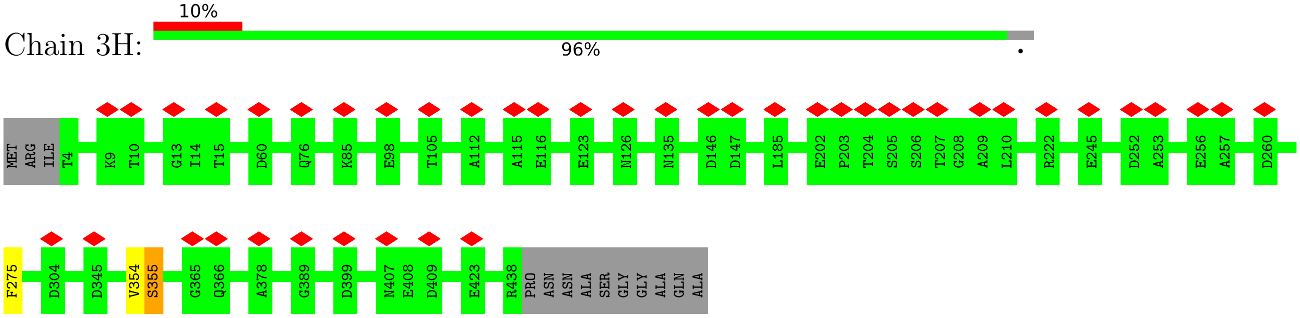
- Molecule 1: Major capsid protein



- Molecule 1: Major capsid protein

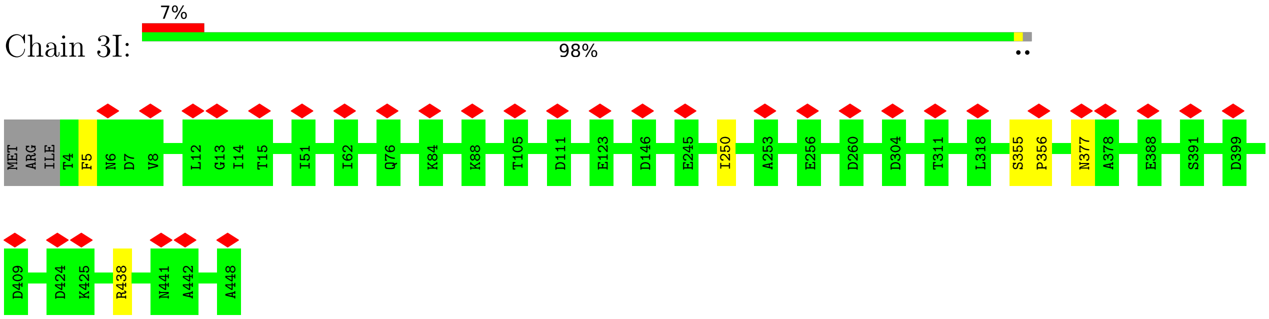


- Molecule 1: Major capsid protein



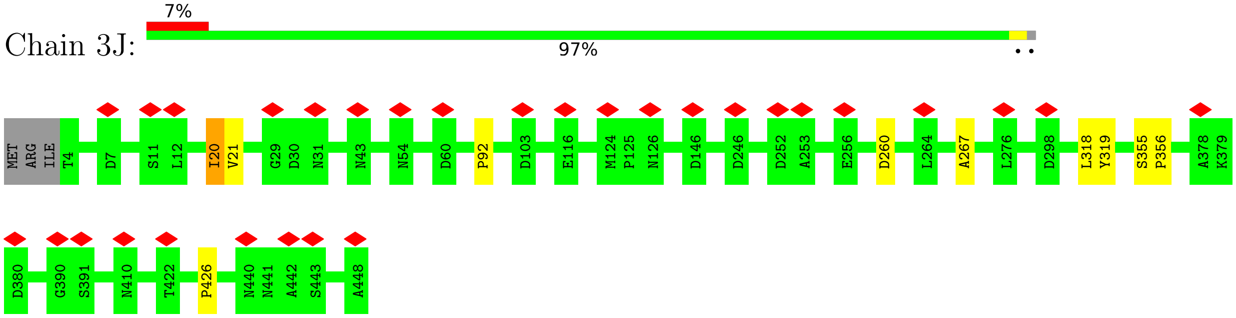
- Molecule 1: Major capsid protein

Chain 3I:



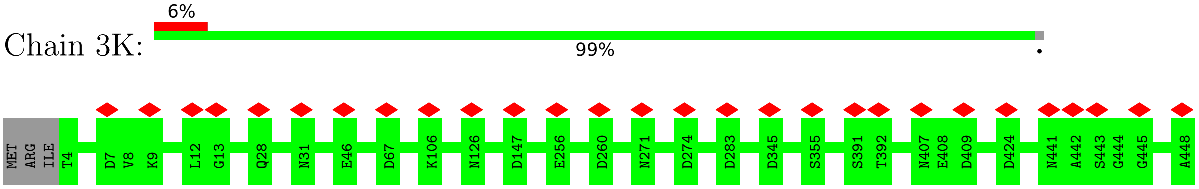
- Molecule 1: Major capsid protein

Chain 3J:



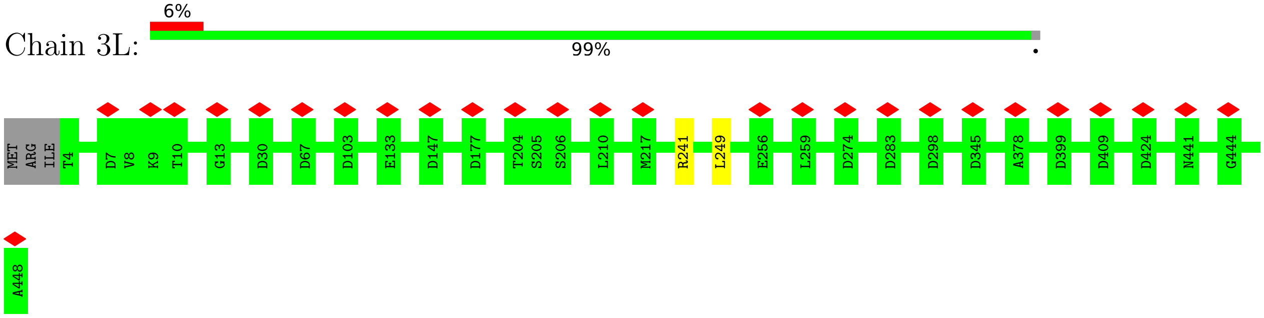
- Molecule 1: Major capsid protein

Chain 3K:



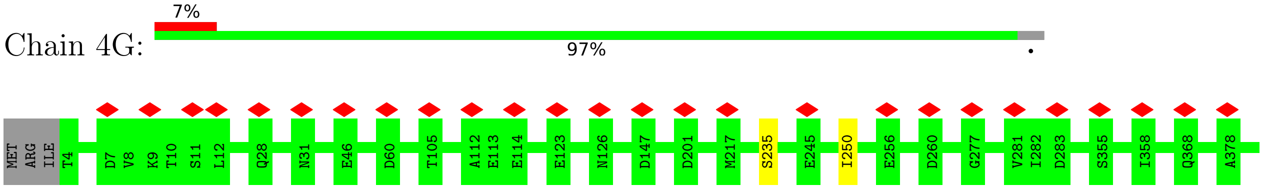
- Molecule 1: Major capsid protein

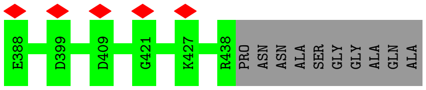
Chain 3L:



- Molecule 1: Major capsid protein

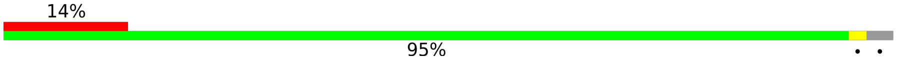
Chain 4G:

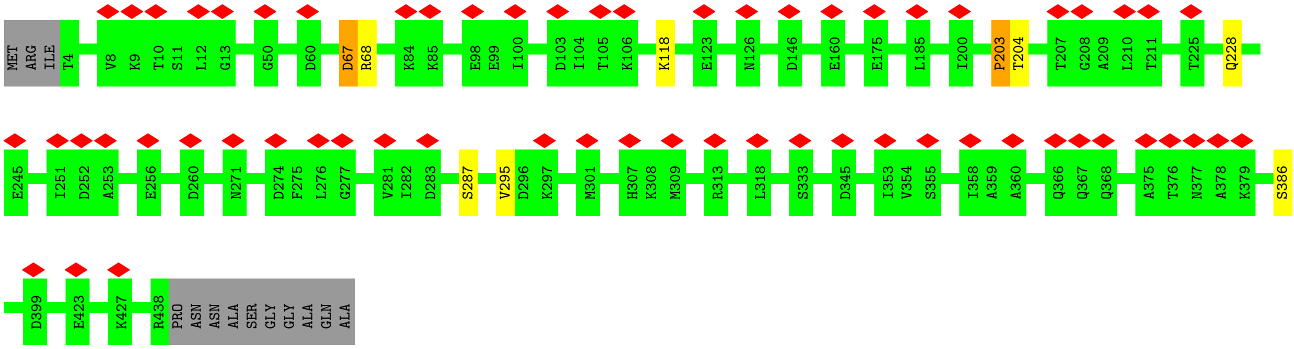




- Molecule 1: Major capsid protein

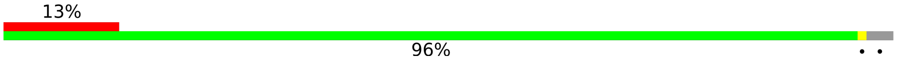
Chain 4H:

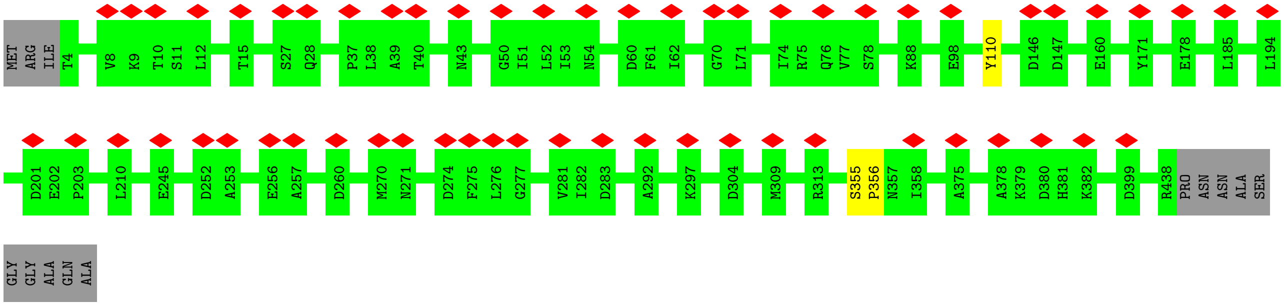




- Molecule 1: Major capsid protein

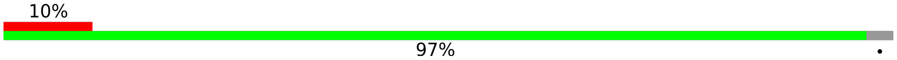
Chain 4I:

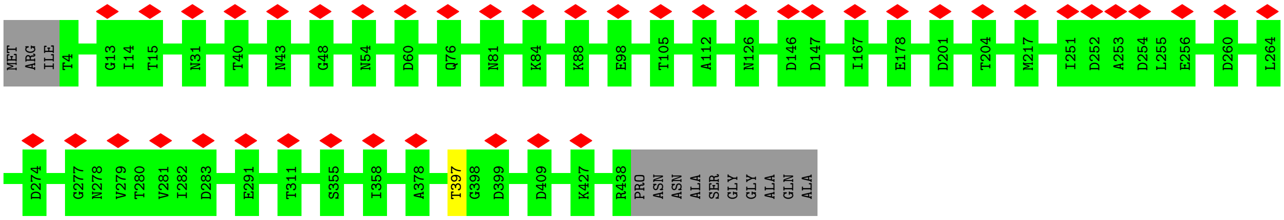




- Molecule 1: Major capsid protein

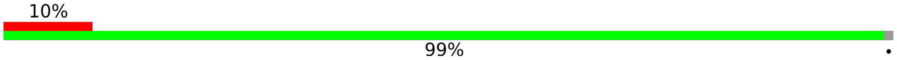
Chain 4J:

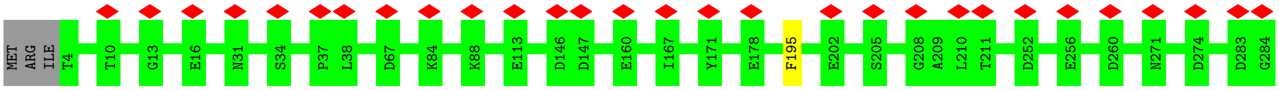


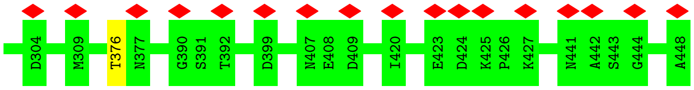


- Molecule 1: Major capsid protein

Chain 4K:

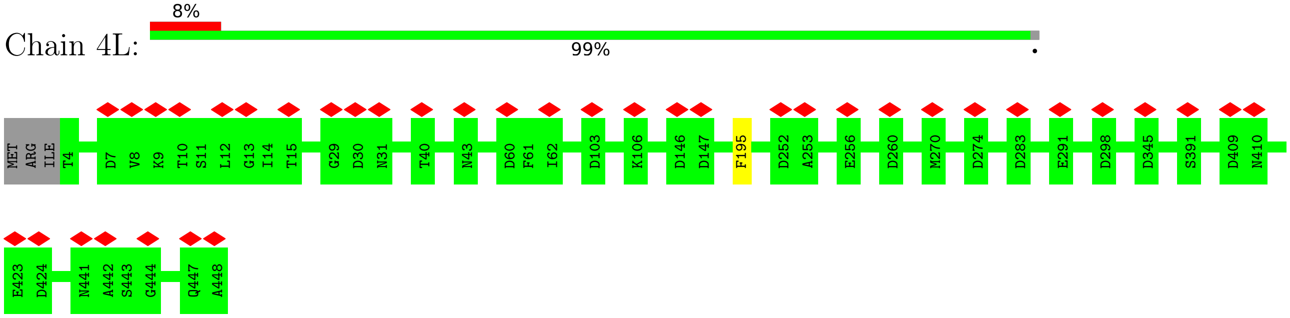






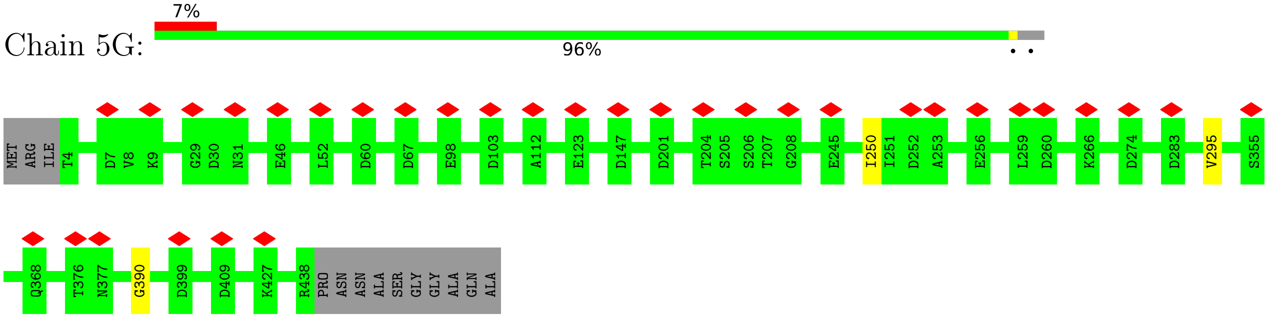
- Molecule 1: Major capsid protein

Chain 4L:



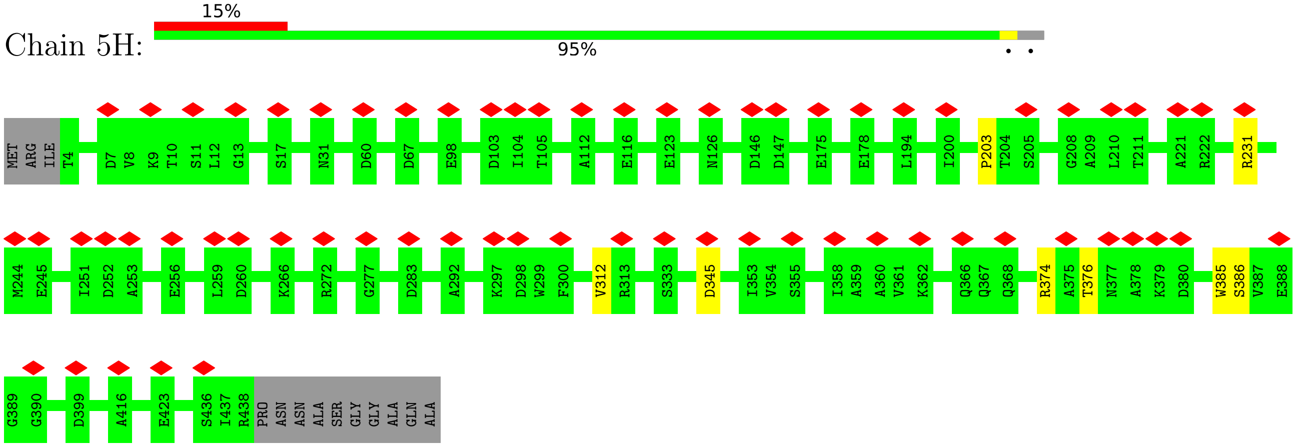
- Molecule 1: Major capsid protein

Chain 5G:



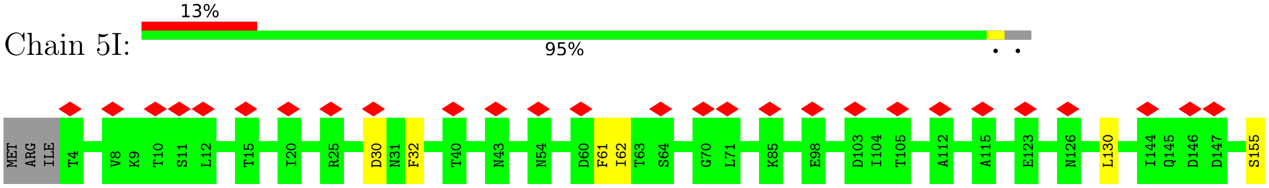
- Molecule 1: Major capsid protein

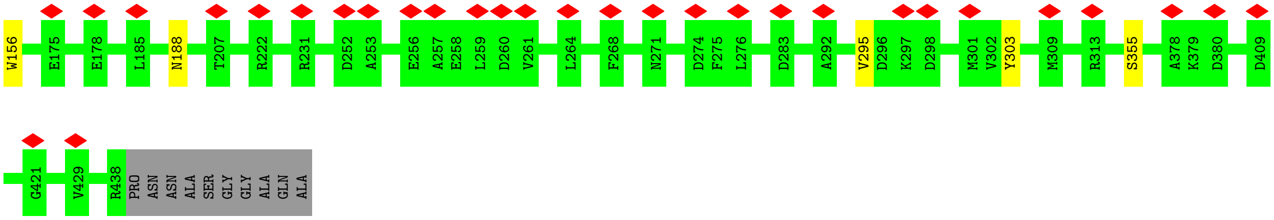
Chain 5H:



- Molecule 1: Major capsid protein

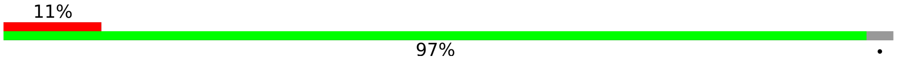
Chain 5I:

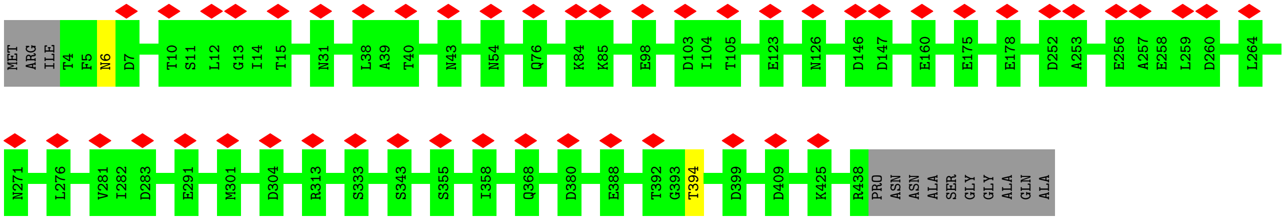




- Molecule 1: Major capsid protein

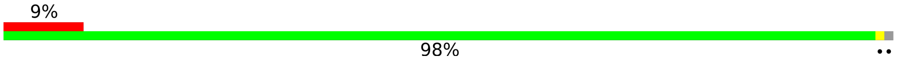
Chain 5J:

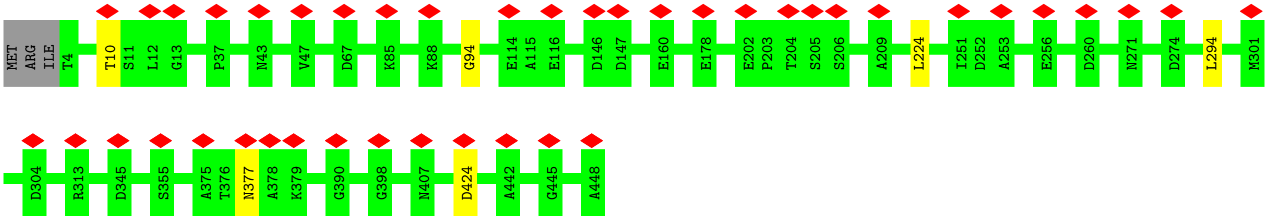




- Molecule 1: Major capsid protein

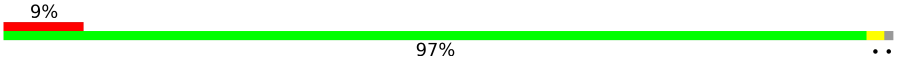
Chain 5K:

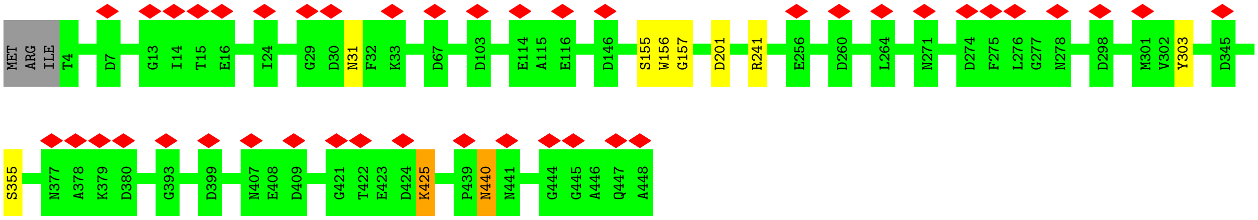




- Molecule 1: Major capsid protein

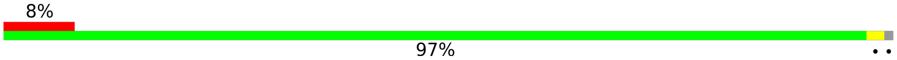
Chain 5L:

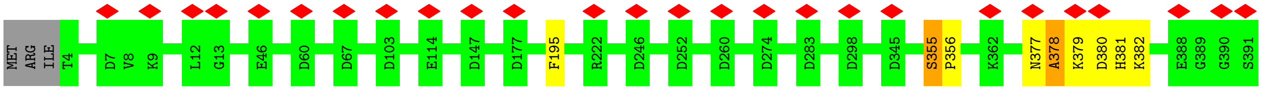


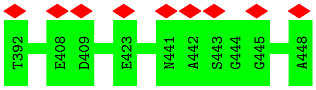


- Molecule 1: Major capsid protein

Chain 6G:

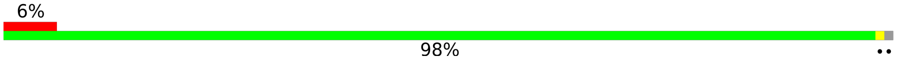


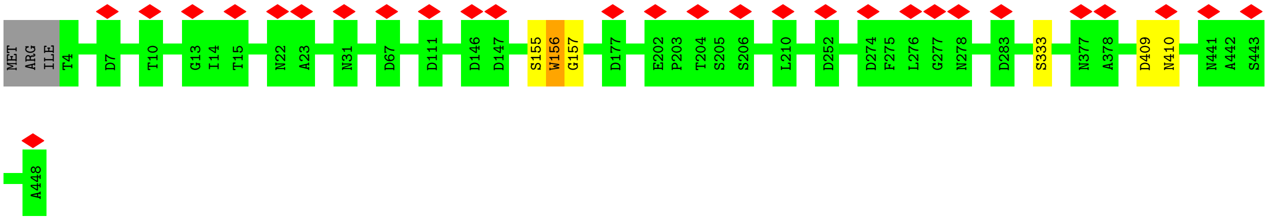




• Molecule 1: Major capsid protein

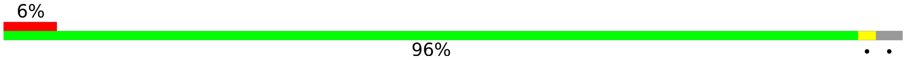
Chain 6H:

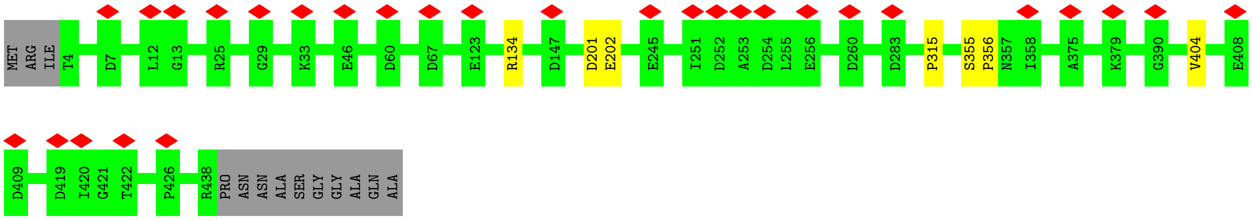




• Molecule 1: Major capsid protein

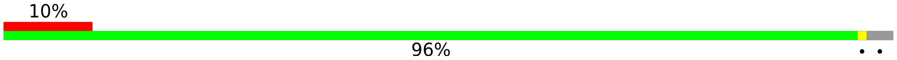
Chain 6I:

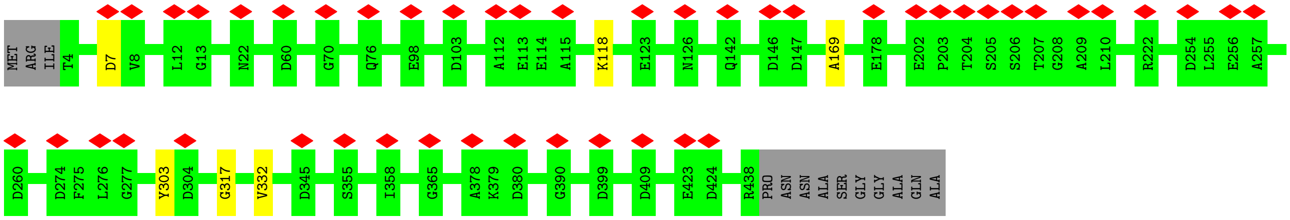




• Molecule 1: Major capsid protein

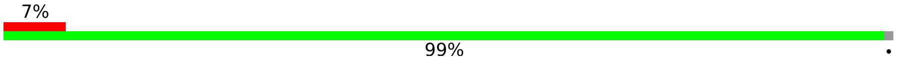
Chain 6J:

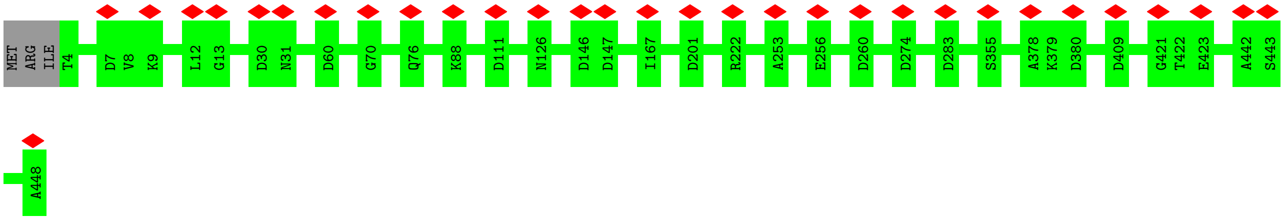




• Molecule 1: Major capsid protein

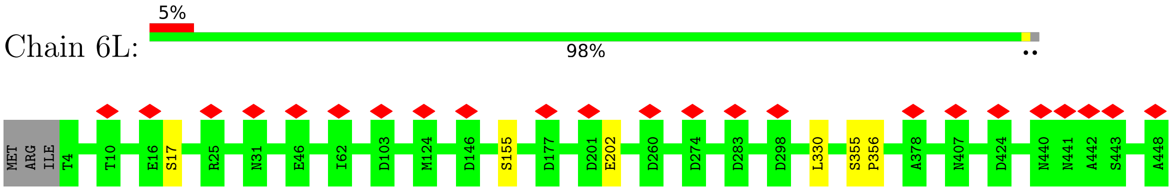
Chain 6K:





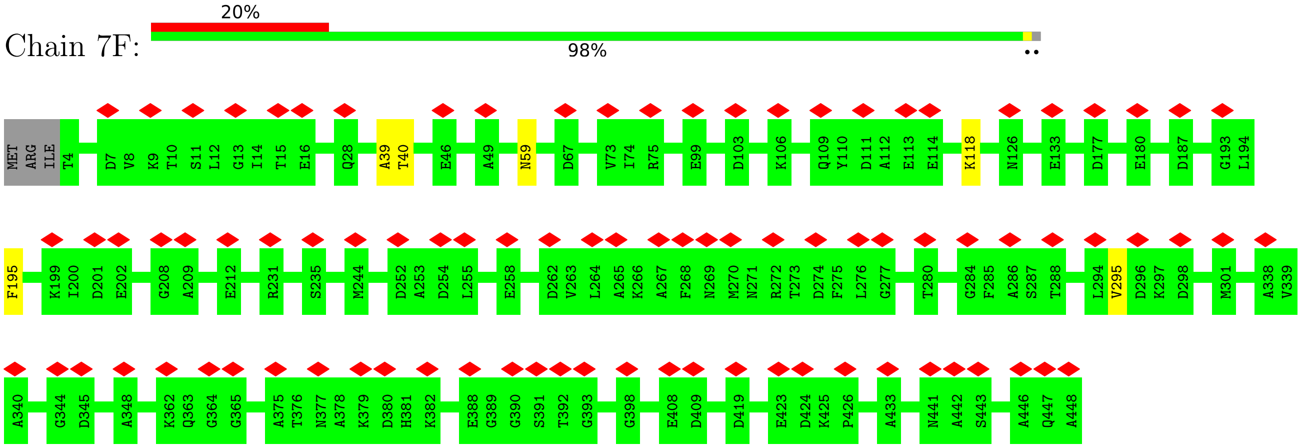
• Molecule 1: Major capsid protein

Chain 6L:



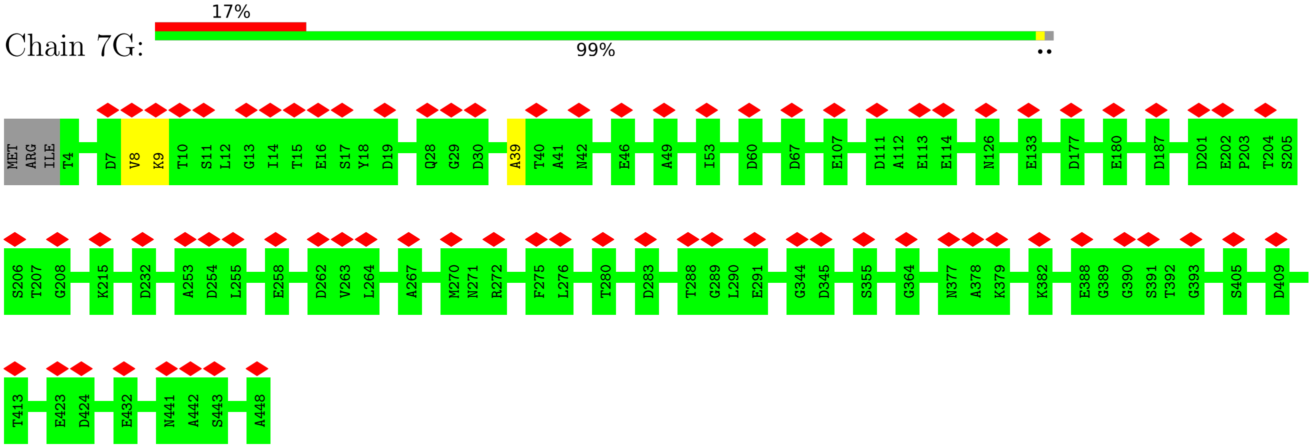
- Molecule 1: Major capsid protein

Chain 7F:



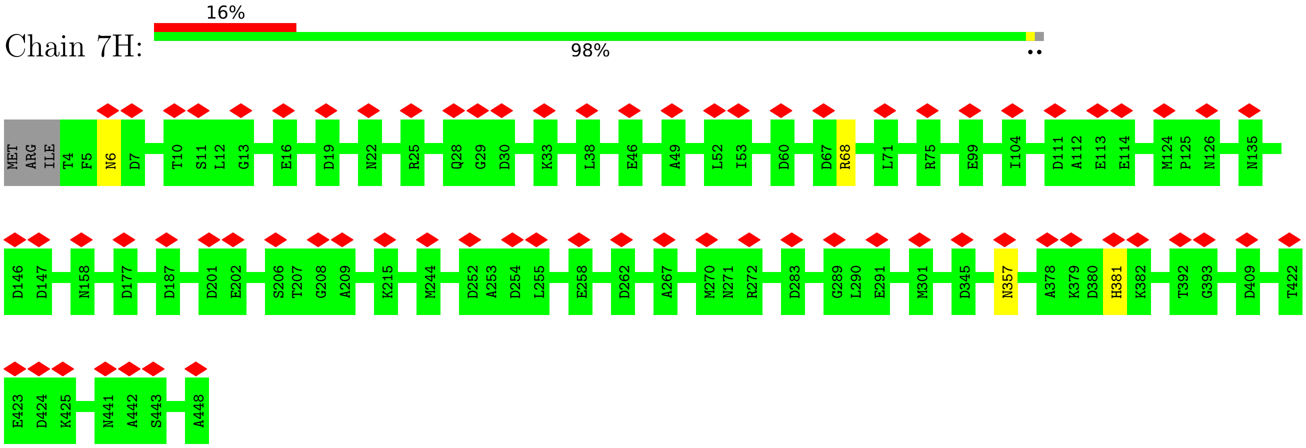
- Molecule 1: Major capsid protein

Chain 7G:



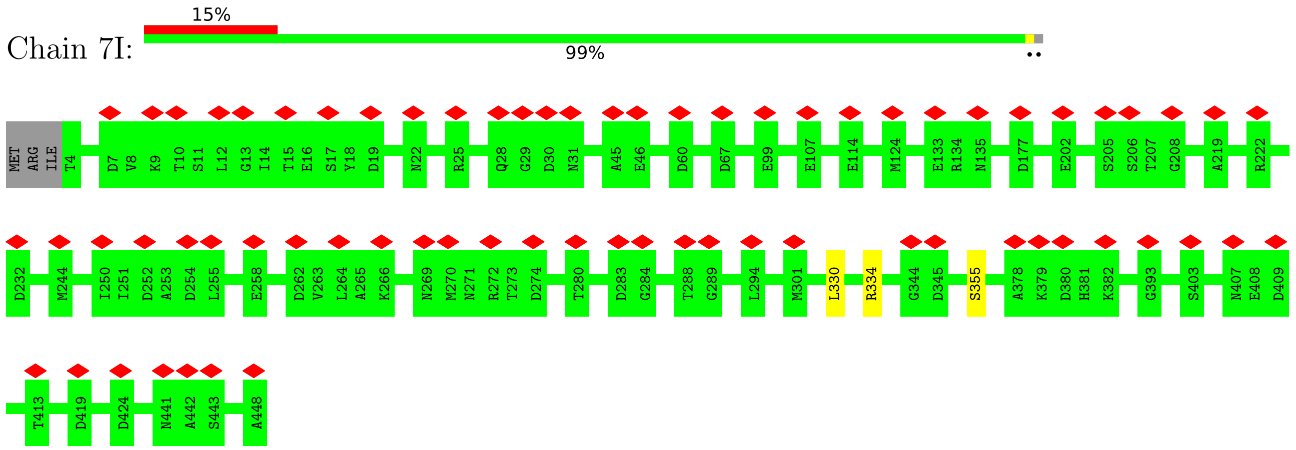
- Molecule 1: Major capsid protein

Chain 7H:



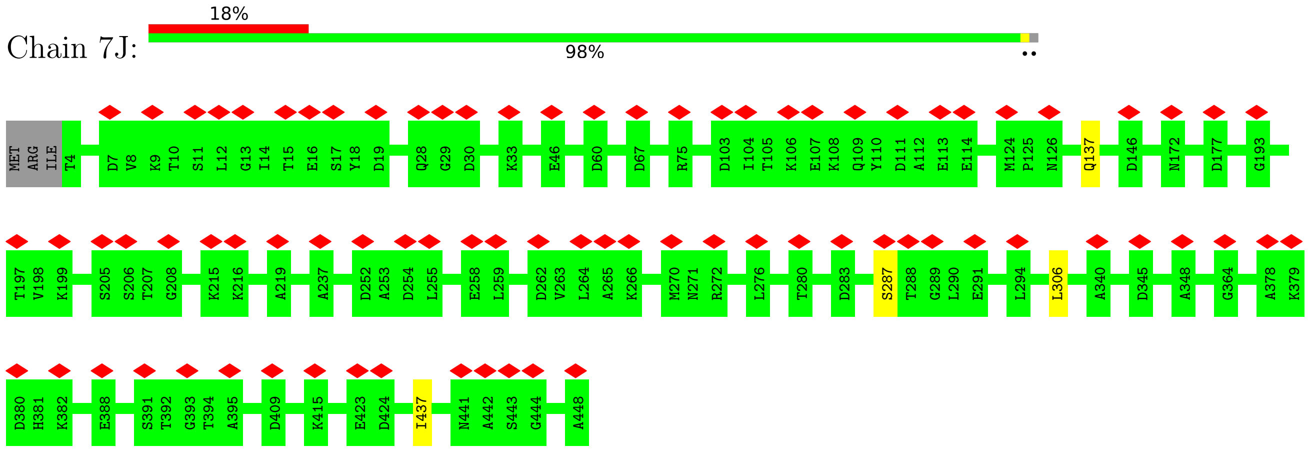
- Molecule 1: Major capsid protein

Chain 7I:



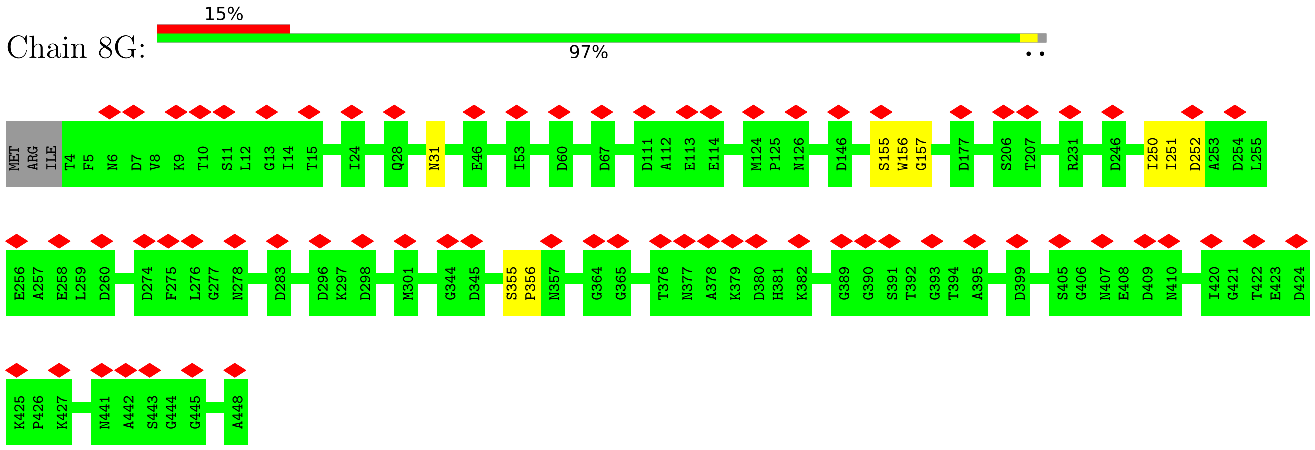
- Molecule 1: Major capsid protein

Chain 7J:



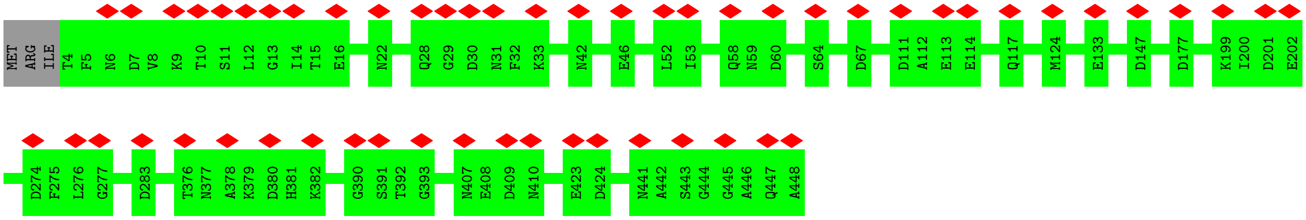
- Molecule 1: Major capsid protein

Chain 8G:



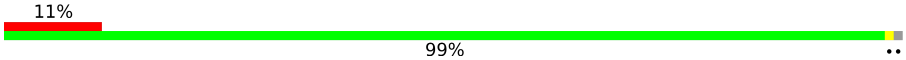
- Molecule 1: Major capsid protein

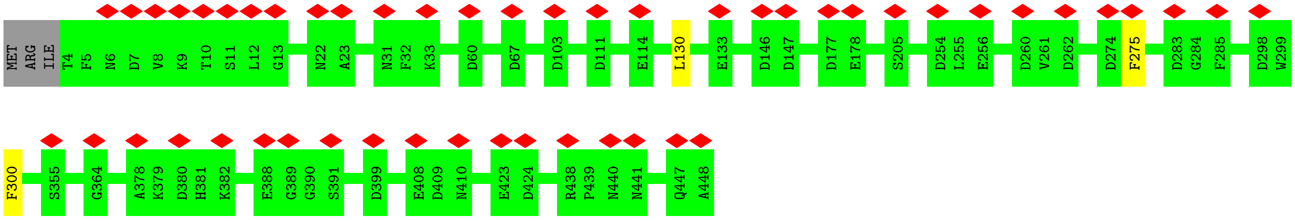
Chain 8H:



- Molecule 1: Major capsid protein

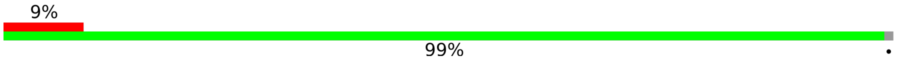
Chain 8I:

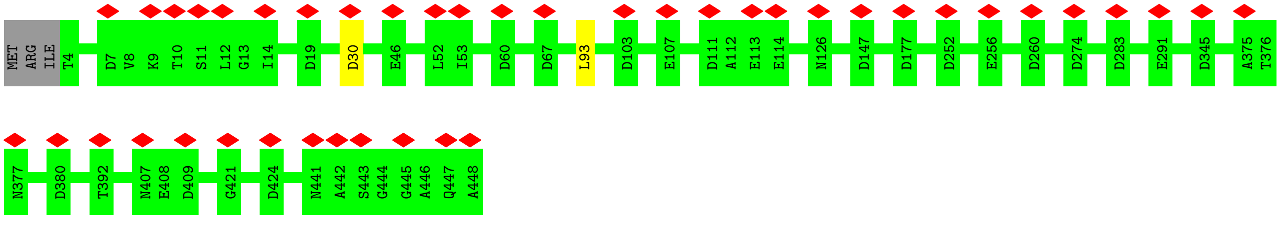




- Molecule 1: Major capsid protein

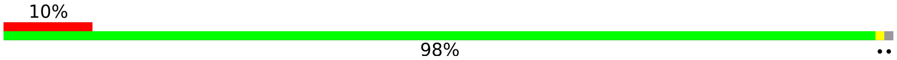
Chain 8J:

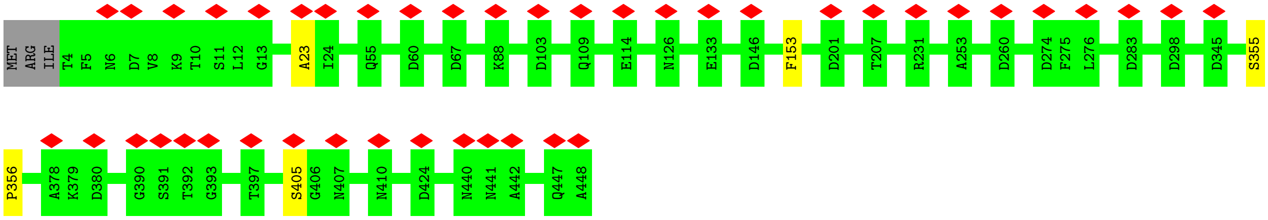




- Molecule 1: Major capsid protein

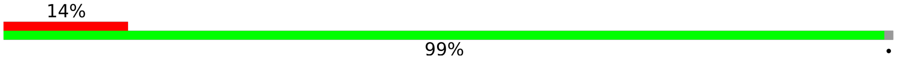
Chain 8K:

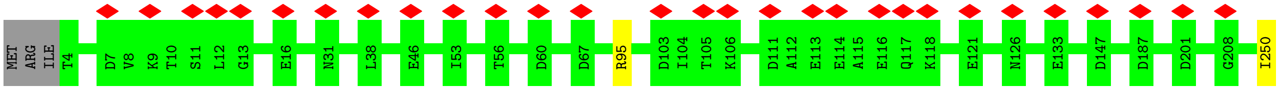


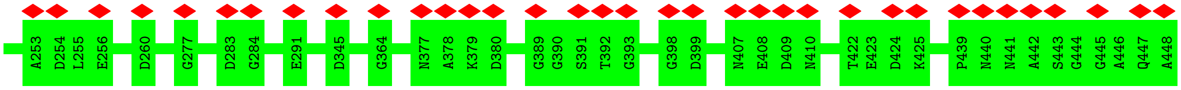


- Molecule 1: Major capsid protein

Chain 8L:

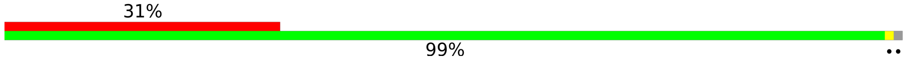


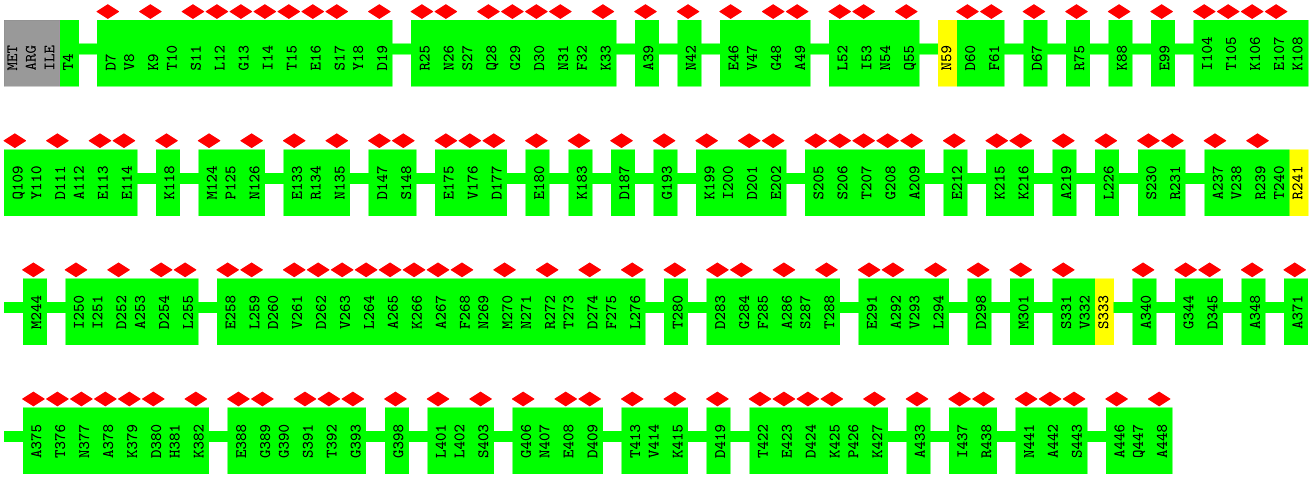




- Molecule 1: Major capsid protein

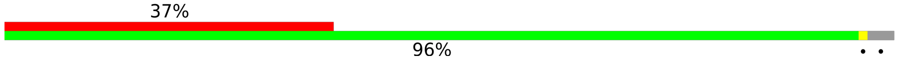
Chain 9B:

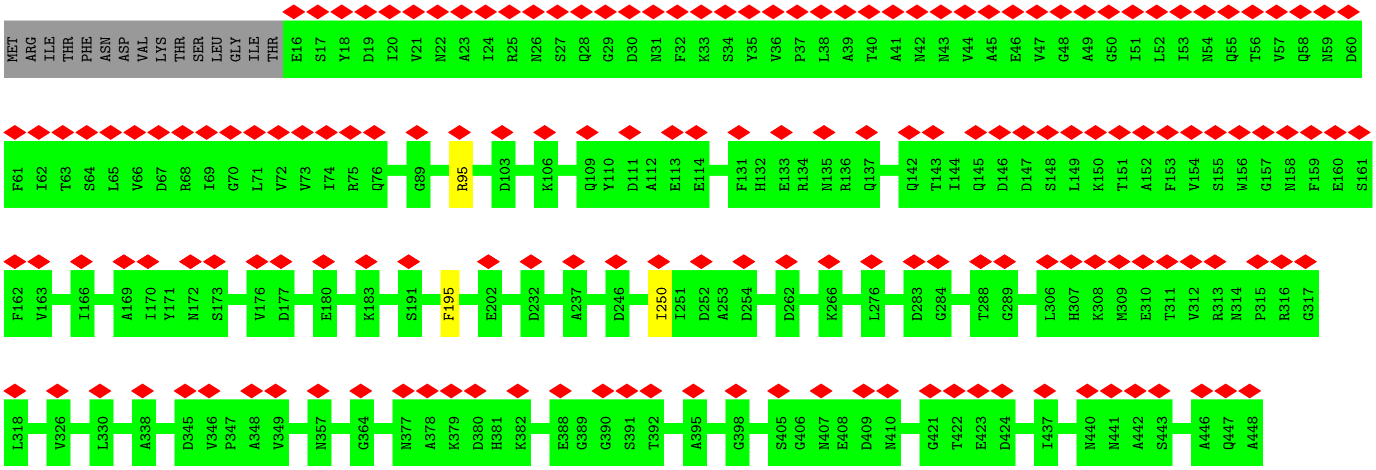




- Molecule 1: Major capsid protein

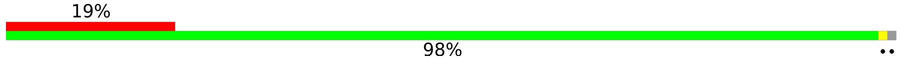
Chain 1M:

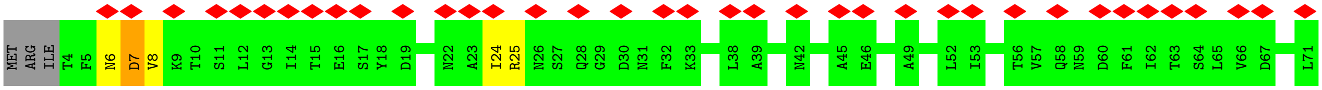


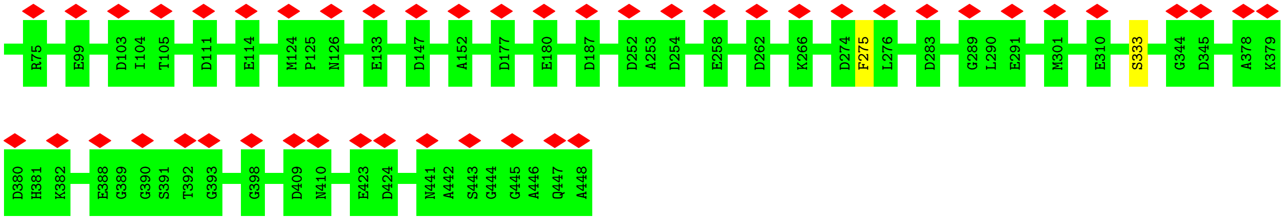


- Molecule 1: Major capsid protein

Chain 1N:

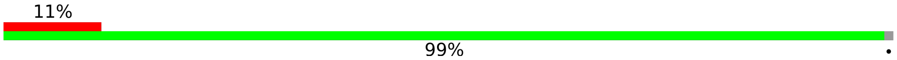


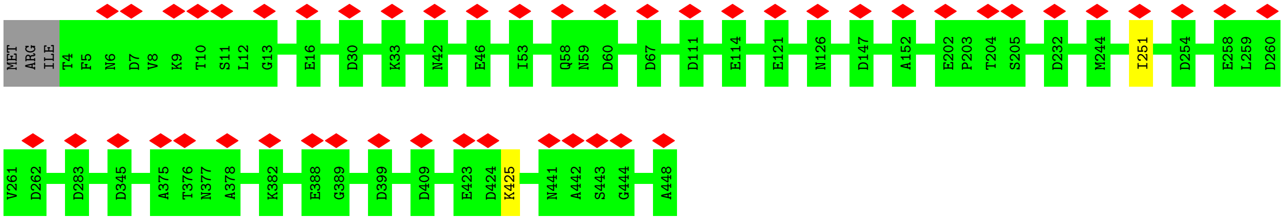




- Molecule 1: Major capsid protein

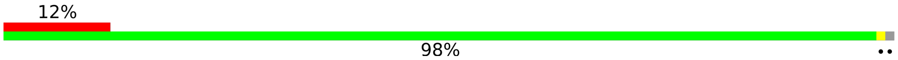
Chain 1O:

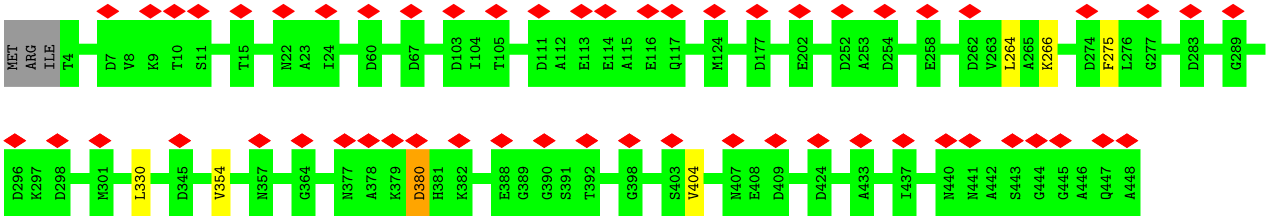




- Molecule 1: Major capsid protein

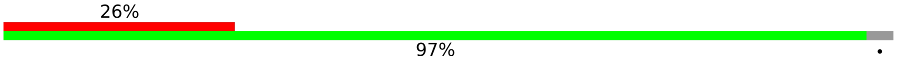
Chain 1P:





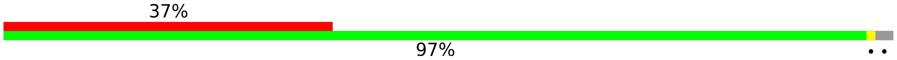
- Molecule 1: Major capsid protein

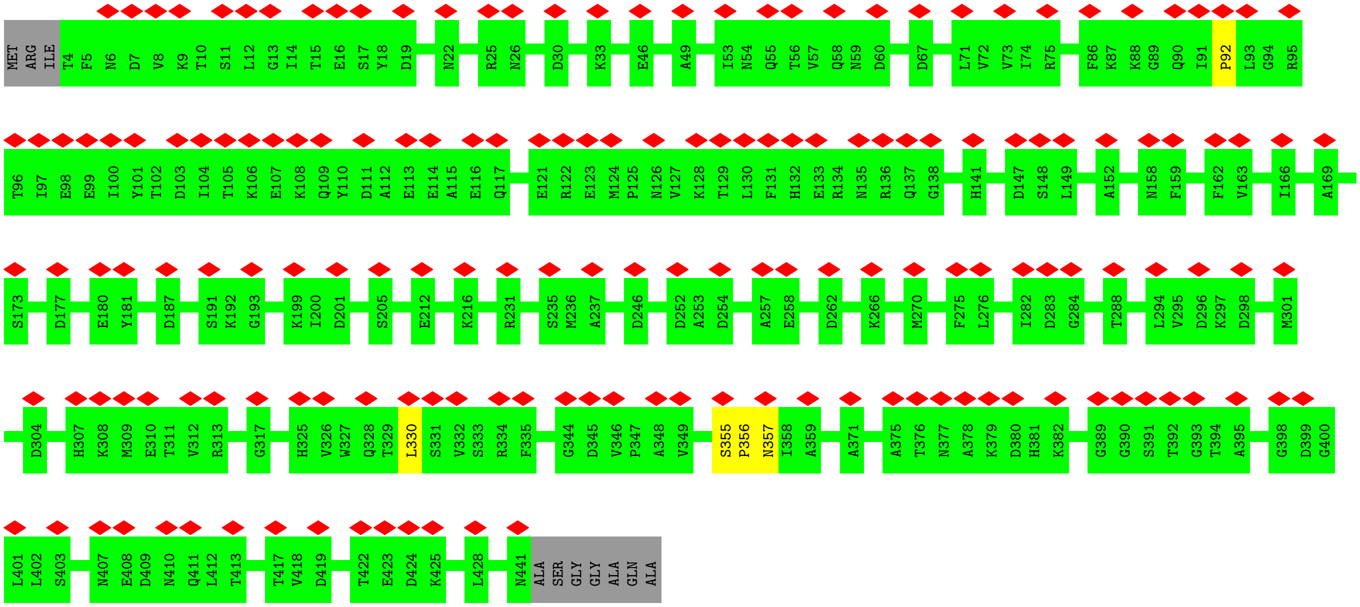
Chain 1Q:



- Molecule 1: Major capsid protein

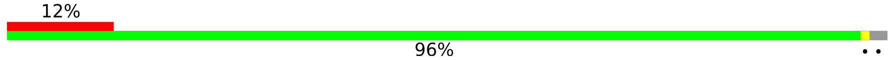
Chain 1R:

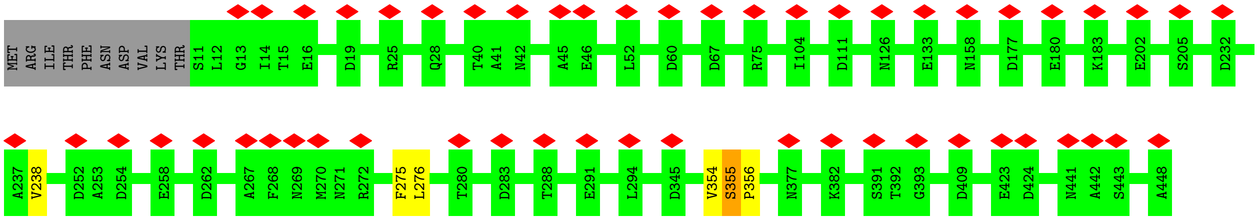




- Molecule 1: Major capsid protein

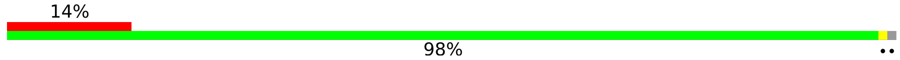
Chain 2K:

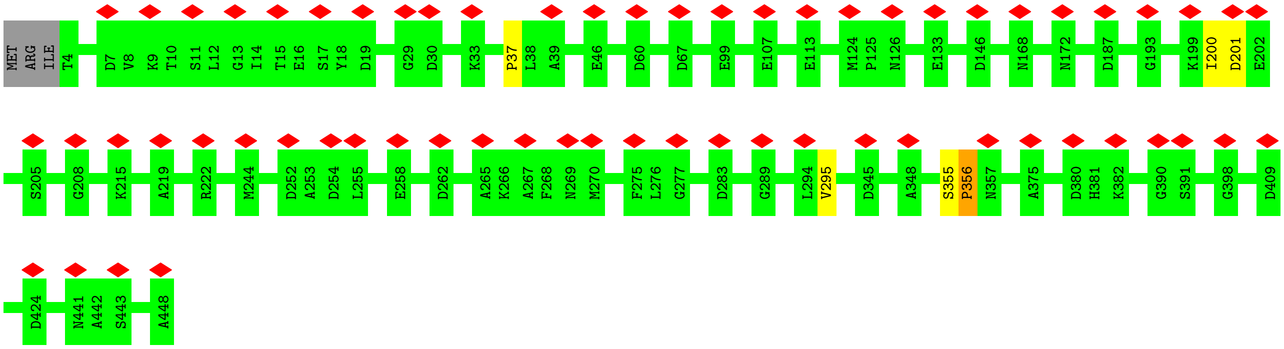




- Molecule 1: Major capsid protein

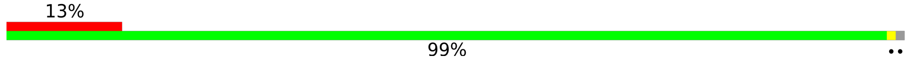
Chain 2L:

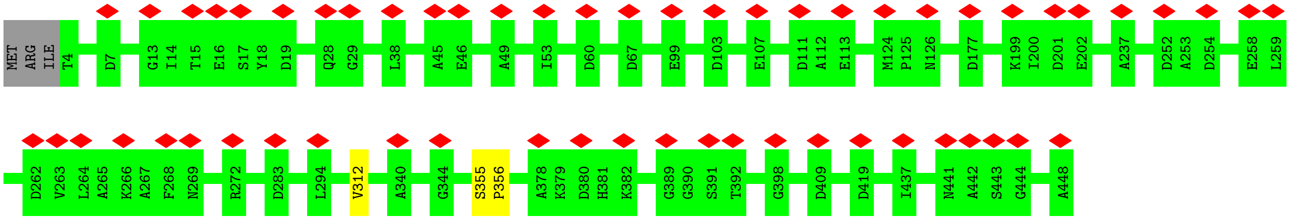




- Molecule 1: Major capsid protein

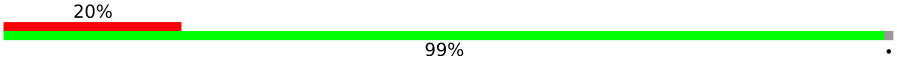
Chain 2M:

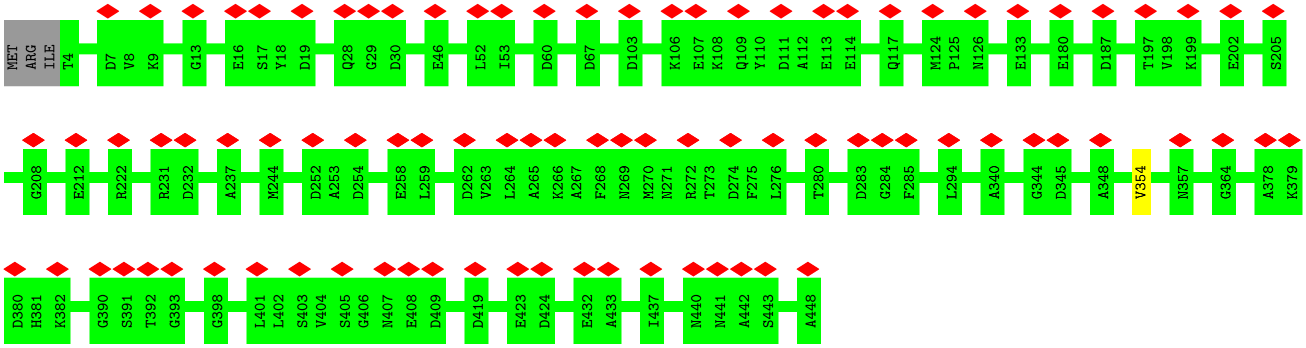




- Molecule 1: Major capsid protein

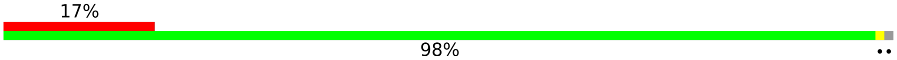
Chain 2N:

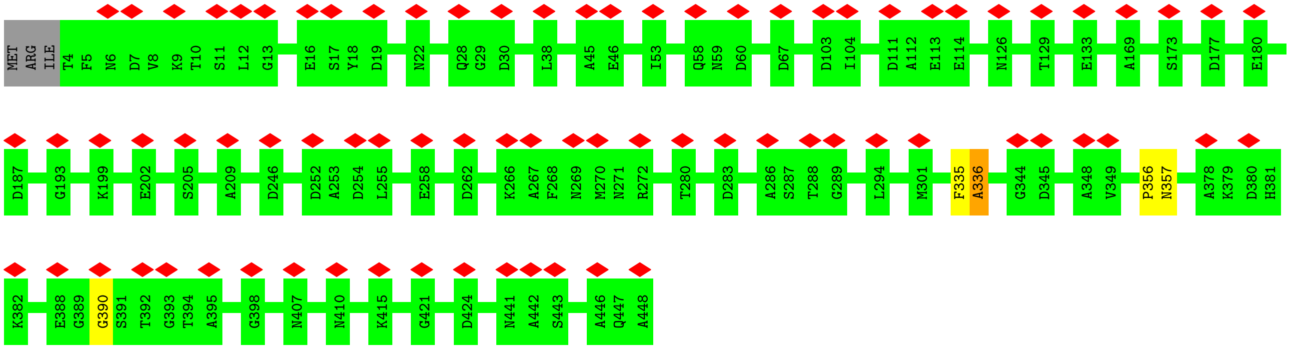




- Molecule 1: Major capsid protein

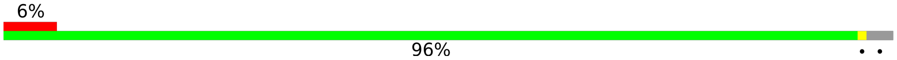
Chain 2O:

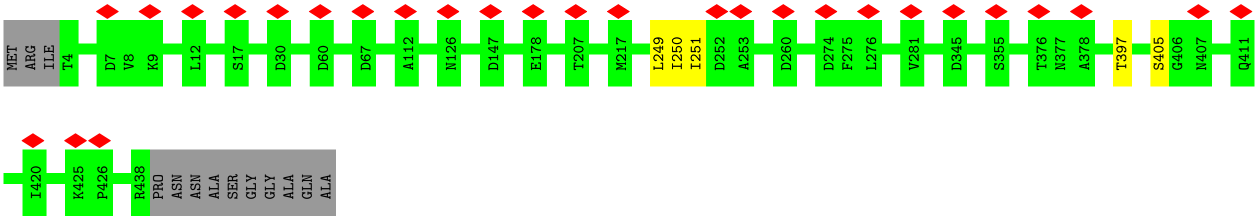




- Molecule 1: Major capsid protein

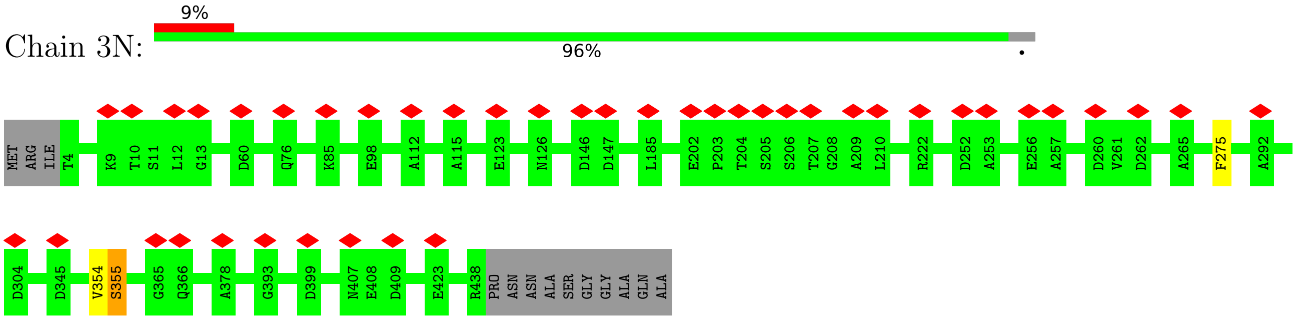
Chain 3M:





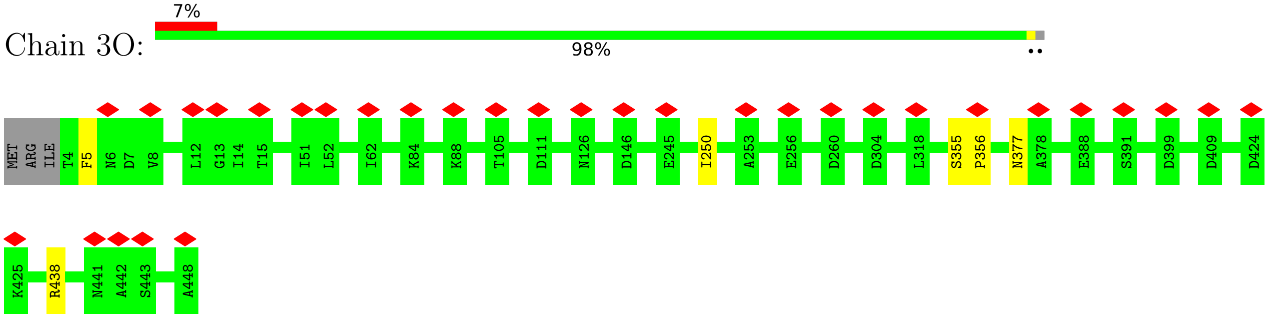
- Molecule 1: Major capsid protein

Chain 3N:



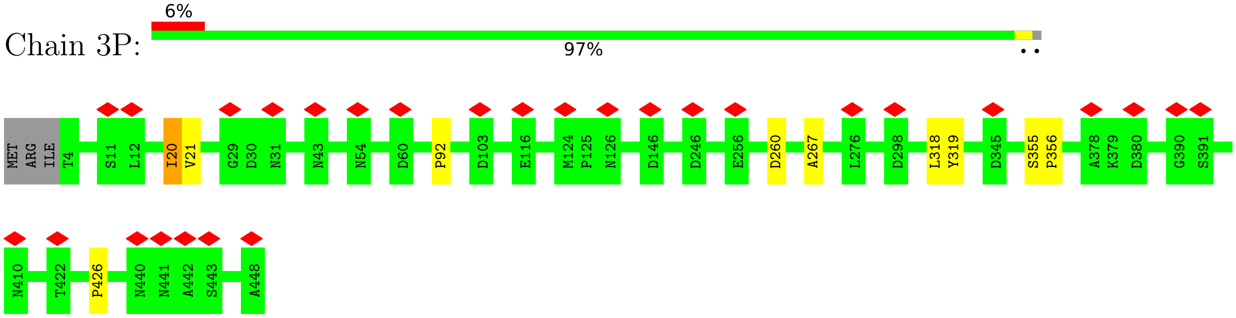
- Molecule 1: Major capsid protein

Chain 3O:



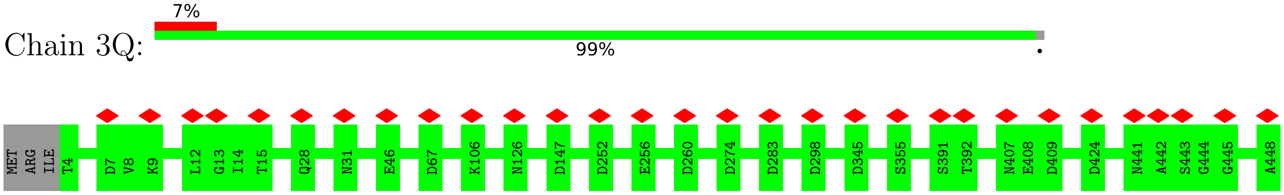
- Molecule 1: Major capsid protein

Chain 3P:



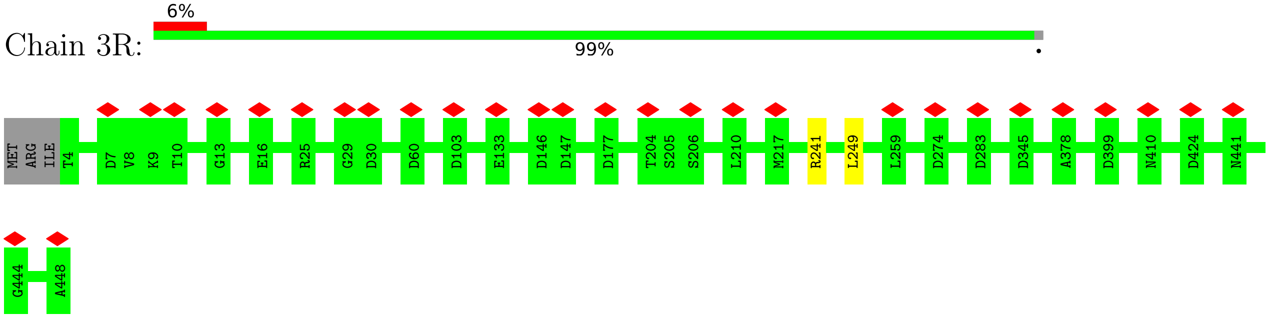
- Molecule 1: Major capsid protein

Chain 3Q:



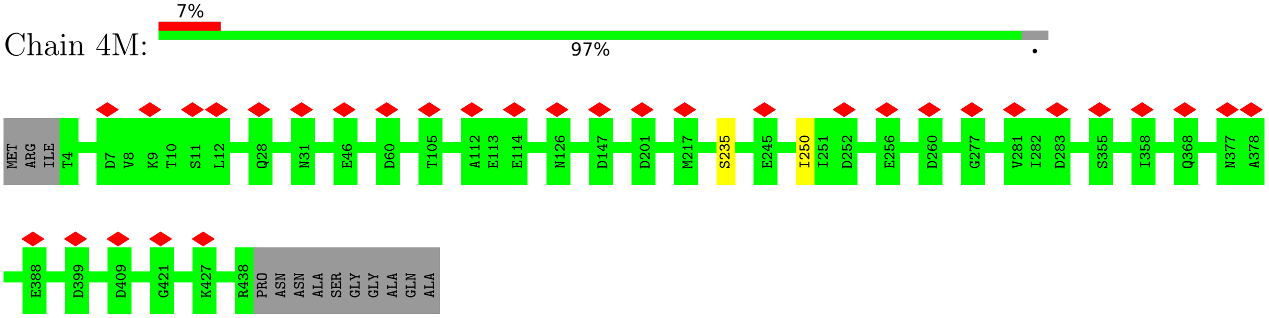
- Molecule 1: Major capsid protein

Chain 3R:



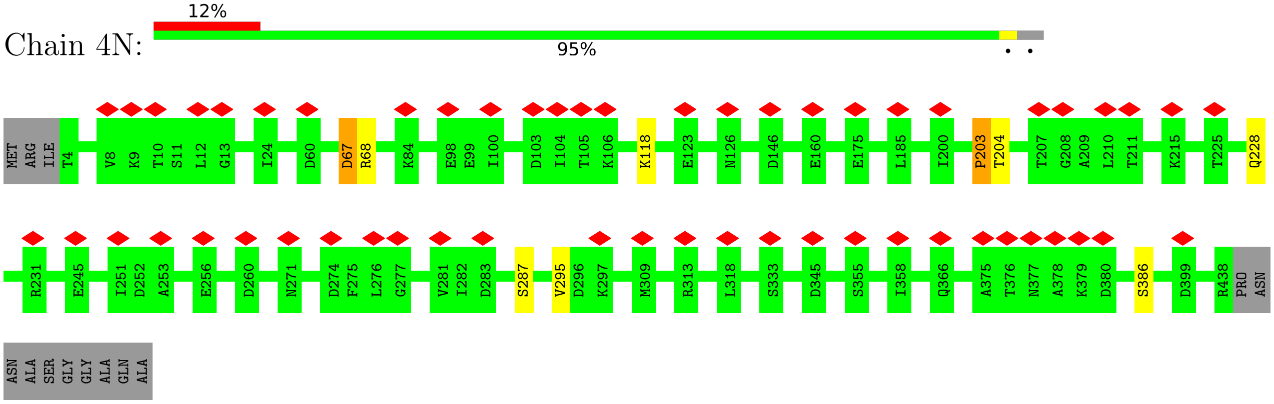
- Molecule 1: Major capsid protein

Chain 4M:



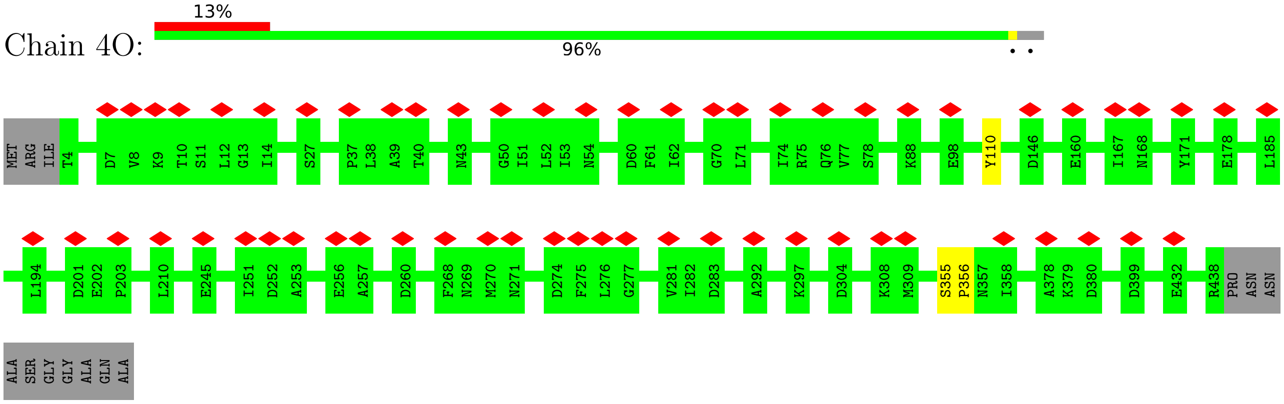
- Molecule 1: Major capsid protein

Chain 4N:



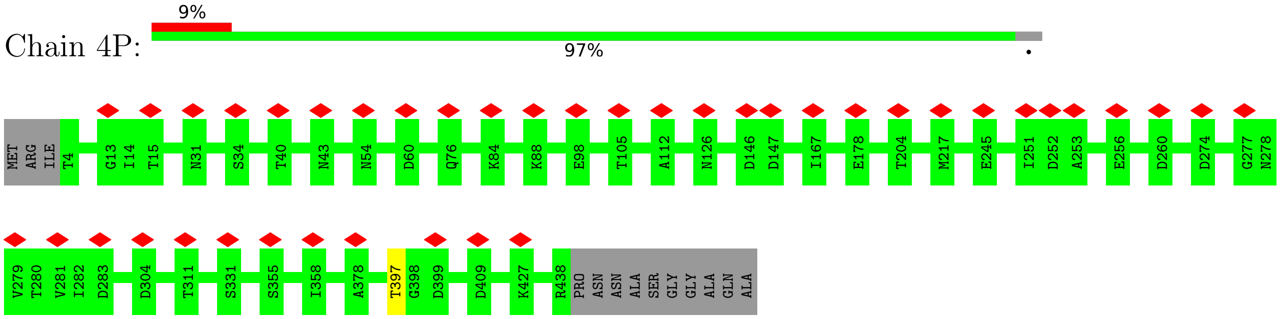
- Molecule 1: Major capsid protein

Chain 4O:



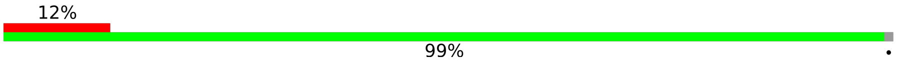
- Molecule 1: Major capsid protein

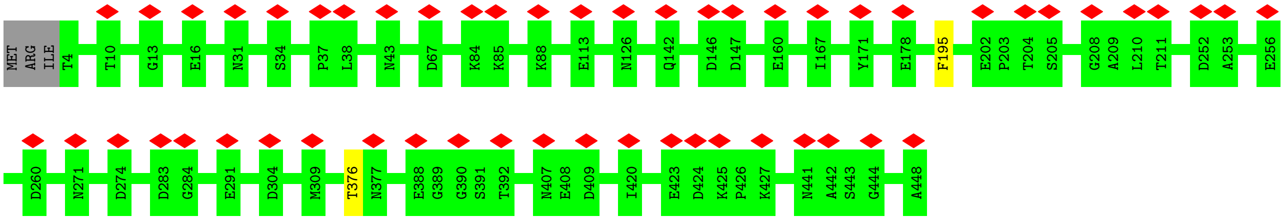
Chain 4P:



- Molecule 1: Major capsid protein

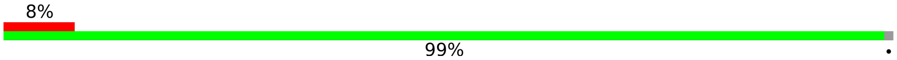
Chain 4Q:

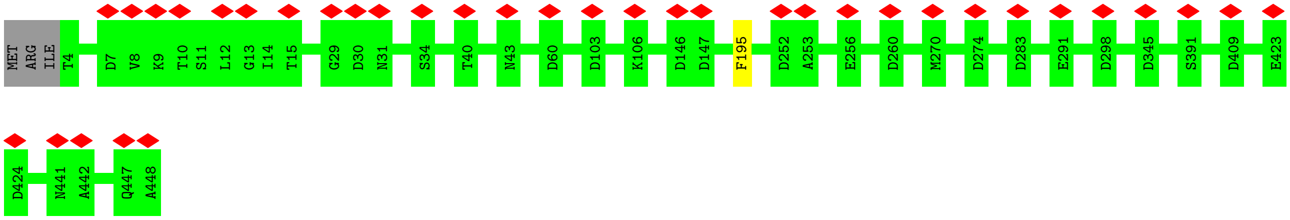




- Molecule 1: Major capsid protein

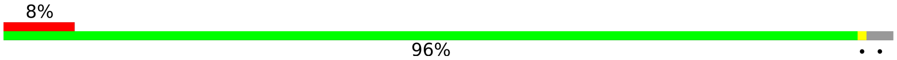
Chain 4R:

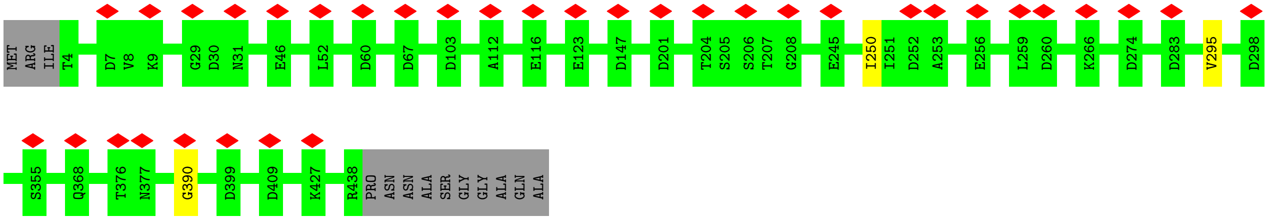




- Molecule 1: Major capsid protein

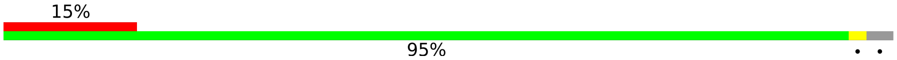
Chain 5M:

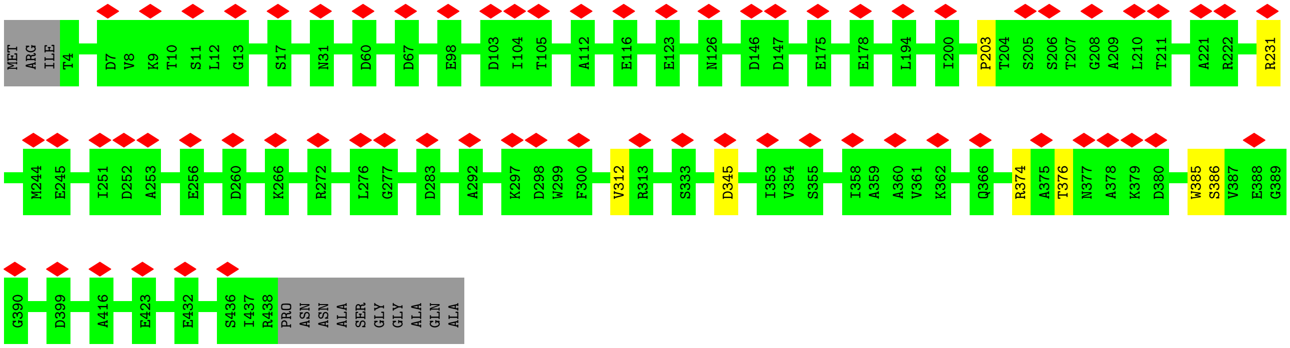




- Molecule 1: Major capsid protein

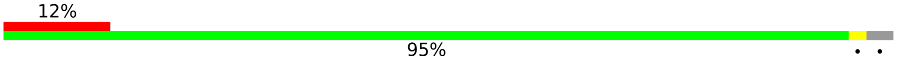
Chain 5N:

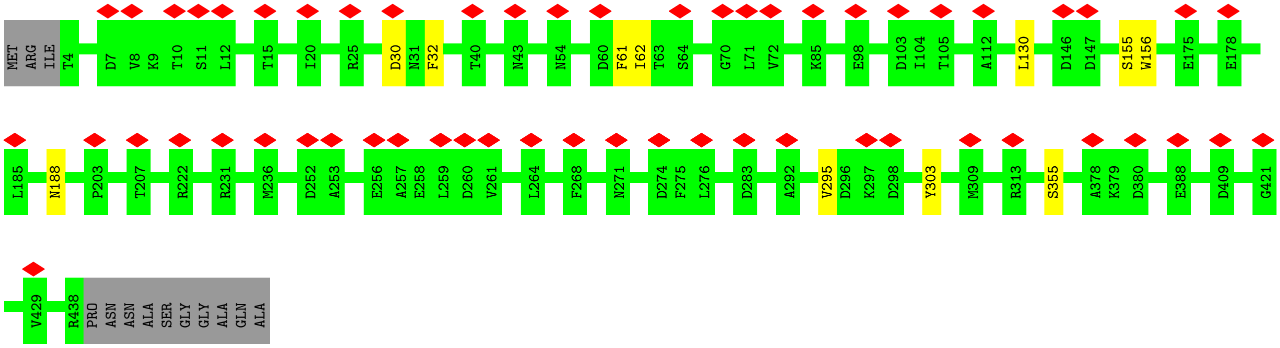




- Molecule 1: Major capsid protein

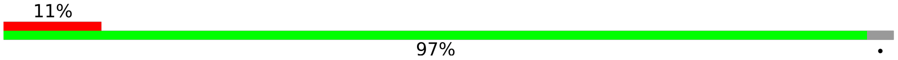
Chain 5O:

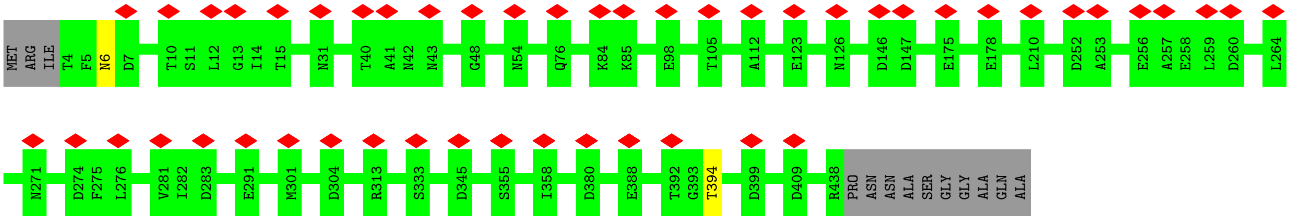




- Molecule 1: Major capsid protein

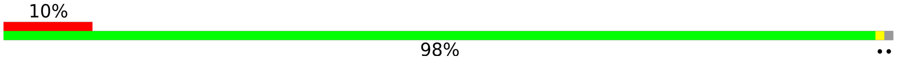
Chain 5P:

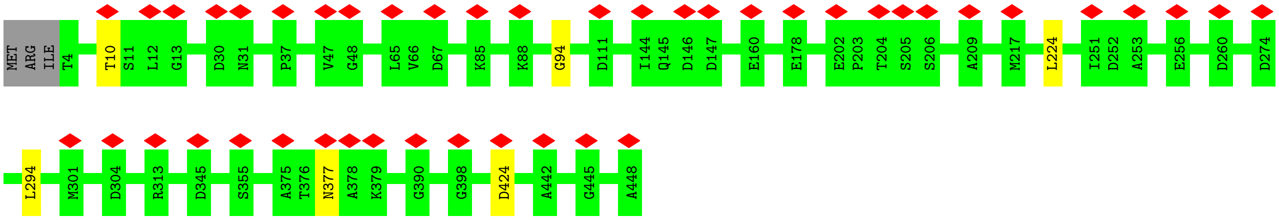




- Molecule 1: Major capsid protein

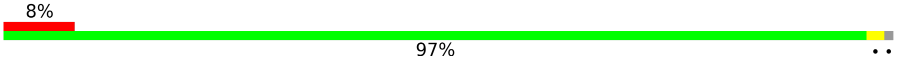
Chain 5Q:

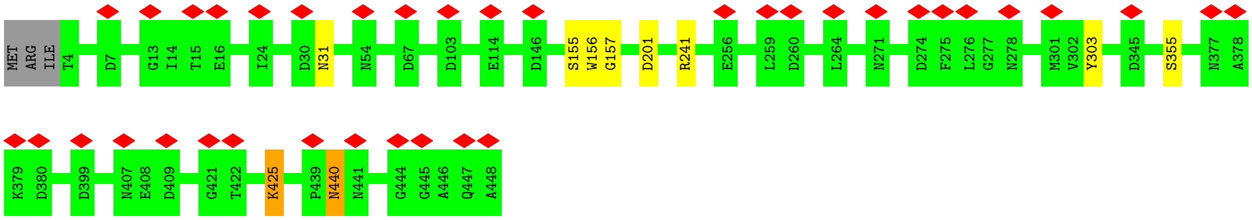




- Molecule 1: Major capsid protein

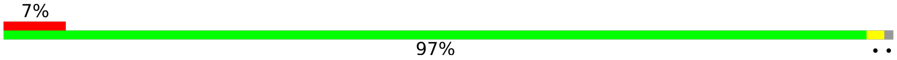
Chain 5R:

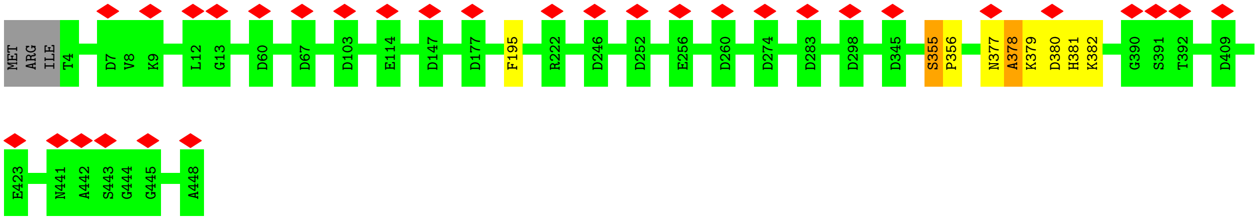




- Molecule 1: Major capsid protein

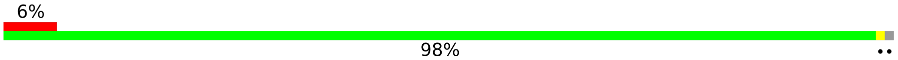
Chain 6M:

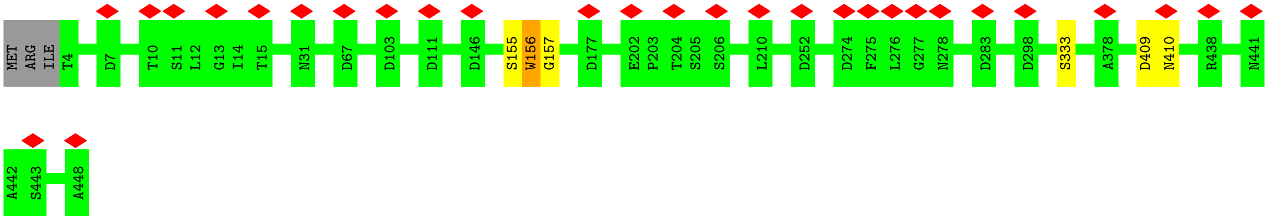




- Molecule 1: Major capsid protein

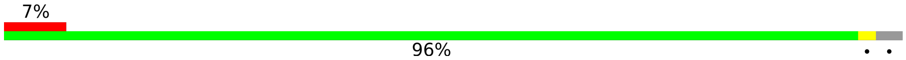
Chain 6N:

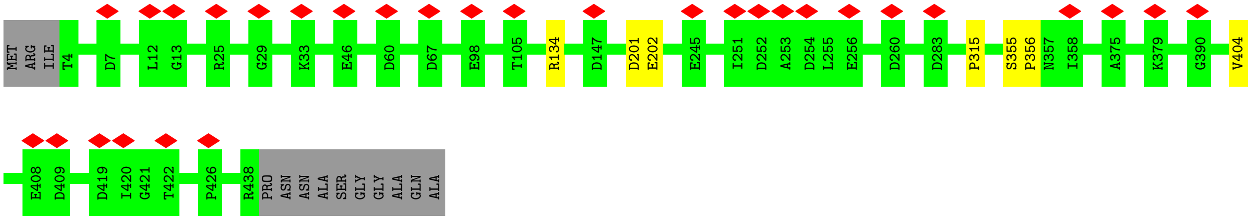




- Molecule 1: Major capsid protein

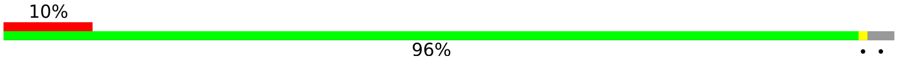
Chain 6O:

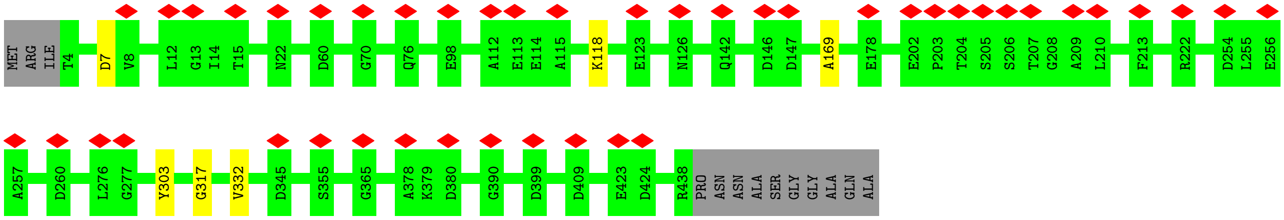




- Molecule 1: Major capsid protein

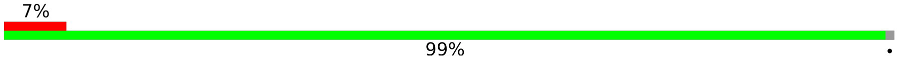
Chain 6P:

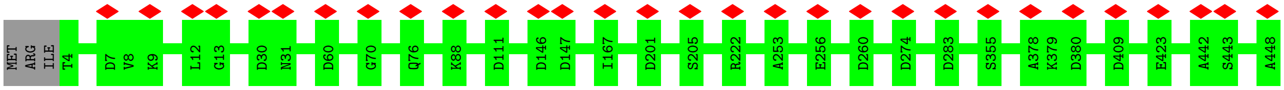




- Molecule 1: Major capsid protein

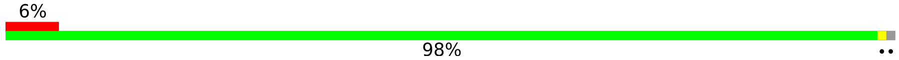
Chain 6Q:

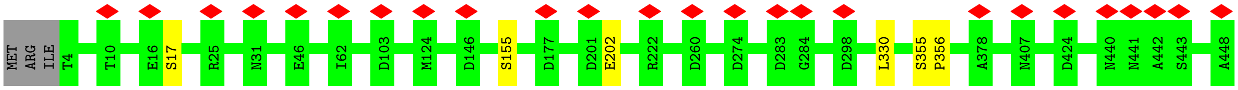




- Molecule 1: Major capsid protein

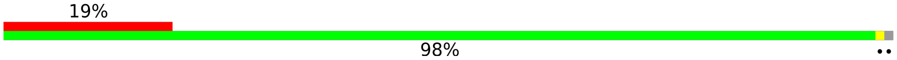
Chain 6R:

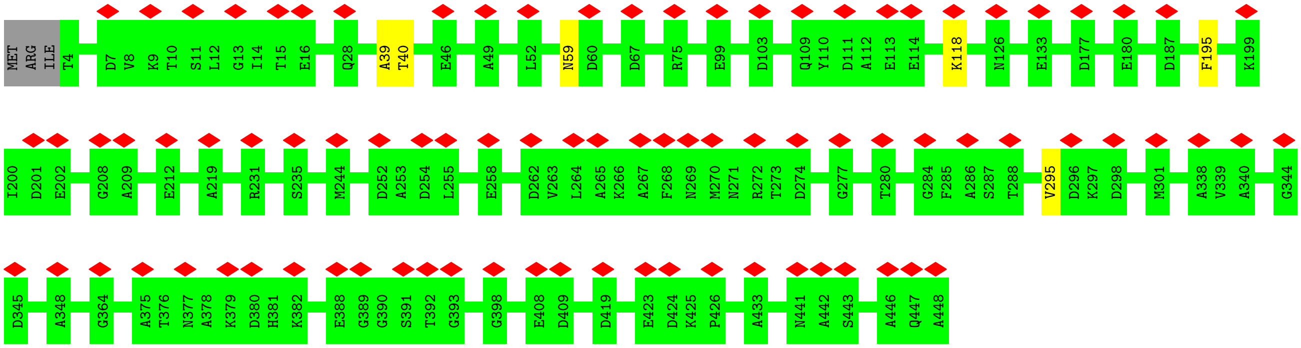




- Molecule 1: Major capsid protein

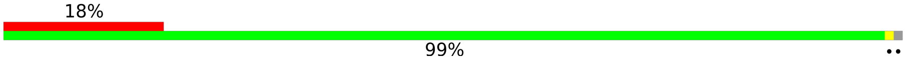
Chain 7K:

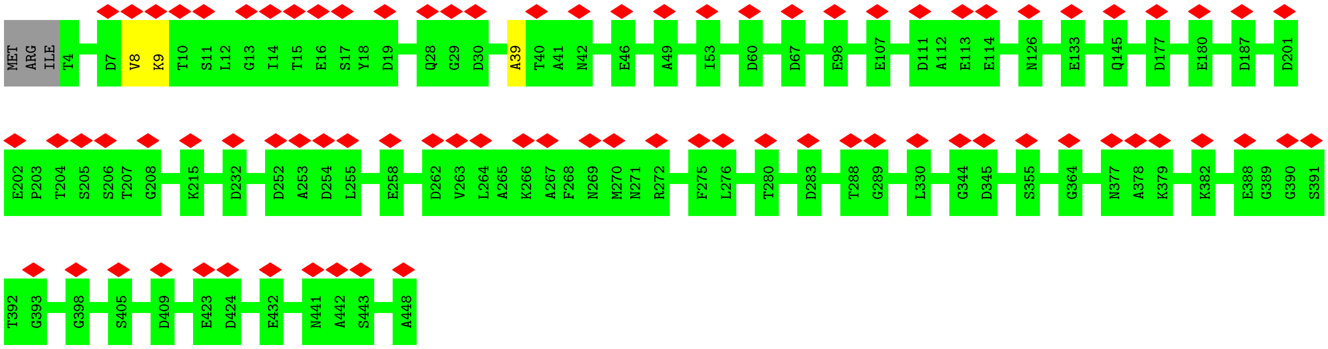




- Molecule 1: Major capsid protein

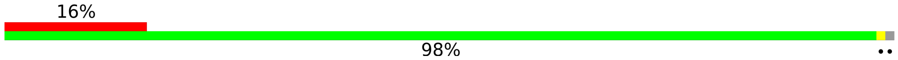
Chain 7L:

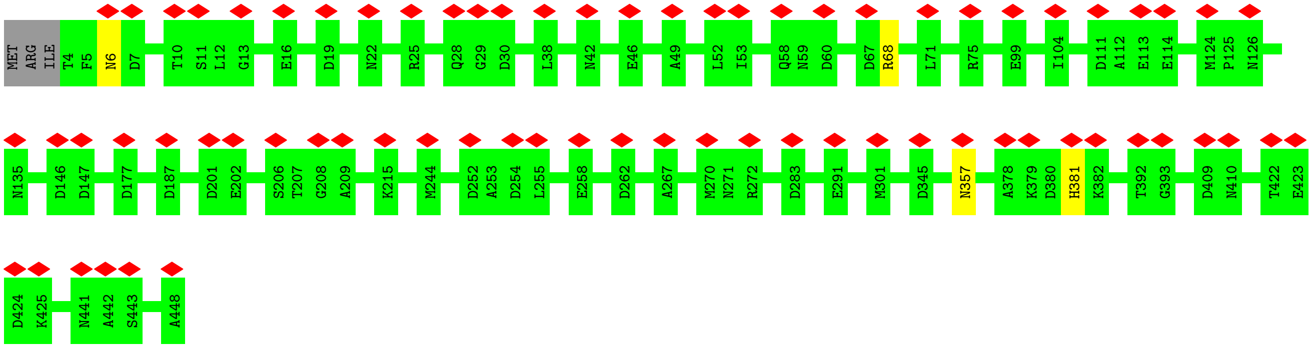




- Molecule 1: Major capsid protein

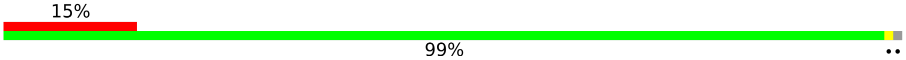
Chain 7M:

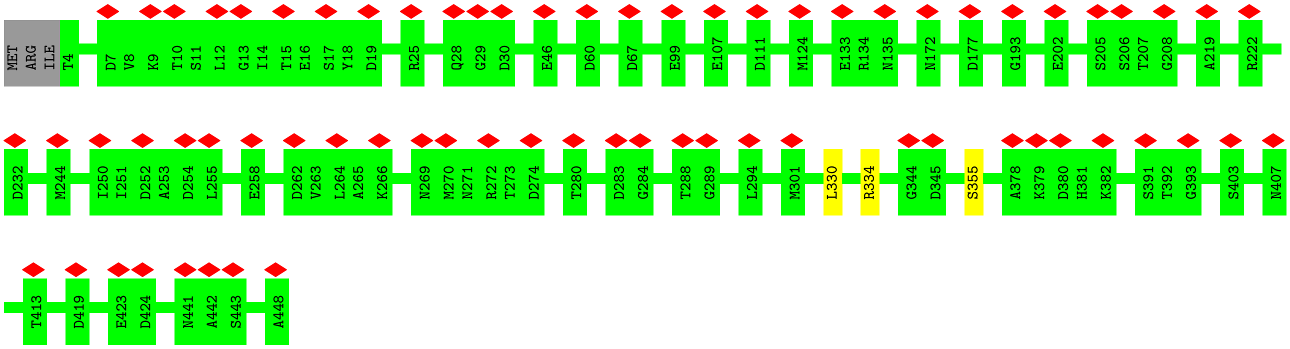




- Molecule 1: Major capsid protein

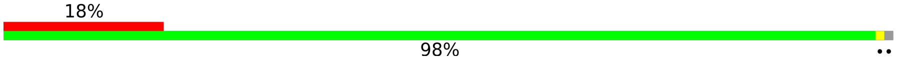
Chain 7N:

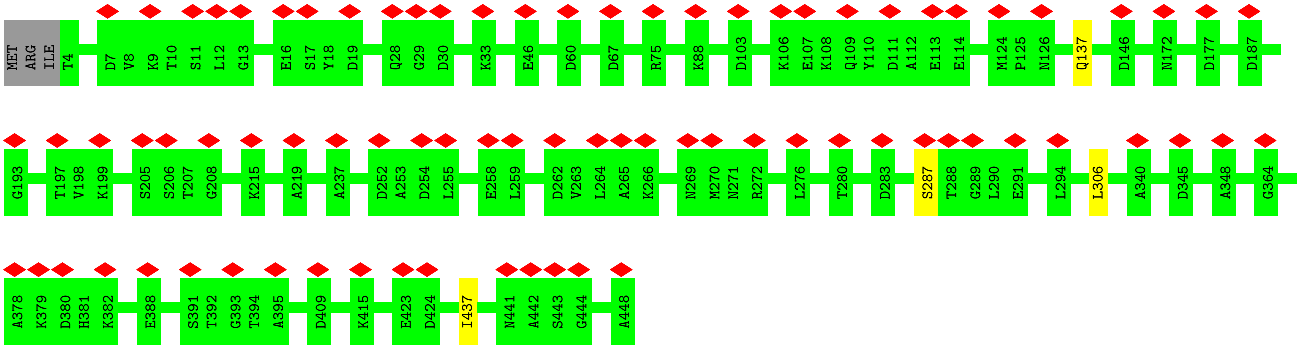




- Molecule 1: Major capsid protein

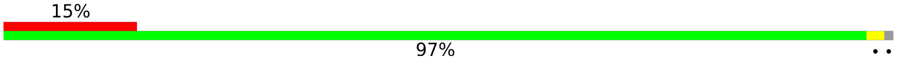
Chain 7O:

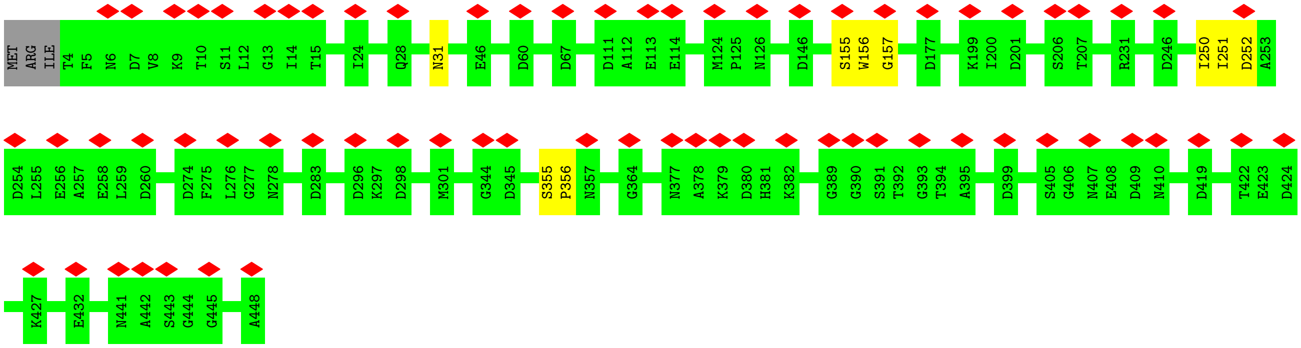




- Molecule 1: Major capsid protein

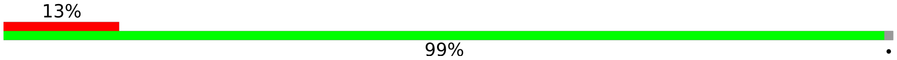
Chain 8M:

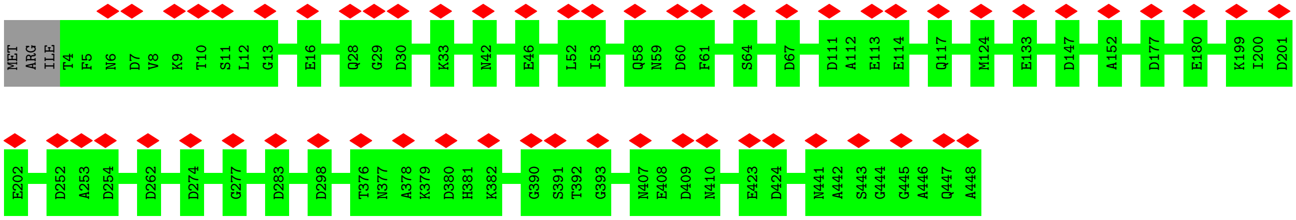




- Molecule 1: Major capsid protein

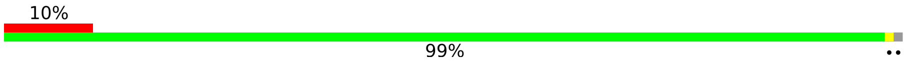
Chain 8N:

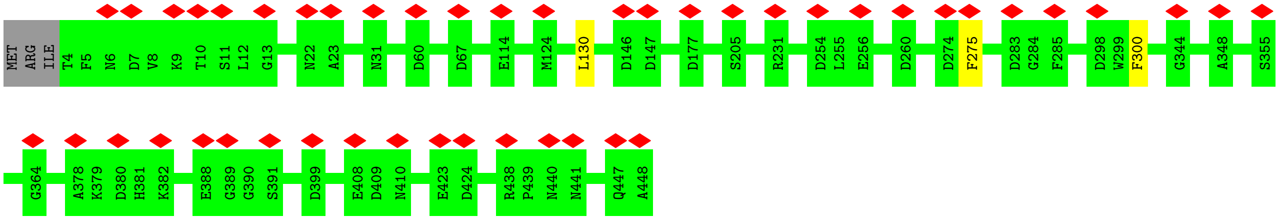




- Molecule 1: Major capsid protein

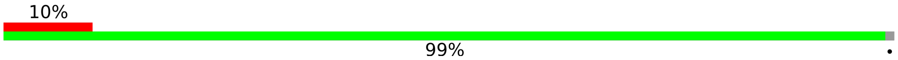
Chain 8O:

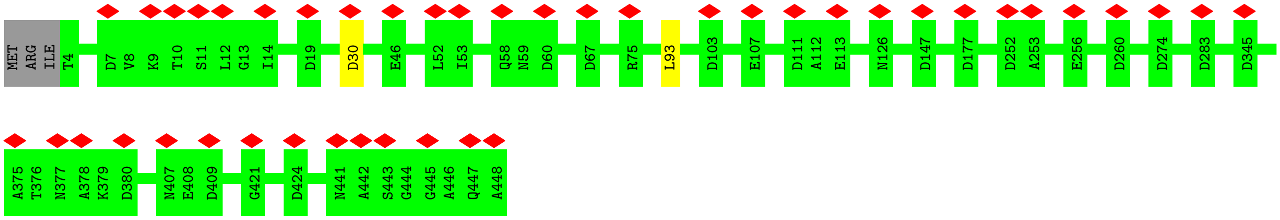




- Molecule 1: Major capsid protein

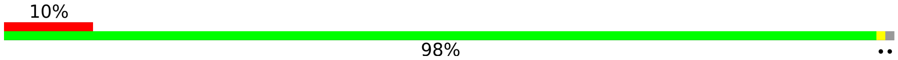
Chain 8P:

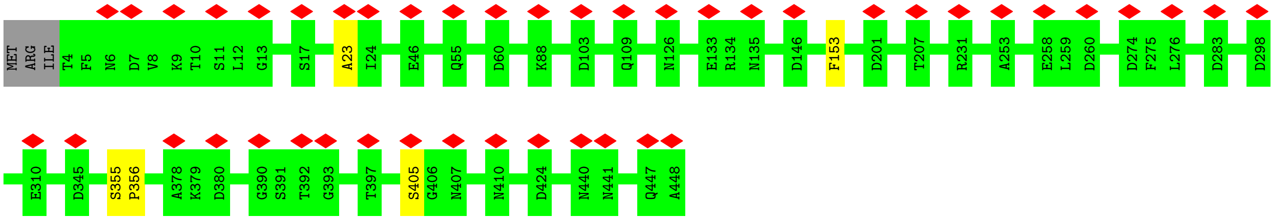




- Molecule 1: Major capsid protein

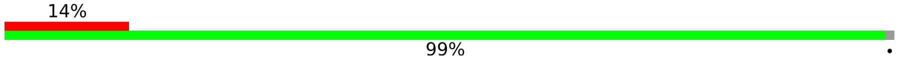
Chain 8Q:

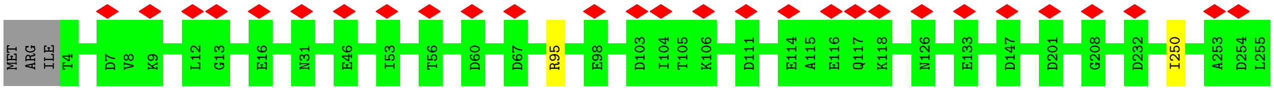


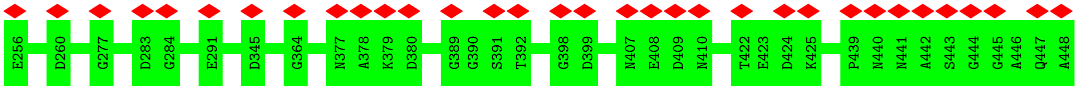


- Molecule 1: Major capsid protein

Chain 8R:

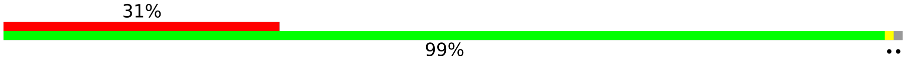


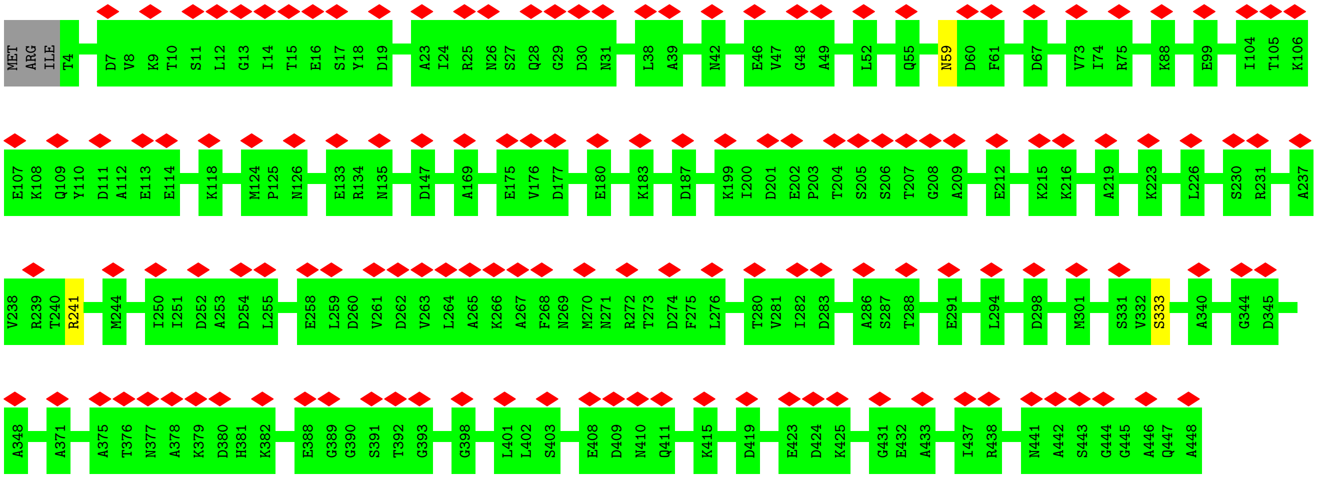




- Molecule 1: Major capsid protein

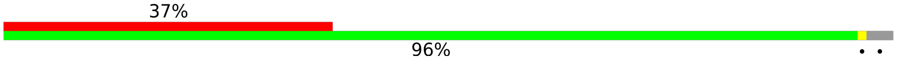
Chain 9C:

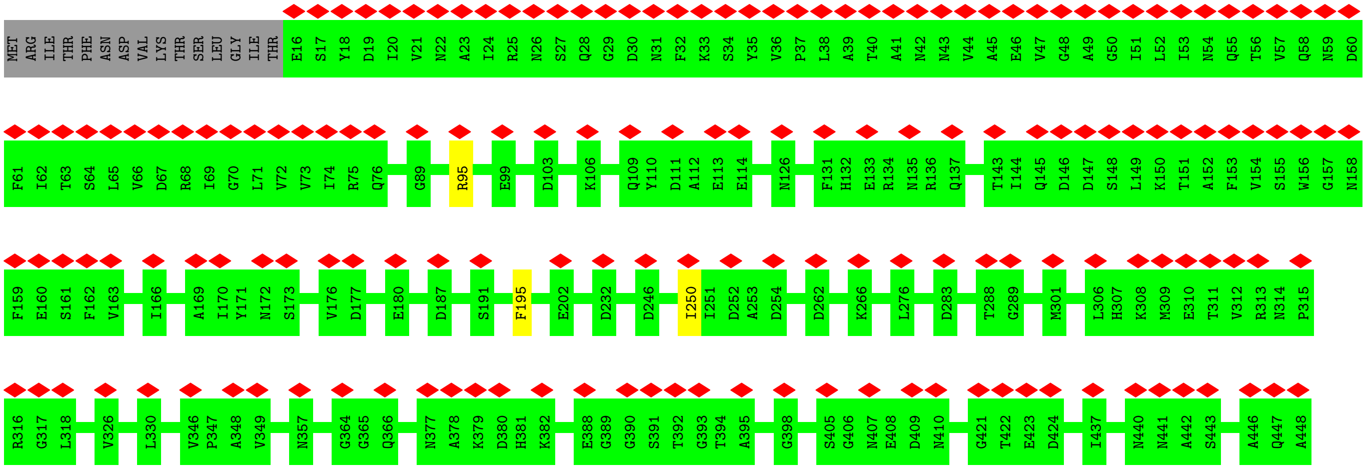




- Molecule 1: Major capsid protein

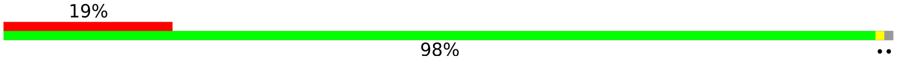
Chain 1S:

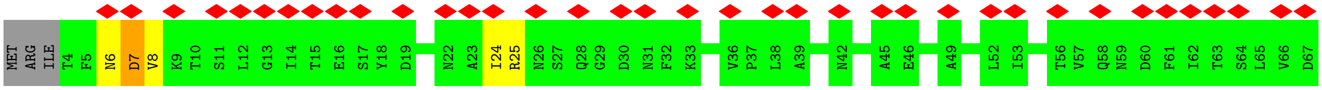


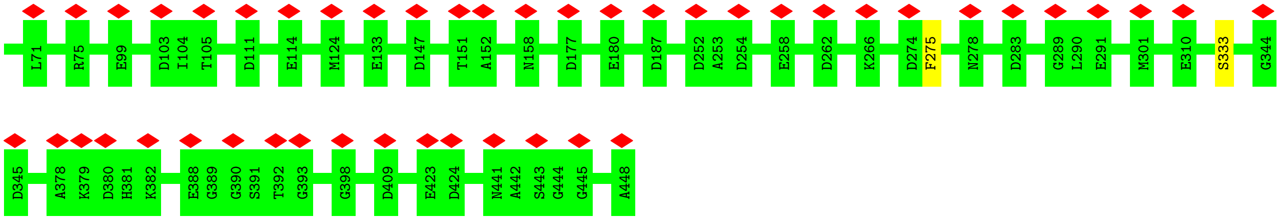


- Molecule 1: Major capsid protein

Chain 1T:

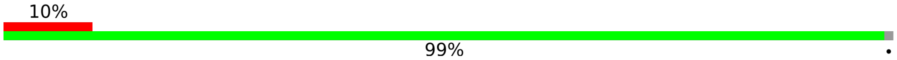


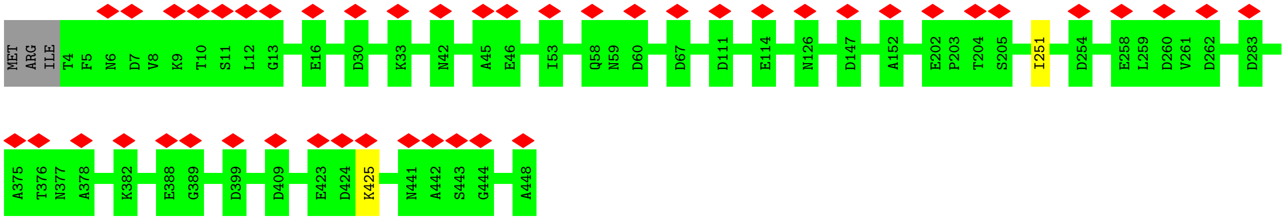




- Molecule 1: Major capsid protein

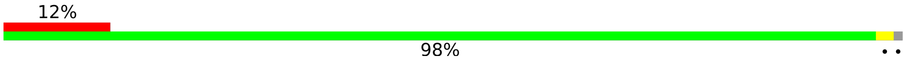
Chain 1U:

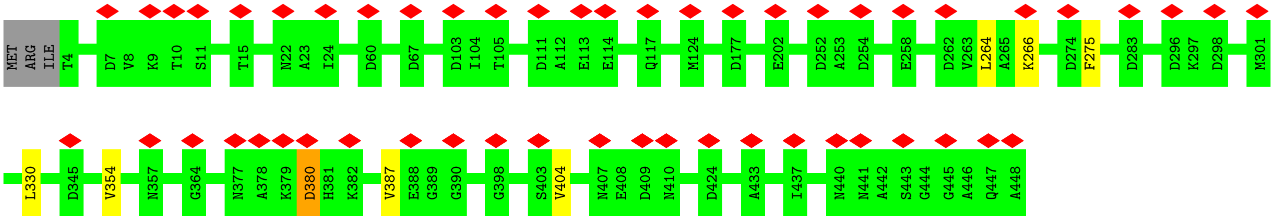




- Molecule 1: Major capsid protein

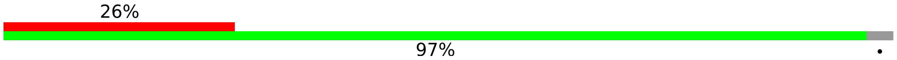
Chain 1V:





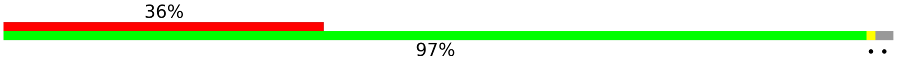
- Molecule 1: Major capsid protein

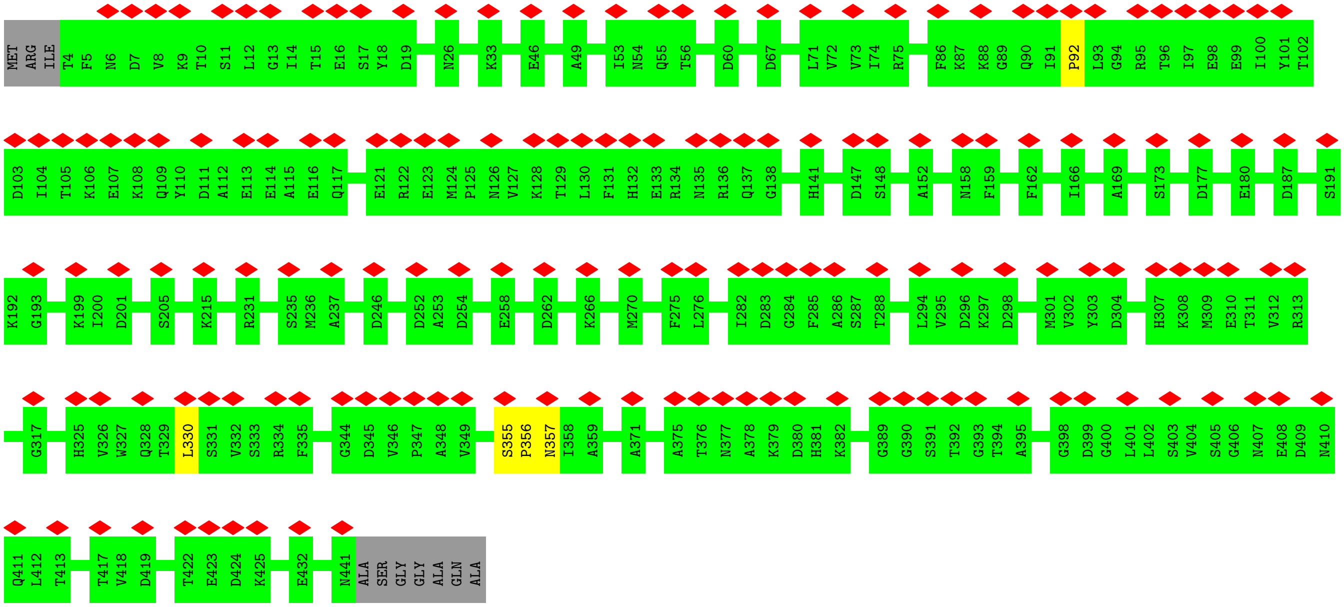
Chain 1W:



- Molecule 1: Major capsid protein

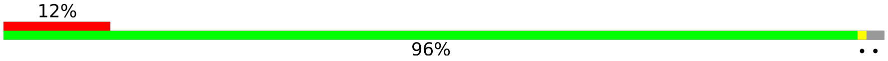
Chain 1X:

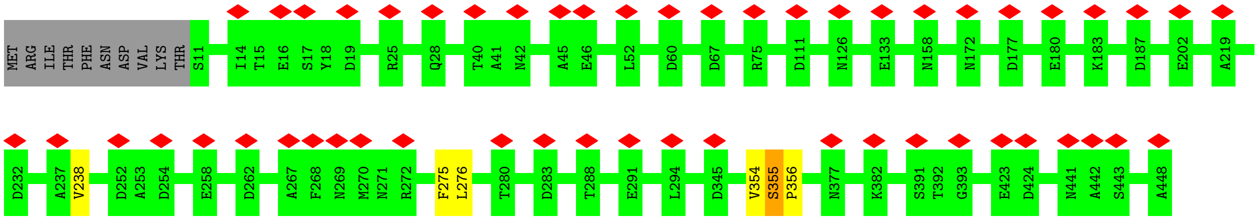




- Molecule 1: Major capsid protein

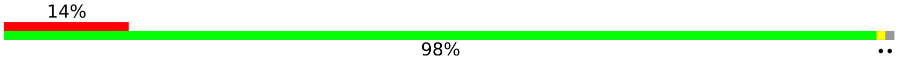
Chain 2P:

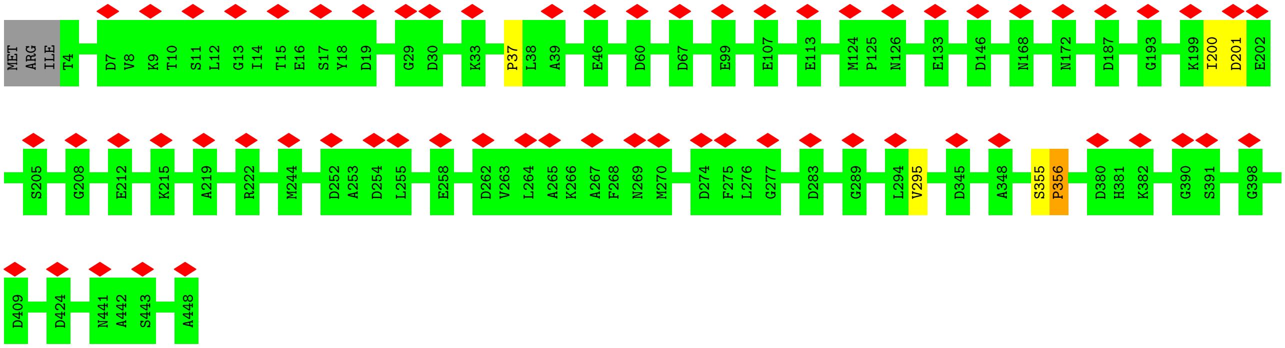




- Molecule 1: Major capsid protein

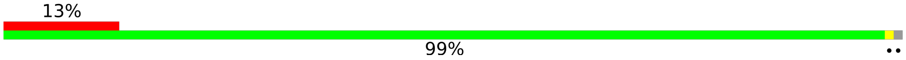
Chain 2Q:

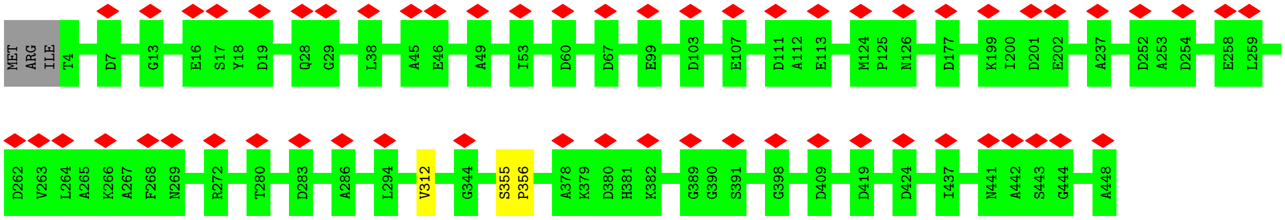




- Molecule 1: Major capsid protein

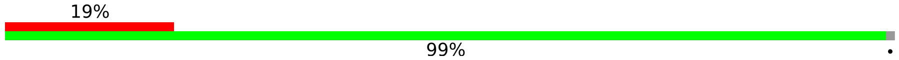
Chain 2R:

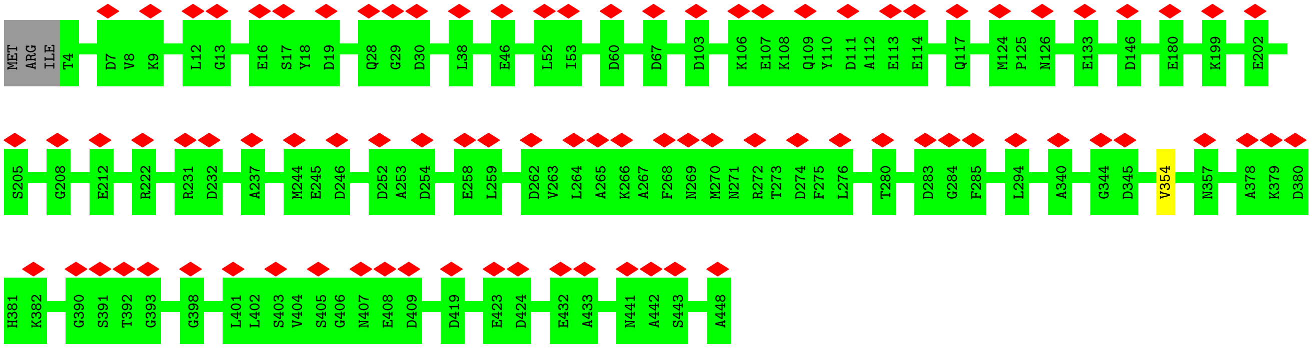




- Molecule 1: Major capsid protein

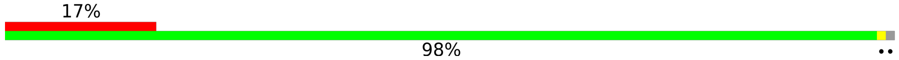
Chain 2S:

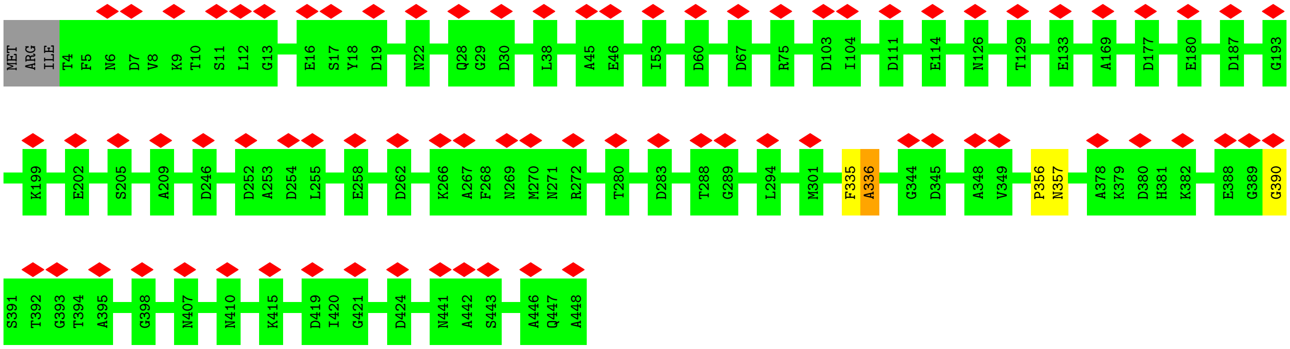




- Molecule 1: Major capsid protein

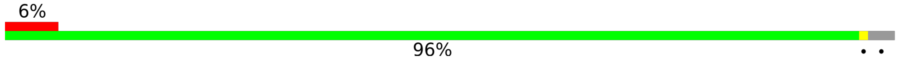
Chain 2T:

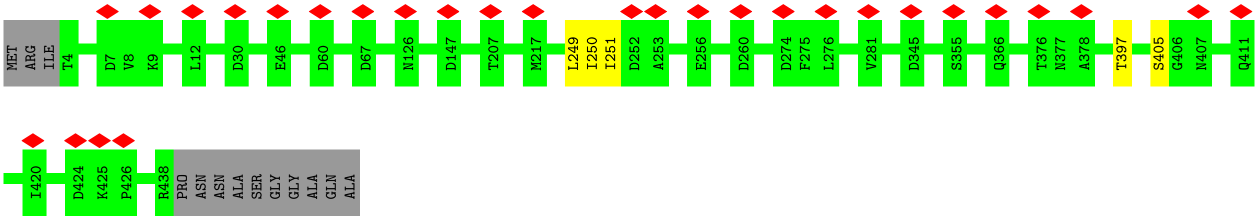




- Molecule 1: Major capsid protein

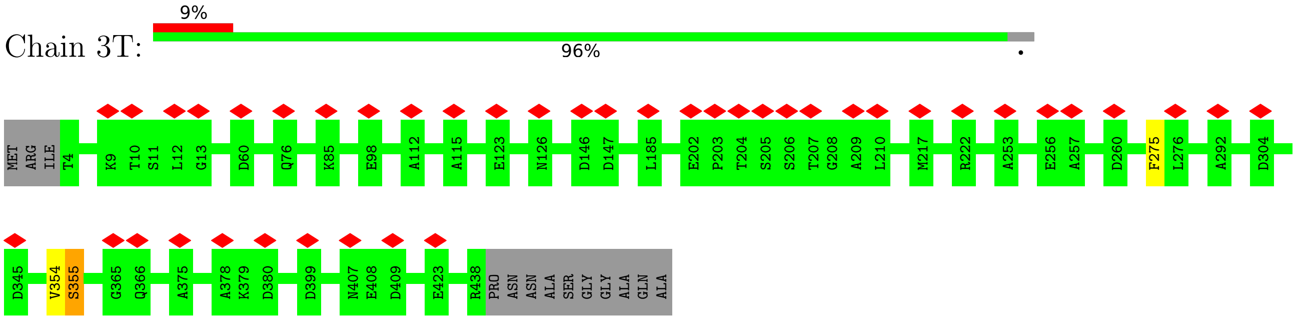
Chain 3S:





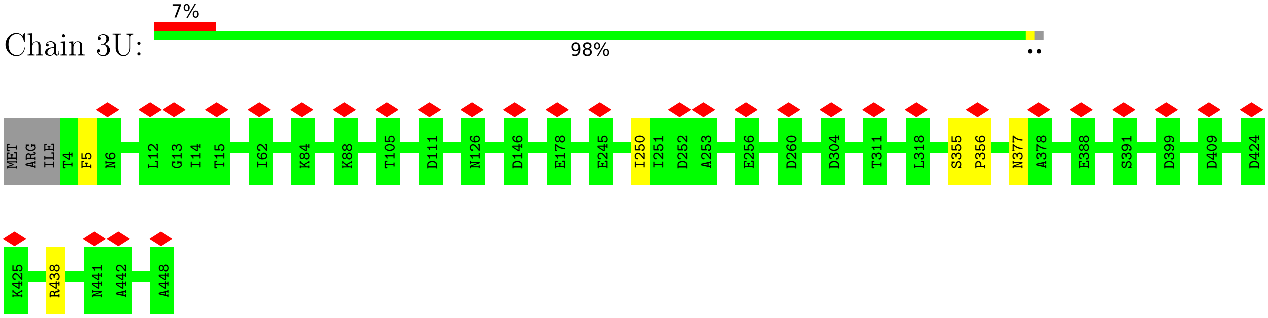
- Molecule 1: Major capsid protein

Chain 3T:



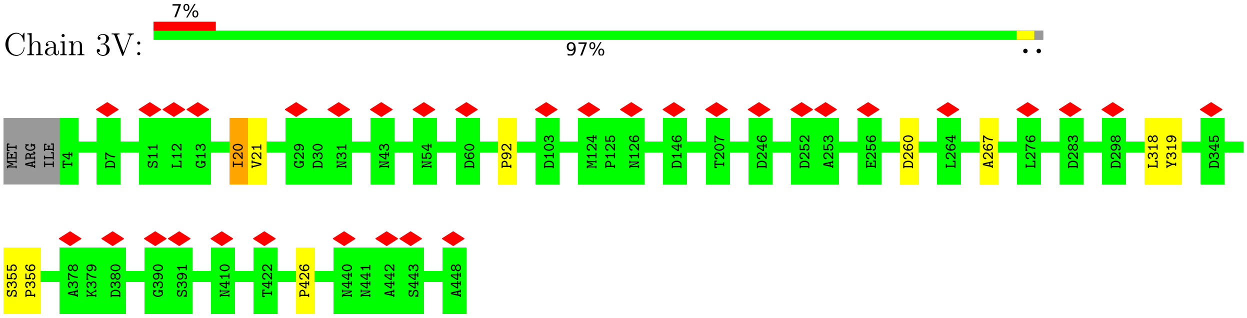
- Molecule 1: Major capsid protein

Chain 3U:



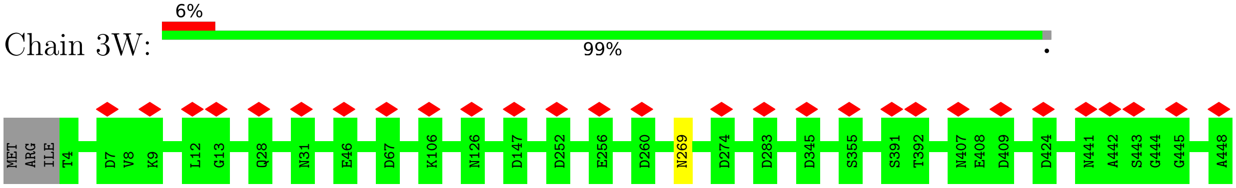
- Molecule 1: Major capsid protein

Chain 3V:



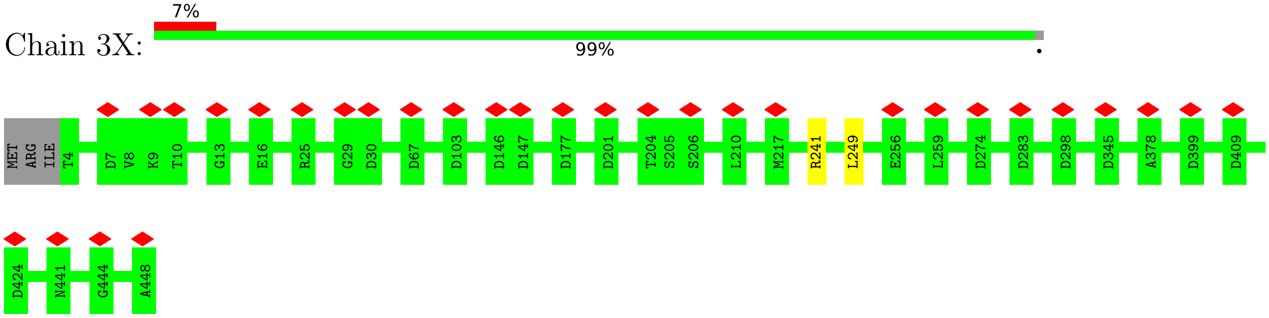
- Molecule 1: Major capsid protein

Chain 3W:

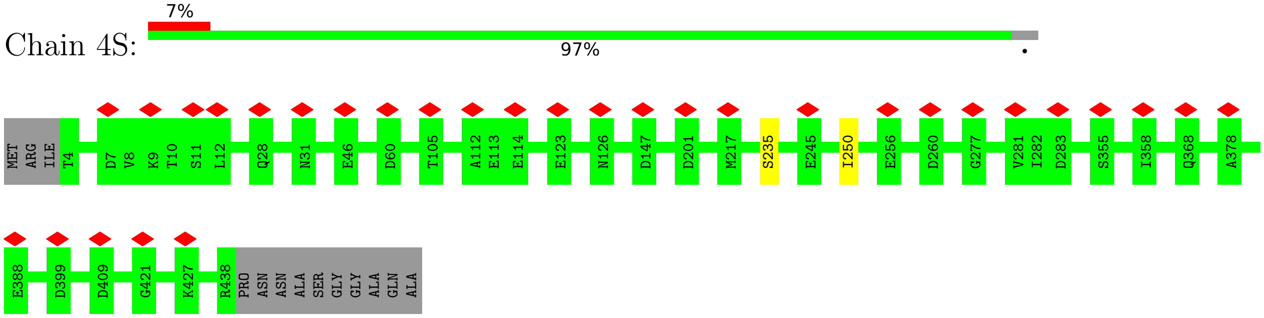


- Molecule 1: Major capsid protein

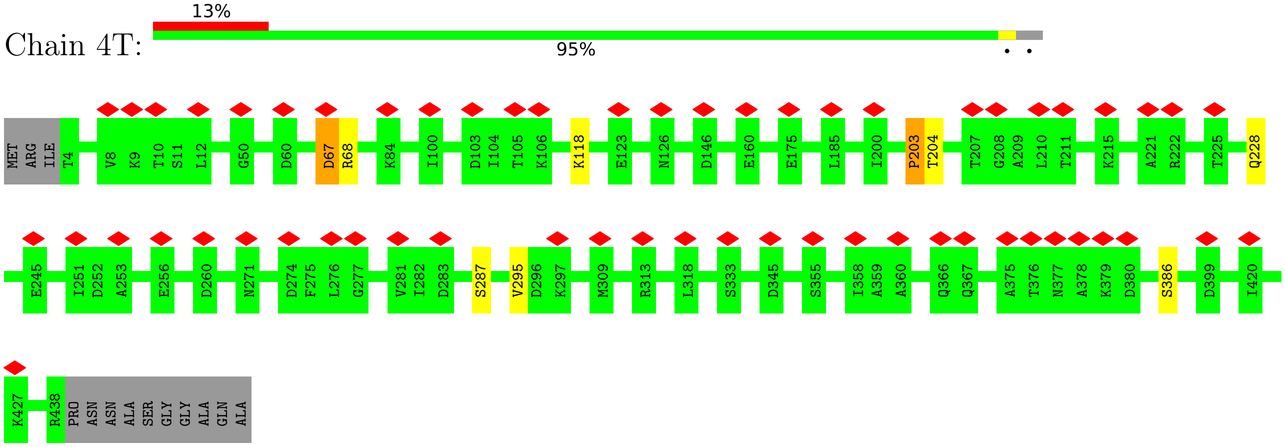
Chain 3X:



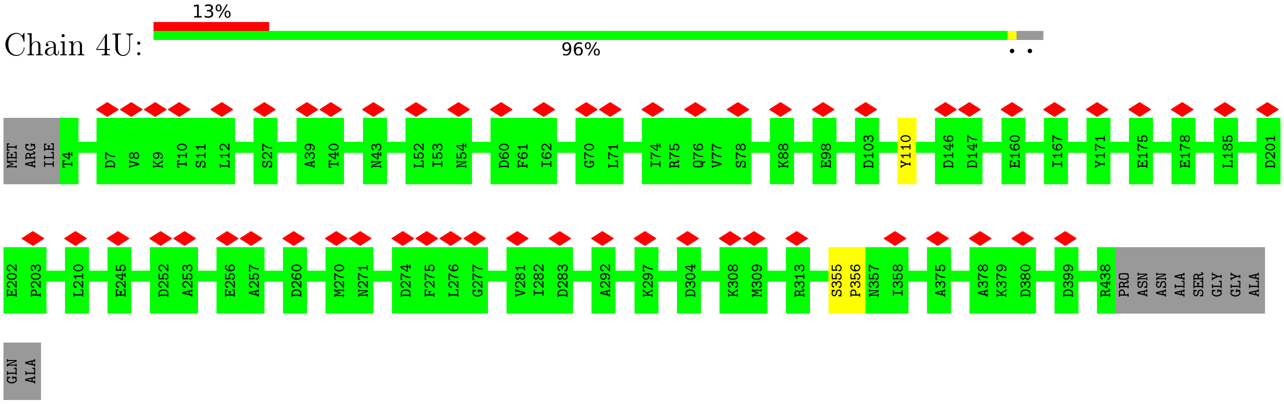
- Molecule 1: Major capsid protein



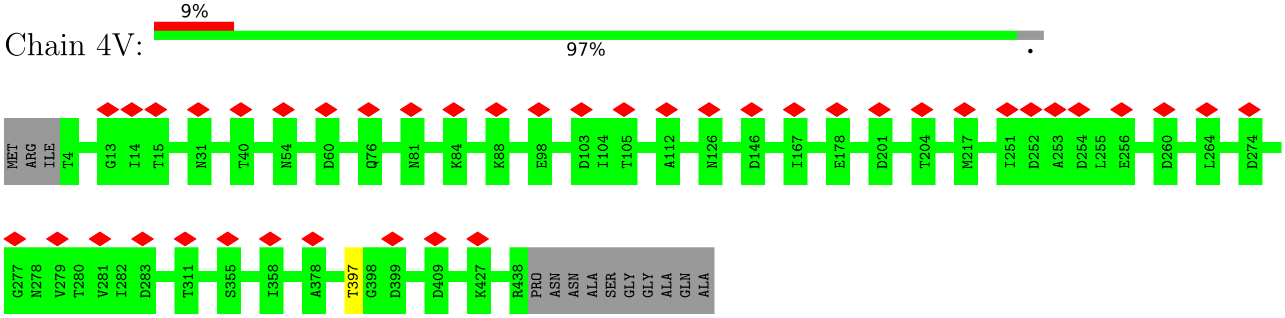
- Molecule 1: Major capsid protein



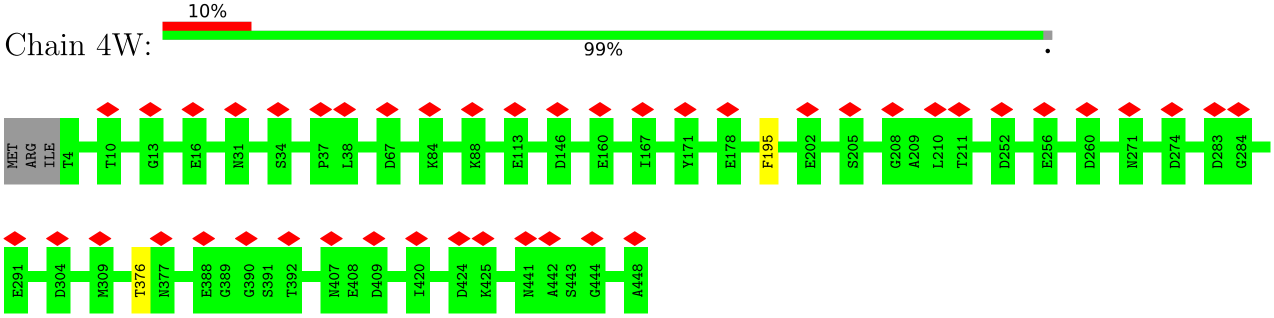
- Molecule 1: Major capsid protein



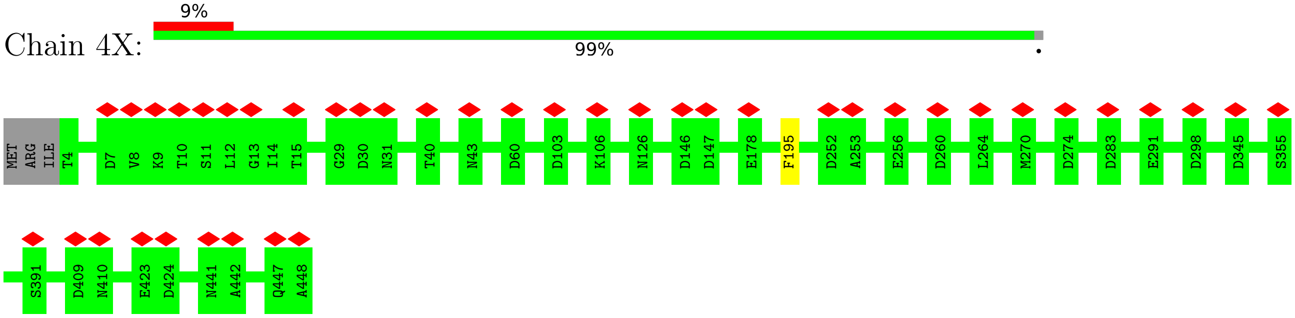
- Molecule 1: Major capsid protein



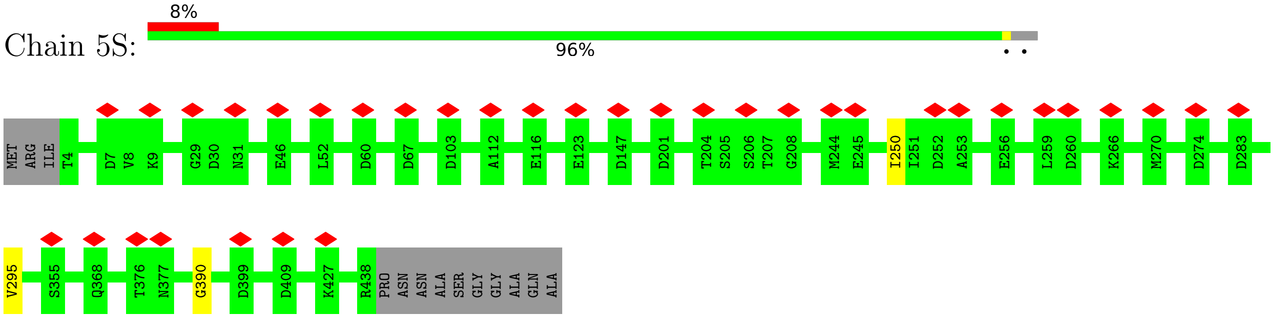
- Molecule 1: Major capsid protein



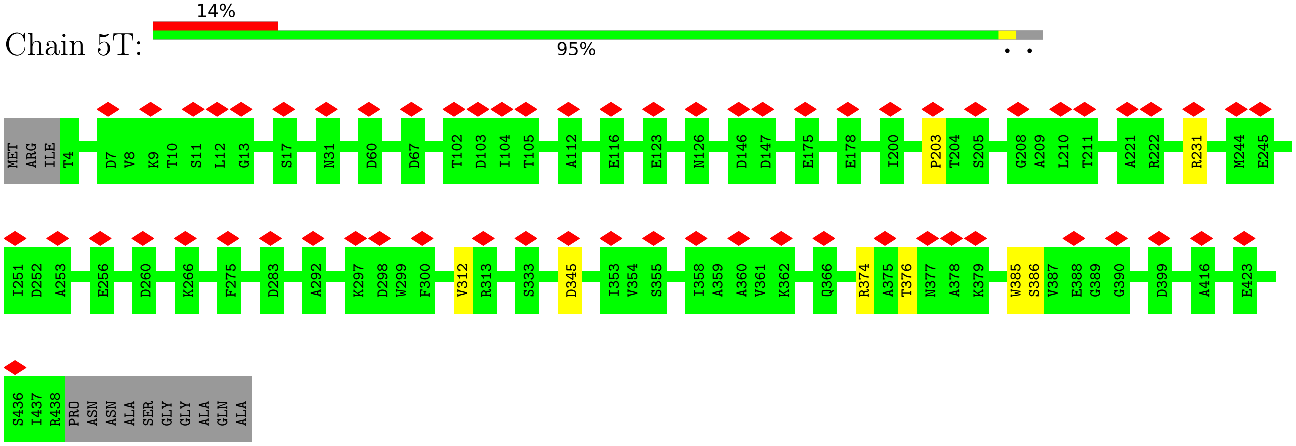
- Molecule 1: Major capsid protein



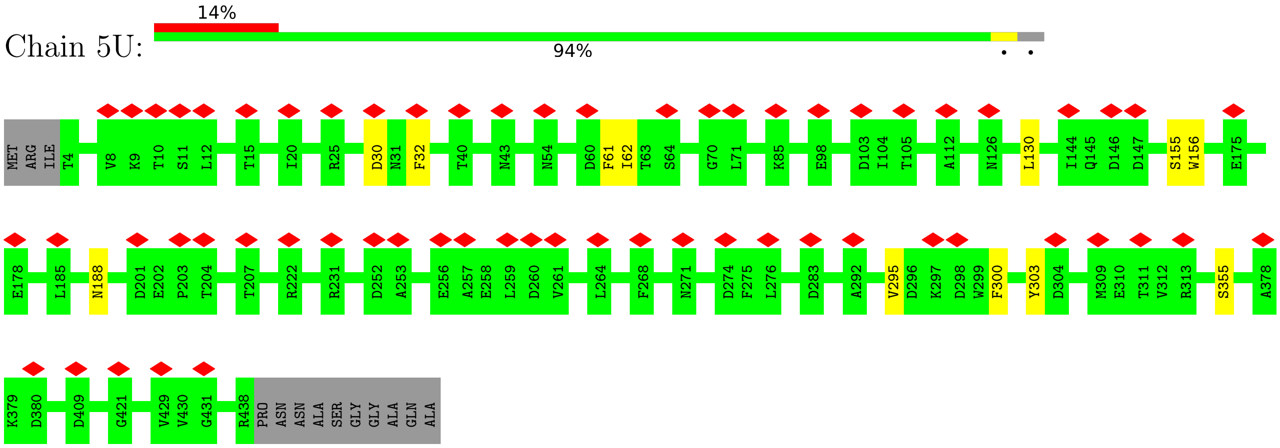
- Molecule 1: Major capsid protein



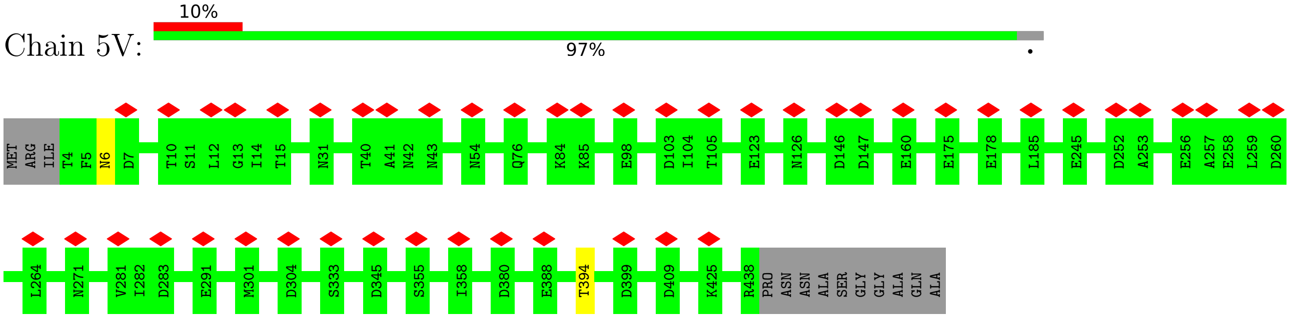
- Molecule 1: Major capsid protein



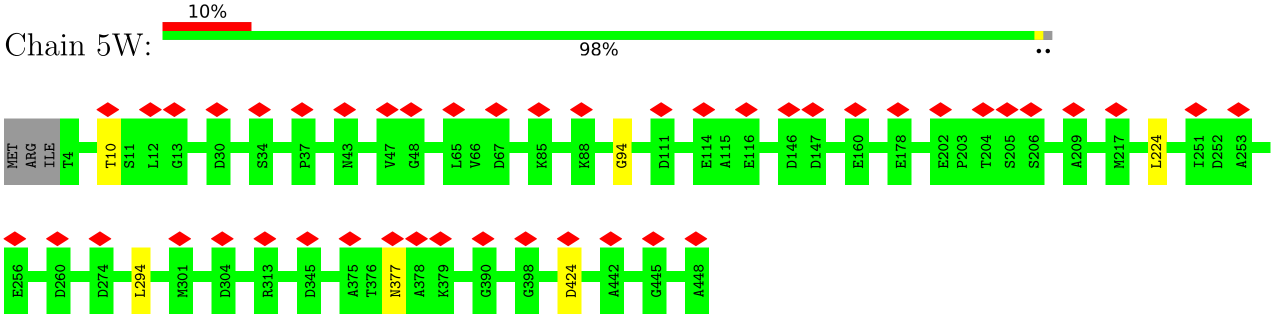
- Molecule 1: Major capsid protein



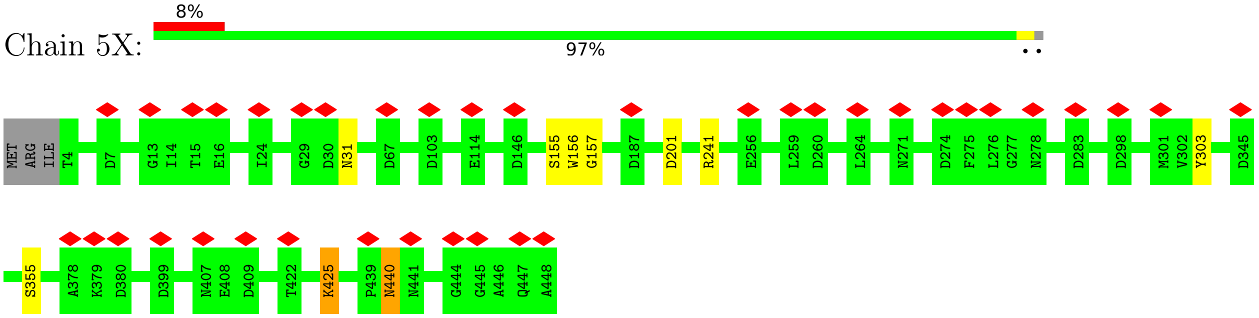
- Molecule 1: Major capsid protein



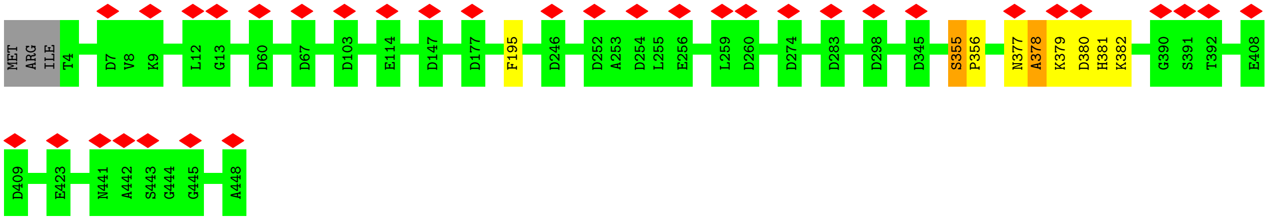
- Molecule 1: Major capsid protein



- Molecule 1: Major capsid protein

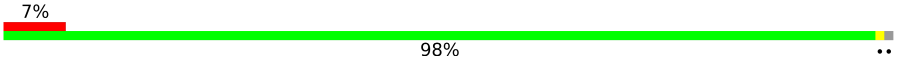


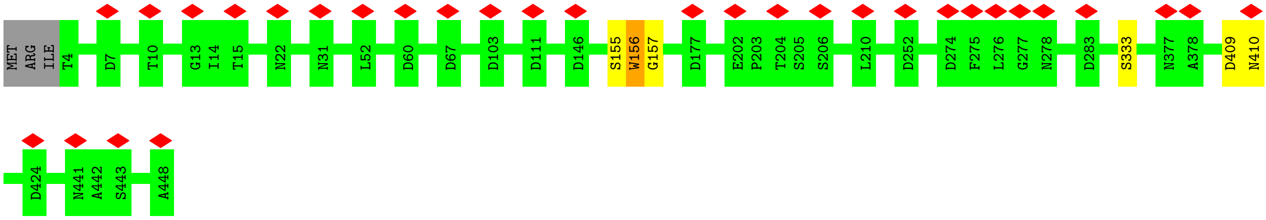
- Molecule 1: Major capsid protein



- Molecule 1: Major capsid protein

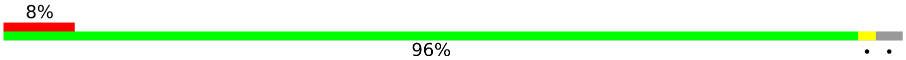
Chain 6T:

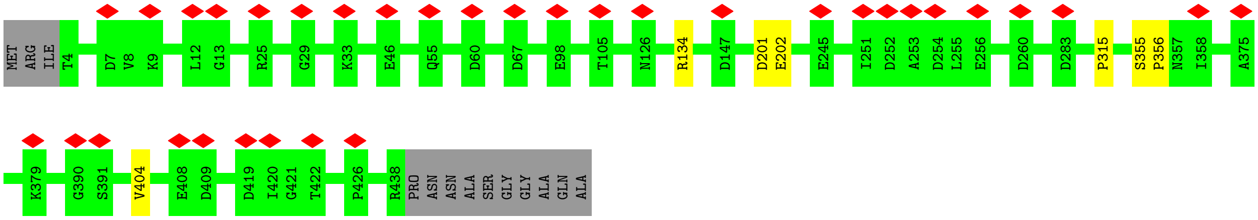




- Molecule 1: Major capsid protein

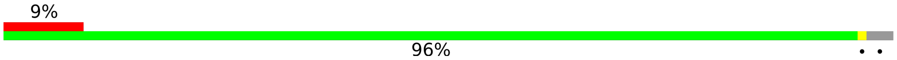
Chain 6U:

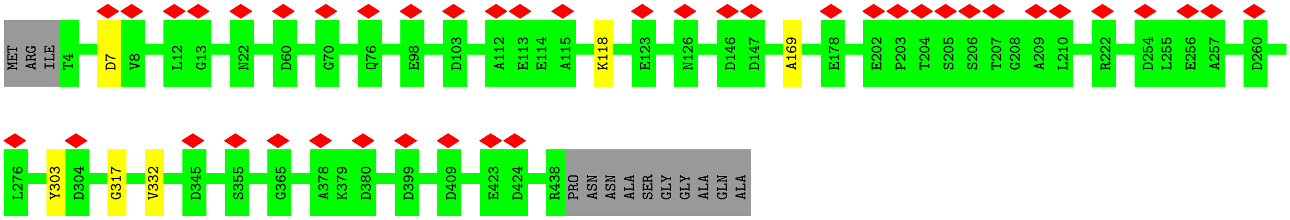




- Molecule 1: Major capsid protein

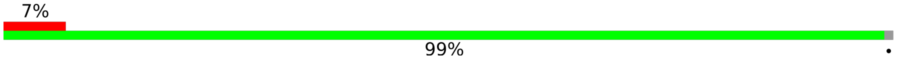
Chain 6V:

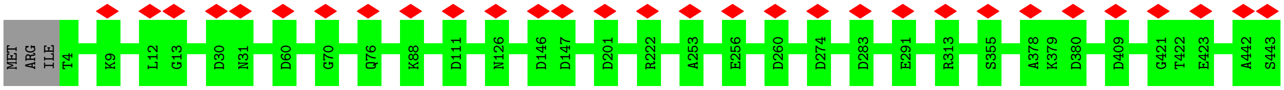


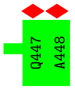


- Molecule 1: Major capsid protein

Chain 6W:

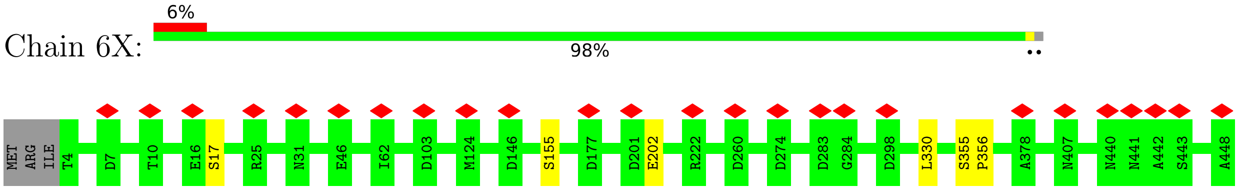






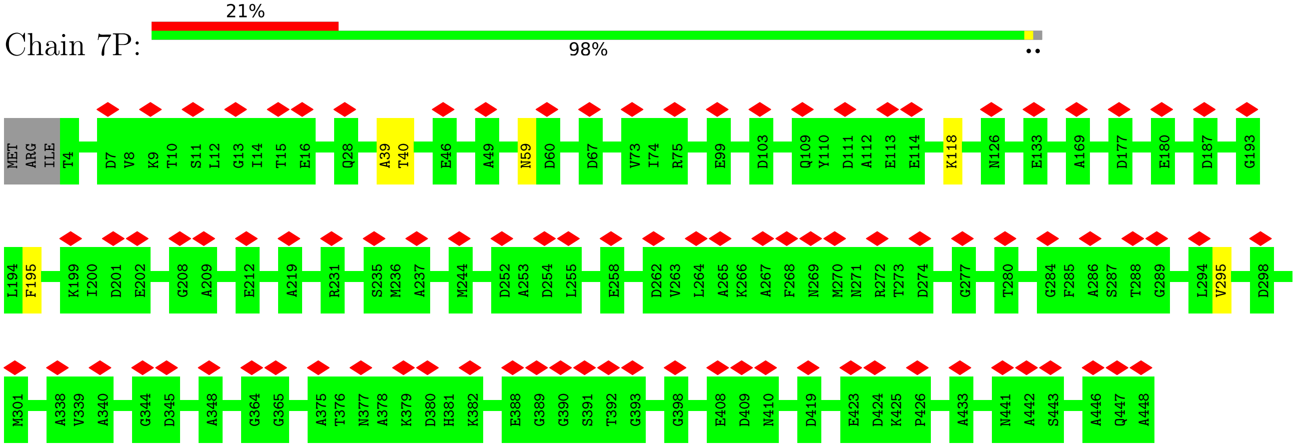
- Molecule 1: Major capsid protein

Chain 6X:



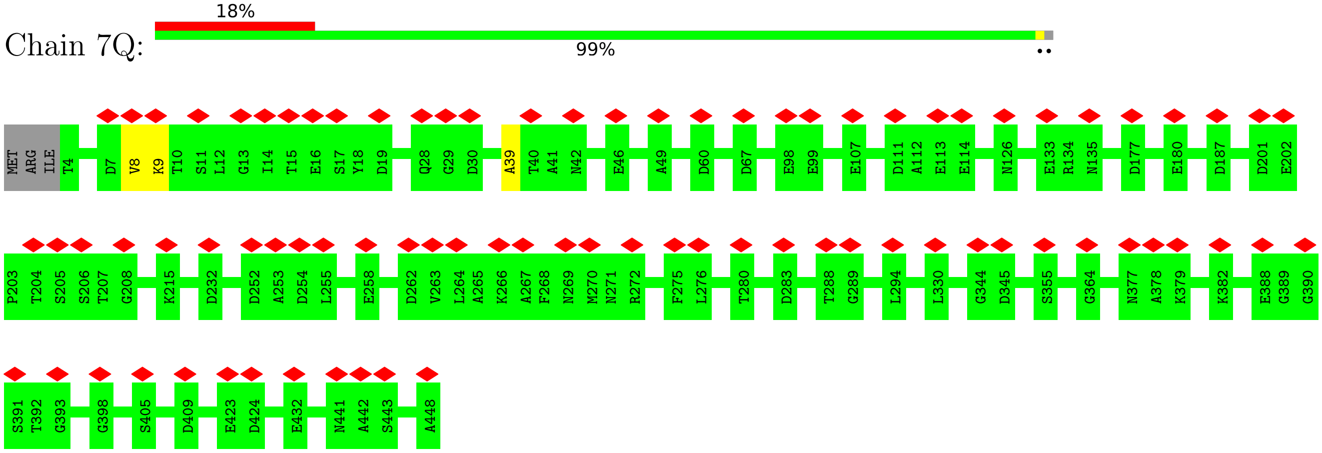
- Molecule 1: Major capsid protein

Chain 7P:



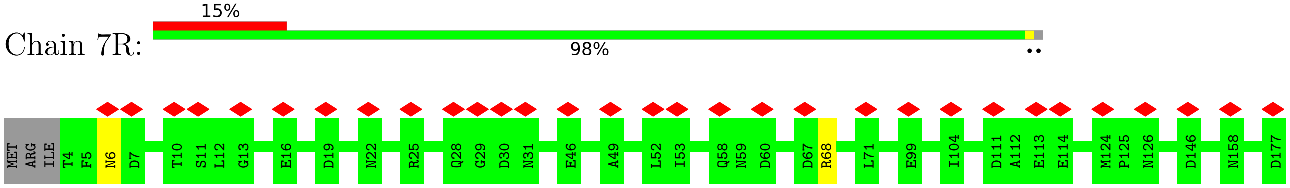
- Molecule 1: Major capsid protein

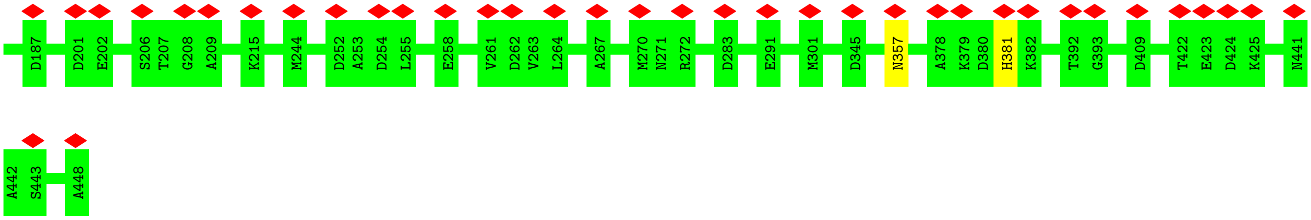
Chain 7Q:



- Molecule 1: Major capsid protein

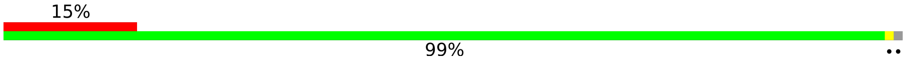
Chain 7R:

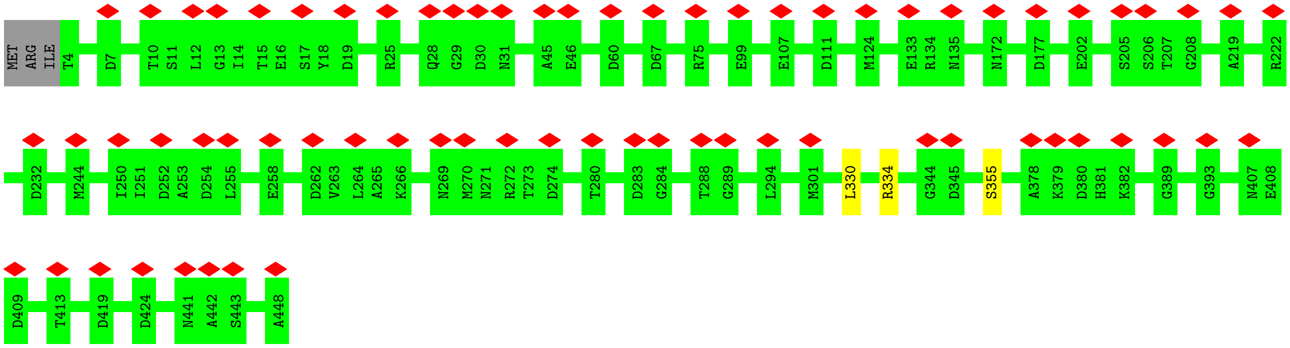




- Molecule 1: Major capsid protein

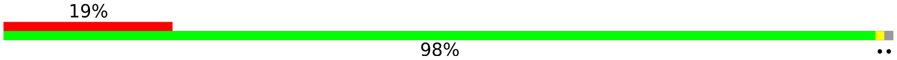
Chain 7S:

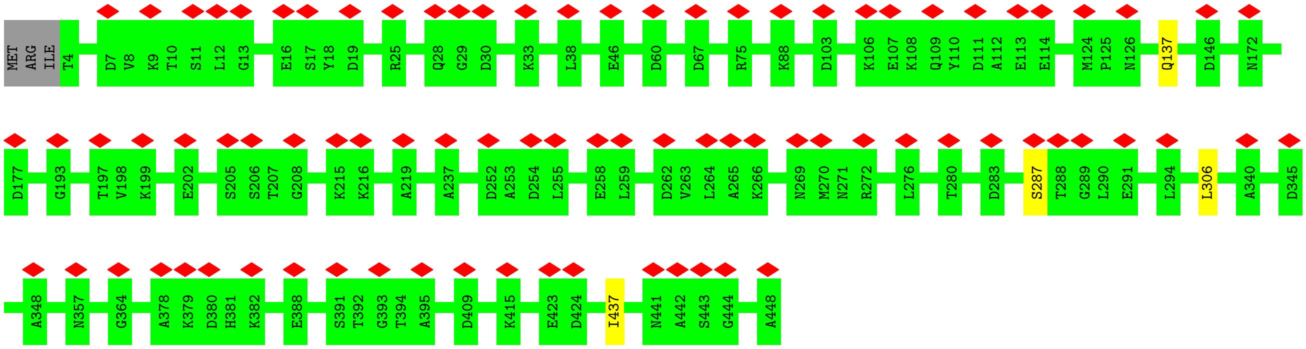




- Molecule 1: Major capsid protein

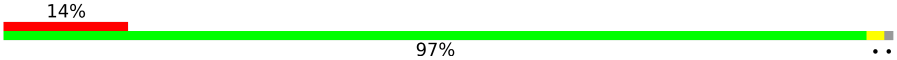
Chain 7T:

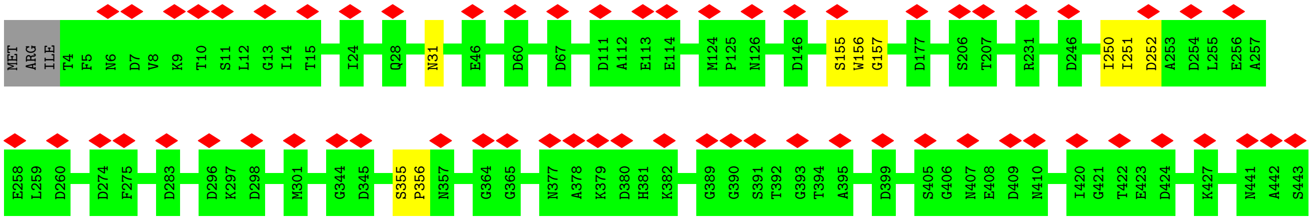


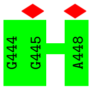


- Molecule 1: Major capsid protein

Chain 8S:

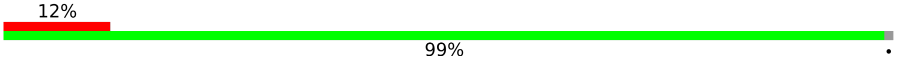


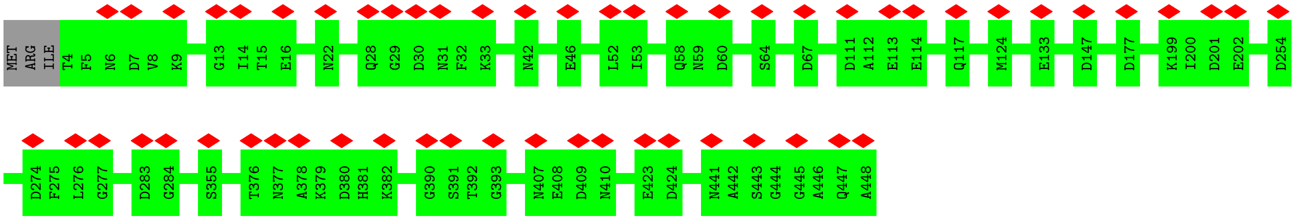




- Molecule 1: Major capsid protein

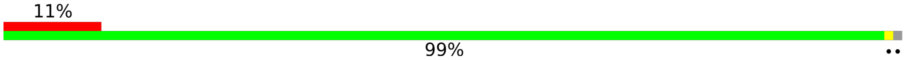
Chain 8T:

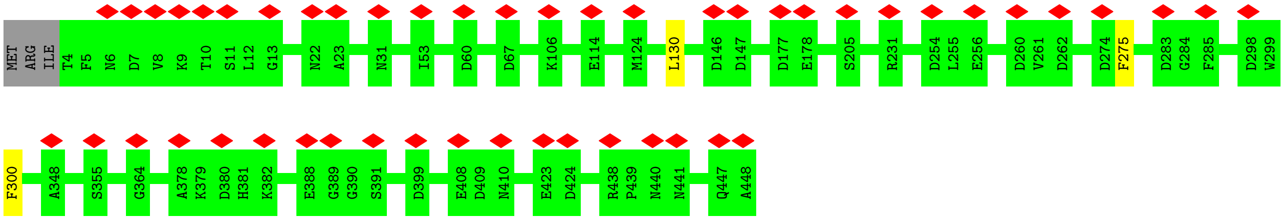




- Molecule 1: Major capsid protein

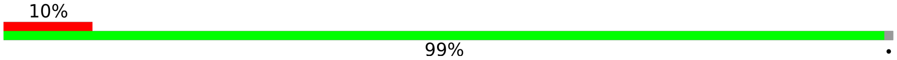
Chain 8U:

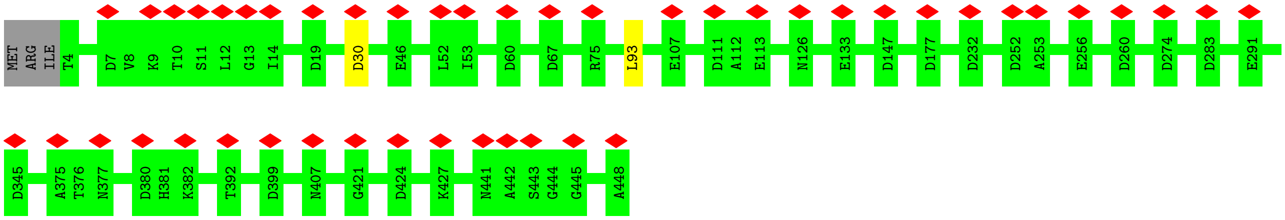




- Molecule 1: Major capsid protein

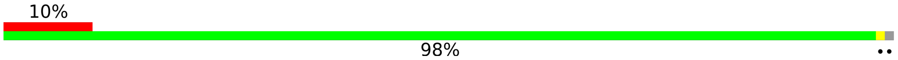
Chain 8V:

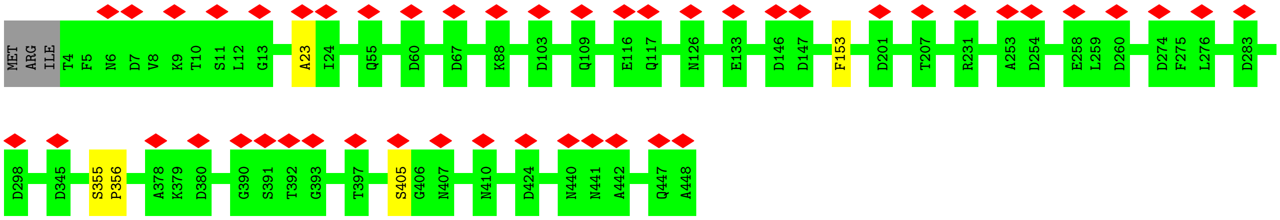




- Molecule 1: Major capsid protein

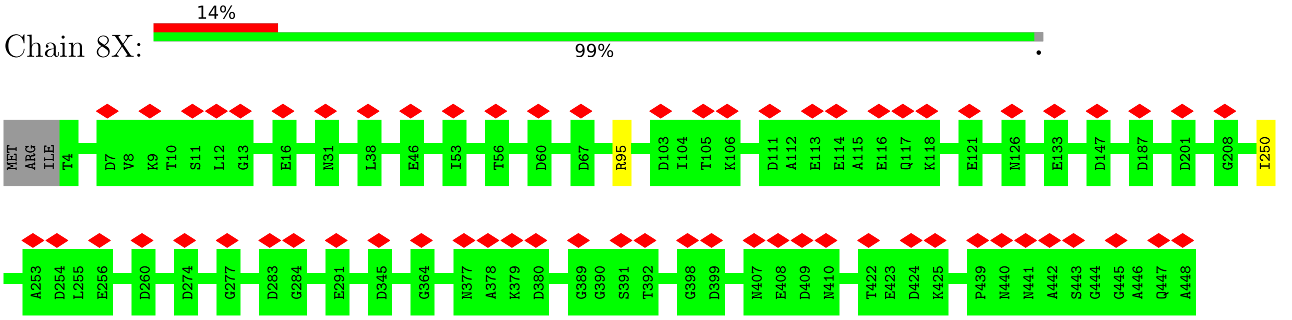
Chain 8W:





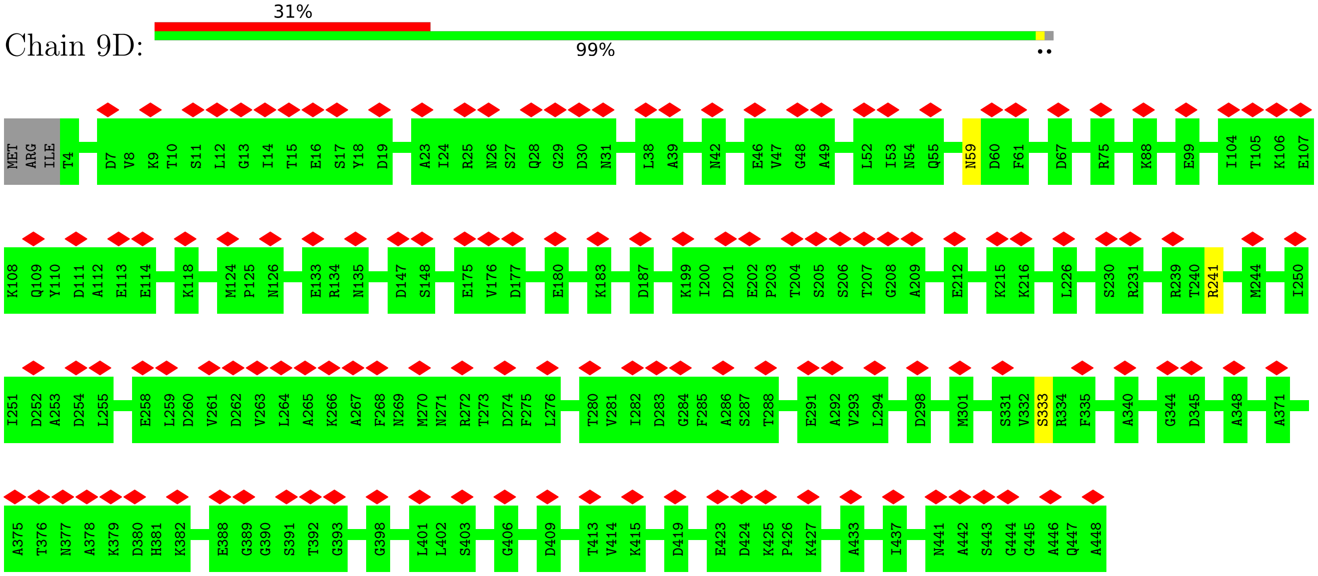
- Molecule 1: Major capsid protein

Chain 8X:



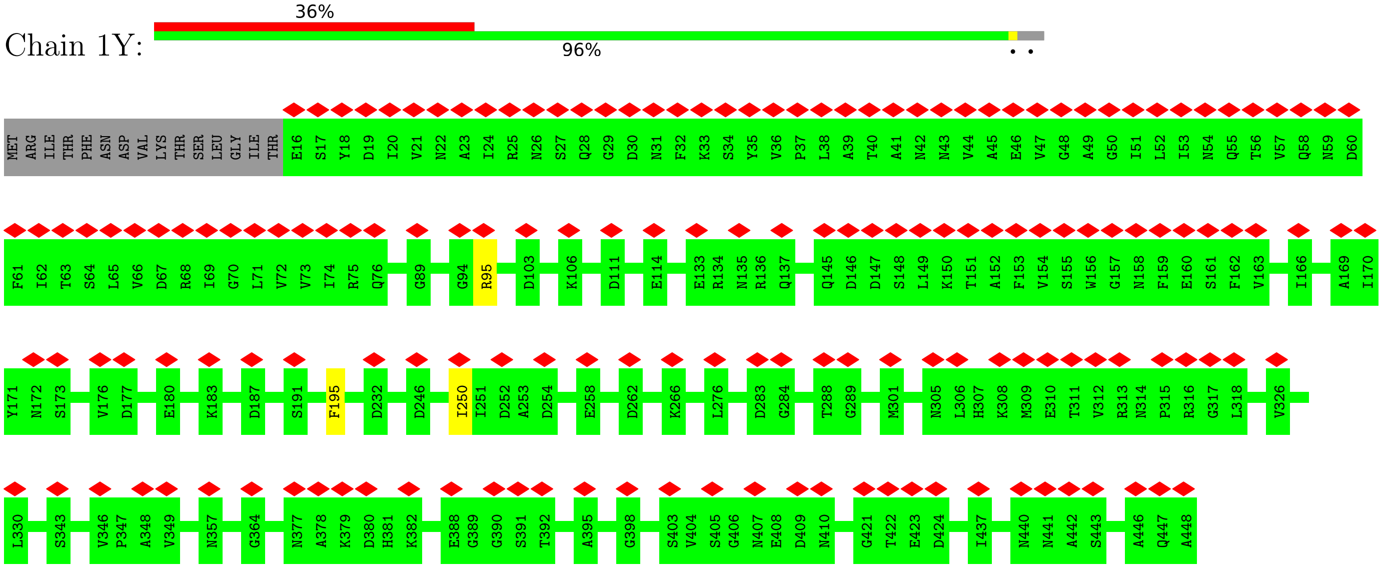
• Molecule 1: Major capsid protein

Chain 9D:



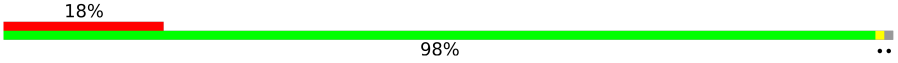
• Molecule 1: Major capsid protein

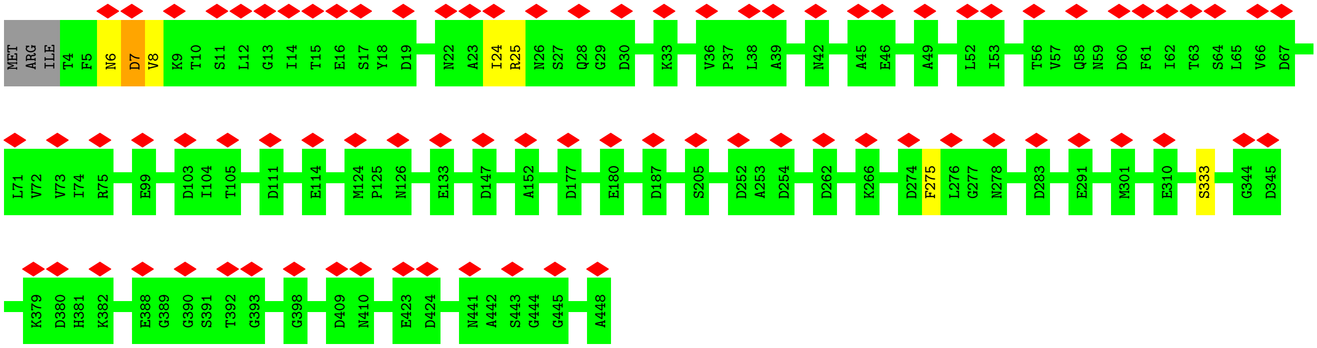
Chain 1Y:



• Molecule 1: Major capsid protein

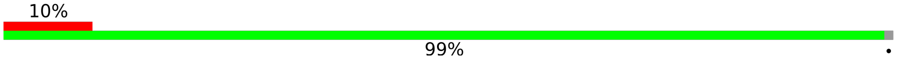
Chain 1Z:

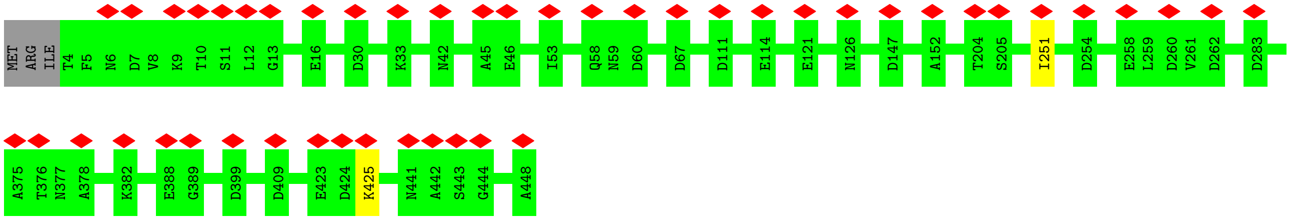




- Molecule 1: Major capsid protein

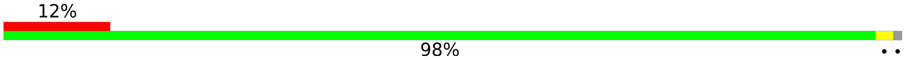
Chain 1a:

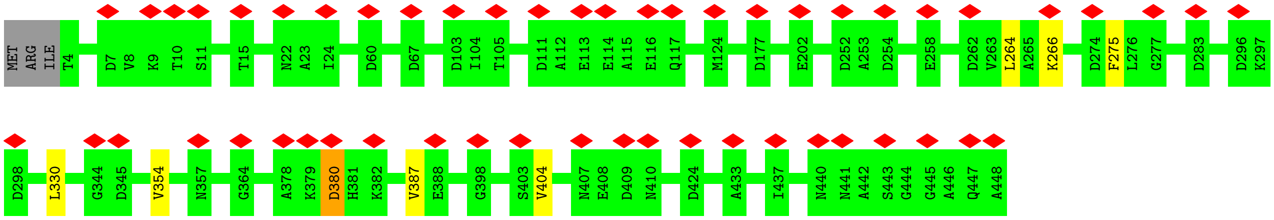




- Molecule 1: Major capsid protein

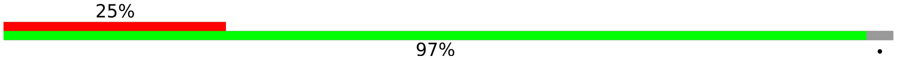
Chain 1b:

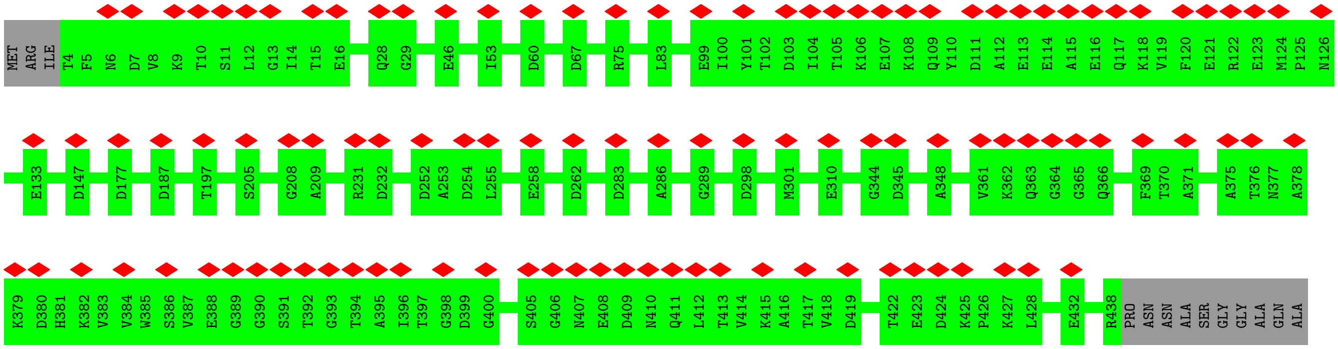




- Molecule 1: Major capsid protein

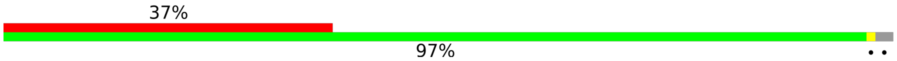
Chain 1c:

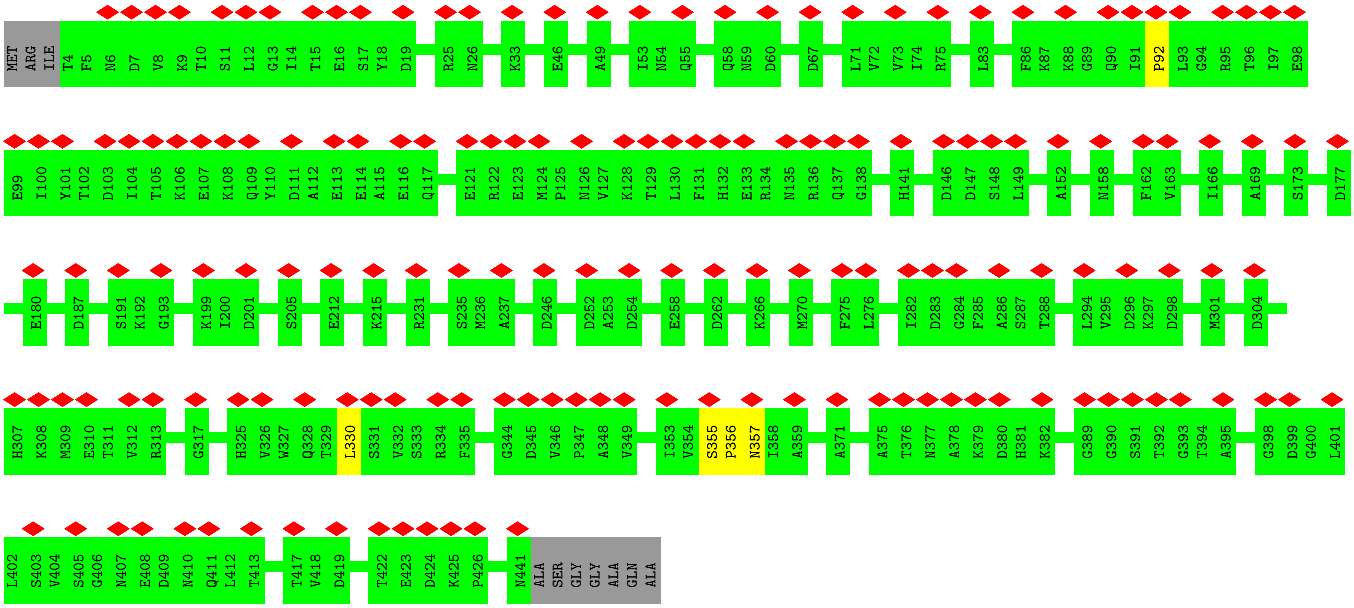




- Molecule 1: Major capsid protein

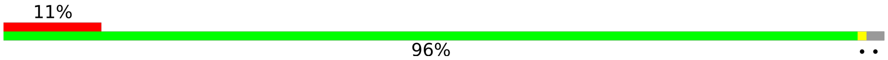
Chain 1d:

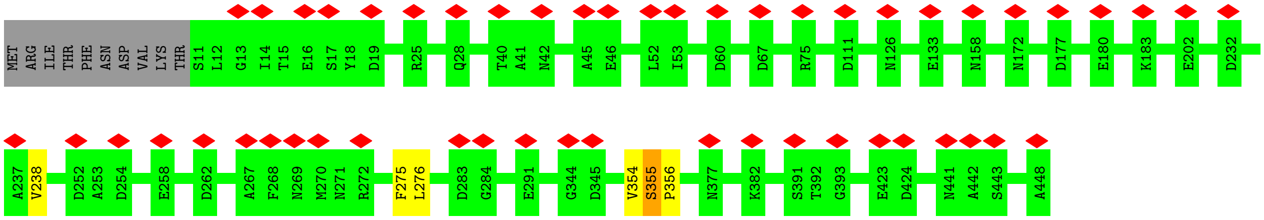




- Molecule 1: Major capsid protein

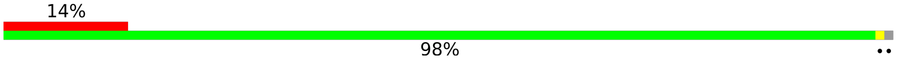
Chain 2U:

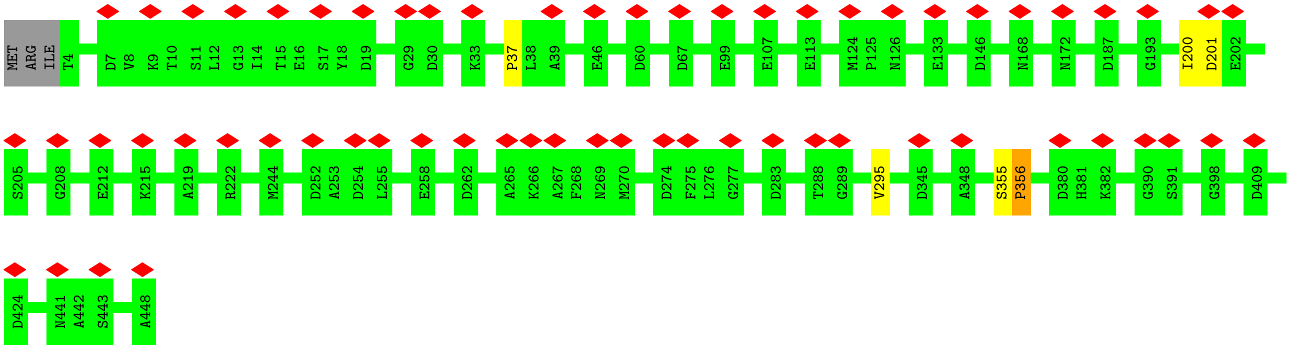




- Molecule 1: Major capsid protein

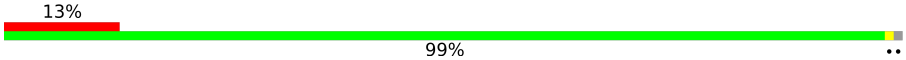
Chain 2V:

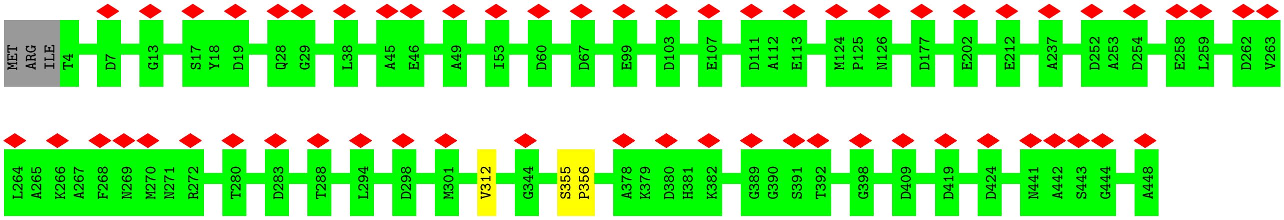




- Molecule 1: Major capsid protein

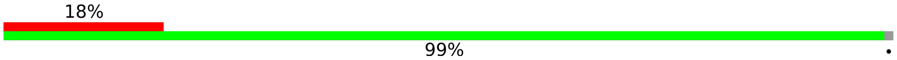
Chain 2W:

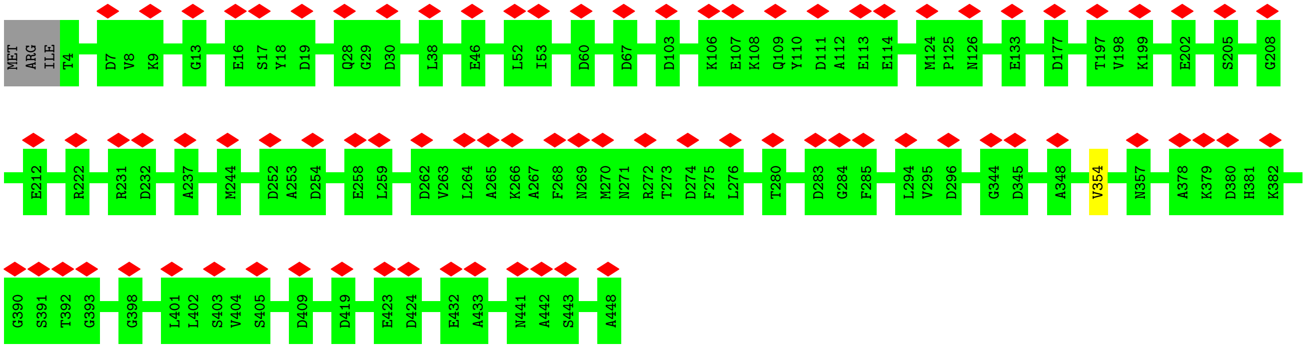




- Molecule 1: Major capsid protein

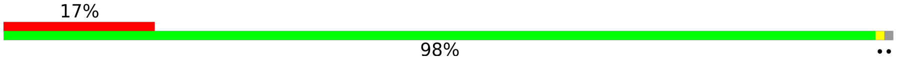
Chain 2X:

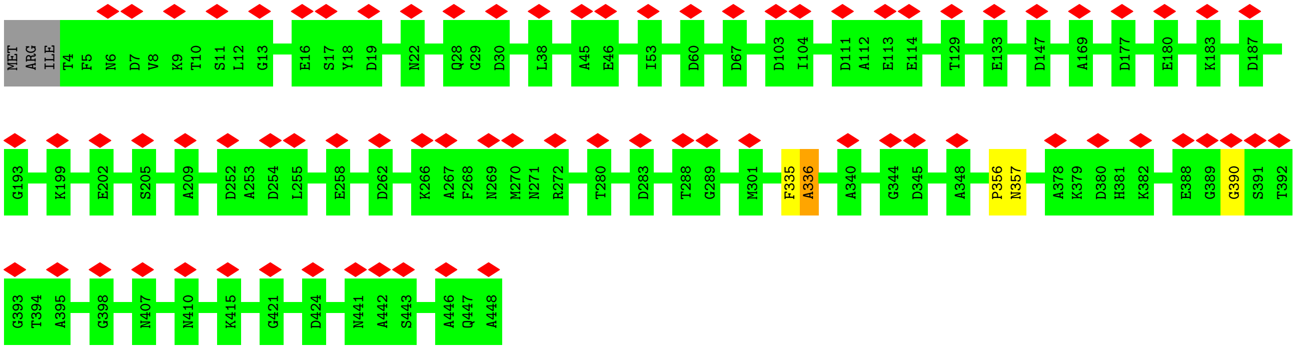




- Molecule 1: Major capsid protein

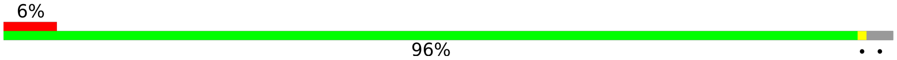
Chain 2Y:

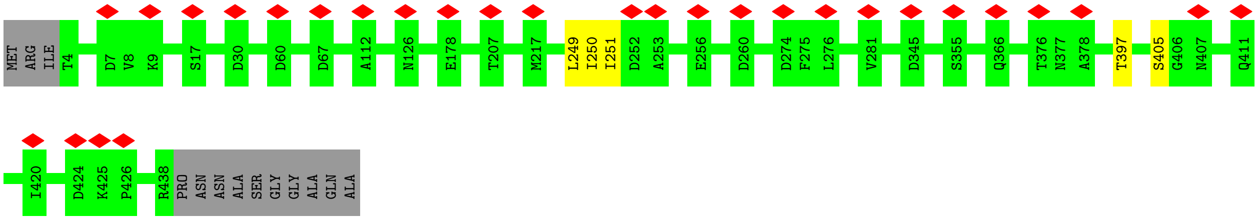




- Molecule 1: Major capsid protein

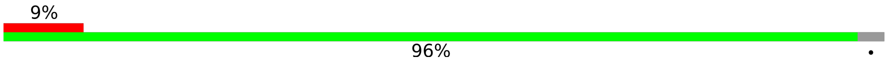
Chain 3Y:

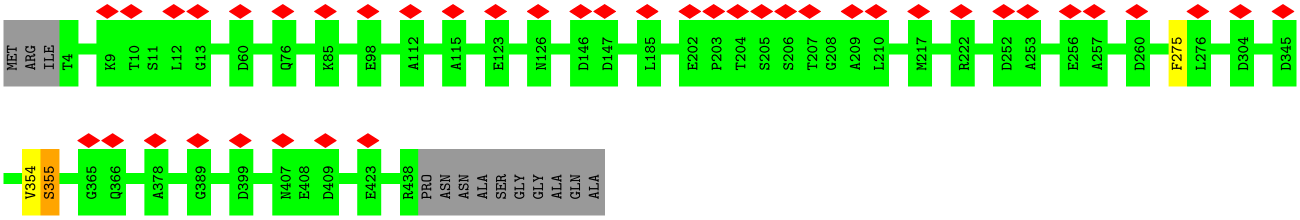




- Molecule 1: Major capsid protein

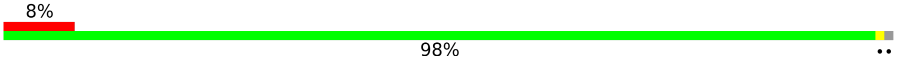
Chain 3Z:

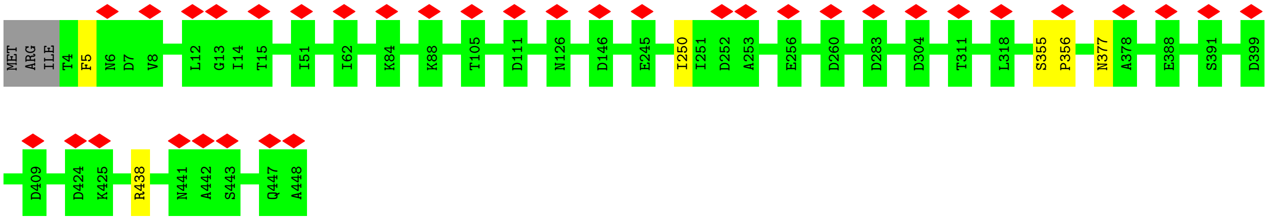




- Molecule 1: Major capsid protein

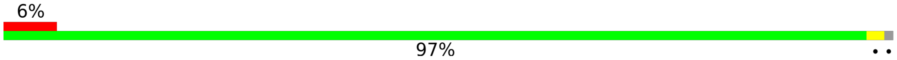
Chain 3a:

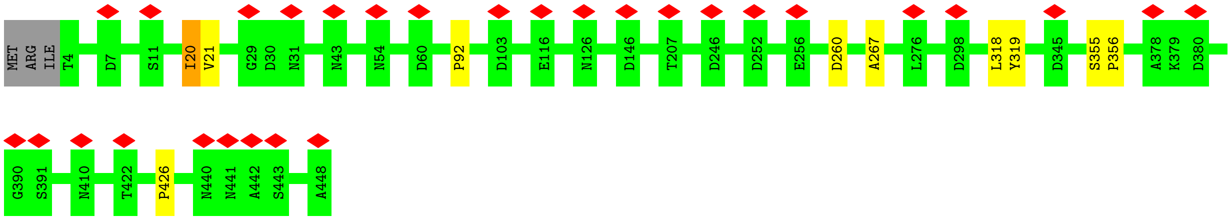




- Molecule 1: Major capsid protein

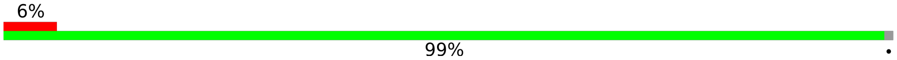
Chain 3b:

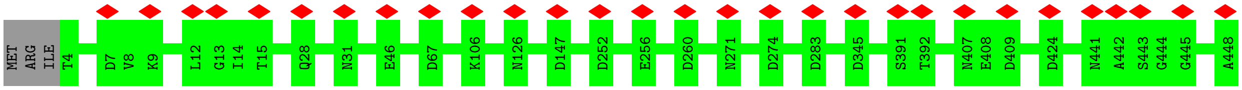




- Molecule 1: Major capsid protein

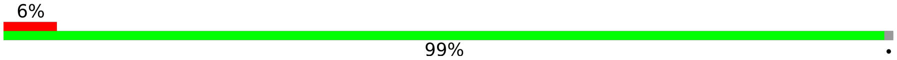
Chain 3c:

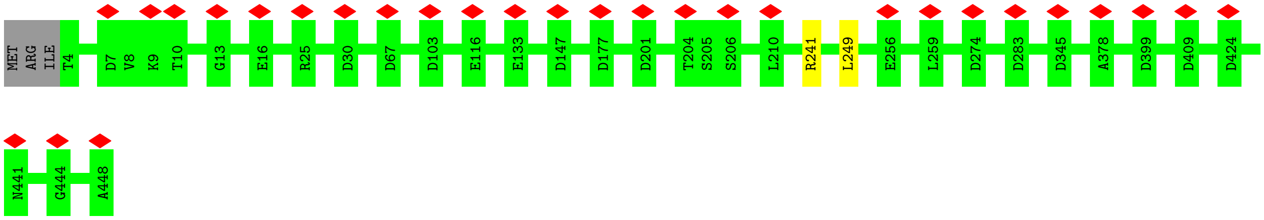




- Molecule 1: Major capsid protein

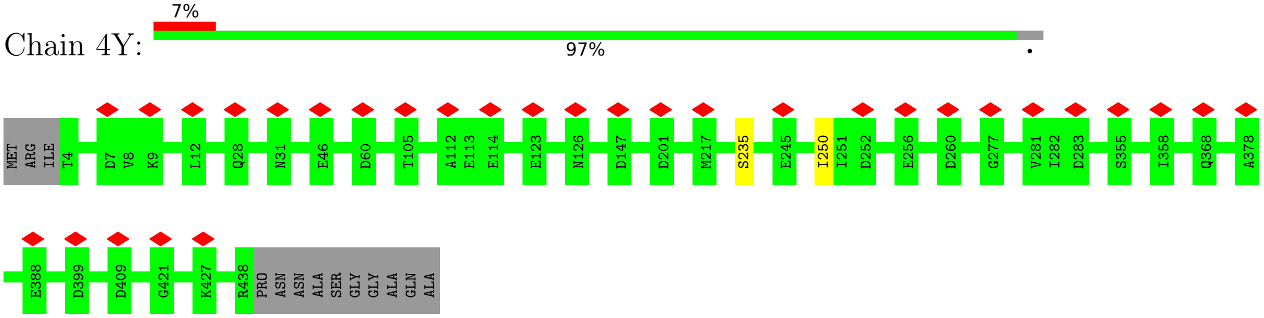
Chain 3d:





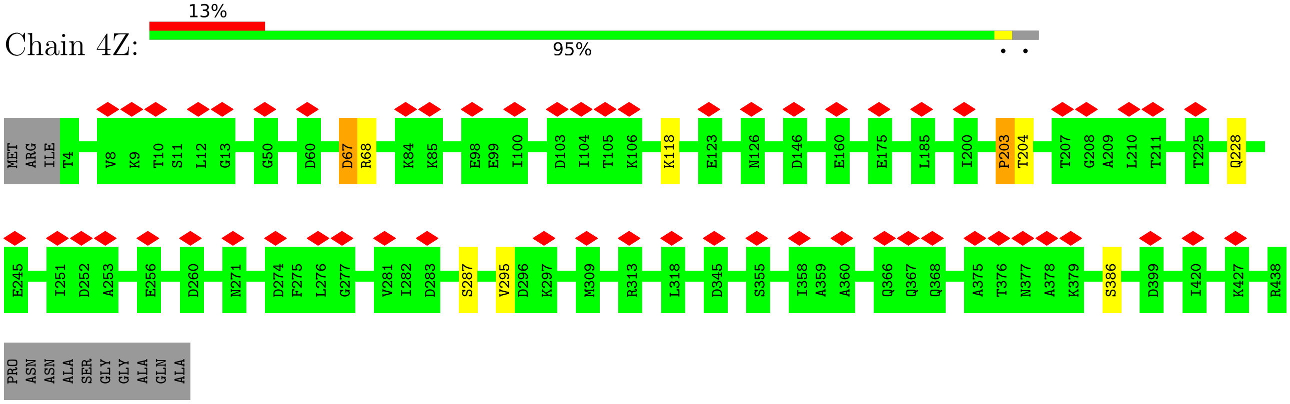
- Molecule 1: Major capsid protein

Chain 4Y:



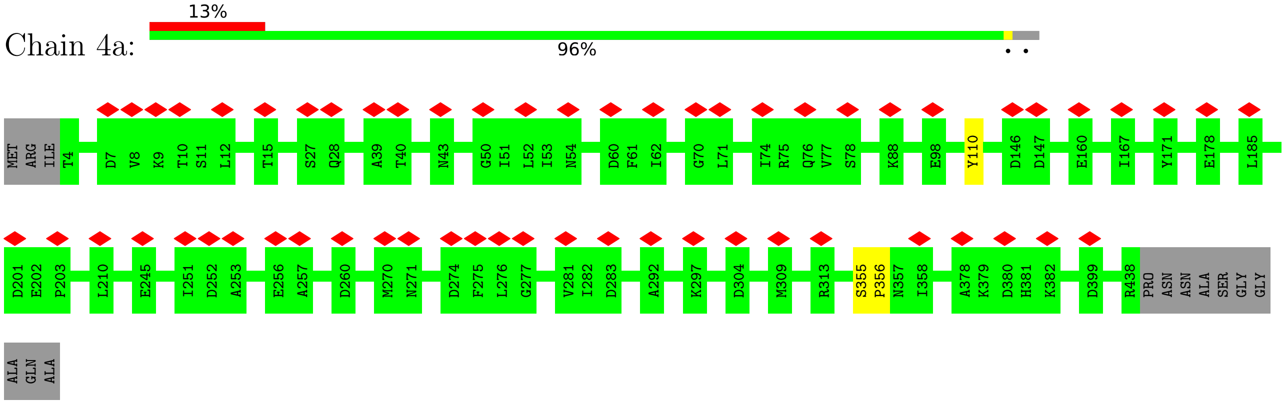
- Molecule 1: Major capsid protein

Chain 4Z:



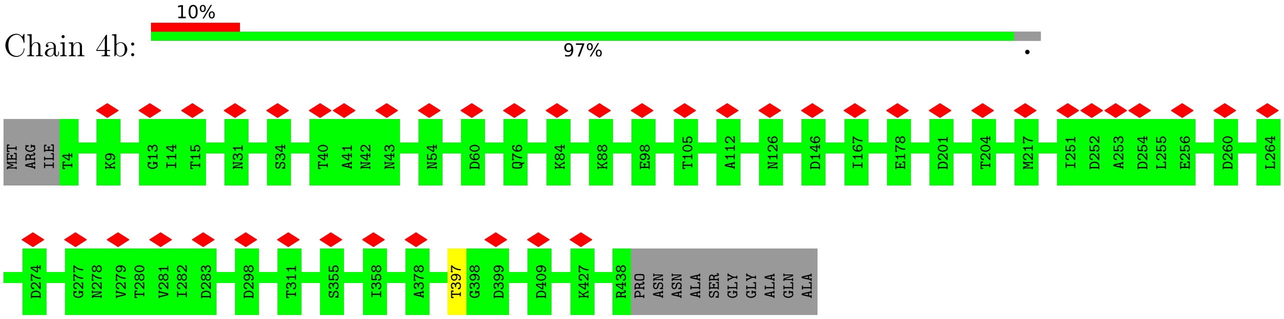
- Molecule 1: Major capsid protein

Chain 4a:



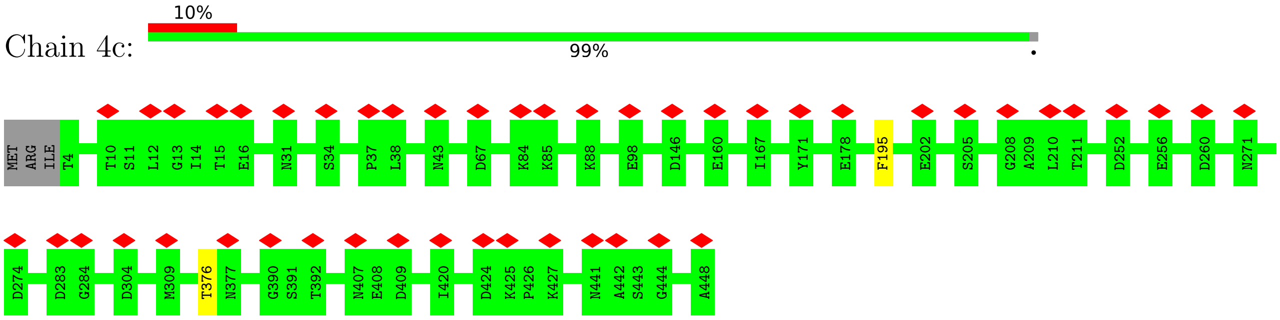
- Molecule 1: Major capsid protein

Chain 4b:



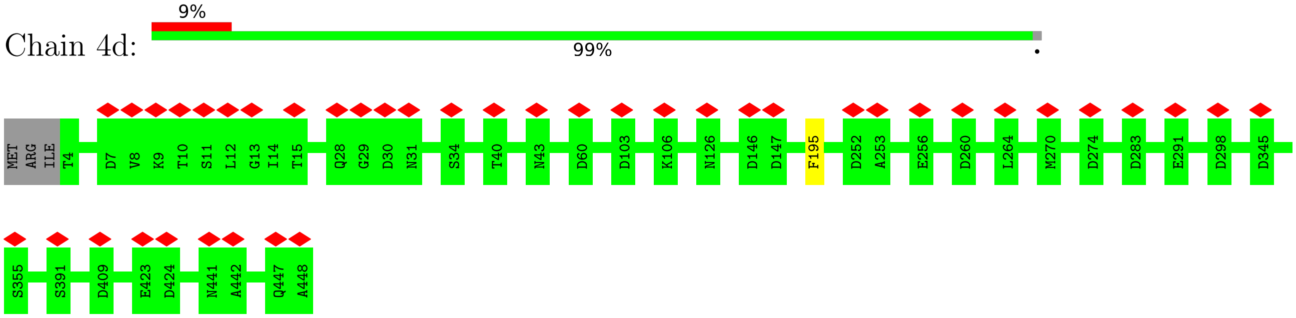
- Molecule 1: Major capsid protein

Chain 4c:



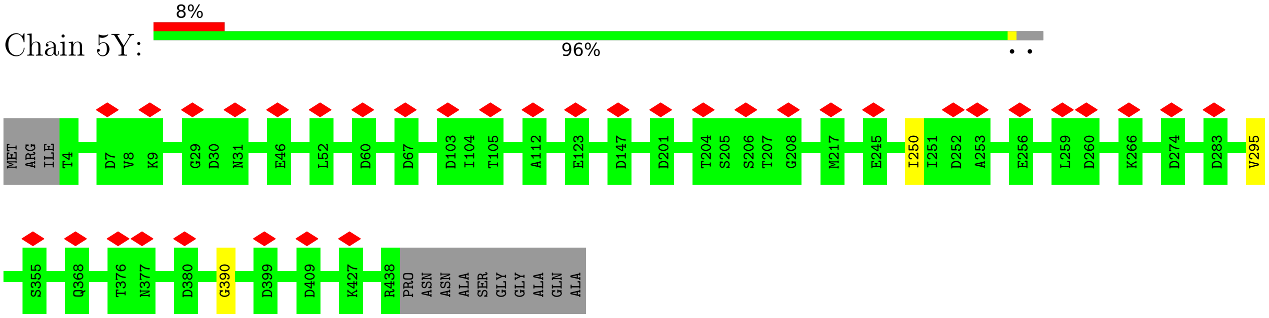
- Molecule 1: Major capsid protein

Chain 4d:



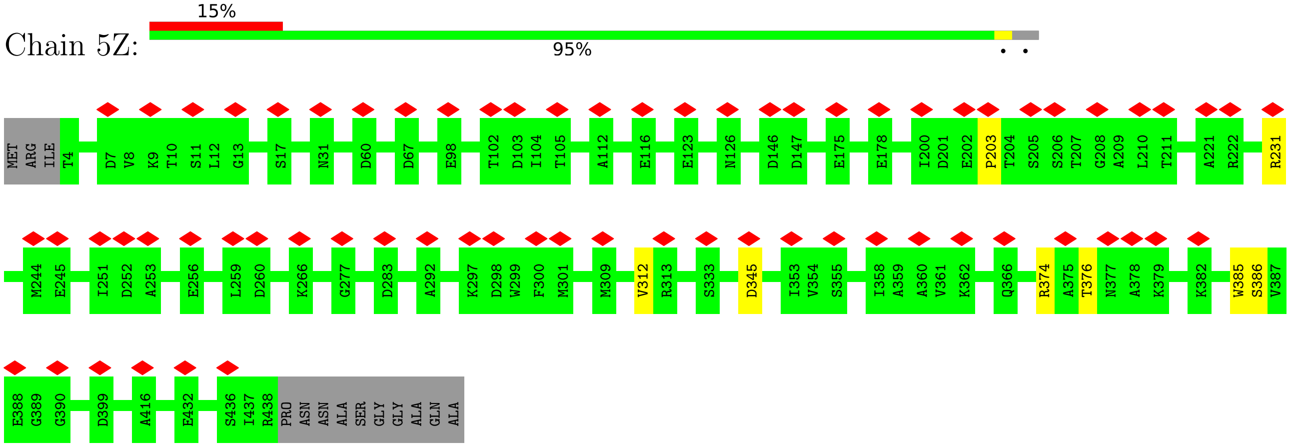
- Molecule 1: Major capsid protein

Chain 5Y:



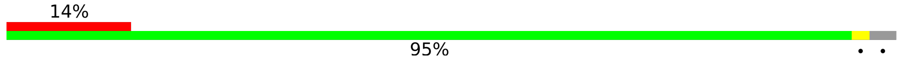
- Molecule 1: Major capsid protein

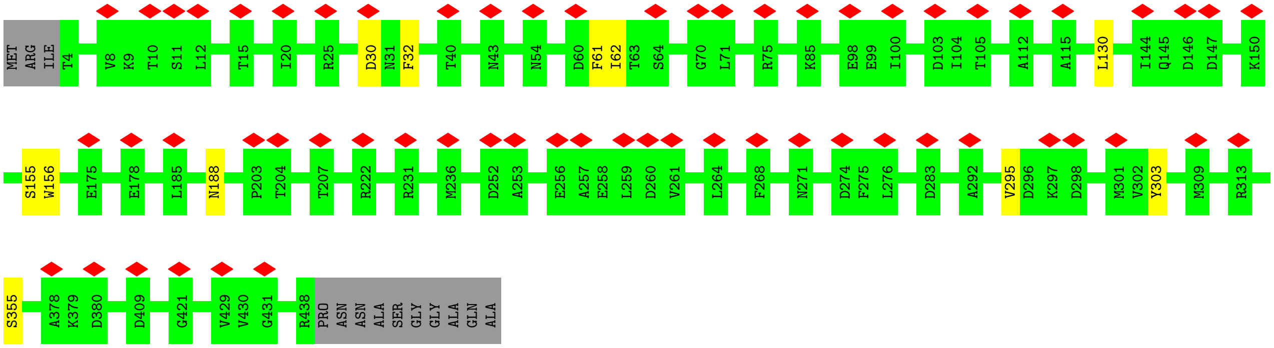
Chain 5Z:



- Molecule 1: Major capsid protein

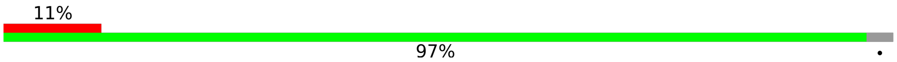
Chain 5a:

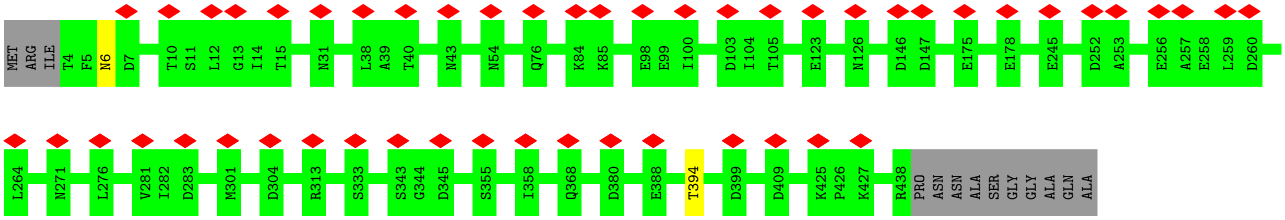




- Molecule 1: Major capsid protein

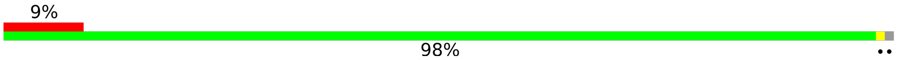
Chain 5b:

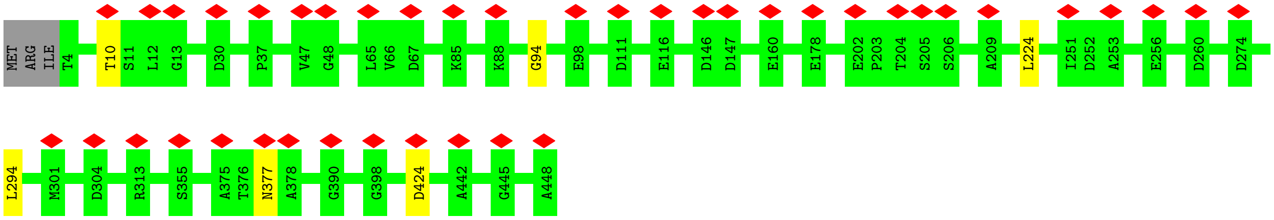




- Molecule 1: Major capsid protein

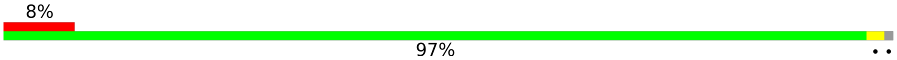
Chain 5c:

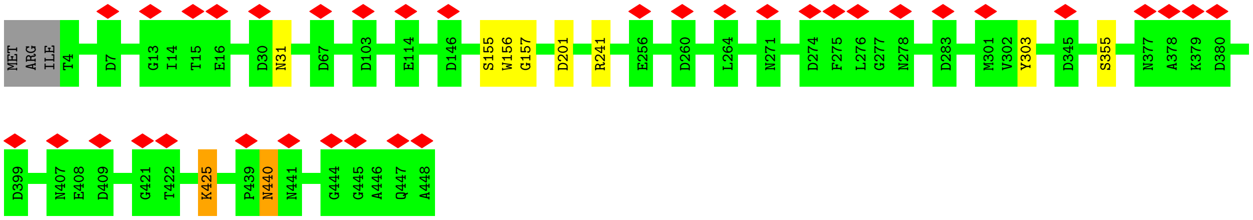




- Molecule 1: Major capsid protein

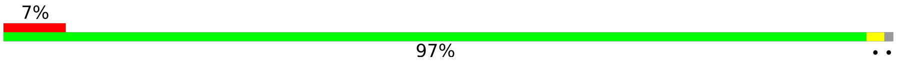
Chain 5d:

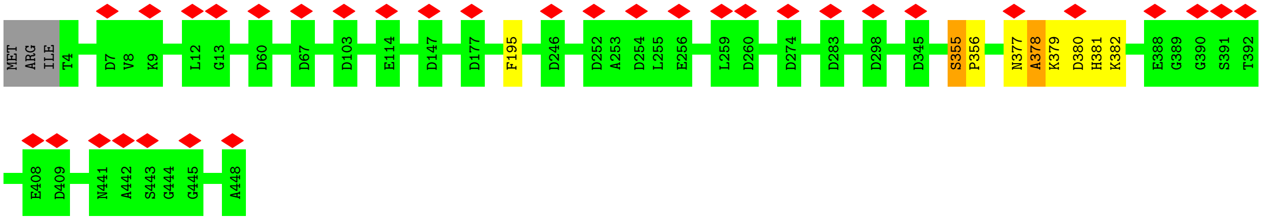




- Molecule 1: Major capsid protein

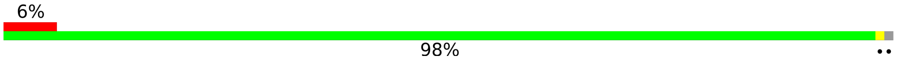
Chain 6Y:

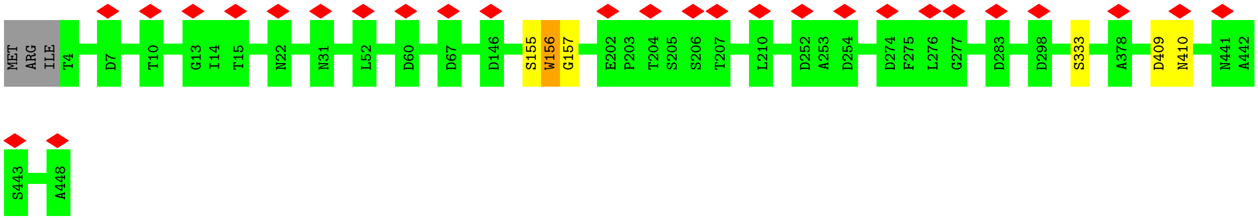




- Molecule 1: Major capsid protein

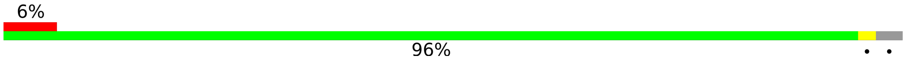
Chain 6Z:

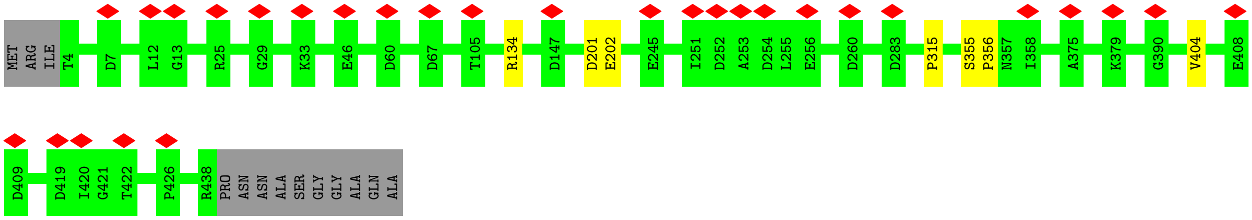




- Molecule 1: Major capsid protein

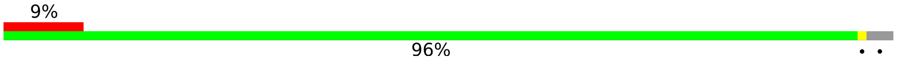
Chain 6a:

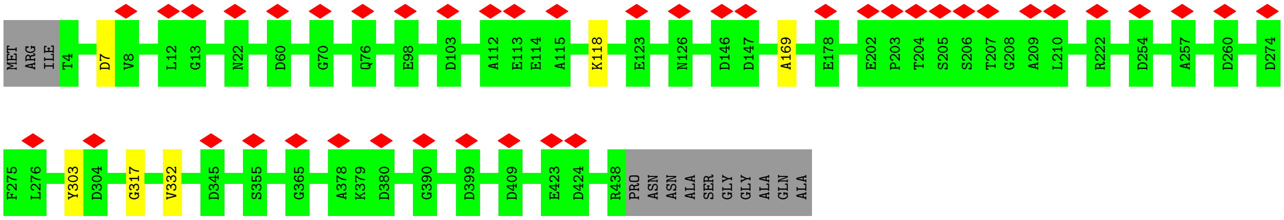




- Molecule 1: Major capsid protein

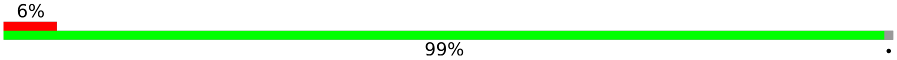
Chain 6b:

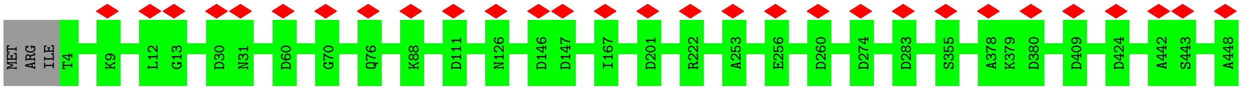




- Molecule 1: Major capsid protein

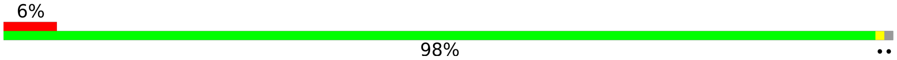
Chain 6c:

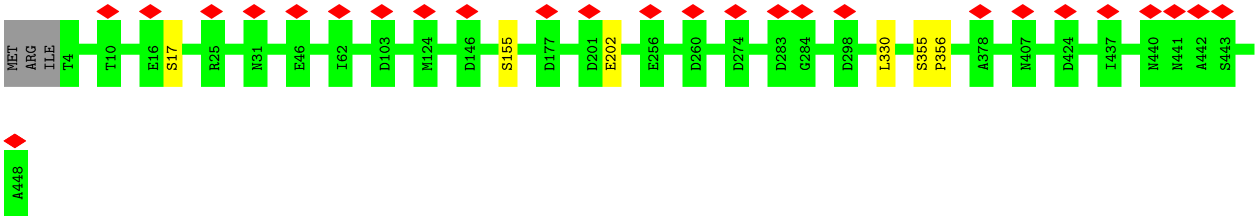




- Molecule 1: Major capsid protein

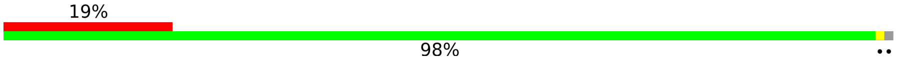
Chain 6d:

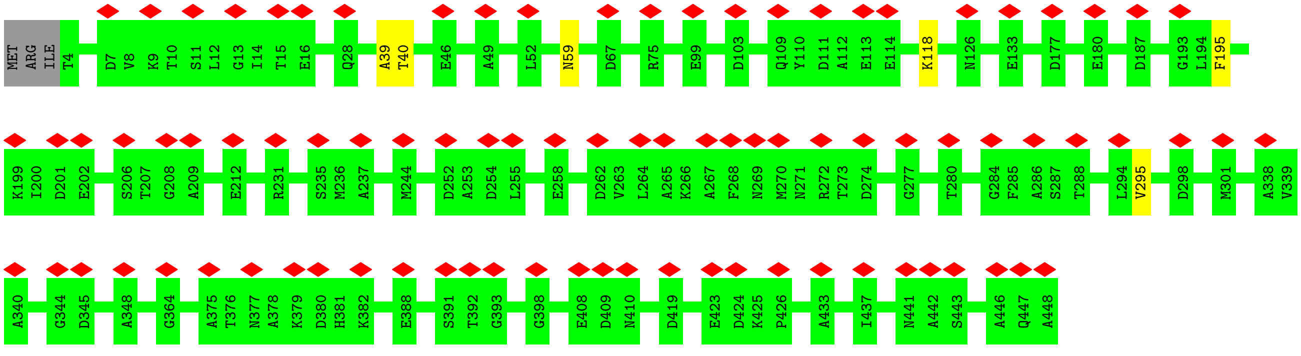




• Molecule 1: Major capsid protein

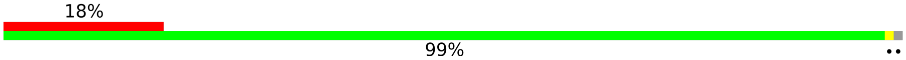
Chain 7U:

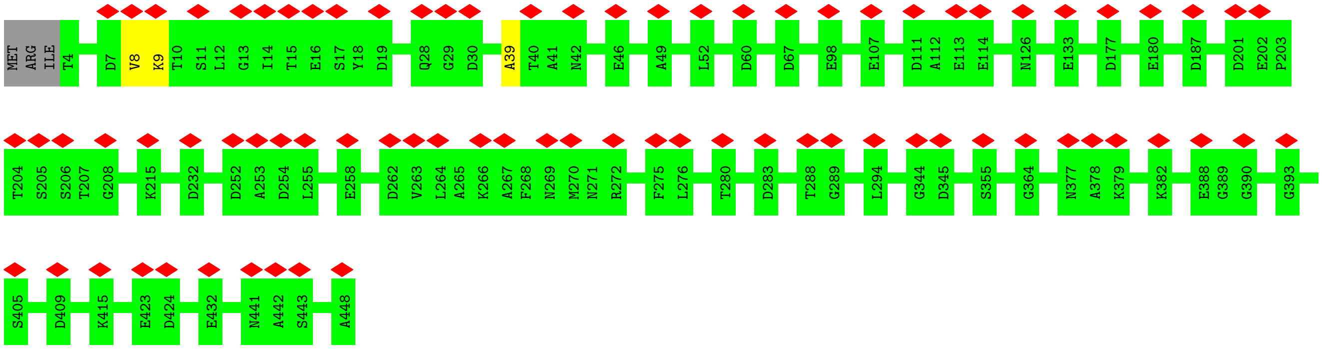




• Molecule 1: Major capsid protein

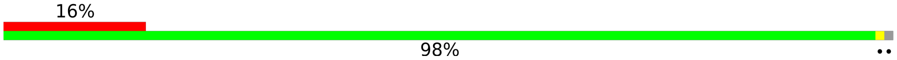
Chain 7V:

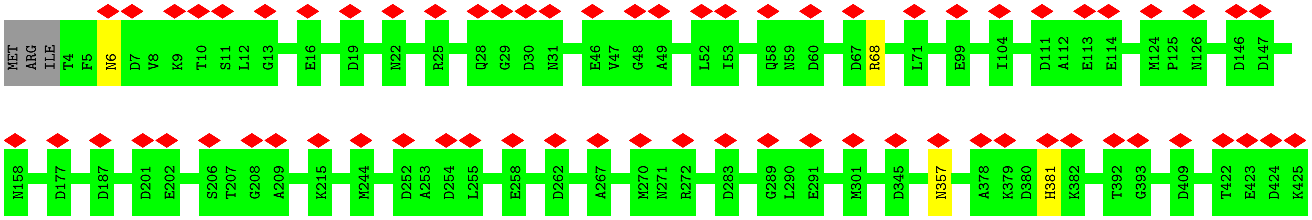


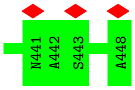


• Molecule 1: Major capsid protein

Chain 7W:

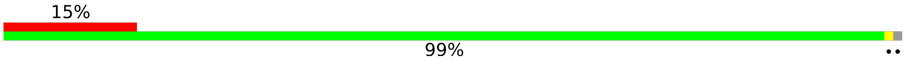


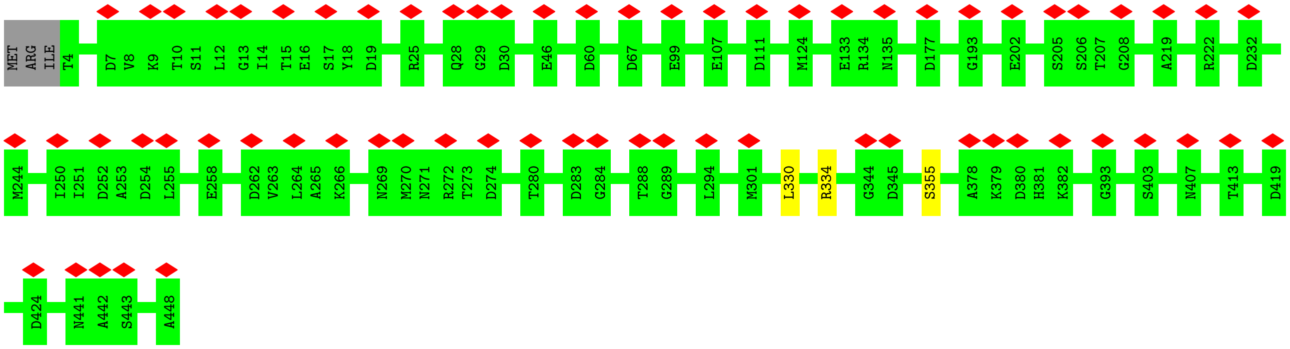




- Molecule 1: Major capsid protein

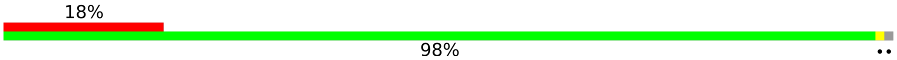
Chain 7X:

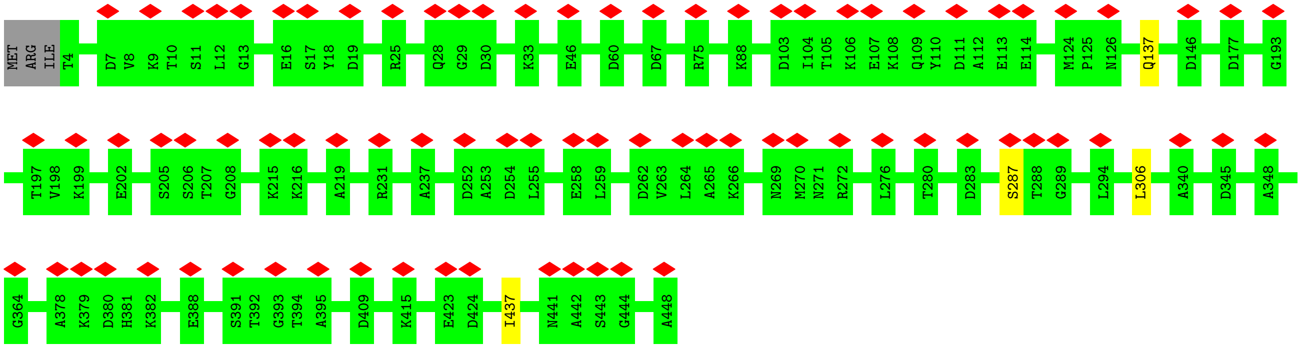




- Molecule 1: Major capsid protein

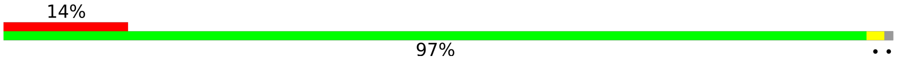
Chain 7Y:

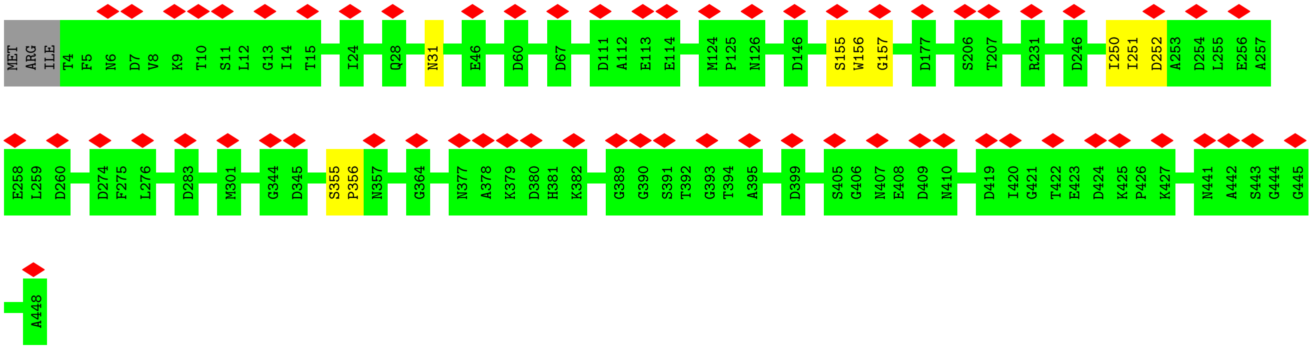




- Molecule 1: Major capsid protein

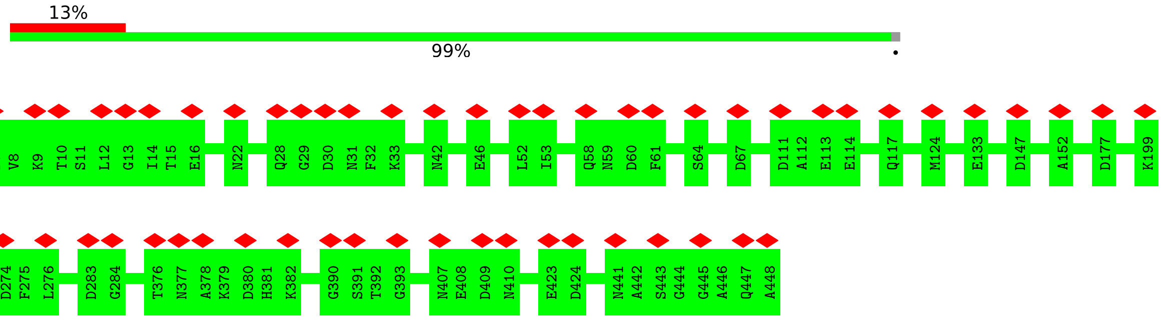
Chain 8Y:





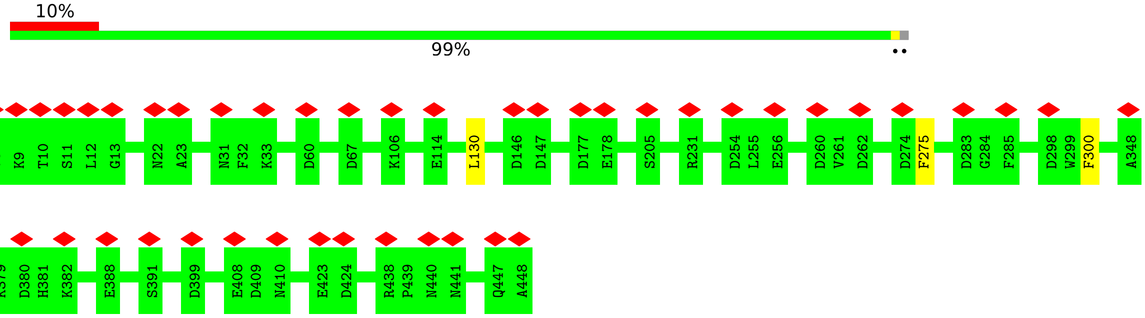
- Molecule 1: Major capsid protein

Chain 8Z:



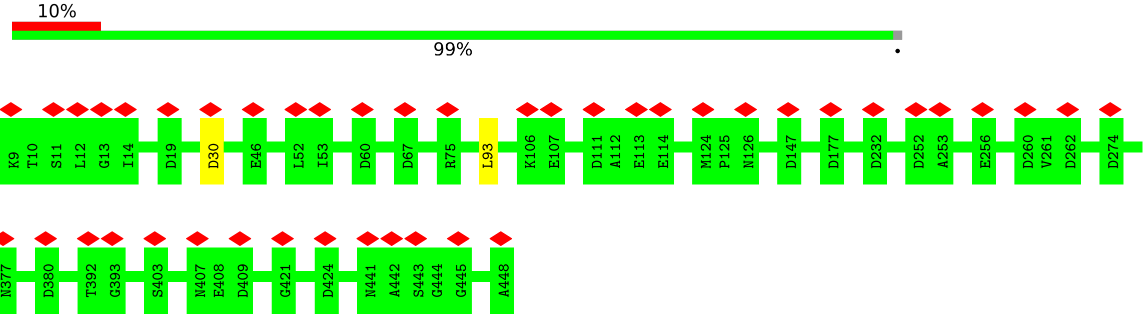
• Molecule 1: Major capsid protein

Chain 8a:



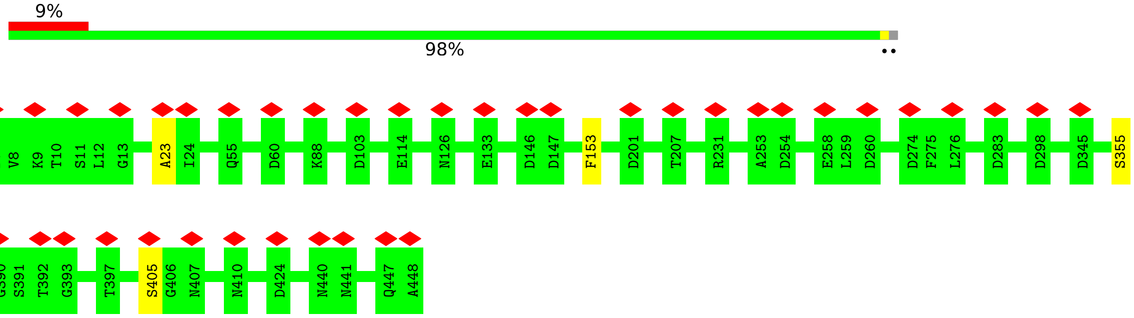
• Molecule 1: Major capsid protein

Chain 8b:



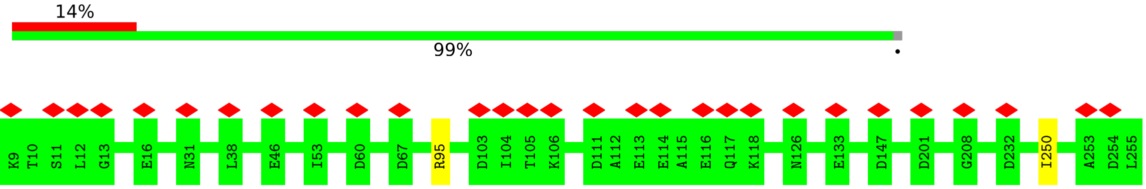
• Molecule 1: Major capsid protein

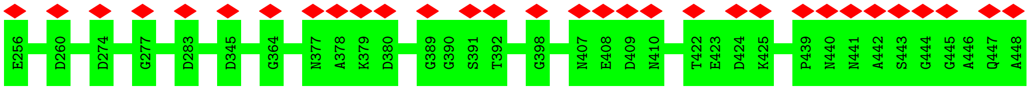
Chain 8c:



• Molecule 1: Major capsid protein

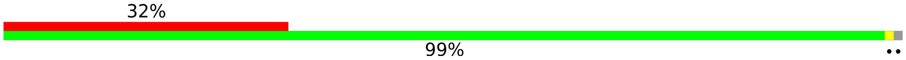
Chain 8d:

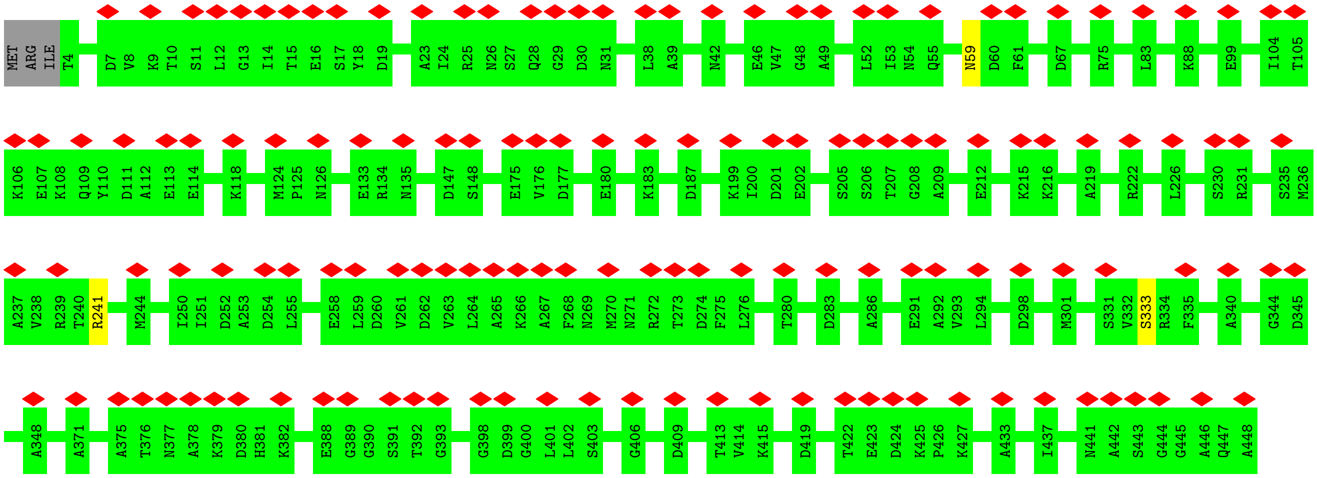




- Molecule 1: Major capsid protein

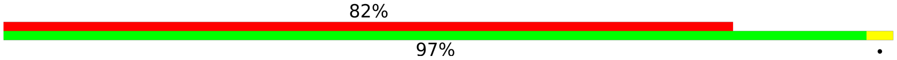
Chain 9E:

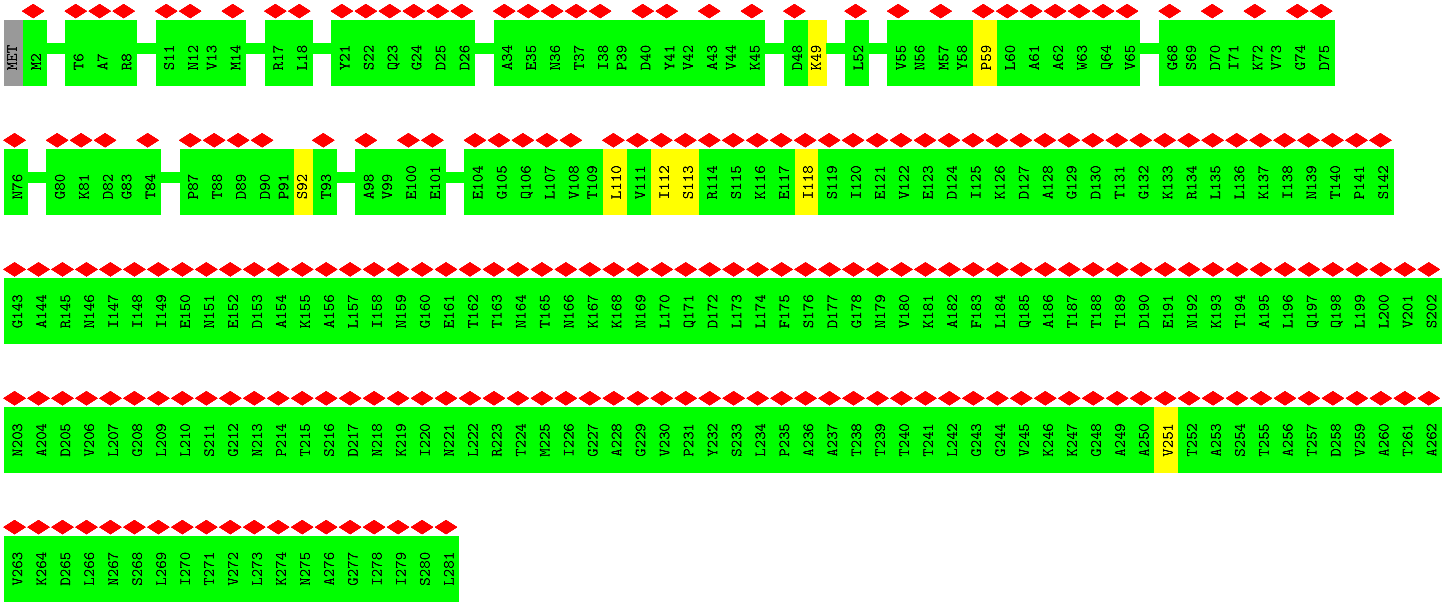




- Molecule 2: Capsid fiber protein

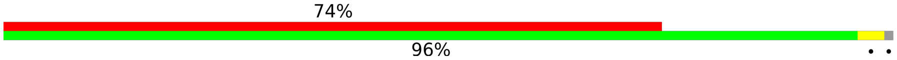
Chain 1e:

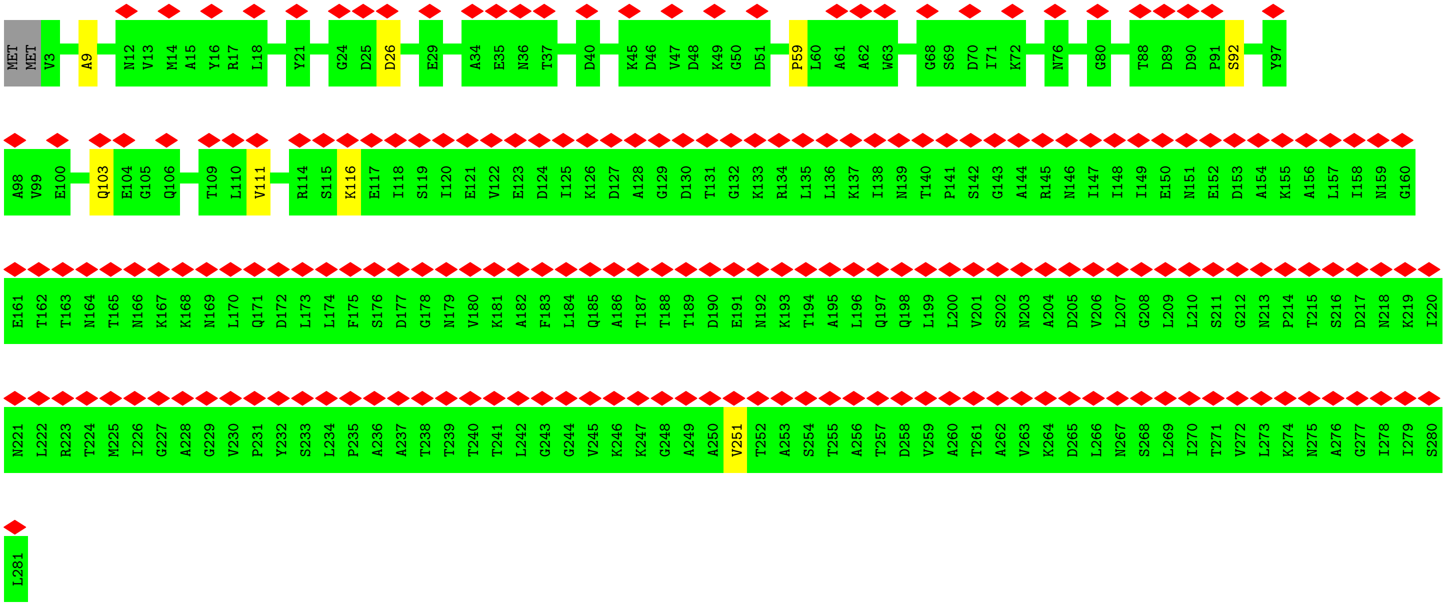




- Molecule 2: Capsid fiber protein

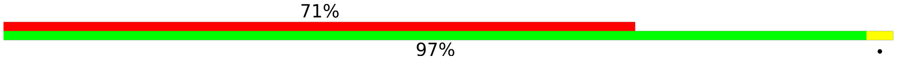
Chain 1f:

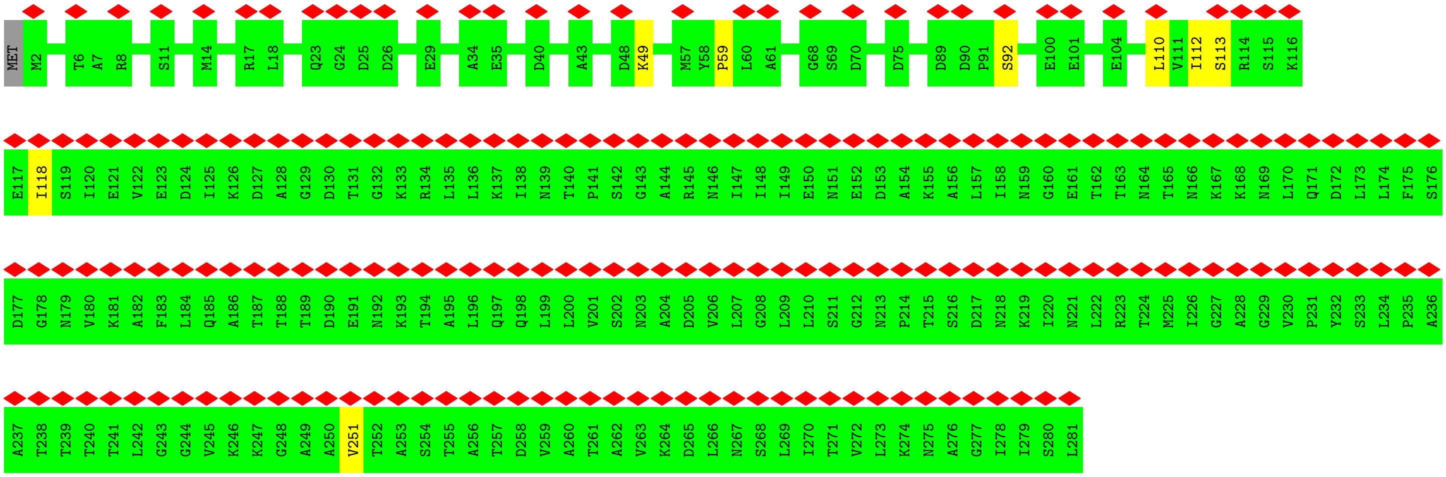




- Molecule 2: Capsid fiber protein

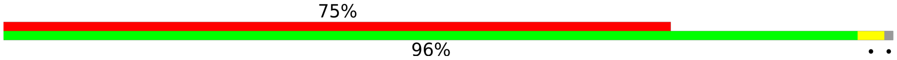
Chain 1g:

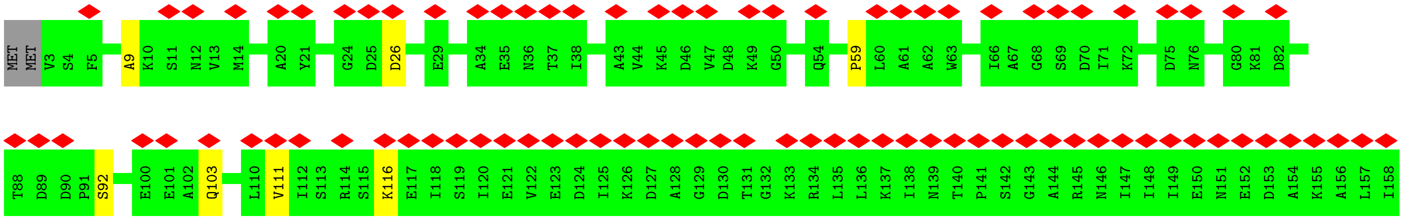


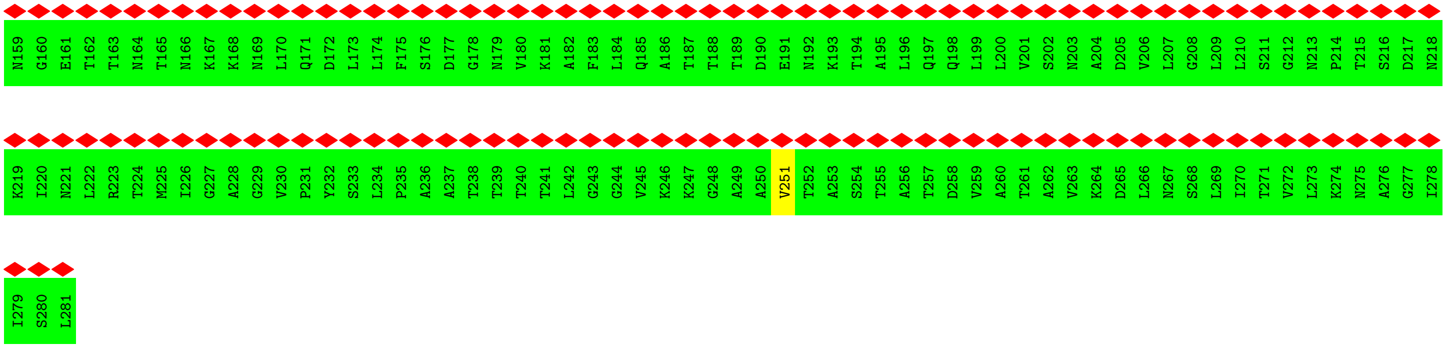


- Molecule 2: Capsid fiber protein

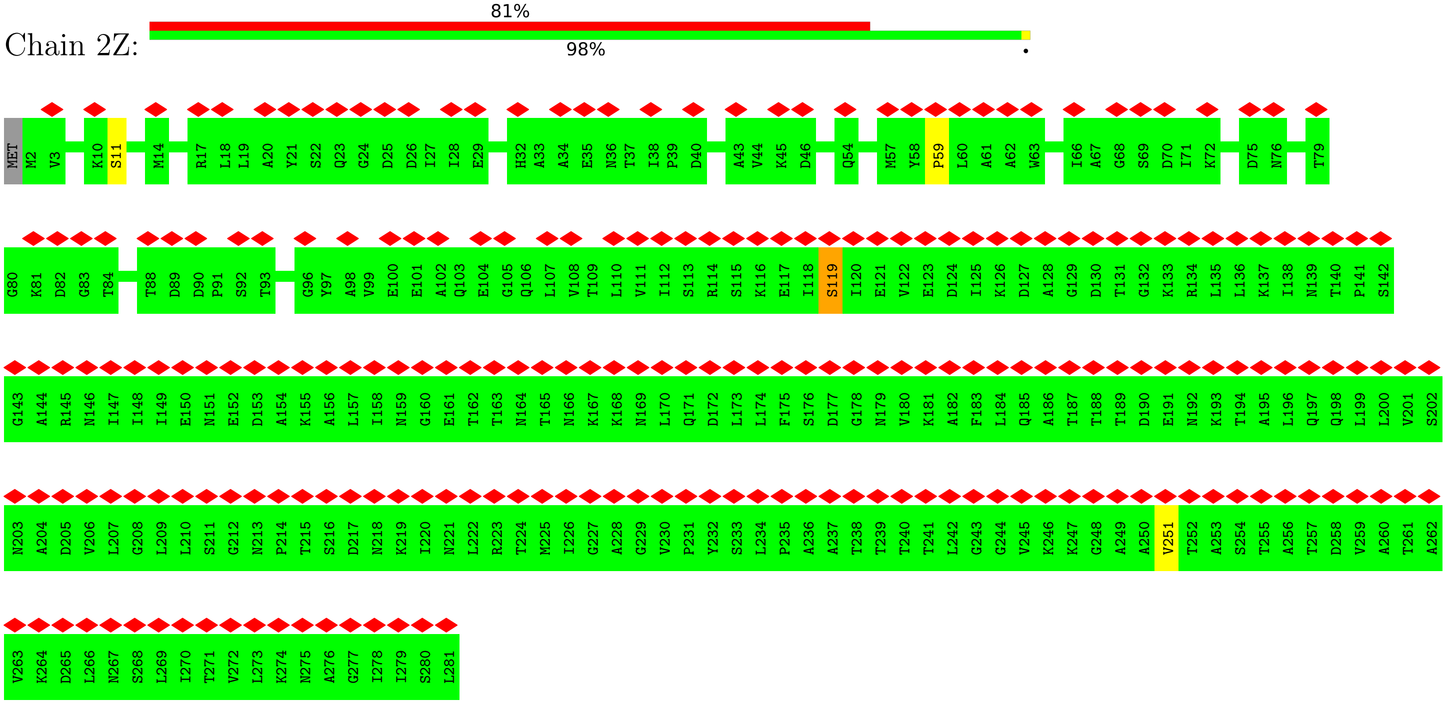
Chain 1h:



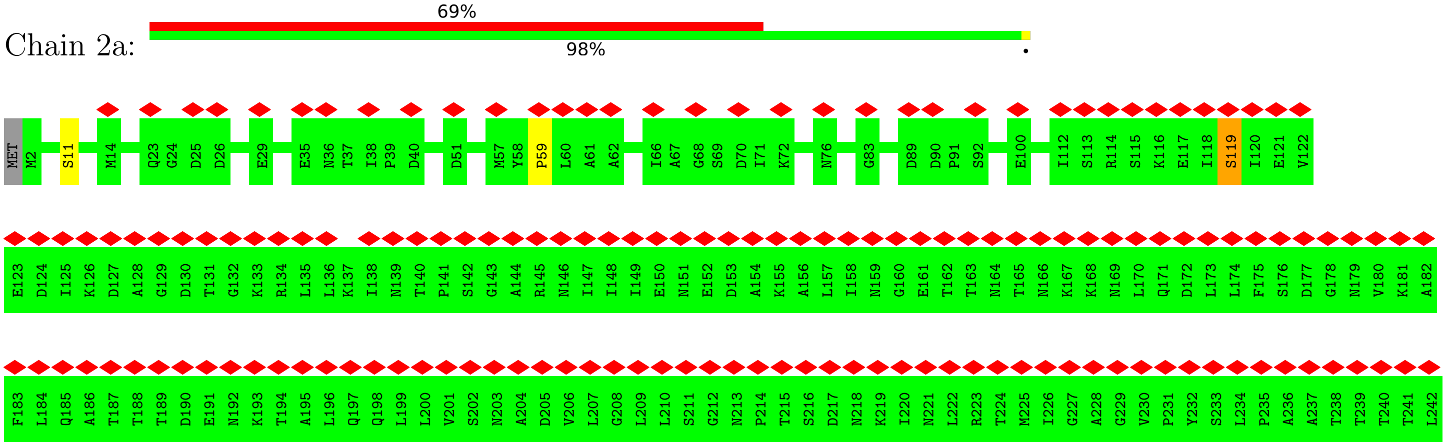


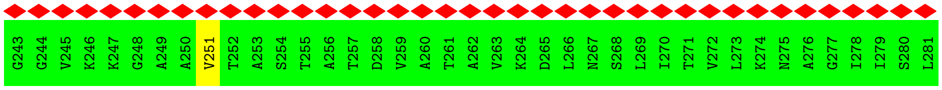


- Molecule 2: Capsid fiber protein



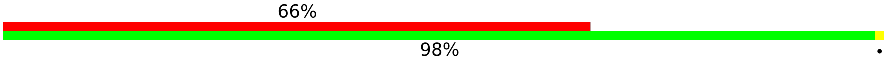
- Molecule 2: Capsid fiber protein

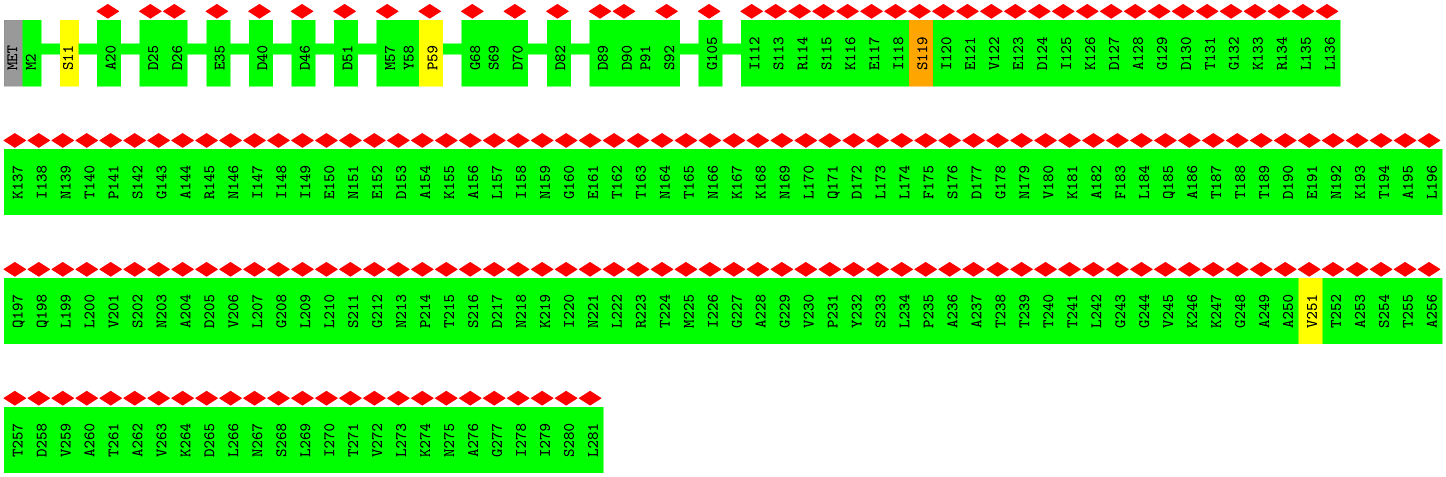




- Molecule 2: Capsid fiber protein

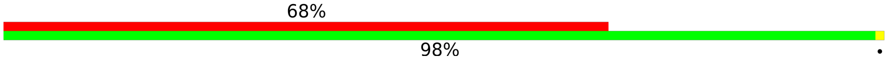
Chain 2b:

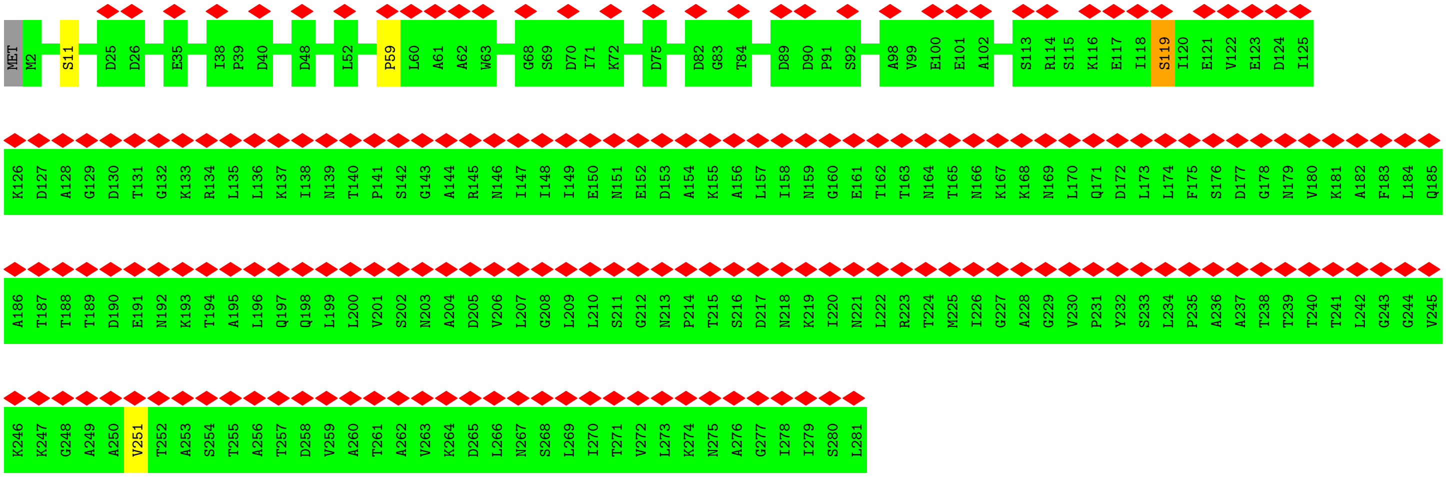




- Molecule 2: Capsid fiber protein

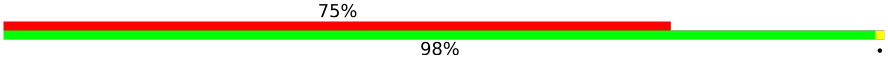
Chain 2c:

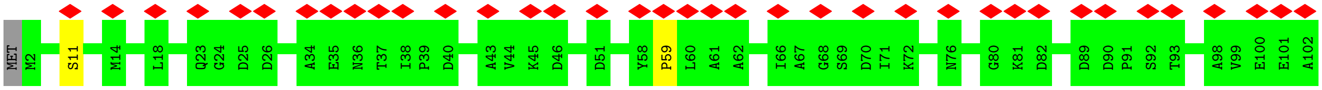


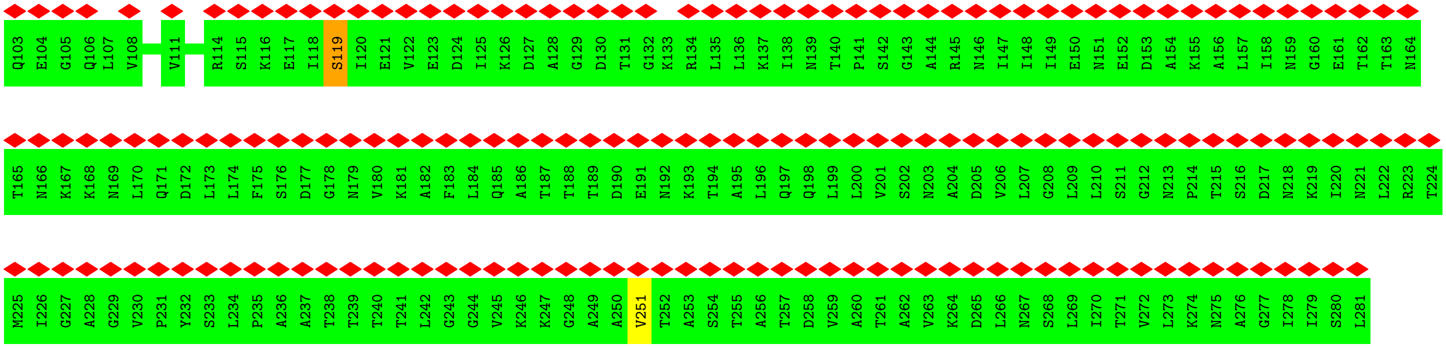


- Molecule 2: Capsid fiber protein

Chain 2d:

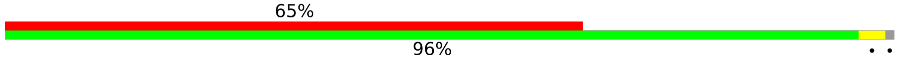


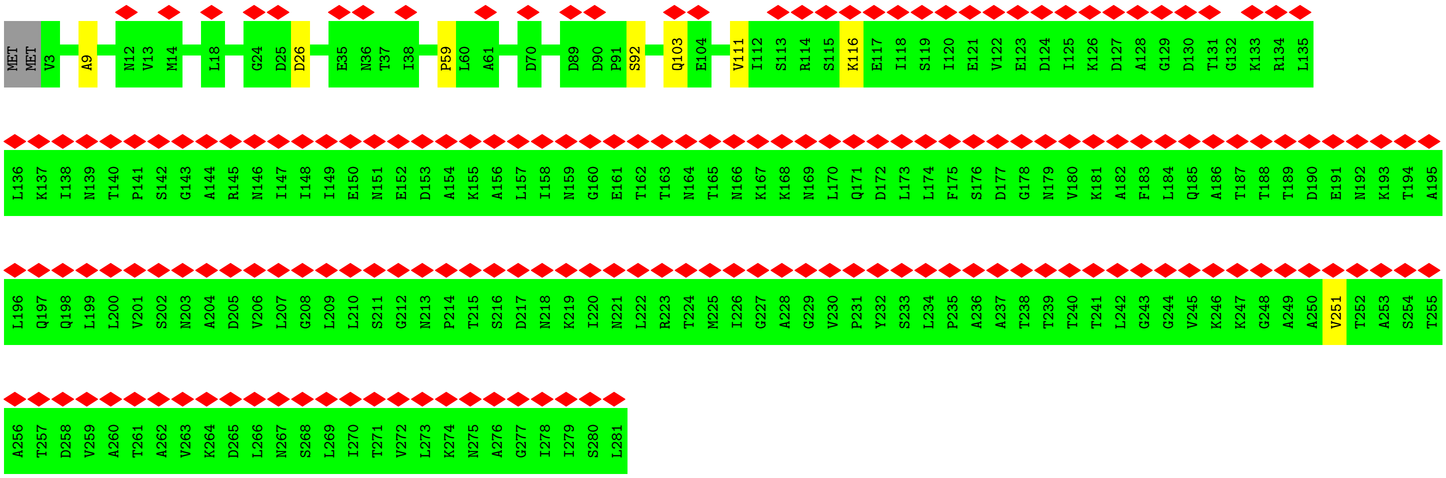




- Molecule 2: Capsid fiber protein

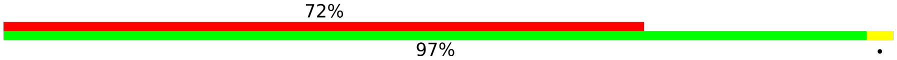
Chain 3e:

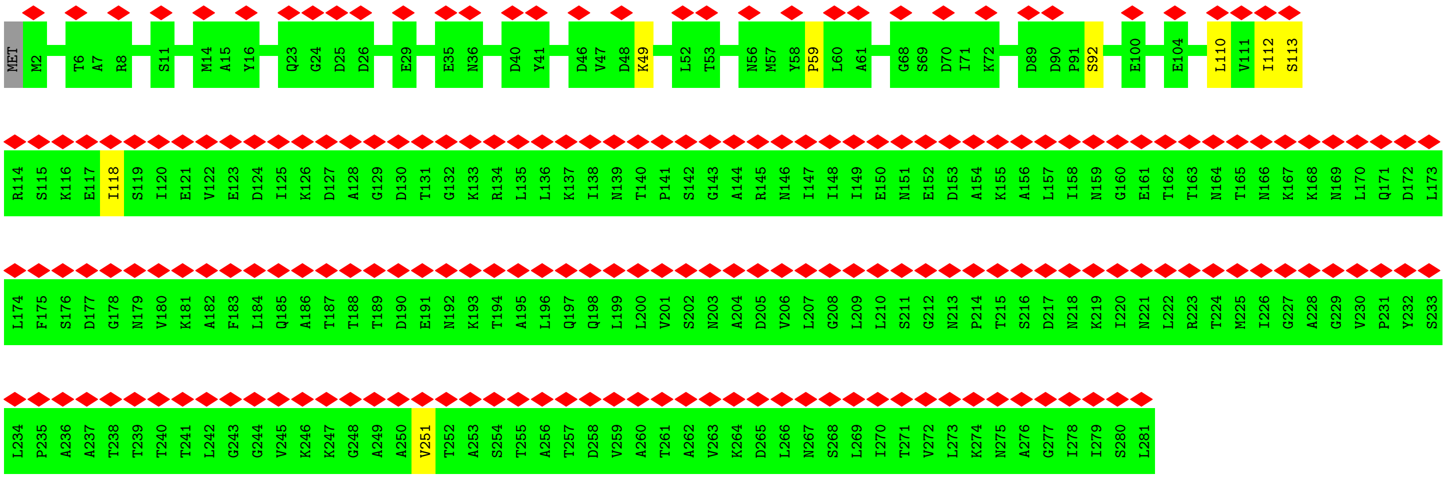




- Molecule 2: Capsid fiber protein

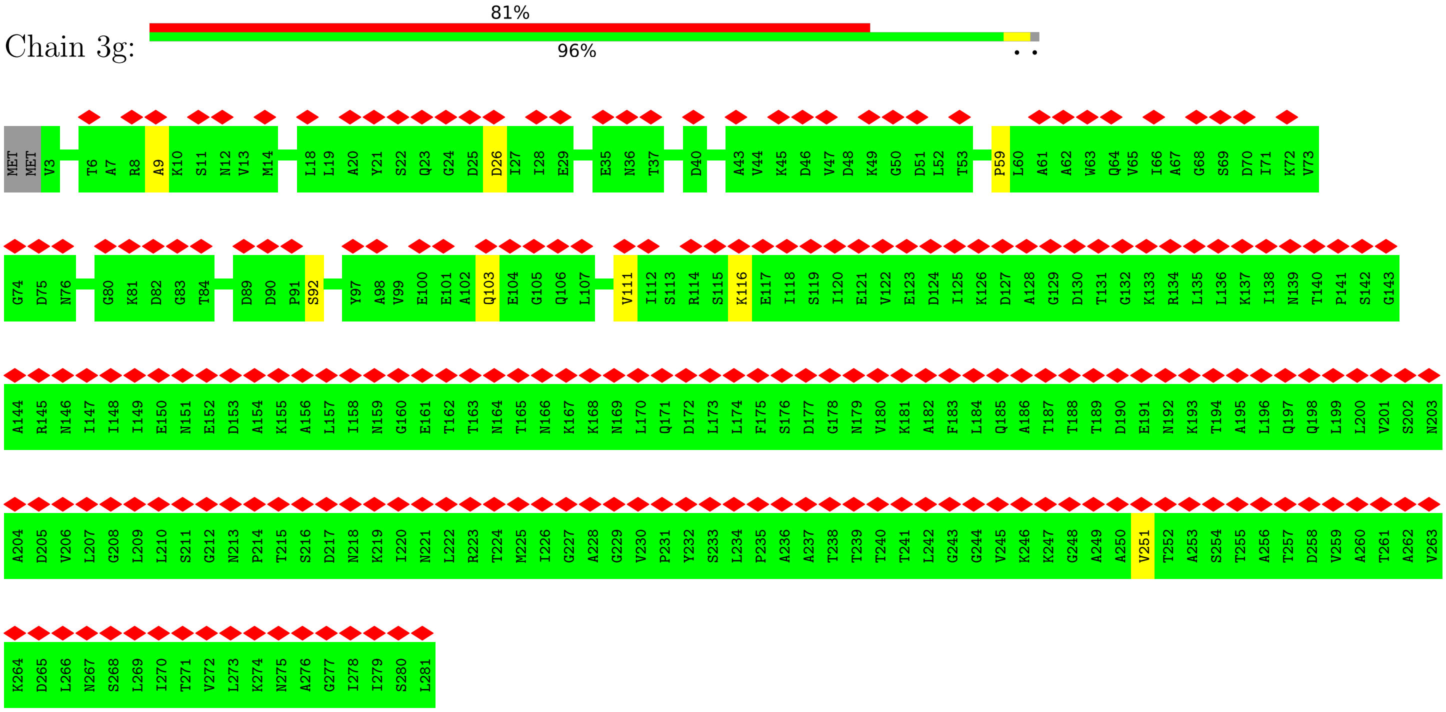
Chain 3f:





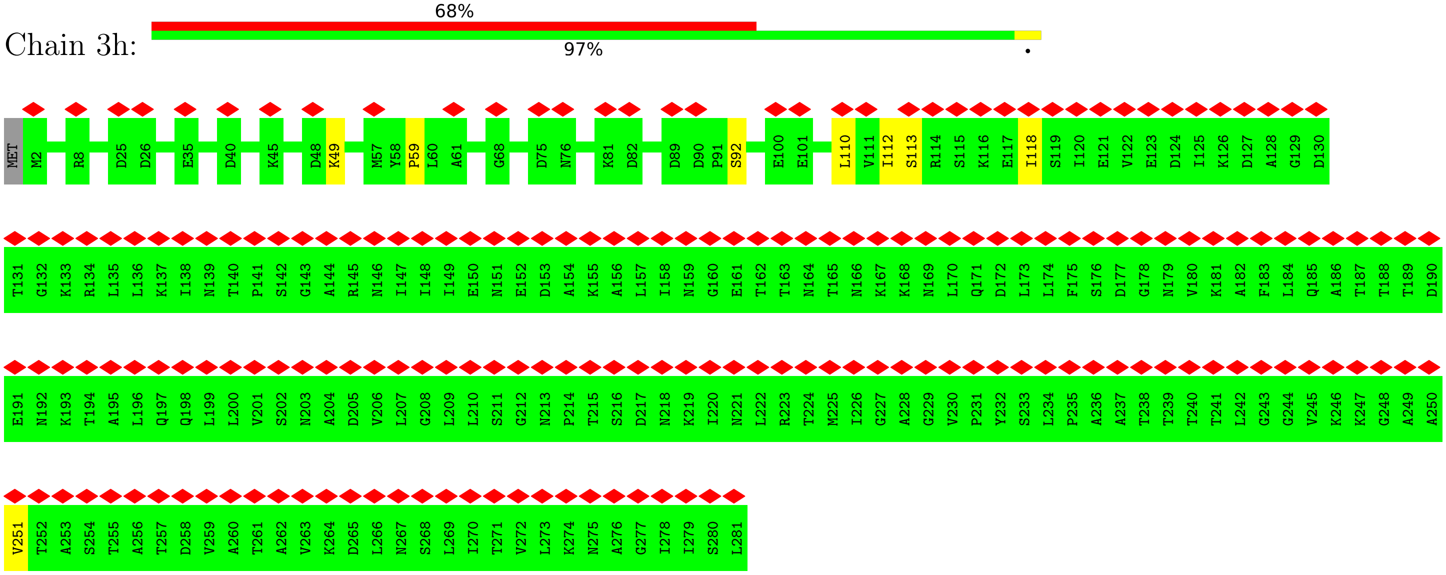
- Molecule 2: Capsid fiber protein

Chain 3g:



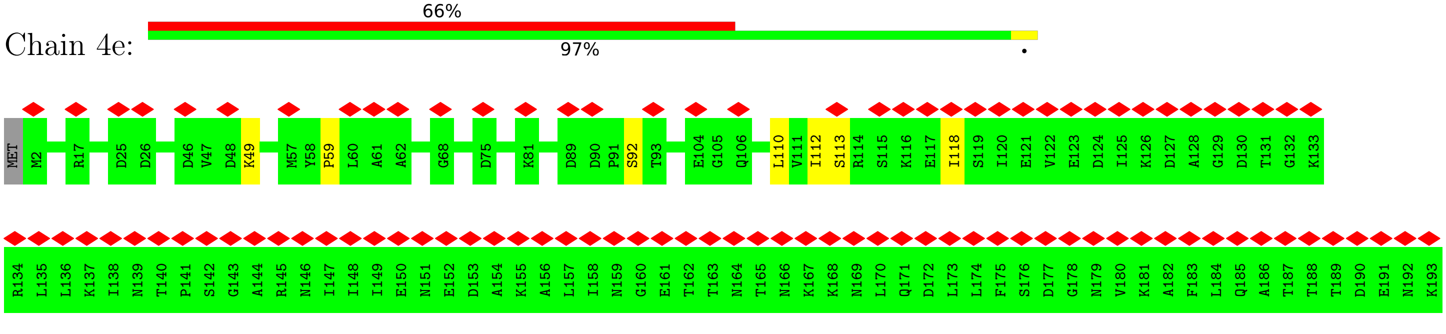
- Molecule 2: Capsid fiber protein

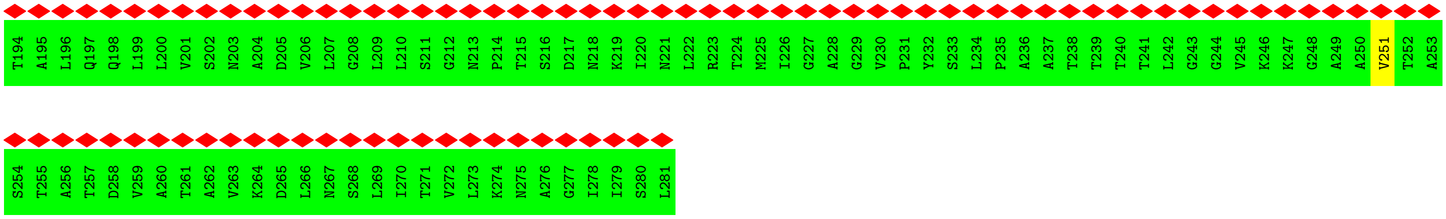
Chain 3h:



- Molecule 2: Capsid fiber protein

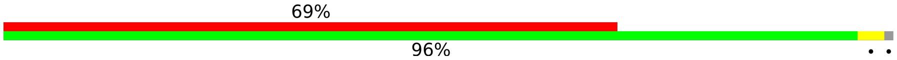
Chain 4e:

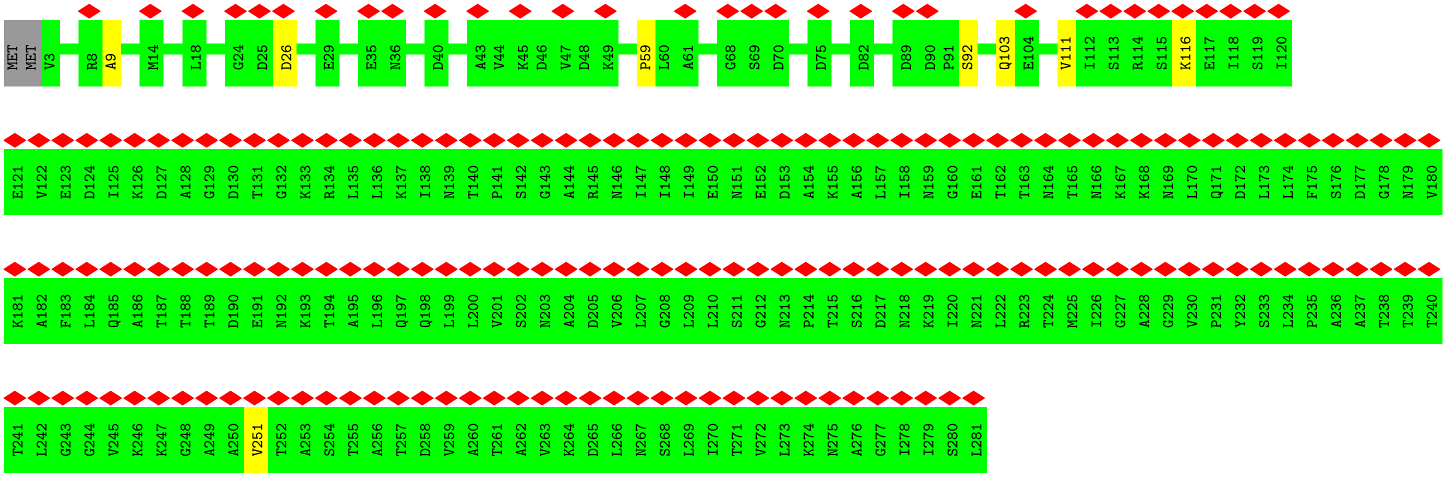




- Molecule 2: Capsid fiber protein

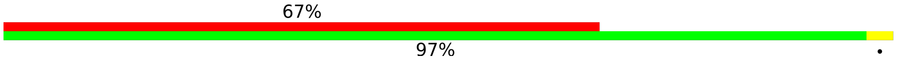
Chain 4f:

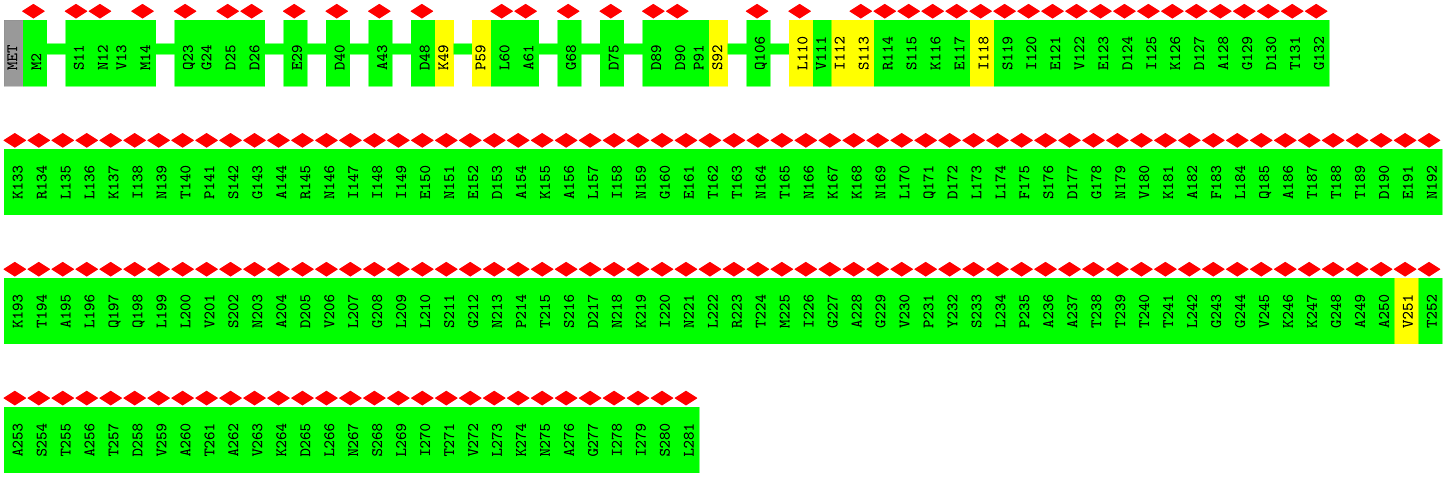




- Molecule 2: Capsid fiber protein

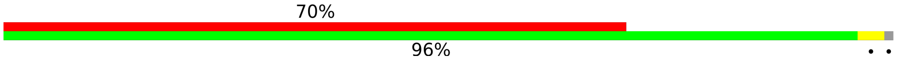
Chain 5e:

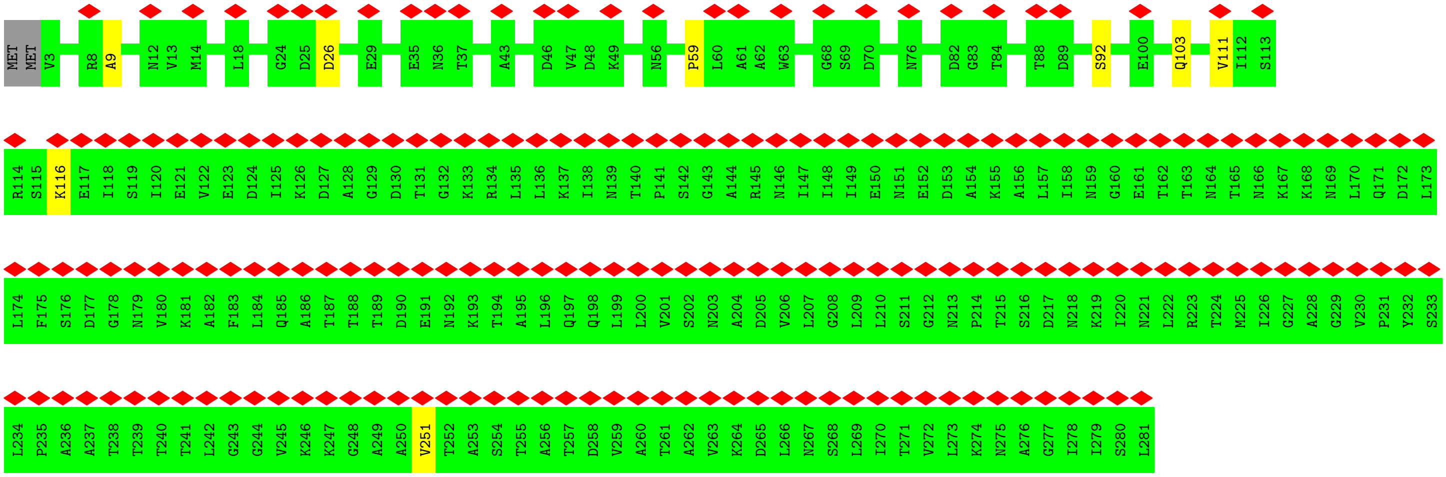




- Molecule 2: Capsid fiber protein

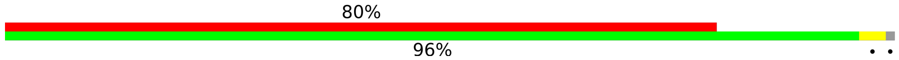
Chain 5f:

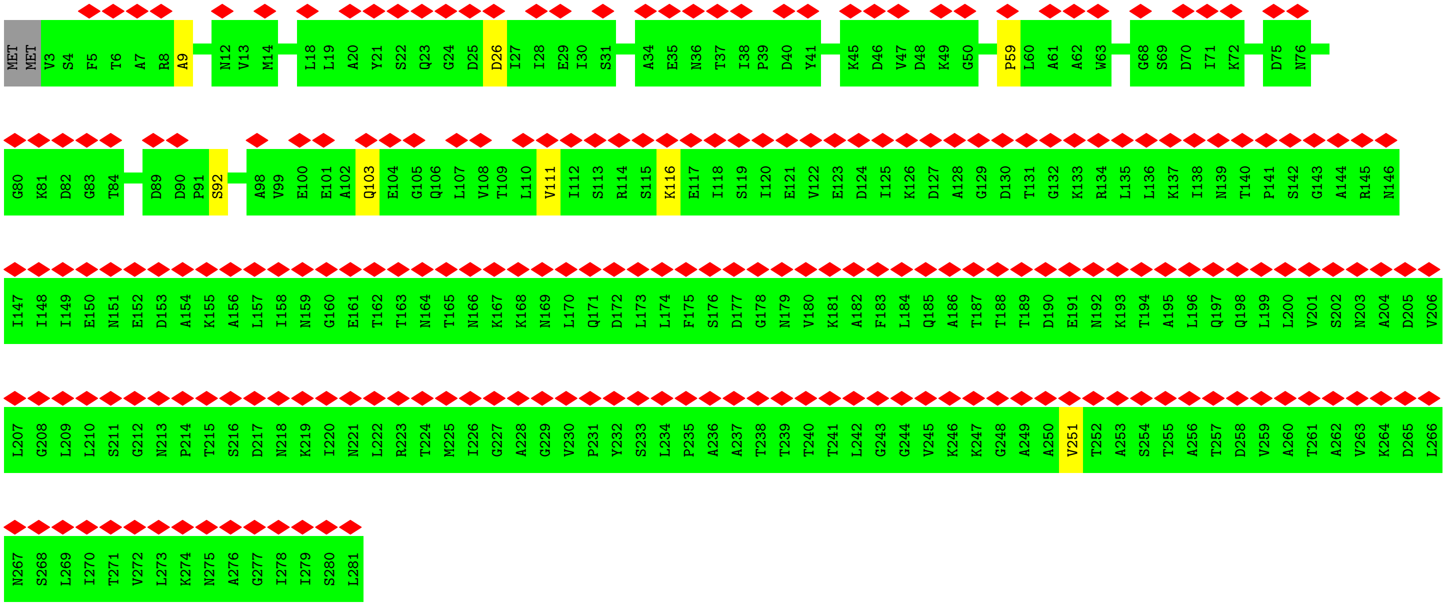




- Molecule 2: Capsid fiber protein

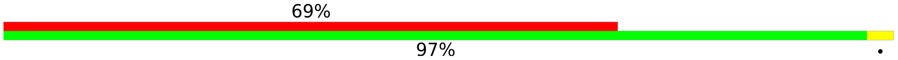
Chain 6e:

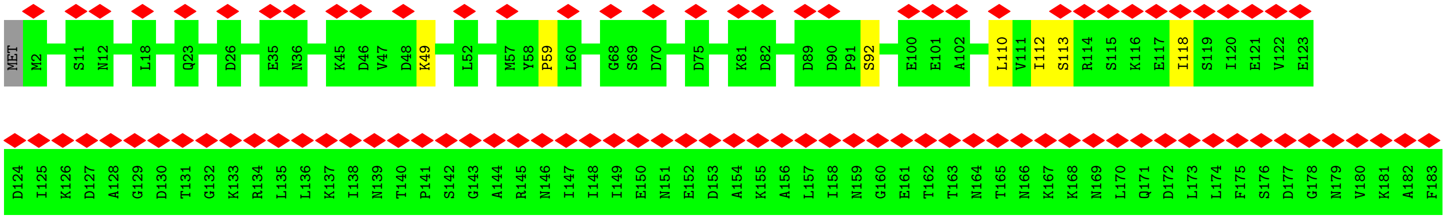


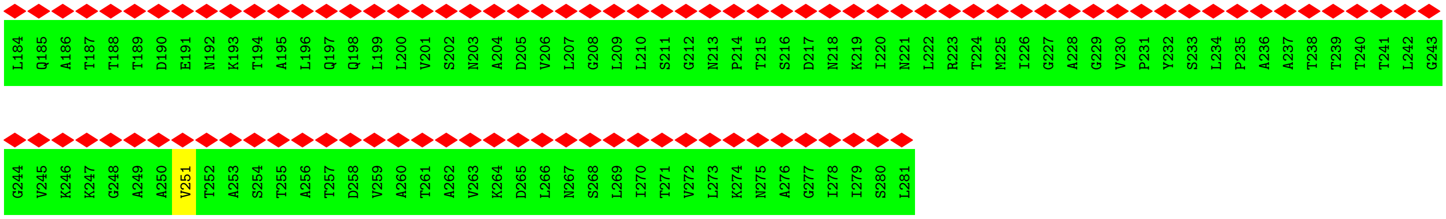


- Molecule 2: Capsid fiber protein

Chain 6f:

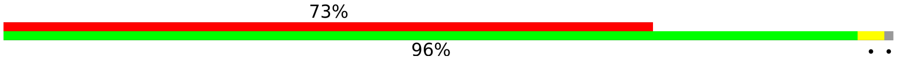


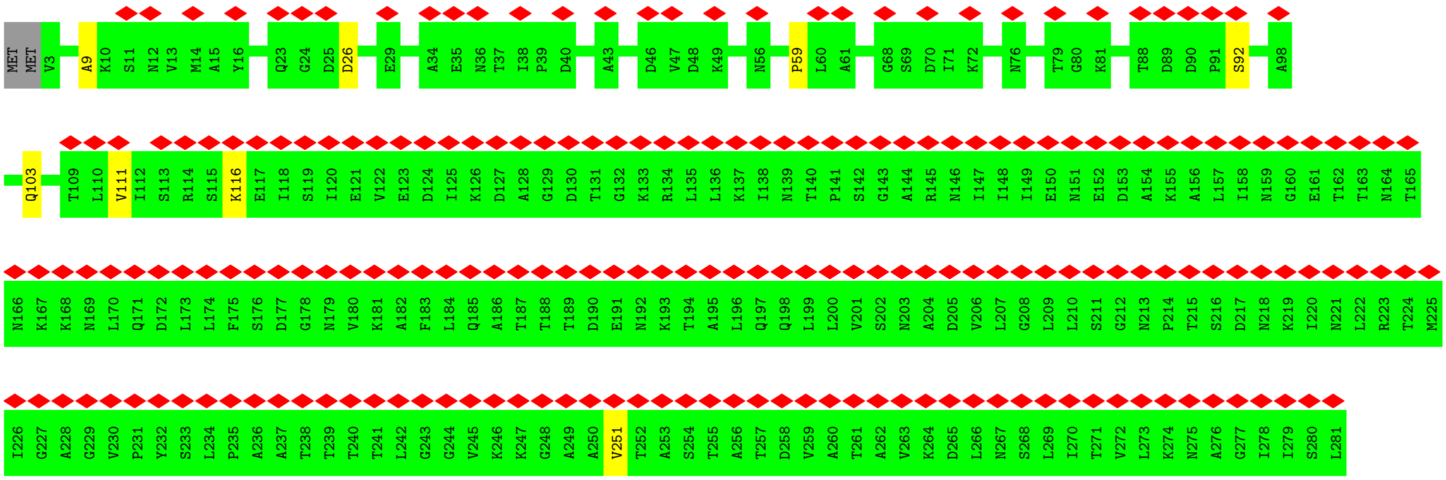




- Molecule 2: Capsid fiber protein

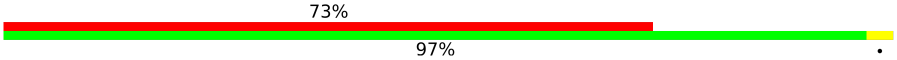
Chain 6g:

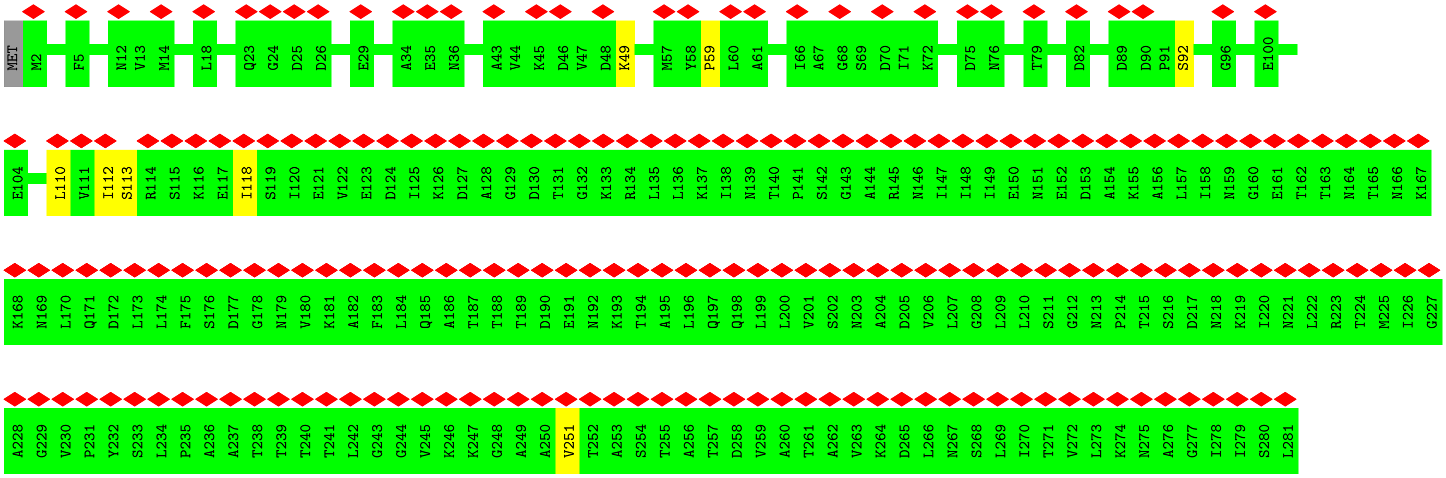




- Molecule 2: Capsid fiber protein

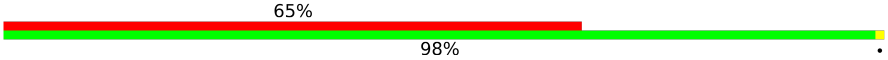
Chain 6h:

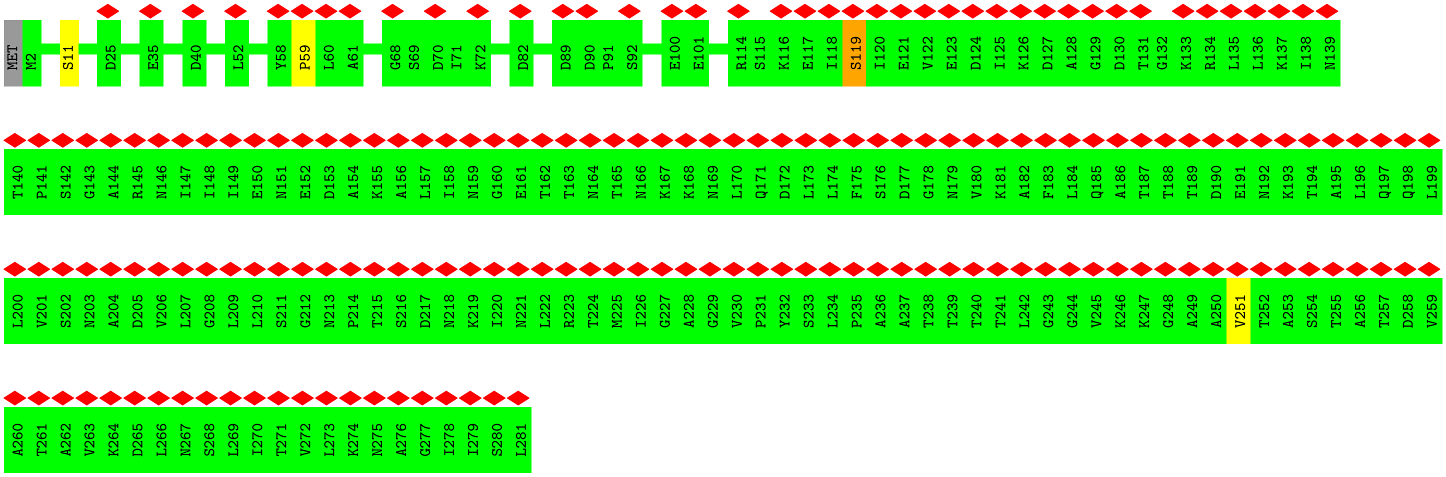




- Molecule 2: Capsid fiber protein

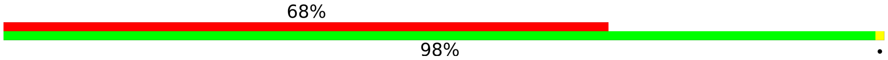
Chain 7Z:

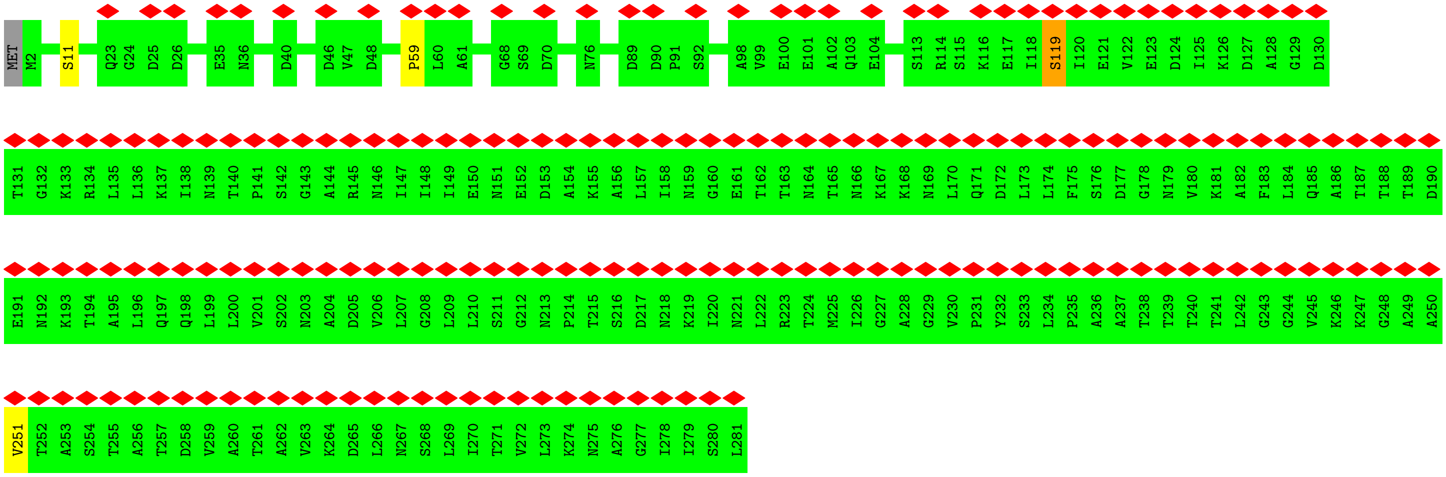




- Molecule 2: Capsid fiber protein

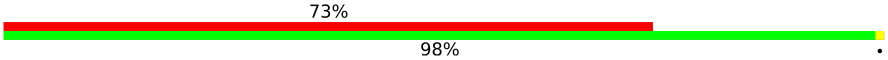
Chain 7a:

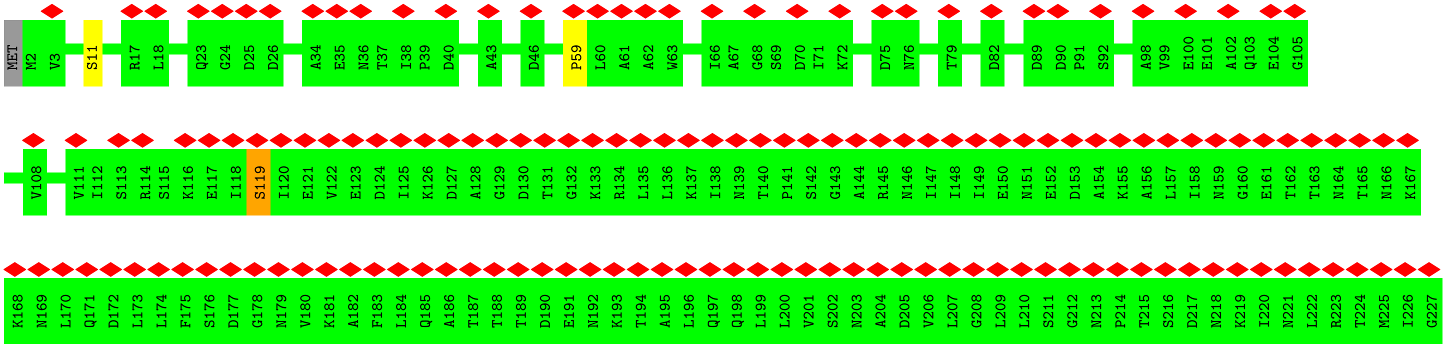


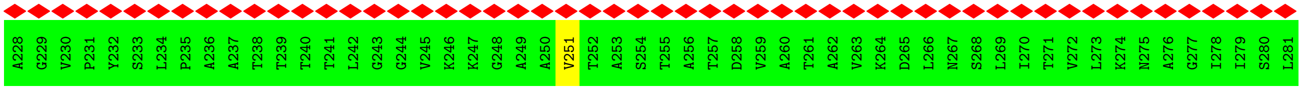


- Molecule 2: Capsid fiber protein

Chain 7b:

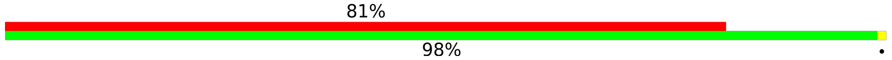


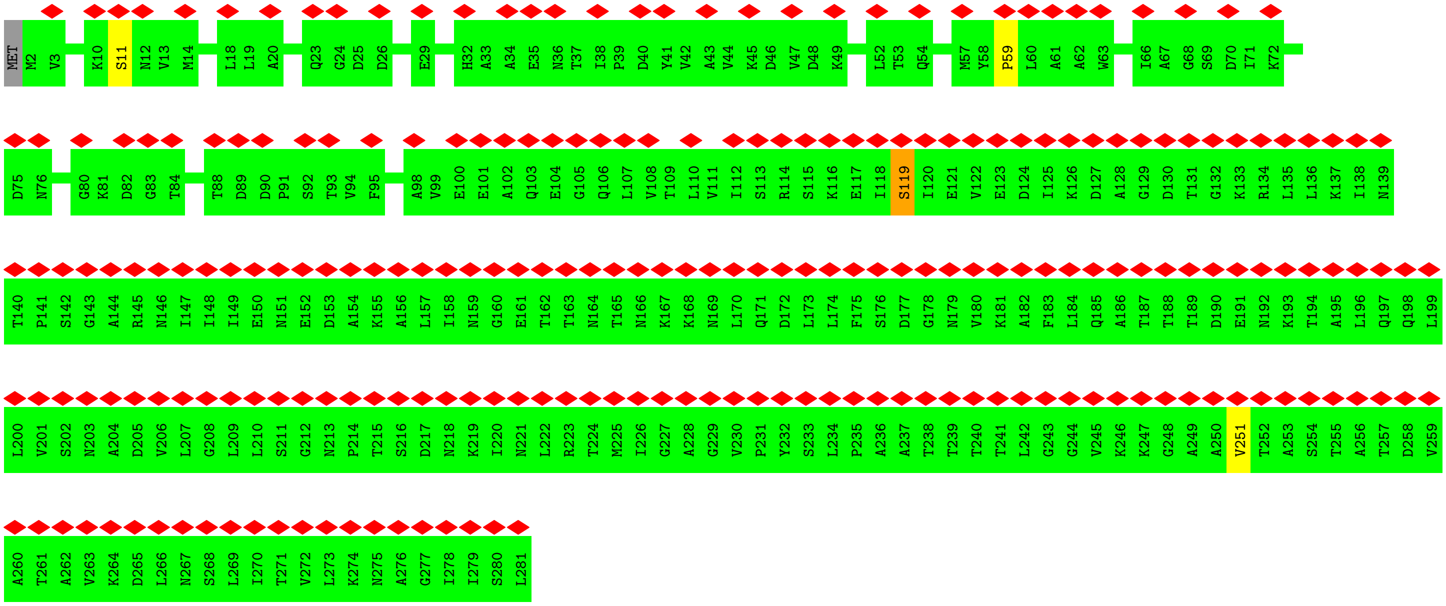




- Molecule 2: Capsid fiber protein

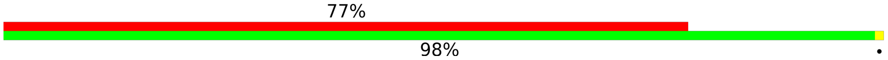
Chain 7c:

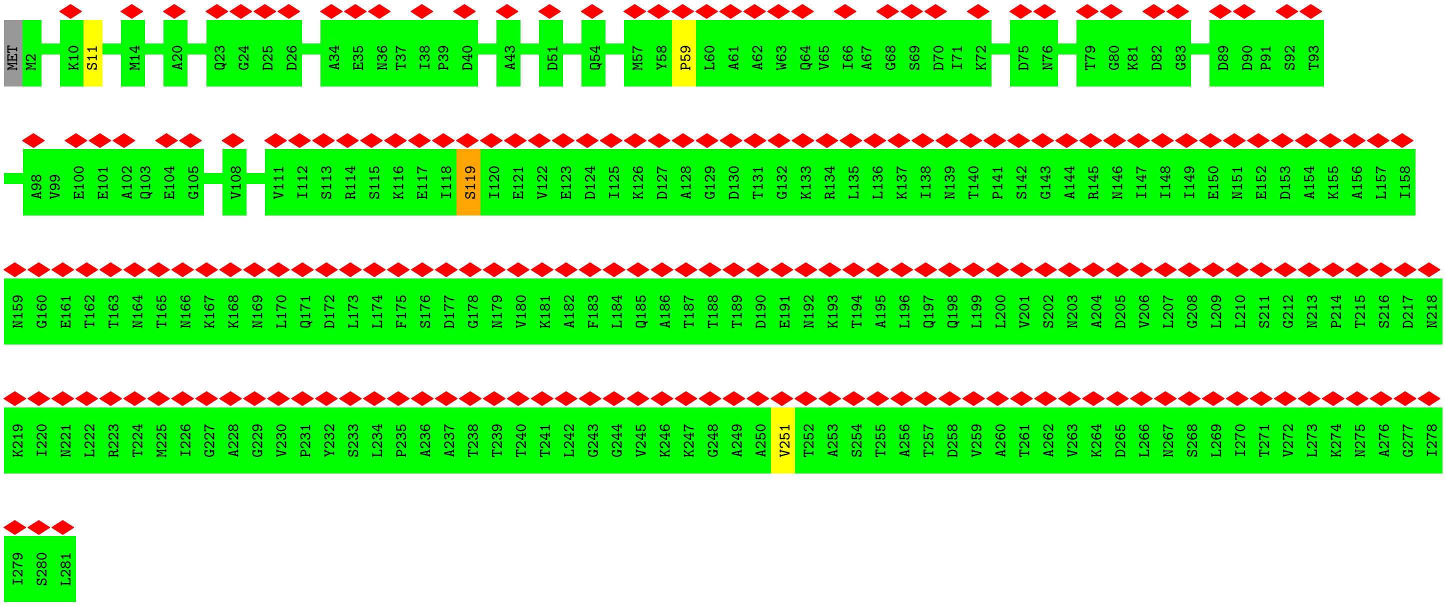




- Molecule 2: Capsid fiber protein

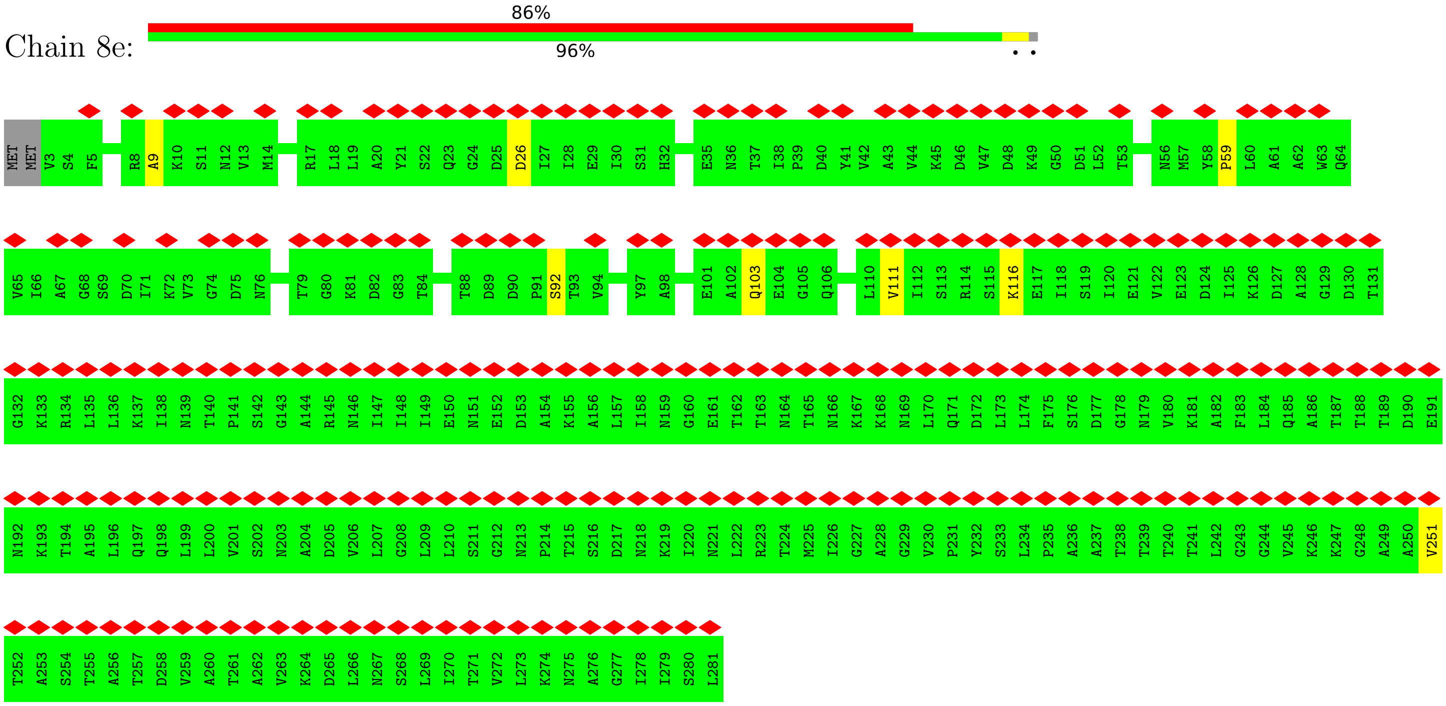
Chain 7d:





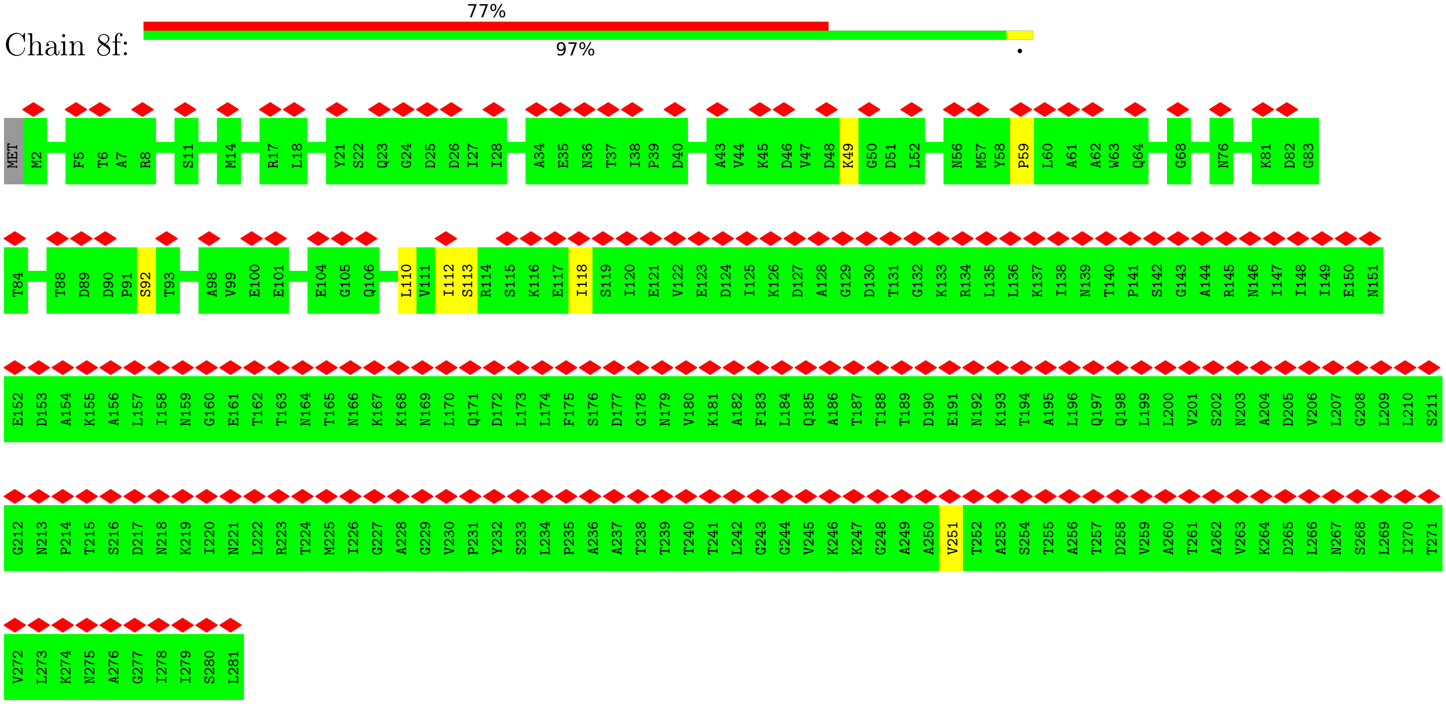
- Molecule 2: Capsid fiber protein

Chain 8e:



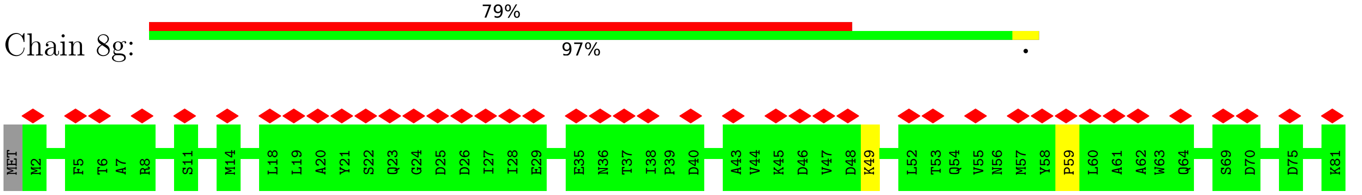
- Molecule 2: Capsid fiber protein

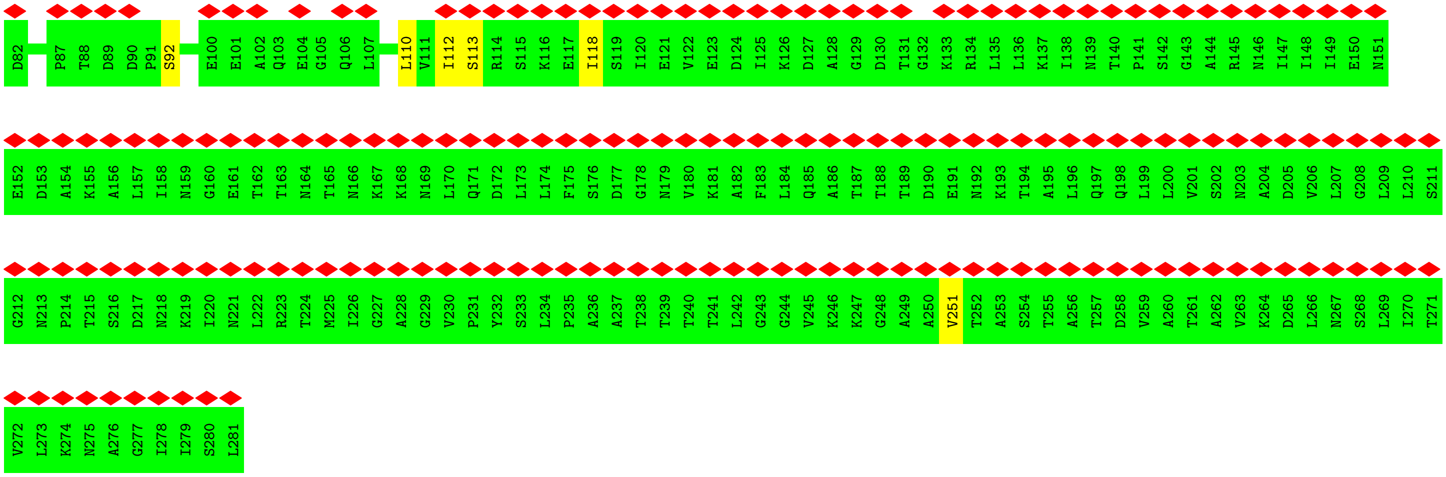
Chain 8f:



- Molecule 2: Capsid fiber protein

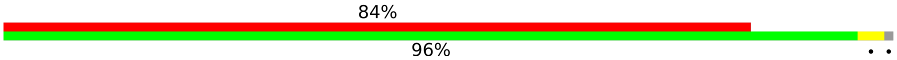
Chain 8g:

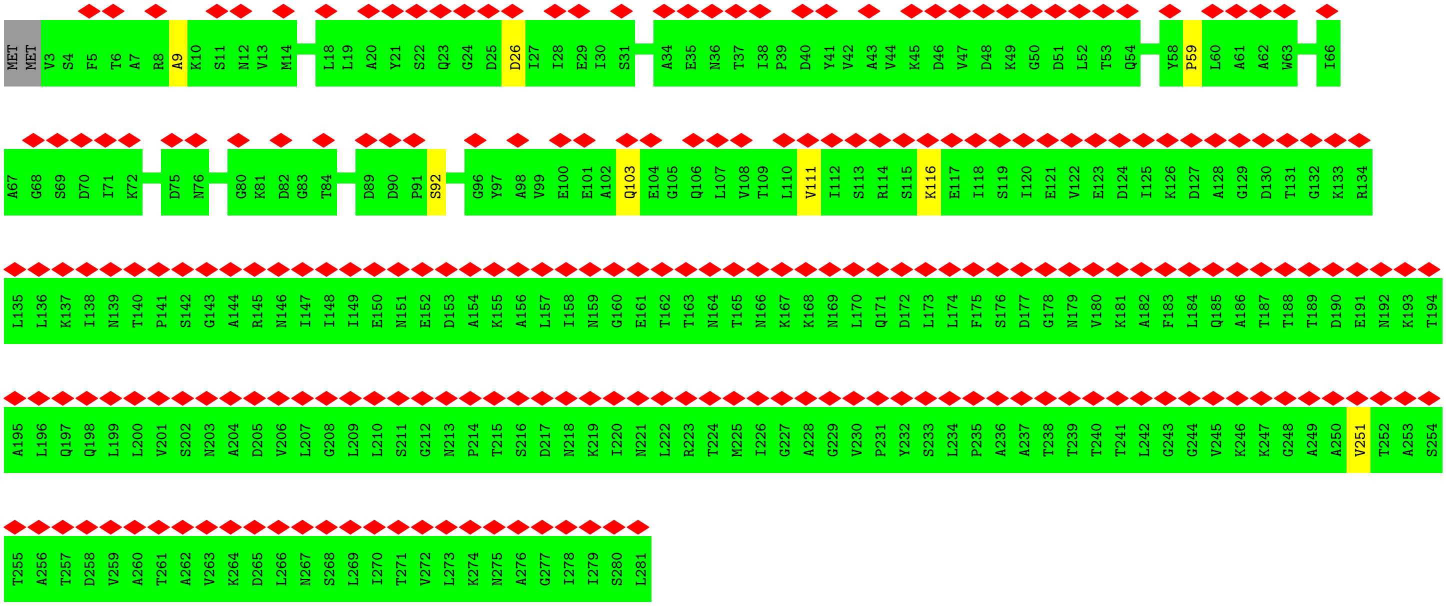




- Molecule 2: Capsid fiber protein

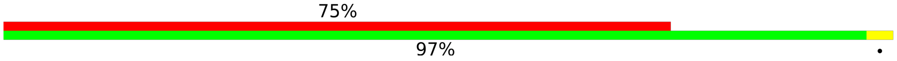
Chain 8h:

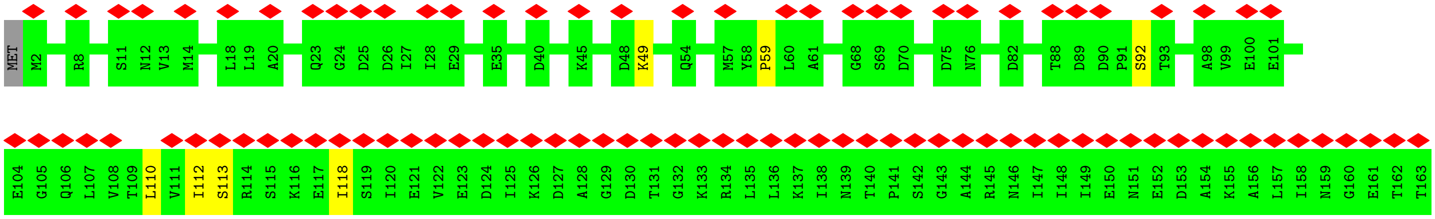


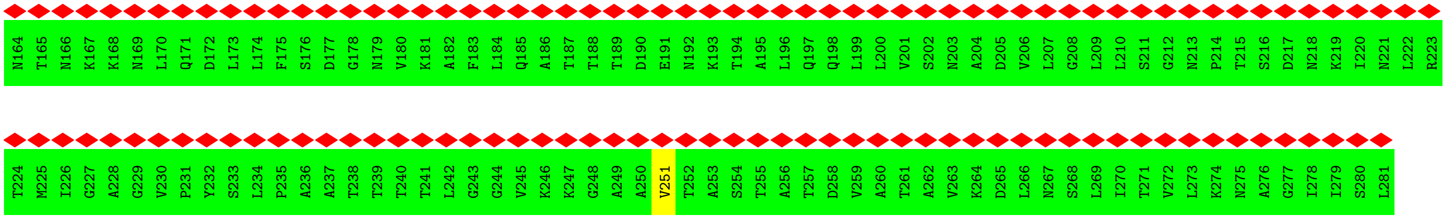


- Molecule 2: Capsid fiber protein

Chain 8i:

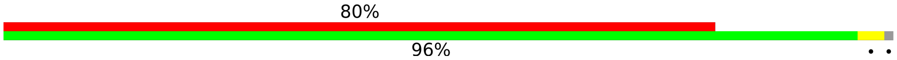


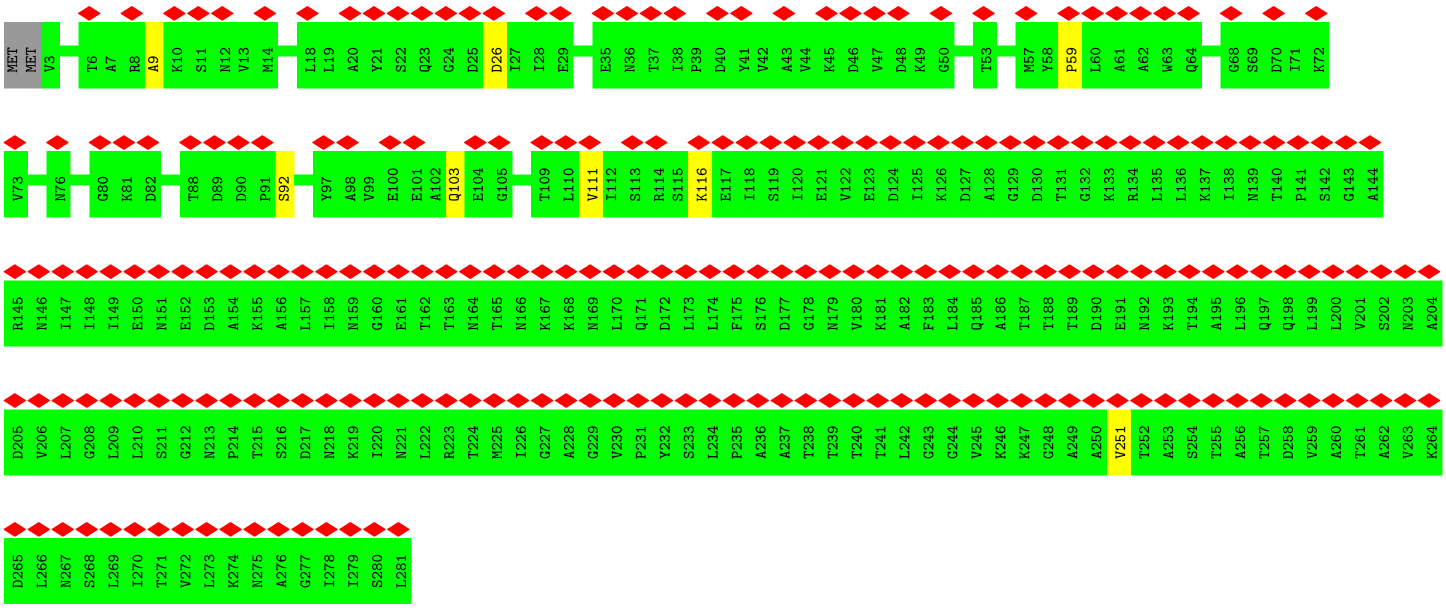




- Molecule 2: Capsid fiber protein

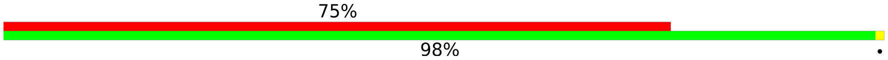
Chain 8j:

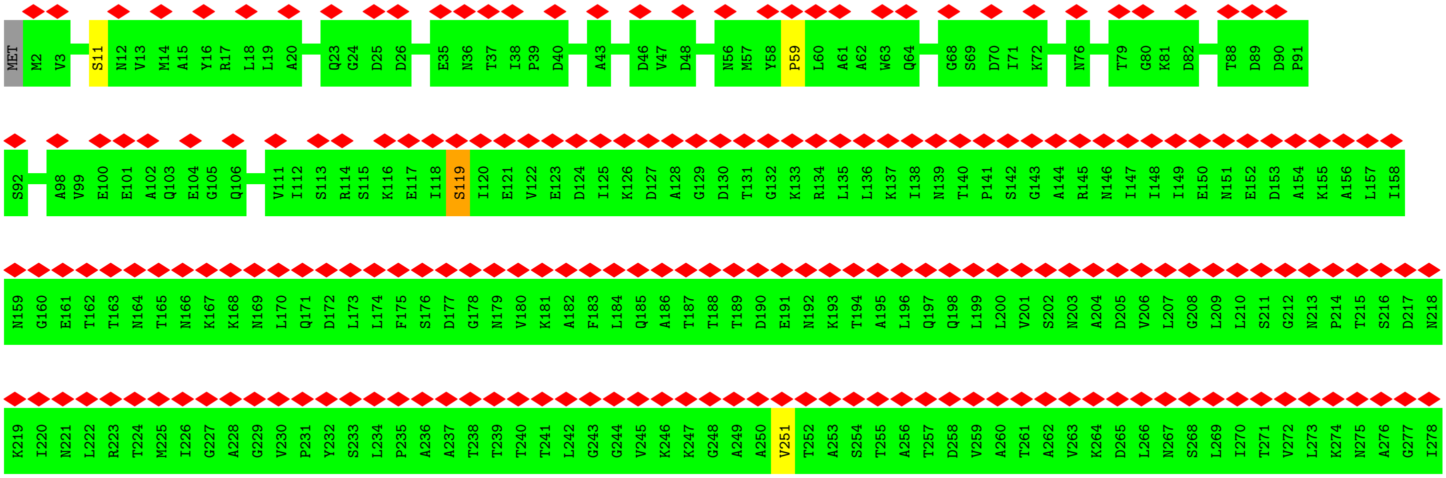


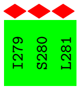


- Molecule 2: Capsid fiber protein

Chain 9F:

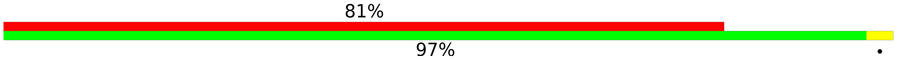


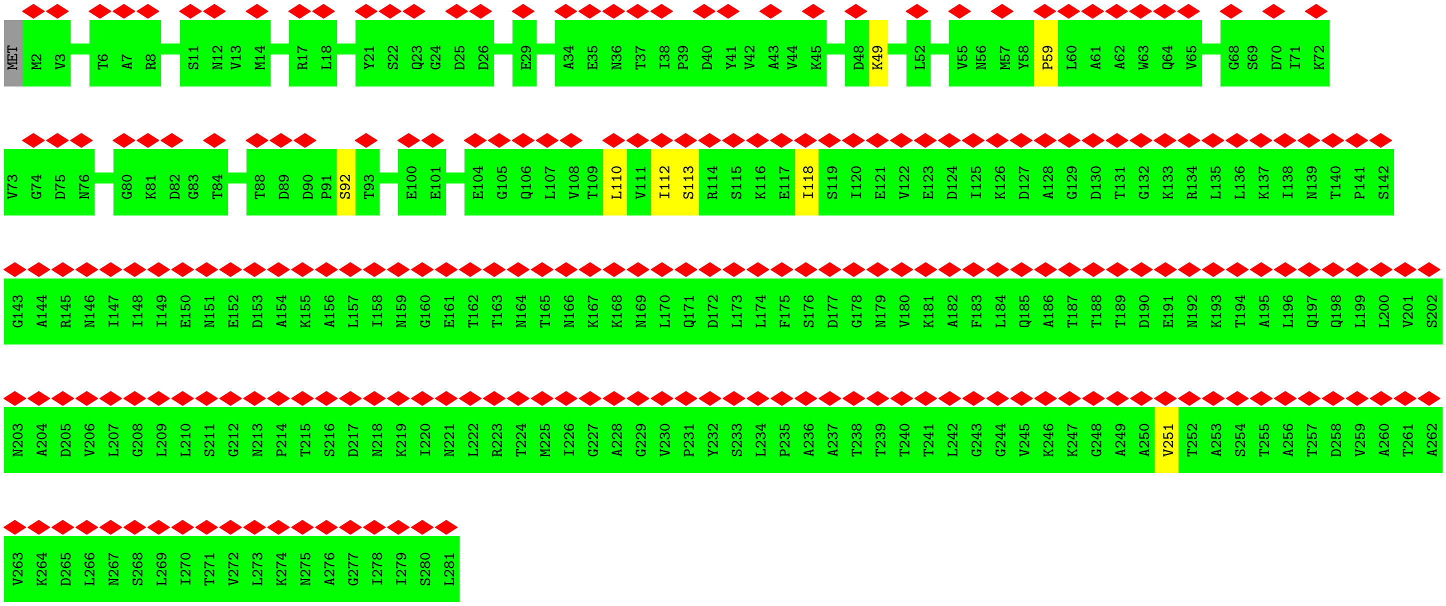




- Molecule 2: Capsid fiber protein

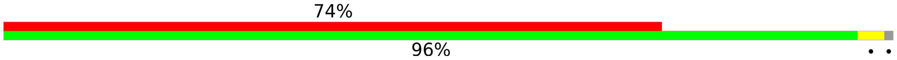
Chain 1i:

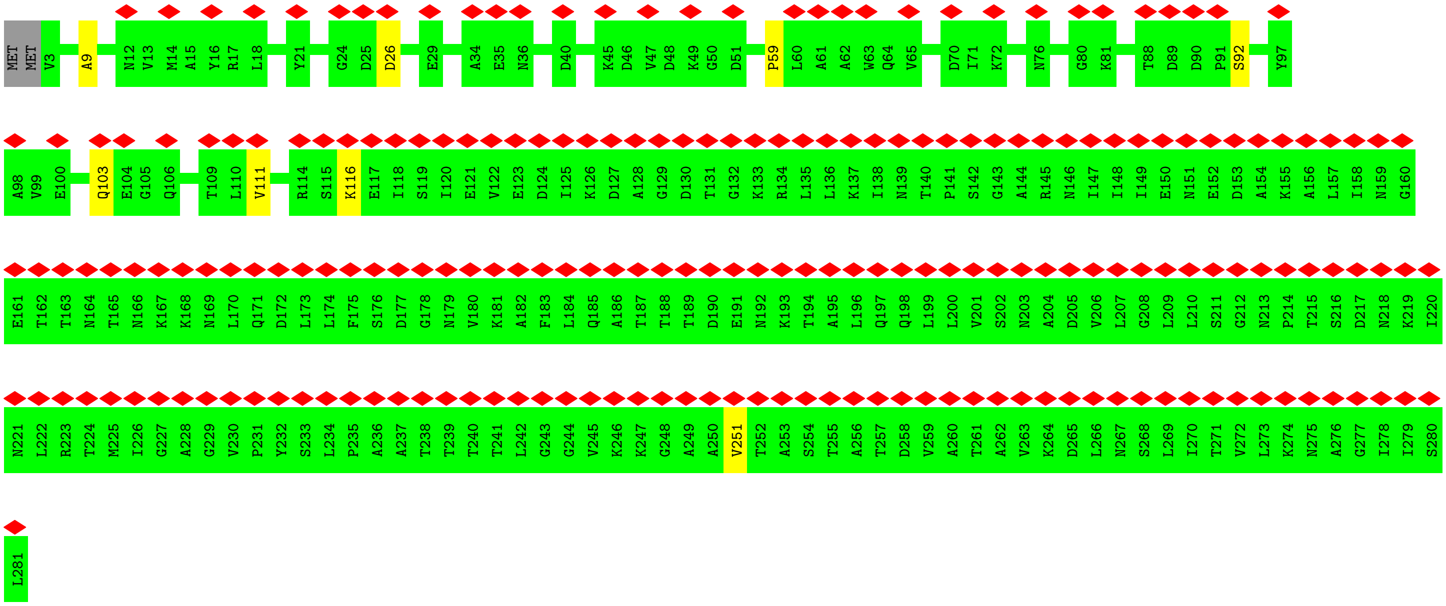




- Molecule 2: Capsid fiber protein

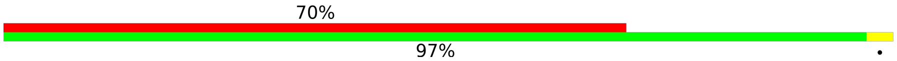
Chain 1j:

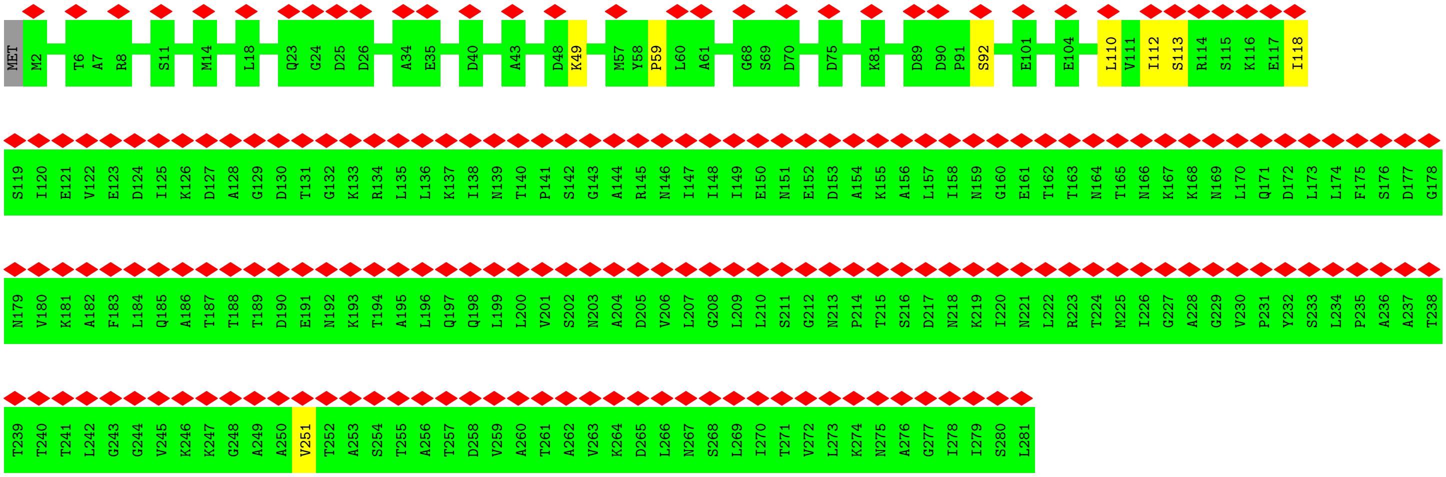




- Molecule 2: Capsid fiber protein

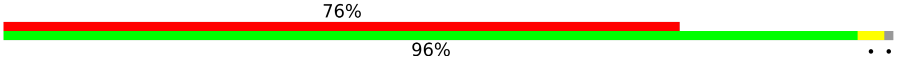
Chain 1k:

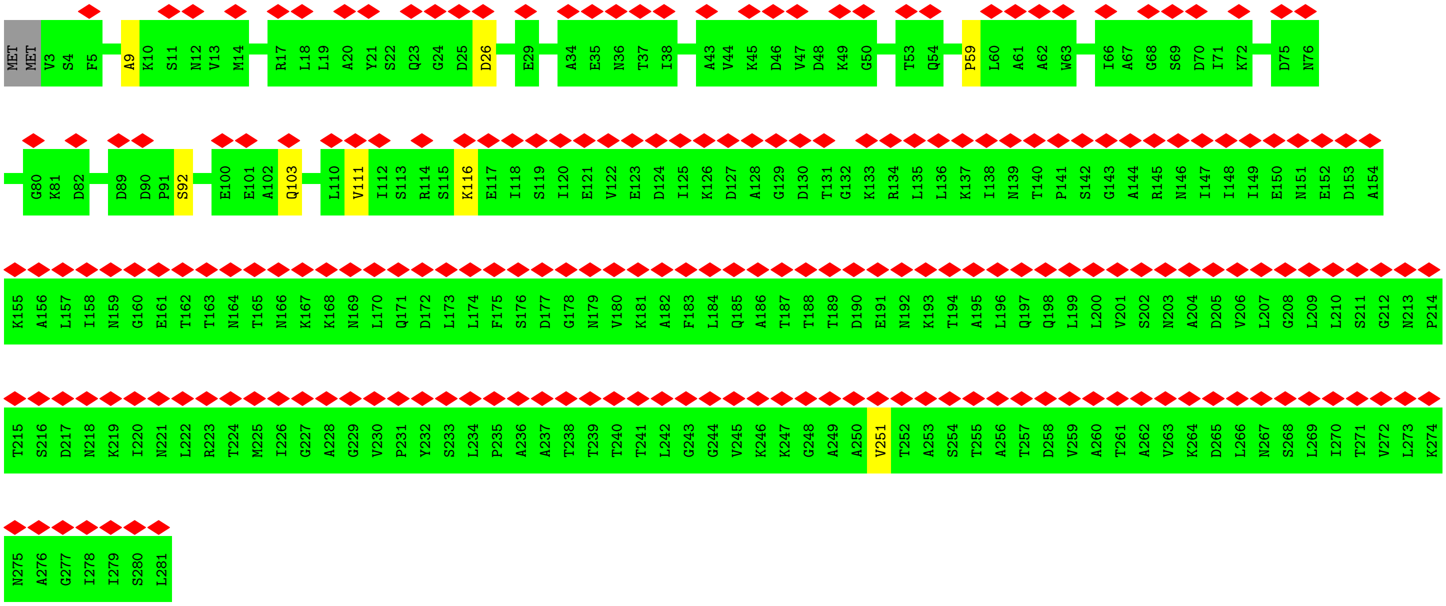




- Molecule 2: Capsid fiber protein

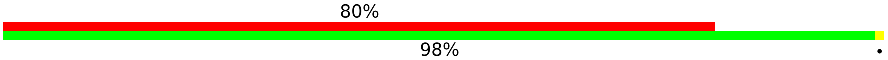
Chain 1l:

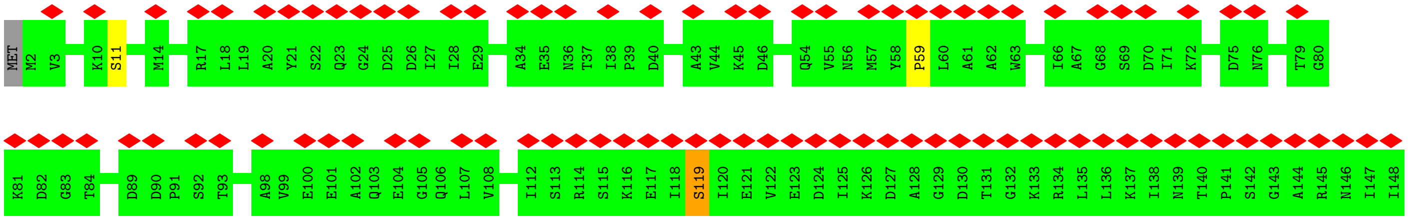


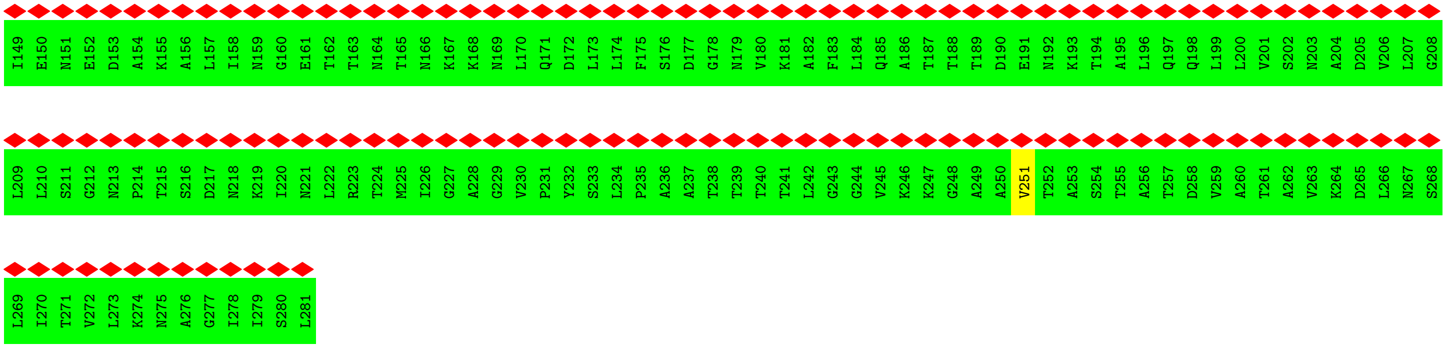


- Molecule 2: Capsid fiber protein

Chain 2e:

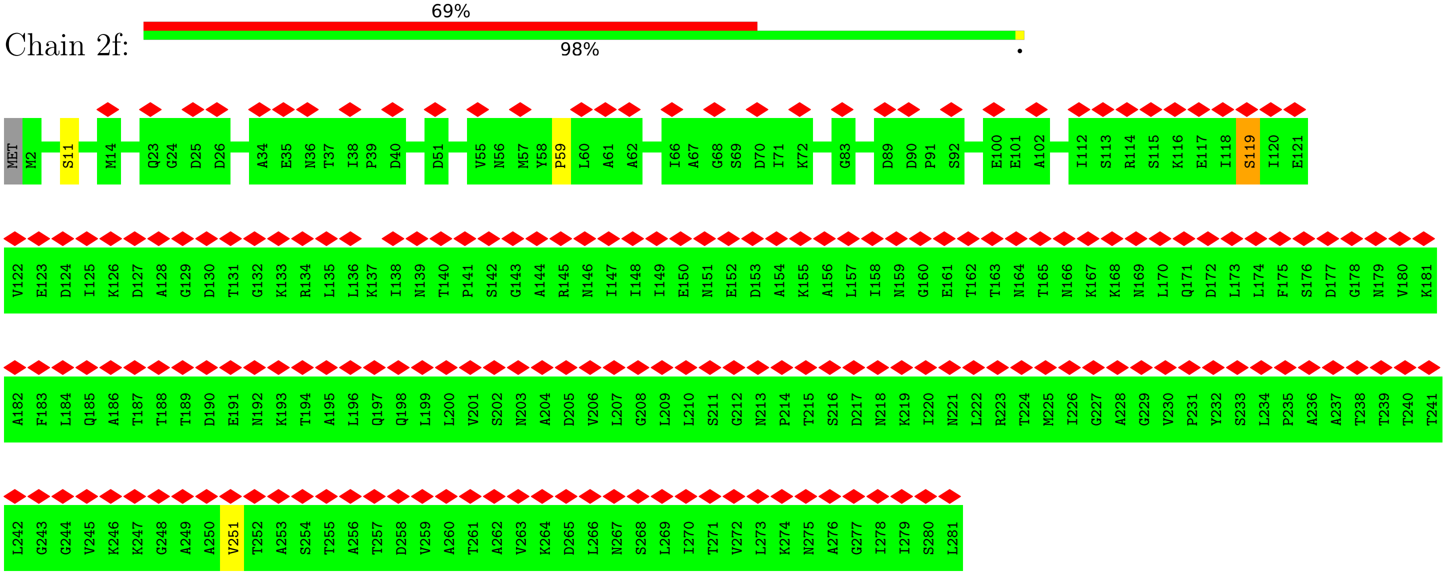






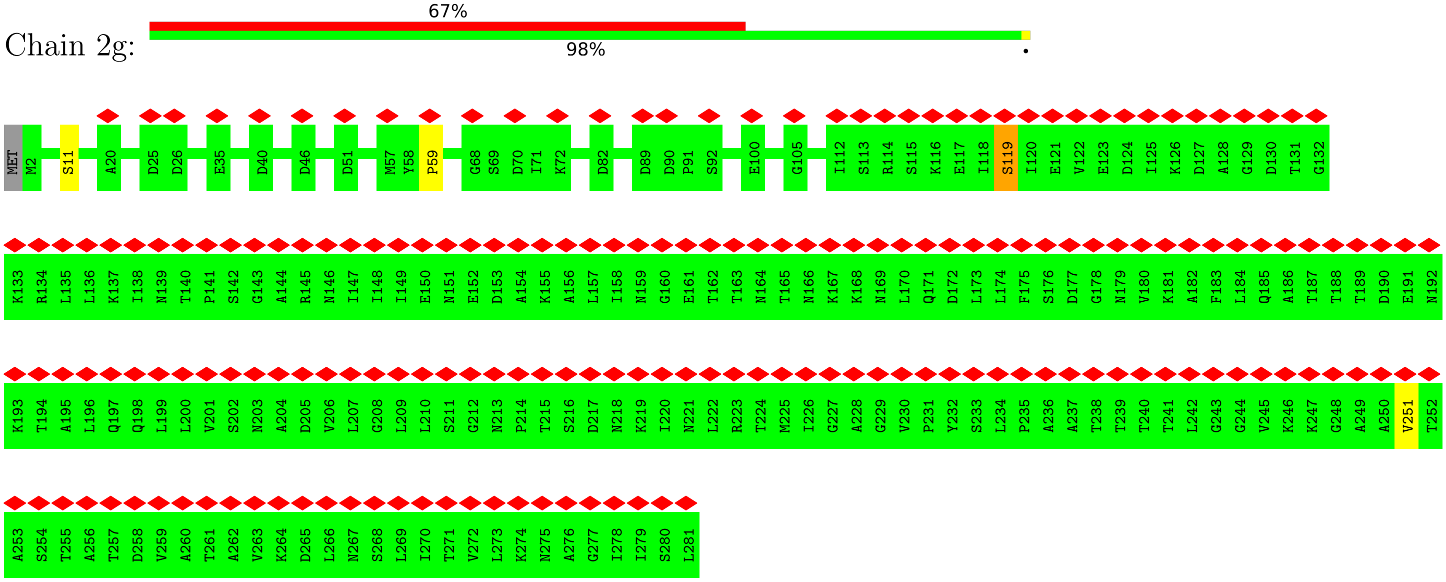
- Molecule 2: Capsid fiber protein

Chain 2f:



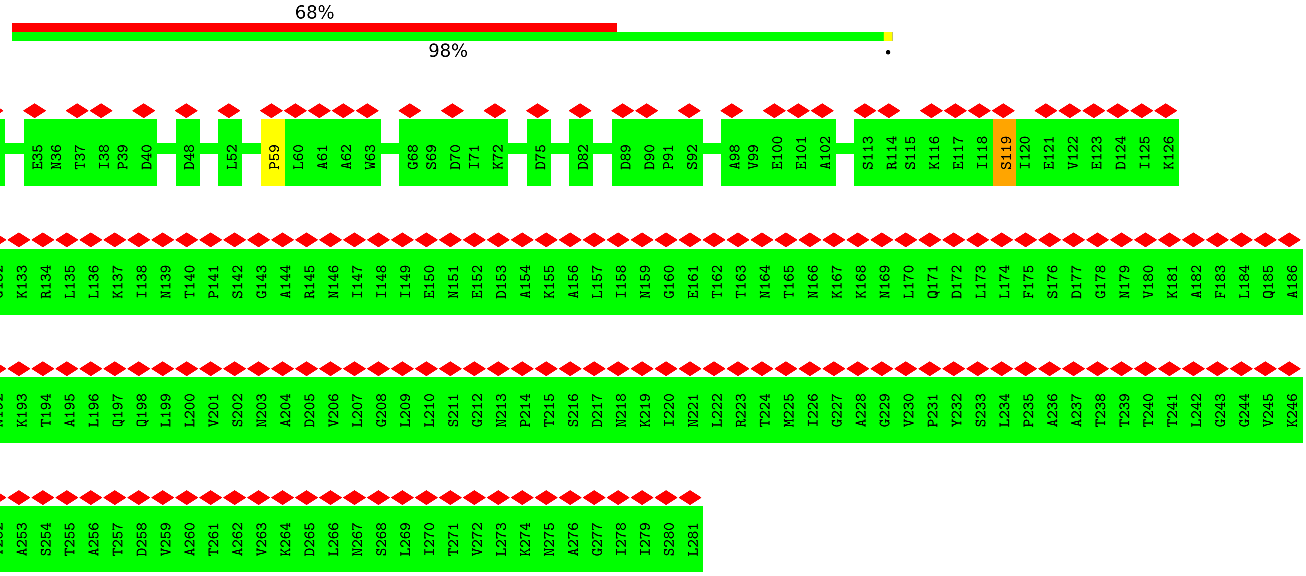
- Molecule 2: Capsid fiber protein

Chain 2g:



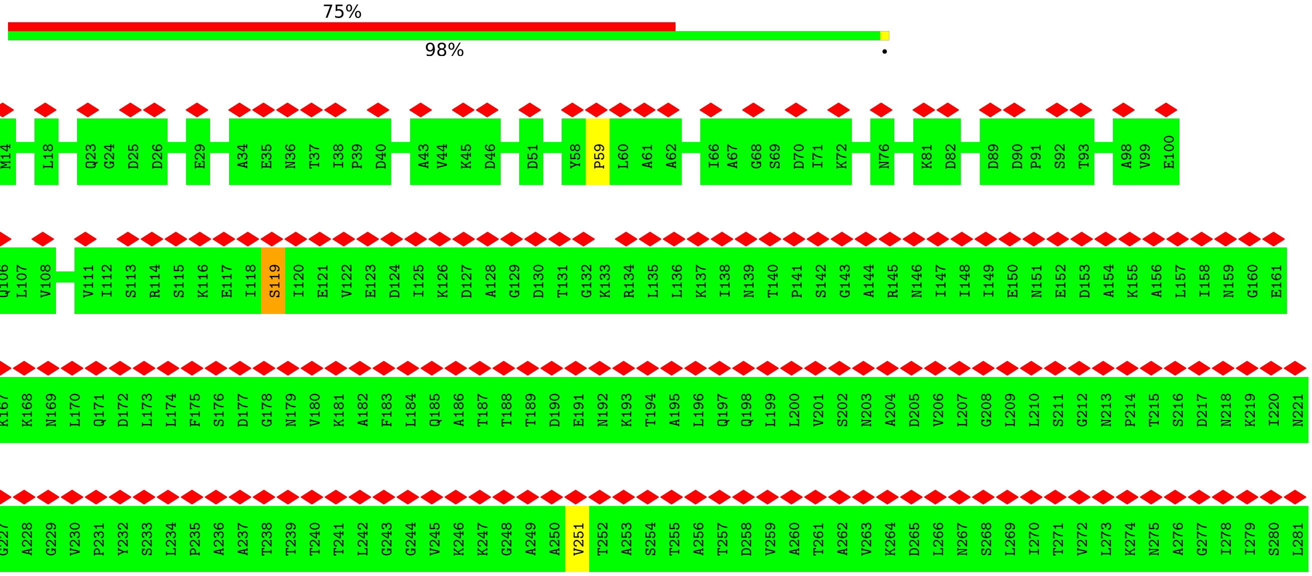
- Molecule 2: Capsid fiber protein

Chain 2h:



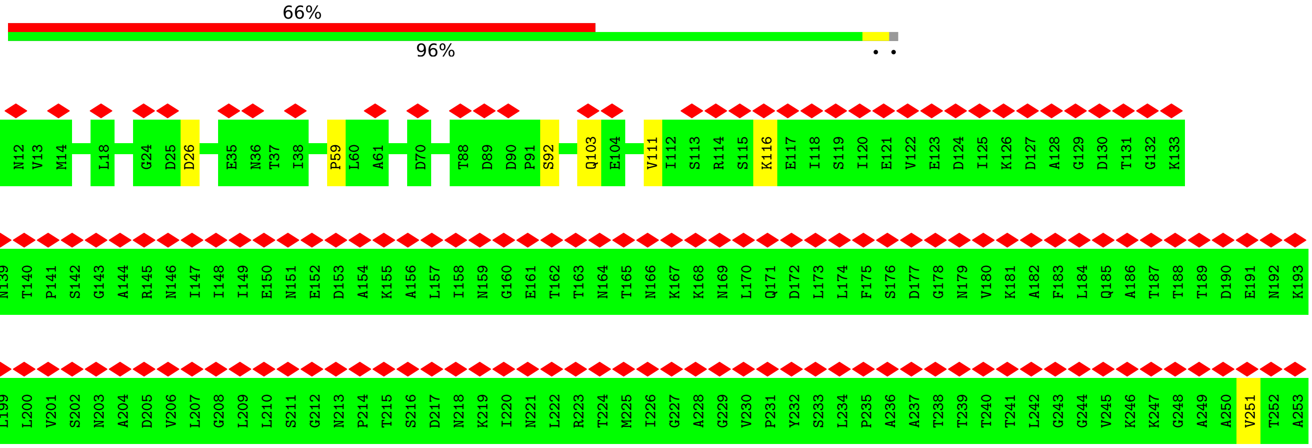
- Molecule 2: Capsid fiber protein

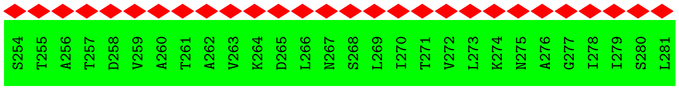
Chain 2i:



- Molecule 2: Capsid fiber protein

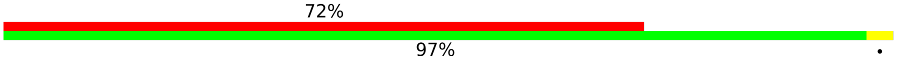
Chain 3i:

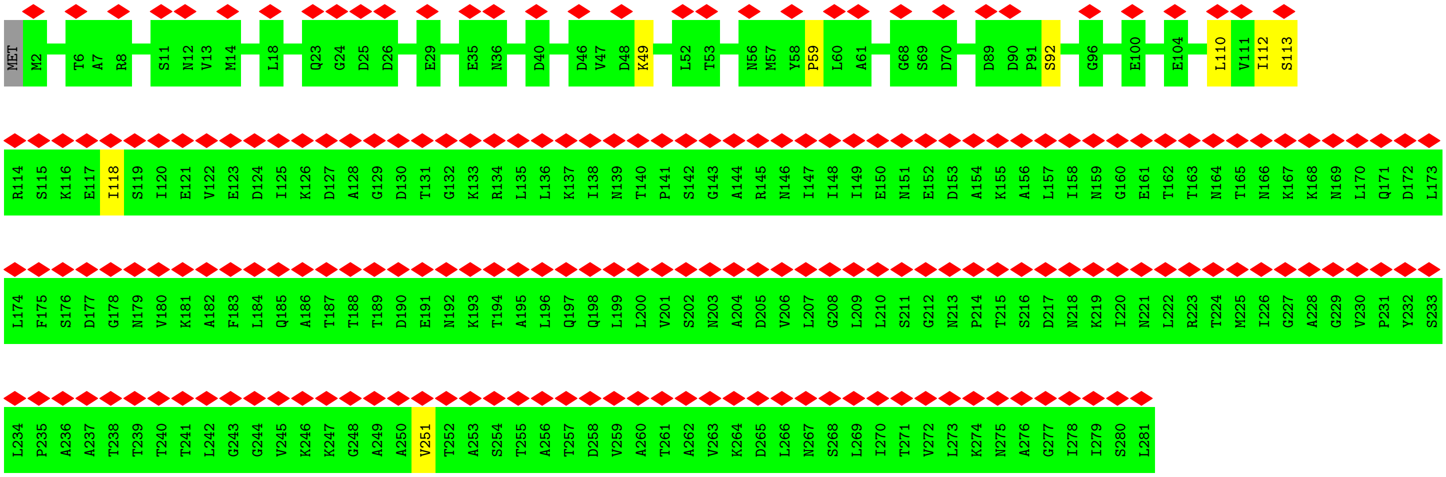




- Molecule 2: Capsid fiber protein

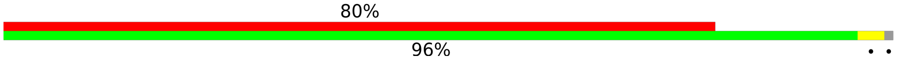
Chain 3j:





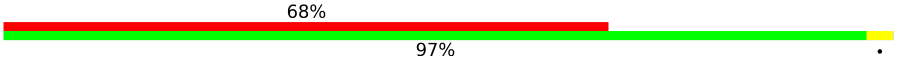
- Molecule 2: Capsid fiber protein

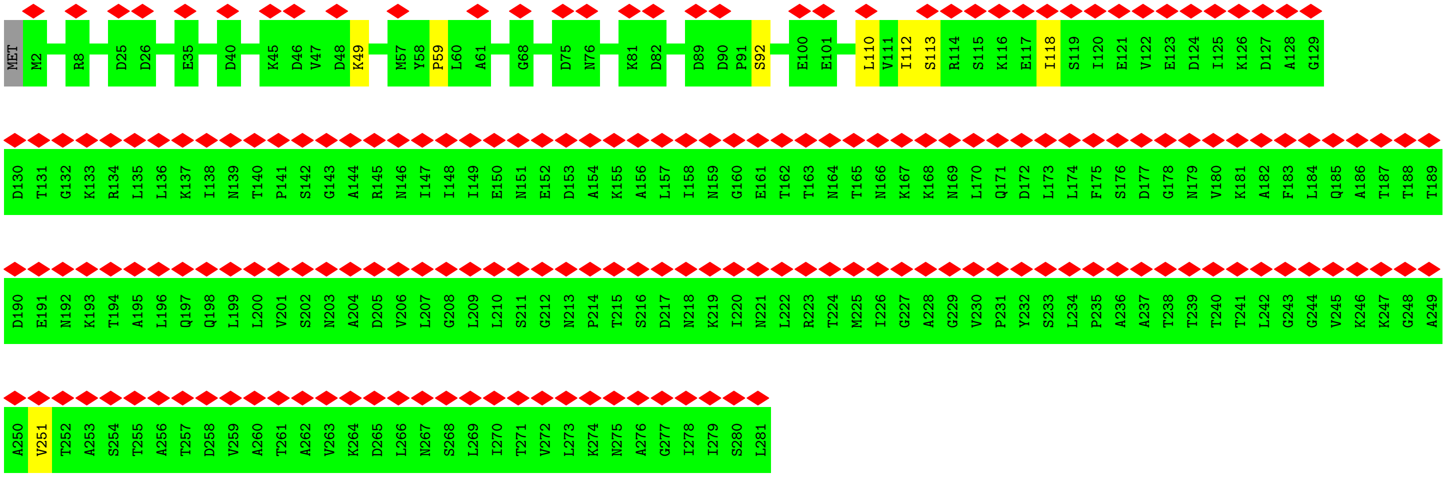
Chain 3k:



- Molecule 2: Capsid fiber protein

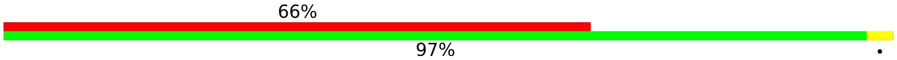
Chain 3l:

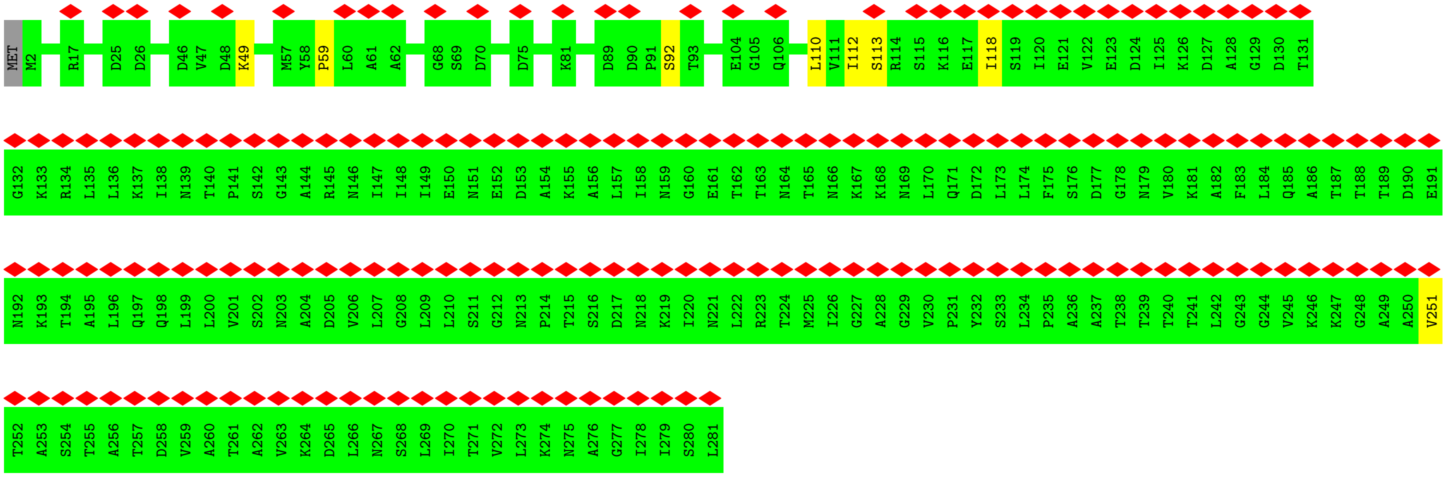




- Molecule 2: Capsid fiber protein

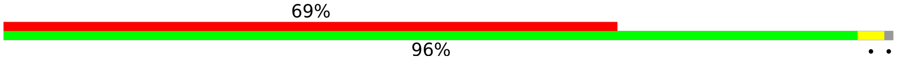
Chain 4g:

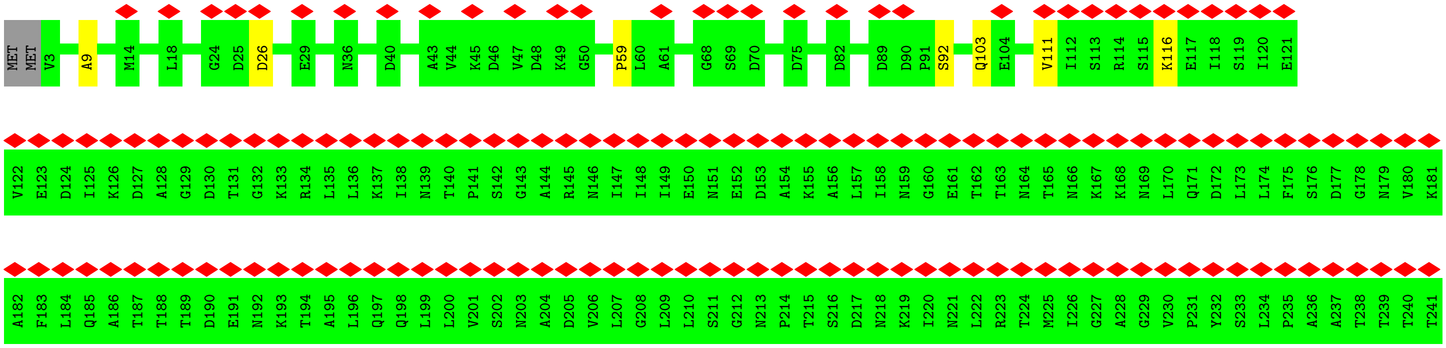


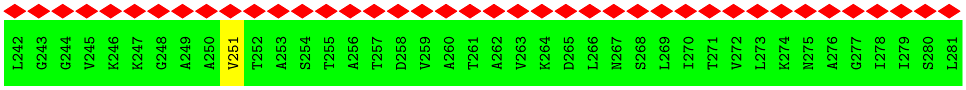


- Molecule 2: Capsid fiber protein

Chain 4h:

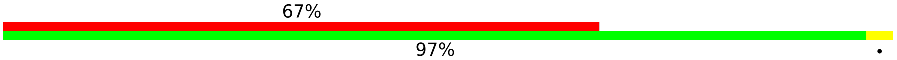


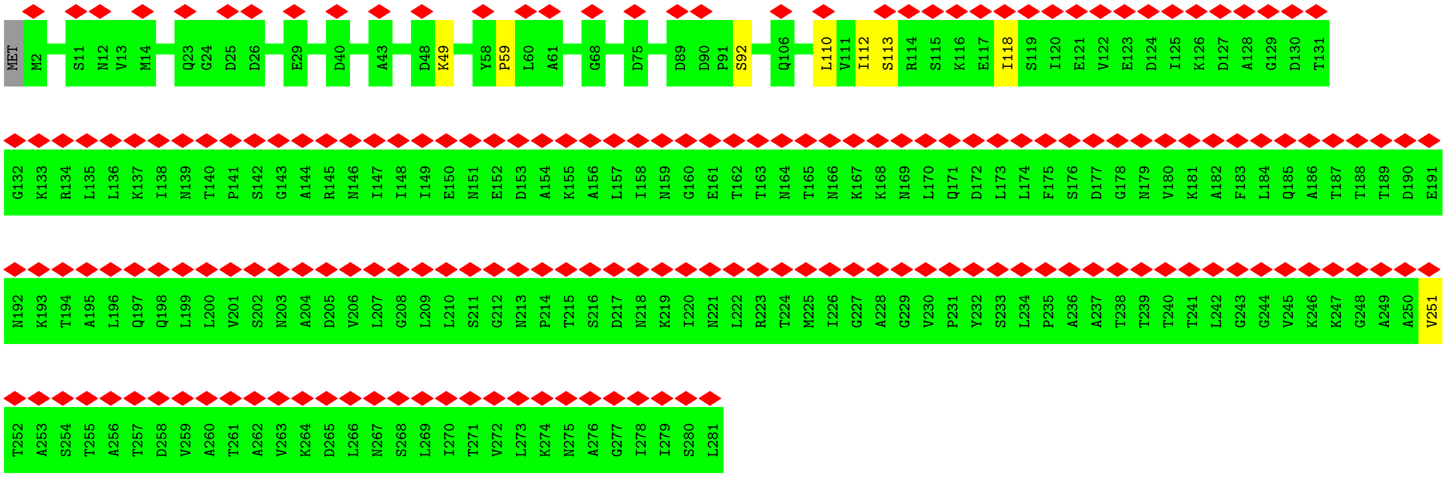




- Molecule 2: Capsid fiber protein

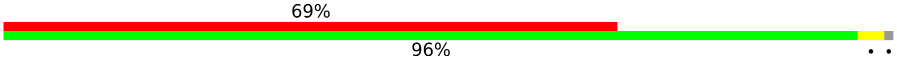
Chain 5g:

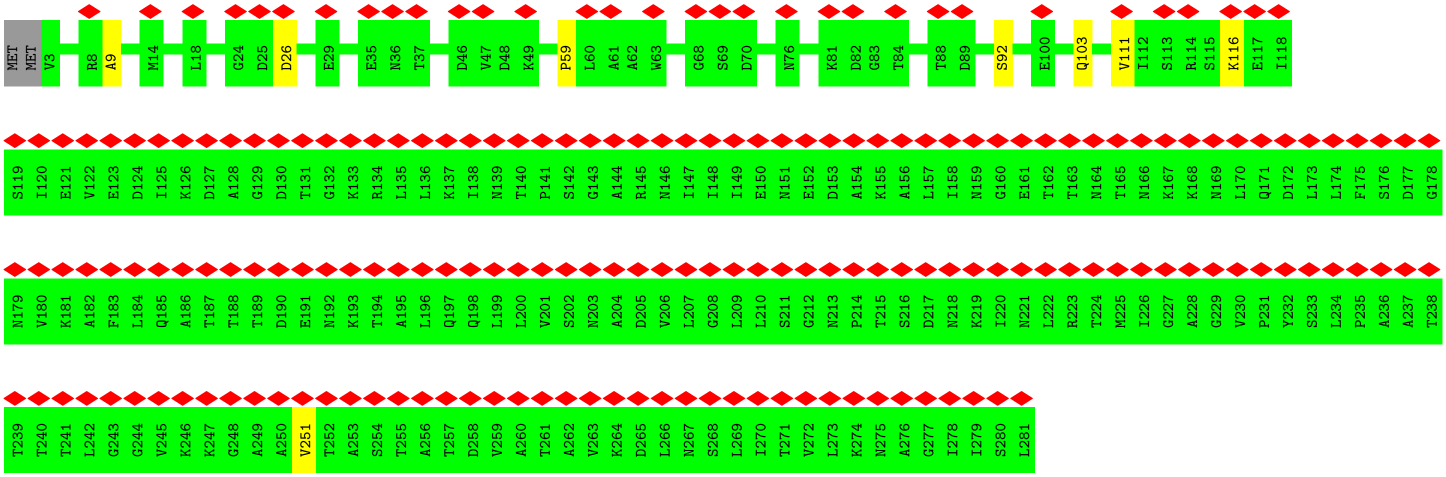




- Molecule 2: Capsid fiber protein

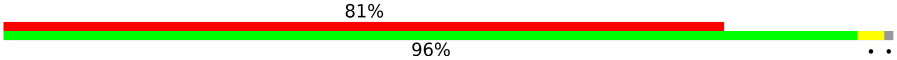
Chain 5h:

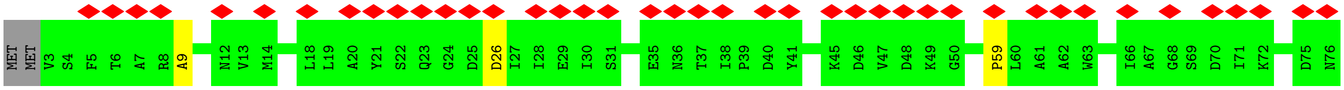


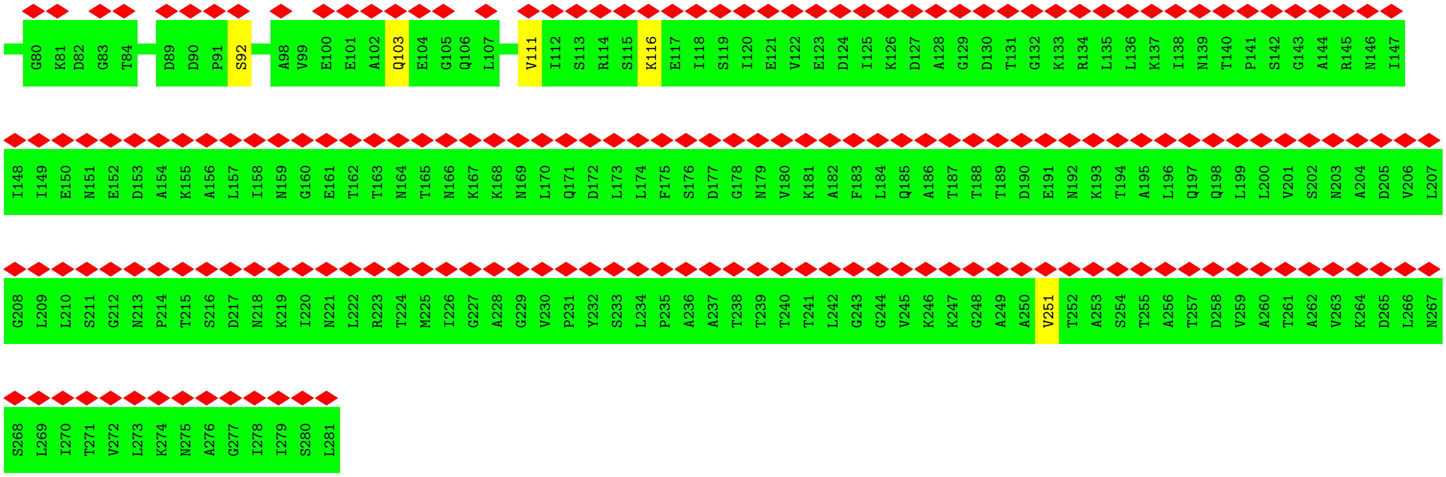


- Molecule 2: Capsid fiber protein

Chain 6i:

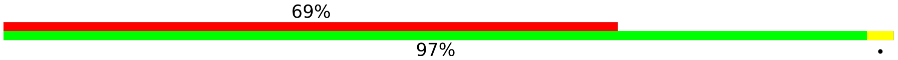


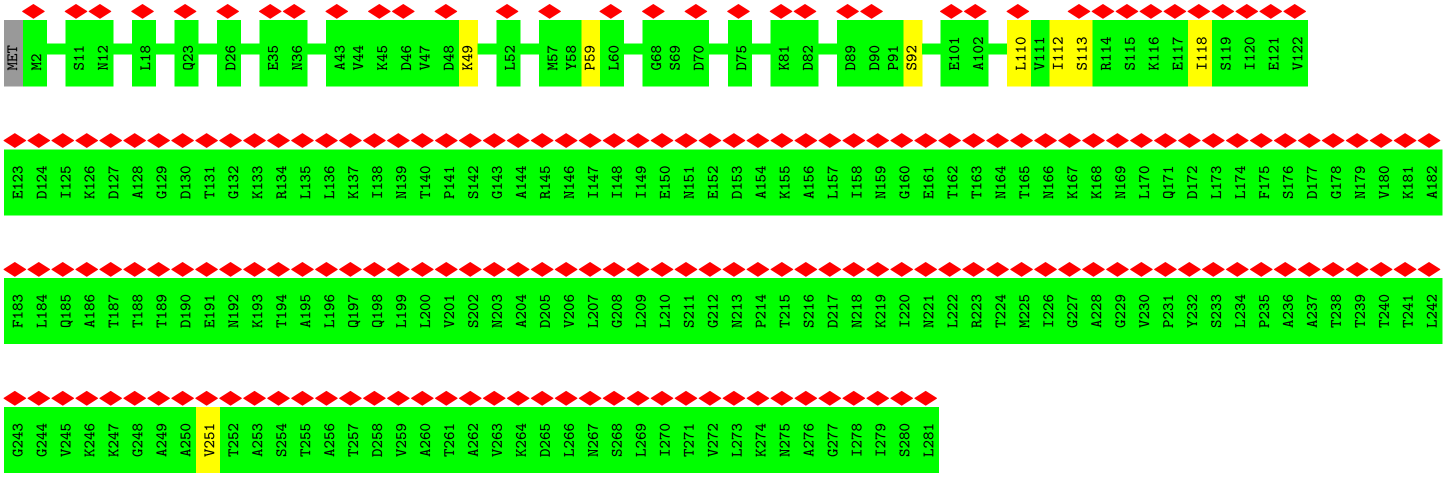




- Molecule 2: Capsid fiber protein

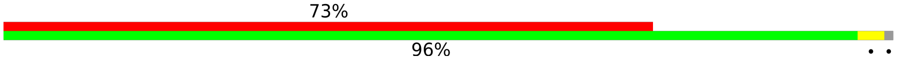
Chain 6j:

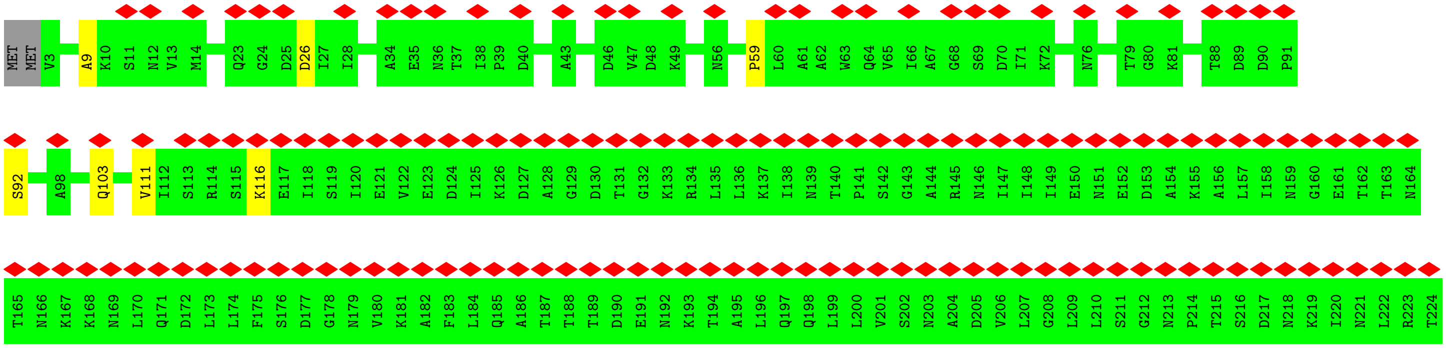


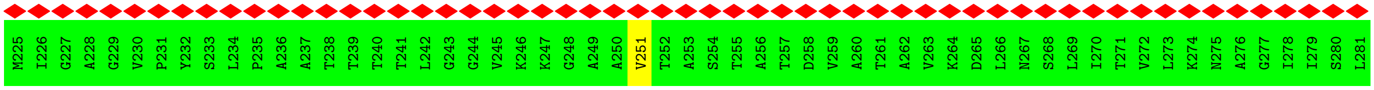


- Molecule 2: Capsid fiber protein

Chain 6k:

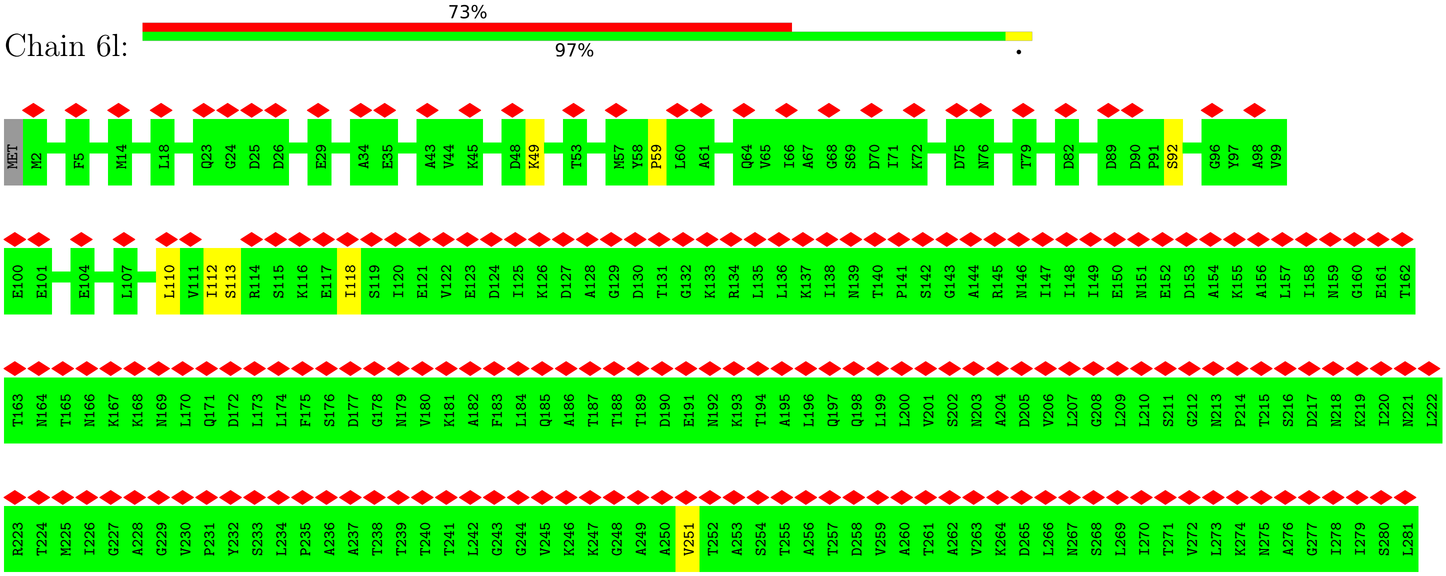






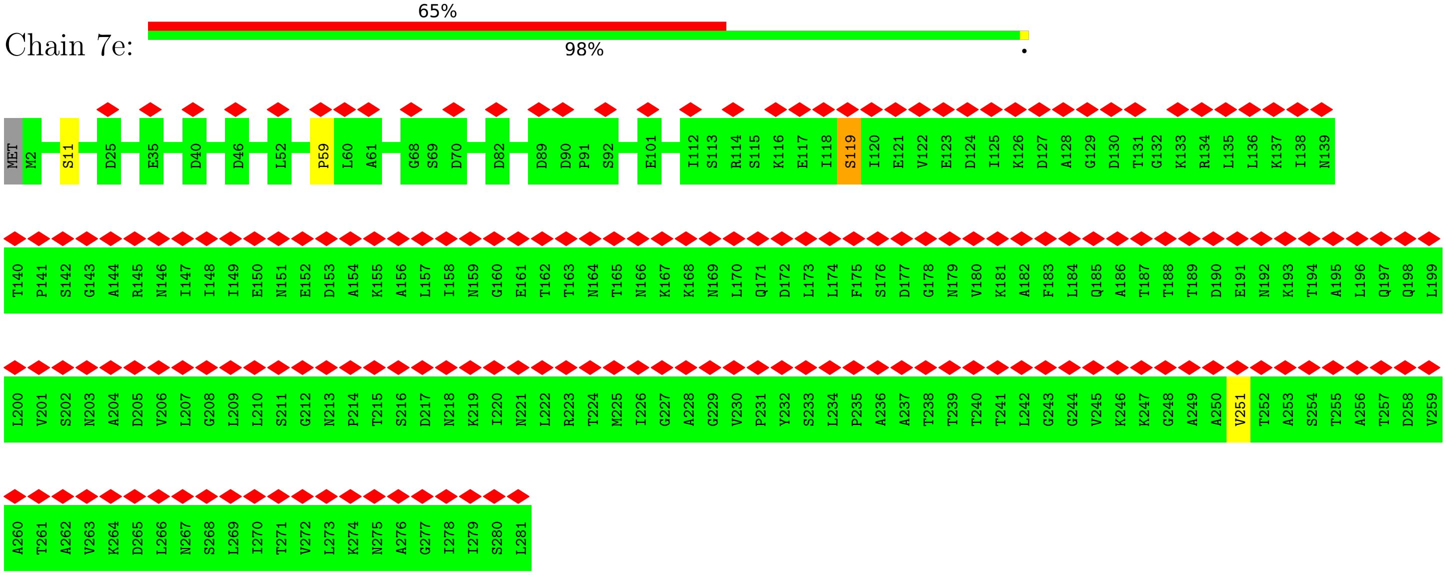
- Molecule 2: Capsid fiber protein

Chain 6l:



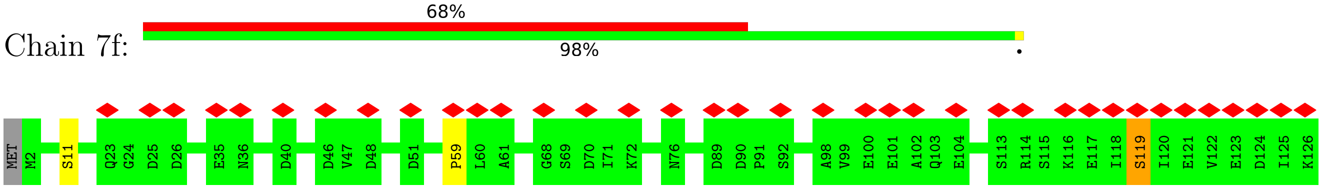
- Molecule 2: Capsid fiber protein

Chain 7e:



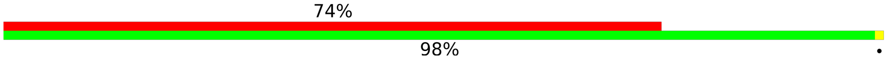
- Molecule 2: Capsid fiber protein

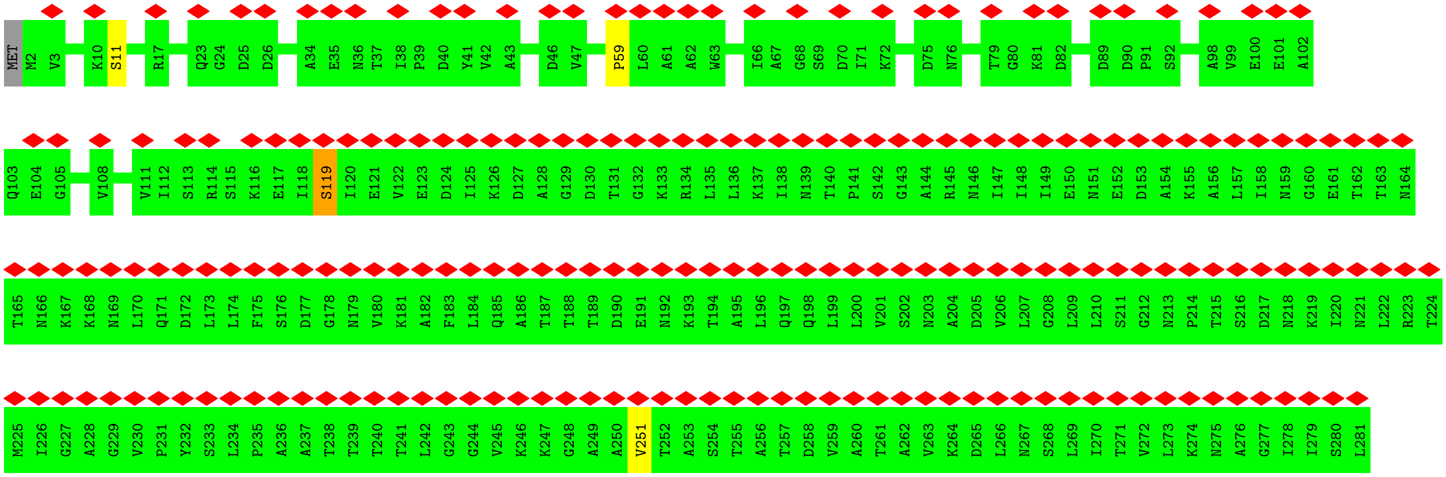
Chain 7f:



• Molecule 2: Capsid fiber protein

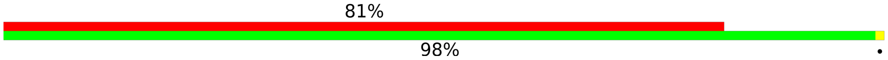
Chain 7g:

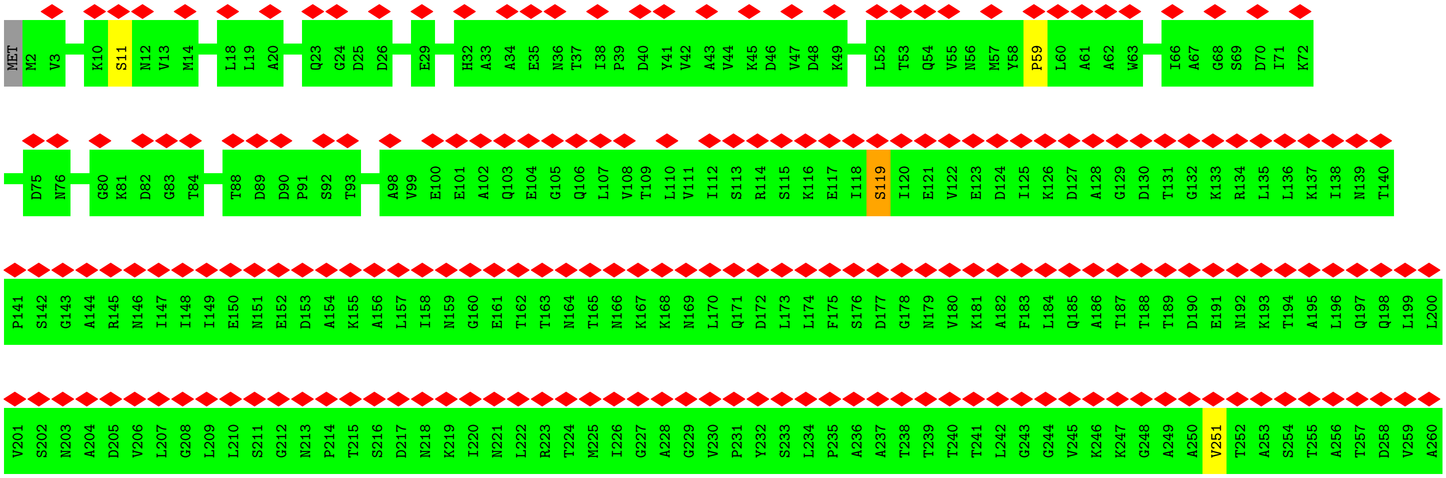


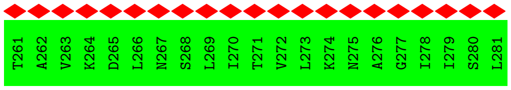


• Molecule 2: Capsid fiber protein

Chain 7h:

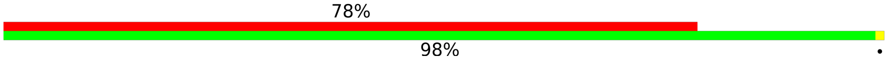


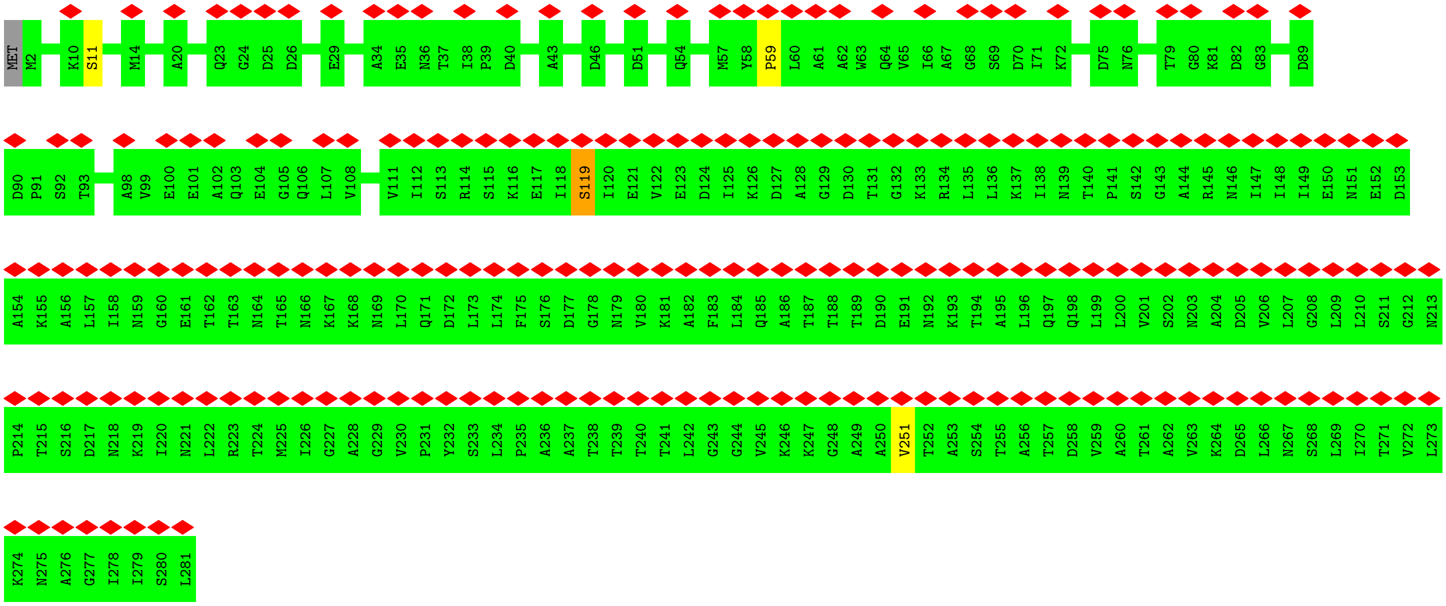




- Molecule 2: Capsid fiber protein

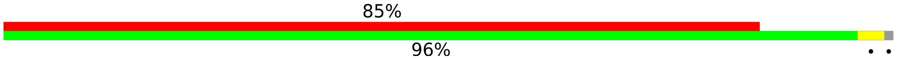
Chain 7i:

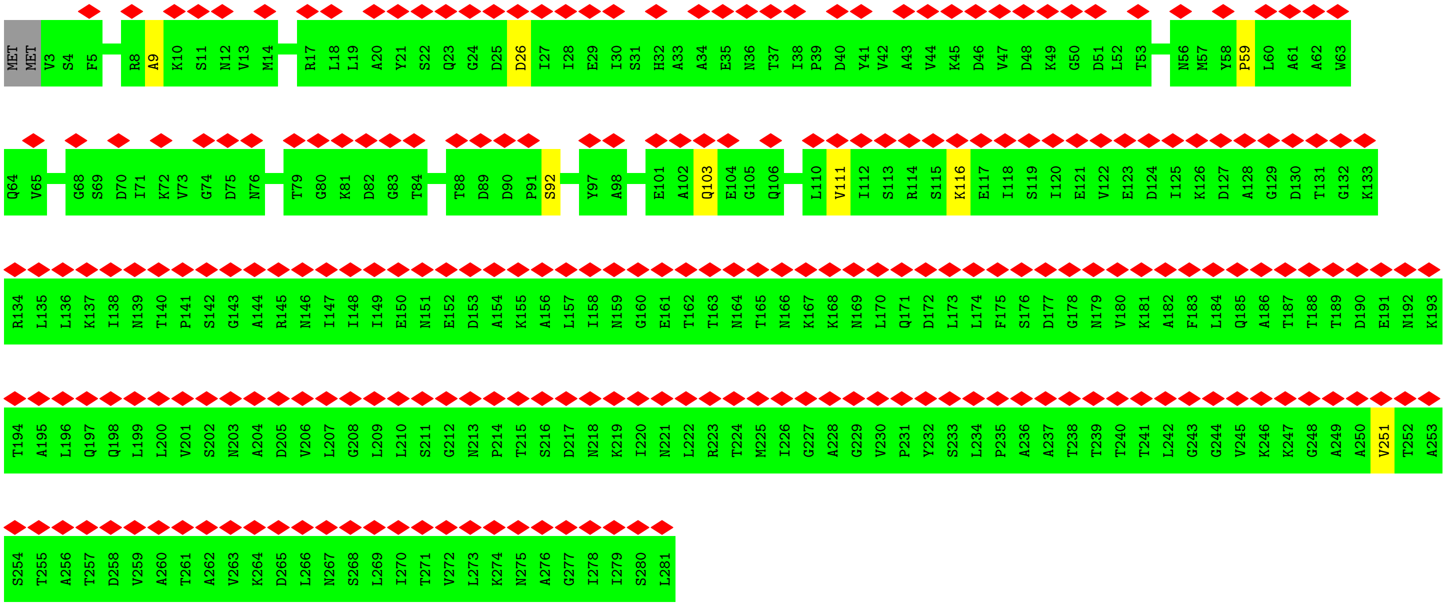




- Molecule 2: Capsid fiber protein

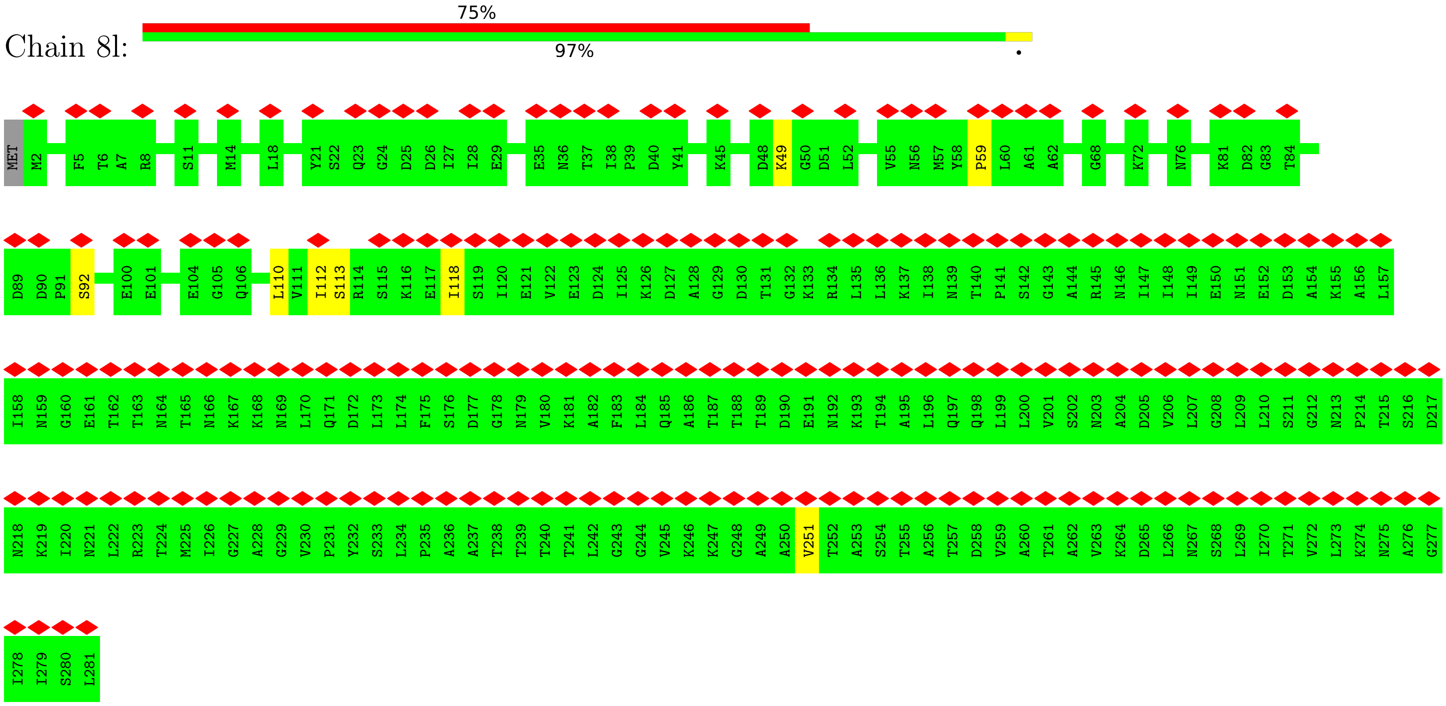
Chain 8k:





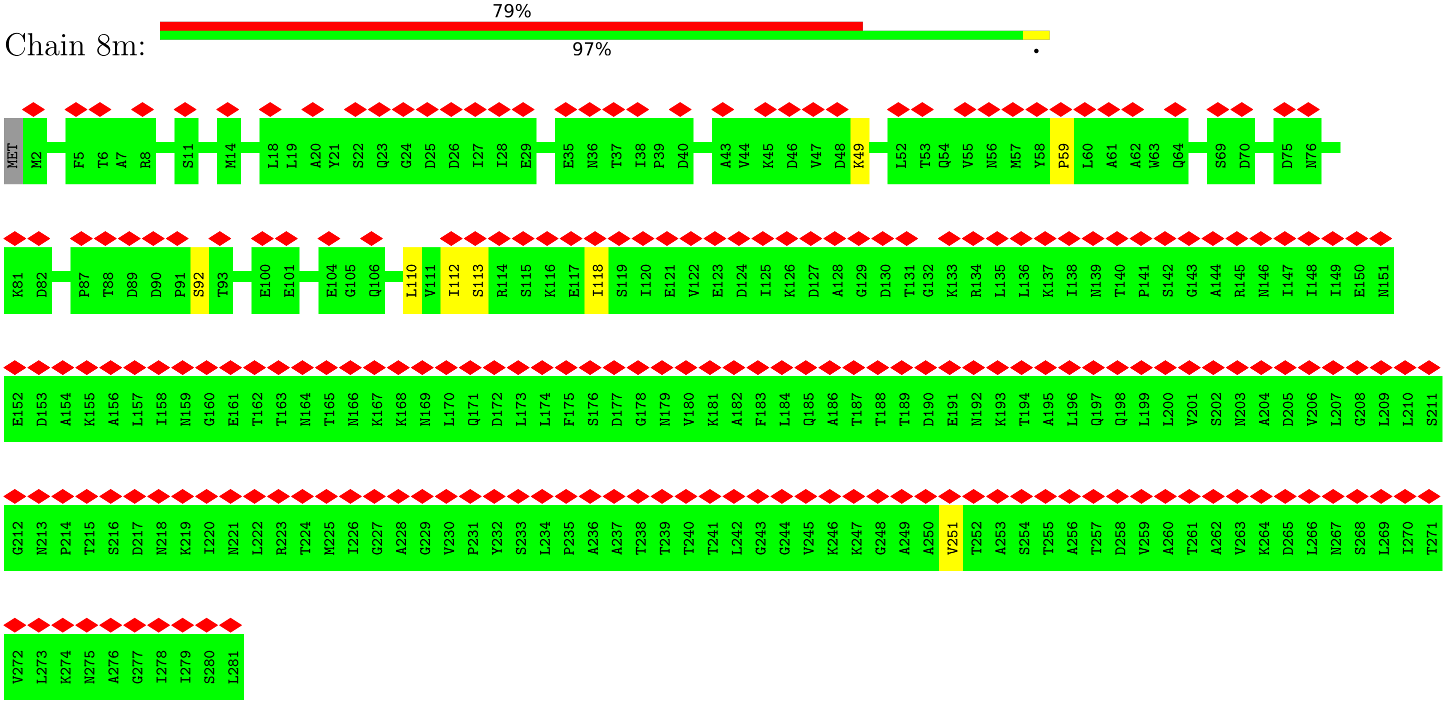
- Molecule 2: Capsid fiber protein

Chain 8l:



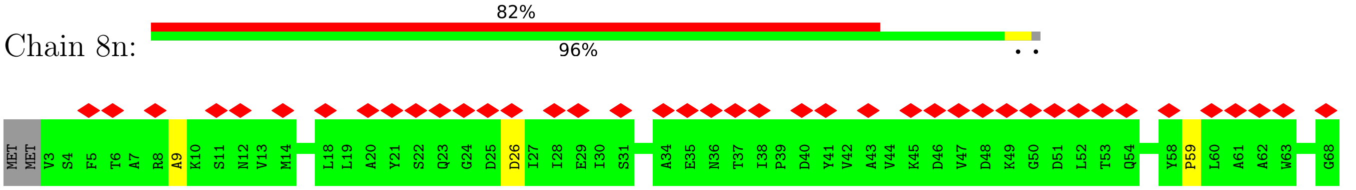
- Molecule 2: Capsid fiber protein

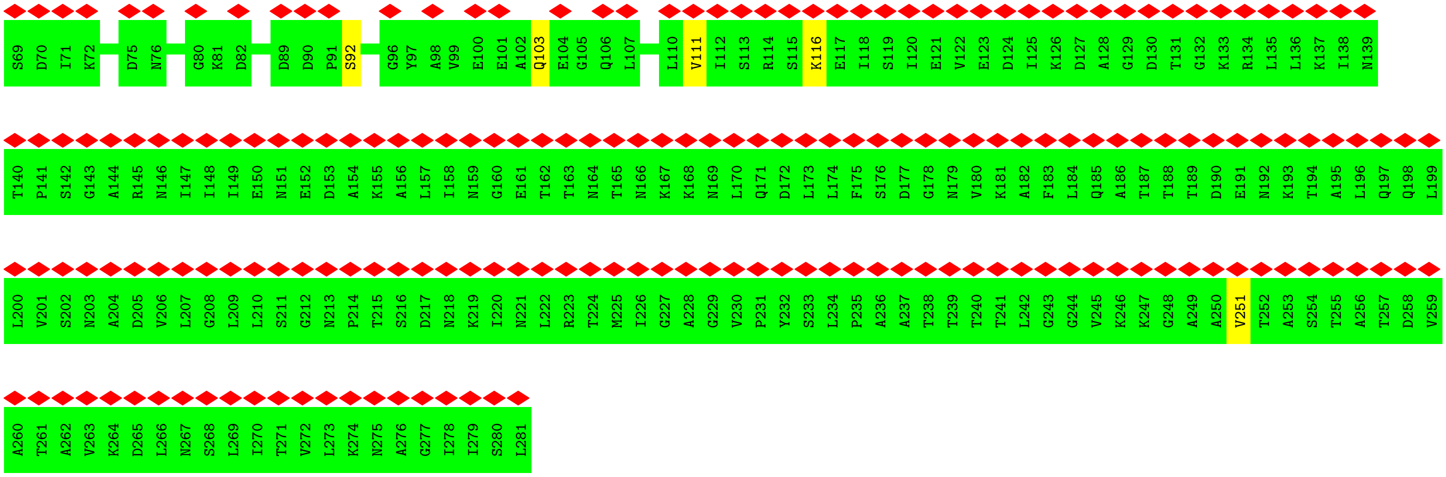
Chain 8m:



- Molecule 2: Capsid fiber protein

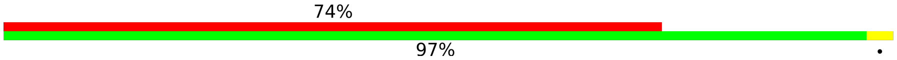
Chain 8n:

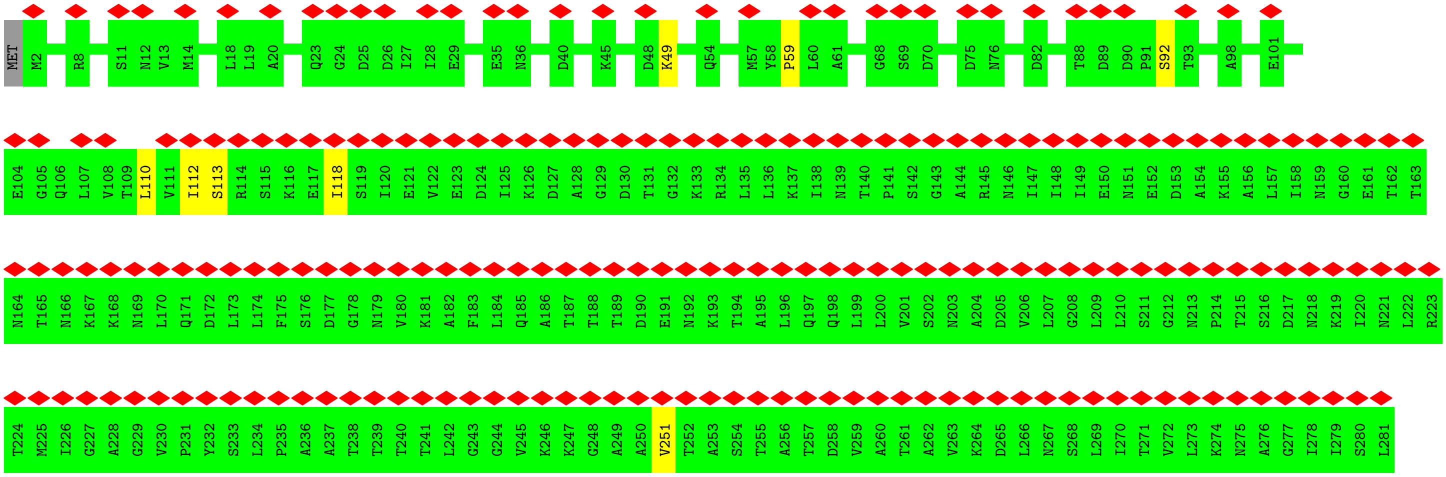




- Molecule 2: Capsid fiber protein

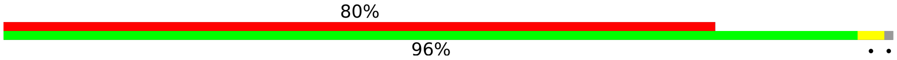
Chain 8o:

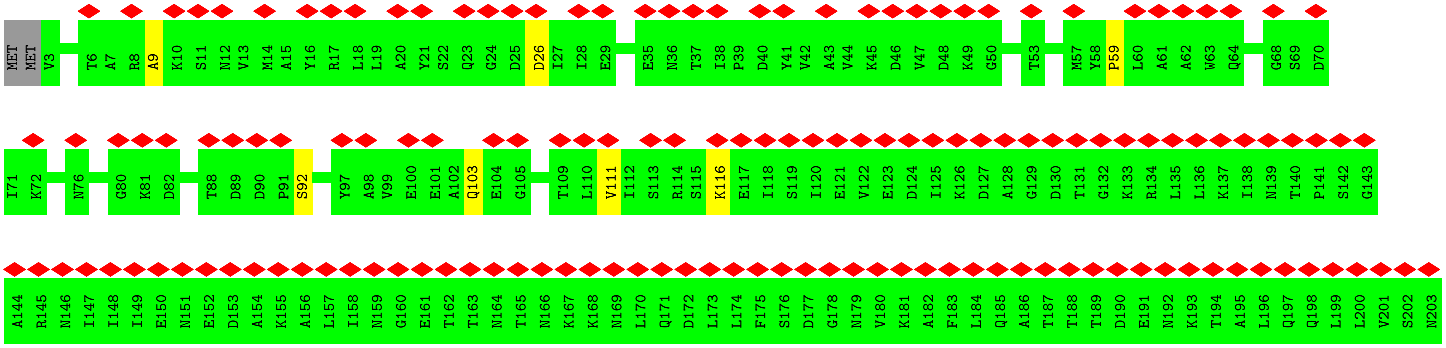


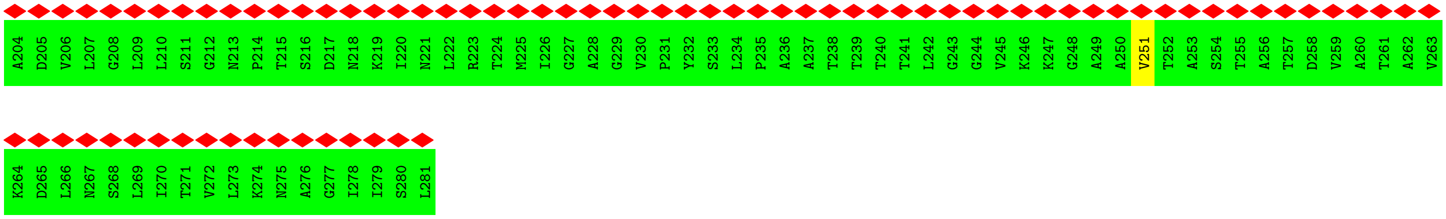


- Molecule 2: Capsid fiber protein

Chain 8p:

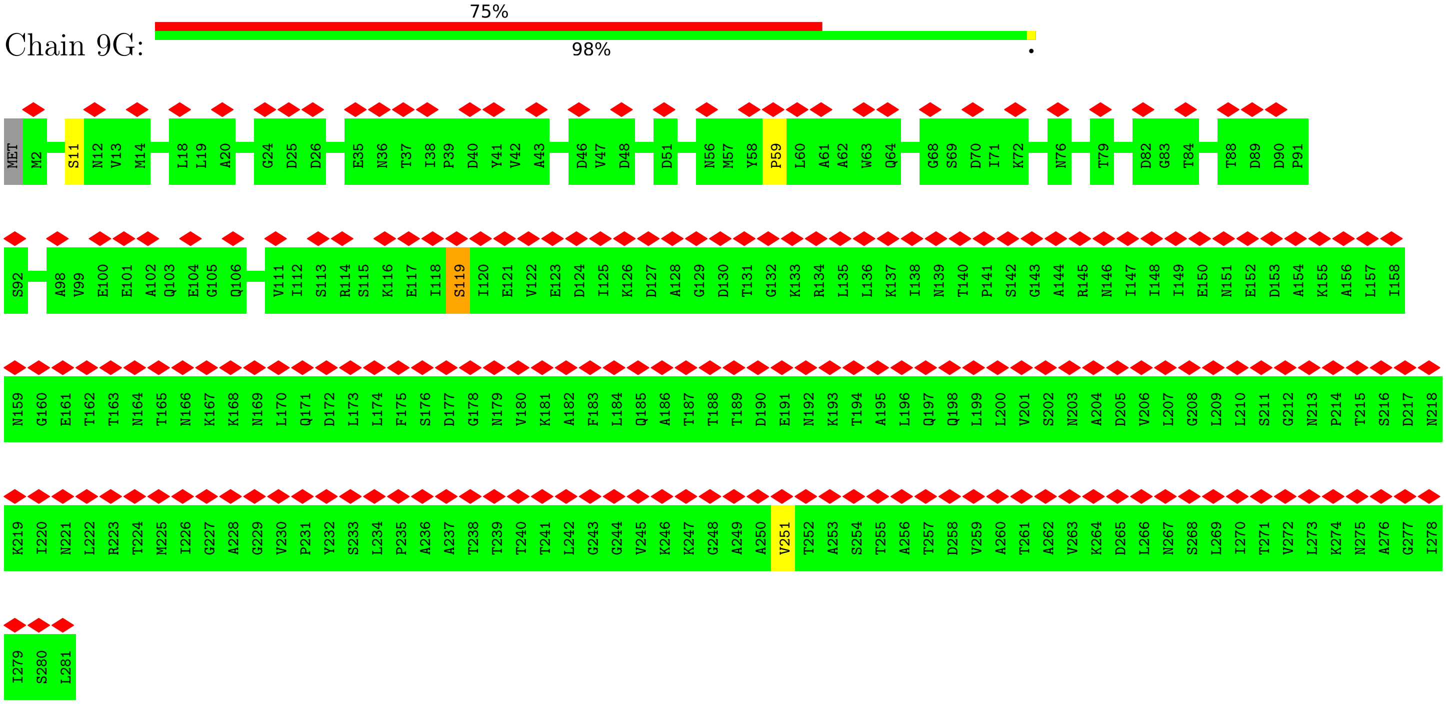






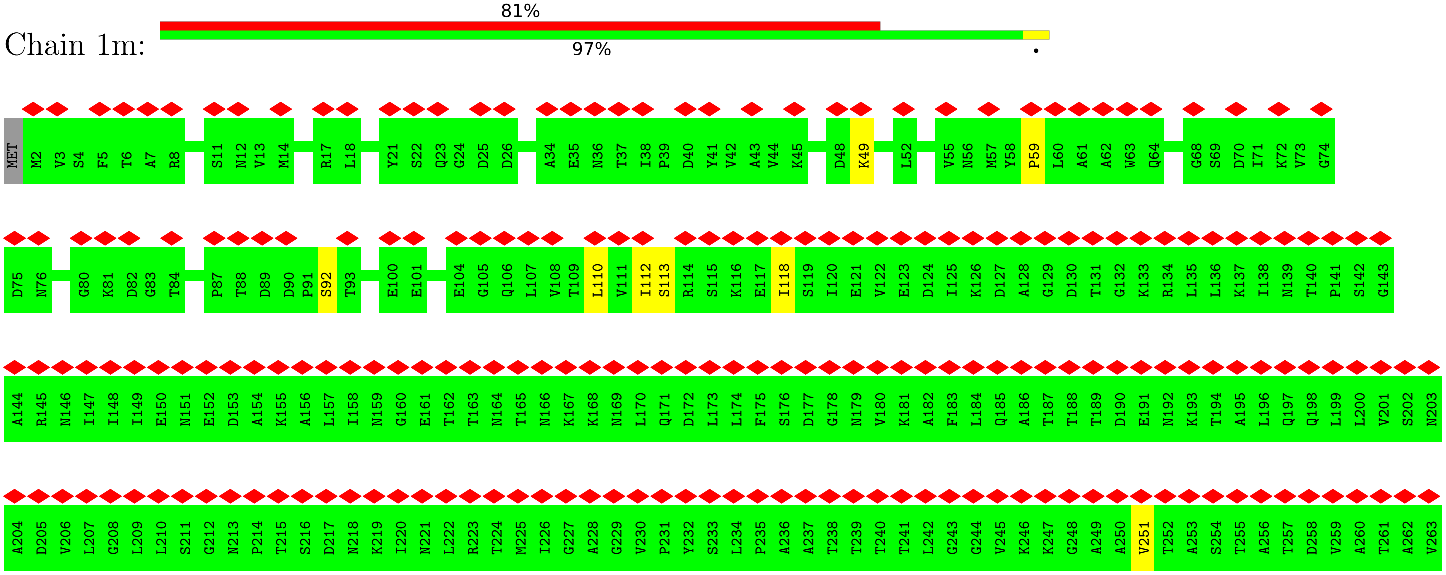
- Molecule 2: Capsid fiber protein

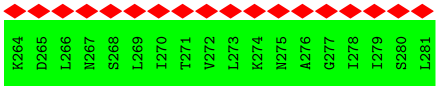
Chain 9G:



- Molecule 2: Capsid fiber protein

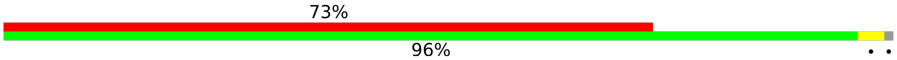
Chain 1m:

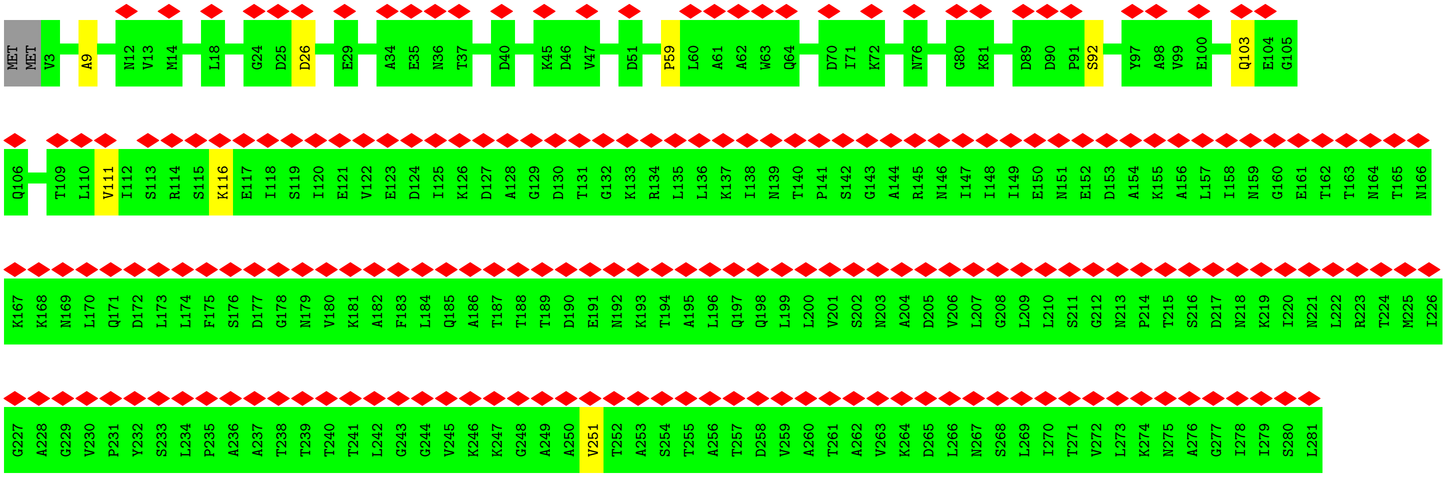




- Molecule 2: Capsid fiber protein

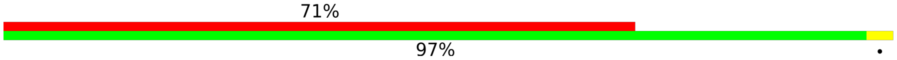
Chain 1n:

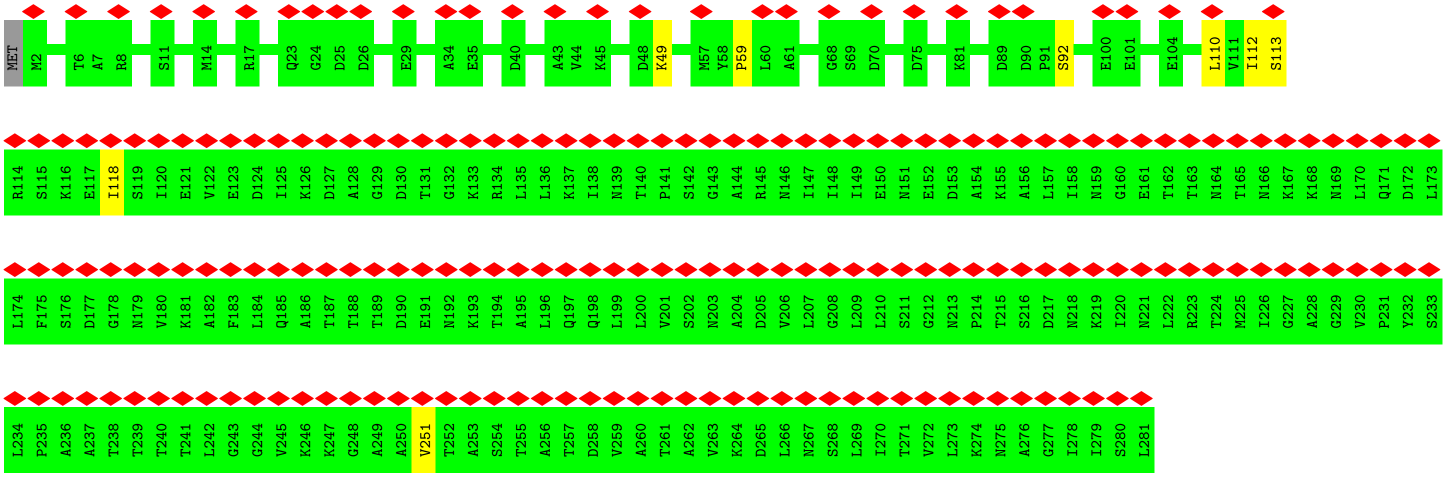




- Molecule 2: Capsid fiber protein

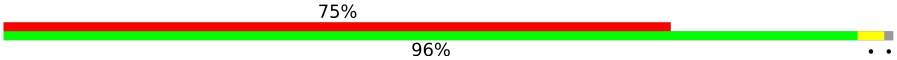
Chain 1o:

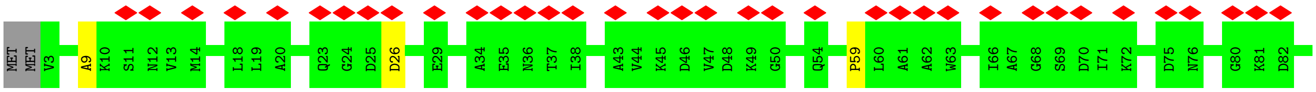


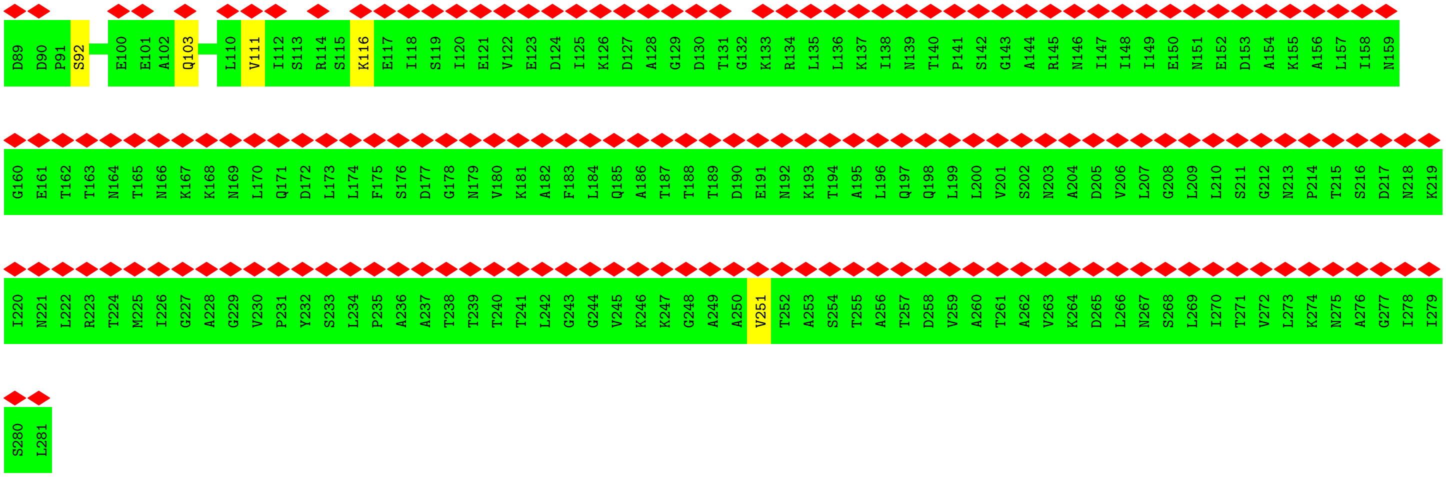


- Molecule 2: Capsid fiber protein

Chain 1p:

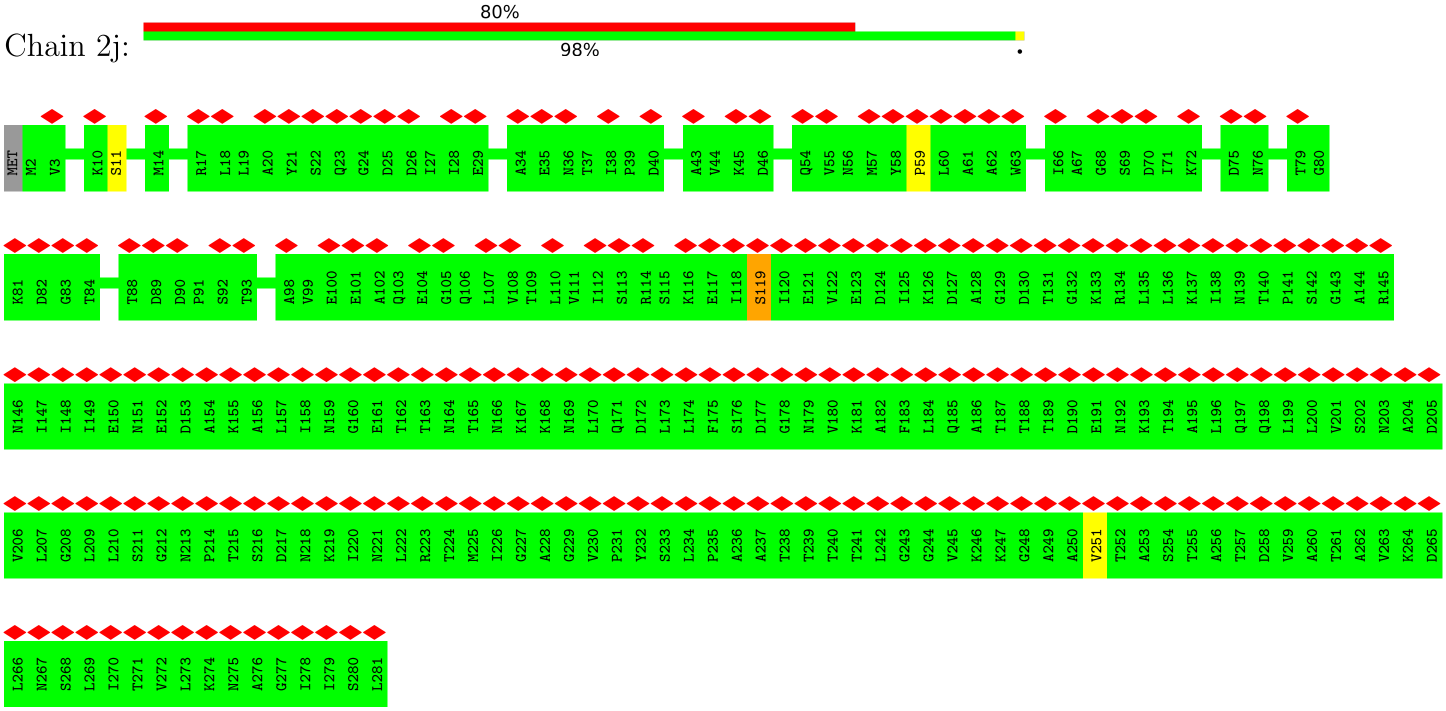






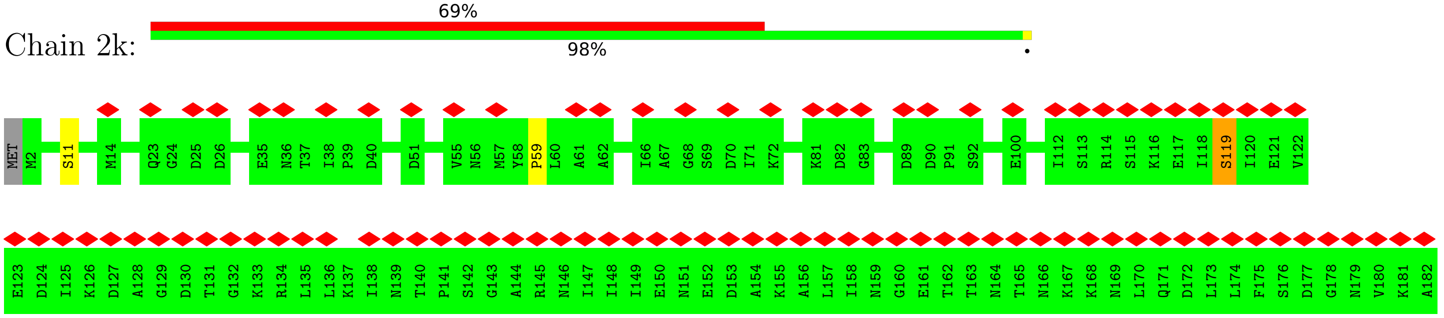
- Molecule 2: Capsid fiber protein

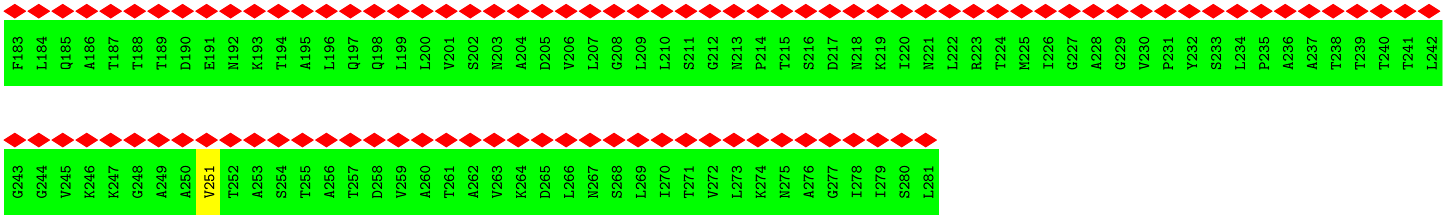
Chain 2j:



- Molecule 2: Capsid fiber protein

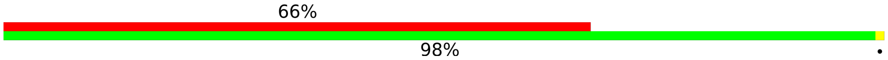
Chain 2k:

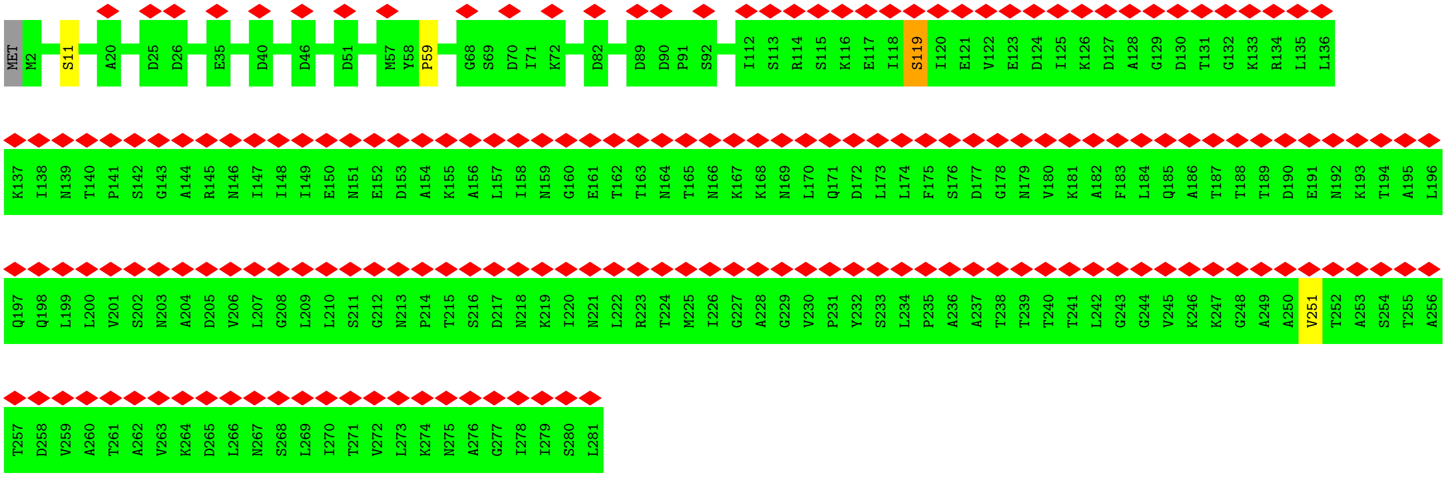




- Molecule 2: Capsid fiber protein

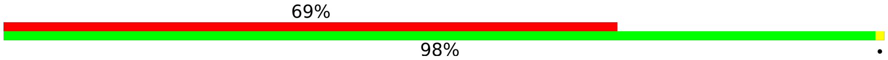
Chain 2l:

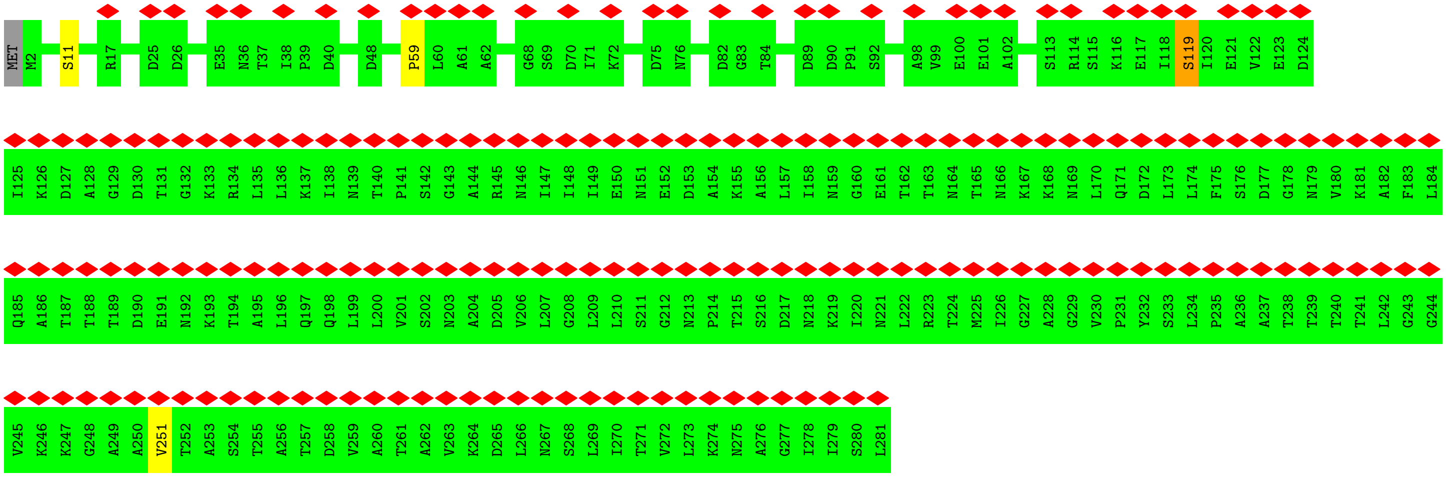




- Molecule 2: Capsid fiber protein

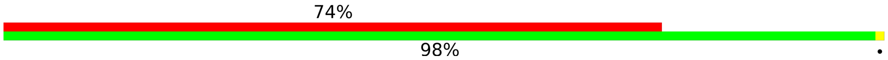
Chain 2m:

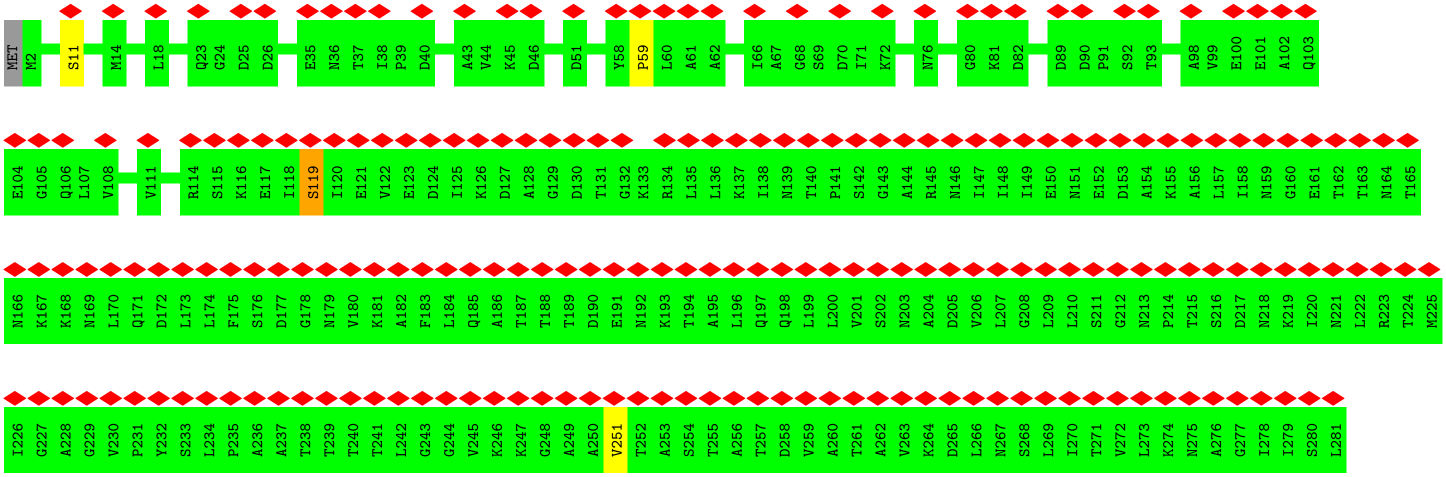




- Molecule 2: Capsid fiber protein

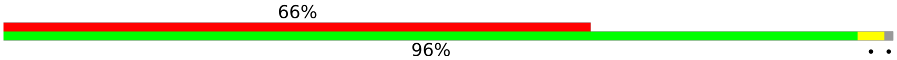
Chain 2n:

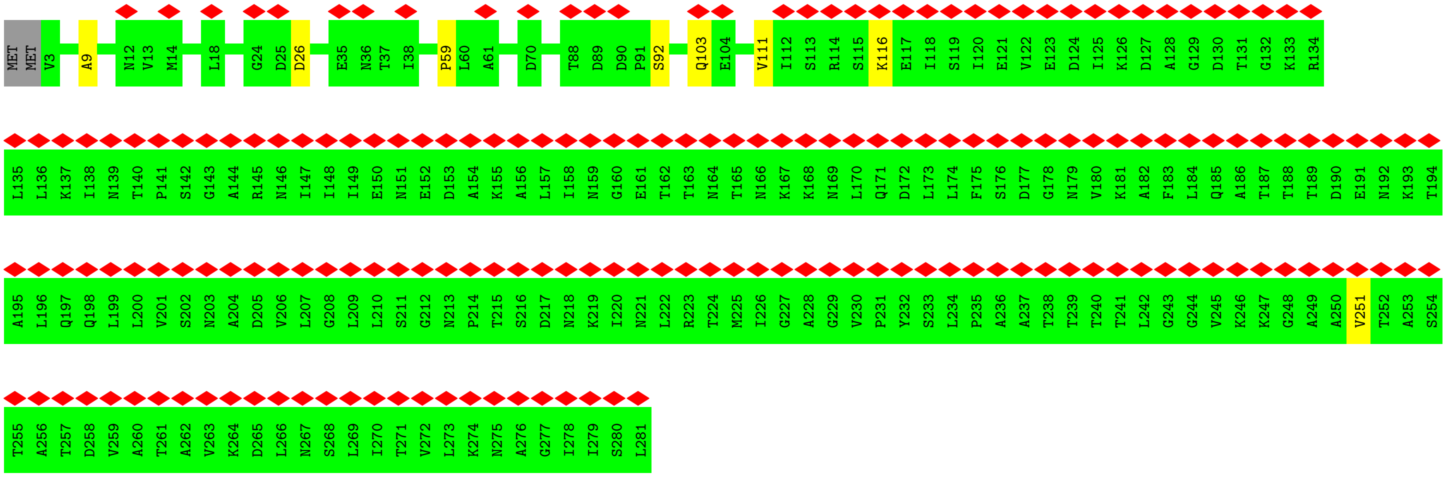




- Molecule 2: Capsid fiber protein

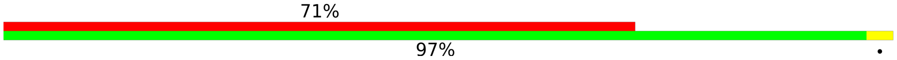
Chain 3m:

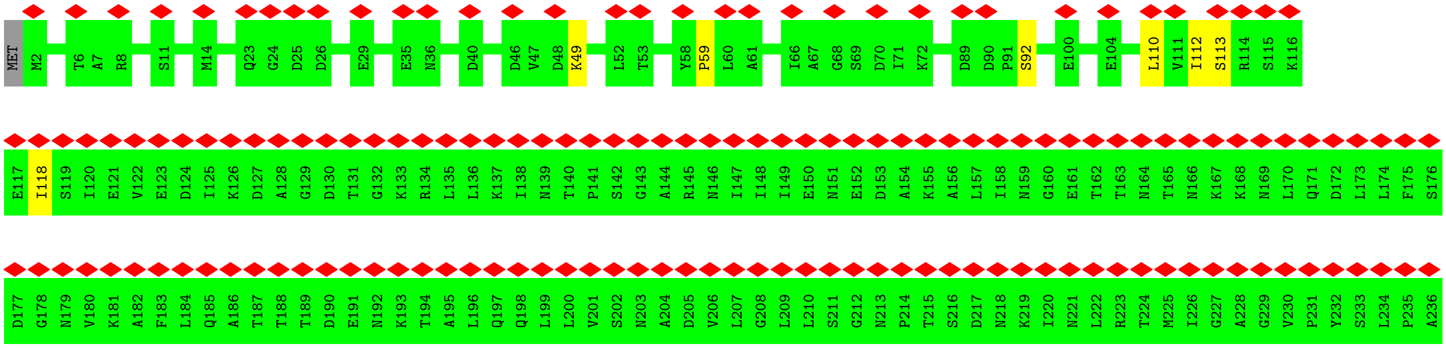


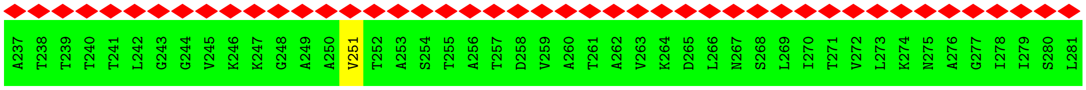


- Molecule 2: Capsid fiber protein

Chain 3n:

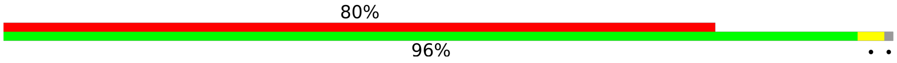


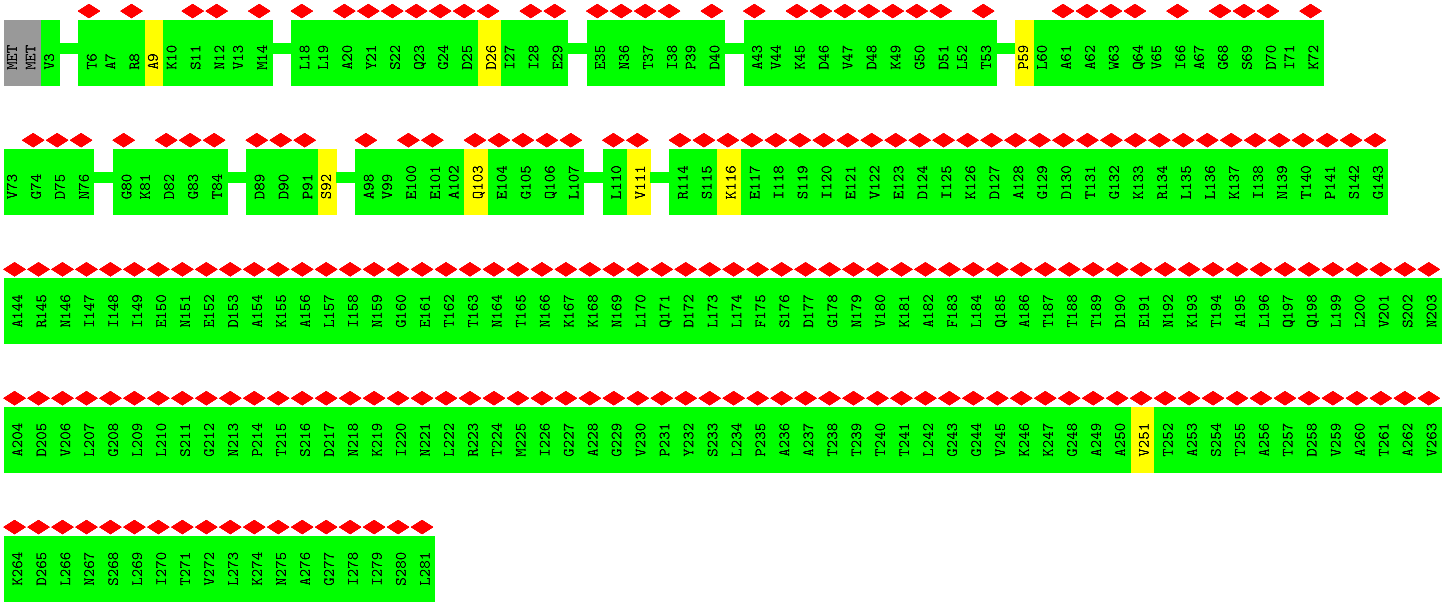




- Molecule 2: Capsid fiber protein

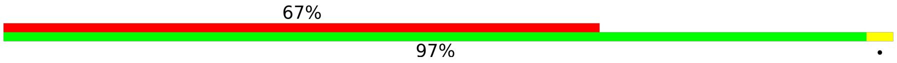
Chain 3o:

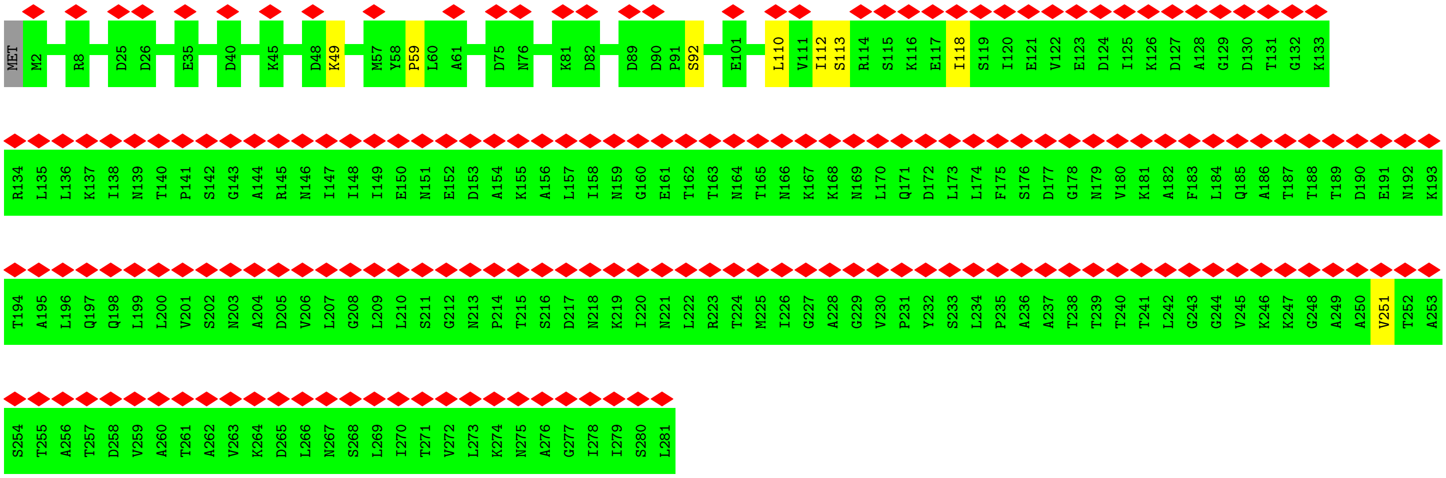




- Molecule 2: Capsid fiber protein

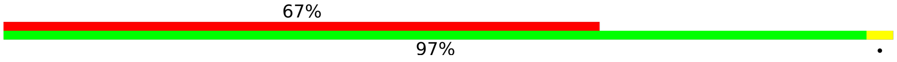
Chain 3p:

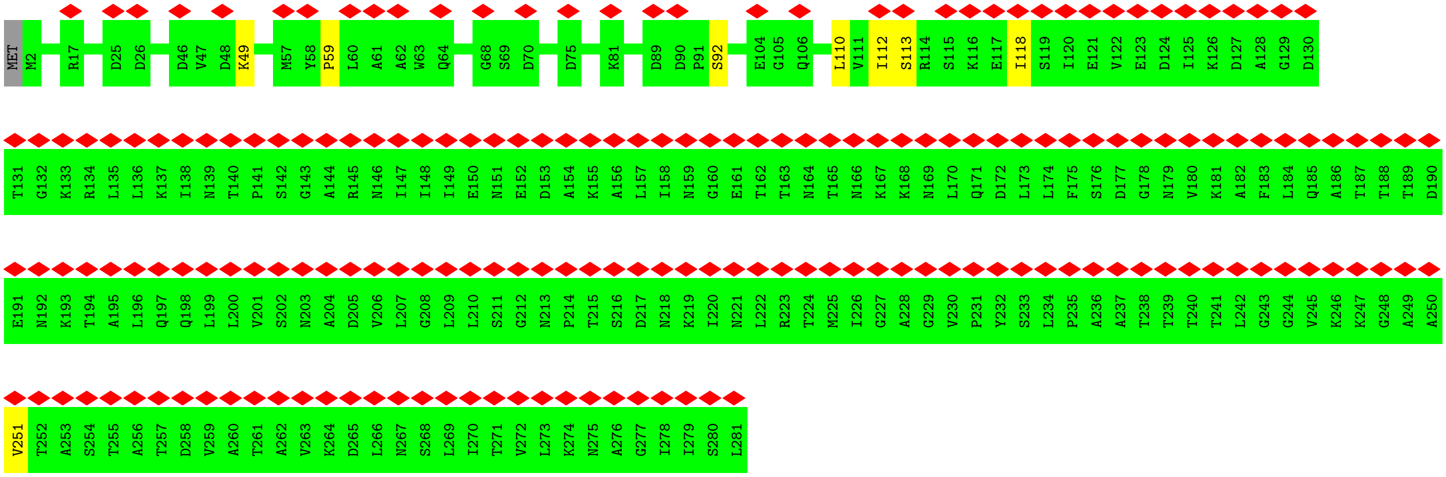




- Molecule 2: Capsid fiber protein

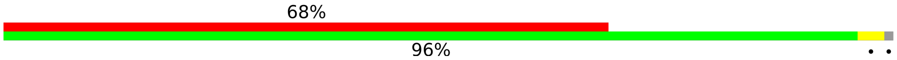
Chain 4i:

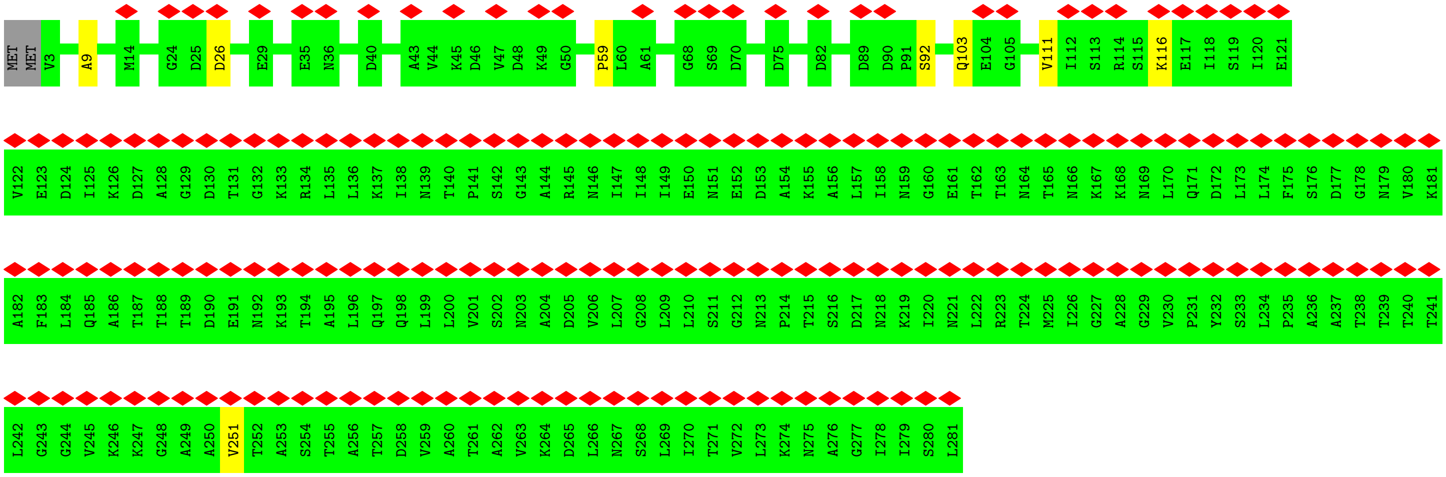




- Molecule 2: Capsid fiber protein

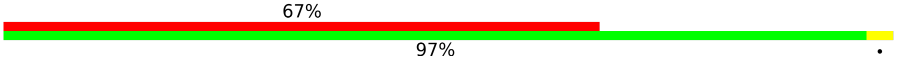
Chain 4j:

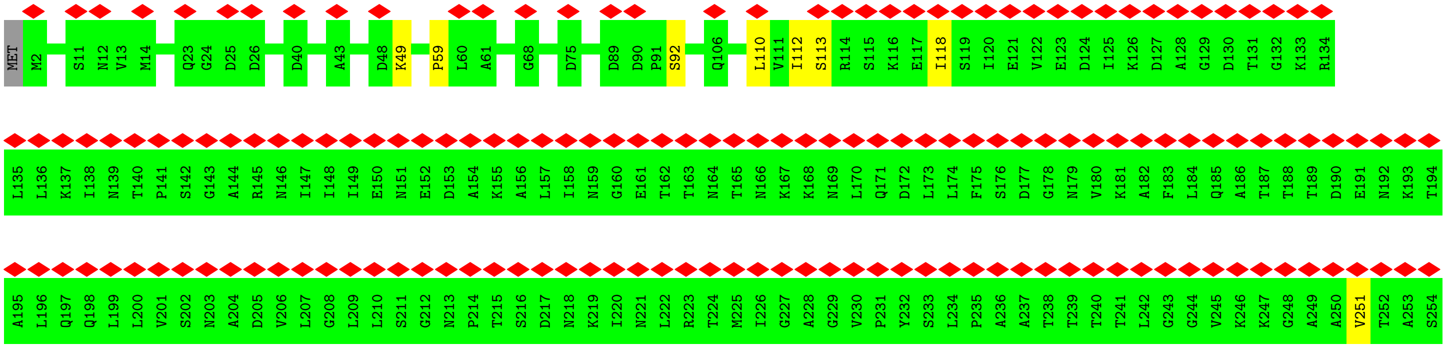


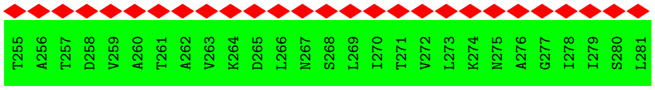


- Molecule 2: Capsid fiber protein

Chain 5i:

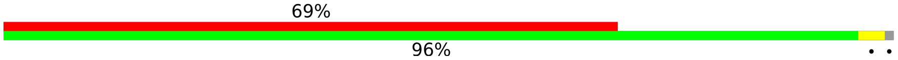


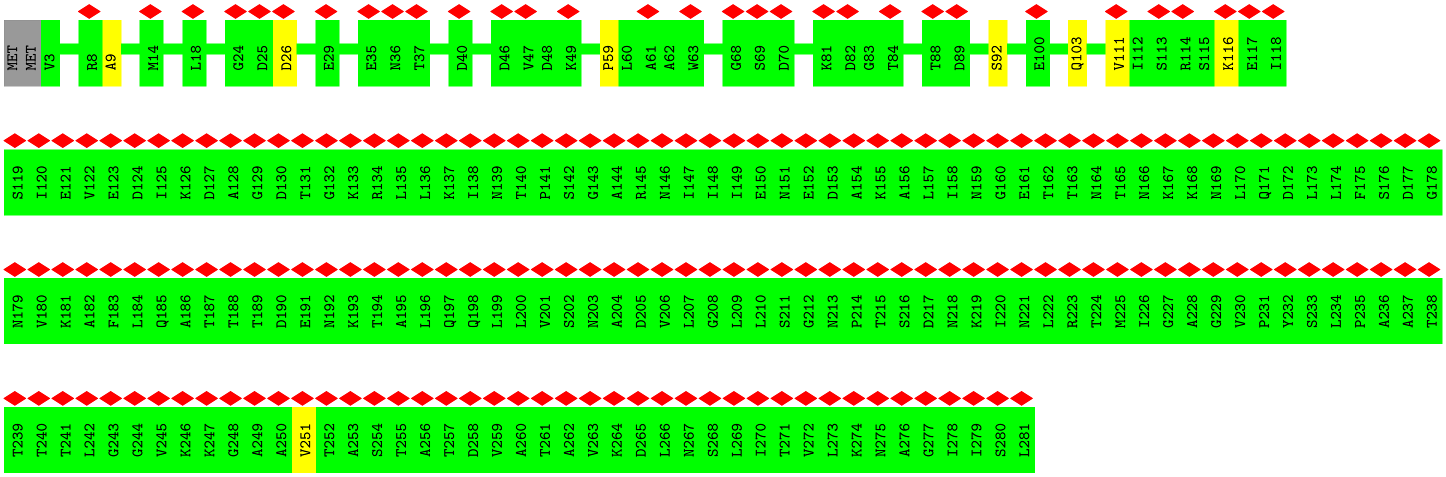




- Molecule 2: Capsid fiber protein

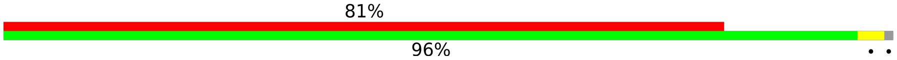
Chain 5j:

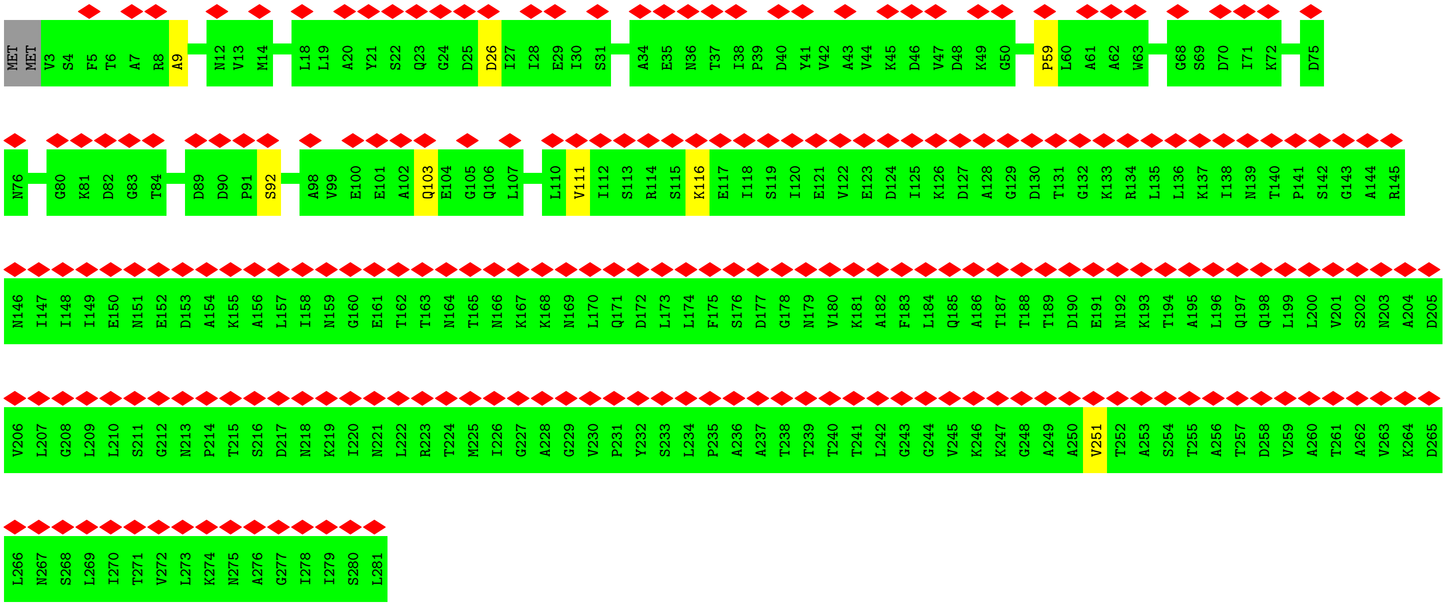




- Molecule 2: Capsid fiber protein

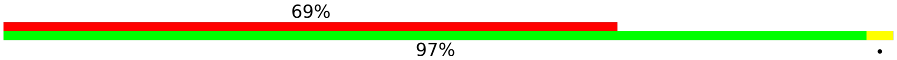
Chain 6m:

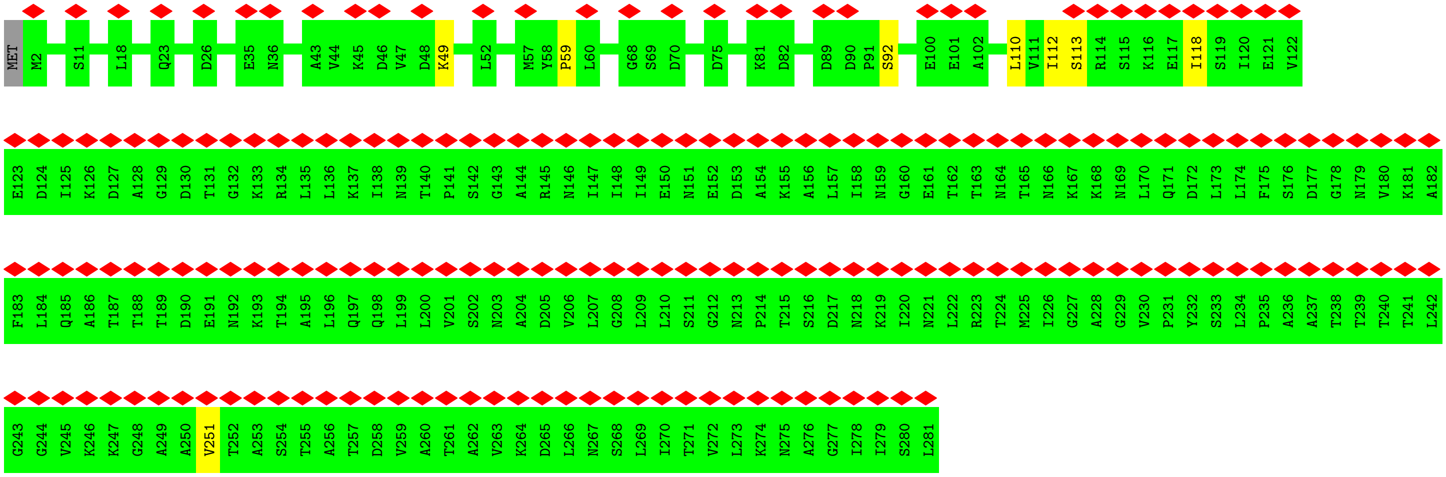




- Molecule 2: Capsid fiber protein

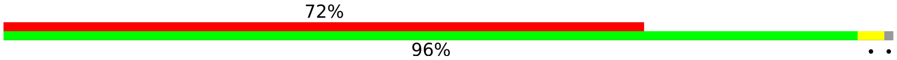
Chain 6n:

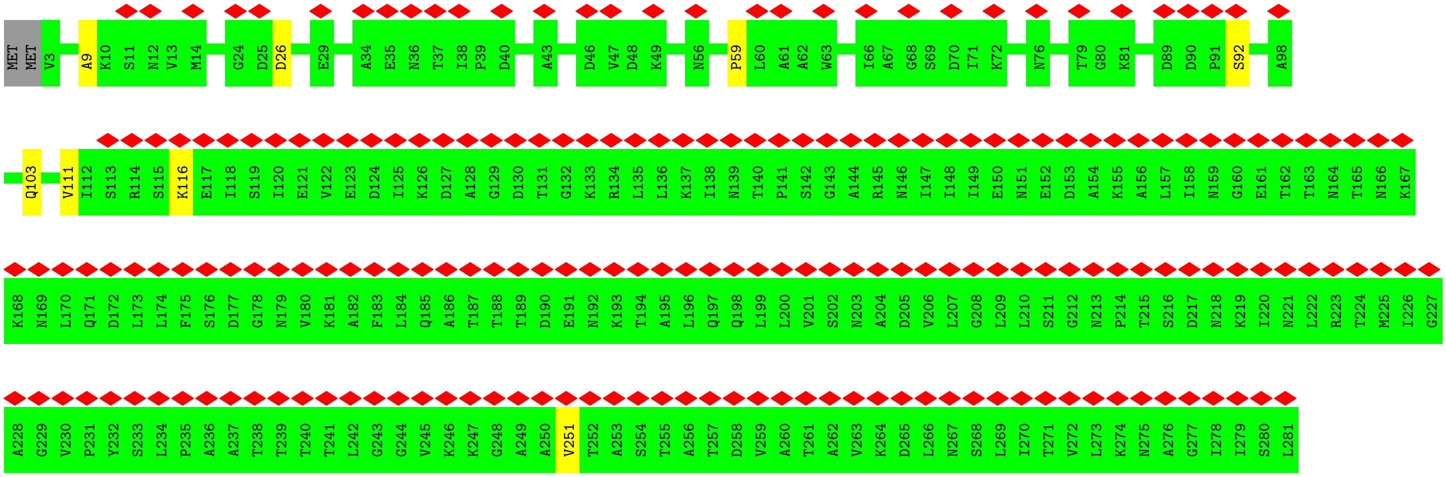




- Molecule 2: Capsid fiber protein

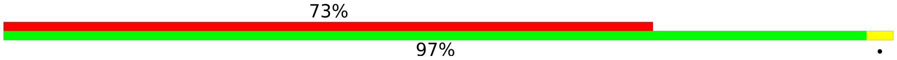
Chain 6o:

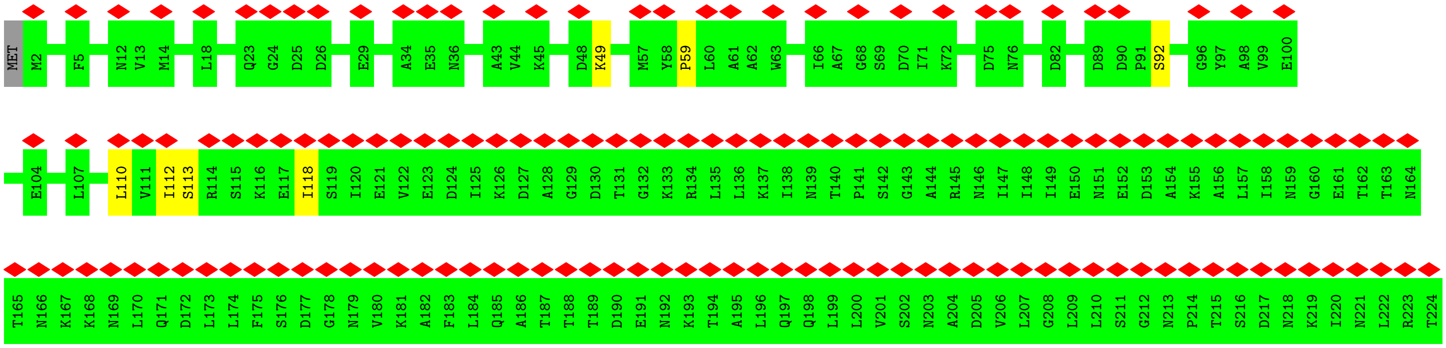


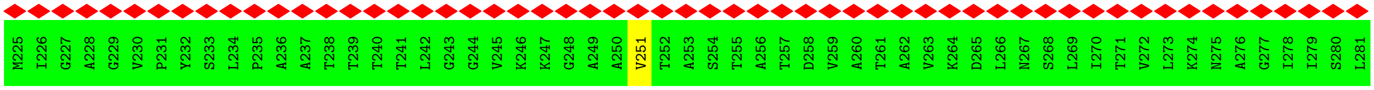


- Molecule 2: Capsid fiber protein

Chain 6p:

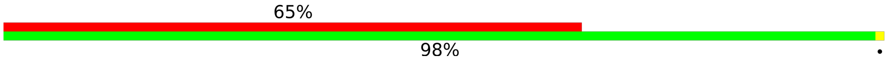


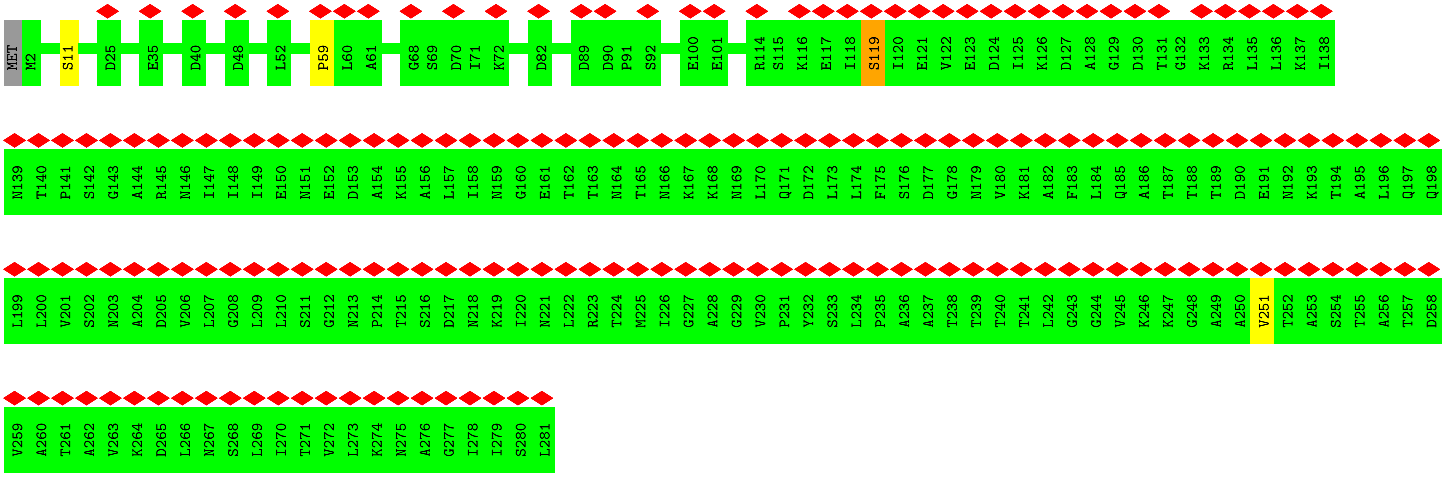




- Molecule 2: Capsid fiber protein

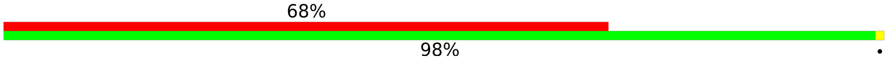
Chain 7j:

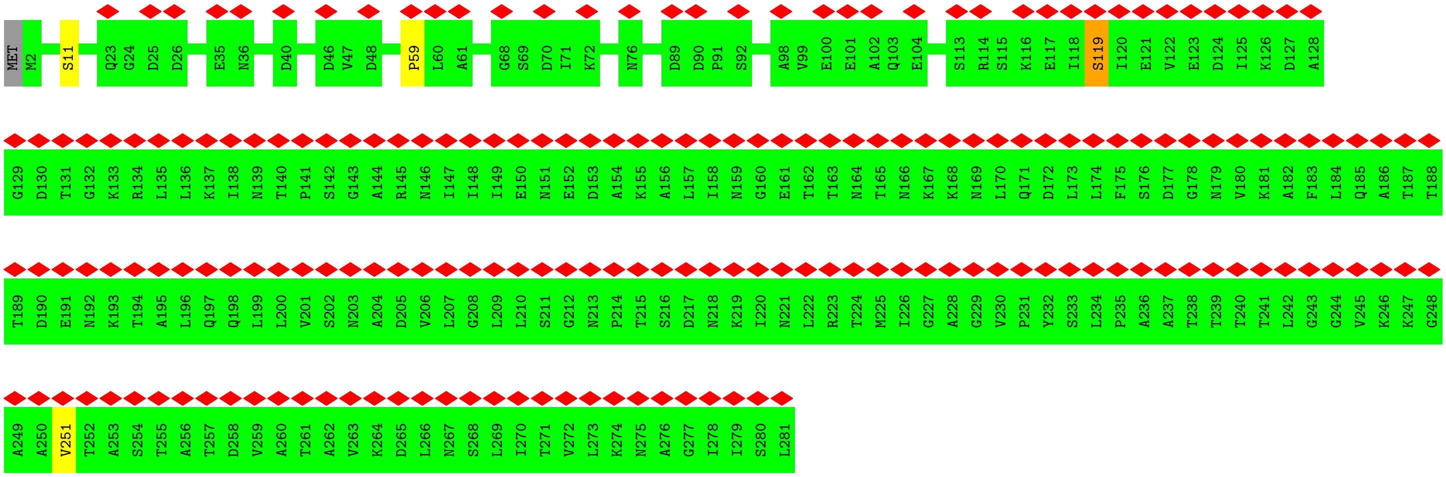




- Molecule 2: Capsid fiber protein

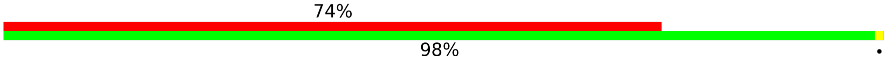
Chain 7k:

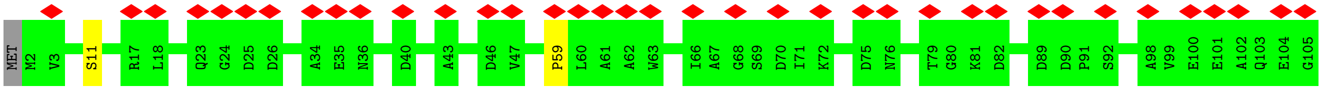


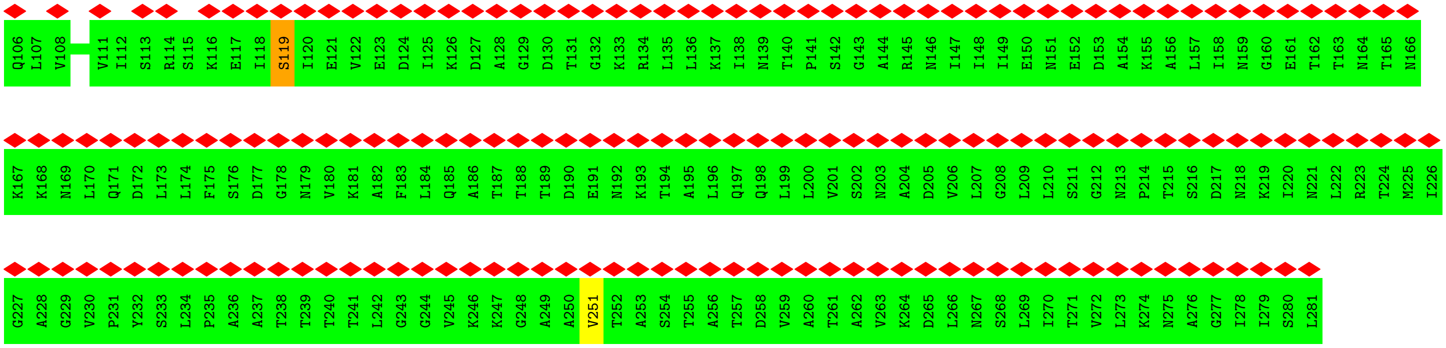


- Molecule 2: Capsid fiber protein

Chain 7l:

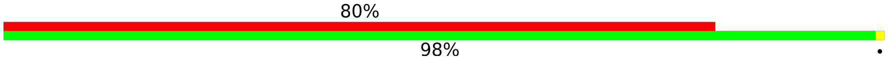


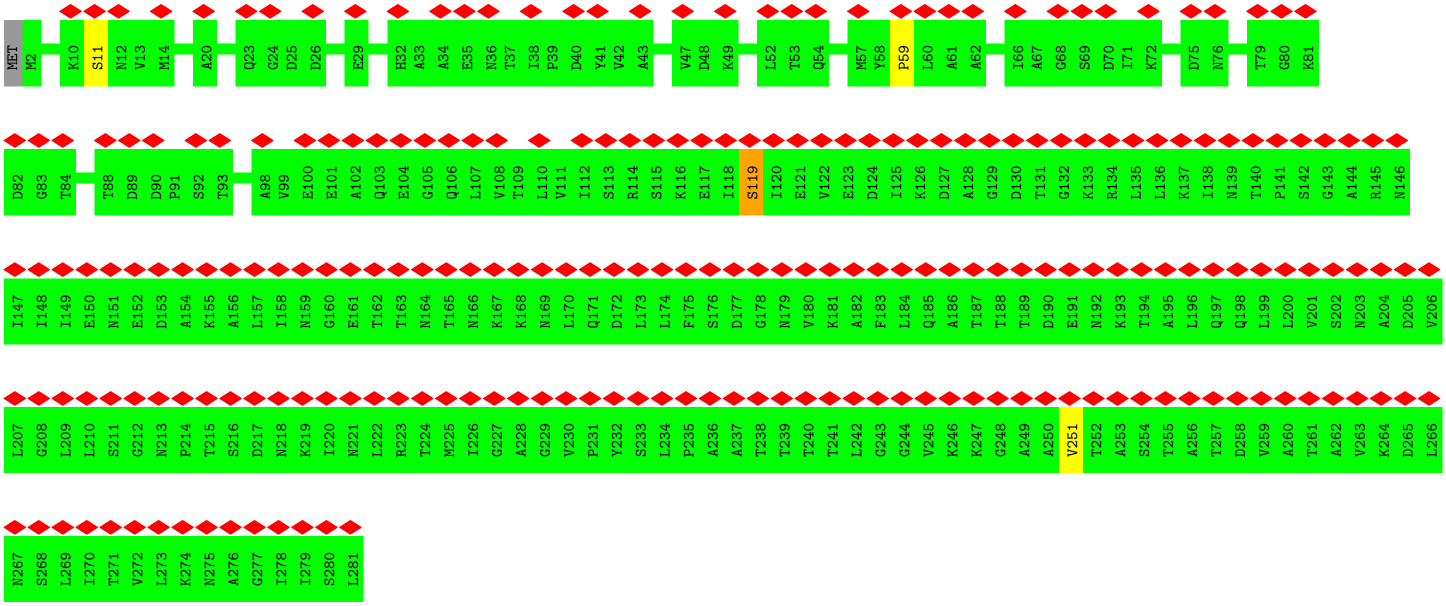




- Molecule 2: Capsid fiber protein

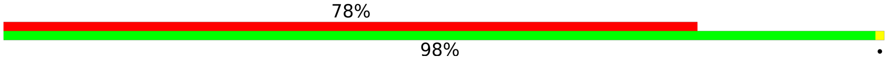
Chain 7m:

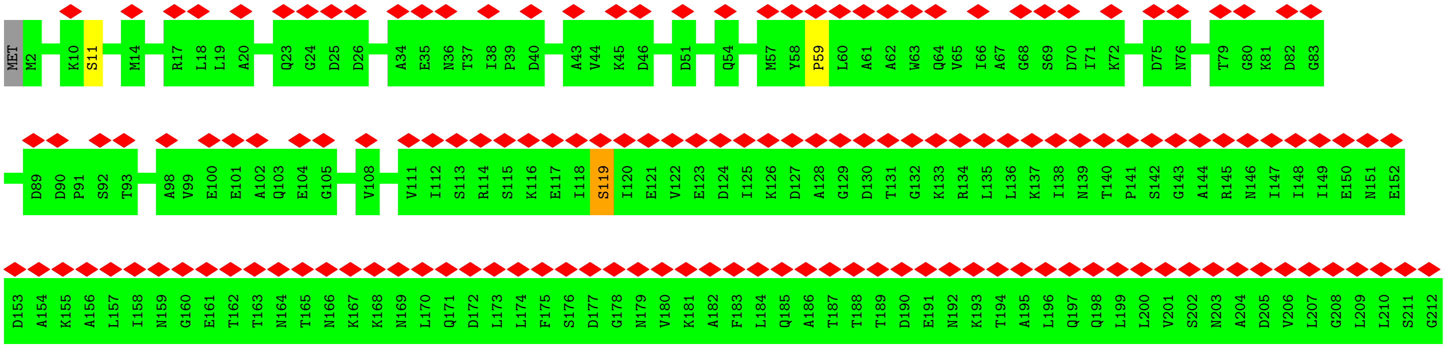


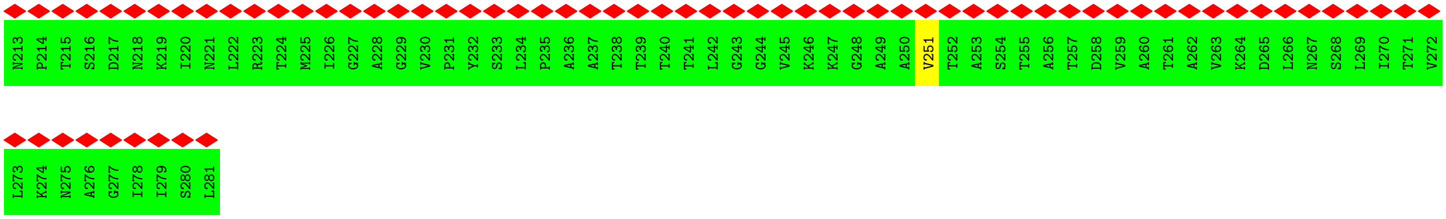


- Molecule 2: Capsid fiber protein

Chain 7n:

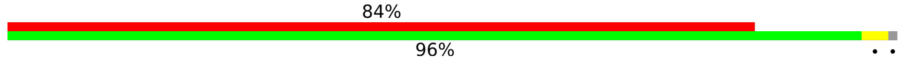


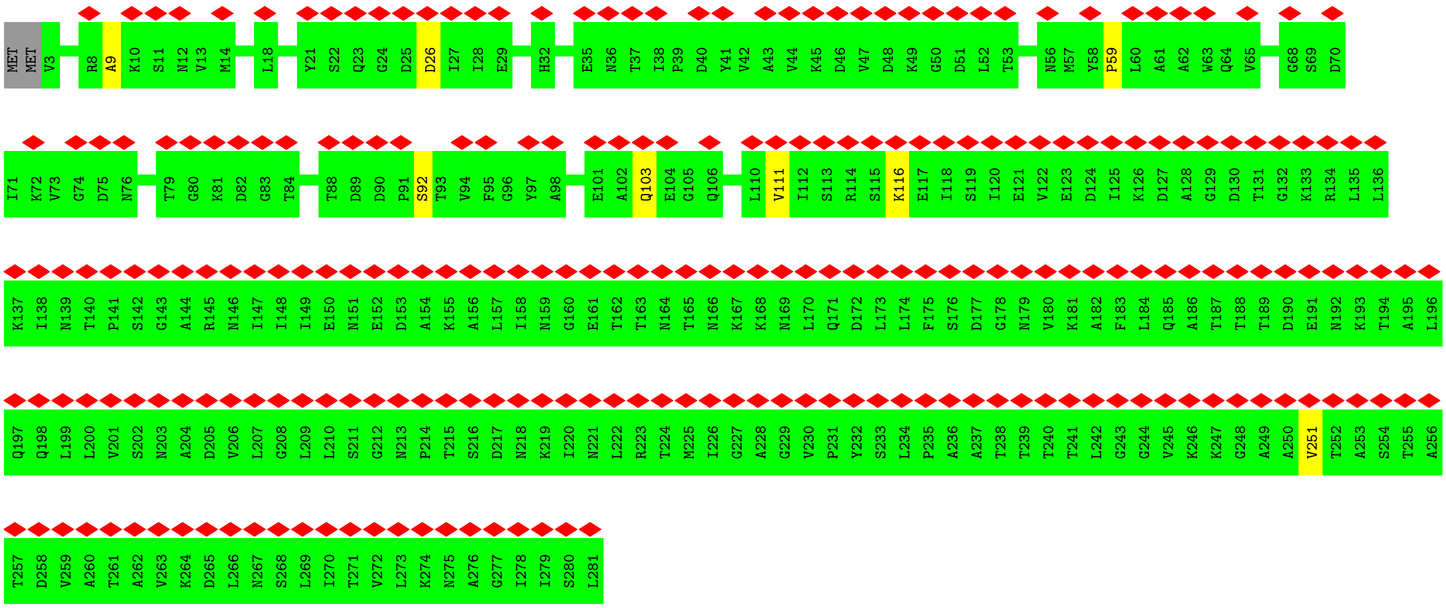




- Molecule 2: Capsid fiber protein

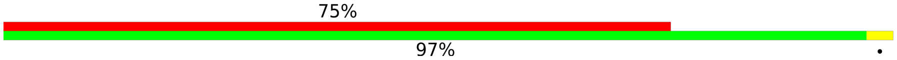
Chain 8q:

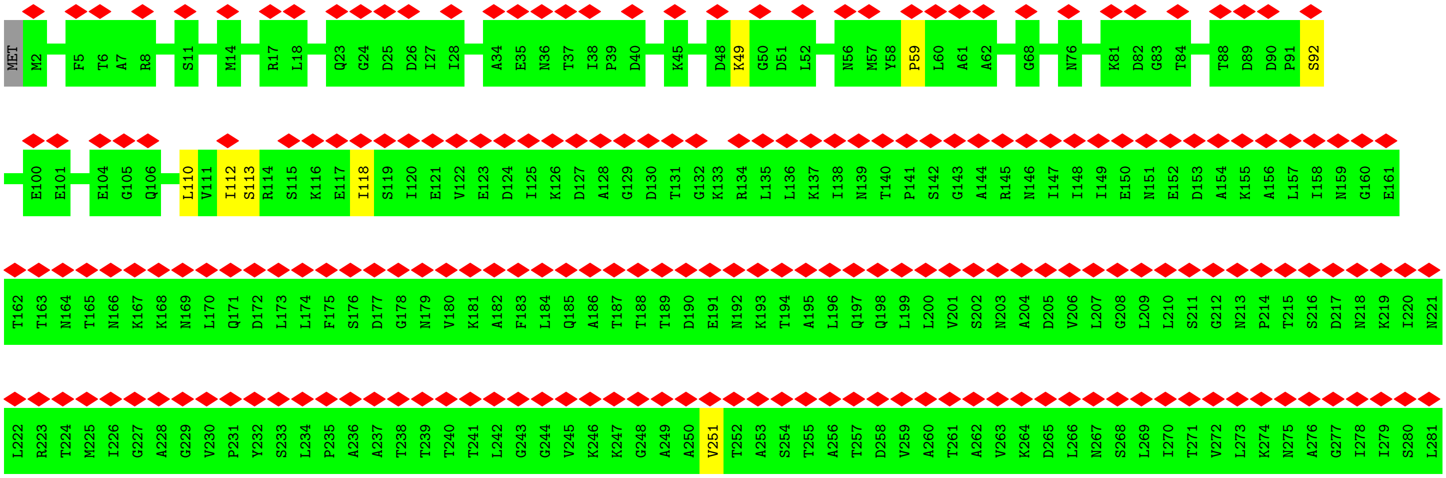




- Molecule 2: Capsid fiber protein

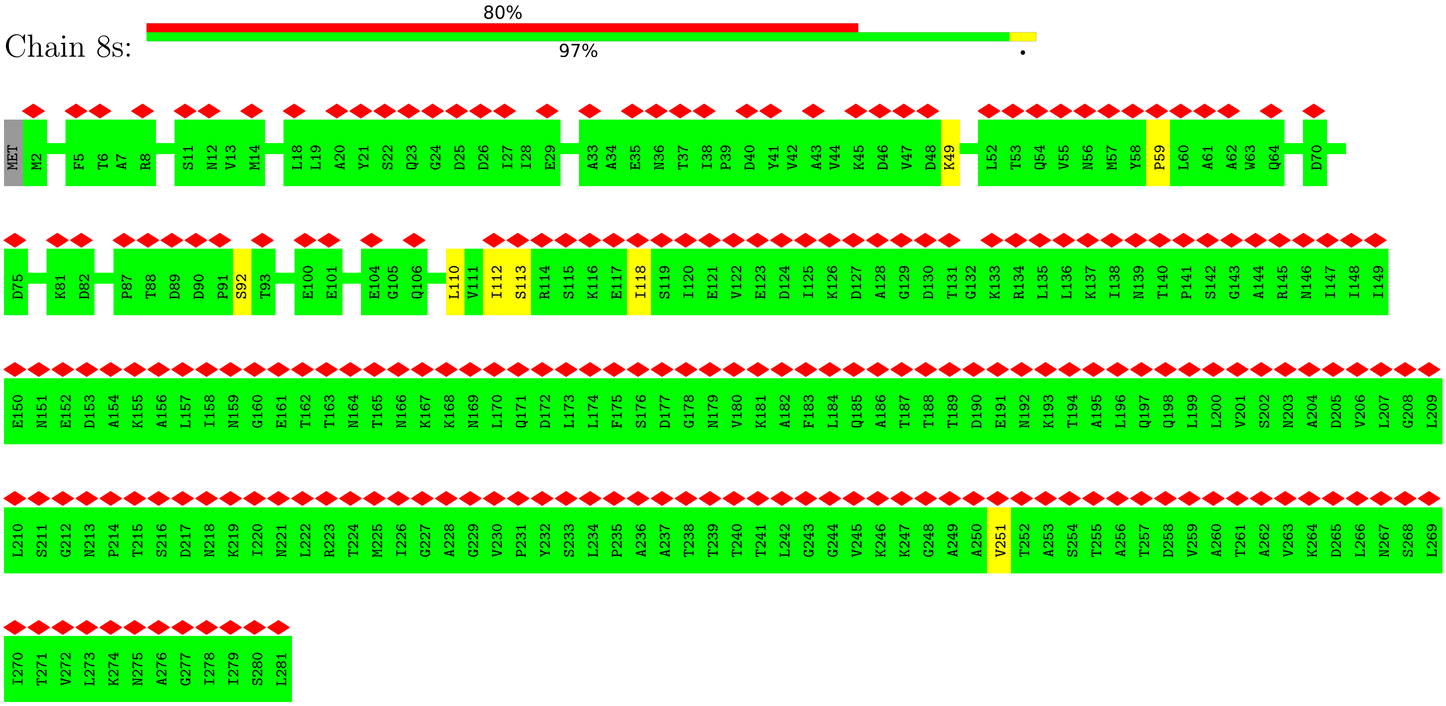
Chain 8r:





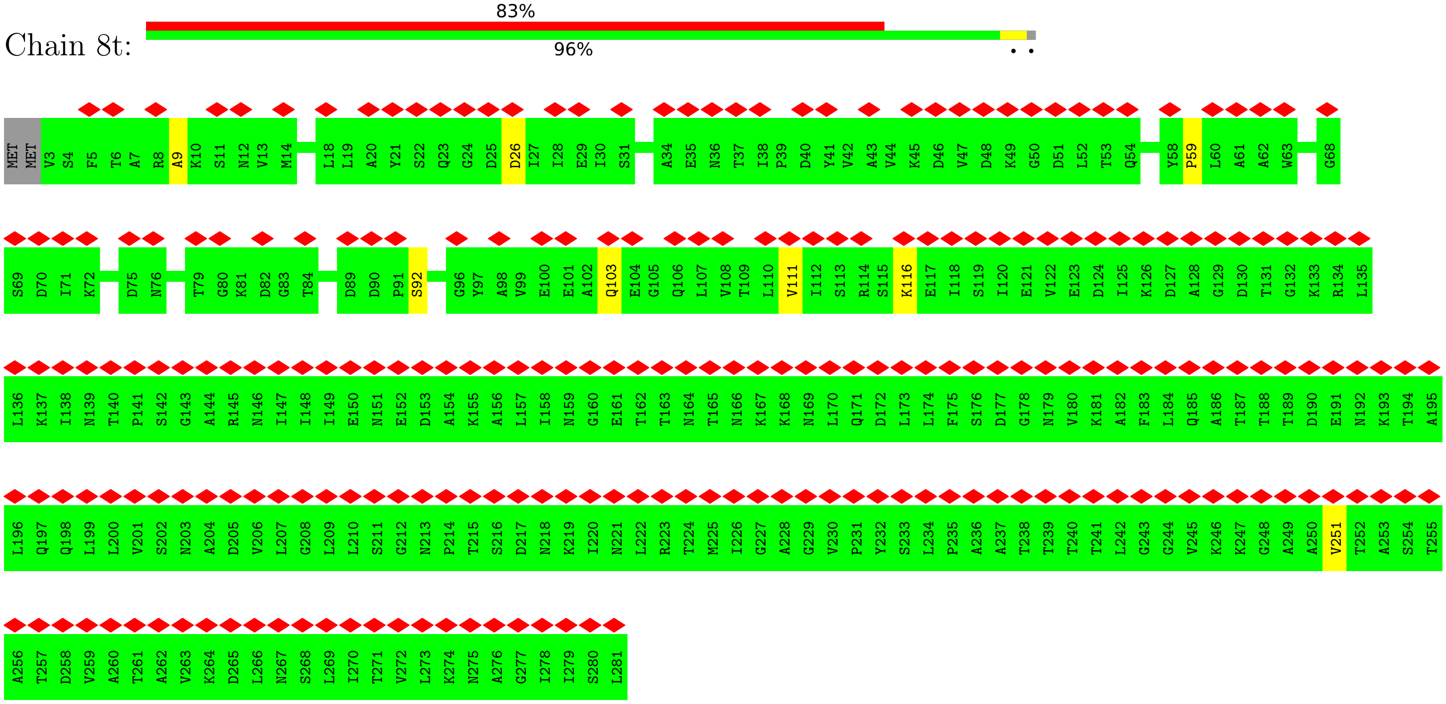
- Molecule 2: Capsid fiber protein

Chain 8s:



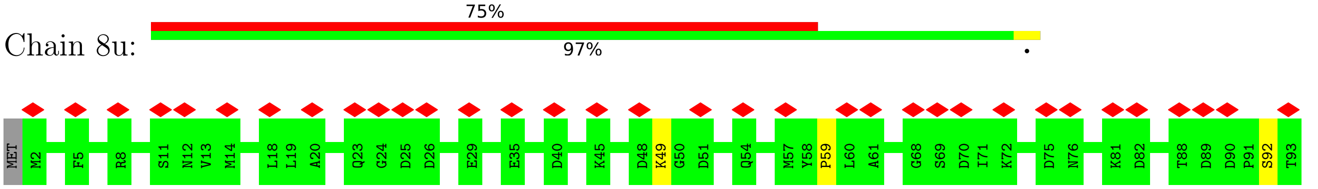
- Molecule 2: Capsid fiber protein

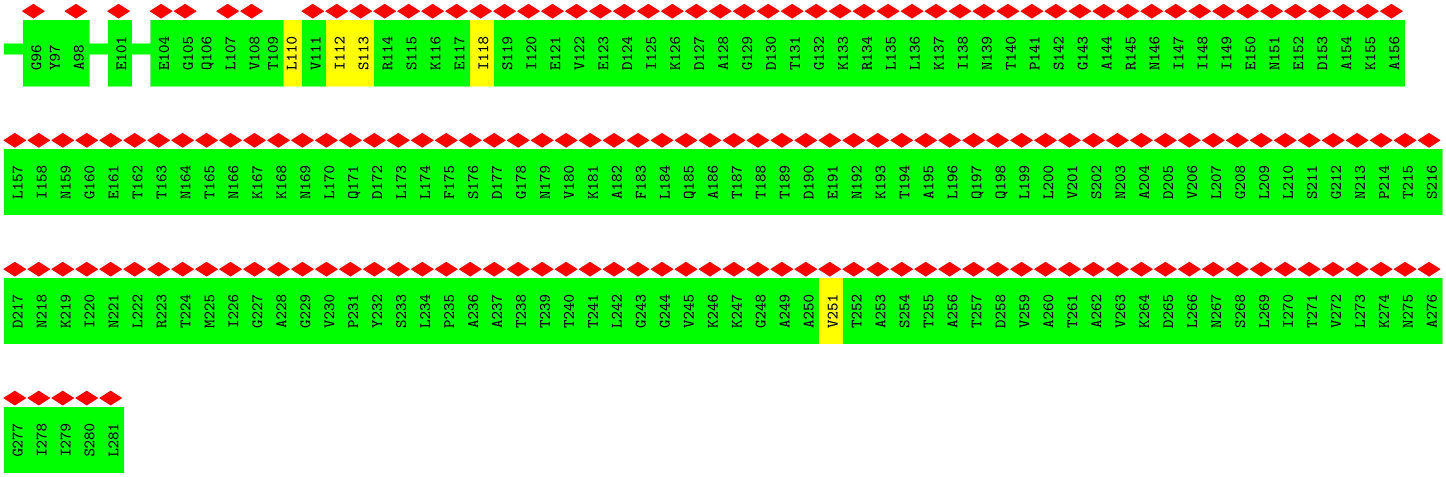
Chain 8t:



- Molecule 2: Capsid fiber protein

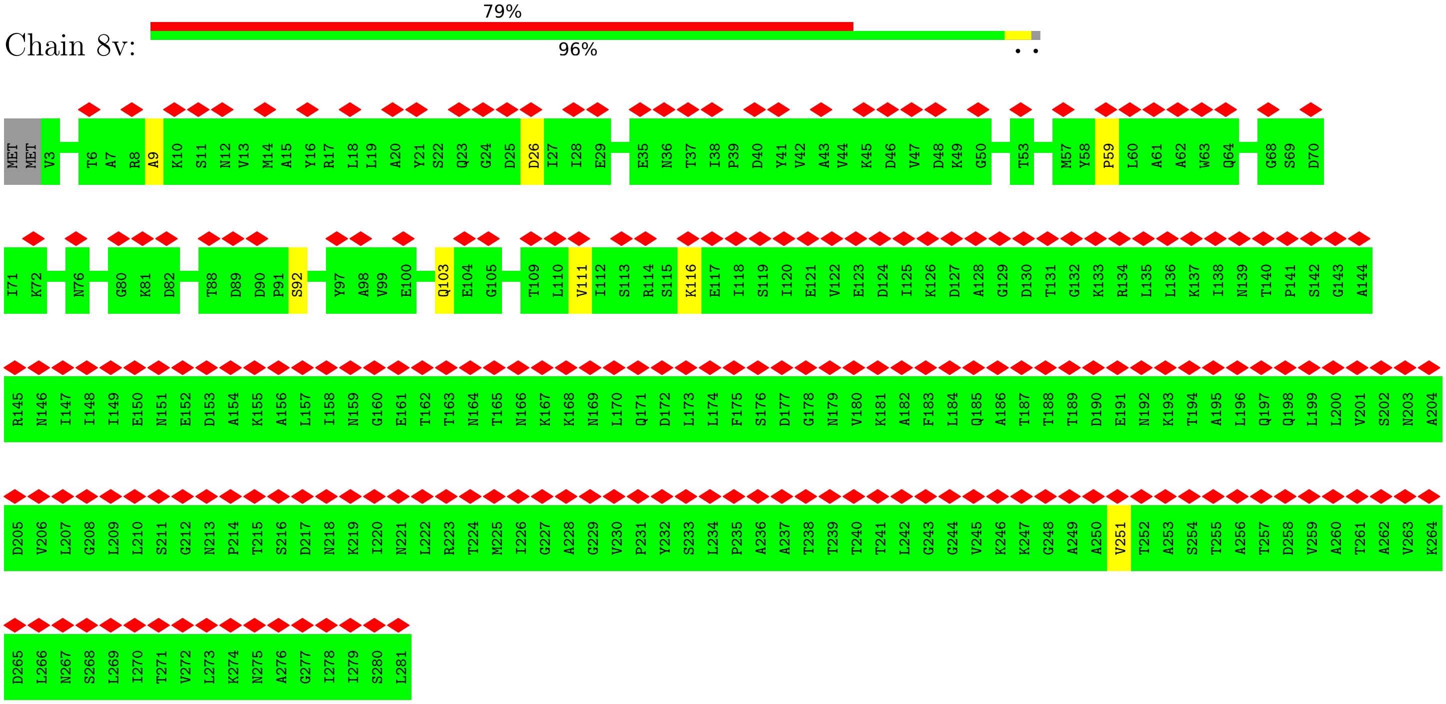
Chain 8u:





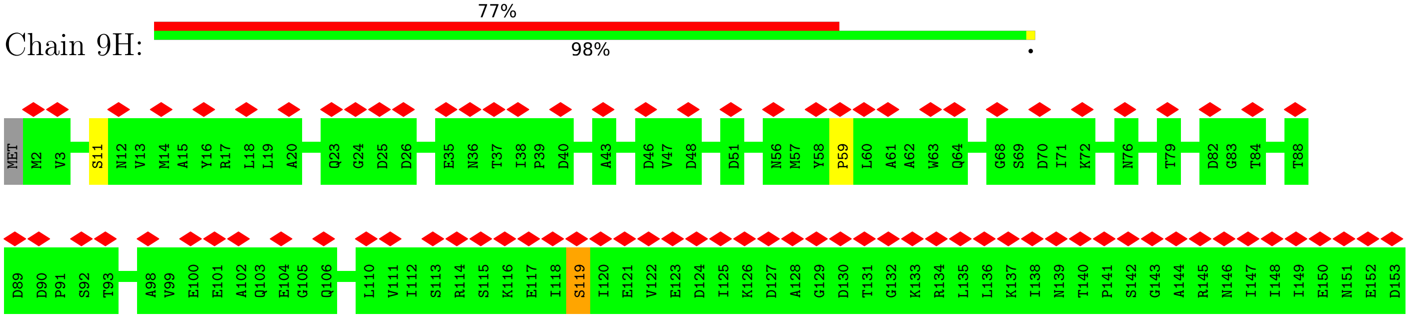
- Molecule 2: Capsid fiber protein

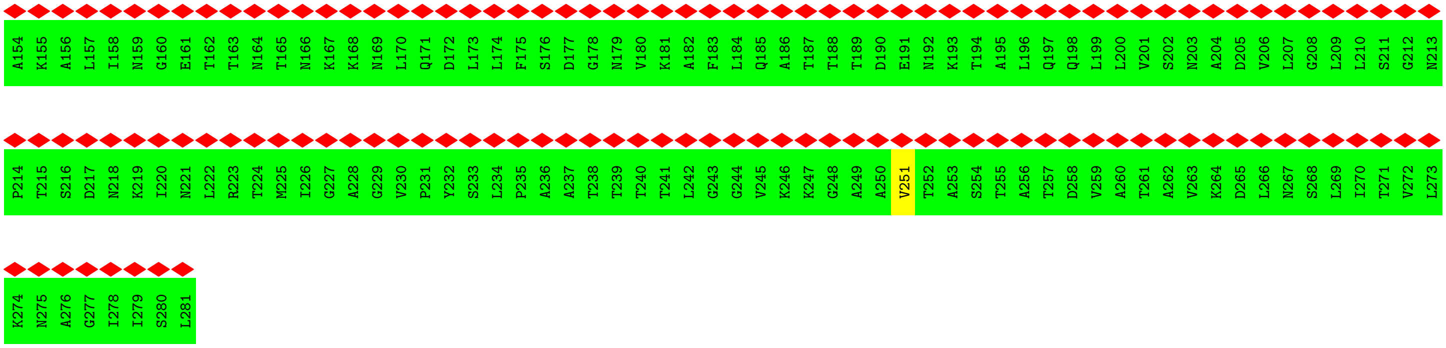
Chain 8v:



- Molecule 2: Capsid fiber protein

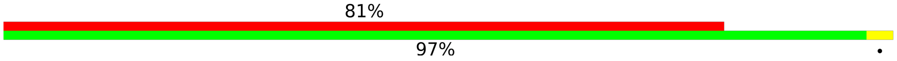
Chain 9H:

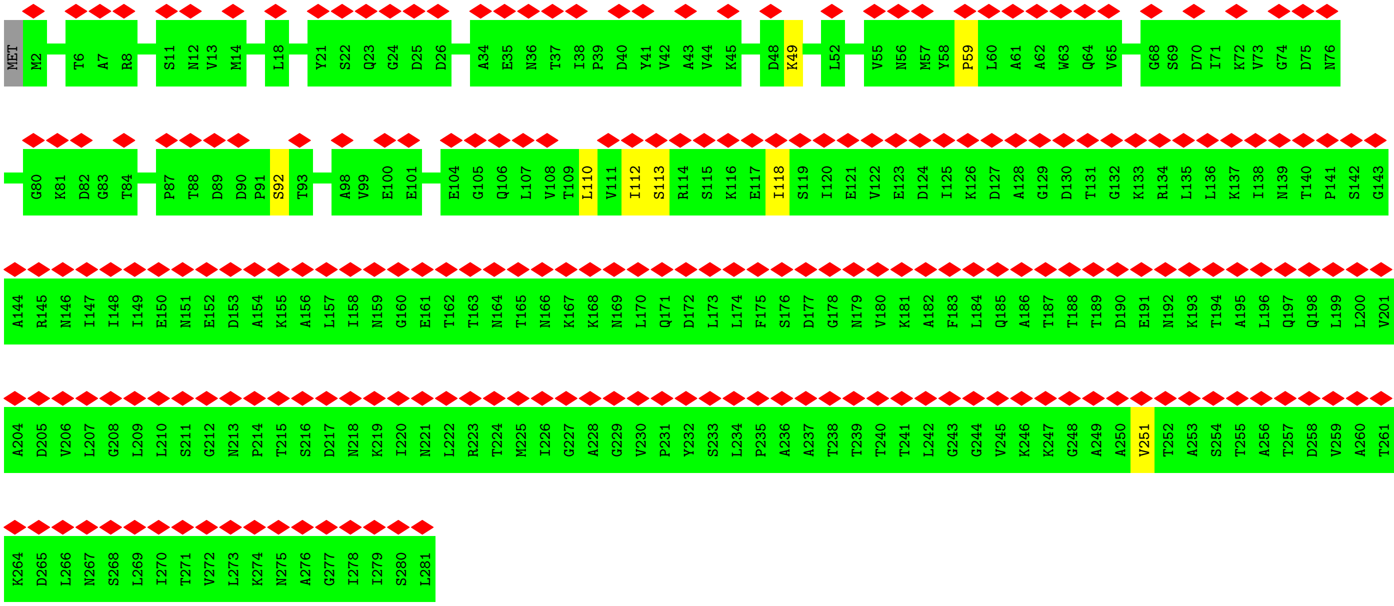




- Molecule 2: Capsid fiber protein

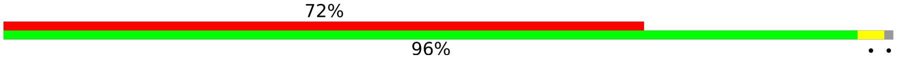
Chain 1q:

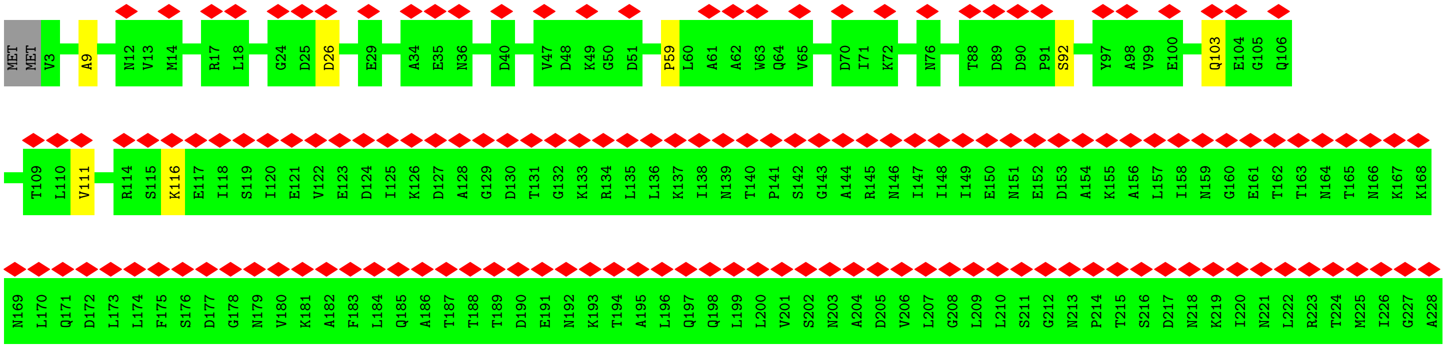


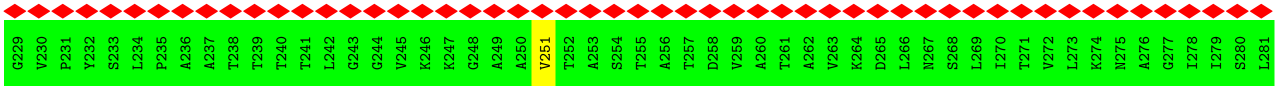


- Molecule 2: Capsid fiber protein

Chain 1r:

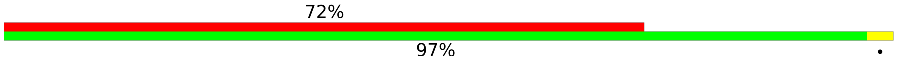


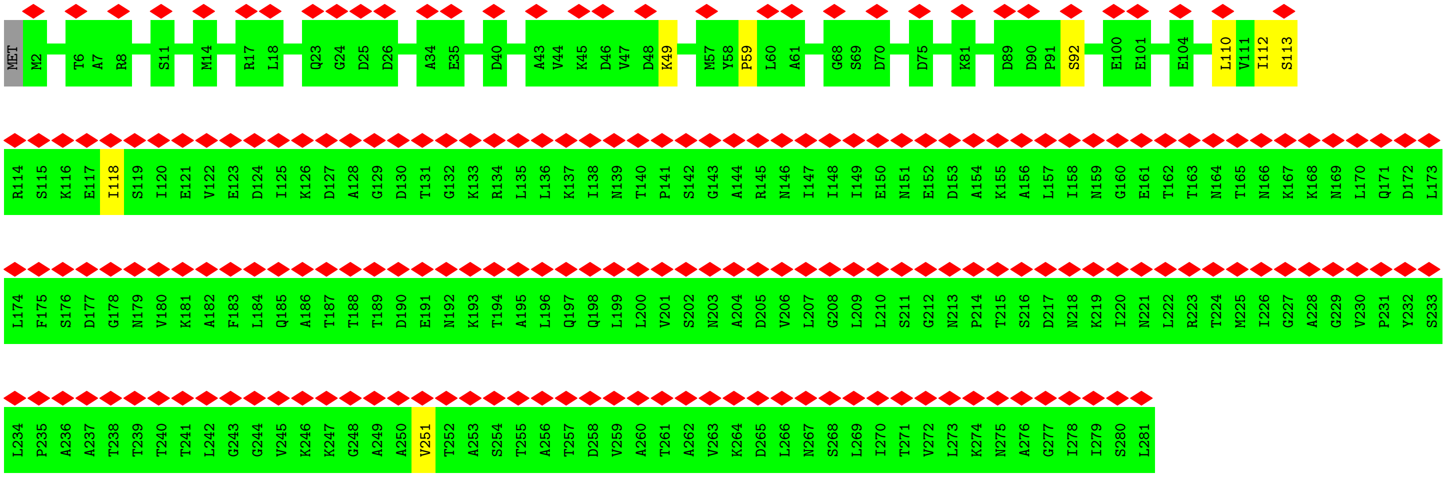




- Molecule 2: Capsid fiber protein

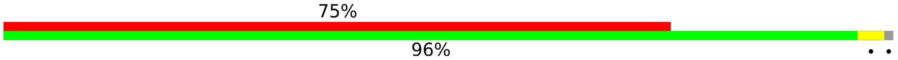
Chain 1s:

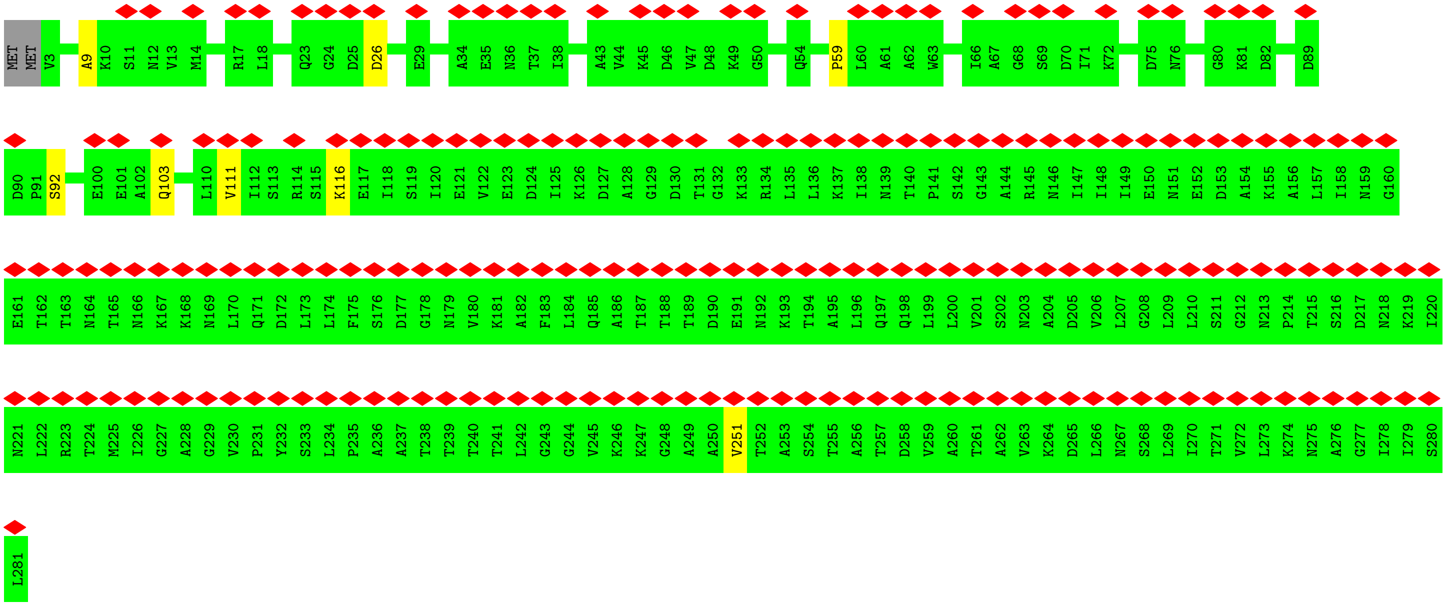




- Molecule 2: Capsid fiber protein

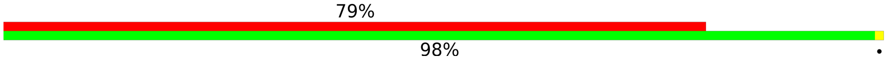
Chain 1t:

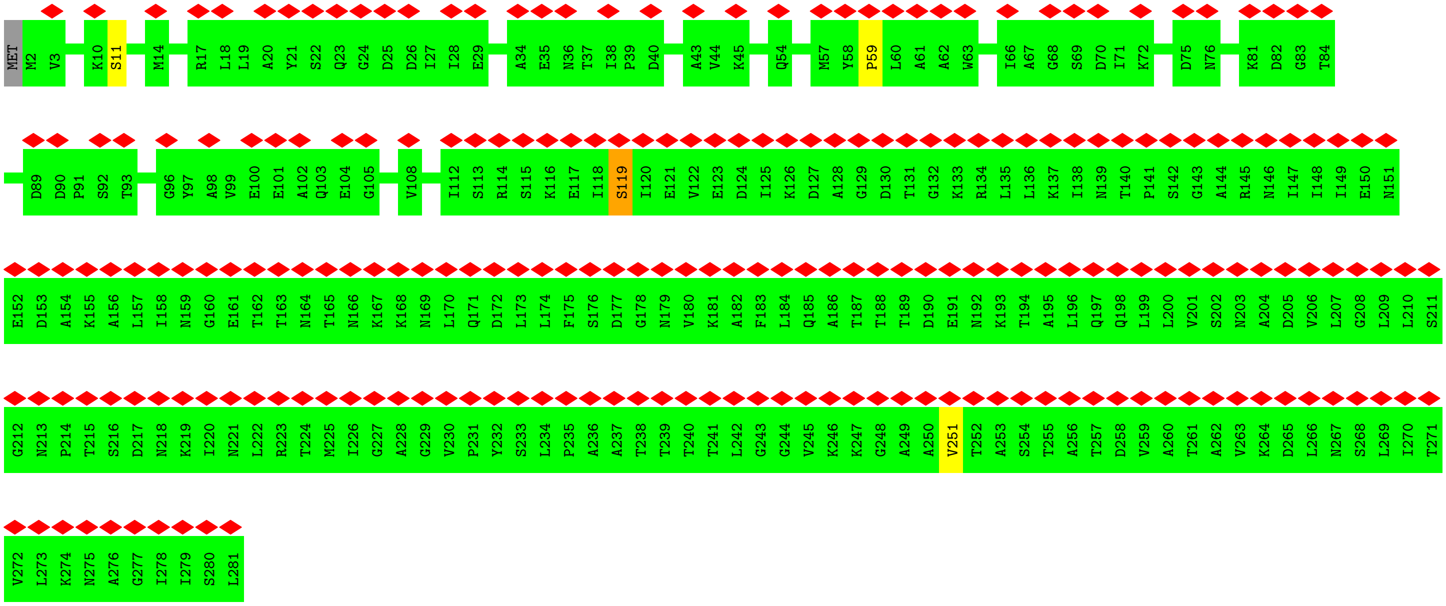




- Molecule 2: Capsid fiber protein

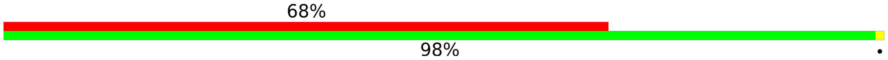
Chain 2o:

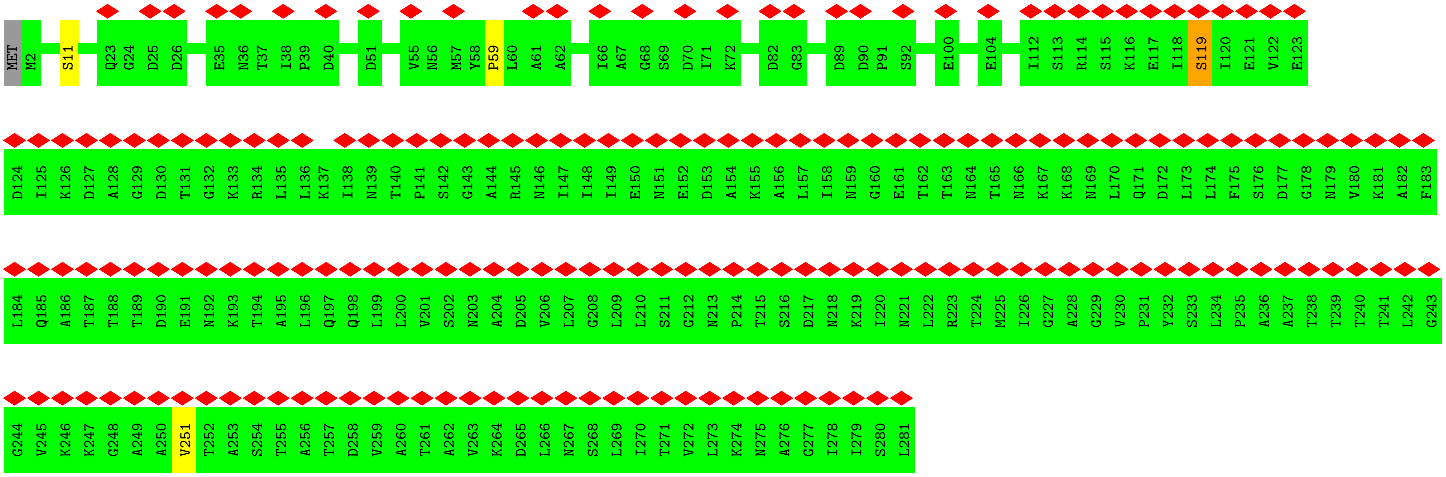




- Molecule 2: Capsid fiber protein

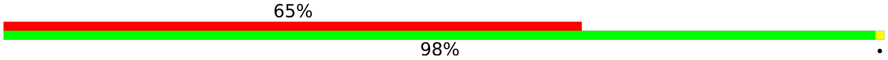
Chain 2p:

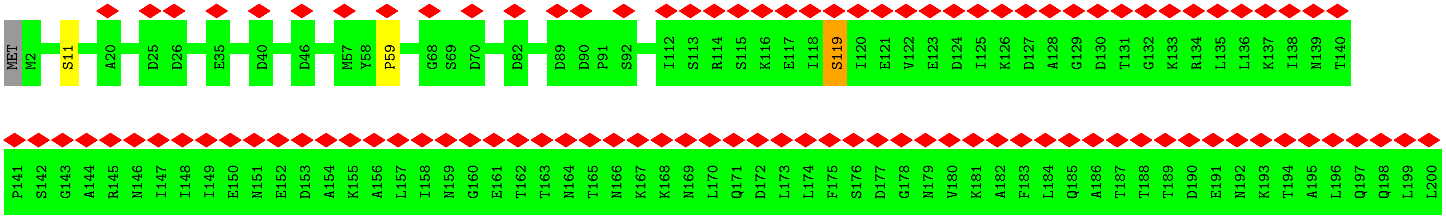


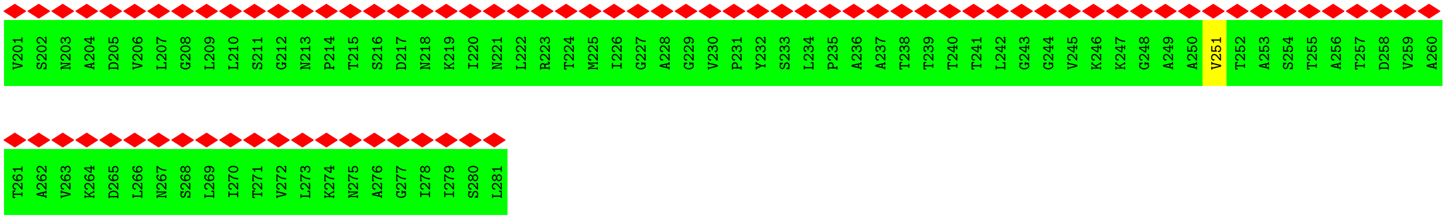


- Molecule 2: Capsid fiber protein

Chain 2q:

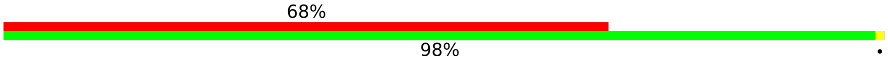


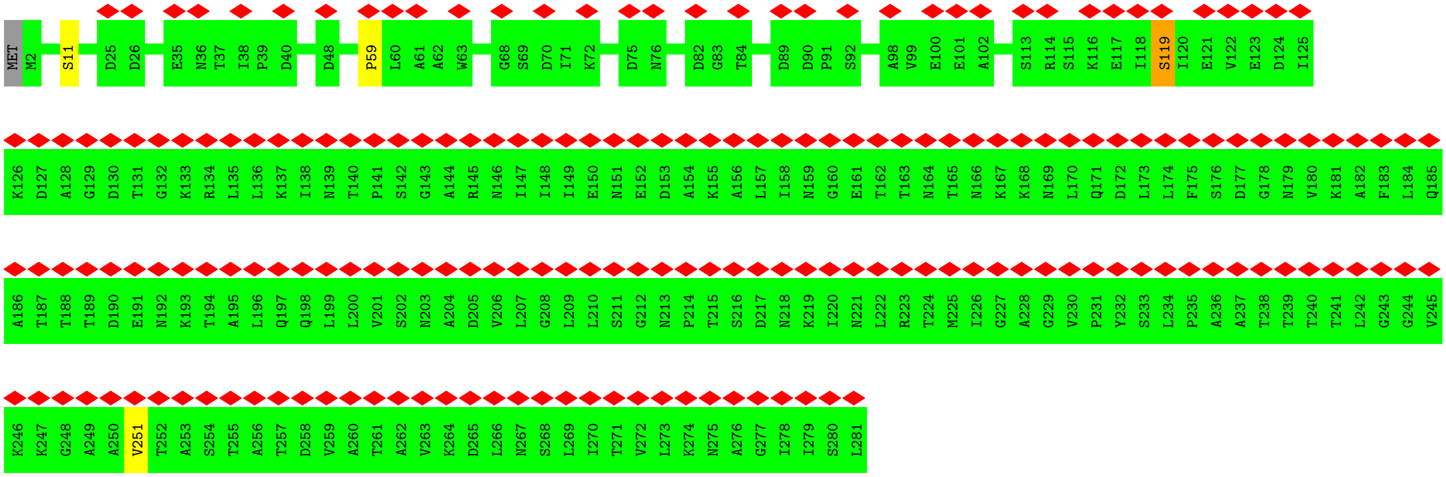




- Molecule 2: Capsid fiber protein

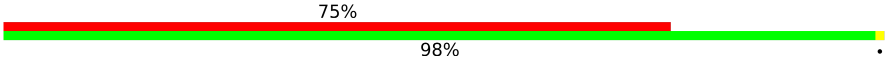
Chain 2r:

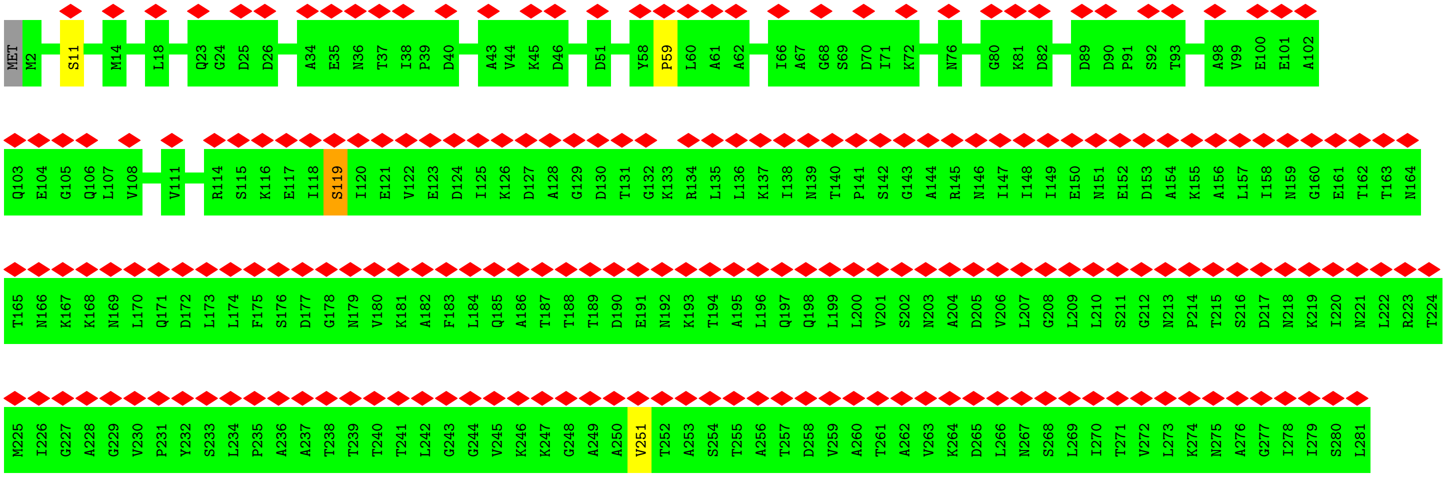




- Molecule 2: Capsid fiber protein

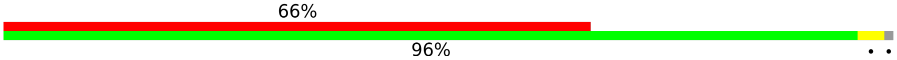
Chain 2s:

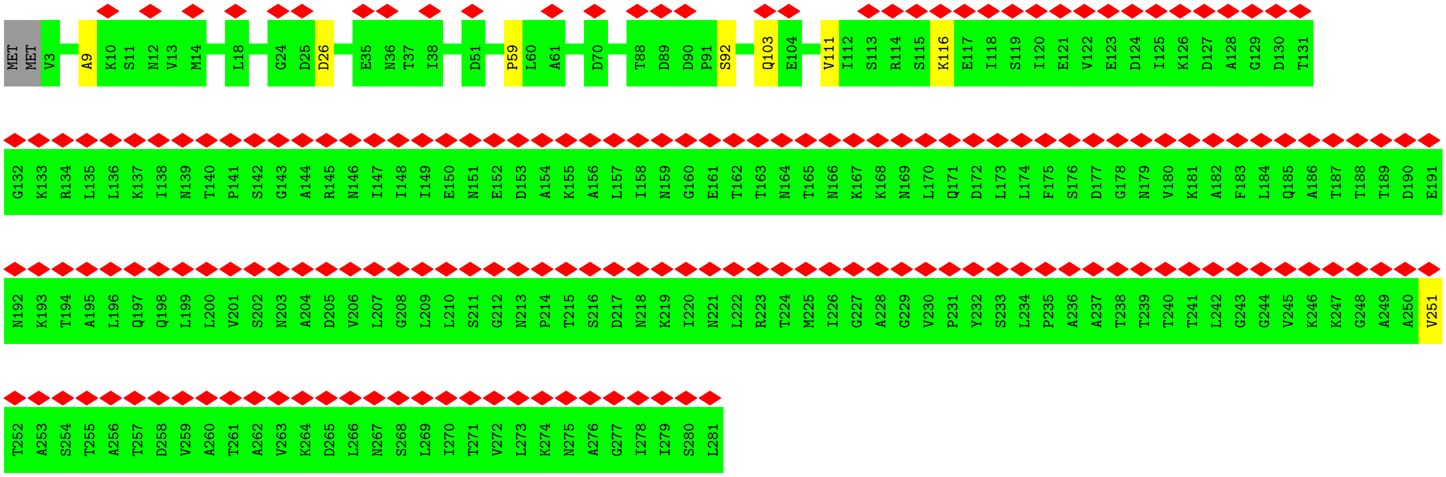




- Molecule 2: Capsid fiber protein

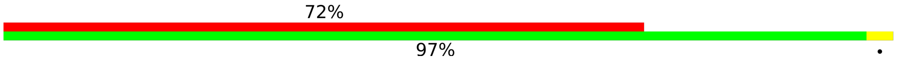
Chain 3q:

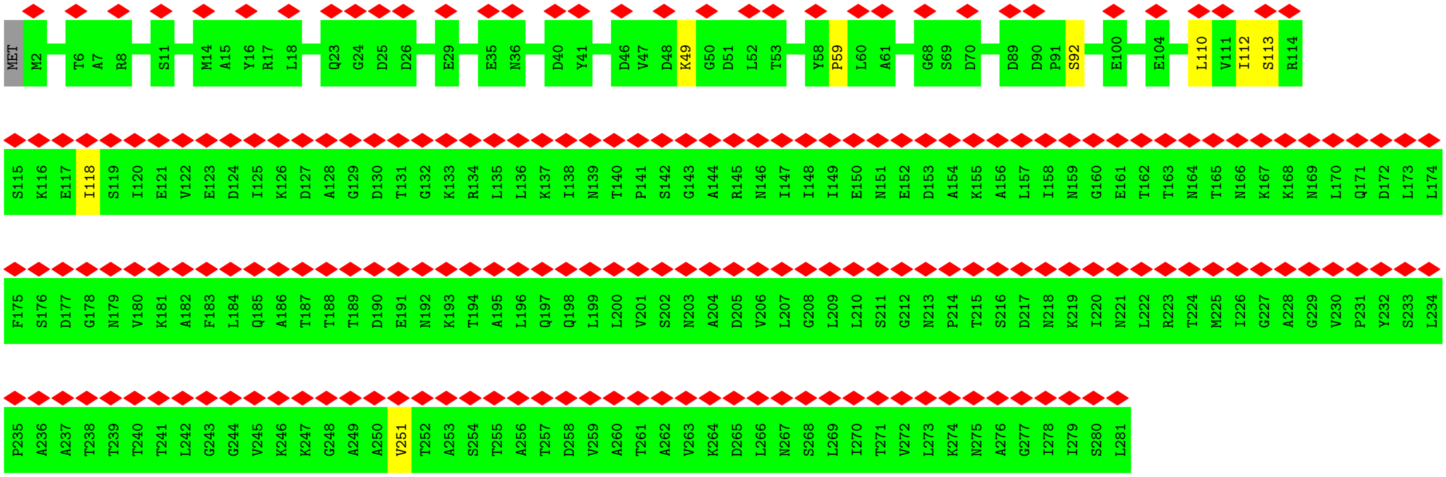




- Molecule 2: Capsid fiber protein

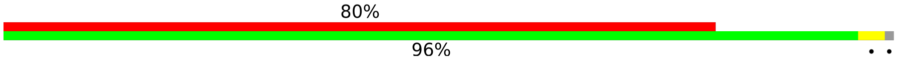
Chain 3r:

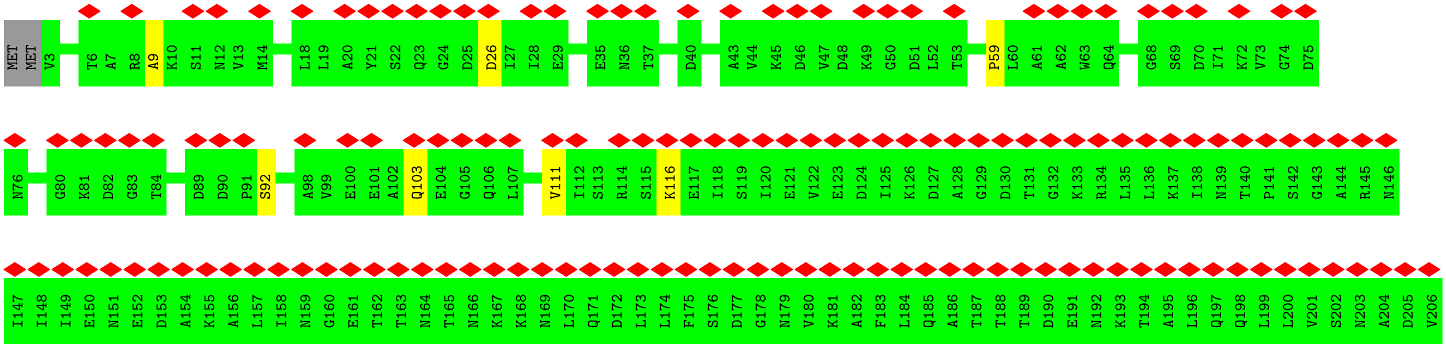


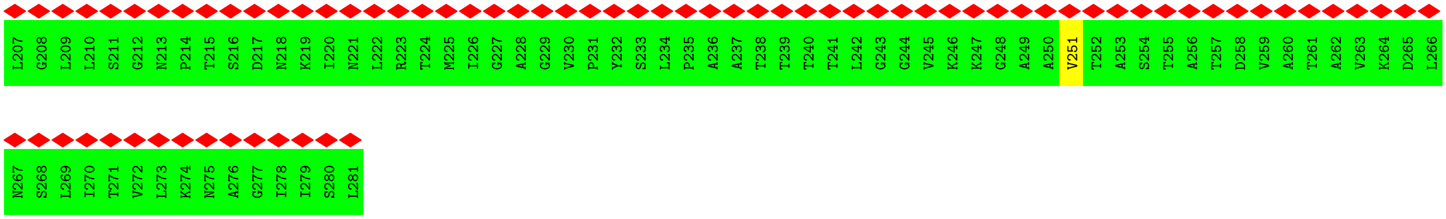


- Molecule 2: Capsid fiber protein

Chain 3s:

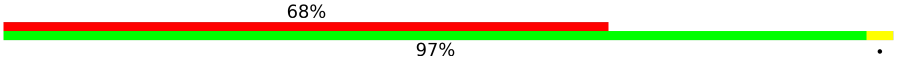


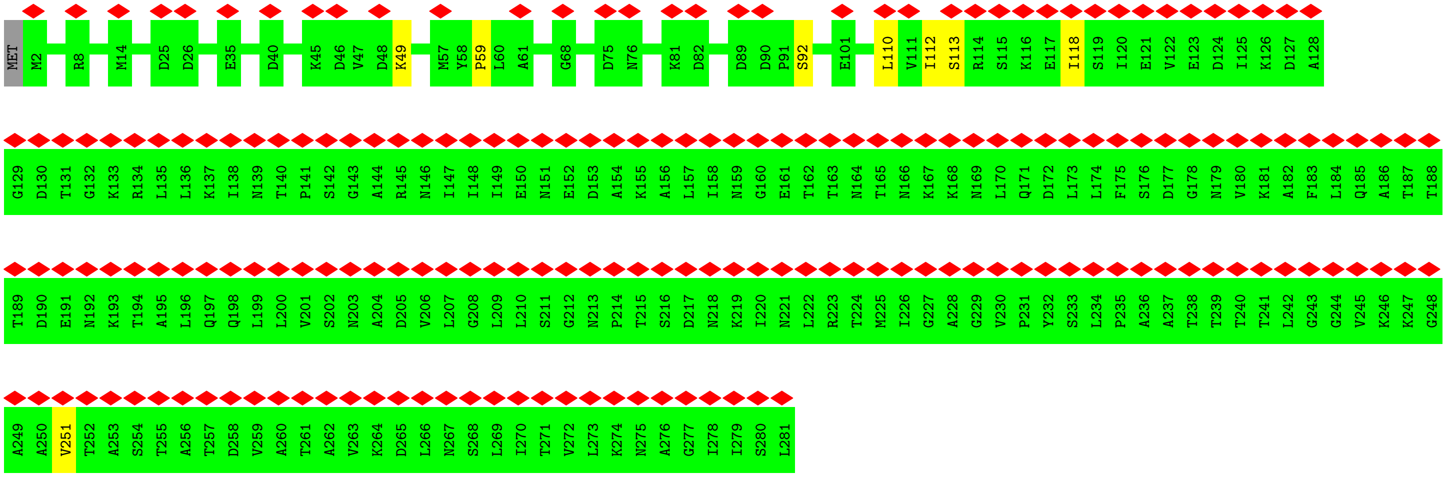




- Molecule 2: Capsid fiber protein

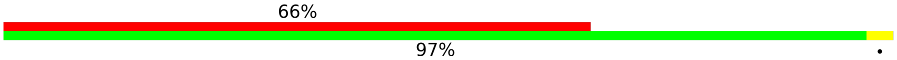
Chain 3t:

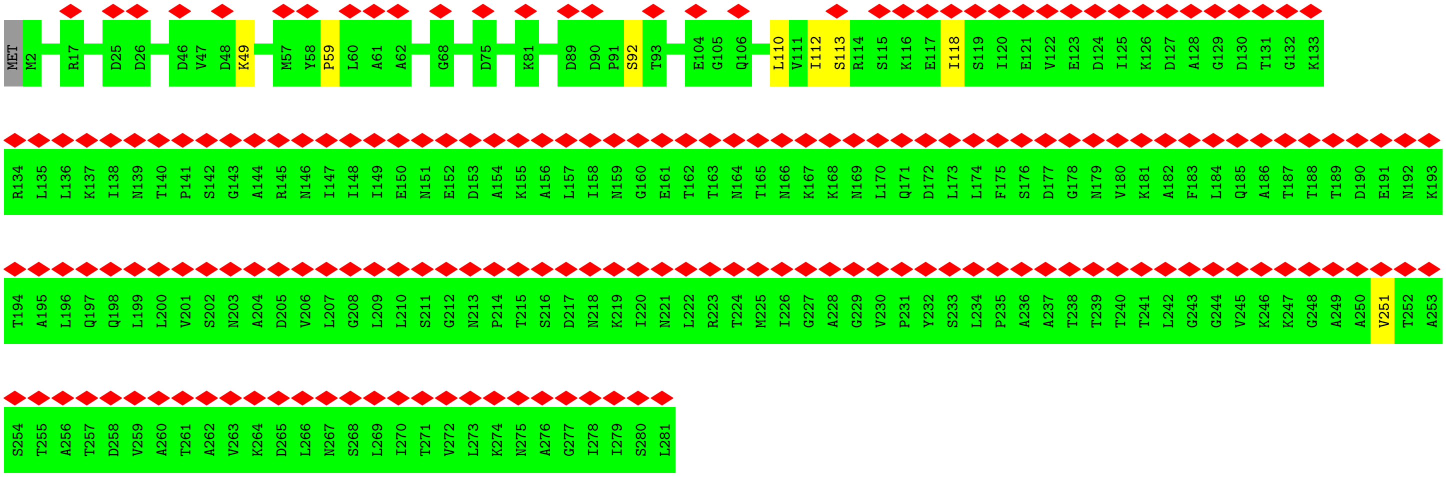




- Molecule 2: Capsid fiber protein

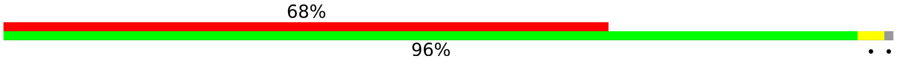
Chain 4k:

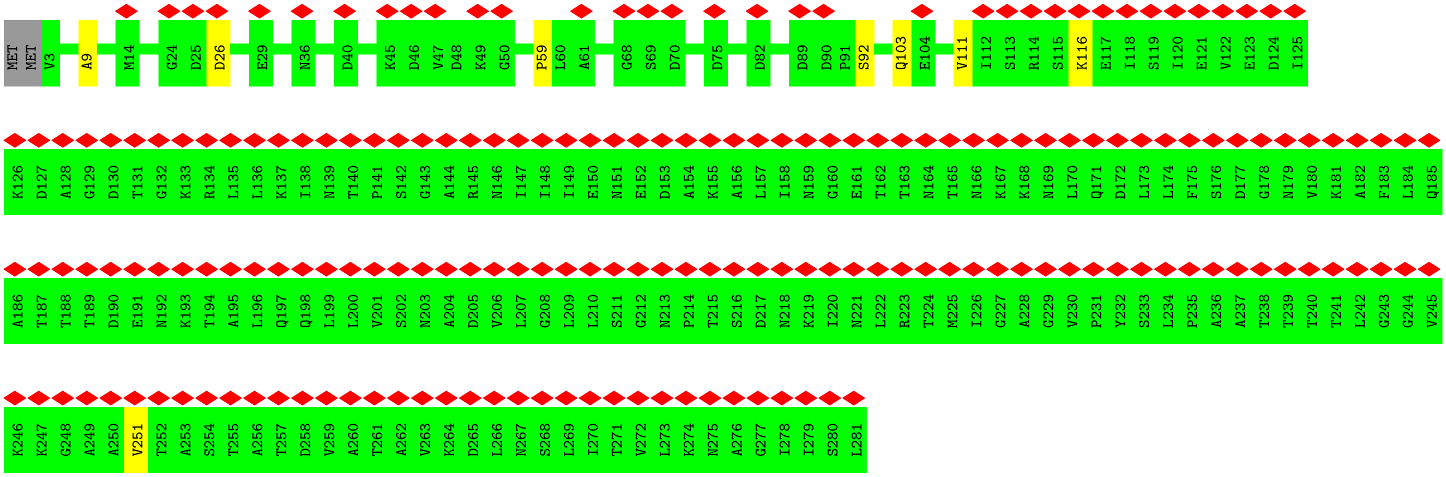




- Molecule 2: Capsid fiber protein

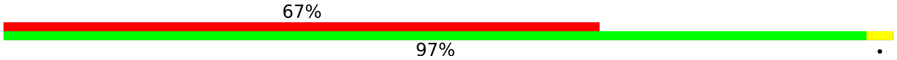
Chain 4l:

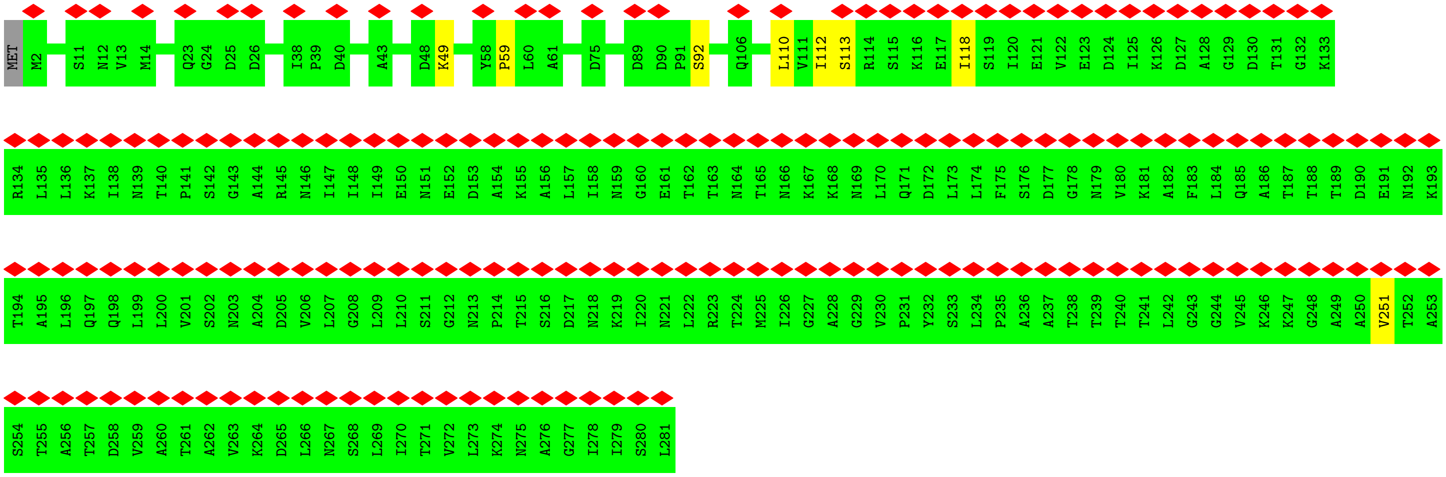




- Molecule 2: Capsid fiber protein

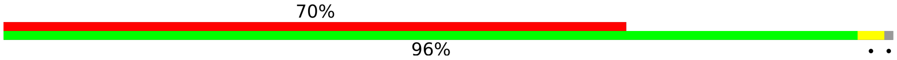
Chain 5k:

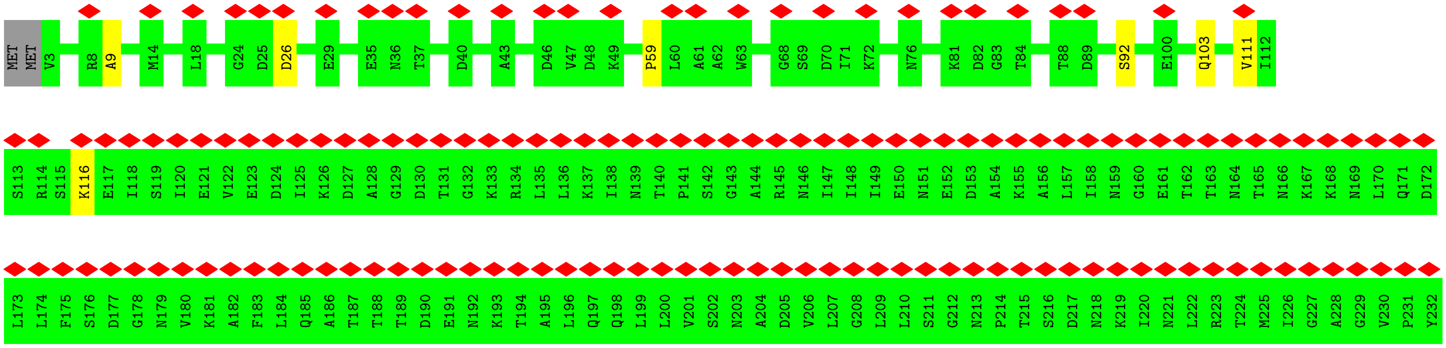


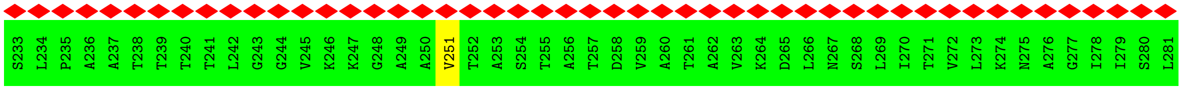


- Molecule 2: Capsid fiber protein

Chain 5l:

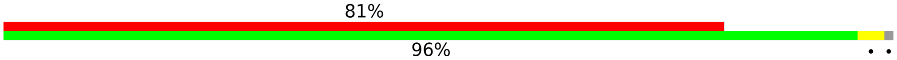


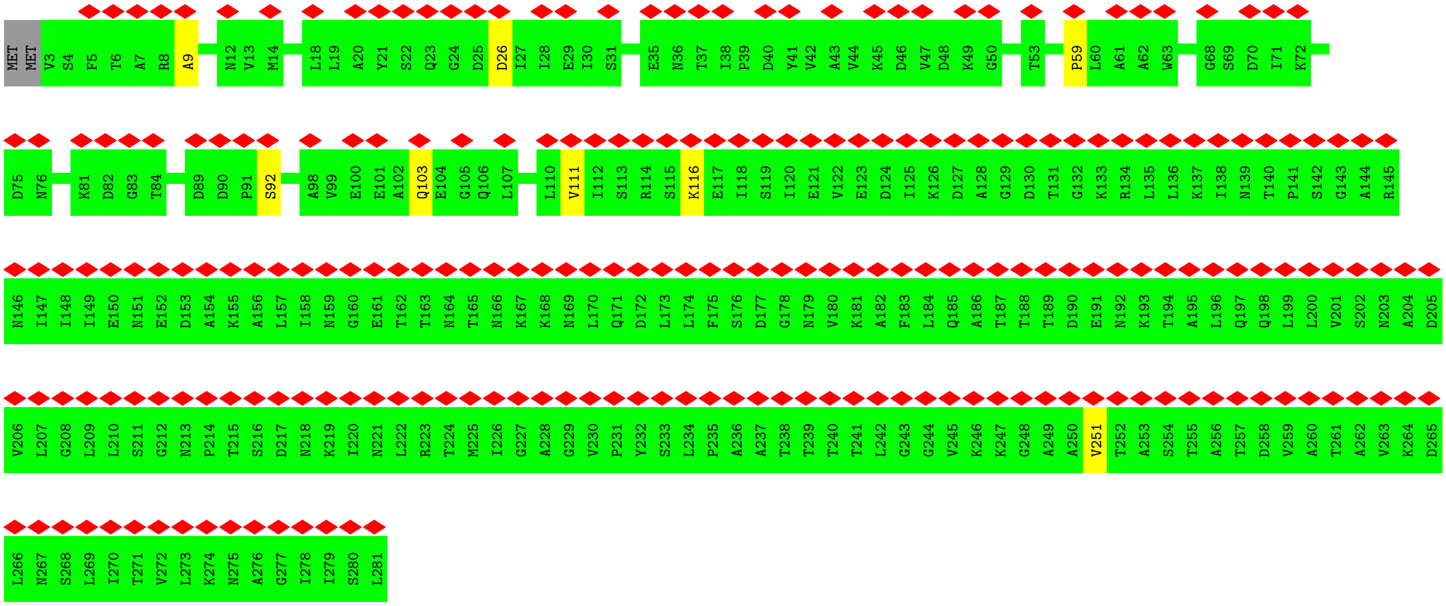




- Molecule 2: Capsid fiber protein

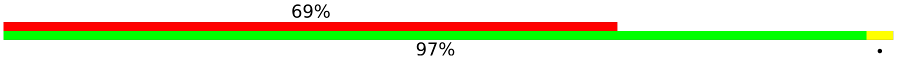
Chain 6q:

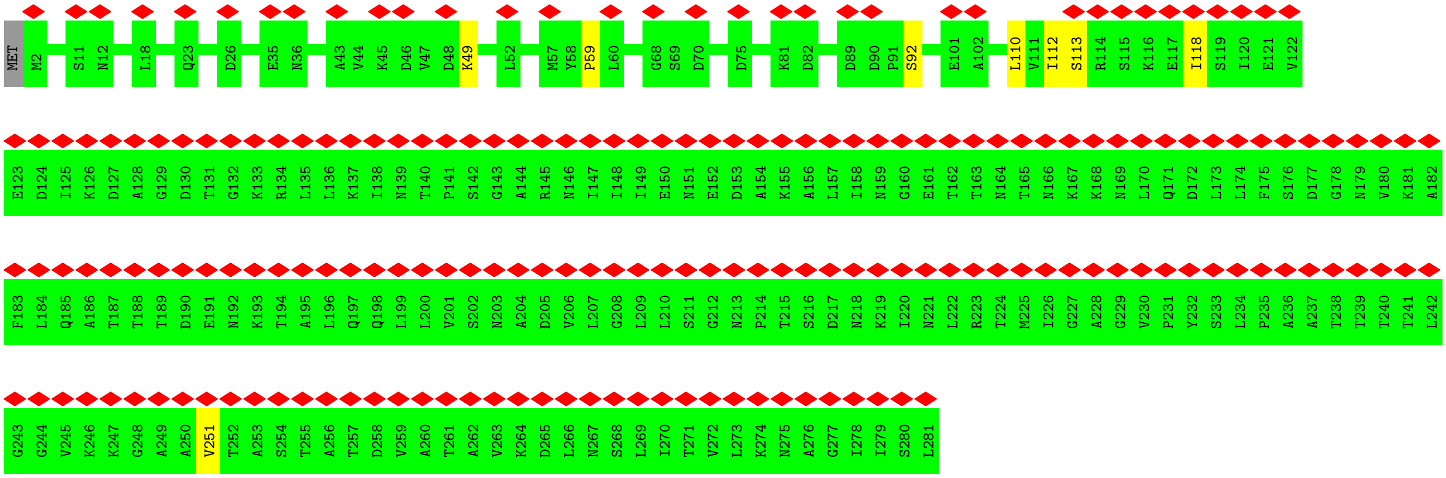




- Molecule 2: Capsid fiber protein

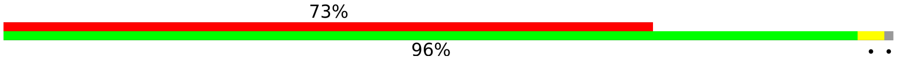
Chain 6r:

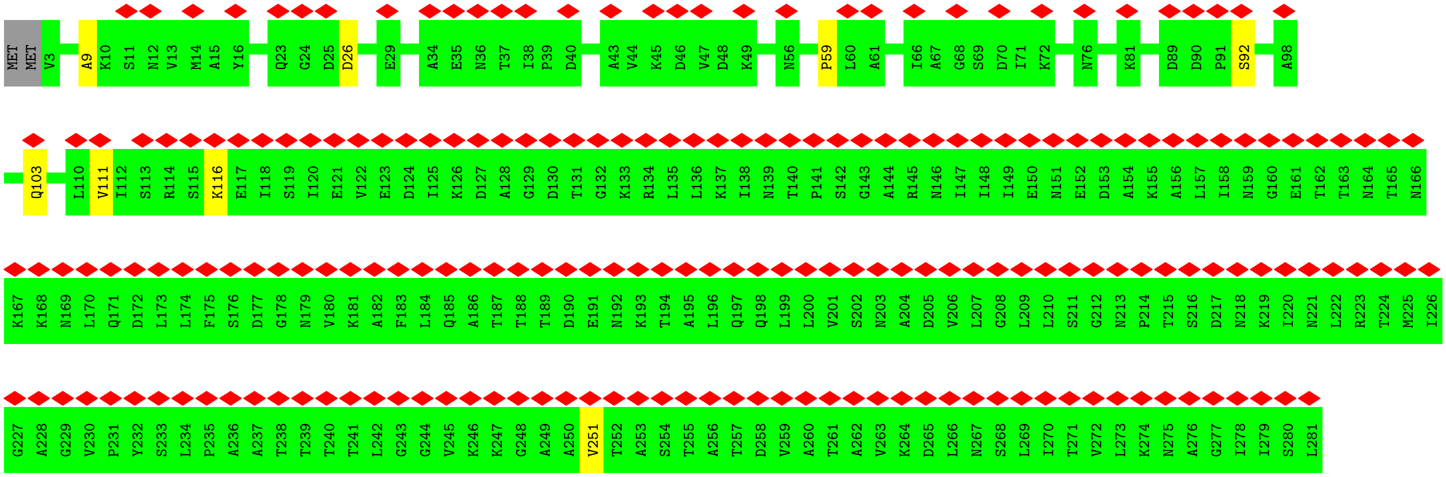




- Molecule 2: Capsid fiber protein

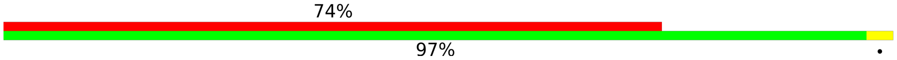
Chain 6s:

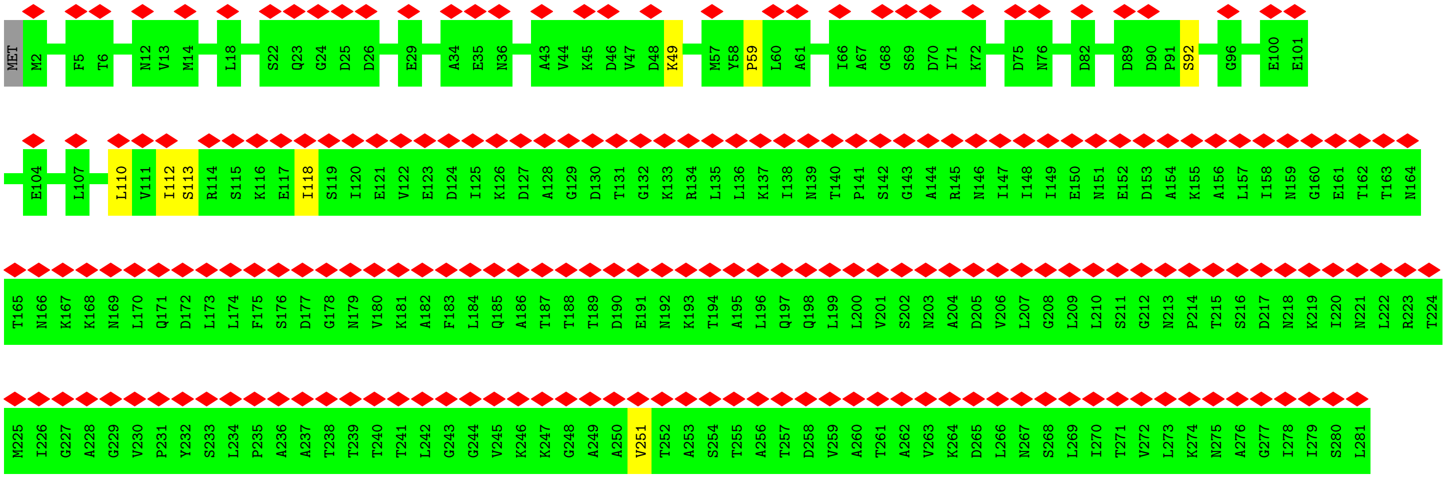




- Molecule 2: Capsid fiber protein

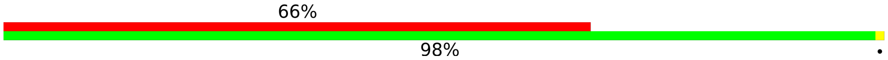
Chain 6t:

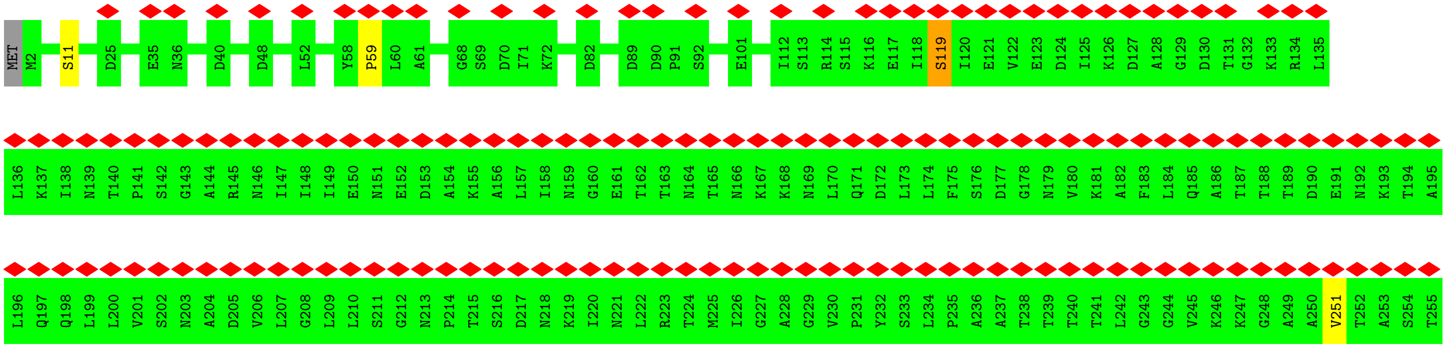


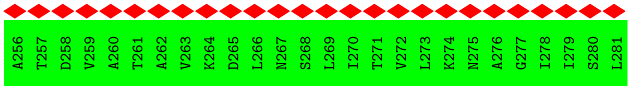


- Molecule 2: Capsid fiber protein

Chain 7o:

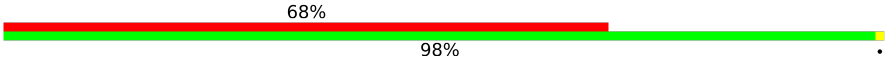


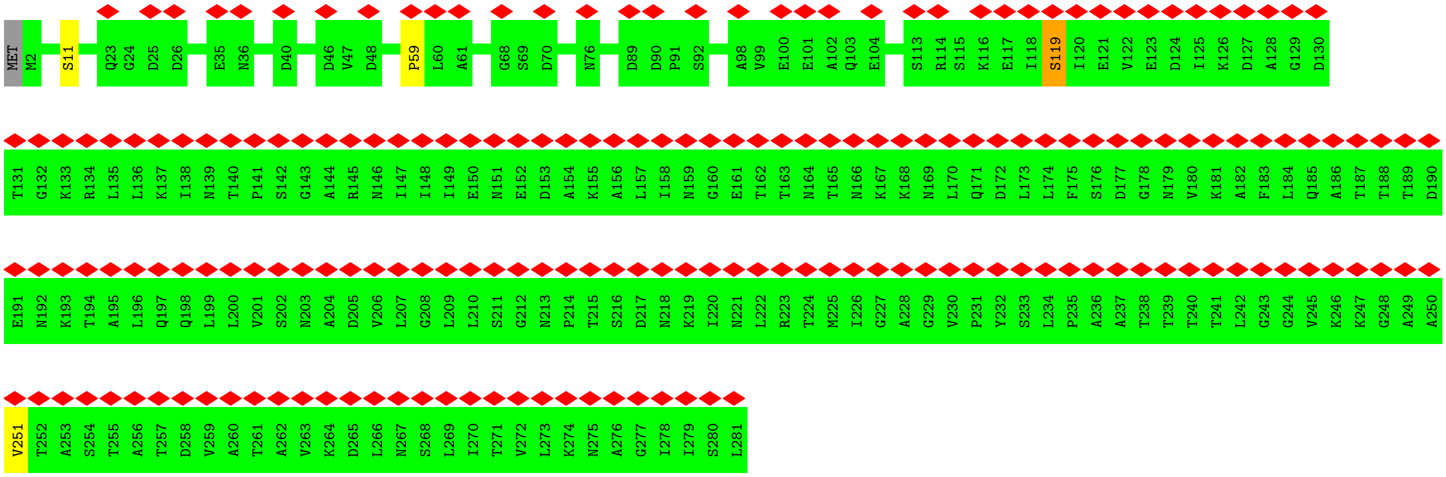




- Molecule 2: Capsid fiber protein

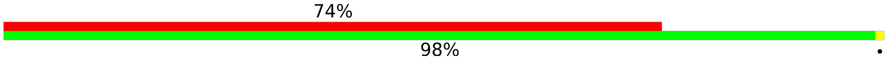
Chain 7p:

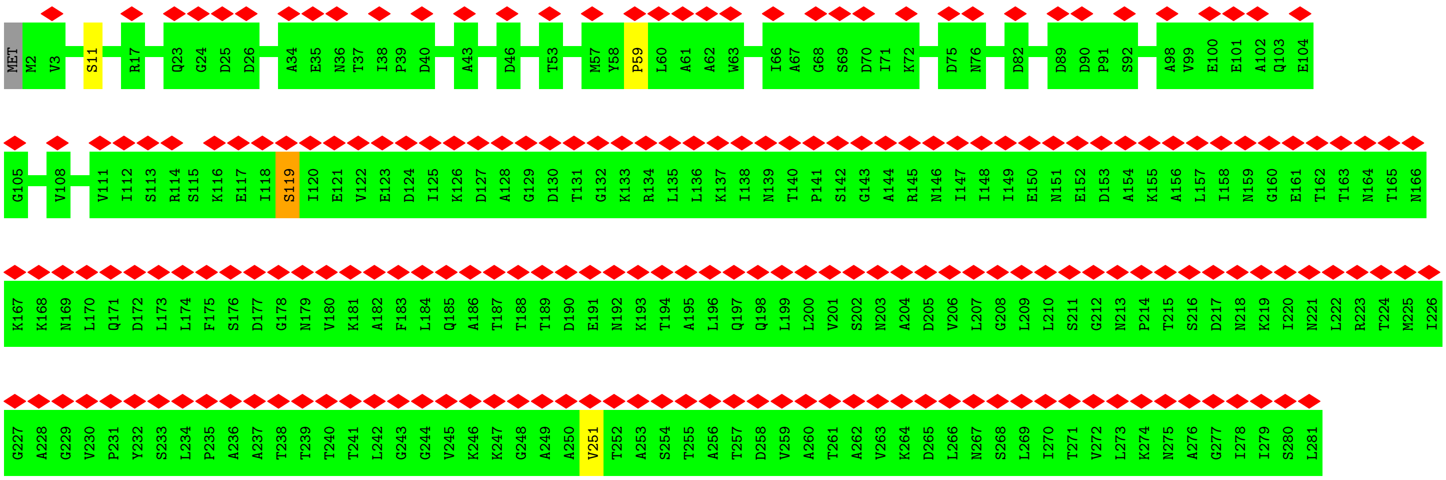




- Molecule 2: Capsid fiber protein

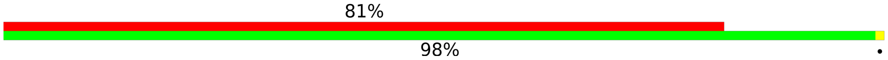
Chain 7q:

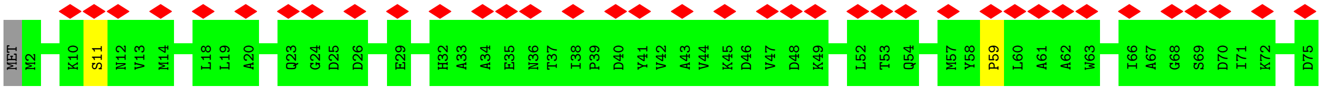


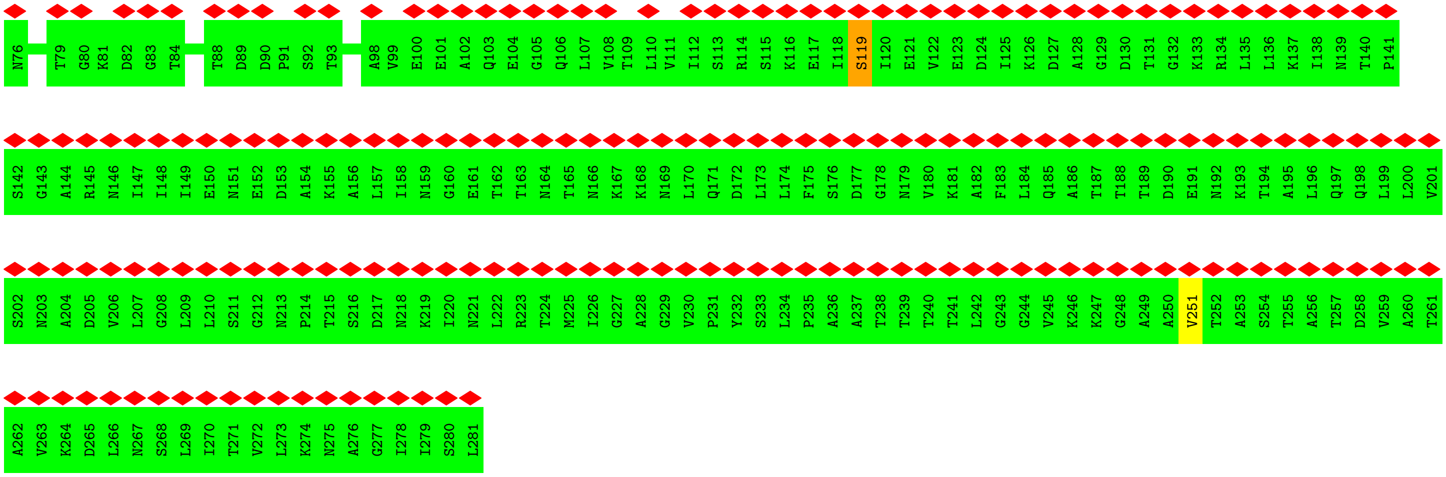


- Molecule 2: Capsid fiber protein

Chain 7r:

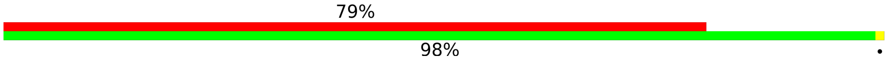


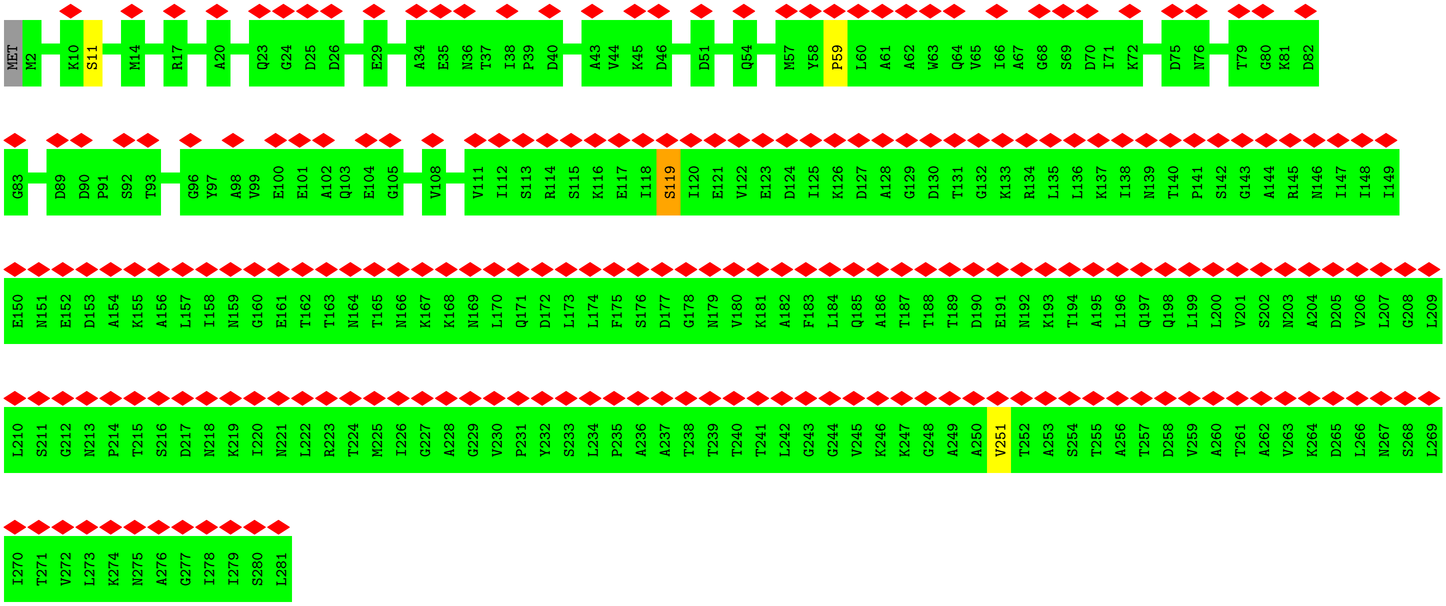




- Molecule 2: Capsid fiber protein

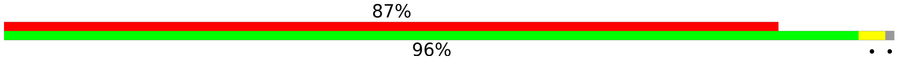
Chain 7s:

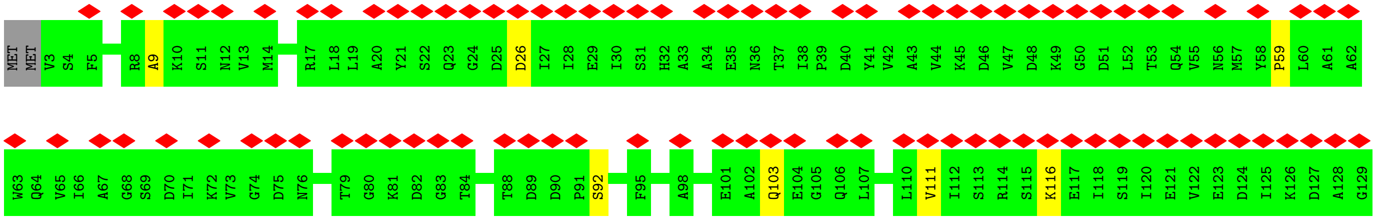


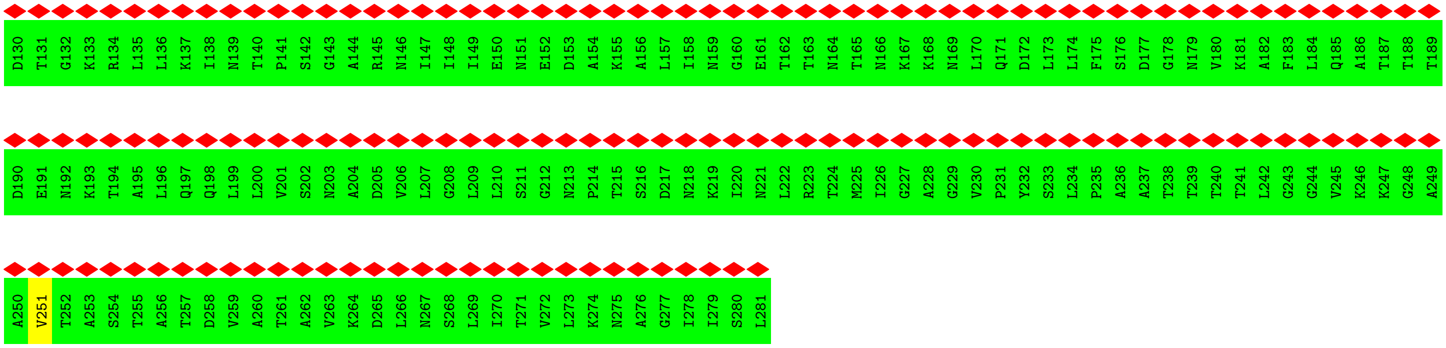


- Molecule 2: Capsid fiber protein

Chain 8w:

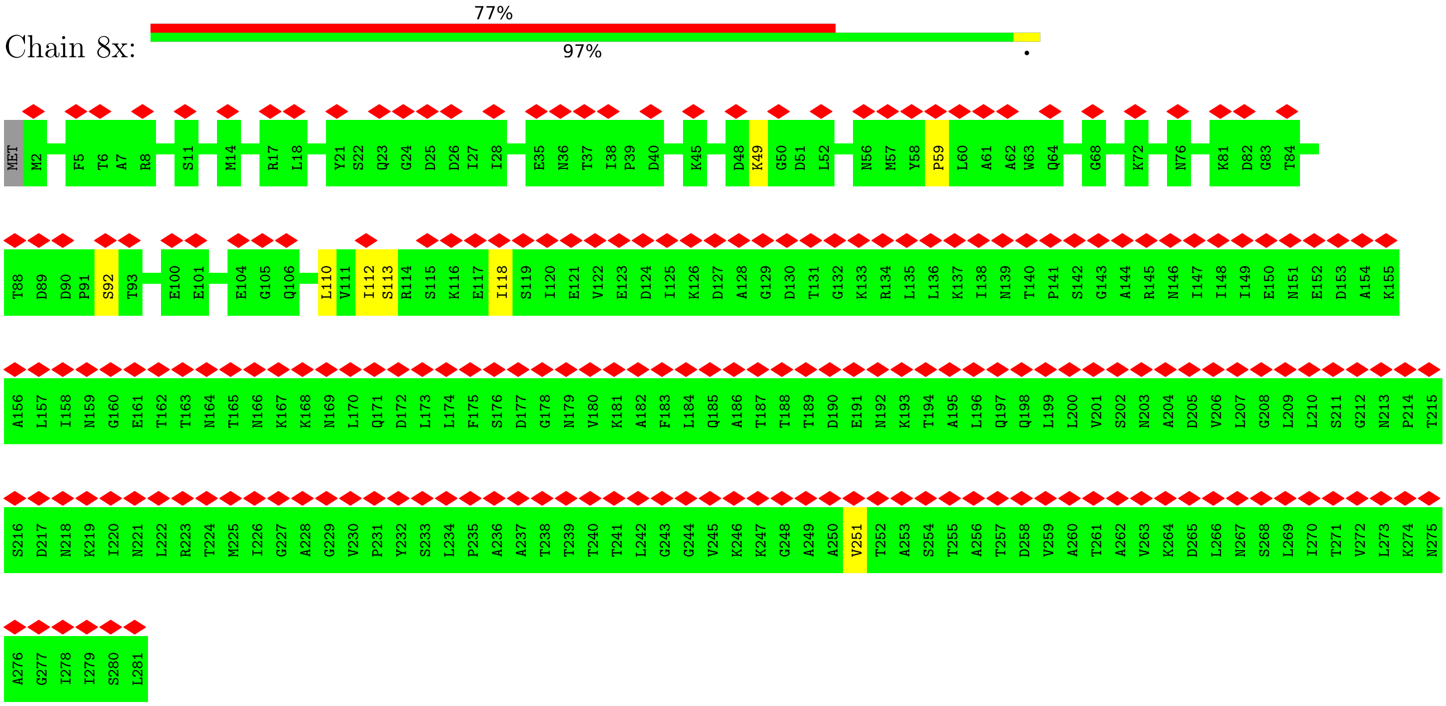






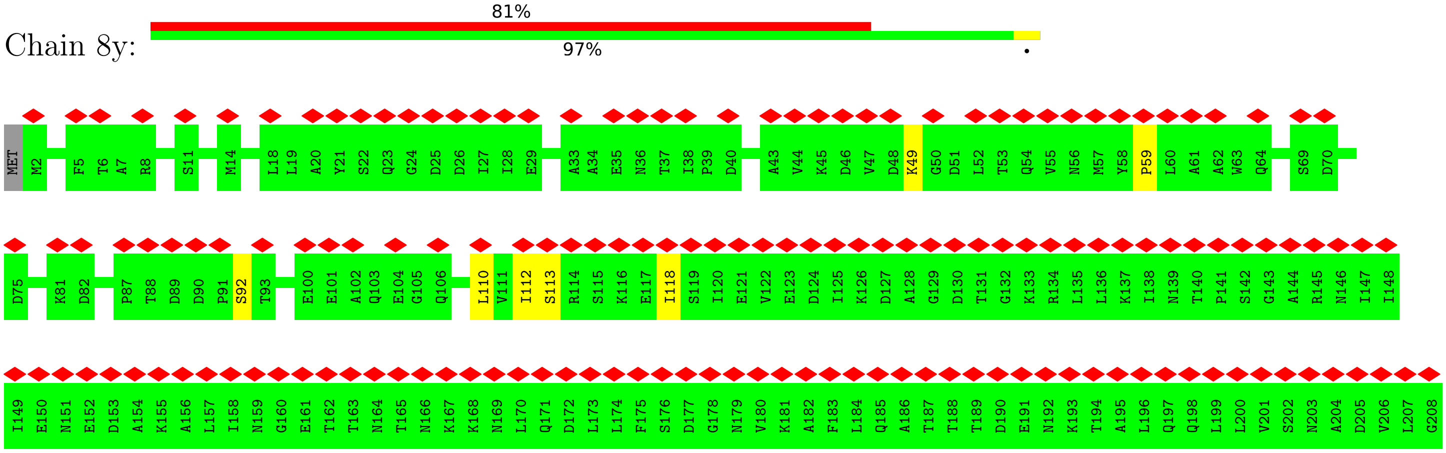
- Molecule 2: Capsid fiber protein

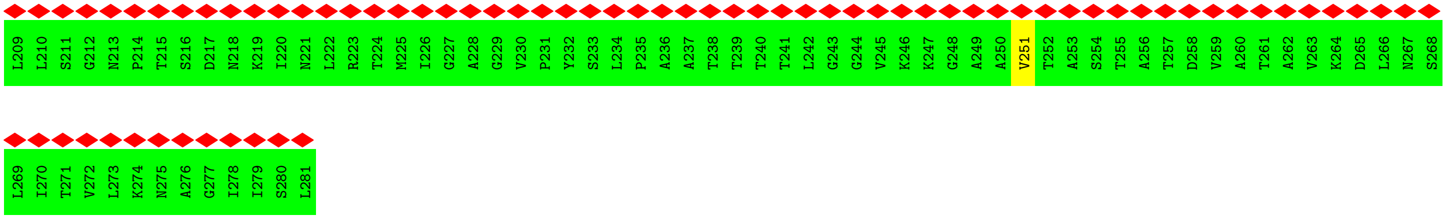
Chain 8x:



- Molecule 2: Capsid fiber protein

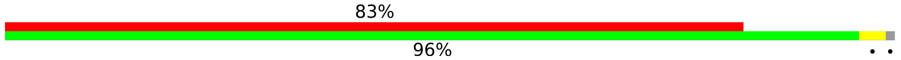
Chain 8y:

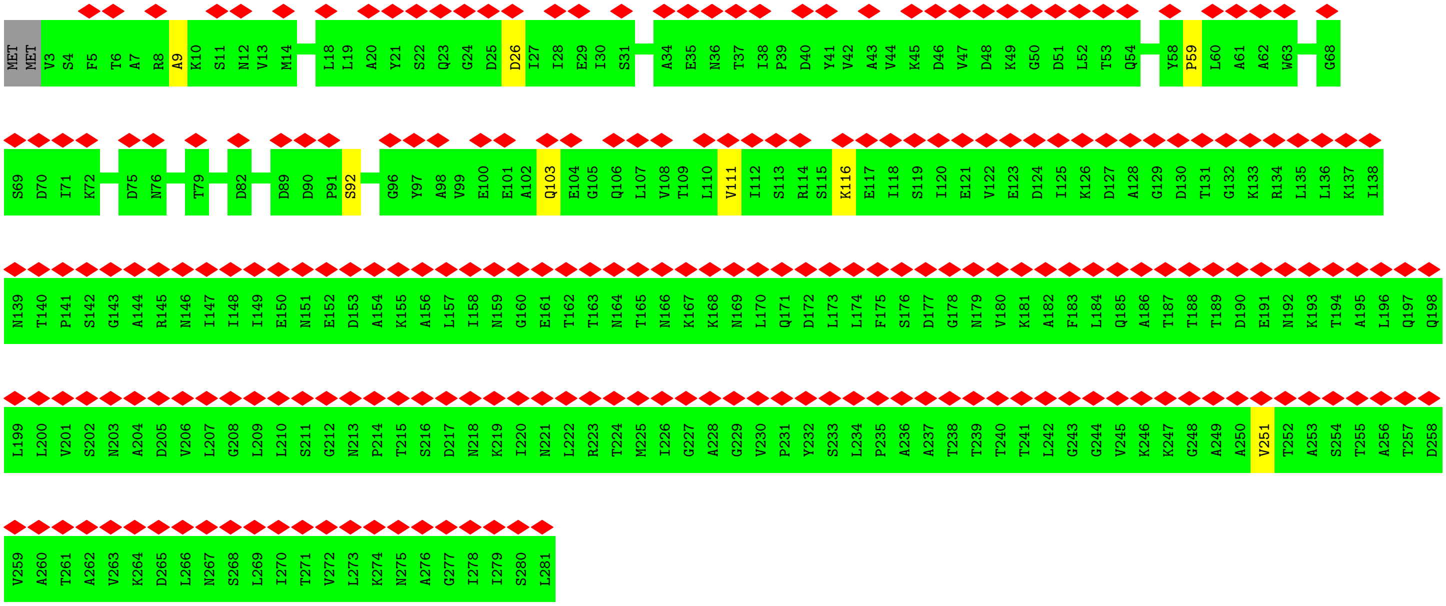




- Molecule 2: Capsid fiber protein

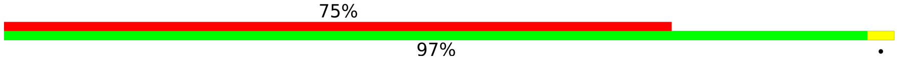
Chain 8z:

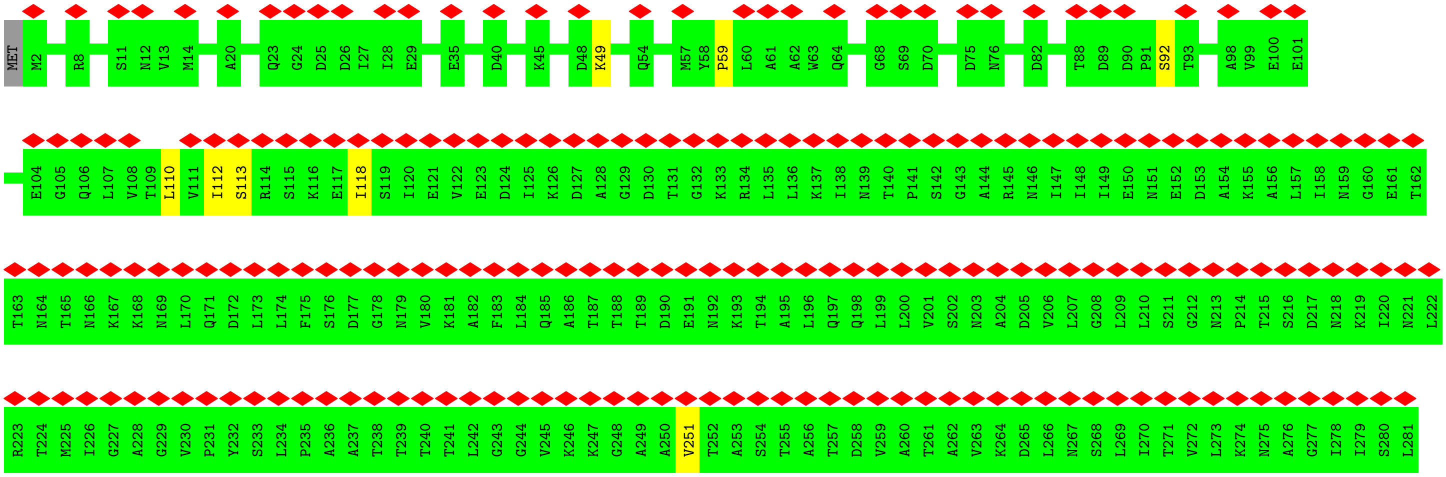




- Molecule 2: Capsid fiber protein

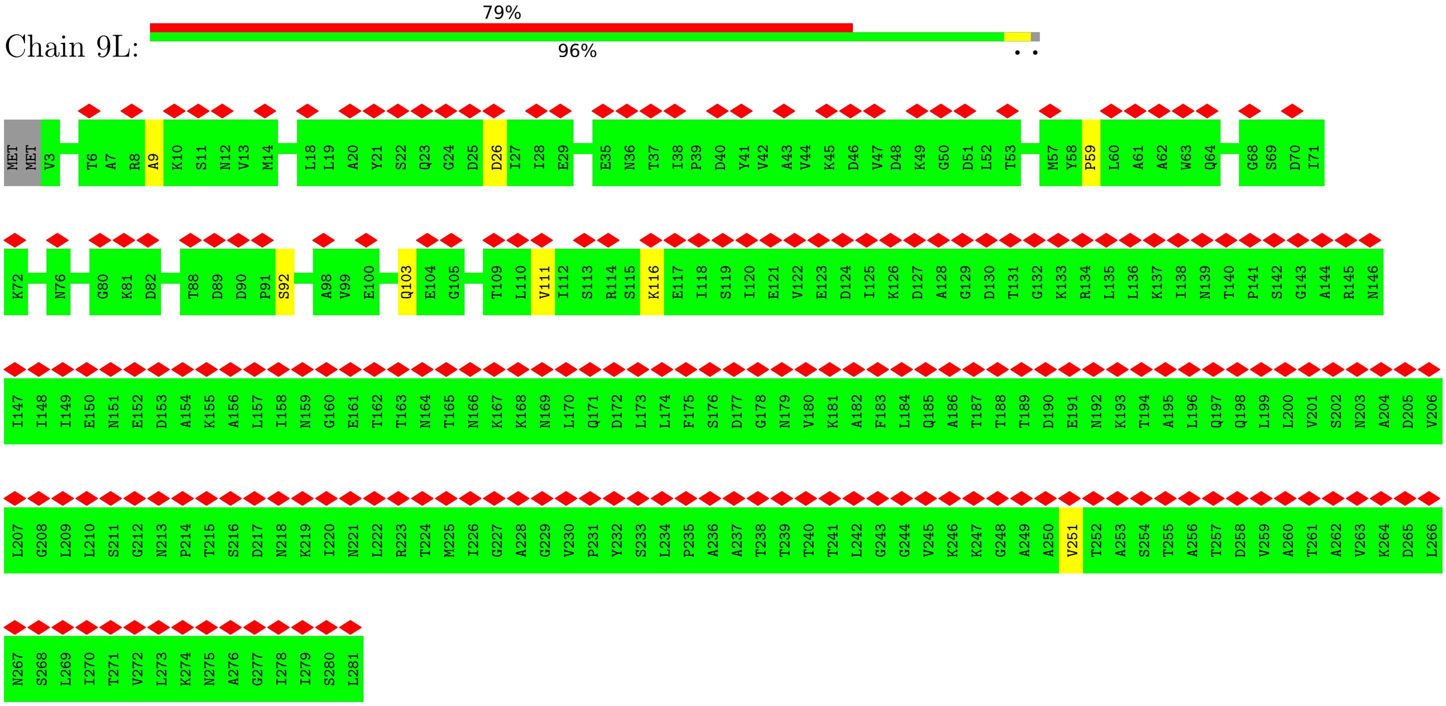
Chain 9K:





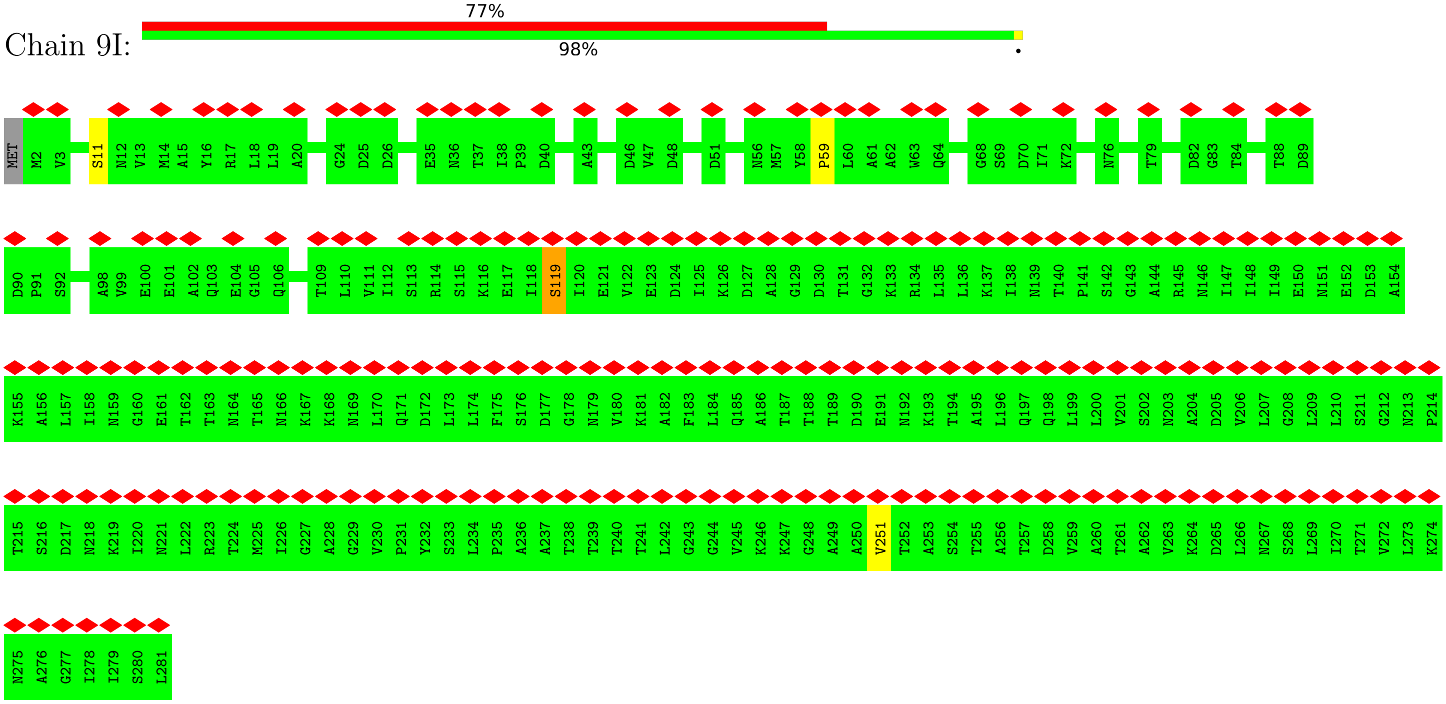
- Molecule 2: Capsid fiber protein

Chain 9L:



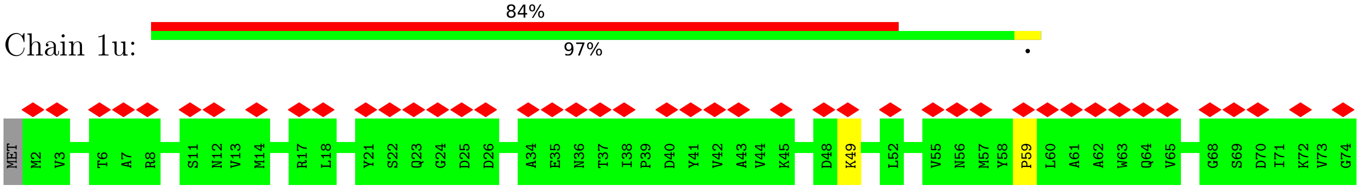
- Molecule 2: Capsid fiber protein

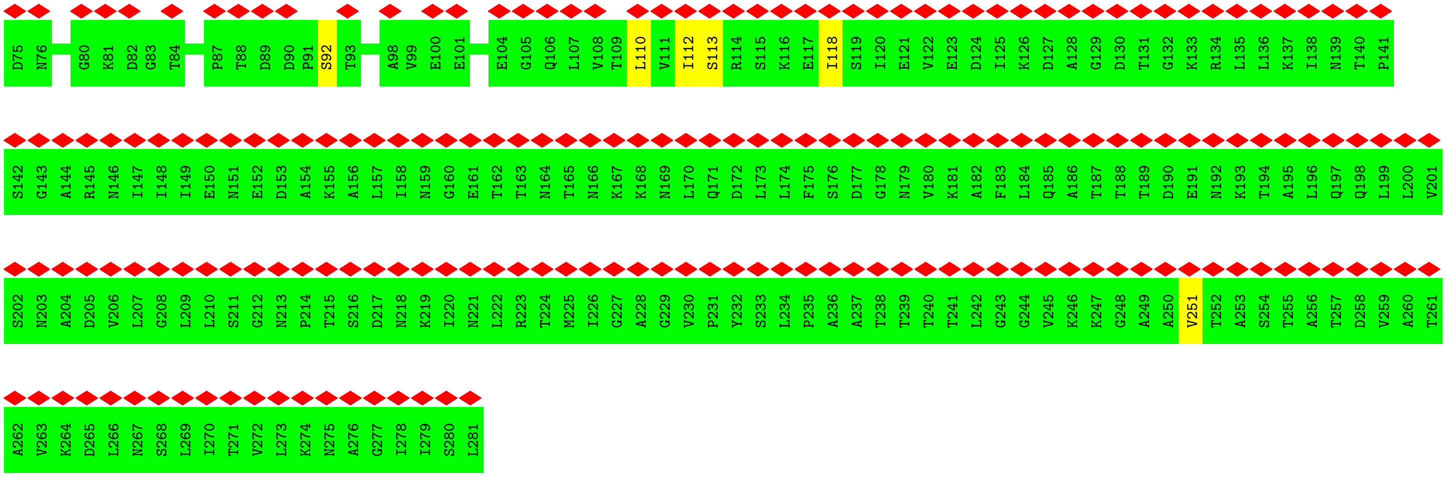
Chain 9I:



- Molecule 2: Capsid fiber protein

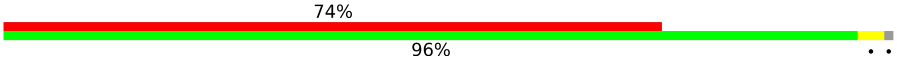
Chain 1u:

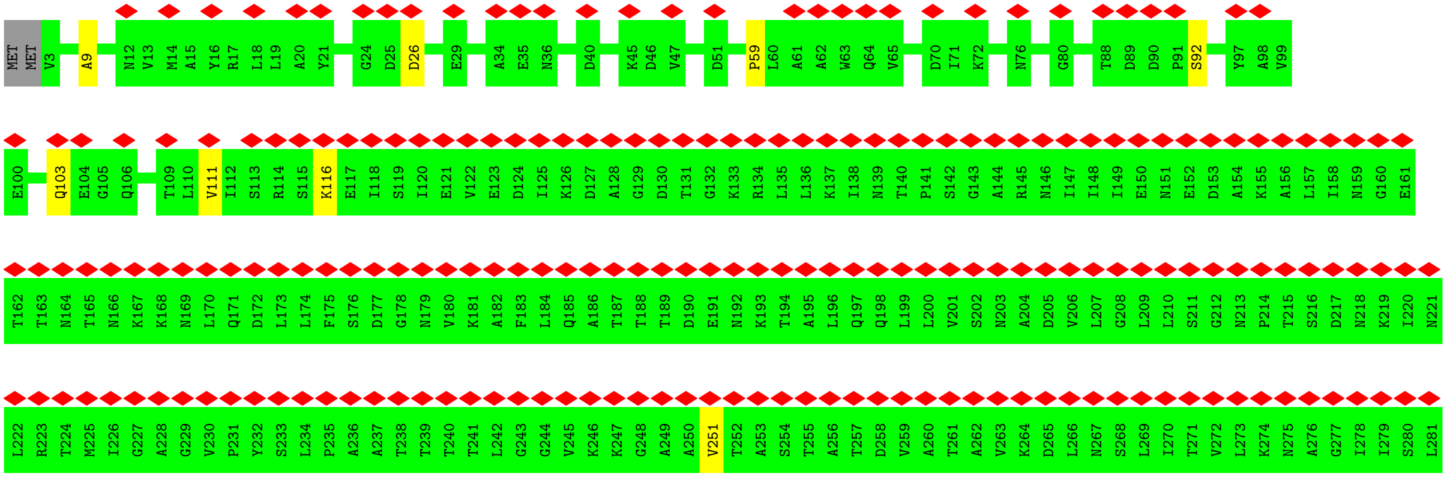




- Molecule 2: Capsid fiber protein

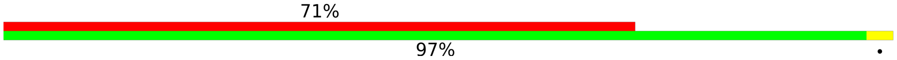
Chain 1v:

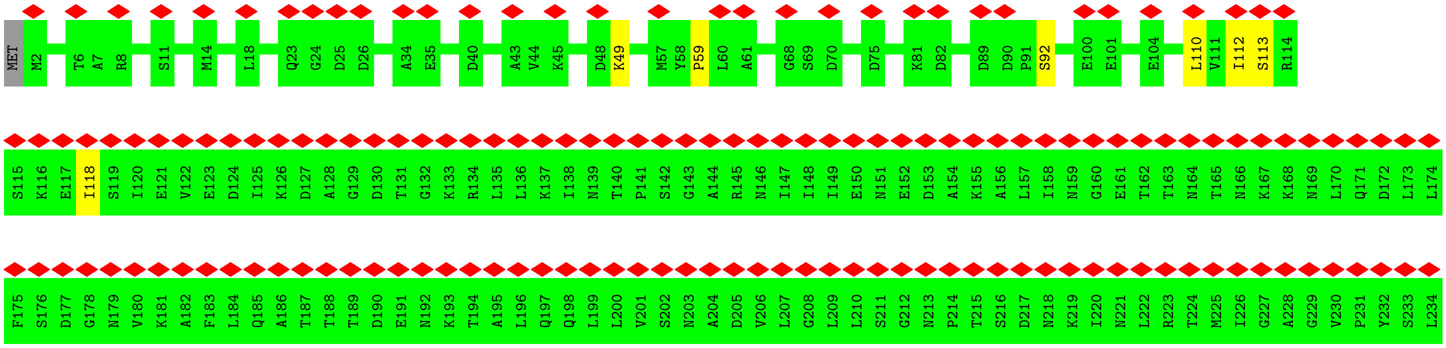


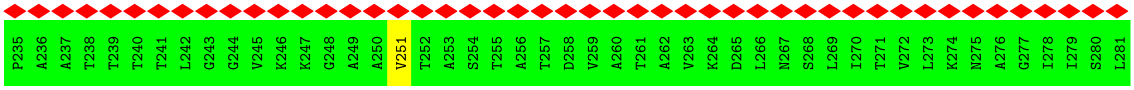


- Molecule 2: Capsid fiber protein

Chain 1w:

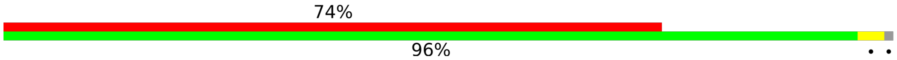


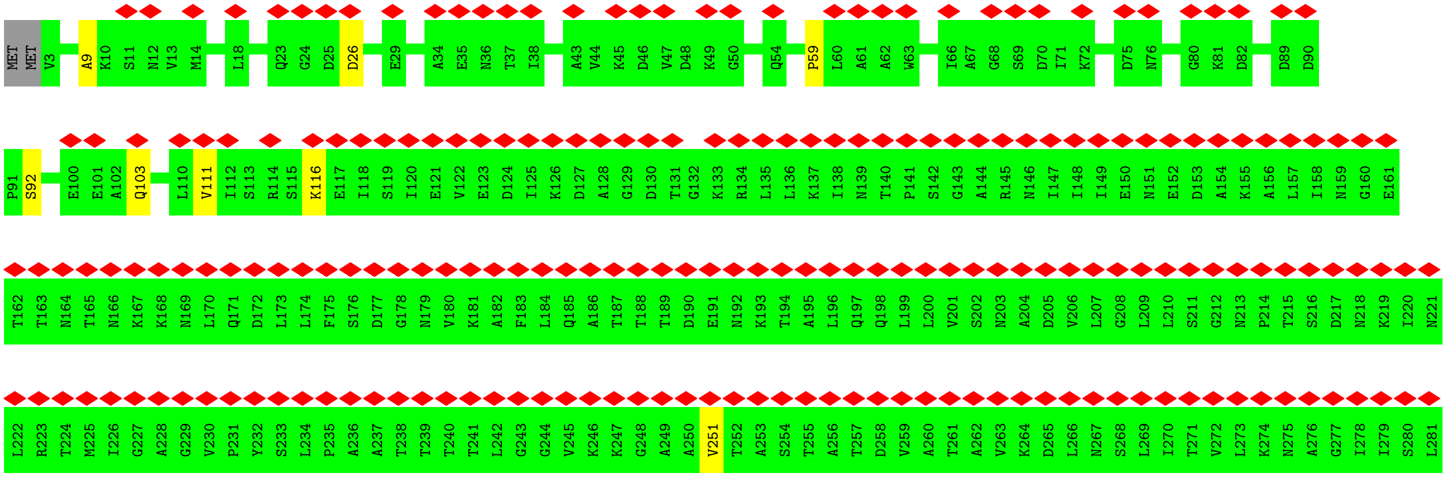




- Molecule 2: Capsid fiber protein

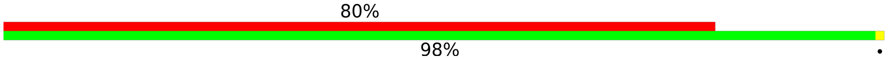
Chain 1x:

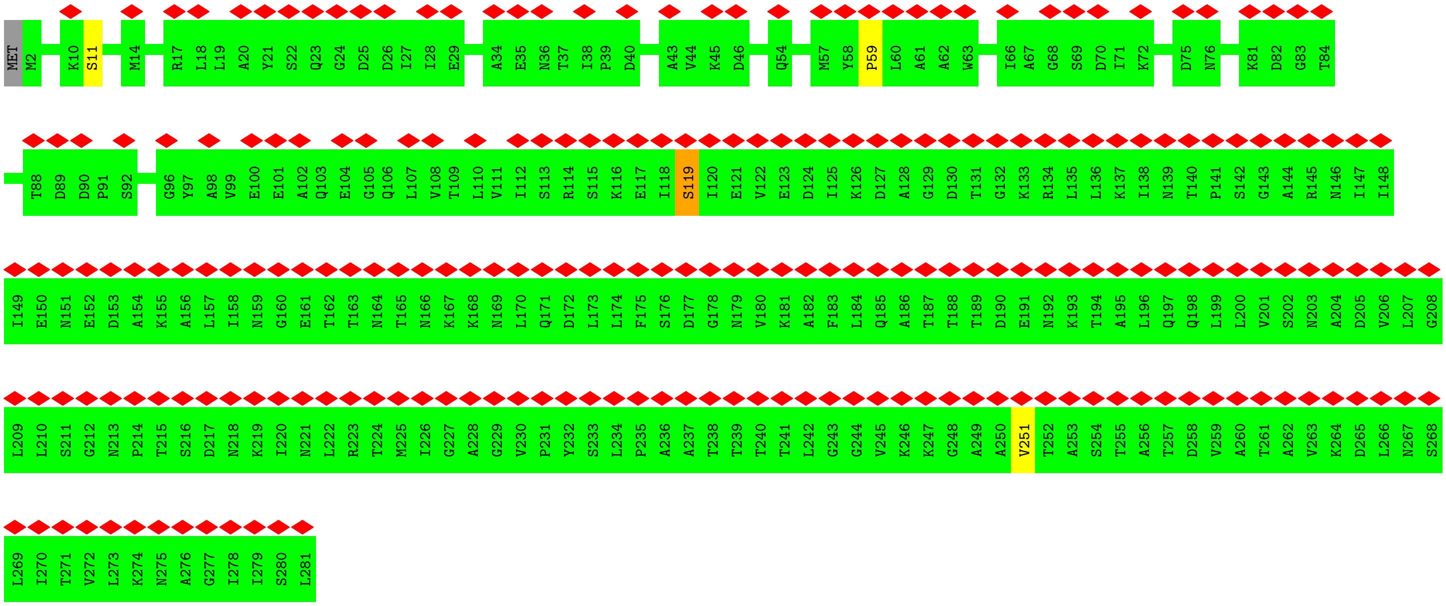




- Molecule 2: Capsid fiber protein

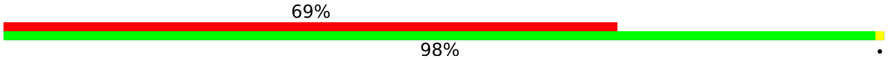
Chain 2t:

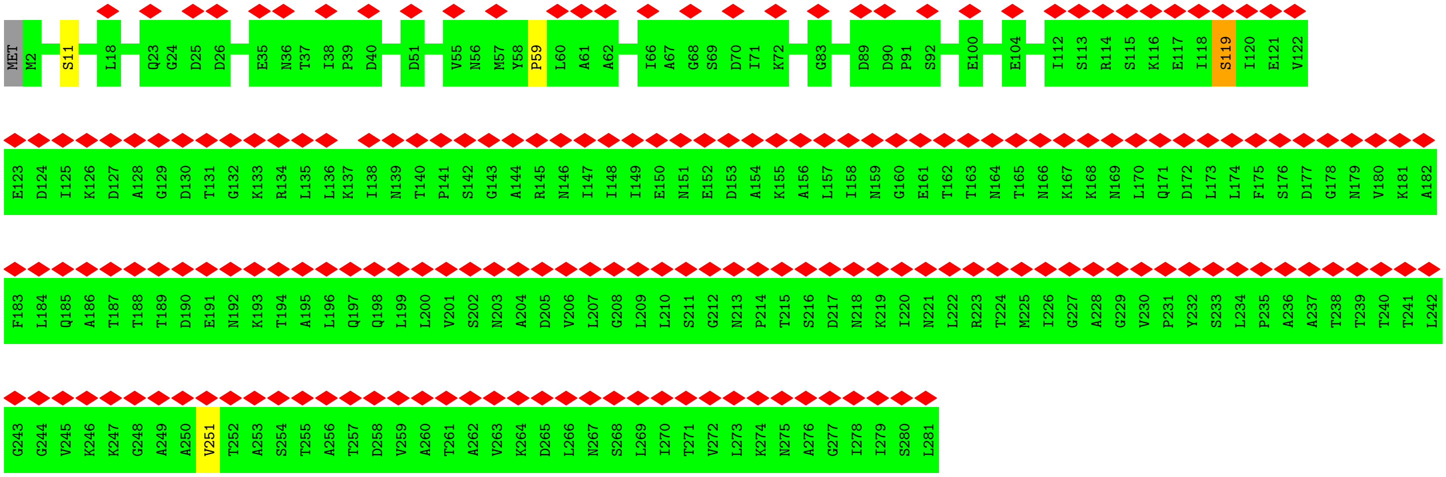




- Molecule 2: Capsid fiber protein

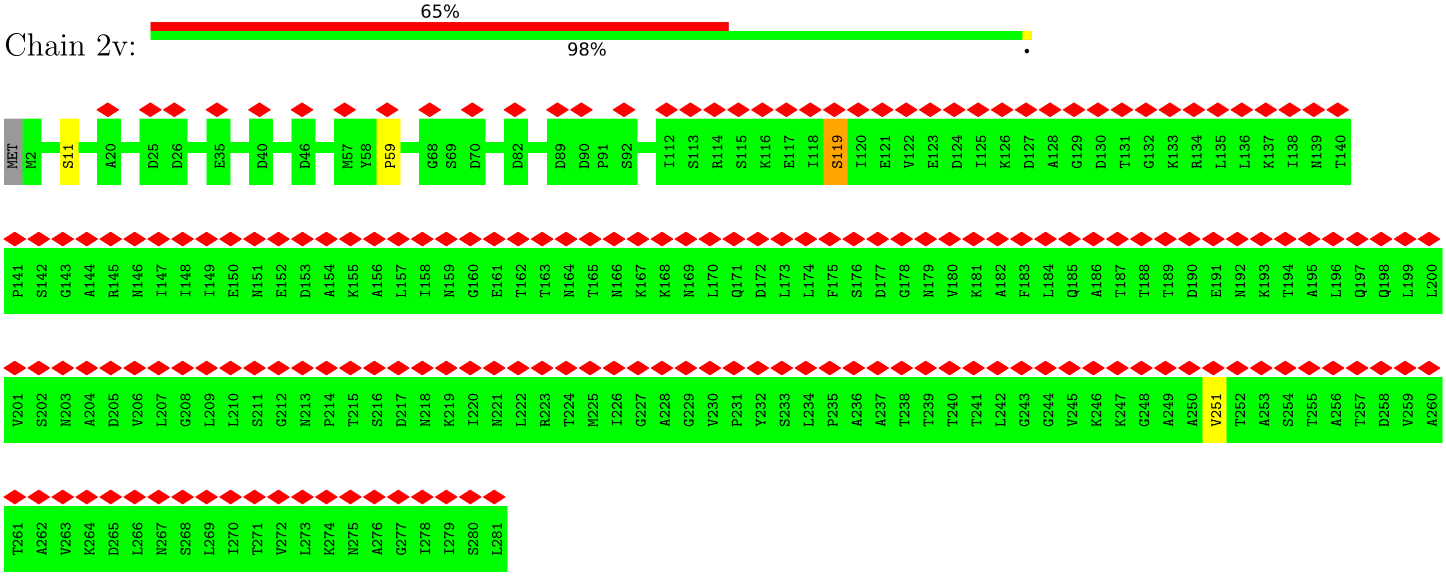
Chain 2u:





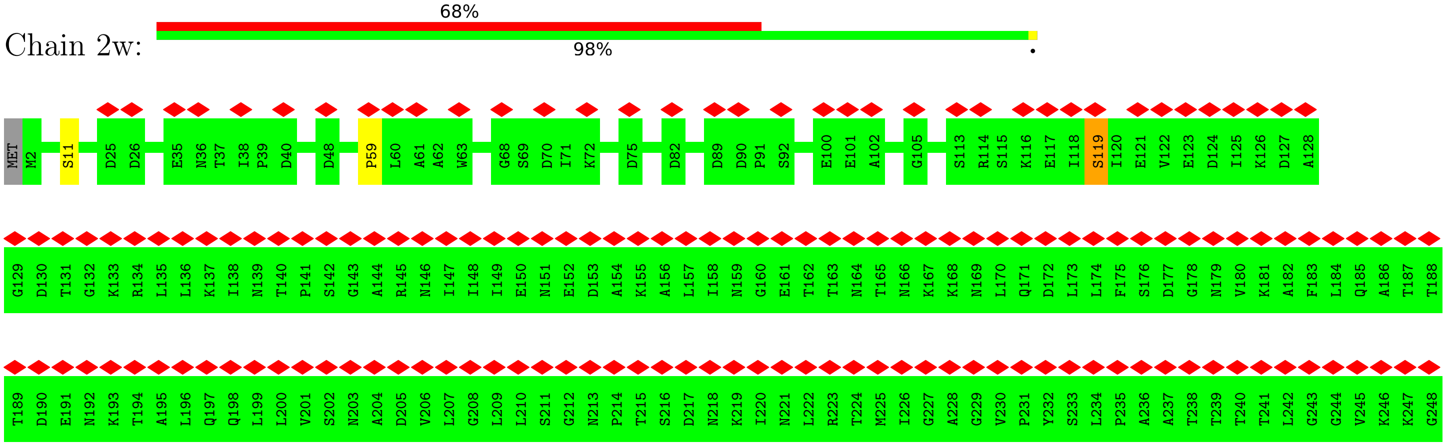
- Molecule 2: Capsid fiber protein

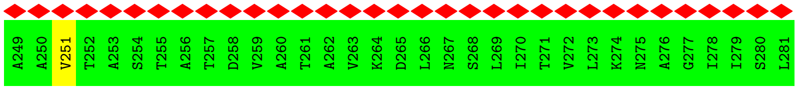
Chain 2v:



- Molecule 2: Capsid fiber protein

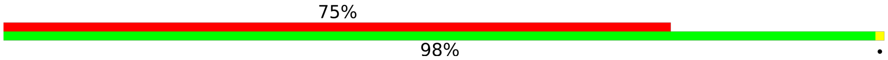
Chain 2w:

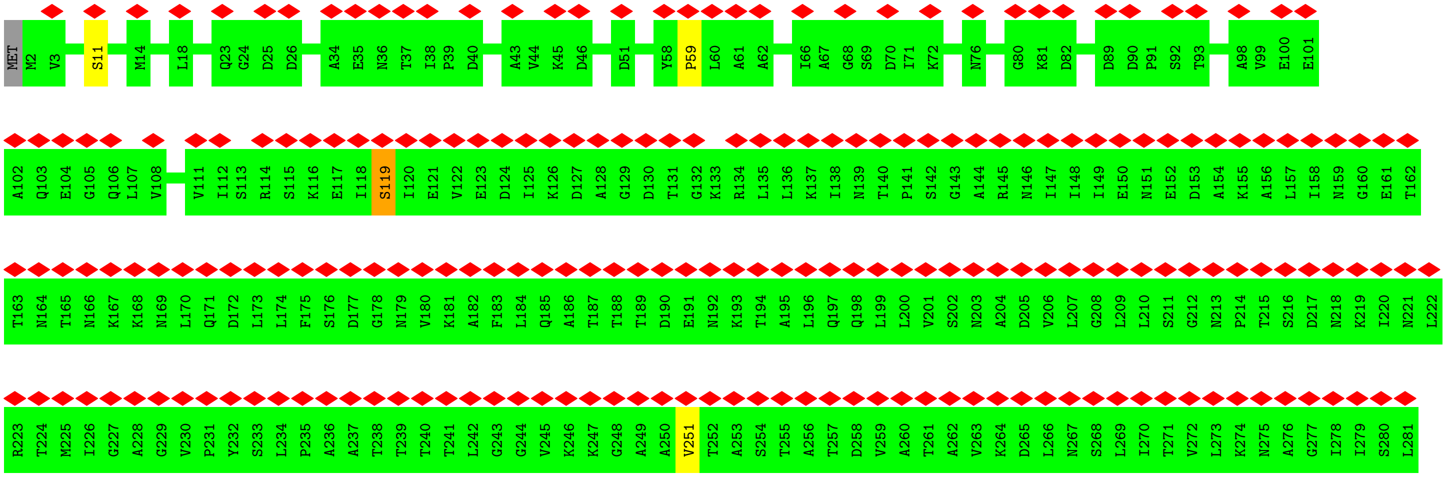




- Molecule 2: Capsid fiber protein

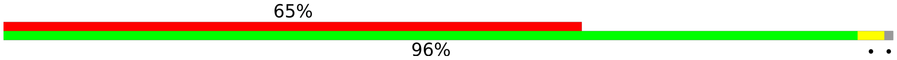
Chain 2x:

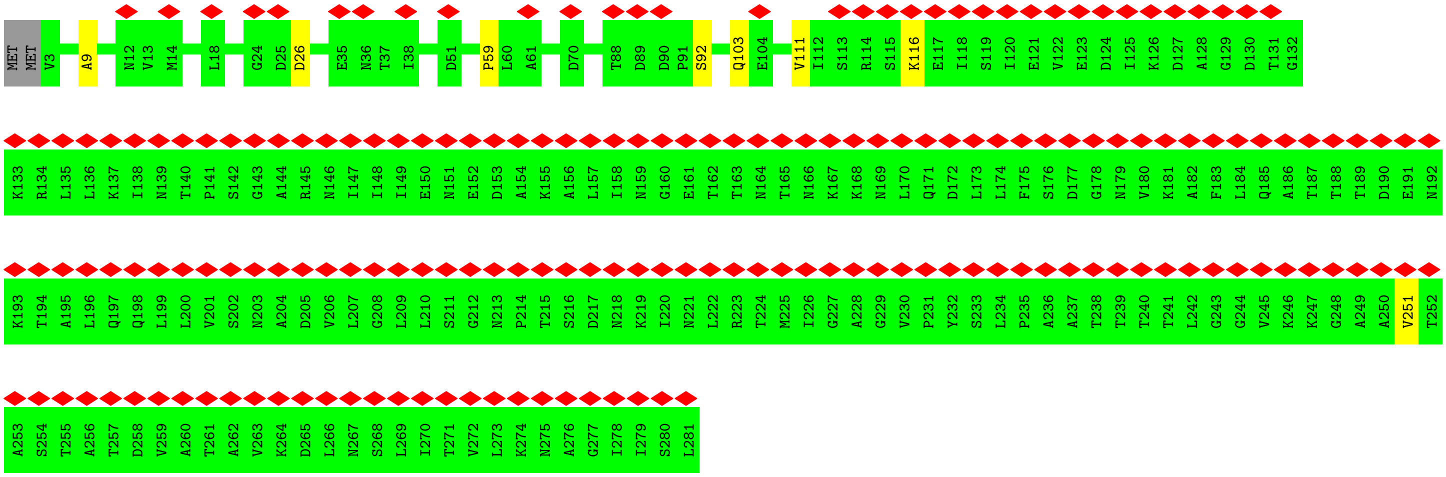




- Molecule 2: Capsid fiber protein

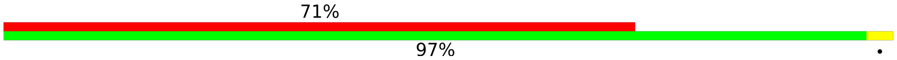
Chain 3u:

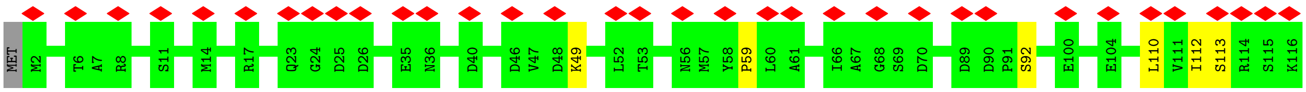


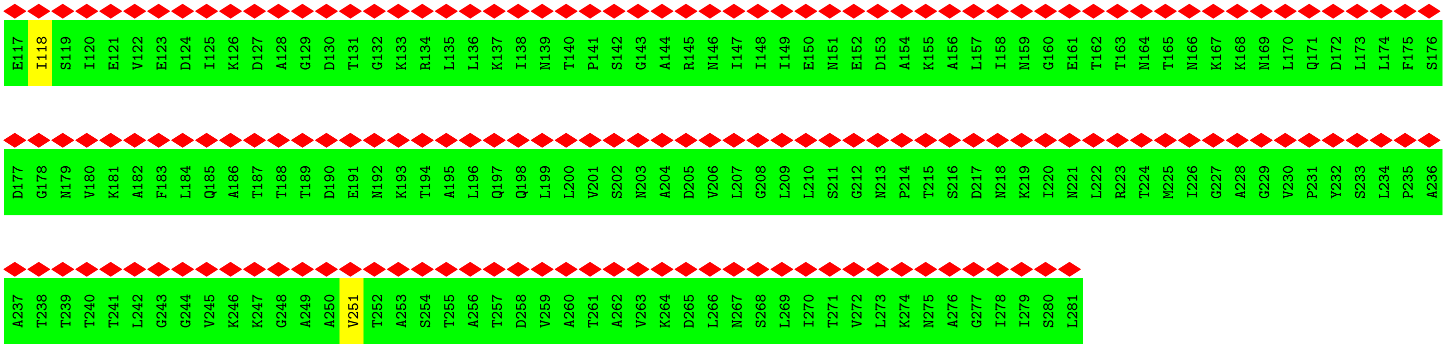


- Molecule 2: Capsid fiber protein

Chain 3v:

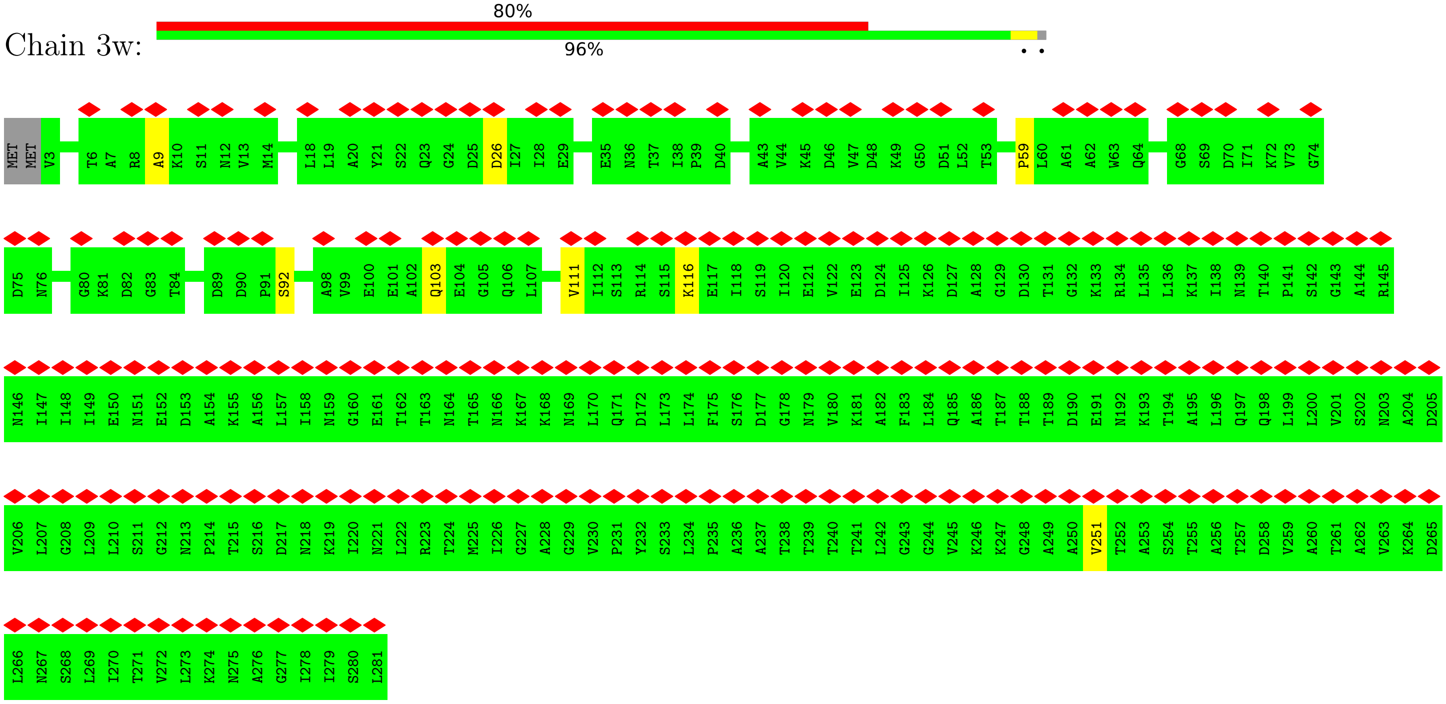






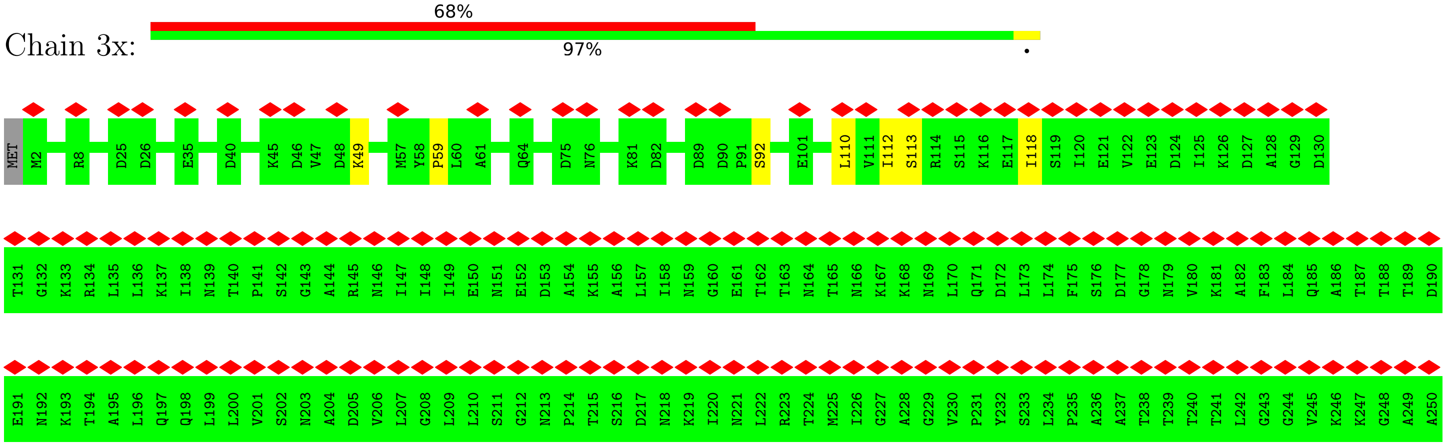
- Molecule 2: Capsid fiber protein

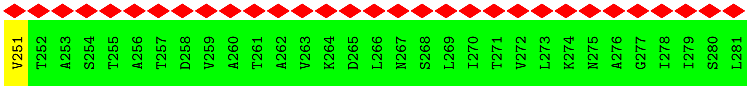
Chain 3w:



- Molecule 2: Capsid fiber protein

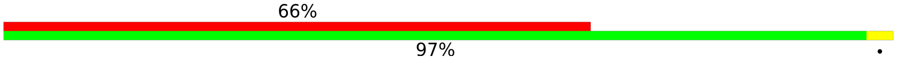
Chain 3x:

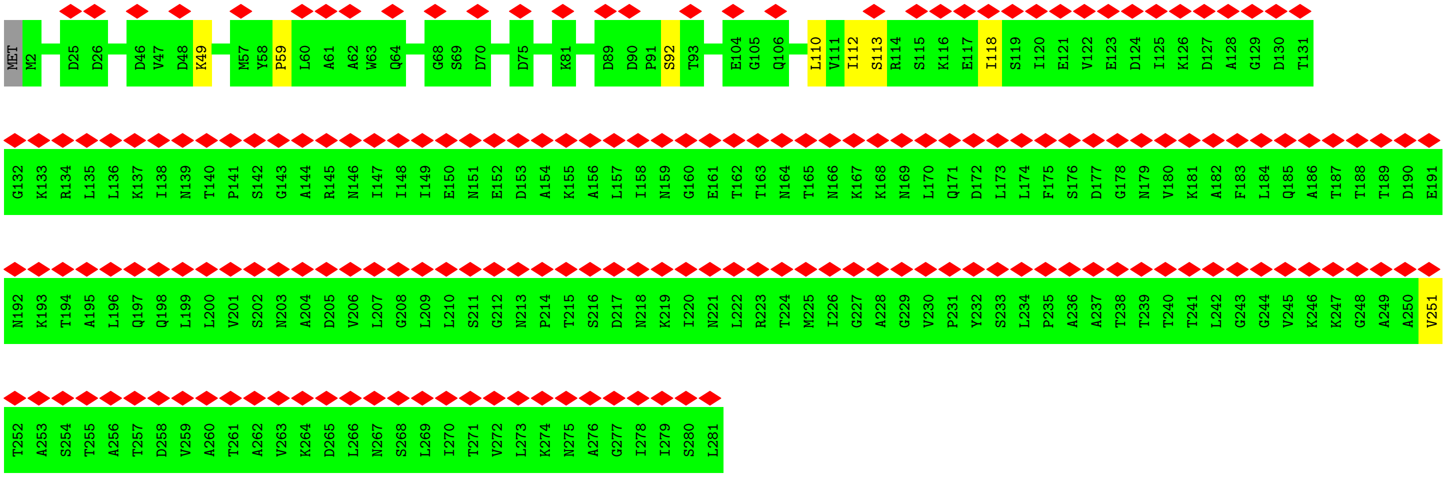




- Molecule 2: Capsid fiber protein

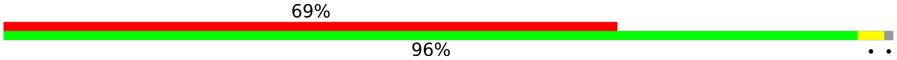
Chain 4m:

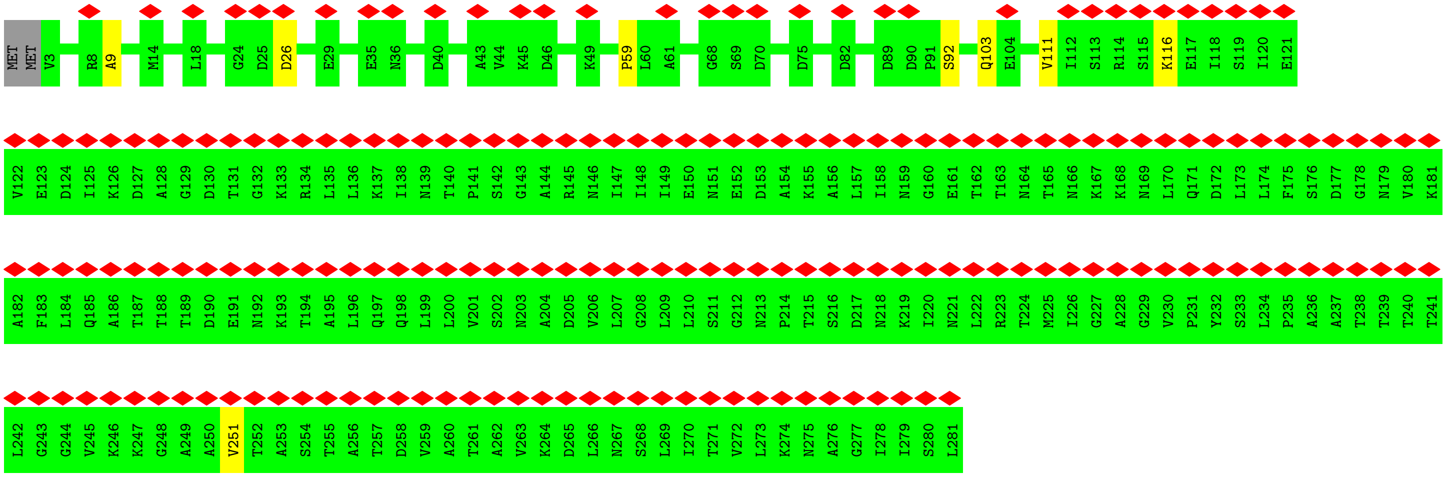




- Molecule 2: Capsid fiber protein

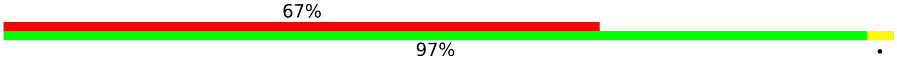
Chain 4n:

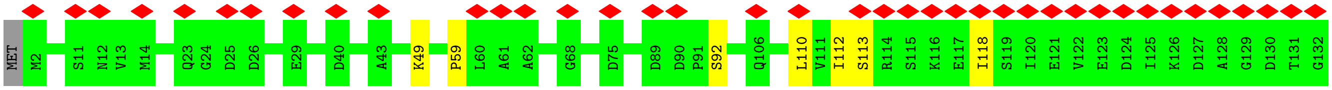




- Molecule 2: Capsid fiber protein

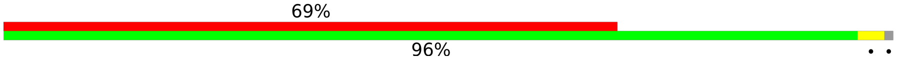
Chain 5m:

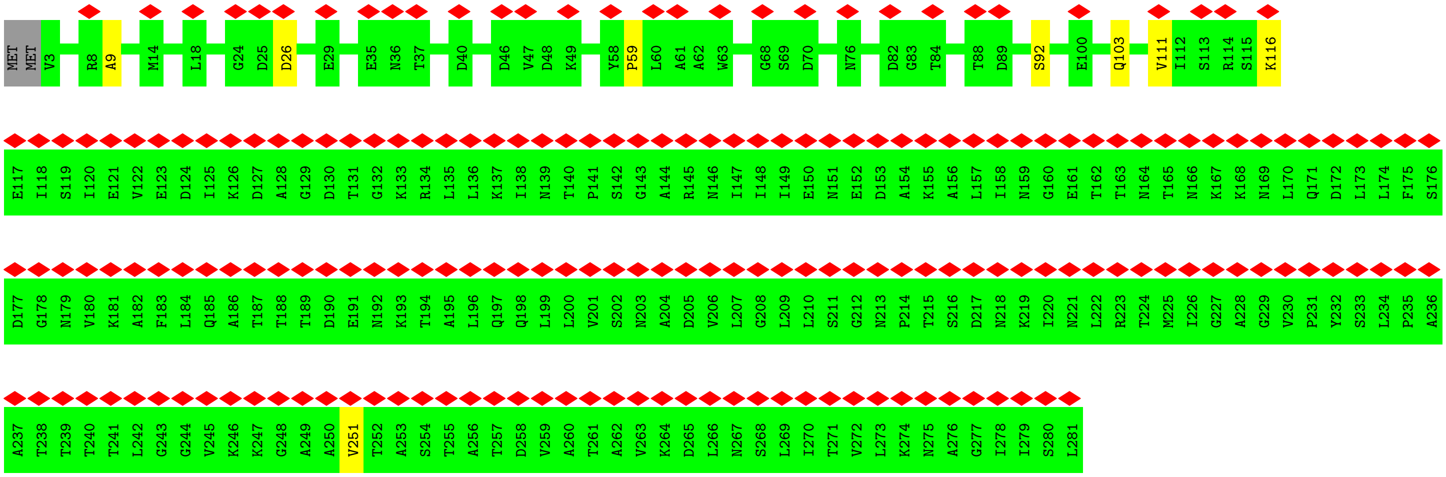




- Molecule 2: Capsid fiber protein

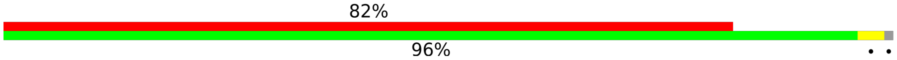
Chain 5n:

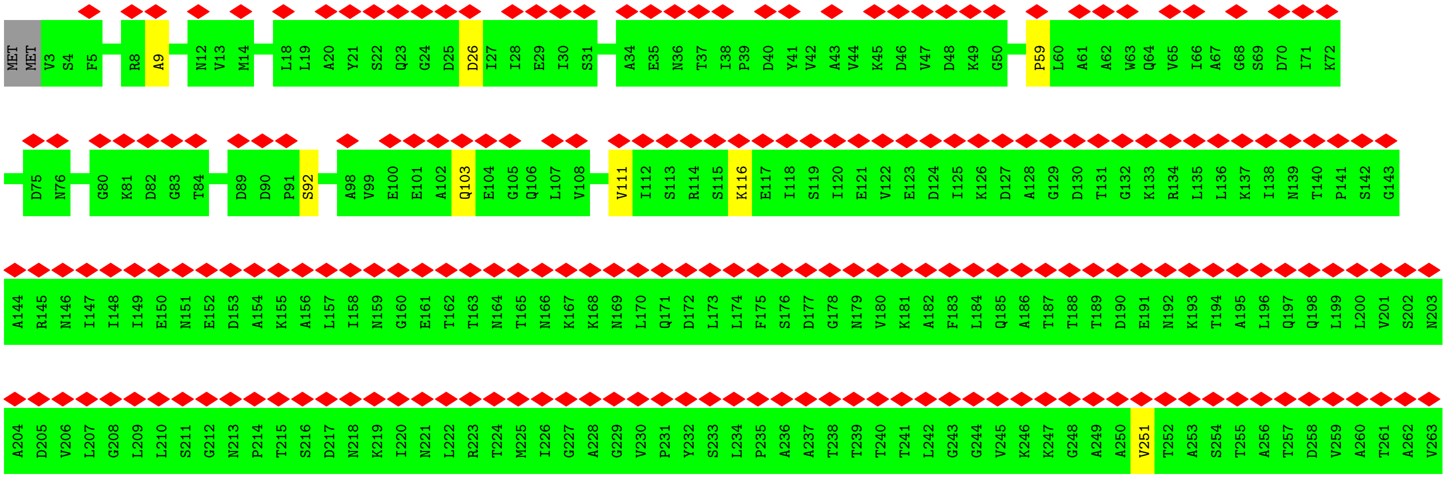


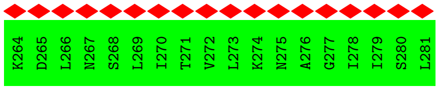


- Molecule 2: Capsid fiber protein

Chain 6u:

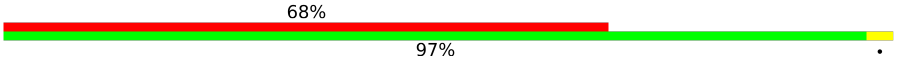


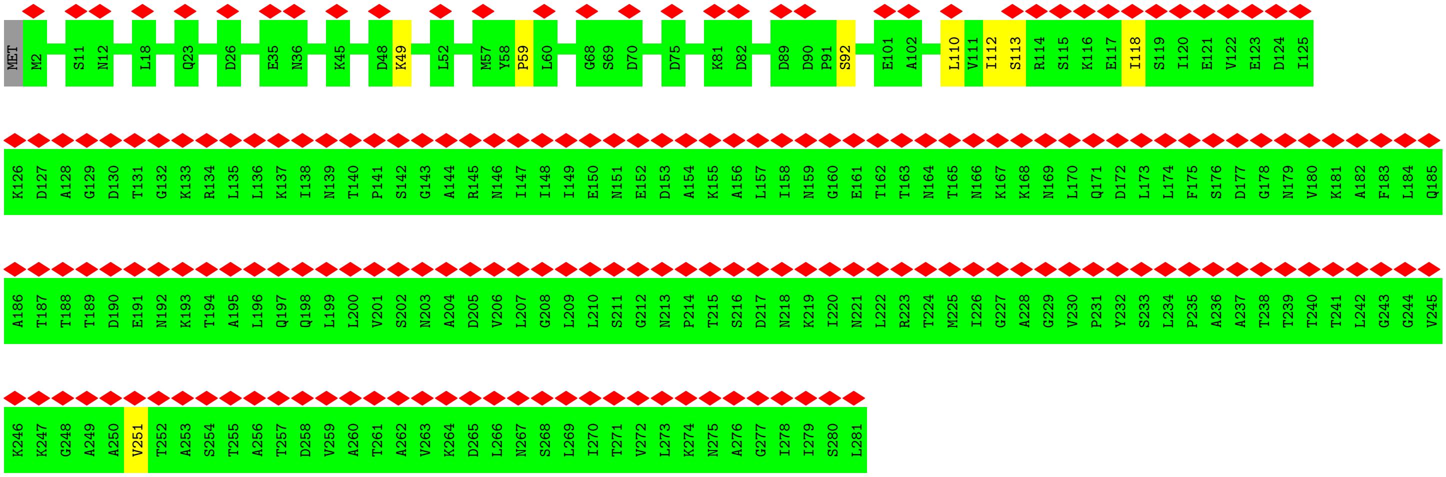




- Molecule 2: Capsid fiber protein

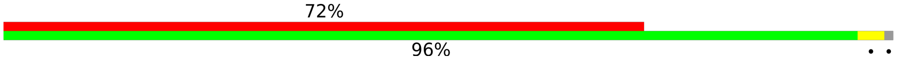
Chain 6v:

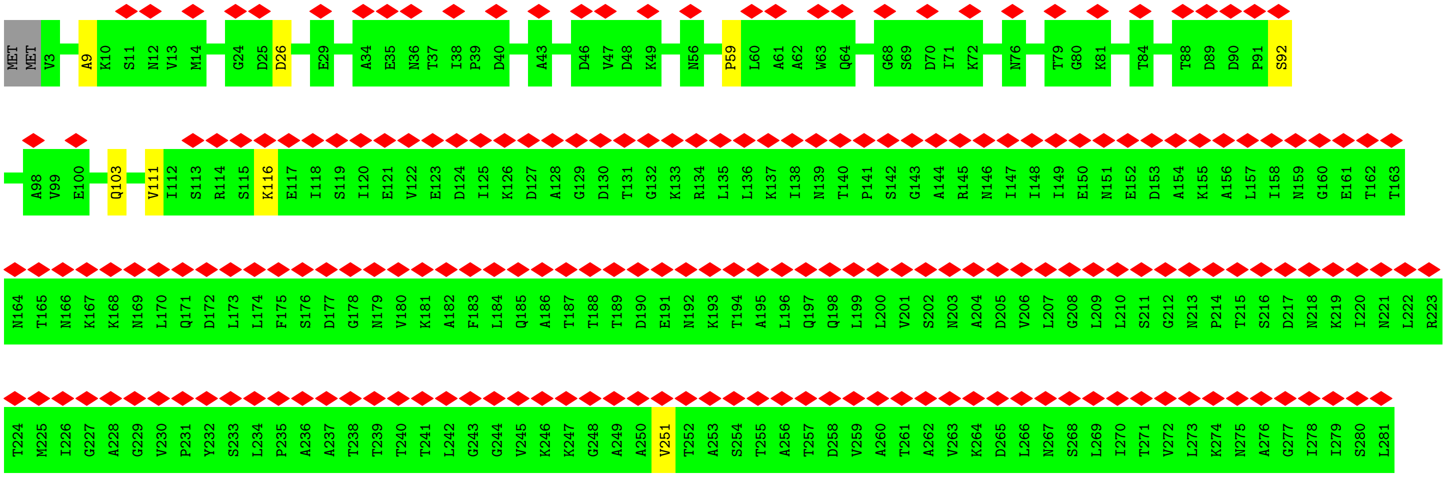




- Molecule 2: Capsid fiber protein

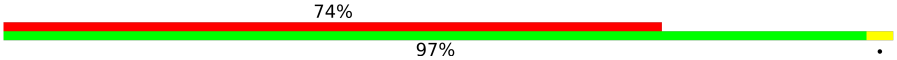
Chain 6w:

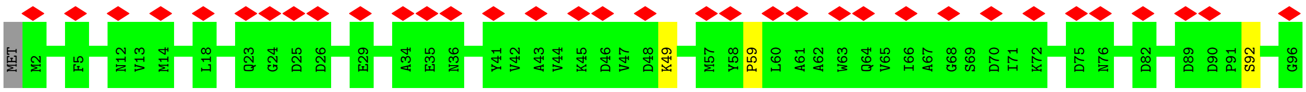


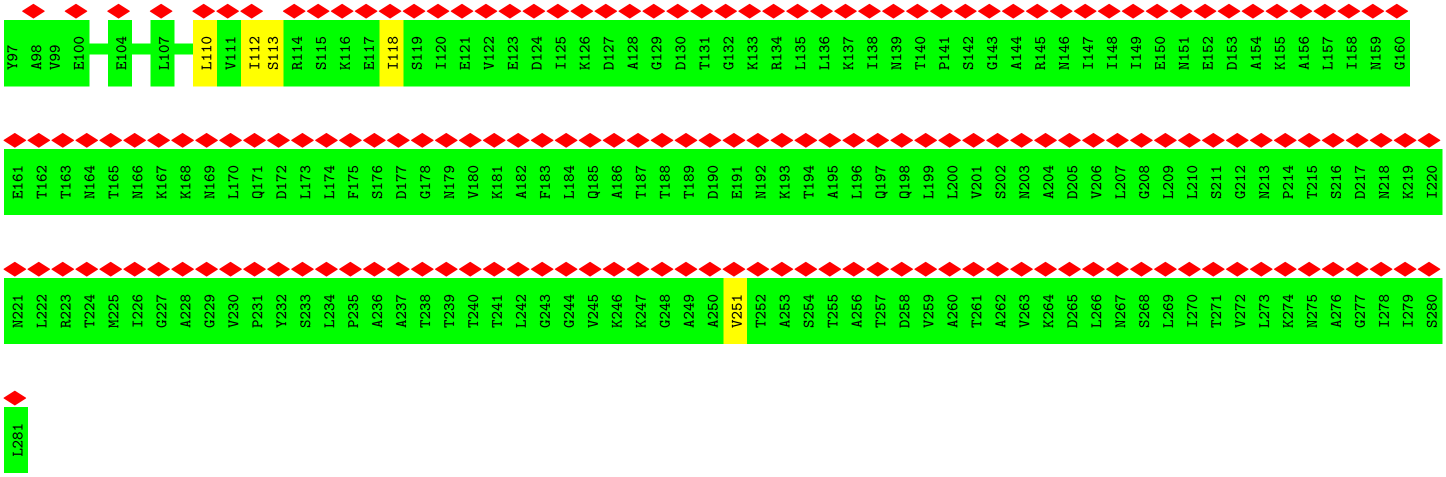


- Molecule 2: Capsid fiber protein

Chain 6x:

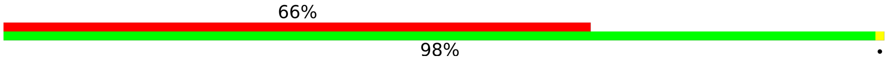


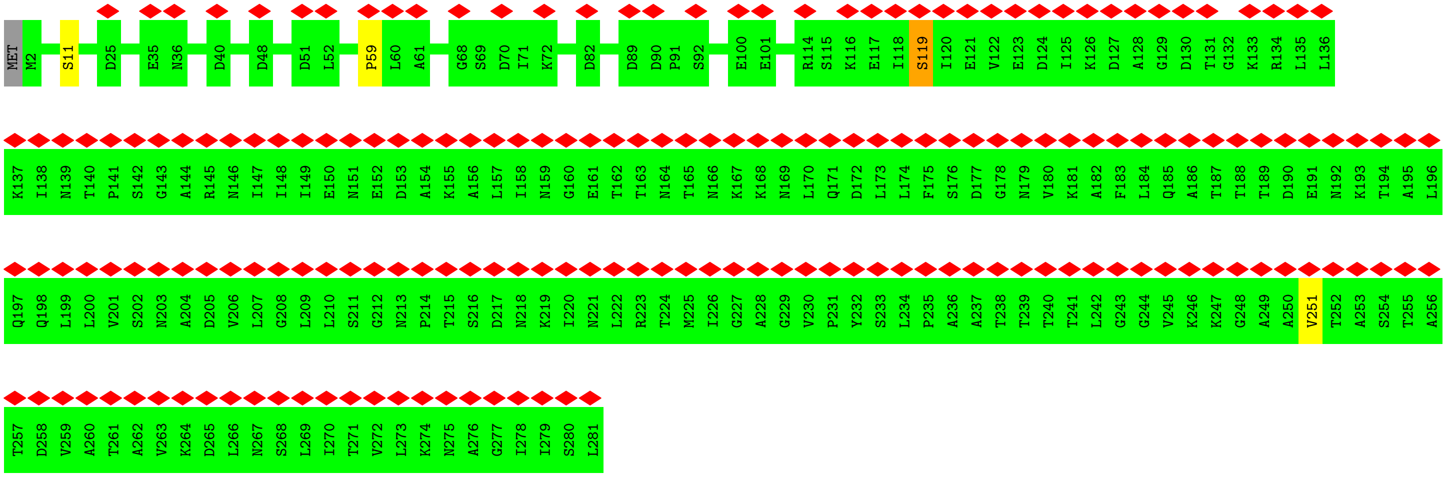




- Molecule 2: Capsid fiber protein

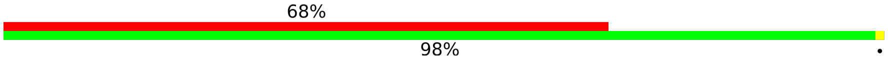
Chain 7t:

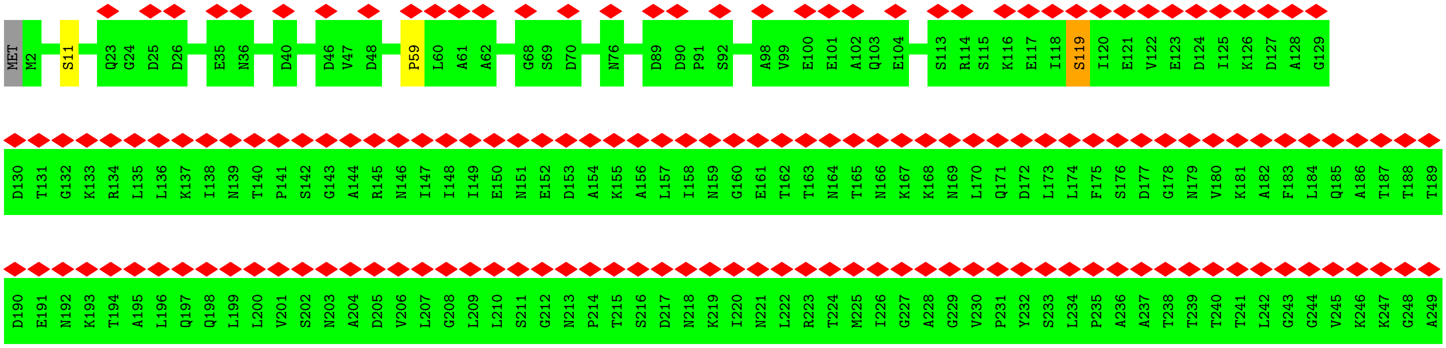


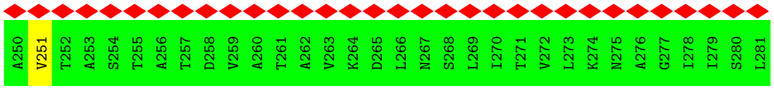


- Molecule 2: Capsid fiber protein

Chain 7u:

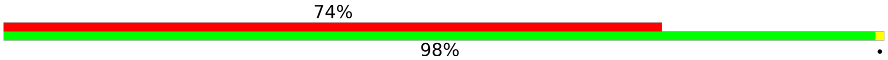


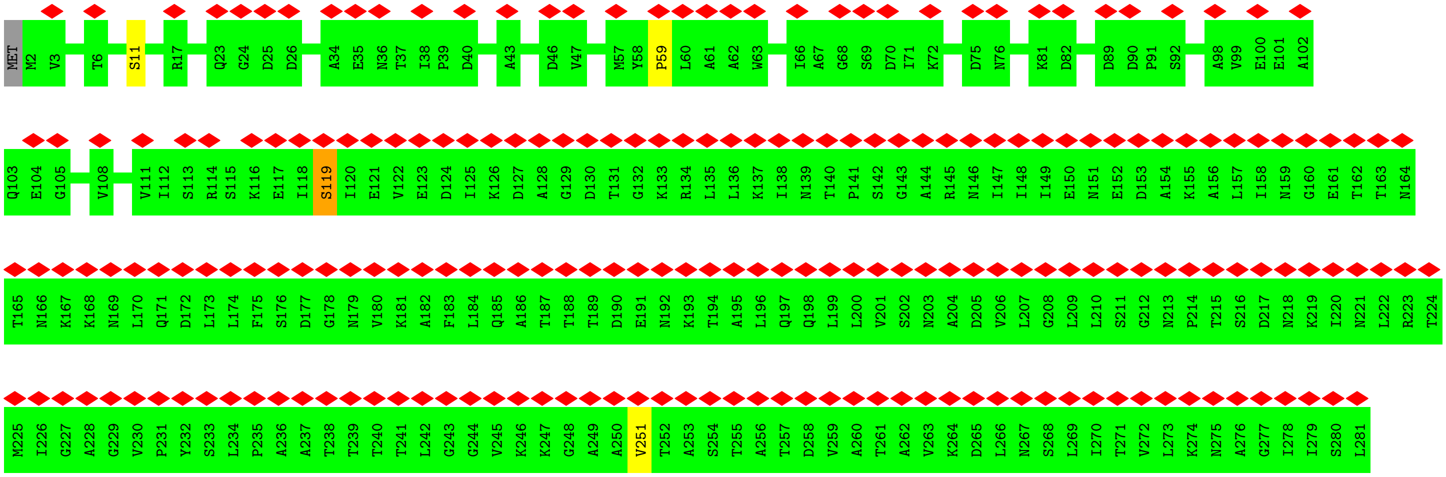




- Molecule 2: Capsid fiber protein

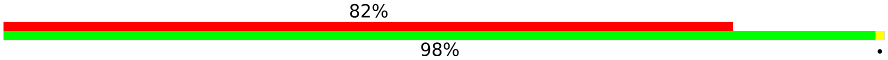
Chain 7v:

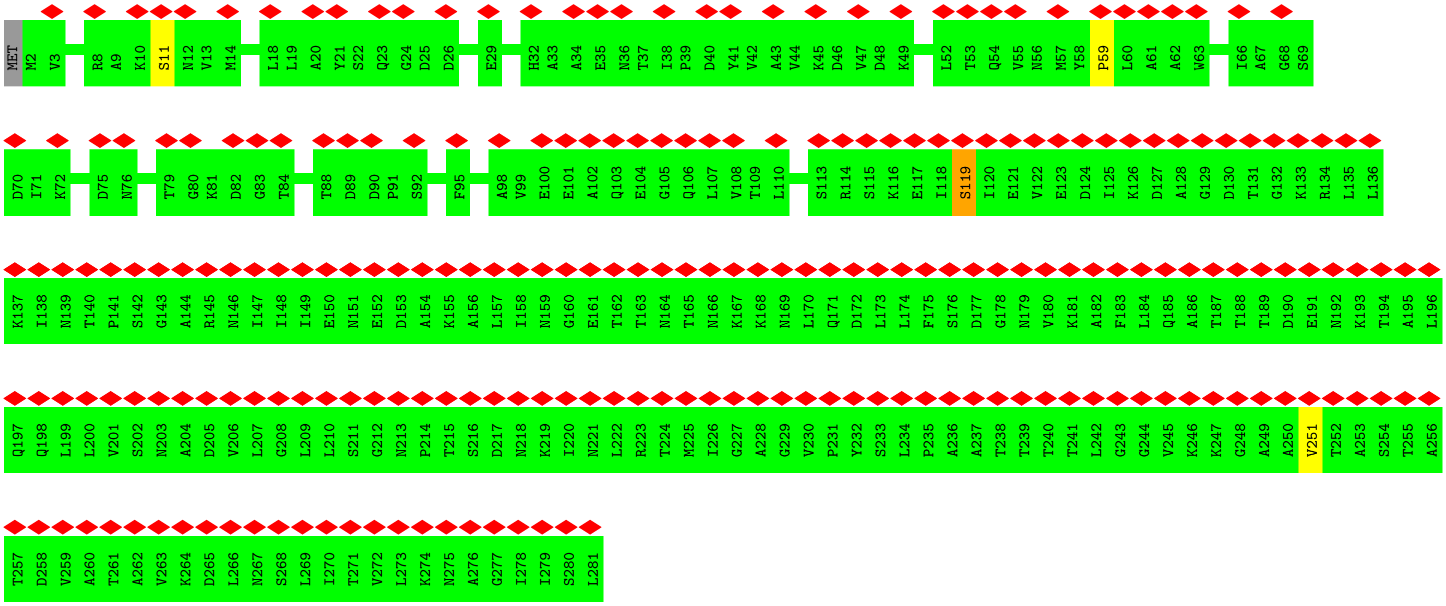




- Molecule 2: Capsid fiber protein

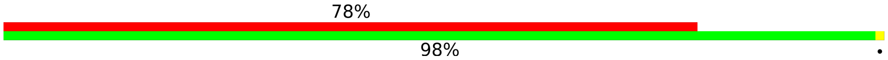
Chain 7w:

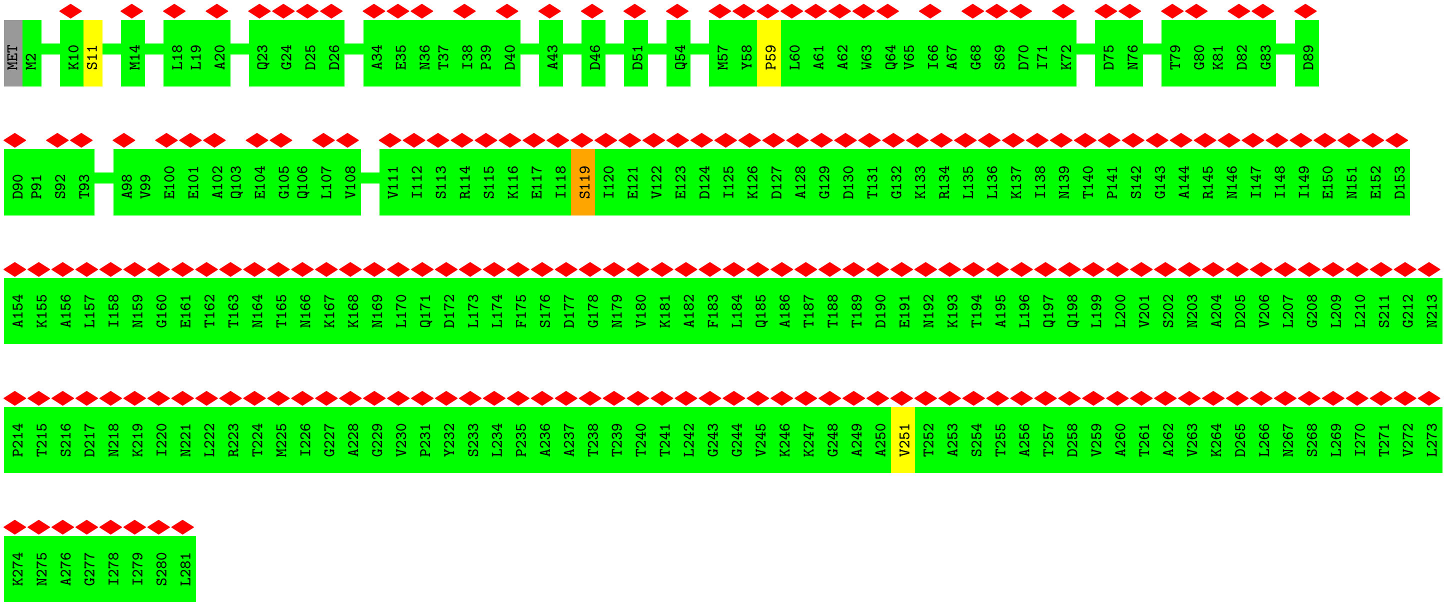




- Molecule 2: Capsid fiber protein

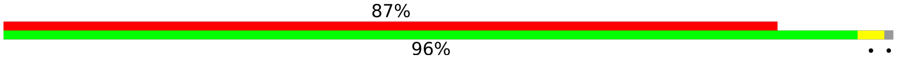
Chain 7x:

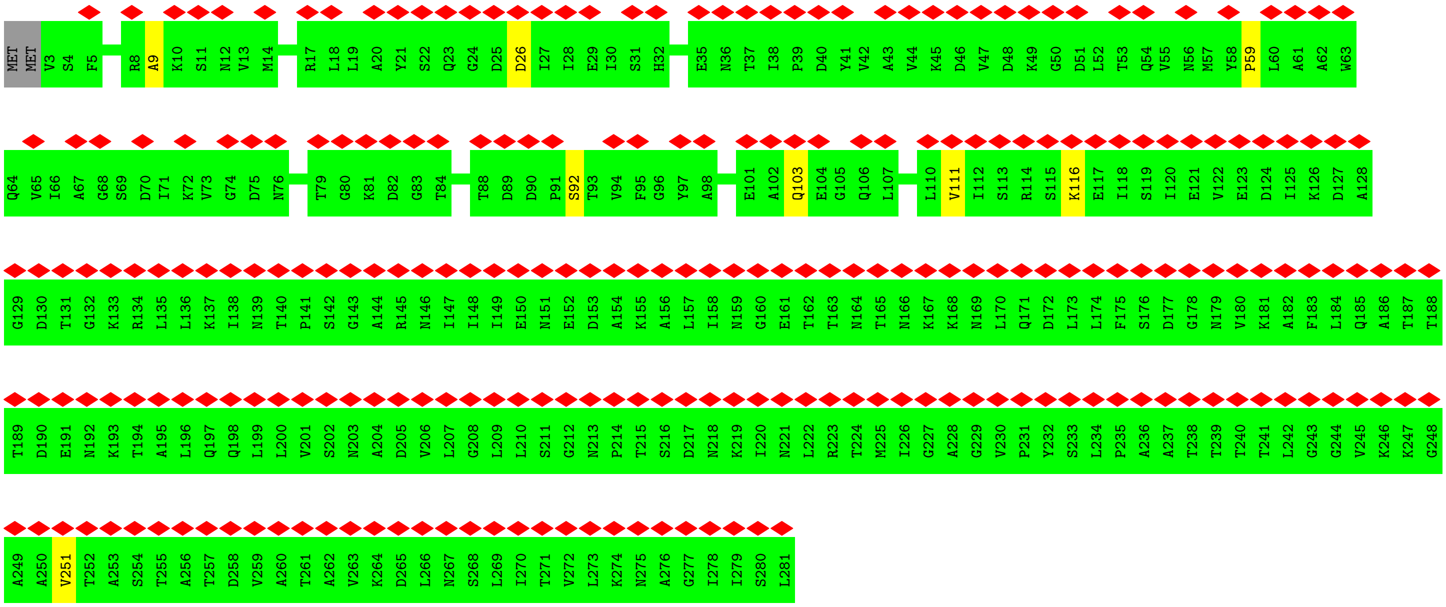




- Molecule 2: Capsid fiber protein

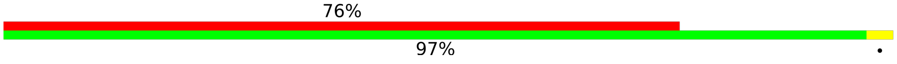
Chain 9M:

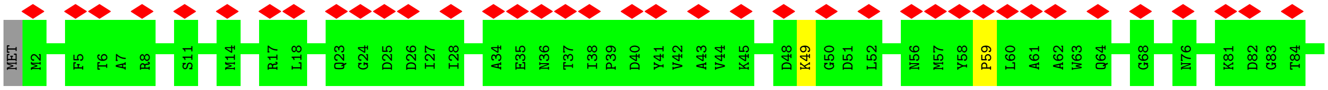


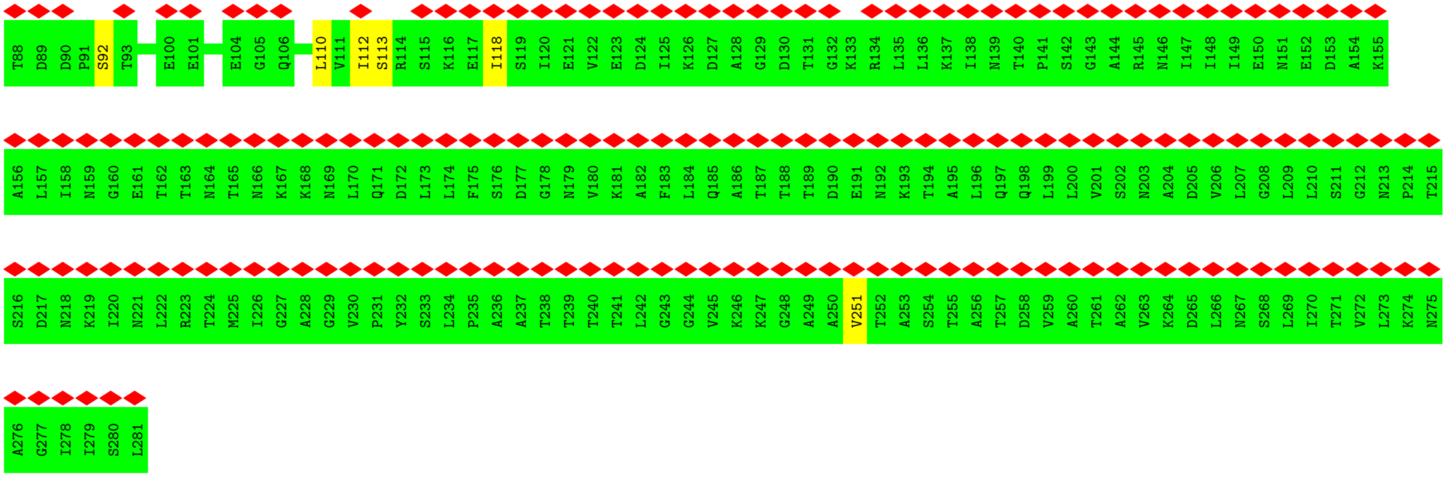


- Molecule 2: Capsid fiber protein

Chain 9N:

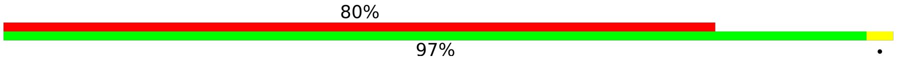


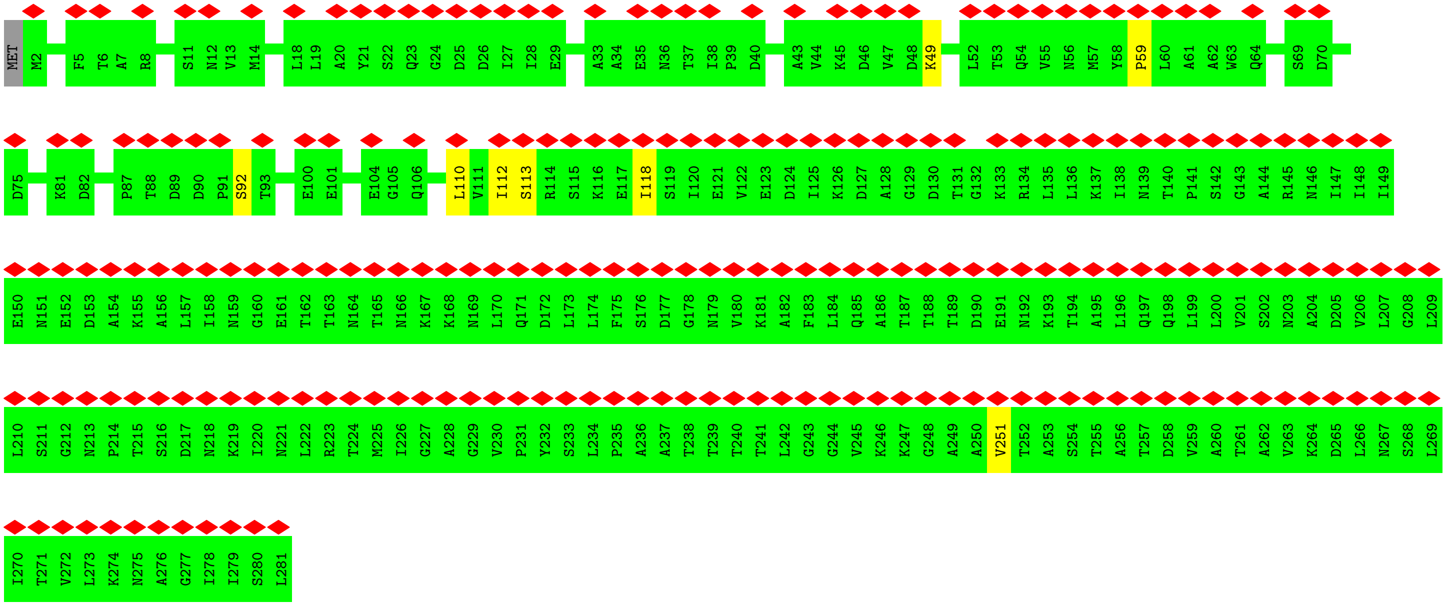




- Molecule 2: Capsid fiber protein

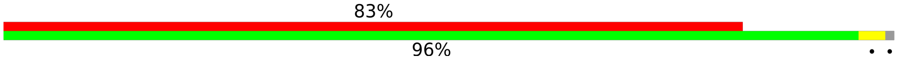
Chain 9O:

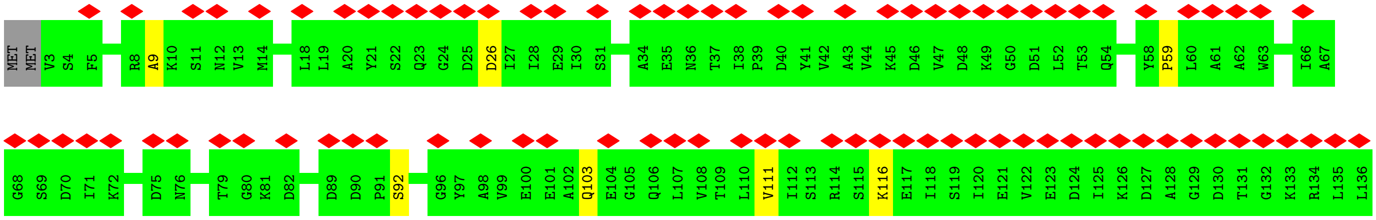


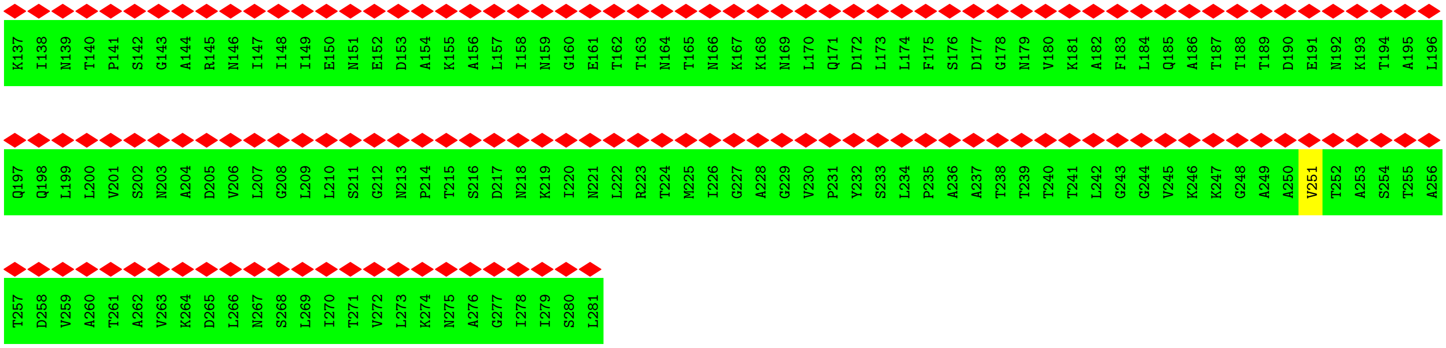


- Molecule 2: Capsid fiber protein

Chain 9P:

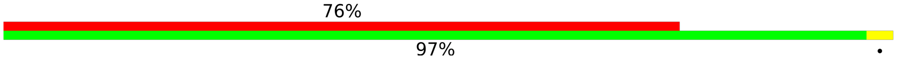


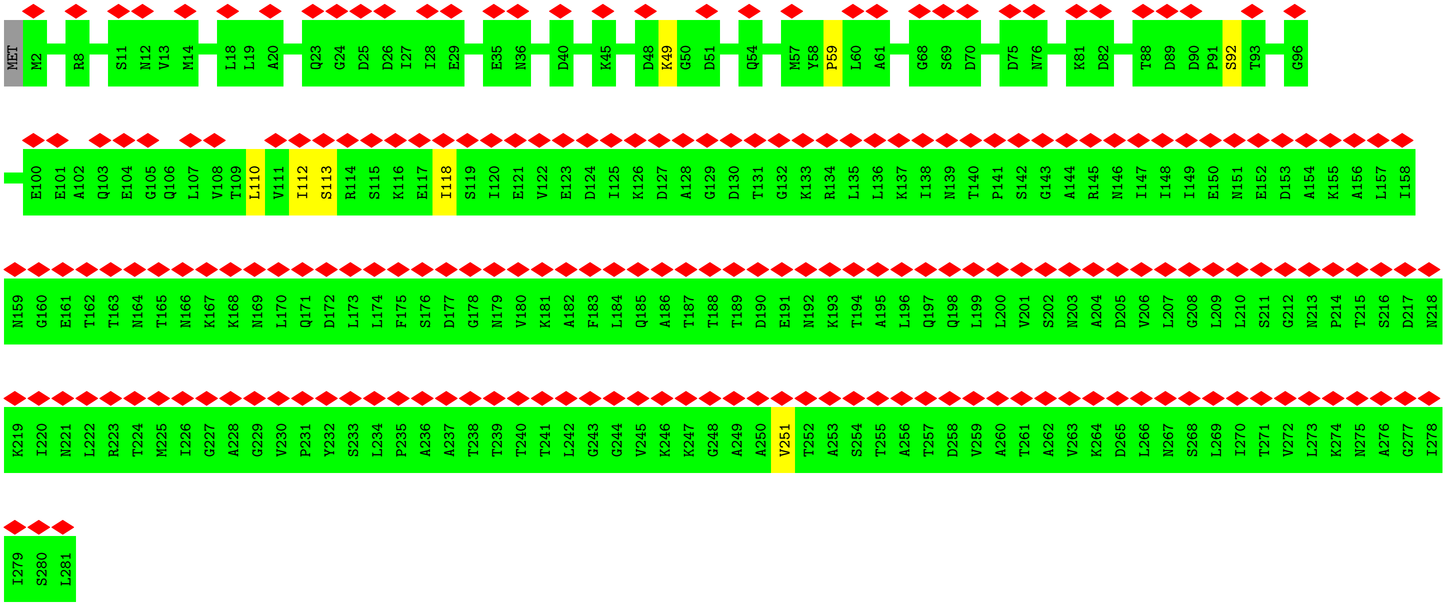




- Molecule 2: Capsid fiber protein

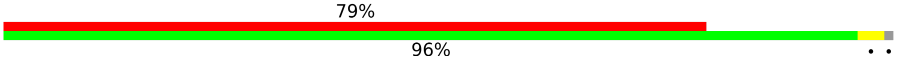
Chain 9Q:

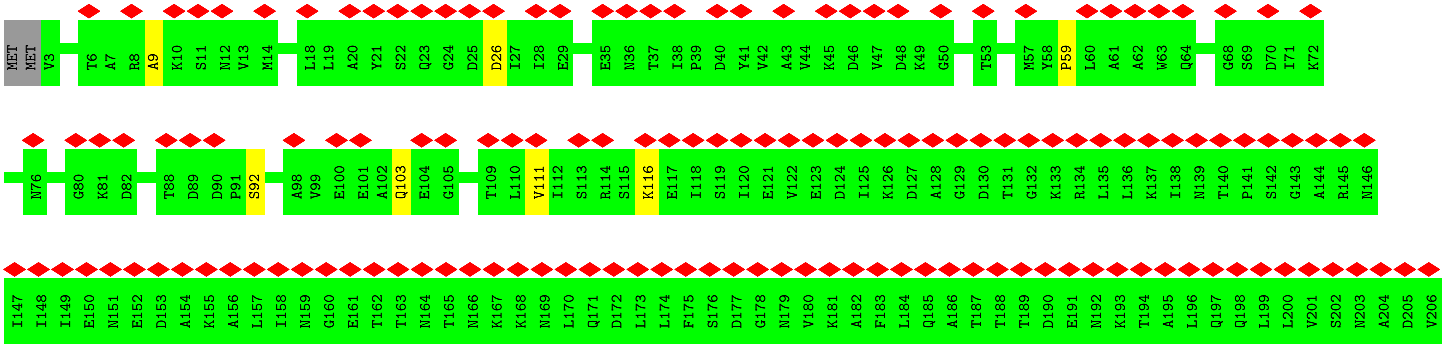


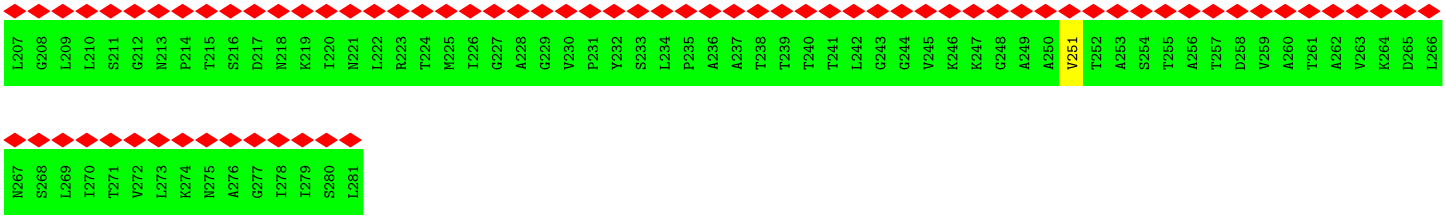


- Molecule 2: Capsid fiber protein

Chain 9R:

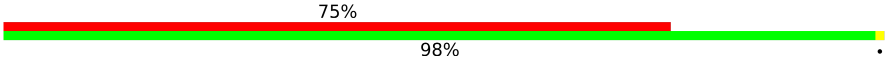


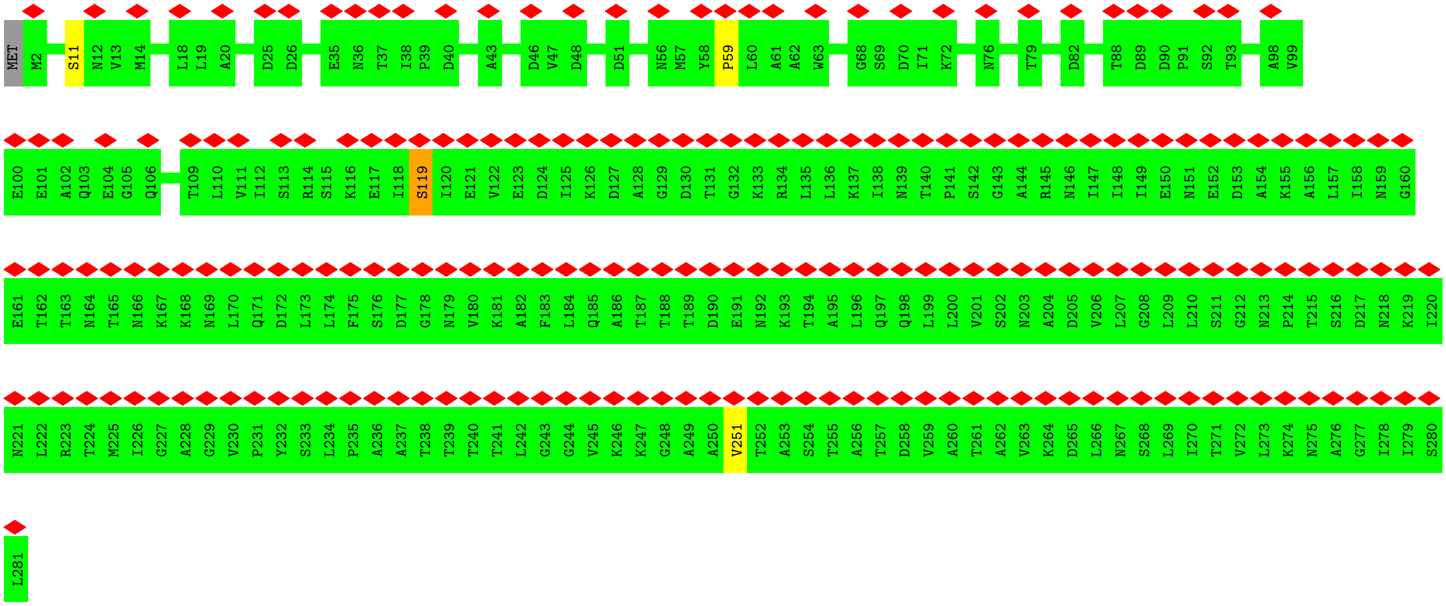




- Molecule 2: Capsid fiber protein

Chain 9J:





4 Experimental information

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	1A	0.53	0/3460	0.60	1/4698 (0.0%)
1	1B	0.61	0/3551	0.66	0/4822
1	1C	0.58	0/3551	0.62	0/4822
1	1D	0.60	0/3551	0.66	2/4822 (0.0%)
1	1E	0.57	0/3489	0.59	0/4737
1	1F	0.54	0/3513	0.64	2/4771 (0.0%)
1	1G	0.53	0/3460	0.60	1/4698 (0.0%)
1	1H	0.61	0/3551	0.66	0/4822
1	1I	0.58	0/3551	0.62	0/4822
1	1J	0.60	0/3551	0.66	2/4822 (0.0%)
1	1K	0.57	0/3489	0.59	0/4737
1	1L	0.54	0/3513	0.64	2/4771 (0.0%)
1	1M	0.53	0/3460	0.60	1/4698 (0.0%)
1	1N	0.61	0/3551	0.66	0/4822
1	1O	0.58	0/3551	0.62	0/4822
1	1P	0.60	0/3551	0.66	2/4822 (0.0%)
1	1Q	0.57	0/3489	0.59	0/4737
1	1R	0.54	0/3513	0.64	2/4771 (0.0%)
1	1S	0.53	0/3460	0.60	1/4698 (0.0%)
1	1T	0.61	0/3551	0.66	0/4822
1	1U	0.58	0/3551	0.62	0/4822
1	1V	0.60	0/3551	0.66	2/4822 (0.0%)
1	1W	0.57	0/3489	0.59	0/4737
1	1X	0.54	0/3513	0.64	2/4771 (0.0%)
1	1Y	0.53	0/3460	0.60	1/4698 (0.0%)
1	1Z	0.61	0/3551	0.66	0/4822
1	1a	0.58	0/3551	0.62	0/4822
1	1b	0.60	0/3551	0.66	2/4822 (0.0%)
1	1c	0.57	0/3489	0.59	0/4737
1	1d	0.54	0/3513	0.64	2/4771 (0.0%)
1	2A	0.63	1/3493 (0.0%)	0.64	1/4743 (0.0%)
1	2B	0.63	0/3551	0.63	1/4822 (0.0%)
1	2C	0.61	0/3551	0.61	0/4822
1	2D	0.62	0/3551	0.61	0/4822

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

The worst 5 of 86 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	7T	137	GLN	CA-CB	-7.06	1.38	1.53
1	7O	137	GLN	CA-CB	-7.06	1.38	1.53
1	7J	137	GLN	CA-CB	-7.05	1.38	1.53
1	7E	137	GLN	CA-CB	-7.05	1.38	1.53
1	7Y	137	GLN	CA-CB	-7.04	1.38	1.53

The worst 5 of 151 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1L	355	SER	C-N-CD	-9.96	98.69	120.60
1	1d	355	SER	C-N-CD	-9.96	98.70	120.60
1	1R	355	SER	C-N-CD	-9.95	98.71	120.60
1	1F	355	SER	C-N-CD	-9.95	98.71	120.60
1	1X	355	SER	C-N-CD	-9.95	98.71	120.60

There are no chirality outliers.

5 of 395 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1B	24	ILE	Peptide
1	1B	333	SER	Peptide
1	1B	6	ASN	Peptide
1	1B	7	ASP	Peptide
1	1C	425	LYS	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1d	436/448 (97%)	399 (92%)	35 (8%)	2 (0%)	29	67
1	2A	436/448 (97%)	411 (94%)	23 (5%)	2 (0%)	29	67
1	2B	443/448 (99%)	410 (93%)	30 (7%)	3 (1%)	22	61
1	2C	443/448 (99%)	414 (94%)	28 (6%)	1 (0%)	47	79
1	2D	443/448 (99%)	407 (92%)	36 (8%)	0	100	100
1	2E	443/448 (99%)	402 (91%)	38 (9%)	3 (1%)	22	61
1	2F	436/448 (97%)	411 (94%)	23 (5%)	2 (0%)	29	67
1	2G	443/448 (99%)	409 (92%)	31 (7%)	3 (1%)	22	61
1	2H	443/448 (99%)	414 (94%)	28 (6%)	1 (0%)	47	79
1	2I	443/448 (99%)	407 (92%)	35 (8%)	1 (0%)	47	79
1	2J	443/448 (99%)	402 (91%)	38 (9%)	3 (1%)	22	61
1	2K	436/448 (97%)	411 (94%)	23 (5%)	2 (0%)	29	67
1	2L	443/448 (99%)	410 (93%)	30 (7%)	3 (1%)	22	61
1	2M	443/448 (99%)	414 (94%)	28 (6%)	1 (0%)	47	79
1	2N	443/448 (99%)	407 (92%)	36 (8%)	0	100	100
1	2O	443/448 (99%)	402 (91%)	38 (9%)	3 (1%)	22	61
1	2P	436/448 (97%)	411 (94%)	23 (5%)	2 (0%)	29	67
1	2Q	443/448 (99%)	410 (93%)	30 (7%)	3 (1%)	22	61
1	2R	443/448 (99%)	414 (94%)	28 (6%)	1 (0%)	47	79
1	2S	443/448 (99%)	407 (92%)	36 (8%)	0	100	100
1	2T	443/448 (99%)	402 (91%)	38 (9%)	3 (1%)	22	61
1	2U	436/448 (97%)	410 (94%)	24 (6%)	2 (0%)	29	67
1	2V	443/448 (99%)	410 (93%)	30 (7%)	3 (1%)	22	61
1	2W	443/448 (99%)	414 (94%)	28 (6%)	1 (0%)	47	79
1	2X	443/448 (99%)	407 (92%)	36 (8%)	0	100	100
1	2Y	443/448 (99%)	402 (91%)	38 (9%)	3 (1%)	22	61
1	3A	433/448 (97%)	389 (90%)	42 (10%)	2 (0%)	29	67
1	3B	433/448 (97%)	393 (91%)	39 (9%)	1 (0%)	47	79
1	3C	443/448 (99%)	407 (92%)	35 (8%)	1 (0%)	47	79
1	3D	443/448 (99%)	398 (90%)	40 (9%)	5 (1%)	14	51
1	3E	443/448 (99%)	411 (93%)	32 (7%)	0	100	100

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	5H	433/448 (97%)	371 (86%)	60 (14%)	2 (0%)	29	67
1	5I	433/448 (97%)	385 (89%)	45 (10%)	3 (1%)	22	61
1	5J	433/448 (97%)	394 (91%)	38 (9%)	1 (0%)	47	79
1	5K	443/448 (99%)	396 (89%)	46 (10%)	1 (0%)	47	79
1	5L	443/448 (99%)	396 (89%)	43 (10%)	4 (1%)	17	56
1	5M	433/448 (97%)	398 (92%)	35 (8%)	0	100	100
1	5N	433/448 (97%)	371 (86%)	60 (14%)	2 (0%)	29	67
1	5O	433/448 (97%)	385 (89%)	45 (10%)	3 (1%)	22	61
1	5P	433/448 (97%)	394 (91%)	38 (9%)	1 (0%)	47	79
1	5Q	443/448 (99%)	396 (89%)	46 (10%)	1 (0%)	47	79
1	5R	443/448 (99%)	396 (89%)	43 (10%)	4 (1%)	17	56
1	5S	433/448 (97%)	399 (92%)	34 (8%)	0	100	100
1	5T	433/448 (97%)	371 (86%)	60 (14%)	2 (0%)	29	67
1	5U	433/448 (97%)	385 (89%)	45 (10%)	3 (1%)	22	61
1	5V	433/448 (97%)	394 (91%)	38 (9%)	1 (0%)	47	79
1	5W	443/448 (99%)	396 (89%)	46 (10%)	1 (0%)	47	79
1	5X	443/448 (99%)	396 (89%)	43 (10%)	4 (1%)	17	56
1	5Y	433/448 (97%)	399 (92%)	34 (8%)	0	100	100
1	5Z	433/448 (97%)	371 (86%)	60 (14%)	2 (0%)	29	67
1	5a	433/448 (97%)	385 (89%)	45 (10%)	3 (1%)	22	61
1	5b	433/448 (97%)	394 (91%)	38 (9%)	1 (0%)	47	79
1	5c	443/448 (99%)	396 (89%)	46 (10%)	1 (0%)	47	79
1	5d	443/448 (99%)	396 (89%)	43 (10%)	4 (1%)	17	56
1	6A	443/448 (99%)	408 (92%)	29 (6%)	6 (1%)	11	46
1	6B	443/448 (99%)	408 (92%)	32 (7%)	3 (1%)	22	61
1	6C	433/448 (97%)	391 (90%)	39 (9%)	3 (1%)	22	61
1	6D	433/448 (97%)	391 (90%)	42 (10%)	0	100	100
1	6E	443/448 (99%)	404 (91%)	39 (9%)	0	100	100
1	6F	443/448 (99%)	399 (90%)	43 (10%)	1 (0%)	47	79
1	6G	443/448 (99%)	408 (92%)	29 (6%)	6 (1%)	11	46
1	6H	443/448 (99%)	407 (92%)	33 (7%)	3 (1%)	22	61

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	8P	443/448 (99%)	423 (96%)	20 (4%)	0	100	100
1	8Q	443/448 (99%)	413 (93%)	28 (6%)	2 (0%)	29	67
1	8R	443/448 (99%)	409 (92%)	34 (8%)	0	100	100
1	8S	443/448 (99%)	407 (92%)	31 (7%)	5 (1%)	14	51
1	8T	443/448 (99%)	413 (93%)	30 (7%)	0	100	100
1	8U	443/448 (99%)	402 (91%)	41 (9%)	0	100	100
1	8V	443/448 (99%)	423 (96%)	20 (4%)	0	100	100
1	8W	443/448 (99%)	414 (94%)	27 (6%)	2 (0%)	29	67
1	8X	443/448 (99%)	409 (92%)	34 (8%)	0	100	100
1	8Y	443/448 (99%)	407 (92%)	31 (7%)	5 (1%)	14	51
1	8Z	443/448 (99%)	413 (93%)	30 (7%)	0	100	100
1	8a	443/448 (99%)	402 (91%)	41 (9%)	0	100	100
1	8b	443/448 (99%)	423 (96%)	20 (4%)	0	100	100
1	8c	443/448 (99%)	414 (94%)	27 (6%)	2 (0%)	29	67
1	8d	443/448 (99%)	409 (92%)	34 (8%)	0	100	100
1	9A	443/448 (99%)	416 (94%)	27 (6%)	0	100	100
1	9B	443/448 (99%)	416 (94%)	27 (6%)	0	100	100
1	9C	443/448 (99%)	416 (94%)	27 (6%)	0	100	100
1	9D	443/448 (99%)	416 (94%)	27 (6%)	0	100	100
1	9E	443/448 (99%)	416 (94%)	27 (6%)	0	100	100
2	1e	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	1f	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	1g	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	1h	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	1i	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	1j	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	1k	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	1l	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	1m	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	1n	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	1o	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	2v	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	54
2	2w	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	54
2	2x	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	54
2	3e	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	3f	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	3g	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	3h	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	3i	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	3j	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	3k	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	3l	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	3m	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	3n	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	3o	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	3p	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	3q	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	3r	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	3s	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	3t	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	3u	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	3v	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	3w	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	3x	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	4e	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	4f	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	4g	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	4h	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	4i	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	4j	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	4k	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	4l	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	4m	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	4n	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	5e	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	5f	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	5g	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	5h	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	5i	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	5j	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	5k	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	5l	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	5m	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	5n	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	6e	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	6f	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	6g	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	6h	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	6i	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	6j	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	6k	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	6l	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	6m	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	6n	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	6o	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	6p	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	6q	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	6r	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	6s	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	6t	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	6u	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	6v	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	6w	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	8j	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	8k	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	8l	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	8m	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	8n	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	8o	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	8p	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	8q	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	8r	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	8s	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	8t	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	8u	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	8v	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	8w	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	8x	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	8y	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	8z	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	9F	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	54
2	9G	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	54
2	9H	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	54
2	9I	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	54
2	9J	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	54
2	9K	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	9L	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	9M	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	9N	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	9O	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	9P	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	9Q	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	9R	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
All	All	150460/151645 (99%)	138708 (92%)	10636 (7%)	1116 (1%)	26	61

5 of 1116 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	6d	381/384 (99%)	381 (100%)	0	100	100
1	7A	381/384 (99%)	378 (99%)	3 (1%)	81	93
1	7B	381/384 (99%)	381 (100%)	0	100	100
1	7C	381/384 (99%)	380 (100%)	1 (0%)	92	96
1	7D	381/384 (99%)	381 (100%)	0	100	100
1	7E	381/384 (99%)	381 (100%)	0	100	100
1	7F	381/384 (99%)	378 (99%)	3 (1%)	81	93
1	7G	381/384 (99%)	381 (100%)	0	100	100
1	7H	381/384 (99%)	380 (100%)	1 (0%)	92	96
1	7I	381/384 (99%)	381 (100%)	0	100	100
1	7J	381/384 (99%)	381 (100%)	0	100	100
1	7K	381/384 (99%)	378 (99%)	3 (1%)	81	93
1	7L	381/384 (99%)	381 (100%)	0	100	100
1	7M	381/384 (99%)	380 (100%)	1 (0%)	92	96
1	7N	381/384 (99%)	381 (100%)	0	100	100
1	7O	381/384 (99%)	381 (100%)	0	100	100
1	7P	381/384 (99%)	378 (99%)	3 (1%)	81	93
1	7Q	381/384 (99%)	381 (100%)	0	100	100
1	7R	381/384 (99%)	380 (100%)	1 (0%)	92	96
1	7S	381/384 (99%)	381 (100%)	0	100	100
1	7T	381/384 (99%)	381 (100%)	0	100	100
1	7U	381/384 (99%)	378 (99%)	3 (1%)	81	93
1	7V	381/384 (99%)	381 (100%)	0	100	100
1	7W	381/384 (99%)	380 (100%)	1 (0%)	92	96
1	7X	381/384 (99%)	381 (100%)	0	100	100
1	7Y	381/384 (99%)	381 (100%)	0	100	100
1	8A	381/384 (99%)	381 (100%)	0	100	100
1	8B	381/384 (99%)	381 (100%)	0	100	100
1	8C	381/384 (99%)	379 (100%)	2 (0%)	88	95
1	8D	381/384 (99%)	381 (100%)	0	100	100
1	8E	381/384 (99%)	381 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	8F	381/384 (99%)	380 (100%)	1 (0%)	92	96
1	8G	381/384 (99%)	381 (100%)	0	100	100
1	8H	381/384 (99%)	381 (100%)	0	100	100
1	8I	381/384 (99%)	379 (100%)	2 (0%)	88	95
1	8J	381/384 (99%)	381 (100%)	0	100	100
1	8K	381/384 (99%)	381 (100%)	0	100	100
1	8L	381/384 (99%)	380 (100%)	1 (0%)	92	96
1	8M	381/384 (99%)	381 (100%)	0	100	100
1	8N	381/384 (99%)	381 (100%)	0	100	100
1	8O	381/384 (99%)	379 (100%)	2 (0%)	88	95
1	8P	381/384 (99%)	381 (100%)	0	100	100
1	8Q	381/384 (99%)	381 (100%)	0	100	100
1	8R	381/384 (99%)	380 (100%)	1 (0%)	92	96
1	8S	381/384 (99%)	381 (100%)	0	100	100
1	8T	381/384 (99%)	381 (100%)	0	100	100
1	8U	381/384 (99%)	379 (100%)	2 (0%)	88	95
1	8V	381/384 (99%)	381 (100%)	0	100	100
1	8W	381/384 (99%)	381 (100%)	0	100	100
1	8X	381/384 (99%)	380 (100%)	1 (0%)	92	96
1	8Y	381/384 (99%)	381 (100%)	0	100	100
1	8Z	381/384 (99%)	381 (100%)	0	100	100
1	8a	381/384 (99%)	379 (100%)	2 (0%)	88	95
1	8b	381/384 (99%)	381 (100%)	0	100	100
1	8c	381/384 (99%)	381 (100%)	0	100	100
1	8d	381/384 (99%)	380 (100%)	1 (0%)	92	96
1	9A	381/384 (99%)	379 (100%)	2 (0%)	88	95
1	9B	381/384 (99%)	379 (100%)	2 (0%)	88	95
1	9C	381/384 (99%)	379 (100%)	2 (0%)	88	95
1	9D	381/384 (99%)	379 (100%)	2 (0%)	88	95
1	9E	381/384 (99%)	379 (100%)	2 (0%)	88	95
2	1e	236/229 (103%)	234 (99%)	2 (1%)	81	93

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	3w	235/229 (103%)	233 (99%)	2 (1%)	78	91
2	3x	236/229 (103%)	234 (99%)	2 (1%)	81	93
2	4e	236/229 (103%)	234 (99%)	2 (1%)	81	93
2	4f	235/229 (103%)	233 (99%)	2 (1%)	78	91
2	4g	236/229 (103%)	234 (99%)	2 (1%)	81	93
2	4h	235/229 (103%)	233 (99%)	2 (1%)	78	91
2	4i	236/229 (103%)	234 (99%)	2 (1%)	81	93
2	4j	235/229 (103%)	233 (99%)	2 (1%)	78	91
2	4k	236/229 (103%)	234 (99%)	2 (1%)	81	93
2	4l	235/229 (103%)	233 (99%)	2 (1%)	78	91
2	4m	236/229 (103%)	234 (99%)	2 (1%)	81	93
2	4n	235/229 (103%)	233 (99%)	2 (1%)	78	91
2	5e	236/229 (103%)	234 (99%)	2 (1%)	81	93
2	5f	235/229 (103%)	233 (99%)	2 (1%)	78	91
2	5g	236/229 (103%)	234 (99%)	2 (1%)	81	93
2	5h	235/229 (103%)	233 (99%)	2 (1%)	78	91
2	5i	236/229 (103%)	234 (99%)	2 (1%)	81	93
2	5j	235/229 (103%)	233 (99%)	2 (1%)	78	91
2	5k	236/229 (103%)	234 (99%)	2 (1%)	81	93
2	5l	235/229 (103%)	233 (99%)	2 (1%)	78	91
2	5m	236/229 (103%)	234 (99%)	2 (1%)	81	93
2	5n	235/229 (103%)	233 (99%)	2 (1%)	78	91
2	6e	235/229 (103%)	233 (99%)	2 (1%)	78	91
2	6f	236/229 (103%)	234 (99%)	2 (1%)	81	93
2	6g	235/229 (103%)	233 (99%)	2 (1%)	78	91
2	6h	236/229 (103%)	234 (99%)	2 (1%)	81	93
2	6i	235/229 (103%)	233 (99%)	2 (1%)	78	91
2	6j	236/229 (103%)	234 (99%)	2 (1%)	81	93
2	6k	235/229 (103%)	233 (99%)	2 (1%)	78	91
2	6l	236/229 (103%)	234 (99%)	2 (1%)	81	93
2	6m	235/229 (103%)	233 (99%)	2 (1%)	78	91

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	7t	236/229 (103%)	234 (99%)	2 (1%)	81	93
2	7u	236/229 (103%)	234 (99%)	2 (1%)	81	93
2	7v	236/229 (103%)	234 (99%)	2 (1%)	81	93
2	7w	236/229 (103%)	234 (99%)	2 (1%)	81	93
2	7x	236/229 (103%)	234 (99%)	2 (1%)	81	93
2	8e	235/229 (103%)	233 (99%)	2 (1%)	78	91
2	8f	236/229 (103%)	234 (99%)	2 (1%)	81	93
2	8g	236/229 (103%)	234 (99%)	2 (1%)	81	93
2	8h	235/229 (103%)	233 (99%)	2 (1%)	78	91
2	8i	236/229 (103%)	234 (99%)	2 (1%)	81	93
2	8j	235/229 (103%)	233 (99%)	2 (1%)	78	91
2	8k	235/229 (103%)	233 (99%)	2 (1%)	78	91
2	8l	236/229 (103%)	234 (99%)	2 (1%)	81	93
2	8m	236/229 (103%)	234 (99%)	2 (1%)	81	93
2	8n	235/229 (103%)	233 (99%)	2 (1%)	78	91
2	8o	236/229 (103%)	234 (99%)	2 (1%)	81	93
2	8p	235/229 (103%)	233 (99%)	2 (1%)	78	91
2	8q	235/229 (103%)	233 (99%)	2 (1%)	78	91
2	8r	236/229 (103%)	234 (99%)	2 (1%)	81	93
2	8s	236/229 (103%)	234 (99%)	2 (1%)	81	93
2	8t	235/229 (103%)	233 (99%)	2 (1%)	78	91
2	8u	236/229 (103%)	234 (99%)	2 (1%)	81	93
2	8v	235/229 (103%)	233 (99%)	2 (1%)	78	91
2	8w	235/229 (103%)	233 (99%)	2 (1%)	78	91
2	8x	236/229 (103%)	234 (99%)	2 (1%)	81	93
2	8y	236/229 (103%)	234 (99%)	2 (1%)	81	93
2	8z	235/229 (103%)	233 (99%)	2 (1%)	78	91
2	9F	236/229 (103%)	234 (99%)	2 (1%)	81	93
2	9G	236/229 (103%)	234 (99%)	2 (1%)	81	93
2	9H	236/229 (103%)	234 (99%)	2 (1%)	81	93
2	9I	236/229 (103%)	234 (99%)	2 (1%)	81	93

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	9J	236/229 (103%)	234 (99%)	2 (1%)	81	93
2	9K	236/229 (103%)	234 (99%)	2 (1%)	81	93
2	9L	235/229 (103%)	233 (99%)	2 (1%)	78	91
2	9M	235/229 (103%)	233 (99%)	2 (1%)	78	91
2	9N	236/229 (103%)	234 (99%)	2 (1%)	81	93
2	9O	236/229 (103%)	234 (99%)	2 (1%)	81	93
2	9P	235/229 (103%)	233 (99%)	2 (1%)	78	91
2	9Q	236/229 (103%)	234 (99%)	2 (1%)	81	93
2	9R	235/229 (103%)	233 (99%)	2 (1%)	78	91
All	All	127985/128025 (100%)	127456 (100%)	529 (0%)	91	95

5 of 529 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1u	110	LEU
2	2v	251	VAL
2	9I	251	VAL
2	9O	251	VAL
1	8a	275	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 1524 such sidechains are listed below:

Mol	Chain	Res	Type
2	2g	103	GLN
2	6o	76	ASN
2	3k	166	ASN
2	2f	218	ASN
2	8o	159	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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.

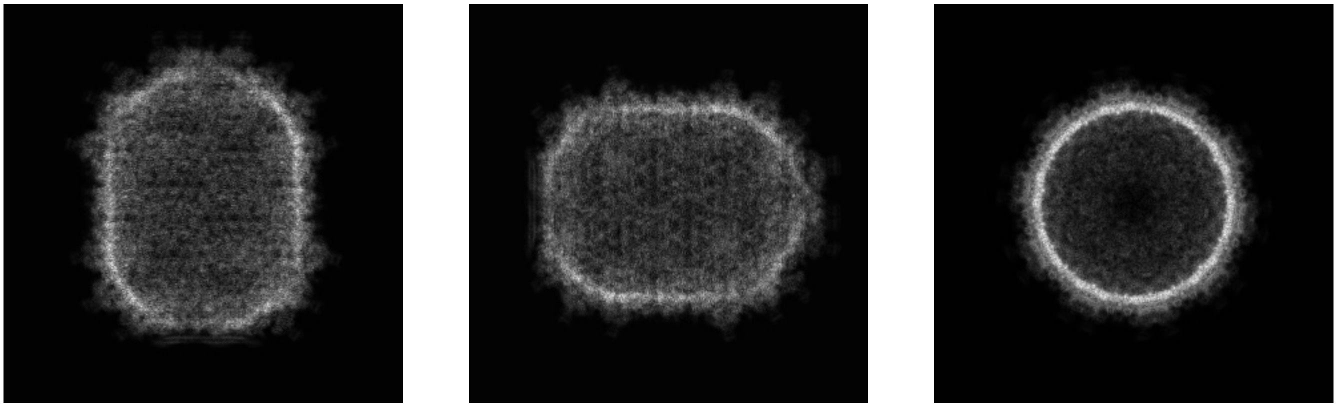
6 Map visualisation ⓘ

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

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

6.1 Orthogonal projections ⓘ

6.1.1 Primary map

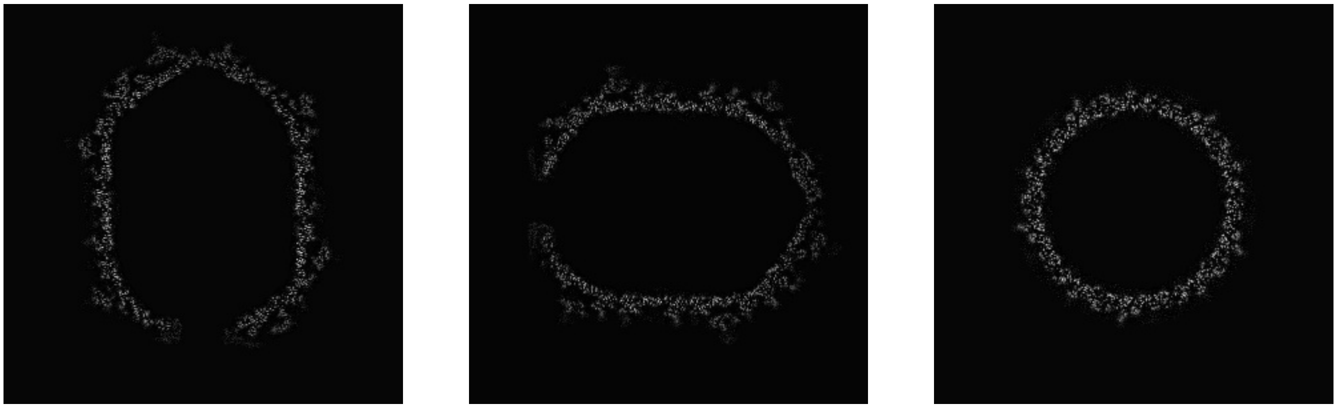


X Y Z

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

6.2 Central slices ⓘ

6.2.1 Primary map

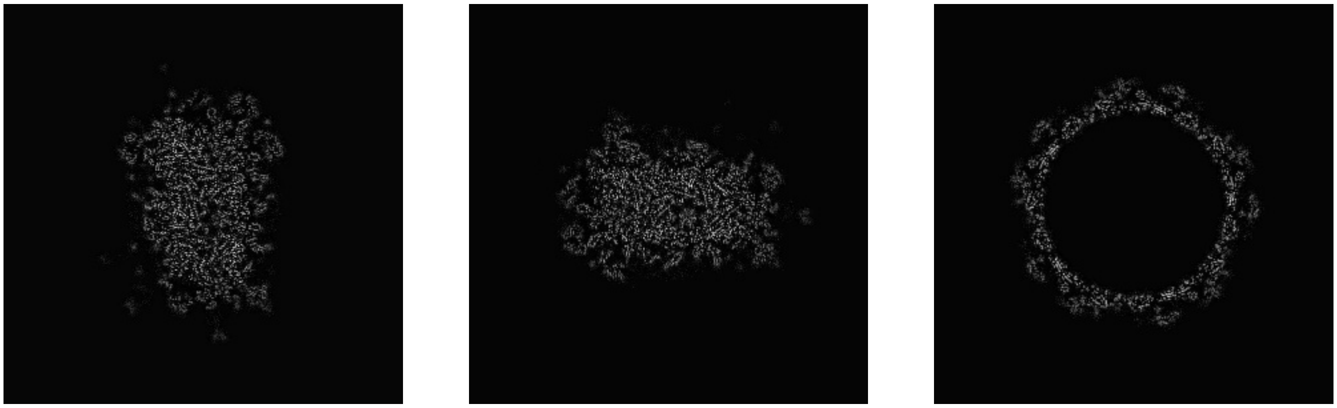


X Index: 270 Y Index: 270 Z Index: 270

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map



X Index: 396 Y Index: 143 Z Index: 212

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

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map

X Y Z

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

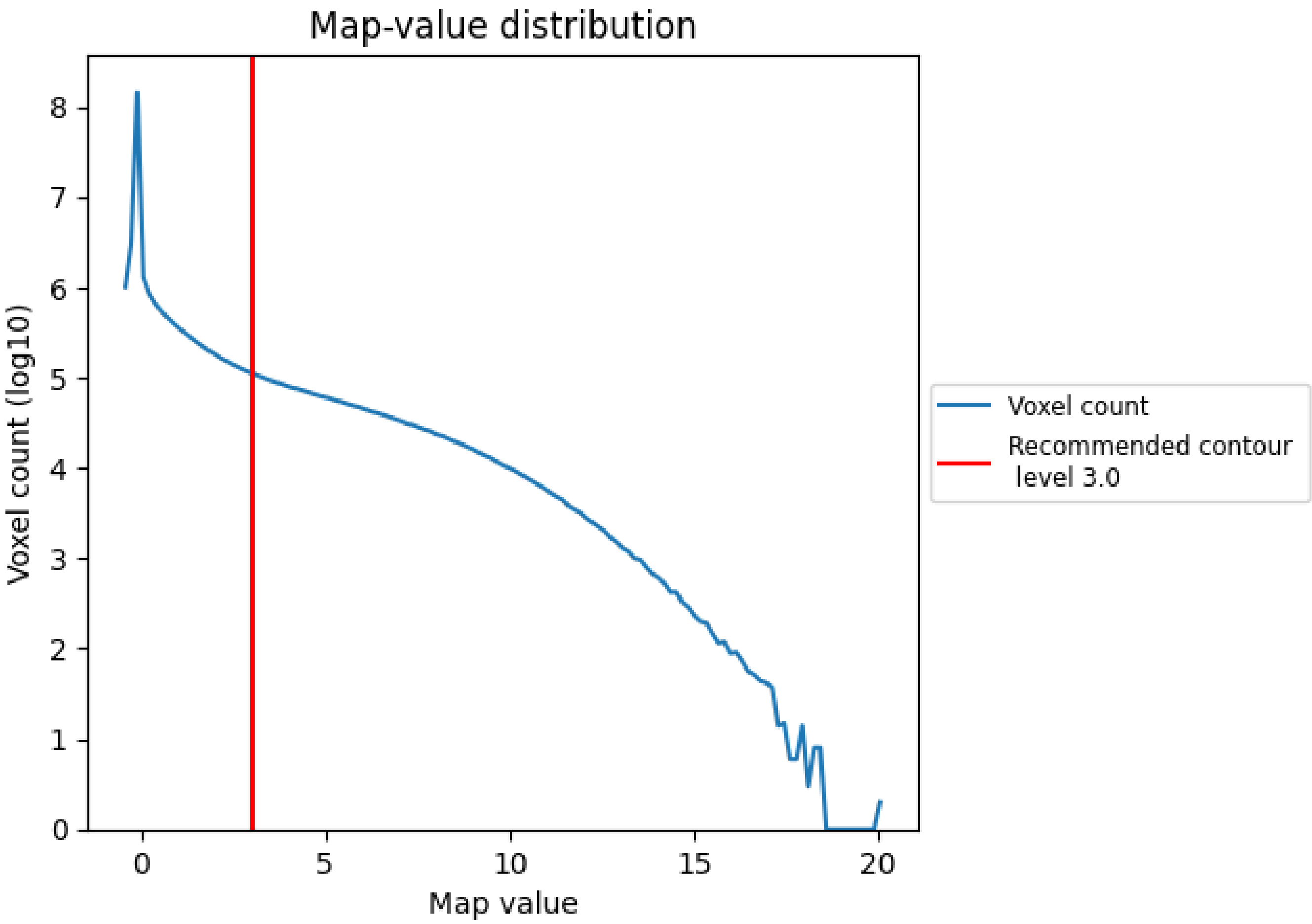
6.5 Mask visualisation ⓘ

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

7 Map analysis ⓘ

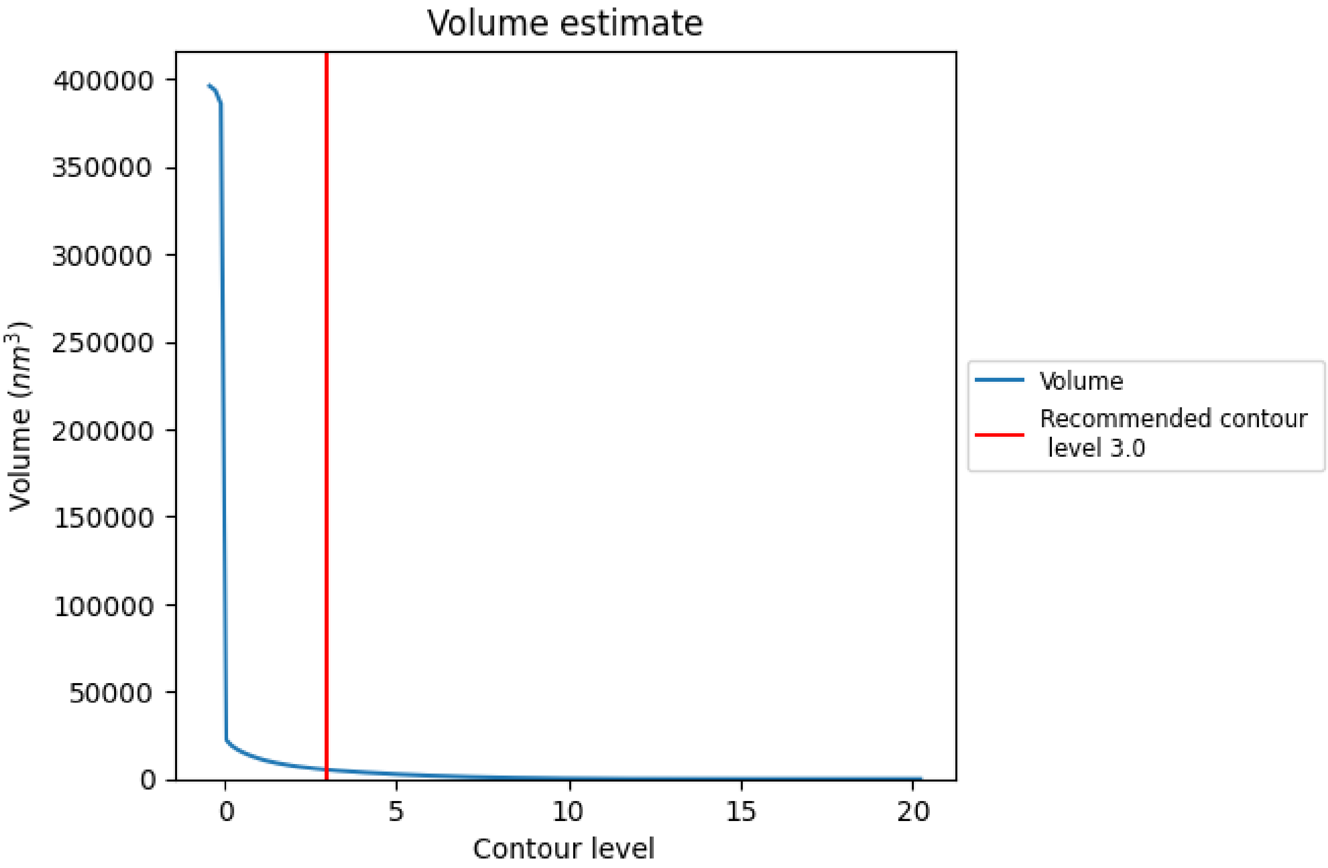
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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.

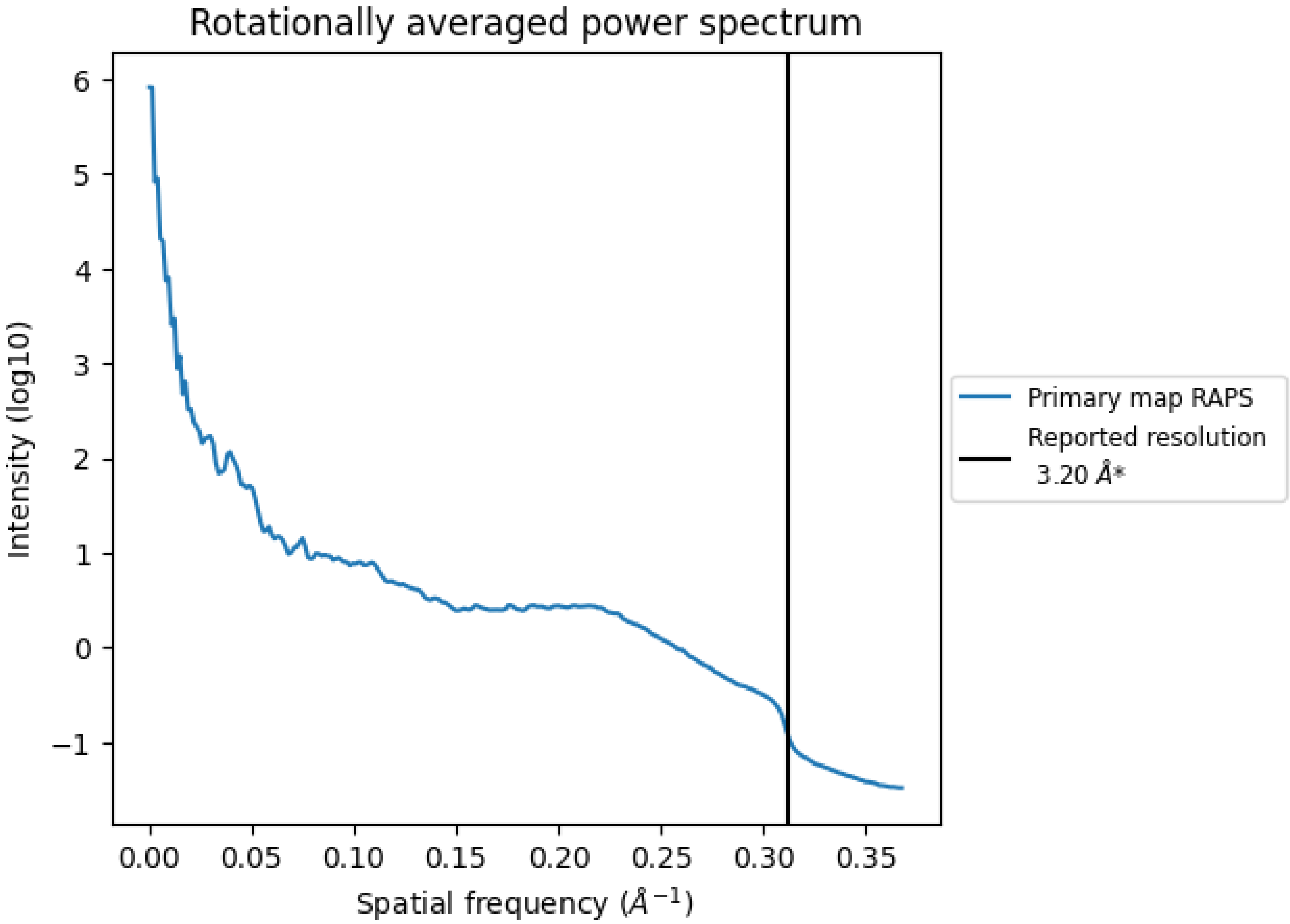
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 5310 nm^3; this corresponds to an approximate mass of 4796 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

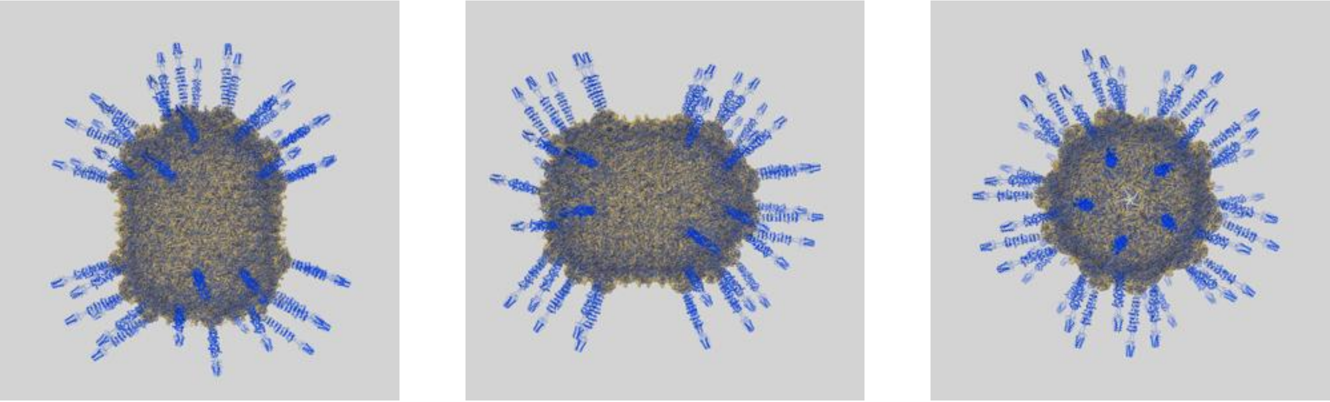
8 Fourier-Shell correlation

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

9 Map-model fit ⓘ

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

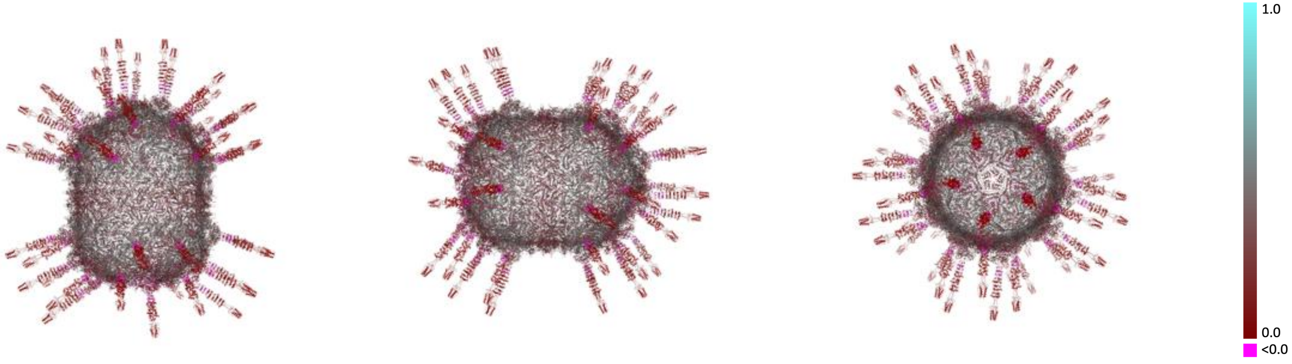
9.1 Map-model overlay ⓘ



X Y Z

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

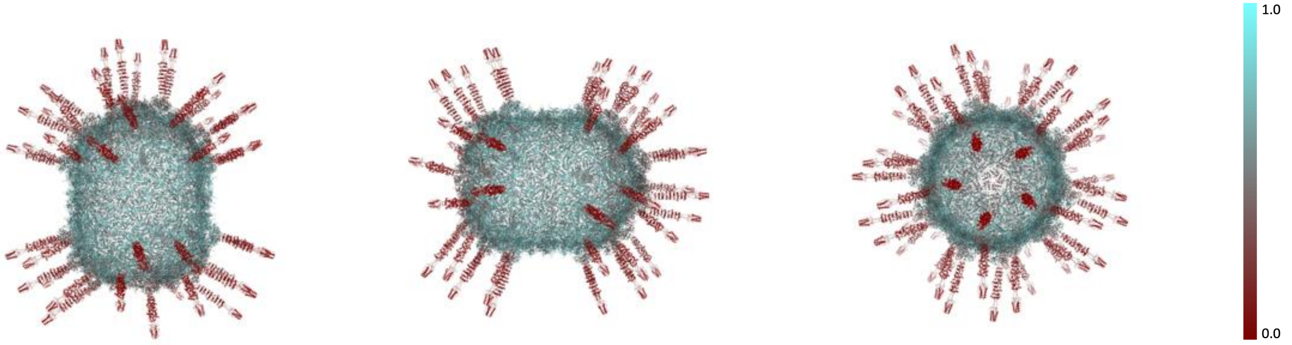
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according 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.

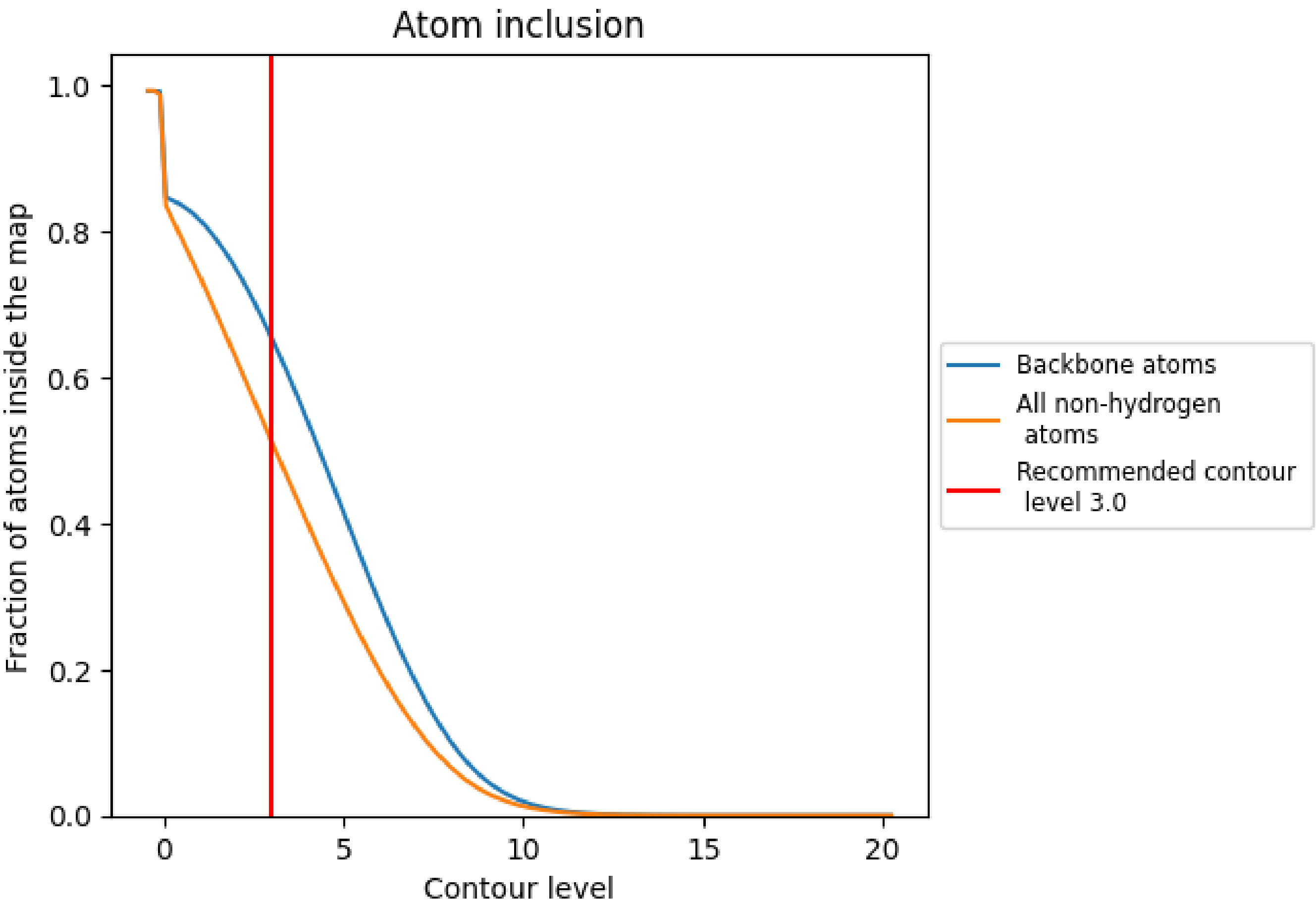
9.3 Atom inclusion mapped to coordinate model



X Y Z

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

9.4 Atom inclusion ⓘ



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

9.5 Map-model fit summary

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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