



## wwPDB EM Validation Summary Report ⓘ

Oct 31, 2024 – 01:01 AM EDT

PDB ID : 3J3Q  
EMDB ID : EMD-5639  
Title : Atomic-level structure of the entire HIV-1 capsid  
Authors : Perilla, J.R.; Zhao, G.; Zhang, P.; Schulten, K.J.  
Deposited on : 2013-04-12  
Resolution : Not provided  
Based on initial model : 3J34

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

# 1 Overall quality at a glance ⓘ











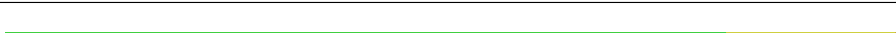

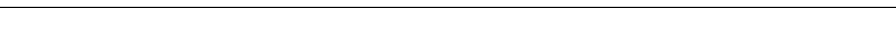
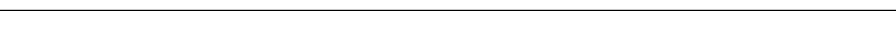
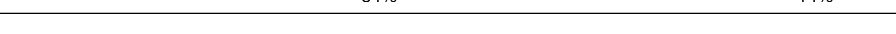
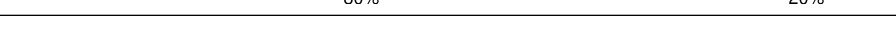
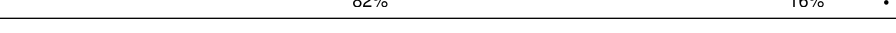
The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is unknown.


























There are no overall percentile quality scores available for this entry.

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	0	231	 78%20%.
1	1	231	 83%17%.
1	10	231	 82%17%.
1	11	231	 84%15%.
1	12	231	 83%16%.
1	13	231	 84%13%.
1	14	231	 81%16%.
1	15	231	 81%19%.
1	16	231	 81%17%.
1	17	231	 84%15%.
1	18	231	 81%19%.
1	19	231	 81%19%.
1	1A	231	 81%18%.
1	1B	231	 84%14%.
1	1C	231	 80%20%.
1	1D	231	 82%16%.
1	1E	231	 86%13%.












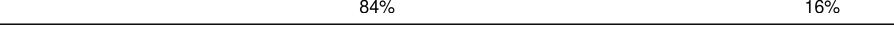







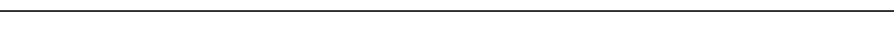

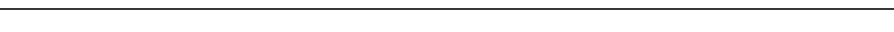
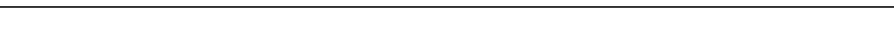


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Mol	Chain	Length	Quality of chain
1	1F	231	 82% 16% .
1	1G	231	 81% 17% .
1	1H	231	 79% 19% .
1	1I	231	 84% 16% .
1	1J	231	 79% 21% .
1	1K	231	 81% 17% .
1	1L	231	 85% 14% .
1	1M	231	 77% 20% .
1	1N	231	 84% 15% .
1	1O	231	 82% 17% .
1	1P	231	 82% 16% .
1	1Q	231	 84% 15% .
1	1R	231	 81% 16% .
1	1S	231	 81% 17% .
1	1T	231	 86% 12% .
1	1U	231	 84% 14% .
1	1V	231	 78% 20% .
1	1W	231	 84% 15% .
1	1X	231	 82% 16% .
1	1Y	231	 78% 21% .
1	1Z	231	 84% 16% .
1	1a	231	 83% 16% .
1	1b	231	 84% 15% .
1	1c	231	 81% 17% .
1	1d	231	 78% 19% .

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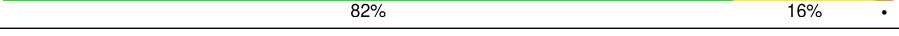

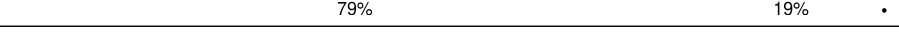
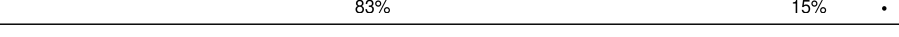

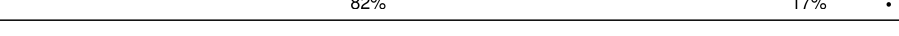


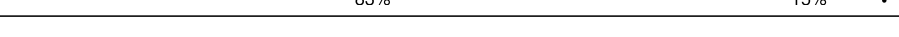

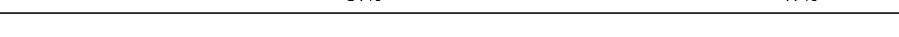






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Mol	Chain	Length	Quality of chain
1	1e	231	 81% 19%
1	1f	231	 80% 19% .
1	1g	231	 82% 17% .
1	1h	231	 79% 19% .
1	1i	231	 84% 15% .
1	1j	231	 82% 16% .
1	1k	231	 83% 16% .
1	1l	231	 82% 17% .
1	1m	231	 82% 16% .
1	1n	231	 84% 15% .
1	1o	231	 80% 16% .
1	1p	231	 84% 16%
1	1q	231	 84% 15% .
1	1r	231	 79% 19% .
1	1s	231	 84% 16%
1	1t	231	 86% 13% .
1	1u	231	 84% 16%
1	1v	231	 84% 15% .
1	1w	231	 83% 16% .
1	1x	231	 82% 17% .
1	1y	231	 82% 16% .
1	1z	231	 80% 19% .
1	2	231	 82% 17% .
1	20	231	 83% 16% .
1	21	231	 81% 16% .

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Mol	Chain	Length	Quality of chain
1	22	231	
1	23	231	
1	24	231	
1	25	231	
1	26	231	
1	27	231	
1	28	231	
1	29	231	
1	2A	231	
1	2B	231	
1	2C	231	
1	2D	231	
1	2E	231	
1	2F	231	
1	2G	231	
1	2H	231	
1	2I	231	
1	2J	231	
1	2K	231	
1	2L	231	
1	2M	231	
1	2N	231	
1	2O	231	
1	2P	231	
1	2Q	231	














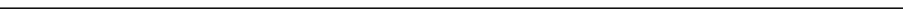











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Mol	Chain	Length	Quality of chain
1	2R	231	 83% 15% .
1	2S	231	 78% 21% .
1	2T	231	 82% 16% .
1	2U	231	 81% 15% .
1	2V	231	 84% 15% .
1	2W	231	 82% 16% .
1	2X	231	 81% 18% .
1	2Y	231	 81% 17% .
1	2Z	231	 80% 17% .
1	2a	231	 82% 17% .
1	2b	231	 85% 15% .
1	2c	231	 79% 19% .
1	2d	231	 86% 12% .
1	2e	231	 81% 18% .
1	2f	231	 83% 16% .
1	2g	231	 82% 17% .
1	2h	231	 83% 15% .
1	2i	231	 83% 16% .
1	2j	231	 81% 17% .
1	2k	231	 80% 19% .
1	2l	231	 79% 18% .
1	2m	231	 79% 19% .
1	2n	231	 84% 15% .
1	2o	231	 81% 16% .
1	2p	231	 81% 18% .














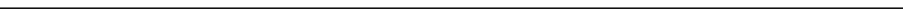











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Mol	Chain	Length	Quality of chain
1	2q	231	 84% 15% .
1	2r	231	 81% 18% .
1	2s	231	 81% 18% .
1	2t	231	 80% 18% .
1	2u	231	 84% 16%
1	2v	231	 83% 15% .
1	2w	231	 81% 18% .
1	2x	231	 80% 19% .
1	2y	231	 78% 21% .
1	2z	231	 80% 18% .
1	3	231	 84% 14% .
1	30	231	 84% 15% .
1	31	231	 82% 16% .
1	32	231	 83% 15% .
1	33	231	 82% 16% .
1	34	231	 84% 15% .
1	35	231	 80% 18% .
1	36	231	 82% 17% .
1	37	231	 85% 13% .
1	38	231	 81% 16% .
1	39	231	 81% 19%
1	3A	231	 80% 20%
1	3B	231	 82% 16% .
1	3C	231	 84% 16%
1	3D	231	 83% 16% .














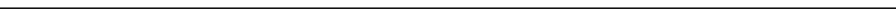











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Mol	Chain	Length	Quality of chain
1	3E	231	 84% 16% .
1	3F	231	 81% 18% .
1	3G	231	 78% 20% .
1	3H	231	 81% 17% .
1	3I	231	 83% 16% .
1	3J	231	 81% 18% .
1	3K	231	 82% 18% .
1	3L	231	 77% 22% .
1	3M	231	 78% 20% .
1	3N	231	 82% 16% .
1	3O	231	 78% 19% .
1	3P	231	 82% 16% .
1	3Q	231	 81% 16% .
1	3R	231	 82% 16% .
1	3S	231	 81% 17% .
1	3T	231	 84% 13% .
1	3U	231	 84% 14% .
1	3V	231	 81% 18% .
1	3W	231	 77% 20% .
1	3X	231	 77% 21% .
1	3Y	231	 83% 15% .
1	3Z	231	 82% 16% .
1	3a	231	 80% 18% .
1	3b	231	 81% 17% .
1	3c	231	 82% 16% .


























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Mol	Chain	Length	Quality of chain
1	3d	231	 81% 16% .
1	3e	231	 79% 19% .
1	3f	231	 80% 19% .
1	3g	231	 83% 16% .
1	3h	231	 84% 15% .
1	3i	231	 85% 13% .
1	3j	231	 81% 18% .
1	3k	231	 80% 19% .
1	3l	231	 80% 19% .
1	3m	231	 86% 12% .
1	3n	231	 83% 16% .
1	3o	231	 82% 16% .
1	3p	231	 80% 19% .
1	3q	231	 80% 19% .
1	3r	231	 87% 11% .
1	3s	231	 84% 13% .
1	3t	231	 85% 13% .
1	3u	231	 83% 15% .
1	3v	231	 80% 19% .
1	3w	231	 84% 14% .
1	3x	231	 86% 14% .
1	3y	231	 80% 18% .
1	3z	231	 83% 16% .
1	4	231	 84% 15% .
1	40	231	 84% 14% .


























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Mol	Chain	Length	Quality of chain
1	41	231	 84% 16%
1	42	231	 84% 13% .
1	43	231	 81% 18% .
1	44	231	 79% 20% .
1	45	231	 83% 17%
1	46	231	 80% 18% .
1	47	231	 85% 12% .
1	48	231	 81% 18%
1	49	231	 84% 15% .
1	4A	231	 84% 14% .
1	4B	231	 84% 16%
1	4C	231	 86% 13% .
1	4D	231	 82% 16% .
1	4E	231	 80% 19% .
1	4F	231	 81% 18% .
1	4G	231	 81% 17% .
1	4H	231	 87% 13%
1	4I	231	 84% 14% .
1	4J	231	 79% 19% .
1	4K	231	 82% 16% .
1	4L	231	 84% 15% .
1	4M	231	 82% 17% .
1	4N	231	 82% 16% .
1	4O	231	 84% 15% .
1	4P	231	 83% 16% .














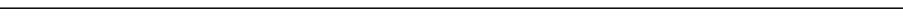











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Mol	Chain	Length	Quality of chain
1	4Q	231	 82% 17% .
1	4R	231	 81% 16% .
1	4S	231	 81% 16% .
1	4T	231	 84% 15% .
1	4U	231	 80% 19% .
1	4V	231	 85% 14% .
1	4W	231	 83% 16% .
1	4X	231	 81% 17% .
1	4Y	231	 79% 19% .
1	4Z	231	 83% 16% .
1	4a	231	 82% 15% .
1	4b	231	 77% 22% .
1	4c	231	 80% 18% .
1	4d	231	 83% 15% .
1	4e	231	 84% 15% .
1	4f	231	 83% 17% .
1	4g	231	 82% 16% .
1	4h	231	 78% 22% .
1	4i	231	 81% 17% .
1	4j	231	 82% 18% .
1	4k	231	 81% 17% .
1	4l	231	 82% 17% .
1	4m	231	 81% 19% .
1	4n	231	 84% 15% .
1	4o	231	 82% 14% .

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Mol	Chain	Length	Quality of chain
1	4p	231	 81% 18% .
1	4q	231	 80% 19% .
1	4r	231	 81% 18% .
1	4s	231	 83% 16% .
1	4t	231	 82% 17% .
1	4u	231	 81% 17% .
1	4v	231	 83% 16% .
1	4w	231	 80% 18% .
1	4x	231	 81% 18% .
1	4y	231	 83% 16% .
1	4z	231	 81% 16% .
1	5	231	 82% 13% 5% .
1	50	231	 83% 15% .
1	51	231	 82% 17% .
1	52	231	 84% 15% .
1	53	231	 84% 16% .
1	54	231	 82% 16% .
1	55	231	 80% 18% .
1	56	231	 85% 13% .
1	57	231	 81% 16% .
1	58	231	 80% 19% .
1	59	231	 83% 15% .
1	5A	231	 81% 16% .
1	5B	231	 88% 11% .
1	5C	231	 82% 17% .

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Mol	Chain	Length	Quality of chain
1	5D	231	 80% 19% .
1	5E	231	 82% 17% .
1	5F	231	 85% 13% .
1	5G	231	 84% 16% .
1	5H	231	 82% 15% .
1	5I	231	 84% 15% .
1	5J	231	 81% 17% .
1	5K	231	 83% 17% .
1	5L	231	 80% 19% .
1	5M	231	 83% 16% .
1	5N	231	 83% 17% .
1	5O	231	 85% 13% .
1	5P	231	 87% 12% .
1	5Q	231	 81% 17% .
1	5R	231	 80% 19% .
1	5S	231	 81% 18% .
1	5T	231	 83% 16% .
1	5U	231	 87% 10% .
1	5V	231	 81% 19% .
1	5W	231	 82% 16% .
1	5X	231	 81% 16% .
1	5Y	231	 82% 18% .
1	5Z	231	 83% 16% .
1	5a	231	 83% 16% .
1	5b	231	 85% 14% .














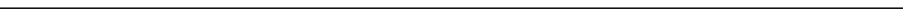











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Mol	Chain	Length	Quality of chain
1	5c	231	 79% 20% .
1	5d	231	 85% 13% .
1	5e	231	 85% 15%
1	5f	231	 85% 13% .
1	5g	231	 81% 18% .
1	5h	231	 82% 18%
1	5i	231	 81% 17% .
1	5j	231	 84% 16%
1	5k	231	 84% 14% .
1	5l	231	 81% 17% .
1	5m	231	 80% 19% .
1	5n	231	 83% 16% .
1	5o	231	 84% 15% .
1	5p	231	 84% 14% .
1	5q	231	 81% 17% .
1	5r	231	 84% 14% .
1	5s	231	 85% 13% .
1	5t	231	 81% 18% .
1	5u	231	 81% 18% .
1	5v	231	 84% 16%
1	5w	231	 82% 17% .
1	5x	231	 80% 18% .
1	5y	231	 78% 20% .
1	5z	231	 85% 14% .
1	6	231	 84% 14% .














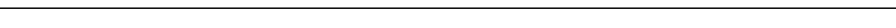











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Mol	Chain	Length	Quality of chain
1	60	231	 81% 19% .
1	61	231	 85% 15% .
1	62	231	 84% 14% .
1	63	231	 84% 15% .
1	64	231	 85% 13% .
1	65	231	 80% 19% .
1	66	231	 84% 15% .
1	67	231	 79% 20% .
1	68	231	 83% 15% .
1	69	231	 84% 16% .
1	6A	231	 78% 21% .
1	6B	231	 82% 17% .
1	6C	231	 76% 22% .
1	6D	231	 84% 16% .
1	6E	231	 84% 14% .
1	6F	231	 87% 12% .
1	6G	231	 85% 14% .
1	6H	231	 83% 16% .
1	6I	231	 80% 18% .
1	6J	231	 82% 17% .
1	6K	231	 86% 13% .
1	6L	231	 84% 15% .
1	6M	231	 81% 17% .
1	6N	231	 84% 15% .
1	6O	231	 83% 16% .


























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Mol	Chain	Length	Quality of chain
1	6P	231	 83% 14% .
1	6Q	231	 83% 16% .
1	6R	231	 81% 17% .
1	6S	231	 84% 14% .
1	6T	231	 77% 20% .
1	6U	231	 84% 14% .
1	6V	231	 84% 16% .
1	6W	231	 83% 16% .
1	6X	231	 83% 16% .
1	6Y	231	 84% 13% .
1	6Z	231	 81% 17% .
1	6a	231	 80% 19% .
1	6b	231	 81% 16% .
1	6c	231	 84% 16%
1	6d	231	 84% 15% .
1	6e	231	 82% 17% .
1	6f	231	 79% 19% .
1	6g	231	 81% 17% .
1	6h	231	 81% 17% .
1	6i	231	 81% 18% .
1	6j	231	 77% 21% .
1	6k	231	 80% 20%
1	6l	231	 82% 15% .
1	6m	231	 84% 15% .
1	6n	231	 77% 23%


























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Mol	Chain	Length	Quality of chain
1	6o	231	 83% 14% .
1	6p	231	 84% 15% .
1	6q	231	 84% 14% .
1	6r	231	 84% 14% .
1	6s	231	 83% 16% .
1	6t	231	 78% 21% .
1	6u	231	 82% 16% .
1	6v	231	 83% 16% .
1	6w	231	 82% 16% .
1	6x	231	 84% 13% .
1	6y	231	 83% 16% .
1	6z	231	 81% 18% .
1	7	231	 83% 16% .
1	70	231	 83% 16% .
1	71	231	 82% 16% .
1	72	231	 81% 17% .
1	73	231	 83% 16% .
1	74	231	 83% 16% .
1	75	231	 78% 20% .
1	76	231	 81% 19% .
1	77	231	 82% 15% .
1	78	231	 81% 18% .
1	79	231	 79% 20% .
1	7A	231	 84% 15% .
1	7B	231	 81% 18% .


























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Mol	Chain	Length	Quality of chain
1	7C	231	 83% 14% .
1	7D	231	 85% 13% .
1	7E	231	 80% 19% .
1	7F	231	 83% 16% .
1	7G	231	 82% 16% .
1	7H	231	 78% 20% .
1	7I	231	 80% 17% .
1	7J	231	 84% 14% .
1	7K	231	 81% 16% .
1	7L	231	 83% 14% .
1	7M	231	 82% 16% .
1	7N	231	 79% 20% .
1	7O	231	 85% 14% .
1	7P	231	 80% 18% .
1	7Q	231	 84% 16% .
1	7R	231	 79% 20% .
1	7S	231	 81% 19% .
1	7T	231	 85% 15% .
1	7U	231	 84% 15% .
1	7V	231	 82% 16% .
1	7W	231	 78% 21% .
1	7X	231	 82% 16% .
1	7Y	231	 83% 17% .
1	7Z	231	 81% 17% .
1	7a	231	 81% 18% .














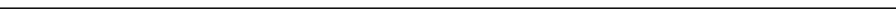











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Mol	Chain	Length	Quality of chain
1	7b	231	 81% 18% .
1	7c	231	 85% 12% .
1	7d	231	 84% 14% .
1	7e	231	 84% 15% .
1	7f	231	 84% 14% .
1	7g	231	 85% 14% .
1	7h	231	 82% 16% .
1	7i	231	 81% 17% .
1	7j	231	 82% 16% .
1	7k	231	 78% 21% .
1	7l	231	 79% 18% .
1	7m	231	 79% 20% .
1	7n	231	 83% 15% .
1	7o	231	 87% 12% .
1	7p	231	 86% 13% .
1	7q	231	 81% 17% .
1	7r	231	 83% 14% .
1	7s	231	 84% 13% .
1	7t	231	 82% 16% .
1	7u	231	 84% 15% .
1	7v	231	 83% 16% .
1	7w	231	 84% 13% .
1	7x	231	 79% 19% .
1	7y	231	 83% 16% .
1	7z	231	 83% 15% .

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Mol	Chain	Length	Quality of chain
1	8	231	 81%17%
1	80	231	 84%15%
1	81	231	 82%16%
1	82	231	 82%16%
1	83	231	 80%19%
1	84	231	 81%16%
1	85	231	 83%17%
1	86	231	 81%17%
1	87	231	 81%16%
1	88	231	 81%17%
1	89	231	 81%18%
1	8A	231	 81%17%
1	8B	231	 81%16%
1	8C	231	 77%22%
1	8D	231	 82%18%
1	8E	231	 80%19%
1	8F	231	 81%16%
1	8G	231	 81%18%
1	8H	231	 81%18%
1	8I	231	 85%14%
1	8J	231	 85%14%
1	8K	231	 81%18%
1	8L	231	 83%16%
1	8M	231	 83%16%
1	8N	231	 79%20%

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Mol	Chain	Length	Quality of chain
1	8O	231	 77% 23%
1	8P	231	 81% 17% .
1	8Q	231	 81% 18% .
1	8R	231	 81% 17% .
1	8S	231	 84% 14% .
1	8T	231	 81% 18% .
1	8U	231	 83% 15% .
1	8V	231	 81% 18% .
1	8W	231	 80% 18% .
1	8X	231	 81% 16% .
1	8Y	231	 84% 15% .
1	8Z	231	 87% 13% .
1	8a	231	 83% 15% .
1	8b	231	 85% 14% .
1	8c	231	 83% 15% .
1	8d	231	 82% 17% .
1	8e	231	 79% 20% .
1	8f	231	 81% 17% .
1	8g	231	 82% 16% .
1	8h	231	 82% 17% .
1	8i	231	 82% 16% .
1	8j	231	 83% 16% .
1	8k	231	 81% 18% .
1	8l	231	 81% 16% .
1	8m	231	 80% 18% .


























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Mol	Chain	Length	Quality of chain
1	8n	231	 81% 18% .
1	8o	231	 84% 15% .
1	8p	231	 81% 17% .
1	8q	231	 81% 17% .
1	8r	231	 85% 13% .
1	8s	231	 83% 16% .
1	8t	231	 79% 18% .
1	8u	231	 83% 16% .
1	8v	231	 84% 13% .
1	8w	231	 84% 16% .
1	8x	231	 82% 17% .
1	8y	231	 82% 18% .
1	8z	231	 84% 15% .
1	9	231	 80% 19% .
1	90	231	 82% 16% .
1	91	231	 85% 14% .
1	92	231	 83% 14% .
1	93	231	 80% 19% .
1	94	231	 80% 18% .
1	95	231	 80% 19% .
1	96	231	 84% 16% .
1	97	231	 84% 15% .
1	98	231	 84% 13% .
1	99	231	 81% 19% .
1	9A	231	 87% 12% .


























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Mol	Chain	Length	Quality of chain
1	9B	231	 82% 15% .
1	9C	231	 81% 18% .
1	9D	231	 81% 18% .
1	9E	231	 85% 14% .
1	9F	231	 84% 15% .
1	9G	231	 79% 19% .
1	9H	231	 81% 18% .
1	9I	231	 84% 15% .
1	9J	231	 87% 13% .
1	9K	231	 75% 24% .
1	9L	231	 81% 18% .
1	9M	231	 78% 20% .
1	9N	231	 77% 22% .
1	9O	231	 80% 17% .
1	9P	231	 85% 13% .
1	9Q	231	 85% 14% .
1	9R	231	 86% 13% .
1	9S	231	 81% 18% .
1	9T	231	 82% 16% .
1	9U	231	 78% 21% .
1	9V	231	 84% 16% .
1	9W	231	 78% 20% .
1	9X	231	 82% 15% .
1	9Y	231	 83% 14% .
1	9Z	231	 84% 15% .


























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Mol	Chain	Length	Quality of chain
1	9a	231	 81% 17% .
1	9b	231	 83% 16% .
1	9c	231	 83% 14% .
1	9d	231	 82% 15% .
1	9e	231	 83% 16% .
1	9f	231	 85% 13% .
1	9g	231	 83% 15% .
1	9h	231	 80% 19% .
1	9i	231	 83% 16% .
1	9j	231	 86% 13% .
1	9k	231	 80% 19% .
1	9l	231	 82% 16% .
1	9m	231	 84% 16% .
1	9n	231	 84% 14% .
1	9o	231	 78% 19% .
1	9p	231	 79% 18% .
1	9q	231	 82% 16% .
1	9r	231	 82% 16% .
1	9s	231	 80% 18% .
1	9t	231	 78% 20% .
1	9u	231	 80% 19% .
1	9v	231	 82% 16% .
1	9w	231	 83% 17% .
1	9x	231	 86% 13% .
1	9y	231	 83% 16% .














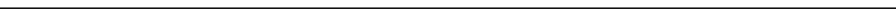











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Mol	Chain	Length	Quality of chain
1	9z	231	 79% 20% .
1	A	231	 82% 16% .
1	B	231	 84% 16%
1	C	231	 80% 19% .
1	D	231	 82% 15% .
1	E	231	 85% 14%
1	F	231	 83% 16%
1	G	231	 85% 13% .
1	H	231	 80% 19% .
1	I	231	 81% 17% .
1	J	231	 82% 17% .
1	K	231	 83% 16% .
1	L	231	 85% 13% .
1	M	231	 81% 16% .
1	N	231	 77% 20% .
1	O	231	 76% 23% .
1	P	231	 79% 20% .
1	Q	231	 81% 17% .
1	R	231	 84% 13% .
1	S	231	 82% 17% .
1	T	231	 81% 18% .
1	U	231	 84% 15% .
1	V	231	 82% 16% .
1	W	231	 84% 15% .
1	X	231	 81% 19%














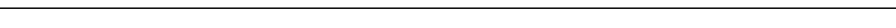











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Mol	Chain	Length	Quality of chain
1	Y	231	 81% 19%
1	Z	231	 81% 19%
1	a	231	 83% 15% .
1	a0	231	 80% 17% .
1	a1	231	 84% 15% .
1	a2	231	 81% 18% .
1	a3	231	 80% 19% .
1	a4	231	 81% 17% .
1	a5	231	 83% 16% .
1	a6	231	 83% 16% .
1	a7	231	 80% 19% .
1	a8	231	 83% 16% .
1	a9	231	 81% 18% .
1	aA	231	 84% 16% .
1	aB	231	 83% 16% .
1	aC	231	 81% 18% .
1	aD	231	 86% 13% .
1	aE	231	 83% 16%
1	aF	231	 80% 19% .
1	aG	231	 82% 16% .
1	aH	231	 82% 16% .
1	aI	231	 81% 18%
1	aJ	231	 85% 14% .
1	aK	231	 83% 14% .
1	aL	231	 81% 18% .














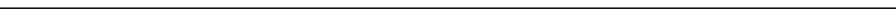











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Mol	Chain	Length	Quality of chain
1	aM	231	 79% 19% .
1	aN	231	 83% 16% .
1	aO	231	 78% 19% .
1	aP	231	 78% 20% .
1	aQ	231	 82% 17% .
1	aR	231	 83% 16% .
1	aS	231	 81% 17% .
1	aT	231	 84% 16%
1	aU	231	 80% 18% .
1	aV	231	 78% 20% .
1	aW	231	 85% 13% .
1	aX	231	 81% 17% .
1	aY	231	 80% 19% .
1	aZ	231	 81% 16% .
1	aa	231	 87% 12% .
1	ab	231	 84% 14% .
1	ac	231	 79% 18% .
1	ad	231	 82% 15% .
1	ae	231	 82% 16% .
1	af	231	 84% 15% .
1	ag	231	 85% 13% .
1	ah	231	 81% 17% .
1	ai	231	 84% 14% .
1	aj	231	 81% 18% .
1	ak	231	 81% 19%

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Mol	Chain	Length	Quality of chain
1	al	231	 81% 17% .
1	am	231	 80% 19% .
1	an	231	 82% 17% .
1	ao	231	 81% 17% .
1	ap	231	 83% 15% .
1	aq	231	 84% 15% .
1	ar	231	 85% 14% .
1	as	231	 82% 17% .
1	at	231	 84% 15% .
1	au	231	 81% 17% .
1	av	231	 81% 16% .
1	aw	231	 82% 16% .
1	ax	231	 81% 16% .
1	ay	231	 86% 13% .
1	az	231	 82% 16% .
1	b	231	 83% 16% .
1	b0	231	 81% 18% .
1	b1	231	 83% 14% .
1	b2	231	 83% 15% .
1	b3	231	 80% 17% .
1	b4	231	 85% 12% .
1	b5	231	 83% 15% .
1	b6	231	 83% 15% .
1	b7	231	 87% 12% .
1	b8	231	 83% 16% .

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Mol	Chain	Length	Quality of chain
1	b9	231	 82% 17% .
1	bA	231	 79% 20% .
1	bB	231	 80% 18% .
1	bC	231	 78% 20% .
1	bD	231	 83% 16% .
1	bE	231	 81% 16% .
1	bF	231	 79% 18% .
1	bG	231	 87% 12% .
1	bH	231	 80% 18% .
1	bI	231	 81% 18% .
1	bJ	231	 83% 16% .
1	bK	231	 79% 19% .
1	bL	231	 84% 15% .
1	bM	231	 83% 16% .
1	bN	231	 83% 15% .
1	bO	231	 79% 21% .
1	bP	231	 81% 18% .
1	bQ	231	 82% 18% .
1	bR	231	 78% 20% .
1	bS	231	 84% 15% .
1	bT	231	 83% 15% .
1	bU	231	 82% 17% .
1	bV	231	 82% 17% .
1	bW	231	 80% 17% .
1	bX	231	 82% 17% .














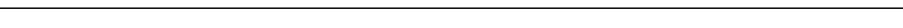











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Mol	Chain	Length	Quality of chain
1	bY	231	
1	bZ	231	
1	ba	231	
1	bb	231	
1	bc	231	
1	bd	231	
1	be	231	
1	bf	231	
1	bg	231	
1	bh	231	
1	bi	231	
1	bj	231	
1	bk	231	
1	bl	231	
1	bm	231	
1	bn	231	
1	bo	231	
1	bp	231	
1	bq	231	
1	br	231	
1	bs	231	
1	bt	231	
1	bu	231	
1	bv	231	
1	bw	231	


























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Mol	Chain	Length	Quality of chain
1	bx	231	 80% 18% .
1	by	231	 81% 17% .
1	bz	231	 81% 17% .
1	c	231	 80% 17% .
1	c0	231	 82% 16% .
1	c1	231	 83% 16% .
1	c2	231	 82% 16% .
1	c3	231	 81% 18% .
1	c4	231	 79% 19% .
1	c5	231	 81% 17% .
1	c6	231	 86% 14% .
1	c7	231	 82% 17% .
1	c8	231	 83% 16% .
1	c9	231	 79% 19% .
1	cA	231	 81% 18% .
1	cB	231	 82% 16% .
1	cC	231	 82% 17% .
1	cD	231	 77% 23% .
1	cE	231	 82% 16% .
1	cF	231	 81% 18% .
1	cG	231	 79% 20% .
1	cH	231	 78% 21% .
1	cI	231	 84% 15% .
1	cJ	231	 86% 13% .
1	cK	231	 80% 19% .

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Mol	Chain	Length	Quality of chain
1	cL	231	 84% 15% .
1	cM	231	 82% 17% .
1	cN	231	 82% 17% .
1	cO	231	 84% 14% .
1	cP	231	 84% 16% .
1	cQ	231	 84% 14% .
1	cR	231	 77% 22% .
1	cS	231	 82% 17% .
1	cT	231	 80% 17% .
1	cU	231	 84% 13% .
1	cV	231	 84% 15% .
1	cW	231	 79% 19% .
1	cX	231	 84% 14% .
1	cY	231	 83% 16% .
1	cZ	231	 84% 14% .
1	ca	231	 80% 17% .
1	cb	231	 81% 18% .
1	cc	231	 80% 18% .
1	cd	231	 81% 18% .
1	ce	231	 82% 17% .
1	cf	231	 79% 20% .
1	cg	231	 85% 12% .
1	ch	231	 84% 15% .
1	ci	231	 79% 19% .
1	cj	231	 83% 16% .


























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Mol	Chain	Length	Quality of chain	
1	ck	231	<div><div></div></div>	78% 21% .
1	cl	231	<div><div></div></div>	79% 20%
1	cm	231	<div><div></div></div>	79% 21%
1	cn	231	<div><div></div></div>	81% 19% .
1	co	231	<div><div></div></div>	82% 18%
1	cp	231	<div><div></div></div>	79% 19% .
1	cq	231	<div><div></div></div>	81% 17% .
1	cr	231	<div><div></div></div>	80% 18% .
1	cs	231	<div><div></div></div>	81% 18% .
1	ct	231	<div><div></div></div>	80% 18% .
1	cu	231	<div><div></div></div>	87% 11% .
1	cv	231	<div><div></div></div>	81% 17% .
1	cw	231	<div><div></div></div>	84% 15% .
1	cx	231	<div><div></div></div>	80% 19% .
1	cy	231	<div><div></div></div>	79% 21%
1	cz	231	<div><div></div></div>	84% 15% .
1	d	231	<div><div></div></div>	84% 14% .
1	d0	231	<div><div></div></div>	81% 18% .
1	d1	231	<div><div></div></div>	81% 17% .
1	d2	231	<div><div></div></div>	81% 16% .
1	d3	231	<div><div></div></div>	84% 15% .
1	d4	231	<div><div></div></div>	79% 19% .
1	d5	231	<div><div></div></div>	81% 18% .
1	d6	231	<div><div></div></div>	82% 16% .
1	d7	231	<div><div></div></div>	82% 17%


























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Mol	Chain	Length	Quality of chain
1	d8	231	 84% 14% .
1	d9	231	 83% 16% .
1	dA	231	 80% 18% .
1	dB	231	 81% 19% .
1	dC	231	 76% 21% .
1	dD	231	 80% 19% .
1	dE	231	 83% 14% .
1	dF	231	 83% 16% .
1	dG	231	 81% 18% .
1	dH	231	 83% 16% .
1	dI	231	 81% 18% .
1	dJ	231	 83% 16% .
1	dK	231	 82% 18% .
1	dL	231	 84% 15% .
1	dM	231	 83% 16% .
1	dN	231	 85% 13% .
1	dO	231	 83% 16% .
1	dP	231	 82% 16% .
1	dQ	231	 84% 14% .
1	dR	231	 86% 12% .
1	dS	231	 84% 13% .
1	dT	231	 82% 16% .
1	dU	231	 84% 14% .
1	dV	231	 81% 18% .
1	dW	231	 81% 16% .


























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Mol	Chain	Length	Quality of chain
1	dX	231	 82% 16% .
1	dY	231	 83% 16% .
1	dZ	231	 79% 19% .
1	da	231	 81% 19% .
1	db	231	 80% 19% .
1	dc	231	 79% 19% .
1	dd	231	 80% 19% .
1	de	231	 85% 13% .
1	df	231	 84% 13% .
1	dg	231	 81% 16% .
1	dh	231	 83% 16% .
1	di	231	 83% 15% .
1	dj	231	 81% 17% .
1	dk	231	 82% 18% .
1	dl	231	 81% 17% .
1	dm	231	 82% 16% .
1	dn	231	 81% 17% .
1	do	231	 79% 19% .
1	dp	231	 84% 16% .
1	dq	231	 84% 16% .
1	dr	231	 84% 14% .
1	ds	231	 81% 18% .
1	dt	231	 83% 16% .
1	du	231	 84% 15% .
1	dv	231	 83% 16% .

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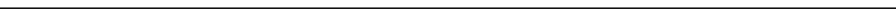











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Mol	Chain	Length	Quality of chain
1	dw	231	 83% 15% .
1	dx	231	 80% 19% .
1	dy	231	 85% 14% .
1	dz	231	 81% 17% .
1	e	231	 81% 18% .
1	e0	231	 81% 19% .
1	e1	231	 80% 19% .
1	e2	231	 83% 16% .
1	e3	231	 84% 16% .
1	e4	231	 81% 18% .
1	e5	231	 81% 17% .
1	e6	231	 80% 19% .
1	e7	231	 84% 15% .
1	e8	231	 84% 15% .
1	e9	231	 80% 19% .
1	eA	231	 79% 19% .
1	eB	231	 84% 15% .
1	eC	231	 81% 16% .
1	eD	231	 81% 17% .
1	eE	231	 81% 17% .
1	eF	231	 83% 15% .
1	eG	231	 85% 14% .
1	eH	231	 81% 18% .
1	eI	231	 81% 17% .
1	eJ	231	 82% 17% .

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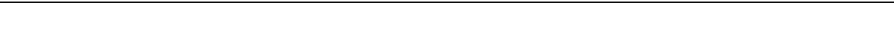

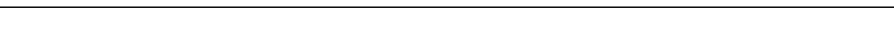
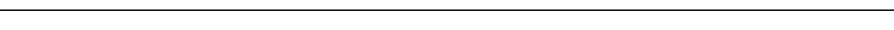













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Mol	Chain	Length	Quality of chain
1	eK	231	 81% 18% .
1	eL	231	 83% 16% .
1	eM	231	 81% 17% .
1	eN	231	 83% 16% .
1	eO	231	 86% 14%
1	eP	231	 82% 16% .
1	eQ	231	 81% 19% .
1	eR	231	 78% 21% .
1	eS	231	 84% 14% .
1	eT	231	 81% 19%
1	eU	231	 84% 15% .
1	eV	231	 85% 14%
1	eW	231	 84% 15% .
1	eX	231	 77% 22% .
1	eY	231	 84% 14% .
1	eZ	231	 82% 16% .
1	ea	231	 84% 14% .
1	eb	231	 83% 17%
1	ec	231	 83% 14% .
1	ed	231	 81% 18% .
1	ee	231	 83% 15% .
1	ef	231	 85% 14% .
1	eg	231	 81% 17% .
1	eh	231	 82% 16% .
1	ei	231	 81% 17% .














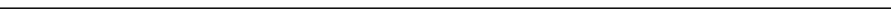











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Mol	Chain	Length	Quality of chain
1	ej	231	 82% 16% .
1	ek	231	 84% 16% .
1	el	231	 84% 13% .
1	em	231	 79% 21% .
1	en	231	 85% 13% .
1	eo	231	 81% 18% .
1	ep	231	 80% 18% .
1	eq	231	 83% 16% .
1	er	231	 81% 16% .
1	es	231	 84% 15% .
1	et	231	 83% 16% .
1	eu	231	 81% 18% .
1	ev	231	 81% 17% .
1	ew	231	 84% 15% .
1	ex	231	 86% 12% .
1	ey	231	 84% 15% .
1	ez	231	 86% 12% .
1	f	231	 83% 16% .
1	f0	231	 83% 17% .
1	f1	231	 81% 18% .
1	f2	231	 87% 12% .
1	f3	231	 80% 18% .
1	f4	231	 79% 20% .
1	f5	231	 84% 15% .
1	f6	231	 83% 16% .











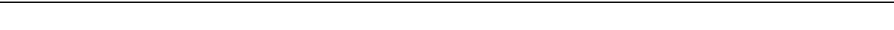

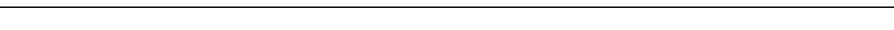
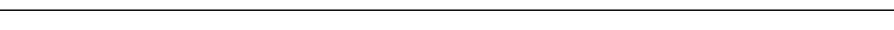











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Mol	Chain	Length	Quality of chain
1	f7	231	 78% 20% .
1	f8	231	 77% 20% .
1	f9	231	 84% 15% .
1	fA	231	 82% 16% .
1	fB	231	 81% 17% .
1	fC	231	 84% 14% .
1	fD	231	 84% 16%
1	fE	231	 84% 15% .
1	fF	231	 81% 17% .
1	fG	231	 83% 16% .
1	fH	231	 82% 16% .
1	fI	231	 80% 19% .
1	fJ	231	 80% 19% .
1	fK	231	 84% 15% .
1	fL	231	 84% 15% .
1	fM	231	 81% 19%
1	fN	231	 83% 15% .
1	fO	231	 83% 16% .
1	fP	231	 82% 16% .
1	fQ	231	 80% 20%
1	fR	231	 81% 18% .
1	fS	231	 84% 15% .
1	fT	231	 81% 19%
1	fU	231	 84% 14% .
1	fV	231	 85% 13% .


























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Mol	Chain	Length	Quality of chain
1	fW	231	 83% 17%
1	fX	231	 83% 15% .
1	fY	231	 84% 15% .
1	fZ	231	 81% 17% .
1	fa	231	 78% 21% .
1	fb	231	 82% 17% .
1	fc	231	 83% 16% .
1	fd	231	 84% 15% .
1	fe	231	 79% 20% .
1	ff	231	 83% 16% .
1	fg	231	 81% 19% .
1	fh	231	 81% 16% .
1	fi	231	 81% 18% .
1	fj	231	 84% 15% .
1	fk	231	 84% 15% .
1	fl	231	 81% 19% .
1	fm	231	 85% 13% .
1	fn	231	 80% 17% .
1	fo	231	 84% 15% .
1	fp	231	 78% 20% .
1	fq	231	 79% 19% .
1	fr	231	 85% 14% .
1	fs	231	 79% 19% .
1	ft	231	 84% 15% .
1	fu	231	 81% 16% .


























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Mol	Chain	Length	Quality of chain
1	fv	231	 84% 15% .
1	fw	231	 85% 13% .
1	fx	231	 87% 12% .
1	fy	231	 81% 15% .
1	fz	231	 80% 18% .
1	g	231	 83% 16% .
1	g0	231	 83% 16% .
1	g1	231	 81% 17% .
1	g2	231	 83% 16% .
1	g3	231	 81% 16% .
1	g4	231	 80% 18% .
1	g5	231	 83% 15% .
1	g6	231	 87% 12% .
1	g7	231	 83% 16% .
1	g8	231	 83% 16% .
1	g9	231	 80% 18% .
1	gA	231	 83% 16% .
1	gB	231	 87% 11% .
1	gC	231	 78% 21% .
1	gD	231	 85% 13% .
1	gE	231	 84% 16% .
1	gF	231	 84% 15% .
1	gG	231	 80% 18% .
1	gH	231	 79% 19% .
1	gI	231	 80% 18% .














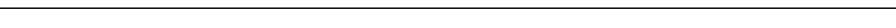











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Mol	Chain	Length	Quality of chain
1	gJ	231	 84% 14%
1	gK	231	 80% 19%
1	gL	231	 81% 17%
1	gM	231	 83% 15%
1	gN	231	 83% 17%
1	gO	231	 81% 16%
1	gP	231	 83% 16%
1	gQ	231	 81% 18%
1	gR	231	 84% 15%
1	gS	231	 84% 14%
1	gT	231	 78% 20%
1	gU	231	 83% 14%
1	gV	231	 84% 16%
1	gW	231	 79% 20%
1	gX	231	 80% 17%
1	gY	231	 82% 17%
1	gZ	231	 85% 14%
1	ga	231	 82% 16%
1	gb	231	 80% 19%
1	gc	231	 85% 14%
1	gd	231	 79% 20%
1	ge	231	 86% 13%
1	gf	231	 82% 16%
1	gg	231	 78% 19%
1	gh	231	 78% 20%













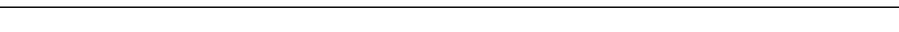

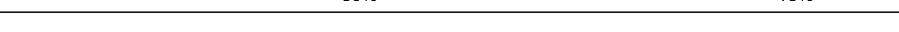

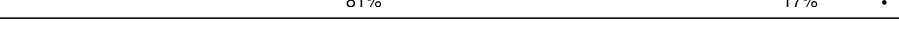








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Mol	Chain	Length	Quality of chain
1	gi	231	 79% 20% .
1	gj	231	 80% 19% .
1	gk	231	 82% 16% .
1	gl	231	 83% 15% .
1	gm	231	 84% 16% .
1	gn	231	 84% 14% .
1	go	231	 81% 18% .
1	gp	231	 79% 19% .
1	gq	231	 81% 16% .
1	gr	231	 79% 19% .
1	gs	231	 83% 15% .
1	gt	231	 81% 18% .
1	gu	231	 84% 16% .
1	gv	231	 82% 17% .
1	gw	231	 83% 15% .
1	gx	231	 82% 17% .
1	gy	231	 82% 16% .
1	gz	231	 80% 19% .
1	h	231	 85% 14% .
1	h0	231	 79% 20% .
1	h1	231	 81% 18% .
1	h2	231	 83% 16% .
1	h3	231	 78% 20% .
1	h4	231	 85% 13% .
1	h5	231	 81% 16% .

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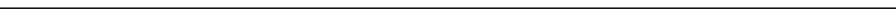











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Mol	Chain	Length	Quality of chain
1	h6	231	 82% 17% .
1	h7	231	 79% 21% .
1	h8	231	 83% 16% .
1	h9	231	 79% 20% .
1	hA	231	 84% 15% .
1	hB	231	 84% 16% .
1	hC	231	 82% 16% .
1	hD	231	 81% 17% .
1	hE	231	 87% 11% .
1	hF	231	 82% 16% .
1	hG	231	 83% 16% .
1	hH	231	 84% 15% .
1	hI	231	 81% 18% .
1	hJ	231	 80% 18% .
1	hK	231	 83% 16% .
1	hL	231	 81% 17% .
1	hM	231	 83% 15% .
1	hN	231	 80% 19% .
1	hO	231	 85% 14% .
1	hP	231	 84% 14% .
1	hQ	231	 77% 23% .
1	hR	231	 78% 21% .
1	hS	231	 84% 15% .
1	hT	231	 84% 15% .
1	hU	231	 81% 17% .

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Mol	Chain	Length	Quality of chain
1	hV	231	 79% 18% .
1	hW	231	 79% 18% .
1	hX	231	 84% 15% .
1	hY	231	 82% 16% .
1	hZ	231	 83% 16% .
1	ha	231	 81% 18% .
1	hb	231	 81% 19% .
1	hc	231	 81% 17% .
1	hd	231	 82% 16% .
1	he	231	 80% 18% .
1	hf	231	 78% 20% .
1	hg	231	 82% 17% .
1	hh	231	 82% 18% .
1	hi	231	 79% 20% .
1	hj	231	 81% 17% .
1	hk	231	 81% 19% .
1	hl	231	 82% 18% .
1	hm	231	 82% 16% .
1	hn	231	 84% 14% .
1	ho	231	 84% 14% .
1	hp	231	 78% 18% .
1	hq	231	 81% 16% .
1	hr	231	 80% 19% .
1	hs	231	 78% 20% .
1	ht	231	 83% 16% .











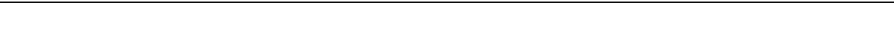

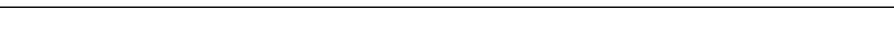
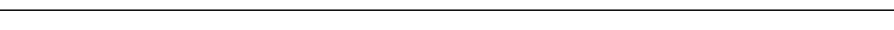











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Mol	Chain	Length	Quality of chain
1	hu	231	 83% 16% .
1	hv	231	 82% 16% .
1	hw	231	 83% 17%
1	hx	231	 84% 14% .
1	hy	231	 80% 18% .
1	hz	231	 80% 17% .
1	i	231	 85% 13% .
1	i0	231	 81% 18% .
1	i1	231	 77% 22% .
1	i2	231	 82% 16% .
1	i3	231	 87% 13% .
1	i4	231	 83% 15% .
1	i5	231	 81% 18% .
1	i6	231	 82% 17% .
1	i7	231	 82% 15% .
1	i8	231	 83% 16% .
1	i9	231	 80% 19% .
1	iA	231	 81% 16% .
1	iB	231	 83% 16% .
1	iC	231	 82% 17%
1	iD	231	 83% 16% .
1	iE	231	 81% 19% .
1	iF	231	 80% 18% .
1	iG	231	 78% 20% .
1	iH	231	 80% 19% .














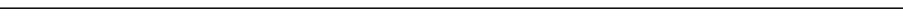











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Mol	Chain	Length	Quality of chain
1	iI	231	 80% 20%
1	iJ	231	 81% 17% •
1	iK	231	 81% 18%
1	iL	231	 81% 18% •
1	iM	231	 81% 18% •
1	iN	231	 81% 16% •
1	iO	231	 85% 13% •
1	iP	231	 82% 17% •
1	iQ	231	 81% 18%
1	iR	231	 81% 17% •
1	iS	231	 82% 16% •
1	iT	231	 78% 20% •
1	iU	231	 85% 14%
1	iV	231	 82% 16% •
1	iW	231	 83% 16% •
1	iX	231	 81% 19%
1	iY	231	 82% 16% •
1	iZ	231	 81% 19% •
1	ia	231	 82% 16% •
1	ib	231	 83% 16% •
1	ic	231	 78% 22%
1	id	231	 84% 15% •
1	ie	231	 82% 16% •
1	if	231	 82% 18%
1	ig	231	 80% 18% •


























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Mol	Chain	Length	Quality of chain
1	ih	231	 81% 16% .
1	ii	231	 81% 18% .
1	ij	231	 82% 16% .
1	ik	231	 80% 18% .
1	il	231	 80% 18% .
1	im	231	 81% 17% .
1	in	231	 81% 17% .
1	io	231	 78% 21% .
1	ip	231	 81% 16% .
1	iq	231	 84% 15% .
1	ir	231	 83% 16% .
1	is	231	 84% 14% .
1	it	231	 80% 19% .
1	iu	231	 83% 15% .
1	iv	231	 81% 18% .
1	iw	231	 83% 16% .
1	ix	231	 82% 15% .
1	iy	231	 83% 16% .
1	iz	231	 80% 18% .
1	j	231	 87% 13% .
1	j0	231	 80% 19% .
1	j1	231	 78% 21% .
1	j2	231	 86% 13% .
1	j3	231	 85% 14% .
1	j4	231	 85% 14% .


























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Mol	Chain	Length	Quality of chain
1	j5	231	 82%16%.
1	j6	231	 82%17%.
1	j7	231	 79%20%.
1	j8	231	 83%16%.
1	j9	231	 78%19%.
1	jA	231	 82%16%.
1	jB	231	 81%18%.
1	jC	231	 81%17%.
1	jD	231	 80%18%.
1	jE	231	 86%13%.
1	jF	231	 81%18%.
1	jG	231	 82%18%.
1	jH	231	 87%13%.
1	jI	231	 82%18%.
1	jJ	231	 83%16%.
1	jK	231	 81%16%.
1	jL	231	 85%13%.
1	jM	231	 81%18%.
1	jN	231	 83%16%.
1	jO	231	 81%16%.
1	jP	231	 82%16%.
1	jQ	231	 78%21%.
1	jR	231	 81%19%.
1	jS	231	 85%14%.
1	jT	231	 81%18%.


























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Mol	Chain	Length	Quality of chain
1	jU	231	 78% 19% .
1	jV	231	 84% 16%
1	jW	231	 81% 18% .
1	jX	231	 84% 15% .
1	jY	231	 84% 13% .
1	jZ	231	 80% 18% .
1	ja	231	 83% 17%
1	jb	231	 77% 20% .
1	jc	231	 83% 16% .
1	jd	231	 86% 13% .
1	je	231	 78% 20% .
1	jf	231	 83% 15% .
1	yg	231	 79% 19% .
1	jh	231	 83% 15% .
1	ji	231	 83% 15% .
1	jj	231	 76% 21% .
1	jk	231	 84% 15% .
1	jl	231	 79% 19% .
1	jm	231	 83% 15% .
1	jn	231	 82% 16% .
1	jo	231	 81% 17% .
1	jp	231	 81% 17% .
1	jq	231	 81% 17% .
1	jr	231	 83% 16% .
1	js	231	 78% 19% .














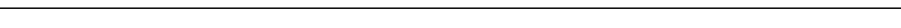











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Mol	Chain	Length	Quality of chain
1	jt	231	
1	ju	231	
1	jv	231	
1	jw	231	
1	jx	231	
1	jy	231	
1	jz	231	
1	k	231	
1	k0	231	
1	k1	231	
1	k2	231	
1	k3	231	
1	k4	231	
1	k5	231	
1	k6	231	
1	k7	231	
1	k8	231	
1	k9	231	
1	kA	231	
1	kB	231	
1	kC	231	
1	kD	231	
1	kE	231	
1	kF	231	
1	kG	231	

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Mol	Chain	Length	Quality of chain
1	kH	231	 81% 17% .
1	kI	231	 81% 19%
1	kJ	231	 81% 16% .
1	kK	231	 81% 18%
1	kL	231	 79% 20%
1	kM	231	 85% 14% .
1	kN	231	 81% 19%
1	kO	231	 83% 16% .
1	kP	231	 82% 16% .
1	kQ	231	 82% 16% .
1	kR	231	 81% 18% .
1	kS	231	 81% 19%
1	kT	231	 83% 15% .
1	kU	231	 83% 15% .
1	kV	231	 82% 17% .
1	kW	231	 82% 15% .
1	kX	231	 79% 20% .
1	kY	231	 85% 14% .
1	kZ	231	 81% 18% .
1	ka	231	 81% 16% .
1	kb	231	 80% 17% .
1	kc	231	 82% 15% .
1	kd	231	 85% 14% .
1	ke	231	 84% 16%
1	kf	231	 82% 17% .

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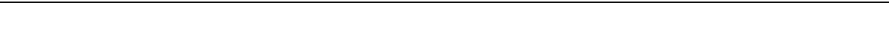

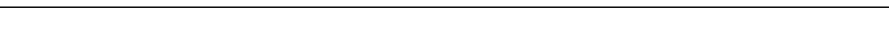
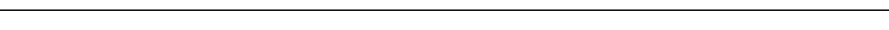













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Mol	Chain	Length	Quality of chain	
1	kg	231	<div><div></div></div>	79%20%
1	kh	231	<div><div></div></div>	81%18%
1	ki	231	<div><div></div></div>	83%15%
1	kj	231	<div><div></div></div>	84%14%
1	kk	231	<div><div></div></div>	81%16%
1	kl	231	<div><div></div></div>	82%17%
1	km	231	<div><div></div></div>	82%16%
1	kn	231	<div><div></div></div>	81%17%
1	ko	231	<div><div></div></div>	81%16%
1	kp	231	<div><div></div></div>	83%16%
1	kq	231	<div><div></div></div>	83%16%
1	kr	231	<div><div></div></div>	77%21%
1	ks	231	<div><div></div></div>	84%15%
1	kt	231	<div><div></div></div>	78%20%
1	ku	231	<div><div></div></div>	83%16%
1	kv	231	<div><div></div></div>	78%20%
1	kw	231	<div><div></div></div>	84%14%
1	kx	231	<div><div></div></div>	80%18%
1	ky	231	<div><div></div></div>	81%17%
1	kz	231	<div><div></div></div>	83%15%
1	l	231	<div><div></div></div>	84%15%
1	l0	231	<div><div></div></div>	80%18%
1	l1	231	<div><div></div></div>	83%16%
1	l2	231	<div><div></div></div>	85%14%
1	l3	231	<div><div></div></div>	82%16%


























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Mol	Chain	Length	Quality of chain
1	l4	231	 79% 20%
1	l5	231	 85% 13% •
1	l6	231	 83% 17%
1	l7	231	 82% 16% •
1	l8	231	 84% 16%
1	l9	231	 81% 19% •
1	lA	231	 80% 20%
1	lB	231	 81% 17% •
1	lC	231	 79% 21%
1	lD	231	 84% 15% •
1	lE	231	 83% 16% •
1	lF	231	 81% 16% •
1	lG	231	 84% 16%
1	lH	231	 78% 19% •
1	lI	231	 81% 17% •
1	lJ	231	 84% 14% •
1	lK	231	 84% 15% •
1	lL	231	 81% 17% •
1	lM	231	 81% 17% •
1	lN	231	 83% 16% •
1	lO	231	 81% 18% •
1	lP	231	 85% 13% •
1	lQ	231	 80% 18% •
1	lR	231	 81% 18%
1	la	231	 84% 13% •

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Mol	Chain	Length	Quality of chain
1	lb	231	 81% 17% .
1	lc	231	 81% 18%
1	ld	231	 84% 15% .
1	le	231	 81% 19% .
1	lf	231	 81% 18% .
1	lg	231	 82% 18%
1	lh	231	 79% 19% .
1	li	231	 84% 15% .
1	lj	231	 80% 18% .
1	lk	231	 81% 18% .
1	ll	231	 83% 14% .
1	lm	231	 83% 17%
1	ln	231	 82% 16% .
1	lo	231	 85% 12% .
1	lp	231	 84% 14% .
1	lq	231	 84% 14% .
1	lr	231	 81% 17% .
1	ls	231	 81% 17% .
1	lt	231	 86% 12% .
1	lu	231	 81% 17% .
1	lv	231	 81% 17% .
1	lw	231	 79% 20% .
1	lx	231	 85% 14% .
1	ly	231	 84% 15% .
1	lz	231	 82% 15% .

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Mol	Chain	Length	Quality of chain
1	m	231	 82% 16% .
1	n	231	 83% 14% .
1	o	231	 82% 16% .
1	p	231	 80% 19%
1	q	231	 83% 16% .
1	r	231	 83% 15% .
1	s	231	 82% 17% .
1	t	231	 82% 17% .
1	u	231	 84% 16%
1	v	231	 81% 17% .
1	w	231	 82% 16% .
1	x	231	 82% 16% .
1	y	231	 82% 18%
1	z	231	 81% 18% .

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2440800 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 capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	g8	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	g9	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ga	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	gb	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	gc	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	gd	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ge	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	gf	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	gg	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	gh	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	1C	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	gi	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	gj	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	gk	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	gl	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	gm	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	gn	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	go	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	gp	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	gq	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	gr	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	1D	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	gs	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	gt	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	gu	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	gv	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	gw	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	gx	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	gy	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	gz	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	gA	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	gB	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	1E	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	gC	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	gD	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	gE	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	gF	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	gG	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	gH	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	gI	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	gJ	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	gK	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	gL	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	1F	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	gM	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	gN	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	gO	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	gP	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	gQ	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	gR	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	gS	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	gT	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	gU	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	gV	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	1G	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	gW	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	gX	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	gY	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	gZ	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	h0	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	h1	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	h2	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	h3	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	h4	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	h5	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	1H	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	h6	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	h7	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	h8	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	h9	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ha	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	hb	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	hc	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	hd	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	he	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	hf	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	1I	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	hg	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	hh	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	hi	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	hj	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	hk	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	hl	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	hm	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	hn	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	ho	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	hp	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	lJ	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	hq	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	hr	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	hs	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	ht	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	hu	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	hv	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	hw	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	hx	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	hy	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	hz	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	lK	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	hA	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	hB	231	Total 1800	C 1134	N 317	O 336	S 13	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	hC	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	hD	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	hE	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	hF	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	hG	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	hH	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	hI	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	hJ	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	1L	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	hK	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	hL	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	hM	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	hN	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	hO	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	hP	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	hQ	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	hR	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	hS	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	hT	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	1M	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	hU	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	hV	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	hW	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	hX	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	hY	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	hZ	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	i0	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	i1	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	i2	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	i3	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	1N	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	i4	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	i5	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	i6	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	i7	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	i8	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	i9	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ia	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ib	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ic	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	id	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	1O	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	ie	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	if	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ig	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ih	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ii	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ij	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ik	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	il	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	im	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	in	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	1P	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	io	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ip	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	iq	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ir	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	is	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	it	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	iu	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	iv	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	iw	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ix	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	1Q	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	iy	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	iz	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	iA	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	iB	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	iC	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	iD	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	iE	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	iF	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	iG	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	iH	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	1R	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	iI	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	iJ	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	iK	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	iL	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	iM	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	iN	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	iO	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	iP	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	iQ	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	iR	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	1S	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	iS	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	iT	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	iU	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	iV	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	iW	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	iX	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	iY	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	iZ	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	j0	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	j1	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	1T	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	j2	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	j3	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	j4	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	j5	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	j6	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	j7	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	j8	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	j9	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	ja	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	jb	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	1U	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	jc	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	jd	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	je	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	jf	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	jg	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	jh	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ji	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	jj	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	jk	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	jl	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	1V	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	jm	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	jn	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	jo	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	jp	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	jq	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	jr	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	js	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	jt	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	ju	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	jv	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	1W	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	jw	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	jx	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	jy	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	jz	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	jA	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	jB	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	jC	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	jD	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	jE	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	jF	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	1X	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	jG	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	jH	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	jI	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	jJ	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	jK	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	jL	231	Total 1800	C 1134	N 317	O 336	S 13	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	jM	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	jN	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	jO	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	jP	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	1Y	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	jQ	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	jR	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	jS	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	jT	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	jU	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	jV	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	jW	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	jX	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	jY	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	jZ	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	1Z	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	k0	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	k1	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	k2	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	k3	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	k4	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	k5	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	k6	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	k7	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	k8	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	k9	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	20	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ka	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	kb	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	kc	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	kd	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ke	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	kf	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	kg	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	kh	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ki	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	kj	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	21	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	kk	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	kl	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	km	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	kn	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	ko	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	kp	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	kq	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	kr	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	ks	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	kt	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	22	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	ku	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	kv	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	kw	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	kx	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	ky	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	kz	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	kA	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	kB	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	kC	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	kD	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	23	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	kE	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	kF	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	kG	231	Total 1800	C 1134	N 317	O 336	S 13	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	kH	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	kI	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	kJ	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	kK	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	kL	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	kM	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	kN	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	24	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	kO	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	kP	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	kQ	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	kR	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	kS	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	kT	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	kU	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	kV	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	kW	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	kX	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	25	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	kY	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	kZ	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	l0	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	l1	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	l2	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	l3	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	l4	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	l5	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	l6	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	l7	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	26	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	l8	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	l9	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	la	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	lb	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	lc	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ld	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	le	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	lf	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	lg	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	lh	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	27	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	li	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	lj	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	lk	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	ll	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	lm	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	ln	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	lo	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	lp	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	lq	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	lr	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	28	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	ls	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	lt	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	lu	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	lv	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	lw	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	lx	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	ly	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	lz	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	lA	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	lB	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	29	231	Total 1800	C 1134	N 317	O 336	S 13	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	lC	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	lD	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	lE	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	lF	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	lG	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	lH	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	lI	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	lJ	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	lK	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	lL	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	2a	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	lM	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	lN	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	lO	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	lP	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	lQ	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	lR	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	2b	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	2c	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	2d	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	2e	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	2f	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	2g	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	2h	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	2i	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	2j	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	2k	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	2l	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	2m	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	2n	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	2o	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	2p	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	2q	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	2r	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	2s	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	2t	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	2u	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	2v	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	2w	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	2x	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	2y	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	2z	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	2A	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	2B	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	2C	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	2D	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	2E	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	2F	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	2G	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	2H	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	2I	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	2J	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	2K	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	2L	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	2M	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	2N	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	2O	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	2P	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	2Q	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	2R	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	2S	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	2T	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	2U	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	2V	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	2W	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	2X	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	2Y	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	2Z	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	30	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	31	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	32	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	33	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	34	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	35	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	36	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	37	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	38	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	39	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	3a	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	3b	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	3c	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	3d	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	3e	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	3f	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	3g	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	3h	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	3i	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	3j	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	3k	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	3l	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	3m	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	3n	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	3o	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	3p	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	3q	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	3r	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	3s	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	3t	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	3u	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	3v	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	3w	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	3x	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	3y	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	3z	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	3A	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	3B	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	3C	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	3D	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	3E	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	3F	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	3G	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	3H	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	3I	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	3J	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	3K	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	3L	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	3M	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	3N	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	3O	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	3P	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	3Q	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	3R	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	3S	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	3T	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	3U	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	3V	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	3W	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	3X	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	3Y	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	3Z	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	40	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	41	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	42	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	43	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	44	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	45	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	46	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	47	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	48	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	49	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	4a	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	4b	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	4c	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	4d	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	4e	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	4f	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	4g	231	Total 1800	C 1134	N 317	O 336	S 13	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	4h	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	4i	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	4j	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	4k	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	4l	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	4m	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	4n	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	4o	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	4p	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	4q	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	4r	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	4s	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	4t	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	4u	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	4v	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	4w	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	4x	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	4y	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	4z	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	4A	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	4B	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	4C	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	4D	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	4E	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	4F	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	4G	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	4H	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	4I	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	4J	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	4K	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	4L	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	4M	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	4N	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	4O	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	4P	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	4Q	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	4R	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	4S	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	4T	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	4U	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	4V	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	4W	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	4X	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	4Y	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	4Z	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	50	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	51	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	52	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	53	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	54	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	55	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	56	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	57	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	58	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	59	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	5a	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	5b	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	5c	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	5d	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	5e	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	5f	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	5g	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	5h	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	5i	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	5j	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	5k	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	5l	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	5m	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	5n	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	5o	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	5p	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	5q	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	5r	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	5s	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	5t	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	5u	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	5v	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	5w	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	5x	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	5y	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	5z	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	5A	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	5B	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	5C	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	5D	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	5E	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	5F	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	5G	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	5H	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	5I	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	5J	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	5K	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	5L	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	5M	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	5N	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	5O	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	5P	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	5Q	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	5R	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	5S	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	5T	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	5U	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	5V	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	5W	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	5X	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	5Y	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	5Z	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	60	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	61	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	62	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	63	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	64	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	65	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	66	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	67	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	68	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	69	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	6a	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	6b	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	6c	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	6d	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	6e	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	6f	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	6g	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	6h	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	6i	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	6j	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	6k	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	6l	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	6m	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	6n	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	6o	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	6p	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	6q	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	6r	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	6s	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	6t	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	6u	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	6v	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	6w	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	6x	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	6y	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	6z	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	6A	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	6B	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	6C	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	6D	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	6E	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	6F	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	6G	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	6H	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	6I	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	6J	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	6K	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	6L	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	6M	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	6N	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	6O	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	6P	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	6Q	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	6R	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	6S	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	6T	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	6U	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	6V	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	6W	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	6X	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	6Y	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	6Z	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	70	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	71	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	72	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	73	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	74	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	75	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	76	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	77	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	78	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	79	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	7a	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	7b	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	7c	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	7d	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	7e	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	7f	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	7g	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	7h	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	7i	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	7j	231	Total 1800	C 1134	N 317	O 336	S 13	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	7k	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	7l	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	7m	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	7n	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	7o	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	7p	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	7q	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	7r	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	7s	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	7t	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	7u	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	7v	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	7w	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	7x	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	7y	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	7z	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	7A	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	7B	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	7C	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	7D	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	7E	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	7F	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	7G	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	7H	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	7I	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	7J	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	7K	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	7L	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	7M	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	7N	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	7O	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	7P	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	7Q	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	7R	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	7S	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	7T	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	7U	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	7V	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	7W	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	7X	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	7Y	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	7Z	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	80	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	81	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	82	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	83	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	84	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	85	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	86	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	87	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	88	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	89	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	8a	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	8b	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	8c	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	8d	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	8e	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	8f	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	8g	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	8h	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	8i	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	8j	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	8k	231	Total 1800	C 1134	N 317	O 336	S 13	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	8l	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	8m	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	8n	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	8o	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	8p	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	8q	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	8r	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	8s	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	8t	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	8u	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	8v	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	8w	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	8x	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	8y	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	8z	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	8A	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	8B	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	8C	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	8D	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	8E	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	8F	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	8G	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	8H	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	8I	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	8J	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	8K	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	8L	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	8M	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	8N	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	8O	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	8P	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	8Q	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	8R	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	8S	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	8T	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	8U	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	8V	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	8W	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	8X	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	8Y	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	8Z	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	90	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	91	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	92	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	93	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	94	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	95	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	96	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	97	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	98	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	99	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	9a	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	9b	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	9c	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	9d	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	9e	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	9f	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	9g	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	9h	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	9i	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	9j	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	9k	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	9l	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	9m	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	9n	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	9o	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	9p	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	9q	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	9r	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	9s	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	9t	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	9u	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	9v	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	9w	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	9x	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	9y	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	9z	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	9A	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	9B	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	9C	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	9D	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	9E	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	9F	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	9G	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	9H	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	9I	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	9J	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	9K	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	9L	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	9M	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	9N	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	9O	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	9P	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	Y	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	9Q	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	9R	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	9S	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	9T	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	9U	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	9V	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	9W	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	9X	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	9Y	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	9Z	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	Z	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	a0	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	a1	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	a2	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	a3	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	a4	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	a5	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	a6	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	a7	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	a8	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	a9	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	10	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	aa	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ab	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ac	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ad	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ae	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	af	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ag	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ah	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ai	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	aj	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	11	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ak	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	al	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	am	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	an	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ao	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ap	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	aq	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ar	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	as	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	at	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	12	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	au	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	av	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	aw	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ax	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ay	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	az	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	aA	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	aB	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	aC	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	aD	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	13	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	aE	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	aF	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	aG	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	aH	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	aI	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	aJ	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	aK	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	aL	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	aM	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	aN	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	14	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	aO	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	aP	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	aQ	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	aR	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	aS	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	aT	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	aU	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	aV	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	aW	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	aX	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	15	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	aY	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	aZ	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	b0	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	b1	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	b2	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	b3	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	b4	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	b5	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	b6	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	b7	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	16	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	b8	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	b9	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ba	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	bb	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	bc	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	bd	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	be	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	bf	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	bg	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	bh	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	17	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	bi	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	bj	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	bk	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	bl	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	bm	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	bn	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	bo	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	bp	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	bq	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	br	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	18	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	bs	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	bt	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	bu	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	bv	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	bw	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	bx	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	by	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	bz	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	bA	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	bB	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	19	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	bC	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	bD	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	bE	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	bF	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	bG	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	bH	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	bI	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	bJ	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	bK	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	bL	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	1a	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	bM	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	bN	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	bO	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	bP	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	bQ	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	bR	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	bS	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	bT	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	bU	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	bV	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	1b	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	bW	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	bX	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	bY	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	bZ	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	c0	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	c1	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	c2	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	c3	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	c4	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	c5	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	1c	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	c6	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	c7	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	c8	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	c9	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	ca	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	cb	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	cc	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	cd	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ce	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	cf	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ld	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	cg	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ch	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ci	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	cj	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ck	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	cl	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	cm	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	cn	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	co	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	cp	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	le	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	cq	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	cr	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	cs	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	ct	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	cu	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	cv	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	cw	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	cx	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	cy	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	cz	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	lf	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	cA	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	cB	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	cC	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	cD	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	cE	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	cF	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	cG	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	cH	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	cI	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	cJ	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	lg	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	cK	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	cL	231	Total 1800	C 1134	N 317	O 336	S 13	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	cM	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	cN	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	cO	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	cP	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	cQ	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	cR	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	cS	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	cT	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	lh	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	cU	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	cV	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	cW	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	cX	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	cY	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	cZ	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	d0	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	d1	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	d2	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	d3	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	li	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	d4	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	d5	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	d6	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	d7	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	d8	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	d9	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	da	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	db	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	dc	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	dd	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	lj	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	de	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	df	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	dg	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	dh	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	di	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	dj	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	dk	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	dl	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	dm	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	dn	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	lk	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	do	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	dp	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	dq	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	dr	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ds	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	dt	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	du	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	dv	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	dw	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	dx	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	dl	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	dy	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	dz	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	dA	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	dB	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	dC	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	dD	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	dE	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	dF	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	dG	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	dH	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	1m	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	dI	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	dJ	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	dK	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	dL	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	dM	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	dN	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	dO	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	dP	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	dQ	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	dR	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	1n	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	dS	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	dT	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	dU	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	dV	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	dW	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	dX	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	dY	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	dZ	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	e0	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	e1	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	lo	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	e2	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	e3	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	e4	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	e5	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	e6	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	e7	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	e8	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	e9	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ea	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	eb	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	lp	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ec	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ed	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ee	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ef	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	eg	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	eh	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ei	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ej	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	ek	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	el	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	lq	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	em	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	en	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	eo	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ep	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	eq	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	er	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	es	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	et	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	eu	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ev	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	lr	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ew	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ex	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ey	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ez	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	eA	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	eB	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	eC	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	eD	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	eE	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	eF	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	1s	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	eG	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	eH	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	eI	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	eJ	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	eK	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	eL	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	eM	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	eN	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	eO	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	eP	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	1t	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	eQ	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	eR	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	eS	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	eT	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	eU	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	eV	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	eW	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	eX	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	eY	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	eZ	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	1u	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	f0	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	f1	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	f2	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	f3	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	f4	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	f5	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	f6	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	f7	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	f8	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	f9	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	1v	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	fa	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	fb	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	fc	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	fd	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	fe	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	ff	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	fg	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	fh	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	fi	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	fj	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	lw	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	fk	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	fl	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	fm	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	fn	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	fo	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	fp	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	fq	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	fr	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	fs	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	ft	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	lx	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	fu	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	fv	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	fw	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	fx	231	Total 1800	C 1134	N 317	O 336	S 13	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	fy	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	fz	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	fA	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	fB	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	fC	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	fD	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	ly	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	fE	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	fF	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	fG	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	fH	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	fI	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	fJ	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	fK	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	fL	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	fM	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	fN	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	lz	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	fO	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	fP	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	fQ	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	fR	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	fS	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	fT	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	fU	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	fV	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	fW	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	fX	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	1A	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	fY	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	fZ	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	g0	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	g1	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	g2	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	g3	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	g4	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	g5	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	g6	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	g7	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	1B	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	0	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	a	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	b	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	c	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	d	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	e	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	f	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	g	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	h	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	i	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	j	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	l	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	k	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	l	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	m	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	n	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	o	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	p	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	q	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	r	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	s	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	t	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	2	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	u	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	v	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	w	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	x	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	y	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	z	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	A	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	B	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	C	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	D	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	3	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	E	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	F	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	G	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	H	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	I	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	J	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	K	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	L	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	M	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	N	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	4	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	O	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	P	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	Q	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	R	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	S	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	T	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	U	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	V	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	W	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	X	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	5	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	6	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	7	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	8	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	9	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		

There are 1356 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g8	92	GLU	ALA	engineered mutation	UNP Q79791
g9	92	GLU	ALA	engineered mutation	UNP Q79791
ga	92	GLU	ALA	engineered mutation	UNP Q79791
gb	92	GLU	ALA	engineered mutation	UNP Q79791
gc	92	GLU	ALA	engineered mutation	UNP Q79791
gd	92	GLU	ALA	engineered mutation	UNP Q79791
ge	92	GLU	ALA	engineered mutation	UNP Q79791

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Chain	Residue	Modelled	Actual	Comment	Reference
gf	92	GLU	ALA	engineered mutation	UNP Q79791
gg	92	GLU	ALA	engineered mutation	UNP Q79791
gh	92	GLU	ALA	engineered mutation	UNP Q79791
1C	92	GLU	ALA	engineered mutation	UNP Q79791
gi	92	GLU	ALA	engineered mutation	UNP Q79791
gj	92	GLU	ALA	engineered mutation	UNP Q79791
gk	92	GLU	ALA	engineered mutation	UNP Q79791
gl	92	GLU	ALA	engineered mutation	UNP Q79791
gm	92	GLU	ALA	engineered mutation	UNP Q79791
gn	92	GLU	ALA	engineered mutation	UNP Q79791
go	92	GLU	ALA	engineered mutation	UNP Q79791
gp	92	GLU	ALA	engineered mutation	UNP Q79791
gq	92	GLU	ALA	engineered mutation	UNP Q79791
gr	92	GLU	ALA	engineered mutation	UNP Q79791
1D	92	GLU	ALA	engineered mutation	UNP Q79791
gs	92	GLU	ALA	engineered mutation	UNP Q79791
gt	92	GLU	ALA	engineered mutation	UNP Q79791
gu	92	GLU	ALA	engineered mutation	UNP Q79791
gv	92	GLU	ALA	engineered mutation	UNP Q79791
gw	92	GLU	ALA	engineered mutation	UNP Q79791
gx	92	GLU	ALA	engineered mutation	UNP Q79791
gy	92	GLU	ALA	engineered mutation	UNP Q79791
gz	92	GLU	ALA	engineered mutation	UNP Q79791
gA	92	GLU	ALA	engineered mutation	UNP Q79791
gB	92	GLU	ALA	engineered mutation	UNP Q79791
1E	92	GLU	ALA	engineered mutation	UNP Q79791
gC	92	GLU	ALA	engineered mutation	UNP Q79791
gD	92	GLU	ALA	engineered mutation	UNP Q79791
gE	92	GLU	ALA	engineered mutation	UNP Q79791
gF	92	GLU	ALA	engineered mutation	UNP Q79791
gG	92	GLU	ALA	engineered mutation	UNP Q79791
gH	92	GLU	ALA	engineered mutation	UNP Q79791
gI	92	GLU	ALA	engineered mutation	UNP Q79791
gJ	92	GLU	ALA	engineered mutation	UNP Q79791
gK	92	GLU	ALA	engineered mutation	UNP Q79791
gL	92	GLU	ALA	engineered mutation	UNP Q79791
1F	92	GLU	ALA	engineered mutation	UNP Q79791
gM	92	GLU	ALA	engineered mutation	UNP Q79791
gN	92	GLU	ALA	engineered mutation	UNP Q79791
gO	92	GLU	ALA	engineered mutation	UNP Q79791
gP	92	GLU	ALA	engineered mutation	UNP Q79791
gQ	92	GLU	ALA	engineered mutation	UNP Q79791

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Chain	Residue	Modelled	Actual	Comment	Reference
gR	92	GLU	ALA	engineered mutation	UNP Q79791
gS	92	GLU	ALA	engineered mutation	UNP Q79791
gT	92	GLU	ALA	engineered mutation	UNP Q79791
gU	92	GLU	ALA	engineered mutation	UNP Q79791
gV	92	GLU	ALA	engineered mutation	UNP Q79791
1G	92	GLU	ALA	engineered mutation	UNP Q79791
gW	92	GLU	ALA	engineered mutation	UNP Q79791
gX	92	GLU	ALA	engineered mutation	UNP Q79791
gY	92	GLU	ALA	engineered mutation	UNP Q79791
gZ	92	GLU	ALA	engineered mutation	UNP Q79791
h0	92	GLU	ALA	engineered mutation	UNP Q79791
h1	92	GLU	ALA	engineered mutation	UNP Q79791
h2	92	GLU	ALA	engineered mutation	UNP Q79791
h3	92	GLU	ALA	engineered mutation	UNP Q79791
h4	92	GLU	ALA	engineered mutation	UNP Q79791
h5	92	GLU	ALA	engineered mutation	UNP Q79791
1H	92	GLU	ALA	engineered mutation	UNP Q79791
h6	92	GLU	ALA	engineered mutation	UNP Q79791
h7	92	GLU	ALA	engineered mutation	UNP Q79791
h8	92	GLU	ALA	engineered mutation	UNP Q79791
h9	92	GLU	ALA	engineered mutation	UNP Q79791
ha	92	GLU	ALA	engineered mutation	UNP Q79791
hb	92	GLU	ALA	engineered mutation	UNP Q79791
hc	92	GLU	ALA	engineered mutation	UNP Q79791
hd	92	GLU	ALA	engineered mutation	UNP Q79791
he	92	GLU	ALA	engineered mutation	UNP Q79791
hf	92	GLU	ALA	engineered mutation	UNP Q79791
1I	92	GLU	ALA	engineered mutation	UNP Q79791
hg	92	GLU	ALA	engineered mutation	UNP Q79791
hh	92	GLU	ALA	engineered mutation	UNP Q79791
hi	92	GLU	ALA	engineered mutation	UNP Q79791
hj	92	GLU	ALA	engineered mutation	UNP Q79791
hk	92	GLU	ALA	engineered mutation	UNP Q79791
hl	92	GLU	ALA	engineered mutation	UNP Q79791
hm	92	GLU	ALA	engineered mutation	UNP Q79791
hn	92	GLU	ALA	engineered mutation	UNP Q79791
ho	92	GLU	ALA	engineered mutation	UNP Q79791
hp	92	GLU	ALA	engineered mutation	UNP Q79791
1J	92	GLU	ALA	engineered mutation	UNP Q79791
hq	92	GLU	ALA	engineered mutation	UNP Q79791
hr	92	GLU	ALA	engineered mutation	UNP Q79791
hs	92	GLU	ALA	engineered mutation	UNP Q79791

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Chain	Residue	Modelled	Actual	Comment	Reference
ht	92	GLU	ALA	engineered mutation	UNP Q79791
hu	92	GLU	ALA	engineered mutation	UNP Q79791
hv	92	GLU	ALA	engineered mutation	UNP Q79791
hw	92	GLU	ALA	engineered mutation	UNP Q79791
hx	92	GLU	ALA	engineered mutation	UNP Q79791
hy	92	GLU	ALA	engineered mutation	UNP Q79791
hz	92	GLU	ALA	engineered mutation	UNP Q79791
1K	92	GLU	ALA	engineered mutation	UNP Q79791
hA	92	GLU	ALA	engineered mutation	UNP Q79791
hB	92	GLU	ALA	engineered mutation	UNP Q79791
hC	92	GLU	ALA	engineered mutation	UNP Q79791
hD	92	GLU	ALA	engineered mutation	UNP Q79791
hE	92	GLU	ALA	engineered mutation	UNP Q79791
hF	92	GLU	ALA	engineered mutation	UNP Q79791
hG	92	GLU	ALA	engineered mutation	UNP Q79791
hH	92	GLU	ALA	engineered mutation	UNP Q79791
hI	92	GLU	ALA	engineered mutation	UNP Q79791
hJ	92	GLU	ALA	engineered mutation	UNP Q79791
1L	92	GLU	ALA	engineered mutation	UNP Q79791
hK	92	GLU	ALA	engineered mutation	UNP Q79791
hL	92	GLU	ALA	engineered mutation	UNP Q79791
hM	92	GLU	ALA	engineered mutation	UNP Q79791
hN	92	GLU	ALA	engineered mutation	UNP Q79791
hO	92	GLU	ALA	engineered mutation	UNP Q79791
hP	92	GLU	ALA	engineered mutation	UNP Q79791
hQ	92	GLU	ALA	engineered mutation	UNP Q79791
hR	92	GLU	ALA	engineered mutation	UNP Q79791
hS	92	GLU	ALA	engineered mutation	UNP Q79791
hT	92	GLU	ALA	engineered mutation	UNP Q79791
1M	92	GLU	ALA	engineered mutation	UNP Q79791
hU	92	GLU	ALA	engineered mutation	UNP Q79791
hV	92	GLU	ALA	engineered mutation	UNP Q79791
hW	92	GLU	ALA	engineered mutation	UNP Q79791
hX	92	GLU	ALA	engineered mutation	UNP Q79791
hY	92	GLU	ALA	engineered mutation	UNP Q79791
hZ	92	GLU	ALA	engineered mutation	UNP Q79791
i0	92	GLU	ALA	engineered mutation	UNP Q79791
i1	92	GLU	ALA	engineered mutation	UNP Q79791
i2	92	GLU	ALA	engineered mutation	UNP Q79791
i3	92	GLU	ALA	engineered mutation	UNP Q79791
1N	92	GLU	ALA	engineered mutation	UNP Q79791
i4	92	GLU	ALA	engineered mutation	UNP Q79791

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Chain	Residue	Modelled	Actual	Comment	Reference
i5	92	GLU	ALA	engineered mutation	UNP Q79791
i6	92	GLU	ALA	engineered mutation	UNP Q79791
i7	92	GLU	ALA	engineered mutation	UNP Q79791
i8	92	GLU	ALA	engineered mutation	UNP Q79791
i9	92	GLU	ALA	engineered mutation	UNP Q79791
ia	92	GLU	ALA	engineered mutation	UNP Q79791
ib	92	GLU	ALA	engineered mutation	UNP Q79791
ic	92	GLU	ALA	engineered mutation	UNP Q79791
id	92	GLU	ALA	engineered mutation	UNP Q79791
1O	92	GLU	ALA	engineered mutation	UNP Q79791
ie	92	GLU	ALA	engineered mutation	UNP Q79791
if	92	GLU	ALA	engineered mutation	UNP Q79791
ig	92	GLU	ALA	engineered mutation	UNP Q79791
ih	92	GLU	ALA	engineered mutation	UNP Q79791
ii	92	GLU	ALA	engineered mutation	UNP Q79791
ij	92	GLU	ALA	engineered mutation	UNP Q79791
ik	92	GLU	ALA	engineered mutation	UNP Q79791
il	92	GLU	ALA	engineered mutation	UNP Q79791
im	92	GLU	ALA	engineered mutation	UNP Q79791
in	92	GLU	ALA	engineered mutation	UNP Q79791
1P	92	GLU	ALA	engineered mutation	UNP Q79791
io	92	GLU	ALA	engineered mutation	UNP Q79791
ip	92	GLU	ALA	engineered mutation	UNP Q79791
iq	92	GLU	ALA	engineered mutation	UNP Q79791
ir	92	GLU	ALA	engineered mutation	UNP Q79791
is	92	GLU	ALA	engineered mutation	UNP Q79791
it	92	GLU	ALA	engineered mutation	UNP Q79791
iu	92	GLU	ALA	engineered mutation	UNP Q79791
iv	92	GLU	ALA	engineered mutation	UNP Q79791
iw	92	GLU	ALA	engineered mutation	UNP Q79791
ix	92	GLU	ALA	engineered mutation	UNP Q79791
1Q	92	GLU	ALA	engineered mutation	UNP Q79791
iy	92	GLU	ALA	engineered mutation	UNP Q79791
iz	92	GLU	ALA	engineered mutation	UNP Q79791
iA	92	GLU	ALA	engineered mutation	UNP Q79791
iB	92	GLU	ALA	engineered mutation	UNP Q79791
iC	92	GLU	ALA	engineered mutation	UNP Q79791
iD	92	GLU	ALA	engineered mutation	UNP Q79791
iE	92	GLU	ALA	engineered mutation	UNP Q79791
iF	92	GLU	ALA	engineered mutation	UNP Q79791
iG	92	GLU	ALA	engineered mutation	UNP Q79791
iH	92	GLU	ALA	engineered mutation	UNP Q79791

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Chain	Residue	Modelled	Actual	Comment	Reference
1R	92	GLU	ALA	engineered mutation	UNP Q79791
iI	92	GLU	ALA	engineered mutation	UNP Q79791
iJ	92	GLU	ALA	engineered mutation	UNP Q79791
iK	92	GLU	ALA	engineered mutation	UNP Q79791
iL	92	GLU	ALA	engineered mutation	UNP Q79791
iM	92	GLU	ALA	engineered mutation	UNP Q79791
iN	92	GLU	ALA	engineered mutation	UNP Q79791
iO	92	GLU	ALA	engineered mutation	UNP Q79791
iP	92	GLU	ALA	engineered mutation	UNP Q79791
iQ	92	GLU	ALA	engineered mutation	UNP Q79791
iR	92	GLU	ALA	engineered mutation	UNP Q79791
1S	92	GLU	ALA	engineered mutation	UNP Q79791
iS	92	GLU	ALA	engineered mutation	UNP Q79791
iT	92	GLU	ALA	engineered mutation	UNP Q79791
iU	92	GLU	ALA	engineered mutation	UNP Q79791
iV	92	GLU	ALA	engineered mutation	UNP Q79791
iW	92	GLU	ALA	engineered mutation	UNP Q79791
iX	92	GLU	ALA	engineered mutation	UNP Q79791
iY	92	GLU	ALA	engineered mutation	UNP Q79791
iZ	92	GLU	ALA	engineered mutation	UNP Q79791
j0	92	GLU	ALA	engineered mutation	UNP Q79791
j1	92	GLU	ALA	engineered mutation	UNP Q79791
1T	92	GLU	ALA	engineered mutation	UNP Q79791
j2	92	GLU	ALA	engineered mutation	UNP Q79791
j3	92	GLU	ALA	engineered mutation	UNP Q79791
j4	92	GLU	ALA	engineered mutation	UNP Q79791
j5	92	GLU	ALA	engineered mutation	UNP Q79791
j6	92	GLU	ALA	engineered mutation	UNP Q79791
j7	92	GLU	ALA	engineered mutation	UNP Q79791
j8	92	GLU	ALA	engineered mutation	UNP Q79791
j9	92	GLU	ALA	engineered mutation	UNP Q79791
ja	92	GLU	ALA	engineered mutation	UNP Q79791
jb	92	GLU	ALA	engineered mutation	UNP Q79791
1U	92	GLU	ALA	engineered mutation	UNP Q79791
jc	92	GLU	ALA	engineered mutation	UNP Q79791
jd	92	GLU	ALA	engineered mutation	UNP Q79791
je	92	GLU	ALA	engineered mutation	UNP Q79791
jf	92	GLU	ALA	engineered mutation	UNP Q79791
jg	92	GLU	ALA	engineered mutation	UNP Q79791
jh	92	GLU	ALA	engineered mutation	UNP Q79791
ji	92	GLU	ALA	engineered mutation	UNP Q79791
jj	92	GLU	ALA	engineered mutation	UNP Q79791

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Chain	Residue	Modelled	Actual	Comment	Reference
jk	92	GLU	ALA	engineered mutation	UNP Q79791
jl	92	GLU	ALA	engineered mutation	UNP Q79791
lV	92	GLU	ALA	engineered mutation	UNP Q79791
jm	92	GLU	ALA	engineered mutation	UNP Q79791
jn	92	GLU	ALA	engineered mutation	UNP Q79791
jo	92	GLU	ALA	engineered mutation	UNP Q79791
jp	92	GLU	ALA	engineered mutation	UNP Q79791
jq	92	GLU	ALA	engineered mutation	UNP Q79791
jr	92	GLU	ALA	engineered mutation	UNP Q79791
js	92	GLU	ALA	engineered mutation	UNP Q79791
jt	92	GLU	ALA	engineered mutation	UNP Q79791
ju	92	GLU	ALA	engineered mutation	UNP Q79791
jv	92	GLU	ALA	engineered mutation	UNP Q79791
lW	92	GLU	ALA	engineered mutation	UNP Q79791
jw	92	GLU	ALA	engineered mutation	UNP Q79791
jx	92	GLU	ALA	engineered mutation	UNP Q79791
jy	92	GLU	ALA	engineered mutation	UNP Q79791
jz	92	GLU	ALA	engineered mutation	UNP Q79791
jA	92	GLU	ALA	engineered mutation	UNP Q79791
jB	92	GLU	ALA	engineered mutation	UNP Q79791
jC	92	GLU	ALA	engineered mutation	UNP Q79791
jD	92	GLU	ALA	engineered mutation	UNP Q79791
jE	92	GLU	ALA	engineered mutation	UNP Q79791
jF	92	GLU	ALA	engineered mutation	UNP Q79791
lX	92	GLU	ALA	engineered mutation	UNP Q79791
jG	92	GLU	ALA	engineered mutation	UNP Q79791
jH	92	GLU	ALA	engineered mutation	UNP Q79791
jI	92	GLU	ALA	engineered mutation	UNP Q79791
jJ	92	GLU	ALA	engineered mutation	UNP Q79791
jK	92	GLU	ALA	engineered mutation	UNP Q79791
jL	92	GLU	ALA	engineered mutation	UNP Q79791
jM	92	GLU	ALA	engineered mutation	UNP Q79791
jN	92	GLU	ALA	engineered mutation	UNP Q79791
jO	92	GLU	ALA	engineered mutation	UNP Q79791
jP	92	GLU	ALA	engineered mutation	UNP Q79791
lY	92	GLU	ALA	engineered mutation	UNP Q79791
jQ	92	GLU	ALA	engineered mutation	UNP Q79791
jR	92	GLU	ALA	engineered mutation	UNP Q79791
jS	92	GLU	ALA	engineered mutation	UNP Q79791
jT	92	GLU	ALA	engineered mutation	UNP Q79791
jU	92	GLU	ALA	engineered mutation	UNP Q79791
jV	92	GLU	ALA	engineered mutation	UNP Q79791

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Chain	Residue	Modelled	Actual	Comment	Reference
jW	92	GLU	ALA	engineered mutation	UNP Q79791
jX	92	GLU	ALA	engineered mutation	UNP Q79791
jY	92	GLU	ALA	engineered mutation	UNP Q79791
jZ	92	GLU	ALA	engineered mutation	UNP Q79791
lZ	92	GLU	ALA	engineered mutation	UNP Q79791
k0	92	GLU	ALA	engineered mutation	UNP Q79791
k1	92	GLU	ALA	engineered mutation	UNP Q79791
k2	92	GLU	ALA	engineered mutation	UNP Q79791
k3	92	GLU	ALA	engineered mutation	UNP Q79791
k4	92	GLU	ALA	engineered mutation	UNP Q79791
k5	92	GLU	ALA	engineered mutation	UNP Q79791
k6	92	GLU	ALA	engineered mutation	UNP Q79791
k7	92	GLU	ALA	engineered mutation	UNP Q79791
k8	92	GLU	ALA	engineered mutation	UNP Q79791
k9	92	GLU	ALA	engineered mutation	UNP Q79791
20	92	GLU	ALA	engineered mutation	UNP Q79791
ka	92	GLU	ALA	engineered mutation	UNP Q79791
kb	92	GLU	ALA	engineered mutation	UNP Q79791
kc	92	GLU	ALA	engineered mutation	UNP Q79791
kd	92	GLU	ALA	engineered mutation	UNP Q79791
ke	92	GLU	ALA	engineered mutation	UNP Q79791
kf	92	GLU	ALA	engineered mutation	UNP Q79791
kg	92	GLU	ALA	engineered mutation	UNP Q79791
kh	92	GLU	ALA	engineered mutation	UNP Q79791
ki	92	GLU	ALA	engineered mutation	UNP Q79791
kj	92	GLU	ALA	engineered mutation	UNP Q79791
21	92	GLU	ALA	engineered mutation	UNP Q79791
kk	92	GLU	ALA	engineered mutation	UNP Q79791
kl	92	GLU	ALA	engineered mutation	UNP Q79791
km	92	GLU	ALA	engineered mutation	UNP Q79791
kn	92	GLU	ALA	engineered mutation	UNP Q79791
ko	92	GLU	ALA	engineered mutation	UNP Q79791
kp	92	GLU	ALA	engineered mutation	UNP Q79791
kq	92	GLU	ALA	engineered mutation	UNP Q79791
kr	92	GLU	ALA	engineered mutation	UNP Q79791
ks	92	GLU	ALA	engineered mutation	UNP Q79791
kt	92	GLU	ALA	engineered mutation	UNP Q79791
22	92	GLU	ALA	engineered mutation	UNP Q79791
ku	92	GLU	ALA	engineered mutation	UNP Q79791
kv	92	GLU	ALA	engineered mutation	UNP Q79791
kW	92	GLU	ALA	engineered mutation	UNP Q79791
kx	92	GLU	ALA	engineered mutation	UNP Q79791

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Chain	Residue	Modelled	Actual	Comment	Reference
ky	92	GLU	ALA	engineered mutation	UNP Q79791
kz	92	GLU	ALA	engineered mutation	UNP Q79791
kA	92	GLU	ALA	engineered mutation	UNP Q79791
kB	92	GLU	ALA	engineered mutation	UNP Q79791
kC	92	GLU	ALA	engineered mutation	UNP Q79791
kD	92	GLU	ALA	engineered mutation	UNP Q79791
23	92	GLU	ALA	engineered mutation	UNP Q79791
kE	92	GLU	ALA	engineered mutation	UNP Q79791
kF	92	GLU	ALA	engineered mutation	UNP Q79791
kG	92	GLU	ALA	engineered mutation	UNP Q79791
kH	92	GLU	ALA	engineered mutation	UNP Q79791
kI	92	GLU	ALA	engineered mutation	UNP Q79791
kJ	92	GLU	ALA	engineered mutation	UNP Q79791
kK	92	GLU	ALA	engineered mutation	UNP Q79791
kL	92	GLU	ALA	engineered mutation	UNP Q79791
kM	92	GLU	ALA	engineered mutation	UNP Q79791
kN	92	GLU	ALA	engineered mutation	UNP Q79791
24	92	GLU	ALA	engineered mutation	UNP Q79791
kO	92	GLU	ALA	engineered mutation	UNP Q79791
kP	92	GLU	ALA	engineered mutation	UNP Q79791
kQ	92	GLU	ALA	engineered mutation	UNP Q79791
kR	92	GLU	ALA	engineered mutation	UNP Q79791
kS	92	GLU	ALA	engineered mutation	UNP Q79791
kT	92	GLU	ALA	engineered mutation	UNP Q79791
kU	92	GLU	ALA	engineered mutation	UNP Q79791
kV	92	GLU	ALA	engineered mutation	UNP Q79791
kW	92	GLU	ALA	engineered mutation	UNP Q79791
kX	92	GLU	ALA	engineered mutation	UNP Q79791
25	92	GLU	ALA	engineered mutation	UNP Q79791
kY	92	GLU	ALA	engineered mutation	UNP Q79791
kZ	92	GLU	ALA	engineered mutation	UNP Q79791
10	92	GLU	ALA	engineered mutation	UNP Q79791
11	92	GLU	ALA	engineered mutation	UNP Q79791
12	92	GLU	ALA	engineered mutation	UNP Q79791
13	92	GLU	ALA	engineered mutation	UNP Q79791
14	92	GLU	ALA	engineered mutation	UNP Q79791
15	92	GLU	ALA	engineered mutation	UNP Q79791
16	92	GLU	ALA	engineered mutation	UNP Q79791
17	92	GLU	ALA	engineered mutation	UNP Q79791
26	92	GLU	ALA	engineered mutation	UNP Q79791
18	92	GLU	ALA	engineered mutation	UNP Q79791
19	92	GLU	ALA	engineered mutation	UNP Q79791

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Chain	Residue	Modelled	Actual	Comment	Reference
la	92	GLU	ALA	engineered mutation	UNP Q79791
lb	92	GLU	ALA	engineered mutation	UNP Q79791
lc	92	GLU	ALA	engineered mutation	UNP Q79791
ld	92	GLU	ALA	engineered mutation	UNP Q79791
le	92	GLU	ALA	engineered mutation	UNP Q79791
lf	92	GLU	ALA	engineered mutation	UNP Q79791
lg	92	GLU	ALA	engineered mutation	UNP Q79791
lh	92	GLU	ALA	engineered mutation	UNP Q79791
27	92	GLU	ALA	engineered mutation	UNP Q79791
li	92	GLU	ALA	engineered mutation	UNP Q79791
lj	92	GLU	ALA	engineered mutation	UNP Q79791
lk	92	GLU	ALA	engineered mutation	UNP Q79791
ll	92	GLU	ALA	engineered mutation	UNP Q79791
lm	92	GLU	ALA	engineered mutation	UNP Q79791
ln	92	GLU	ALA	engineered mutation	UNP Q79791
lo	92	GLU	ALA	engineered mutation	UNP Q79791
lp	92	GLU	ALA	engineered mutation	UNP Q79791
lq	92	GLU	ALA	engineered mutation	UNP Q79791
lr	92	GLU	ALA	engineered mutation	UNP Q79791
28	92	GLU	ALA	engineered mutation	UNP Q79791
ls	92	GLU	ALA	engineered mutation	UNP Q79791
lt	92	GLU	ALA	engineered mutation	UNP Q79791
lu	92	GLU	ALA	engineered mutation	UNP Q79791
lv	92	GLU	ALA	engineered mutation	UNP Q79791
lw	92	GLU	ALA	engineered mutation	UNP Q79791
lx	92	GLU	ALA	engineered mutation	UNP Q79791
ly	92	GLU	ALA	engineered mutation	UNP Q79791
lz	92	GLU	ALA	engineered mutation	UNP Q79791
lA	92	GLU	ALA	engineered mutation	UNP Q79791
lB	92	GLU	ALA	engineered mutation	UNP Q79791
29	92	GLU	ALA	engineered mutation	UNP Q79791
lC	92	GLU	ALA	engineered mutation	UNP Q79791
lD	92	GLU	ALA	engineered mutation	UNP Q79791
lE	92	GLU	ALA	engineered mutation	UNP Q79791
lF	92	GLU	ALA	engineered mutation	UNP Q79791
lG	92	GLU	ALA	engineered mutation	UNP Q79791
lH	92	GLU	ALA	engineered mutation	UNP Q79791
lI	92	GLU	ALA	engineered mutation	UNP Q79791
lJ	92	GLU	ALA	engineered mutation	UNP Q79791
lK	92	GLU	ALA	engineered mutation	UNP Q79791
lL	92	GLU	ALA	engineered mutation	UNP Q79791
2a	92	GLU	ALA	engineered mutation	UNP Q79791

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Chain	Residue	Modelled	Actual	Comment	Reference
1M	92	GLU	ALA	engineered mutation	UNP Q79791
1N	92	GLU	ALA	engineered mutation	UNP Q79791
1O	92	GLU	ALA	engineered mutation	UNP Q79791
1P	92	GLU	ALA	engineered mutation	UNP Q79791
1Q	92	GLU	ALA	engineered mutation	UNP Q79791
1R	92	GLU	ALA	engineered mutation	UNP Q79791
2b	92	GLU	ALA	engineered mutation	UNP Q79791
2c	92	GLU	ALA	engineered mutation	UNP Q79791
2d	92	GLU	ALA	engineered mutation	UNP Q79791
2e	92	GLU	ALA	engineered mutation	UNP Q79791
2f	92	GLU	ALA	engineered mutation	UNP Q79791
2g	92	GLU	ALA	engineered mutation	UNP Q79791
2h	92	GLU	ALA	engineered mutation	UNP Q79791
2i	92	GLU	ALA	engineered mutation	UNP Q79791
2j	92	GLU	ALA	engineered mutation	UNP Q79791
2k	92	GLU	ALA	engineered mutation	UNP Q79791
2l	92	GLU	ALA	engineered mutation	UNP Q79791
2m	92	GLU	ALA	engineered mutation	UNP Q79791
2n	92	GLU	ALA	engineered mutation	UNP Q79791
2o	92	GLU	ALA	engineered mutation	UNP Q79791
2p	92	GLU	ALA	engineered mutation	UNP Q79791
2q	92	GLU	ALA	engineered mutation	UNP Q79791
2r	92	GLU	ALA	engineered mutation	UNP Q79791
2s	92	GLU	ALA	engineered mutation	UNP Q79791
2t	92	GLU	ALA	engineered mutation	UNP Q79791
2u	92	GLU	ALA	engineered mutation	UNP Q79791
2v	92	GLU	ALA	engineered mutation	UNP Q79791
2w	92	GLU	ALA	engineered mutation	UNP Q79791
2x	92	GLU	ALA	engineered mutation	UNP Q79791
2y	92	GLU	ALA	engineered mutation	UNP Q79791
2z	92	GLU	ALA	engineered mutation	UNP Q79791
2A	92	GLU	ALA	engineered mutation	UNP Q79791
2B	92	GLU	ALA	engineered mutation	UNP Q79791
2C	92	GLU	ALA	engineered mutation	UNP Q79791
2D	92	GLU	ALA	engineered mutation	UNP Q79791
2E	92	GLU	ALA	engineered mutation	UNP Q79791
2F	92	GLU	ALA	engineered mutation	UNP Q79791
2G	92	GLU	ALA	engineered mutation	UNP Q79791
2H	92	GLU	ALA	engineered mutation	UNP Q79791
2I	92	GLU	ALA	engineered mutation	UNP Q79791
2J	92	GLU	ALA	engineered mutation	UNP Q79791
2K	92	GLU	ALA	engineered mutation	UNP Q79791

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Chain	Residue	Modelled	Actual	Comment	Reference
2L	92	GLU	ALA	engineered mutation	UNP Q79791
2M	92	GLU	ALA	engineered mutation	UNP Q79791
2N	92	GLU	ALA	engineered mutation	UNP Q79791
2O	92	GLU	ALA	engineered mutation	UNP Q79791
2P	92	GLU	ALA	engineered mutation	UNP Q79791
2Q	92	GLU	ALA	engineered mutation	UNP Q79791
2R	92	GLU	ALA	engineered mutation	UNP Q79791
2S	92	GLU	ALA	engineered mutation	UNP Q79791
2T	92	GLU	ALA	engineered mutation	UNP Q79791
2U	92	GLU	ALA	engineered mutation	UNP Q79791
2V	92	GLU	ALA	engineered mutation	UNP Q79791
2W	92	GLU	ALA	engineered mutation	UNP Q79791
2X	92	GLU	ALA	engineered mutation	UNP Q79791
2Y	92	GLU	ALA	engineered mutation	UNP Q79791
2Z	92	GLU	ALA	engineered mutation	UNP Q79791
30	92	GLU	ALA	engineered mutation	UNP Q79791
31	92	GLU	ALA	engineered mutation	UNP Q79791
32	92	GLU	ALA	engineered mutation	UNP Q79791
33	92	GLU	ALA	engineered mutation	UNP Q79791
34	92	GLU	ALA	engineered mutation	UNP Q79791
35	92	GLU	ALA	engineered mutation	UNP Q79791
36	92	GLU	ALA	engineered mutation	UNP Q79791
37	92	GLU	ALA	engineered mutation	UNP Q79791
38	92	GLU	ALA	engineered mutation	UNP Q79791
39	92	GLU	ALA	engineered mutation	UNP Q79791
3a	92	GLU	ALA	engineered mutation	UNP Q79791
3b	92	GLU	ALA	engineered mutation	UNP Q79791
3c	92	GLU	ALA	engineered mutation	UNP Q79791
3d	92	GLU	ALA	engineered mutation	UNP Q79791
3e	92	GLU	ALA	engineered mutation	UNP Q79791
3f	92	GLU	ALA	engineered mutation	UNP Q79791
3g	92	GLU	ALA	engineered mutation	UNP Q79791
3h	92	GLU	ALA	engineered mutation	UNP Q79791
3i	92	GLU	ALA	engineered mutation	UNP Q79791
3j	92	GLU	ALA	engineered mutation	UNP Q79791
3k	92	GLU	ALA	engineered mutation	UNP Q79791
3l	92	GLU	ALA	engineered mutation	UNP Q79791
3m	92	GLU	ALA	engineered mutation	UNP Q79791
3n	92	GLU	ALA	engineered mutation	UNP Q79791
3o	92	GLU	ALA	engineered mutation	UNP Q79791
3p	92	GLU	ALA	engineered mutation	UNP Q79791
3q	92	GLU	ALA	engineered mutation	UNP Q79791

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Chain	Residue	Modelled	Actual	Comment	Reference
3r	92	GLU	ALA	engineered mutation	UNP Q79791
3s	92	GLU	ALA	engineered mutation	UNP Q79791
3t	92	GLU	ALA	engineered mutation	UNP Q79791
3u	92	GLU	ALA	engineered mutation	UNP Q79791
3v	92	GLU	ALA	engineered mutation	UNP Q79791
3w	92	GLU	ALA	engineered mutation	UNP Q79791
3x	92	GLU	ALA	engineered mutation	UNP Q79791
3y	92	GLU	ALA	engineered mutation	UNP Q79791
3z	92	GLU	ALA	engineered mutation	UNP Q79791
3A	92	GLU	ALA	engineered mutation	UNP Q79791
3B	92	GLU	ALA	engineered mutation	UNP Q79791
3C	92	GLU	ALA	engineered mutation	UNP Q79791
3D	92	GLU	ALA	engineered mutation	UNP Q79791
3E	92	GLU	ALA	engineered mutation	UNP Q79791
3F	92	GLU	ALA	engineered mutation	UNP Q79791
3G	92	GLU	ALA	engineered mutation	UNP Q79791
3H	92	GLU	ALA	engineered mutation	UNP Q79791
3I	92	GLU	ALA	engineered mutation	UNP Q79791
3J	92	GLU	ALA	engineered mutation	UNP Q79791
3K	92	GLU	ALA	engineered mutation	UNP Q79791
3L	92	GLU	ALA	engineered mutation	UNP Q79791
3M	92	GLU	ALA	engineered mutation	UNP Q79791
3N	92	GLU	ALA	engineered mutation	UNP Q79791
3O	92	GLU	ALA	engineered mutation	UNP Q79791
3P	92	GLU	ALA	engineered mutation	UNP Q79791
3Q	92	GLU	ALA	engineered mutation	UNP Q79791
3R	92	GLU	ALA	engineered mutation	UNP Q79791
3S	92	GLU	ALA	engineered mutation	UNP Q79791
3T	92	GLU	ALA	engineered mutation	UNP Q79791
3U	92	GLU	ALA	engineered mutation	UNP Q79791
3V	92	GLU	ALA	engineered mutation	UNP Q79791
3W	92	GLU	ALA	engineered mutation	UNP Q79791
3X	92	GLU	ALA	engineered mutation	UNP Q79791
3Y	92	GLU	ALA	engineered mutation	UNP Q79791
3Z	92	GLU	ALA	engineered mutation	UNP Q79791
40	92	GLU	ALA	engineered mutation	UNP Q79791
41	92	GLU	ALA	engineered mutation	UNP Q79791
42	92	GLU	ALA	engineered mutation	UNP Q79791
43	92	GLU	ALA	engineered mutation	UNP Q79791
44	92	GLU	ALA	engineered mutation	UNP Q79791
45	92	GLU	ALA	engineered mutation	UNP Q79791
46	92	GLU	ALA	engineered mutation	UNP Q79791

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Chain	Residue	Modelled	Actual	Comment	Reference
47	92	GLU	ALA	engineered mutation	UNP Q79791
48	92	GLU	ALA	engineered mutation	UNP Q79791
49	92	GLU	ALA	engineered mutation	UNP Q79791
4a	92	GLU	ALA	engineered mutation	UNP Q79791
4b	92	GLU	ALA	engineered mutation	UNP Q79791
4c	92	GLU	ALA	engineered mutation	UNP Q79791
4d	92	GLU	ALA	engineered mutation	UNP Q79791
4e	92	GLU	ALA	engineered mutation	UNP Q79791
4f	92	GLU	ALA	engineered mutation	UNP Q79791
4g	92	GLU	ALA	engineered mutation	UNP Q79791
4h	92	GLU	ALA	engineered mutation	UNP Q79791
4i	92	GLU	ALA	engineered mutation	UNP Q79791
4j	92	GLU	ALA	engineered mutation	UNP Q79791
4k	92	GLU	ALA	engineered mutation	UNP Q79791
4l	92	GLU	ALA	engineered mutation	UNP Q79791
4m	92	GLU	ALA	engineered mutation	UNP Q79791
4n	92	GLU	ALA	engineered mutation	UNP Q79791
4o	92	GLU	ALA	engineered mutation	UNP Q79791
4p	92	GLU	ALA	engineered mutation	UNP Q79791
4q	92	GLU	ALA	engineered mutation	UNP Q79791
4r	92	GLU	ALA	engineered mutation	UNP Q79791
4s	92	GLU	ALA	engineered mutation	UNP Q79791
4t	92	GLU	ALA	engineered mutation	UNP Q79791
4u	92	GLU	ALA	engineered mutation	UNP Q79791
4v	92	GLU	ALA	engineered mutation	UNP Q79791
4w	92	GLU	ALA	engineered mutation	UNP Q79791
4x	92	GLU	ALA	engineered mutation	UNP Q79791
4y	92	GLU	ALA	engineered mutation	UNP Q79791
4z	92	GLU	ALA	engineered mutation	UNP Q79791
4A	92	GLU	ALA	engineered mutation	UNP Q79791
4B	92	GLU	ALA	engineered mutation	UNP Q79791
4C	92	GLU	ALA	engineered mutation	UNP Q79791
4D	92	GLU	ALA	engineered mutation	UNP Q79791
4E	92	GLU	ALA	engineered mutation	UNP Q79791
4F	92	GLU	ALA	engineered mutation	UNP Q79791
4G	92	GLU	ALA	engineered mutation	UNP Q79791
4H	92	GLU	ALA	engineered mutation	UNP Q79791
4I	92	GLU	ALA	engineered mutation	UNP Q79791
4J	92	GLU	ALA	engineered mutation	UNP Q79791
4K	92	GLU	ALA	engineered mutation	UNP Q79791
4L	92	GLU	ALA	engineered mutation	UNP Q79791
4M	92	GLU	ALA	engineered mutation	UNP Q79791

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Chain	Residue	Modelled	Actual	Comment	Reference
4N	92	GLU	ALA	engineered mutation	UNP Q79791
4O	92	GLU	ALA	engineered mutation	UNP Q79791
4P	92	GLU	ALA	engineered mutation	UNP Q79791
4Q	92	GLU	ALA	engineered mutation	UNP Q79791
4R	92	GLU	ALA	engineered mutation	UNP Q79791
4S	92	GLU	ALA	engineered mutation	UNP Q79791
4T	92	GLU	ALA	engineered mutation	UNP Q79791
4U	92	GLU	ALA	engineered mutation	UNP Q79791
4V	92	GLU	ALA	engineered mutation	UNP Q79791
4W	92	GLU	ALA	engineered mutation	UNP Q79791
4X	92	GLU	ALA	engineered mutation	UNP Q79791
4Y	92	GLU	ALA	engineered mutation	UNP Q79791
4Z	92	GLU	ALA	engineered mutation	UNP Q79791
50	92	GLU	ALA	engineered mutation	UNP Q79791
51	92	GLU	ALA	engineered mutation	UNP Q79791
52	92	GLU	ALA	engineered mutation	UNP Q79791
53	92	GLU	ALA	engineered mutation	UNP Q79791
54	92	GLU	ALA	engineered mutation	UNP Q79791
55	92	GLU	ALA	engineered mutation	UNP Q79791
56	92	GLU	ALA	engineered mutation	UNP Q79791
57	92	GLU	ALA	engineered mutation	UNP Q79791
58	92	GLU	ALA	engineered mutation	UNP Q79791
59	92	GLU	ALA	engineered mutation	UNP Q79791
5a	92	GLU	ALA	engineered mutation	UNP Q79791
5b	92	GLU	ALA	engineered mutation	UNP Q79791
5c	92	GLU	ALA	engineered mutation	UNP Q79791
5d	92	GLU	ALA	engineered mutation	UNP Q79791
5e	92	GLU	ALA	engineered mutation	UNP Q79791
5f	92	GLU	ALA	engineered mutation	UNP Q79791
5g	92	GLU	ALA	engineered mutation	UNP Q79791
5h	92	GLU	ALA	engineered mutation	UNP Q79791
5i	92	GLU	ALA	engineered mutation	UNP Q79791
5j	92	GLU	ALA	engineered mutation	UNP Q79791
5k	92	GLU	ALA	engineered mutation	UNP Q79791
5l	92	GLU	ALA	engineered mutation	UNP Q79791
5m	92	GLU	ALA	engineered mutation	UNP Q79791
5n	92	GLU	ALA	engineered mutation	UNP Q79791
5o	92	GLU	ALA	engineered mutation	UNP Q79791
5p	92	GLU	ALA	engineered mutation	UNP Q79791
5q	92	GLU	ALA	engineered mutation	UNP Q79791
5r	92	GLU	ALA	engineered mutation	UNP Q79791
5s	92	GLU	ALA	engineered mutation	UNP Q79791

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Chain	Residue	Modelled	Actual	Comment	Reference
5t	92	GLU	ALA	engineered mutation	UNP Q79791
5u	92	GLU	ALA	engineered mutation	UNP Q79791
5v	92	GLU	ALA	engineered mutation	UNP Q79791
5w	92	GLU	ALA	engineered mutation	UNP Q79791
5x	92	GLU	ALA	engineered mutation	UNP Q79791
5y	92	GLU	ALA	engineered mutation	UNP Q79791
5z	92	GLU	ALA	engineered mutation	UNP Q79791
5A	92	GLU	ALA	engineered mutation	UNP Q79791
5B	92	GLU	ALA	engineered mutation	UNP Q79791
5C	92	GLU	ALA	engineered mutation	UNP Q79791
5D	92	GLU	ALA	engineered mutation	UNP Q79791
5E	92	GLU	ALA	engineered mutation	UNP Q79791
5F	92	GLU	ALA	engineered mutation	UNP Q79791
5G	92	GLU	ALA	engineered mutation	UNP Q79791
5H	92	GLU	ALA	engineered mutation	UNP Q79791
5I	92	GLU	ALA	engineered mutation	UNP Q79791
5J	92	GLU	ALA	engineered mutation	UNP Q79791
5K	92	GLU	ALA	engineered mutation	UNP Q79791
5L	92	GLU	ALA	engineered mutation	UNP Q79791
5M	92	GLU	ALA	engineered mutation	UNP Q79791
5N	92	GLU	ALA	engineered mutation	UNP Q79791
5O	92	GLU	ALA	engineered mutation	UNP Q79791
5P	92	GLU	ALA	engineered mutation	UNP Q79791
5Q	92	GLU	ALA	engineered mutation	UNP Q79791
5R	92	GLU	ALA	engineered mutation	UNP Q79791
5S	92	GLU	ALA	engineered mutation	UNP Q79791
5T	92	GLU	ALA	engineered mutation	UNP Q79791
5U	92	GLU	ALA	engineered mutation	UNP Q79791
5V	92	GLU	ALA	engineered mutation	UNP Q79791
5W	92	GLU	ALA	engineered mutation	UNP Q79791
5X	92	GLU	ALA	engineered mutation	UNP Q79791
5Y	92	GLU	ALA	engineered mutation	UNP Q79791
5Z	92	GLU	ALA	engineered mutation	UNP Q79791
60	92	GLU	ALA	engineered mutation	UNP Q79791
61	92	GLU	ALA	engineered mutation	UNP Q79791
62	92	GLU	ALA	engineered mutation	UNP Q79791
63	92	GLU	ALA	engineered mutation	UNP Q79791
64	92	GLU	ALA	engineered mutation	UNP Q79791
65	92	GLU	ALA	engineered mutation	UNP Q79791
66	92	GLU	ALA	engineered mutation	UNP Q79791
67	92	GLU	ALA	engineered mutation	UNP Q79791
68	92	GLU	ALA	engineered mutation	UNP Q79791

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Chain	Residue	Modelled	Actual	Comment	Reference
69	92	GLU	ALA	engineered mutation	UNP Q79791
6a	92	GLU	ALA	engineered mutation	UNP Q79791
6b	92	GLU	ALA	engineered mutation	UNP Q79791
6c	92	GLU	ALA	engineered mutation	UNP Q79791
6d	92	GLU	ALA	engineered mutation	UNP Q79791
6e	92	GLU	ALA	engineered mutation	UNP Q79791
6f	92	GLU	ALA	engineered mutation	UNP Q79791
6g	92	GLU	ALA	engineered mutation	UNP Q79791
6h	92	GLU	ALA	engineered mutation	UNP Q79791
6i	92	GLU	ALA	engineered mutation	UNP Q79791
6j	92	GLU	ALA	engineered mutation	UNP Q79791
6k	92	GLU	ALA	engineered mutation	UNP Q79791
6l	92	GLU	ALA	engineered mutation	UNP Q79791
6m	92	GLU	ALA	engineered mutation	UNP Q79791
6n	92	GLU	ALA	engineered mutation	UNP Q79791
6o	92	GLU	ALA	engineered mutation	UNP Q79791
6p	92	GLU	ALA	engineered mutation	UNP Q79791
6q	92	GLU	ALA	engineered mutation	UNP Q79791
6r	92	GLU	ALA	engineered mutation	UNP Q79791
6s	92	GLU	ALA	engineered mutation	UNP Q79791
6t	92	GLU	ALA	engineered mutation	UNP Q79791
6u	92	GLU	ALA	engineered mutation	UNP Q79791
6v	92	GLU	ALA	engineered mutation	UNP Q79791
6w	92	GLU	ALA	engineered mutation	UNP Q79791
6x	92	GLU	ALA	engineered mutation	UNP Q79791
6y	92	GLU	ALA	engineered mutation	UNP Q79791
6z	92	GLU	ALA	engineered mutation	UNP Q79791
6A	92	GLU	ALA	engineered mutation	UNP Q79791
6B	92	GLU	ALA	engineered mutation	UNP Q79791
6C	92	GLU	ALA	engineered mutation	UNP Q79791
6D	92	GLU	ALA	engineered mutation	UNP Q79791
6E	92	GLU	ALA	engineered mutation	UNP Q79791
6F	92	GLU	ALA	engineered mutation	UNP Q79791
6G	92	GLU	ALA	engineered mutation	UNP Q79791
6H	92	GLU	ALA	engineered mutation	UNP Q79791
6I	92	GLU	ALA	engineered mutation	UNP Q79791
6J	92	GLU	ALA	engineered mutation	UNP Q79791
6K	92	GLU	ALA	engineered mutation	UNP Q79791
6L	92	GLU	ALA	engineered mutation	UNP Q79791
6M	92	GLU	ALA	engineered mutation	UNP Q79791
6N	92	GLU	ALA	engineered mutation	UNP Q79791
6O	92	GLU	ALA	engineered mutation	UNP Q79791

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Chain	Residue	Modelled	Actual	Comment	Reference
6P	92	GLU	ALA	engineered mutation	UNP Q79791
6Q	92	GLU	ALA	engineered mutation	UNP Q79791
6R	92	GLU	ALA	engineered mutation	UNP Q79791
6S	92	GLU	ALA	engineered mutation	UNP Q79791
6T	92	GLU	ALA	engineered mutation	UNP Q79791
6U	92	GLU	ALA	engineered mutation	UNP Q79791
6V	92	GLU	ALA	engineered mutation	UNP Q79791
6W	92	GLU	ALA	engineered mutation	UNP Q79791
6X	92	GLU	ALA	engineered mutation	UNP Q79791
6Y	92	GLU	ALA	engineered mutation	UNP Q79791
6Z	92	GLU	ALA	engineered mutation	UNP Q79791
70	92	GLU	ALA	engineered mutation	UNP Q79791
71	92	GLU	ALA	engineered mutation	UNP Q79791
72	92	GLU	ALA	engineered mutation	UNP Q79791
73	92	GLU	ALA	engineered mutation	UNP Q79791
74	92	GLU	ALA	engineered mutation	UNP Q79791
75	92	GLU	ALA	engineered mutation	UNP Q79791
76	92	GLU	ALA	engineered mutation	UNP Q79791
77	92	GLU	ALA	engineered mutation	UNP Q79791
78	92	GLU	ALA	engineered mutation	UNP Q79791
79	92	GLU	ALA	engineered mutation	UNP Q79791
7a	92	GLU	ALA	engineered mutation	UNP Q79791
7b	92	GLU	ALA	engineered mutation	UNP Q79791
7c	92	GLU	ALA	engineered mutation	UNP Q79791
7d	92	GLU	ALA	engineered mutation	UNP Q79791
7e	92	GLU	ALA	engineered mutation	UNP Q79791
7f	92	GLU	ALA	engineered mutation	UNP Q79791
7g	92	GLU	ALA	engineered mutation	UNP Q79791
7h	92	GLU	ALA	engineered mutation	UNP Q79791
7i	92	GLU	ALA	engineered mutation	UNP Q79791
7j	92	GLU	ALA	engineered mutation	UNP Q79791
7k	92	GLU	ALA	engineered mutation	UNP Q79791
7l	92	GLU	ALA	engineered mutation	UNP Q79791
7m	92	GLU	ALA	engineered mutation	UNP Q79791
7n	92	GLU	ALA	engineered mutation	UNP Q79791
7o	92	GLU	ALA	engineered mutation	UNP Q79791
7p	92	GLU	ALA	engineered mutation	UNP Q79791
7q	92	GLU	ALA	engineered mutation	UNP Q79791
7r	92	GLU	ALA	engineered mutation	UNP Q79791
7s	92	GLU	ALA	engineered mutation	UNP Q79791
7t	92	GLU	ALA	engineered mutation	UNP Q79791
7u	92	GLU	ALA	engineered mutation	UNP Q79791

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Chain	Residue	Modelled	Actual	Comment	Reference
7v	92	GLU	ALA	engineered mutation	UNP Q79791
7w	92	GLU	ALA	engineered mutation	UNP Q79791
7x	92	GLU	ALA	engineered mutation	UNP Q79791
7y	92	GLU	ALA	engineered mutation	UNP Q79791
7z	92	GLU	ALA	engineered mutation	UNP Q79791
7A	92	GLU	ALA	engineered mutation	UNP Q79791
7B	92	GLU	ALA	engineered mutation	UNP Q79791
7C	92	GLU	ALA	engineered mutation	UNP Q79791
7D	92	GLU	ALA	engineered mutation	UNP Q79791
7E	92	GLU	ALA	engineered mutation	UNP Q79791
7F	92	GLU	ALA	engineered mutation	UNP Q79791
7G	92	GLU	ALA	engineered mutation	UNP Q79791
7H	92	GLU	ALA	engineered mutation	UNP Q79791
7I	92	GLU	ALA	engineered mutation	UNP Q79791
7J	92	GLU	ALA	engineered mutation	UNP Q79791
7K	92	GLU	ALA	engineered mutation	UNP Q79791
7L	92	GLU	ALA	engineered mutation	UNP Q79791
7M	92	GLU	ALA	engineered mutation	UNP Q79791
7N	92	GLU	ALA	engineered mutation	UNP Q79791
7O	92	GLU	ALA	engineered mutation	UNP Q79791
7P	92	GLU	ALA	engineered mutation	UNP Q79791
7Q	92	GLU	ALA	engineered mutation	UNP Q79791
7R	92	GLU	ALA	engineered mutation	UNP Q79791
7S	92	GLU	ALA	engineered mutation	UNP Q79791
7T	92	GLU	ALA	engineered mutation	UNP Q79791
7U	92	GLU	ALA	engineered mutation	UNP Q79791
7V	92	GLU	ALA	engineered mutation	UNP Q79791
7W	92	GLU	ALA	engineered mutation	UNP Q79791
7X	92	GLU	ALA	engineered mutation	UNP Q79791
7Y	92	GLU	ALA	engineered mutation	UNP Q79791
7Z	92	GLU	ALA	engineered mutation	UNP Q79791
80	92	GLU	ALA	engineered mutation	UNP Q79791
81	92	GLU	ALA	engineered mutation	UNP Q79791
82	92	GLU	ALA	engineered mutation	UNP Q79791
83	92	GLU	ALA	engineered mutation	UNP Q79791
84	92	GLU	ALA	engineered mutation	UNP Q79791
85	92	GLU	ALA	engineered mutation	UNP Q79791
86	92	GLU	ALA	engineered mutation	UNP Q79791
87	92	GLU	ALA	engineered mutation	UNP Q79791
88	92	GLU	ALA	engineered mutation	UNP Q79791
89	92	GLU	ALA	engineered mutation	UNP Q79791
8a	92	GLU	ALA	engineered mutation	UNP Q79791

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Chain	Residue	Modelled	Actual	Comment	Reference
8b	92	GLU	ALA	engineered mutation	UNP Q79791
8c	92	GLU	ALA	engineered mutation	UNP Q79791
8d	92	GLU	ALA	engineered mutation	UNP Q79791
8e	92	GLU	ALA	engineered mutation	UNP Q79791
8f	92	GLU	ALA	engineered mutation	UNP Q79791
8g	92	GLU	ALA	engineered mutation	UNP Q79791
8h	92	GLU	ALA	engineered mutation	UNP Q79791
8i	92	GLU	ALA	engineered mutation	UNP Q79791
8j	92	GLU	ALA	engineered mutation	UNP Q79791
8k	92	GLU	ALA	engineered mutation	UNP Q79791
8l	92	GLU	ALA	engineered mutation	UNP Q79791
8m	92	GLU	ALA	engineered mutation	UNP Q79791
8n	92	GLU	ALA	engineered mutation	UNP Q79791
8o	92	GLU	ALA	engineered mutation	UNP Q79791
8p	92	GLU	ALA	engineered mutation	UNP Q79791
8q	92	GLU	ALA	engineered mutation	UNP Q79791
8r	92	GLU	ALA	engineered mutation	UNP Q79791
8s	92	GLU	ALA	engineered mutation	UNP Q79791
8t	92	GLU	ALA	engineered mutation	UNP Q79791
8u	92	GLU	ALA	engineered mutation	UNP Q79791
8v	92	GLU	ALA	engineered mutation	UNP Q79791
8w	92	GLU	ALA	engineered mutation	UNP Q79791
8x	92	GLU	ALA	engineered mutation	UNP Q79791
8y	92	GLU	ALA	engineered mutation	UNP Q79791
8z	92	GLU	ALA	engineered mutation	UNP Q79791
8A	92	GLU	ALA	engineered mutation	UNP Q79791
8B	92	GLU	ALA	engineered mutation	UNP Q79791
8C	92	GLU	ALA	engineered mutation	UNP Q79791
8D	92	GLU	ALA	engineered mutation	UNP Q79791
8E	92	GLU	ALA	engineered mutation	UNP Q79791
8F	92	GLU	ALA	engineered mutation	UNP Q79791
8G	92	GLU	ALA	engineered mutation	UNP Q79791
8H	92	GLU	ALA	engineered mutation	UNP Q79791
8I	92	GLU	ALA	engineered mutation	UNP Q79791
8J	92	GLU	ALA	engineered mutation	UNP Q79791
8K	92	GLU	ALA	engineered mutation	UNP Q79791
8L	92	GLU	ALA	engineered mutation	UNP Q79791
8M	92	GLU	ALA	engineered mutation	UNP Q79791
8N	92	GLU	ALA	engineered mutation	UNP Q79791
8O	92	GLU	ALA	engineered mutation	UNP Q79791
8P	92	GLU	ALA	engineered mutation	UNP Q79791
8Q	92	GLU	ALA	engineered mutation	UNP Q79791

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Chain	Residue	Modelled	Actual	Comment	Reference
8R	92	GLU	ALA	engineered mutation	UNP Q79791
8S	92	GLU	ALA	engineered mutation	UNP Q79791
8T	92	GLU	ALA	engineered mutation	UNP Q79791
8U	92	GLU	ALA	engineered mutation	UNP Q79791
8V	92	GLU	ALA	engineered mutation	UNP Q79791
8W	92	GLU	ALA	engineered mutation	UNP Q79791
8X	92	GLU	ALA	engineered mutation	UNP Q79791
8Y	92	GLU	ALA	engineered mutation	UNP Q79791
8Z	92	GLU	ALA	engineered mutation	UNP Q79791
90	92	GLU	ALA	engineered mutation	UNP Q79791
91	92	GLU	ALA	engineered mutation	UNP Q79791
92	92	GLU	ALA	engineered mutation	UNP Q79791
93	92	GLU	ALA	engineered mutation	UNP Q79791
94	92	GLU	ALA	engineered mutation	UNP Q79791
95	92	GLU	ALA	engineered mutation	UNP Q79791
96	92	GLU	ALA	engineered mutation	UNP Q79791
97	92	GLU	ALA	engineered mutation	UNP Q79791
98	92	GLU	ALA	engineered mutation	UNP Q79791
99	92	GLU	ALA	engineered mutation	UNP Q79791
9a	92	GLU	ALA	engineered mutation	UNP Q79791
9b	92	GLU	ALA	engineered mutation	UNP Q79791
9c	92	GLU	ALA	engineered mutation	UNP Q79791
9d	92	GLU	ALA	engineered mutation	UNP Q79791
9e	92	GLU	ALA	engineered mutation	UNP Q79791
9f	92	GLU	ALA	engineered mutation	UNP Q79791
9g	92	GLU	ALA	engineered mutation	UNP Q79791
9h	92	GLU	ALA	engineered mutation	UNP Q79791
9i	92	GLU	ALA	engineered mutation	UNP Q79791
9j	92	GLU	ALA	engineered mutation	UNP Q79791
9k	92	GLU	ALA	engineered mutation	UNP Q79791
9l	92	GLU	ALA	engineered mutation	UNP Q79791
9m	92	GLU	ALA	engineered mutation	UNP Q79791
9n	92	GLU	ALA	engineered mutation	UNP Q79791
9o	92	GLU	ALA	engineered mutation	UNP Q79791
9p	92	GLU	ALA	engineered mutation	UNP Q79791
9q	92	GLU	ALA	engineered mutation	UNP Q79791
9r	92	GLU	ALA	engineered mutation	UNP Q79791
9s	92	GLU	ALA	engineered mutation	UNP Q79791
9t	92	GLU	ALA	engineered mutation	UNP Q79791
9u	92	GLU	ALA	engineered mutation	UNP Q79791
9v	92	GLU	ALA	engineered mutation	UNP Q79791
9w	92	GLU	ALA	engineered mutation	UNP Q79791

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Chain	Residue	Modelled	Actual	Comment	Reference
9x	92	GLU	ALA	engineered mutation	UNP Q79791
9y	92	GLU	ALA	engineered mutation	UNP Q79791
9z	92	GLU	ALA	engineered mutation	UNP Q79791
9A	92	GLU	ALA	engineered mutation	UNP Q79791
9B	92	GLU	ALA	engineered mutation	UNP Q79791
9C	92	GLU	ALA	engineered mutation	UNP Q79791
9D	92	GLU	ALA	engineered mutation	UNP Q79791
9E	92	GLU	ALA	engineered mutation	UNP Q79791
9F	92	GLU	ALA	engineered mutation	UNP Q79791
9G	92	GLU	ALA	engineered mutation	UNP Q79791
9H	92	GLU	ALA	engineered mutation	UNP Q79791
9I	92	GLU	ALA	engineered mutation	UNP Q79791
9J	92	GLU	ALA	engineered mutation	UNP Q79791
9K	92	GLU	ALA	engineered mutation	UNP Q79791
9L	92	GLU	ALA	engineered mutation	UNP Q79791
9M	92	GLU	ALA	engineered mutation	UNP Q79791
9N	92	GLU	ALA	engineered mutation	UNP Q79791
9O	92	GLU	ALA	engineered mutation	UNP Q79791
9P	92	GLU	ALA	engineered mutation	UNP Q79791
Y	92	GLU	ALA	engineered mutation	UNP Q79791
9Q	92	GLU	ALA	engineered mutation	UNP Q79791
9R	92	GLU	ALA	engineered mutation	UNP Q79791
9S	92	GLU	ALA	engineered mutation	UNP Q79791
9T	92	GLU	ALA	engineered mutation	UNP Q79791
9U	92	GLU	ALA	engineered mutation	UNP Q79791
9V	92	GLU	ALA	engineered mutation	UNP Q79791
9W	92	GLU	ALA	engineered mutation	UNP Q79791
9X	92	GLU	ALA	engineered mutation	UNP Q79791
9Y	92	GLU	ALA	engineered mutation	UNP Q79791
9Z	92	GLU	ALA	engineered mutation	UNP Q79791
Z	92	GLU	ALA	engineered mutation	UNP Q79791
a0	92	GLU	ALA	engineered mutation	UNP Q79791
a1	92	GLU	ALA	engineered mutation	UNP Q79791
a2	92	GLU	ALA	engineered mutation	UNP Q79791
a3	92	GLU	ALA	engineered mutation	UNP Q79791
a4	92	GLU	ALA	engineered mutation	UNP Q79791
a5	92	GLU	ALA	engineered mutation	UNP Q79791
a6	92	GLU	ALA	engineered mutation	UNP Q79791
a7	92	GLU	ALA	engineered mutation	UNP Q79791
a8	92	GLU	ALA	engineered mutation	UNP Q79791
a9	92	GLU	ALA	engineered mutation	UNP Q79791
10	92	GLU	ALA	engineered mutation	UNP Q79791

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Chain	Residue	Modelled	Actual	Comment	Reference
aa	92	GLU	ALA	engineered mutation	UNP Q79791
ab	92	GLU	ALA	engineered mutation	UNP Q79791
ac	92	GLU	ALA	engineered mutation	UNP Q79791
ad	92	GLU	ALA	engineered mutation	UNP Q79791
ae	92	GLU	ALA	engineered mutation	UNP Q79791
af	92	GLU	ALA	engineered mutation	UNP Q79791
ag	92	GLU	ALA	engineered mutation	UNP Q79791
ah	92	GLU	ALA	engineered mutation	UNP Q79791
ai	92	GLU	ALA	engineered mutation	UNP Q79791
aj	92	GLU	ALA	engineered mutation	UNP Q79791
11	92	GLU	ALA	engineered mutation	UNP Q79791
ak	92	GLU	ALA	engineered mutation	UNP Q79791
al	92	GLU	ALA	engineered mutation	UNP Q79791
am	92	GLU	ALA	engineered mutation	UNP Q79791
an	92	GLU	ALA	engineered mutation	UNP Q79791
ao	92	GLU	ALA	engineered mutation	UNP Q79791
ap	92	GLU	ALA	engineered mutation	UNP Q79791
aq	92	GLU	ALA	engineered mutation	UNP Q79791
ar	92	GLU	ALA	engineered mutation	UNP Q79791
as	92	GLU	ALA	engineered mutation	UNP Q79791
at	92	GLU	ALA	engineered mutation	UNP Q79791
12	92	GLU	ALA	engineered mutation	UNP Q79791
au	92	GLU	ALA	engineered mutation	UNP Q79791
av	92	GLU	ALA	engineered mutation	UNP Q79791
aw	92	GLU	ALA	engineered mutation	UNP Q79791
ax	92	GLU	ALA	engineered mutation	UNP Q79791
ay	92	GLU	ALA	engineered mutation	UNP Q79791
az	92	GLU	ALA	engineered mutation	UNP Q79791
aA	92	GLU	ALA	engineered mutation	UNP Q79791
aB	92	GLU	ALA	engineered mutation	UNP Q79791
aC	92	GLU	ALA	engineered mutation	UNP Q79791
aD	92	GLU	ALA	engineered mutation	UNP Q79791
13	92	GLU	ALA	engineered mutation	UNP Q79791
aE	92	GLU	ALA	engineered mutation	UNP Q79791
aF	92	GLU	ALA	engineered mutation	UNP Q79791
aG	92	GLU	ALA	engineered mutation	UNP Q79791
aH	92	GLU	ALA	engineered mutation	UNP Q79791
aI	92	GLU	ALA	engineered mutation	UNP Q79791
aJ	92	GLU	ALA	engineered mutation	UNP Q79791
aK	92	GLU	ALA	engineered mutation	UNP Q79791
aL	92	GLU	ALA	engineered mutation	UNP Q79791
aM	92	GLU	ALA	engineered mutation	UNP Q79791

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Chain	Residue	Modelled	Actual	Comment	Reference
aN	92	GLU	ALA	engineered mutation	UNP Q79791
14	92	GLU	ALA	engineered mutation	UNP Q79791
aO	92	GLU	ALA	engineered mutation	UNP Q79791
aP	92	GLU	ALA	engineered mutation	UNP Q79791
aQ	92	GLU	ALA	engineered mutation	UNP Q79791
aR	92	GLU	ALA	engineered mutation	UNP Q79791
aS	92	GLU	ALA	engineered mutation	UNP Q79791
aT	92	GLU	ALA	engineered mutation	UNP Q79791
aU	92	GLU	ALA	engineered mutation	UNP Q79791
aV	92	GLU	ALA	engineered mutation	UNP Q79791
aW	92	GLU	ALA	engineered mutation	UNP Q79791
aX	92	GLU	ALA	engineered mutation	UNP Q79791
15	92	GLU	ALA	engineered mutation	UNP Q79791
aY	92	GLU	ALA	engineered mutation	UNP Q79791
aZ	92	GLU	ALA	engineered mutation	UNP Q79791
b0	92	GLU	ALA	engineered mutation	UNP Q79791
b1	92	GLU	ALA	engineered mutation	UNP Q79791
b2	92	GLU	ALA	engineered mutation	UNP Q79791
b3	92	GLU	ALA	engineered mutation	UNP Q79791
b4	92	GLU	ALA	engineered mutation	UNP Q79791
b5	92	GLU	ALA	engineered mutation	UNP Q79791
b6	92	GLU	ALA	engineered mutation	UNP Q79791
b7	92	GLU	ALA	engineered mutation	UNP Q79791
16	92	GLU	ALA	engineered mutation	UNP Q79791
b8	92	GLU	ALA	engineered mutation	UNP Q79791
b9	92	GLU	ALA	engineered mutation	UNP Q79791
ba	92	GLU	ALA	engineered mutation	UNP Q79791
bb	92	GLU	ALA	engineered mutation	UNP Q79791
bc	92	GLU	ALA	engineered mutation	UNP Q79791
bd	92	GLU	ALA	engineered mutation	UNP Q79791
be	92	GLU	ALA	engineered mutation	UNP Q79791
bf	92	GLU	ALA	engineered mutation	UNP Q79791
bg	92	GLU	ALA	engineered mutation	UNP Q79791
bh	92	GLU	ALA	engineered mutation	UNP Q79791
17	92	GLU	ALA	engineered mutation	UNP Q79791
bi	92	GLU	ALA	engineered mutation	UNP Q79791
bj	92	GLU	ALA	engineered mutation	UNP Q79791
bk	92	GLU	ALA	engineered mutation	UNP Q79791
bl	92	GLU	ALA	engineered mutation	UNP Q79791
bm	92	GLU	ALA	engineered mutation	UNP Q79791
bn	92	GLU	ALA	engineered mutation	UNP Q79791
bo	92	GLU	ALA	engineered mutation	UNP Q79791

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Chain	Residue	Modelled	Actual	Comment	Reference
bp	92	GLU	ALA	engineered mutation	UNP Q79791
bq	92	GLU	ALA	engineered mutation	UNP Q79791
br	92	GLU	ALA	engineered mutation	UNP Q79791
18	92	GLU	ALA	engineered mutation	UNP Q79791
bs	92	GLU	ALA	engineered mutation	UNP Q79791
bt	92	GLU	ALA	engineered mutation	UNP Q79791
bu	92	GLU	ALA	engineered mutation	UNP Q79791
bv	92	GLU	ALA	engineered mutation	UNP Q79791
bw	92	GLU	ALA	engineered mutation	UNP Q79791
bx	92	GLU	ALA	engineered mutation	UNP Q79791
by	92	GLU	ALA	engineered mutation	UNP Q79791
bz	92	GLU	ALA	engineered mutation	UNP Q79791
bA	92	GLU	ALA	engineered mutation	UNP Q79791
bB	92	GLU	ALA	engineered mutation	UNP Q79791
19	92	GLU	ALA	engineered mutation	UNP Q79791
bC	92	GLU	ALA	engineered mutation	UNP Q79791
bD	92	GLU	ALA	engineered mutation	UNP Q79791
bE	92	GLU	ALA	engineered mutation	UNP Q79791
bF	92	GLU	ALA	engineered mutation	UNP Q79791
bG	92	GLU	ALA	engineered mutation	UNP Q79791
bH	92	GLU	ALA	engineered mutation	UNP Q79791
bI	92	GLU	ALA	engineered mutation	UNP Q79791
bJ	92	GLU	ALA	engineered mutation	UNP Q79791
bK	92	GLU	ALA	engineered mutation	UNP Q79791
bL	92	GLU	ALA	engineered mutation	UNP Q79791
1a	92	GLU	ALA	engineered mutation	UNP Q79791
bM	92	GLU	ALA	engineered mutation	UNP Q79791
bN	92	GLU	ALA	engineered mutation	UNP Q79791
bO	92	GLU	ALA	engineered mutation	UNP Q79791
bP	92	GLU	ALA	engineered mutation	UNP Q79791
bQ	92	GLU	ALA	engineered mutation	UNP Q79791
bR	92	GLU	ALA	engineered mutation	UNP Q79791
bS	92	GLU	ALA	engineered mutation	UNP Q79791
bT	92	GLU	ALA	engineered mutation	UNP Q79791
bU	92	GLU	ALA	engineered mutation	UNP Q79791
bV	92	GLU	ALA	engineered mutation	UNP Q79791
1b	92	GLU	ALA	engineered mutation	UNP Q79791
bW	92	GLU	ALA	engineered mutation	UNP Q79791
bX	92	GLU	ALA	engineered mutation	UNP Q79791
bY	92	GLU	ALA	engineered mutation	UNP Q79791
bZ	92	GLU	ALA	engineered mutation	UNP Q79791
c0	92	GLU	ALA	engineered mutation	UNP Q79791

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Chain	Residue	Modelled	Actual	Comment	Reference
c1	92	GLU	ALA	engineered mutation	UNP Q79791
c2	92	GLU	ALA	engineered mutation	UNP Q79791
c3	92	GLU	ALA	engineered mutation	UNP Q79791
c4	92	GLU	ALA	engineered mutation	UNP Q79791
c5	92	GLU	ALA	engineered mutation	UNP Q79791
1c	92	GLU	ALA	engineered mutation	UNP Q79791
c6	92	GLU	ALA	engineered mutation	UNP Q79791
c7	92	GLU	ALA	engineered mutation	UNP Q79791
c8	92	GLU	ALA	engineered mutation	UNP Q79791
c9	92	GLU	ALA	engineered mutation	UNP Q79791
ca	92	GLU	ALA	engineered mutation	UNP Q79791
cb	92	GLU	ALA	engineered mutation	UNP Q79791
cc	92	GLU	ALA	engineered mutation	UNP Q79791
cd	92	GLU	ALA	engineered mutation	UNP Q79791
ce	92	GLU	ALA	engineered mutation	UNP Q79791
cf	92	GLU	ALA	engineered mutation	UNP Q79791
1d	92	GLU	ALA	engineered mutation	UNP Q79791
cg	92	GLU	ALA	engineered mutation	UNP Q79791
ch	92	GLU	ALA	engineered mutation	UNP Q79791
ci	92	GLU	ALA	engineered mutation	UNP Q79791
cj	92	GLU	ALA	engineered mutation	UNP Q79791
ck	92	GLU	ALA	engineered mutation	UNP Q79791
cl	92	GLU	ALA	engineered mutation	UNP Q79791
cm	92	GLU	ALA	engineered mutation	UNP Q79791
cn	92	GLU	ALA	engineered mutation	UNP Q79791
co	92	GLU	ALA	engineered mutation	UNP Q79791
cp	92	GLU	ALA	engineered mutation	UNP Q79791
1e	92	GLU	ALA	engineered mutation	UNP Q79791
cq	92	GLU	ALA	engineered mutation	UNP Q79791
cr	92	GLU	ALA	engineered mutation	UNP Q79791
cs	92	GLU	ALA	engineered mutation	UNP Q79791
ct	92	GLU	ALA	engineered mutation	UNP Q79791
cu	92	GLU	ALA	engineered mutation	UNP Q79791
cv	92	GLU	ALA	engineered mutation	UNP Q79791
cw	92	GLU	ALA	engineered mutation	UNP Q79791
cx	92	GLU	ALA	engineered mutation	UNP Q79791
cy	92	GLU	ALA	engineered mutation	UNP Q79791
cz	92	GLU	ALA	engineered mutation	UNP Q79791
1f	92	GLU	ALA	engineered mutation	UNP Q79791
cA	92	GLU	ALA	engineered mutation	UNP Q79791
cB	92	GLU	ALA	engineered mutation	UNP Q79791
cC	92	GLU	ALA	engineered mutation	UNP Q79791

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Chain	Residue	Modelled	Actual	Comment	Reference
cD	92	GLU	ALA	engineered mutation	UNP Q79791
cE	92	GLU	ALA	engineered mutation	UNP Q79791
cF	92	GLU	ALA	engineered mutation	UNP Q79791
cG	92	GLU	ALA	engineered mutation	UNP Q79791
cH	92	GLU	ALA	engineered mutation	UNP Q79791
cI	92	GLU	ALA	engineered mutation	UNP Q79791
cJ	92	GLU	ALA	engineered mutation	UNP Q79791
lg	92	GLU	ALA	engineered mutation	UNP Q79791
cK	92	GLU	ALA	engineered mutation	UNP Q79791
cL	92	GLU	ALA	engineered mutation	UNP Q79791
cM	92	GLU	ALA	engineered mutation	UNP Q79791
cN	92	GLU	ALA	engineered mutation	UNP Q79791
cO	92	GLU	ALA	engineered mutation	UNP Q79791
cP	92	GLU	ALA	engineered mutation	UNP Q79791
cQ	92	GLU	ALA	engineered mutation	UNP Q79791
cR	92	GLU	ALA	engineered mutation	UNP Q79791
cS	92	GLU	ALA	engineered mutation	UNP Q79791
cT	92	GLU	ALA	engineered mutation	UNP Q79791
lh	92	GLU	ALA	engineered mutation	UNP Q79791
cU	92	GLU	ALA	engineered mutation	UNP Q79791
cV	92	GLU	ALA	engineered mutation	UNP Q79791
cW	92	GLU	ALA	engineered mutation	UNP Q79791
cX	92	GLU	ALA	engineered mutation	UNP Q79791
cY	92	GLU	ALA	engineered mutation	UNP Q79791
cZ	92	GLU	ALA	engineered mutation	UNP Q79791
d0	92	GLU	ALA	engineered mutation	UNP Q79791
d1	92	GLU	ALA	engineered mutation	UNP Q79791
d2	92	GLU	ALA	engineered mutation	UNP Q79791
d3	92	GLU	ALA	engineered mutation	UNP Q79791
li	92	GLU	ALA	engineered mutation	UNP Q79791
d4	92	GLU	ALA	engineered mutation	UNP Q79791
d5	92	GLU	ALA	engineered mutation	UNP Q79791
d6	92	GLU	ALA	engineered mutation	UNP Q79791
d7	92	GLU	ALA	engineered mutation	UNP Q79791
d8	92	GLU	ALA	engineered mutation	UNP Q79791
d9	92	GLU	ALA	engineered mutation	UNP Q79791
da	92	GLU	ALA	engineered mutation	UNP Q79791
db	92	GLU	ALA	engineered mutation	UNP Q79791
dc	92	GLU	ALA	engineered mutation	UNP Q79791
dd	92	GLU	ALA	engineered mutation	UNP Q79791
lj	92	GLU	ALA	engineered mutation	UNP Q79791
de	92	GLU	ALA	engineered mutation	UNP Q79791

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Chain	Residue	Modelled	Actual	Comment	Reference
df	92	GLU	ALA	engineered mutation	UNP Q79791
dg	92	GLU	ALA	engineered mutation	UNP Q79791
dh	92	GLU	ALA	engineered mutation	UNP Q79791
di	92	GLU	ALA	engineered mutation	UNP Q79791
dj	92	GLU	ALA	engineered mutation	UNP Q79791
dk	92	GLU	ALA	engineered mutation	UNP Q79791
dl	92	GLU	ALA	engineered mutation	UNP Q79791
dm	92	GLU	ALA	engineered mutation	UNP Q79791
dn	92	GLU	ALA	engineered mutation	UNP Q79791
lk	92	GLU	ALA	engineered mutation	UNP Q79791
do	92	GLU	ALA	engineered mutation	UNP Q79791
dp	92	GLU	ALA	engineered mutation	UNP Q79791
dq	92	GLU	ALA	engineered mutation	UNP Q79791
dr	92	GLU	ALA	engineered mutation	UNP Q79791
ds	92	GLU	ALA	engineered mutation	UNP Q79791
dt	92	GLU	ALA	engineered mutation	UNP Q79791
du	92	GLU	ALA	engineered mutation	UNP Q79791
dv	92	GLU	ALA	engineered mutation	UNP Q79791
dw	92	GLU	ALA	engineered mutation	UNP Q79791
dx	92	GLU	ALA	engineered mutation	UNP Q79791
1l	92	GLU	ALA	engineered mutation	UNP Q79791
dy	92	GLU	ALA	engineered mutation	UNP Q79791
dz	92	GLU	ALA	engineered mutation	UNP Q79791
dA	92	GLU	ALA	engineered mutation	UNP Q79791
dB	92	GLU	ALA	engineered mutation	UNP Q79791
dC	92	GLU	ALA	engineered mutation	UNP Q79791
dD	92	GLU	ALA	engineered mutation	UNP Q79791
dE	92	GLU	ALA	engineered mutation	UNP Q79791
dF	92	GLU	ALA	engineered mutation	UNP Q79791
dG	92	GLU	ALA	engineered mutation	UNP Q79791
dH	92	GLU	ALA	engineered mutation	UNP Q79791
1m	92	GLU	ALA	engineered mutation	UNP Q79791
dI	92	GLU	ALA	engineered mutation	UNP Q79791
dJ	92	GLU	ALA	engineered mutation	UNP Q79791
dK	92	GLU	ALA	engineered mutation	UNP Q79791
dL	92	GLU	ALA	engineered mutation	UNP Q79791
dM	92	GLU	ALA	engineered mutation	UNP Q79791
dN	92	GLU	ALA	engineered mutation	UNP Q79791
dO	92	GLU	ALA	engineered mutation	UNP Q79791
dP	92	GLU	ALA	engineered mutation	UNP Q79791
dQ	92	GLU	ALA	engineered mutation	UNP Q79791
dR	92	GLU	ALA	engineered mutation	UNP Q79791

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Chain	Residue	Modelled	Actual	Comment	Reference
1n	92	GLU	ALA	engineered mutation	UNP Q79791
dS	92	GLU	ALA	engineered mutation	UNP Q79791
dT	92	GLU	ALA	engineered mutation	UNP Q79791
dU	92	GLU	ALA	engineered mutation	UNP Q79791
dV	92	GLU	ALA	engineered mutation	UNP Q79791
dW	92	GLU	ALA	engineered mutation	UNP Q79791
dX	92	GLU	ALA	engineered mutation	UNP Q79791
dY	92	GLU	ALA	engineered mutation	UNP Q79791
dZ	92	GLU	ALA	engineered mutation	UNP Q79791
e0	92	GLU	ALA	engineered mutation	UNP Q79791
e1	92	GLU	ALA	engineered mutation	UNP Q79791
1o	92	GLU	ALA	engineered mutation	UNP Q79791
e2	92	GLU	ALA	engineered mutation	UNP Q79791
e3	92	GLU	ALA	engineered mutation	UNP Q79791
e4	92	GLU	ALA	engineered mutation	UNP Q79791
e5	92	GLU	ALA	engineered mutation	UNP Q79791
e6	92	GLU	ALA	engineered mutation	UNP Q79791
e7	92	GLU	ALA	engineered mutation	UNP Q79791
e8	92	GLU	ALA	engineered mutation	UNP Q79791
e9	92	GLU	ALA	engineered mutation	UNP Q79791
ea	92	GLU	ALA	engineered mutation	UNP Q79791
eb	92	GLU	ALA	engineered mutation	UNP Q79791
1p	92	GLU	ALA	engineered mutation	UNP Q79791
ec	92	GLU	ALA	engineered mutation	UNP Q79791
ed	92	GLU	ALA	engineered mutation	UNP Q79791
ee	92	GLU	ALA	engineered mutation	UNP Q79791
ef	92	GLU	ALA	engineered mutation	UNP Q79791
eg	92	GLU	ALA	engineered mutation	UNP Q79791
eh	92	GLU	ALA	engineered mutation	UNP Q79791
ei	92	GLU	ALA	engineered mutation	UNP Q79791
ej	92	GLU	ALA	engineered mutation	UNP Q79791
ek	92	GLU	ALA	engineered mutation	UNP Q79791
el	92	GLU	ALA	engineered mutation	UNP Q79791
1q	92	GLU	ALA	engineered mutation	UNP Q79791
em	92	GLU	ALA	engineered mutation	UNP Q79791
en	92	GLU	ALA	engineered mutation	UNP Q79791
eo	92	GLU	ALA	engineered mutation	UNP Q79791
ep	92	GLU	ALA	engineered mutation	UNP Q79791
eq	92	GLU	ALA	engineered mutation	UNP Q79791
er	92	GLU	ALA	engineered mutation	UNP Q79791
es	92	GLU	ALA	engineered mutation	UNP Q79791
et	92	GLU	ALA	engineered mutation	UNP Q79791

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Chain	Residue	Modelled	Actual	Comment	Reference
eu	92	GLU	ALA	engineered mutation	UNP Q79791
ev	92	GLU	ALA	engineered mutation	UNP Q79791
lr	92	GLU	ALA	engineered mutation	UNP Q79791
ew	92	GLU	ALA	engineered mutation	UNP Q79791
ex	92	GLU	ALA	engineered mutation	UNP Q79791
ey	92	GLU	ALA	engineered mutation	UNP Q79791
ez	92	GLU	ALA	engineered mutation	UNP Q79791
eA	92	GLU	ALA	engineered mutation	UNP Q79791
eB	92	GLU	ALA	engineered mutation	UNP Q79791
eC	92	GLU	ALA	engineered mutation	UNP Q79791
eD	92	GLU	ALA	engineered mutation	UNP Q79791
eE	92	GLU	ALA	engineered mutation	UNP Q79791
eF	92	GLU	ALA	engineered mutation	UNP Q79791
ls	92	GLU	ALA	engineered mutation	UNP Q79791
eG	92	GLU	ALA	engineered mutation	UNP Q79791
eH	92	GLU	ALA	engineered mutation	UNP Q79791
eI	92	GLU	ALA	engineered mutation	UNP Q79791
eJ	92	GLU	ALA	engineered mutation	UNP Q79791
eK	92	GLU	ALA	engineered mutation	UNP Q79791
eL	92	GLU	ALA	engineered mutation	UNP Q79791
eM	92	GLU	ALA	engineered mutation	UNP Q79791
eN	92	GLU	ALA	engineered mutation	UNP Q79791
eO	92	GLU	ALA	engineered mutation	UNP Q79791
eP	92	GLU	ALA	engineered mutation	UNP Q79791
lt	92	GLU	ALA	engineered mutation	UNP Q79791
eQ	92	GLU	ALA	engineered mutation	UNP Q79791
eR	92	GLU	ALA	engineered mutation	UNP Q79791
eS	92	GLU	ALA	engineered mutation	UNP Q79791
eT	92	GLU	ALA	engineered mutation	UNP Q79791
eU	92	GLU	ALA	engineered mutation	UNP Q79791
eV	92	GLU	ALA	engineered mutation	UNP Q79791
eW	92	GLU	ALA	engineered mutation	UNP Q79791
eX	92	GLU	ALA	engineered mutation	UNP Q79791
eY	92	GLU	ALA	engineered mutation	UNP Q79791
eZ	92	GLU	ALA	engineered mutation	UNP Q79791
lu	92	GLU	ALA	engineered mutation	UNP Q79791
f0	92	GLU	ALA	engineered mutation	UNP Q79791
f1	92	GLU	ALA	engineered mutation	UNP Q79791
f2	92	GLU	ALA	engineered mutation	UNP Q79791
f3	92	GLU	ALA	engineered mutation	UNP Q79791
f4	92	GLU	ALA	engineered mutation	UNP Q79791
f5	92	GLU	ALA	engineered mutation	UNP Q79791

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Chain	Residue	Modelled	Actual	Comment	Reference
f6	92	GLU	ALA	engineered mutation	UNP Q79791
f7	92	GLU	ALA	engineered mutation	UNP Q79791
f8	92	GLU	ALA	engineered mutation	UNP Q79791
f9	92	GLU	ALA	engineered mutation	UNP Q79791
lv	92	GLU	ALA	engineered mutation	UNP Q79791
fa	92	GLU	ALA	engineered mutation	UNP Q79791
fb	92	GLU	ALA	engineered mutation	UNP Q79791
fc	92	GLU	ALA	engineered mutation	UNP Q79791
fd	92	GLU	ALA	engineered mutation	UNP Q79791
fe	92	GLU	ALA	engineered mutation	UNP Q79791
ff	92	GLU	ALA	engineered mutation	UNP Q79791
fg	92	GLU	ALA	engineered mutation	UNP Q79791
fh	92	GLU	ALA	engineered mutation	UNP Q79791
fi	92	GLU	ALA	engineered mutation	UNP Q79791
fj	92	GLU	ALA	engineered mutation	UNP Q79791
lw	92	GLU	ALA	engineered mutation	UNP Q79791
fk	92	GLU	ALA	engineered mutation	UNP Q79791
fl	92	GLU	ALA	engineered mutation	UNP Q79791
fm	92	GLU	ALA	engineered mutation	UNP Q79791
fn	92	GLU	ALA	engineered mutation	UNP Q79791
fo	92	GLU	ALA	engineered mutation	UNP Q79791
fp	92	GLU	ALA	engineered mutation	UNP Q79791
fq	92	GLU	ALA	engineered mutation	UNP Q79791
fr	92	GLU	ALA	engineered mutation	UNP Q79791
fs	92	GLU	ALA	engineered mutation	UNP Q79791
ft	92	GLU	ALA	engineered mutation	UNP Q79791
lx	92	GLU	ALA	engineered mutation	UNP Q79791
fu	92	GLU	ALA	engineered mutation	UNP Q79791
fv	92	GLU	ALA	engineered mutation	UNP Q79791
fw	92	GLU	ALA	engineered mutation	UNP Q79791
fx	92	GLU	ALA	engineered mutation	UNP Q79791
fy	92	GLU	ALA	engineered mutation	UNP Q79791
fz	92	GLU	ALA	engineered mutation	UNP Q79791
fA	92	GLU	ALA	engineered mutation	UNP Q79791
fB	92	GLU	ALA	engineered mutation	UNP Q79791
fC	92	GLU	ALA	engineered mutation	UNP Q79791
fD	92	GLU	ALA	engineered mutation	UNP Q79791
ly	92	GLU	ALA	engineered mutation	UNP Q79791
fE	92	GLU	ALA	engineered mutation	UNP Q79791
fF	92	GLU	ALA	engineered mutation	UNP Q79791
fG	92	GLU	ALA	engineered mutation	UNP Q79791
fH	92	GLU	ALA	engineered mutation	UNP Q79791

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Chain	Residue	Modelled	Actual	Comment	Reference
fI	92	GLU	ALA	engineered mutation	UNP Q79791
fJ	92	GLU	ALA	engineered mutation	UNP Q79791
fK	92	GLU	ALA	engineered mutation	UNP Q79791
fL	92	GLU	ALA	engineered mutation	UNP Q79791
fM	92	GLU	ALA	engineered mutation	UNP Q79791
fN	92	GLU	ALA	engineered mutation	UNP Q79791
1z	92	GLU	ALA	engineered mutation	UNP Q79791
fO	92	GLU	ALA	engineered mutation	UNP Q79791
fP	92	GLU	ALA	engineered mutation	UNP Q79791
fQ	92	GLU	ALA	engineered mutation	UNP Q79791
fR	92	GLU	ALA	engineered mutation	UNP Q79791
fS	92	GLU	ALA	engineered mutation	UNP Q79791
fT	92	GLU	ALA	engineered mutation	UNP Q79791
fU	92	GLU	ALA	engineered mutation	UNP Q79791
fV	92	GLU	ALA	engineered mutation	UNP Q79791
fW	92	GLU	ALA	engineered mutation	UNP Q79791
fX	92	GLU	ALA	engineered mutation	UNP Q79791
1A	92	GLU	ALA	engineered mutation	UNP Q79791
fY	92	GLU	ALA	engineered mutation	UNP Q79791
fZ	92	GLU	ALA	engineered mutation	UNP Q79791
g0	92	GLU	ALA	engineered mutation	UNP Q79791
g1	92	GLU	ALA	engineered mutation	UNP Q79791
g2	92	GLU	ALA	engineered mutation	UNP Q79791
g3	92	GLU	ALA	engineered mutation	UNP Q79791
g4	92	GLU	ALA	engineered mutation	UNP Q79791
g5	92	GLU	ALA	engineered mutation	UNP Q79791
g6	92	GLU	ALA	engineered mutation	UNP Q79791
g7	92	GLU	ALA	engineered mutation	UNP Q79791
1B	92	GLU	ALA	engineered mutation	UNP Q79791
0	92	GLU	ALA	engineered mutation	UNP Q79791
a	92	GLU	ALA	engineered mutation	UNP Q79791
b	92	GLU	ALA	engineered mutation	UNP Q79791
c	92	GLU	ALA	engineered mutation	UNP Q79791
d	92	GLU	ALA	engineered mutation	UNP Q79791
e	92	GLU	ALA	engineered mutation	UNP Q79791
f	92	GLU	ALA	engineered mutation	UNP Q79791
g	92	GLU	ALA	engineered mutation	UNP Q79791
h	92	GLU	ALA	engineered mutation	UNP Q79791
i	92	GLU	ALA	engineered mutation	UNP Q79791
j	92	GLU	ALA	engineered mutation	UNP Q79791
l	92	GLU	ALA	engineered mutation	UNP Q79791
k	92	GLU	ALA	engineered mutation	UNP Q79791

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Chain	Residue	Modelled	Actual	Comment	Reference
l	92	GLU	ALA	engineered mutation	UNP Q79791
m	92	GLU	ALA	engineered mutation	UNP Q79791
n	92	GLU	ALA	engineered mutation	UNP Q79791
o	92	GLU	ALA	engineered mutation	UNP Q79791
p	92	GLU	ALA	engineered mutation	UNP Q79791
q	92	GLU	ALA	engineered mutation	UNP Q79791
r	92	GLU	ALA	engineered mutation	UNP Q79791
s	92	GLU	ALA	engineered mutation	UNP Q79791
t	92	GLU	ALA	engineered mutation	UNP Q79791
2	92	GLU	ALA	engineered mutation	UNP Q79791
u	92	GLU	ALA	engineered mutation	UNP Q79791
v	92	GLU	ALA	engineered mutation	UNP Q79791
w	92	GLU	ALA	engineered mutation	UNP Q79791
x	92	GLU	ALA	engineered mutation	UNP Q79791
y	92	GLU	ALA	engineered mutation	UNP Q79791
z	92	GLU	ALA	engineered mutation	UNP Q79791
A	92	GLU	ALA	engineered mutation	UNP Q79791
B	92	GLU	ALA	engineered mutation	UNP Q79791
C	92	GLU	ALA	engineered mutation	UNP Q79791
D	92	GLU	ALA	engineered mutation	UNP Q79791
3	92	GLU	ALA	engineered mutation	UNP Q79791
E	92	GLU	ALA	engineered mutation	UNP Q79791
F	92	GLU	ALA	engineered mutation	UNP Q79791
G	92	GLU	ALA	engineered mutation	UNP Q79791
H	92	GLU	ALA	engineered mutation	UNP Q79791
I	92	GLU	ALA	engineered mutation	UNP Q79791
J	92	GLU	ALA	engineered mutation	UNP Q79791
K	92	GLU	ALA	engineered mutation	UNP Q79791
L	92	GLU	ALA	engineered mutation	UNP Q79791
M	92	GLU	ALA	engineered mutation	UNP Q79791
N	92	GLU	ALA	engineered mutation	UNP Q79791
4	92	GLU	ALA	engineered mutation	UNP Q79791
O	92	GLU	ALA	engineered mutation	UNP Q79791
P	92	GLU	ALA	engineered mutation	UNP Q79791
Q	92	GLU	ALA	engineered mutation	UNP Q79791
R	92	GLU	ALA	engineered mutation	UNP Q79791
S	92	GLU	ALA	engineered mutation	UNP Q79791
T	92	GLU	ALA	engineered mutation	UNP Q79791
U	92	GLU	ALA	engineered mutation	UNP Q79791
V	92	GLU	ALA	engineered mutation	UNP Q79791
W	92	GLU	ALA	engineered mutation	UNP Q79791
X	92	GLU	ALA	engineered mutation	UNP Q79791

*Continued on next page...*


*Continued from previous page...*

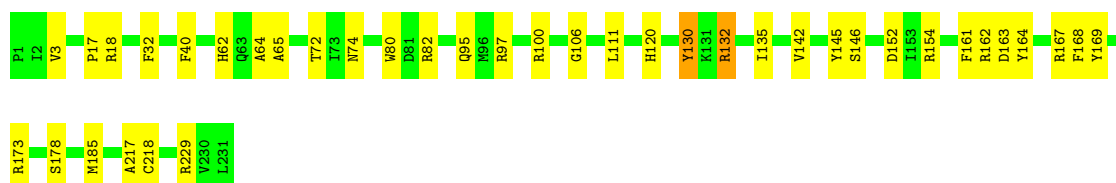
Chain	Residue	Modelled	Actual	Comment	Reference
5	92	GLU	ALA	engineered mutation	UNP Q79791
6	92	GLU	ALA	engineered mutation	UNP Q79791
7	92	GLU	ALA	engineered mutation	UNP Q79791
8	92	GLU	ALA	engineered mutation	UNP Q79791
9	92	GLU	ALA	engineered mutation	UNP Q79791

### 3 Residue-property plots [i](#)


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

Chain g8:  83% 16% .




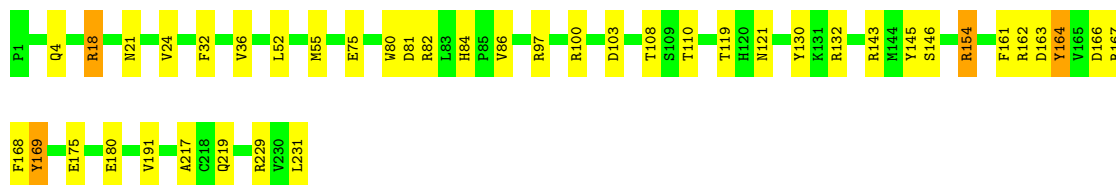
- Molecule 1: capsid protein

Chain g9:  80% 18% .




- Molecule 1: capsid protein

Chain ga:  82% 16% .



- Molecule 1: capsid protein

Chain gb:  80% 19% .





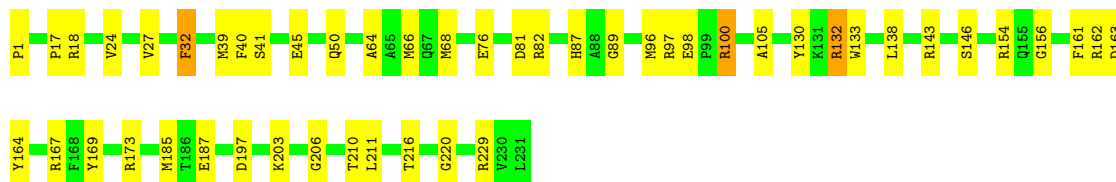
- Molecule 1: capsid protein

Chain gc: 85% 14%



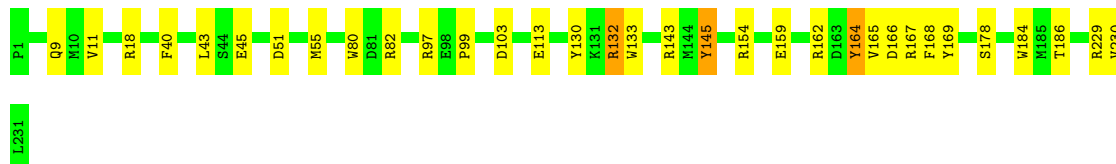
- Molecule 1: capsid protein

Chain gd: 79% 20%



- Molecule 1: capsid protein

Chain ge: 86% 13%



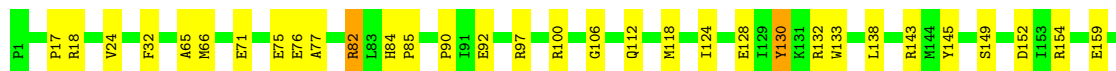
- Molecule 1: capsid protein

Chain gf: 82% 16%



- Molecule 1: capsid protein

Chain gg: 78% 19%







- Molecule 1: capsid protein

Chain gh: 78% 20%



- Molecule 1: capsid protein

Chain 1C: 80% 20%



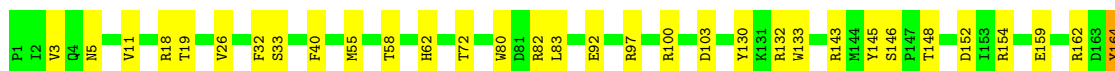
- Molecule 1: capsid protein

Chain gi: 79% 20%



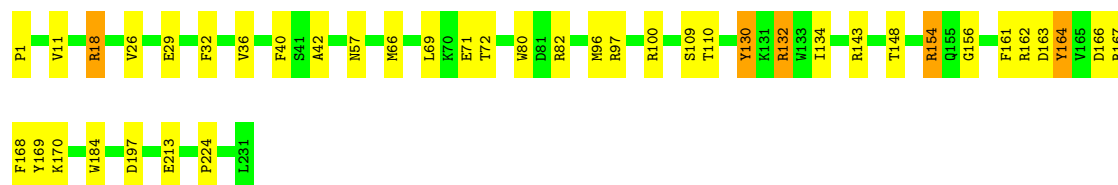
- Molecule 1: capsid protein

Chain gj: 80% 19%



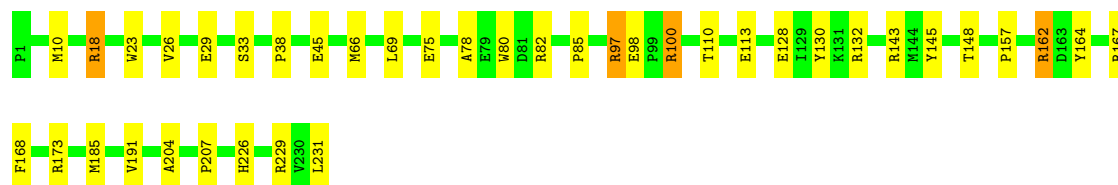
- Molecule 1: capsid protein

Chain gk: 82% 16%



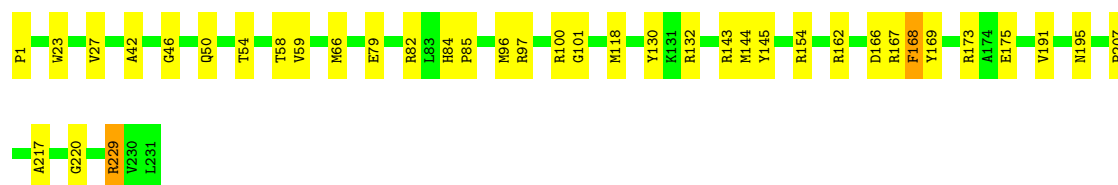
- Molecule 1: capsid protein

Chain gl: 83% 15% .



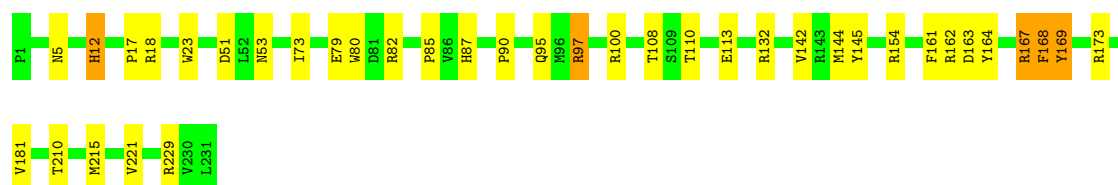
- Molecule 1: capsid protein

Chain gm: 84% 16% .



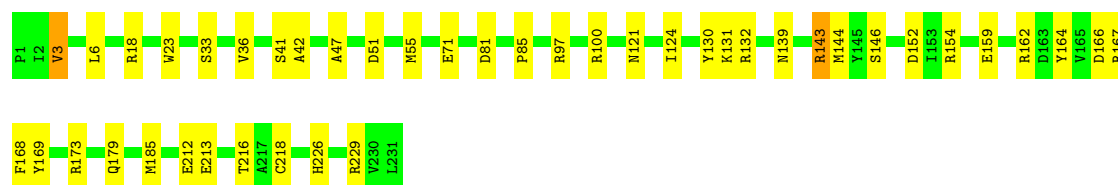
- Molecule 1: capsid protein

Chain gn: 84% 14% .




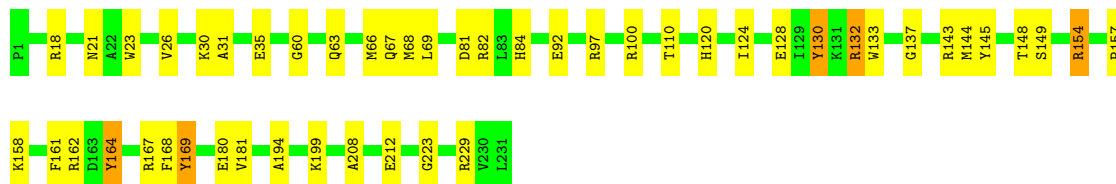
- Molecule 1: capsid protein

Chain go: 81% 18% .




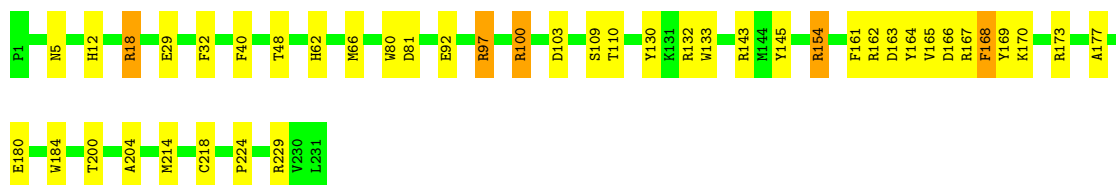
- Molecule 1: capsid protein

Chain gp:  79% 19%




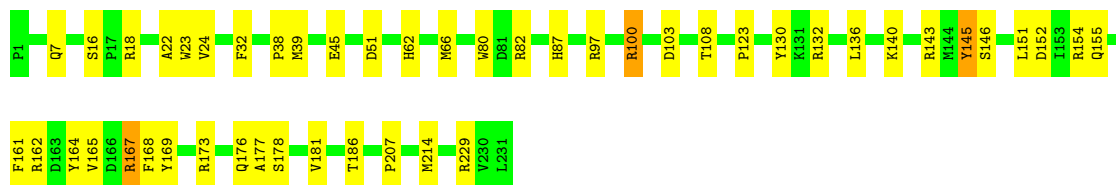
- Molecule 1: capsid protein

Chain gq:  81% 16%




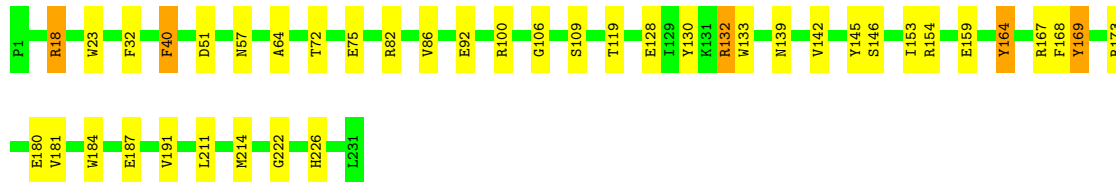
- Molecule 1: capsid protein

Chain gr:  79% 19%




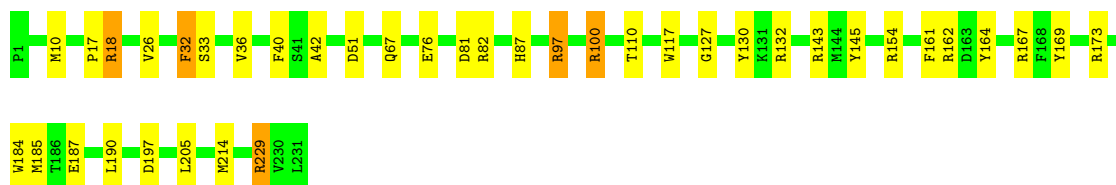
- Molecule 1: capsid protein

Chain 1D:  82% 16%




- Molecule 1: capsid protein


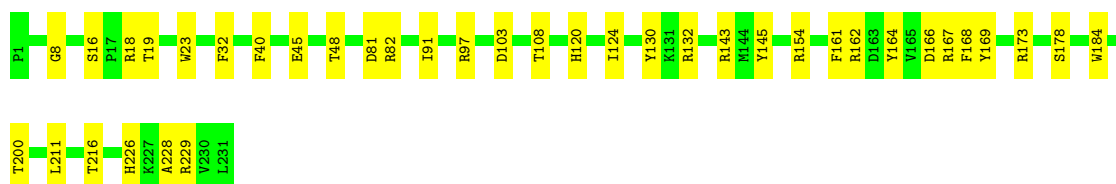
Chain gs:  83% 15%




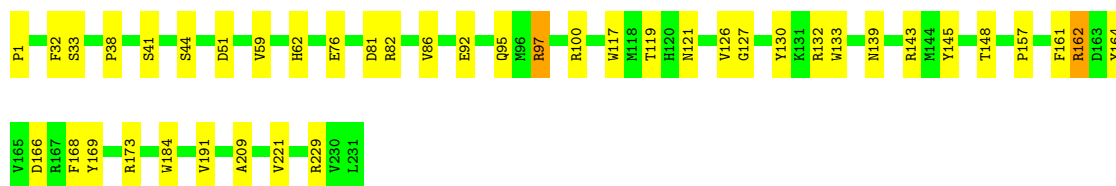
## • Molecule 1: capsid protein

Chain gt:  81% 18%


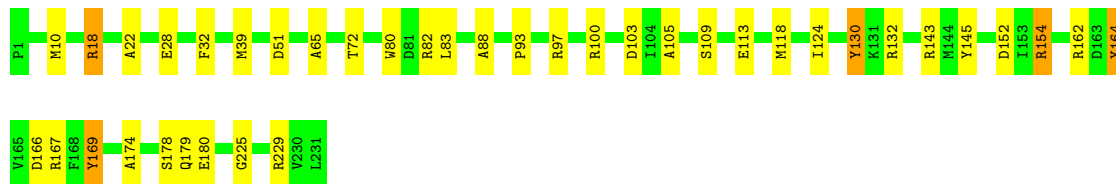
## • Molecule 1: capsid protein

Chain gu:  84% 16%


## • Molecule 1: capsid protein

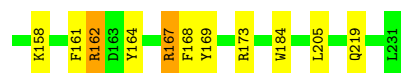
Chain gv:  82% 17%

## • Molecule 1: capsid protein

Chain gw:  83% 15%

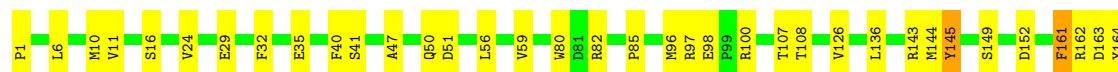
## • Molecule 1: capsid protein

Chain gx:  82% 17%



- Molecule 1: capsid protein

Chain gy: 82% 16% .



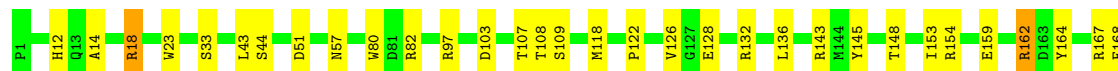
- Molecule 1: capsid protein

Chain gz: 80% 19% .



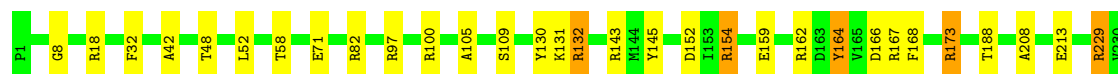
- Molecule 1: capsid protein

Chain gA: 83% 16% .



- Molecule 1: capsid protein

Chain gB: 87% 11% .




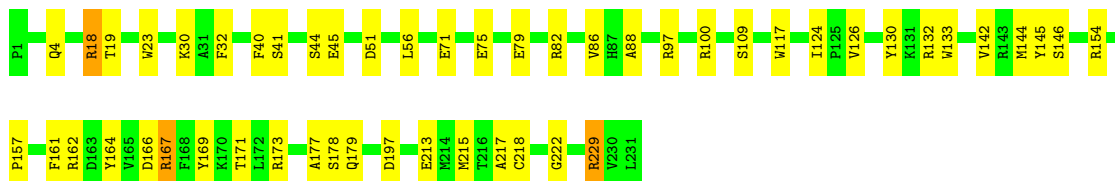
- Molecule 1: capsid protein

Chain 1E: 86% 13% .




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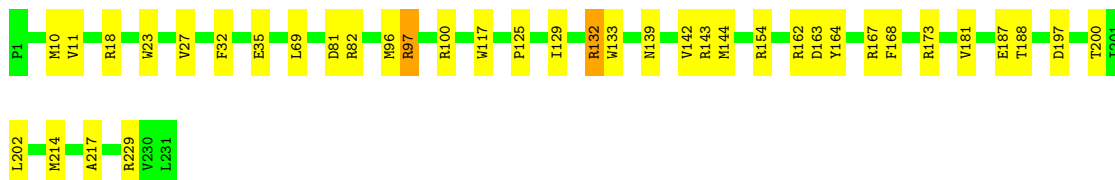
- Molecule 1: capsid protein

Chain gC:  78% 21%


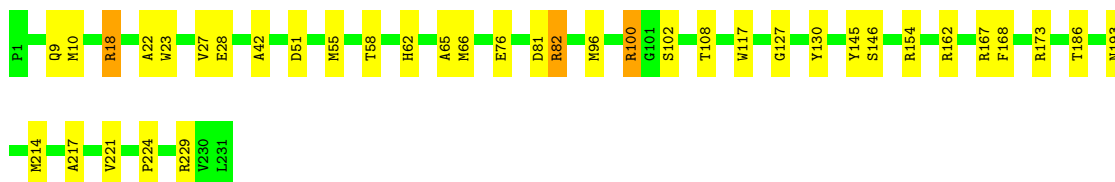
- Molecule 1: capsid protein

Chain gD:  85% 13%


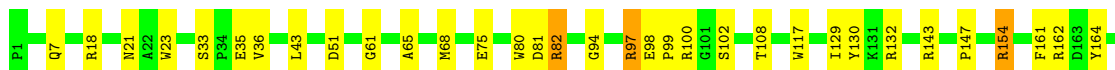
- Molecule 1: capsid protein

Chain gE:  84% 16%

- Molecule 1: capsid protein


Chain gF:  84% 15%

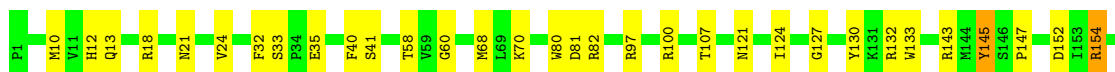
- Molecule 1: capsid protein

Chain gG:  80% 18%




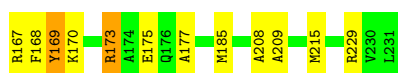
- Molecule 1: capsid protein

Chain gH:  79% 19% •




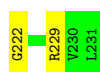
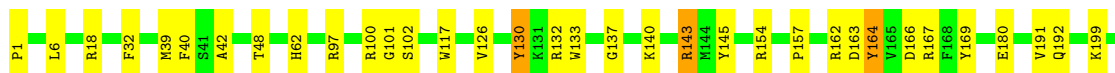
- Molecule 1: capsid protein

Chain gI:  80% 18% •




- Molecule 1: capsid protein

Chain gJ:  84% 14% •




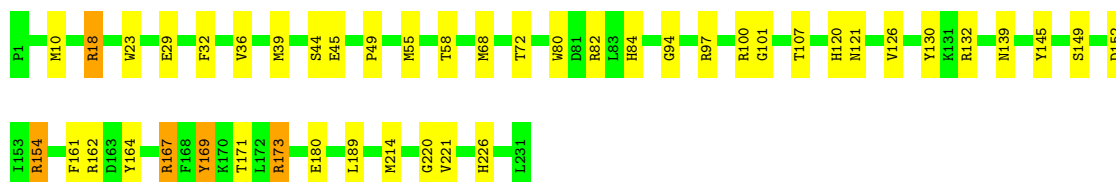
- Molecule 1: capsid protein

Chain gK:  80% 19% •



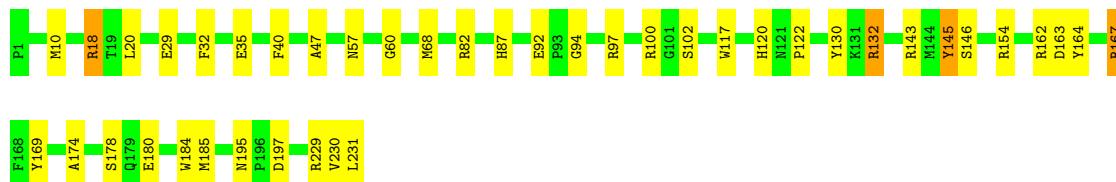
- Molecule 1: capsid protein

Chain gL:  81% 17% •



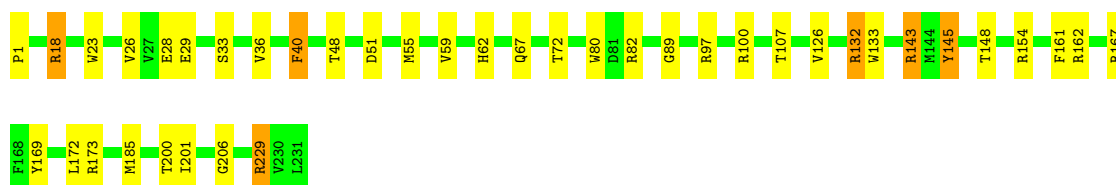
- Molecule 1: capsid protein

Chain 1F: 82% 16% •



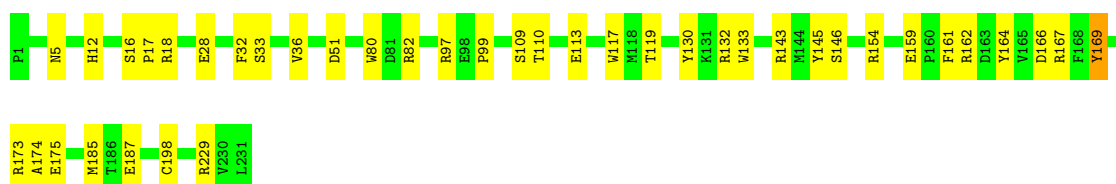
- Molecule 1: capsid protein

Chain gM: 83% 15% •



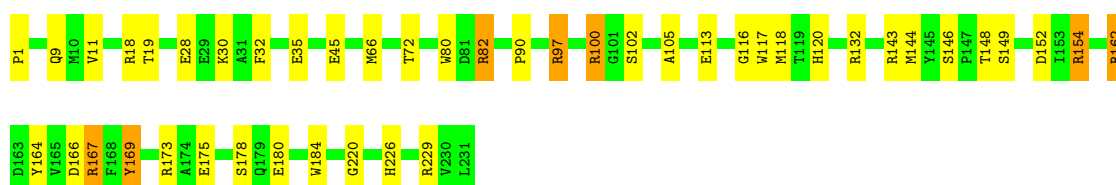
- Molecule 1: capsid protein

Chain gN: 83% 17% •




- Molecule 1: capsid protein

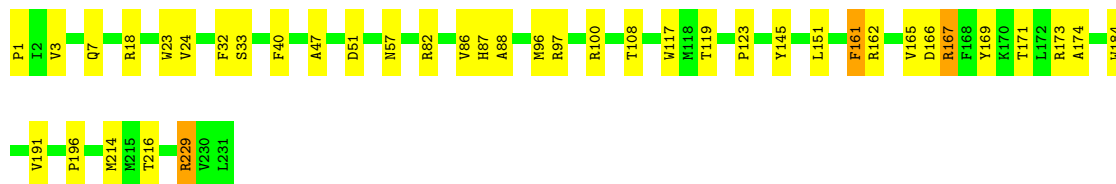
Chain gO: 81% 16% •




- Molecule 1: capsid protein

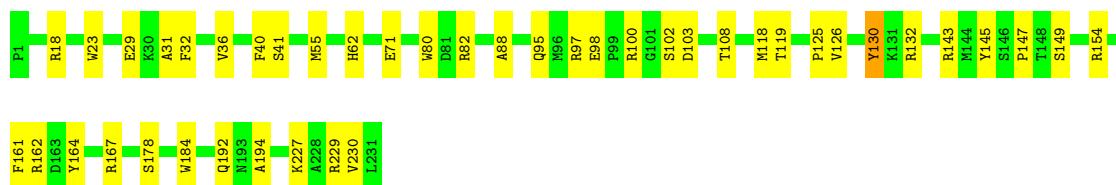


Chain gP:  83% 16%




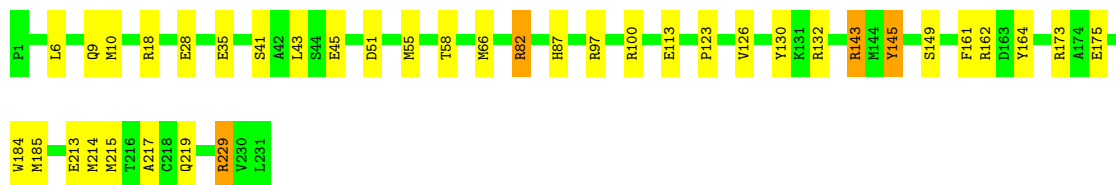
- Molecule 1: capsid protein

Chain gQ:  81% 18%




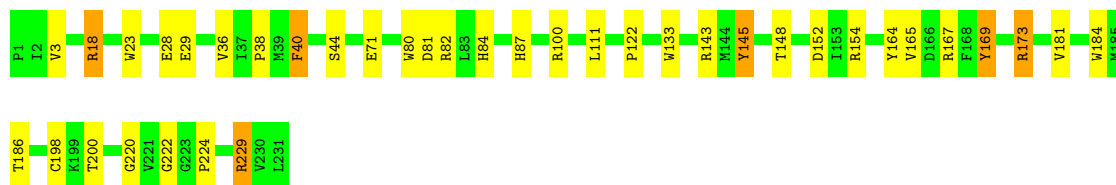
- Molecule 1: capsid protein

Chain gR:  84% 15%




- Molecule 1: capsid protein

Chain gS:  84% 14%


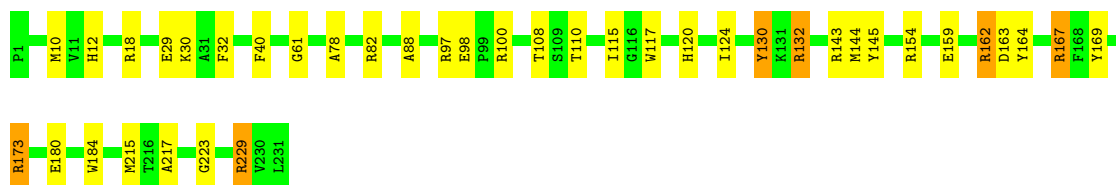


- Molecule 1: capsid protein


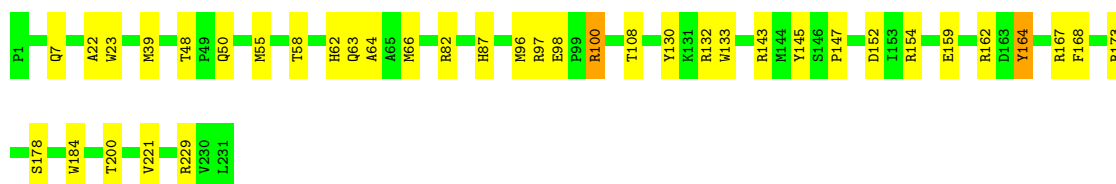
Chain gT:  78% 20%




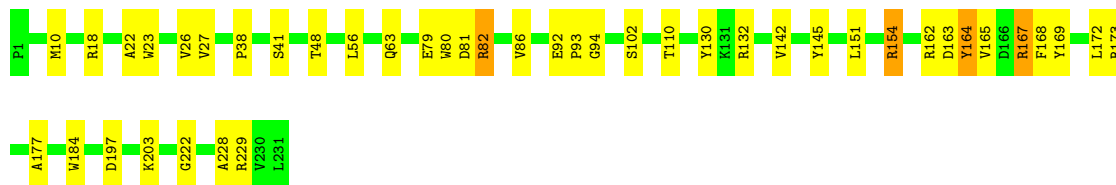
## • Molecule 1: capsid protein

Chain gU:  83% 14% .


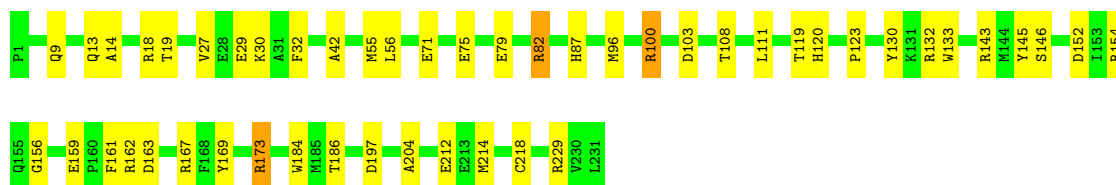
## • Molecule 1: capsid protein

Chain gV:  84% 16% .


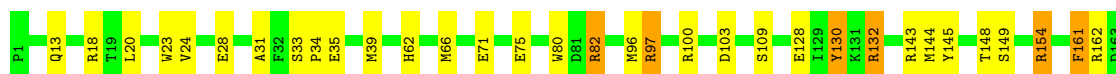
## • Molecule 1: capsid protein

Chain 1G:  81% 17% .

## • Molecule 1: capsid protein

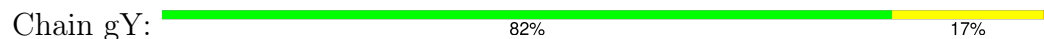
Chain gW:  79% 20% .

## • Molecule 1: capsid protein

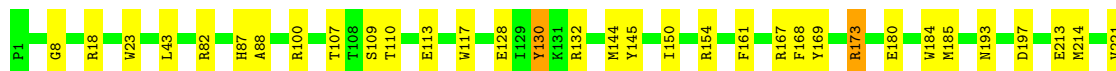
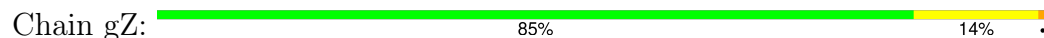
Chain gX:  80% 17% .



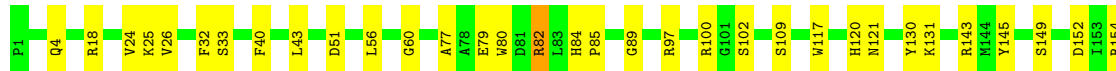
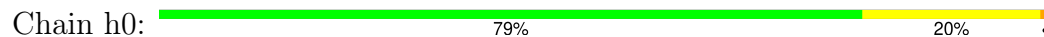
- Molecule 1: capsid protein



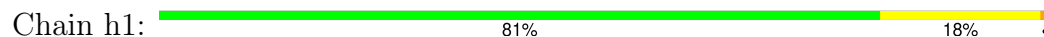
- Molecule 1: capsid protein



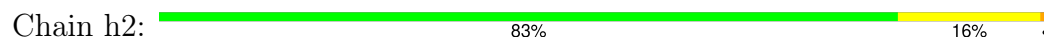
- Molecule 1: capsid protein

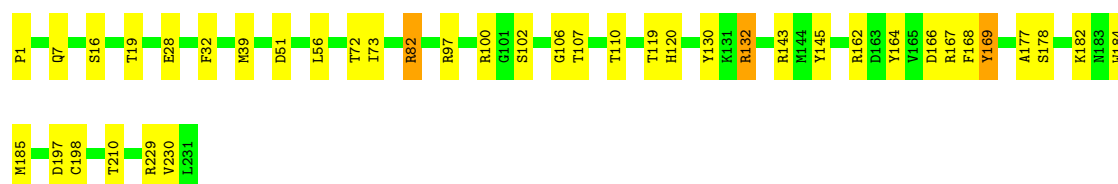


- Molecule 1: capsid protein



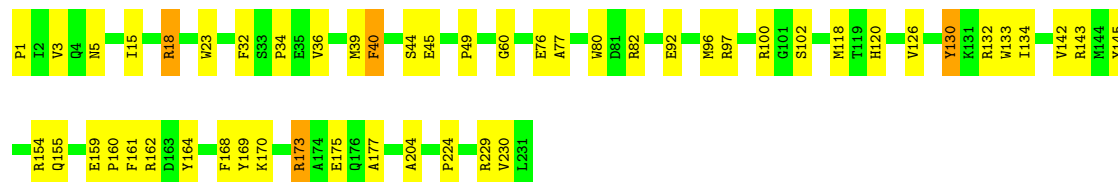
- Molecule 1: capsid protein





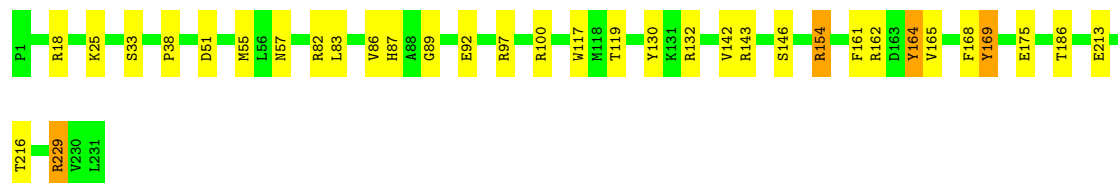
- Molecule 1: capsid protein

Chain h3: 78% 20% .



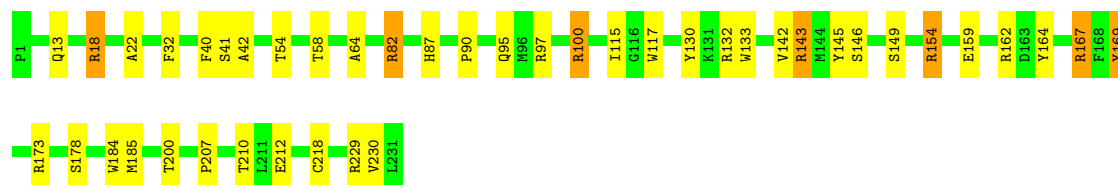
- Molecule 1: capsid protein

Chain h4: 85% 13% .



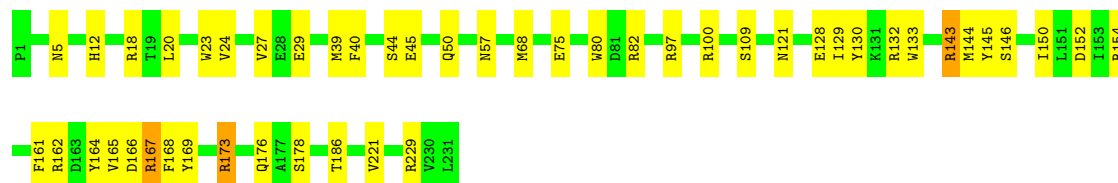
- Molecule 1: capsid protein

Chain h5: 81% 16% .



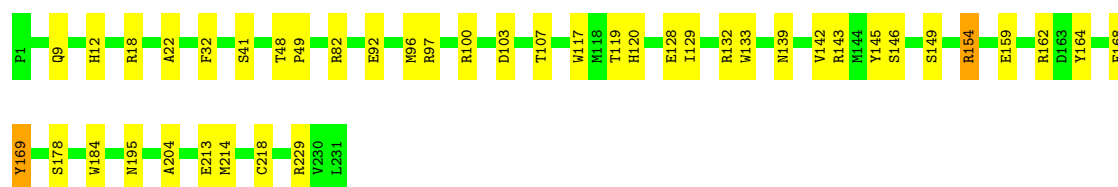
- Molecule 1: capsid protein

Chain 1H: 79% 19% .




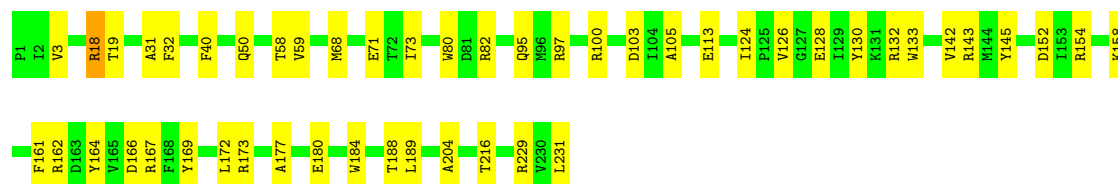
- Molecule 1: capsid protein

Chain h6: 82% 17% .




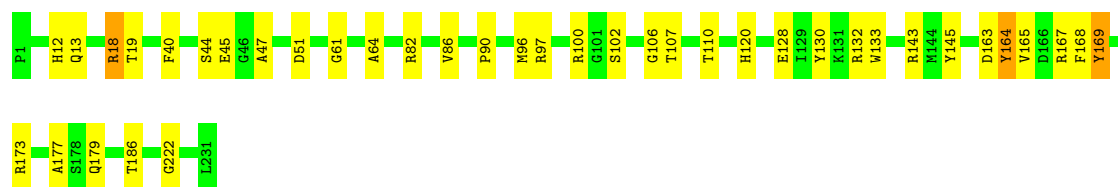
- Molecule 1: capsid protein

Chain h7:  79% 21%




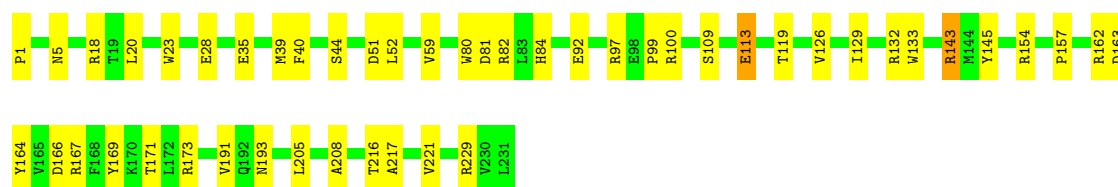
- Molecule 1: capsid protein

Chain h8:  83% 16%




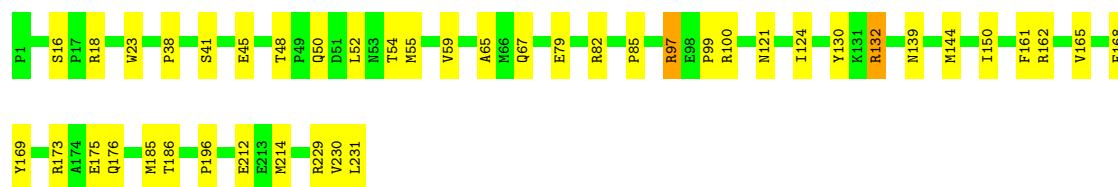
- Molecule 1: capsid protein

Chain h9:  79% 20%




- Molecule 1: capsid protein

Chain ha:  81% 18%



- Molecule 1: capsid protein

Chain hb:  81% 19%



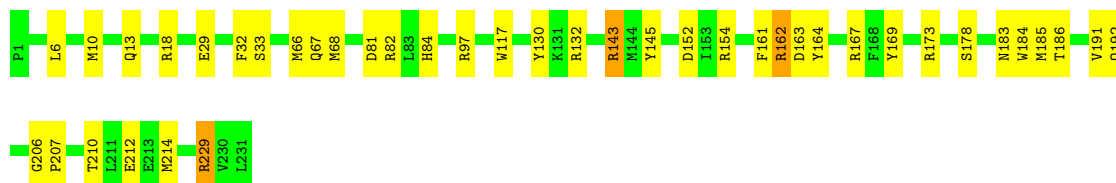
- Molecule 1: capsid protein

Chain hc: 81% 17% •



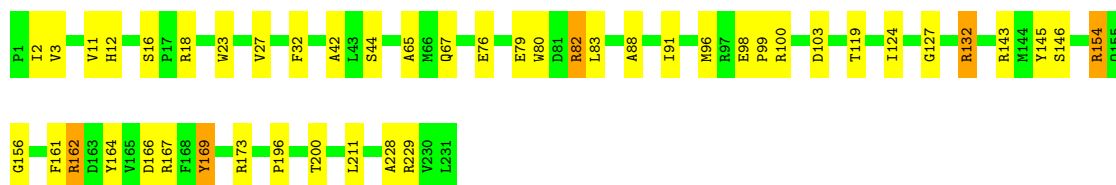
- Molecule 1: capsid protein

Chain hd: 82% 16% •



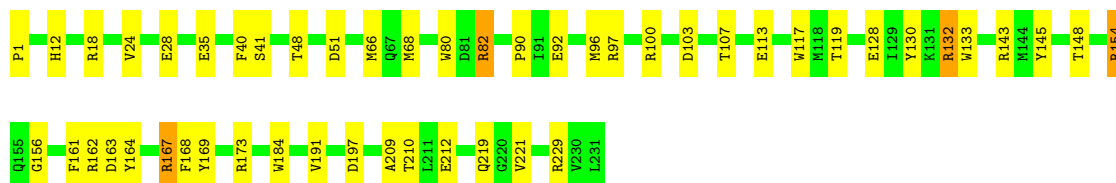
- Molecule 1: capsid protein

Chain he: 80% 18% •



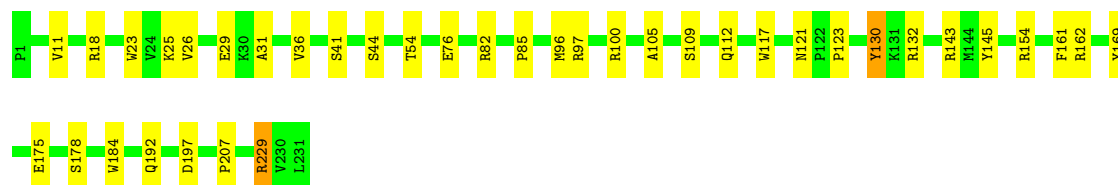
- Molecule 1: capsid protein

Chain hf: 78% 20% •

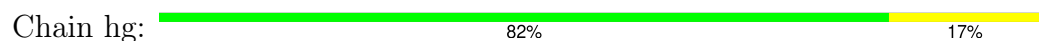


- Molecule 1: capsid protein

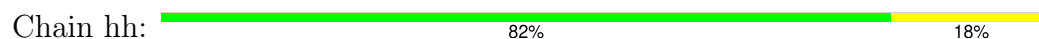
Chain 1I: 84% 16% •



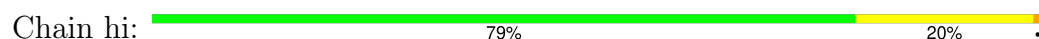
- Molecule 1: capsid protein



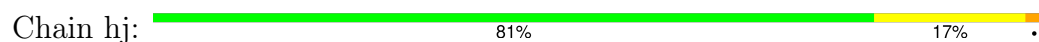
- Molecule 1: capsid protein




- Molecule 1: capsid protein

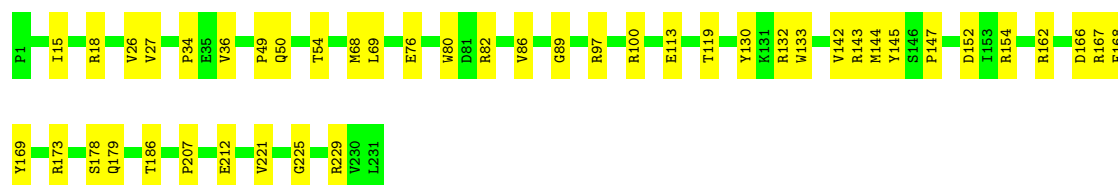


- Molecule 1: capsid protein




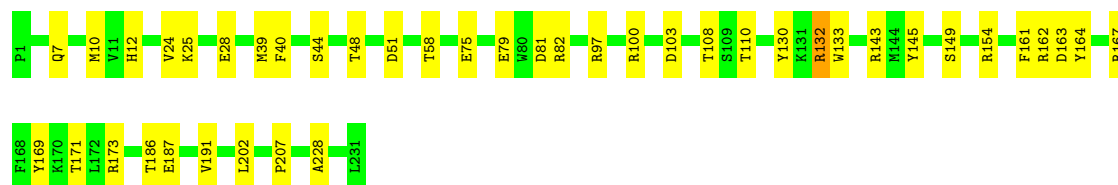
- Molecule 1: capsid protein

Chain hk:  81% 19%




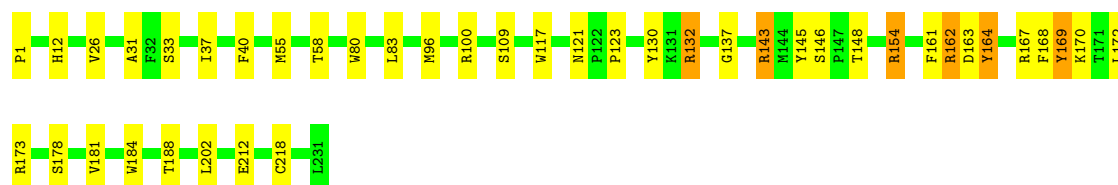
- Molecule 1: capsid protein

Chain hl:  82% 18%




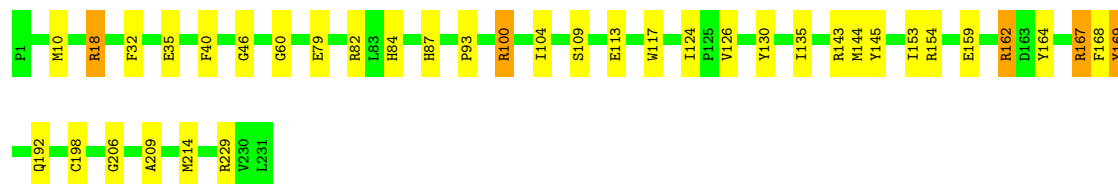
- Molecule 1: capsid protein

Chain hm:  82% 16% •




- Molecule 1: capsid protein

Chain hn:  84% 14% •




- Molecule 1: capsid protein

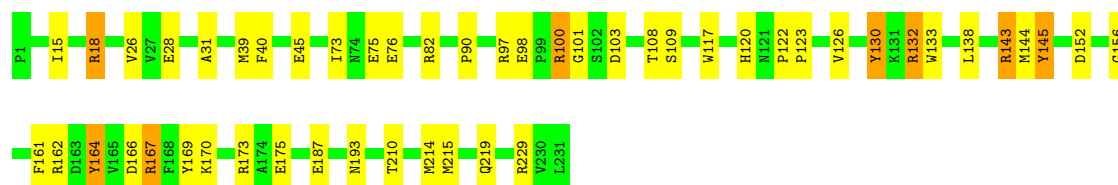
Chain ho:  84% 14% •




- Molecule 1: capsid protein

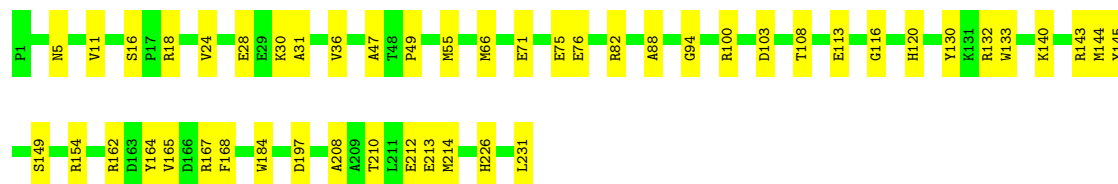


Chain hp:  78% 18%




- Molecule 1: capsid protein

Chain 1J:  79% 21%




- Molecule 1: capsid protein

Chain hq:  81% 16%




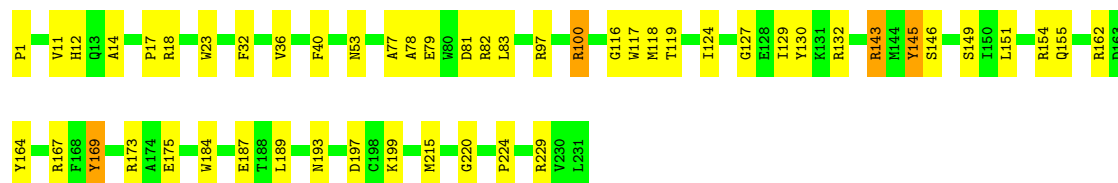
- Molecule 1: capsid protein

Chain hr:  80% 19%




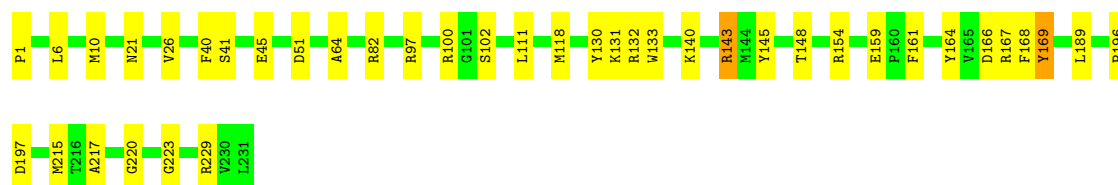
- Molecule 1: capsid protein

Chain hs:  78% 20%




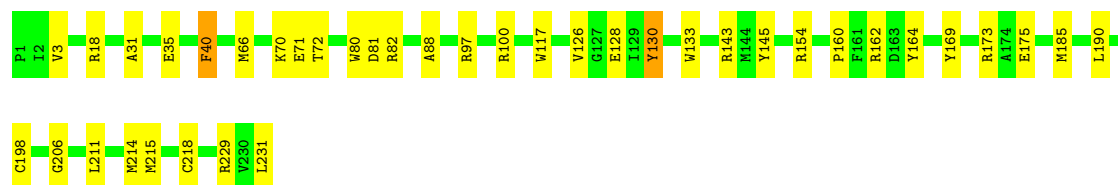
- Molecule 1: capsid protein

Chain ht:  83% 16% •




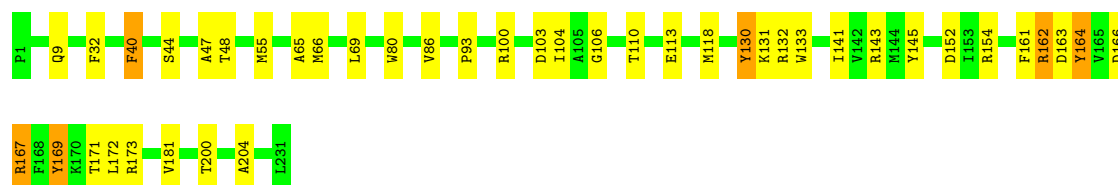
- Molecule 1: capsid protein

Chain hu:  83% 16% •




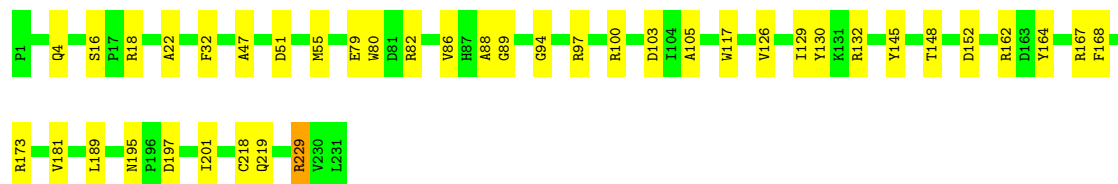
- Molecule 1: capsid protein

Chain hv:  82% 16% •




- Molecule 1: capsid protein

Chain hw:  83% 17% •




- Molecule 1: capsid protein

Chain hx:  84% 14% •




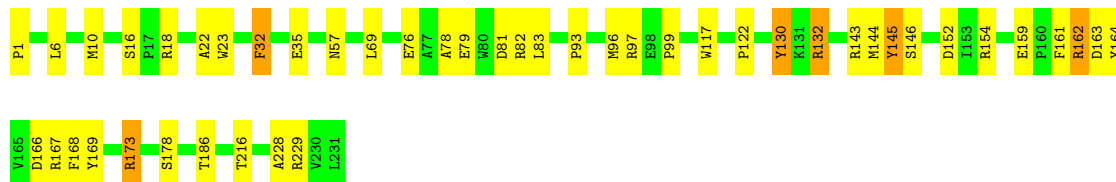
- Molecule 1: capsid protein

Chain hy:  80% 18% .




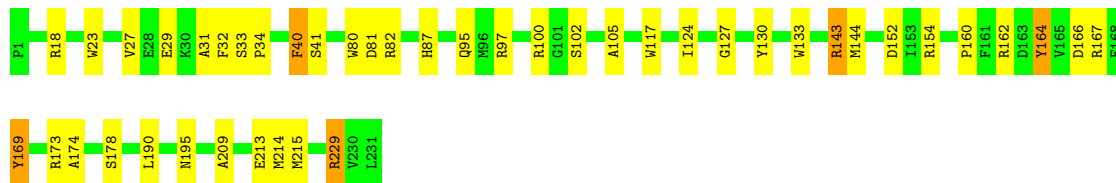
- Molecule 1: capsid protein

Chain hz:  80% 17% .




- Molecule 1: capsid protein

Chain 1K:  81% 17% .




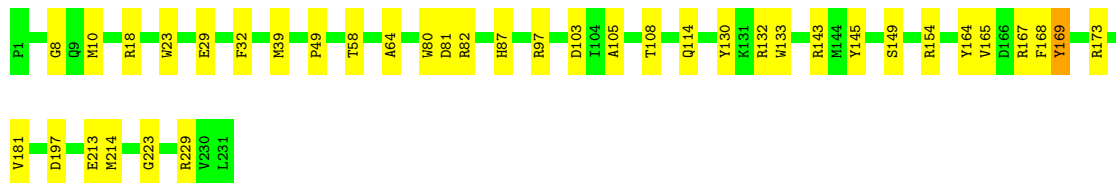
- Molecule 1: capsid protein

Chain hA:  84% 15% .




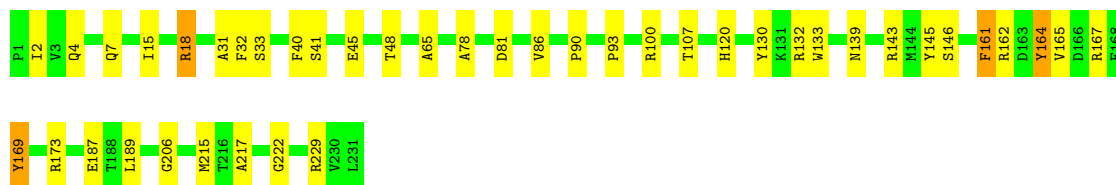
- Molecule 1: capsid protein

Chain hB:  84% 16% .




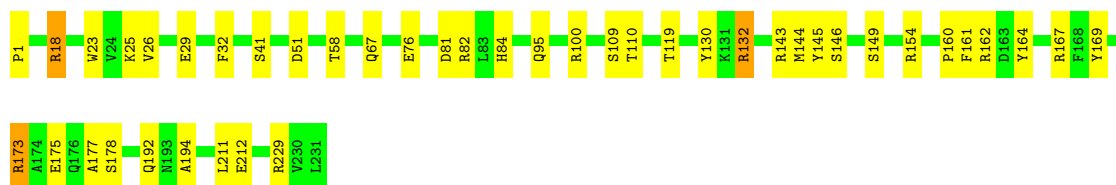
- Molecule 1: capsid protein

Chain hC:  82% 16% •




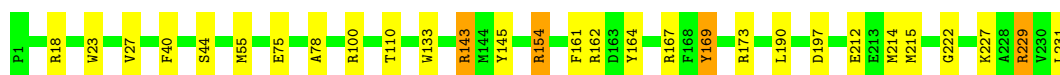
- Molecule 1: capsid protein

Chain hD:  81% 17% •




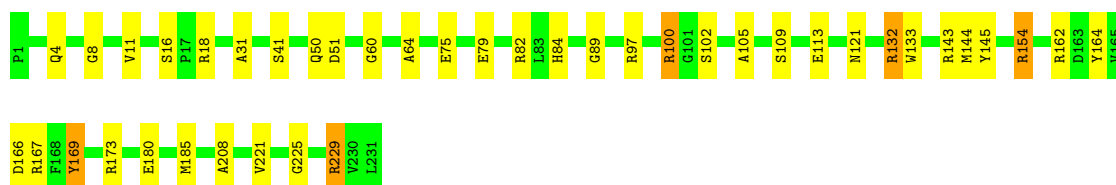
- Molecule 1: capsid protein

Chain hE:  87% 11% •




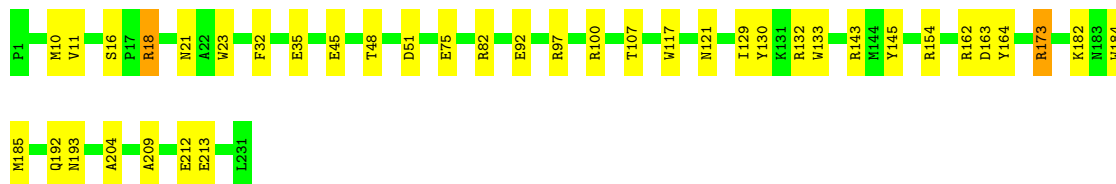
- Molecule 1: capsid protein

Chain hF:  82% 16% •




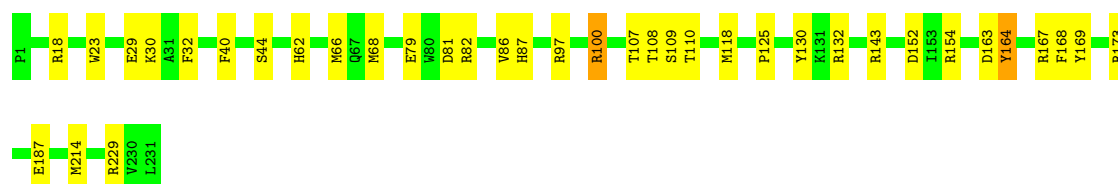
- Molecule 1: capsid protein

Chain hG:  83% 16% •



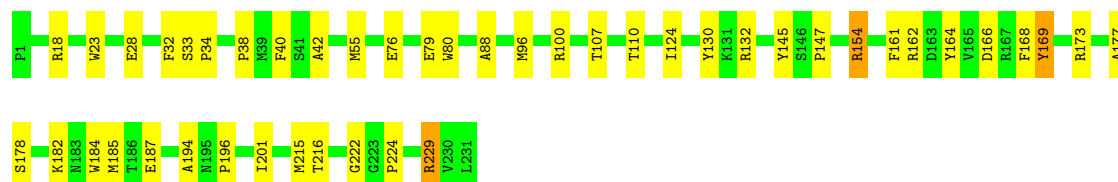
- Molecule 1: capsid protein

Chain hH:  84% 15% •



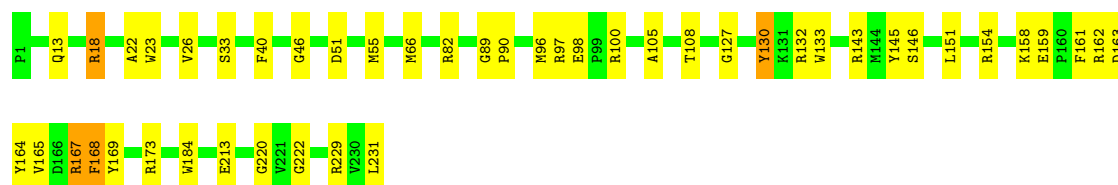
- Molecule 1: capsid protein

Chain hI: 81% 18% •



- Molecule 1: capsid protein

Chain hJ: 80% 18% •



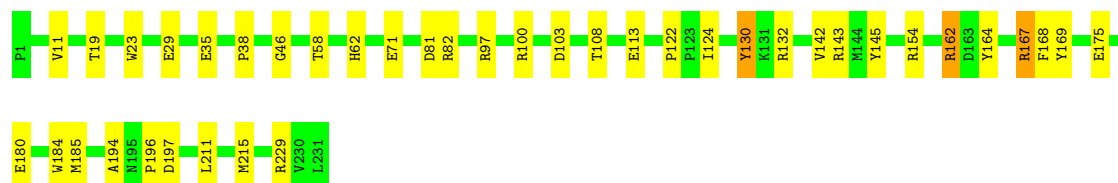
- Molecule 1: capsid protein

Chain 1L: 85% 14% •



- Molecule 1: capsid protein

Chain hK: 83% 16% •



- Molecule 1: capsid protein

Chain hL: 81% 17% •





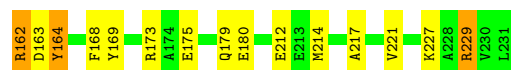
- Molecule 1: capsid protein

Chain hM: 83% 15% •



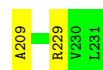
- Molecule 1: capsid protein

Chain hN: 80% 19% •



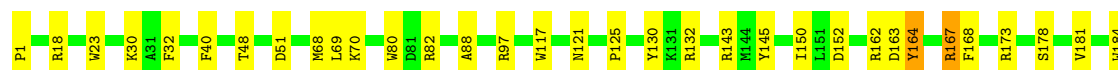
- Molecule 1: capsid protein

Chain hO: 85% 14% •



- Molecule 1: capsid protein

Chain hP: 84% 14% •



- Molecule 1: capsid protein

Chain hQ: 77% 23% •





- Molecule 1: capsid protein

Chain hR: 78% 21% •



- Molecule 1: capsid protein

Chain hS: 84% 15% •



- Molecule 1: capsid protein

Chain hT: 84% 15% •



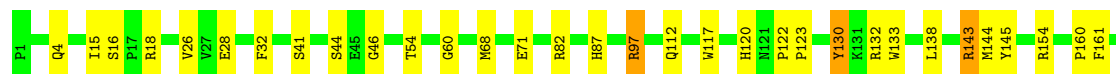
- Molecule 1: capsid protein

Chain 1M: 77% 20% •



- Molecule 1: capsid protein

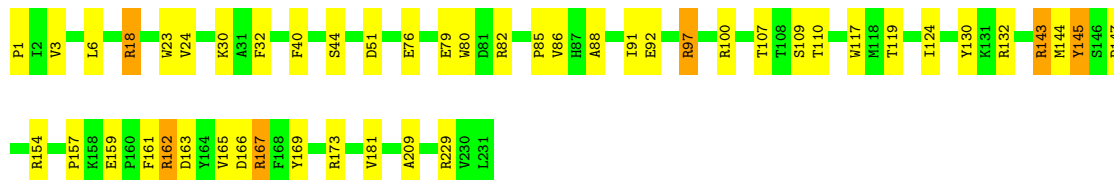
Chain hU: 81% 17% •





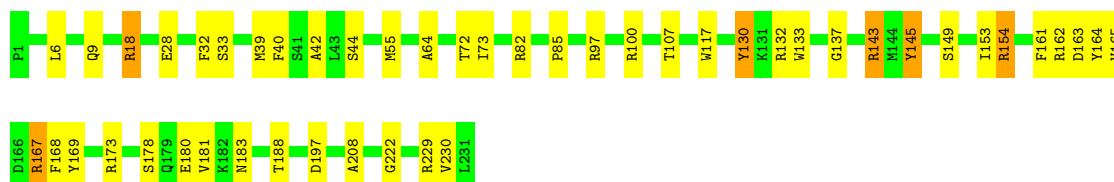
- Molecule 1: capsid protein

Chain hV:   
79% 18%



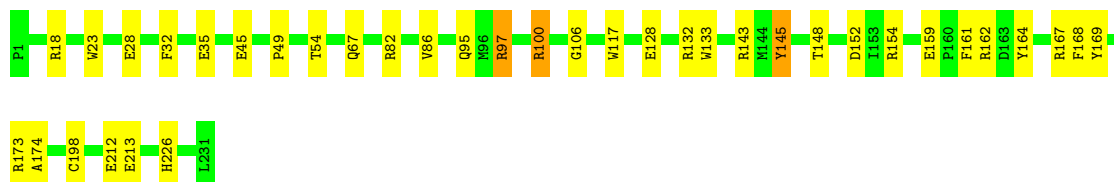
- Molecule 1: capsid protein

Chain hW:   
79% 18%



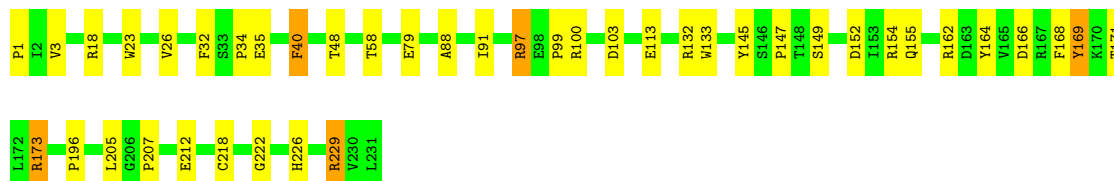
- Molecule 1: capsid protein

Chain hX:   
84% 15%



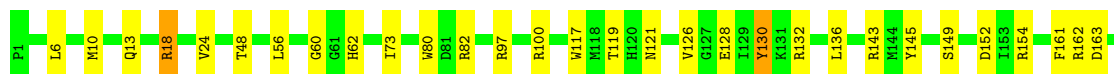
- Molecule 1: capsid protein

Chain hY:   
82% 16%



- Molecule 1: capsid protein

Chain hZ:   
83% 16%







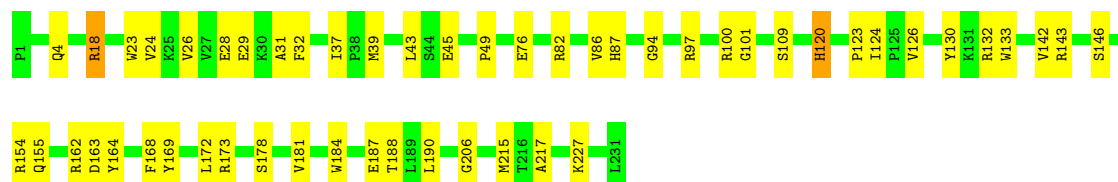
- Molecule 1: capsid protein

Chain i0: 81% 18%



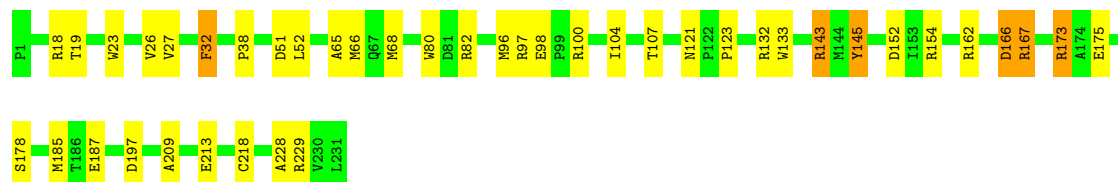
- Molecule 1: capsid protein

Chain i1: 77% 22%



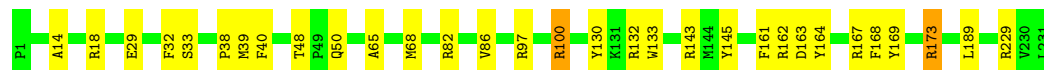
- Molecule 1: capsid protein

Chain i2: 82% 16%



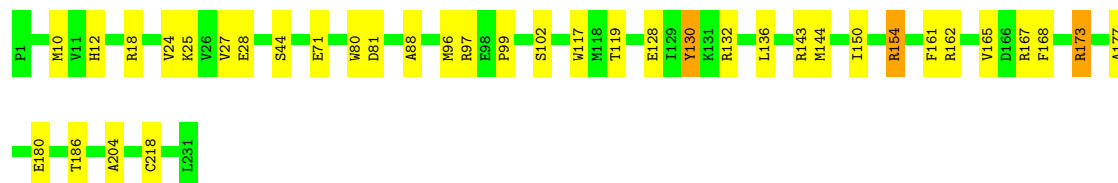
- Molecule 1: capsid protein

Chain i3: 87% 13%

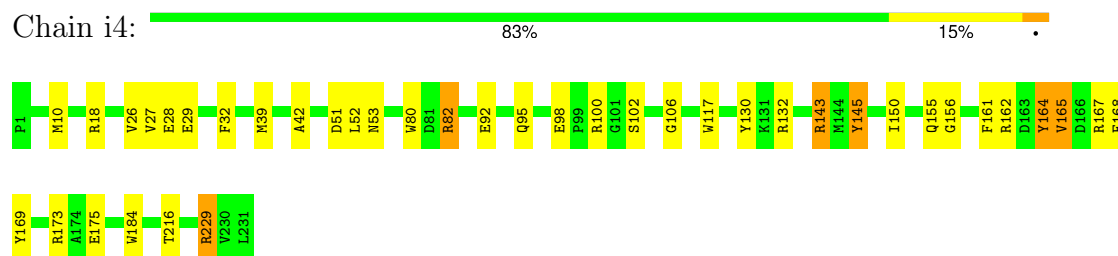


- Molecule 1: capsid protein

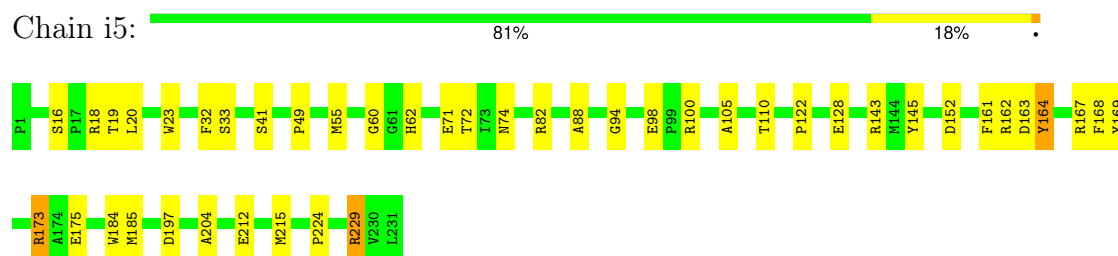
Chain 1N: 84% 15%



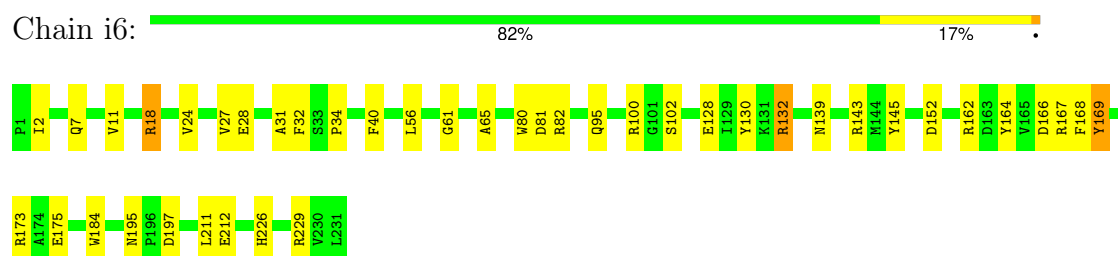
## • Molecule 1: capsid protein



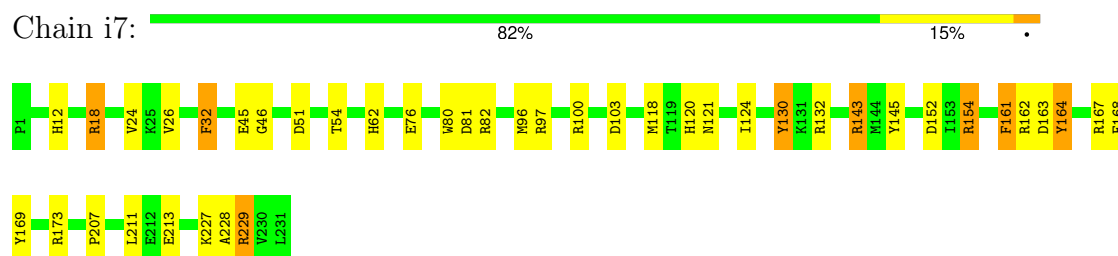
## • Molecule 1: capsid protein



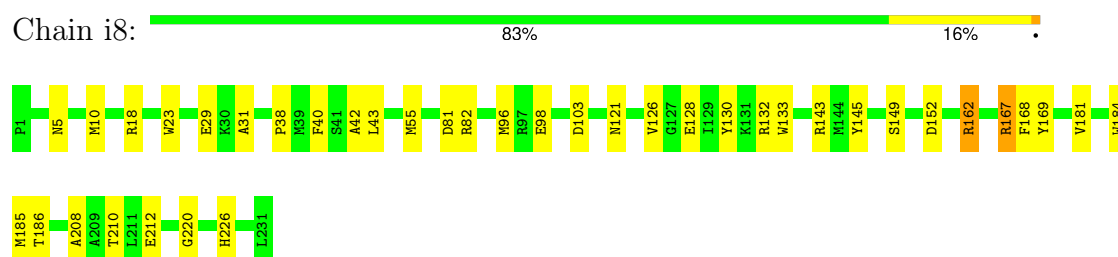
## • Molecule 1: capsid protein




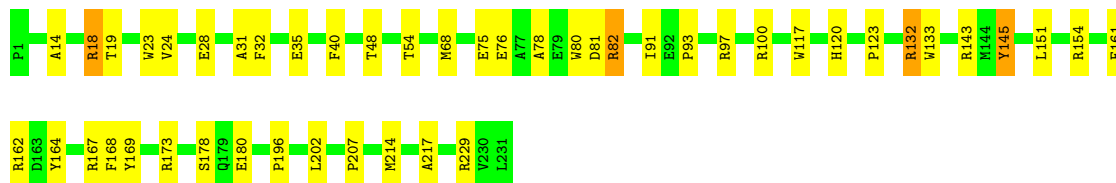
## • Molecule 1: capsid protein




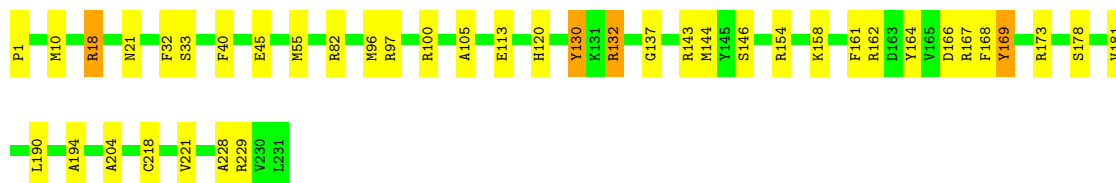
## • Molecule 1: capsid protein




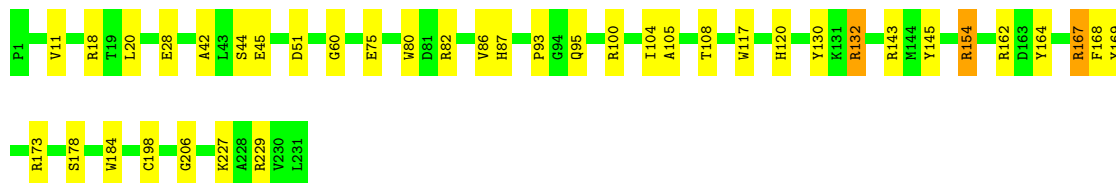
## • Molecule 1: capsid protein

Chain i9:  80% 19%


## • Molecule 1: capsid protein

Chain ia:  82% 16%


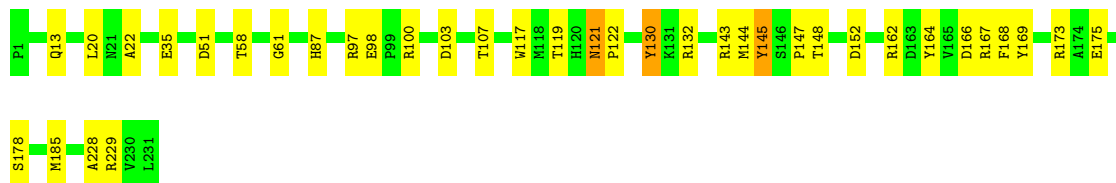
## • Molecule 1: capsid protein

Chain ib:  83% 16%


## • Molecule 1: capsid protein

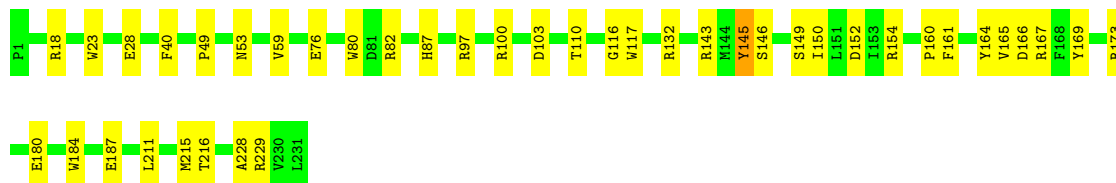
Chain ic:  78% 22%

## • Molecule 1: capsid protein


Chain id:  84% 15%

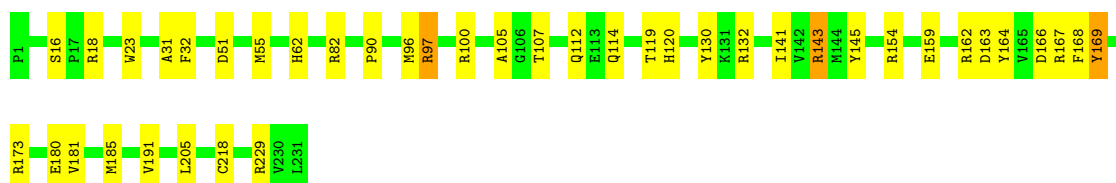
- Molecule 1: capsid protein

Chain 10:  82% 17%




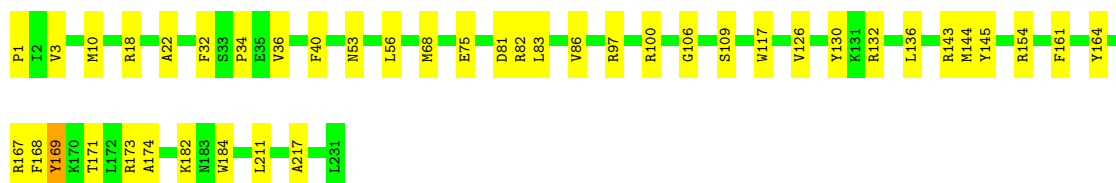
- Molecule 1: capsid protein

Chain ie:  82% 16%




- Molecule 1: capsid protein

Chain if:  82% 18%




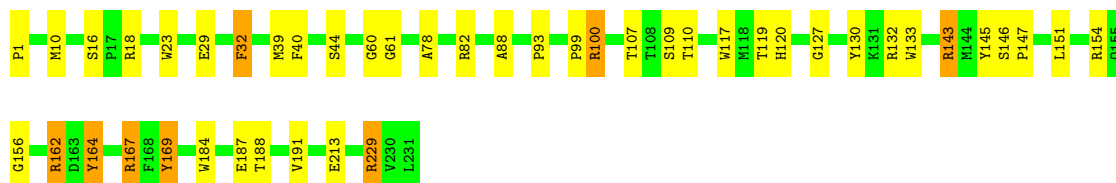
- Molecule 1: capsid protein

Chain ig:  80% 18%

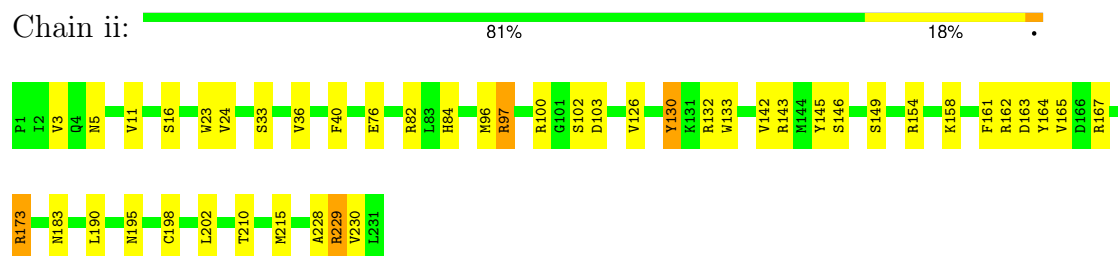


- Molecule 1: capsid protein

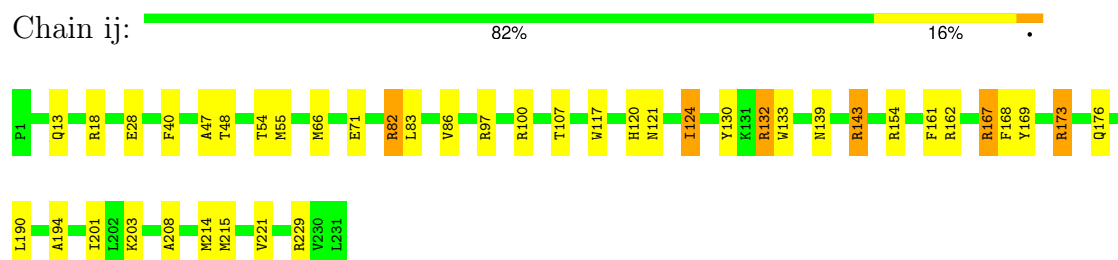
Chain ih:  81% 16%



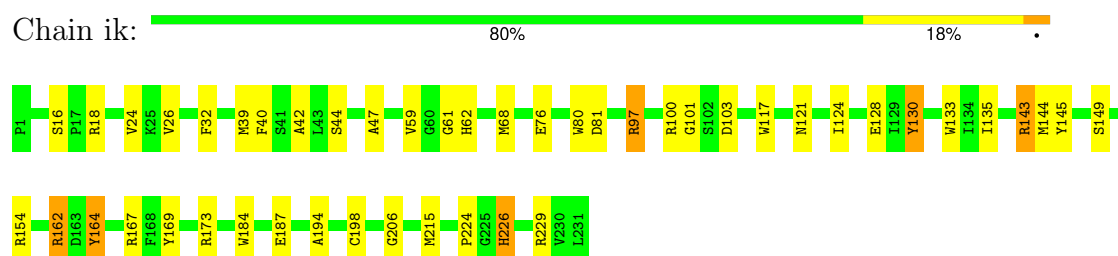
- Molecule 1: capsid protein



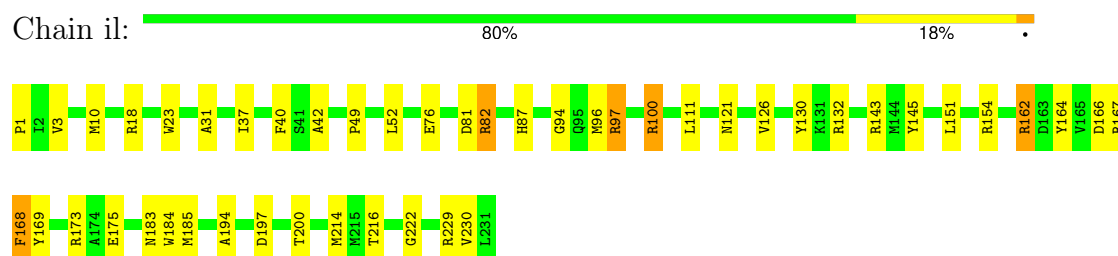
- Molecule 1: capsid protein



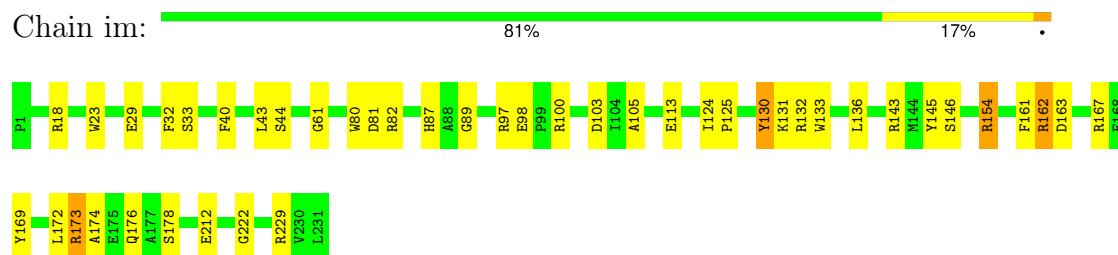
- Molecule 1: capsid protein



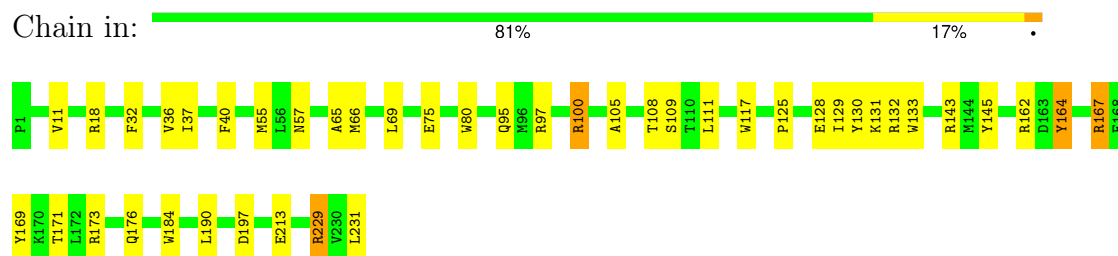
- Molecule 1: capsid protein



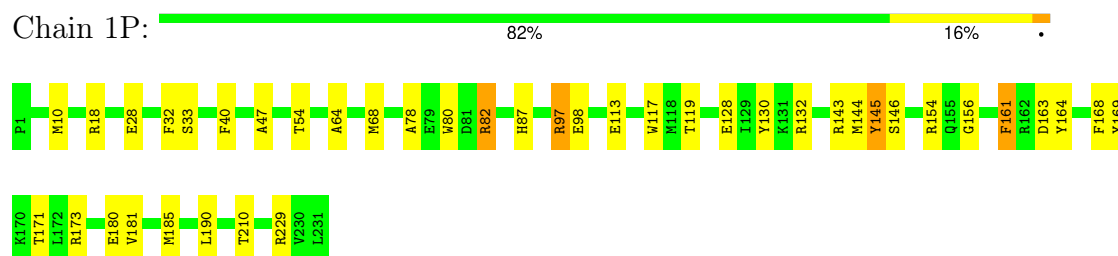
- Molecule 1: capsid protein



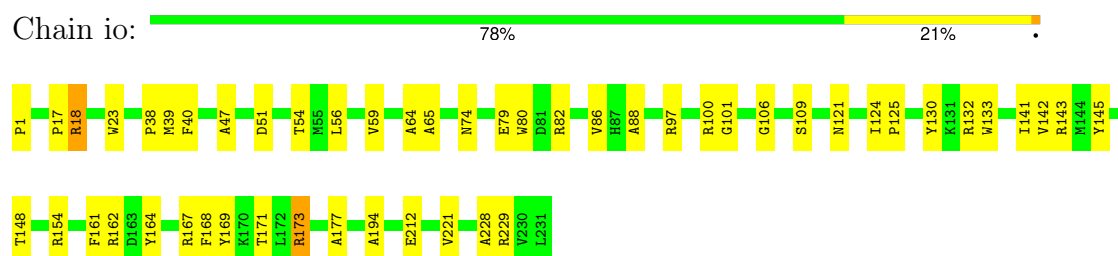
## • Molecule 1: capsid protein



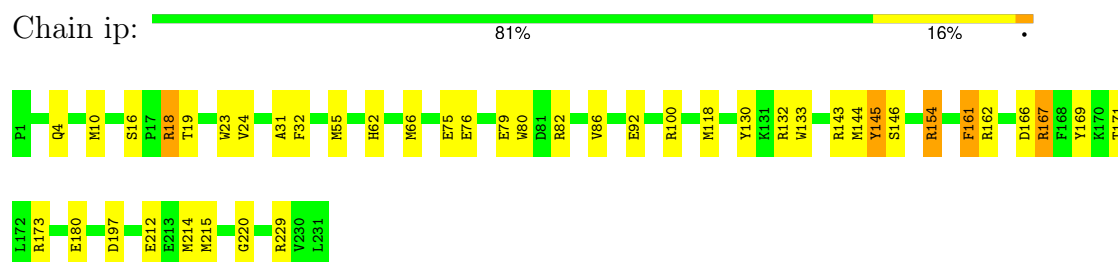
## • Molecule 1: capsid protein



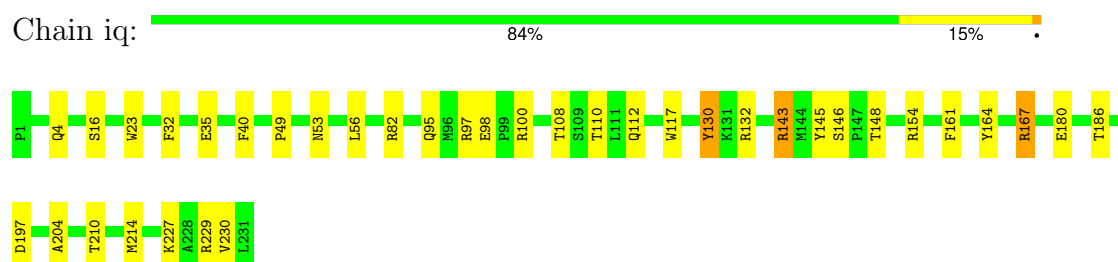
## • Molecule 1: capsid protein



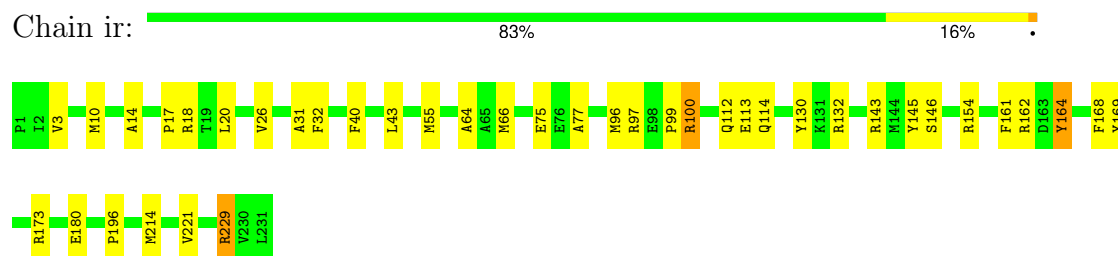
## • Molecule 1: capsid protein



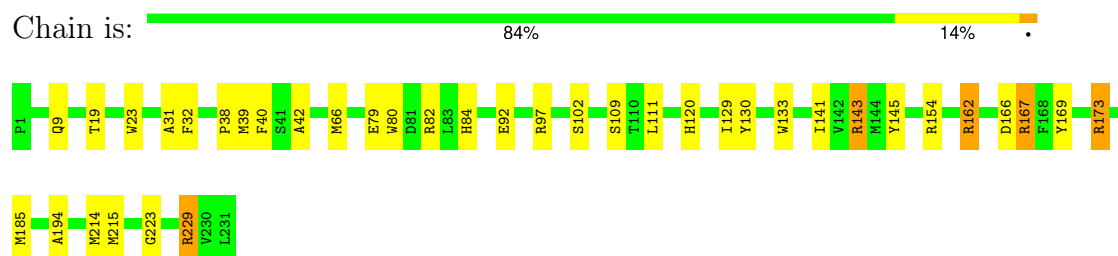
## • Molecule 1: capsid protein



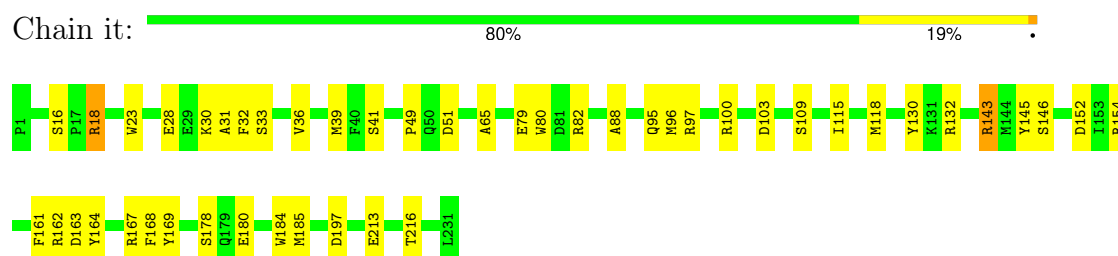
## • Molecule 1: capsid protein



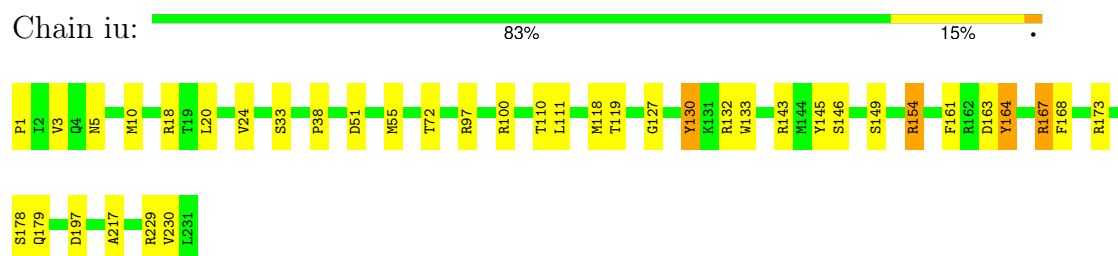
## • Molecule 1: capsid protein



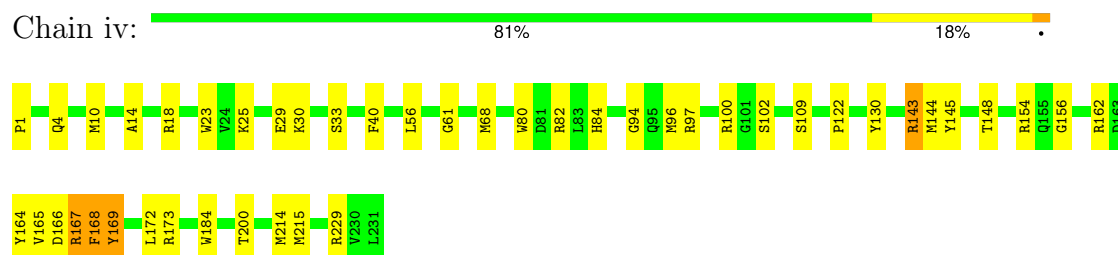
## • Molecule 1: capsid protein




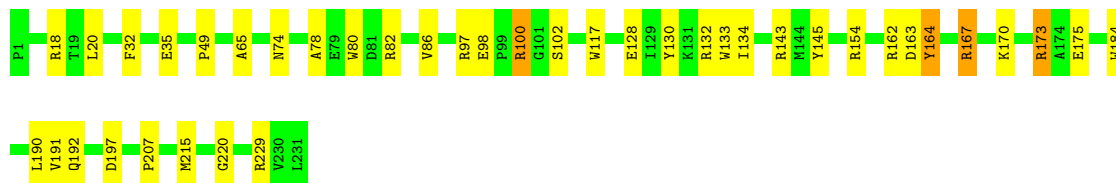
## • Molecule 1: capsid protein




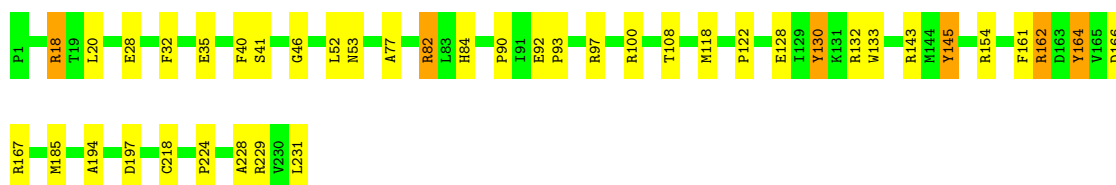
## • Molecule 1: capsid protein




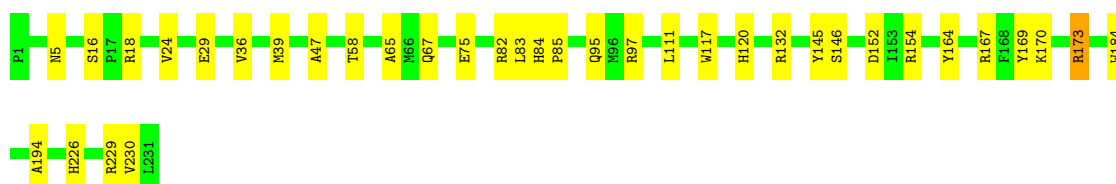
## • Molecule 1: capsid protein

Chain iw:  83% 16%


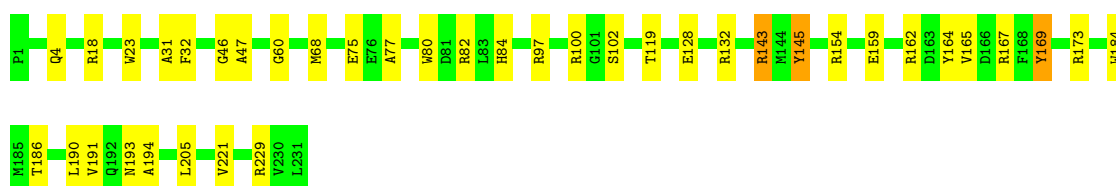
## • Molecule 1: capsid protein

Chain ix:  82% 15%

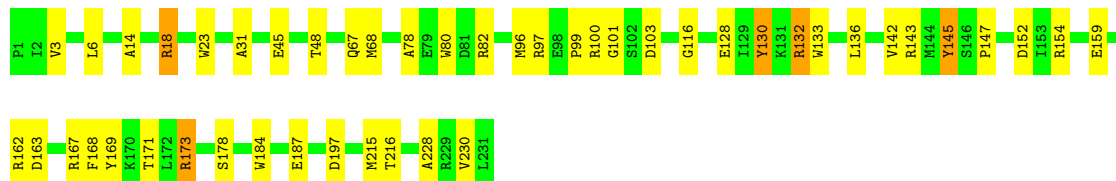
## • Molecule 1: capsid protein

Chain 1Q:  84% 15%

## • Molecule 1: capsid protein

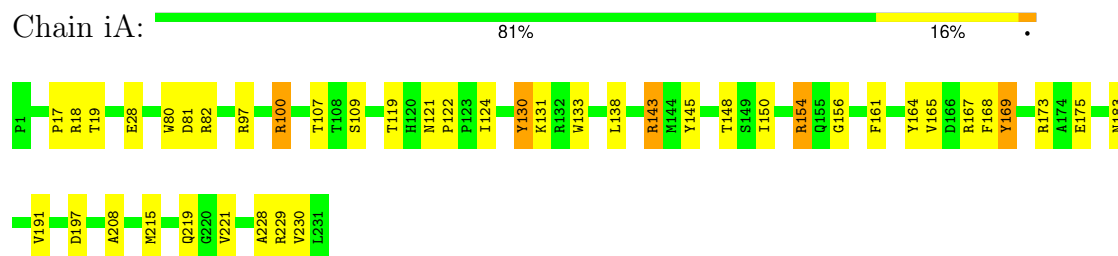
Chain iy:  83% 16%

## • Molecule 1: capsid protein

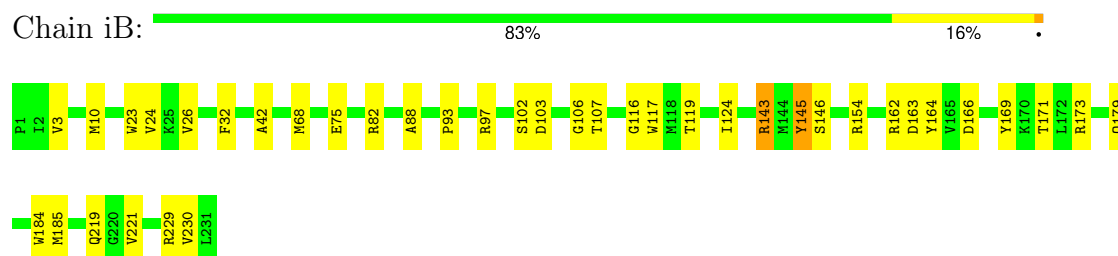
Chain iz:  80% 18%



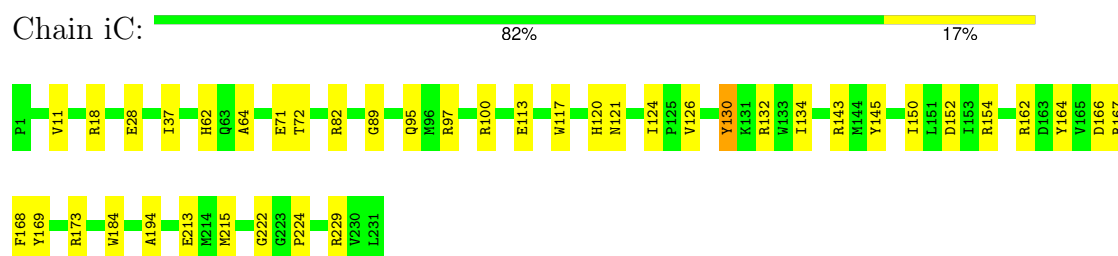
- Molecule 1: capsid protein



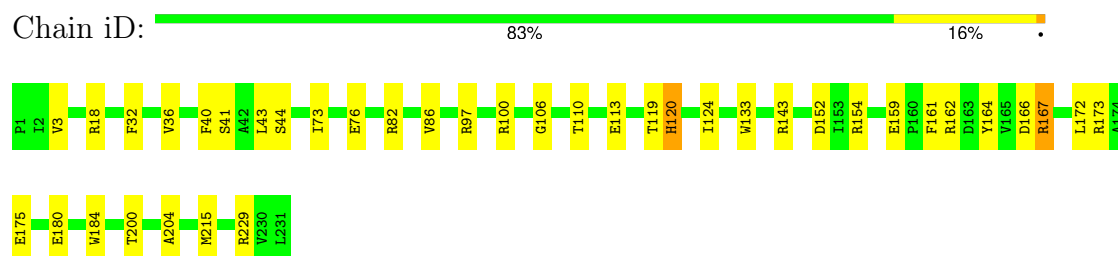
- Molecule 1: capsid protein



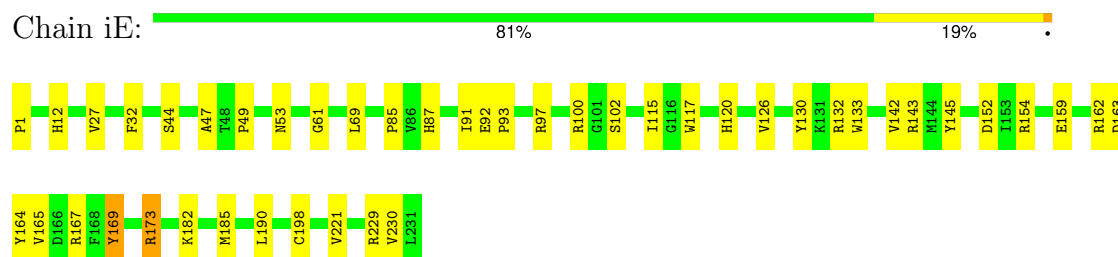
- Molecule 1: capsid protein



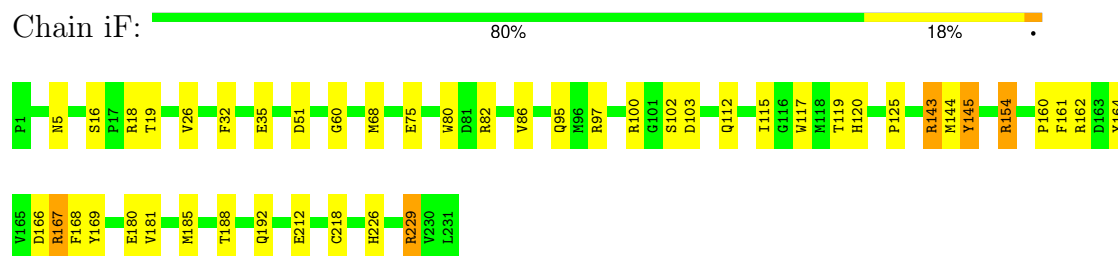
- Molecule 1: capsid protein



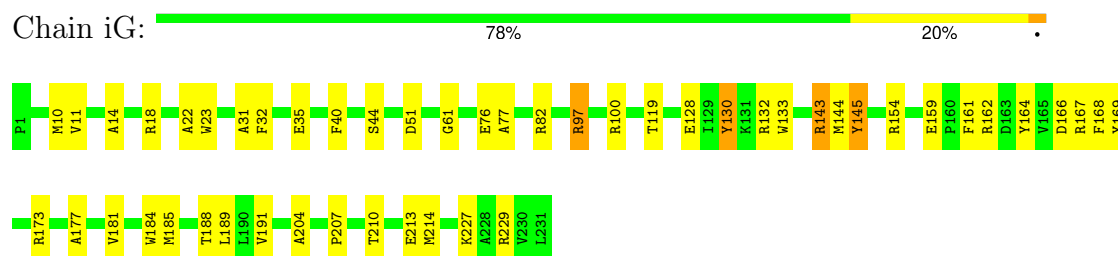
- Molecule 1: capsid protein



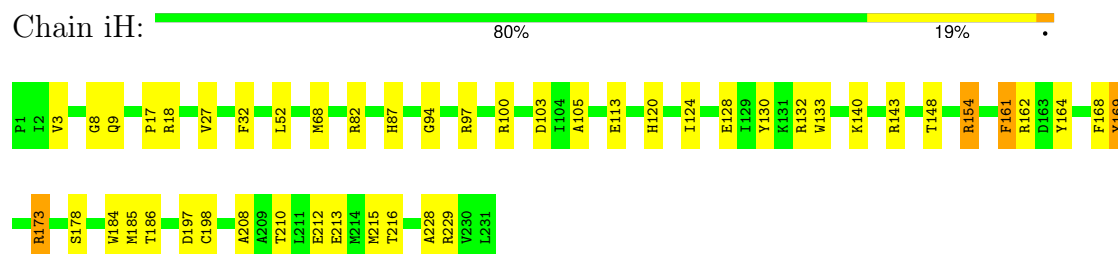
## • Molecule 1: capsid protein



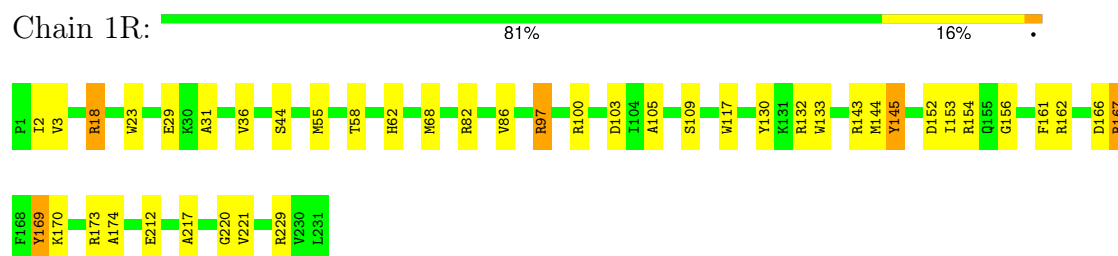
## • Molecule 1: capsid protein



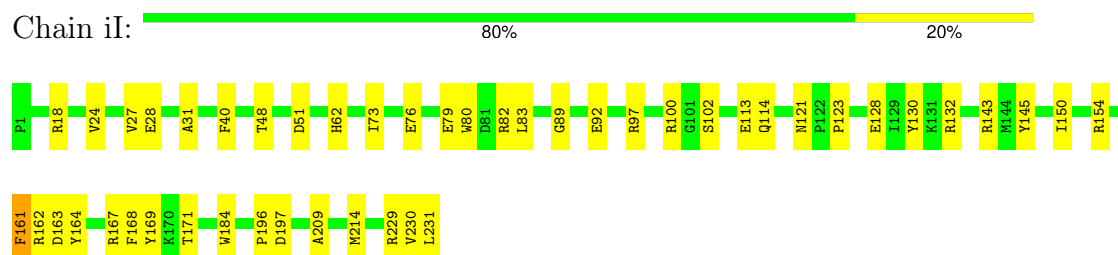
## • Molecule 1: capsid protein



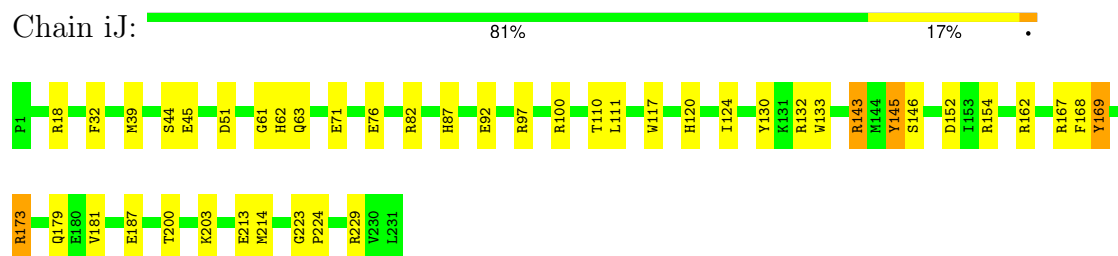
## • Molecule 1: capsid protein



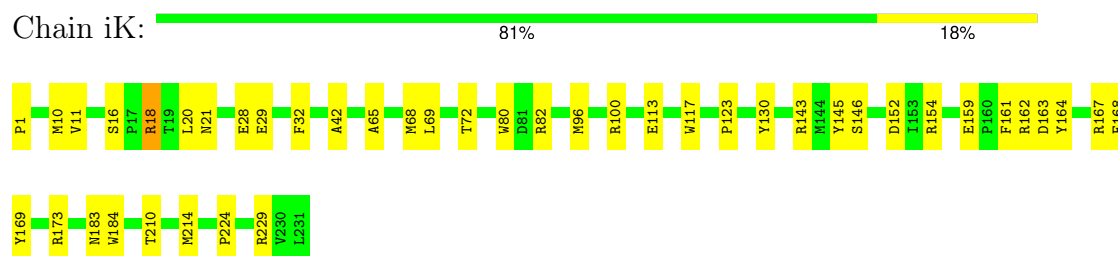
## • Molecule 1: capsid protein



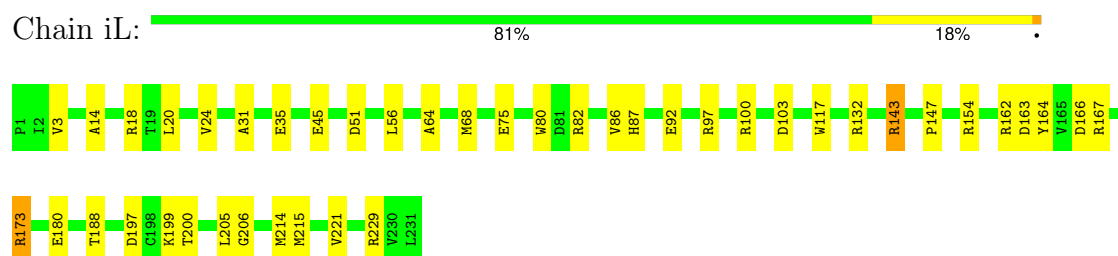
## • Molecule 1: capsid protein



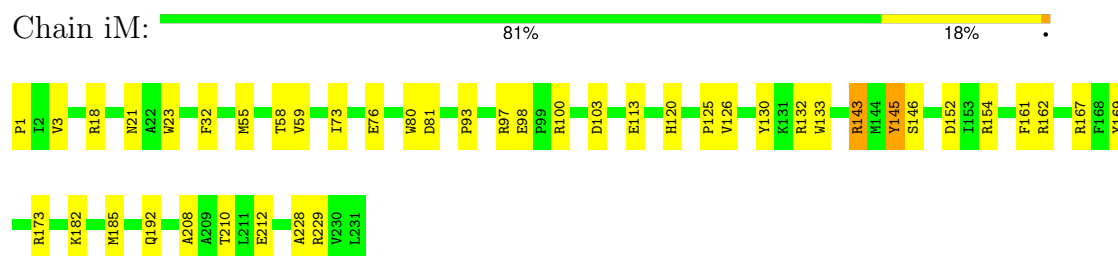
## • Molecule 1: capsid protein



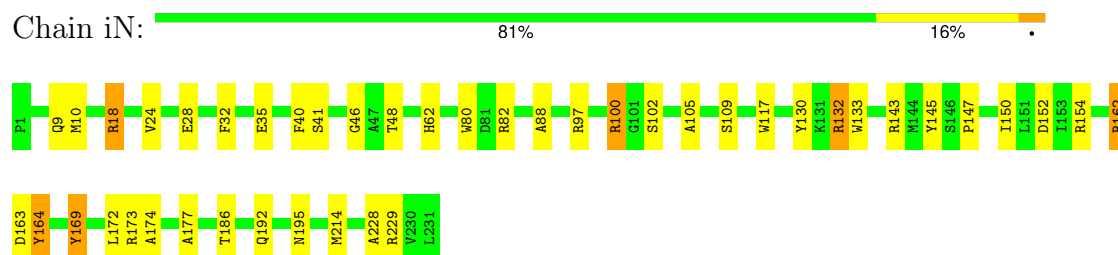
## • Molecule 1: capsid protein



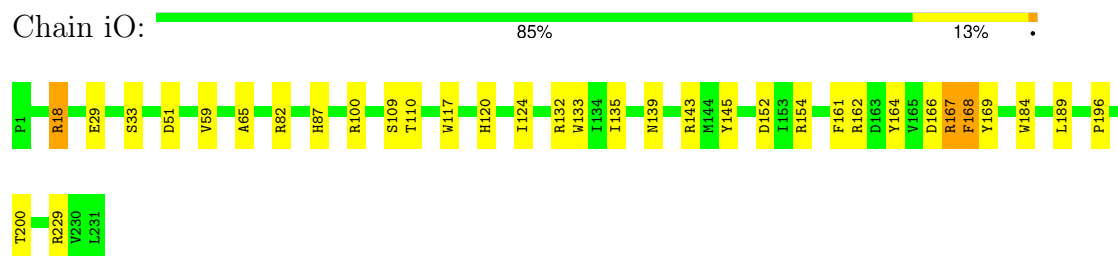
## • Molecule 1: capsid protein



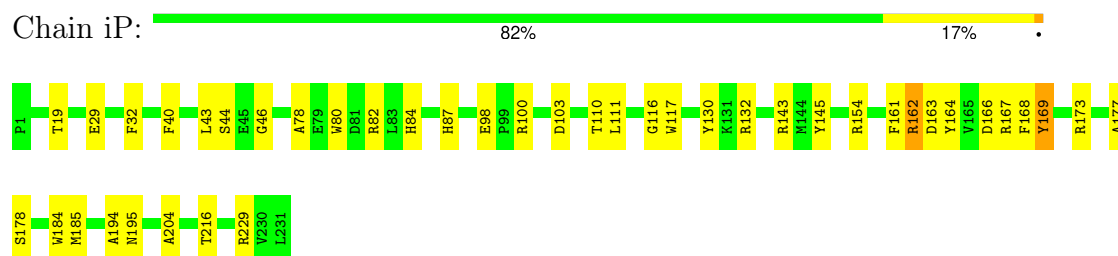
## • Molecule 1: capsid protein



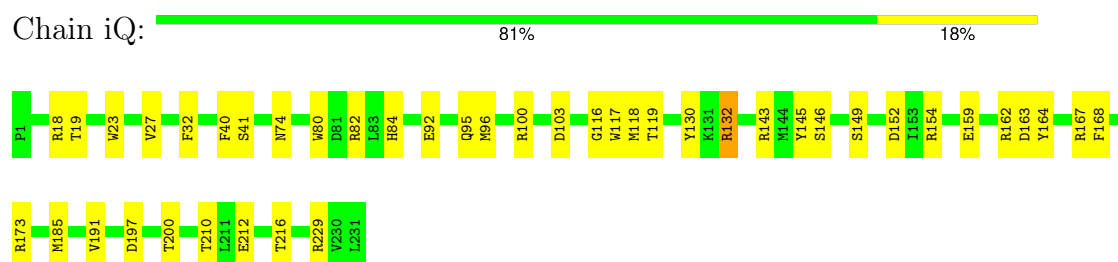
## • Molecule 1: capsid protein



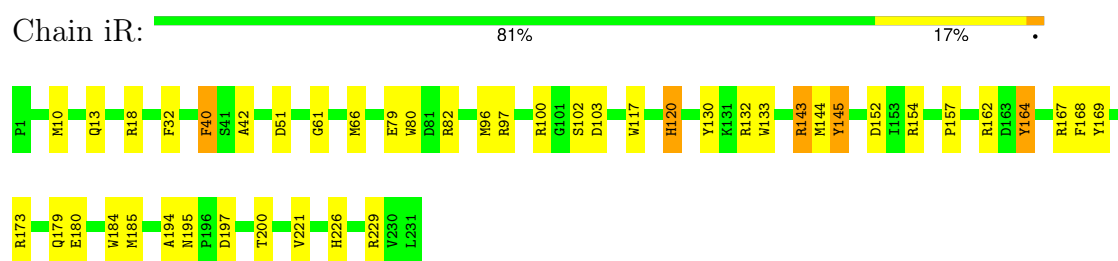
## • Molecule 1: capsid protein



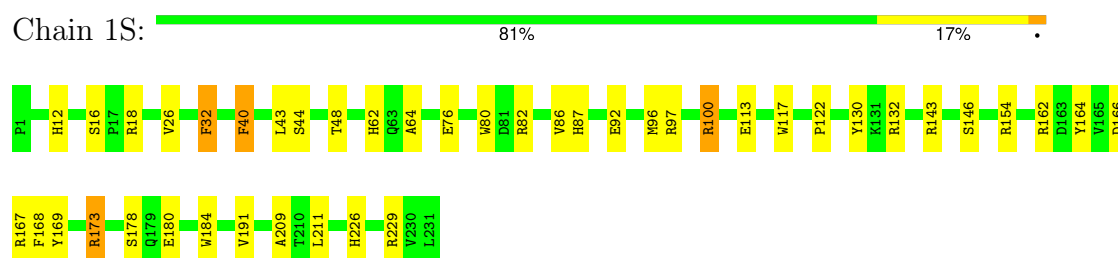
## • Molecule 1: capsid protein



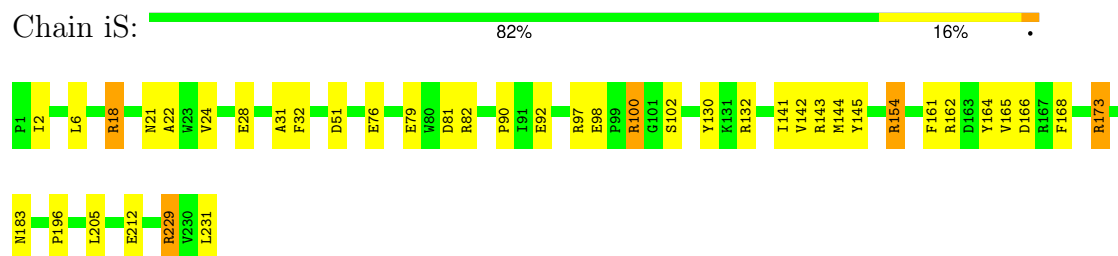
## • Molecule 1: capsid protein



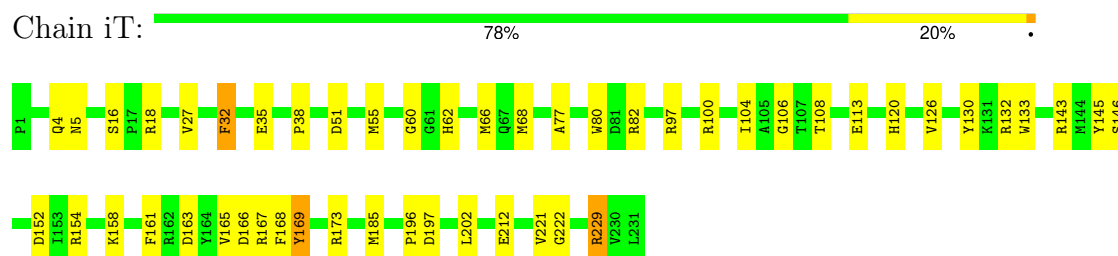
## • Molecule 1: capsid protein



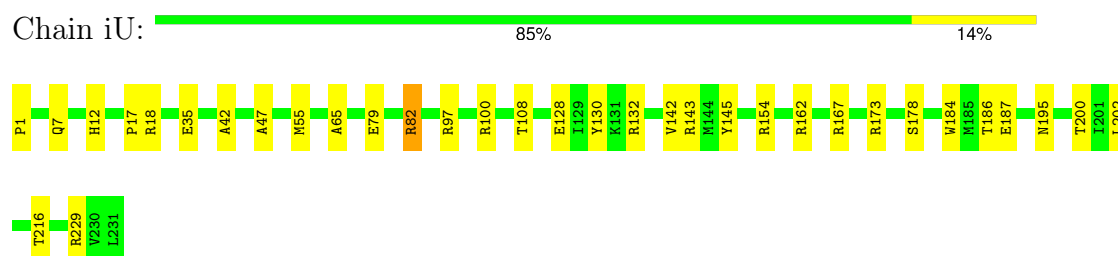
## • Molecule 1: capsid protein



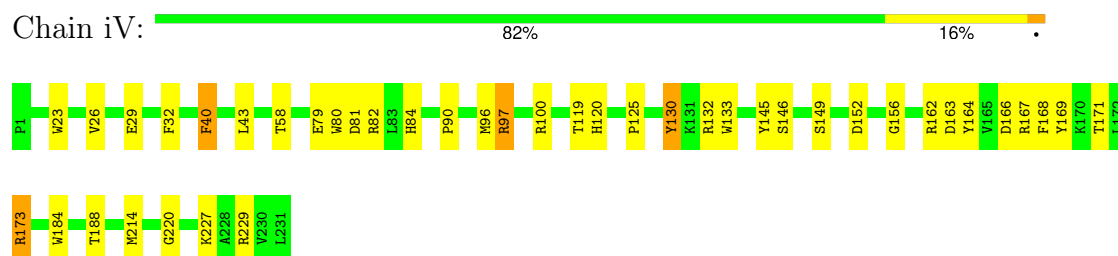
## • Molecule 1: capsid protein



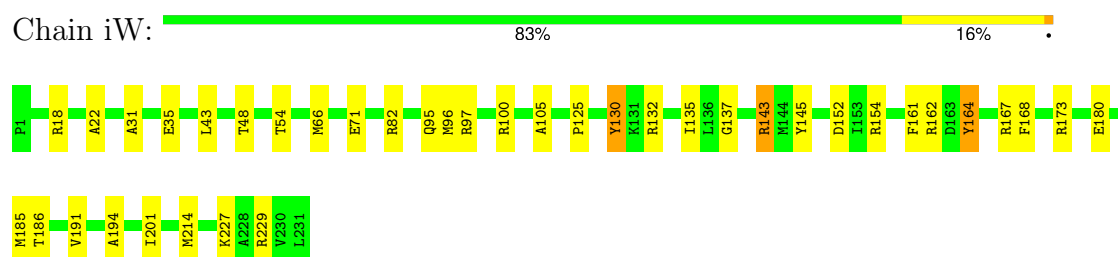
## • Molecule 1: capsid protein



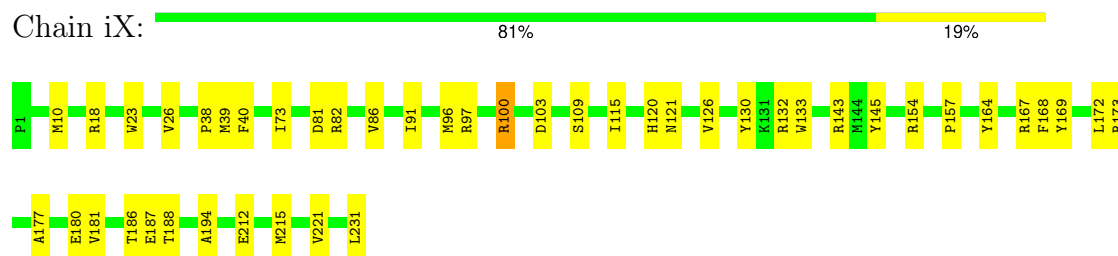
## • Molecule 1: capsid protein



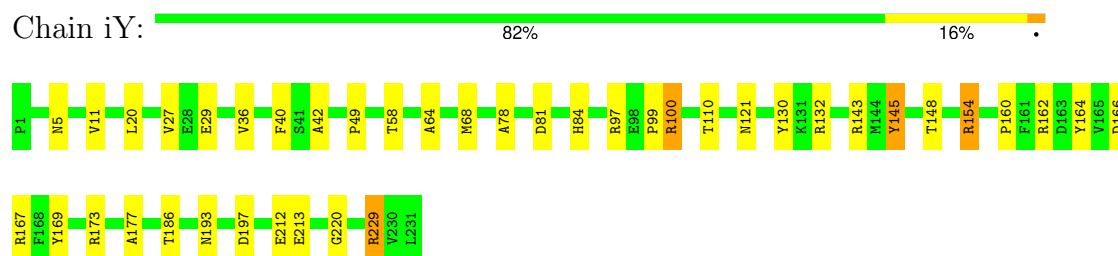
## • Molecule 1: capsid protein



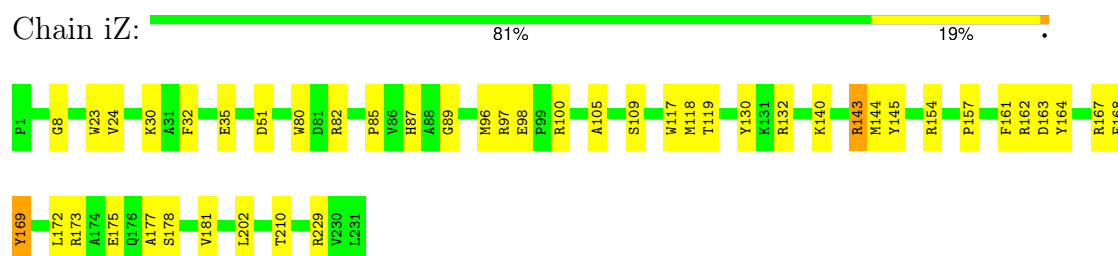
## • Molecule 1: capsid protein



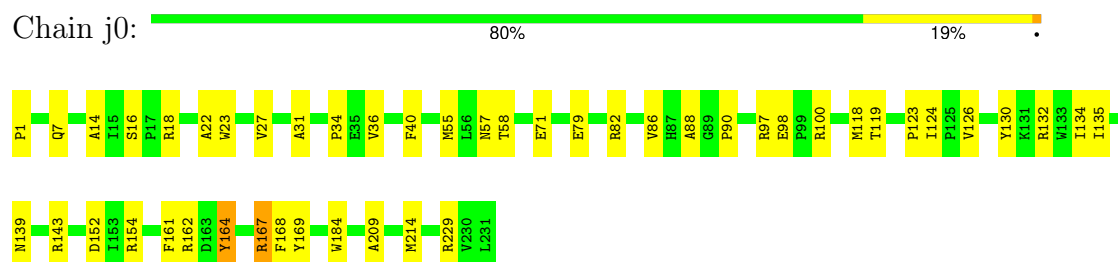
## • Molecule 1: capsid protein



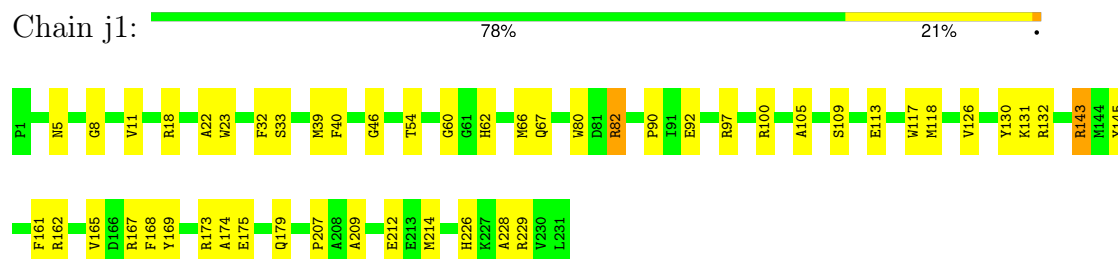
## • Molecule 1: capsid protein



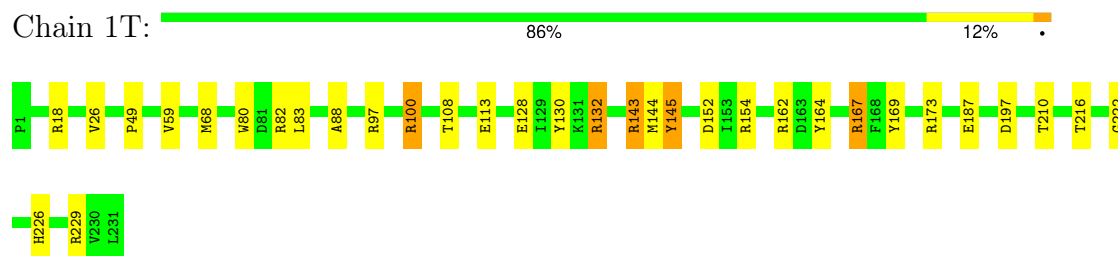
## • Molecule 1: capsid protein



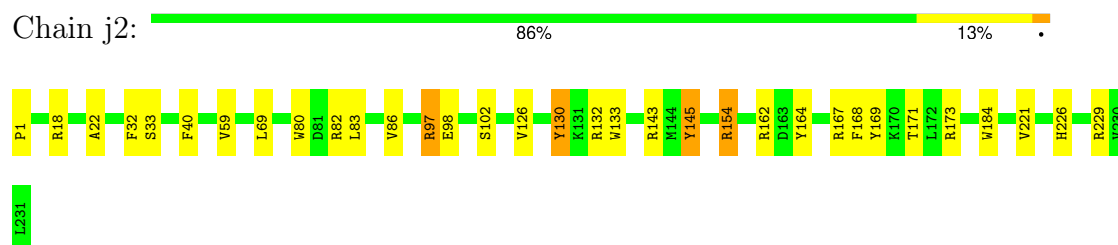
## • Molecule 1: capsid protein



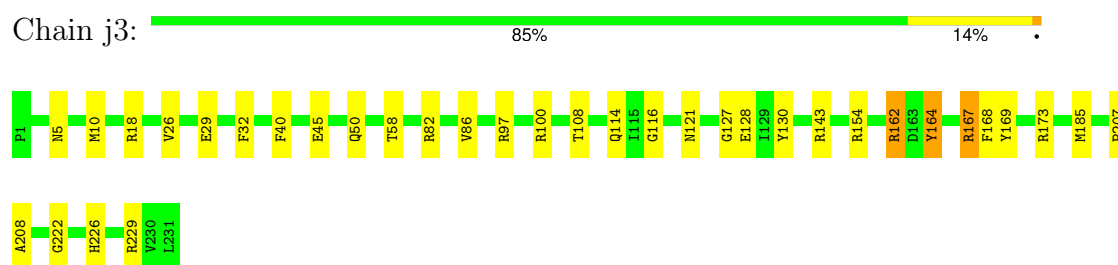
- Molecule 1: capsid protein



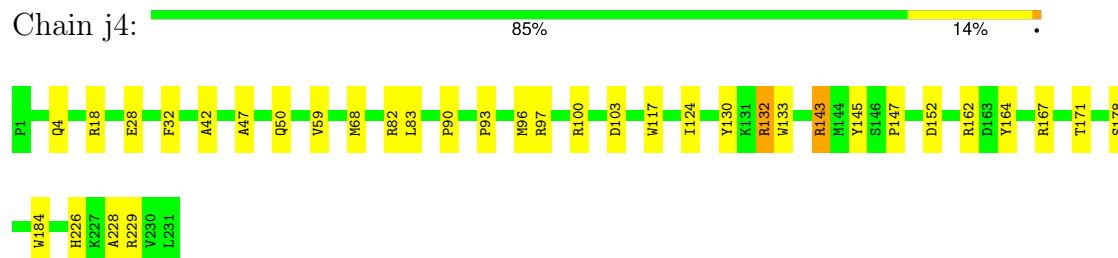
- Molecule 1: capsid protein



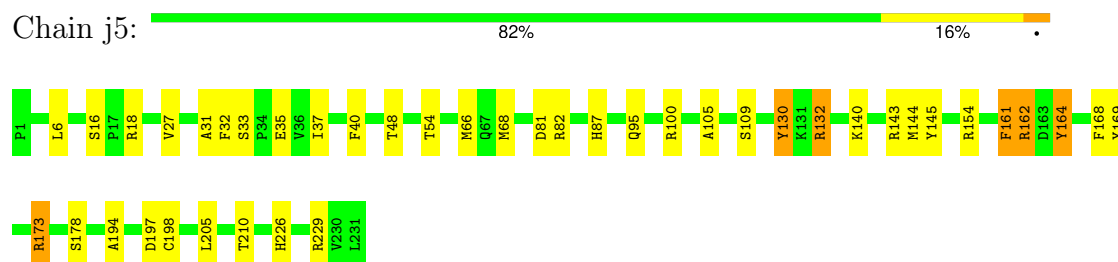
- Molecule 1: capsid protein



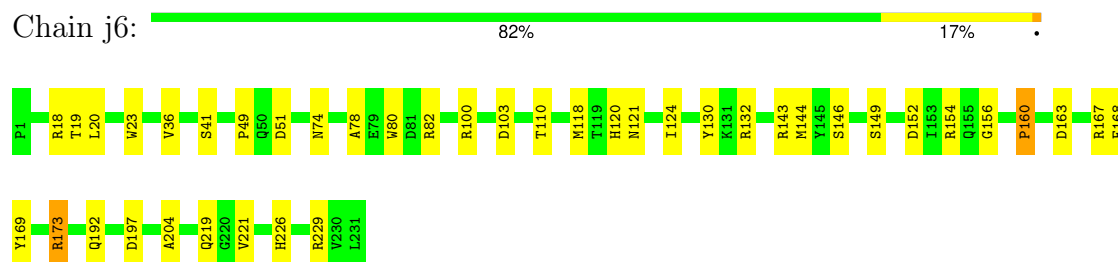
- Molecule 1: capsid protein



- Molecule 1: capsid protein



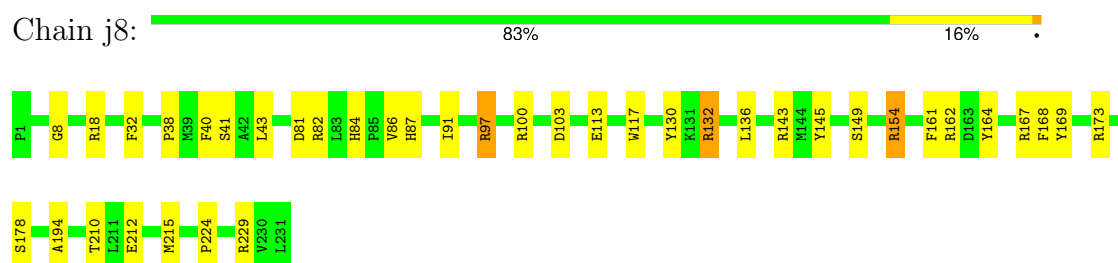
- Molecule 1: capsid protein



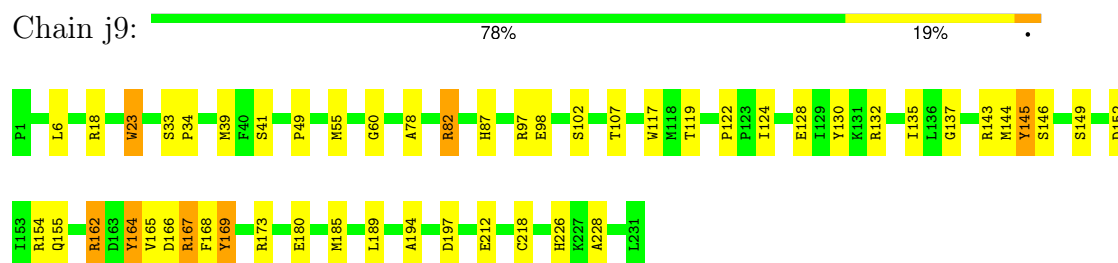
- Molecule 1: capsid protein



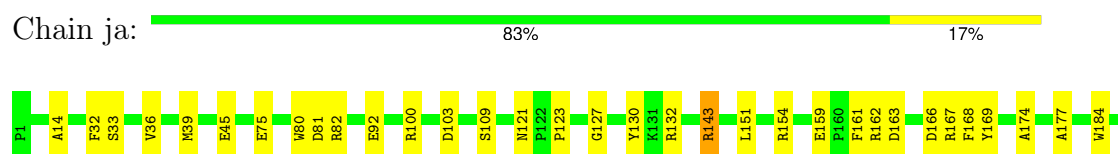
- Molecule 1: capsid protein



- Molecule 1: capsid protein



- Molecule 1: capsid protein







- Molecule 1: capsid protein

Chain jb: 77% 20% .



- Molecule 1: capsid protein

Chain 1U: 84% 14% .



- Molecule 1: capsid protein

Chain jc: 83% 16% .



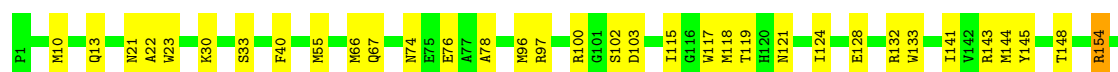
- Molecule 1: capsid protein

Chain jd: 86% 13% .



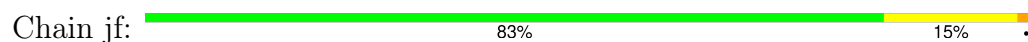
- Molecule 1: capsid protein

Chain je: 78% 20% .

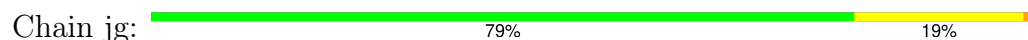




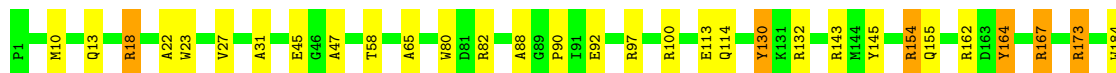
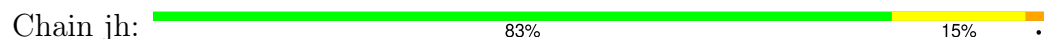
- Molecule 1: capsid protein



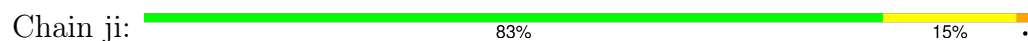
- Molecule 1: capsid protein



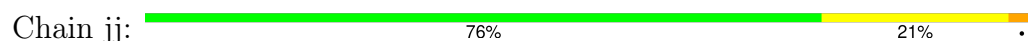
- Molecule 1: capsid protein

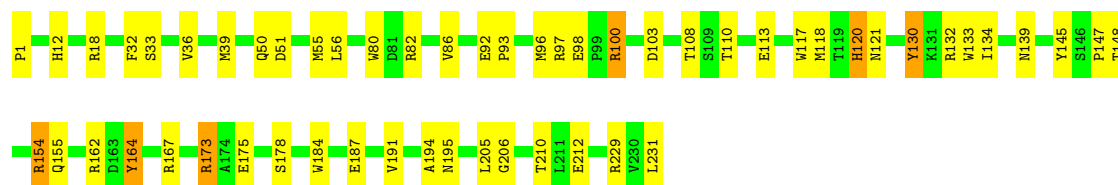


- Molecule 1: capsid protein



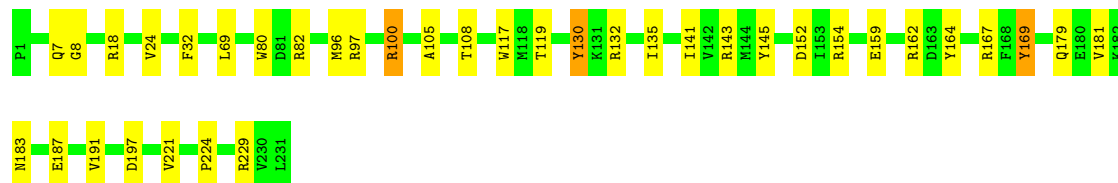
- Molecule 1: capsid protein





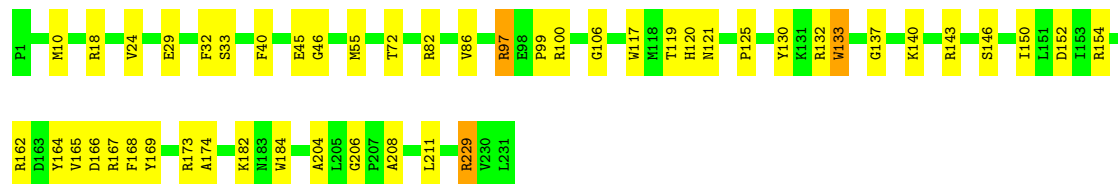
- Molecule 1: capsid protein

Chain jk: 84% 15% •



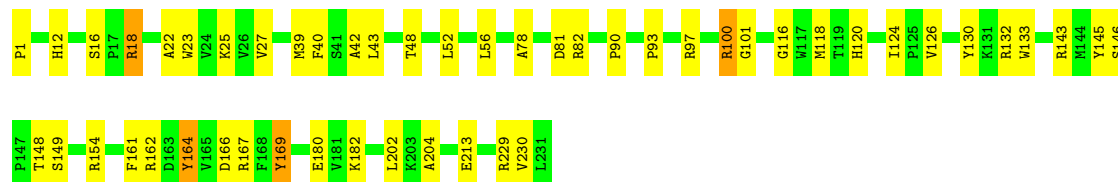
- Molecule 1: capsid protein

Chain jl: 79% 19% •



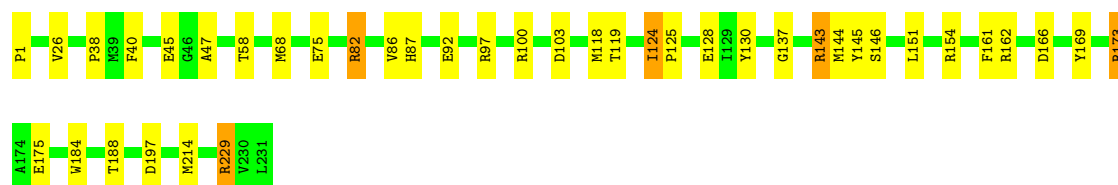
- Molecule 1: capsid protein

Chain 1V: 78% 20% •




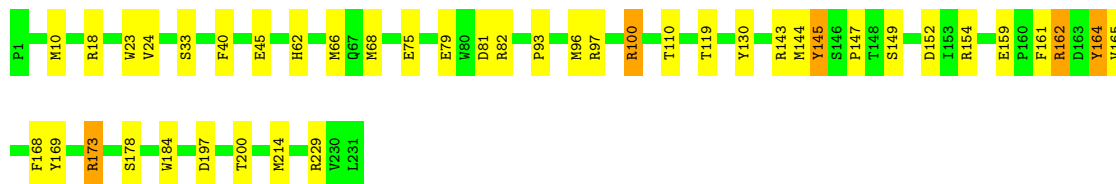
- Molecule 1: capsid protein

Chain jm: 83% 15% •




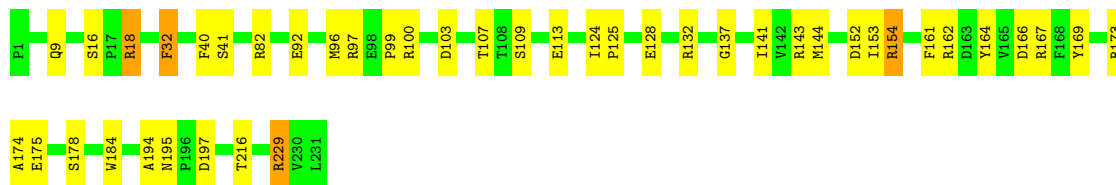
- Molecule 1: capsid protein

Chain jn:  82% 16%




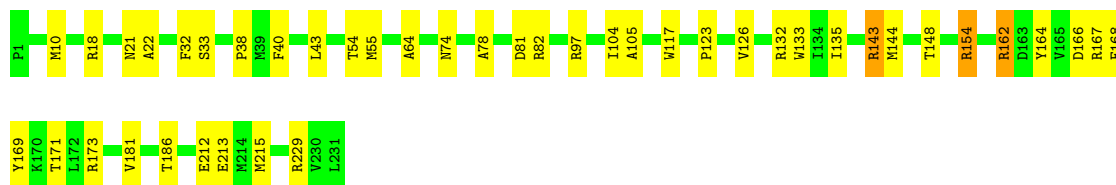
- Molecule 1: capsid protein

Chain jo:  81% 17%




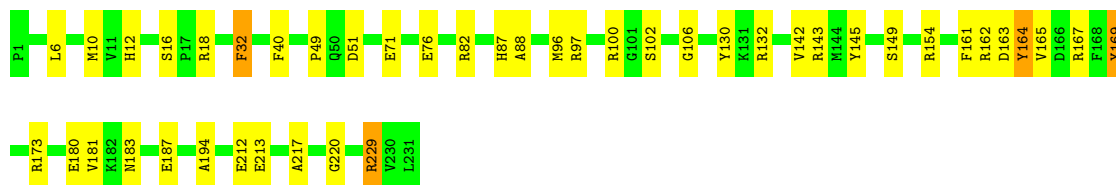
- Molecule 1: capsid protein

Chain jp:  81% 17%




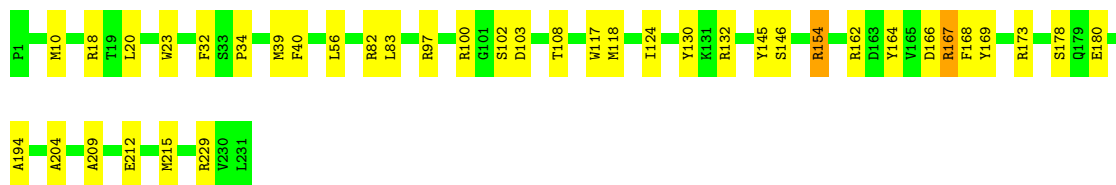
- Molecule 1: capsid protein

Chain jq:  81% 17%

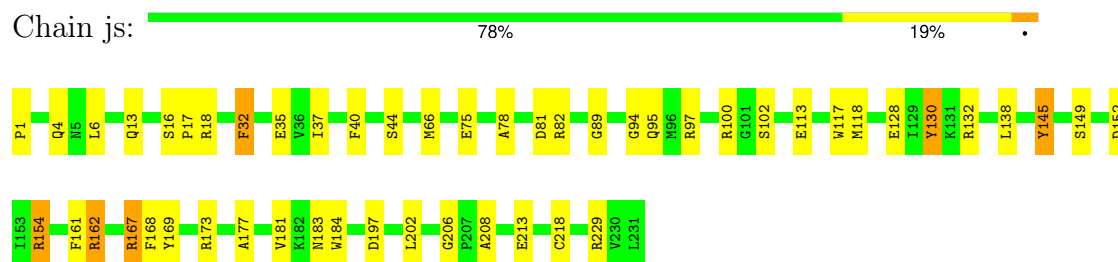


- Molecule 1: capsid protein

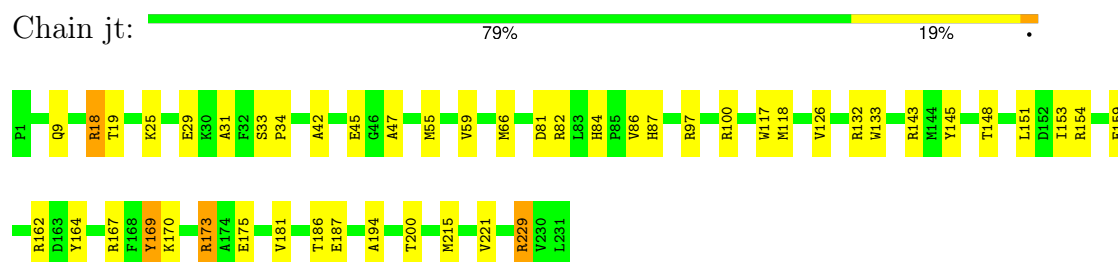
Chain jr:  83% 16%



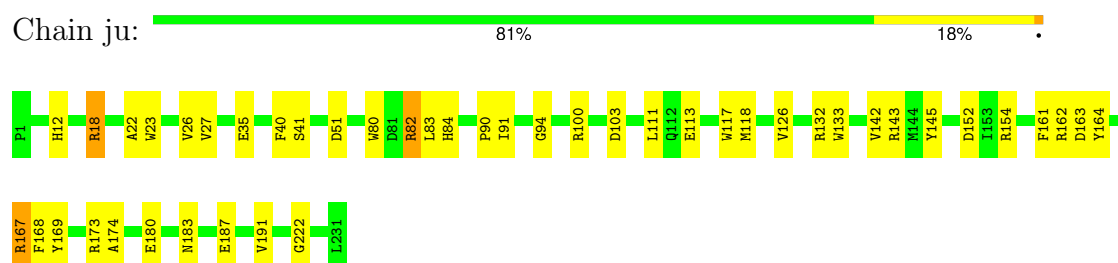
## • Molecule 1: capsid protein



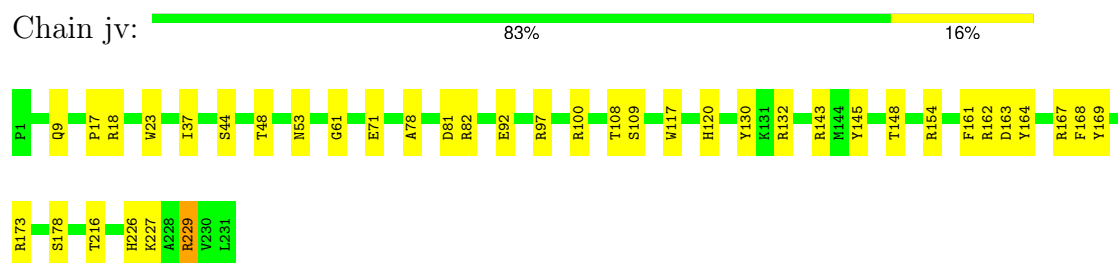
## • Molecule 1: capsid protein



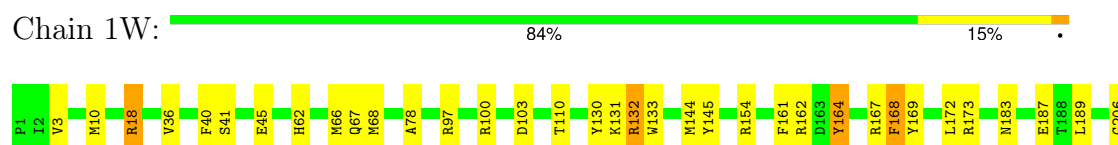
## • Molecule 1: capsid protein



## • Molecule 1: capsid protein



## • Molecule 1: capsid protein





- Molecule 1: capsid protein

Chain jw: 83% 15% •



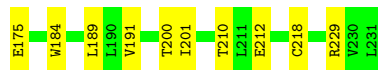
- Molecule 1: capsid protein

Chain jx: 81% 17% •



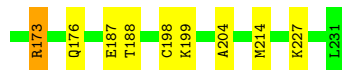
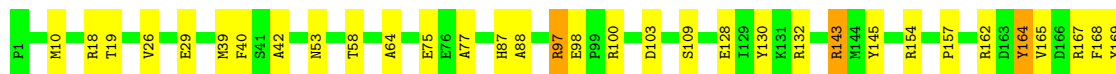
- Molecule 1: capsid protein

Chain jy: 81% 18%



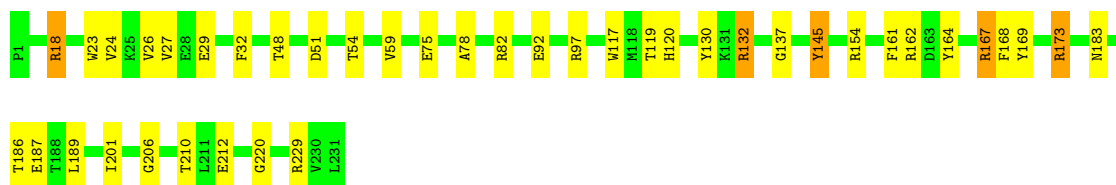
- Molecule 1: capsid protein

Chain jz: 82% 16% •



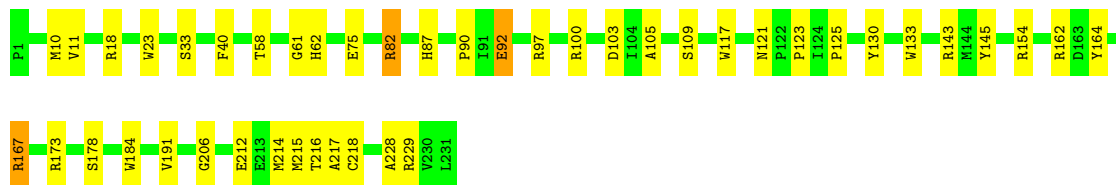
- Molecule 1: capsid protein

Chain jA: 82% 16% •



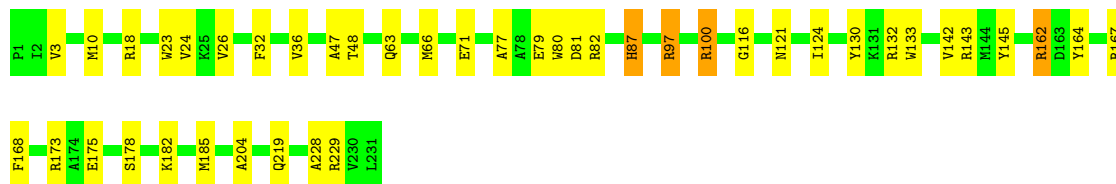
- Molecule 1: capsid protein

Chain jB: 81% 18% .



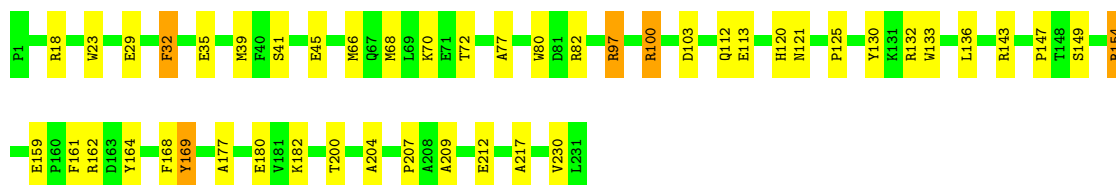
- Molecule 1: capsid protein

Chain jC: 81% 17% .



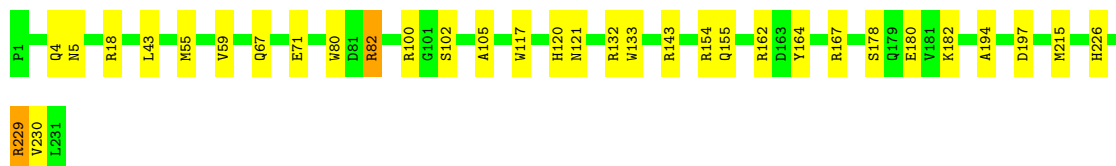
- Molecule 1: capsid protein

Chain jD: 80% 18% .



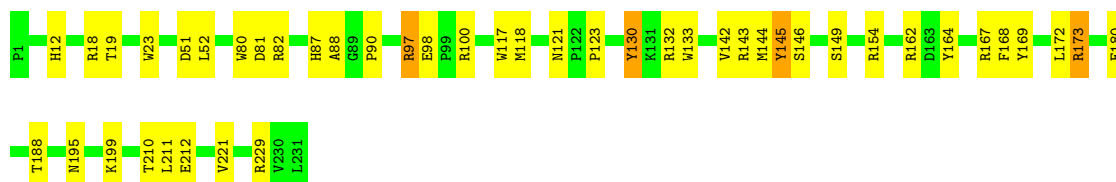
- Molecule 1: capsid protein

Chain jE: 86% 13% .



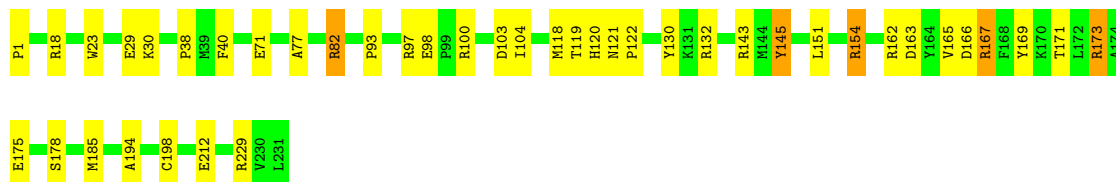
- Molecule 1: capsid protein

Chain jF: 81% 18% .



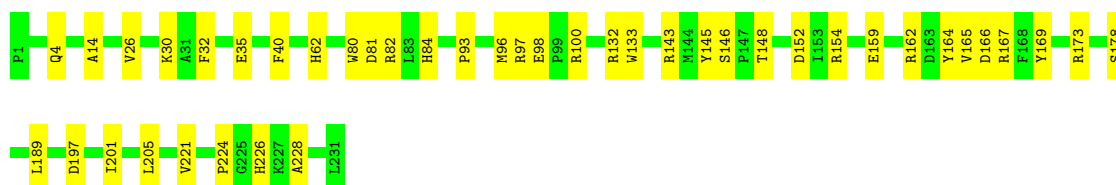
- Molecule 1: capsid protein

Chain 1X: 82% 16%



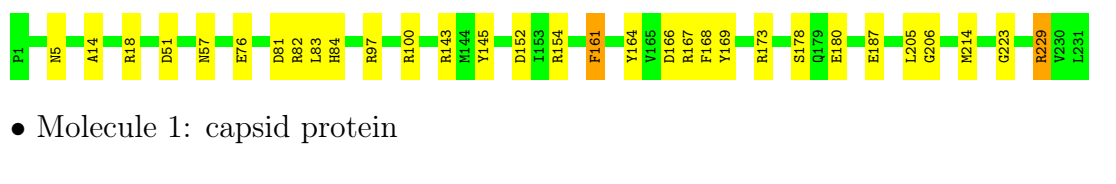
- Molecule 1: capsid protein

Chain jG: 82% 18%



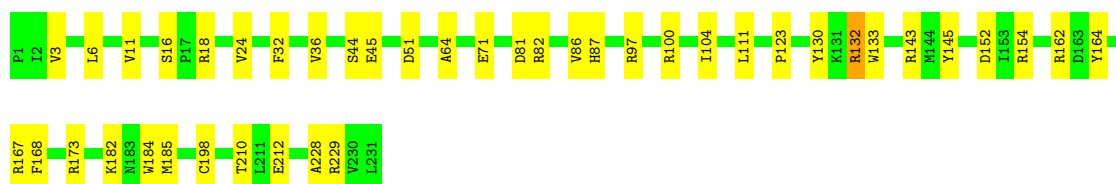
- Molecule 1: capsid protein

Chain jH: 87% 13%



- Molecule 1: capsid protein

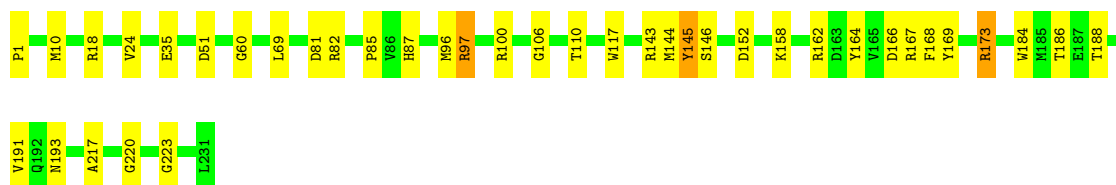
Chain jI: 82% 18%



- Molecule 1: capsid protein

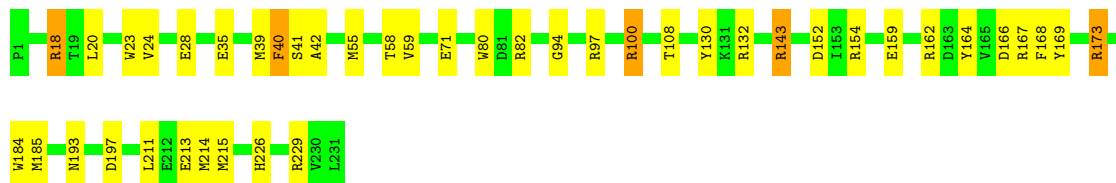
Chain jJ: 83% 16%





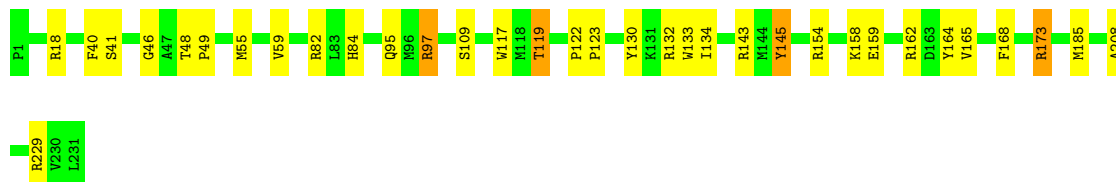
- Molecule 1: capsid protein

Chain jK: 81% 16%



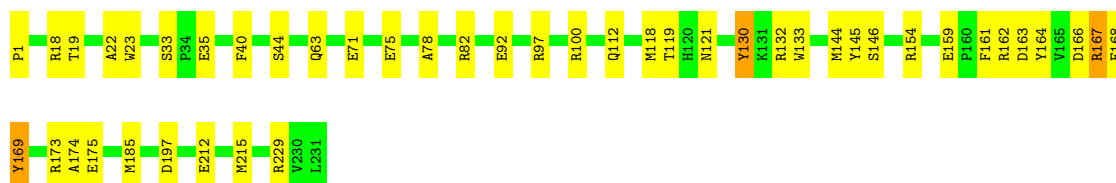
- Molecule 1: capsid protein

Chain jL: 85% 13%



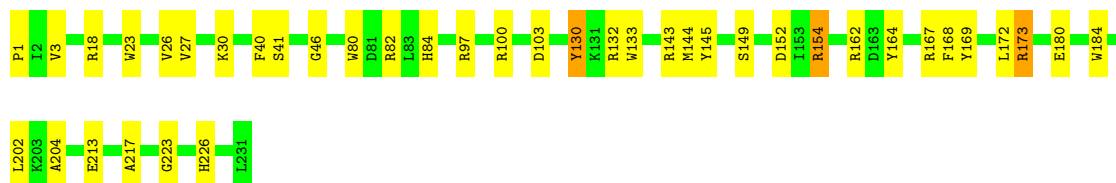
- Molecule 1: capsid protein

Chain jM: 81% 18%




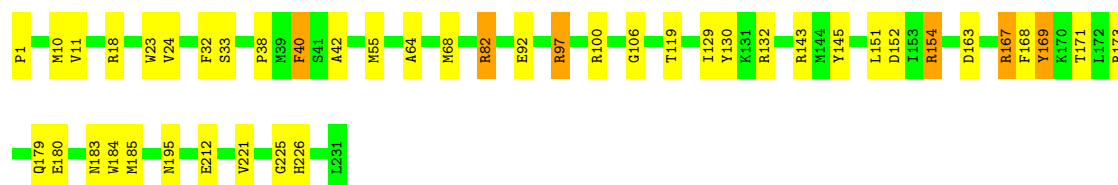
- Molecule 1: capsid protein

Chain jN: 83% 16%




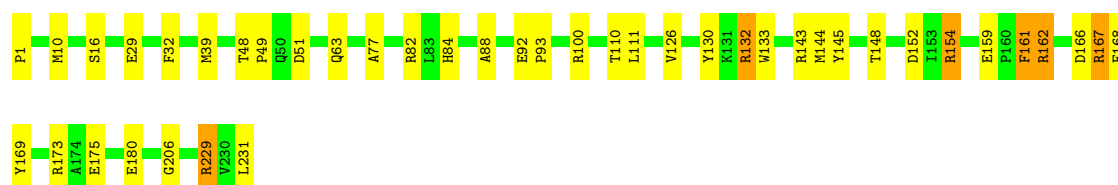
- Molecule 1: capsid protein

Chain jO:  81% 16% .




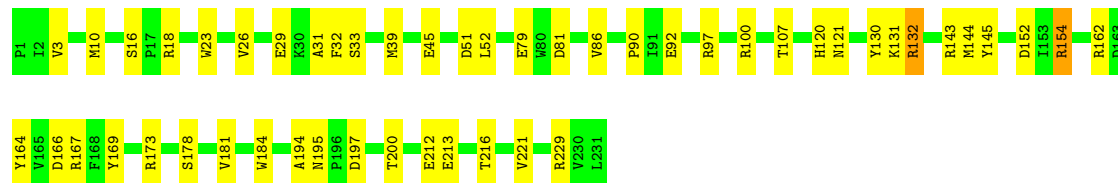
- Molecule 1: capsid protein

Chain jP:  82% 16% .




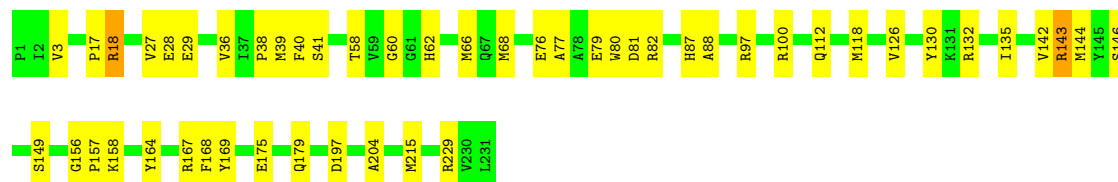
- Molecule 1: capsid protein

Chain 1Y:  78% 21% .




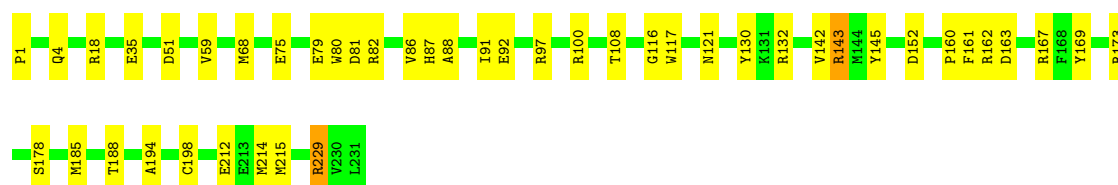
- Molecule 1: capsid protein

Chain jQ:  78% 21% .

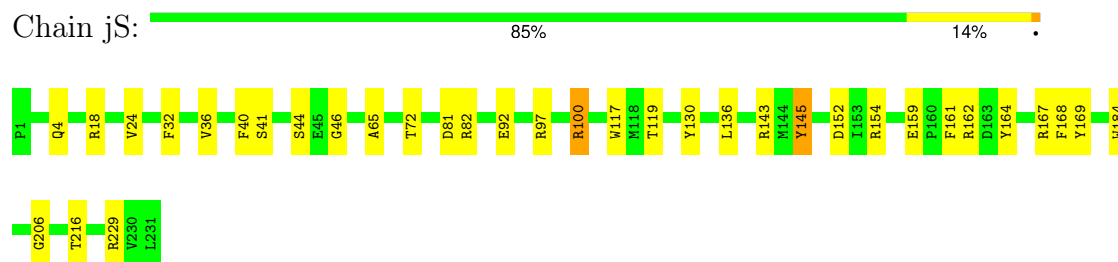


- Molecule 1: capsid protein

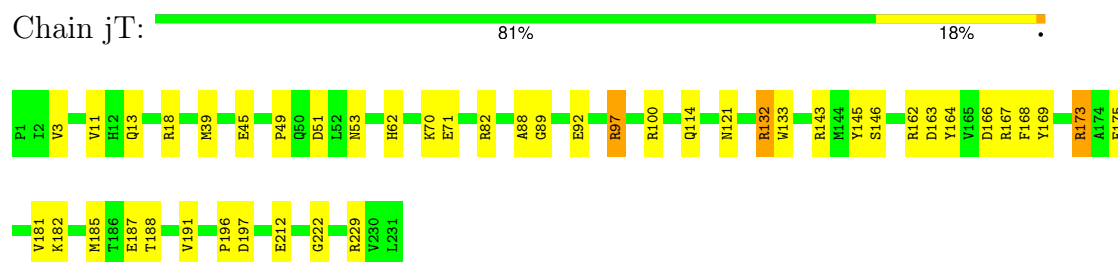
Chain jR:  81% 19% .



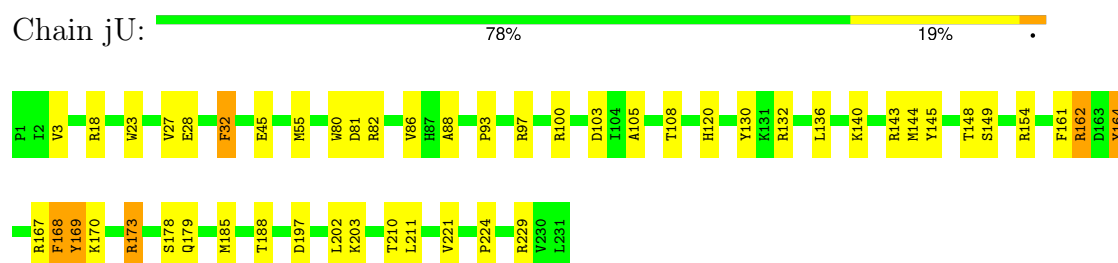
## • Molecule 1: capsid protein



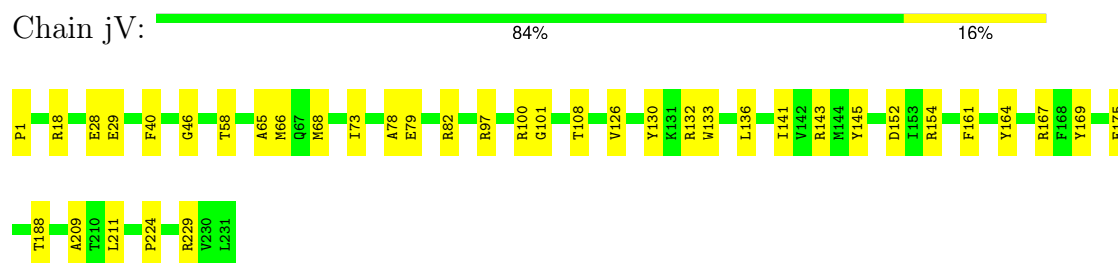
## • Molecule 1: capsid protein



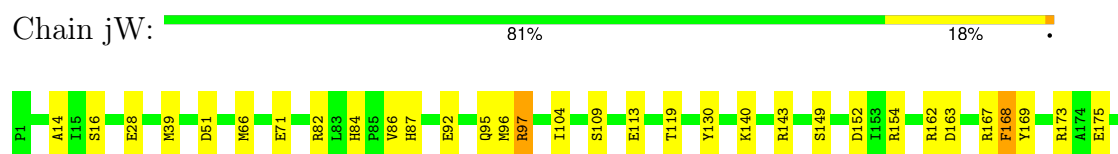
## • Molecule 1: capsid protein

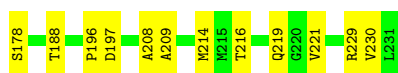


## • Molecule 1: capsid protein




## • Molecule 1: capsid protein






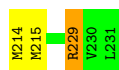
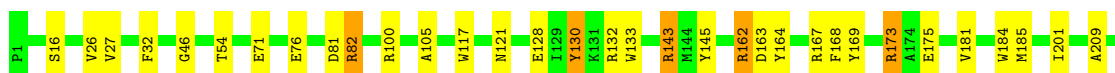
- Molecule 1: capsid protein

Chain jX:  84% 15%




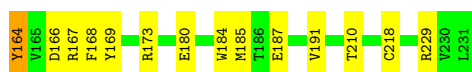
- Molecule 1: capsid protein

Chain jY:  84% 13%




- Molecule 1: capsid protein

Chain jZ:  80% 18%




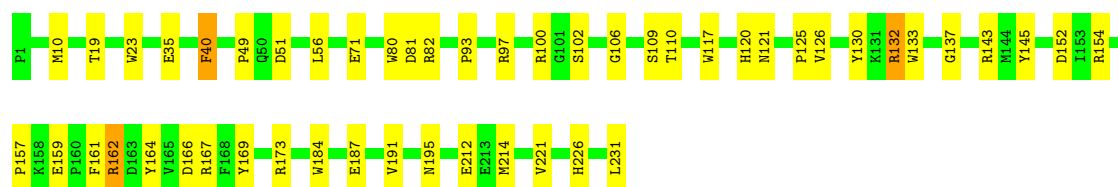
- Molecule 1: capsid protein

Chain 1Z:  84% 16%



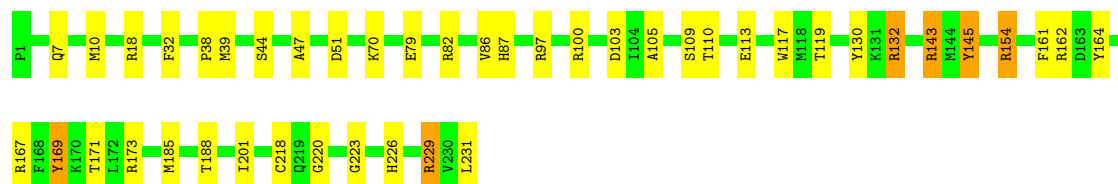
- Molecule 1: capsid protein

Chain k0:  78% 20%



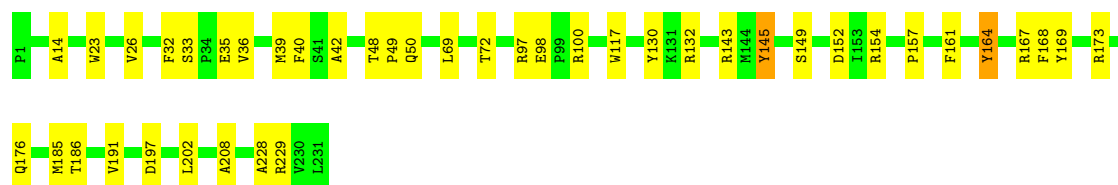
- Molecule 1: capsid protein

Chain k1: 81% 16% •



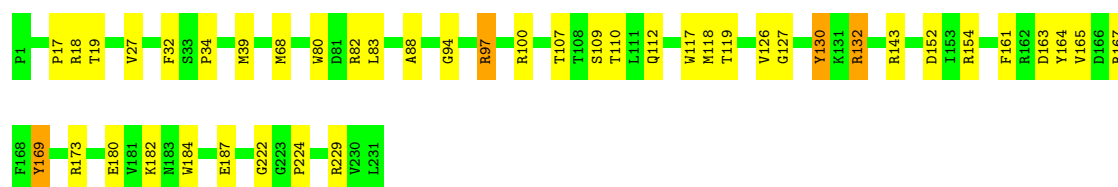
- Molecule 1: capsid protein

Chain k2: 82% 17% •



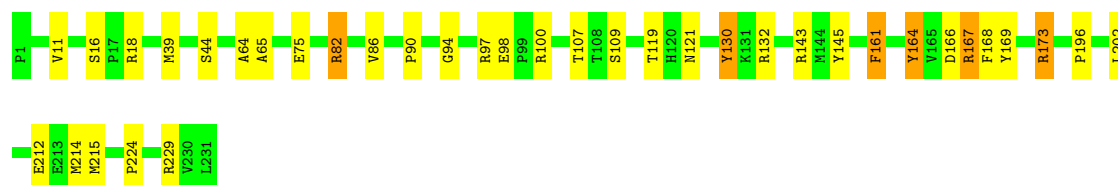
- Molecule 1: capsid protein

Chain k3: 81% 17% •



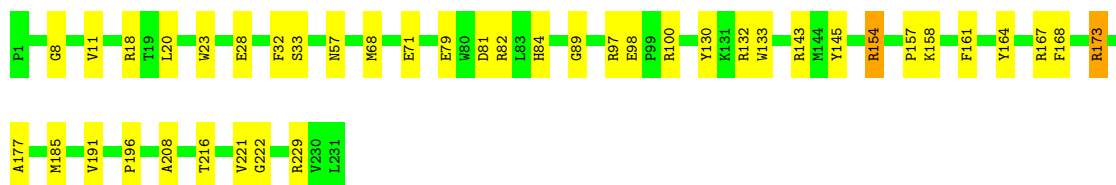
- Molecule 1: capsid protein

Chain k4: 84% 13% •



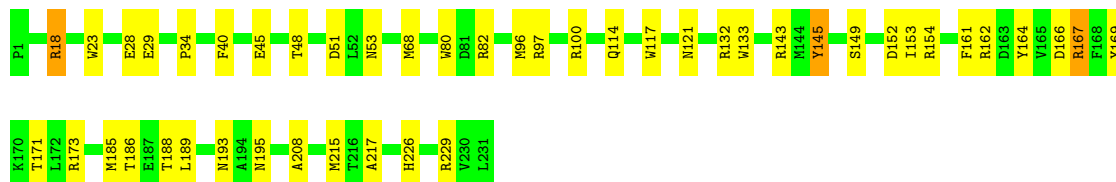
- Molecule 1: capsid protein

Chain k5: 82% 17% •



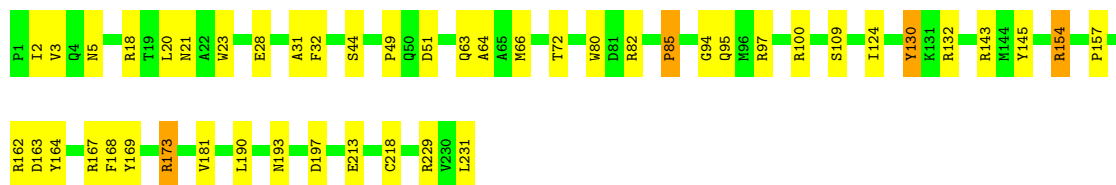
- Molecule 1: capsid protein

Chain k6: 80% 19% •



- Molecule 1: capsid protein

Chain k7: 80% 19% •



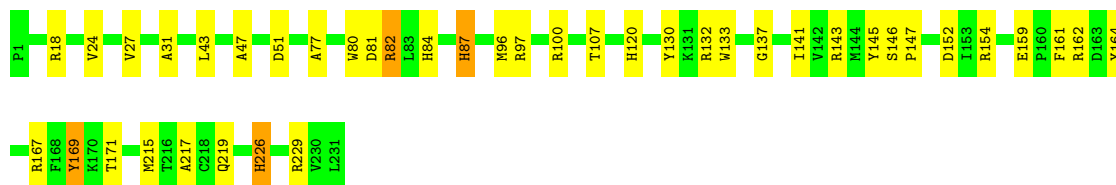
- Molecule 1: capsid protein

Chain k8: 83% 15% •



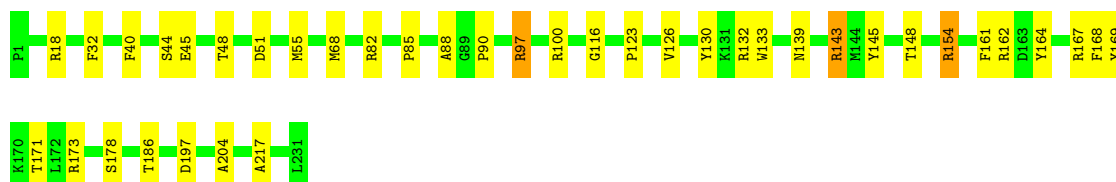
- Molecule 1: capsid protein

Chain k9: 82% 16% •



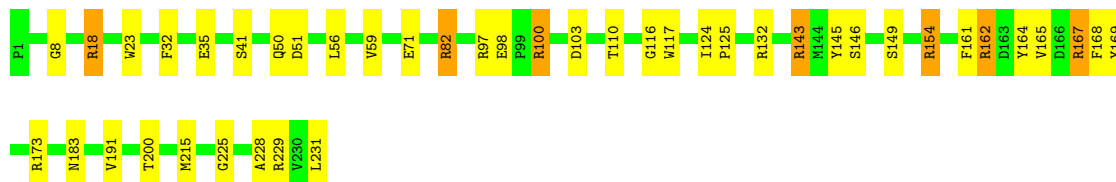
- Molecule 1: capsid protein

Chain 20: 83% 16% •



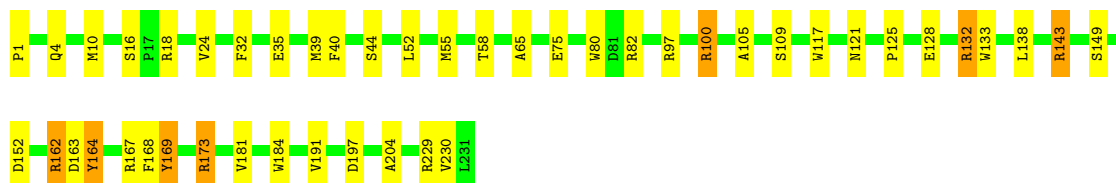
- Molecule 1: capsid protein

Chain ka: 81% 16% .



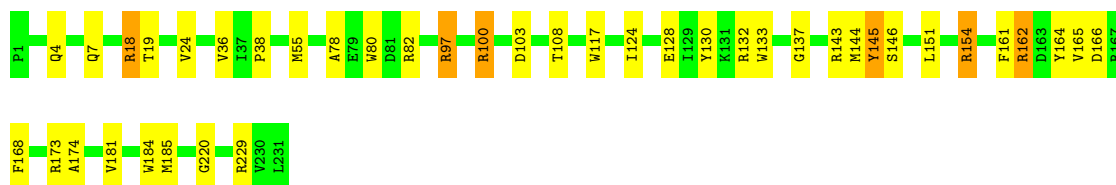
- Molecule 1: capsid protein

Chain kb: 80% 17% .



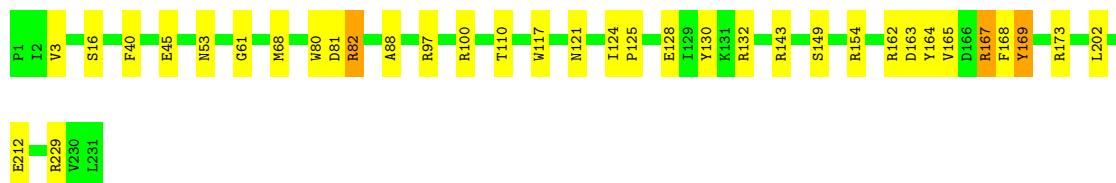
- Molecule 1: capsid protein

Chain kc: 82% 15% .



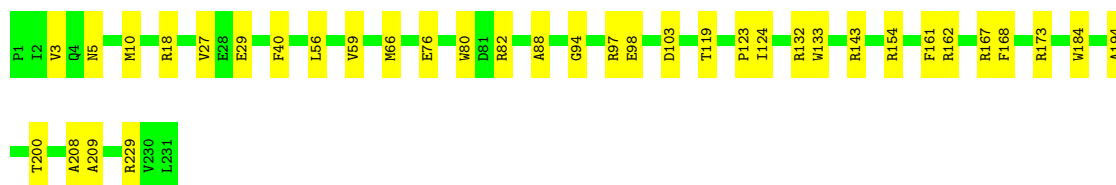
- Molecule 1: capsid protein

Chain kd: 85% 14% .



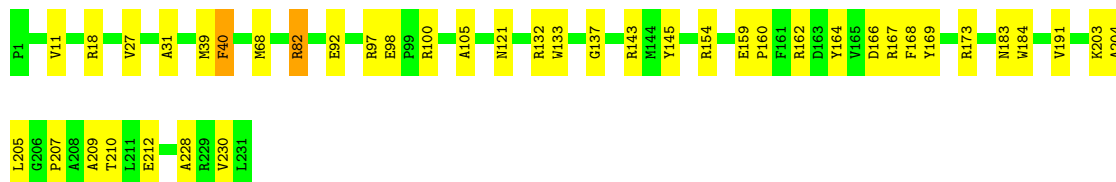
- Molecule 1: capsid protein

Chain ke: 84% 16%



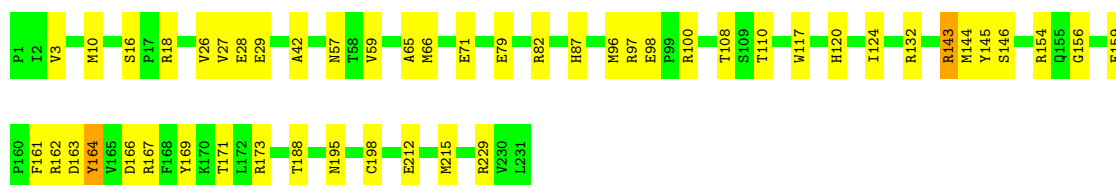
- Molecule 1: capsid protein

Chain kf: 82% 17% •



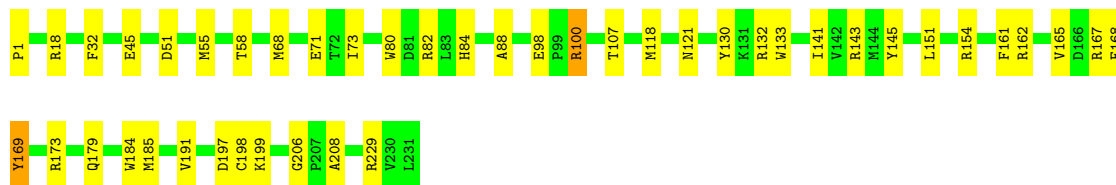
- Molecule 1: capsid protein

Chain kg: 79% 20% •



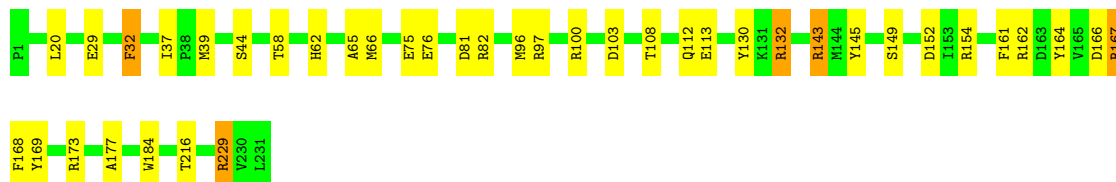
- Molecule 1: capsid protein

Chain kh: 81% 18% •



- Molecule 1: capsid protein

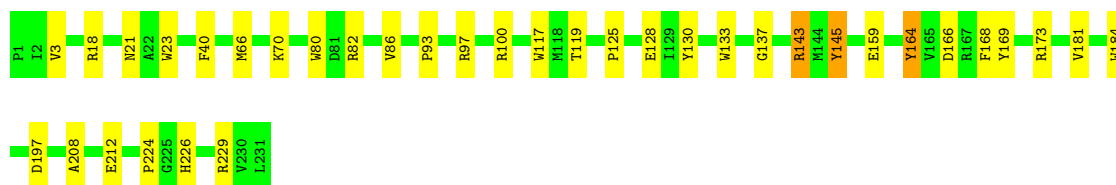
Chain ki: 83% 15% •




- Molecule 1: capsid protein

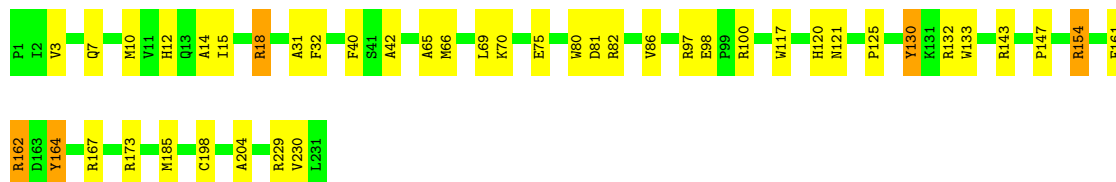
Chain kj: 84% 14% •






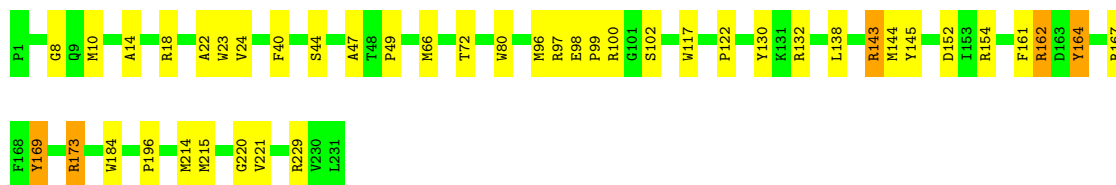
- Molecule 1: capsid protein

Chain 21:  81% 16%




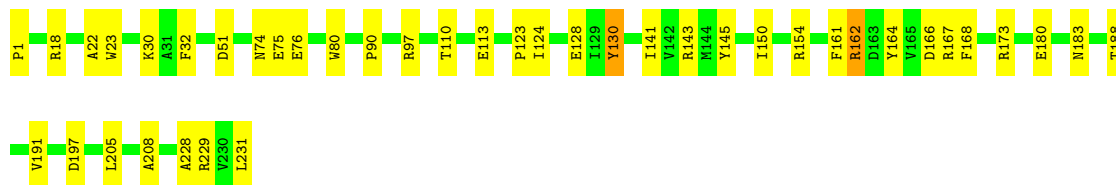
- Molecule 1: capsid protein

Chain kk:  81% 16%




- Molecule 1: capsid protein

Chain kl:  82% 17%




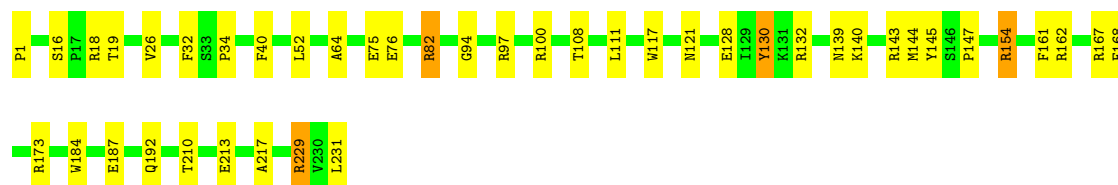
- Molecule 1: capsid protein

Chain km:  82% 16%



- Molecule 1: capsid protein

Chain kn:  81% 17%



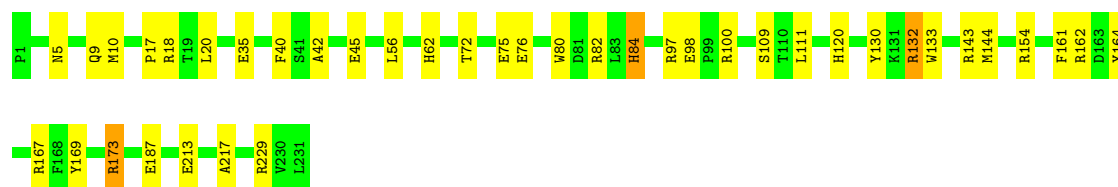
- Molecule 1: capsid protein

Chain ko: 81% 16% .



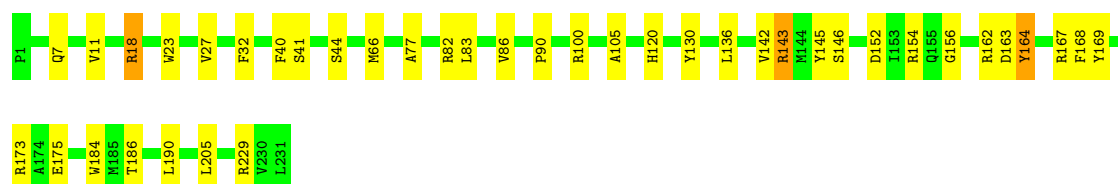
- Molecule 1: capsid protein

Chain kp: 83% 16% .



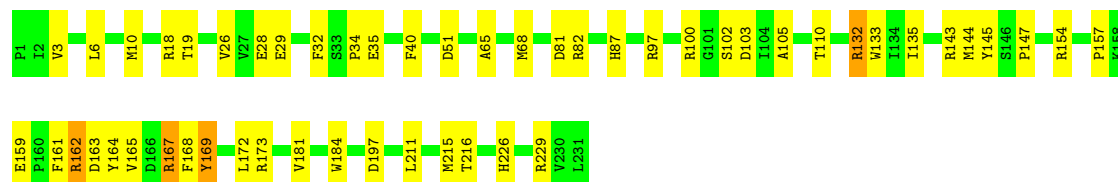
- Molecule 1: capsid protein

Chain kq: 83% 16% .




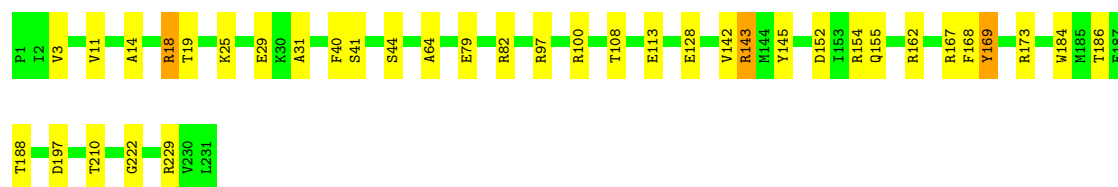
- Molecule 1: capsid protein

Chain kr: 77% 21% .




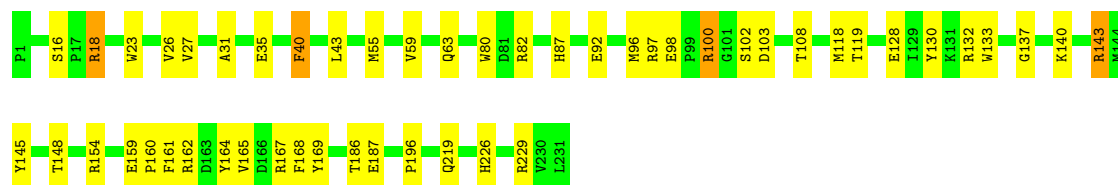
- Molecule 1: capsid protein

Chain ks:  84% 15%



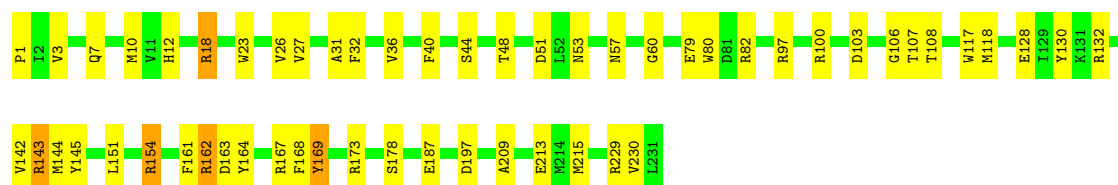
- Molecule 1: capsid protein

Chain kt:  78% 20%




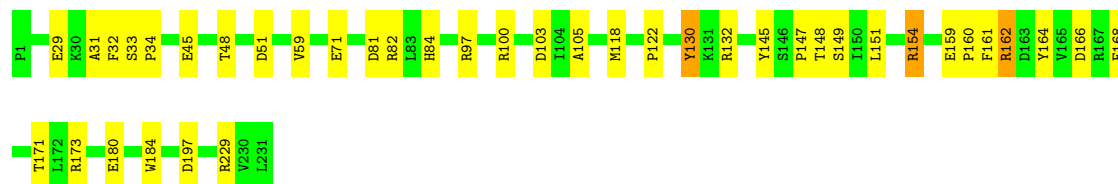
- Molecule 1: capsid protein

Chain 22:  76% 22%




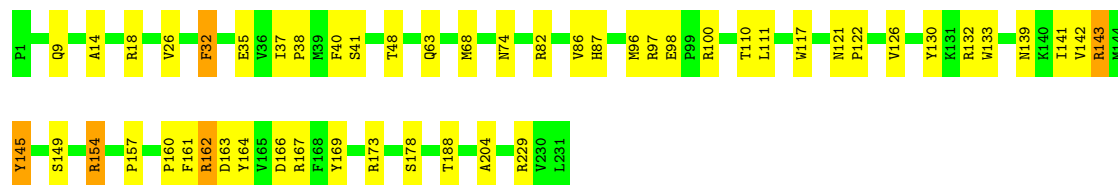
- Molecule 1: capsid protein

Chain ku:  83% 16%




- Molecule 1: capsid protein

Chain kv:  78% 20%




- Molecule 1: capsid protein

Chain kw:  84% 14%




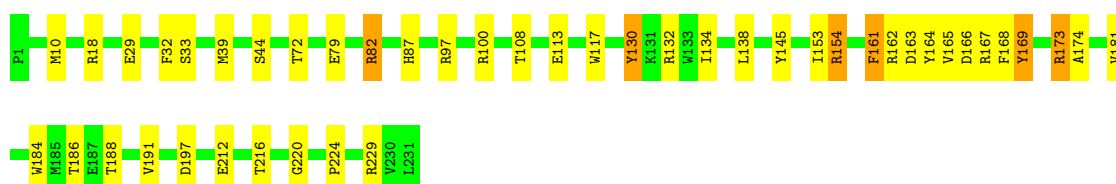
- Molecule 1: capsid protein

Chain kx:  80% 18%




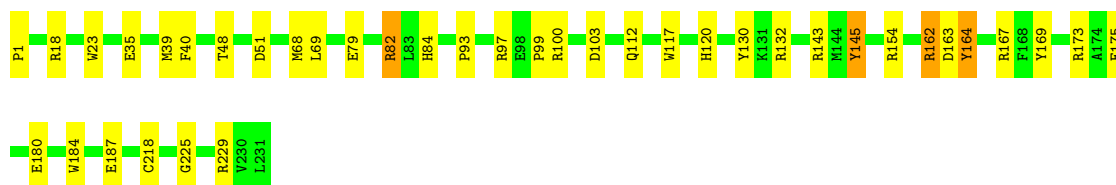
- Molecule 1: capsid protein

Chain ky:  81% 17%




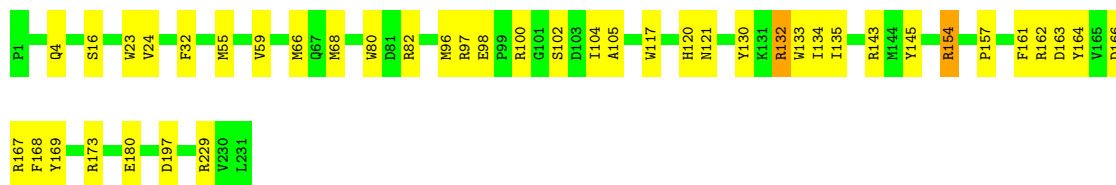
- Molecule 1: capsid protein

Chain kz:  83% 15%




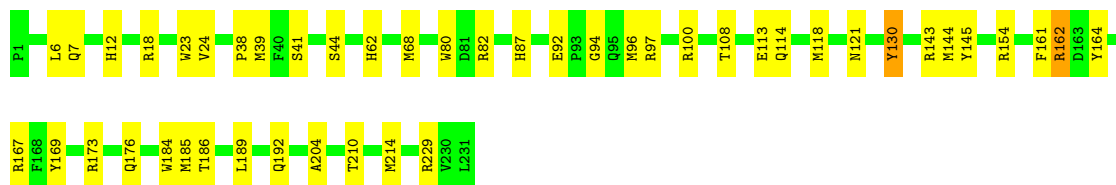
- Molecule 1: capsid protein

Chain kA:  82% 17%




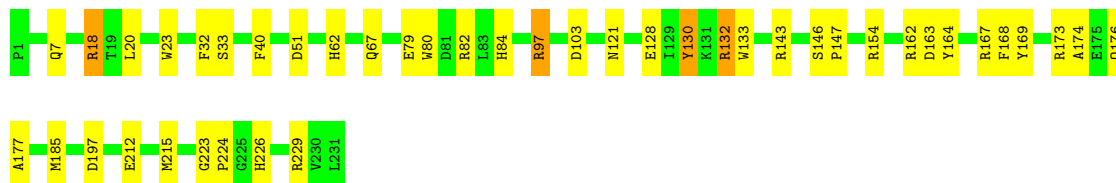
- Molecule 1: capsid protein

Chain kB:  80% 19% .




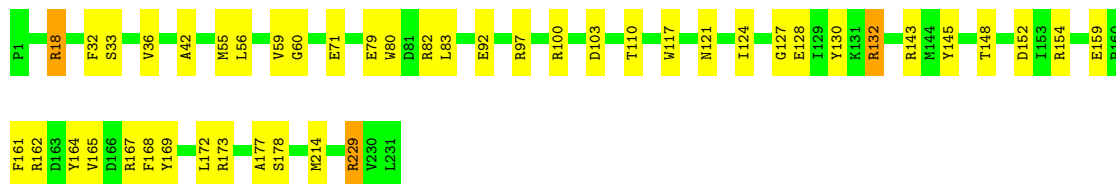
- Molecule 1: capsid protein

Chain kC:  81% 17% .




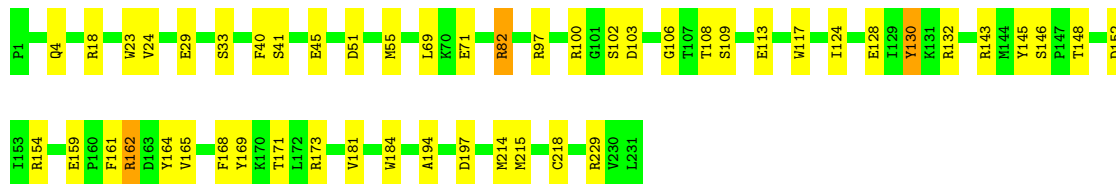
- Molecule 1: capsid protein

Chain kD:  81% 18% .




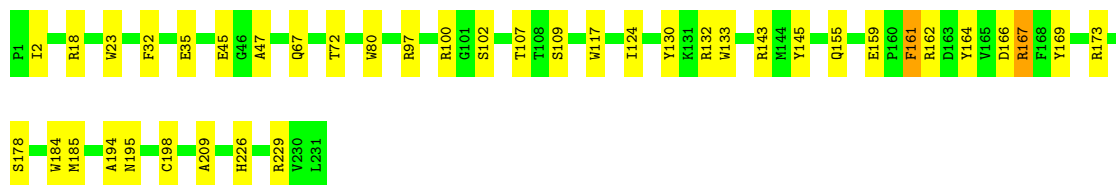
- Molecule 1: capsid protein

Chain 23:  78% 20% .




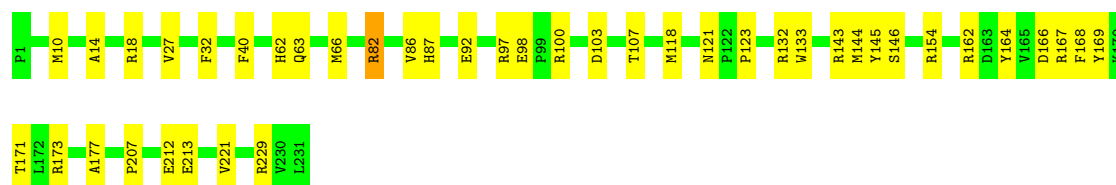
- Molecule 1: capsid protein

Chain kE:  83% 16% .




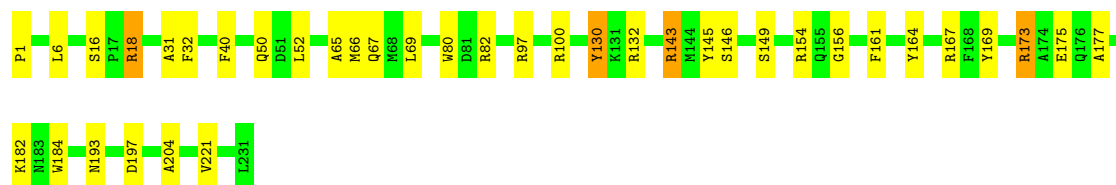
- Molecule 1: capsid protein

Chain kF:  82% 18%




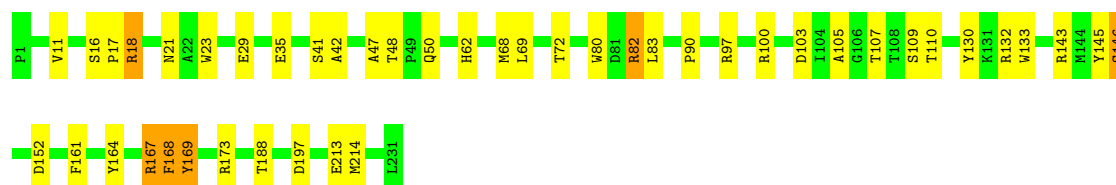
- Molecule 1: capsid protein

Chain kG:  84% 15%




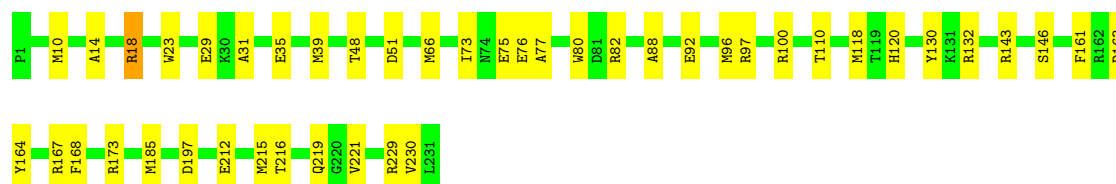
- Molecule 1: capsid protein

Chain kH:  81% 17%




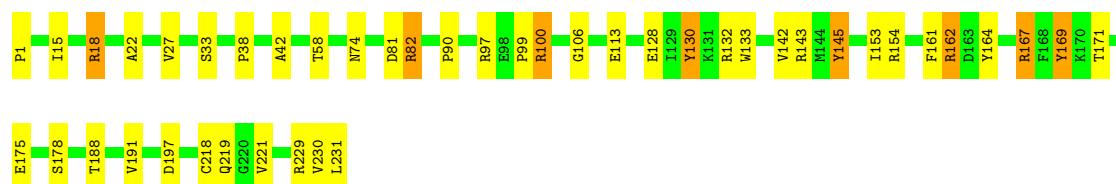
- Molecule 1: capsid protein

Chain kI:  81% 19%




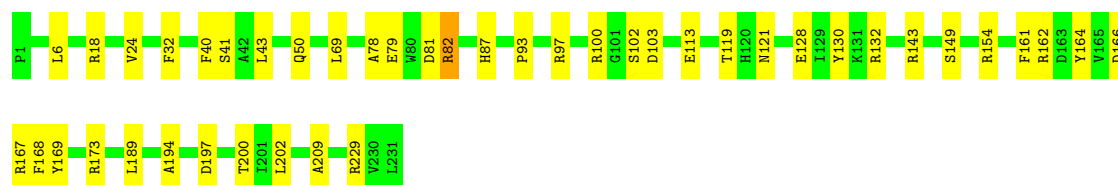
- Molecule 1: capsid protein

Chain kJ:  81% 16%




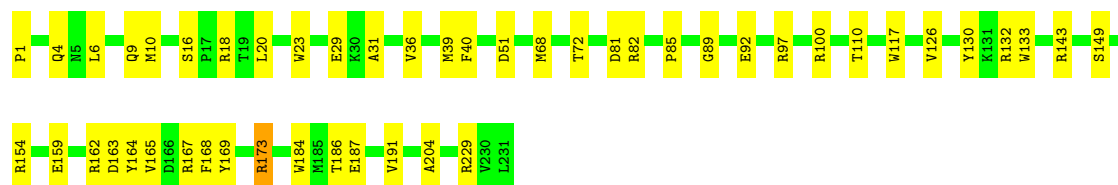
- Molecule 1: capsid protein

Chain kK:  81% 18%




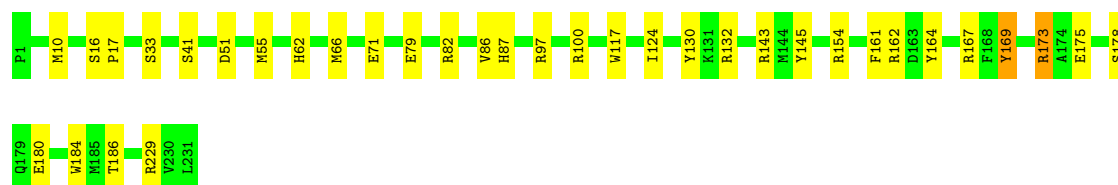
- Molecule 1: capsid protein

Chain kL:  79% 20%




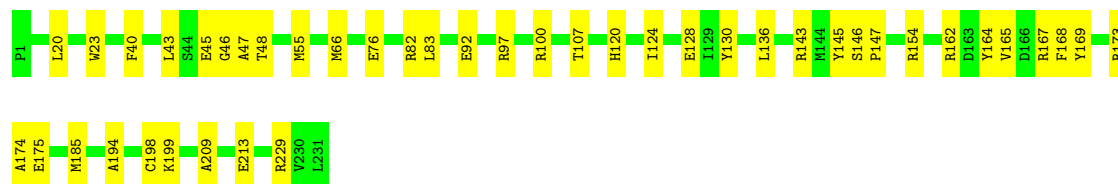
- Molecule 1: capsid protein

Chain kM:  85% 14%




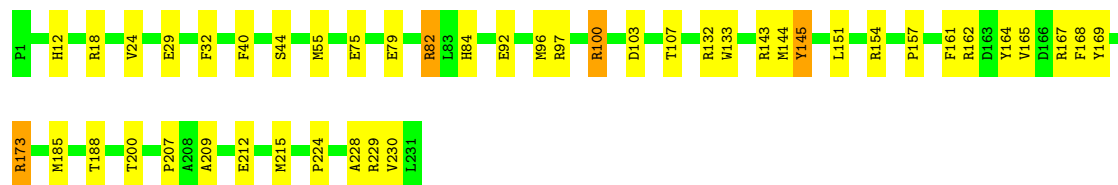
- Molecule 1: capsid protein

Chain kN:  81% 19%




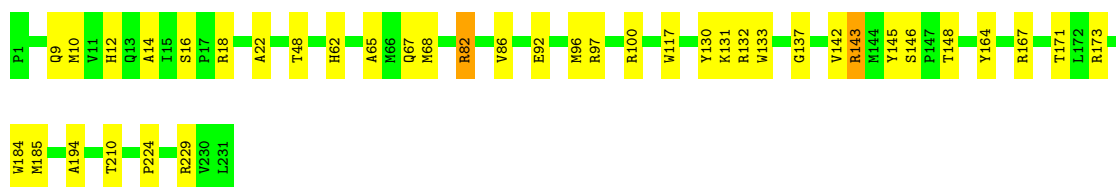
- Molecule 1: capsid protein

Chain 24:  81% 18%




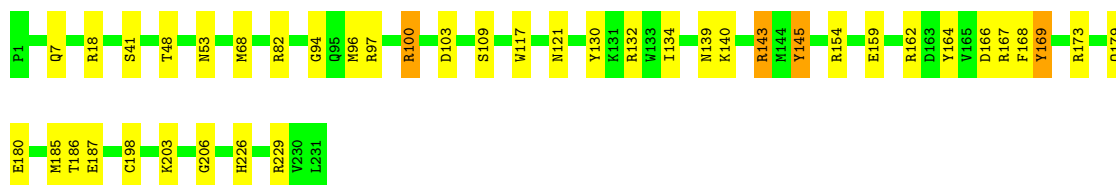
- Molecule 1: capsid protein

Chain kO:  83% 16% .




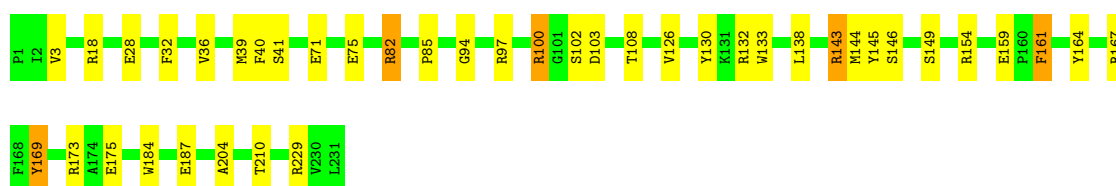
- Molecule 1: capsid protein

Chain kP:  82% 16% .




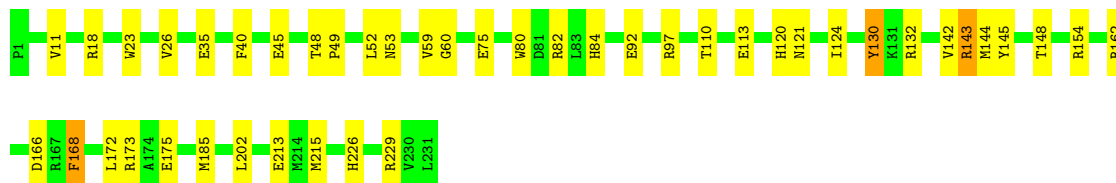
- Molecule 1: capsid protein

Chain kQ:  82% 16% .




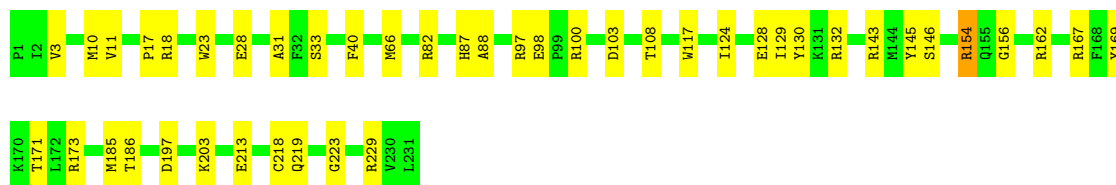
- Molecule 1: capsid protein

Chain kR:  81% 18% .




- Molecule 1: capsid protein

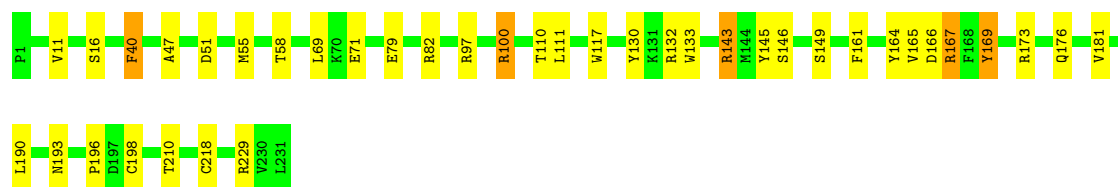
Chain kS:  81% 19% .




- Molecule 1: capsid protein

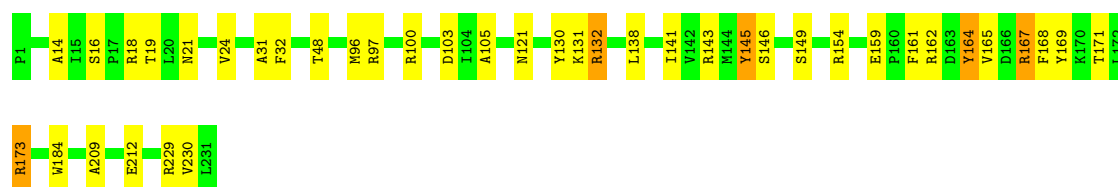


Chain kT:  83% 15% •




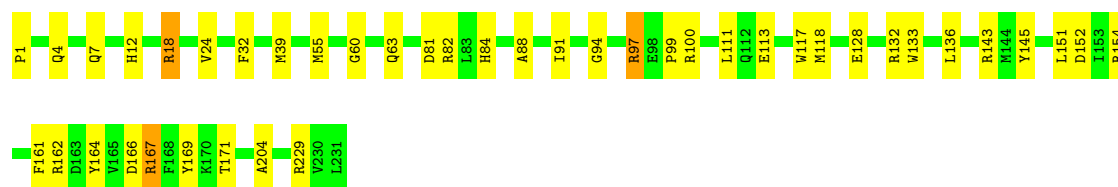
- Molecule 1: capsid protein

Chain kU:  83% 15% •




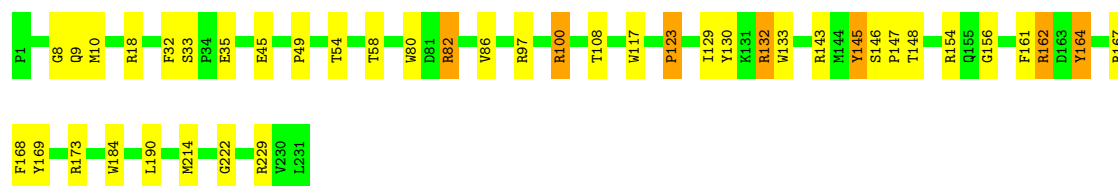
- Molecule 1: capsid protein

Chain kV:  82% 17% •




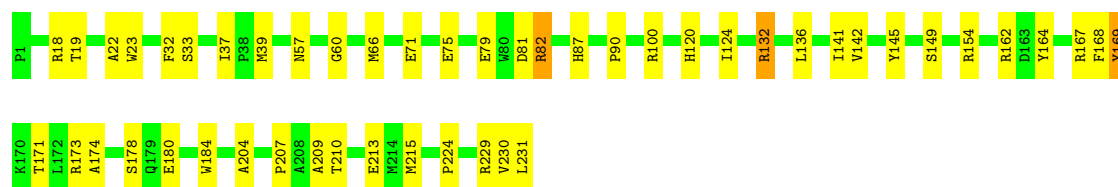
- Molecule 1: capsid protein

Chain kW:  82% 15% •




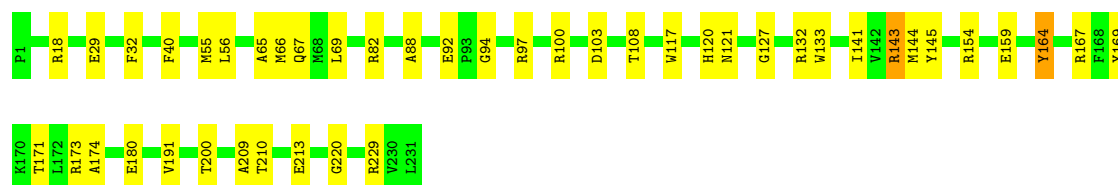
- Molecule 1: capsid protein

Chain kX:  79% 20% •




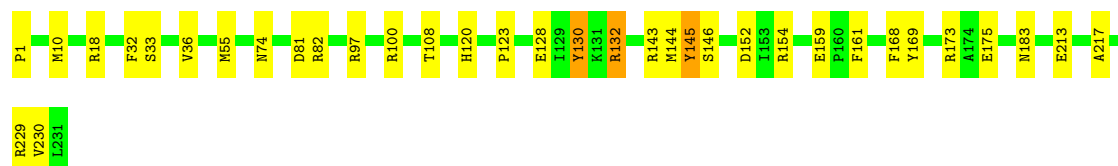
- Molecule 1: capsid protein

Chain 25:  81% 18% •




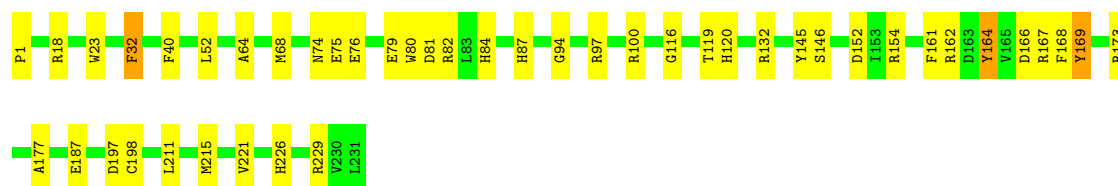
- Molecule 1: capsid protein

Chain kY:  85% 14% •




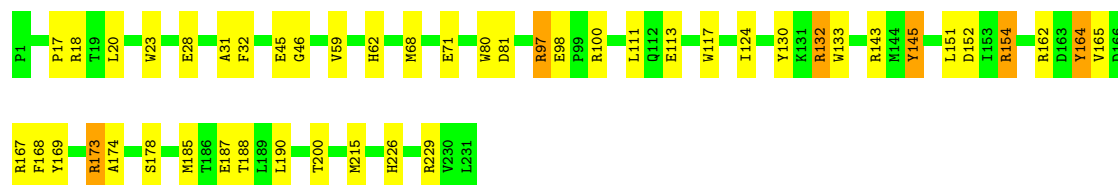
- Molecule 1: capsid protein

Chain kZ:  81% 18% •




- Molecule 1: capsid protein

Chain l0:  80% 18% •




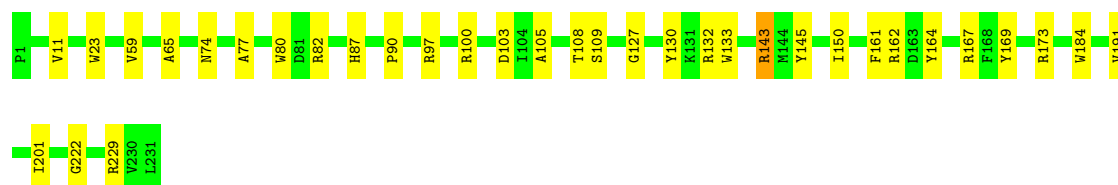
- Molecule 1: capsid protein

Chain l1:  83% 16% •




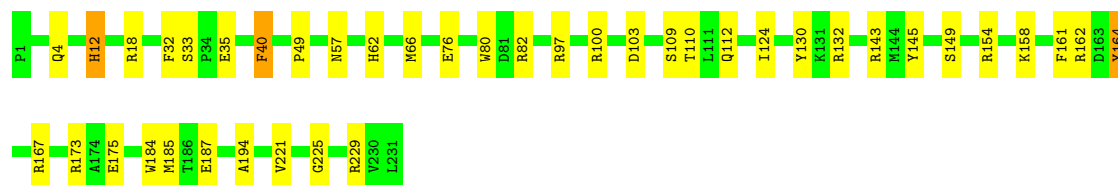
- Molecule 1: capsid protein

Chain l2:  85% 14%




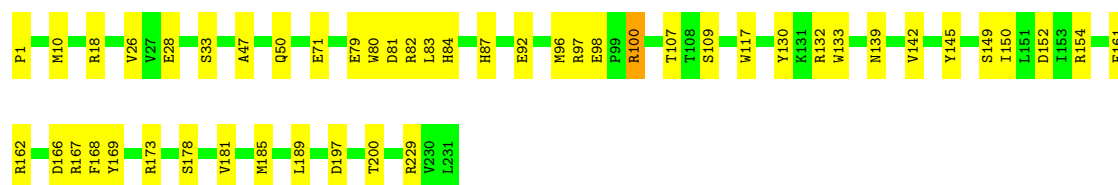
- Molecule 1: capsid protein

Chain l3:  82% 16%




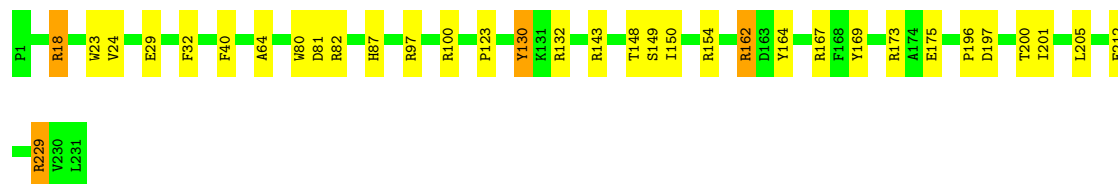
- Molecule 1: capsid protein

Chain l4:  79% 20%




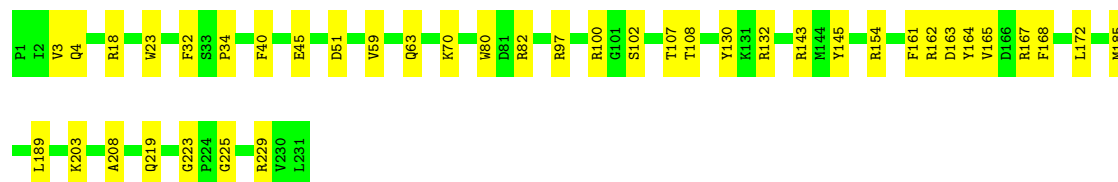
- Molecule 1: capsid protein

Chain l5:  85% 13%

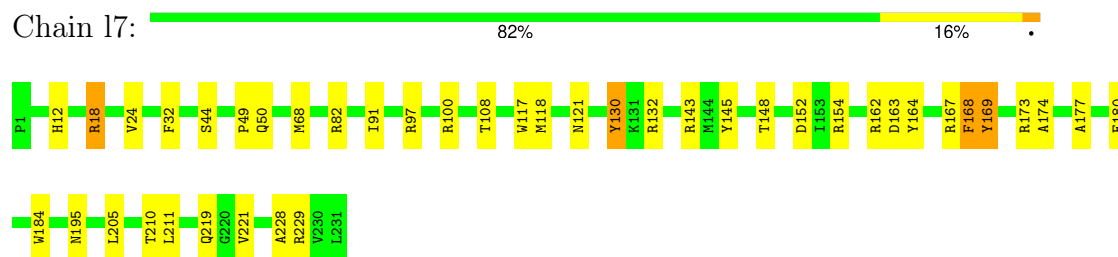


- Molecule 1: capsid protein

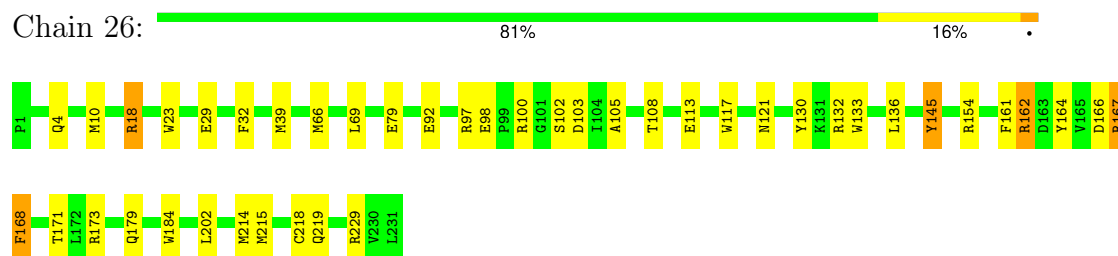
Chain l6:  83% 17%



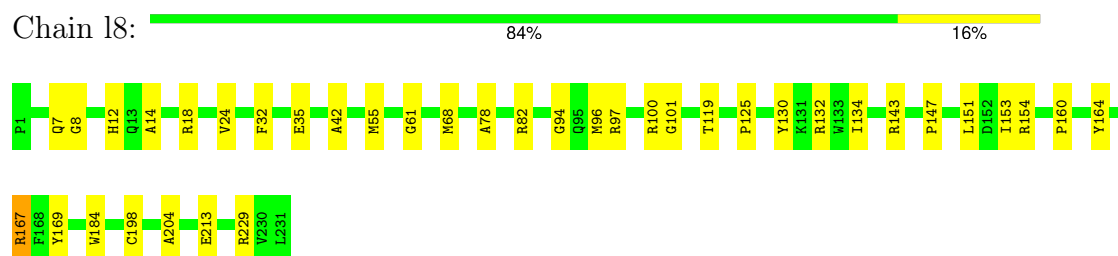
- Molecule 1: capsid protein



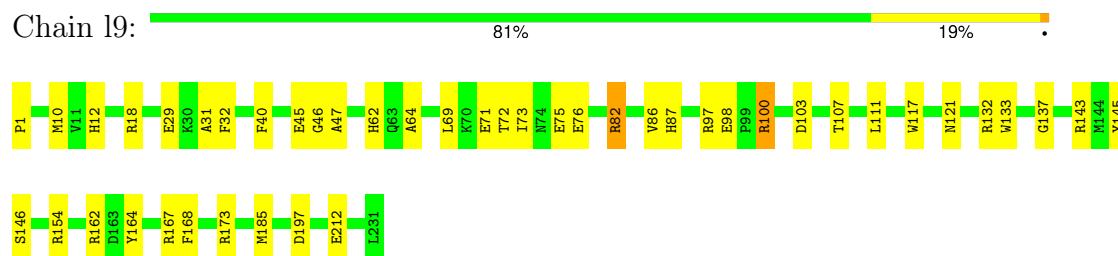
- Molecule 1: capsid protein



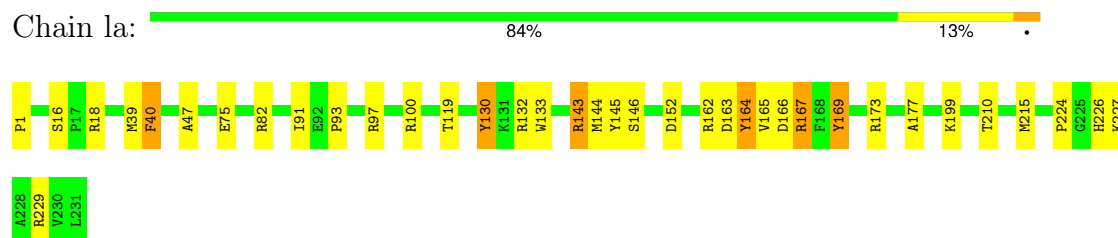
- Molecule 1: capsid protein




- Molecule 1: capsid protein

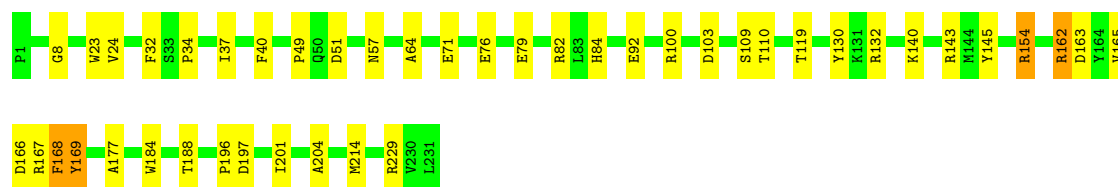


- Molecule 1: capsid protein




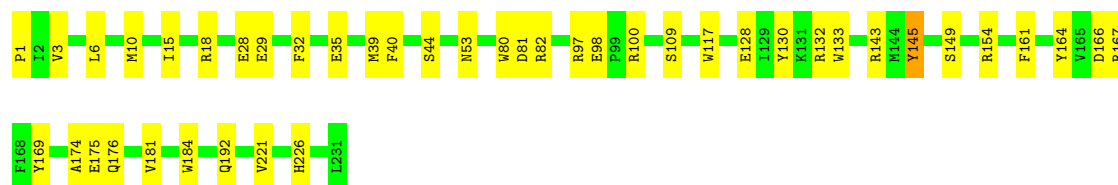
- Molecule 1: capsid protein

Chain lb:  81% 17%




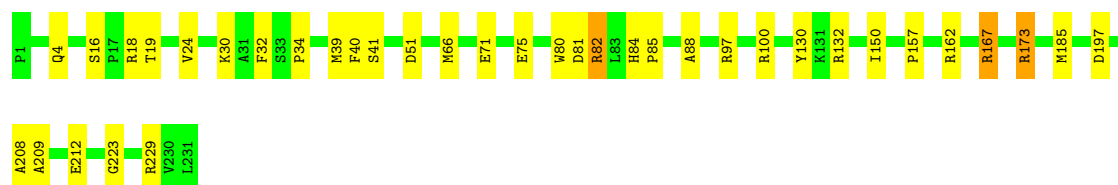
- Molecule 1: capsid protein

Chain lc:  81% 18%




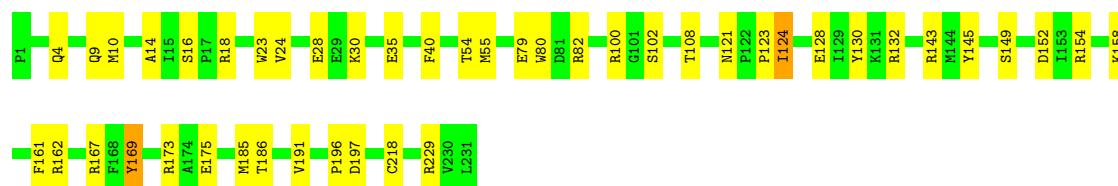
- Molecule 1: capsid protein

Chain ld:  84% 15%




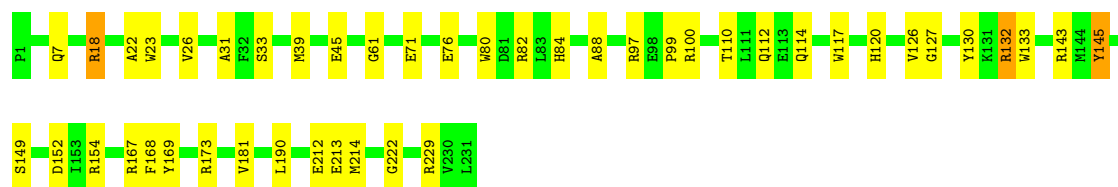
- Molecule 1: capsid protein

Chain le:  81% 19%




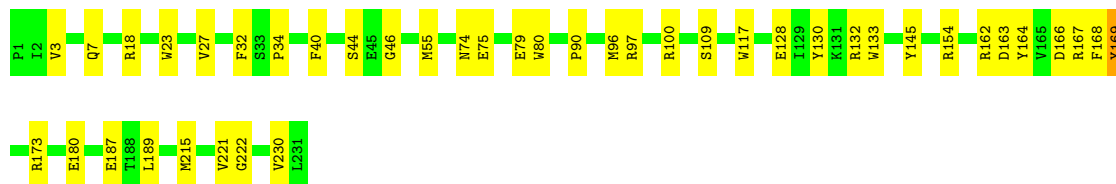
- Molecule 1: capsid protein

Chain lf:  81% 18%




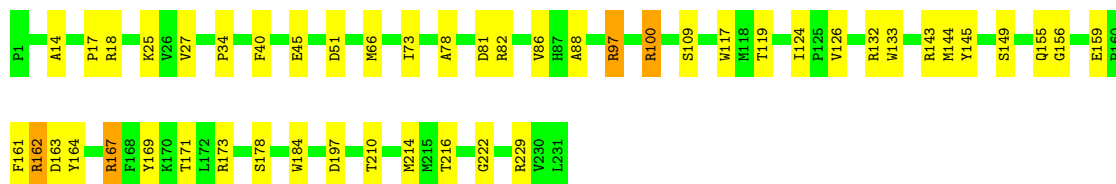
- Molecule 1: capsid protein

Chain lg:  82% 18%




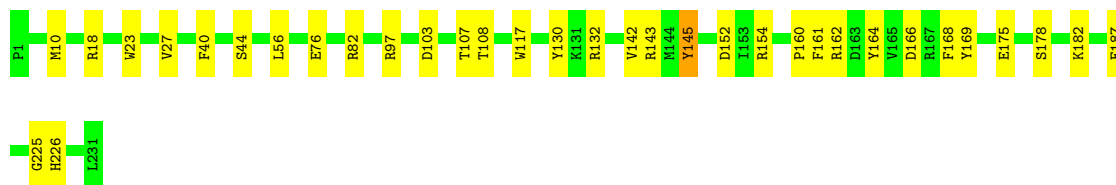
- Molecule 1: capsid protein

Chain lh:  79% 19% .




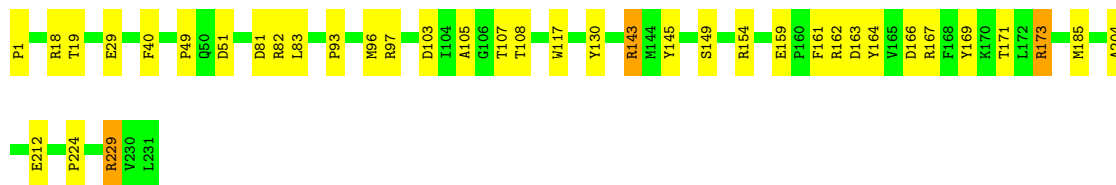
- Molecule 1: capsid protein

Chain 27:  85% 14%




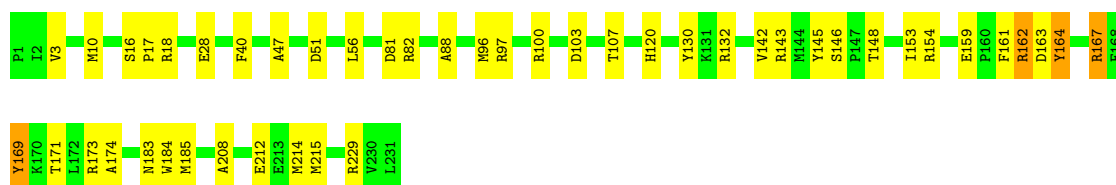
- Molecule 1: capsid protein

Chain li:  84% 15% .



- Molecule 1: capsid protein

Chain lj:  80% 18% .



- Molecule 1: capsid protein


- Molecule 1: capsid protein

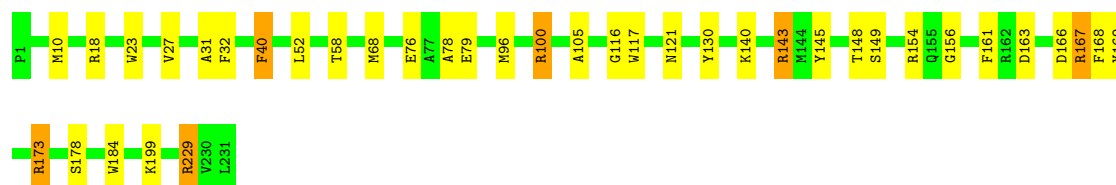
- Molecule 1: capsid protein

- Molecule 1: capsid protein


- Molecule 1: capsid protein

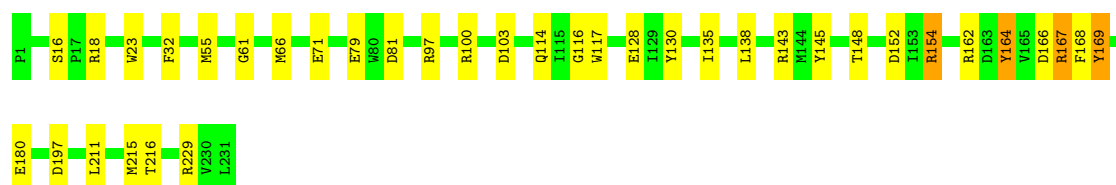
- Molecule 1: capsid protein

Chain lp:  84% 14%




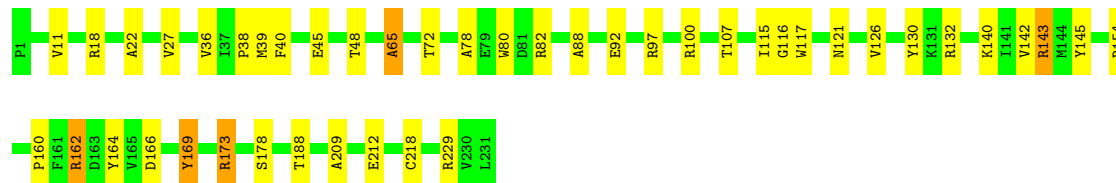
- Molecule 1: capsid protein

Chain lq:  84% 14%




- Molecule 1: capsid protein

Chain lr:  81% 17%




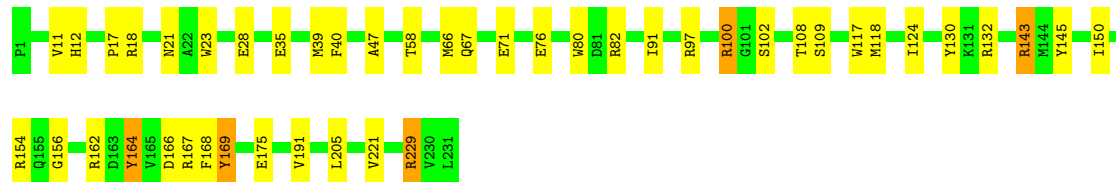
- Molecule 1: capsid protein

Chain 28:  81% 19%




- Molecule 1: capsid protein

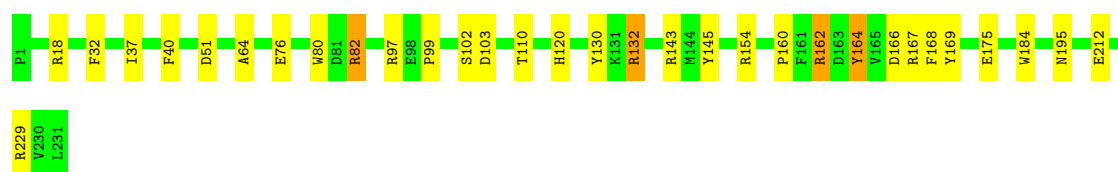
Chain ls:  81% 17%




- Molecule 1: capsid protein



Chain lt:  86% 12%




- Molecule 1: capsid protein

Chain lu:  81% 17%




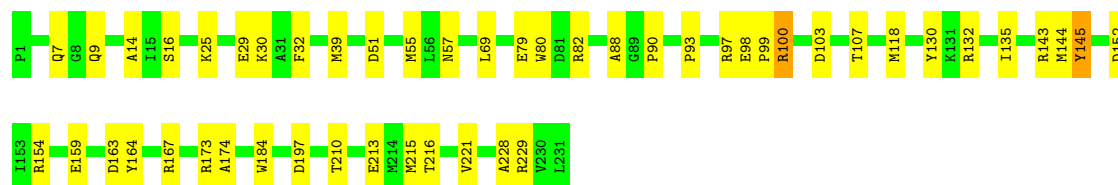
- Molecule 1: capsid protein

Chain lv:  81% 17%




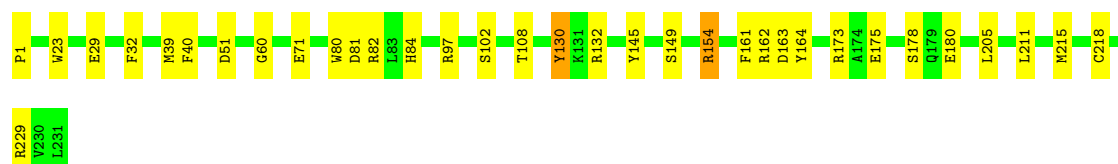
- Molecule 1: capsid protein

Chain lw:  79% 20%




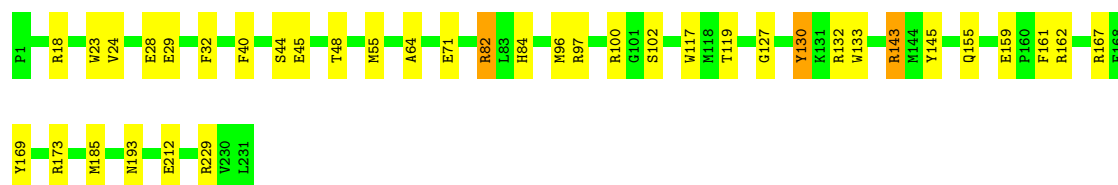
- Molecule 1: capsid protein

Chain lx:  85% 14%




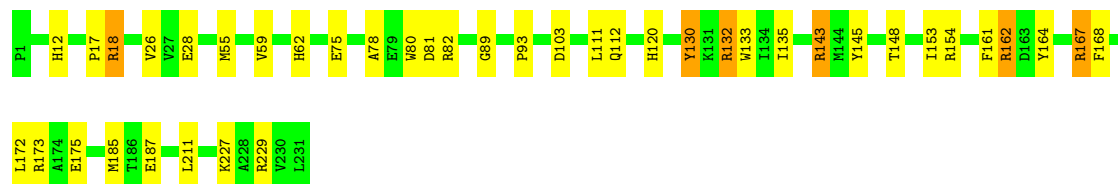
- Molecule 1: capsid protein

Chain ly:  84% 15%




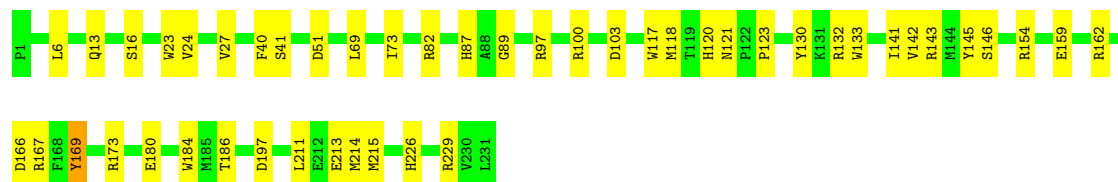
- Molecule 1: capsid protein

Chain lz:  82% 15%




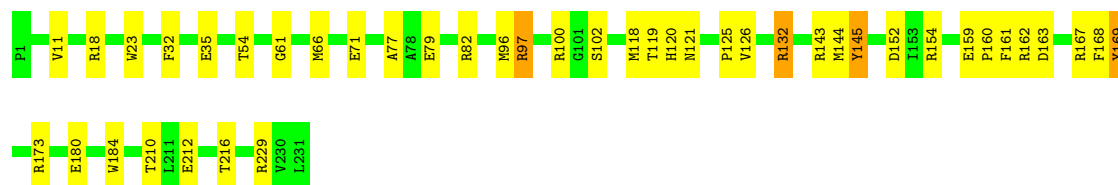
- Molecule 1: capsid protein

Chain lA:  80% 20%




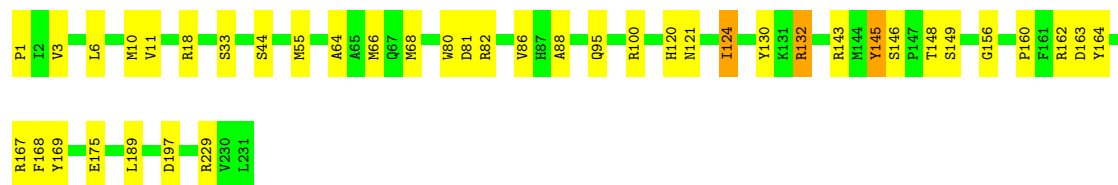
- Molecule 1: capsid protein

Chain lB:  81% 17%




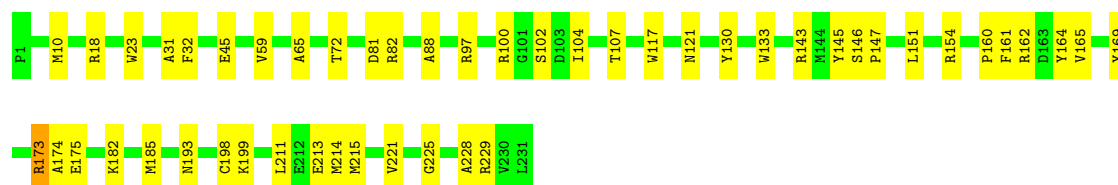
- Molecule 1: capsid protein

Chain 29:  82% 16%




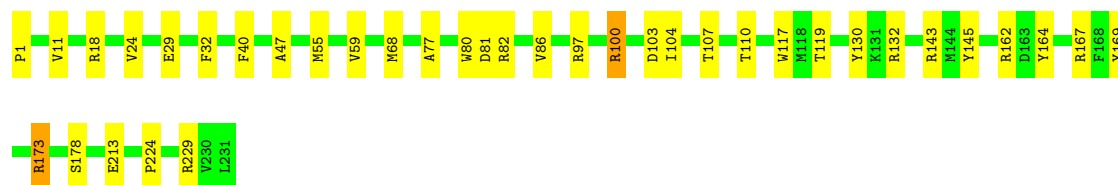
- Molecule 1: capsid protein

Chain IC:  79% 21%




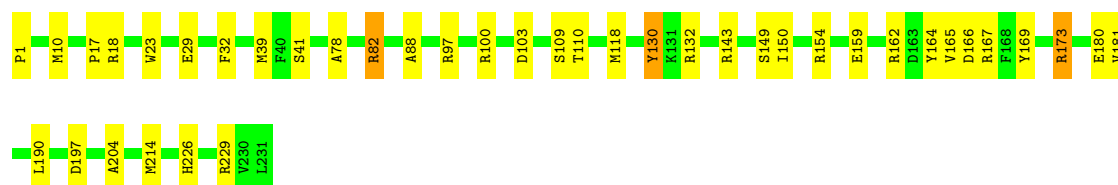
- Molecule 1: capsid protein

Chain ID:  84% 15% •




- Molecule 1: capsid protein

Chain IE:  83% 16% •




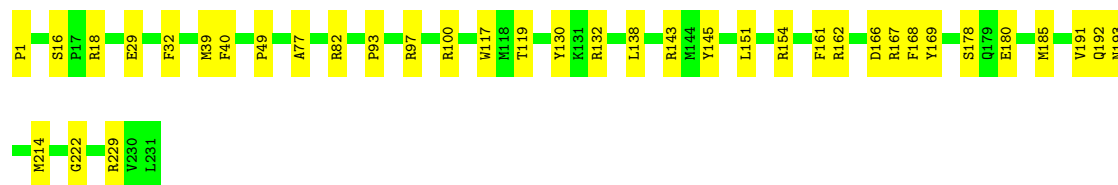
- Molecule 1: capsid protein

Chain IF:  81% 16% •




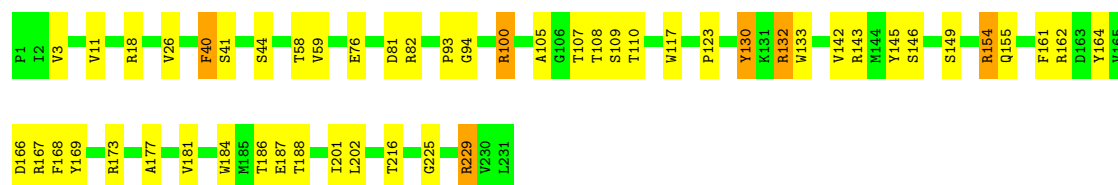
- Molecule 1: capsid protein

Chain IG:  84% 16%




- Molecule 1: capsid protein

Chain IH:  78% 19%




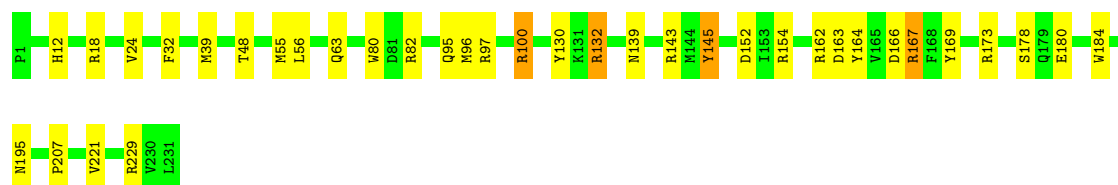
- Molecule 1: capsid protein

Chain II:  81% 17%




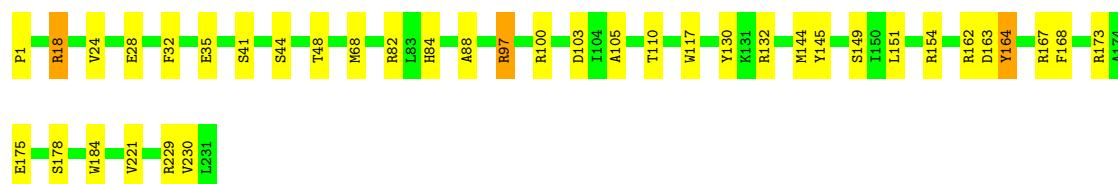
- Molecule 1: capsid protein

Chain IJ:  84% 14%




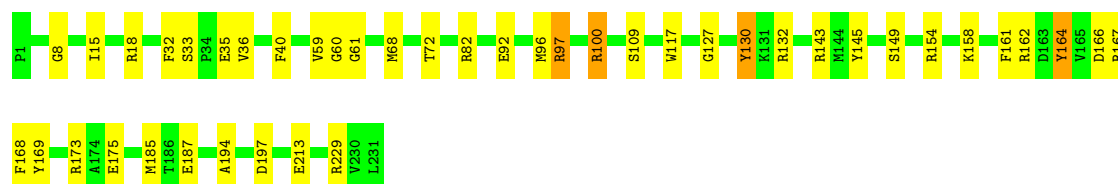
- Molecule 1: capsid protein

Chain IK:  84% 15%




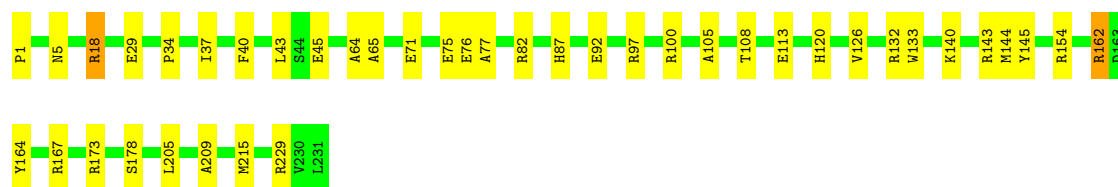
- Molecule 1: capsid protein

Chain IL:  81% 17%




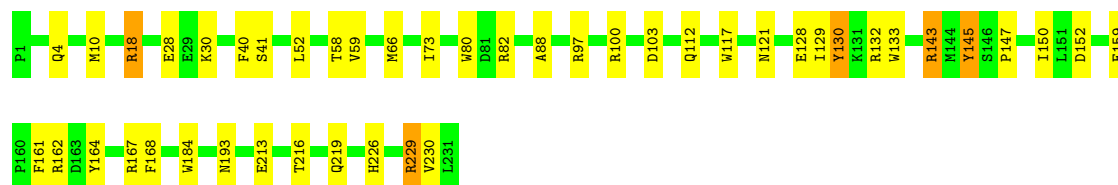
- Molecule 1: capsid protein

Chain 2a:  82% 17%




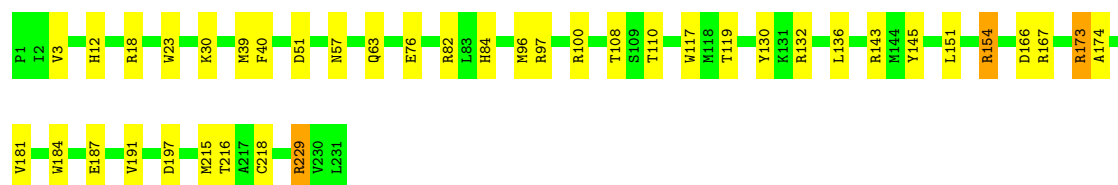
- Molecule 1: capsid protein

Chain 1M:  81% 17%




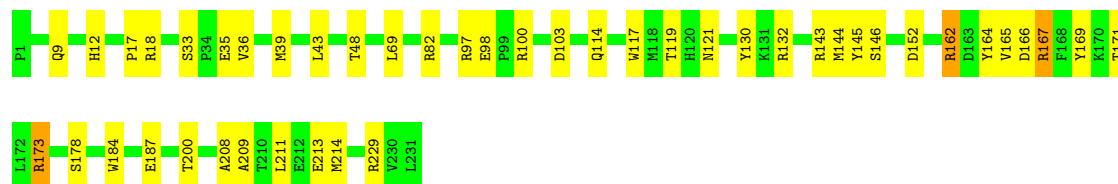
- Molecule 1: capsid protein

Chain 1N:  83% 16%




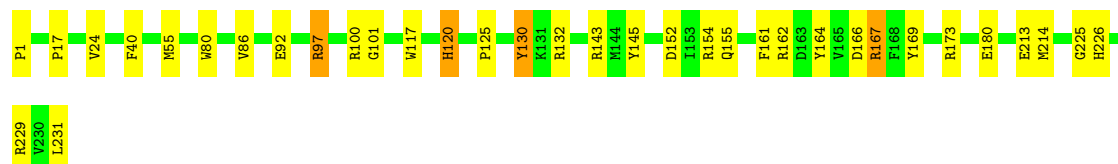
- Molecule 1: capsid protein

Chain 1O:  81% 18%




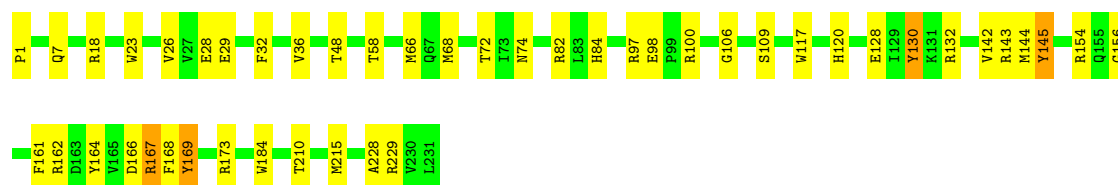
- Molecule 1: capsid protein

Chain 1P:  85% 13%




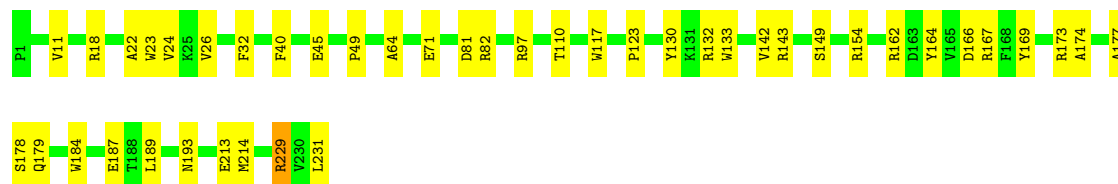
- Molecule 1: capsid protein

Chain 1Q:  80% 18% •




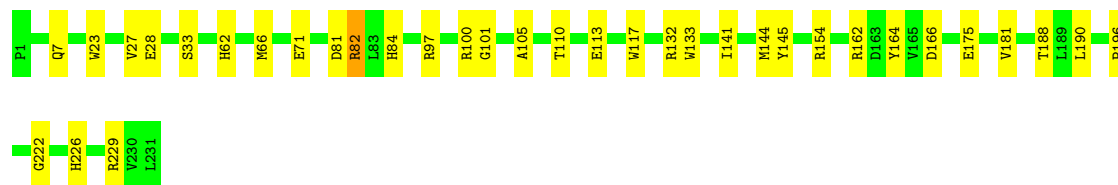
- Molecule 1: capsid protein

Chain 1R:  81% 18%




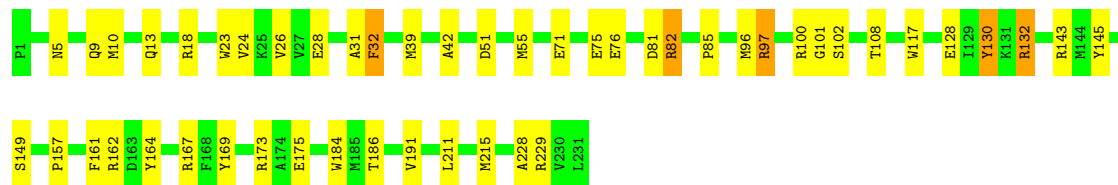
- Molecule 1: capsid protein

Chain 2b:  85% 15%



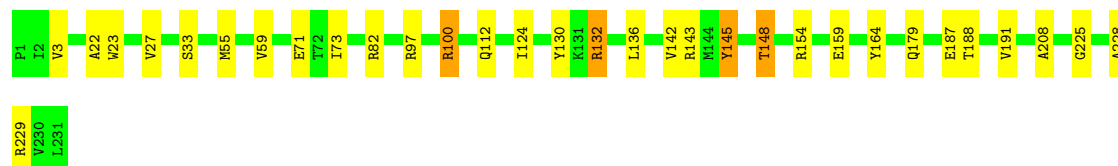
- Molecule 1: capsid protein

Chain 2c:  79% 19% •




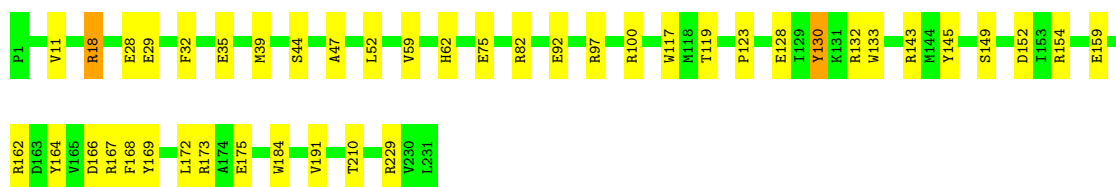
- Molecule 1: capsid protein

Chain 2d:  86% 12% •




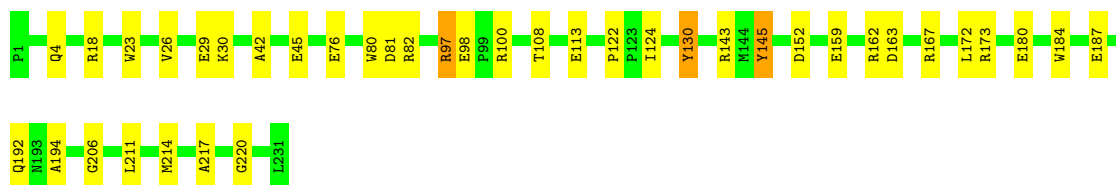
- Molecule 1: capsid protein

Chain 2e:  81% 18% .




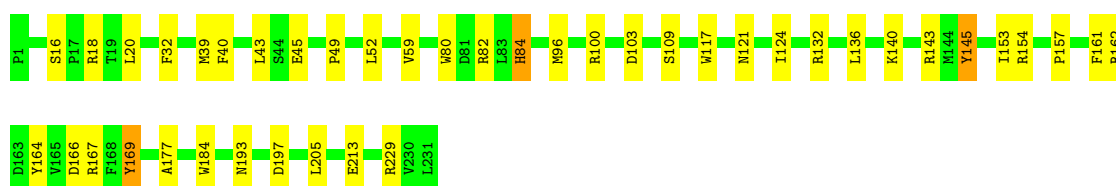
- Molecule 1: capsid protein

Chain 2f:  83% 16% .




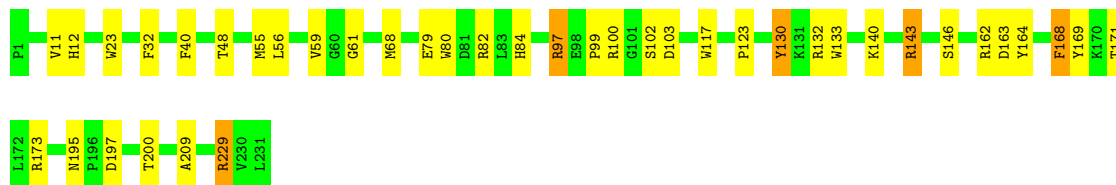
- Molecule 1: capsid protein

Chain 2g:  82% 17% .




- Molecule 1: capsid protein

Chain 2h:  83% 15% .




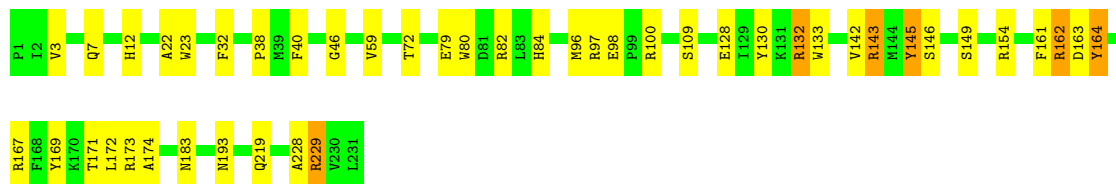
- Molecule 1: capsid protein

Chain 2i:  83% 16% .




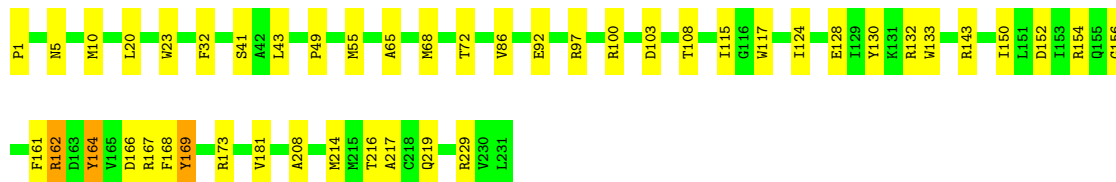
- Molecule 1: capsid protein

Chain 2j:  81% 17%




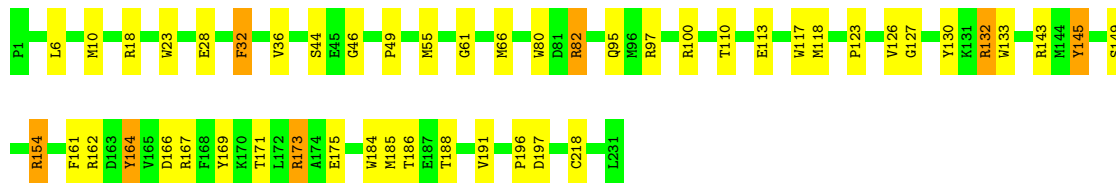
- Molecule 1: capsid protein

Chain 2k:  80% 19%




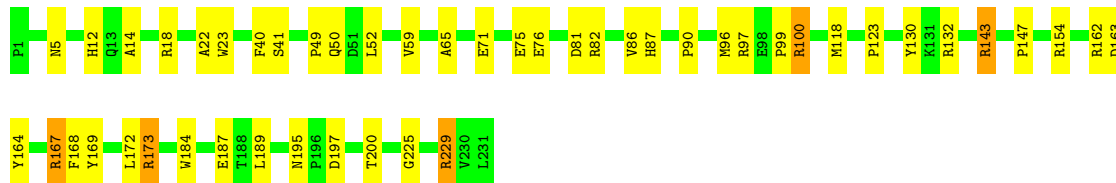
- Molecule 1: capsid protein

Chain 2l:  79% 18%




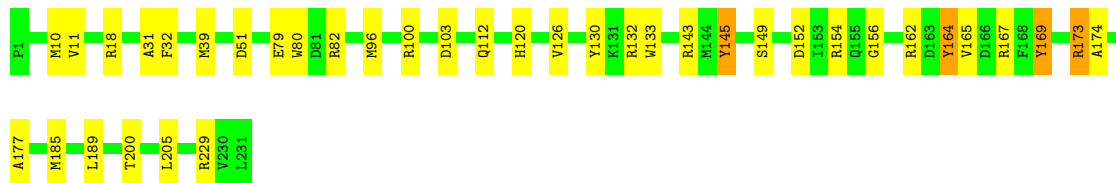
- Molecule 1: capsid protein

Chain 2m:  79% 19%



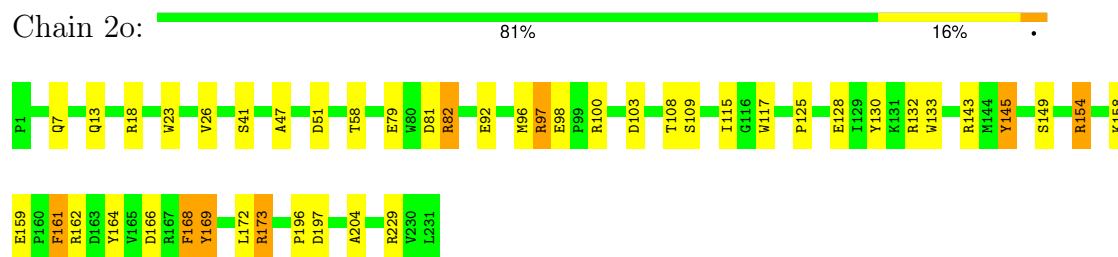
- Molecule 1: capsid protein

Chain 2n:  84% 15%

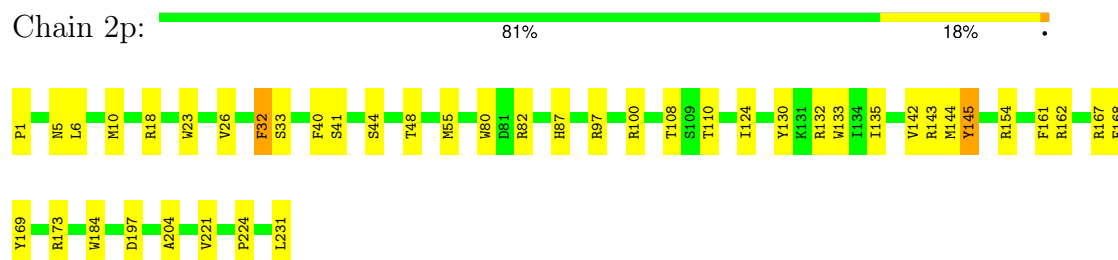


- Molecule 1: capsid protein

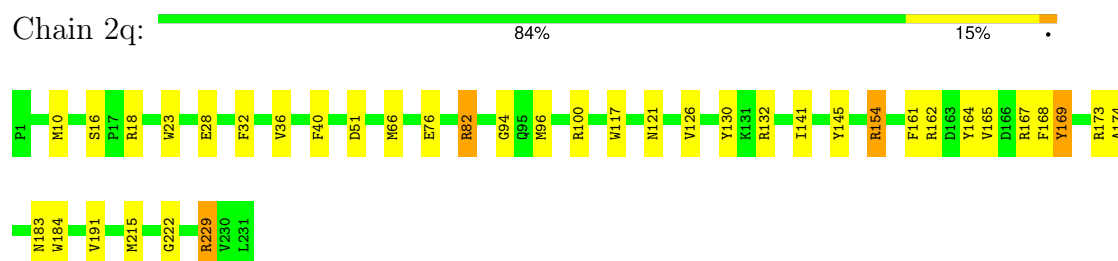




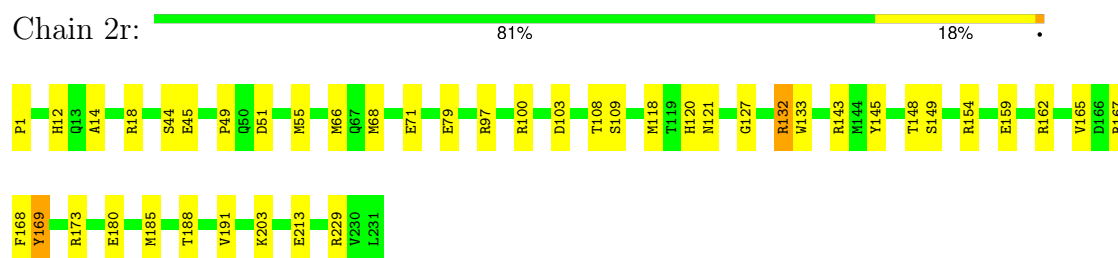
- Molecule 1: capsid protein



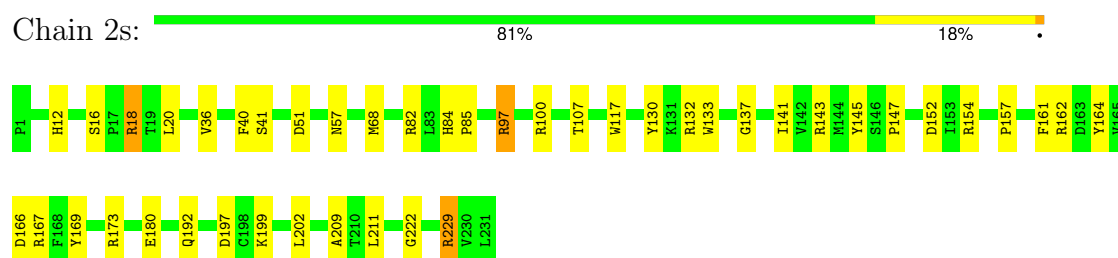
- Molecule 1: capsid protein




- Molecule 1: capsid protein

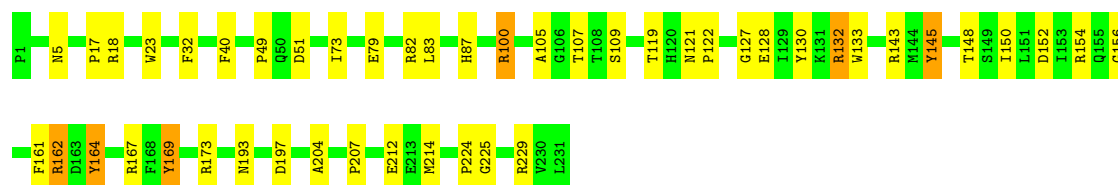


- Molecule 1: capsid protein




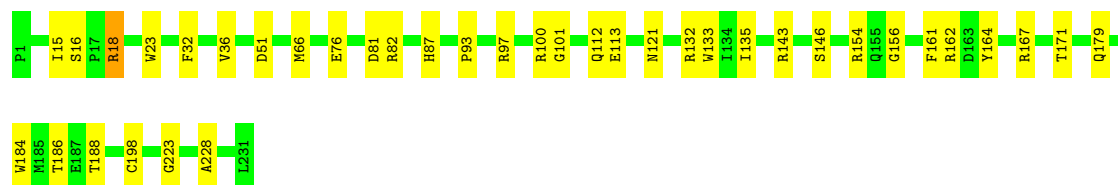
- Molecule 1: capsid protein

Chain 2t:  80% 18% •




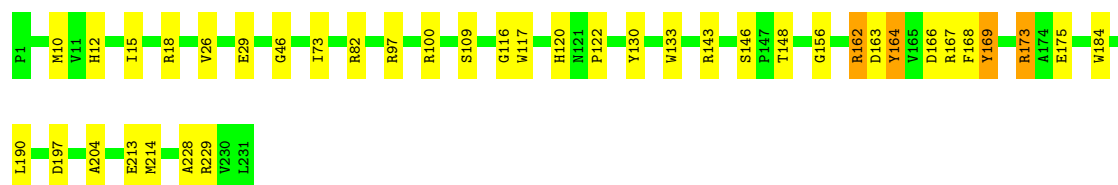
- Molecule 1: capsid protein

Chain 2u:  84% 16%




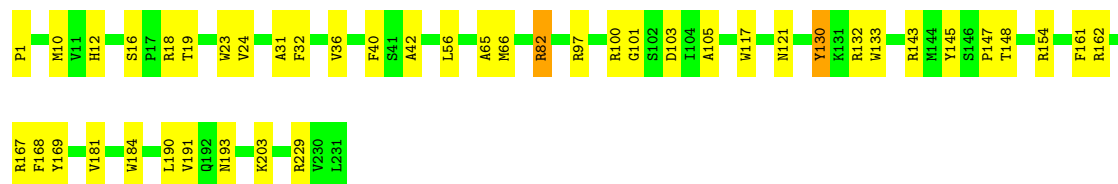
- Molecule 1: capsid protein

Chain 2v:  83% 15% •




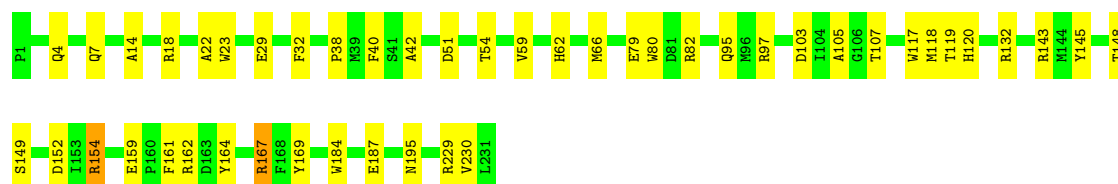
- Molecule 1: capsid protein

Chain 2w:  81% 18% •




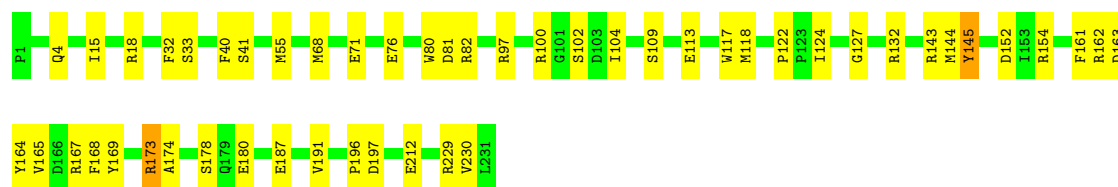
- Molecule 1: capsid protein

Chain 2x:  80% 19% •




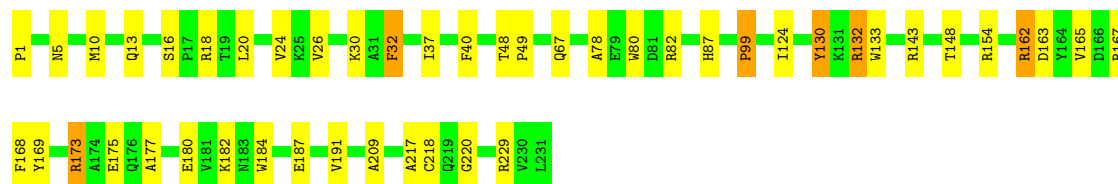
- Molecule 1: capsid protein

Chain 2y:  78% 21% .




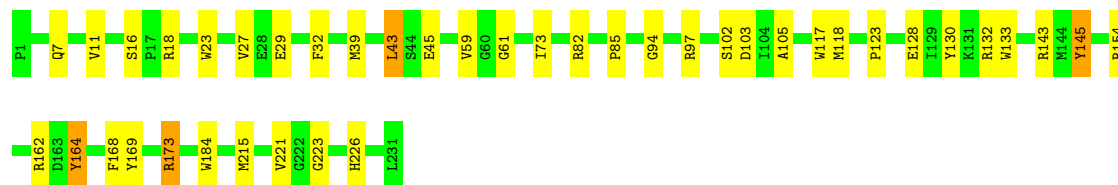
- Molecule 1: capsid protein

Chain 2z:  80% 18% .




- Molecule 1: capsid protein

Chain 2A:  82% 16% .




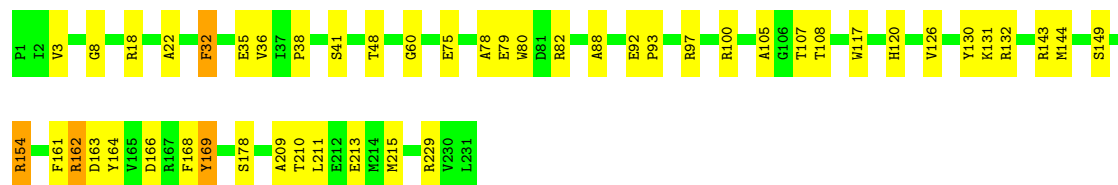
- Molecule 1: capsid protein

Chain 2B:  83% 16% .




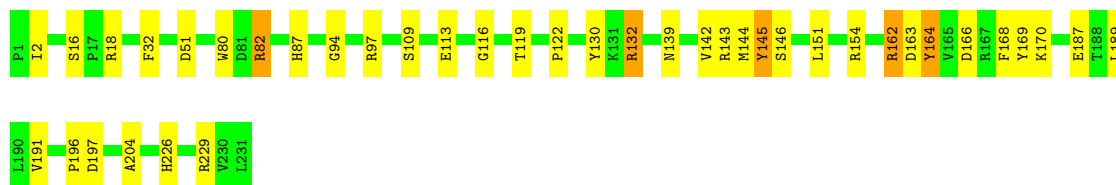
- Molecule 1: capsid protein

Chain 2C:  79% 19% .




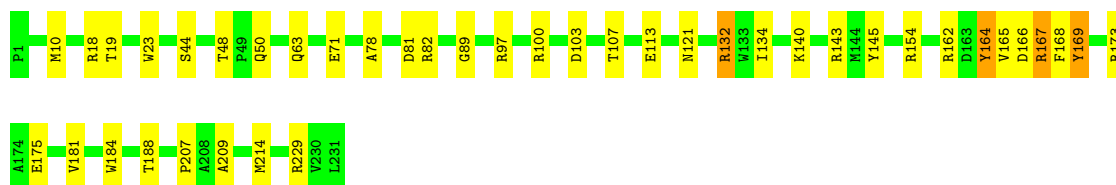
- Molecule 1: capsid protein

Chain 2D:  83% 15% •




- Molecule 1: capsid protein

Chain 2E:  82% 16% •




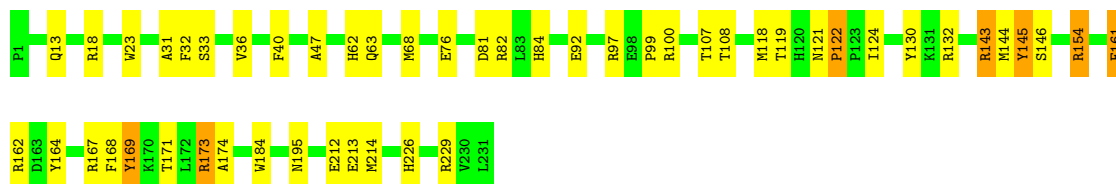
- Molecule 1: capsid protein

Chain 2F:  82% 17% •




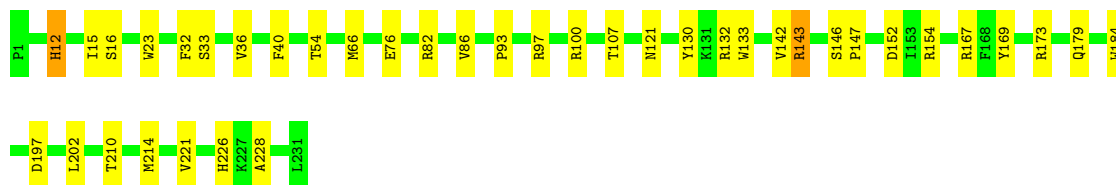
- Molecule 1: capsid protein

Chain 2G:  78% 19% •



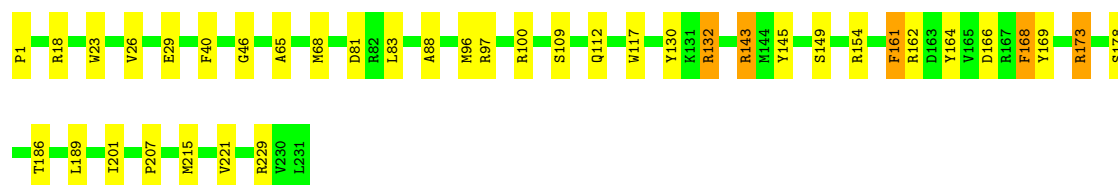
- Molecule 1: capsid protein

Chain 2H:  83% 16% •




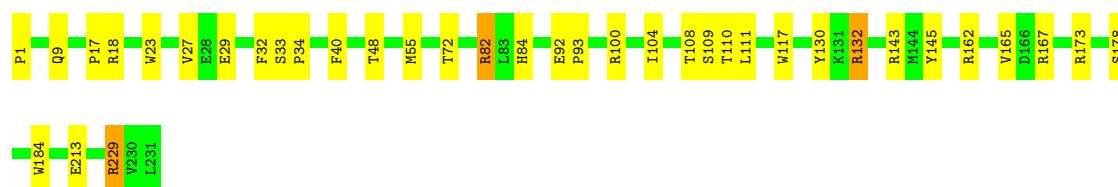
- Molecule 1: capsid protein

Chain 2I:  83% 15% .




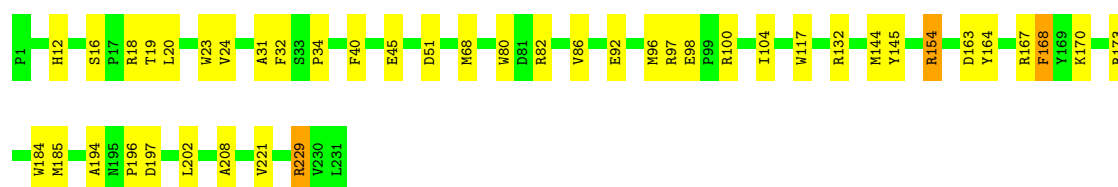
- Molecule 1: capsid protein

Chain 2J:  84% 15% .




- Molecule 1: capsid protein

Chain 2K:  81% 17% .




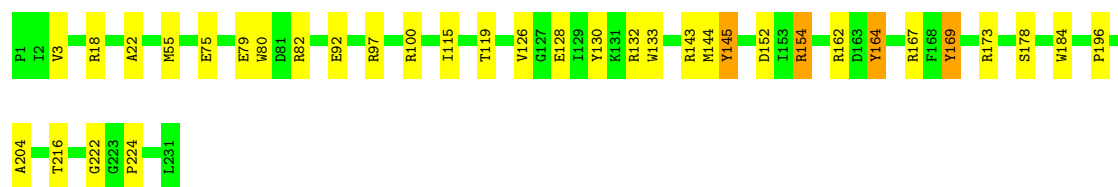
- Molecule 1: capsid protein

Chain 2L:  84% 16% .




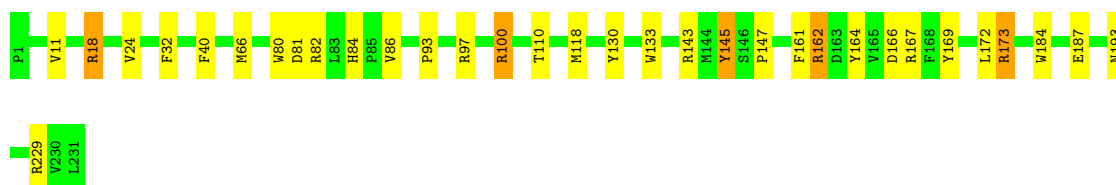
- Molecule 1: capsid protein

Chain 2M:  85% 13% .




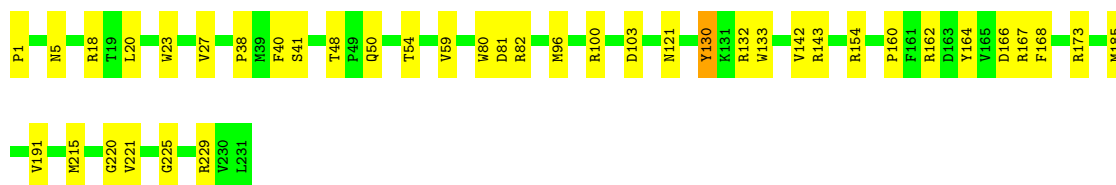
- Molecule 1: capsid protein

Chain 2N:  86% 12% •




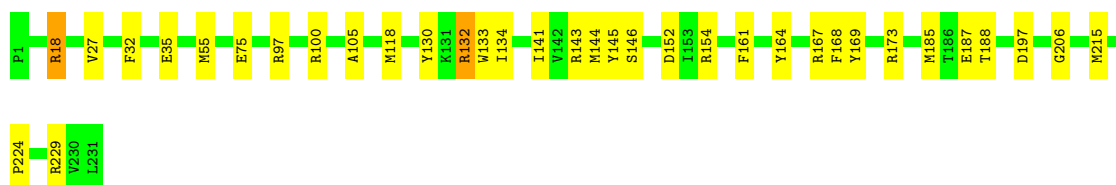
- Molecule 1: capsid protein

Chain 2O:  83% 17% •




- Molecule 1: capsid protein

Chain 2P:  85% 14% •




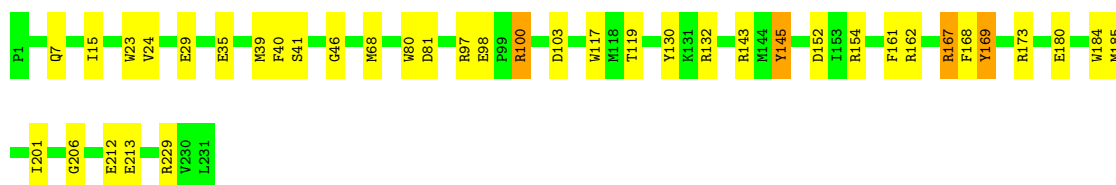
- Molecule 1: capsid protein

Chain 2Q:  81% 18% •




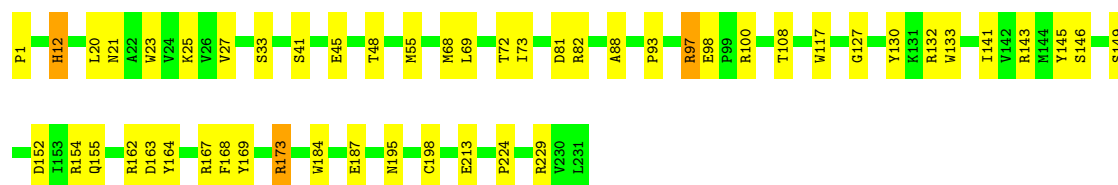
- Molecule 1: capsid protein

Chain 2R:  83% 15% •




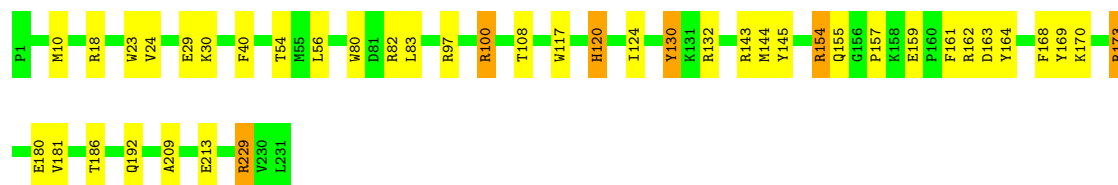
- Molecule 1: capsid protein

Chain 2S:  78% 21%




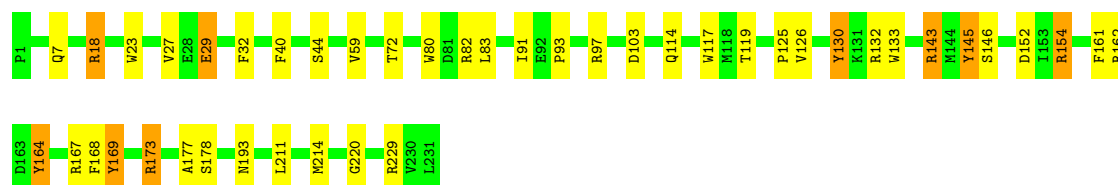
- Molecule 1: capsid protein

Chain 2T:  82% 16%




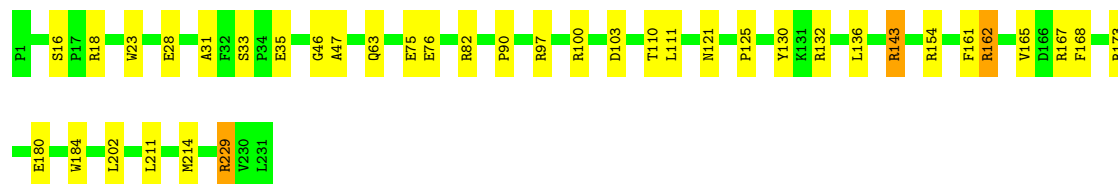
- Molecule 1: capsid protein

Chain 2U:  81% 15%




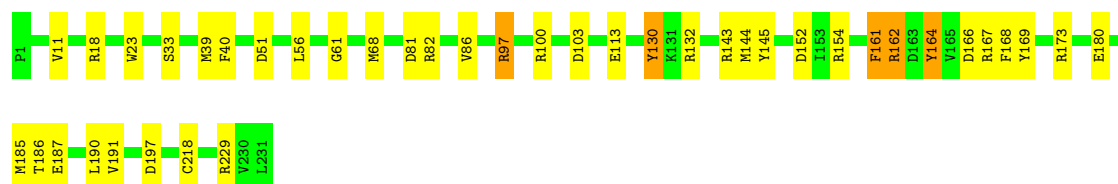
- Molecule 1: capsid protein

Chain 2V:  84% 15%




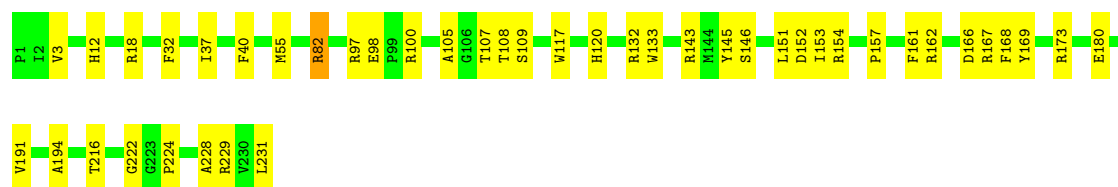
- Molecule 1: capsid protein

Chain 2W:  82% 16%




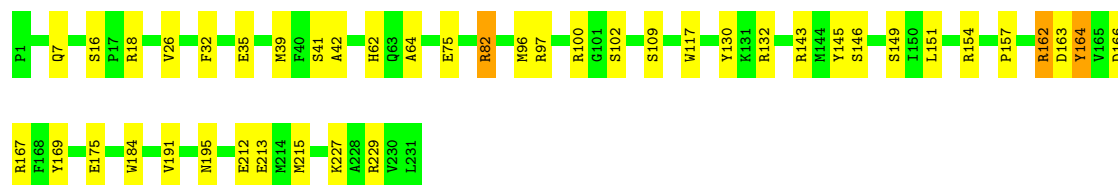
- Molecule 1: capsid protein

Chain 2X:  81% 18%




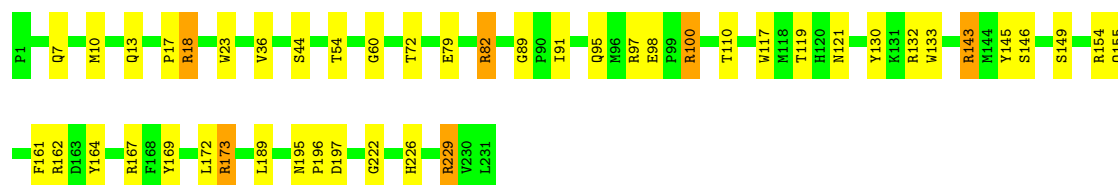
- Molecule 1: capsid protein

Chain 2Y:  81% 17%




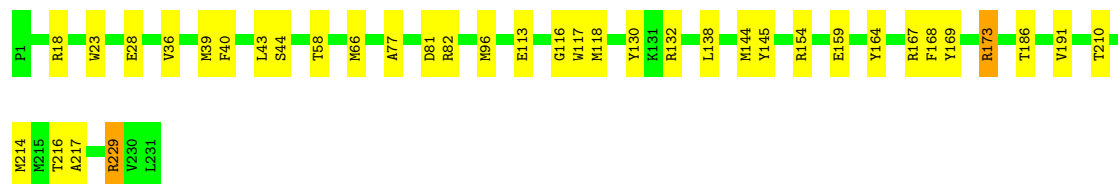
- Molecule 1: capsid protein

Chain 2Z:  80% 17%




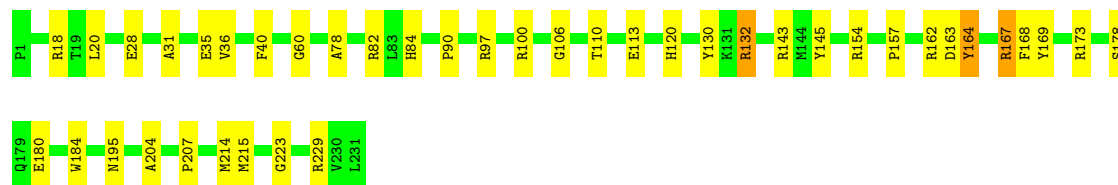
- Molecule 1: capsid protein

Chain 30:  84% 15%




- Molecule 1: capsid protein

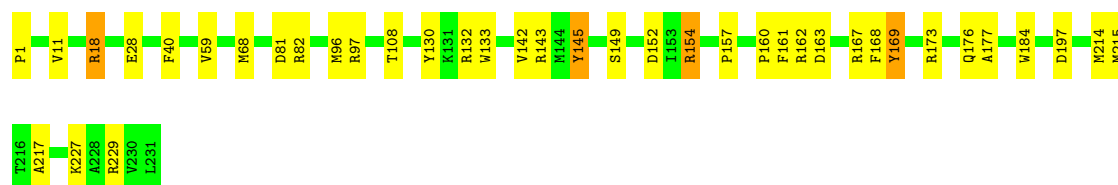
Chain 31:  82% 16%




- Molecule 1: capsid protein

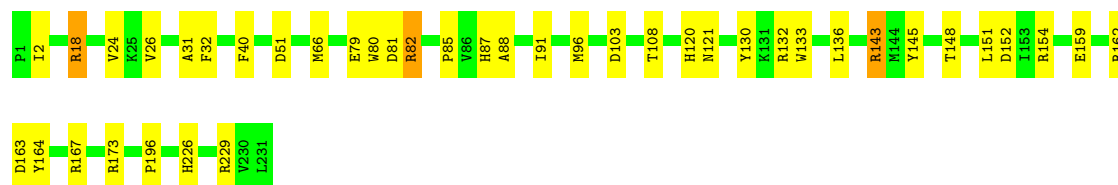


Chain 32:  83% 15%




- Molecule 1: capsid protein

Chain 33:  82% 16%




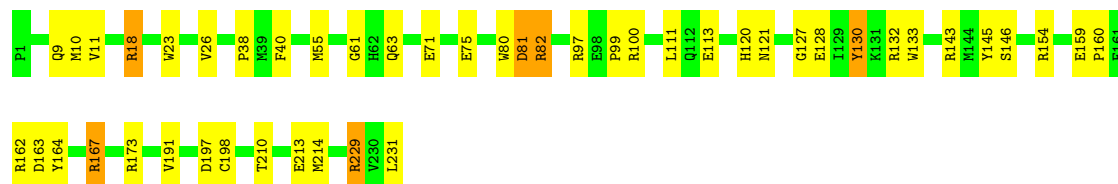
- Molecule 1: capsid protein

Chain 34:  84% 15%




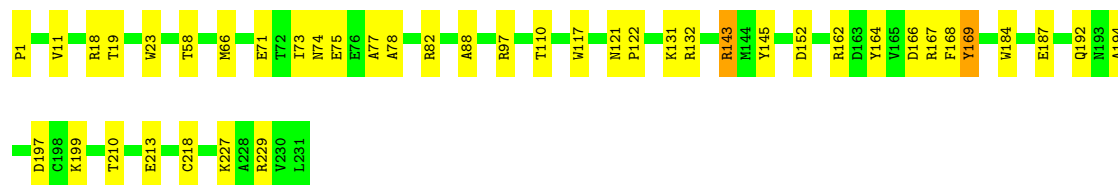
- Molecule 1: capsid protein

Chain 35:  80% 18%

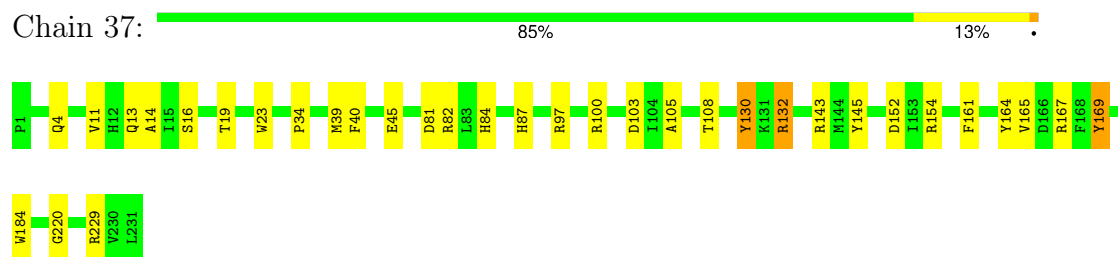


- Molecule 1: capsid protein

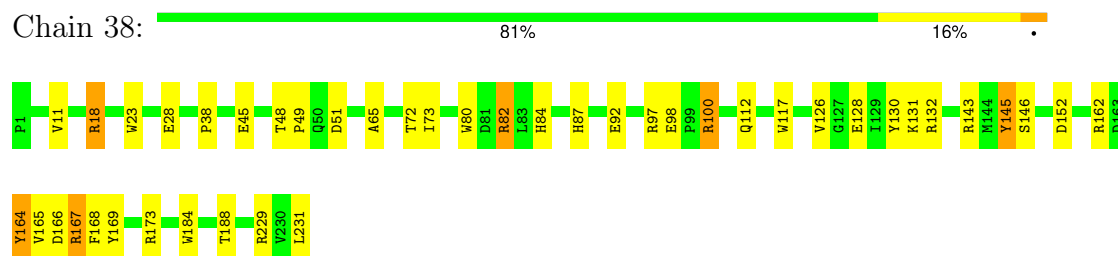
Chain 36:  82% 17%



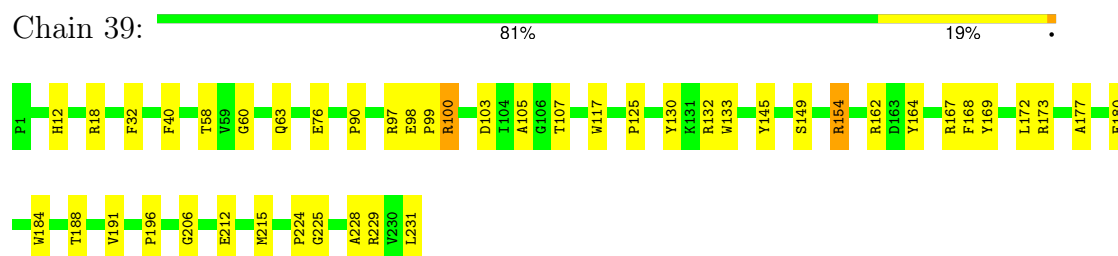
- Molecule 1: capsid protein



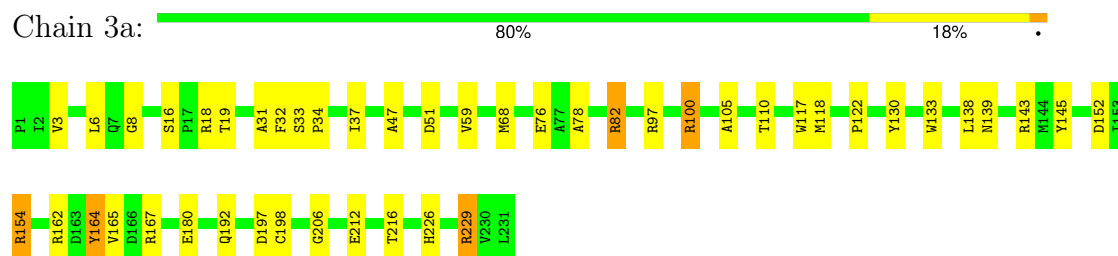
- Molecule 1: capsid protein



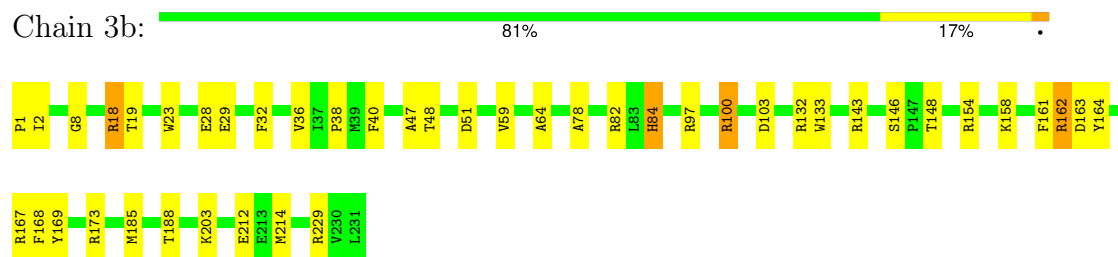
- Molecule 1: capsid protein



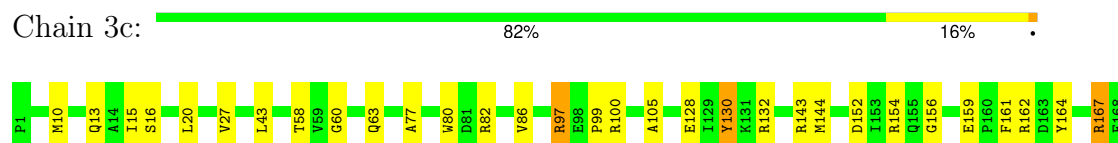
- Molecule 1: capsid protein



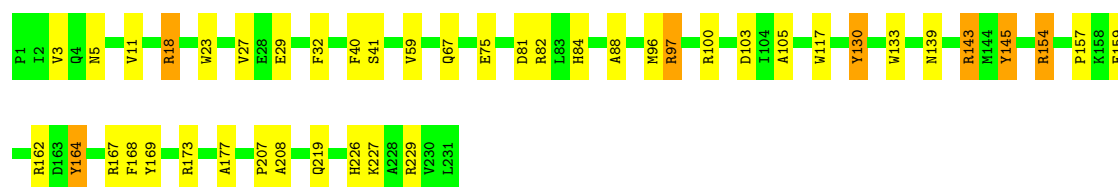
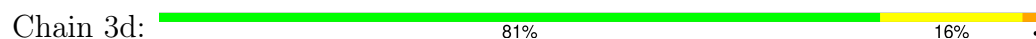
- Molecule 1: capsid protein



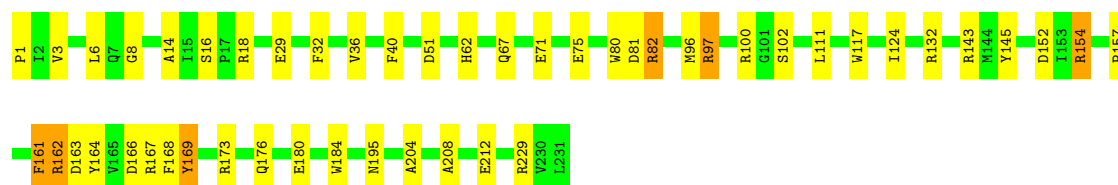
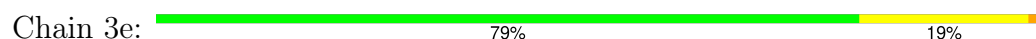
- Molecule 1: capsid protein



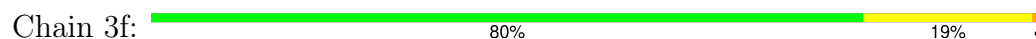
- Molecule 1: capsid protein



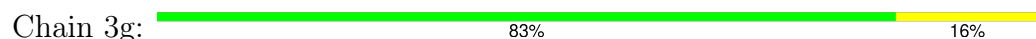
- Molecule 1: capsid protein




- Molecule 1: capsid protein

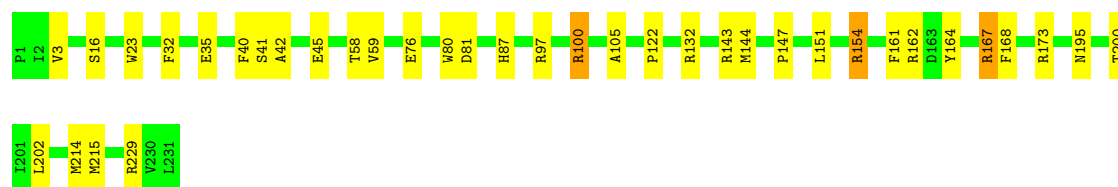


- Molecule 1: capsid protein




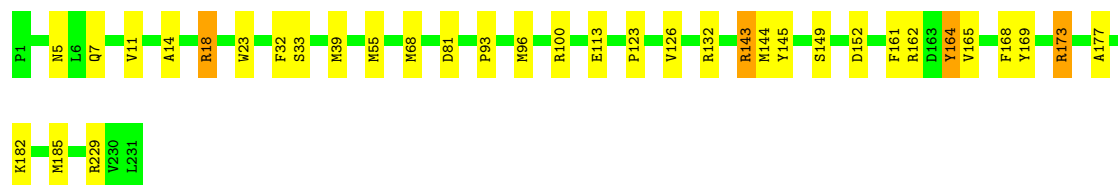
- Molecule 1: capsid protein

Chain 3h:  84% 15% •




- Molecule 1: capsid protein

Chain 3i:  85% 13% •




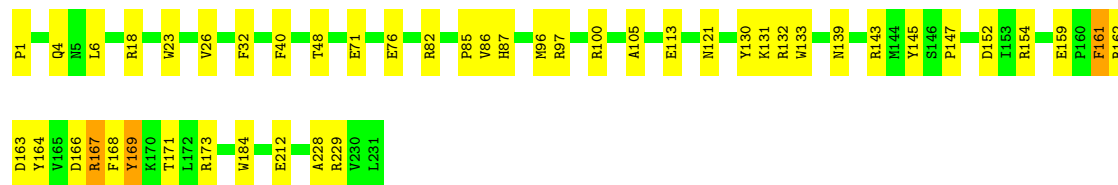
- Molecule 1: capsid protein

Chain 3j:  81% 18% •




- Molecule 1: capsid protein

Chain 3k:  80% 19% •




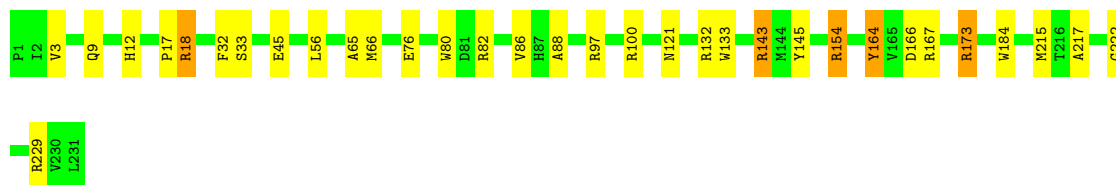
- Molecule 1: capsid protein

Chain 3l:  80% 19%




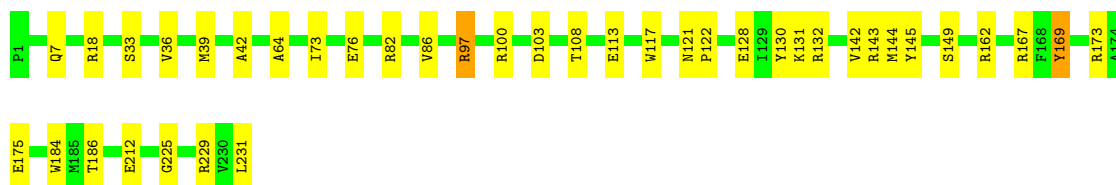
- Molecule 1: capsid protein

Chain 3m:  86% 12%




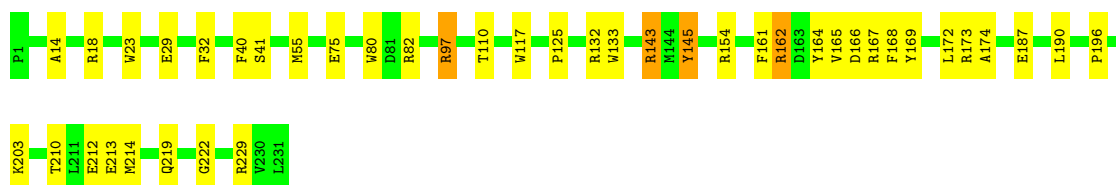
- Molecule 1: capsid protein

Chain 3n:  83% 16%




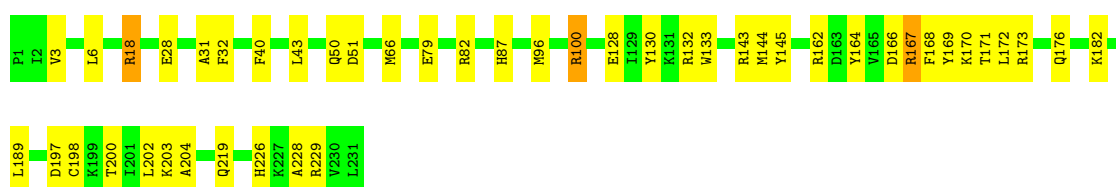
- Molecule 1: capsid protein

Chain 3o:  82% 16%




- Molecule 1: capsid protein

Chain 3p:  80% 19%




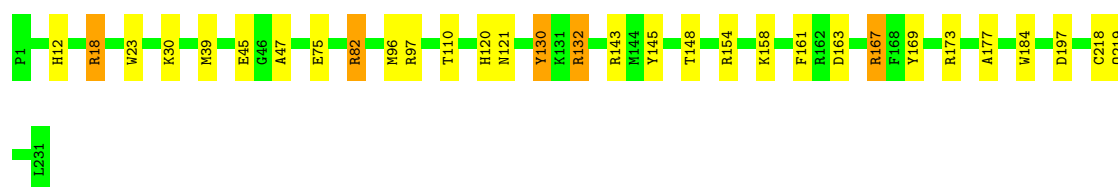
- Molecule 1: capsid protein

Chain 3q:  80% 19%




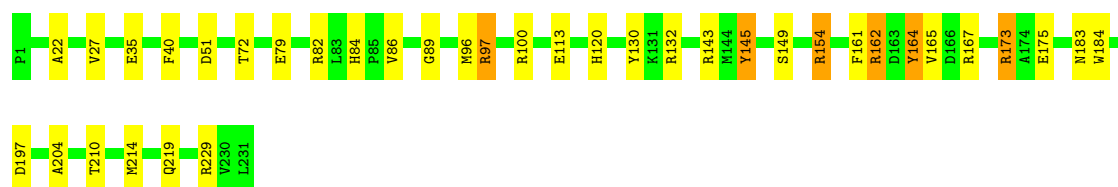
- Molecule 1: capsid protein

Chain 3r:  87% 11% •




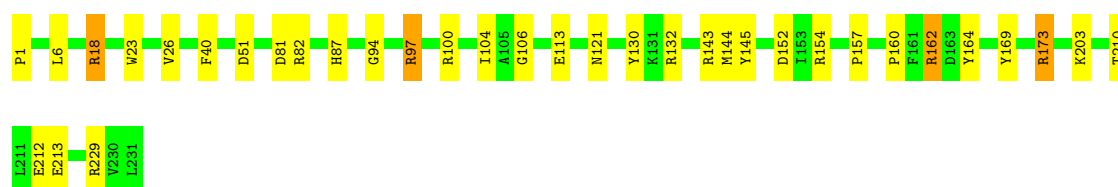
- Molecule 1: capsid protein

Chain 3s:  84% 13% •




- Molecule 1: capsid protein

Chain 3t:  85% 13% •




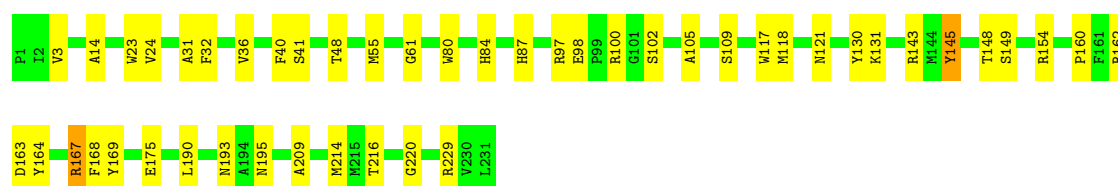
- Molecule 1: capsid protein

Chain 3u:  83% 15% •




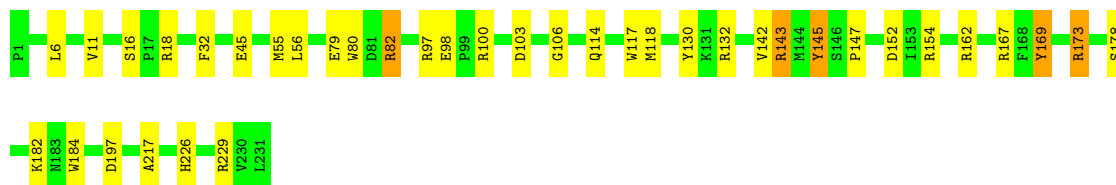
- Molecule 1: capsid protein

Chain 3v:  80% 19% •




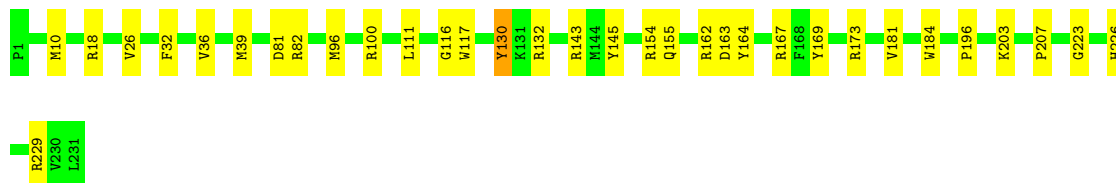
- Molecule 1: capsid protein

Chain 3w:  84% 14%




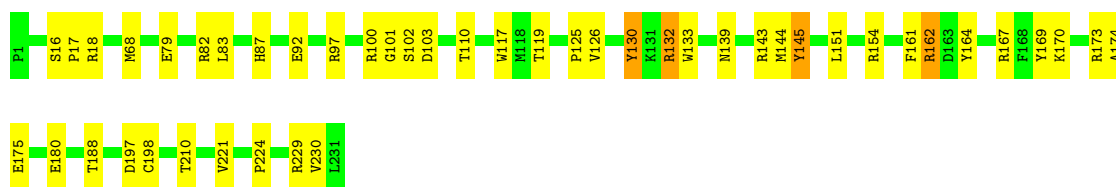
- Molecule 1: capsid protein

Chain 3x:  86% 14%




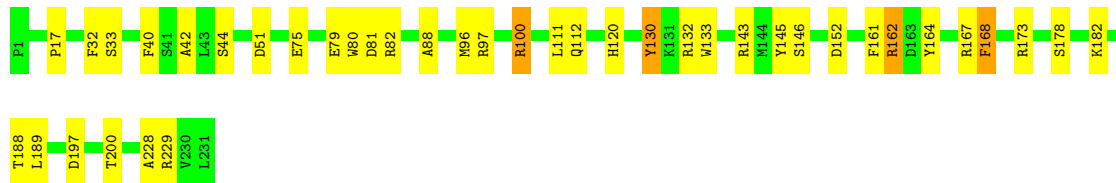
- Molecule 1: capsid protein

Chain 3y:  80% 18%




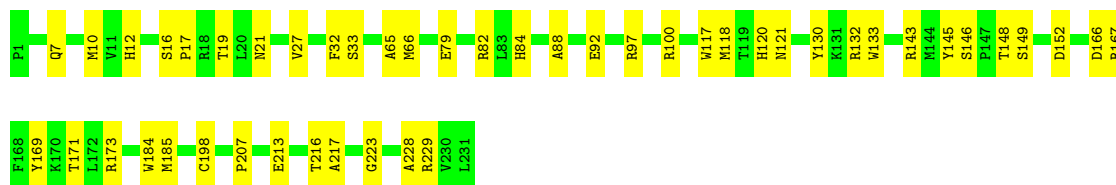
- Molecule 1: capsid protein

Chain 3z:  83% 16%




- Molecule 1: capsid protein

Chain 3A:  80% 20%




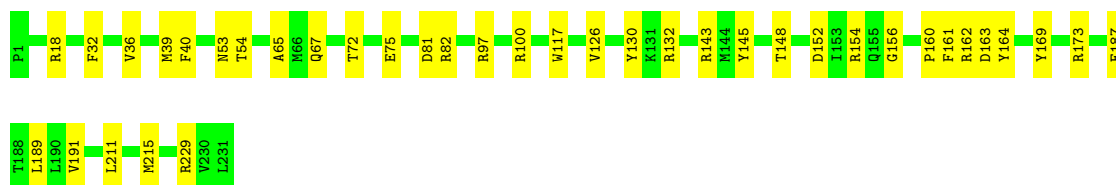
- Molecule 1: capsid protein

Chain 3B:  82% 16% .




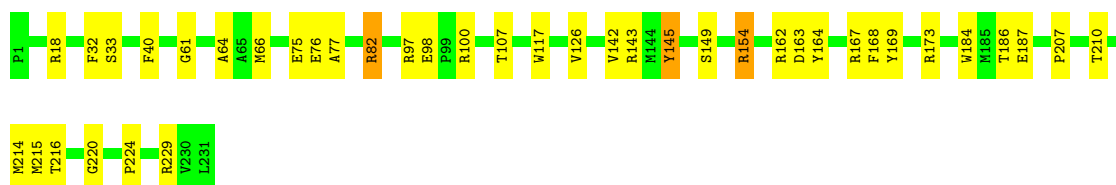
- Molecule 1: capsid protein

Chain 3C:  84% 16% .




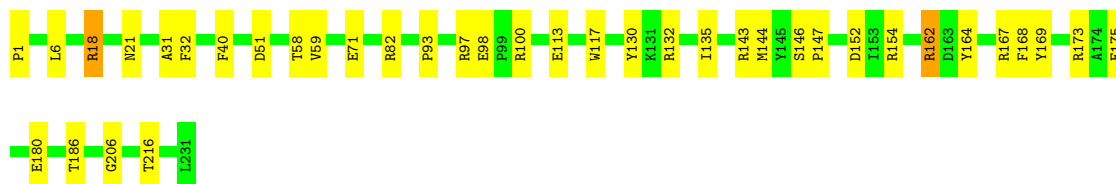
- Molecule 1: capsid protein

Chain 3D:  83% 16% .




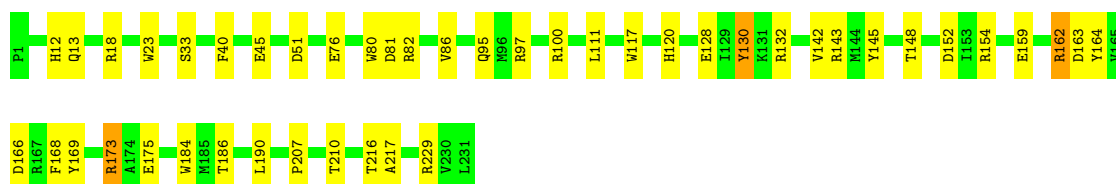
- Molecule 1: capsid protein

Chain 3E:  84% 16% .




- Molecule 1: capsid protein

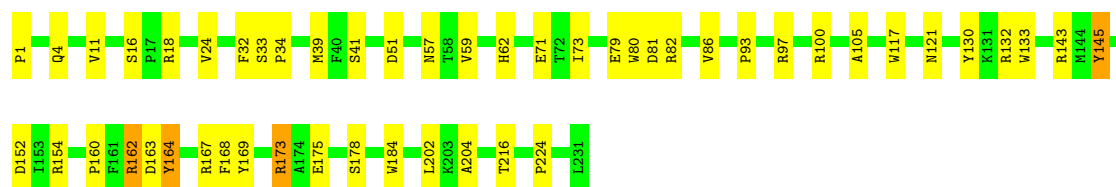
Chain 3F:  81% 18% .




- Molecule 1: capsid protein

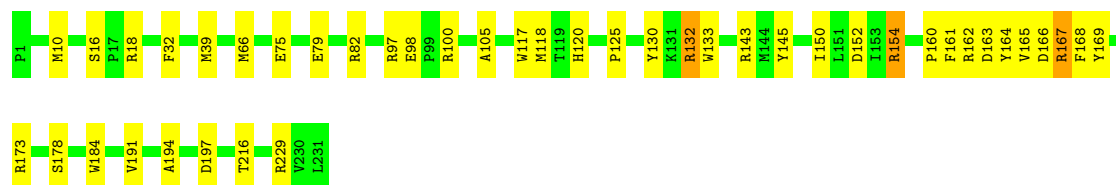


Chain 3G:  78% 20%




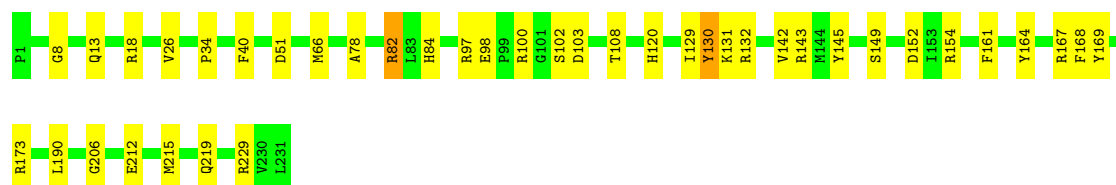
- Molecule 1: capsid protein

Chain 3H:  81% 17%




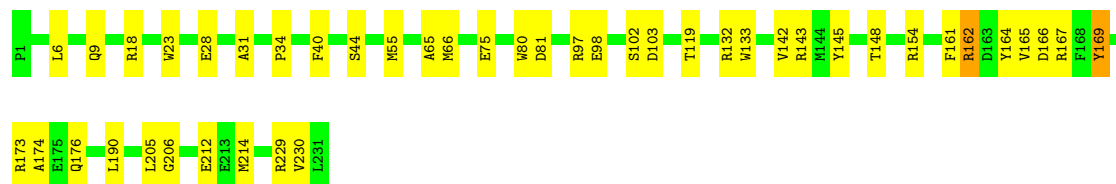
- Molecule 1: capsid protein

Chain 3I:  83% 16%




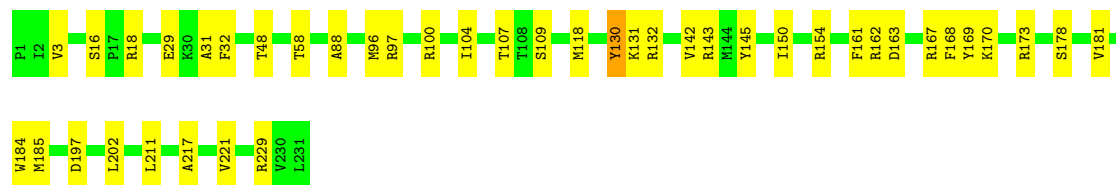
- Molecule 1: capsid protein

Chain 3J:  81% 18%




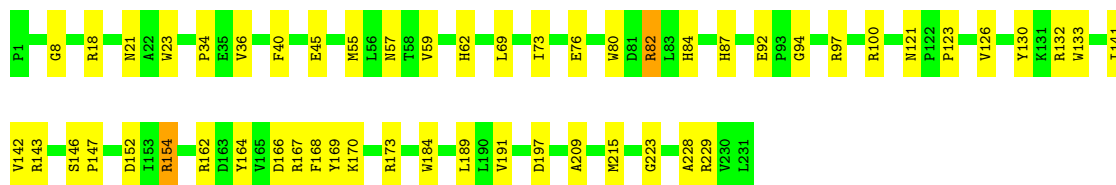
- Molecule 1: capsid protein

Chain 3K:  82% 18%




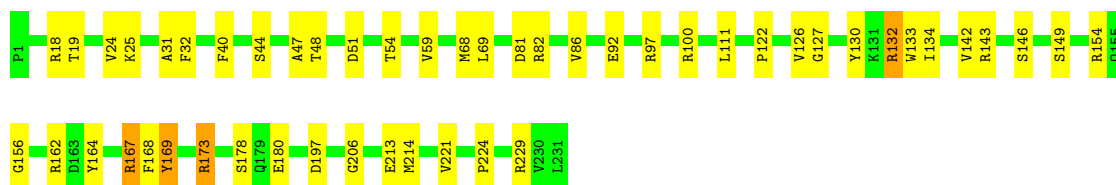
- Molecule 1: capsid protein

Chain 3L:  77% 22% .




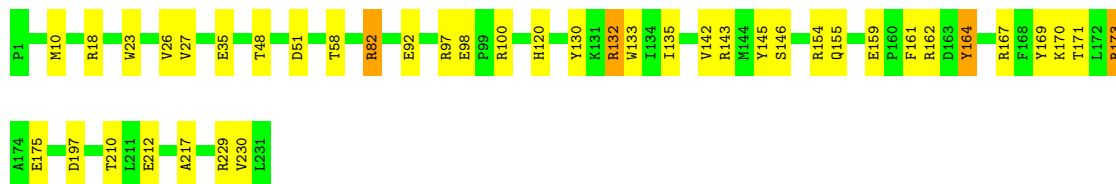
- Molecule 1: capsid protein

Chain 3M:  78% 20% .




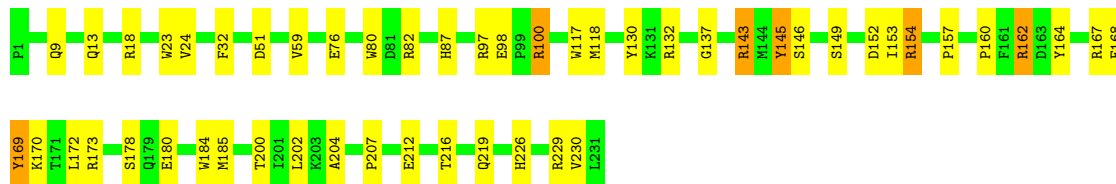
- Molecule 1: capsid protein

Chain 3N:  82% 16% .




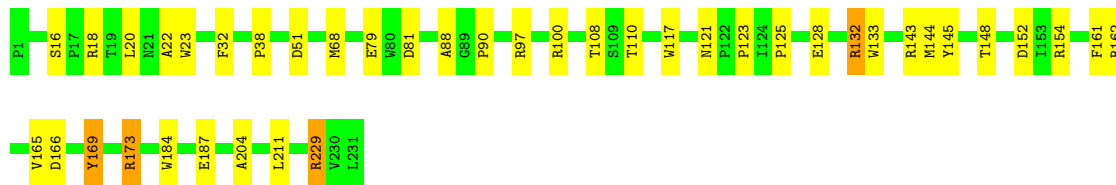
- Molecule 1: capsid protein

Chain 3O:  78% 19% .




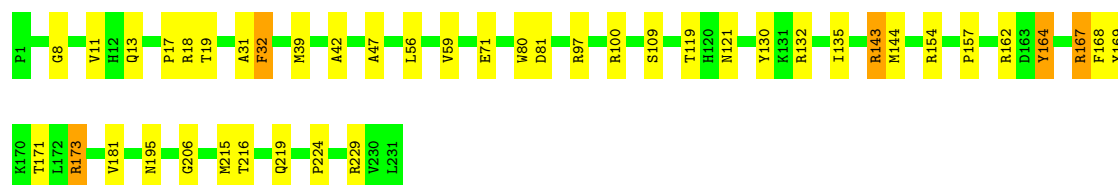
- Molecule 1: capsid protein

Chain 3P:  82% 16% .




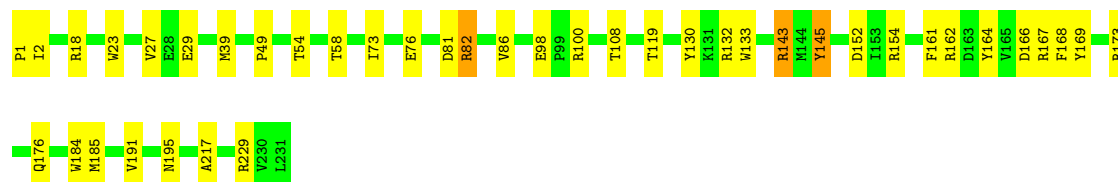
- Molecule 1: capsid protein

Chain 3Q:  81% 16%




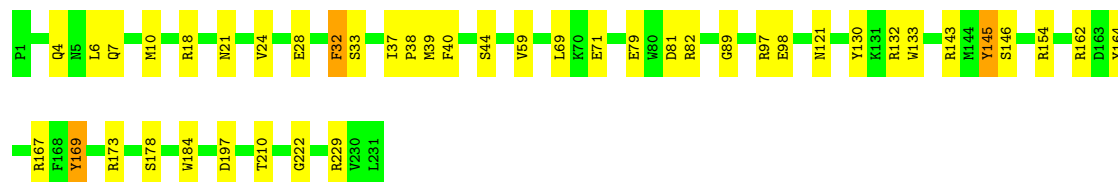
- Molecule 1: capsid protein

Chain 3R:  82% 16%




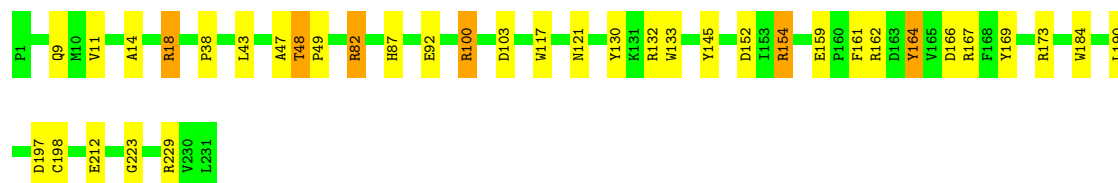
- Molecule 1: capsid protein

Chain 3S:  81% 17%




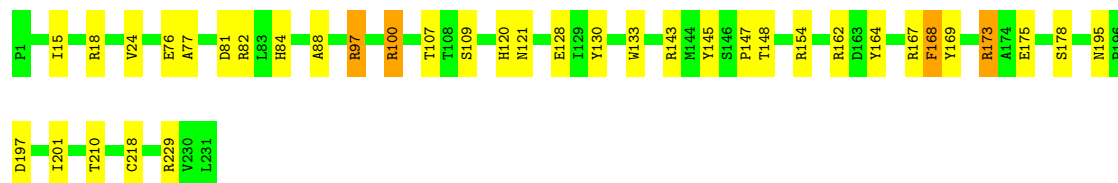
- Molecule 1: capsid protein

Chain 3T:  84% 13%




- Molecule 1: capsid protein

Chain 3U:  84% 14%




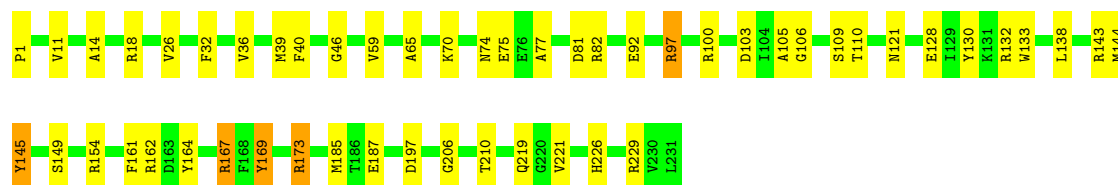
- Molecule 1: capsid protein

Chain 3V:  81% 18% .




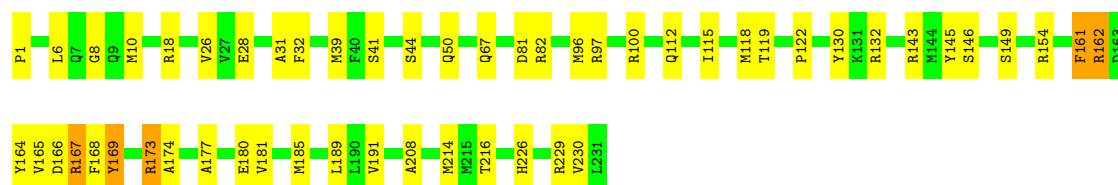
- Molecule 1: capsid protein

Chain 3W:  77% 20% .




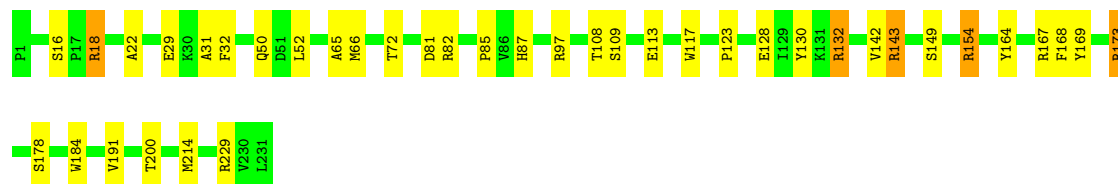
- Molecule 1: capsid protein

Chain 3X:  77% 21% .




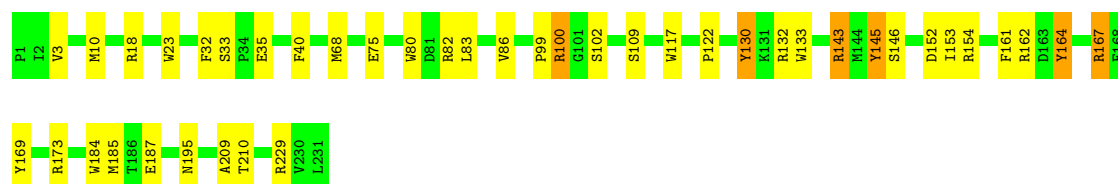
- Molecule 1: capsid protein

Chain 3Y:  83% 15% .

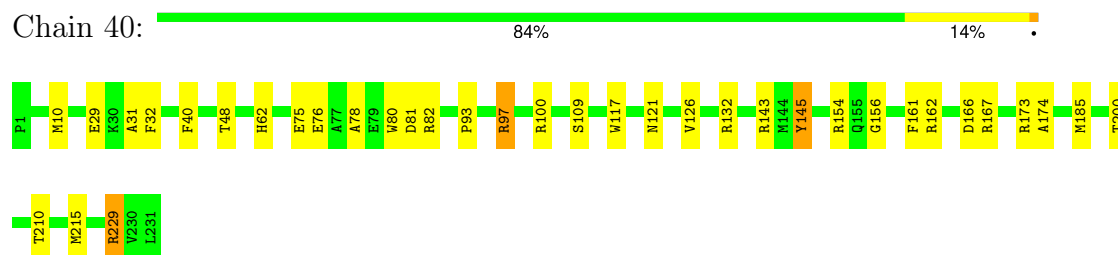


- Molecule 1: capsid protein

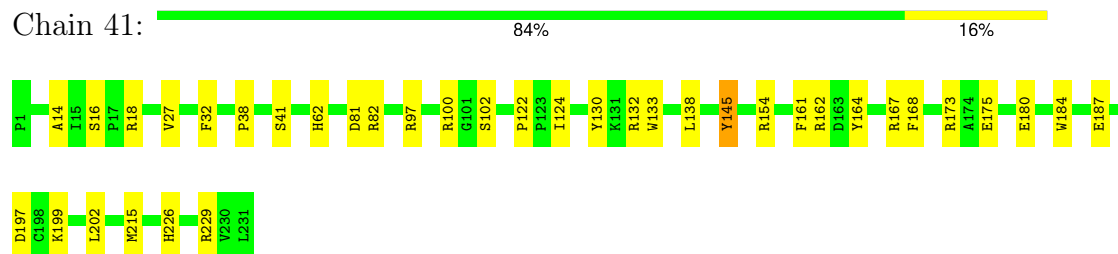
Chain 3Z:  82% 16% .



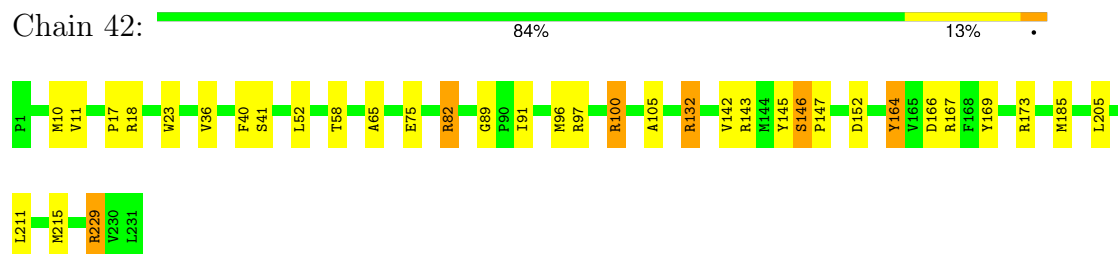
- Molecule 1: capsid protein



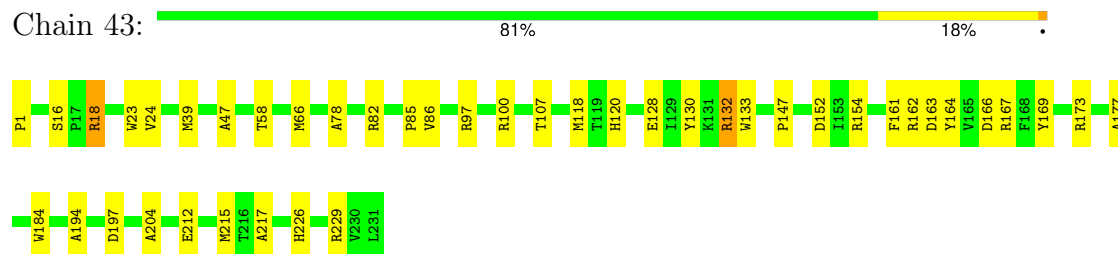
- Molecule 1: capsid protein



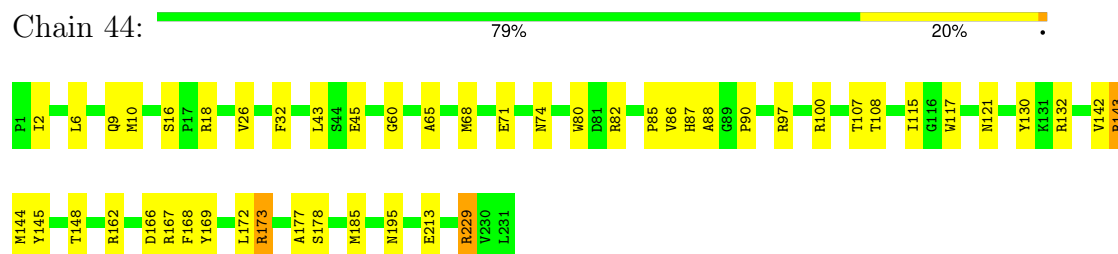
- Molecule 1: capsid protein




- Molecule 1: capsid protein

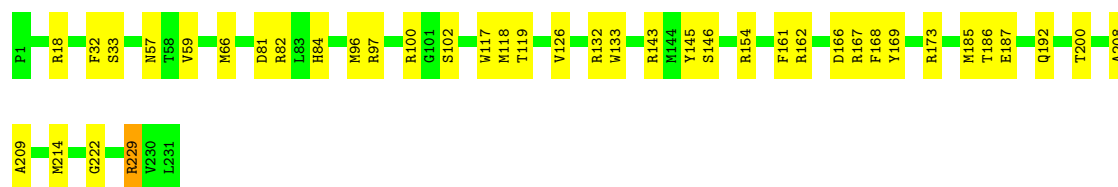


- Molecule 1: capsid protein




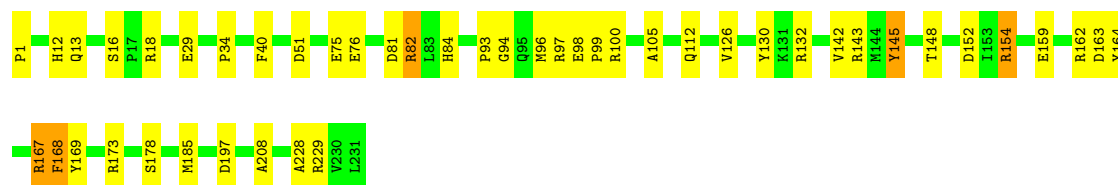
- Molecule 1: capsid protein

Chain 45:  83% 17%




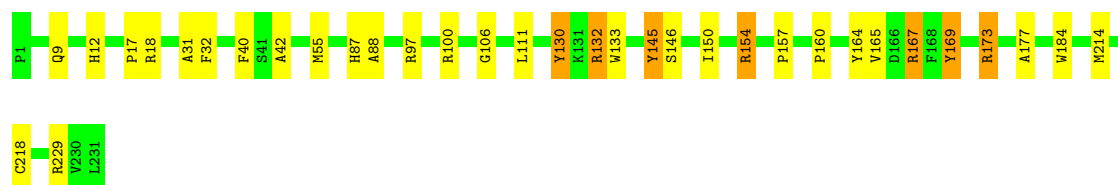
- Molecule 1: capsid protein

Chain 46:  80% 18%




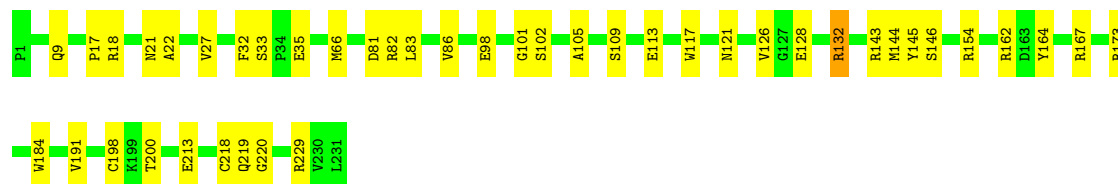
- Molecule 1: capsid protein

Chain 47:  85% 12%




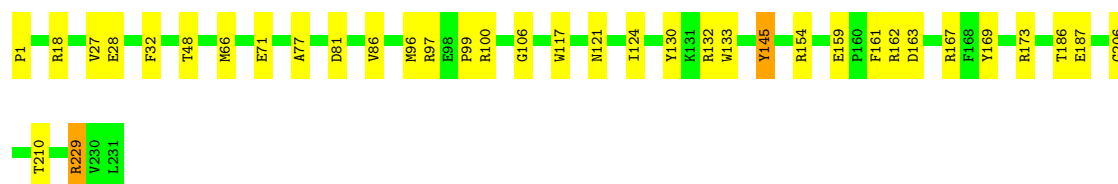
- Molecule 1: capsid protein

Chain 48:  81% 18%

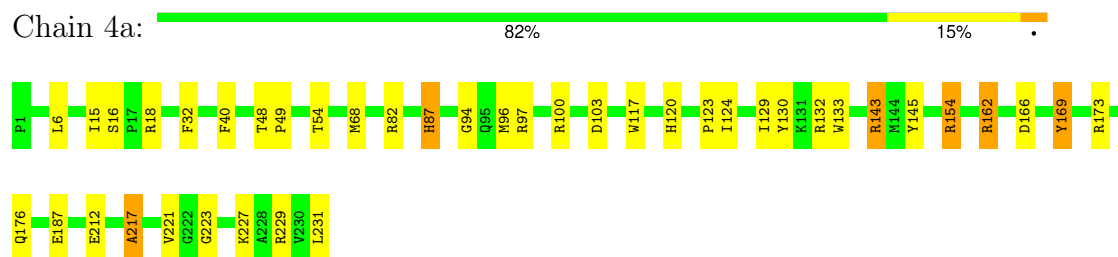


- Molecule 1: capsid protein

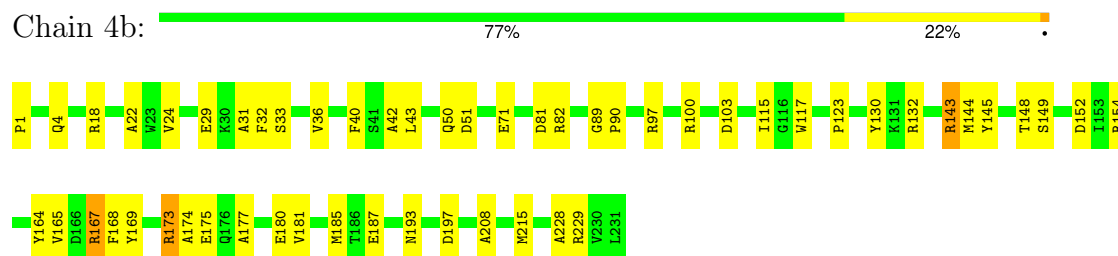
Chain 49:  84% 15%



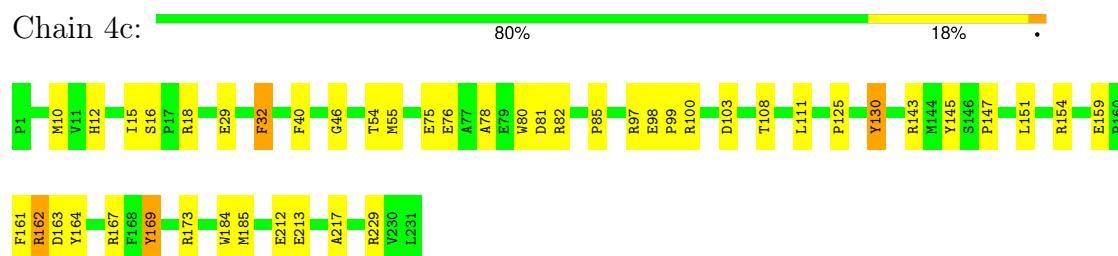
- Molecule 1: capsid protein



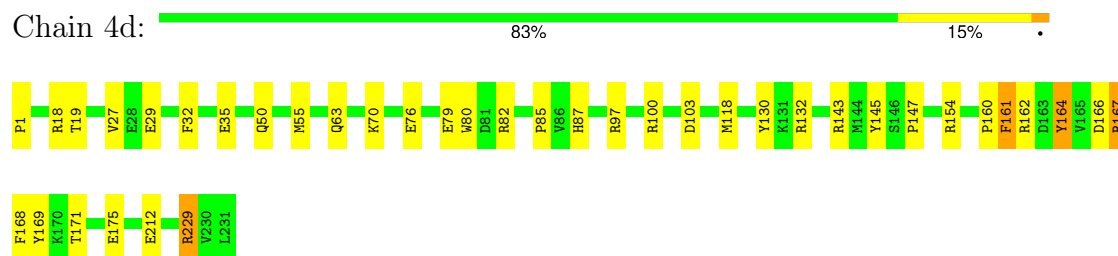
- Molecule 1: capsid protein



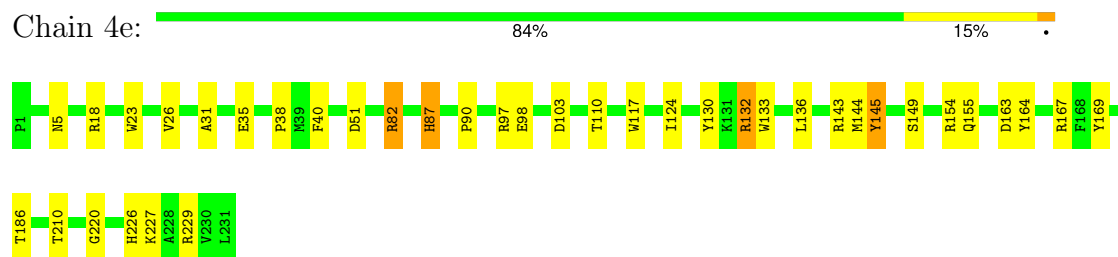
- Molecule 1: capsid protein




- Molecule 1: capsid protein

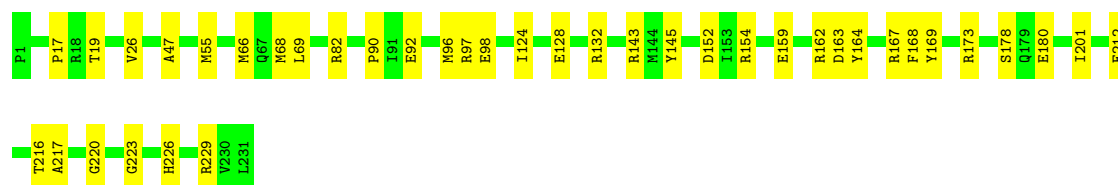


- Molecule 1: capsid protein




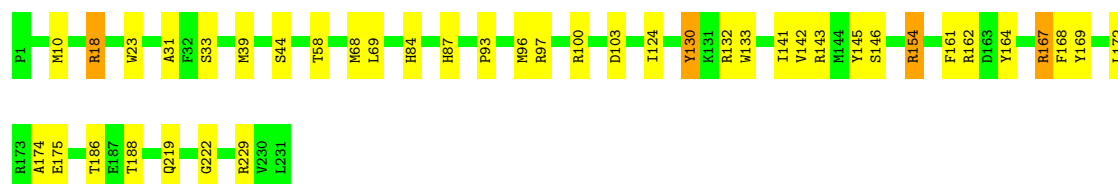
- Molecule 1: capsid protein

Chain 4f:  83% 17%




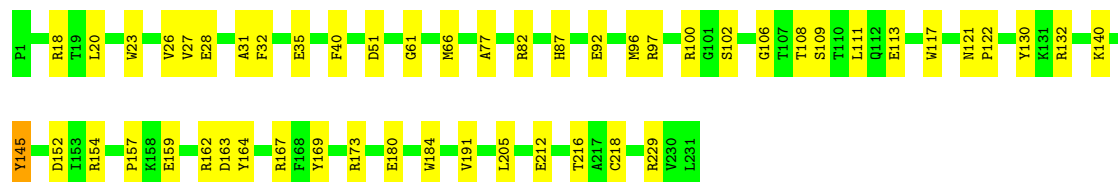
- Molecule 1: capsid protein

Chain 4g:  82% 16% •




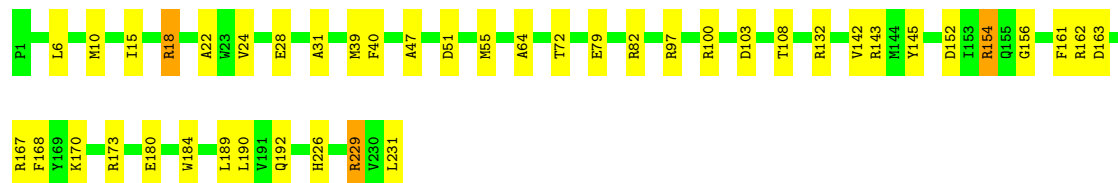
- Molecule 1: capsid protein

Chain 4h:  78% 22%




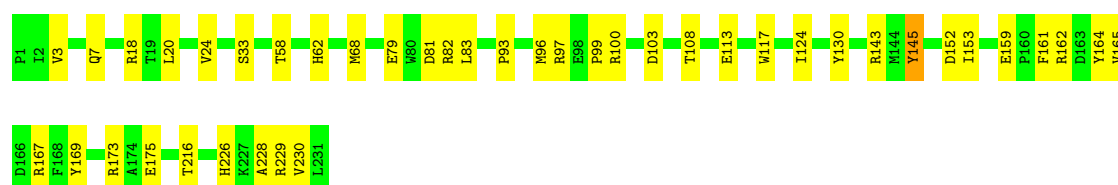
- Molecule 1: capsid protein

Chain 4i:  81% 17% •



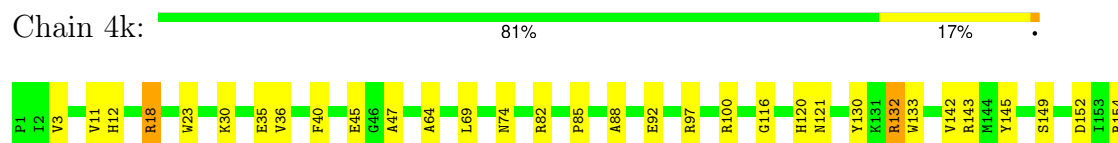
- Molecule 1: capsid protein

Chain 4j:  82% 18%

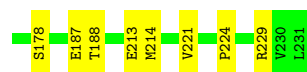
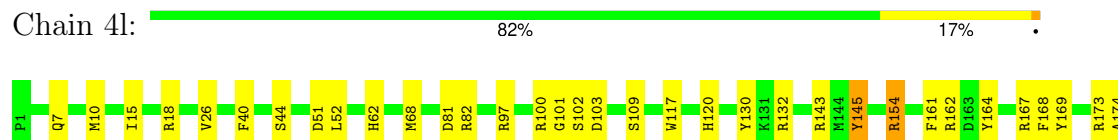


- Molecule 1: capsid protein

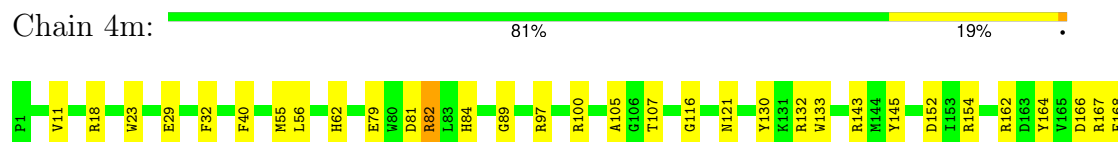




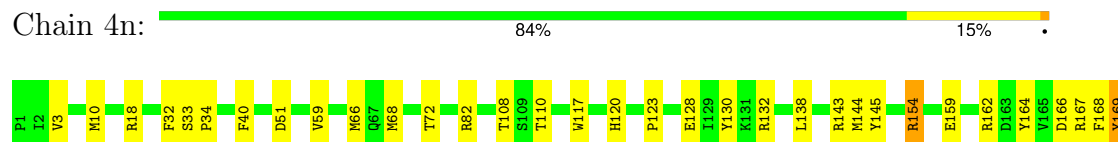
- Molecule 1: capsid protein



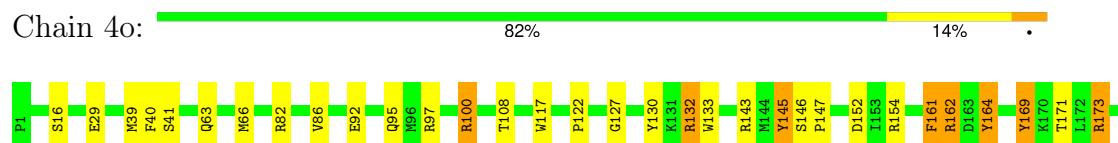
- Molecule 1: capsid protein




- Molecule 1: capsid protein

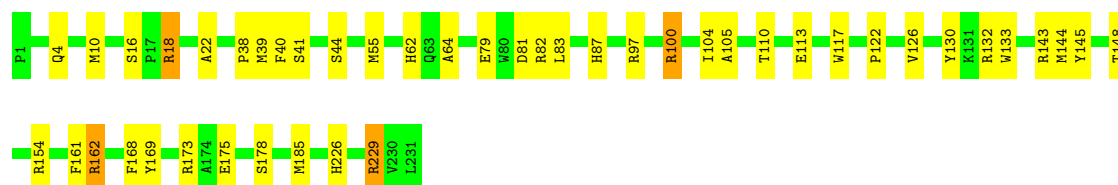


- Molecule 1: capsid protein




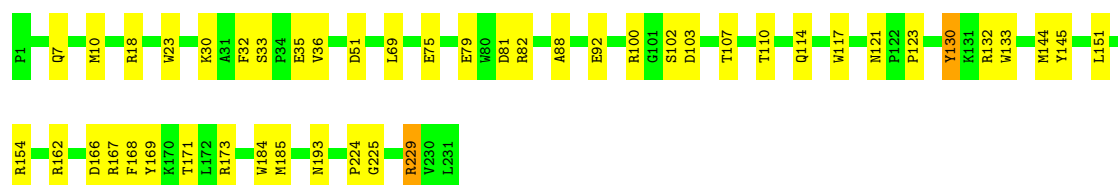
- Molecule 1: capsid protein

Chain 4p:  81% 18%




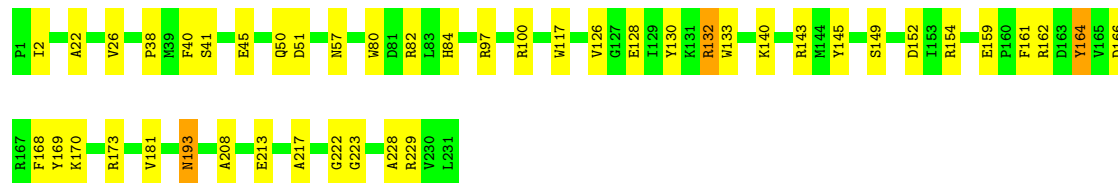
- Molecule 1: capsid protein

Chain 4q:  80% 19%




- Molecule 1: capsid protein

Chain 4r:  81% 18%




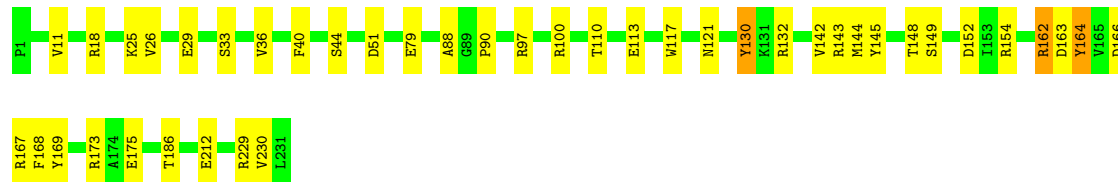
- Molecule 1: capsid protein

Chain 4s:  83% 16%




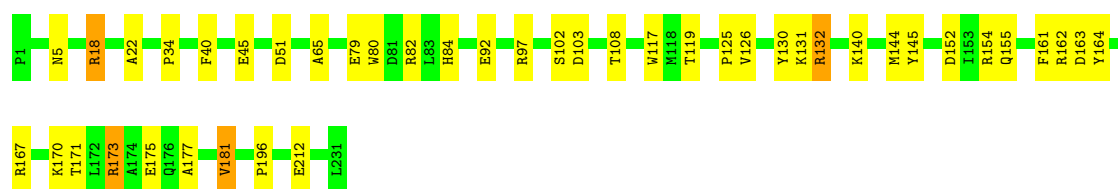
- Molecule 1: capsid protein

Chain 4t:  82% 17%




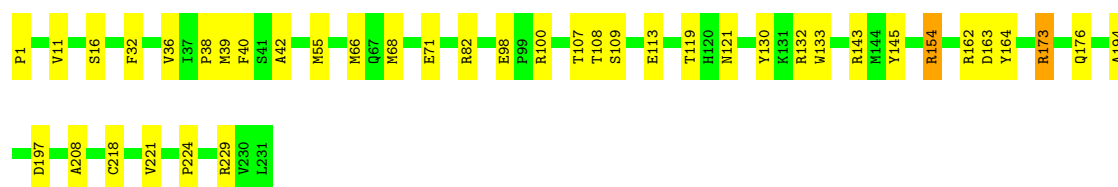
- Molecule 1: capsid protein

Chain 4u:  81% 17%



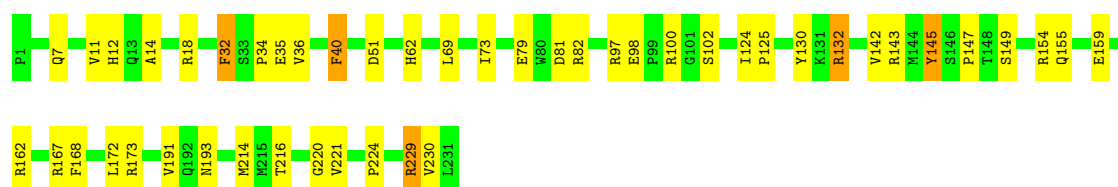
- Molecule 1: capsid protein

Chain 4v:  83% 16%




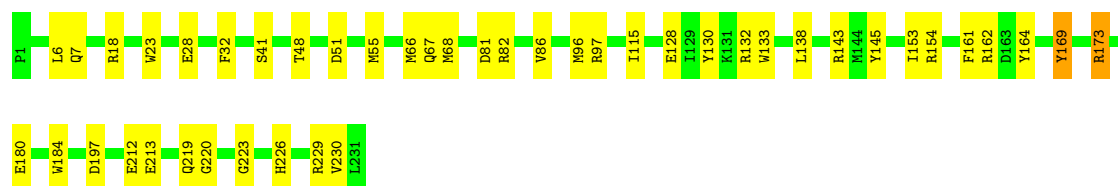
- Molecule 1: capsid protein

Chain 4w:  80% 18%




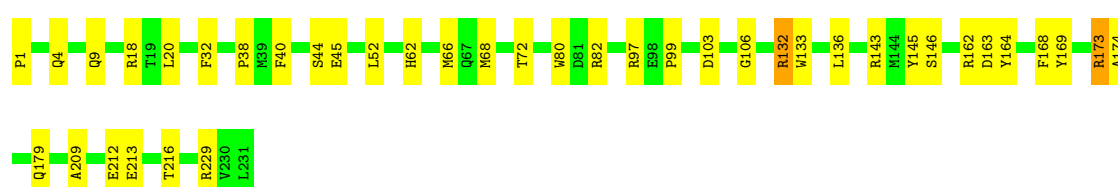
- Molecule 1: capsid protein

Chain 4x:  81% 18%

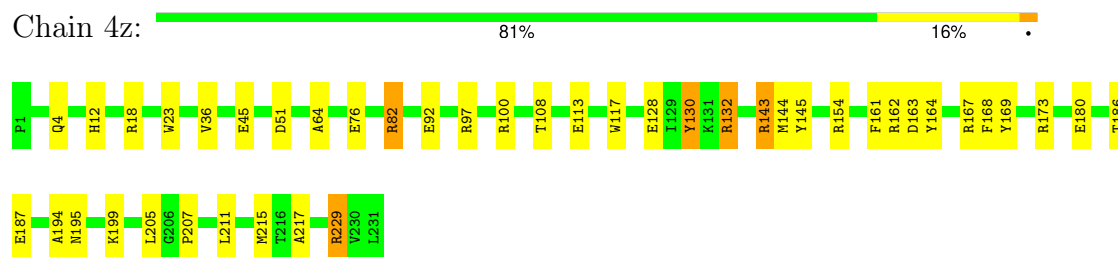


- Molecule 1: capsid protein

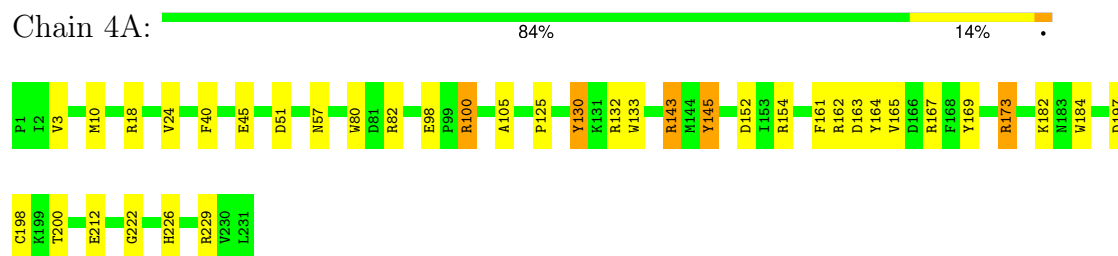
Chain 4y:  83% 16%



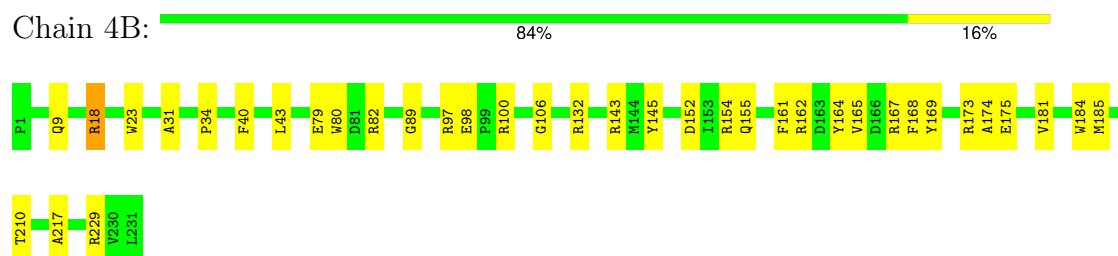
- Molecule 1: capsid protein



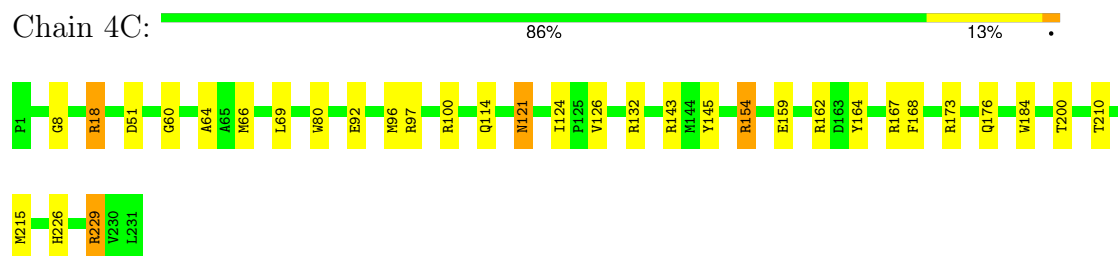
- Molecule 1: capsid protein



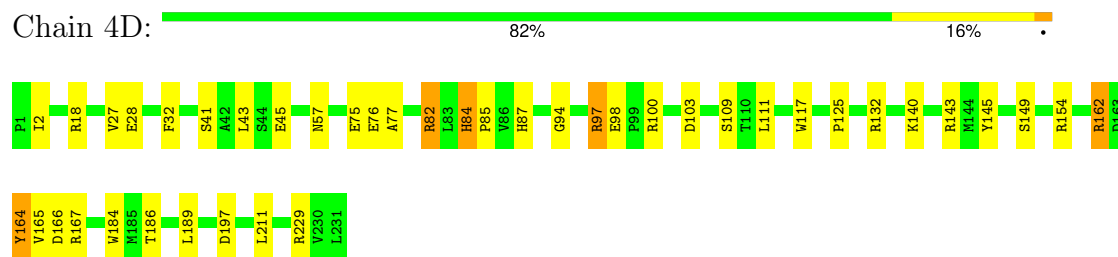
- Molecule 1: capsid protein



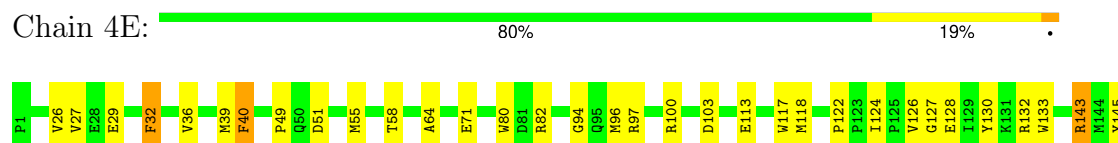
- Molecule 1: capsid protein



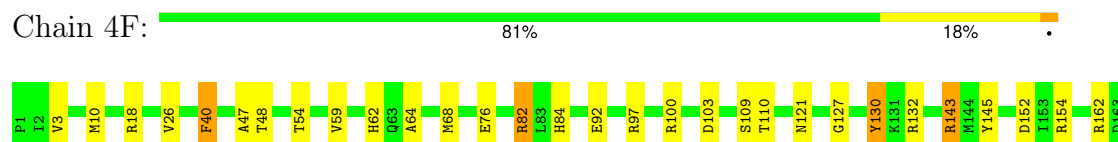
- Molecule 1: capsid protein



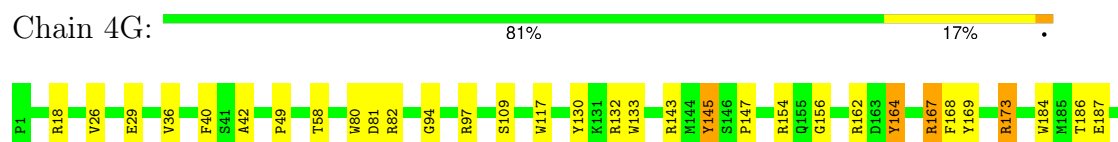
- Molecule 1: capsid protein



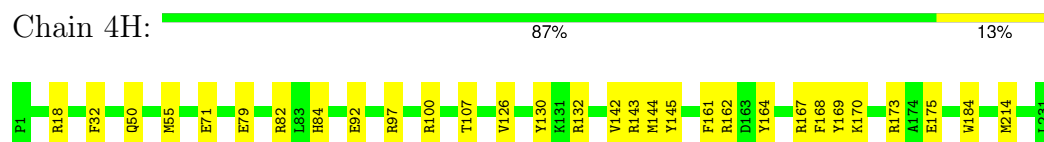
- Molecule 1: capsid protein



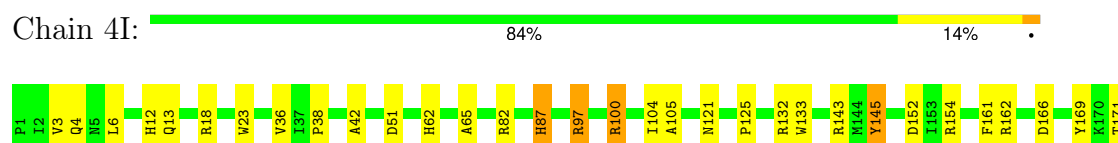
- Molecule 1: capsid protein



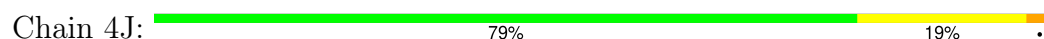
- Molecule 1: capsid protein

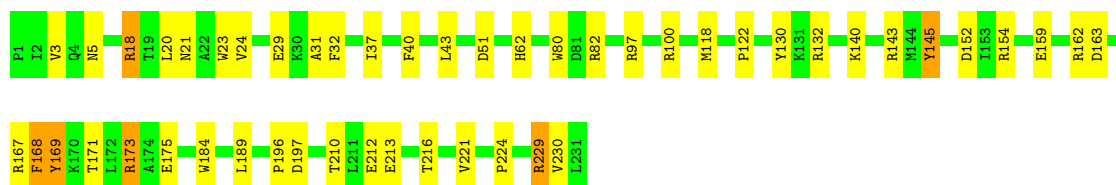


- Molecule 1: capsid protein



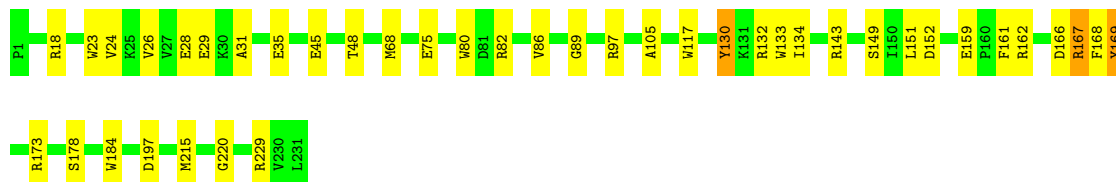
- Molecule 1: capsid protein





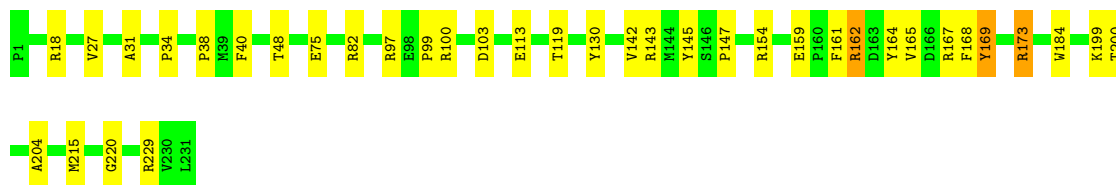
- Molecule 1: capsid protein

Chain 4K: 82% 16% .



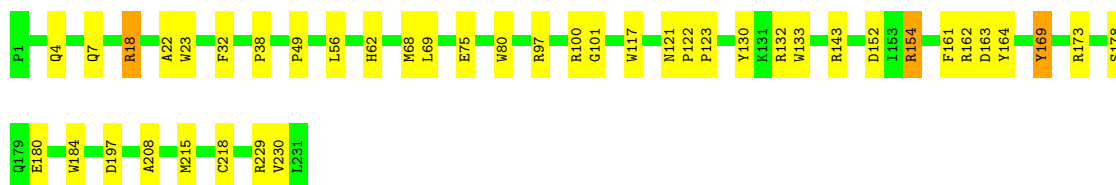
- Molecule 1: capsid protein

Chain 4L: 84% 15% .



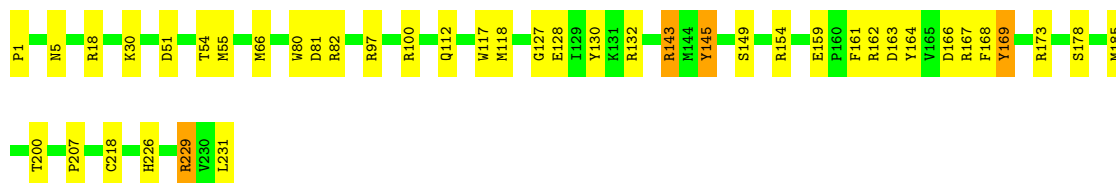
- Molecule 1: capsid protein

Chain 4M: 82% 17% .



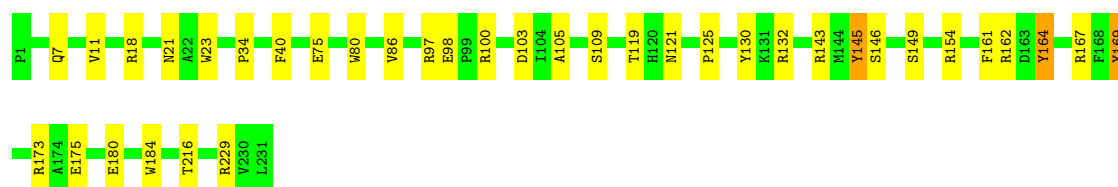
- Molecule 1: capsid protein

Chain 4N: 82% 16% .



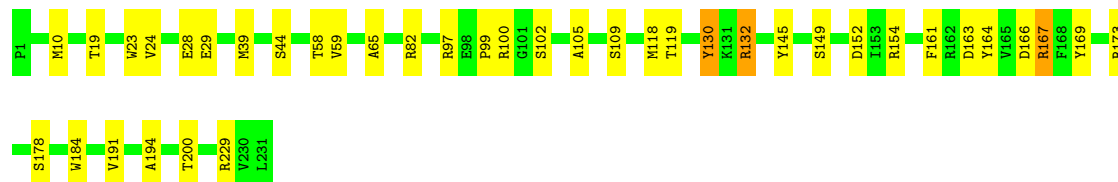
- Molecule 1: capsid protein

Chain 4O: 84% 15% .



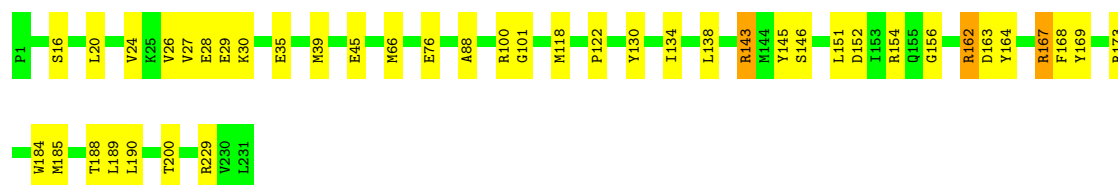
- Molecule 1: capsid protein

Chain 4P: 83% 16%



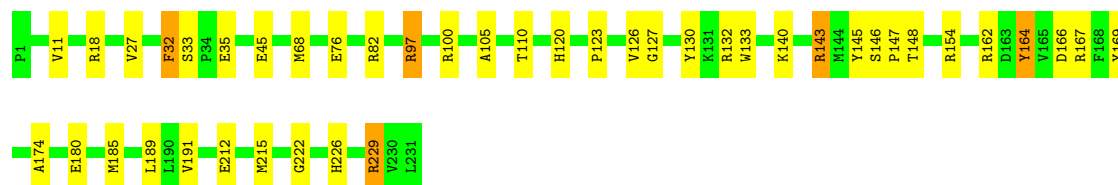
- Molecule 1: capsid protein

Chain 4Q: 82% 17%



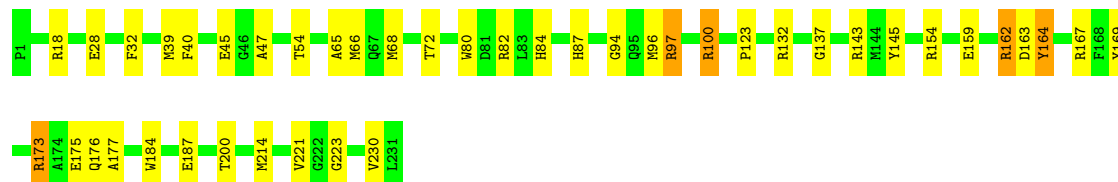
- Molecule 1: capsid protein

Chain 4R: 81% 16%



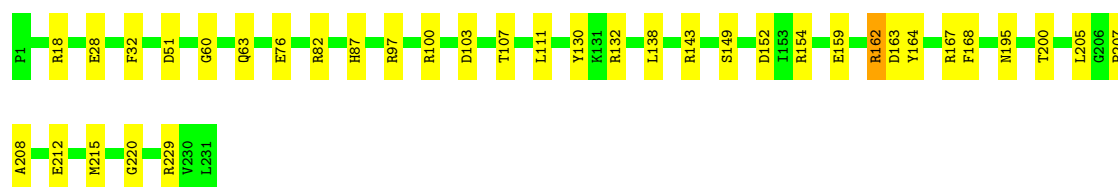
- Molecule 1: capsid protein

Chain 4S: 81% 16%




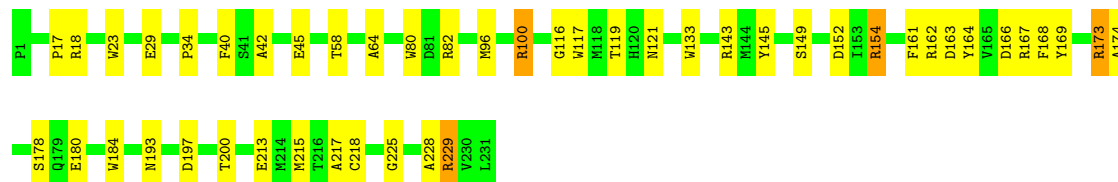
- Molecule 1: capsid protein

Chain 4T: 84% 15%




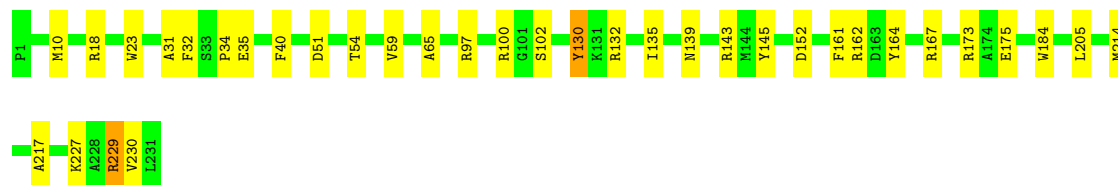
- Molecule 1: capsid protein

Chain 4U:  80% 19% .




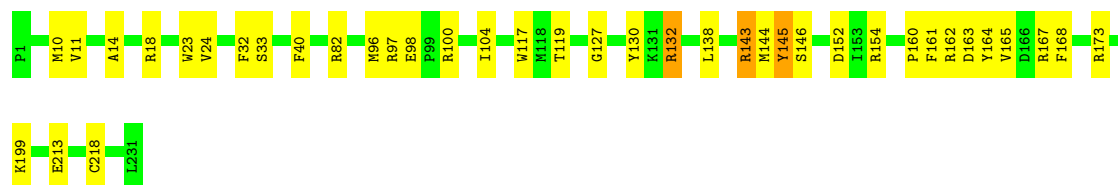
- Molecule 1: capsid protein

Chain 4V:  85% 14% .




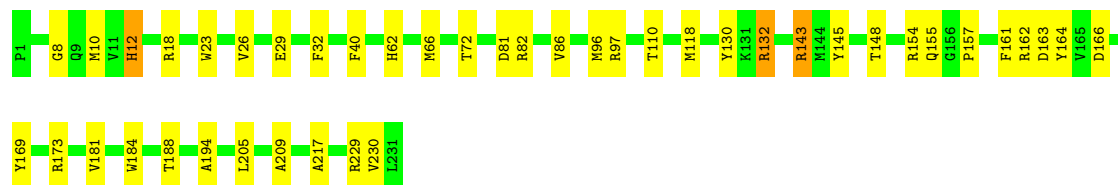
- Molecule 1: capsid protein

Chain 4W:  83% 16% .




- Molecule 1: capsid protein

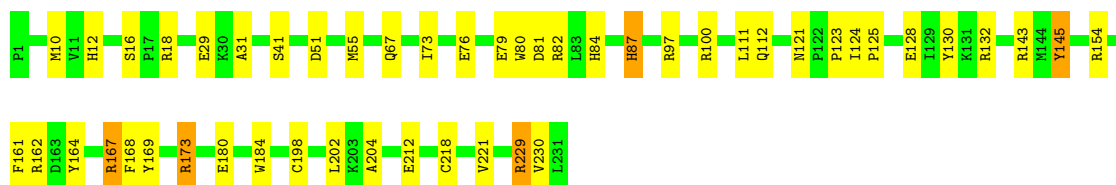
Chain 4X:  81% 17% .



- Molecule 1: capsid protein

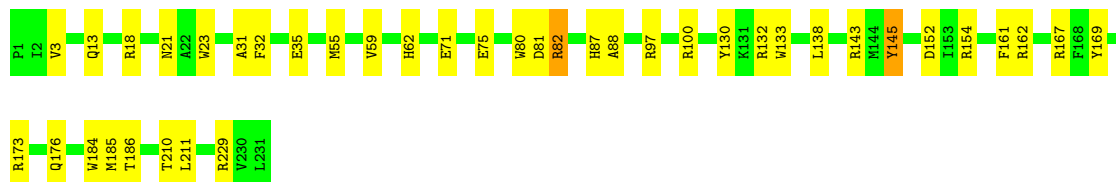
Chain 4Y:  79% 19% .





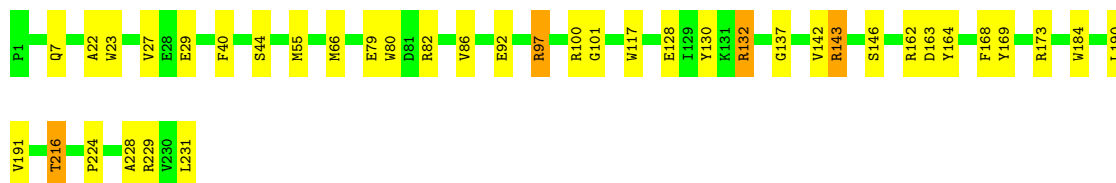
- Molecule 1: capsid protein

Chain 4Z: 83% 16% .



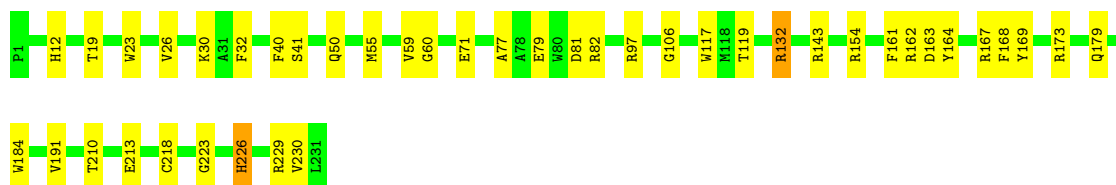
- Molecule 1: capsid protein

Chain 50: 83% 15% .



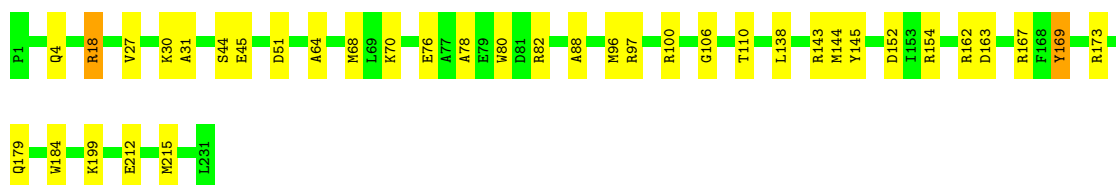
- Molecule 1: capsid protein

Chain 51: 82% 17% .



- Molecule 1: capsid protein

Chain 52: 84% 15% .



- Molecule 1: capsid protein

Chain 53: 84% 16% .



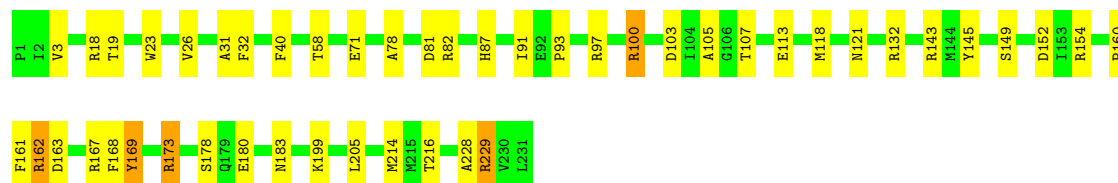
- Molecule 1: capsid protein

Chain 54: 82% 16% •



- Molecule 1: capsid protein

Chain 55: 80% 18% •



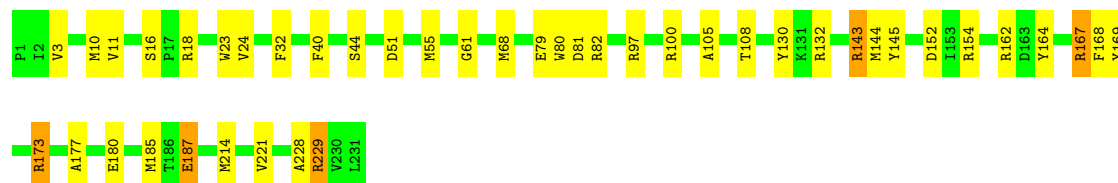
- Molecule 1: capsid protein

Chain 56: 85% 13% •



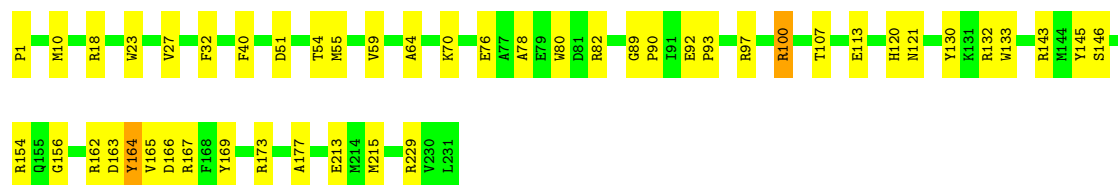
- Molecule 1: capsid protein

Chain 57: 81% 16% •



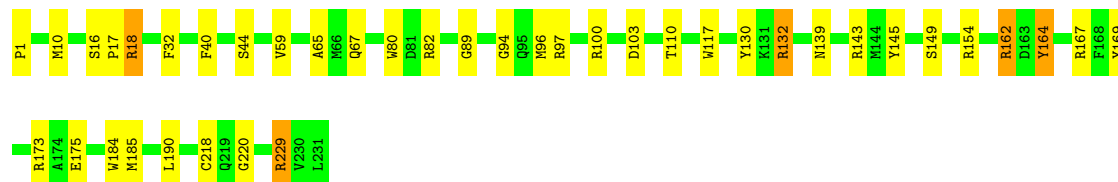
- Molecule 1: capsid protein

Chain 58: 80% 19% •



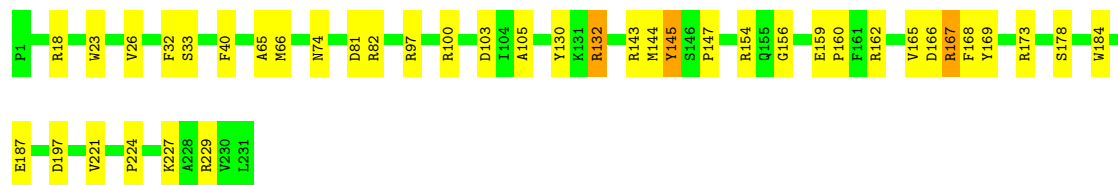
- Molecule 1: capsid protein

Chain 59: 83% 15%



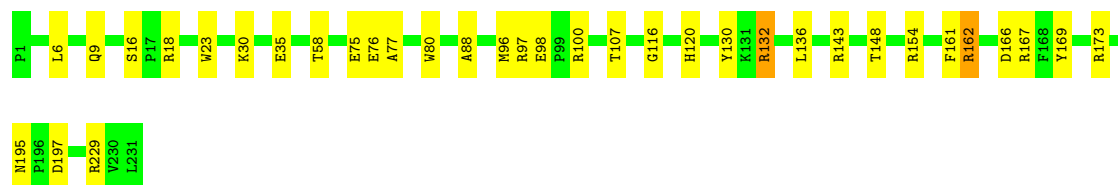
- Molecule 1: capsid protein

Chain 5a: 83% 16%



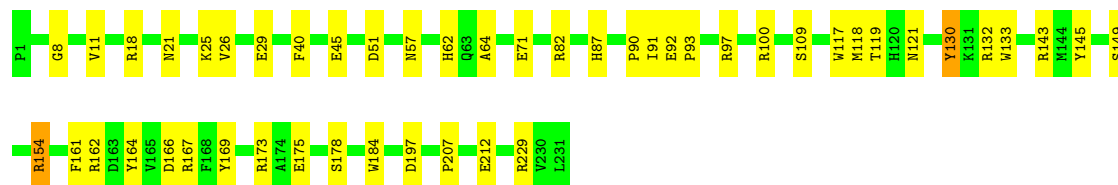
- Molecule 1: capsid protein

Chain 5b: 85% 14%



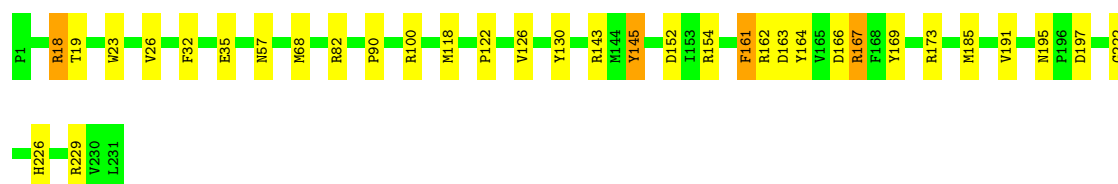
- Molecule 1: capsid protein

Chain 5c: 79% 20%



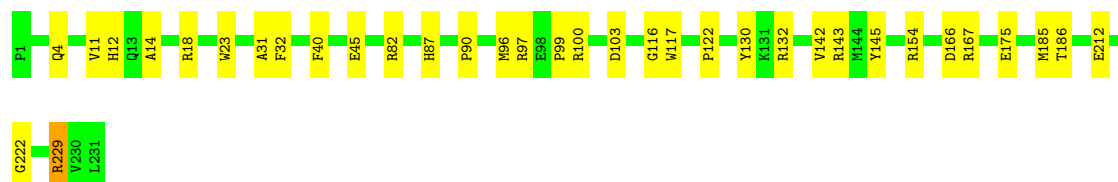
- Molecule 1: capsid protein

Chain 5d: 85% 13%



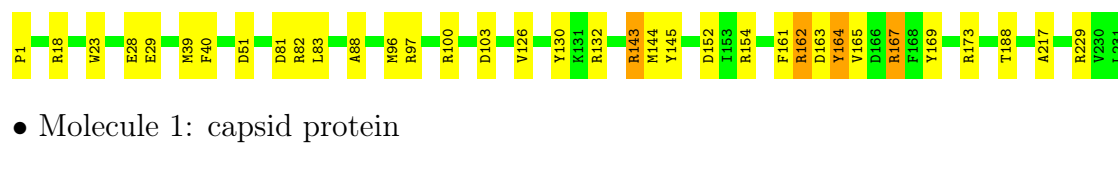
- Molecule 1: capsid protein

Chain 5e:  85% 15%



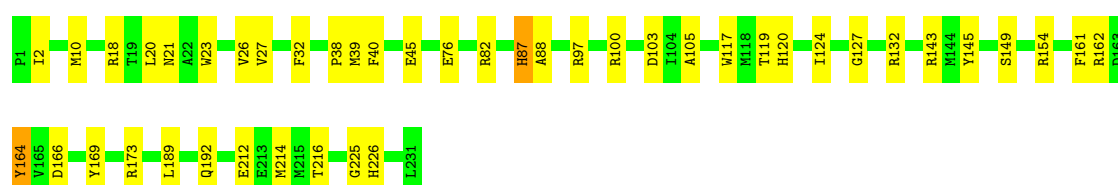
- Molecule 1: capsid protein

Chain 5f:  85% 13%



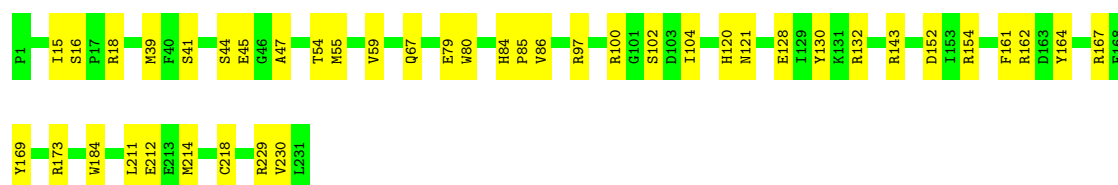
- Molecule 1: capsid protein

Chain 5g:  81% 18%



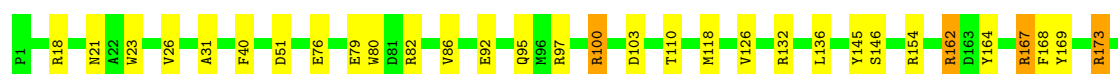
- Molecule 1: capsid protein

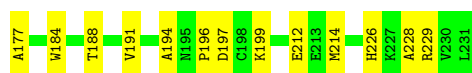
Chain 5h:  82% 18%



- Molecule 1: capsid protein

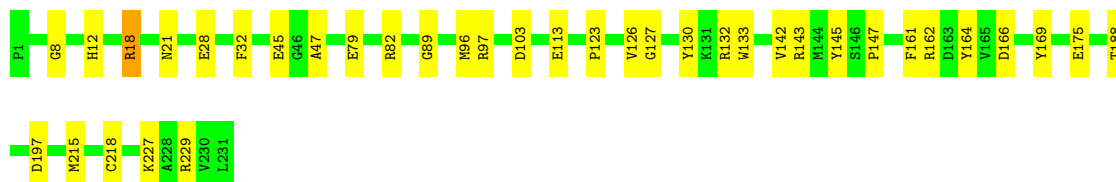
Chain 5i:  81% 17%





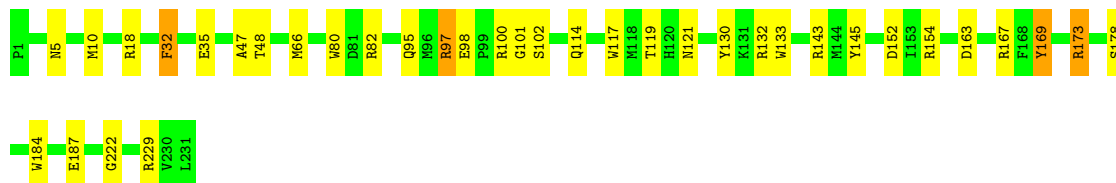
- Molecule 1: capsid protein

Chain 5j: 84% 16%



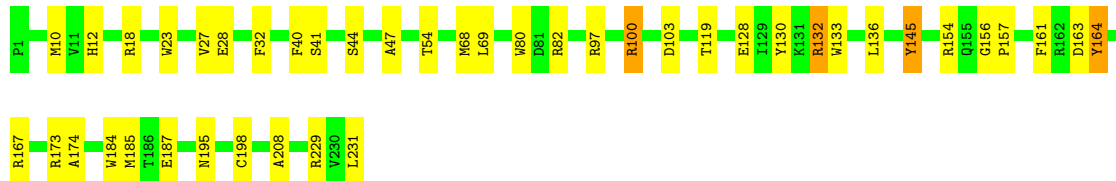
- Molecule 1: capsid protein

Chain 5k: 84% 14%



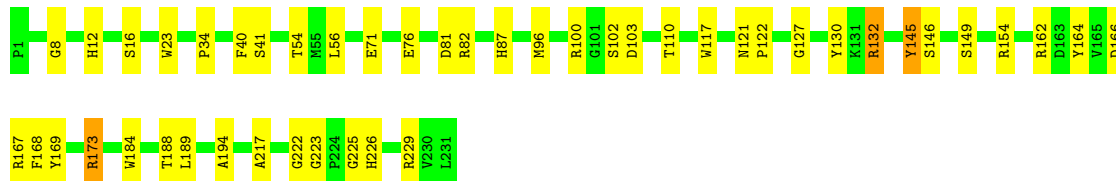
- Molecule 1: capsid protein

Chain 5l: 81% 17%



- Molecule 1: capsid protein

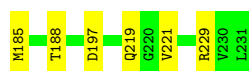
Chain 5m: 80% 19%



- Molecule 1: capsid protein

Chain 5n: 83% 16%





- Molecule 1: capsid protein

Chain 5o: 84% 15%



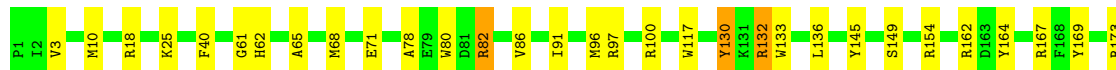
- Molecule 1: capsid protein

Chain 5p: 84% 14%



- Molecule 1: capsid protein

Chain 5q: 81% 17%



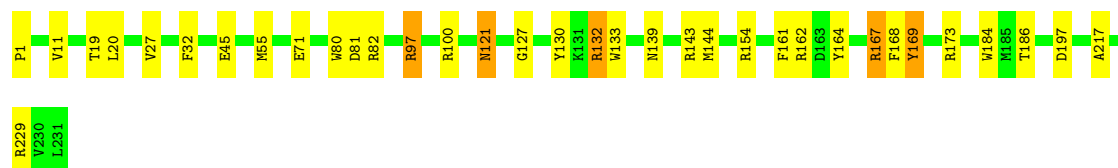
- Molecule 1: capsid protein

Chain 5r: 84% 14%



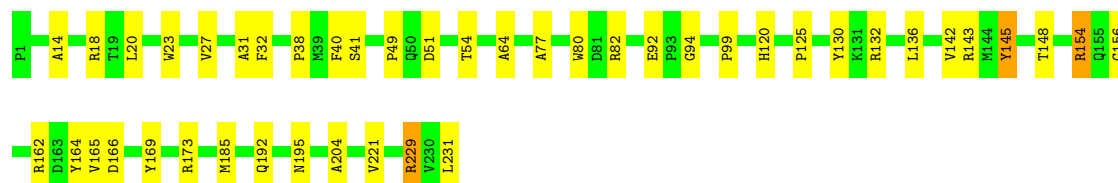
- Molecule 1: capsid protein

Chain 5s: 85% 13%



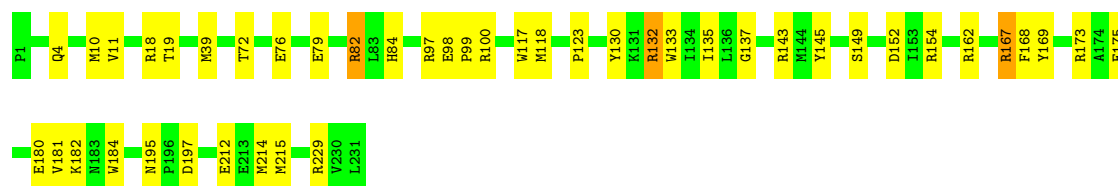
- Molecule 1: capsid protein

Chain 5t: 81% 18%



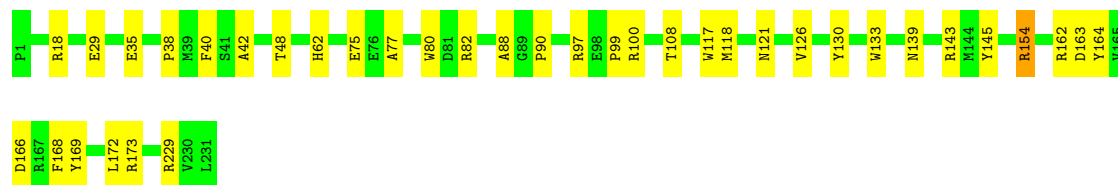
- Molecule 1: capsid protein

Chain 5u: 81% 18%



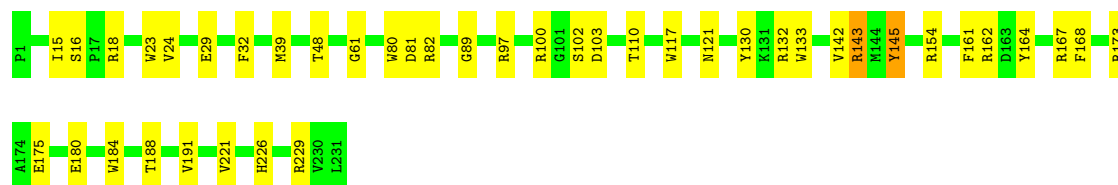
- Molecule 1: capsid protein

Chain 5v: 84% 16%



- Molecule 1: capsid protein

Chain 5w: 82% 17%



- Molecule 1: capsid protein

Chain 5x: 80% 18%

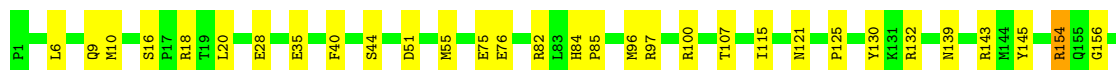






- Molecule 1: capsid protein

Chain 5D: 80% 19% .



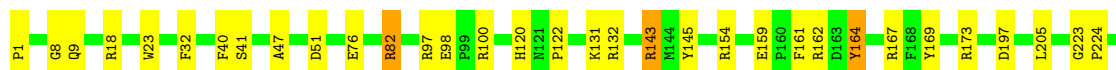
- Molecule 1: capsid protein

Chain 5E: 82% 17% .



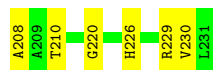
- Molecule 1: capsid protein

Chain 5F: 85% 13% .



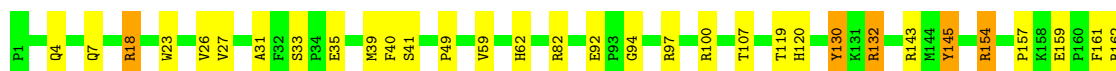
- Molecule 1: capsid protein

Chain 5G: 84% 16% .



- Molecule 1: capsid protein

Chain 5H: 82% 15% .





- Molecule 1: capsid protein

Chain 5I: 84% 15%



- Molecule 1: capsid protein

Chain 5J: 81% 17%



- Molecule 1: capsid protein

Chain 5K: 83% 17%



- Molecule 1: capsid protein

Chain 5L: 80% 19%



- Molecule 1: capsid protein

Chain 5M: 83% 16%





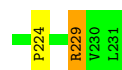
- Molecule 1: capsid protein

Chain 5N: 83% 17%



- Molecule 1: capsid protein

Chain 5O: 85% 13%



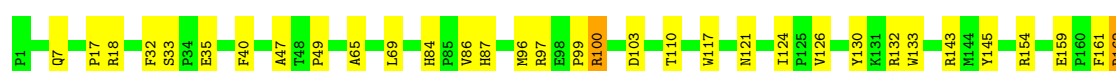
- Molecule 1: capsid protein

Chain 5P: 87% 12%



- Molecule 1: capsid protein

Chain 5Q: 81% 17%



- Molecule 1: capsid protein

Chain 5R: 80% 19%





- Molecule 1: capsid protein

Chain 5S: 81% 18%



- Molecule 1: capsid protein

Chain 5T: 83% 16%



- Molecule 1: capsid protein

Chain 5U: 87% 10%



- Molecule 1: capsid protein

Chain 5V: 81% 19%

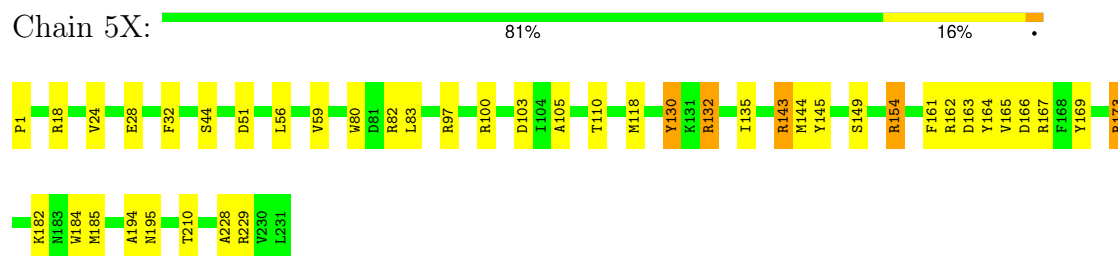


- Molecule 1: capsid protein

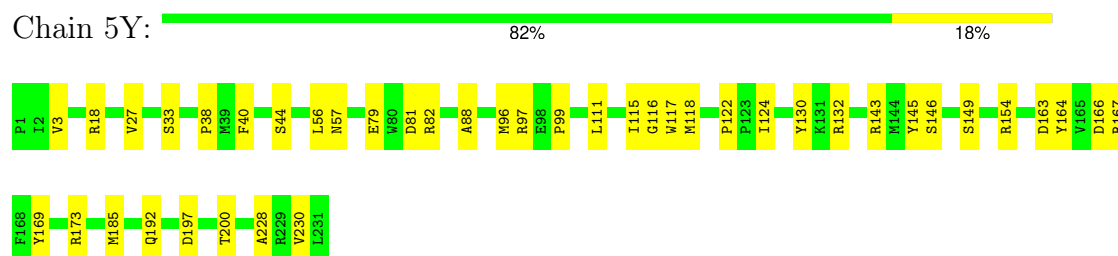
Chain 5W: 82% 16%



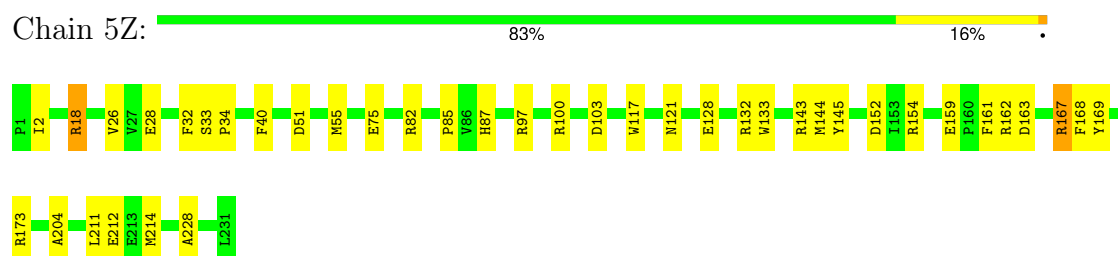
- Molecule 1: capsid protein



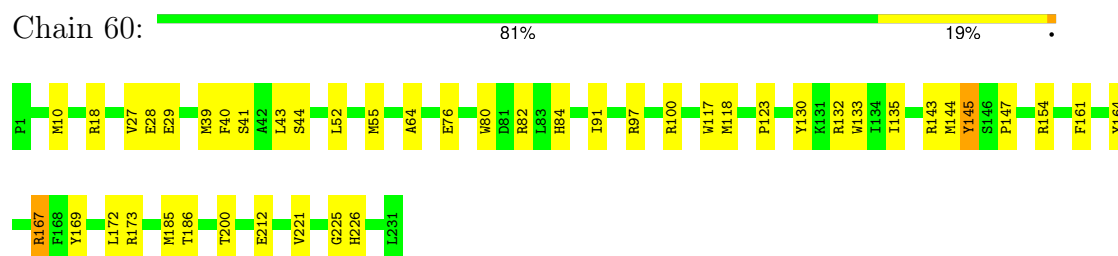
- Molecule 1: capsid protein



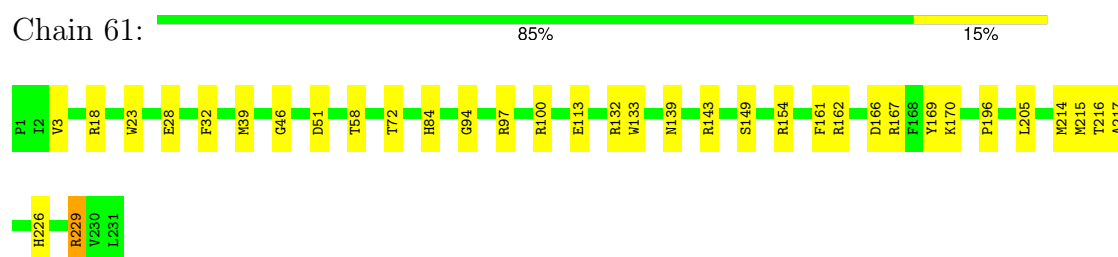
- Molecule 1: capsid protein



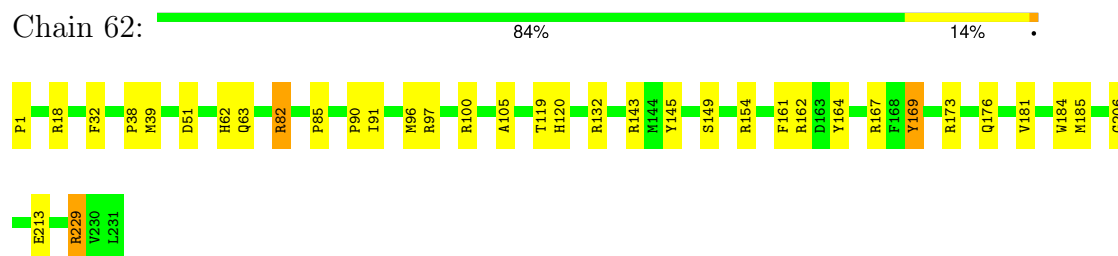
- Molecule 1: capsid protein



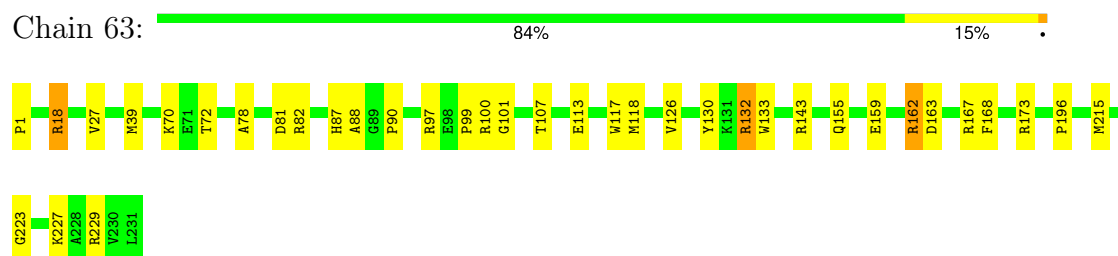
- Molecule 1: capsid protein



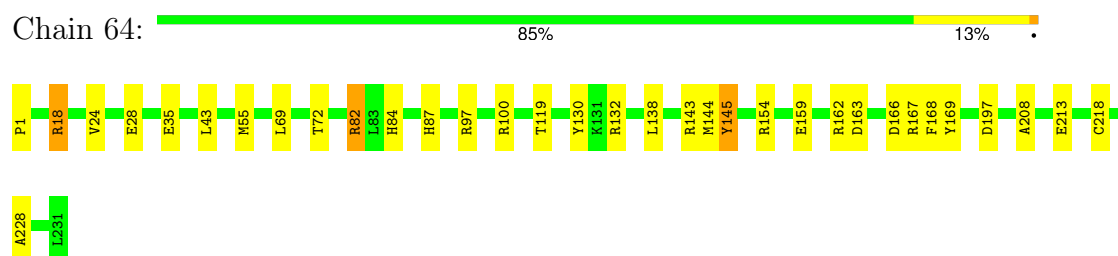
## • Molecule 1: capsid protein



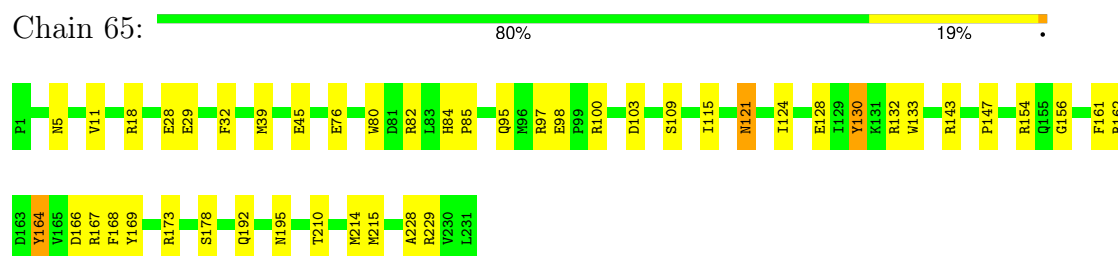
## • Molecule 1: capsid protein



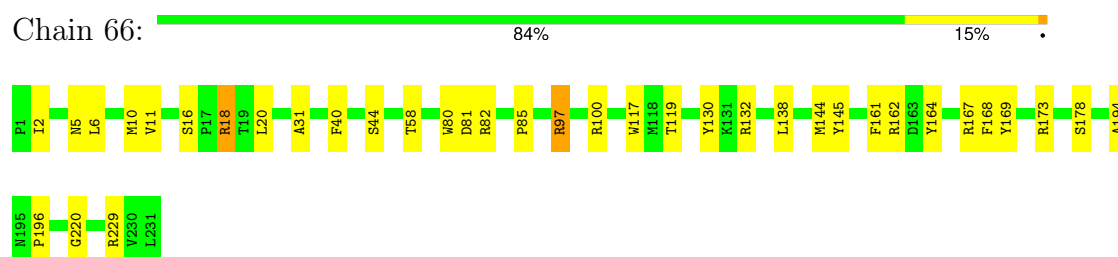
## • Molecule 1: capsid protein



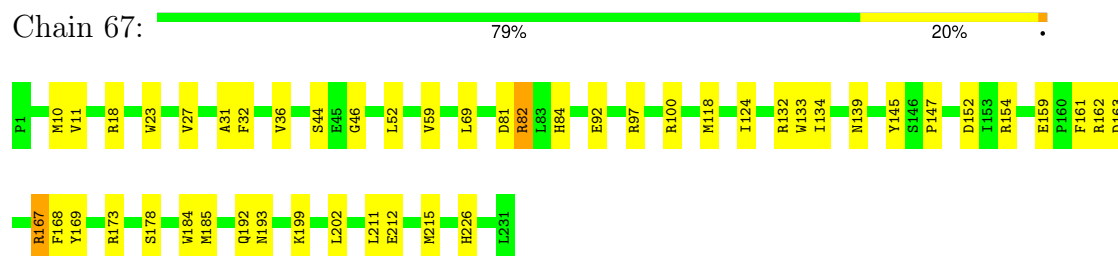
## • Molecule 1: capsid protein



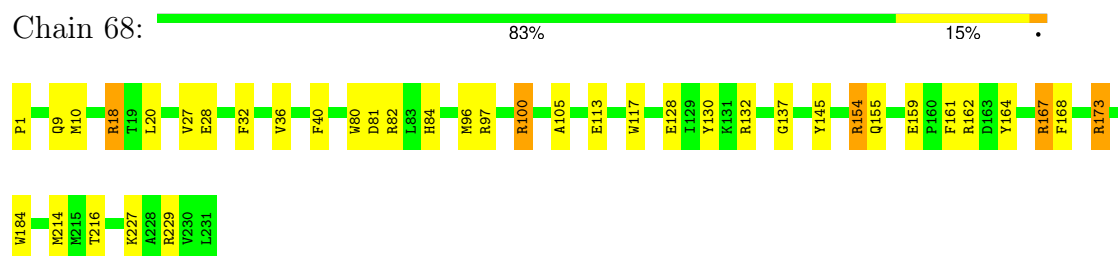
## • Molecule 1: capsid protein



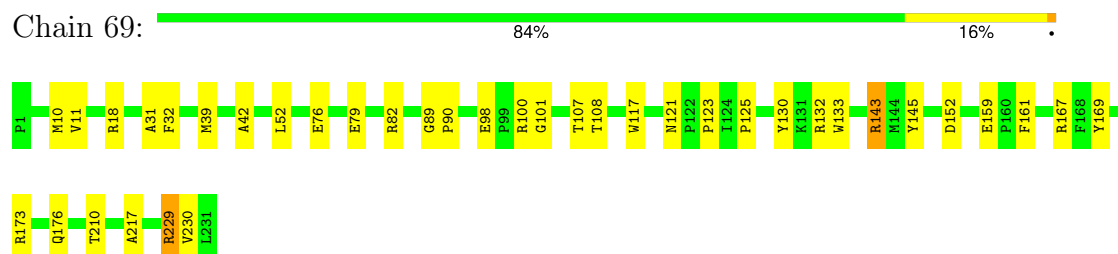
- Molecule 1: capsid protein



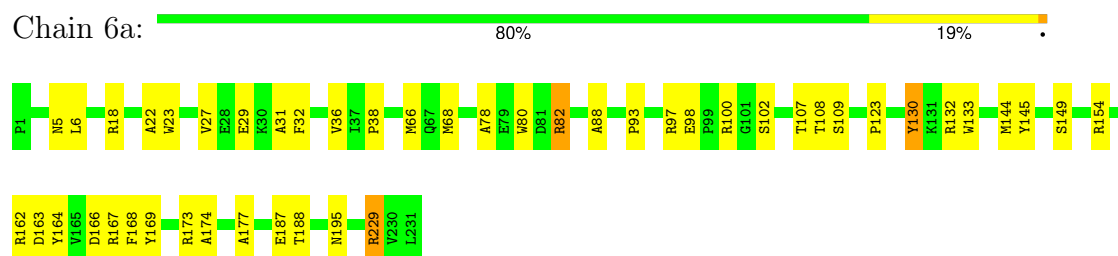
- Molecule 1: capsid protein



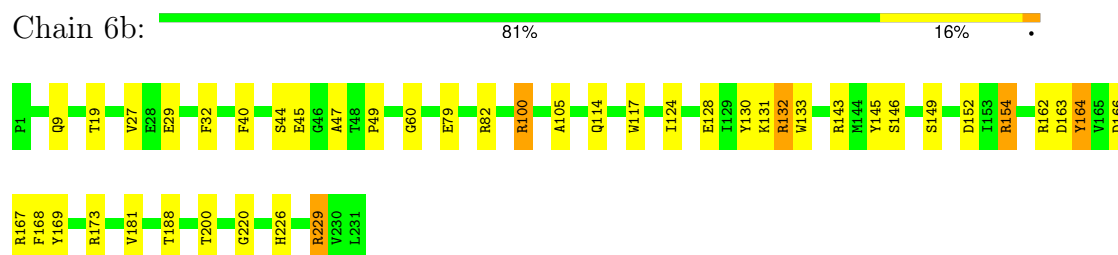
- Molecule 1: capsid protein



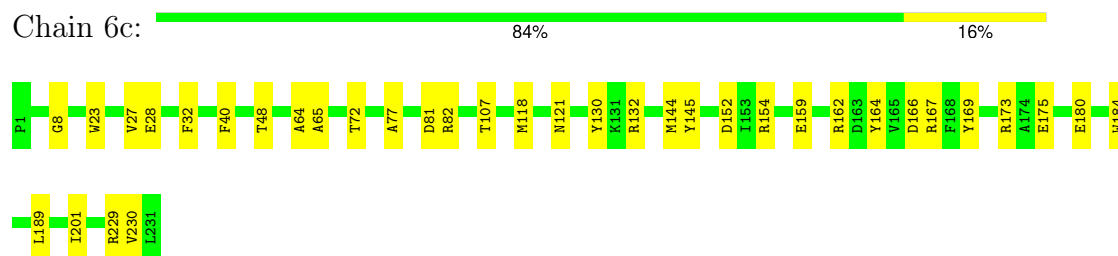
- Molecule 1: capsid protein



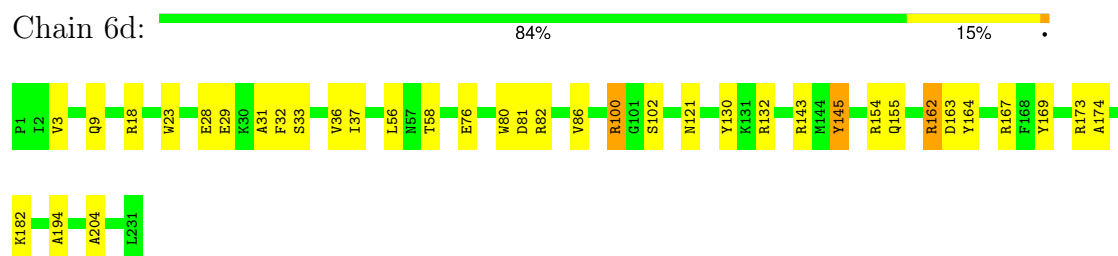
- Molecule 1: capsid protein



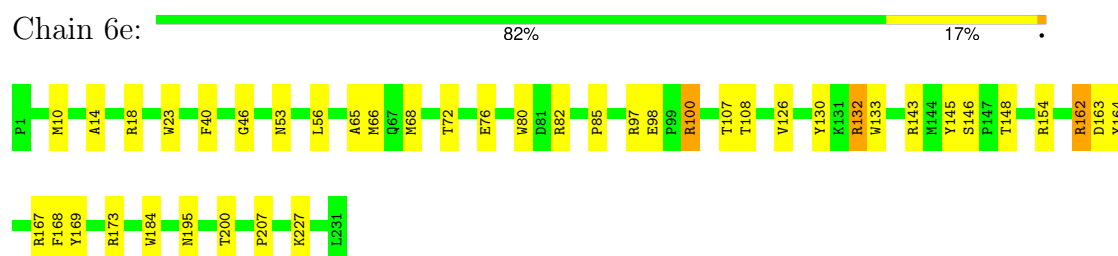
## • Molecule 1: capsid protein



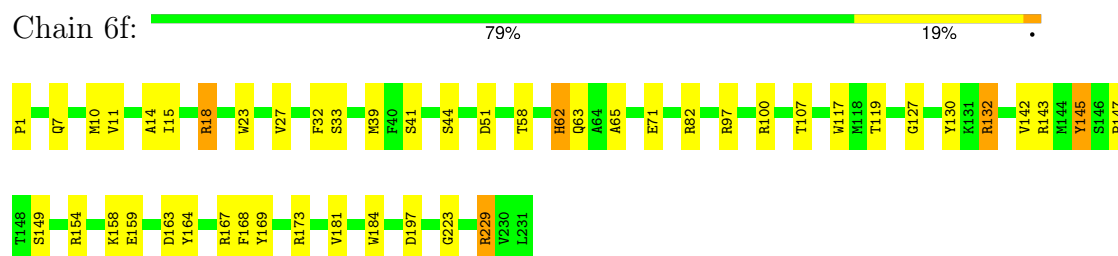
## • Molecule 1: capsid protein



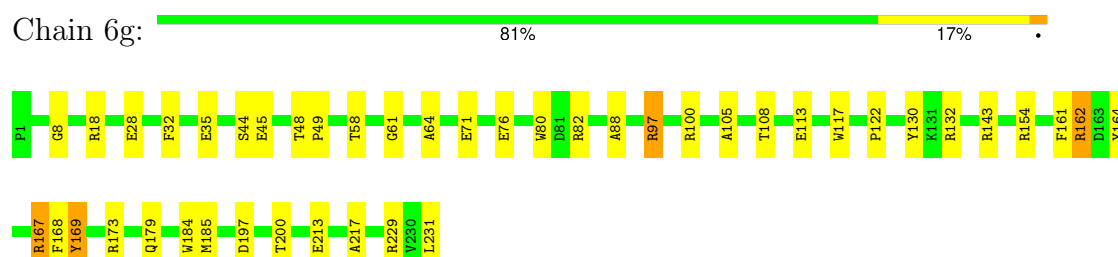
## • Molecule 1: capsid protein



## • Molecule 1: capsid protein

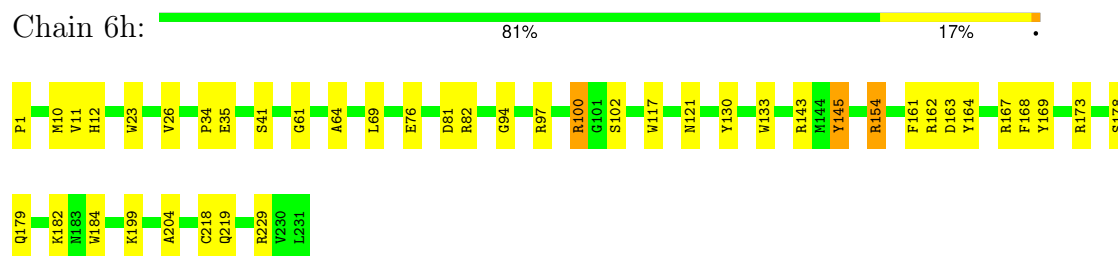


## • Molecule 1: capsid protein

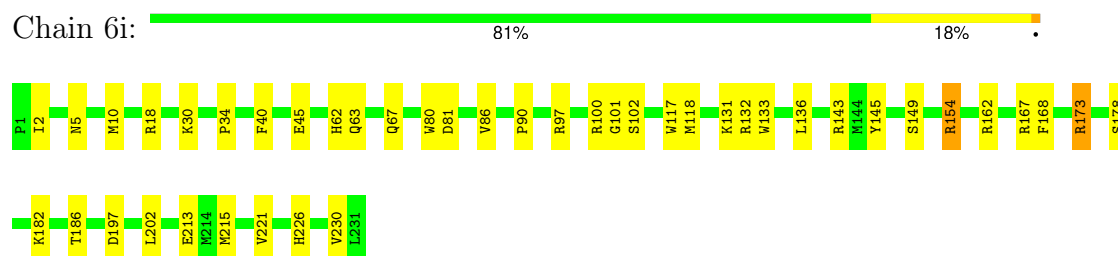




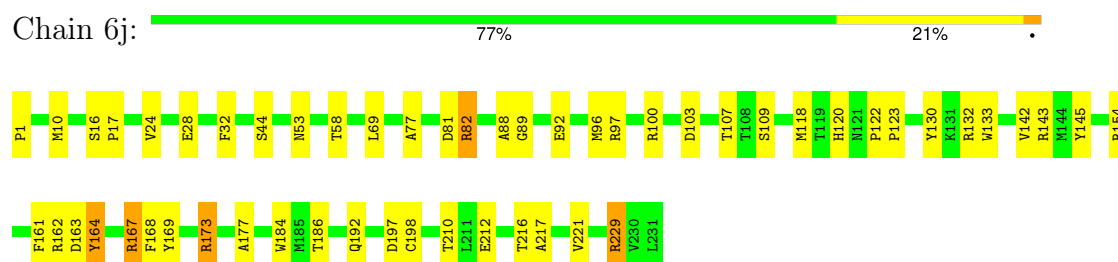
- Molecule 1: capsid protein



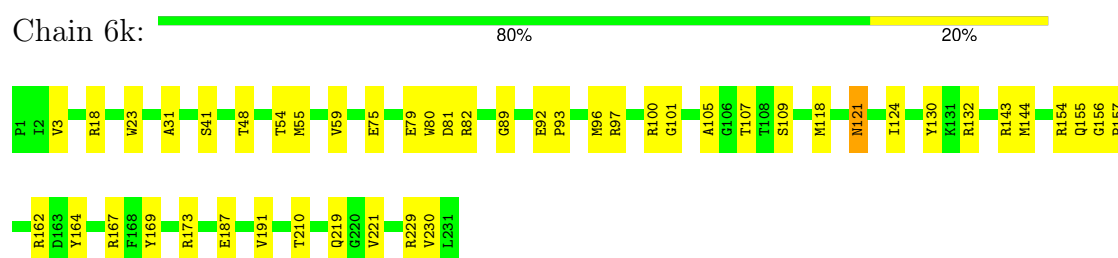
- Molecule 1: capsid protein



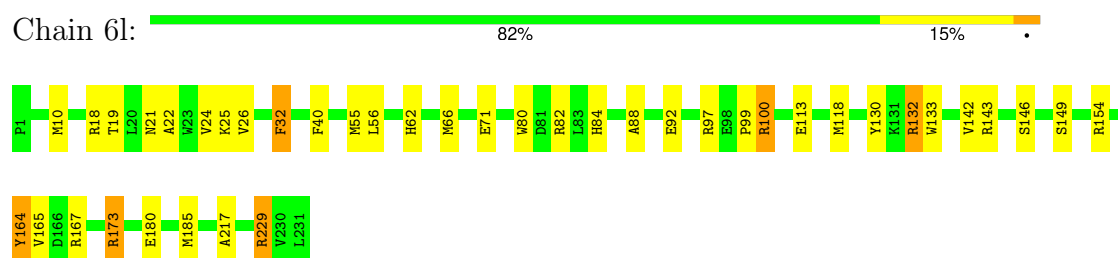
- Molecule 1: capsid protein



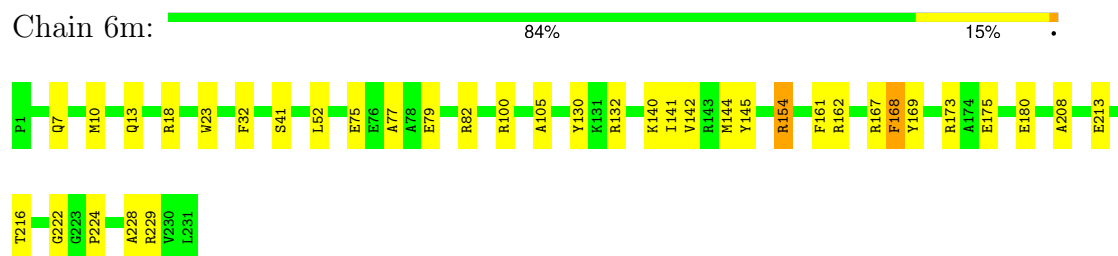
- Molecule 1: capsid protein



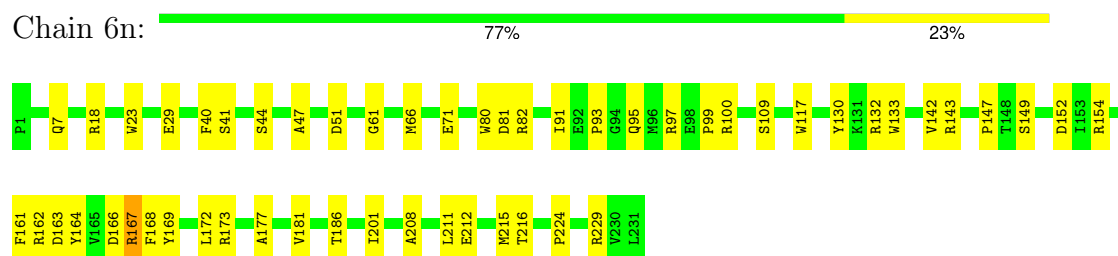
- Molecule 1: capsid protein



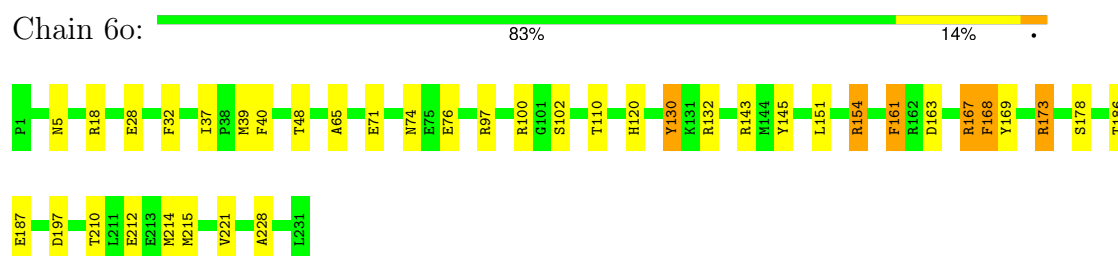
## • Molecule 1: capsid protein



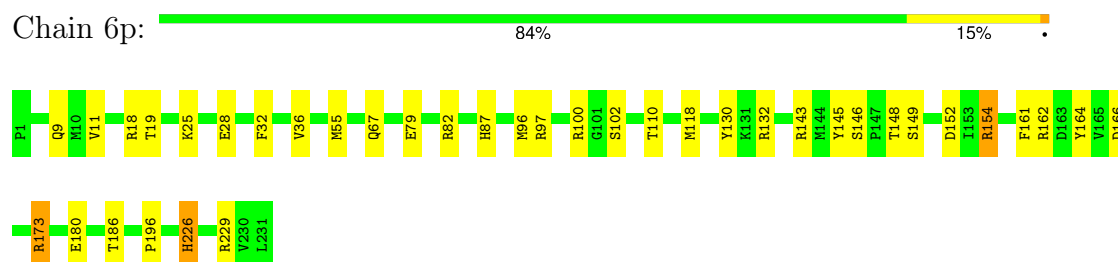
## • Molecule 1: capsid protein



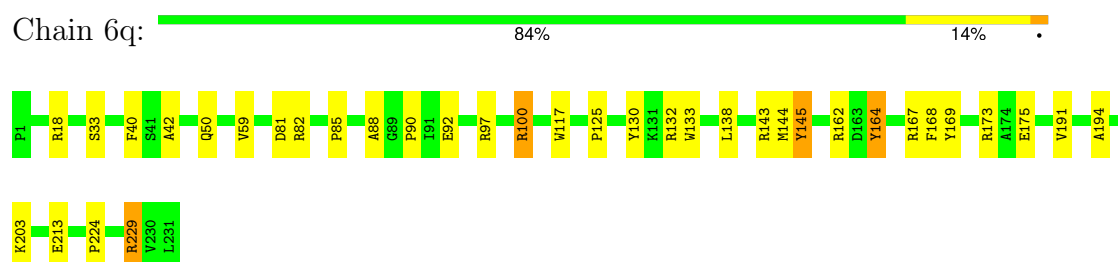
## • Molecule 1: capsid protein



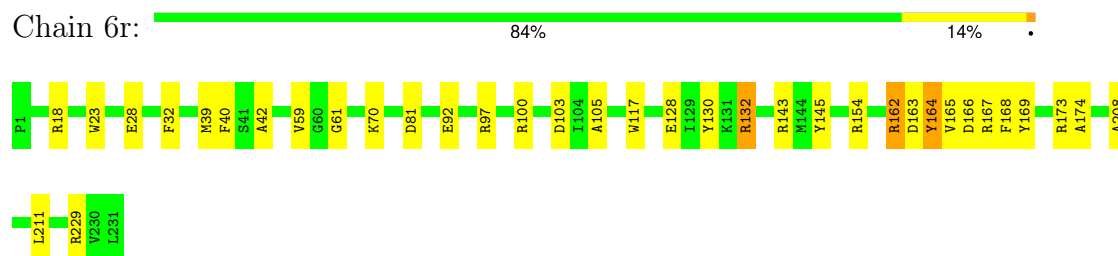
## • Molecule 1: capsid protein



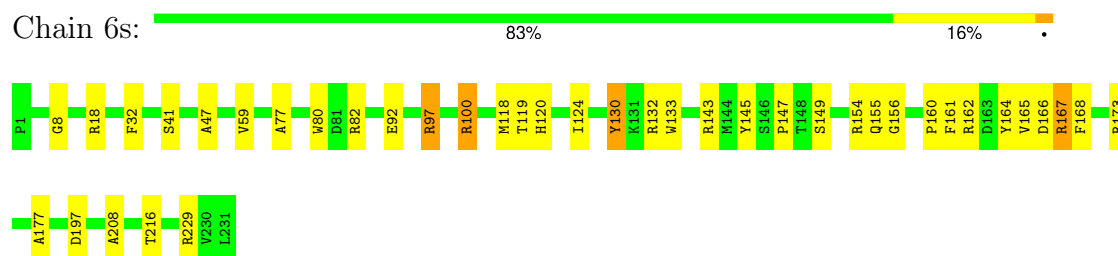
## • Molecule 1: capsid protein



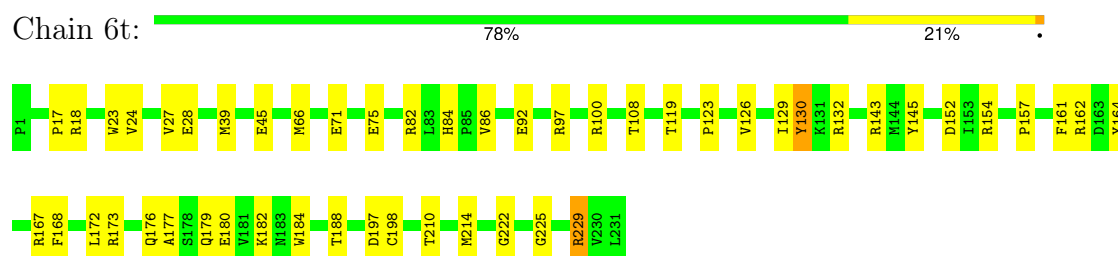
## • Molecule 1: capsid protein



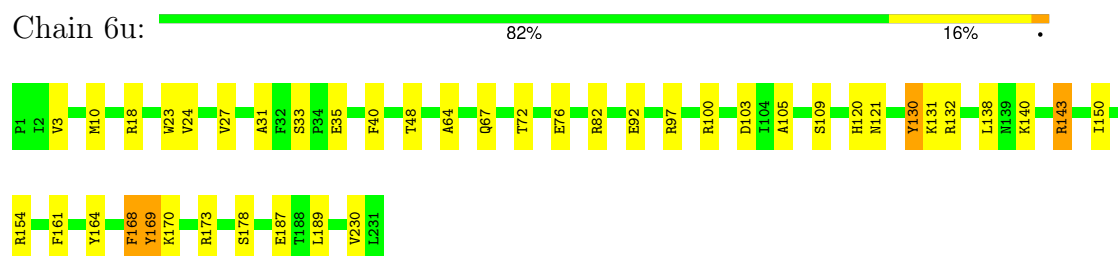
## • Molecule 1: capsid protein



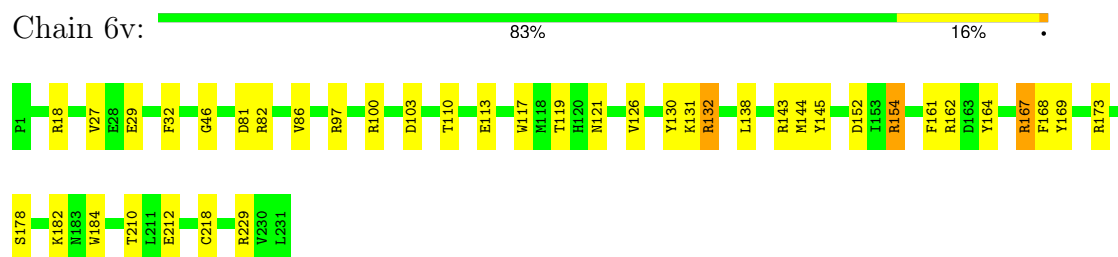
## • Molecule 1: capsid protein




## • Molecule 1: capsid protein

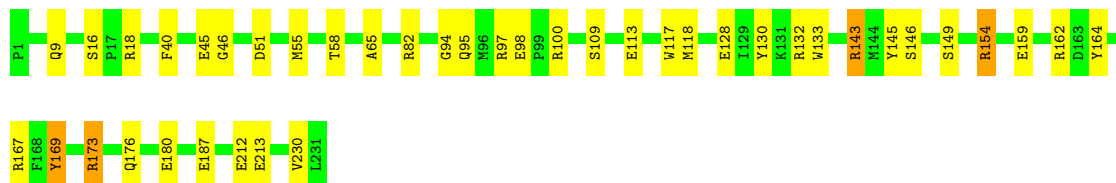


## • Molecule 1: capsid protein




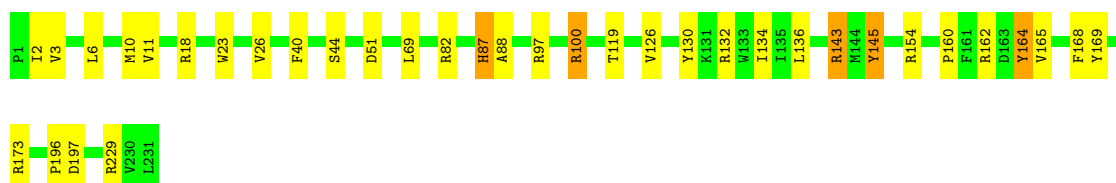
- Molecule 1: capsid protein

Chain 6w:  82% 16%




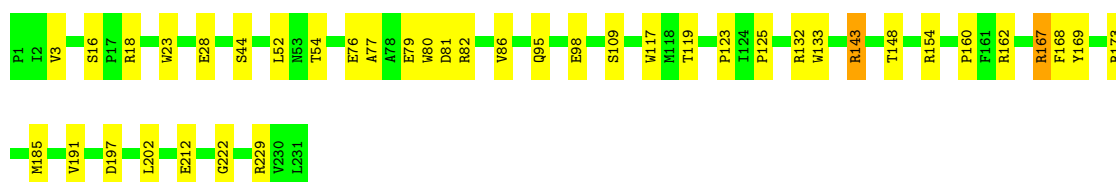
- Molecule 1: capsid protein

Chain 6x:  84% 13%




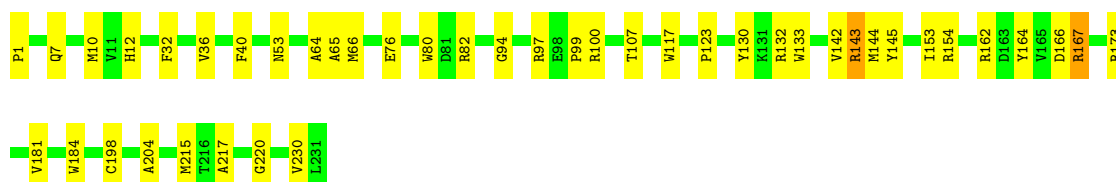
- Molecule 1: capsid protein

Chain 6y:  83% 16%




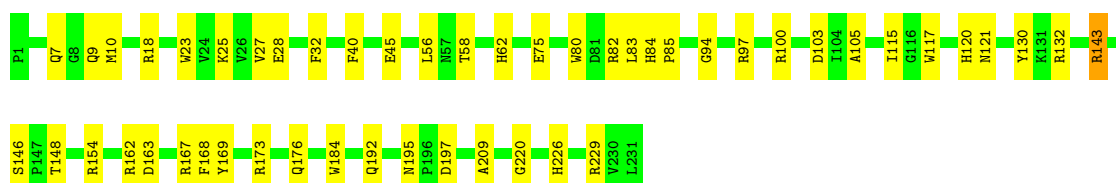
- Molecule 1: capsid protein

Chain 6z:  81% 18%

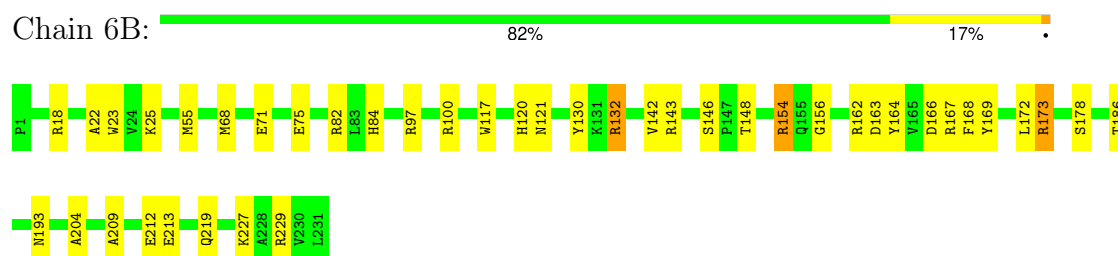


- Molecule 1: capsid protein

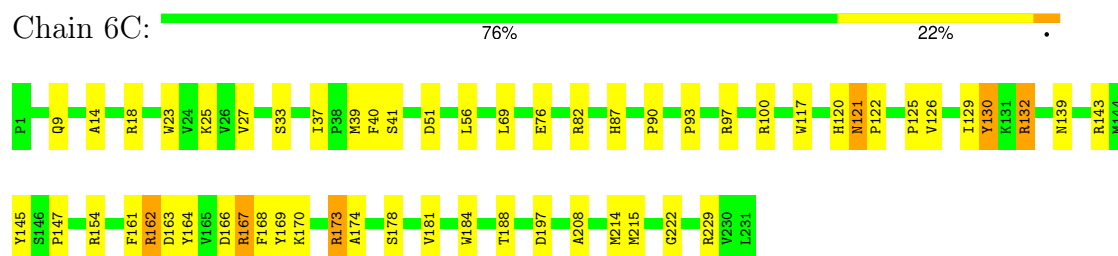
Chain 6A:  78% 21%



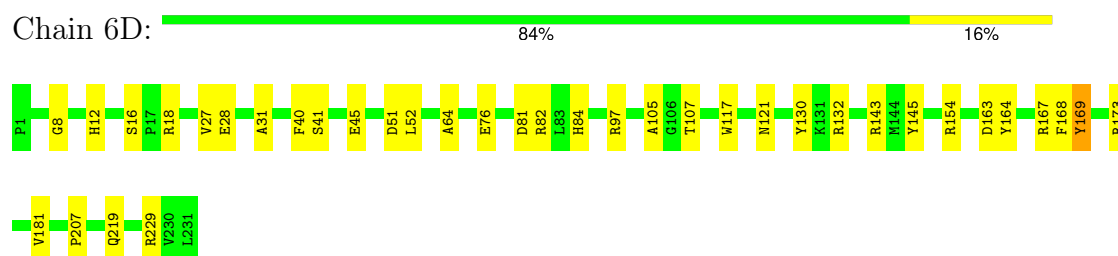
## • Molecule 1: capsid protein



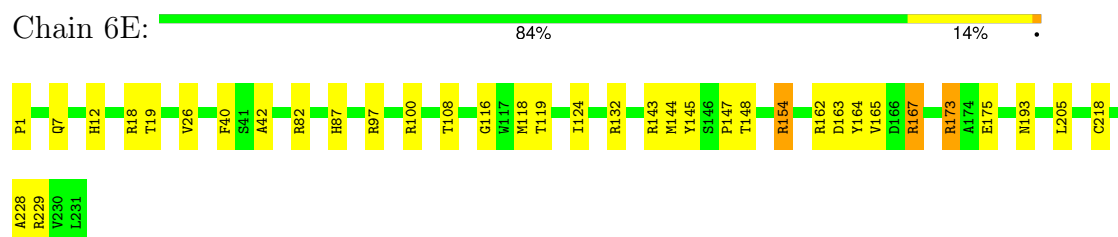
## • Molecule 1: capsid protein



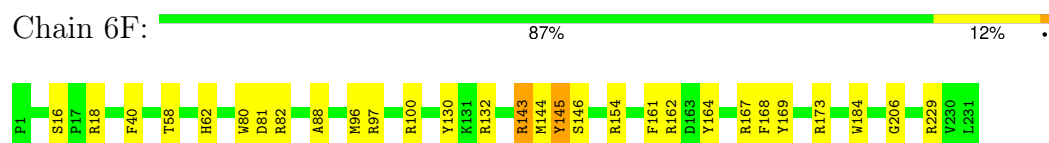
## • Molecule 1: capsid protein



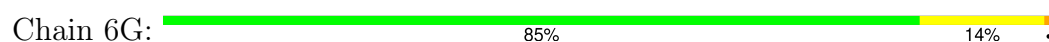
## • Molecule 1: capsid protein

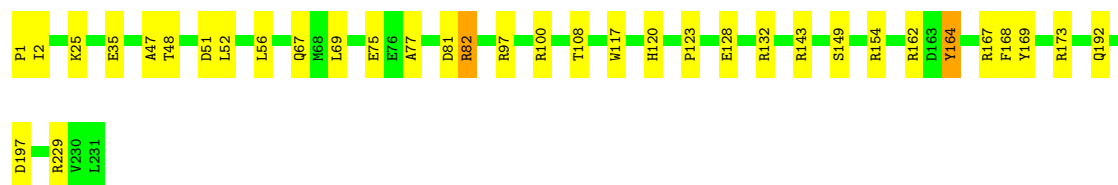


## • Molecule 1: capsid protein



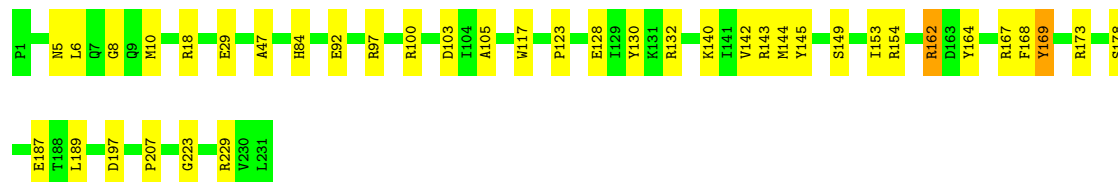
## • Molecule 1: capsid protein





- Molecule 1: capsid protein

Chain 6H: 83% 16%



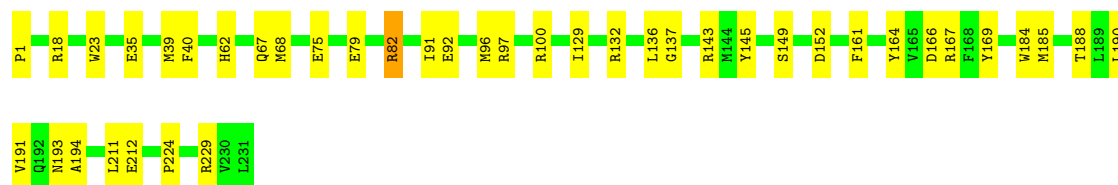
- Molecule 1: capsid protein

Chain 6I: 80% 18%



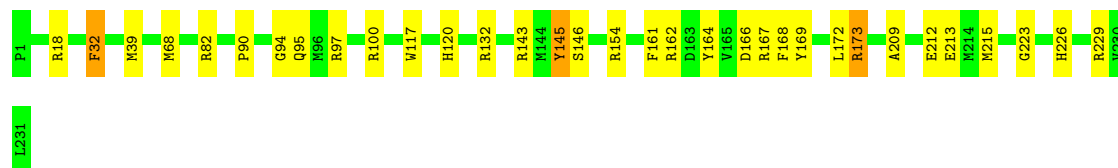
- Molecule 1: capsid protein

Chain 6J: 82% 17%



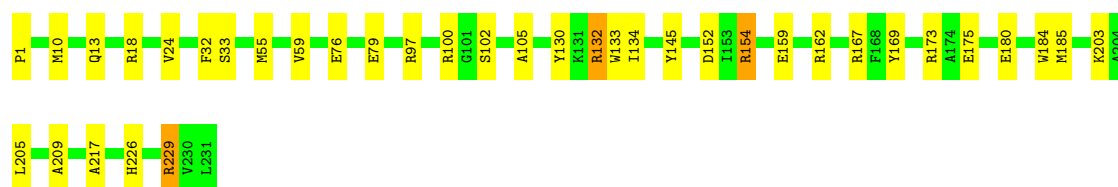
- Molecule 1: capsid protein

Chain 6K: 86% 13%



- Molecule 1: capsid protein

Chain 6L: 84% 15%



- Molecule 1: capsid protein

Chain 6M: 81% 17% •



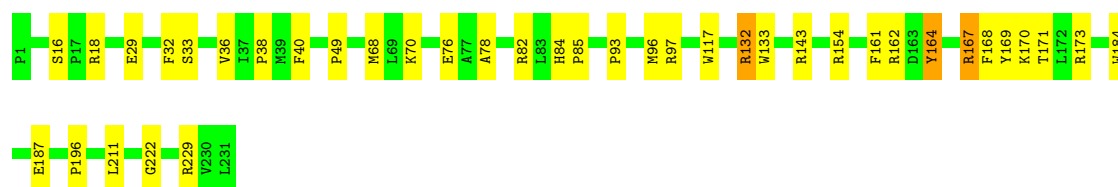
- Molecule 1: capsid protein

Chain 6N: 84% 15% •



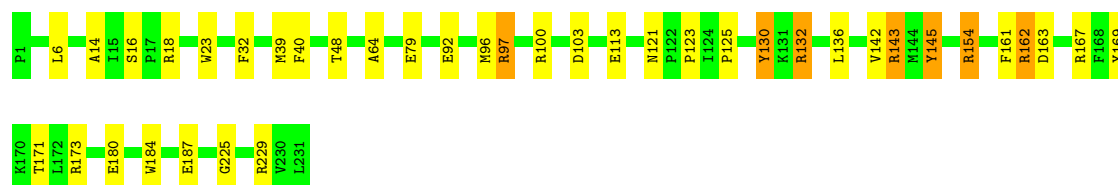
- Molecule 1: capsid protein

Chain 6O: 83% 16% •



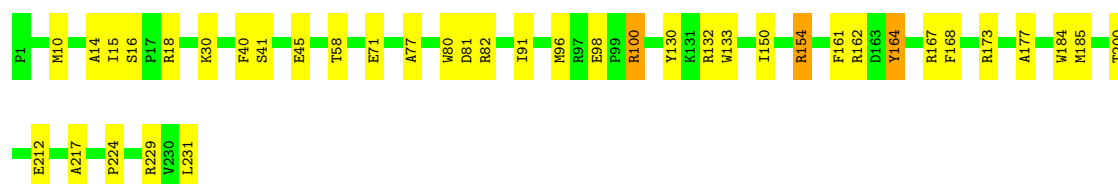
- Molecule 1: capsid protein

Chain 6P: 83% 14% •



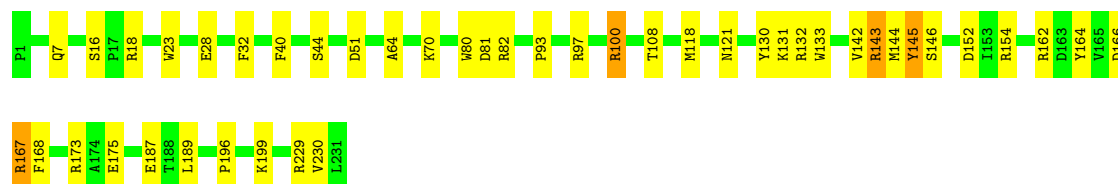
- Molecule 1: capsid protein

Chain 6Q: 83% 16% •



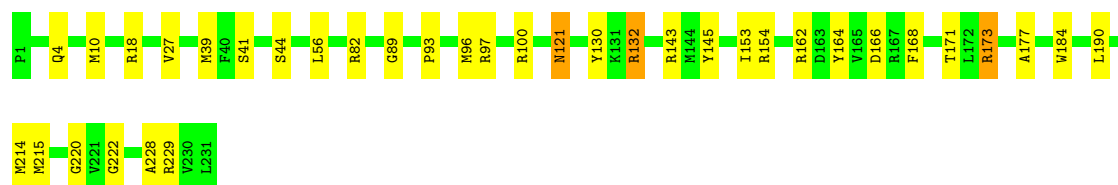
- Molecule 1: capsid protein

Chain 6R: 81% 17%



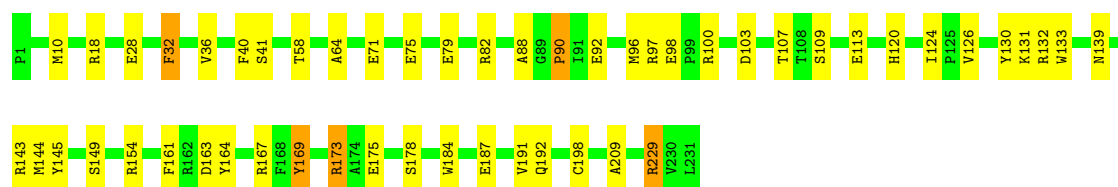
- Molecule 1: capsid protein

Chain 6S: 84% 14%



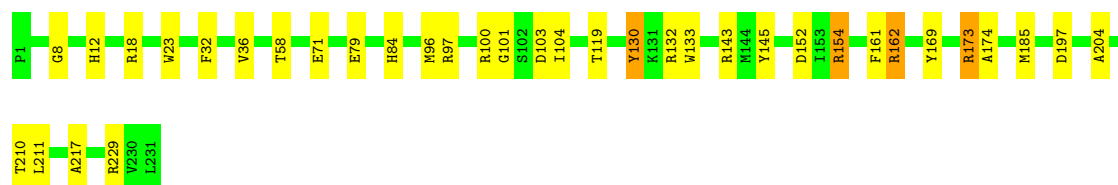
- Molecule 1: capsid protein

Chain 6T: 77% 20%



- Molecule 1: capsid protein

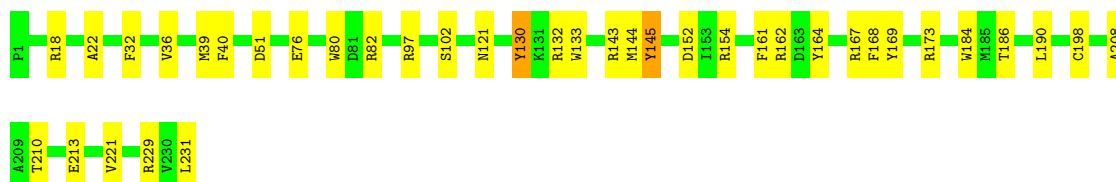
Chain 6U: 84% 14%



- Molecule 1: capsid protein

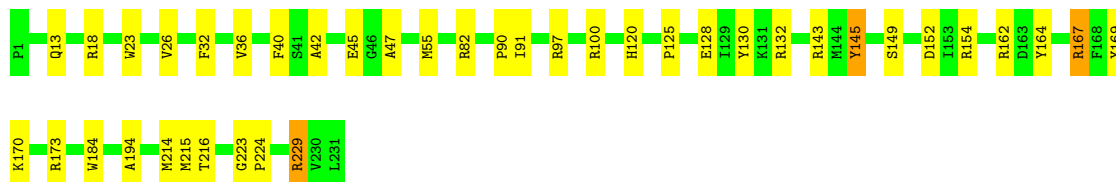
Chain 6V: 84% 16%





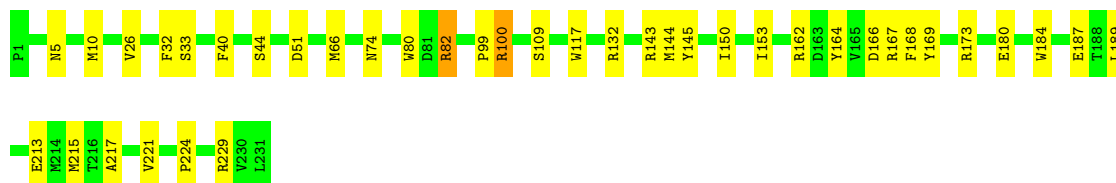
- Molecule 1: capsid protein

Chain 6W: 83% 16%



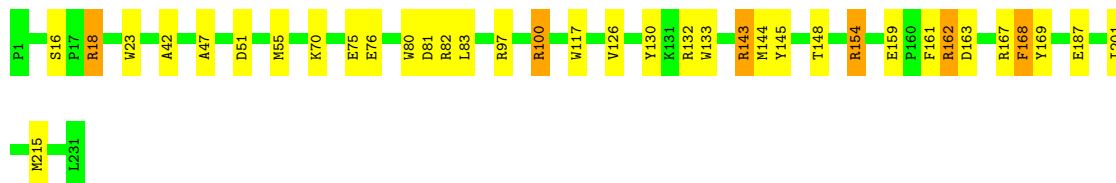
- Molecule 1: capsid protein

Chain 6X: 83% 16%



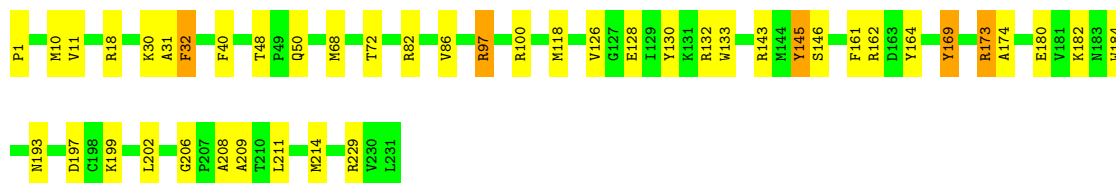
- Molecule 1: capsid protein

Chain 6Y: 84% 13%



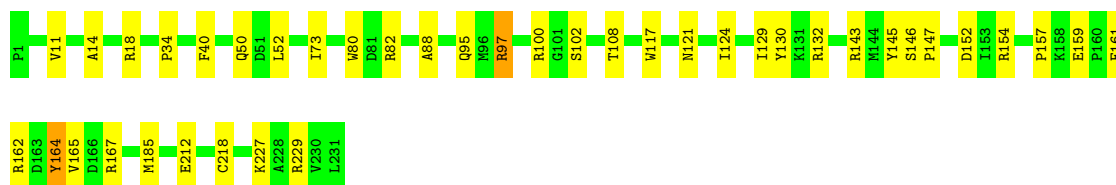
- Molecule 1: capsid protein

Chain 6Z: 81% 17%



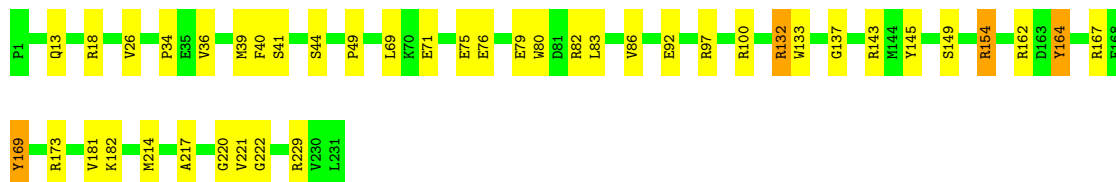
- Molecule 1: capsid protein

Chain 70: 83% 16%



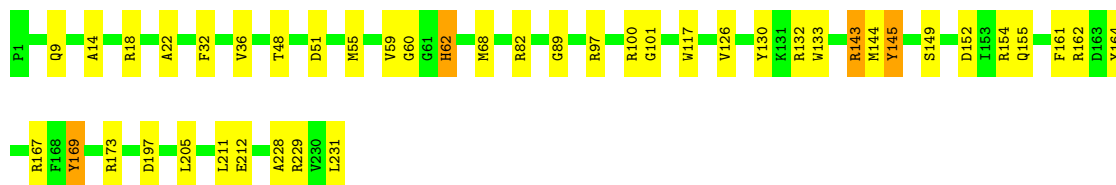
- Molecule 1: capsid protein

Chain 71: 82% 16% •



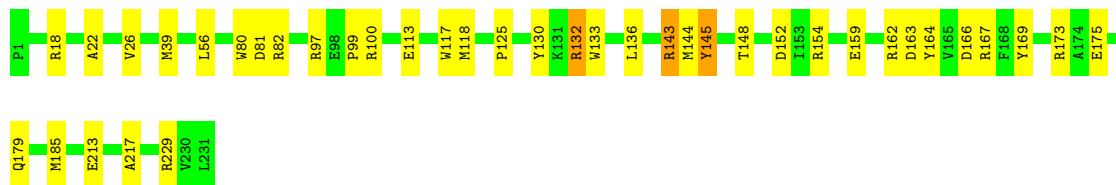
- Molecule 1: capsid protein

Chain 72: 81% 17% •



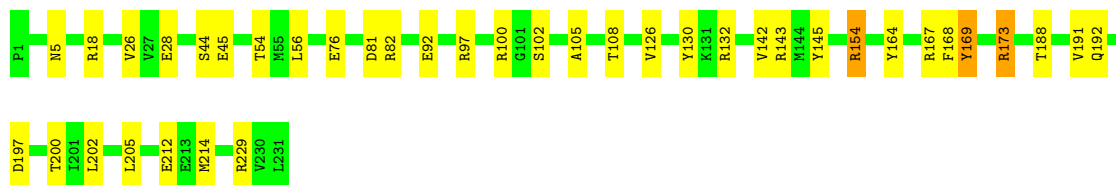
- Molecule 1: capsid protein

Chain 73: 83% 16% •



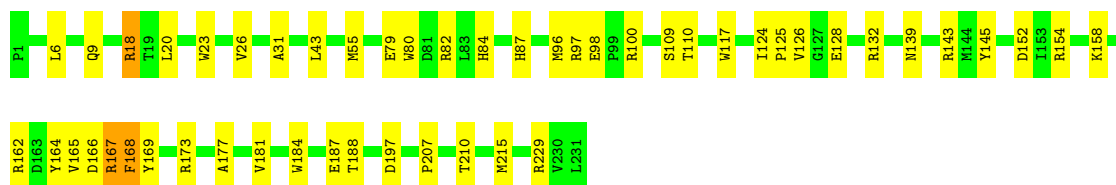
- Molecule 1: capsid protein

Chain 74: 83% 16% •



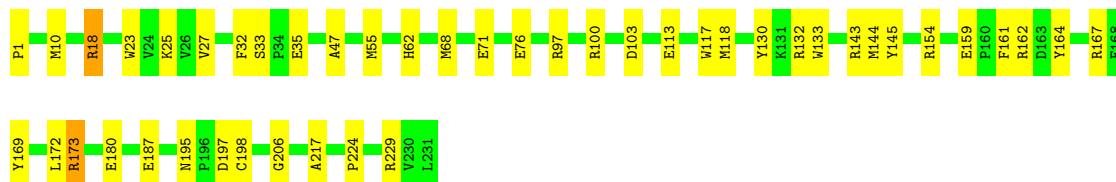
- Molecule 1: capsid protein

Chain 75: 78% 20% •



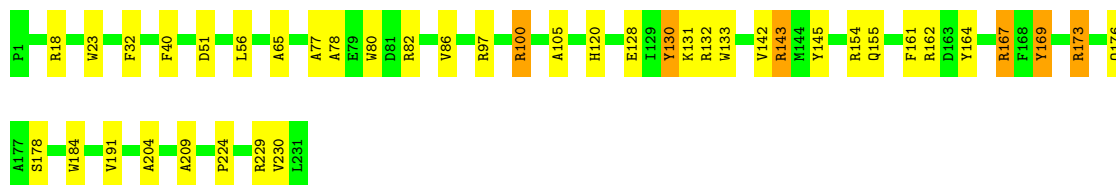
- Molecule 1: capsid protein

Chain 76: 81% 19%



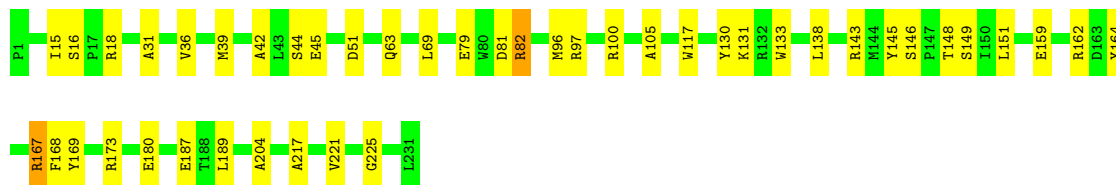
- Molecule 1: capsid protein

Chain 77: 82% 15%



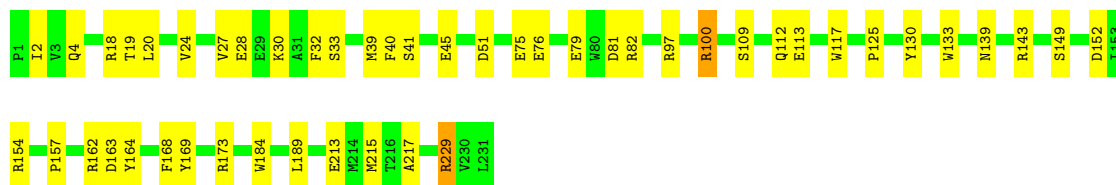
- Molecule 1: capsid protein

Chain 78: 81% 18%



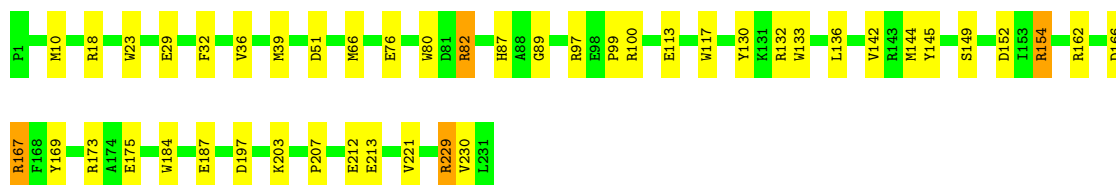
- Molecule 1: capsid protein

Chain 79: 79% 20%



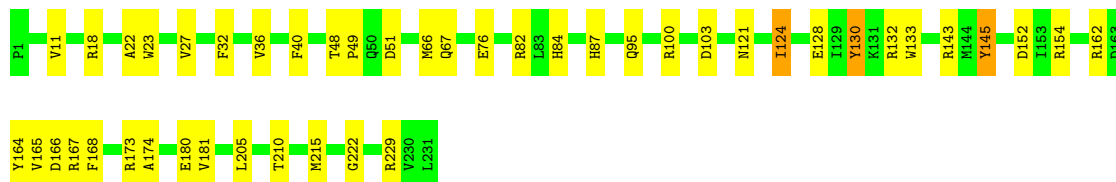
- Molecule 1: capsid protein

Chain 7a: 81% 18%



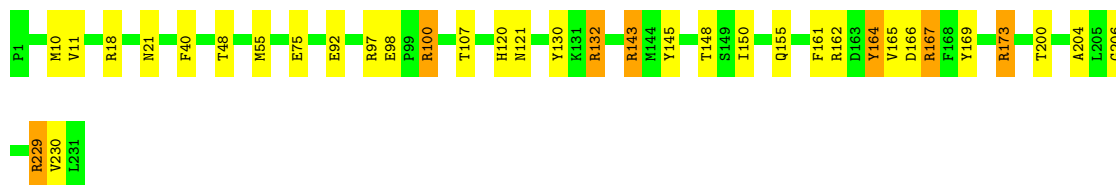
- Molecule 1: capsid protein

Chain 7b: 81% 18% •



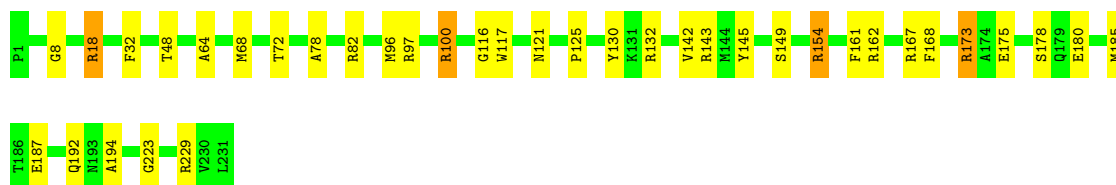
- Molecule 1: capsid protein

Chain 7c: 85% 12% •



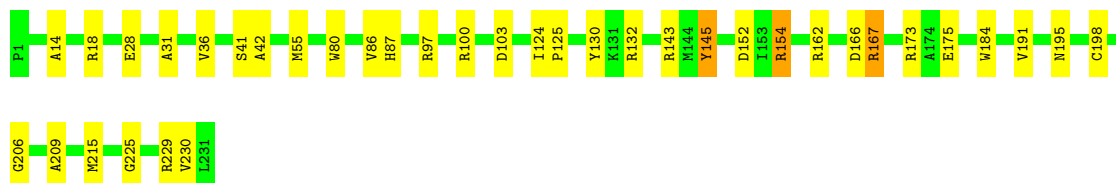
- Molecule 1: capsid protein

Chain 7d: 84% 14% •



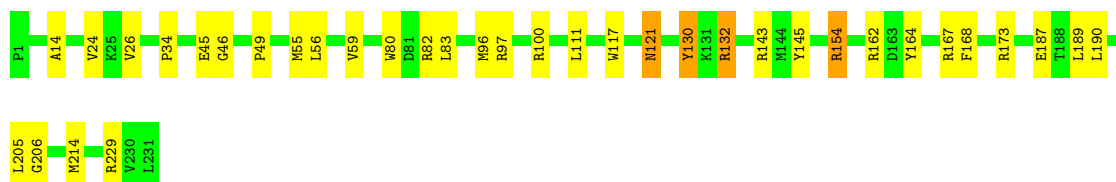
- Molecule 1: capsid protein

Chain 7e: 84% 15% •



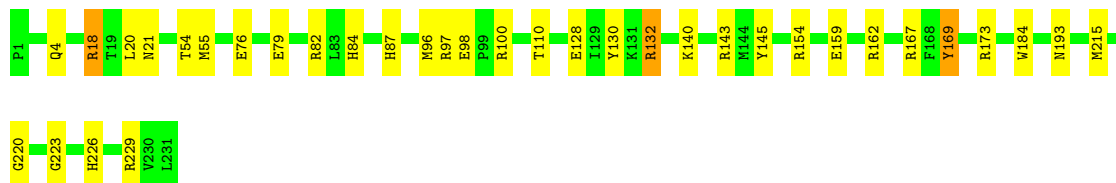
- Molecule 1: capsid protein

Chain 7f: 84% 14% •



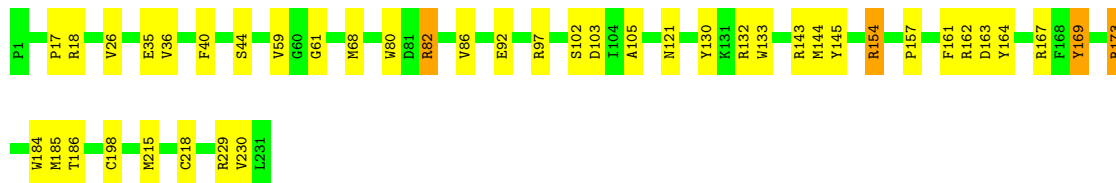
- Molecule 1: capsid protein

Chain 7g: 85% 14%



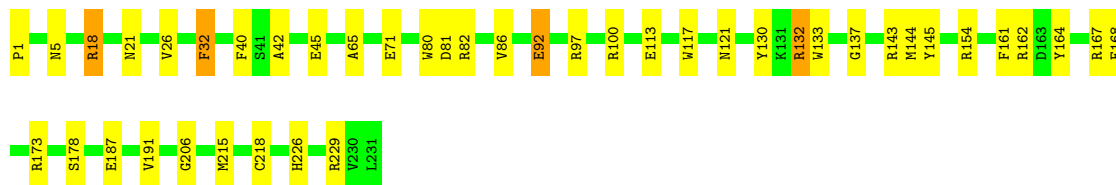
- Molecule 1: capsid protein

Chain 7h: 82% 16%



- Molecule 1: capsid protein

Chain 7i: 81% 17%




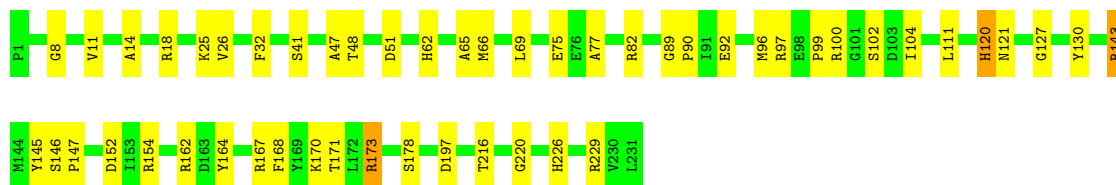
- Molecule 1: capsid protein

Chain 7j: 82% 16%




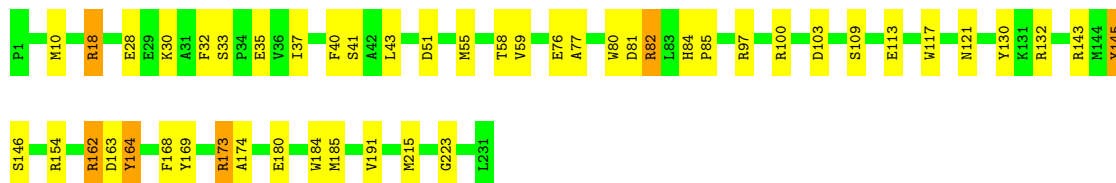
- Molecule 1: capsid protein

Chain 7k:  78% 21% .




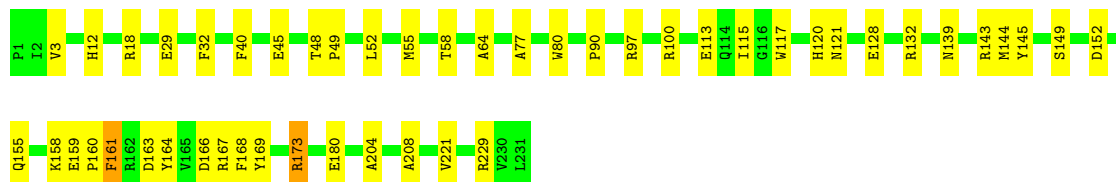
- Molecule 1: capsid protein

Chain 7l:  79% 18% .




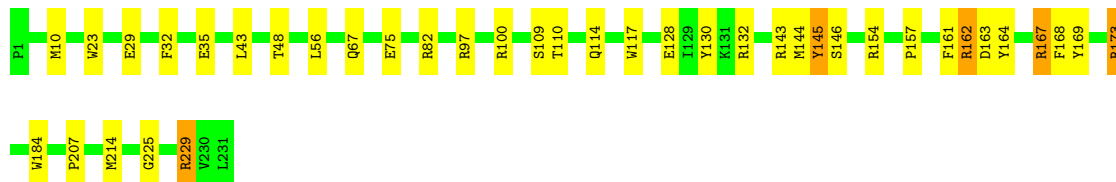
- Molecule 1: capsid protein

Chain 7m:  79% 20% .




- Molecule 1: capsid protein

Chain 7n:  83% 15% .




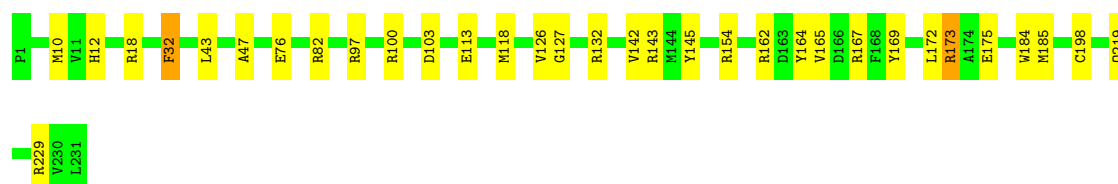
- Molecule 1: capsid protein

Chain 7o:  87% 12% .



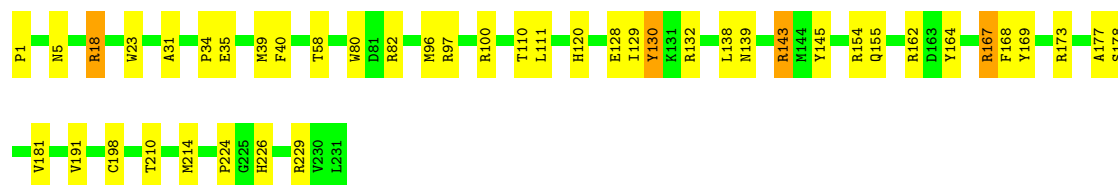
- Molecule 1: capsid protein

Chain 7p:  86% 13% .



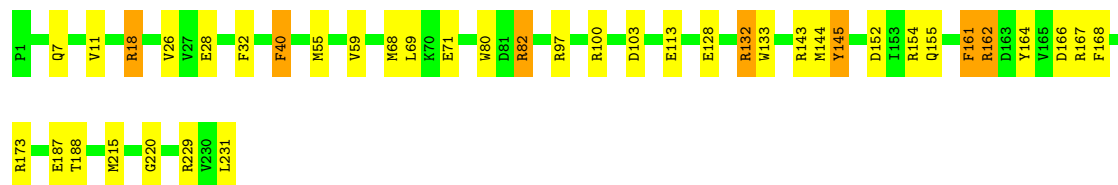
- Molecule 1: capsid protein

Chain 7q: 81% 17% .



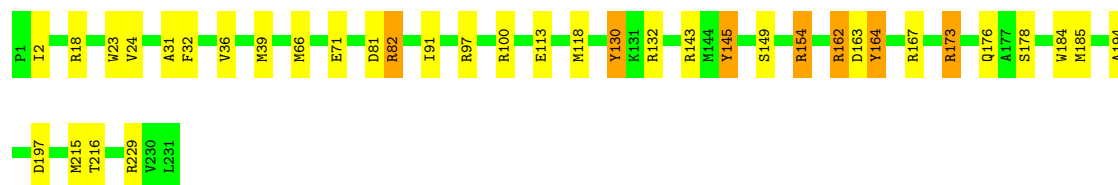
- Molecule 1: capsid protein

Chain 7r: 83% 14% .



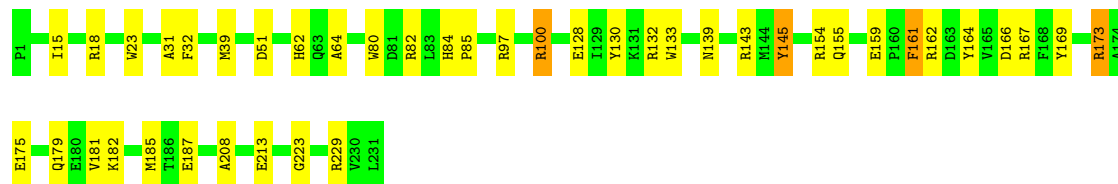
- Molecule 1: capsid protein

Chain 7s: 84% 13% .



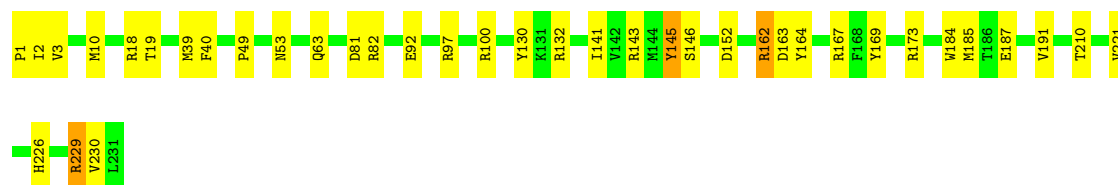
- Molecule 1: capsid protein

Chain 7t: 82% 16% .



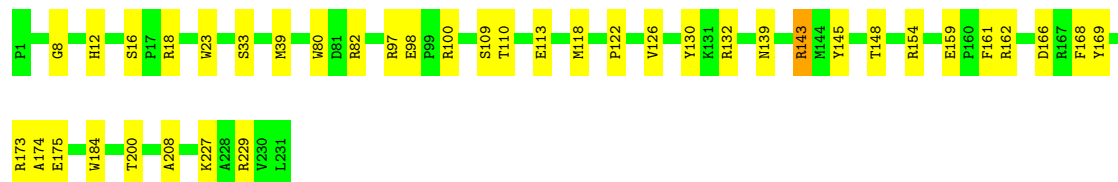
- Molecule 1: capsid protein

Chain 7u: 84% 15% .



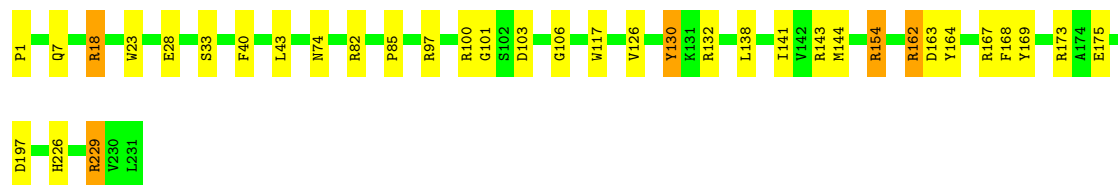
- Molecule 1: capsid protein

Chain 7v: 83% 16%



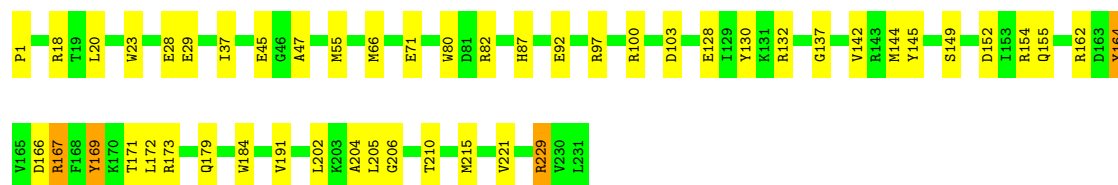
- Molecule 1: capsid protein

Chain 7w: 84% 13%



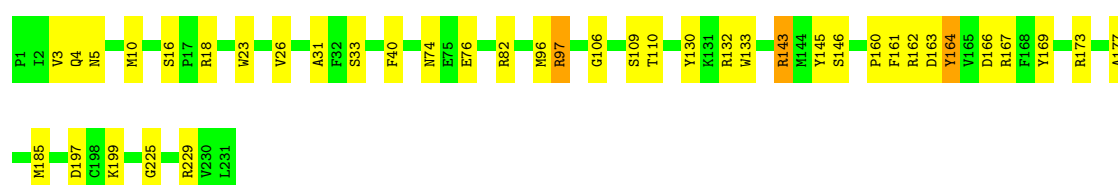
- Molecule 1: capsid protein

Chain 7x: 79% 19%



- Molecule 1: capsid protein

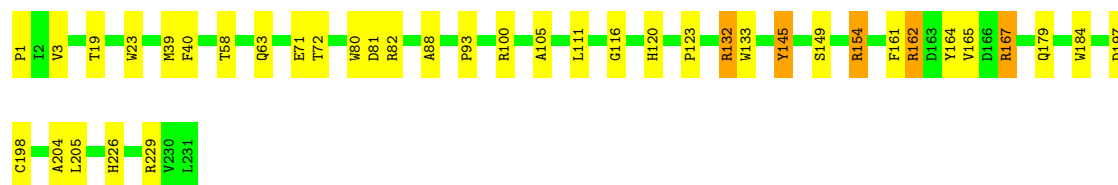
Chain 7y: 83% 16%



- Molecule 1: capsid protein

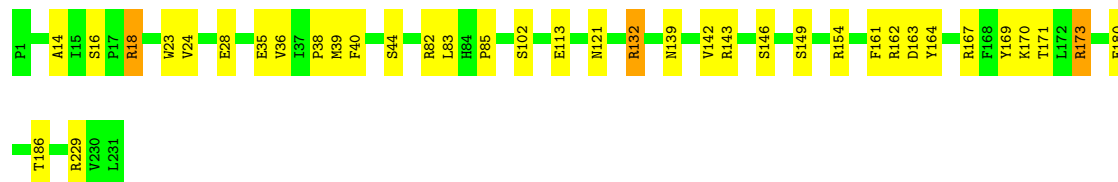
Chain 7z: 83% 15%





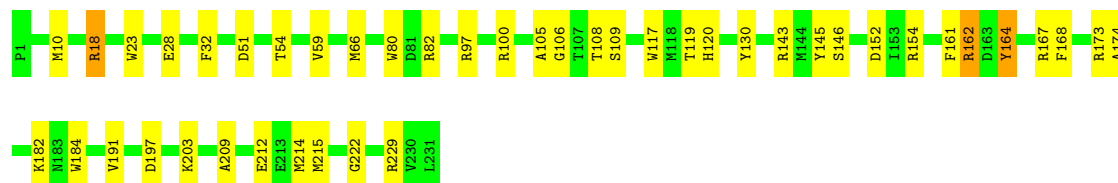
- Molecule 1: capsid protein

Chain 7A: 84% 15% •



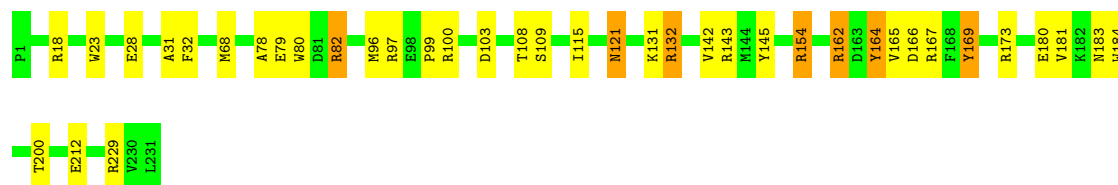
- Molecule 1: capsid protein

Chain 7B: 81% 18% •



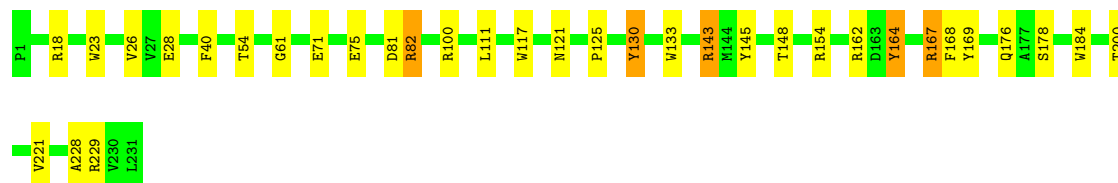
- Molecule 1: capsid protein

Chain 7C: 83% 14% •



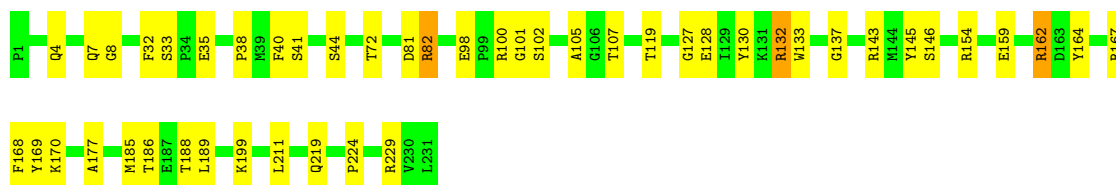
- Molecule 1: capsid protein

Chain 7D: 85% 13% •



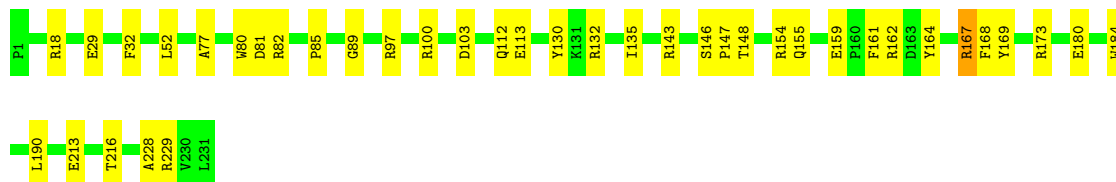
- Molecule 1: capsid protein

Chain 7E: 80% 19% •



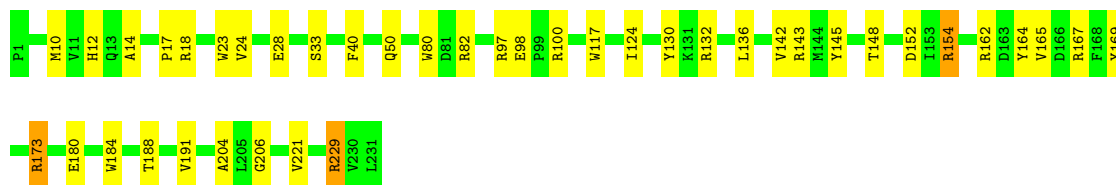
- Molecule 1: capsid protein

Chain 7F: 83% 16%



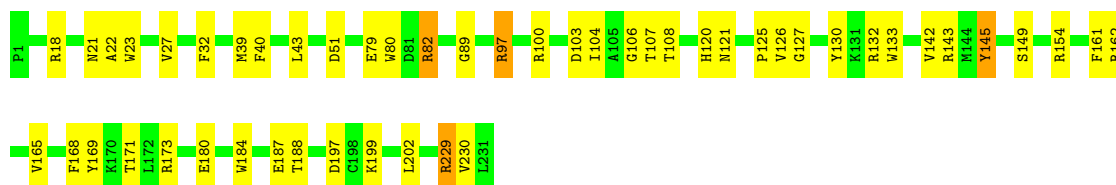
- Molecule 1: capsid protein

Chain 7G: 82% 16%



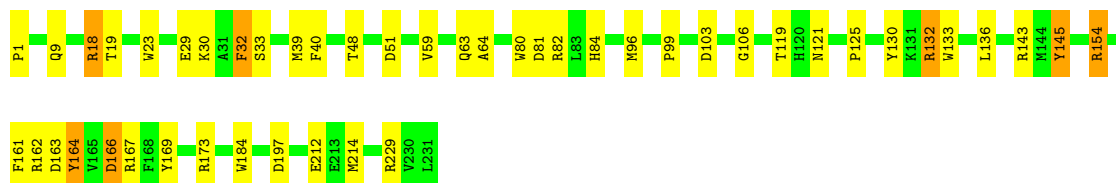
- Molecule 1: capsid protein

Chain 7H: 78% 20%



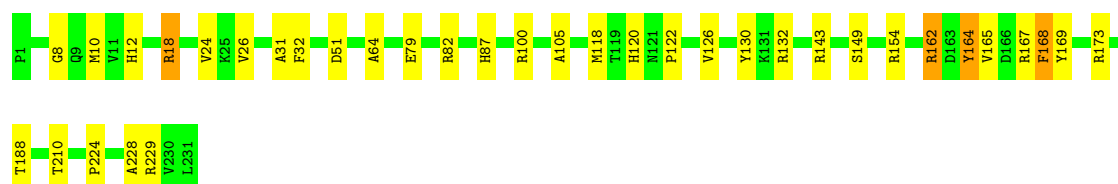
- Molecule 1: capsid protein

Chain 7I: 80% 17%

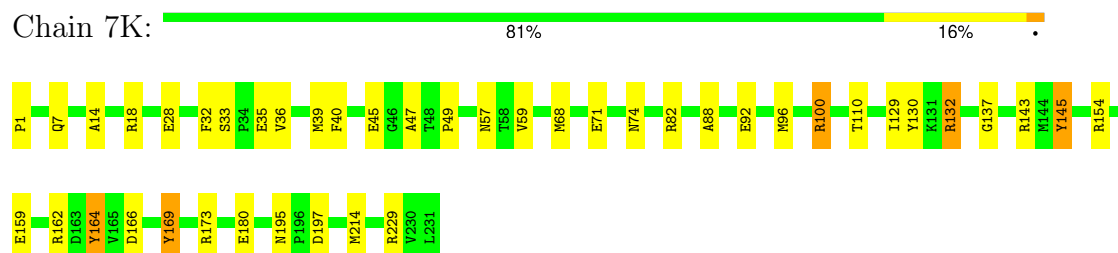


- Molecule 1: capsid protein

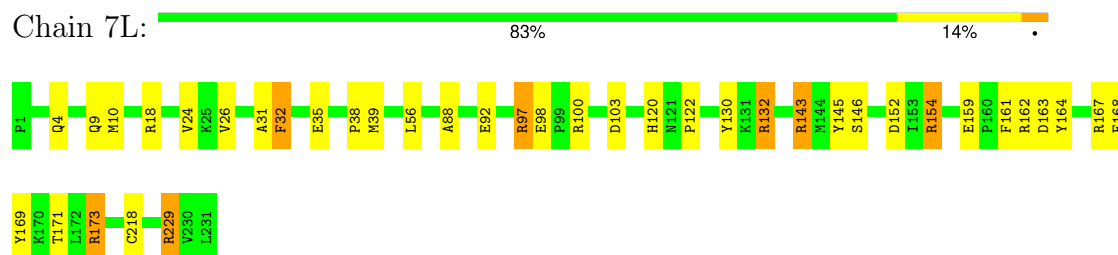
Chain 7J: 84% 14%



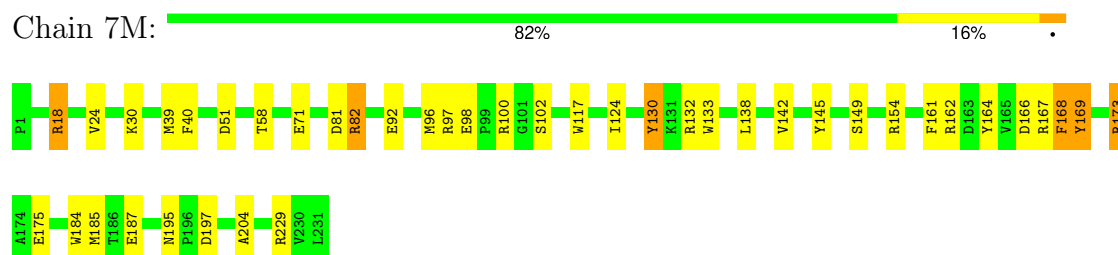
- Molecule 1: capsid protein



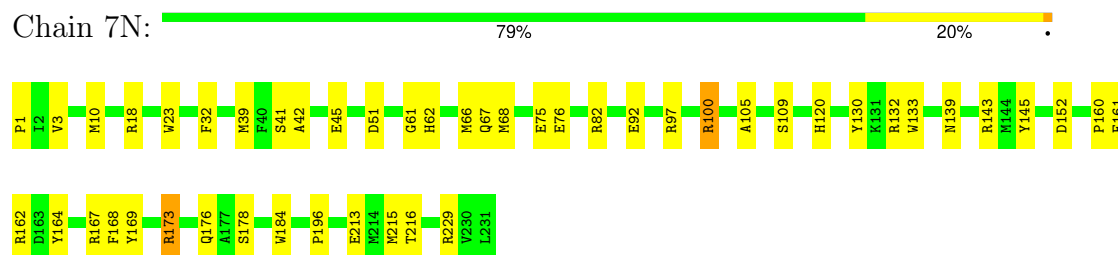
- Molecule 1: capsid protein



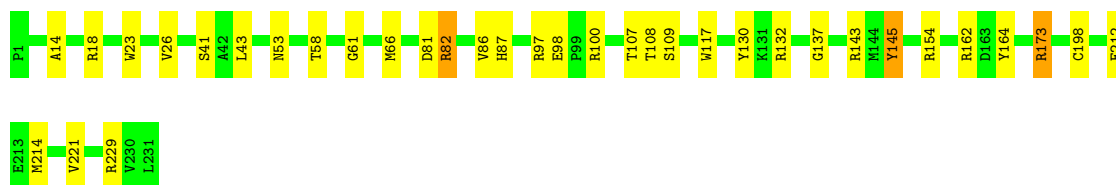
- Molecule 1: capsid protein



- Molecule 1: capsid protein

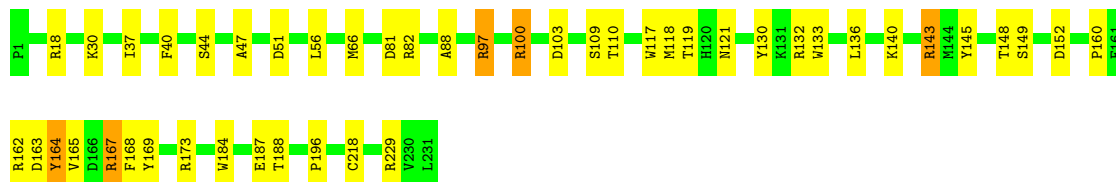


- Molecule 1: capsid protein



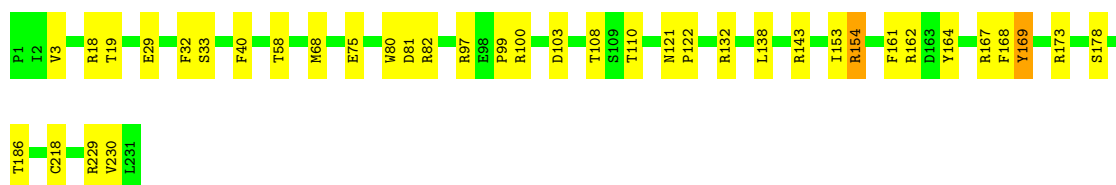
- Molecule 1: capsid protein

Chain 7P: 80% 18% .



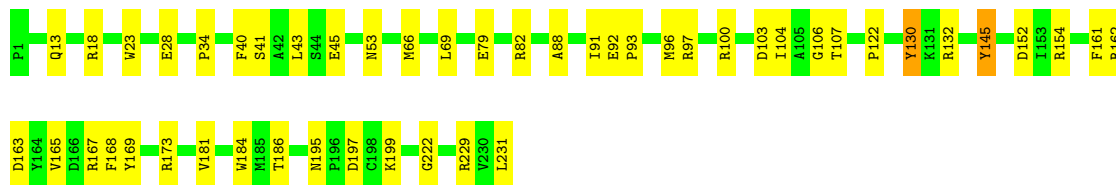
- Molecule 1: capsid protein

Chain 7Q: 84% 16% .



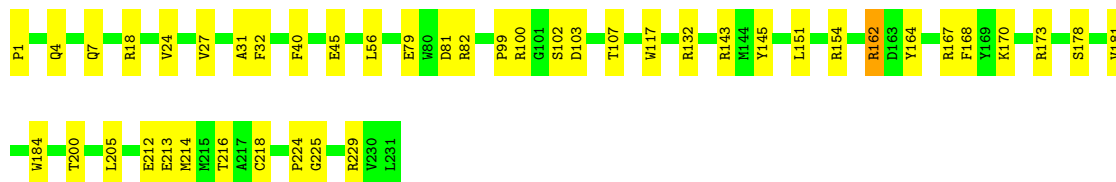
- Molecule 1: capsid protein

Chain 7R: 79% 20% .



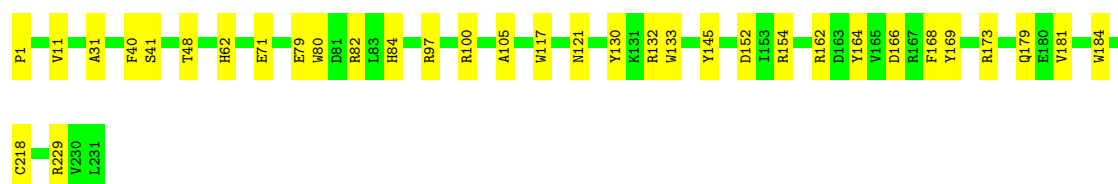
- Molecule 1: capsid protein

Chain 7S: 81% 19%



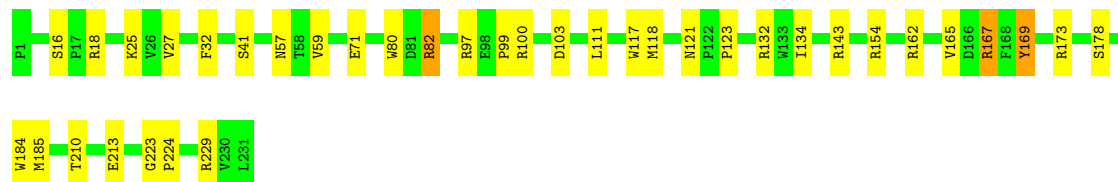
- Molecule 1: capsid protein

Chain 7T: 85% 15%



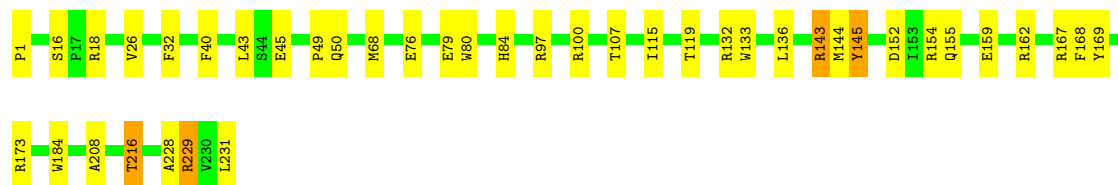
- Molecule 1: capsid protein

Chain 7U: 84% 15% .



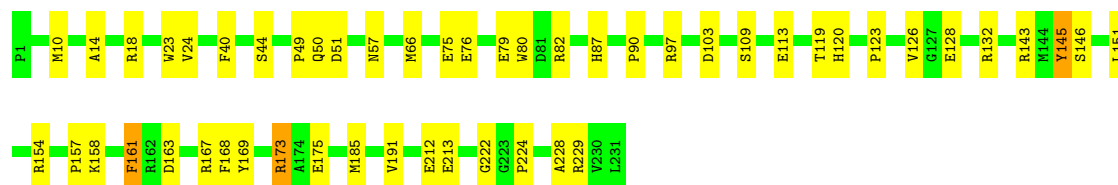
- Molecule 1: capsid protein

Chain 7V: 82% 16% .



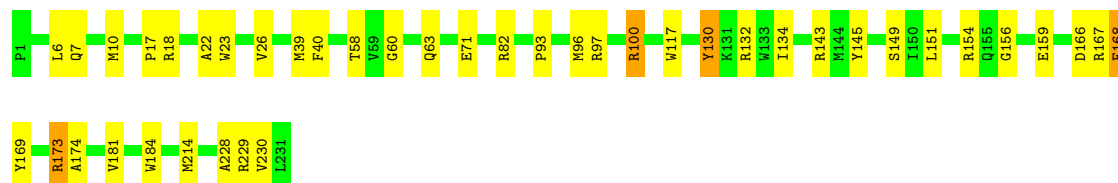
- Molecule 1: capsid protein

Chain 7W: 78% 21% .



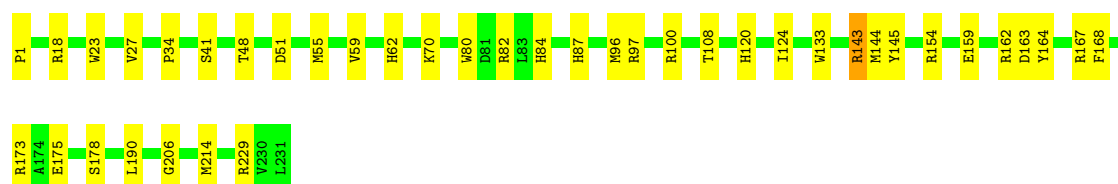
- Molecule 1: capsid protein

Chain 7X: 82% 16% .



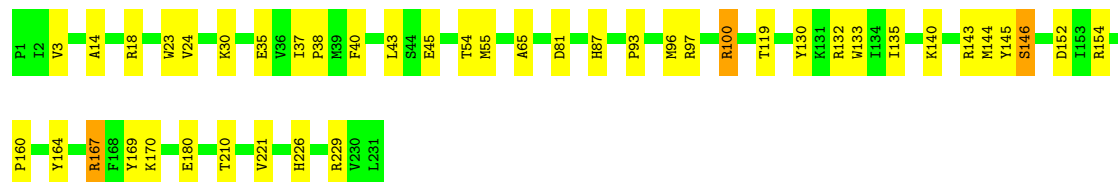
- Molecule 1: capsid protein

Chain 7Y: 83% 17% .



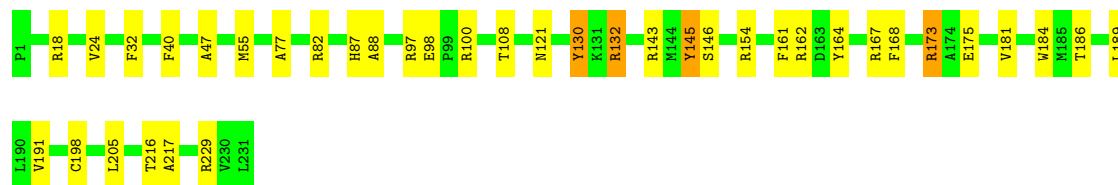
- Molecule 1: capsid protein

Chain 7Z: 81% 17% •



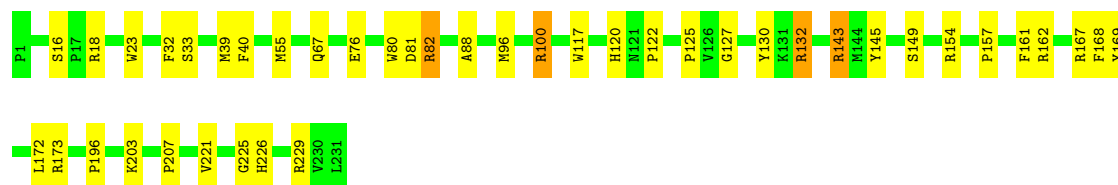
- Molecule 1: capsid protein

Chain 80: 84% 15% •



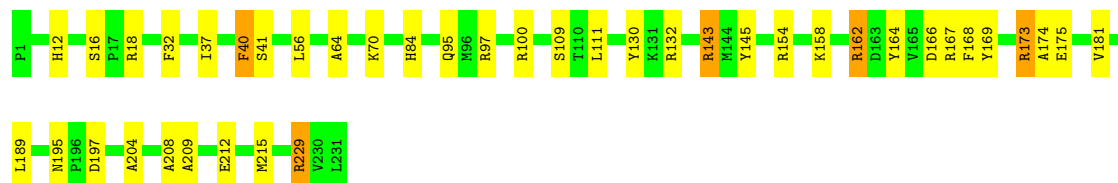
- Molecule 1: capsid protein

Chain 81: 82% 16% •



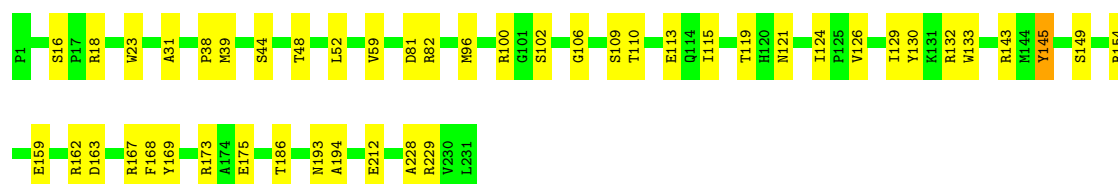
- Molecule 1: capsid protein

Chain 82: 82% 16% •



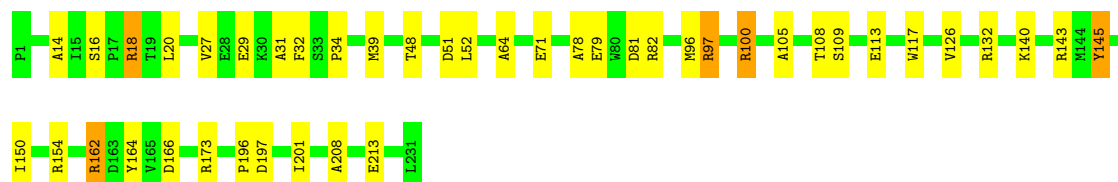
- Molecule 1: capsid protein

Chain 83: 80% 19% •



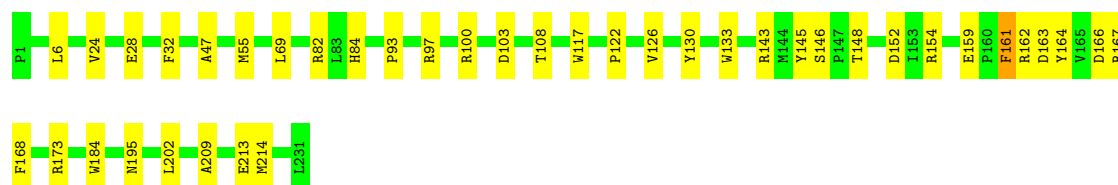
- Molecule 1: capsid protein

Chain 84: 81% 16%



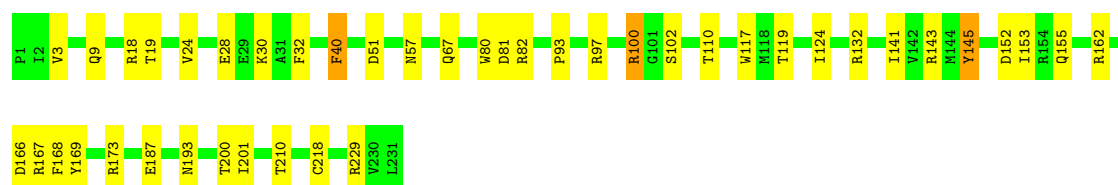
- Molecule 1: capsid protein

Chain 85: 83% 17%



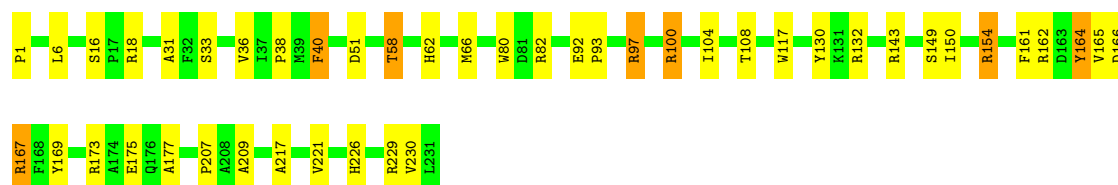
- Molecule 1: capsid protein

Chain 86: 81% 17%



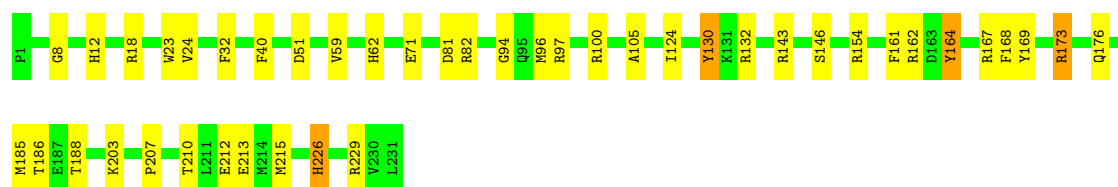
- Molecule 1: capsid protein

Chain 87: 81% 16%



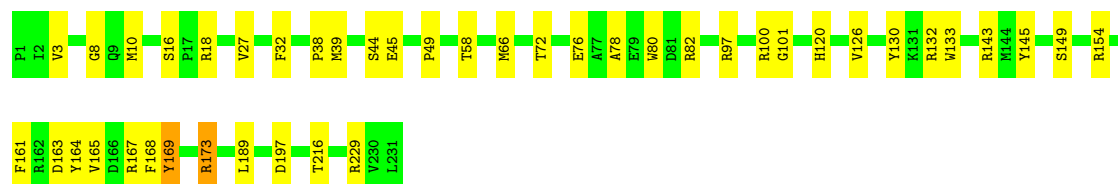
- Molecule 1: capsid protein

Chain 88: 81% 17%



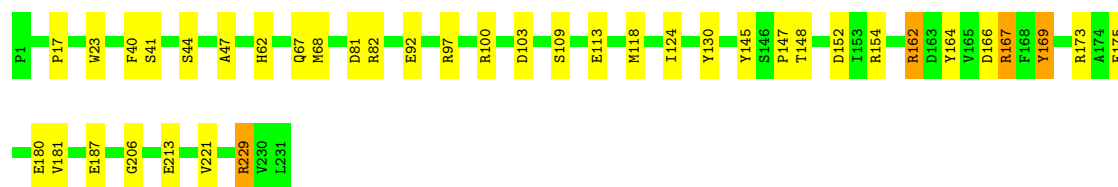
- Molecule 1: capsid protein

Chain 89: 81% 18% .



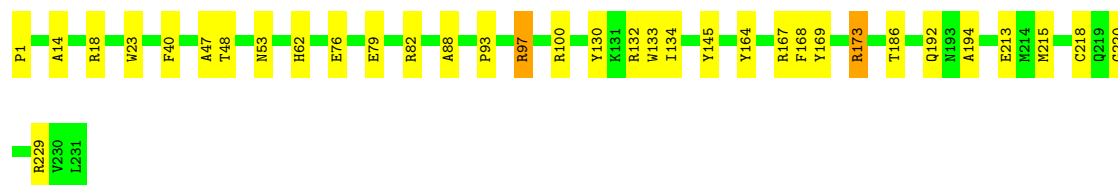
- Molecule 1: capsid protein

Chain 8a: 83% 15% .



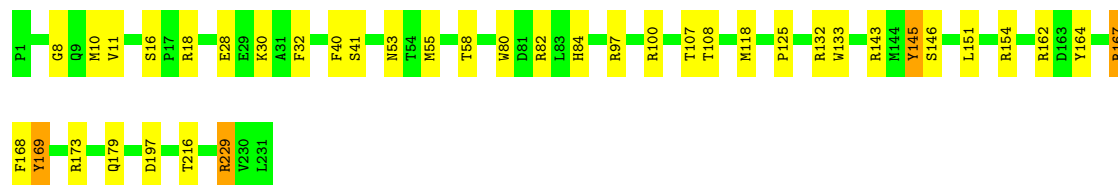
- Molecule 1: capsid protein

Chain 8b: 85% 14% .



- Molecule 1: capsid protein

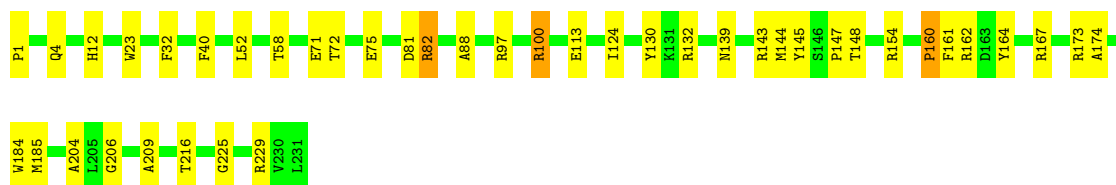
Chain 8c: 83% 15% .



- Molecule 1: capsid protein

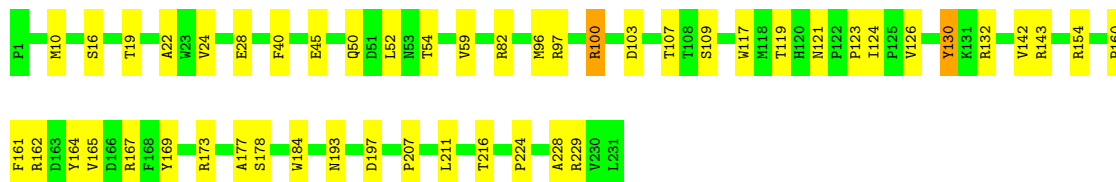
Chain 8d: 82% 17% .





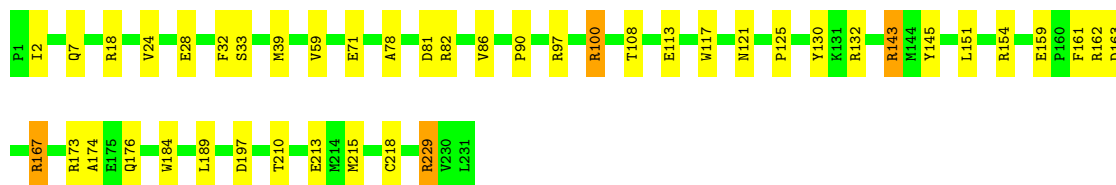
- Molecule 1: capsid protein

Chain 8e: 79% 20% •



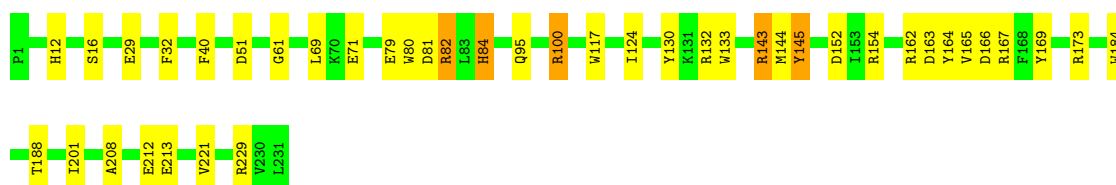
- Molecule 1: capsid protein

Chain 8f: 81% 17% •



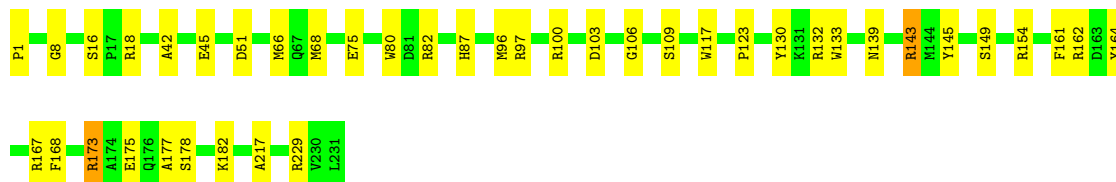
- Molecule 1: capsid protein

Chain 8g: 82% 16% •



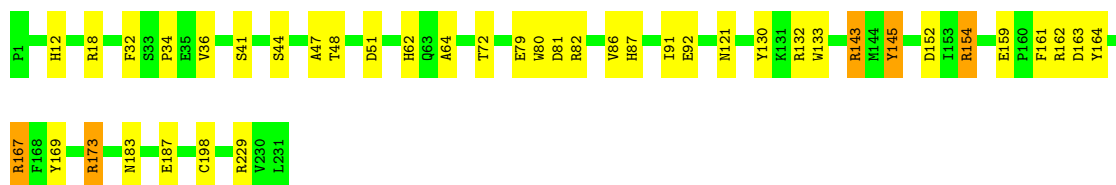
- Molecule 1: capsid protein

Chain 8h: 82% 17% •



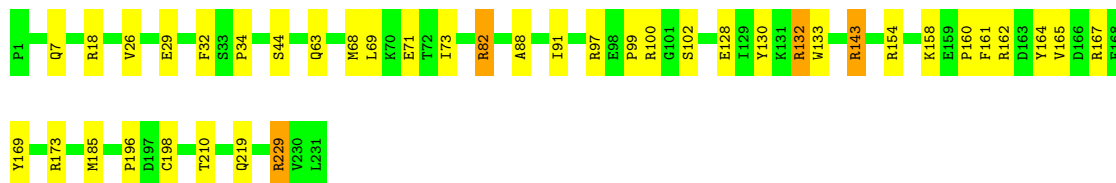
- Molecule 1: capsid protein

Chain 8i: 82% 16% •



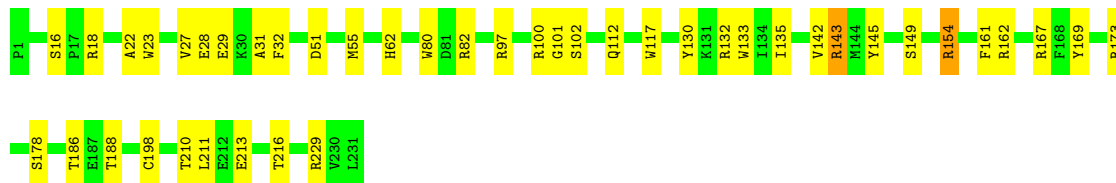
- Molecule 1: capsid protein

Chain 8j: 83% 16% •



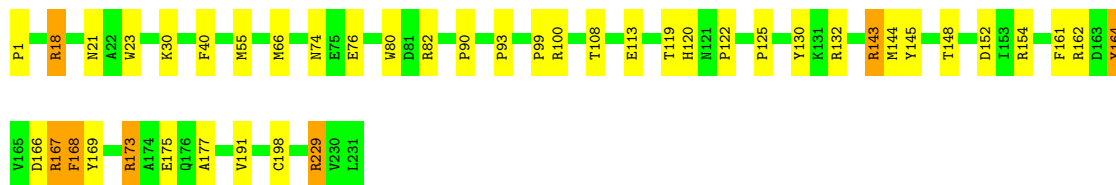
- Molecule 1: capsid protein

Chain 8k: 81% 18% •



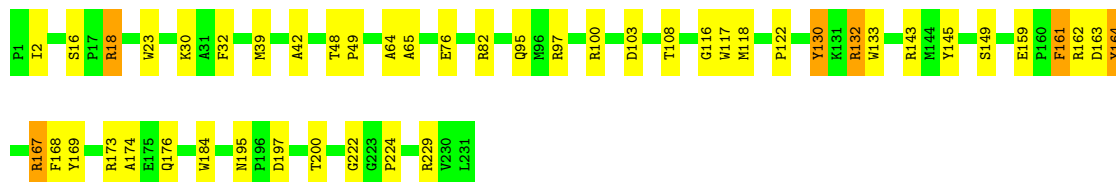
- Molecule 1: capsid protein

Chain 8l: 81% 16% •



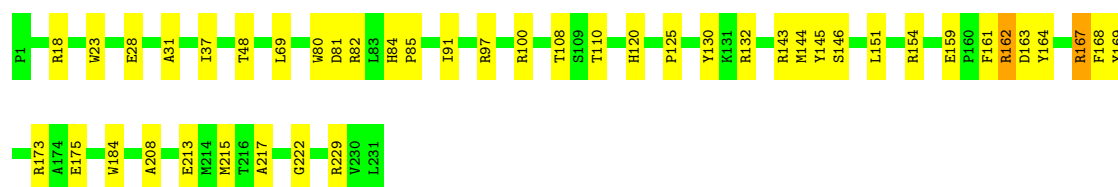
- Molecule 1: capsid protein

Chain 8m: 80% 18% •



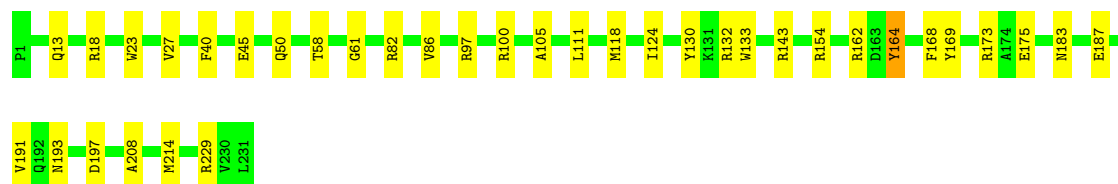
- Molecule 1: capsid protein

Chain 8n: 81% 18% •



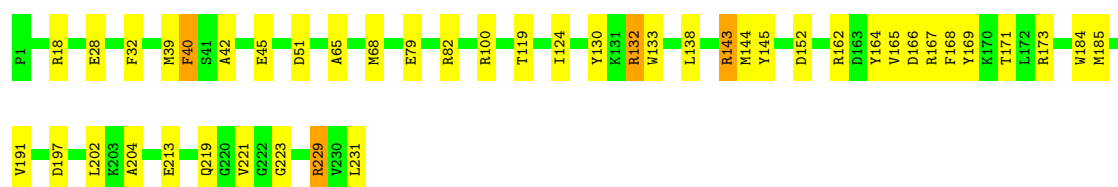
- Molecule 1: capsid protein

Chain 8o:   84% 15%



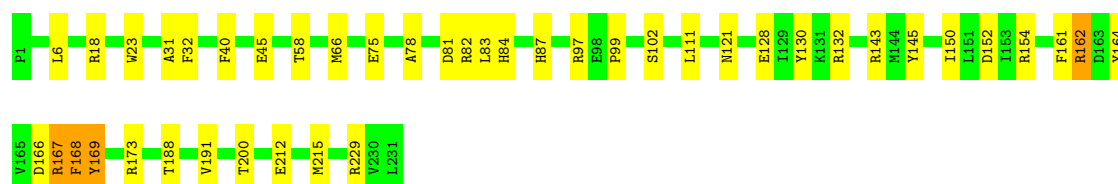
- Molecule 1: capsid protein

Chain 8p:   81% 17%



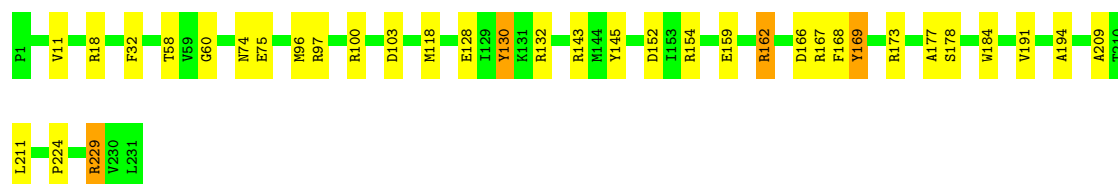
- Molecule 1: capsid protein

Chain 8q:   81% 17%




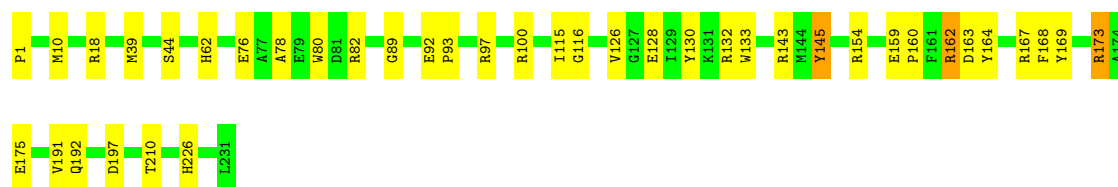
- Molecule 1: capsid protein

Chain 8r:   85% 13%




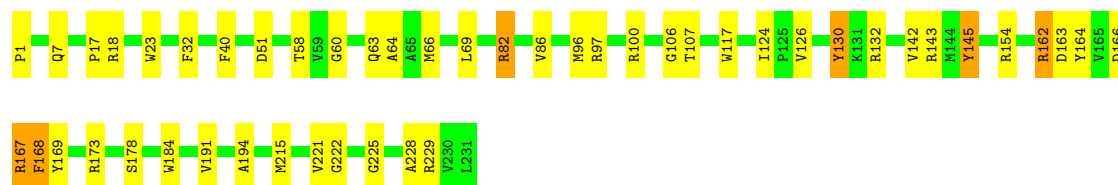
- Molecule 1: capsid protein

Chain 8s:  83% 16%




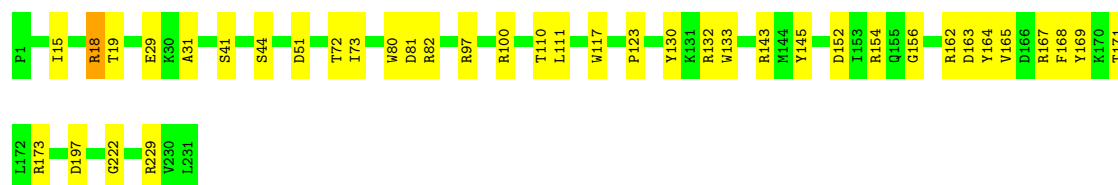
- Molecule 1: capsid protein

Chain 8t:  79% 18%




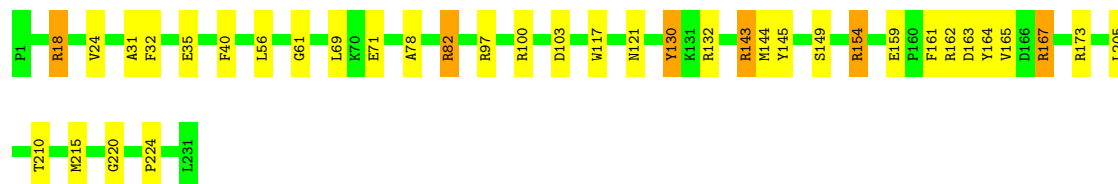
- Molecule 1: capsid protein

Chain 8u:  83% 16%




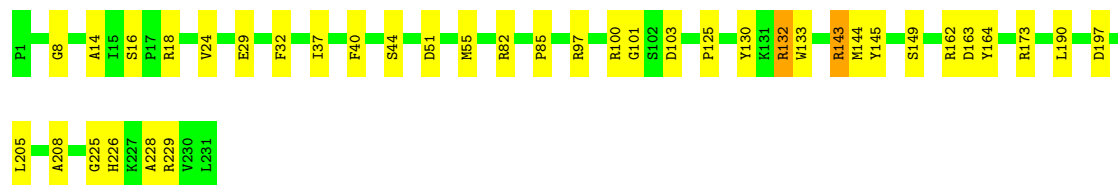
- Molecule 1: capsid protein

Chain 8v:  84% 13%




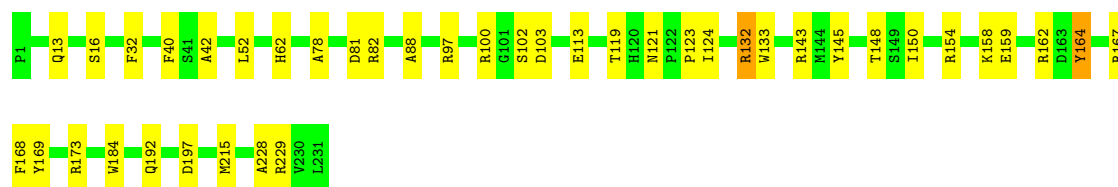
- Molecule 1: capsid protein

Chain 8w:  84% 16%




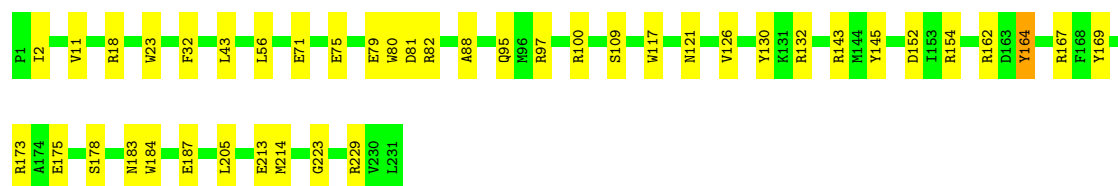
- Molecule 1: capsid protein

Chain 8x:  82% 17% •




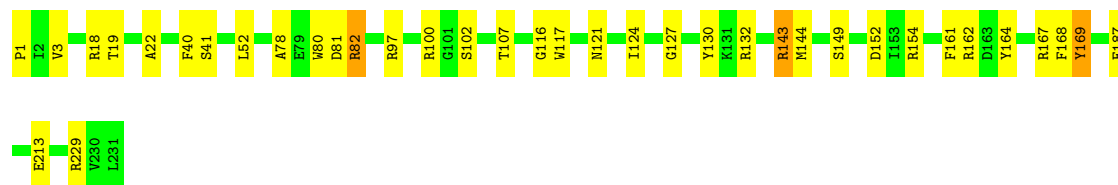
- Molecule 1: capsid protein

Chain 8y:  82% 18%




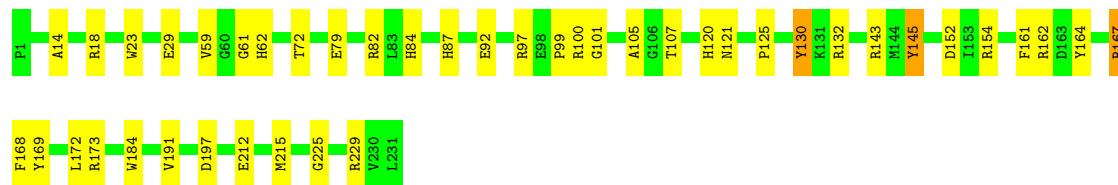
- Molecule 1: capsid protein

Chain 8z:  84% 15% •




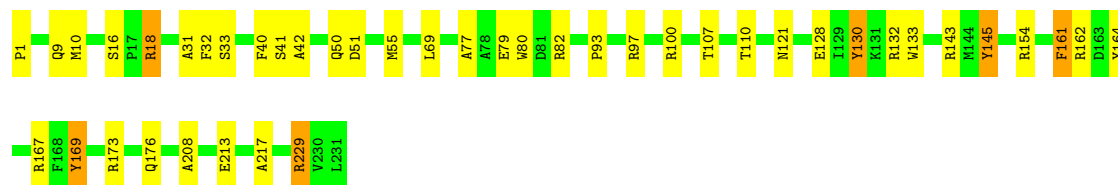
- Molecule 1: capsid protein

Chain 8A:  81% 17% •




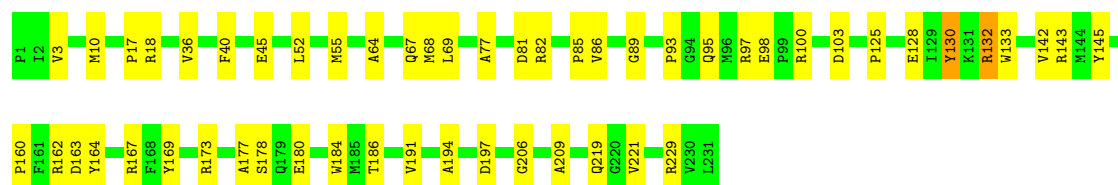
- Molecule 1: capsid protein

Chain 8B:  81% 16% •




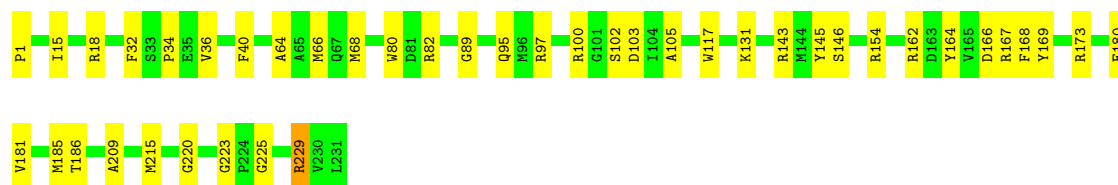
- Molecule 1: capsid protein

Chain 8C:  77% 22%




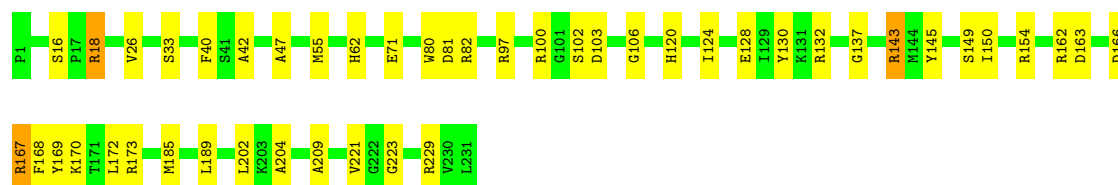
- Molecule 1: capsid protein

Chain 8D:  82% 18%




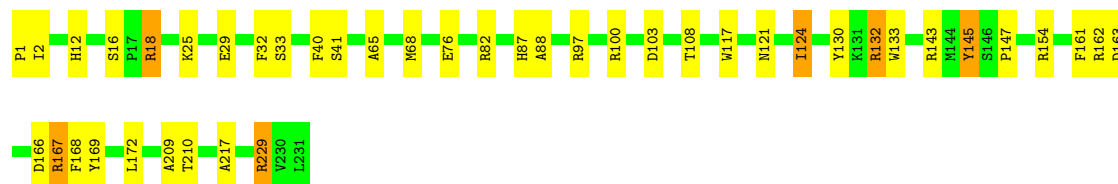
- Molecule 1: capsid protein

Chain 8E:  80% 19%




- Molecule 1: capsid protein

Chain 8F:  81% 16%




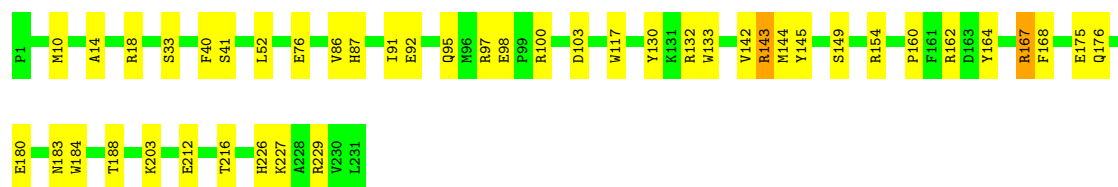
- Molecule 1: capsid protein

Chain 8G:  81% 18%




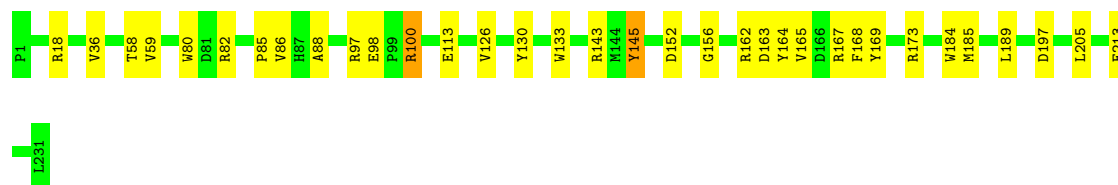
- Molecule 1: capsid protein

Chain 8H:  81% 18%




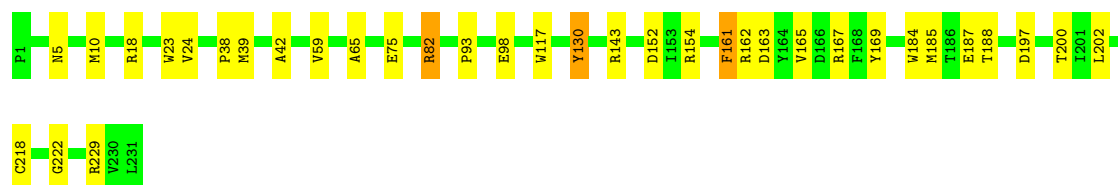
- Molecule 1: capsid protein

Chain 8I:  85% 14%




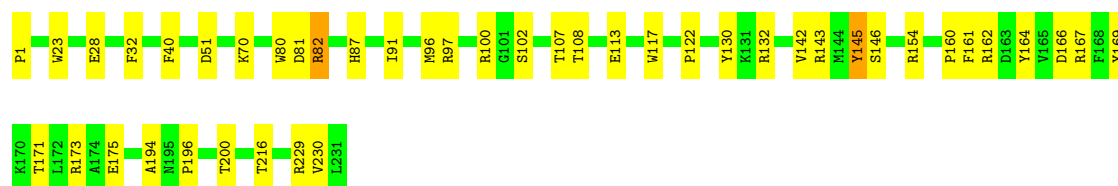
- Molecule 1: capsid protein

Chain 8J:  85% 14%




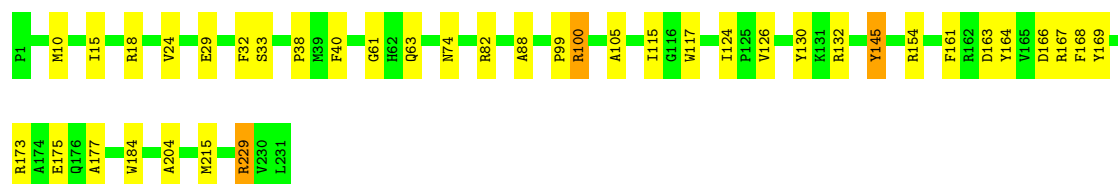
- Molecule 1: capsid protein

Chain 8K:  81% 18%




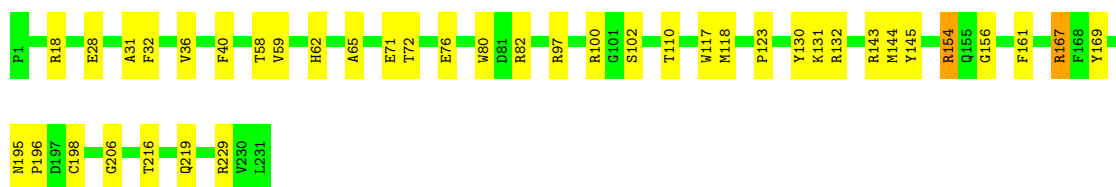
- Molecule 1: capsid protein

Chain 8L:  83% 16%




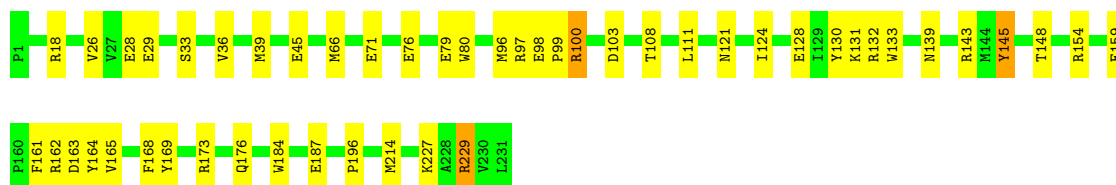
- Molecule 1: capsid protein

Chain 8M:  83% 16% .




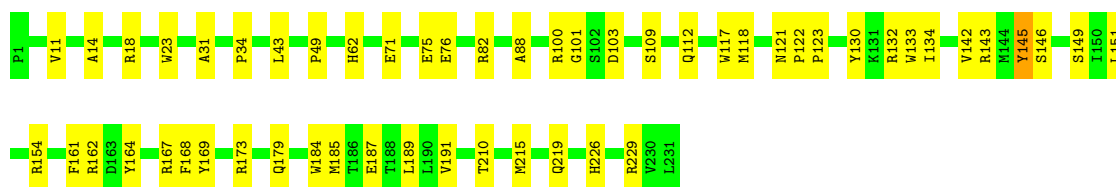
- Molecule 1: capsid protein

Chain 8N:  79% 20% .




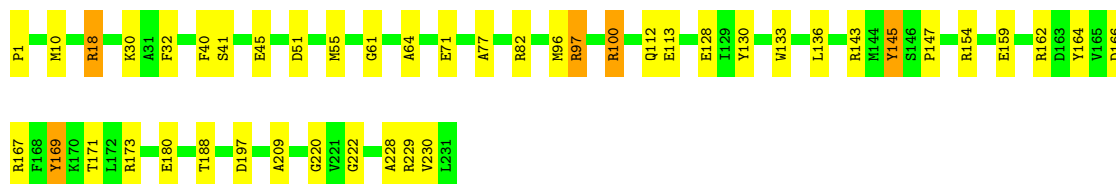
- Molecule 1: capsid protein

Chain 8O:  77% 23% .




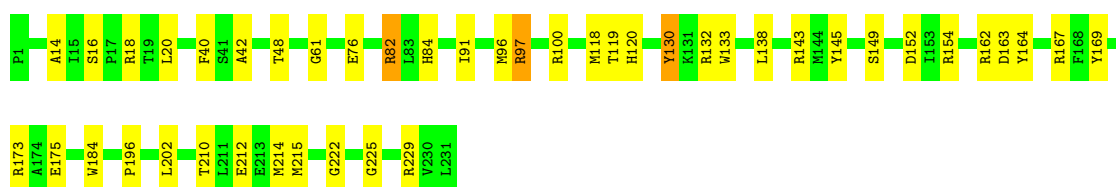
- Molecule 1: capsid protein

Chain 8P:  81% 17% .




- Molecule 1: capsid protein

Chain 8Q:  81% 18% .




- Molecule 1: capsid protein

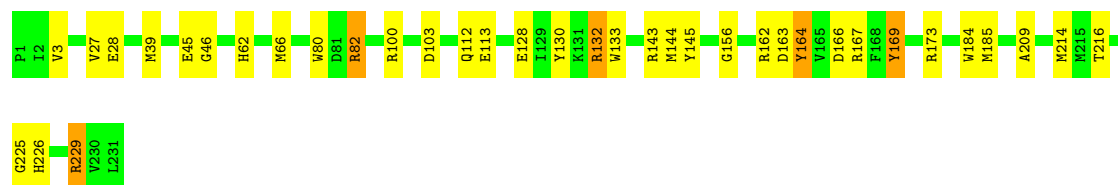


Chain 8R:  81% 17% •




- Molecule 1: capsid protein

Chain 8S:  84% 14% •




- Molecule 1: capsid protein

Chain 8T:  81% 18% •




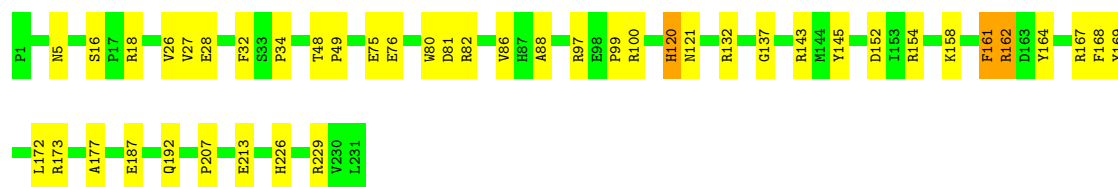
- Molecule 1: capsid protein

Chain 8U:  83% 15% •




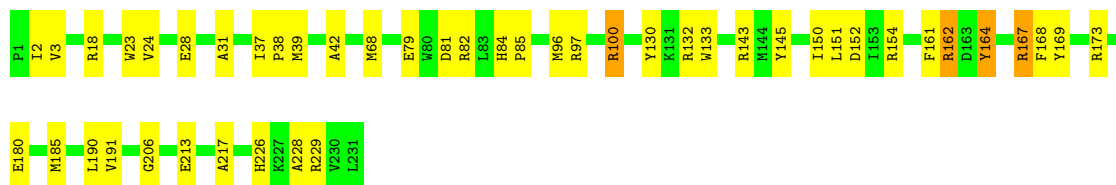
- Molecule 1: capsid protein

Chain 8V:  81% 18% •




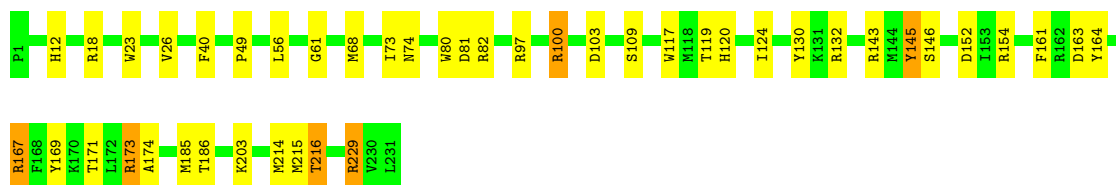
- Molecule 1: capsid protein

Chain 8W:  80% 18% .




- Molecule 1: capsid protein

Chain 8X:  81% 16% .



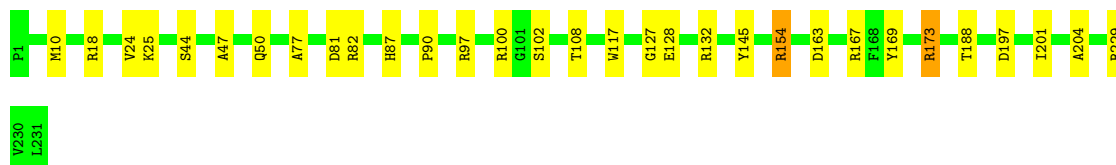
- Molecule 1: capsid protein

Chain 8Y:  84% 15% .




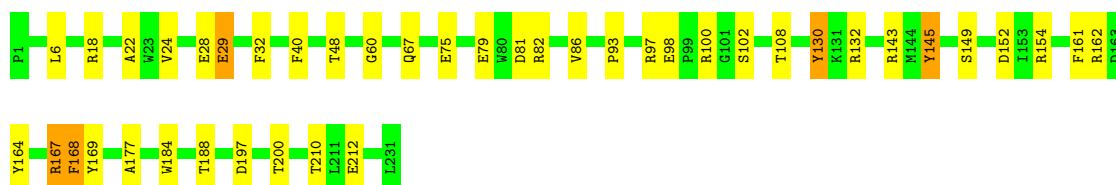
- Molecule 1: capsid protein

Chain 8Z:  87% 13% .

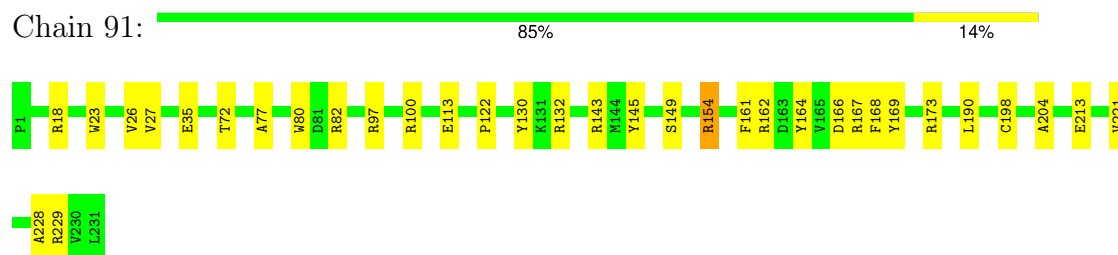


- Molecule 1: capsid protein

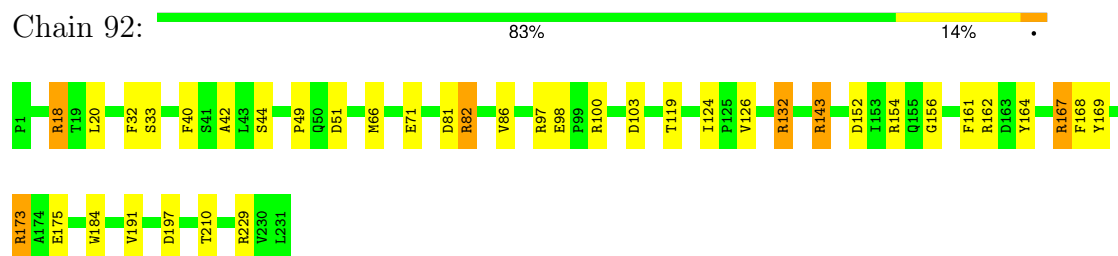
Chain 90:  82% 16% .



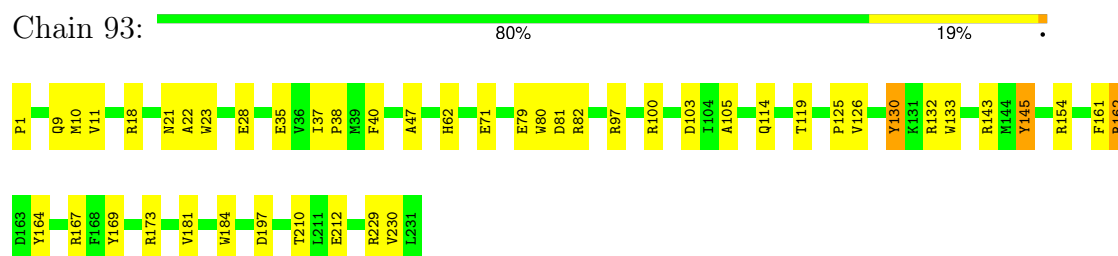
- Molecule 1: capsid protein



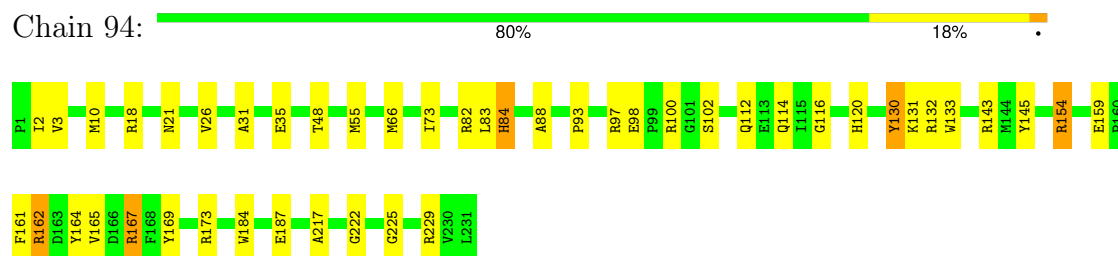
- Molecule 1: capsid protein



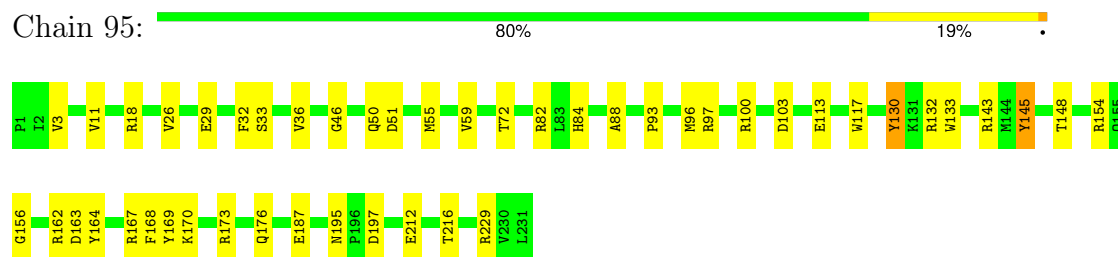
- Molecule 1: capsid protein




- Molecule 1: capsid protein



- Molecule 1: capsid protein




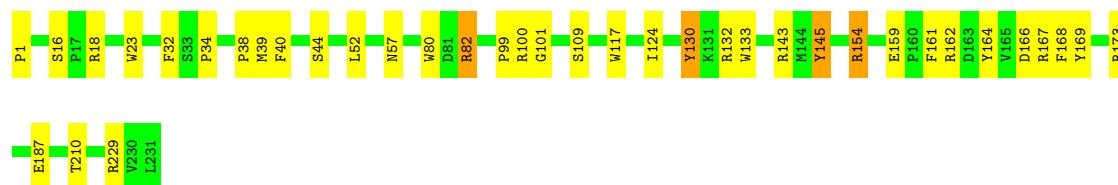
- Molecule 1: capsid protein

Chain 96:  84% 16%




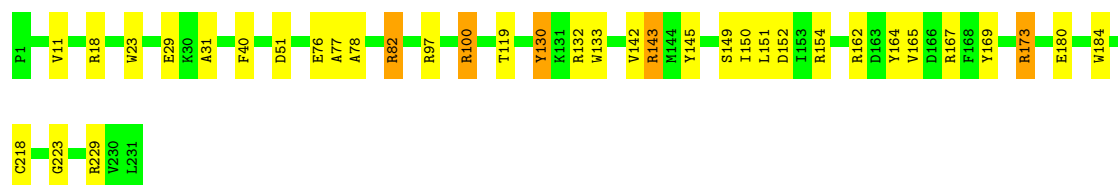
- Molecule 1: capsid protein

Chain 97:  84% 15% •




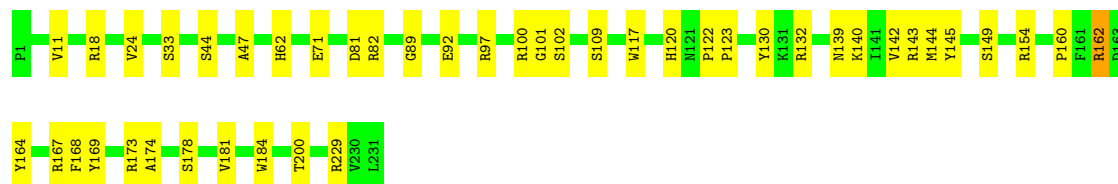
- Molecule 1: capsid protein

Chain 98:  84% 13% •




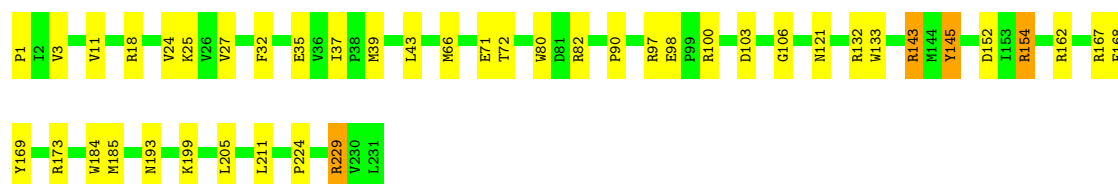
- Molecule 1: capsid protein

Chain 99:  81% 19%




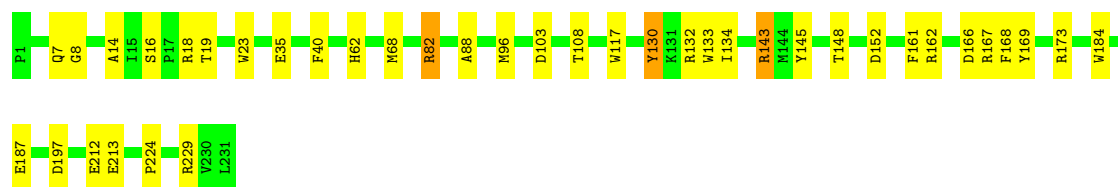
- Molecule 1: capsid protein

Chain 9a:  81% 17% •




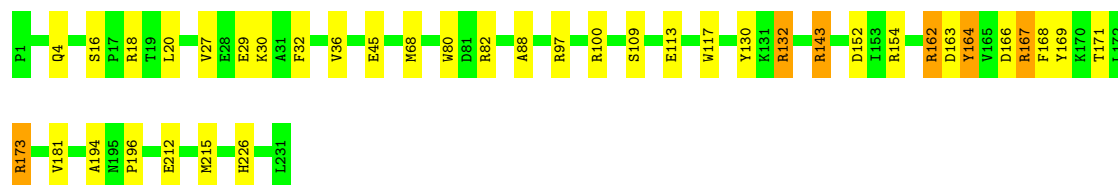
- Molecule 1: capsid protein

Chain 9b:  83% 16%




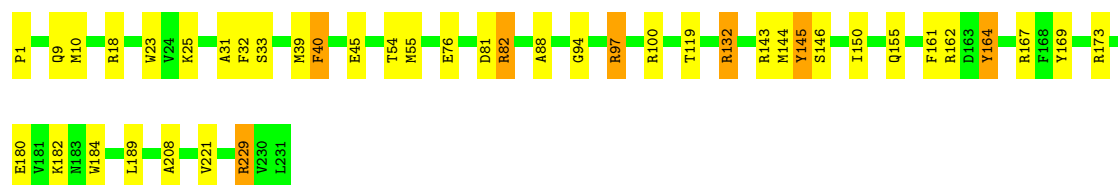
- Molecule 1: capsid protein

Chain 9c:  83% 14%




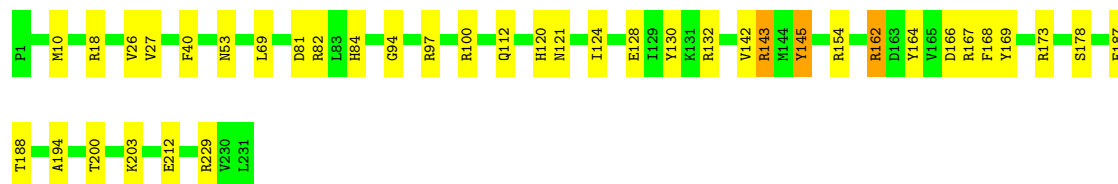
- Molecule 1: capsid protein

Chain 9d:  82% 15%




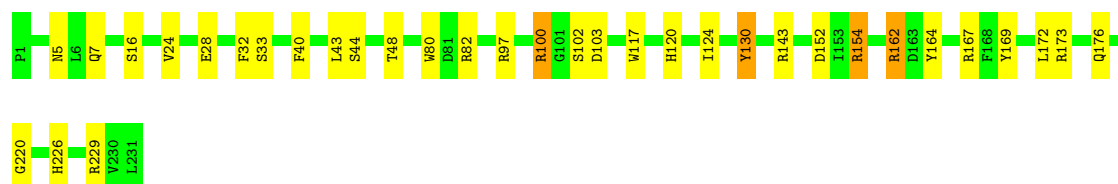
- Molecule 1: capsid protein

Chain 9e:  83% 16%




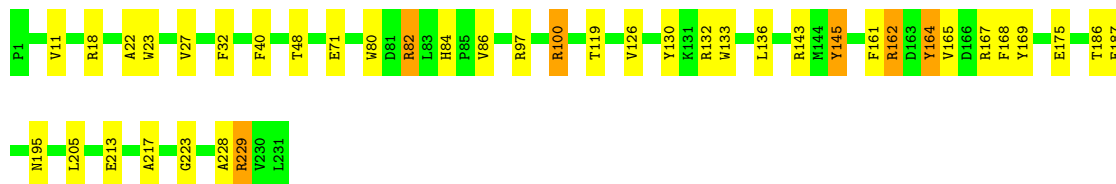
- Molecule 1: capsid protein

Chain 9f:  85% 13%




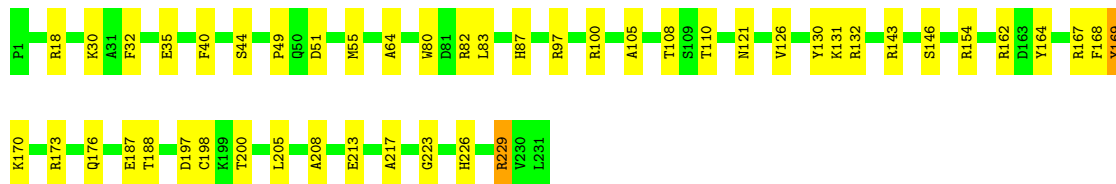
- Molecule 1: capsid protein

Chain 9g:  83% 15% •




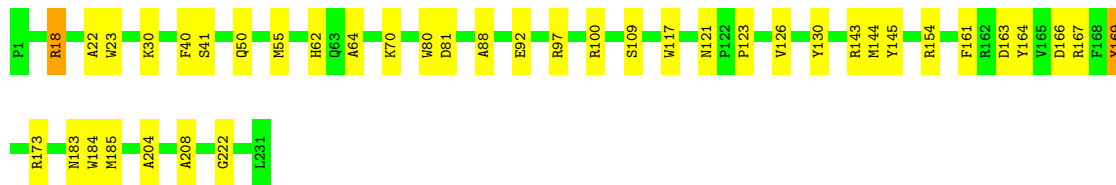
- Molecule 1: capsid protein

Chain 9h:  80% 19% •




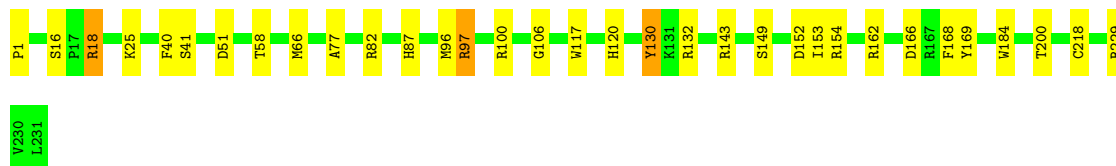
- Molecule 1: capsid protein

Chain 9i:  83% 16% •




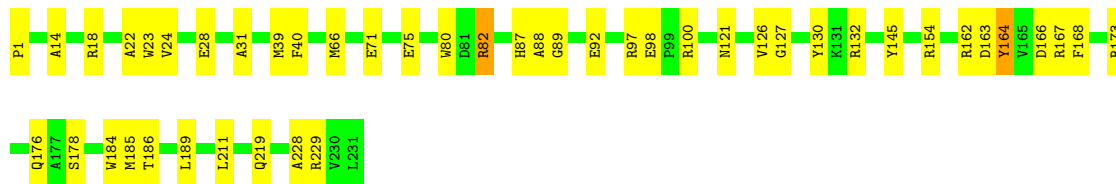
- Molecule 1: capsid protein

Chain 9j:  86% 13% •

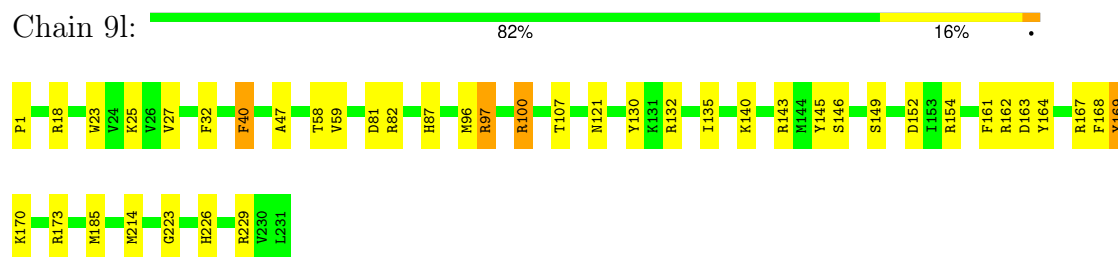


- Molecule 1: capsid protein

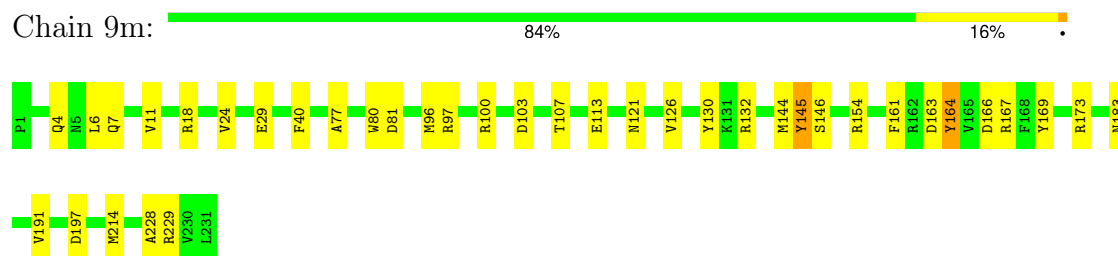
Chain 9k:  80% 19% •



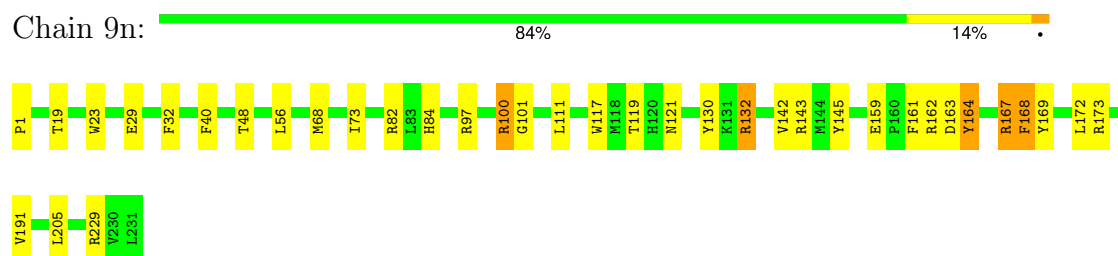
- Molecule 1: capsid protein



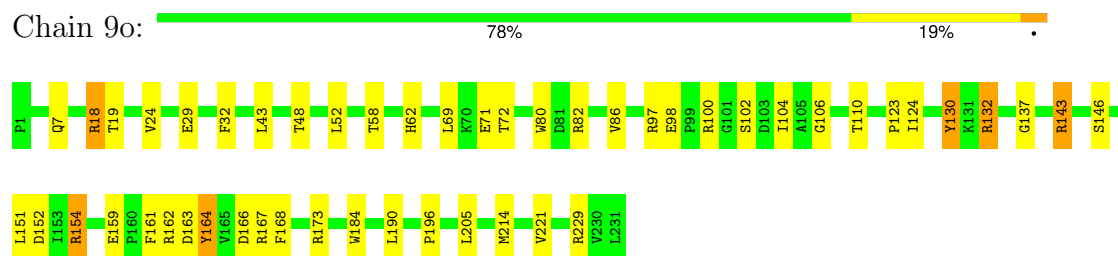
- Molecule 1: capsid protein



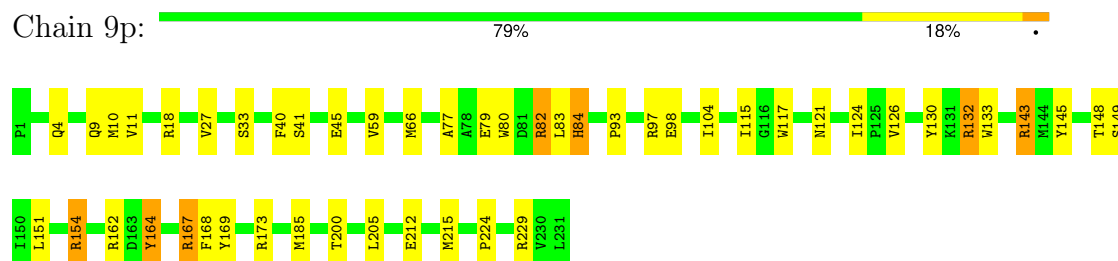
- Molecule 1: capsid protein




- Molecule 1: capsid protein

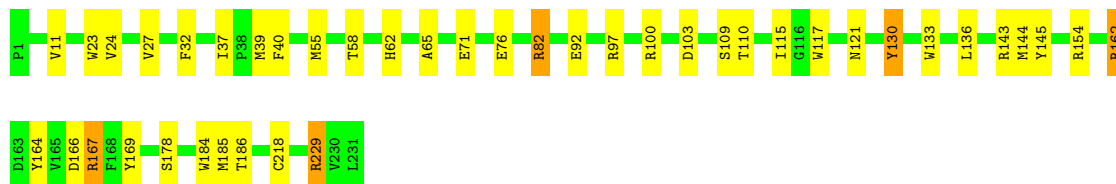


- Molecule 1: capsid protein




- Molecule 1: capsid protein

Chain 9q:  82% 16% •




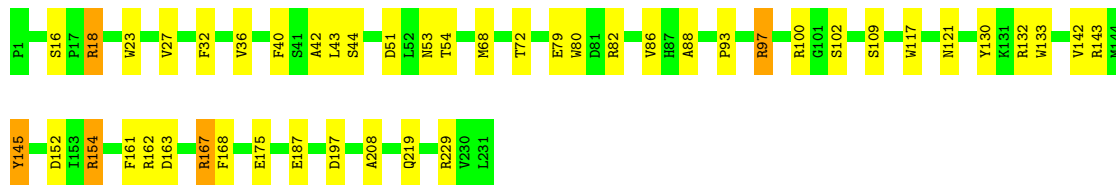
- Molecule 1: capsid protein

Chain 9r:  82% 16% •




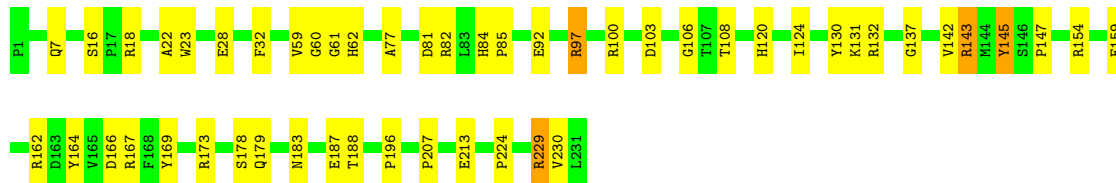
- Molecule 1: capsid protein

Chain 9s:  80% 18% •




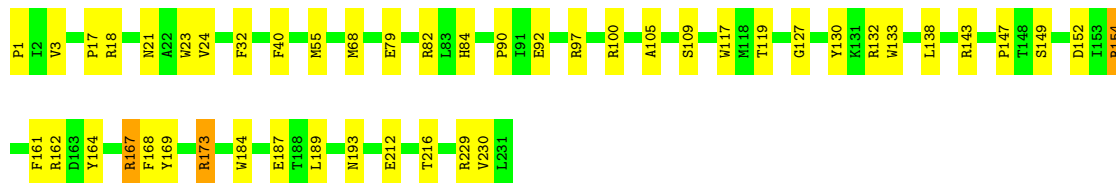
- Molecule 1: capsid protein

Chain 9t:  78% 20% •




- Molecule 1: capsid protein

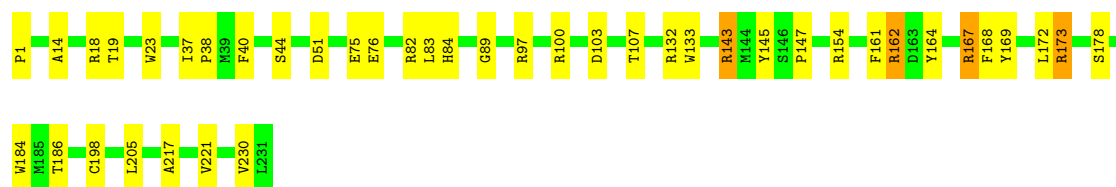
Chain 9u:  80% 19% •




- Molecule 1: capsid protein

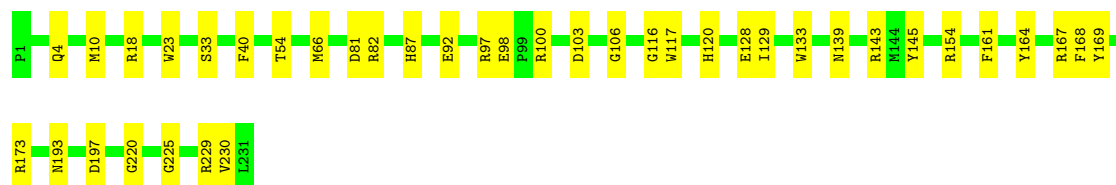


Chain 9v:  82% 16% •




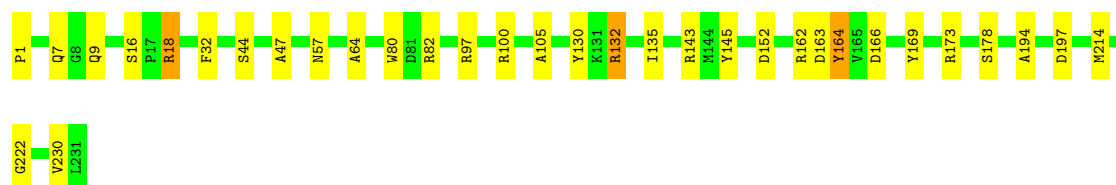
- Molecule 1: capsid protein

Chain 9w:  83% 17%




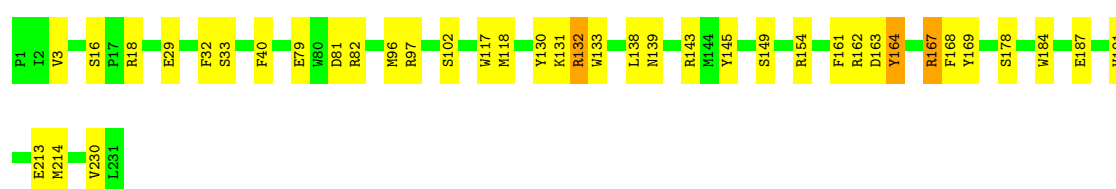
- Molecule 1: capsid protein

Chain 9x:  86% 13% •




- Molecule 1: capsid protein

Chain 9y:  83% 16% •




- Molecule 1: capsid protein

Chain 9z:  79% 20% •




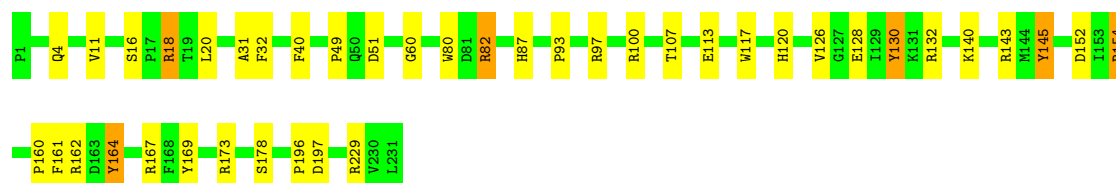
- Molecule 1: capsid protein

Chain 9A:  87% 12%




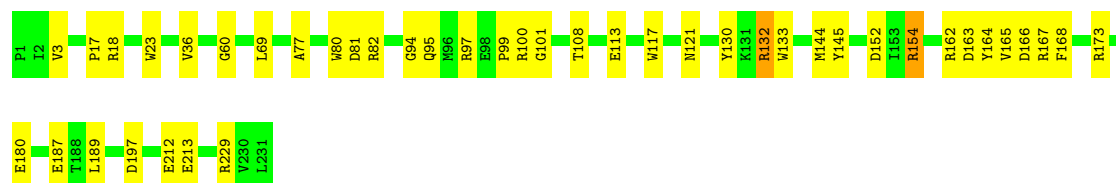
- Molecule 1: capsid protein

Chain 9B:  82% 15%




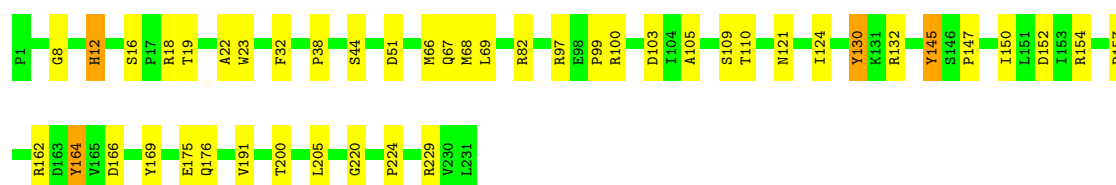
- Molecule 1: capsid protein

Chain 9C:  81% 18%




- Molecule 1: capsid protein

Chain 9D:  81% 18%




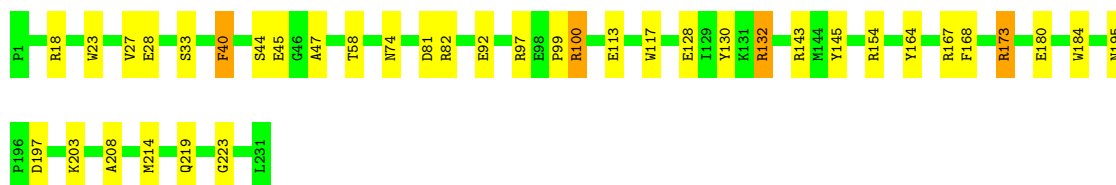
- Molecule 1: capsid protein

Chain 9E:  85% 14%



- Molecule 1: capsid protein

Chain 9F:  84% 15%



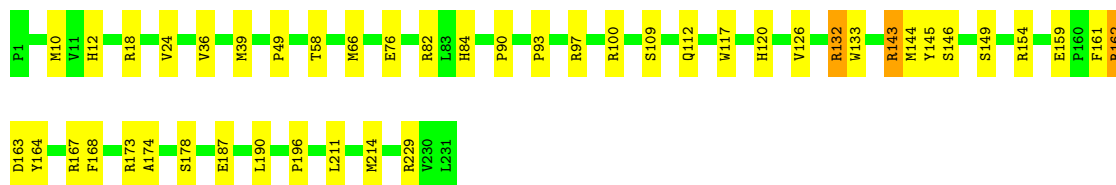
- Molecule 1: capsid protein

Chain 9G: 79% 19%



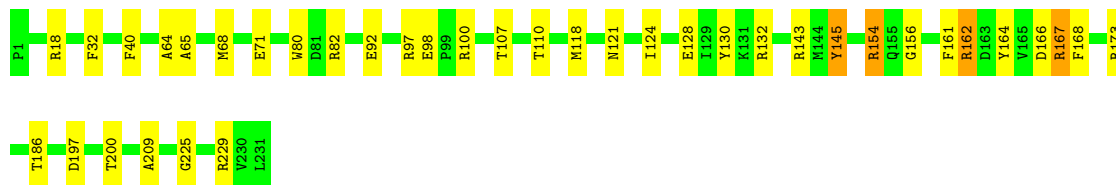
- Molecule 1: capsid protein

Chain 9H: 81% 18%



- Molecule 1: capsid protein

Chain 9I: 84% 15%



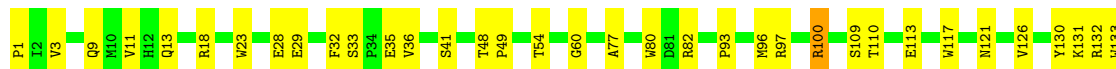
- Molecule 1: capsid protein

Chain 9J: 87% 13%



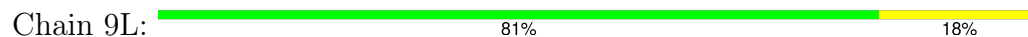
- Molecule 1: capsid protein

Chain 9K: 75% 24%

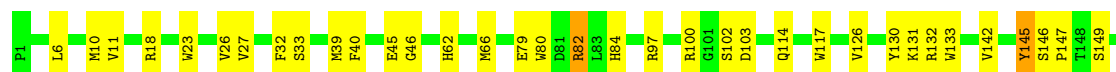
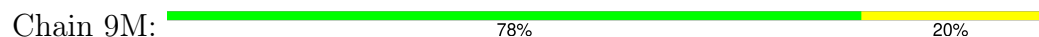




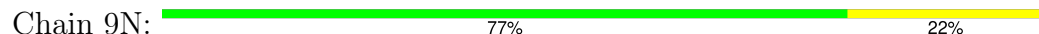
- Molecule 1: capsid protein



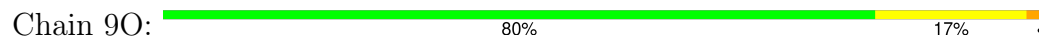
- Molecule 1: capsid protein



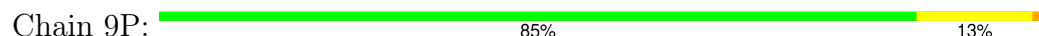
- Molecule 1: capsid protein

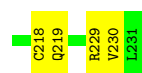


- Molecule 1: capsid protein



- Molecule 1: capsid protein





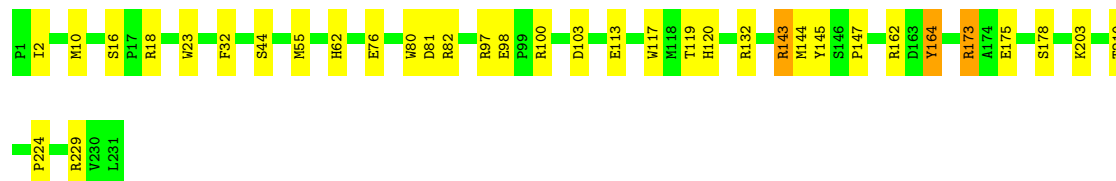
- Molecule 1: capsid protein

Chain Y: 81% 19%



- Molecule 1: capsid protein

Chain 9Q: 85% 14%



- Molecule 1: capsid protein

Chain 9R: 86% 13%



- Molecule 1: capsid protein

Chain 9S: 81% 18%



- Molecule 1: capsid protein

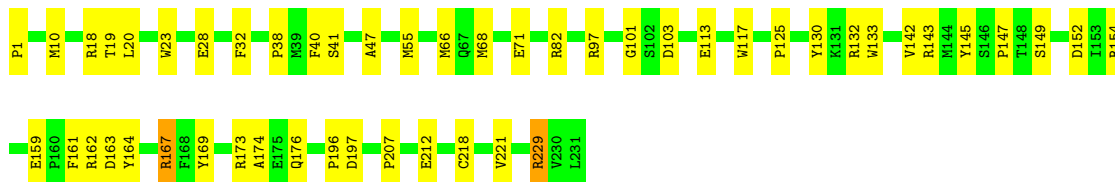
Chain 9T: 82% 16%





- Molecule 1: capsid protein

Chain 9U: 78% 21% •



- Molecule 1: capsid protein

Chain 9V: 84% 16% •



- Molecule 1: capsid protein

Chain 9W: 78% 20% •



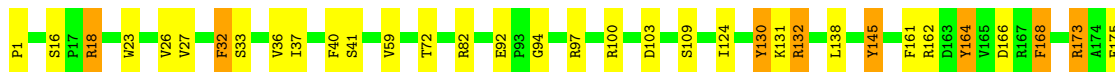
- Molecule 1: capsid protein

Chain 9X: 82% 15% •



- Molecule 1: capsid protein

Chain 9Y: 83% 14% •





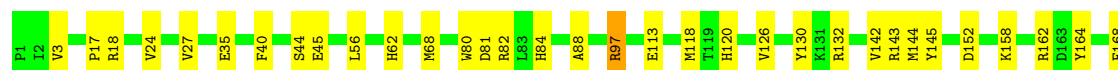
- Molecule 1: capsid protein

Chain 9Z: 84% 15%



- Molecule 1: capsid protein

Chain Z: 81% 19%



- Molecule 1: capsid protein

Chain a0: 80% 17%



- Molecule 1: capsid protein

Chain a1: 84% 15%



- Molecule 1: capsid protein

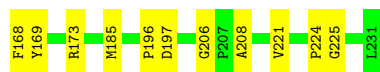
Chain a2: 81% 18%





- Molecule 1: capsid protein

Chain a3: 80% 19%



- Molecule 1: capsid protein

Chain a4: 81% 17%



- Molecule 1: capsid protein

Chain a5: 83% 16%



- Molecule 1: capsid protein

Chain a6: 83% 16%

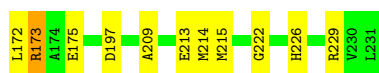


- Molecule 1: capsid protein

Chain a7: 80% 19%

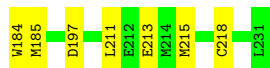
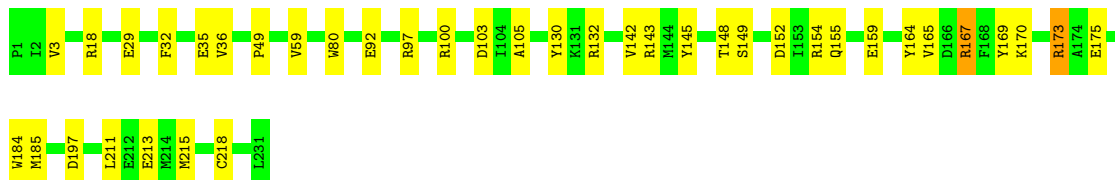






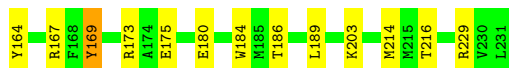
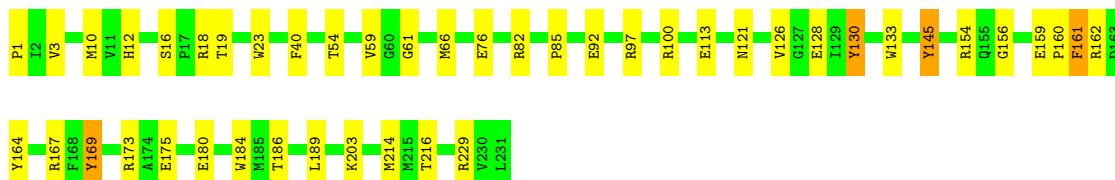
- Molecule 1: capsid protein

Chain a8: 83% 16% •



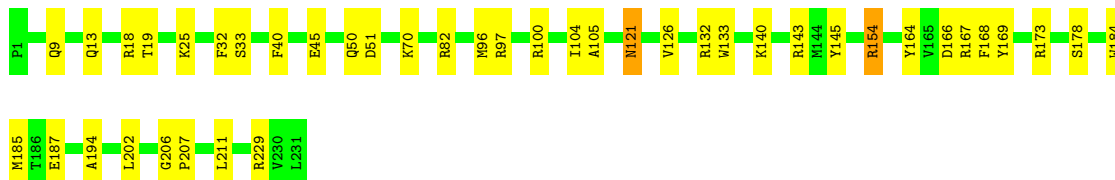
- Molecule 1: capsid protein

Chain a9: 81% 18% •



- Molecule 1: capsid protein

Chain 10: 82% 17% •



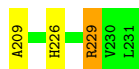
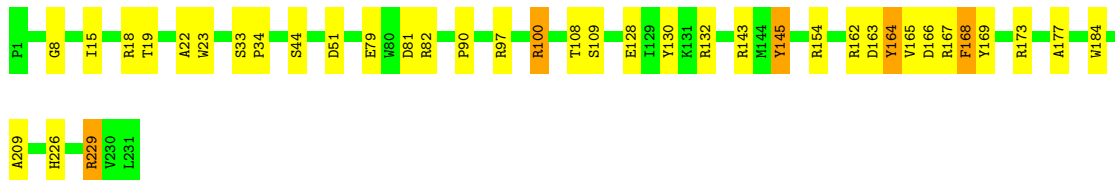
- Molecule 1: capsid protein

Chain aa: 87% 12% •


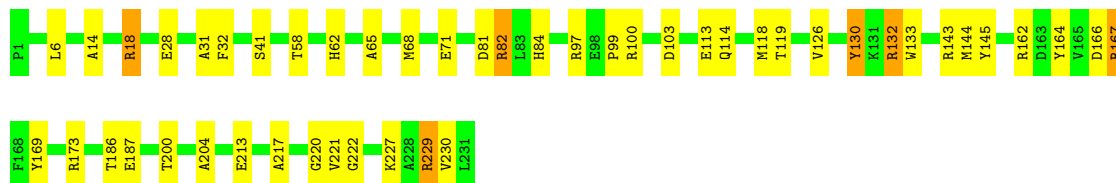


- Molecule 1: capsid protein


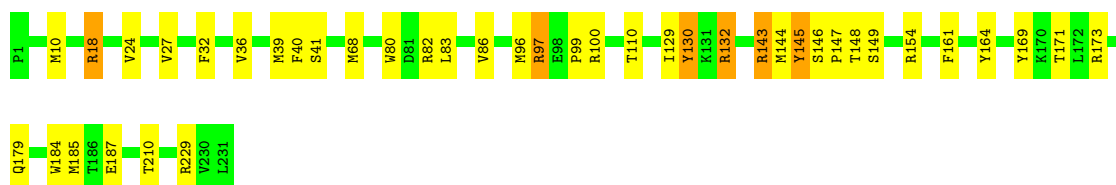
Chain ab: 84% 14% •




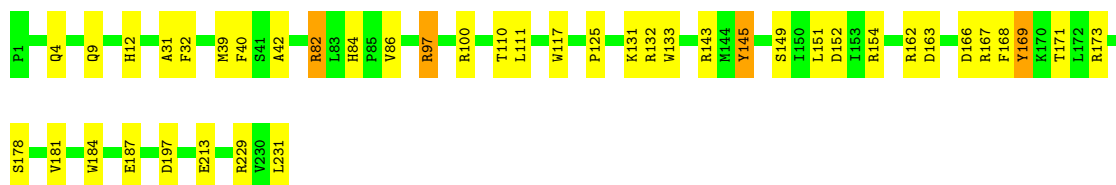
## • Molecule 1: capsid protein

Chain ac:  79% 18%


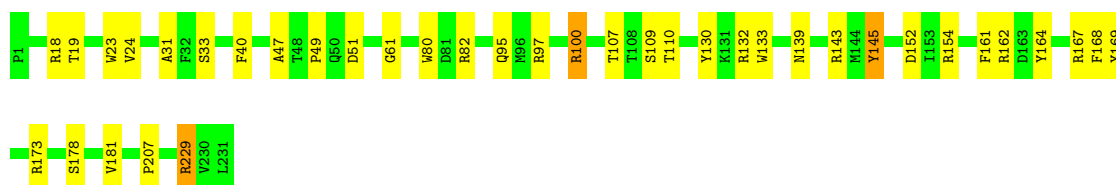
## • Molecule 1: capsid protein

Chain ad:  82% 15%


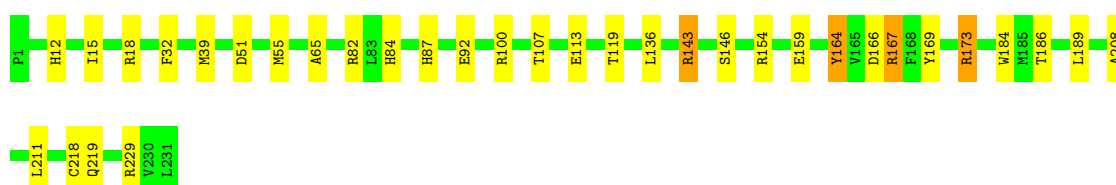
## • Molecule 1: capsid protein

Chain ae:  82% 16%


## • Molecule 1: capsid protein

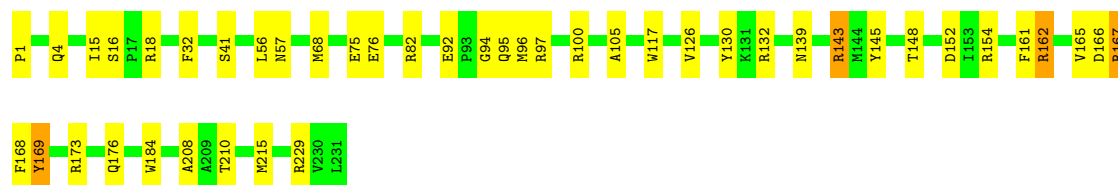
Chain af:  84% 15%

## • Molecule 1: capsid protein


Chain ag:  85% 13%

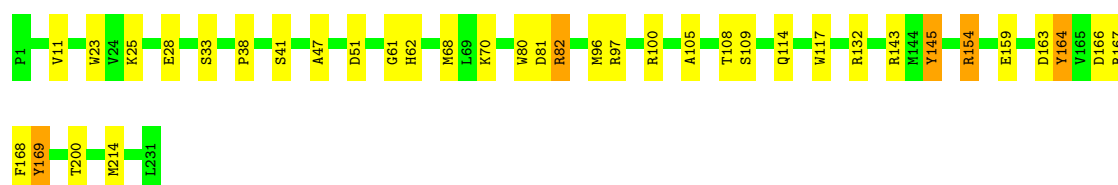
- Molecule 1: capsid protein

Chain ah:  81% 17%




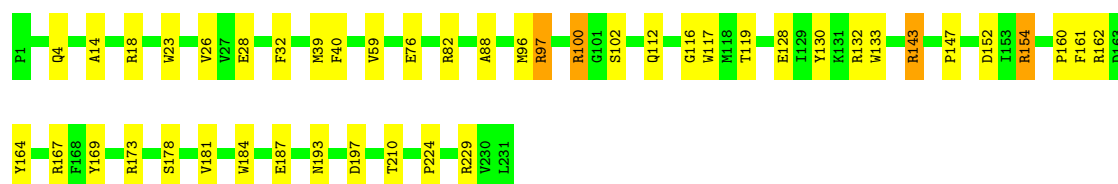
- Molecule 1: capsid protein

Chain ai:  84% 14%




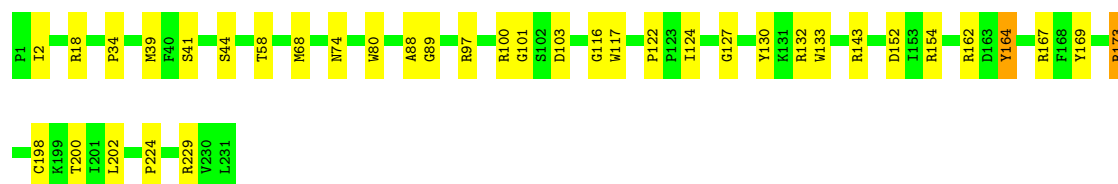
- Molecule 1: capsid protein

Chain aj:  81% 18%




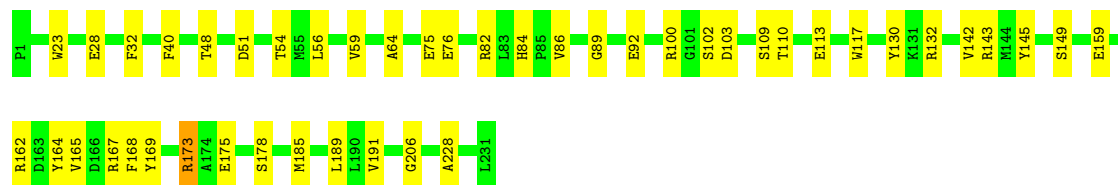
- Molecule 1: capsid protein

Chain 11:  84% 15%


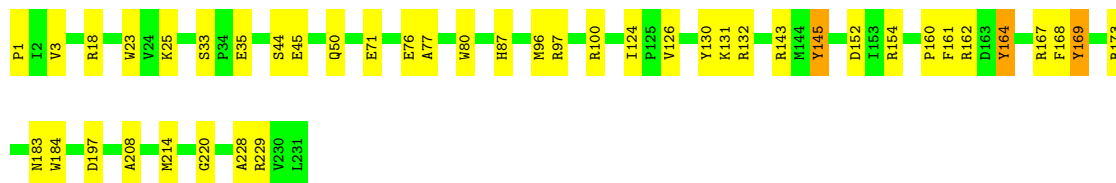


- Molecule 1: capsid protein


Chain ak:  81% 19%




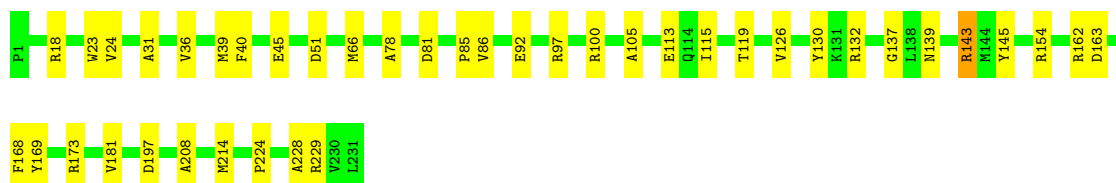
## • Molecule 1: capsid protein

Chain al:  81% 17%


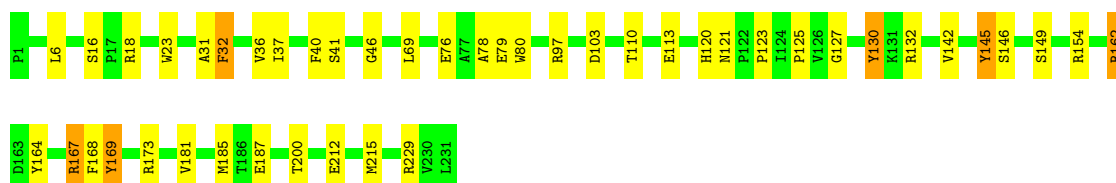
## • Molecule 1: capsid protein

Chain am:  80% 19%


## • Molecule 1: capsid protein

Chain an:  82% 17%


## • Molecule 1: capsid protein

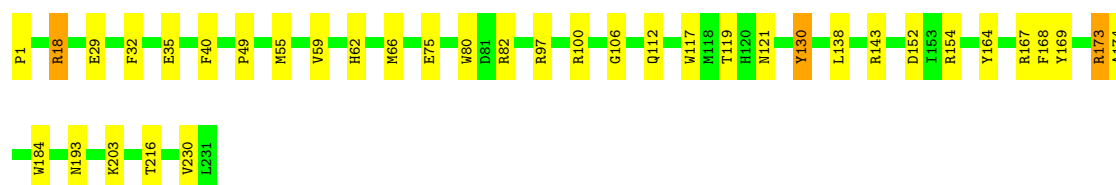
Chain ao:  81% 17%

## • Molecule 1: capsid protein


Chain ap:  83% 15%

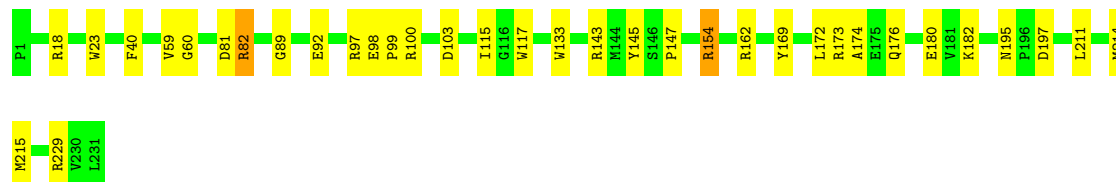
- Molecule 1: capsid protein

Chain aq:  84% 15% .




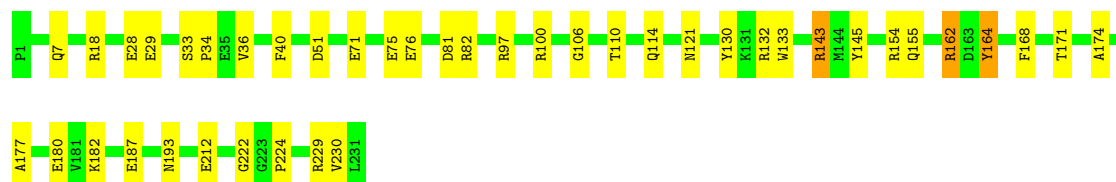
- Molecule 1: capsid protein

Chain ar:  85% 14% .




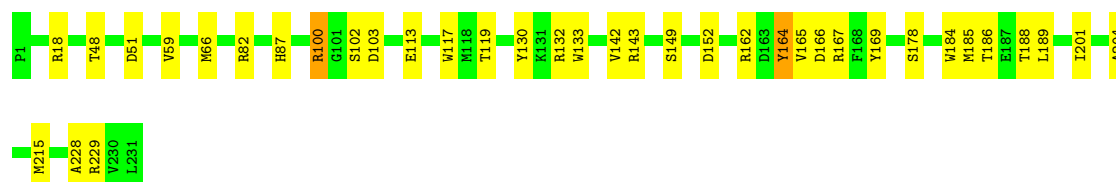
- Molecule 1: capsid protein

Chain as:  82% 17% .




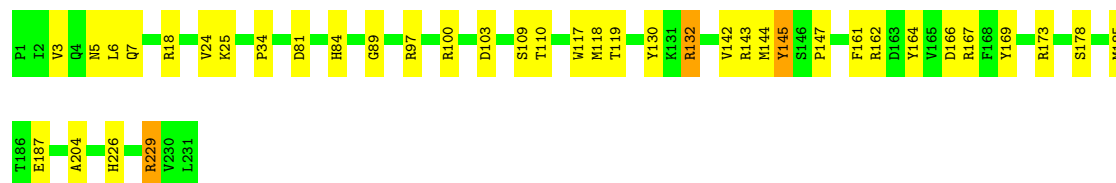
- Molecule 1: capsid protein

Chain at:  84% 15% .

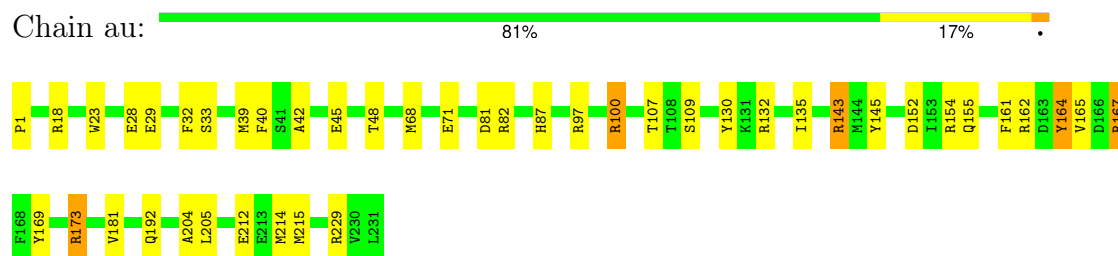


- Molecule 1: capsid protein

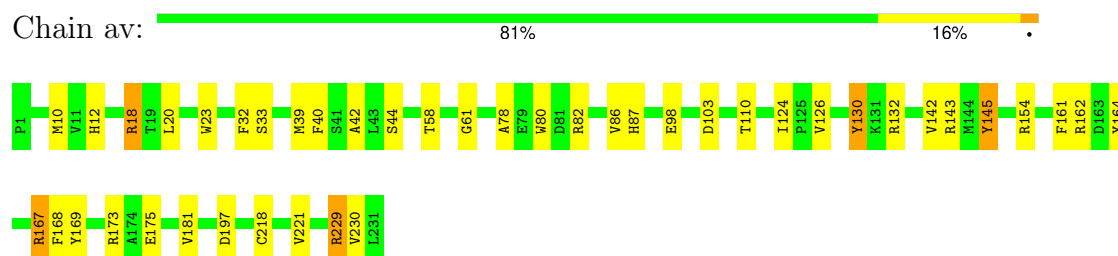
Chain 12:  83% 16% .



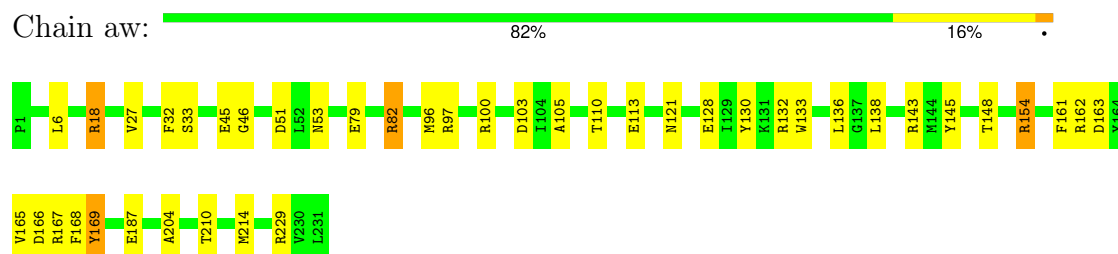
## • Molecule 1: capsid protein



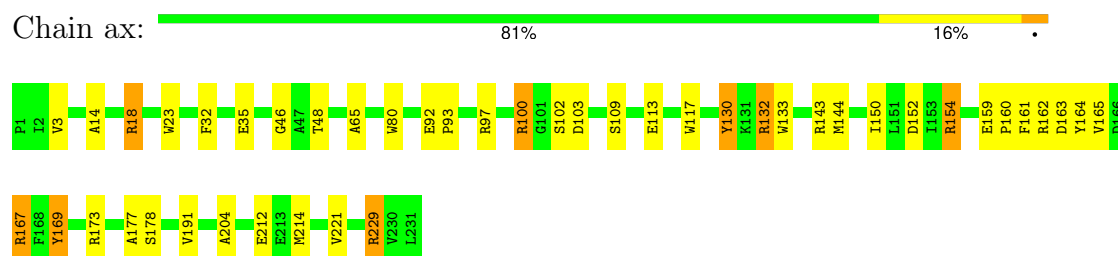
## • Molecule 1: capsid protein



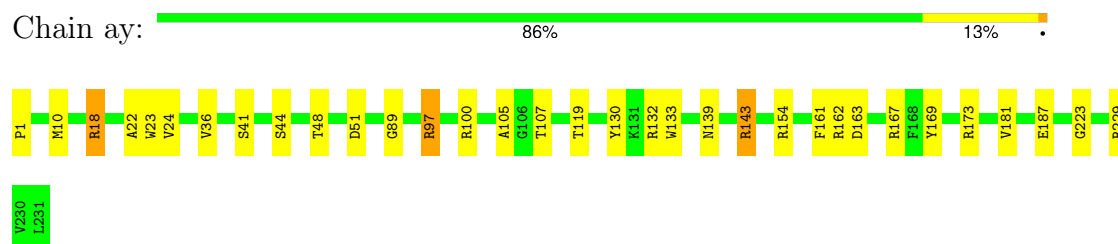
## • Molecule 1: capsid protein




## • Molecule 1: capsid protein



## • Molecule 1: capsid protein




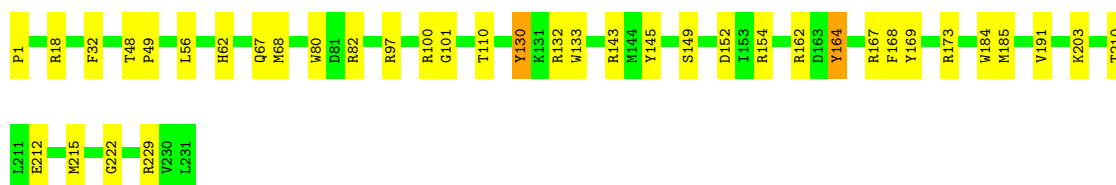
- Molecule 1: capsid protein

Chain az:  82% 16%




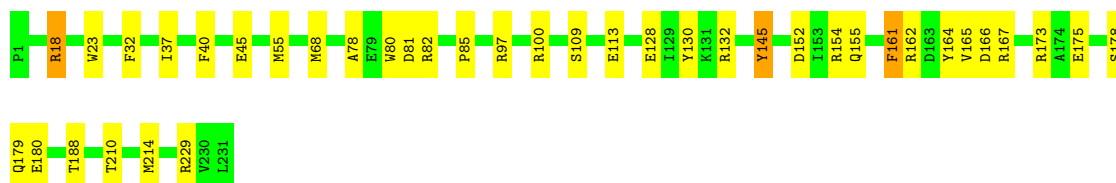
- Molecule 1: capsid protein

Chain aA:  84% 16%




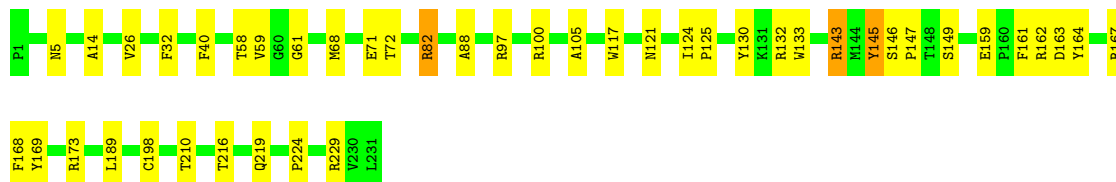
- Molecule 1: capsid protein

Chain aB:  83% 16%




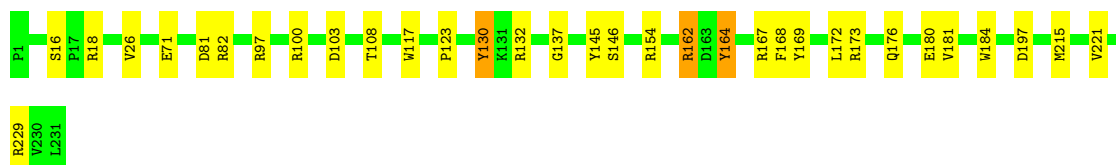
- Molecule 1: capsid protein

Chain aC:  81% 18%

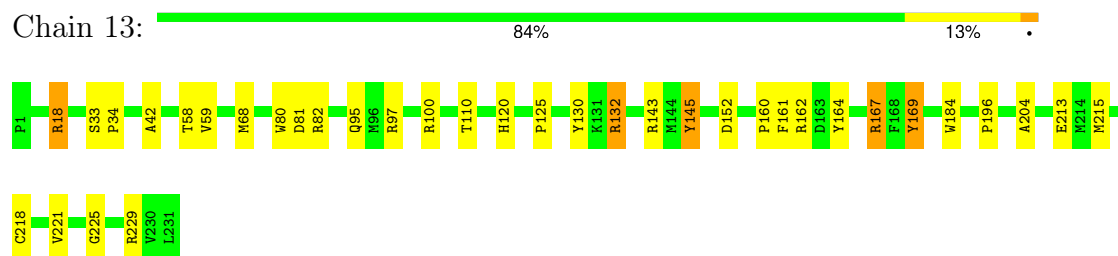


- Molecule 1: capsid protein

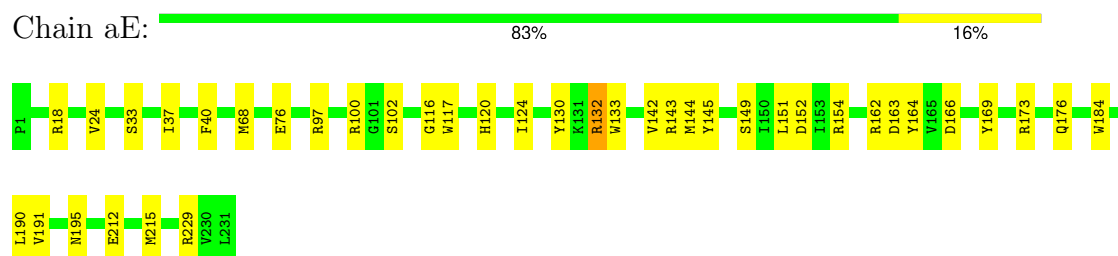
Chain aD:  86% 13%



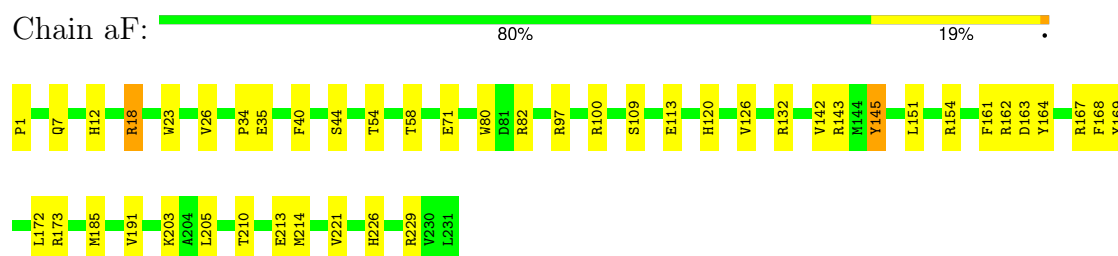
- Molecule 1: capsid protein



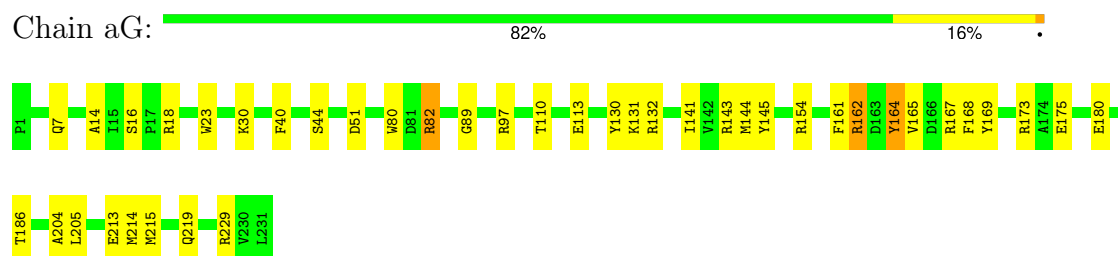
- Molecule 1: capsid protein



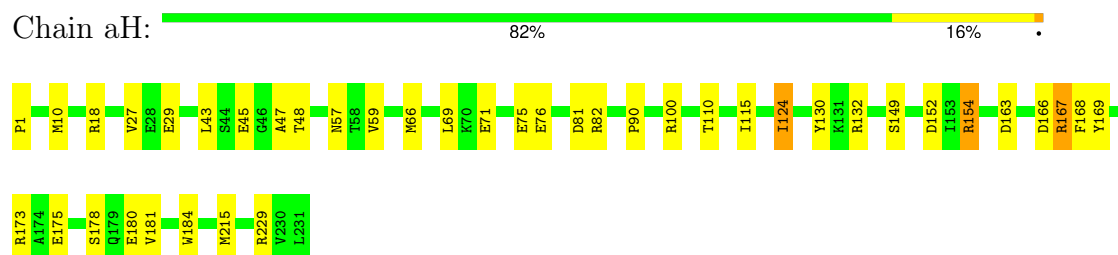
- Molecule 1: capsid protein



- Molecule 1: capsid protein

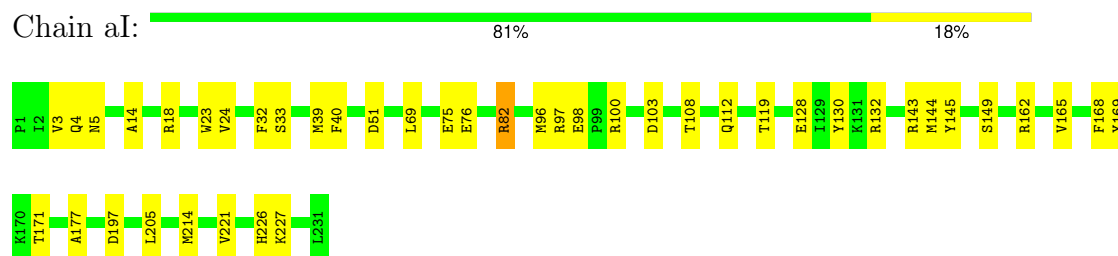


- Molecule 1: capsid protein

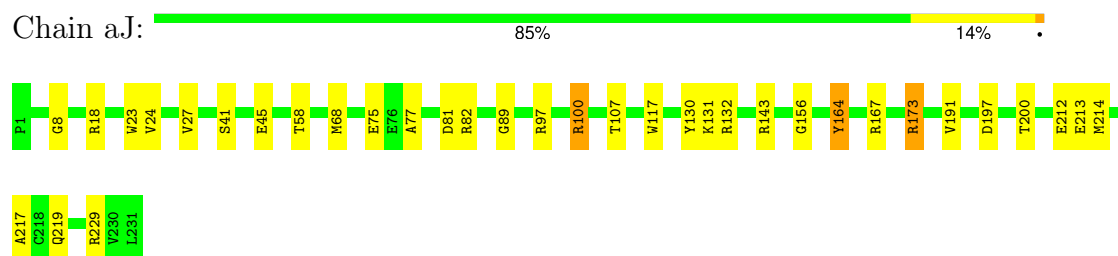




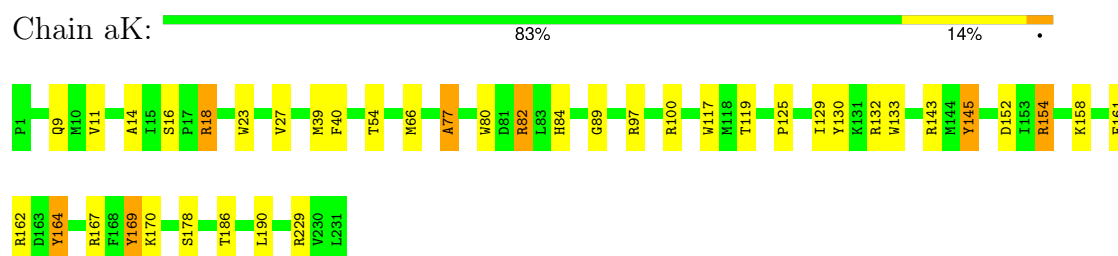
## • Molecule 1: capsid protein



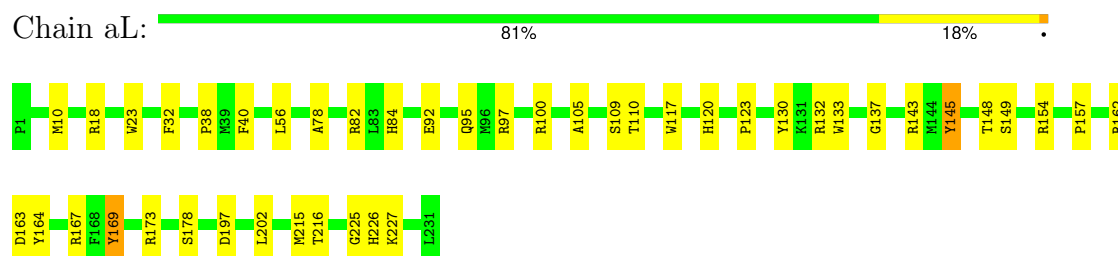
## • Molecule 1: capsid protein



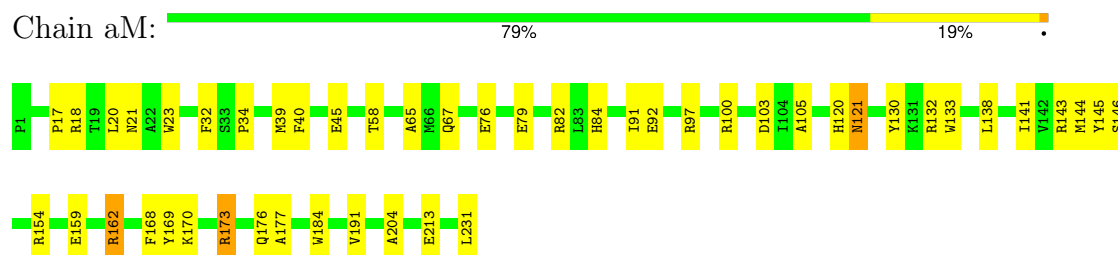
## • Molecule 1: capsid protein




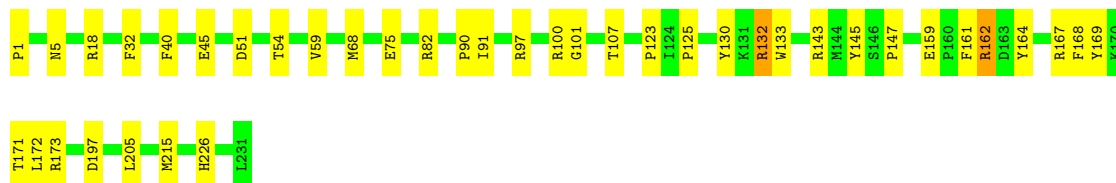
## • Molecule 1: capsid protein




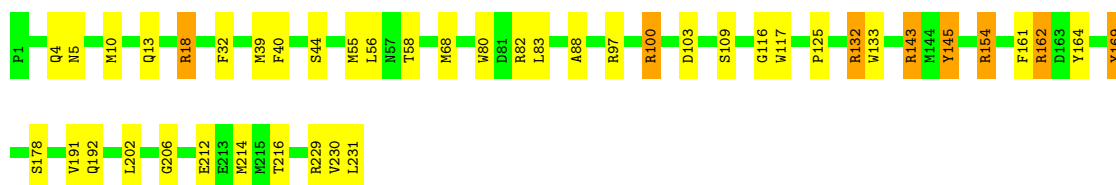
## • Molecule 1: capsid protein




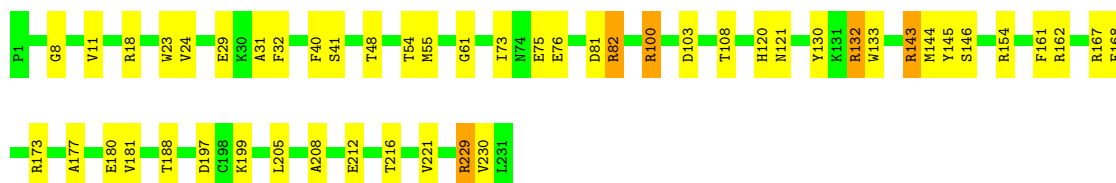
## • Molecule 1: capsid protein

Chain aN:  83% 16%


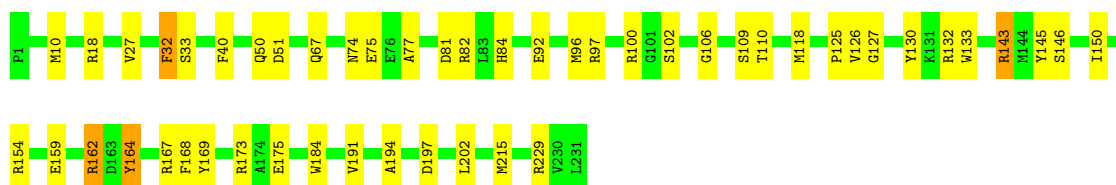
## • Molecule 1: capsid protein

Chain 14:  81% 16%


## • Molecule 1: capsid protein

Chain aO:  78% 19%


## • Molecule 1: capsid protein

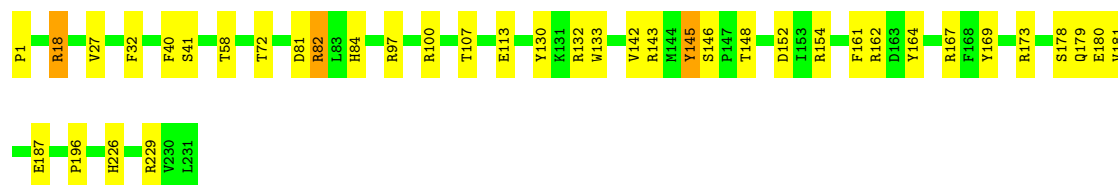
Chain aP:  78% 20%

## • Molecule 1: capsid protein


Chain aQ:  82% 17%

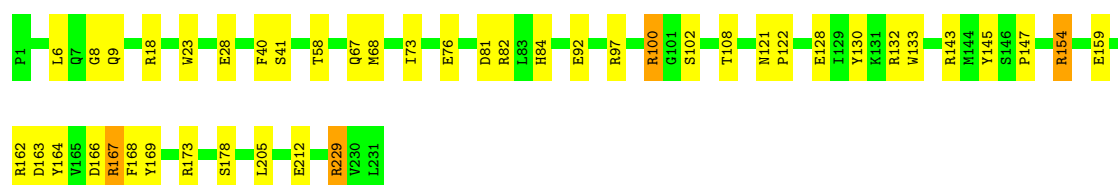
- Molecule 1: capsid protein

Chain aR:  83% 16%




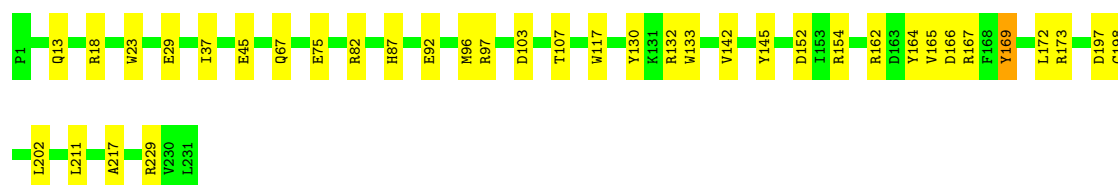
- Molecule 1: capsid protein

Chain aS:  81% 17%




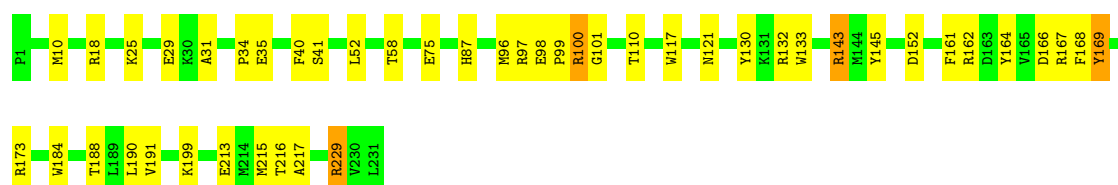
- Molecule 1: capsid protein

Chain aT:  84% 16%




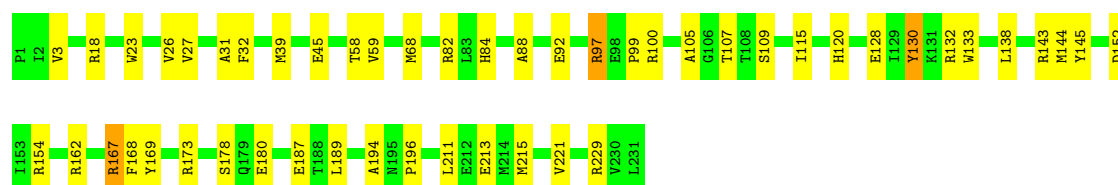
- Molecule 1: capsid protein

Chain aU:  80% 18%

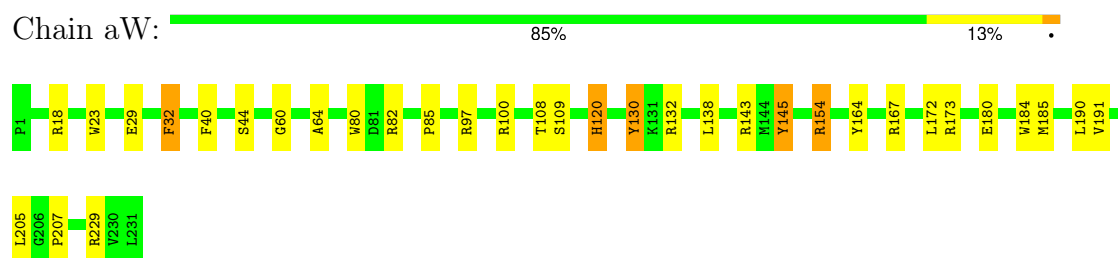


- Molecule 1: capsid protein

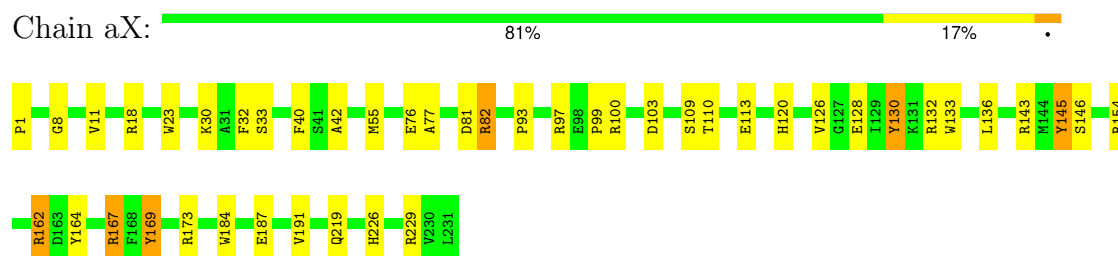
Chain aV:  78% 20%



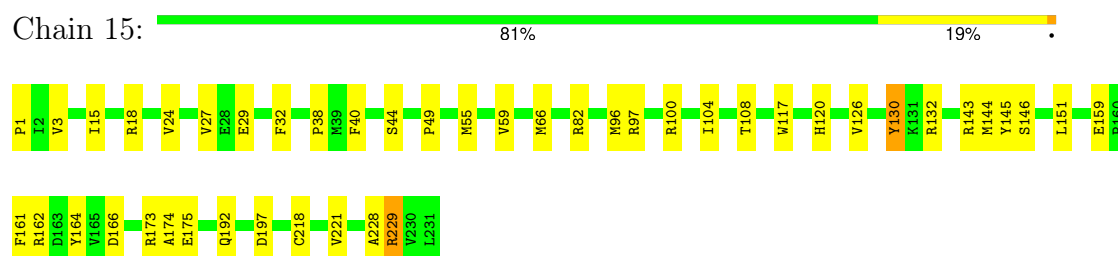
- Molecule 1: capsid protein



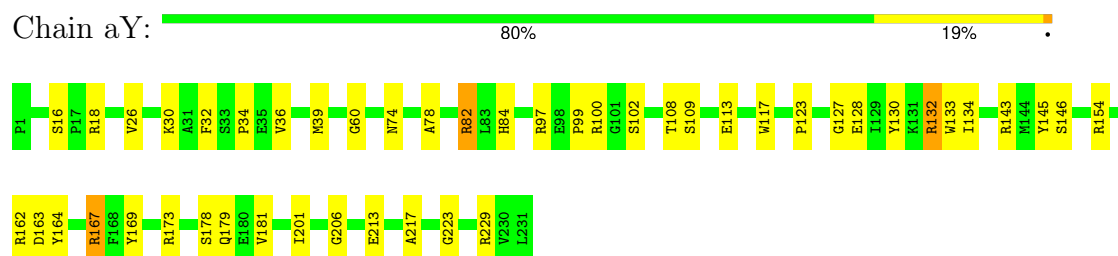
- Molecule 1: capsid protein



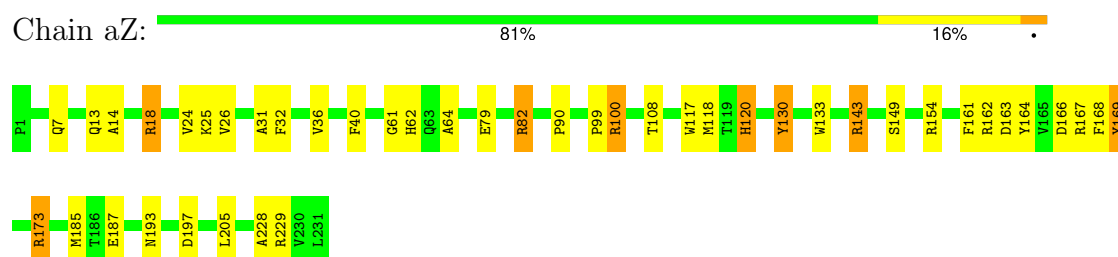
- Molecule 1: capsid protein



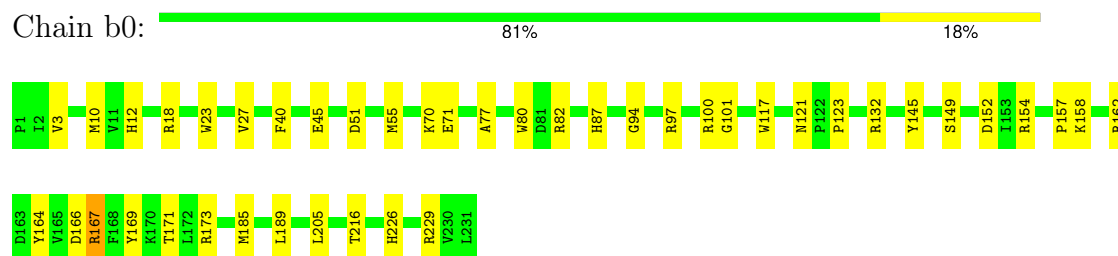
- Molecule 1: capsid protein



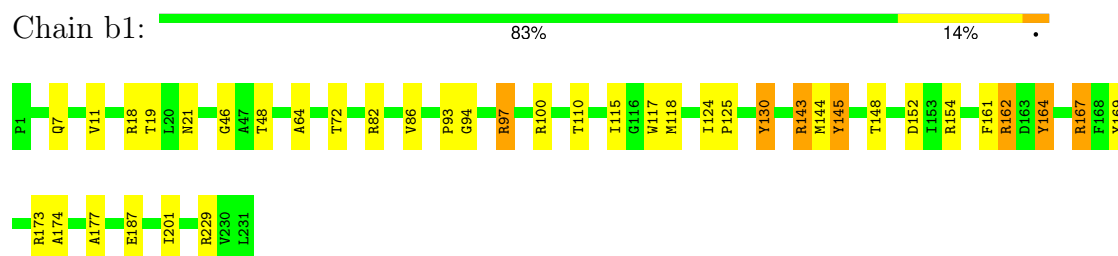
- Molecule 1: capsid protein



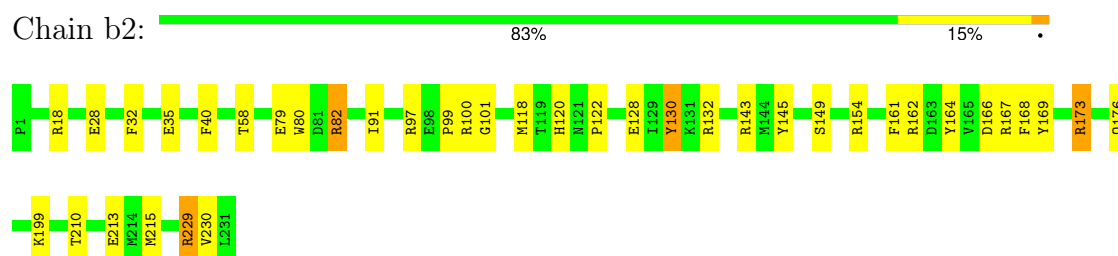
## • Molecule 1: capsid protein



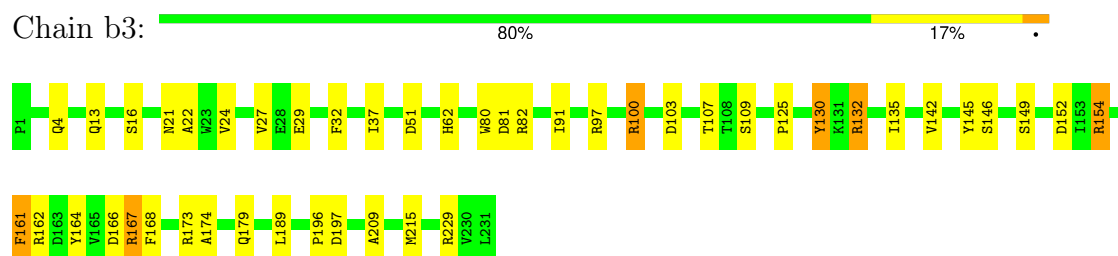
## • Molecule 1: capsid protein



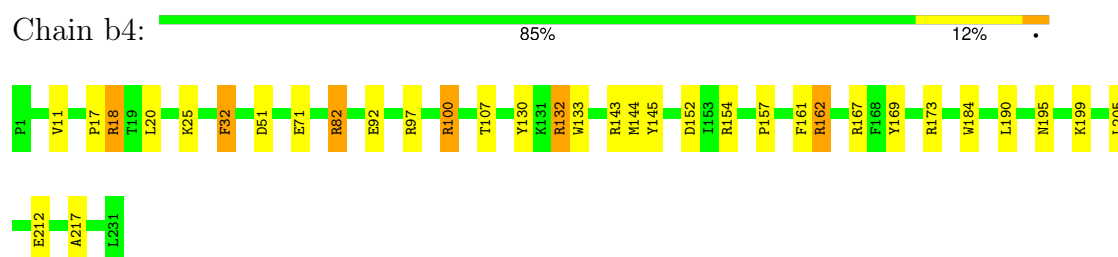
## • Molecule 1: capsid protein



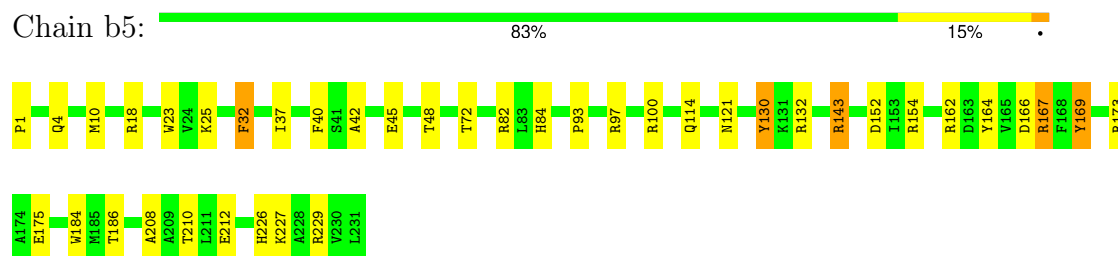
## • Molecule 1: capsid protein



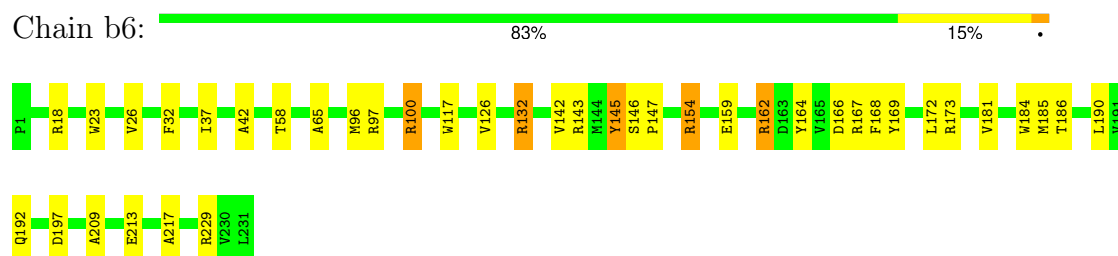
## • Molecule 1: capsid protein



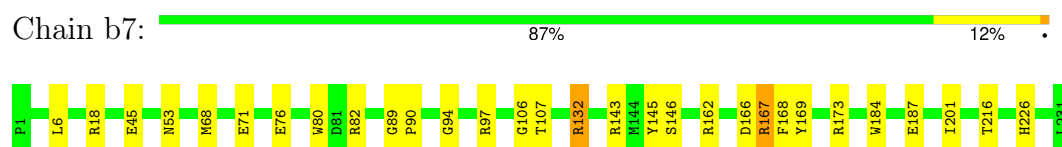
## • Molecule 1: capsid protein



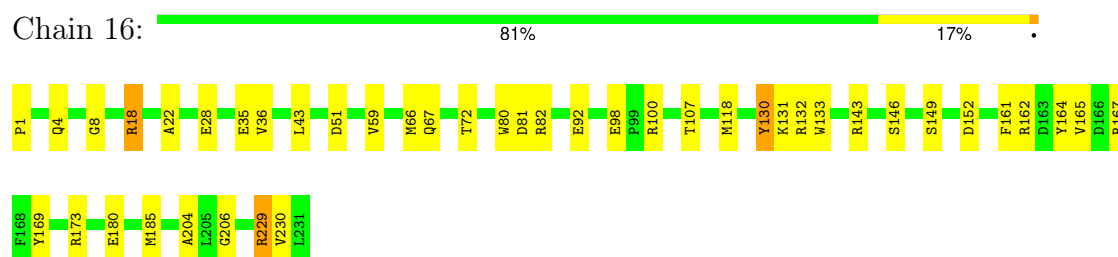
## • Molecule 1: capsid protein



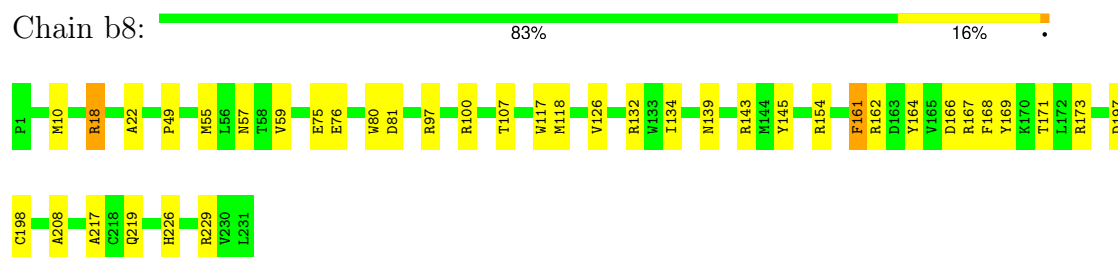
## • Molecule 1: capsid protein




## • Molecule 1: capsid protein

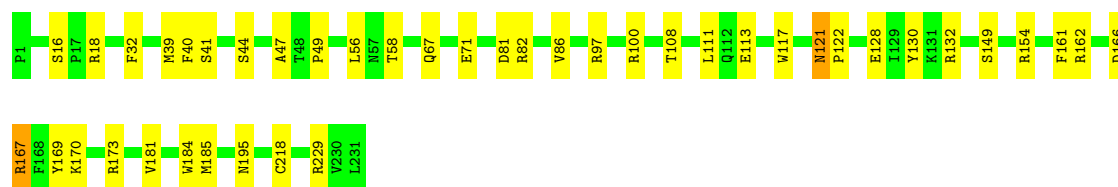


## • Molecule 1: capsid protein




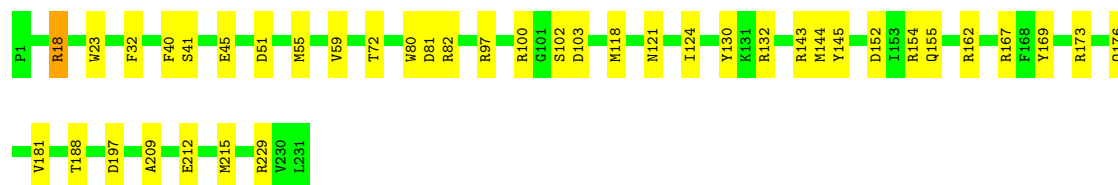
## • Molecule 1: capsid protein

Chain b9:  82% 17%




- Molecule 1: capsid protein

Chain ba:  83% 17%




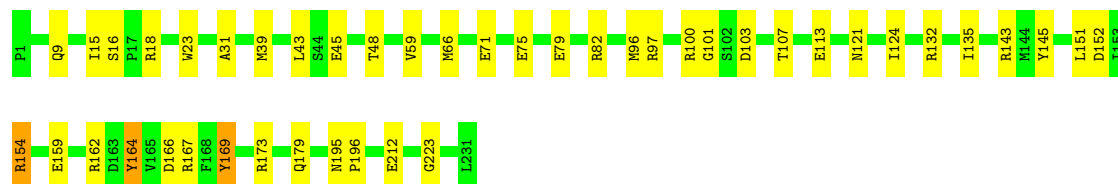
- Molecule 1: capsid protein

Chain bb:  81% 16%




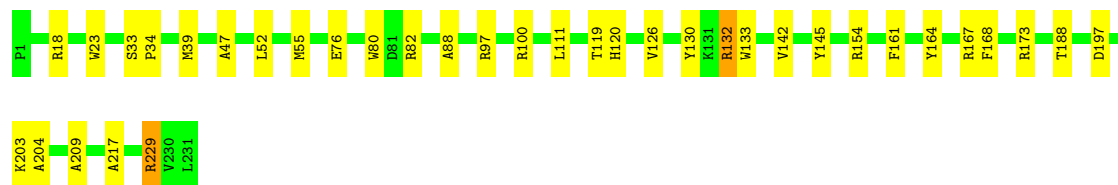
- Molecule 1: capsid protein

Chain bc:  81% 18%




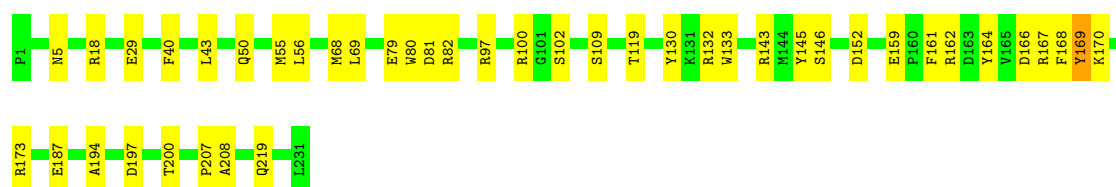
- Molecule 1: capsid protein

Chain bd:  84% 15%




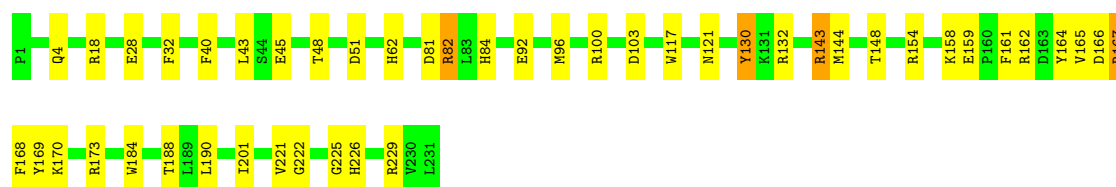
- Molecule 1: capsid protein

Chain be:  81% 18%




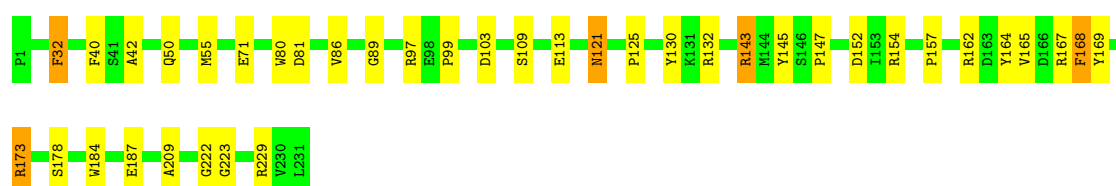
- Molecule 1: capsid protein

Chain bf:  80% 18%




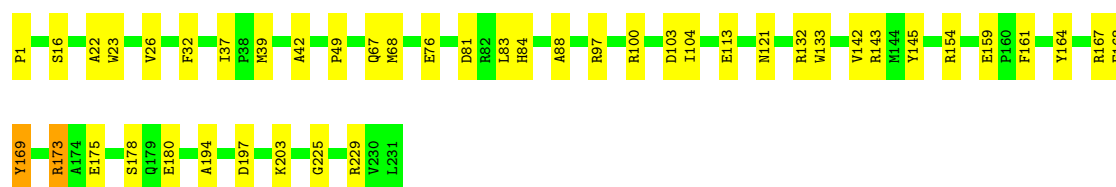
- Molecule 1: capsid protein

Chain bg:  83% 15%



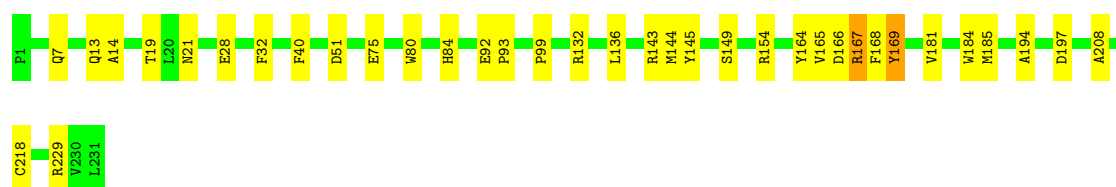
- Molecule 1: capsid protein

Chain bh:  81% 18%




- Molecule 1: capsid protein

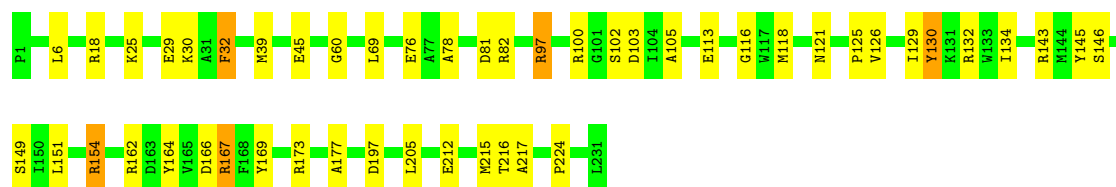
Chain 17:  84% 15%




- Molecule 1: capsid protein



Chain bi:  79% 19%




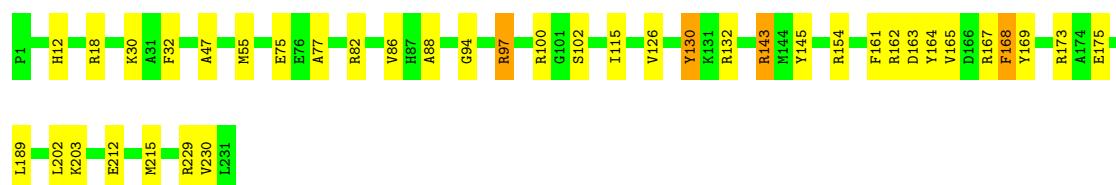
- Molecule 1: capsid protein

Chain bj:  86% 13%



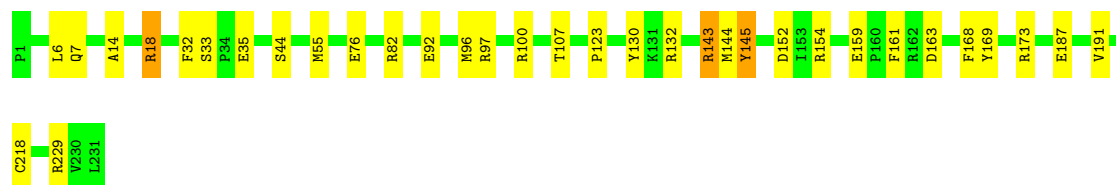
- Molecule 1: capsid protein

Chain bk:  83% 15%



- Molecule 1: capsid protein

Chain bl:  85% 13%




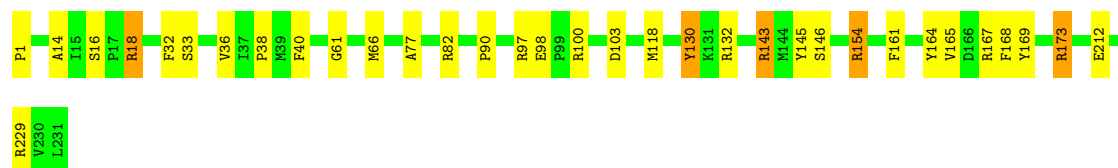
- Molecule 1: capsid protein

Chain bm:  83% 15%



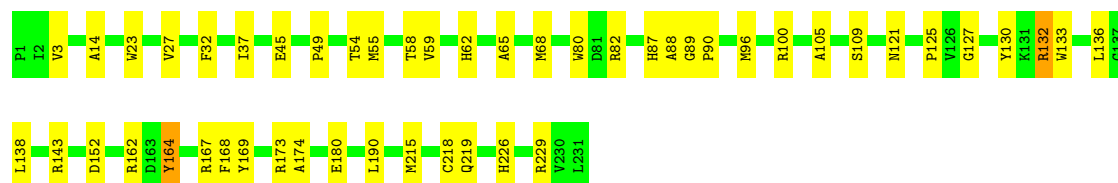
- Molecule 1: capsid protein

Chain bn:  85% 13%



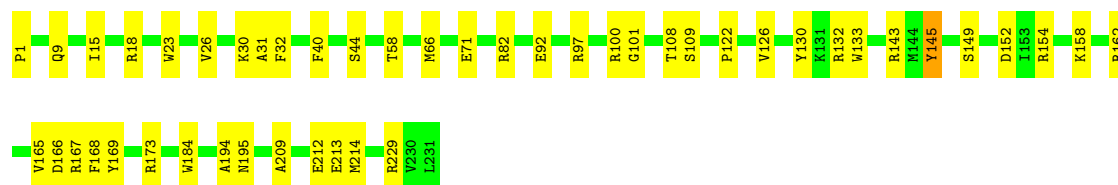
- Molecule 1: capsid protein

Chain bo: 79% 20%



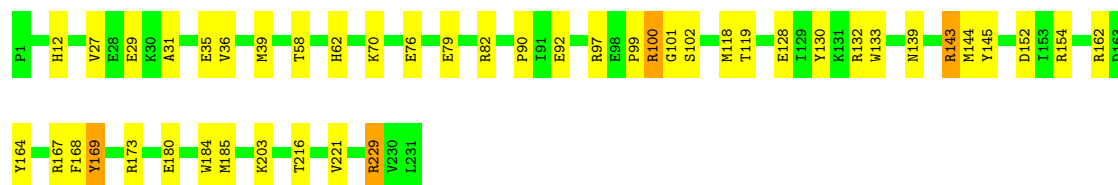
- Molecule 1: capsid protein

Chain bp: 80% 20%



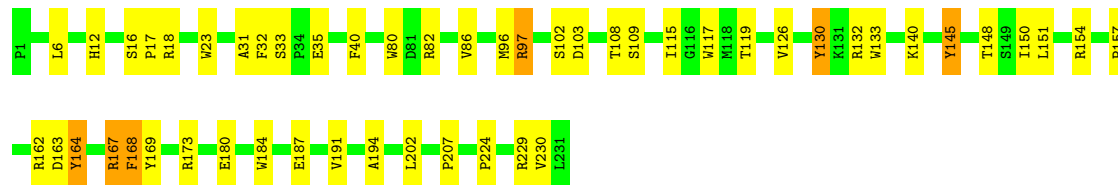
- Molecule 1: capsid protein

Chain bq: 81% 18%



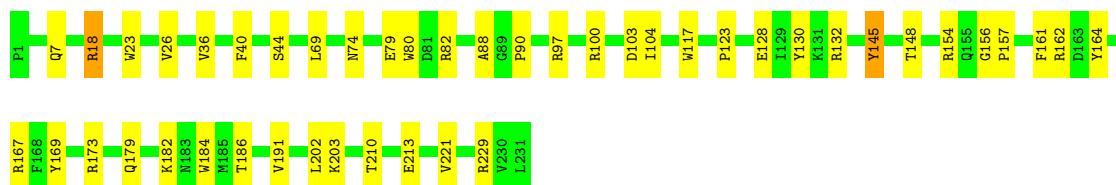
- Molecule 1: capsid protein

Chain br: 78% 19%




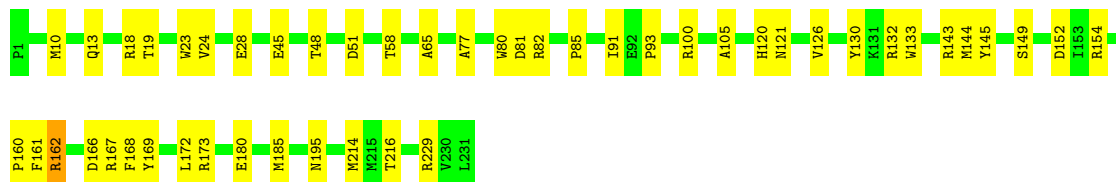
- Molecule 1: capsid protein

Chain 18: 81% 19%




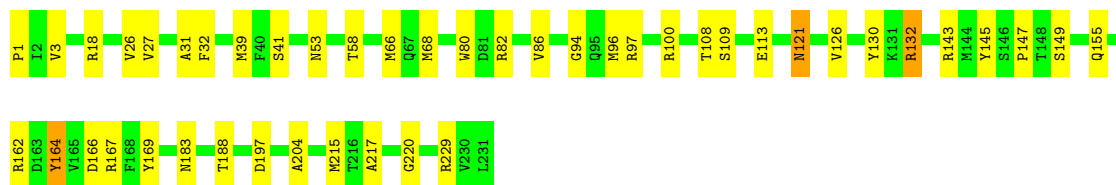
- Molecule 1: capsid protein

Chain bs:  79% 20%




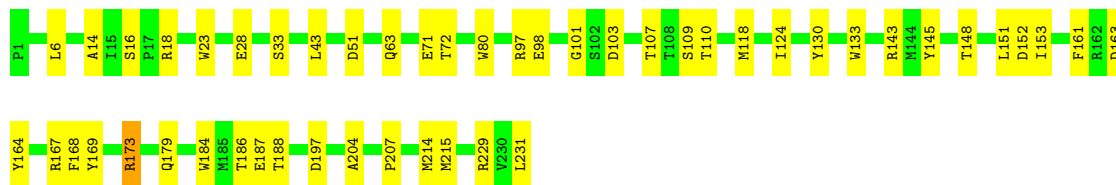
- Molecule 1: capsid protein

Chain bt:  81% 18%




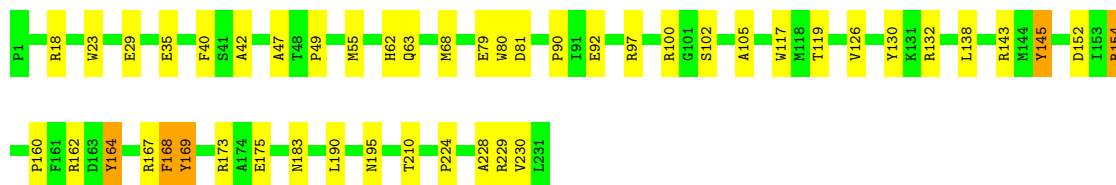
- Molecule 1: capsid protein

Chain bu:  79% 21%




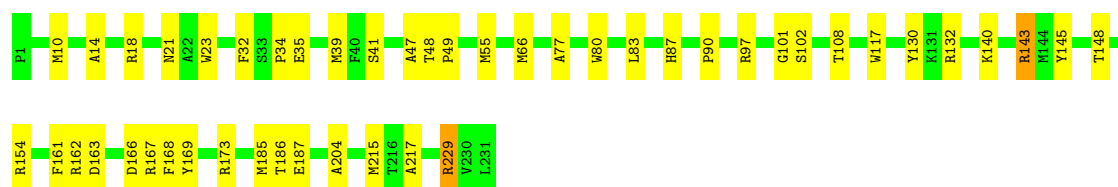
- Molecule 1: capsid protein

Chain bv:  80% 18%

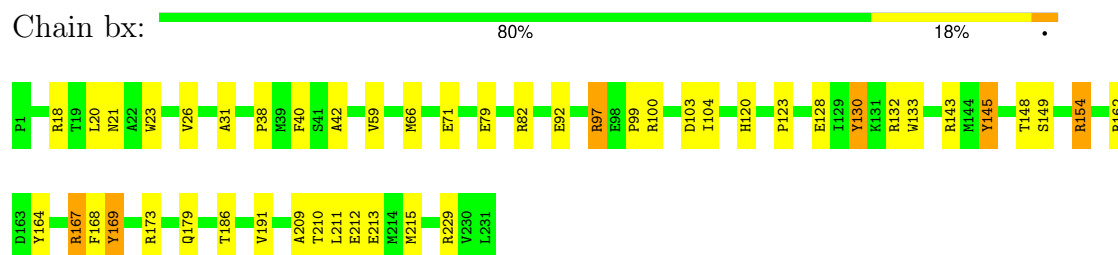


- Molecule 1: capsid protein

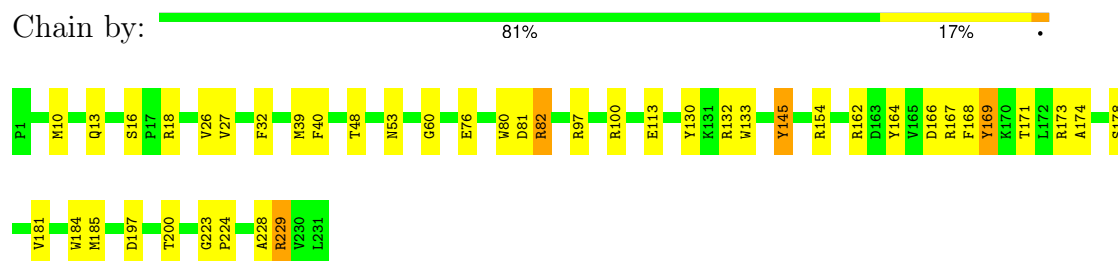
Chain bw:  80% 19%



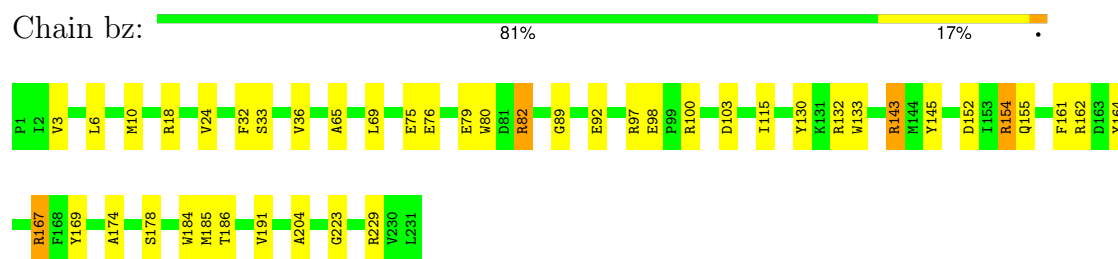
- Molecule 1: capsid protein



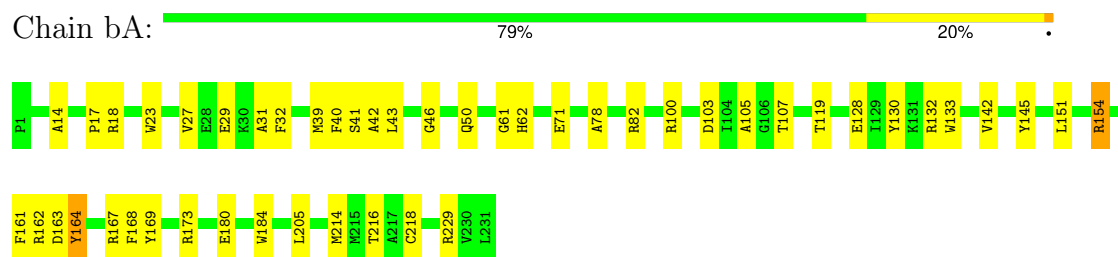
- Molecule 1: capsid protein



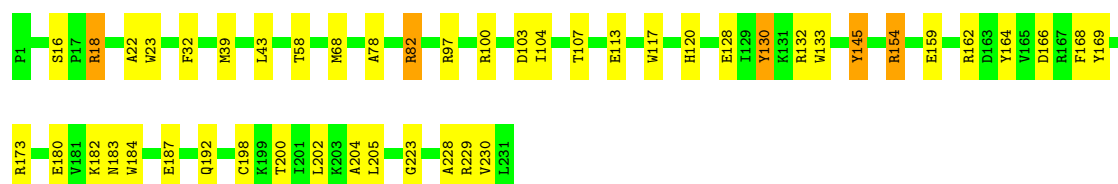
- Molecule 1: capsid protein



- Molecule 1: capsid protein



- Molecule 1: capsid protein



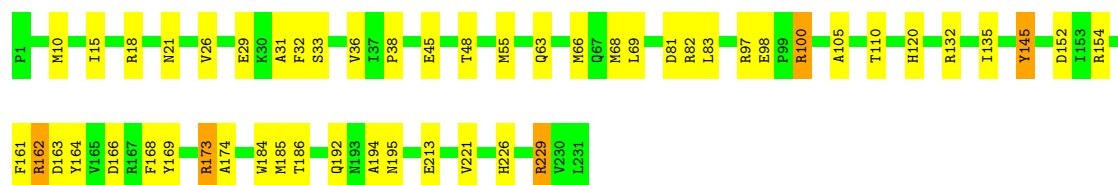
- Molecule 1: capsid protein

Chain 19: 81% 19%



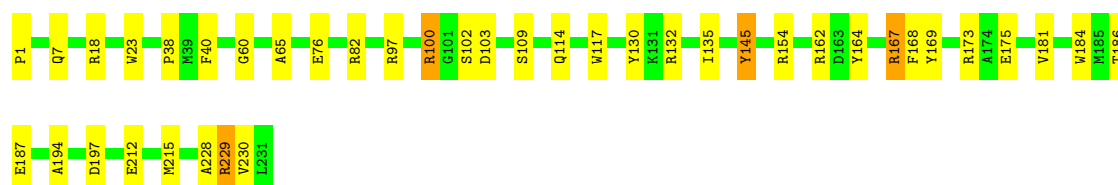
- Molecule 1: capsid protein

Chain bC: 78% 20%



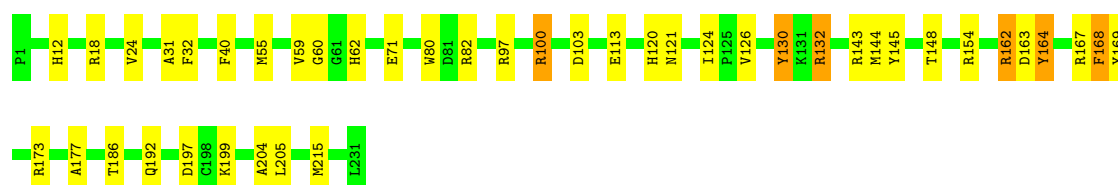
- Molecule 1: capsid protein

Chain bD: 83% 16%



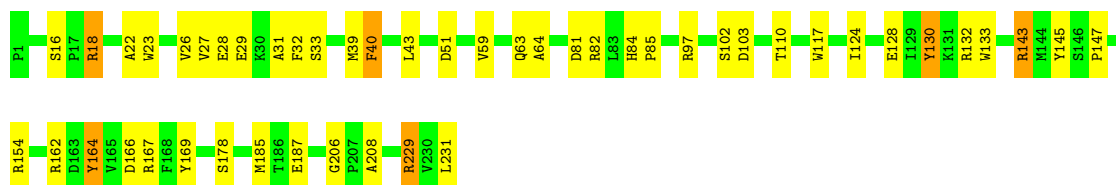
- Molecule 1: capsid protein

Chain bE: 81% 16%



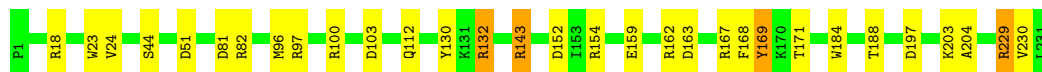
- Molecule 1: capsid protein

Chain bF: 79% 18%



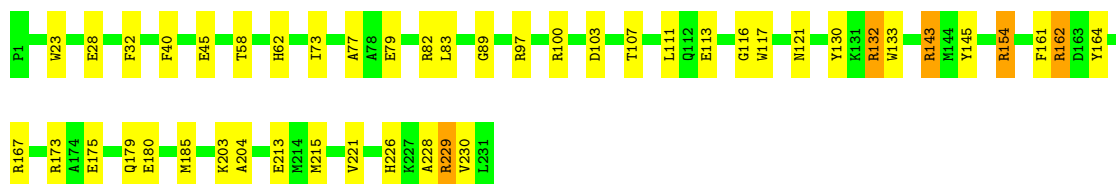
- Molecule 1: capsid protein

Chain bG: 87% 12%



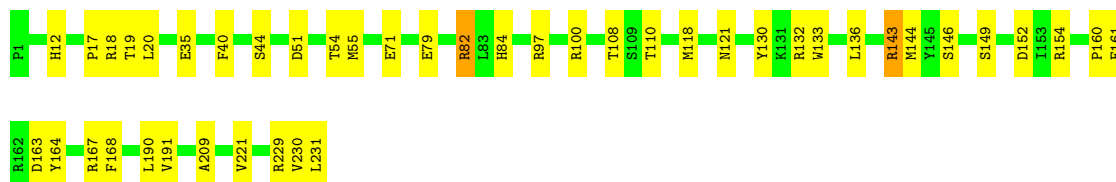
- Molecule 1: capsid protein

Chain bH: 80% 18%



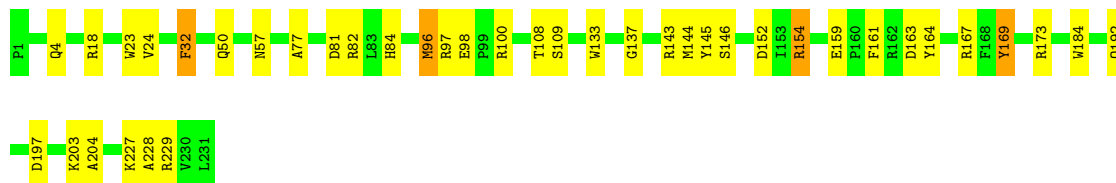
- Molecule 1: capsid protein

Chain bI: 81% 18%



- Molecule 1: capsid protein

Chain bJ: 83% 16%



- Molecule 1: capsid protein

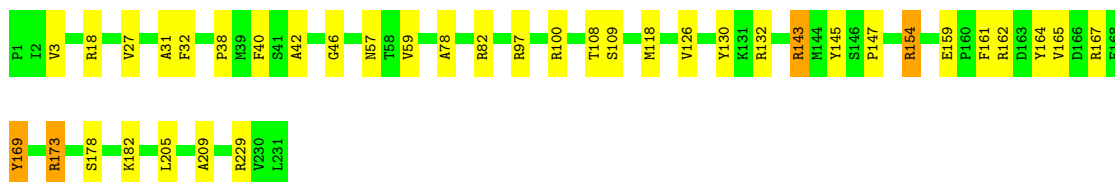
Chain bK: 79% 19%





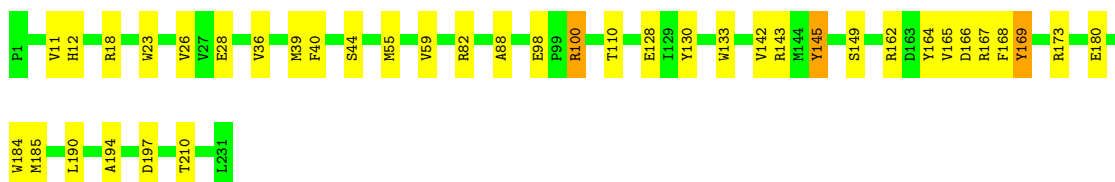
- Molecule 1: capsid protein

Chain bL: 84% 15% •



- Molecule 1: capsid protein

Chain 1a: 83% 16% •



- Molecule 1: capsid protein

Chain bM: 83% 16% •



- Molecule 1: capsid protein

Chain bN: 83% 15% •



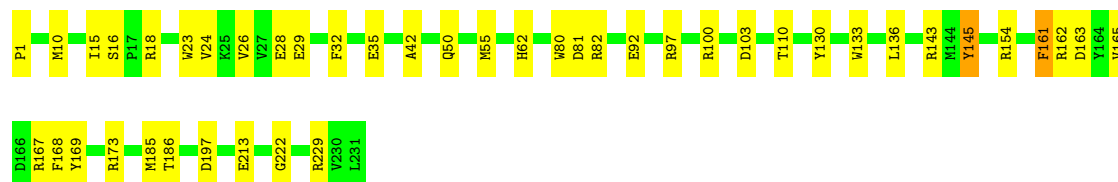
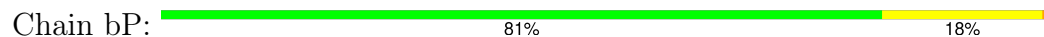
- Molecule 1: capsid protein

Chain bO: 79% 21% •

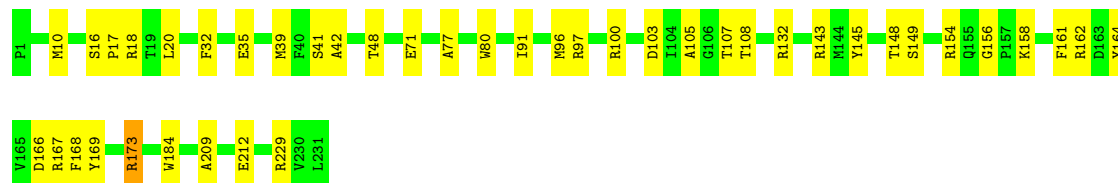
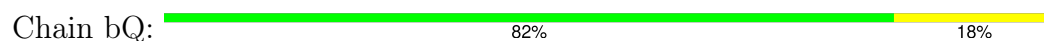




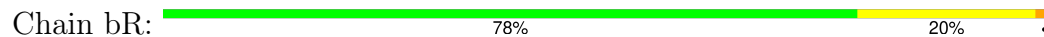
- Molecule 1: capsid protein



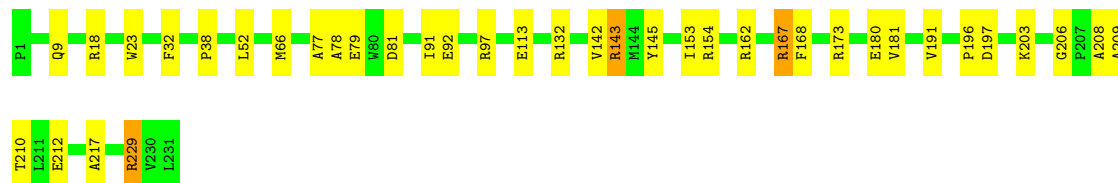
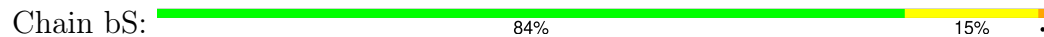
- Molecule 1: capsid protein



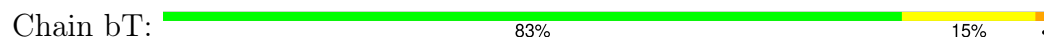
- Molecule 1: capsid protein



- Molecule 1: capsid protein



- Molecule 1: capsid protein







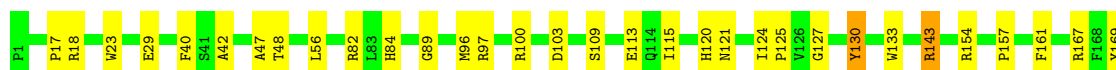
- Molecule 1: capsid protein

Chain bU: 82% 17% •



- Molecule 1: capsid protein

Chain bV: 82% 17% •



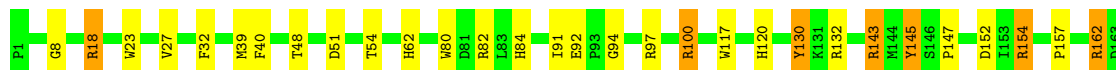
- Molecule 1: capsid protein

Chain 1b: 84% 15% •



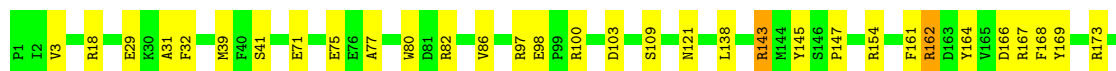
- Molecule 1: capsid protein

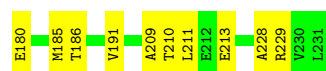
Chain bW: 80% 17% •



- Molecule 1: capsid protein

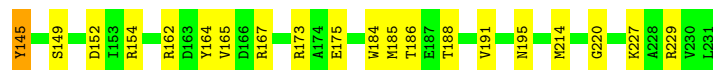
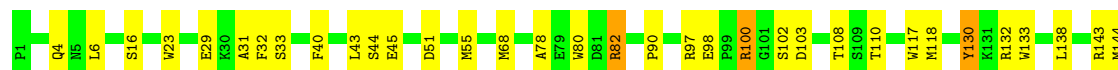
Chain bX: 82% 17% •





- Molecule 1: capsid protein

Chain bY: 77% 22%



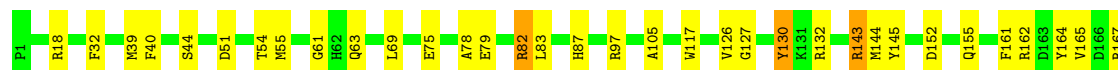
- Molecule 1: capsid protein

Chain bZ: 80% 18%



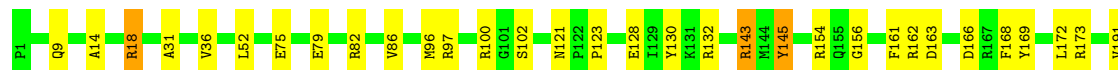
- Molecule 1: capsid protein

Chain c0: 82% 16%



- Molecule 1: capsid protein

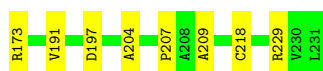
Chain c1: 83% 16%



- Molecule 1: capsid protein

Chain c2: 82% 16%





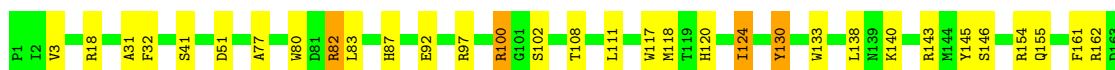
- Molecule 1: capsid protein

Chain c3: 81% 18% •



- Molecule 1: capsid protein

Chain c4: 79% 19% •



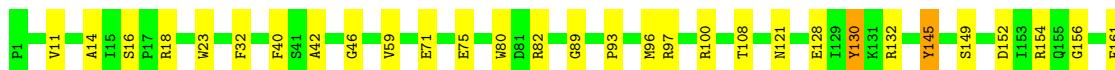
- Molecule 1: capsid protein

Chain c5: 81% 17% •



- Molecule 1: capsid protein

Chain 1c: 81% 17% •




- Molecule 1: capsid protein

Chain c6: 86% 14%






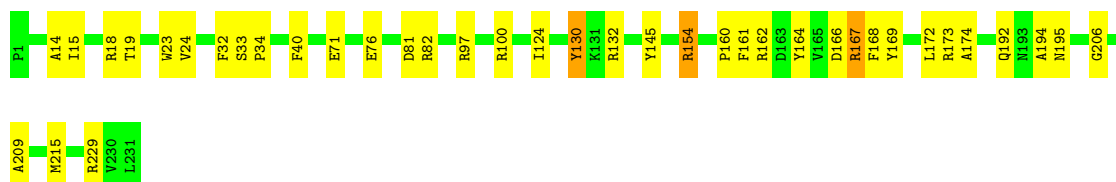
- Molecule 1: capsid protein

Chain c7:  82% 17%




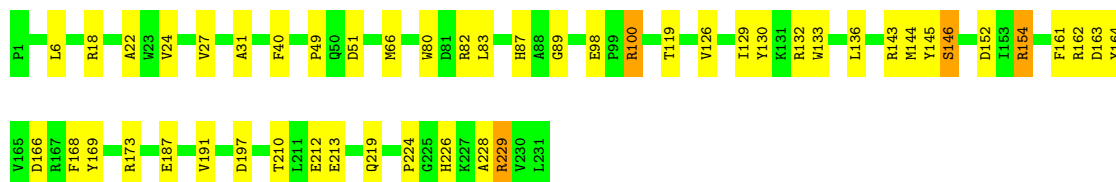
- Molecule 1: capsid protein

Chain c8:  83% 16%




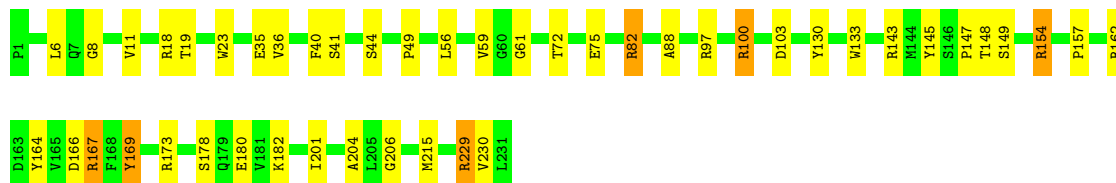
- Molecule 1: capsid protein

Chain c9:  79% 19%




- Molecule 1: capsid protein

Chain ca:  80% 17%



- Molecule 1: capsid protein

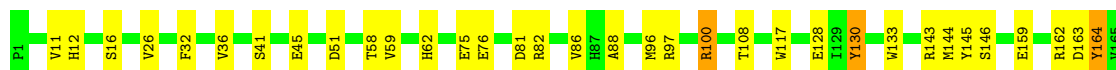
Chain cb:  81% 18%





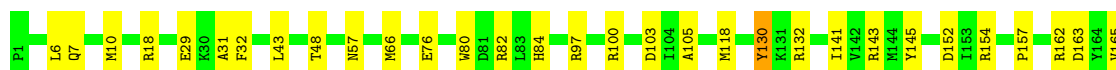
- Molecule 1: capsid protein

Chain cc: 80% 18% •



- Molecule 1: capsid protein

Chain cd: 81% 18%



- Molecule 1: capsid protein

Chain ce: 82% 17%



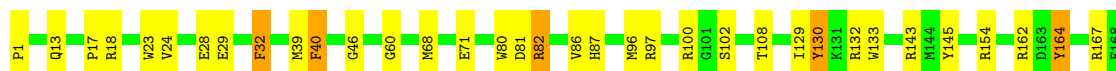
- Molecule 1: capsid protein

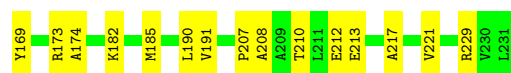
Chain cf: 79% 20% •



- Molecule 1: capsid protein

Chain 1d: 78% 19% •





- Molecule 1: capsid protein

Chain cg: 85% 12% .



- Molecule 1: capsid protein

Chain ch: 84% 15% .



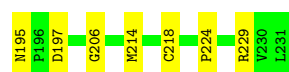
- Molecule 1: capsid protein

Chain ci: 79% 19% .



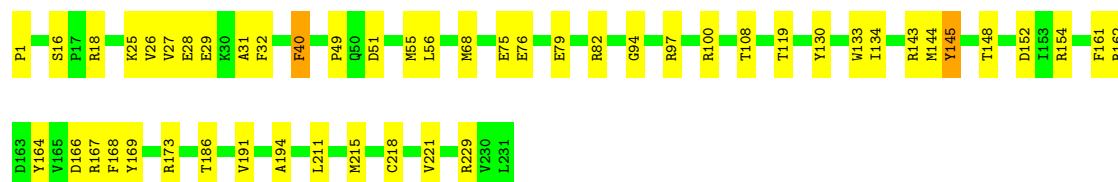
- Molecule 1: capsid protein

Chain cj: 83% 16% .



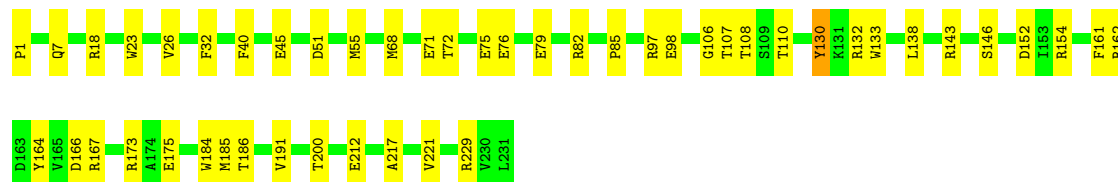
- Molecule 1: capsid protein

Chain ck: 78% 21% .



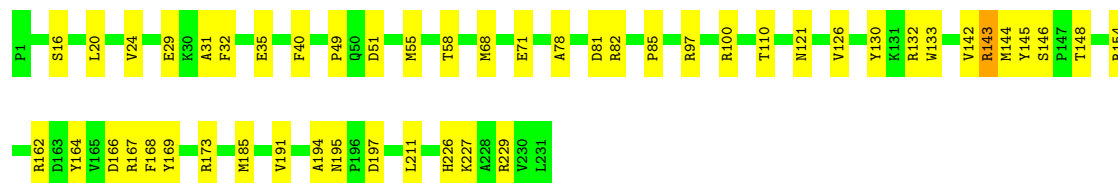
- Molecule 1: capsid protein

Chain cl: 79% 20%



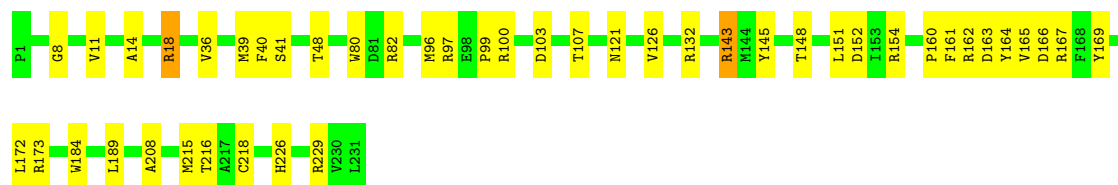
- Molecule 1: capsid protein

Chain cm: 79% 21%



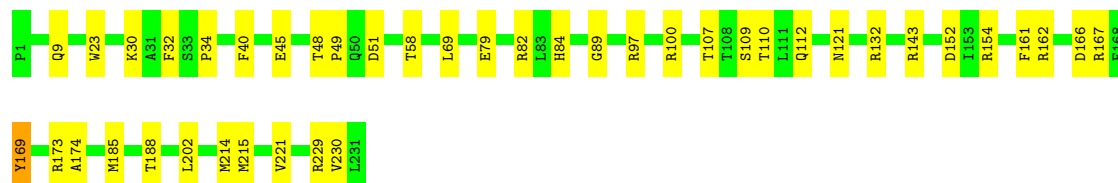
- Molecule 1: capsid protein

Chain cn: 81% 19%



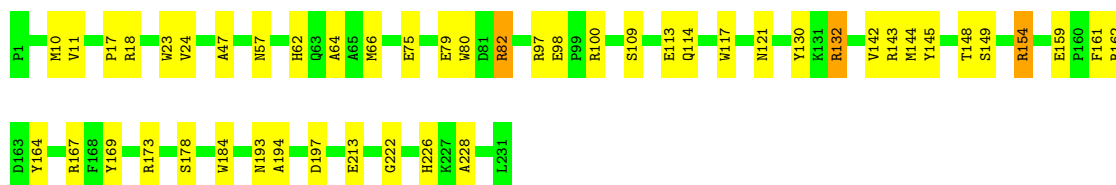
- Molecule 1: capsid protein

Chain co: 82% 18%



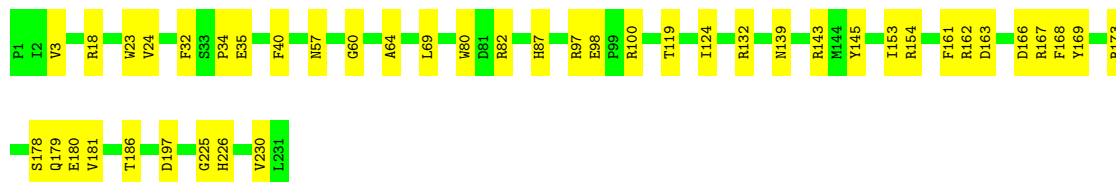
- Molecule 1: capsid protein

Chain cp: 79% 19%



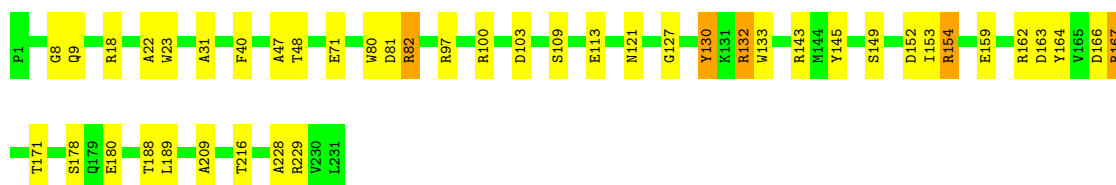
- Molecule 1: capsid protein

Chain 1e: 81% 19%



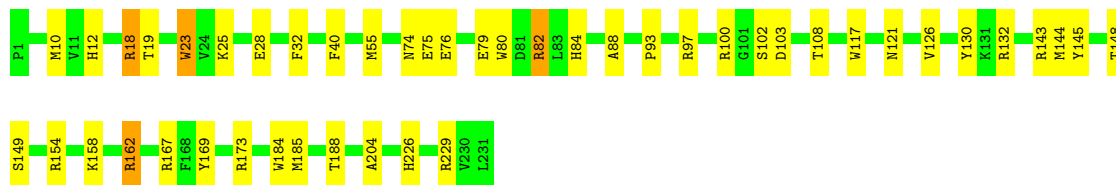
- Molecule 1: capsid protein

Chain cq: 81% 17%



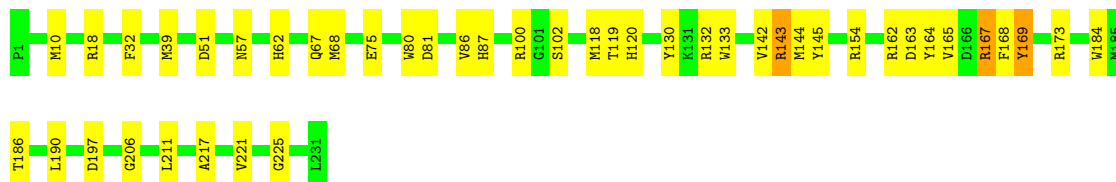
- Molecule 1: capsid protein

Chain cr: 80% 18%



- Molecule 1: capsid protein

Chain cs: 81% 18%

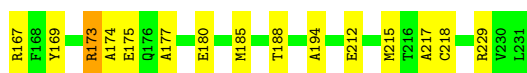


- Molecule 1: capsid protein

Chain ct: 80% 18%

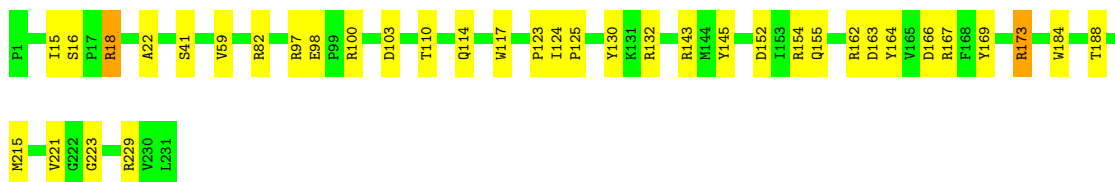






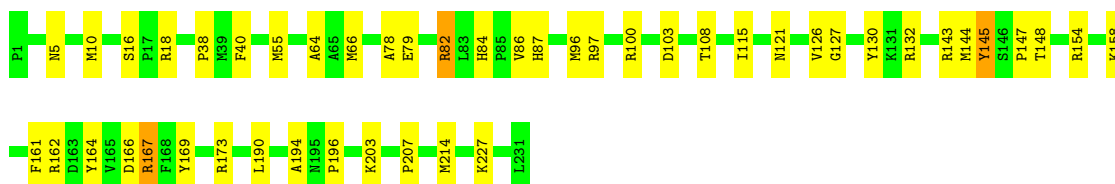
- Molecule 1: capsid protein

Chain cz: 84% 15%



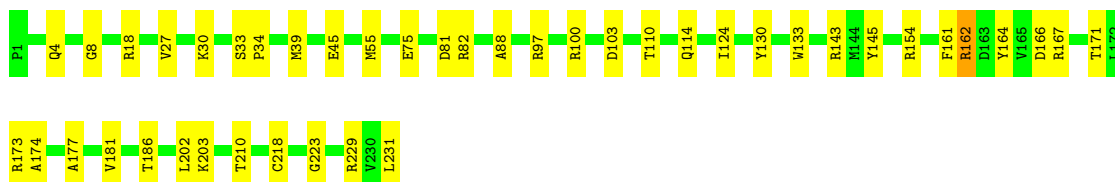
- Molecule 1: capsid protein

Chain 1f: 80% 19%



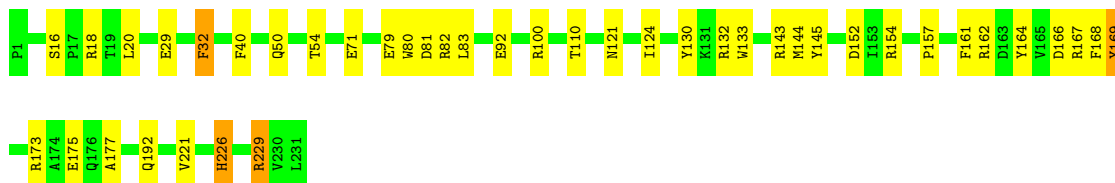
- Molecule 1: capsid protein

Chain cA: 81% 18%



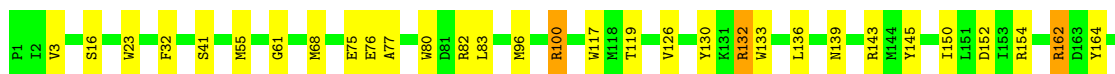
- Molecule 1: capsid protein

Chain cB: 82% 16%



- Molecule 1: capsid protein

Chain cC: 82% 17%





- Molecule 1: capsid protein

Chain cD: 77% 23%



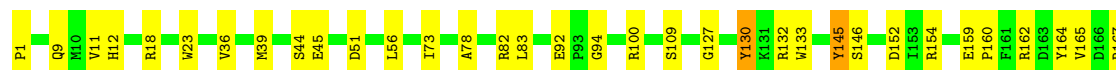
- Molecule 1: capsid protein

Chain cE: 82% 16%



- Molecule 1: capsid protein

Chain cF: 81% 18%



- Molecule 1: capsid protein

Chain cG: 79% 20%




- Molecule 1: capsid protein

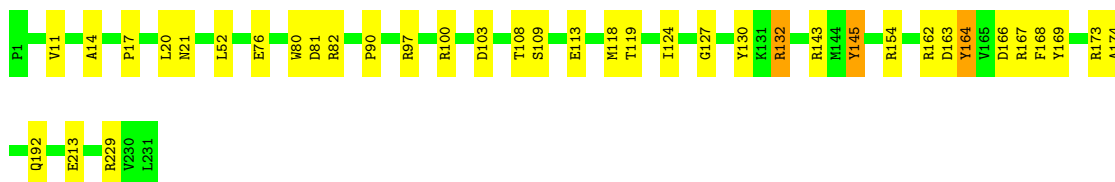
Chain cH: 78% 21%






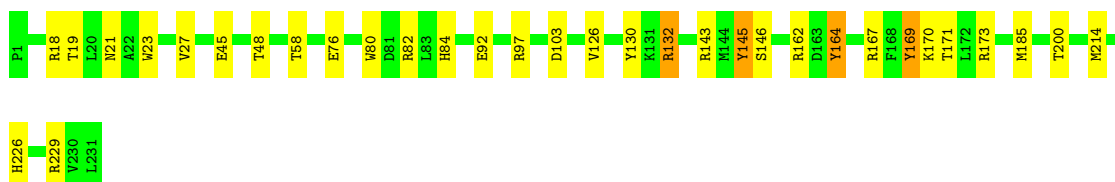
- Molecule 1: capsid protein

Chain cI:  84% 15% •




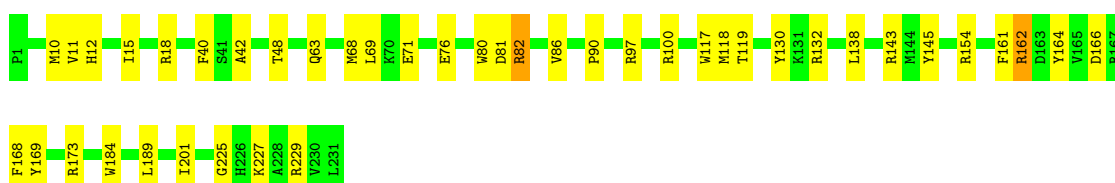
- Molecule 1: capsid protein

Chain cJ:  86% 13% •




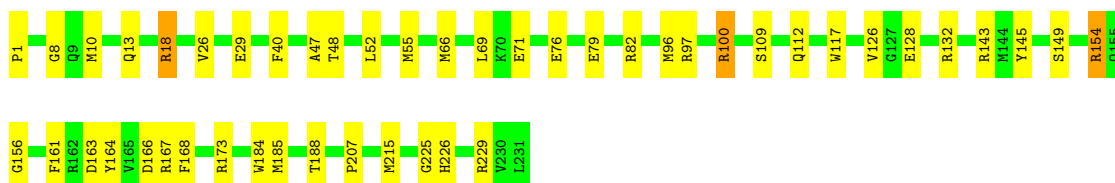
- Molecule 1: capsid protein

Chain 1g:  82% 17% •




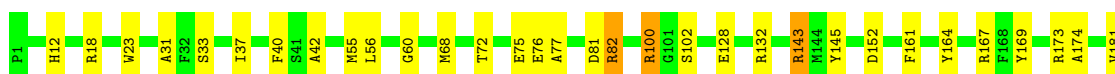
- Molecule 1: capsid protein

Chain cK:  80% 19% •




- Molecule 1: capsid protein

Chain cL:  84% 15% •






- Molecule 1: capsid protein

Chain cM:  82% 17%




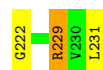
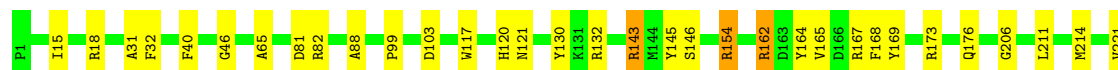
- Molecule 1: capsid protein

Chain cN:  82% 17%




- Molecule 1: capsid protein

Chain cO:  84% 14%




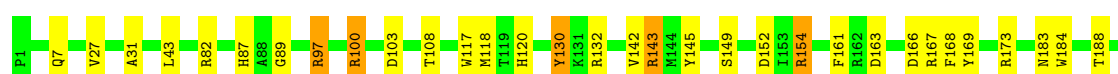
- Molecule 1: capsid protein

Chain cP:  84% 16%



- Molecule 1: capsid protein

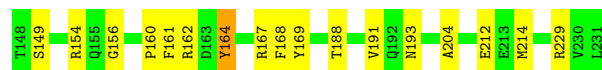
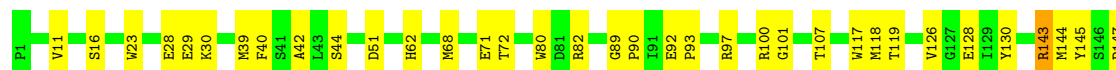
Chain cQ:  84% 14%





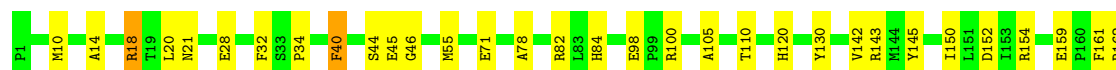
- Molecule 1: capsid protein

Chain cR: 77% 22%



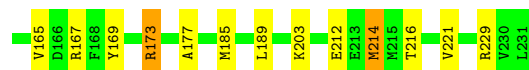
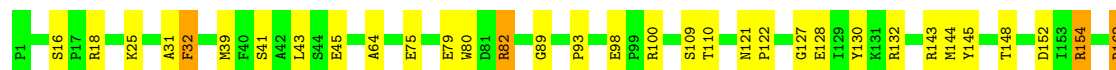
- Molecule 1: capsid protein

Chain cS: 82% 17%



- Molecule 1: capsid protein

Chain cT: 80% 17%



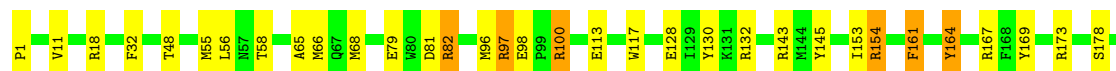
- Molecule 1: capsid protein

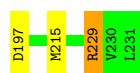
Chain 1h: 79% 19%




- Molecule 1: capsid protein

Chain cU: 84% 13%






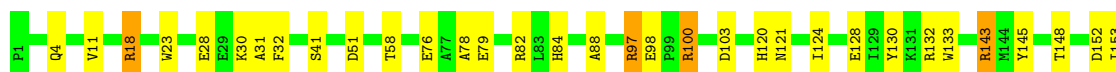
- Molecule 1: capsid protein

Chain cV:  84% 15%




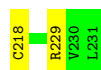
- Molecule 1: capsid protein

Chain cW:  79% 19%




- Molecule 1: capsid protein

Chain cX:  84% 14%




- Molecule 1: capsid protein

Chain cY:  83% 16%



- Molecule 1: capsid protein

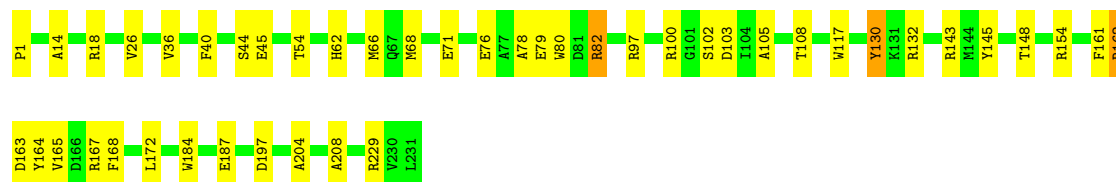
Chain cZ:  84% 14%





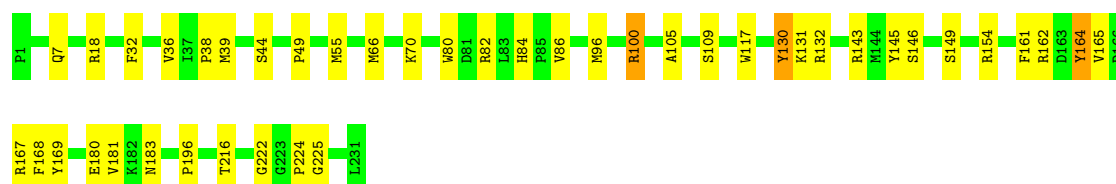
- Molecule 1: capsid protein

Chain d0: 81% 18%



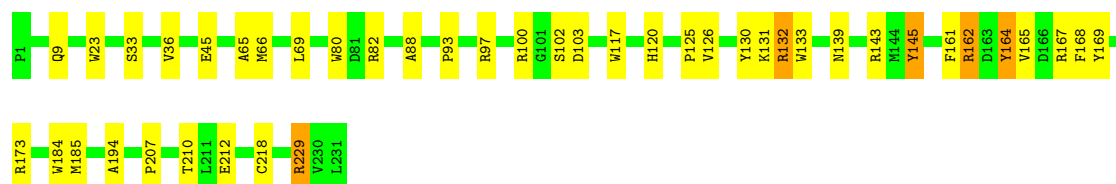
- Molecule 1: capsid protein

Chain d1: 81% 17%



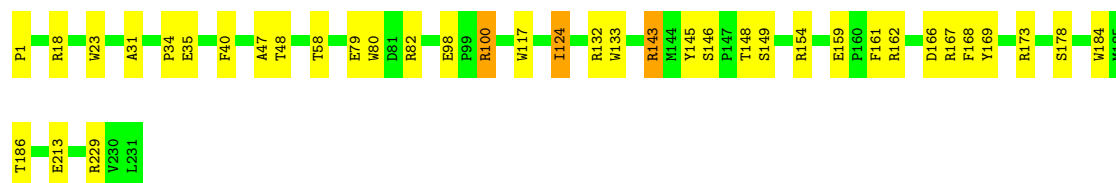
- Molecule 1: capsid protein

Chain d2: 81% 16%



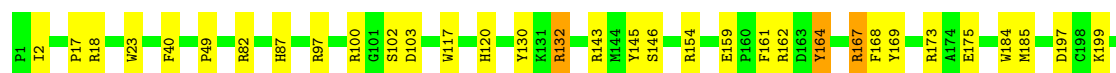
- Molecule 1: capsid protein

Chain d3: 84% 15%



- Molecule 1: capsid protein

Chain 1i: 84% 15%







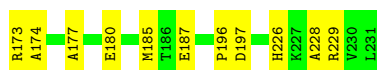
- Molecule 1: capsid protein

Chain d4: 79% 19%



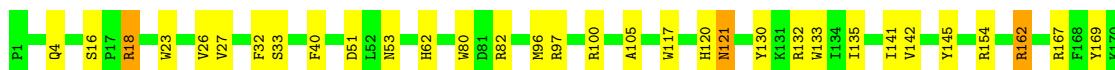
- Molecule 1: capsid protein

Chain d5: 81% 18%



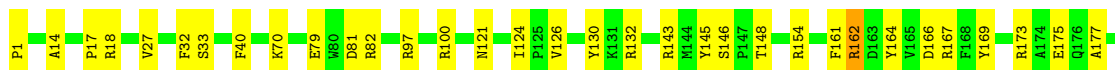
- Molecule 1: capsid protein

Chain d6: 82% 16%



- Molecule 1: capsid protein

Chain d7: 82% 17%



- Molecule 1: capsid protein

Chain d8: 84% 14%





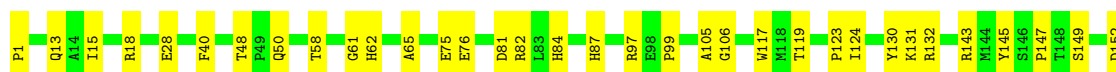
- Molecule 1: capsid protein

Chain d9: 83% 16%



- Molecule 1: capsid protein

Chain da: 81% 19%



- Molecule 1: capsid protein

Chain db: 80% 19%



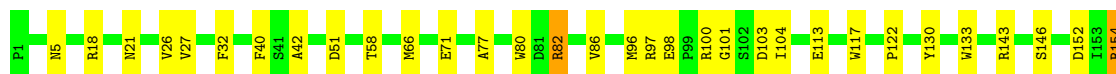
- Molecule 1: capsid protein

Chain dc: 79% 19%



- Molecule 1: capsid protein

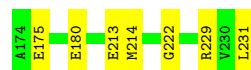
Chain dd: 80% 19%





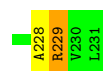
- Molecule 1: capsid protein

Chain 1j: 82% 16% .



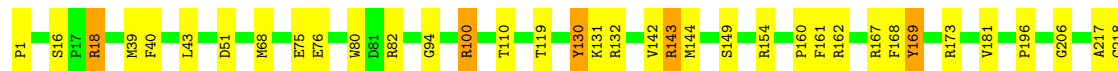
- Molecule 1: capsid protein

Chain de: 85% 13% .



- Molecule 1: capsid protein

Chain df: 84% 13% .



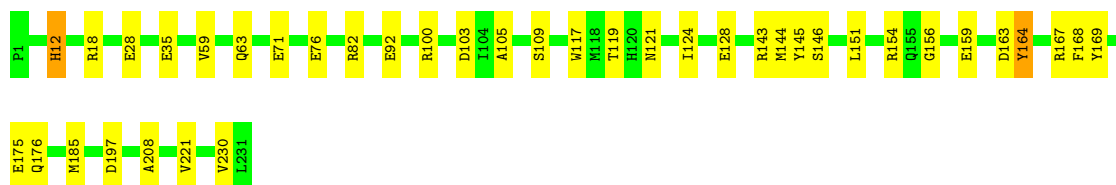
- Molecule 1: capsid protein

Chain dg: 81% 16% .



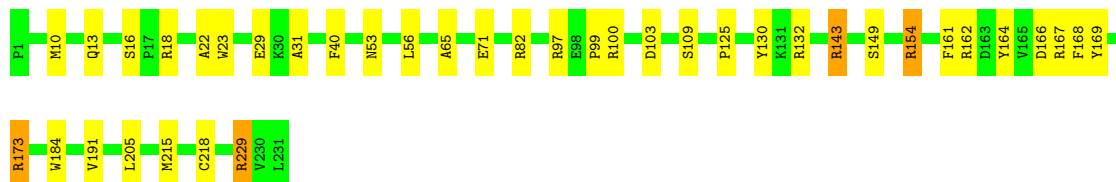
- Molecule 1: capsid protein

Chain dh: 83% 16% .



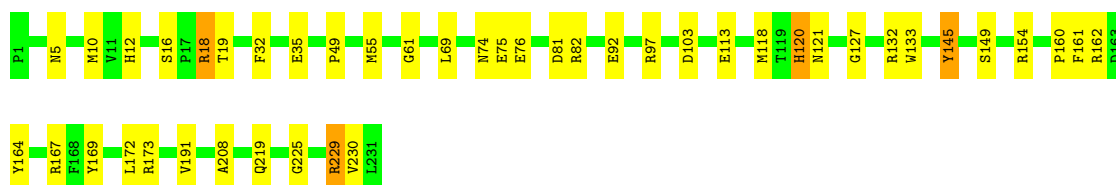
- Molecule 1: capsid protein

Chain di: 83% 15% .



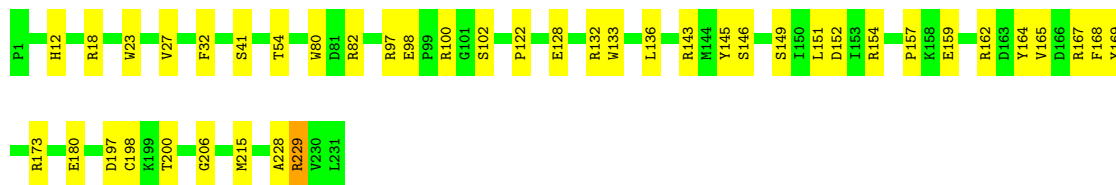
- Molecule 1: capsid protein

Chain dj: 81% 17% .



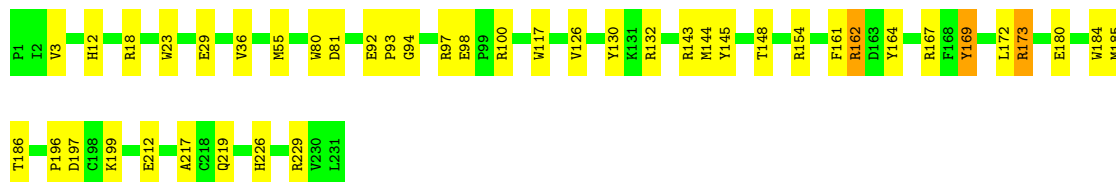
- Molecule 1: capsid protein

Chain dk: 82% 18% .



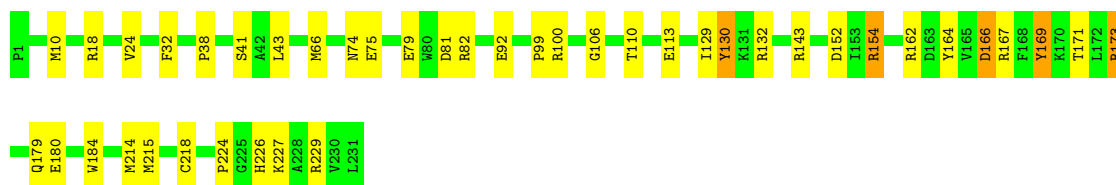
- Molecule 1: capsid protein

Chain dl: 81% 17% .




- Molecule 1: capsid protein

Chain dm: 82% 16% .




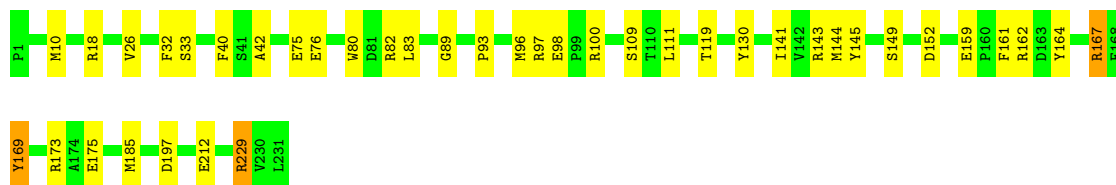
- Molecule 1: capsid protein

Chain dn:  81% 17% .




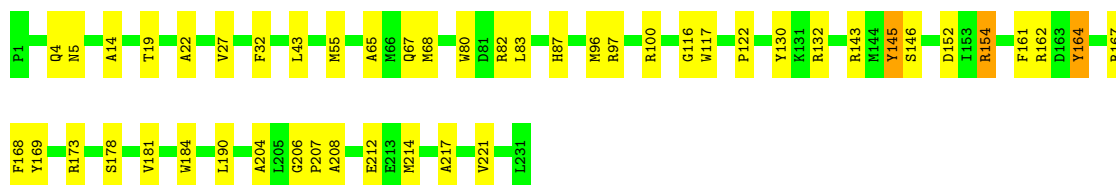
- Molecule 1: capsid protein

Chain 1k:  83% 16% .




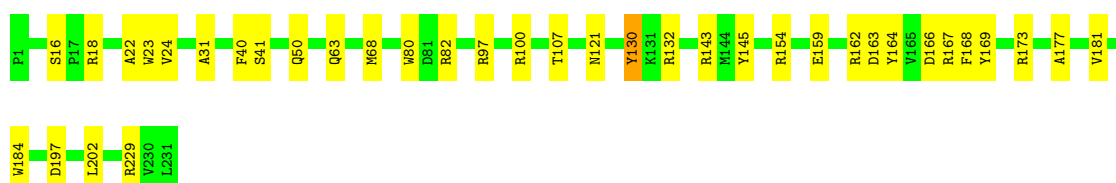
- Molecule 1: capsid protein

Chain do:  79% 19% .




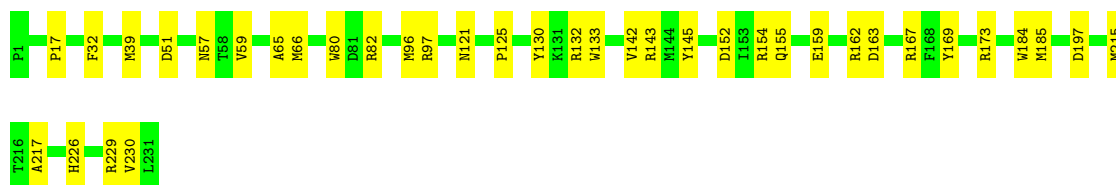
- Molecule 1: capsid protein

Chain dp:  84% 16% .



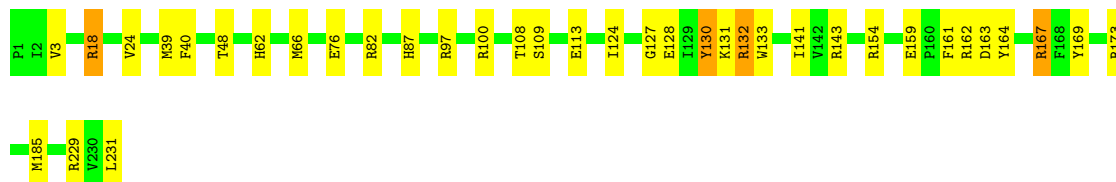
- Molecule 1: capsid protein

Chain dq:  84% 16% .



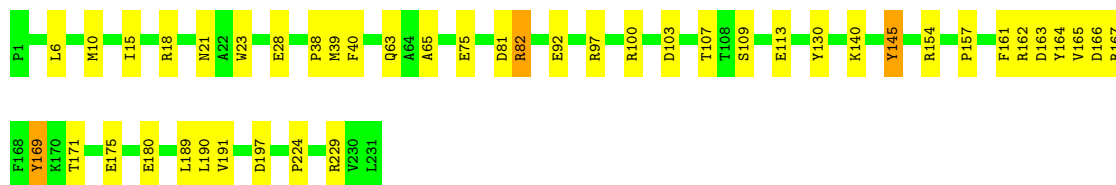
- Molecule 1: capsid protein

Chain dr: 84% 14%



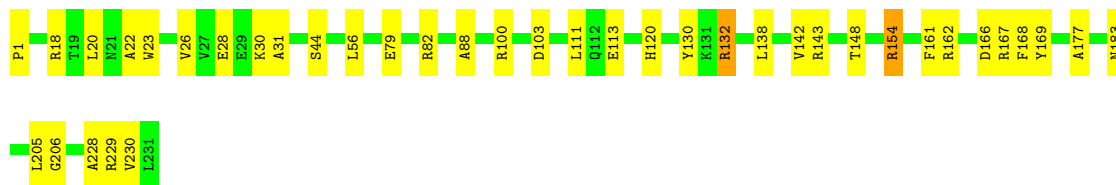
- Molecule 1: capsid protein

Chain ds: 81% 18%



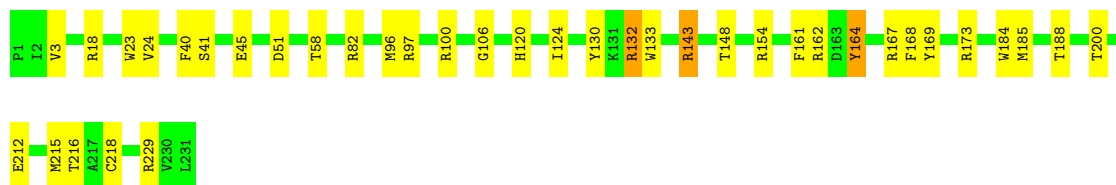
- Molecule 1: capsid protein

Chain dt: 83% 16%



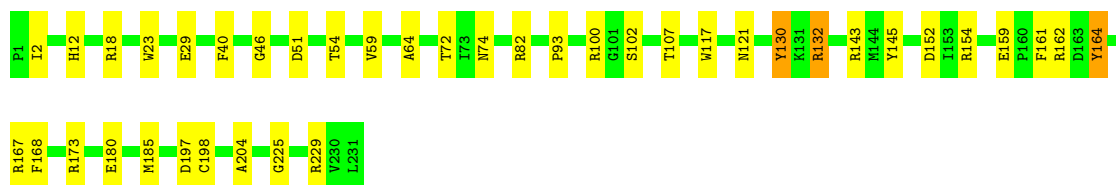
- Molecule 1: capsid protein

Chain du: 84% 15%



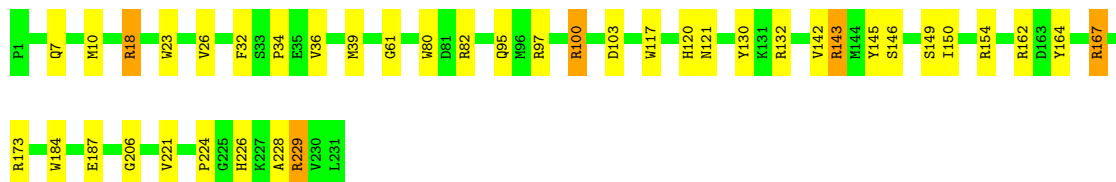
- Molecule 1: capsid protein

Chain dv: 83% 16%



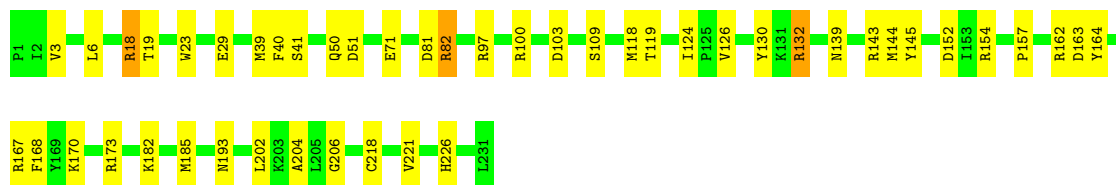
- Molecule 1: capsid protein

Chain dw: 83% 15% .



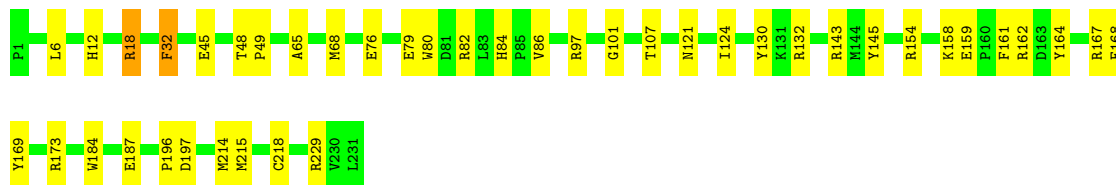
- Molecule 1: capsid protein

Chain dx: 80% 19% .



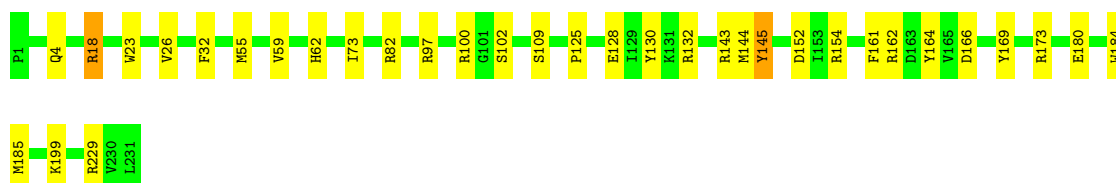
- Molecule 1: capsid protein

Chain 1l: 82% 17% .



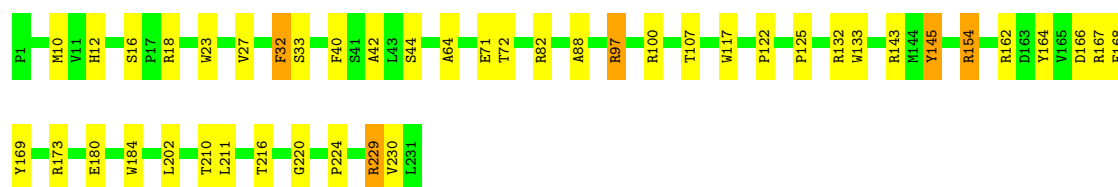
- Molecule 1: capsid protein

Chain dy: 85% 14% .



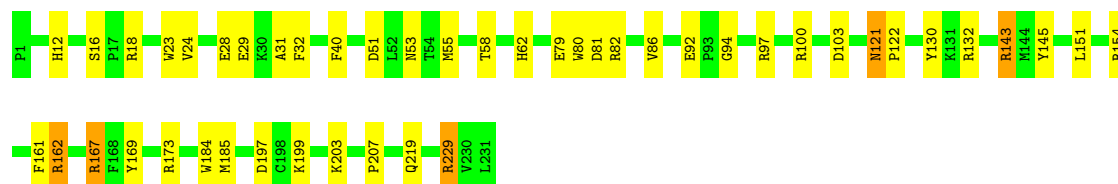
- Molecule 1: capsid protein

Chain dz: 81% 17% .



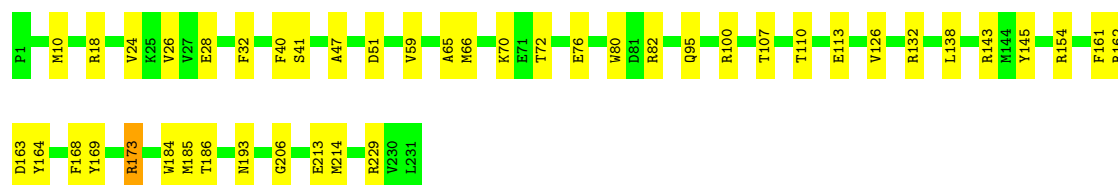
- Molecule 1: capsid protein

Chain dA: 80% 18%



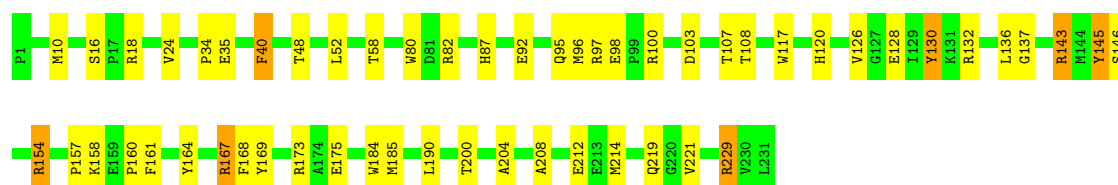
- Molecule 1: capsid protein

Chain dB: 81% 19%



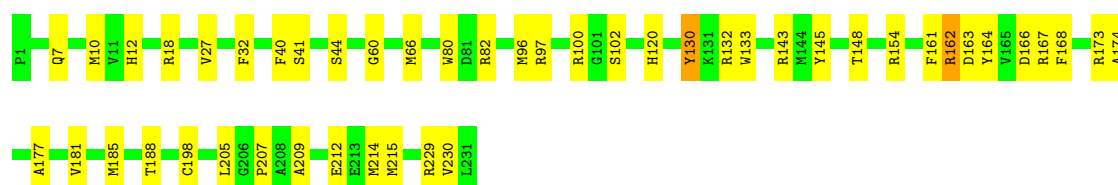
- Molecule 1: capsid protein

Chain dC: 76% 21%



- Molecule 1: capsid protein

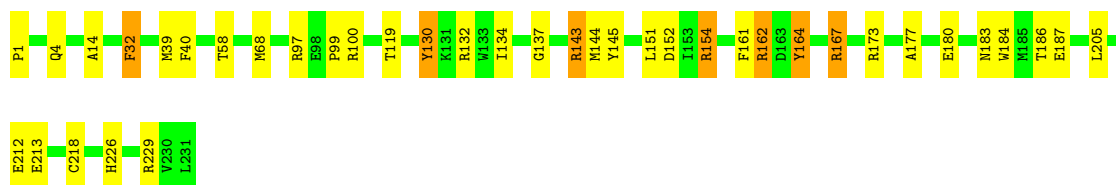
Chain dD: 80% 19%




- Molecule 1: capsid protein

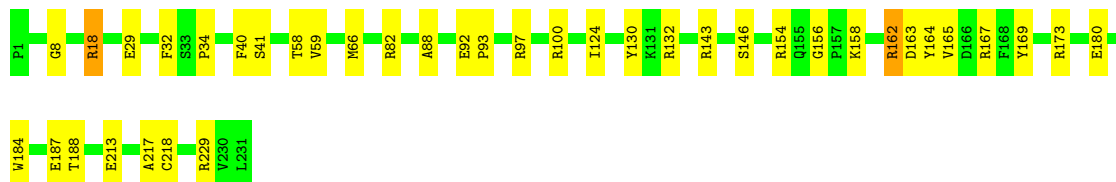
Chain dE: 83% 14%






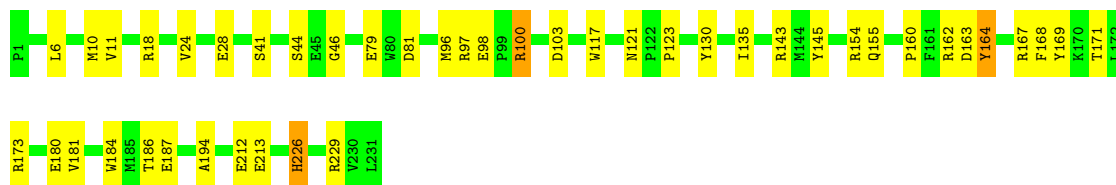
- Molecule 1: capsid protein

Chain dF:  83% 16% .




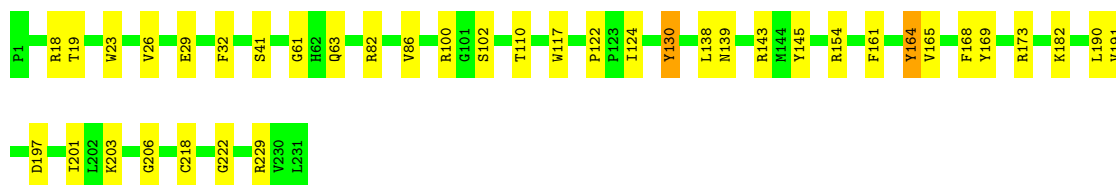
- Molecule 1: capsid protein

Chain dG:  81% 18% .




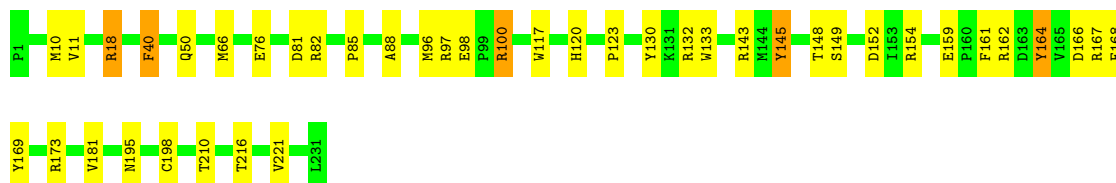
- Molecule 1: capsid protein

Chain dH:  83% 16% .




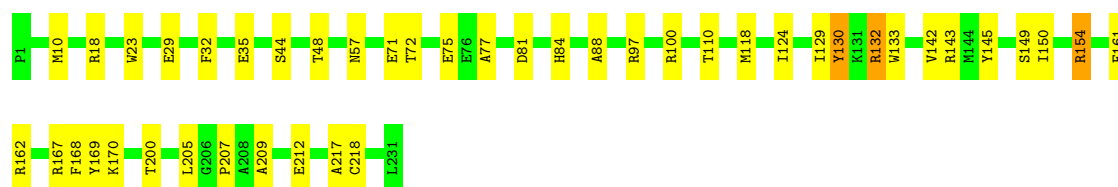
- Molecule 1: capsid protein

Chain 1m:  82% 16% .



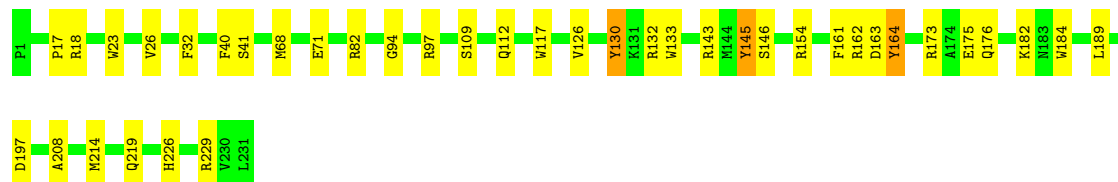
- Molecule 1: capsid protein

Chain dI:  81% 18% .



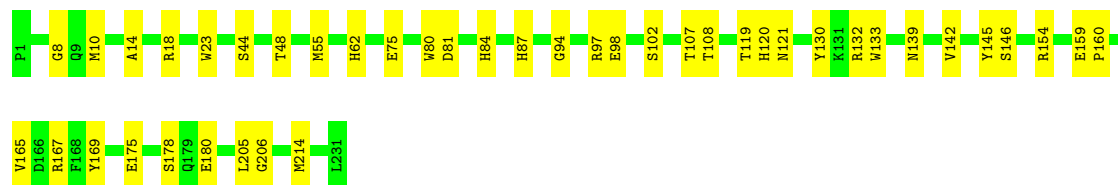
- Molecule 1: capsid protein

Chain dJ: 83% 16%



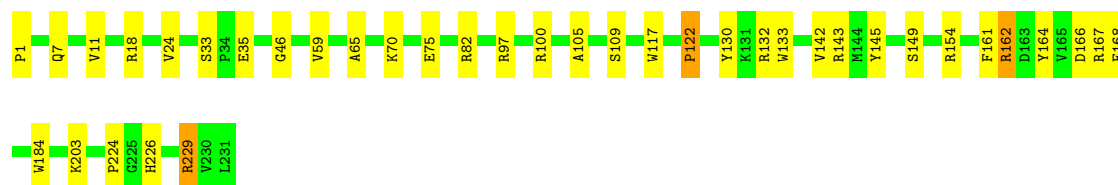
- Molecule 1: capsid protein

Chain dK: 82% 18%



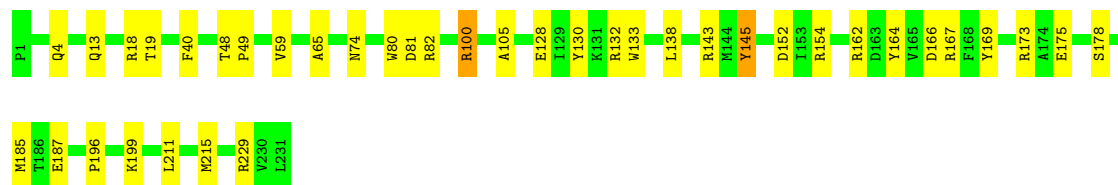
- Molecule 1: capsid protein

Chain dL: 84% 15%



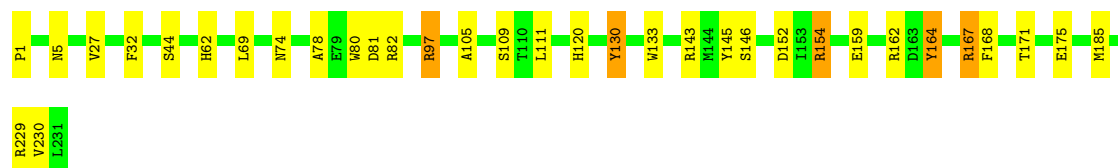
- Molecule 1: capsid protein

Chain dM: 83% 16%



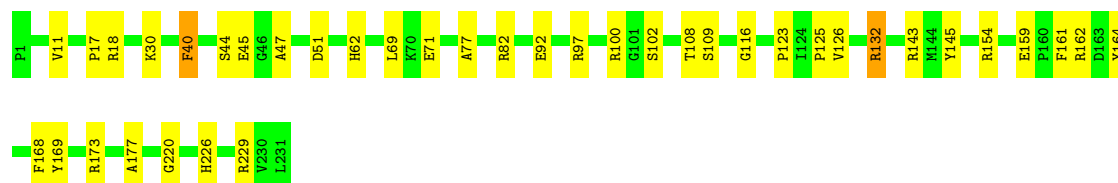
- Molecule 1: capsid protein

Chain dN: 85% 13%



- Molecule 1: capsid protein

Chain dO: 83% 16% •



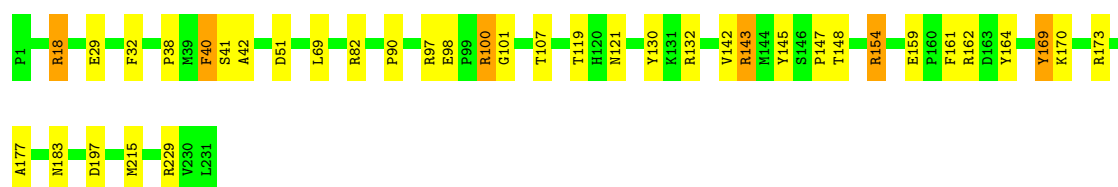
- Molecule 1: capsid protein

Chain dP: 82% 16% •



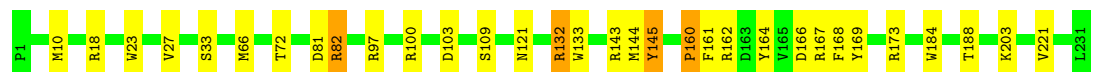
- Molecule 1: capsid protein

Chain dQ: 84% 14% •



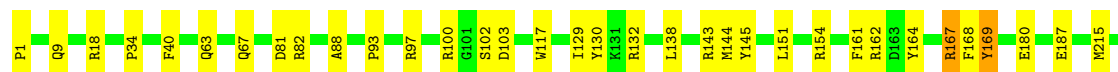
- Molecule 1: capsid protein

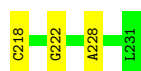
Chain dR: 86% 12% •




- Molecule 1: capsid protein

Chain 1n: 84% 15% •






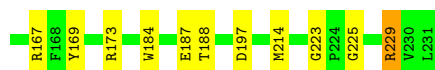
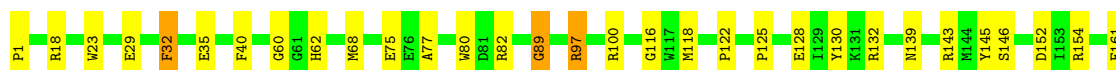
- Molecule 1: capsid protein

Chain dS:  84% 13% •




- Molecule 1: capsid protein

Chain dT:  82% 16% •




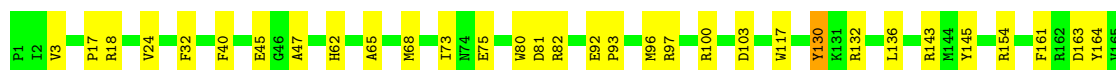
- Molecule 1: capsid protein

Chain dU:  84% 14% •




- Molecule 1: capsid protein

Chain dV:  81% 18% •



- Molecule 1: capsid protein

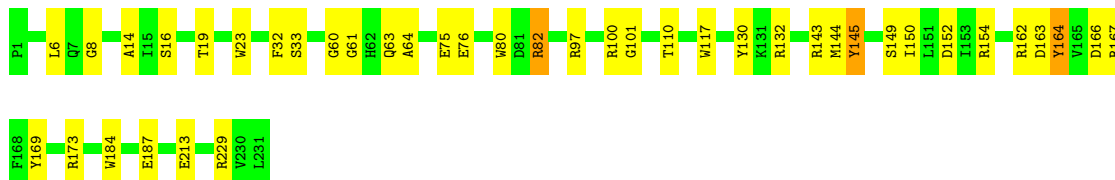
Chain dW:  81% 16% •





- Molecule 1: capsid protein

Chain dX: 82% 16%



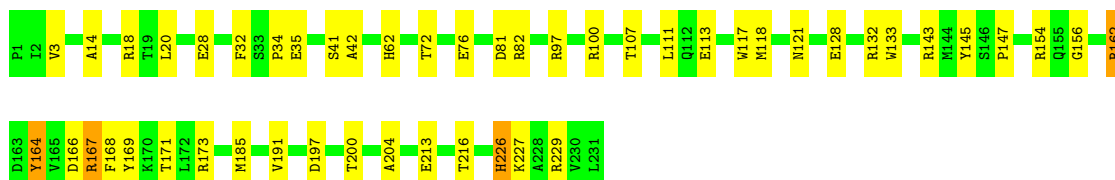
- Molecule 1: capsid protein

Chain dY: 83% 16%



- Molecule 1: capsid protein

Chain dZ: 79% 19%



- Molecule 1: capsid protein

Chain e0: 81% 19%



- Molecule 1: capsid protein

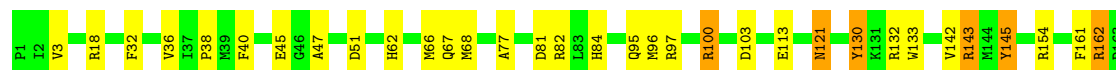
Chain e1: 80% 19%





- Molecule 1: capsid protein

Chain 1o: 80% 16%



- Molecule 1: capsid protein

Chain e2: 83% 16%



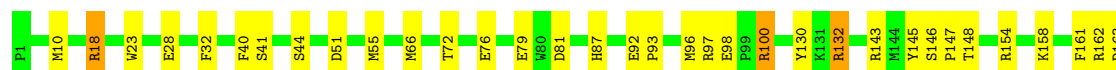
- Molecule 1: capsid protein

Chain e3: 84% 16%



- Molecule 1: capsid protein

Chain e4: 81% 18%



- Molecule 1: capsid protein

Chain e5: 81% 17%





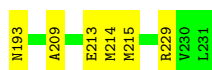
- Molecule 1: capsid protein

Chain e6: 80% 19%



- Molecule 1: capsid protein

Chain e7: 84% 15%



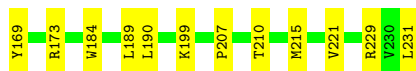
- Molecule 1: capsid protein

Chain e8: 84% 15%



- Molecule 1: capsid protein

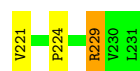
Chain e9: 80% 19%




- Molecule 1: capsid protein

Chain ea: 84% 14%






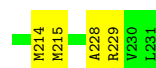
- Molecule 1: capsid protein

Chain eb:  83% 17%




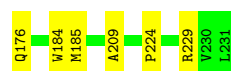
- Molecule 1: capsid protein

Chain 1p:  84% 16%




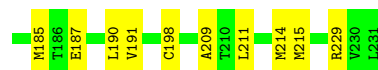
- Molecule 1: capsid protein

Chain ec:  83% 14%




- Molecule 1: capsid protein

Chain ed:  81% 18%



- Molecule 1: capsid protein

Chain ee:  83% 15%







- Molecule 1: capsid protein

Chain ef: 85% 14% •



- Molecule 1: capsid protein

Chain eg: 81% 17% •



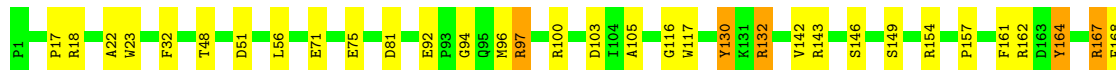
- Molecule 1: capsid protein

Chain eh: 82% 16% •



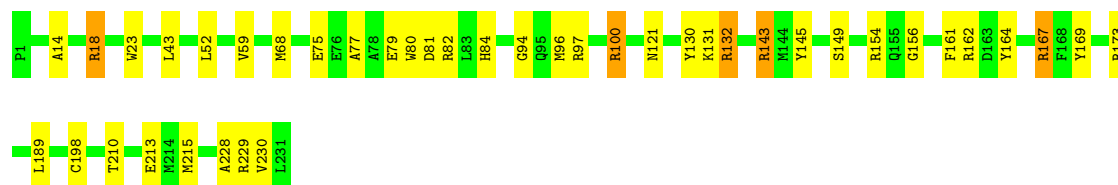
- Molecule 1: capsid protein

Chain ei: 81% 17% •




- Molecule 1: capsid protein

Chain ej: 82% 16% •




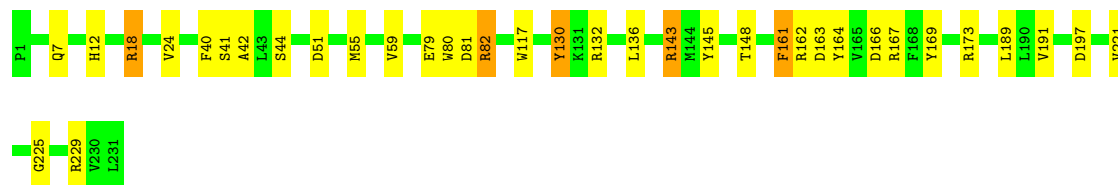
- Molecule 1: capsid protein

Chain ek:  84% 16% .




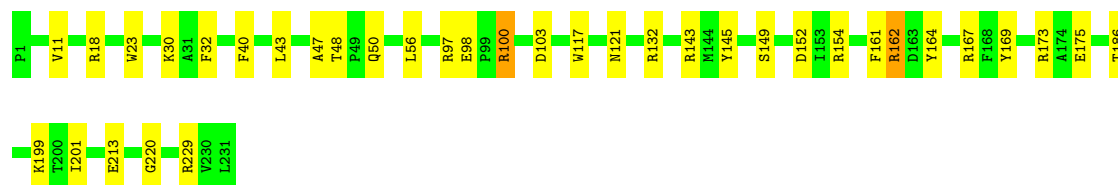
- Molecule 1: capsid protein

Chain el:  84% 13% .




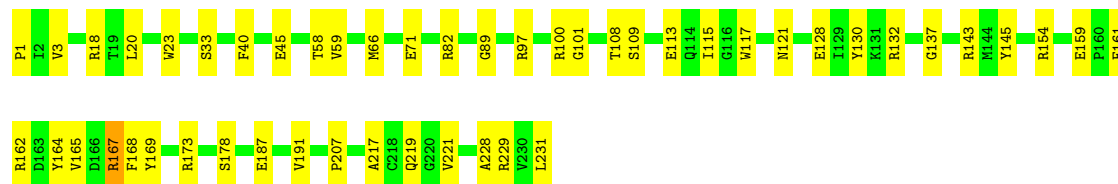
- Molecule 1: capsid protein

Chain 1q:  84% 15% .




- Molecule 1: capsid protein

Chain em:  79% 21% .



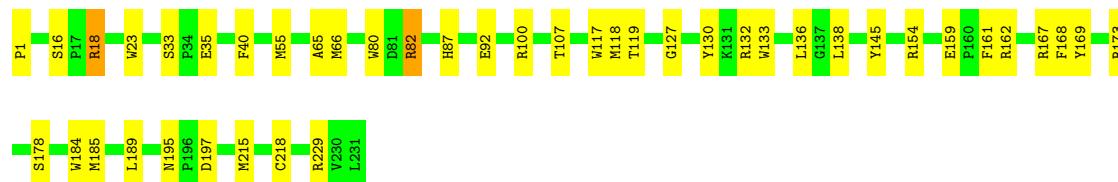
- Molecule 1: capsid protein

Chain en:  85% 13% .



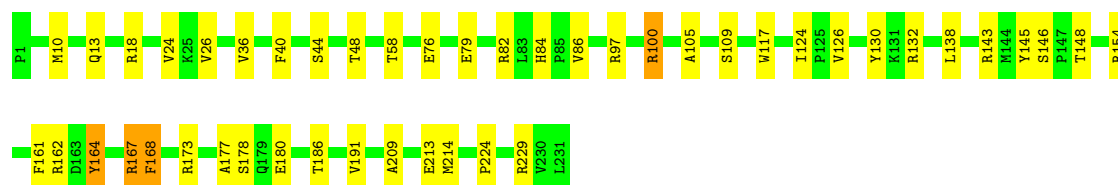
- Molecule 1: capsid protein

Chain eo: 81% 18% .



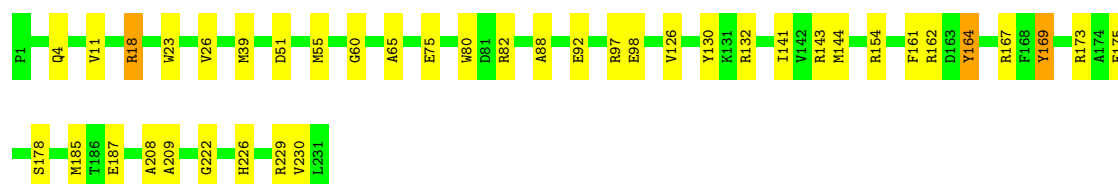
- Molecule 1: capsid protein

Chain ep: 80% 18% .



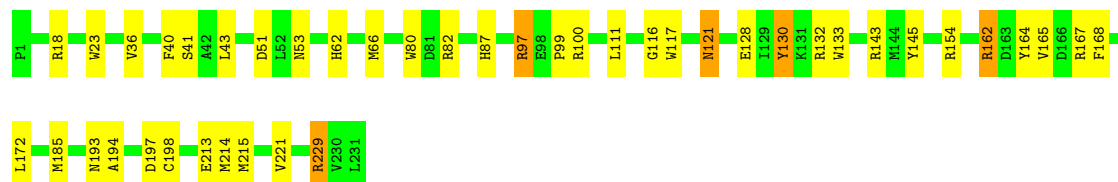
- Molecule 1: capsid protein

Chain eq: 83% 16% .




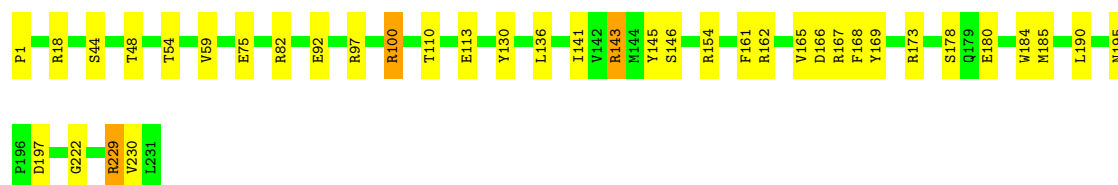
- Molecule 1: capsid protein

Chain er: 81% 16% .




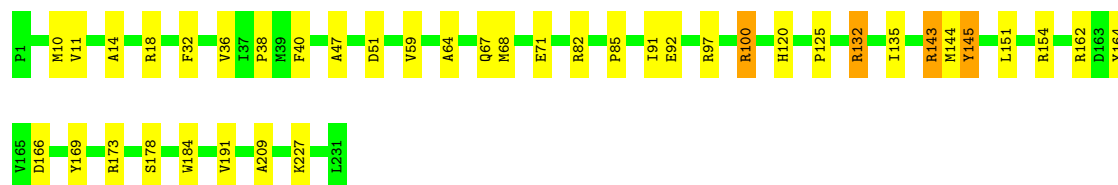
- Molecule 1: capsid protein

Chain es:  84% 15% •




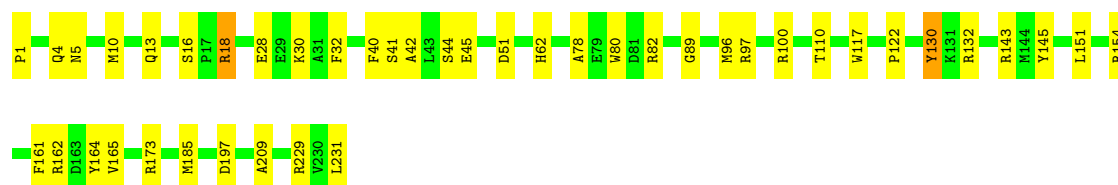
- Molecule 1: capsid protein

Chain et:  83% 16% •




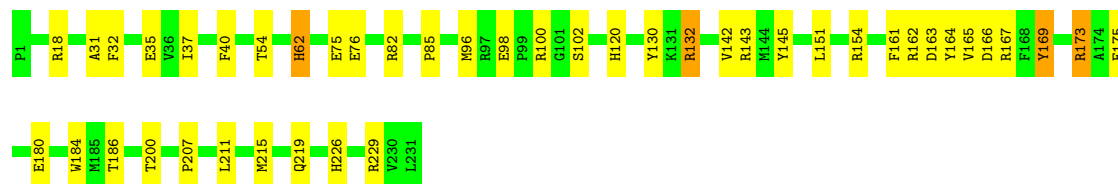
- Molecule 1: capsid protein

Chain eu:  81% 18% •




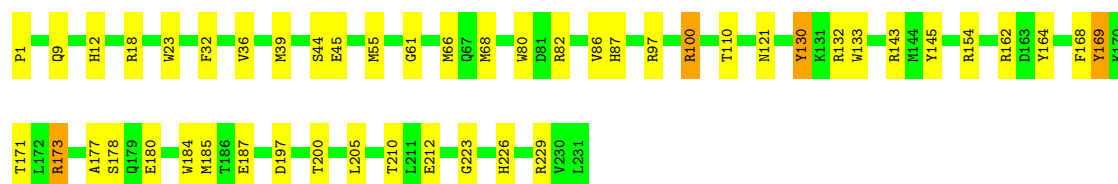
- Molecule 1: capsid protein

Chain ev:  81% 17% •




- Molecule 1: capsid protein

Chain 1r:  79% 19% •




- Molecule 1: capsid protein

Chain ew:  84% 15%




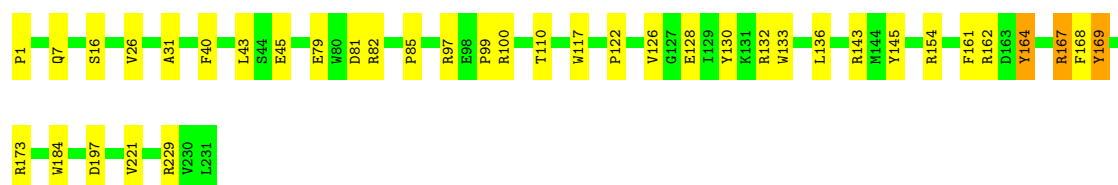
- Molecule 1: capsid protein

Chain ex:  86% 12%




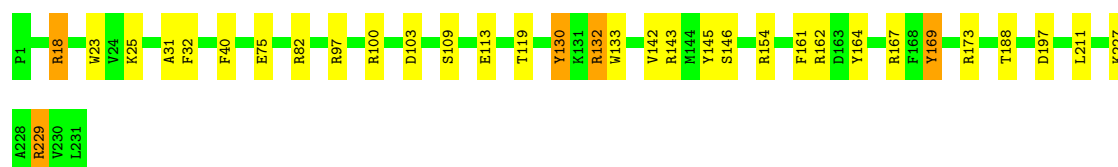
- Molecule 1: capsid protein

Chain ey:  84% 15%




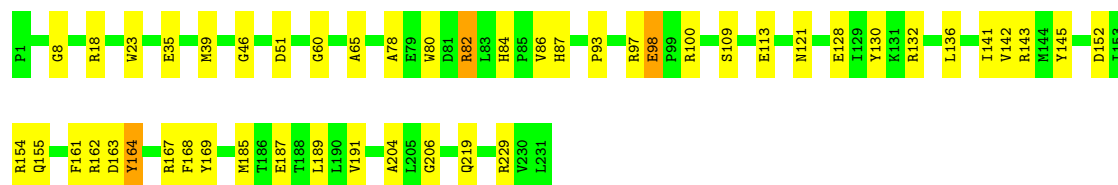
- Molecule 1: capsid protein

Chain ez:  86% 12%




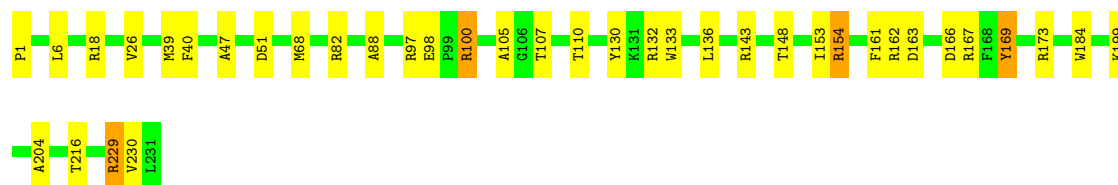
- Molecule 1: capsid protein

Chain eA:  79% 19%



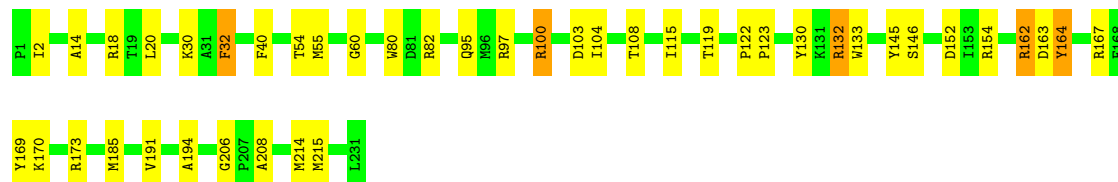
- Molecule 1: capsid protein

Chain eB:  84% 15%



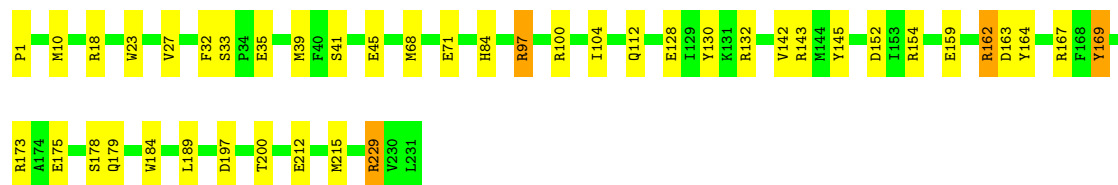
- Molecule 1: capsid protein

Chain eC: 81% 16% •



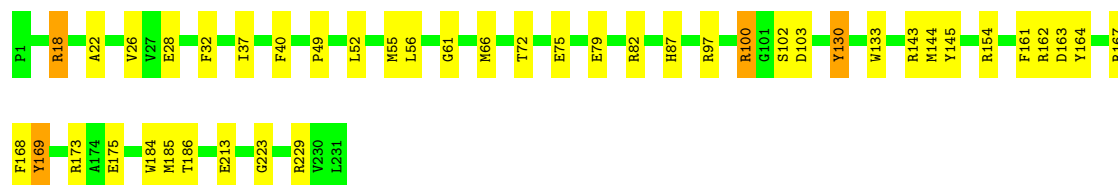
- Molecule 1: capsid protein

Chain eD: 81% 17% •



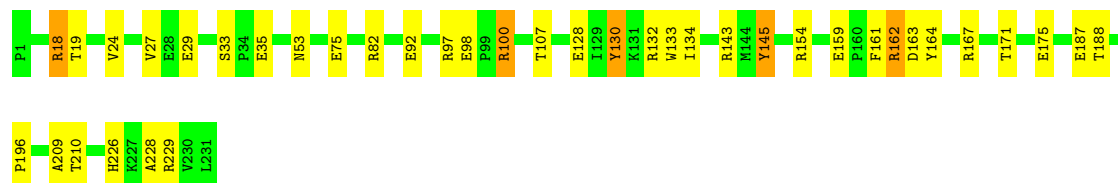
- Molecule 1: capsid protein

Chain eE: 81% 17% •



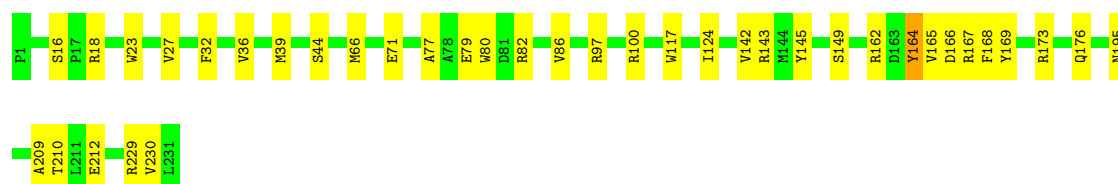
- Molecule 1: capsid protein

Chain eF: 83% 15% •



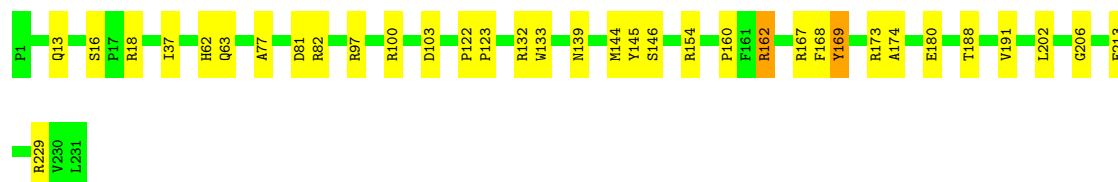
- Molecule 1: capsid protein

Chain 1s: 84% 16% •



- Molecule 1: capsid protein

Chain eG: 85% 14%



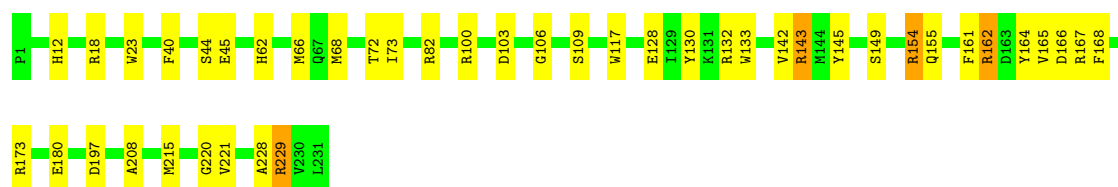
- Molecule 1: capsid protein

Chain eH: 81% 18%



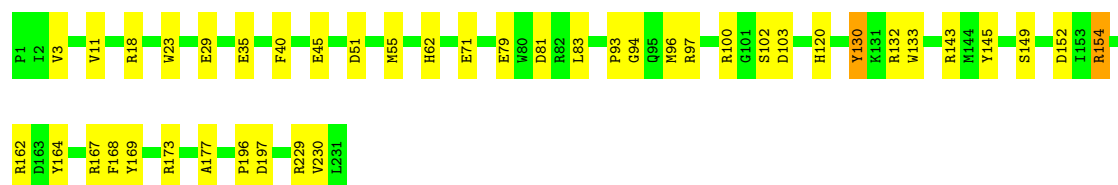
- Molecule 1: capsid protein

Chain eI: 81% 17%



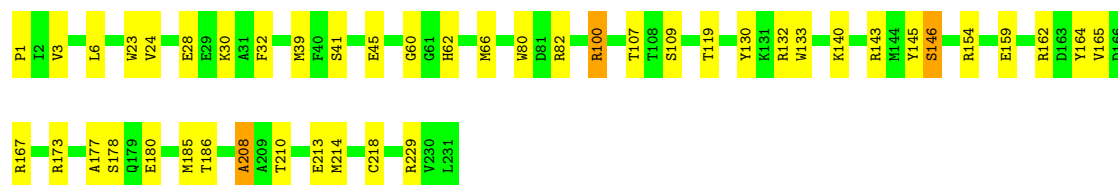
- Molecule 1: capsid protein

Chain eJ: 82% 17%



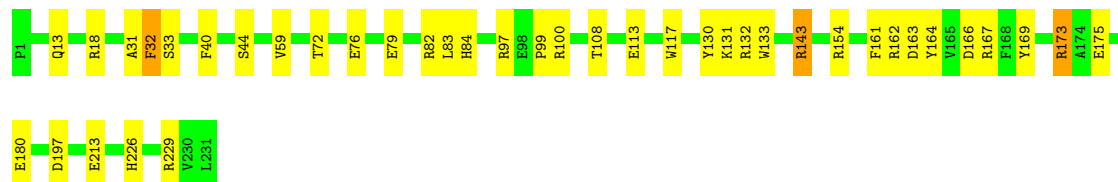
- Molecule 1: capsid protein

Chain eK: 81% 18%



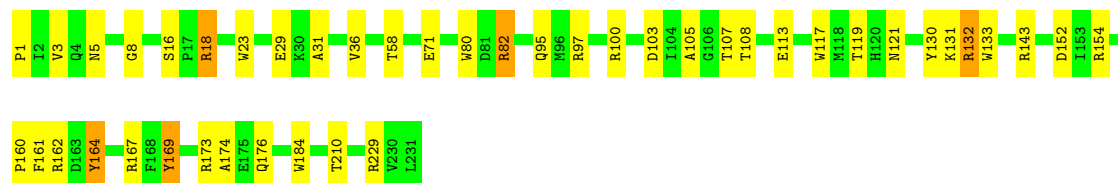
- Molecule 1: capsid protein

Chain eL: 83% 16% .



- Molecule 1: capsid protein

Chain eM: 81% 17% .



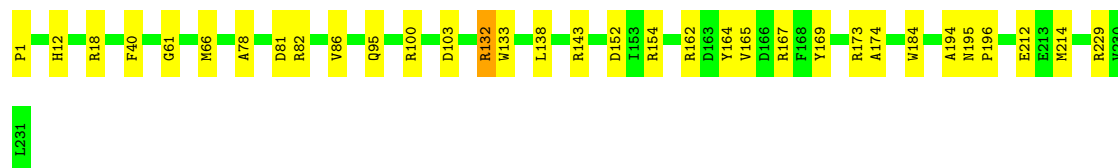
- Molecule 1: capsid protein

Chain eN: 83% 16% .



- Molecule 1: capsid protein

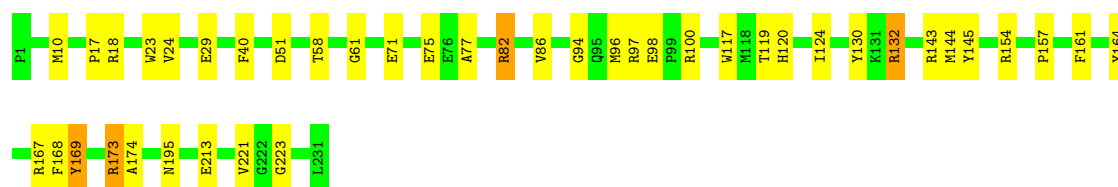
Chain eO: 86% 14% .



- Molecule 1: capsid protein

Chain eP: 82% 16% .





- Molecule 1: capsid protein

Chain 1t: 86% 13%



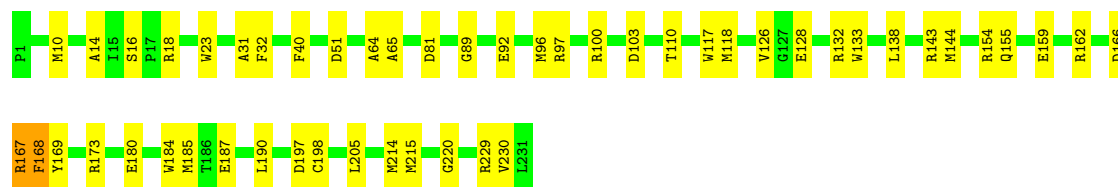
- Molecule 1: capsid protein

Chain eQ: 81% 19%



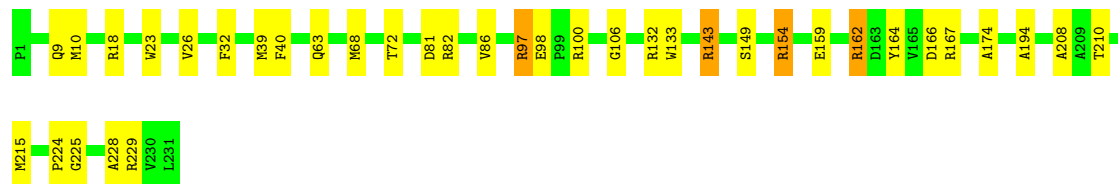
- Molecule 1: capsid protein

Chain eR: 78% 21%



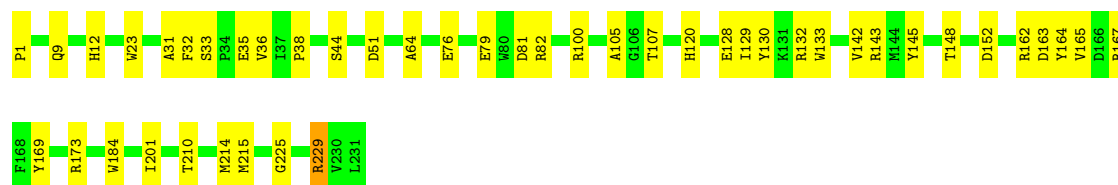
- Molecule 1: capsid protein

Chain eS: 84% 14%



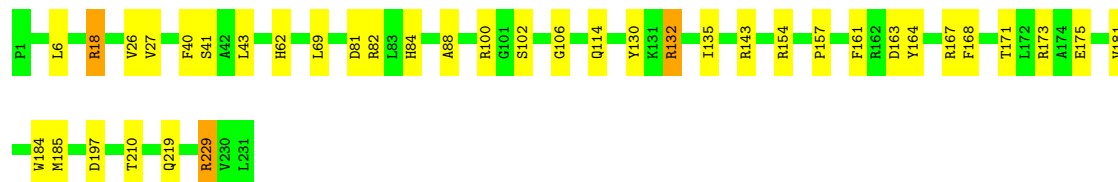
- Molecule 1: capsid protein

Chain eT: 81% 19%



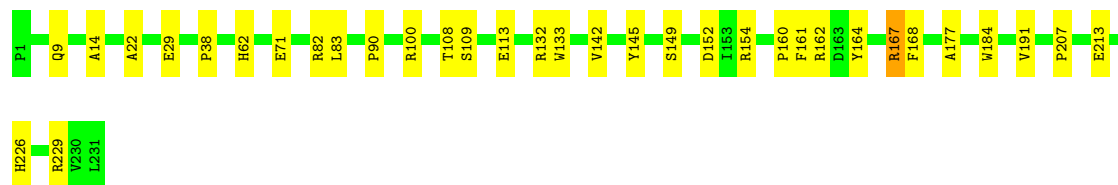
- Molecule 1: capsid protein

Chain eU: 84% 15% .



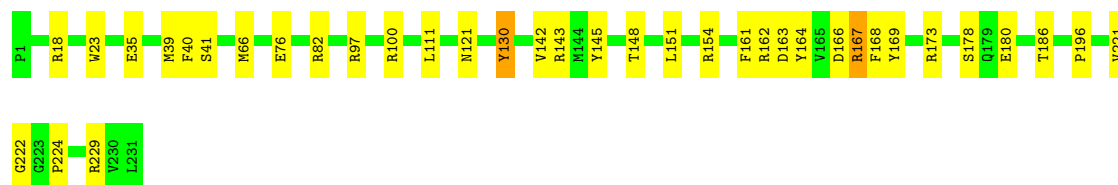
- Molecule 1: capsid protein

Chain eV: 85% 14% .



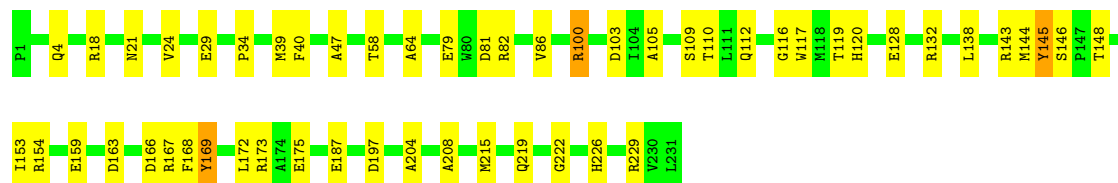
- Molecule 1: capsid protein

Chain eW: 84% 15% .



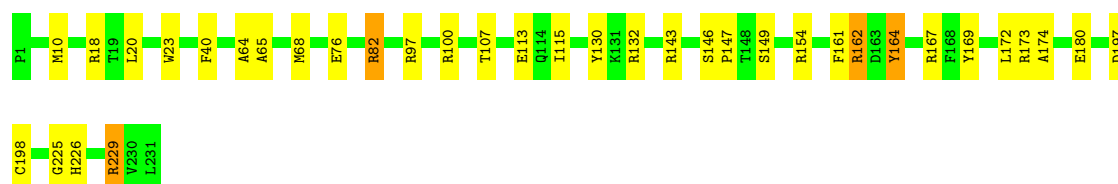
- Molecule 1: capsid protein

Chain eX: 77% 22% .



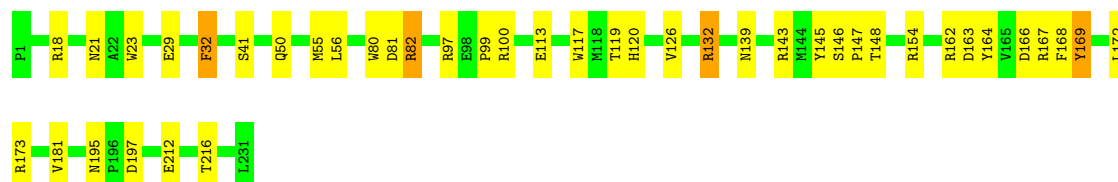
- Molecule 1: capsid protein

Chain eY: 84% 14% .



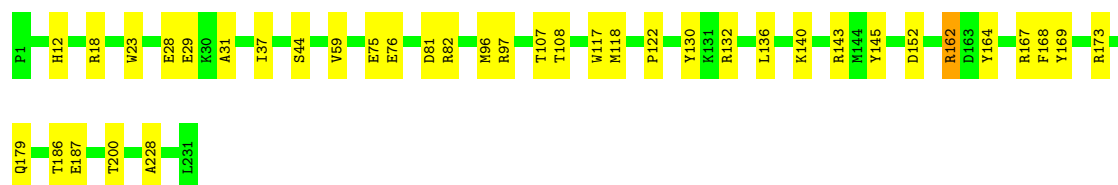
- Molecule 1: capsid protein

Chain eZ: 82% 16% •



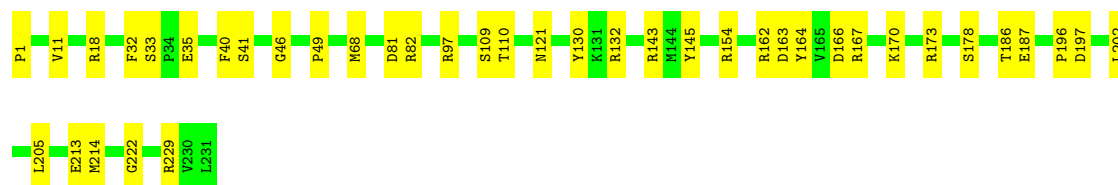
- Molecule 1: capsid protein

Chain 1u: 84% 16% •



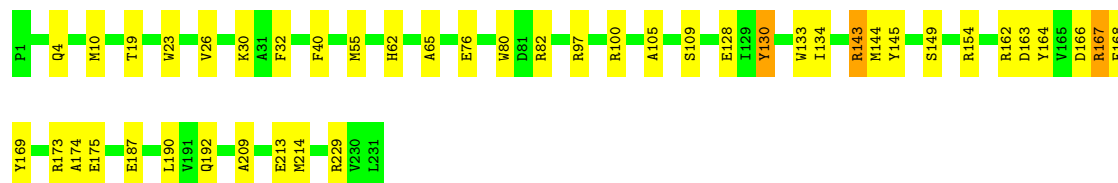
- Molecule 1: capsid protein

Chain f0: 83% 17% •



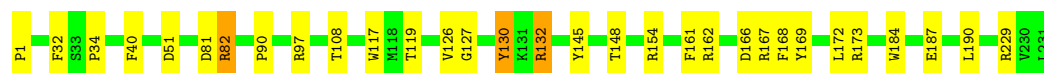
- Molecule 1: capsid protein

Chain f1: 81% 18% •



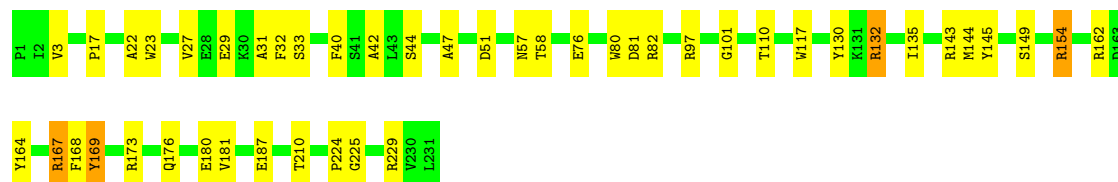
- Molecule 1: capsid protein

Chain f2: 87% 12% •



- Molecule 1: capsid protein

Chain f3: 80% 18%



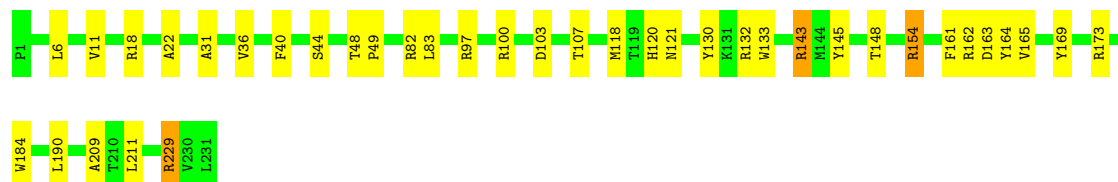
- Molecule 1: capsid protein

Chain f4: 79% 20%



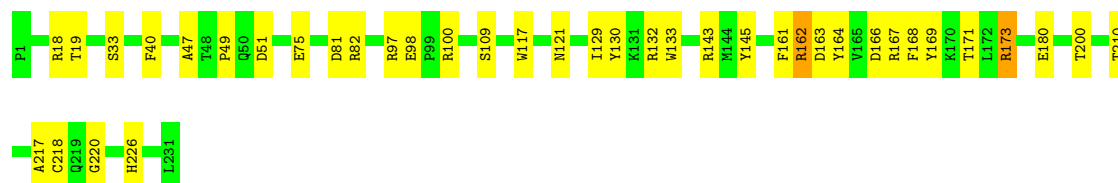
- Molecule 1: capsid protein

Chain f5: 84% 15%



- Molecule 1: capsid protein

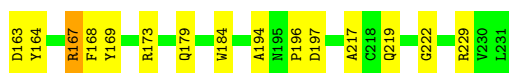
Chain f6: 83% 16%



- Molecule 1: capsid protein

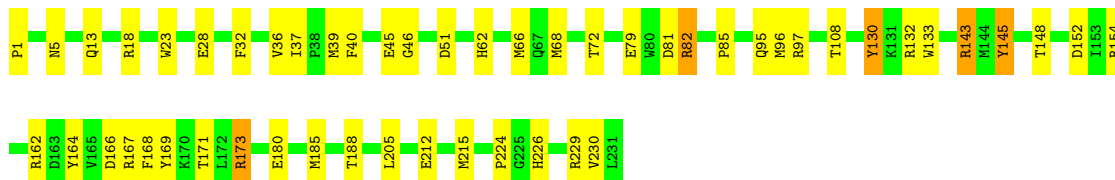
Chain f7: 78% 20%





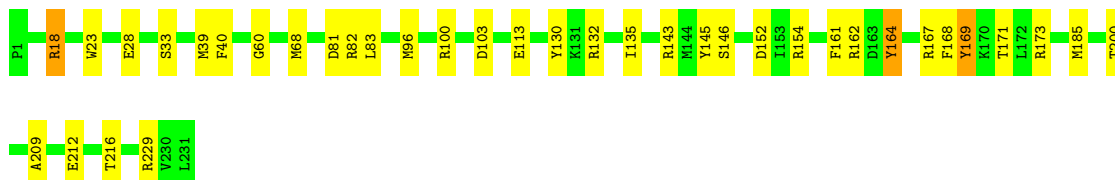
- Molecule 1: capsid protein

Chain f8: 77% 20% .



- Molecule 1: capsid protein

Chain f9: 84% 15% .



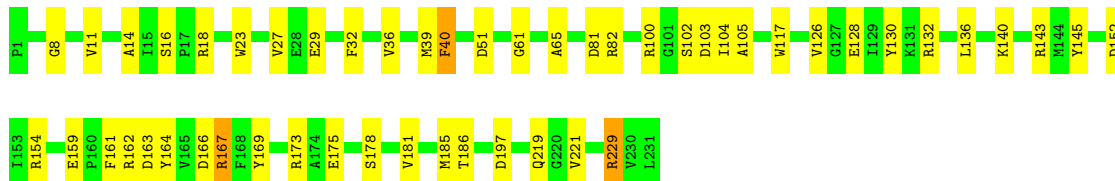
- Molecule 1: capsid protein

Chain 1v: 84% 15% .



- Molecule 1: capsid protein

Chain fa: 78% 21% .



- Molecule 1: capsid protein

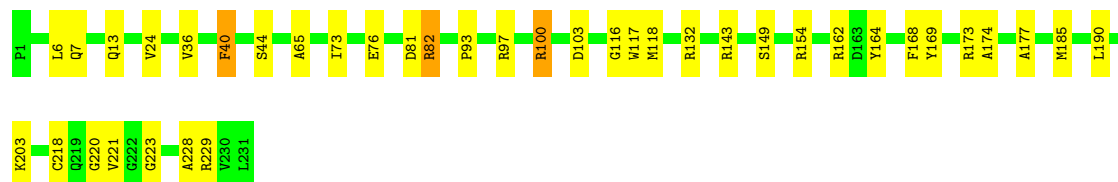
Chain fb: 82% 17% .





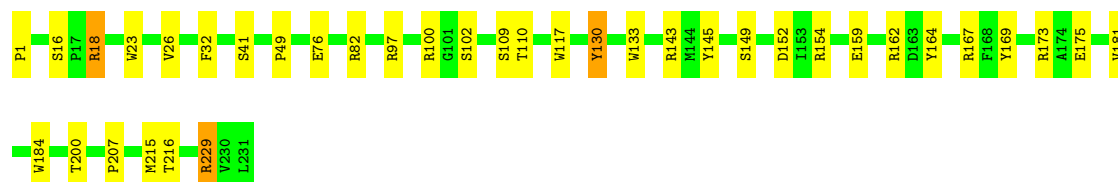
- Molecule 1: capsid protein

Chain fc: 83% 16%



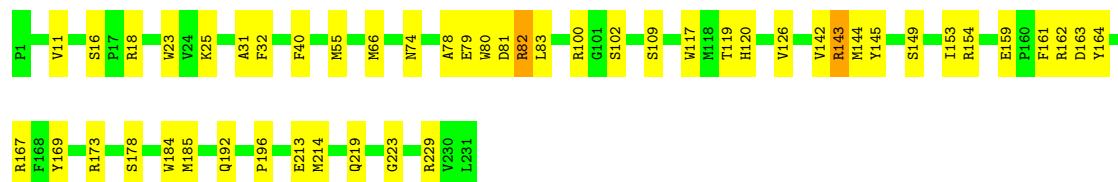
- Molecule 1: capsid protein

Chain fd: 84% 15%



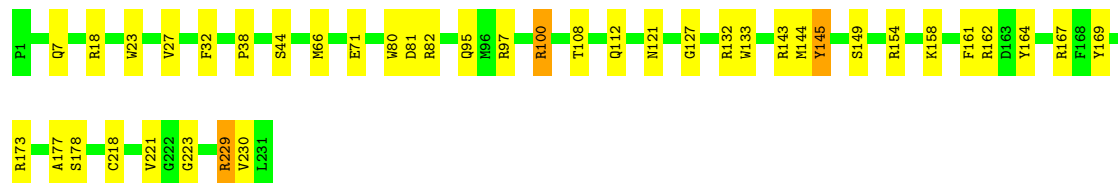
- Molecule 1: capsid protein

Chain fe: 79% 20%



- Molecule 1: capsid protein

Chain ff: 83% 16%



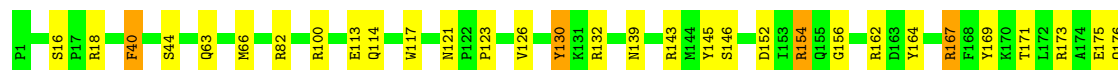
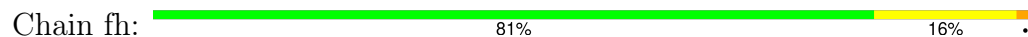
- Molecule 1: capsid protein

Chain fg: 81% 19%

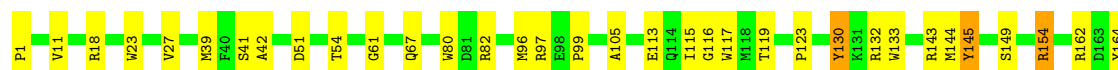
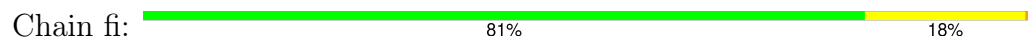




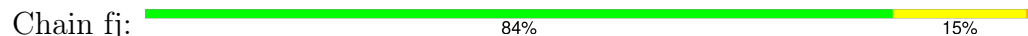
- Molecule 1: capsid protein



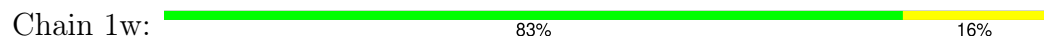
- Molecule 1: capsid protein



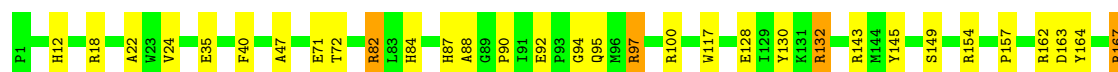
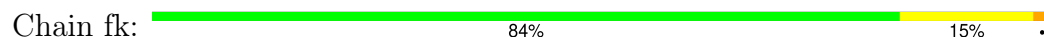
- Molecule 1: capsid protein



- Molecule 1: capsid protein

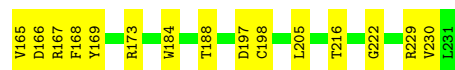
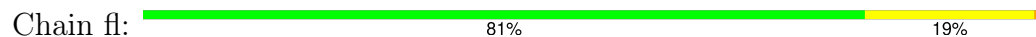


- Molecule 1: capsid protein

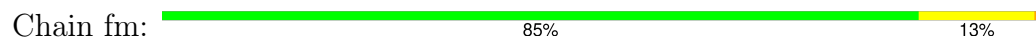




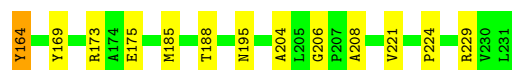
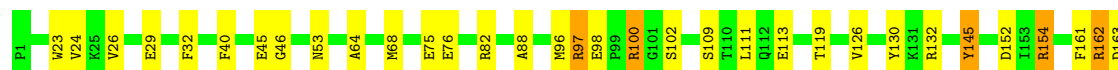
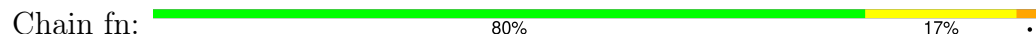
- Molecule 1: capsid protein



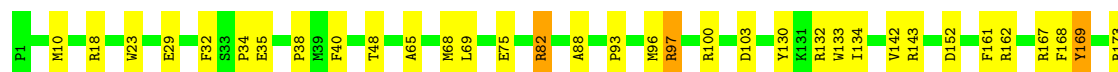
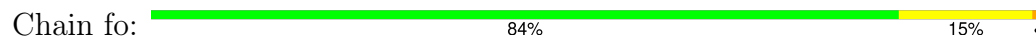
- Molecule 1: capsid protein



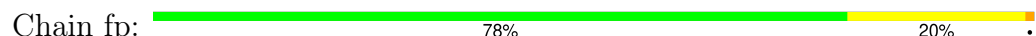
- Molecule 1: capsid protein



- Molecule 1: capsid protein



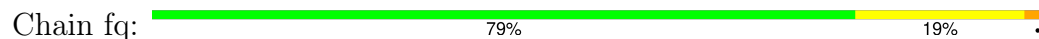
- Molecule 1: capsid protein



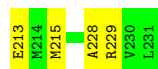
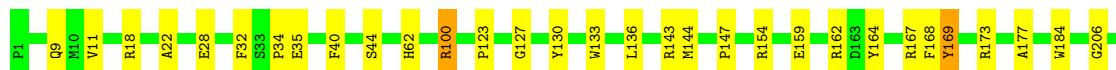
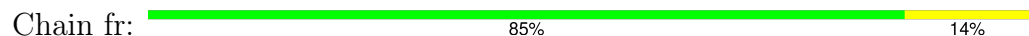




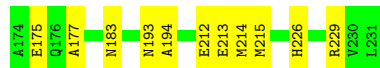
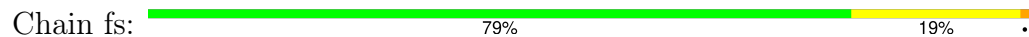
- Molecule 1: capsid protein



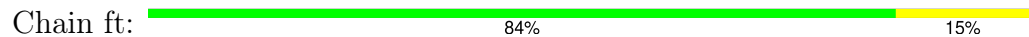
- Molecule 1: capsid protein



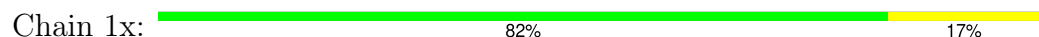
- Molecule 1: capsid protein

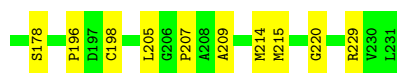


- Molecule 1: capsid protein



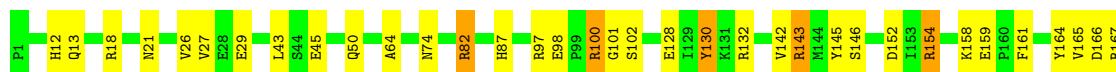
- Molecule 1: capsid protein





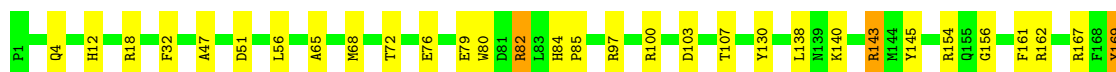
- Molecule 1: capsid protein

Chain fu: 81% 16%



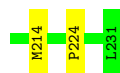
- Molecule 1: capsid protein

Chain fv: 84% 15%



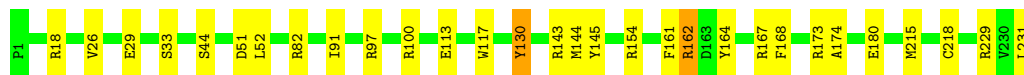
- Molecule 1: capsid protein

Chain fw: 85% 13%



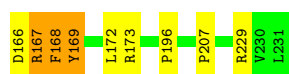
- Molecule 1: capsid protein

Chain fx: 87% 12%

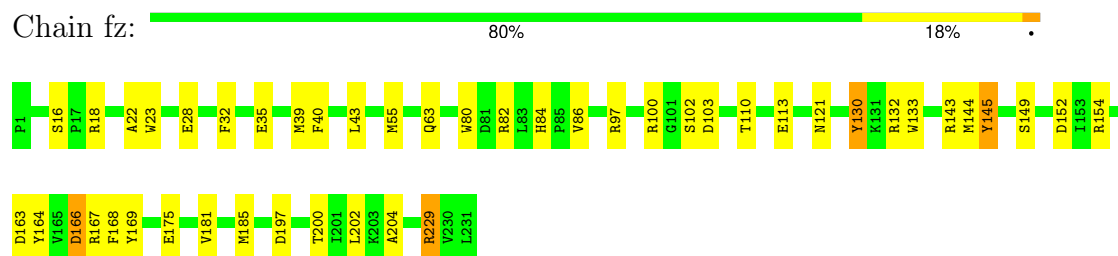


- Molecule 1: capsid protein

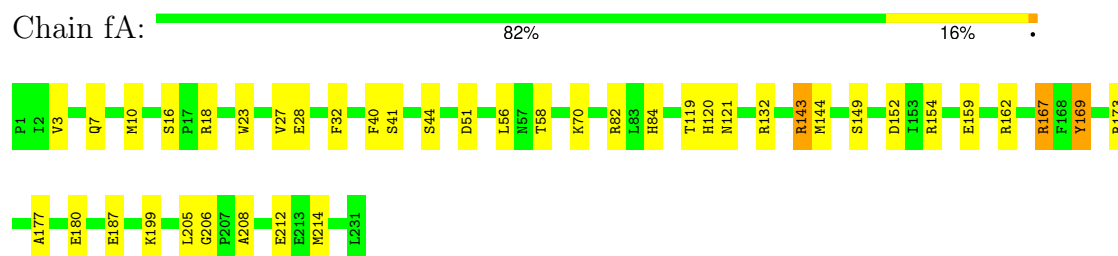
Chain fy: 81% 15%



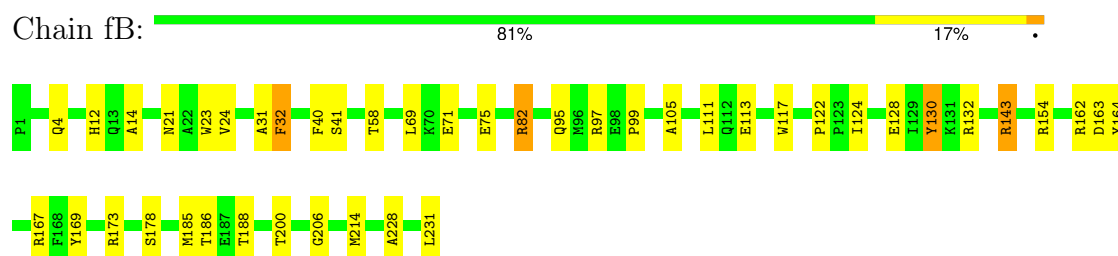
- Molecule 1: capsid protein



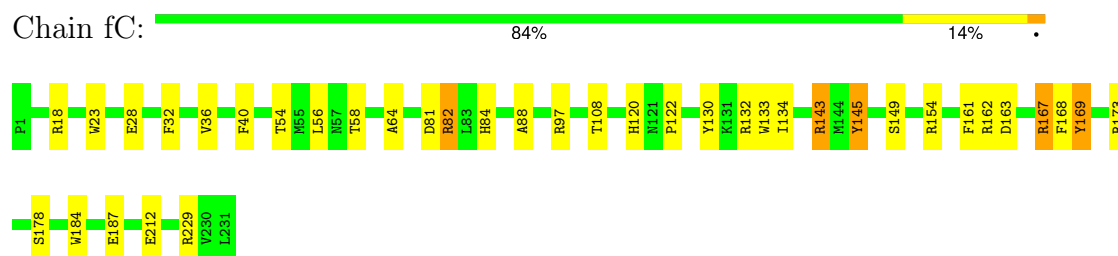
- Molecule 1: capsid protein



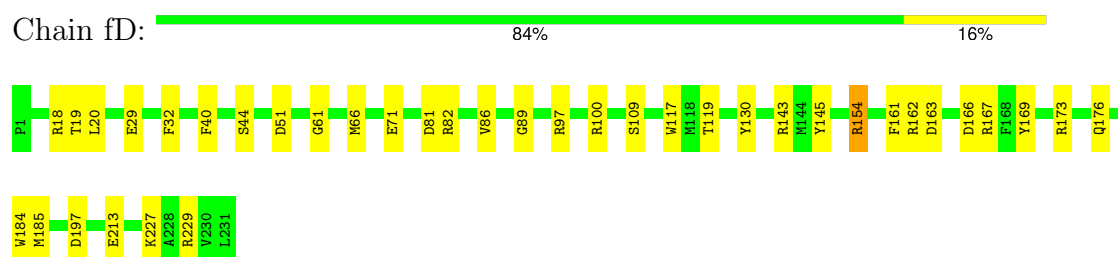
- Molecule 1: capsid protein




- Molecule 1: capsid protein



- Molecule 1: capsid protein




- Molecule 1: capsid protein

Chain 1y:  82% 16% .




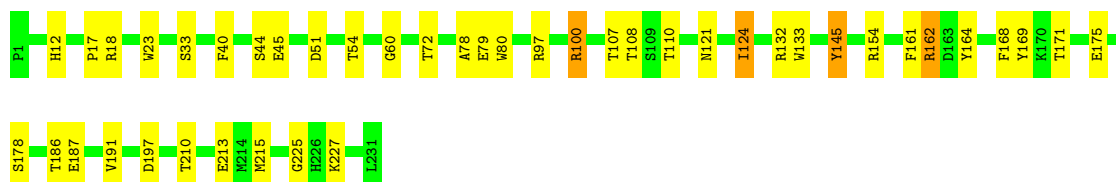
- Molecule 1: capsid protein

Chain fE:  84% 15% .




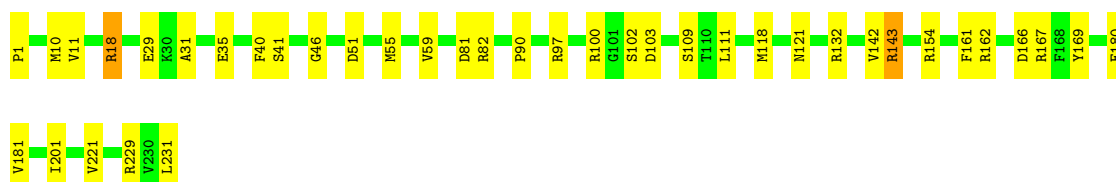
- Molecule 1: capsid protein

Chain fF:  81% 17% .




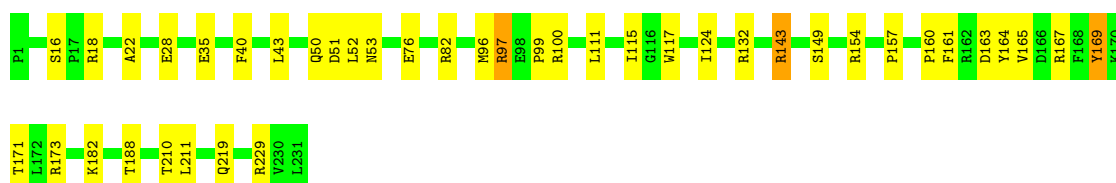
- Molecule 1: capsid protein

Chain fG:  83% 16% .

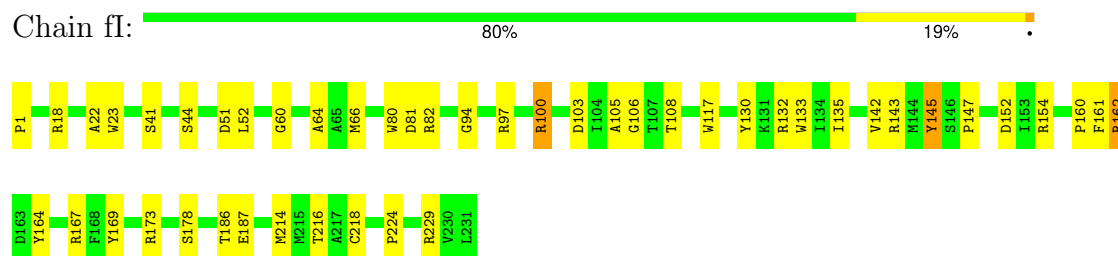


- Molecule 1: capsid protein

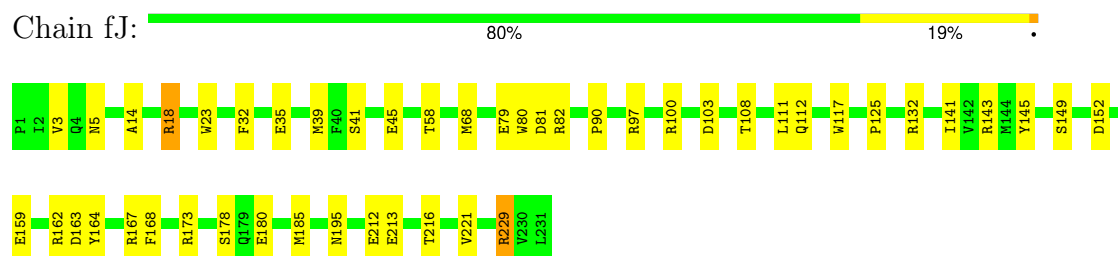
Chain fH:  82% 16% .



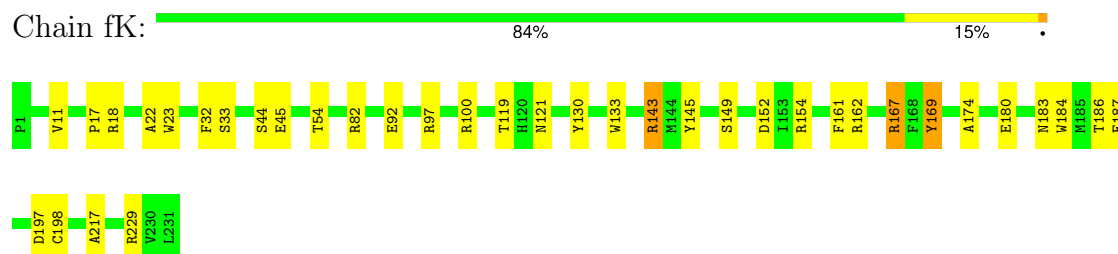
## • Molecule 1: capsid protein



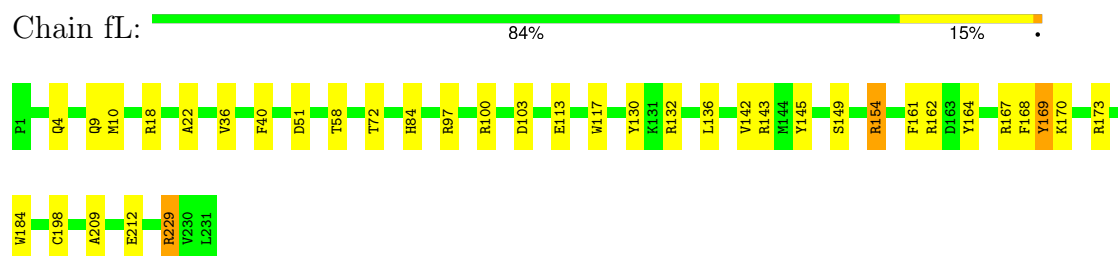
## • Molecule 1: capsid protein



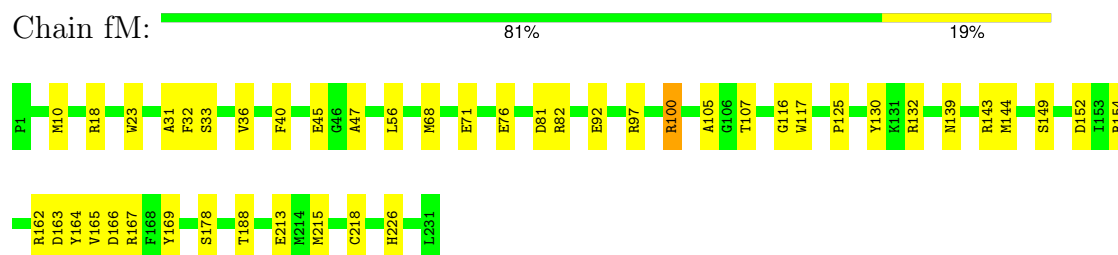
## • Molecule 1: capsid protein




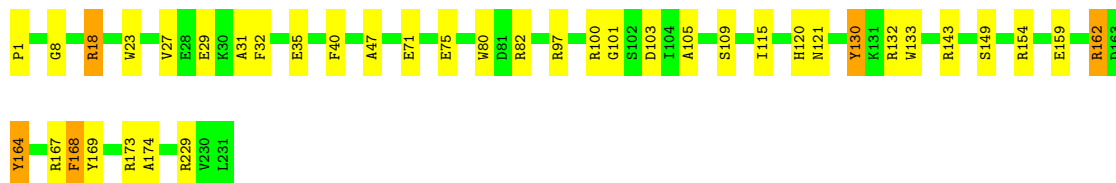
## • Molecule 1: capsid protein




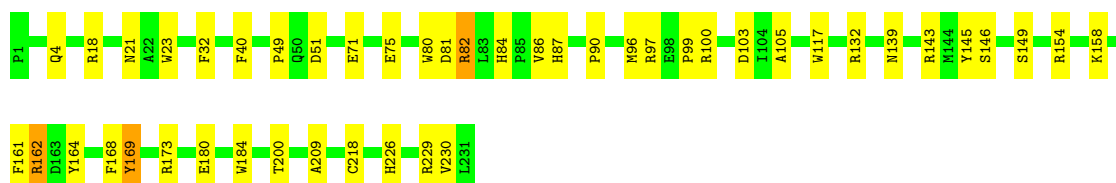
## • Molecule 1: capsid protein




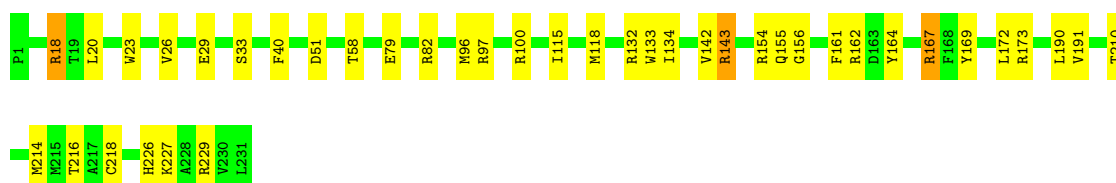
## • Molecule 1: capsid protein

Chain fN:  83% 15%


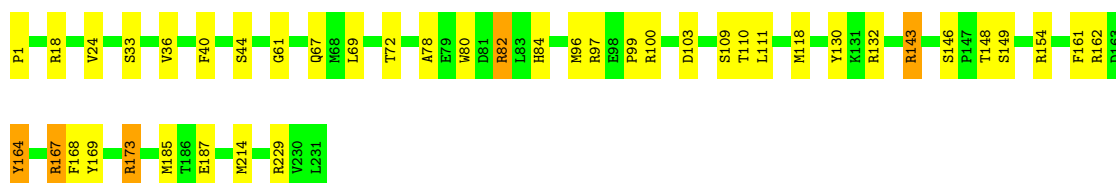
## • Molecule 1: capsid protein

Chain 1z:  80% 19%


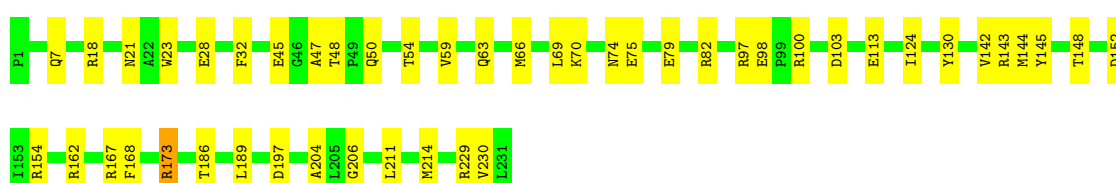
## • Molecule 1: capsid protein

Chain fO:  83% 16%

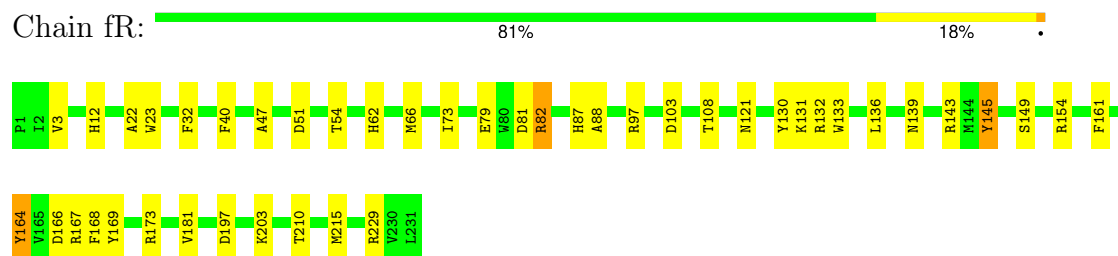
## • Molecule 1: capsid protein

Chain fP:  82% 16%

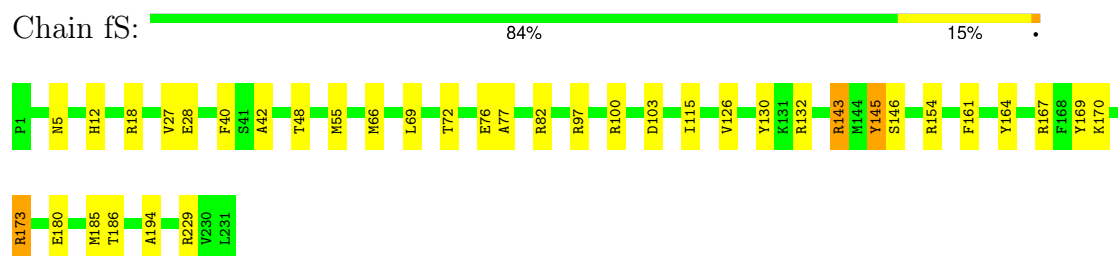
## • Molecule 1: capsid protein

Chain fQ:  80% 20%

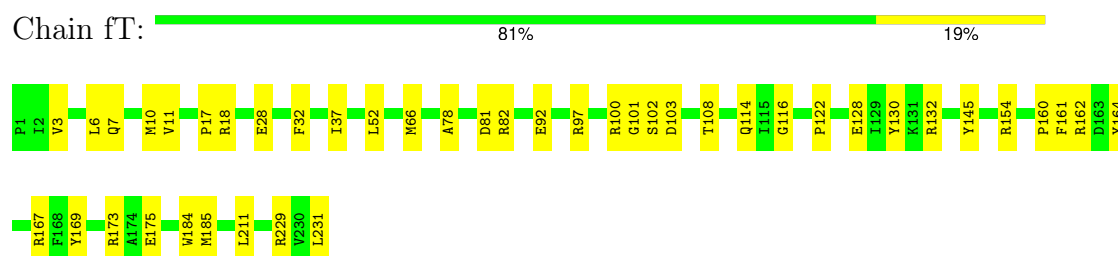
- Molecule 1: capsid protein



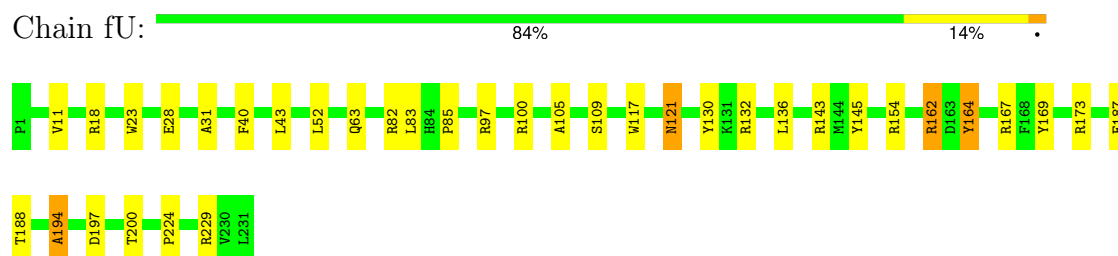
- Molecule 1: capsid protein



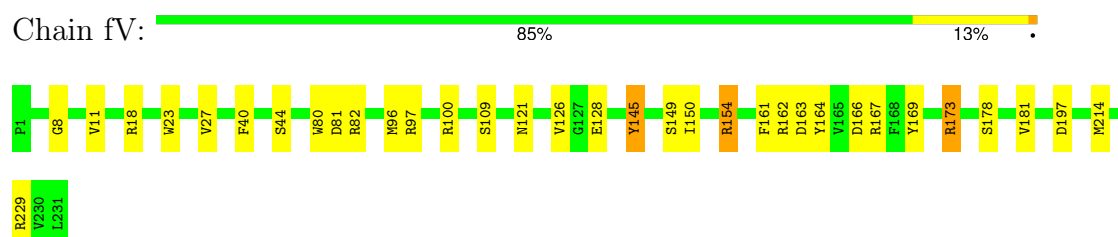
- Molecule 1: capsid protein




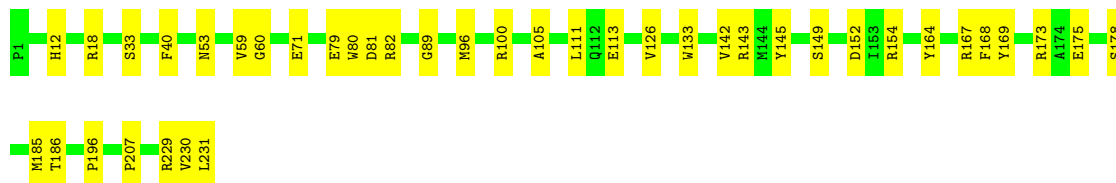
- Molecule 1: capsid protein




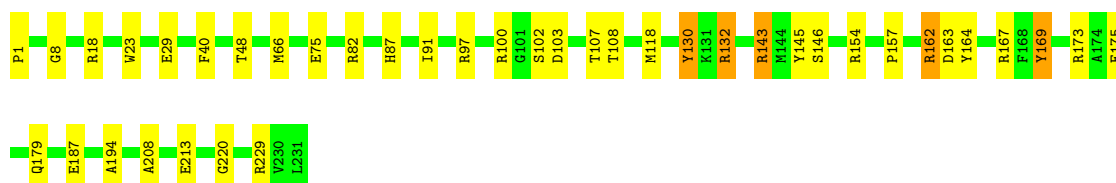
- Molecule 1: capsid protein




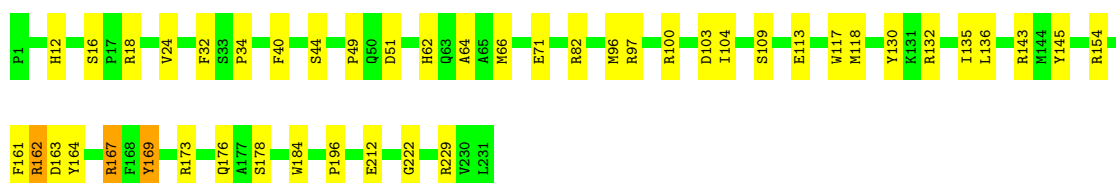
## • Molecule 1: capsid protein

Chain fW:  83% 17%


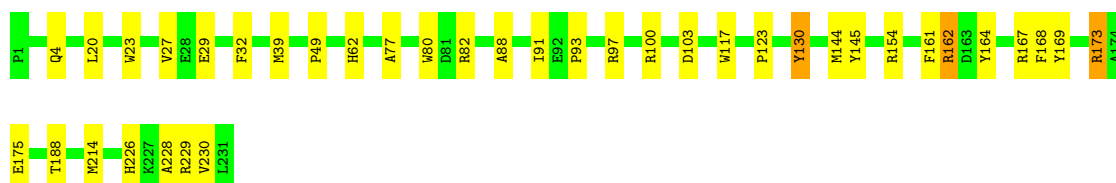
## • Molecule 1: capsid protein

Chain fX:  83% 15% •


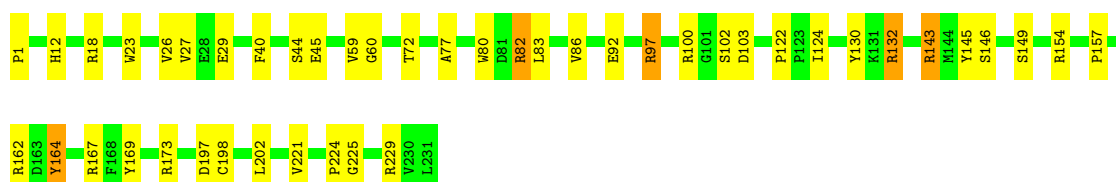
## • Molecule 1: capsid protein

Chain 1A:  81% 18% •

## • Molecule 1: capsid protein


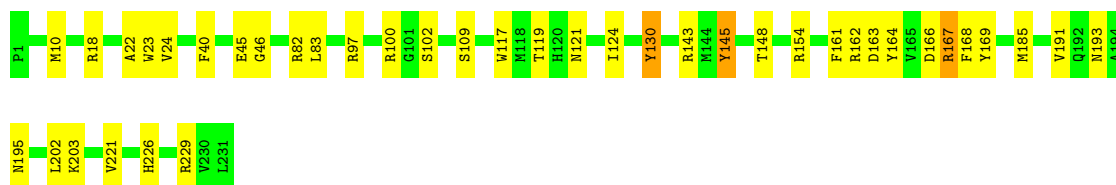
Chain fY:  84% 15% •

## • Molecule 1: capsid protein


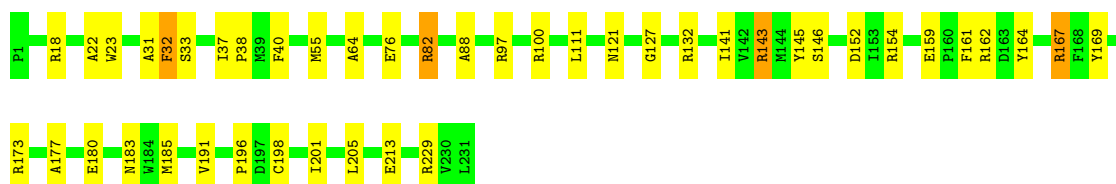
Chain fZ:  81% 17% •




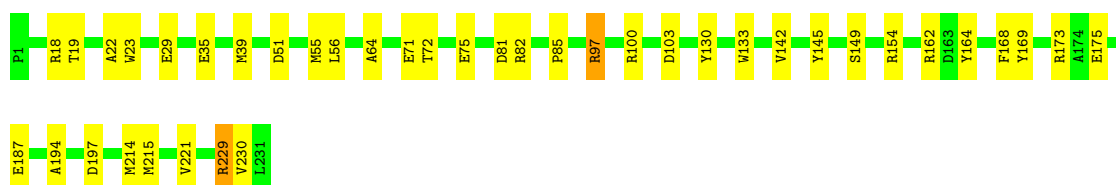
## • Molecule 1: capsid protein

Chain g0:  83% 16% •


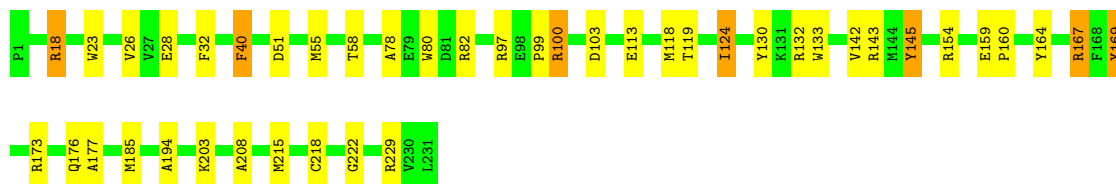
## • Molecule 1: capsid protein

Chain g1:  81% 17% •


## • Molecule 1: capsid protein

Chain g2:  83% 16% •

## • Molecule 1: capsid protein

Chain g3:  81% 16% •

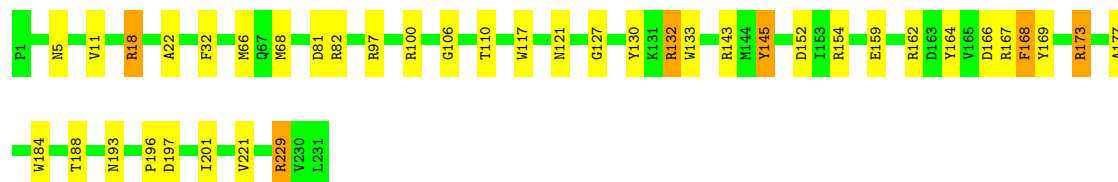
## • Molecule 1: capsid protein

Chain g4:  80% 18% •



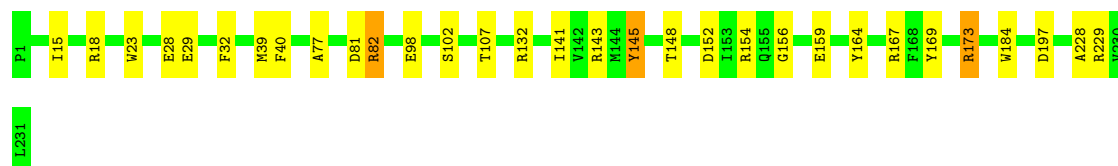
- Molecule 1: capsid protein

Chain g5: 83% 15% •



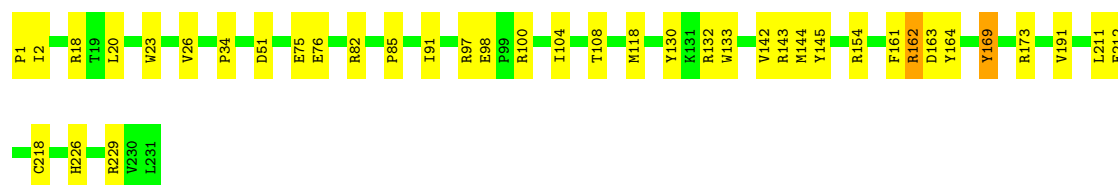
- Molecule 1: capsid protein

Chain g6: 87% 12% •



- Molecule 1: capsid protein

Chain g7: 83% 16% •



- Molecule 1: capsid protein

Chain 1B: 84% 14% •



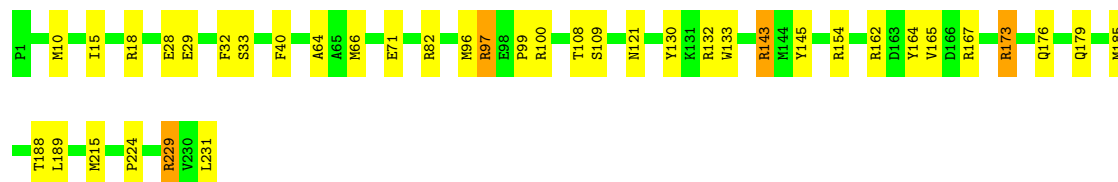
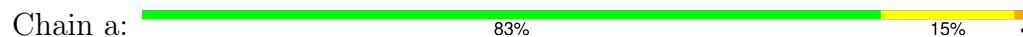
- Molecule 1: capsid protein

Chain 0: 78% 20% •

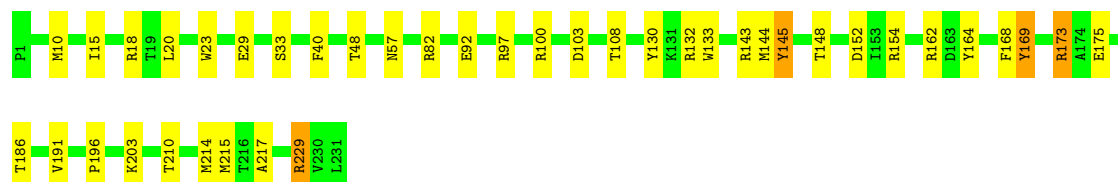
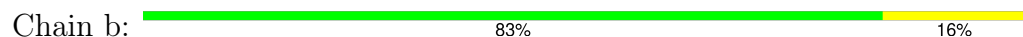




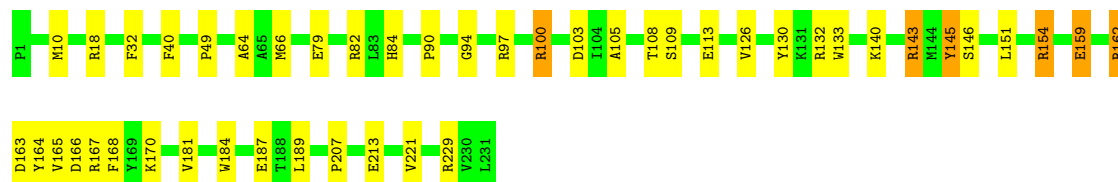
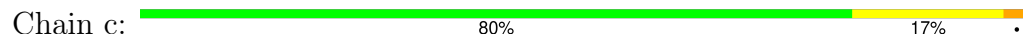
- Molecule 1: capsid protein



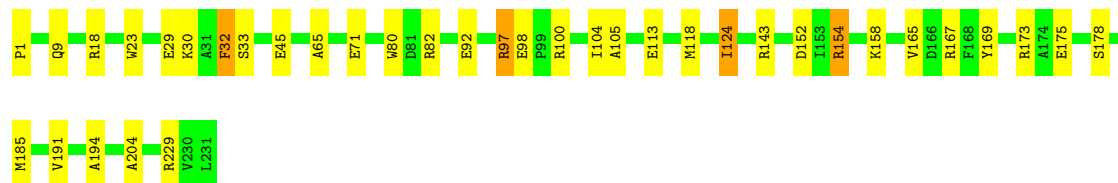
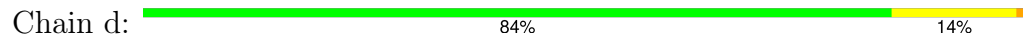
- Molecule 1: capsid protein



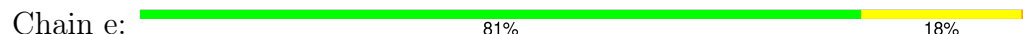
- Molecule 1: capsid protein



- Molecule 1: capsid protein



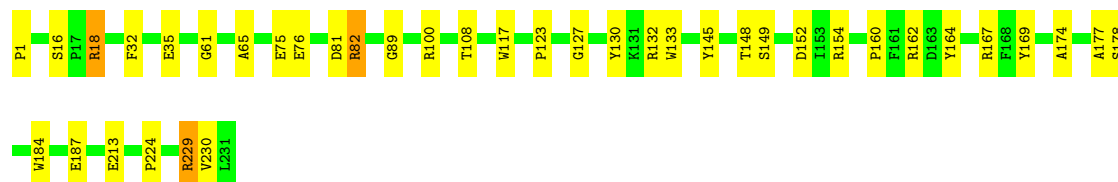
- Molecule 1: capsid protein





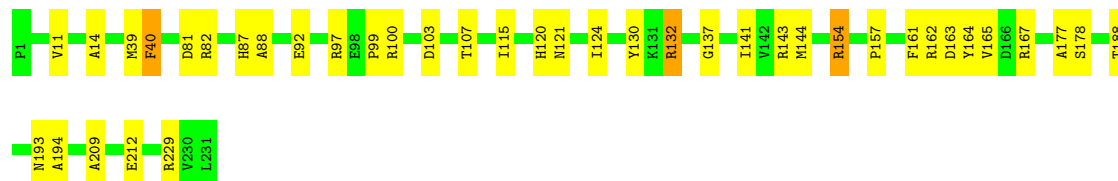
- Molecule 1: capsid protein

Chain f: 83% 16% •



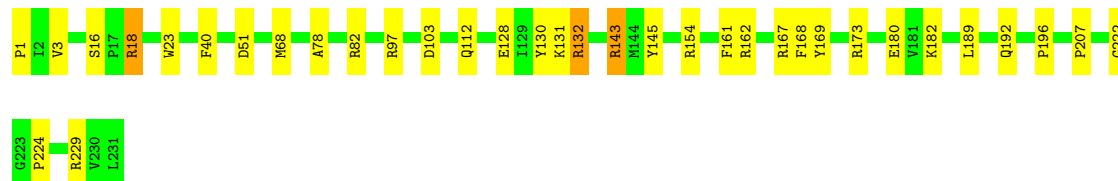
- Molecule 1: capsid protein

Chain g: 83% 16% •



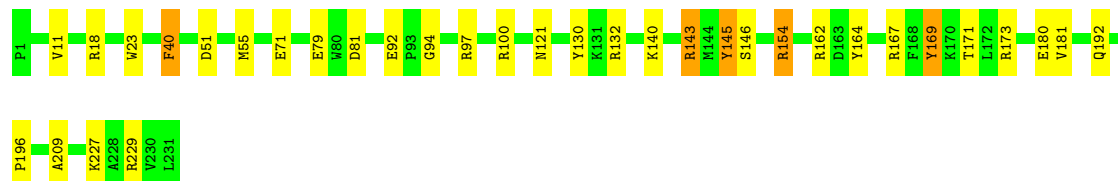
- Molecule 1: capsid protein

Chain h: 85% 14% •



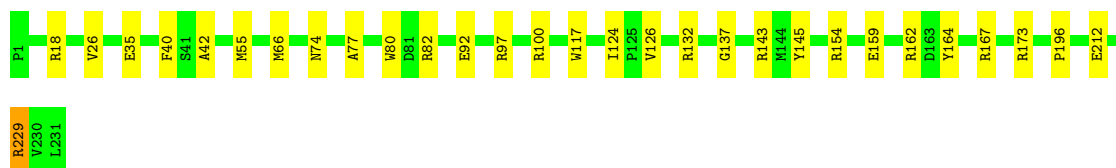
- Molecule 1: capsid protein

Chain i: 85% 13% •

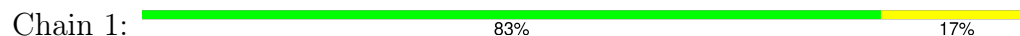


- Molecule 1: capsid protein

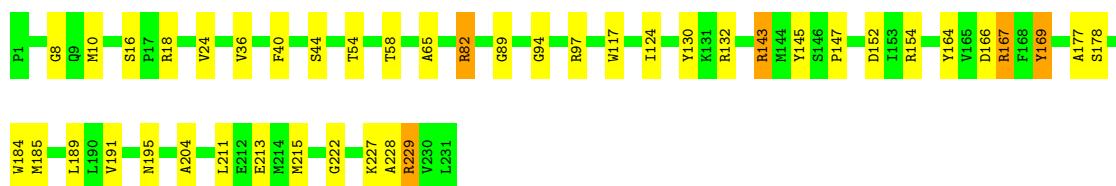
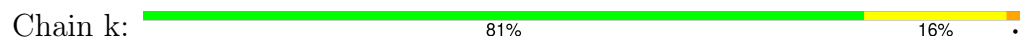
Chain j: 87% 13%



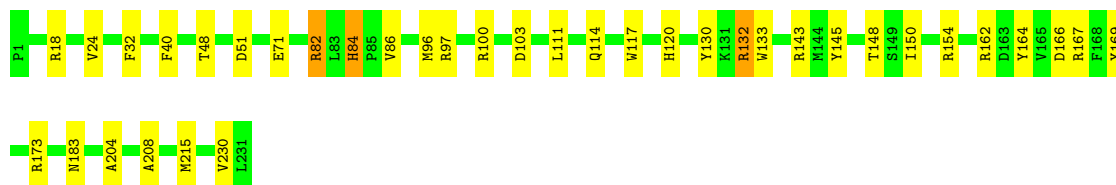
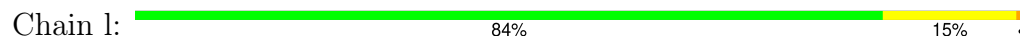
- Molecule 1: capsid protein



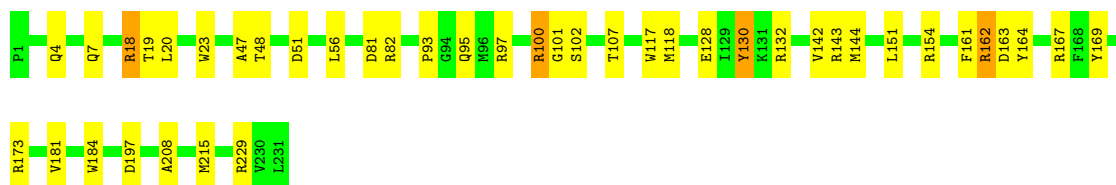
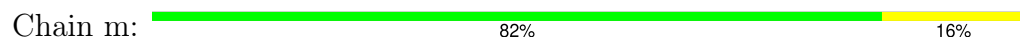
- Molecule 1: capsid protein



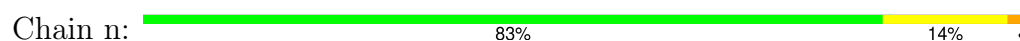
- Molecule 1: capsid protein

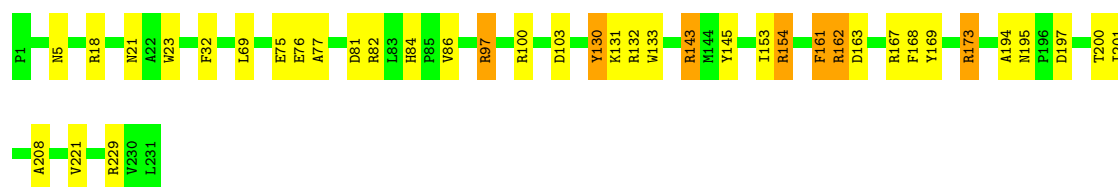


- Molecule 1: capsid protein



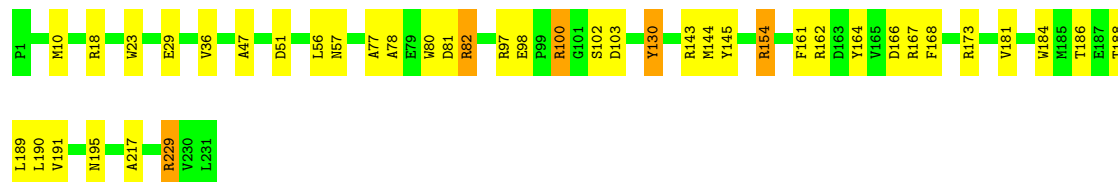
- Molecule 1: capsid protein





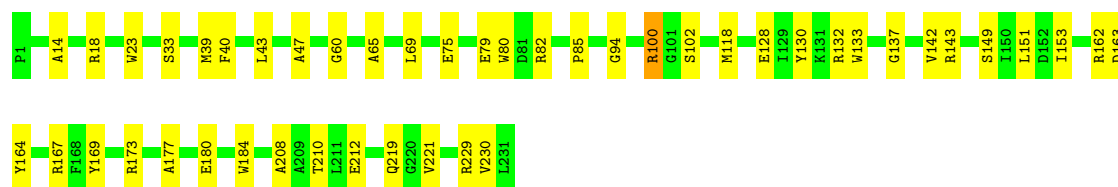
- Molecule 1: capsid protein

Chain o: 82% 16% .



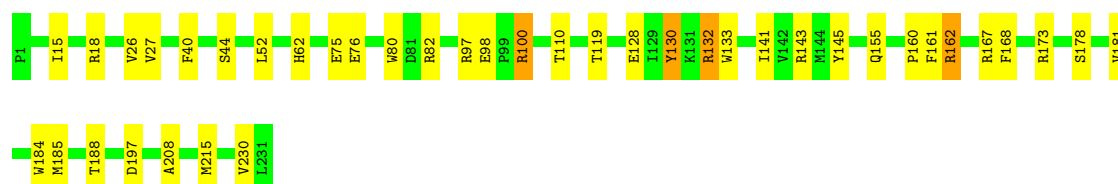
- Molecule 1: capsid protein

Chain p: 80% 19% .



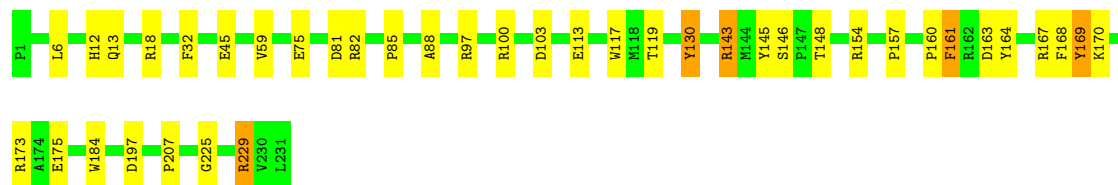
- Molecule 1: capsid protein

Chain q: 83% 16% .




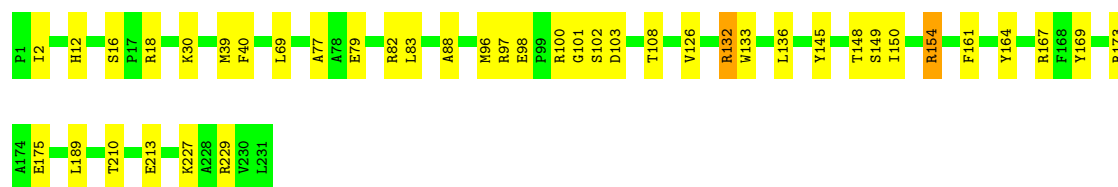
- Molecule 1: capsid protein

Chain r: 83% 15% .




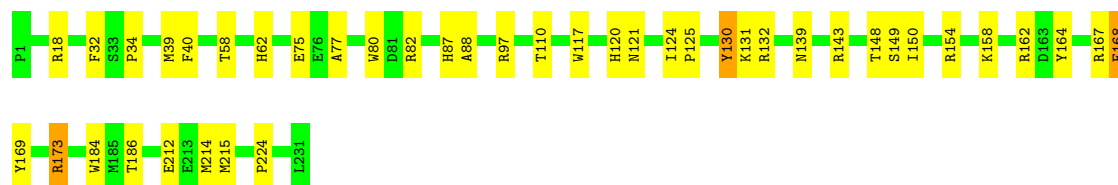
- Molecule 1: capsid protein

Chain s:  82% 17%




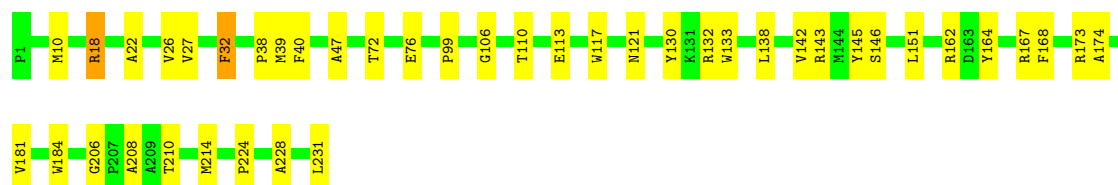
- Molecule 1: capsid protein

Chain t:  82% 17%




- Molecule 1: capsid protein

Chain 2:  82% 17%




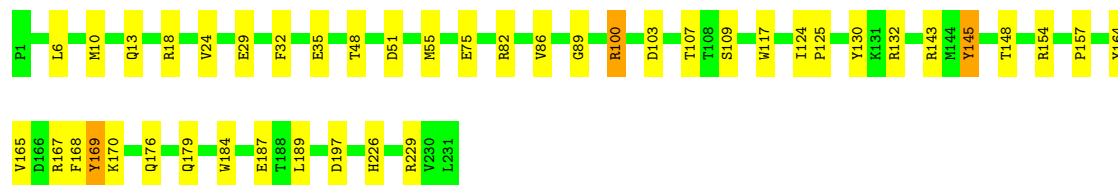
- Molecule 1: capsid protein

Chain u:  84% 16%




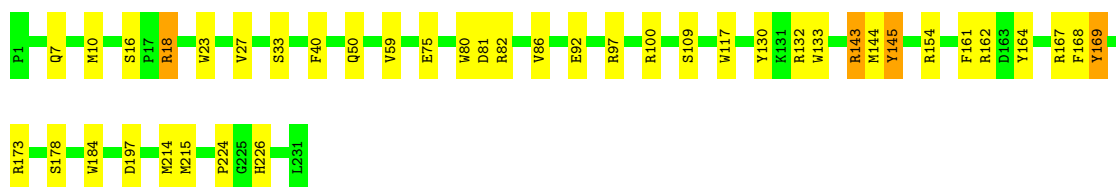
- Molecule 1: capsid protein

Chain v:  81% 17%




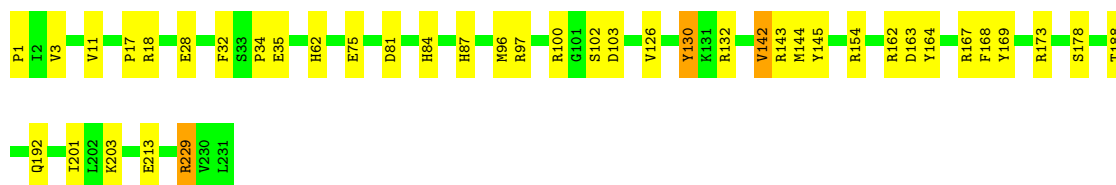
- Molecule 1: capsid protein

Chain w:  82% 16%




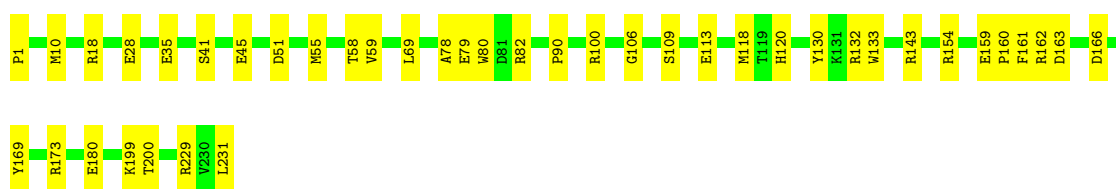
- Molecule 1: capsid protein

Chain x:  82% 16%




- Molecule 1: capsid protein

Chain y:  82% 18%




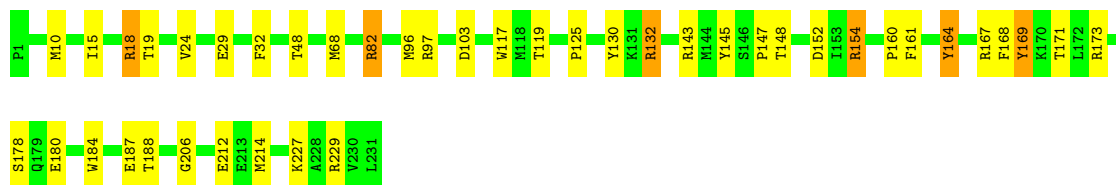
- Molecule 1: capsid protein

Chain z:  81% 18%




- Molecule 1: capsid protein

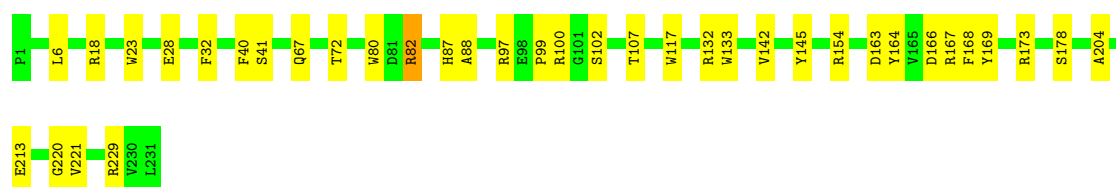
Chain A:  82% 16%




- Molecule 1: capsid protein

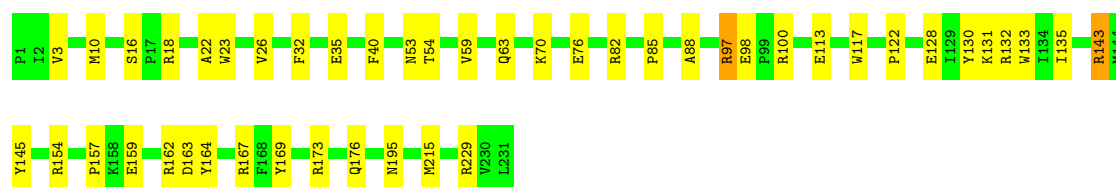


Chain B:  84% 16%




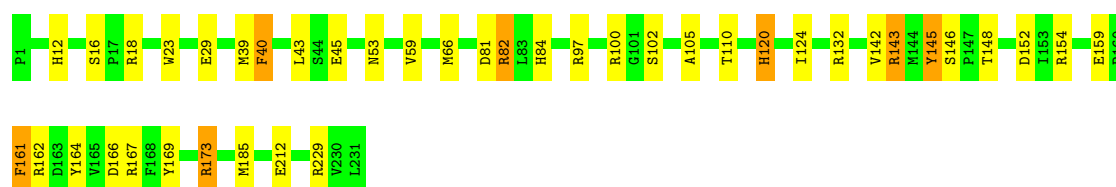
- Molecule 1: capsid protein

Chain C:  80% 19% •




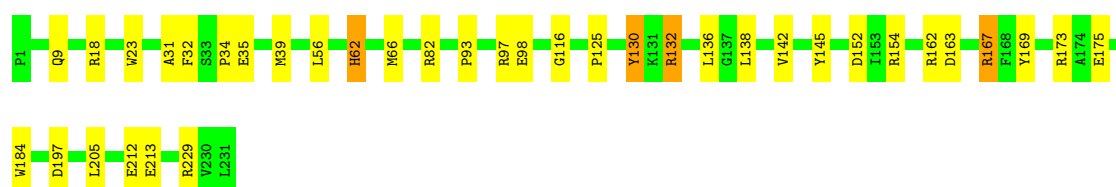
- Molecule 1: capsid protein

Chain D:  82% 15% •




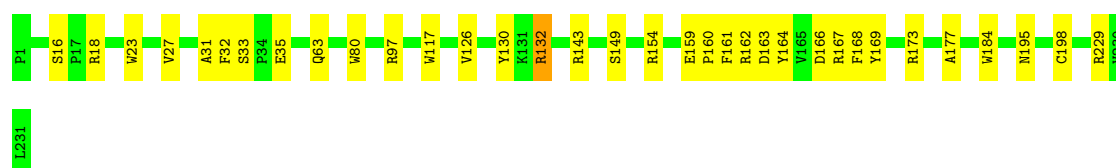
- Molecule 1: capsid protein

Chain 3:  84% 14% •




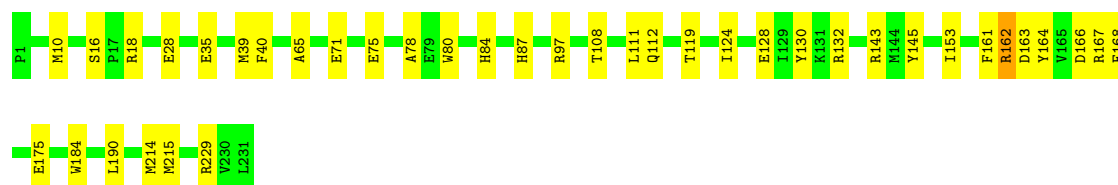
- Molecule 1: capsid protein

Chain E:  85% 14%




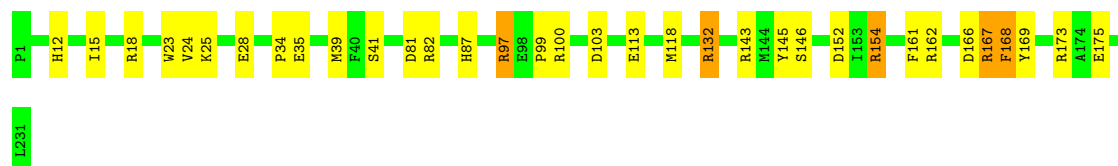
- Molecule 1: capsid protein

Chain F:  83% 16%




- Molecule 1: capsid protein

Chain G:  85% 13%




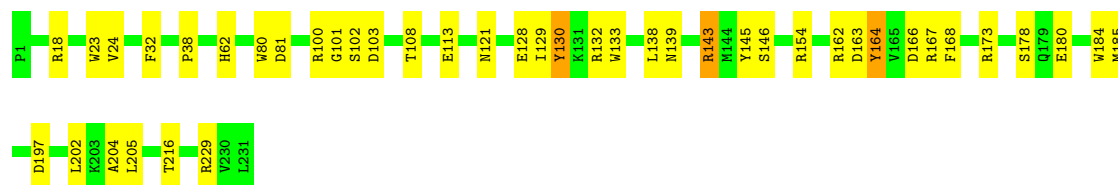
- Molecule 1: capsid protein

Chain H:  80% 19%




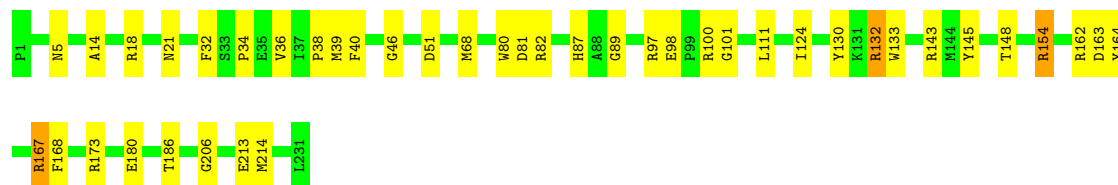
- Molecule 1: capsid protein

Chain I:  81% 17%




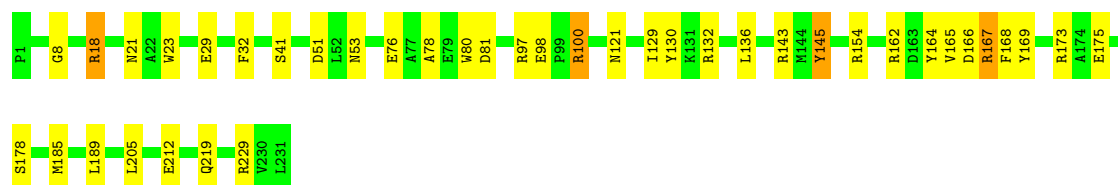
- Molecule 1: capsid protein

Chain J:  82% 17%




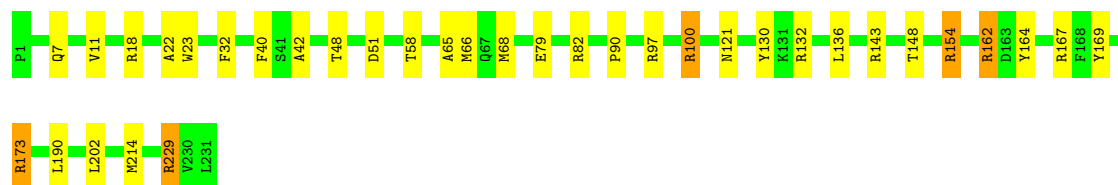
- Molecule 1: capsid protein

Chain K:  83% 16% •




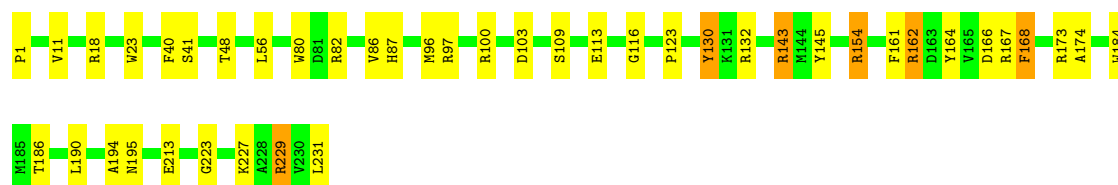
- Molecule 1: capsid protein

Chain L:  85% 13% •




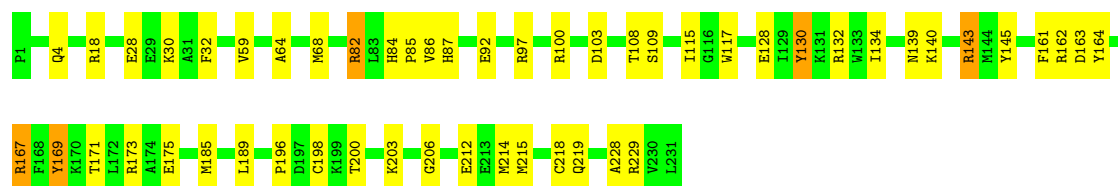
- Molecule 1: capsid protein

Chain M:  81% 16% •




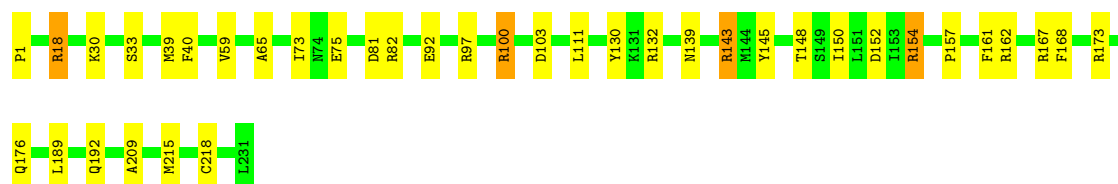
- Molecule 1: capsid protein

Chain N:  77% 20% •




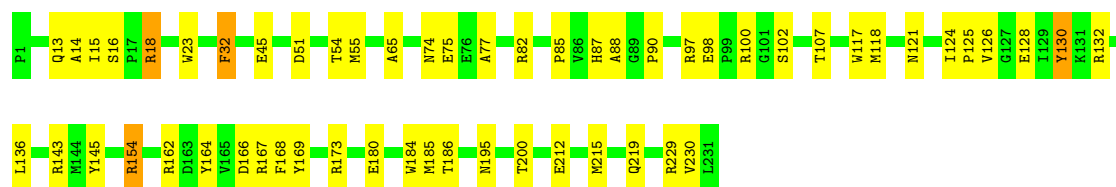
- Molecule 1: capsid protein

Chain 4:  84% 15% •




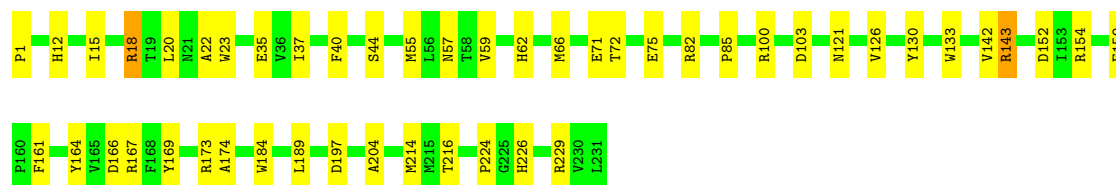
- Molecule 1: capsid protein

Chain O:  76% 23% .




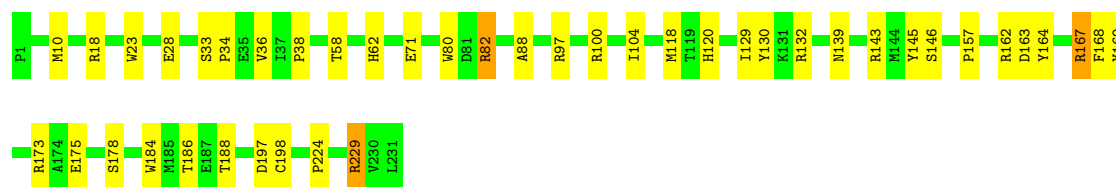
- Molecule 1: capsid protein

Chain P:  79% 20% .




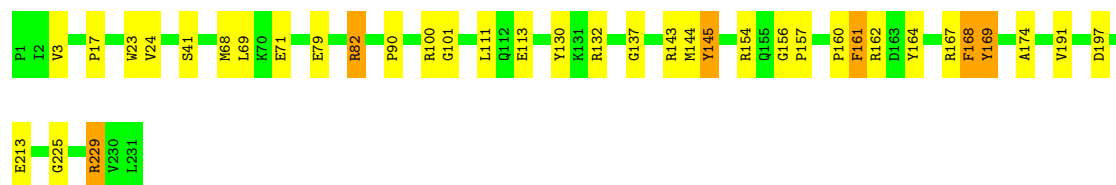
- Molecule 1: capsid protein

Chain Q:  81% 17% .




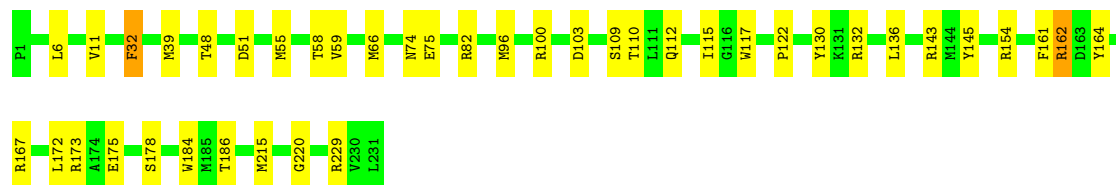
- Molecule 1: capsid protein

Chain R:  84% 13% .

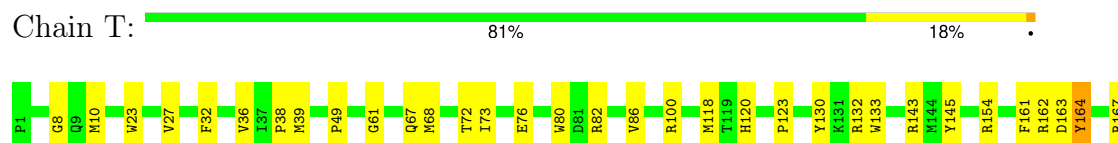


- Molecule 1: capsid protein

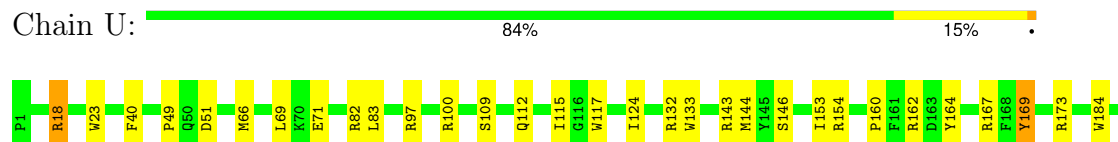
Chain S:  82% 17% .



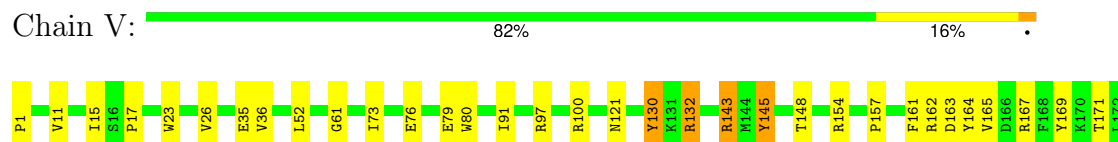
- Molecule 1: capsid protein



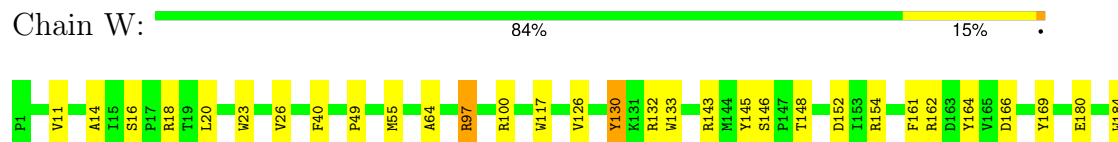
- Molecule 1: capsid protein



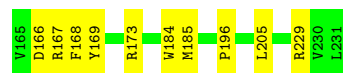
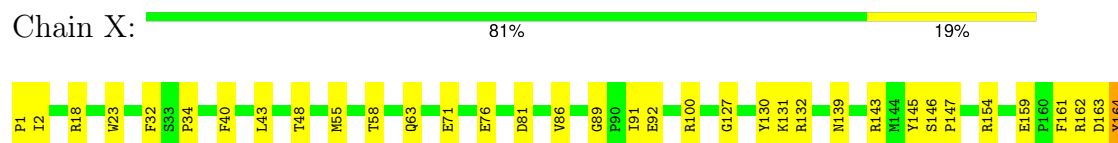
- Molecule 1: capsid protein




- Molecule 1: capsid protein



- Molecule 1: capsid protein




- Molecule 1: capsid protein

Chain 5: 




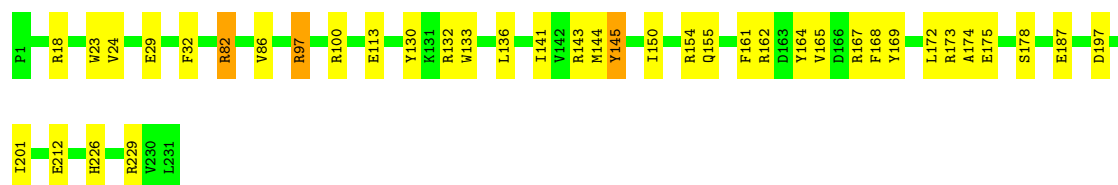
• Molecule 1: capsid protein

Chain 6: 




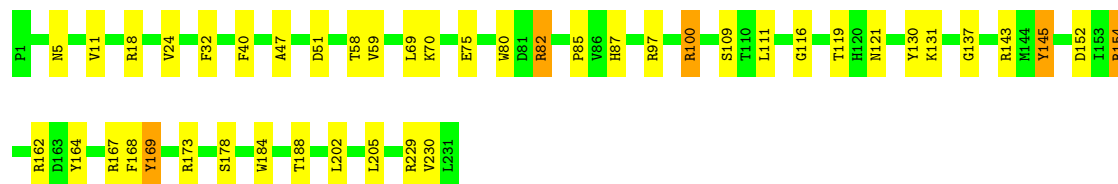
• Molecule 1: capsid protein

Chain 7: 




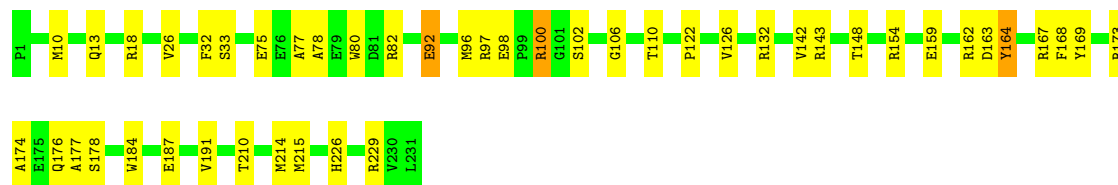
• Molecule 1: capsid protein

Chain 8: 



• Molecule 1: capsid protein

Chain 9: 



## 4 Experimental information

Property	Value	Source
EM reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of tilted images used	Not provided	
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	120	Depositor
Minimum defocus (nm)	8000	Depositor
Maximum defocus (nm)	8000	Depositor
Magnification	39000	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	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	0	1.63	8/1841 (0.4%)	2.10	56/2500 (2.2%)
1	1	1.64	12/1841 (0.7%)	2.01	50/2500 (2.0%)
1	10	1.64	12/1841 (0.7%)	2.16	47/2500 (1.9%)
1	11	1.65	14/1841 (0.8%)	2.02	35/2500 (1.4%)
1	12	1.61	5/1841 (0.3%)	2.07	44/2500 (1.8%)
1	13	1.62	12/1841 (0.7%)	1.98	34/2500 (1.4%)
1	14	1.64	9/1841 (0.5%)	2.02	43/2500 (1.7%)
1	15	1.65	14/1841 (0.8%)	2.00	44/2500 (1.8%)
1	16	1.63	12/1841 (0.7%)	1.97	46/2500 (1.8%)
1	17	1.57	9/1841 (0.5%)	1.96	35/2500 (1.4%)
1	18	1.63	15/1841 (0.8%)	2.00	46/2500 (1.8%)
1	19	1.60	13/1841 (0.7%)	2.03	50/2500 (2.0%)
1	1A	1.59	5/1841 (0.3%)	2.01	51/2500 (2.0%)
1	1B	1.67	14/1841 (0.8%)	1.89	34/2500 (1.4%)
1	1C	1.59	11/1841 (0.6%)	1.99	43/2500 (1.7%)
1	1D	1.65	12/1841 (0.7%)	2.01	48/2500 (1.9%)
1	1E	1.57	5/1841 (0.3%)	1.92	36/2500 (1.4%)
1	1F	1.66	12/1841 (0.7%)	2.03	47/2500 (1.9%)
1	1G	1.68	12/1841 (0.7%)	2.00	50/2500 (2.0%)
1	1H	1.64	17/1841 (0.9%)	2.11	51/2500 (2.0%)
1	1I	1.66	17/1841 (0.9%)	2.08	41/2500 (1.6%)
1	1J	1.68	18/1841 (1.0%)	1.93	38/2500 (1.5%)
1	1K	1.64	15/1841 (0.8%)	1.94	40/2500 (1.6%)
1	1L	1.64	9/1841 (0.5%)	2.01	40/2500 (1.6%)
1	1M	1.62	8/1841 (0.4%)	2.01	52/2500 (2.1%)
1	1N	1.62	8/1841 (0.4%)	1.98	41/2500 (1.6%)
1	1O	1.64	11/1841 (0.6%)	1.98	47/2500 (1.9%)
1	1P	1.62	13/1841 (0.7%)	1.98	41/2500 (1.6%)
1	1Q	1.64	10/1841 (0.5%)	2.04	38/2500 (1.5%)
1	1R	1.64	14/1841 (0.8%)	2.12	49/2500 (2.0%)
1	1S	1.70	14/1841 (0.8%)	2.08	42/2500 (1.7%)
1	1T	1.60	7/1841 (0.4%)	1.98	39/2500 (1.6%)
1	1U	1.61	8/1841 (0.4%)	2.03	41/2500 (1.6%)
1	1V	1.66	17/1841 (0.9%)	2.10	43/2500 (1.7%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	1W	1.63	8/1841 (0.4%)	1.94	41/2500 (1.6%)
1	1X	1.64	15/1841 (0.8%)	2.04	44/2500 (1.8%)
1	1Y	1.64	11/1841 (0.6%)	2.02	49/2500 (2.0%)
1	1Z	1.63	10/1841 (0.5%)	2.02	41/2500 (1.6%)
1	1a	1.62	9/1841 (0.5%)	1.98	41/2500 (1.6%)
1	1b	1.60	7/1841 (0.4%)	1.97	42/2500 (1.7%)
1	1c	1.67	18/1841 (1.0%)	2.04	43/2500 (1.7%)
1	1d	1.68	20/1841 (1.1%)	2.00	55/2500 (2.2%)
1	1e	1.60	10/1841 (0.5%)	2.08	44/2500 (1.8%)
1	1f	1.60	10/1841 (0.5%)	1.98	50/2500 (2.0%)
1	1g	1.64	10/1841 (0.5%)	2.04	48/2500 (1.9%)
1	1h	1.62	9/1841 (0.5%)	2.01	51/2500 (2.0%)
1	1i	1.68	15/1841 (0.8%)	2.02	43/2500 (1.7%)
1	1j	1.64	12/1841 (0.7%)	1.98	46/2500 (1.8%)
1	1k	1.69	14/1841 (0.8%)	2.09	40/2500 (1.6%)
1	1l	1.65	9/1841 (0.5%)	2.04	45/2500 (1.8%)
1	1m	1.67	9/1841 (0.5%)	2.02	52/2500 (2.1%)
1	1n	1.68	13/1841 (0.7%)	2.06	48/2500 (1.9%)
1	1o	1.65	10/1841 (0.5%)	1.94	51/2500 (2.0%)
1	1p	1.63	6/1841 (0.3%)	1.98	39/2500 (1.6%)
1	1q	1.56	3/1841 (0.2%)	1.94	40/2500 (1.6%)
1	1r	1.62	21/1841 (1.1%)	1.91	41/2500 (1.6%)
1	1s	1.62	12/1841 (0.7%)	1.99	33/2500 (1.3%)
1	1t	1.66	10/1841 (0.5%)	1.91	29/2500 (1.2%)
1	1u	1.63	9/1841 (0.5%)	2.02	40/2500 (1.6%)
1	1v	1.59	9/1841 (0.5%)	1.91	36/2500 (1.4%)
1	1w	1.66	11/1841 (0.6%)	2.08	39/2500 (1.6%)
1	1x	1.66	13/1841 (0.7%)	2.02	41/2500 (1.6%)
1	1y	1.62	8/1841 (0.4%)	1.99	44/2500 (1.8%)
1	1z	1.59	9/1841 (0.5%)	2.11	58/2500 (2.3%)
1	2	1.62	13/1841 (0.7%)	1.97	41/2500 (1.6%)
1	20	1.63	12/1841 (0.7%)	1.97	35/2500 (1.4%)
1	21	1.65	11/1841 (0.6%)	1.98	39/2500 (1.6%)
1	22	1.66	14/1841 (0.8%)	2.08	63/2500 (2.5%)
1	23	1.69	19/1841 (1.0%)	2.04	44/2500 (1.8%)
1	24	1.64	11/1841 (0.6%)	2.02	45/2500 (1.8%)
1	25	1.65	9/1841 (0.5%)	2.10	49/2500 (2.0%)
1	26	1.62	12/1841 (0.7%)	1.91	43/2500 (1.7%)
1	27	1.64	8/1841 (0.4%)	1.97	36/2500 (1.4%)
1	28	1.61	10/1841 (0.5%)	1.97	46/2500 (1.8%)
1	29	1.71	8/1841 (0.4%)	2.01	43/2500 (1.7%)
1	2A	1.68	15/1841 (0.8%)	2.01	42/2500 (1.7%)
1	2B	1.63	12/1841 (0.7%)	1.97	36/2500 (1.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	2C	1.63	13/1841 (0.7%)	2.01	46/2500 (1.8%)
1	2D	1.64	12/1841 (0.7%)	2.00	39/2500 (1.6%)
1	2E	1.66	11/1841 (0.6%)	2.07	47/2500 (1.9%)
1	2F	1.62	8/1841 (0.4%)	2.06	48/2500 (1.9%)
1	2G	1.65	13/1841 (0.7%)	1.98	51/2500 (2.0%)
1	2H	1.60	8/1841 (0.4%)	1.89	38/2500 (1.5%)
1	2I	1.61	9/1841 (0.5%)	1.93	43/2500 (1.7%)
1	2J	1.61	10/1841 (0.5%)	2.04	41/2500 (1.6%)
1	2K	1.59	7/1841 (0.4%)	1.99	47/2500 (1.9%)
1	2L	1.63	13/1841 (0.7%)	1.98	37/2500 (1.5%)
1	2M	1.62	9/1841 (0.5%)	2.10	39/2500 (1.6%)
1	2N	1.63	9/1841 (0.5%)	2.12	41/2500 (1.6%)
1	2O	1.64	11/1841 (0.6%)	2.14	47/2500 (1.9%)
1	2P	1.63	8/1841 (0.4%)	1.98	44/2500 (1.8%)
1	2Q	1.66	13/1841 (0.7%)	1.96	41/2500 (1.6%)
1	2R	1.62	8/1841 (0.4%)	2.03	45/2500 (1.8%)
1	2S	1.69	18/1841 (1.0%)	2.16	60/2500 (2.4%)
1	2T	1.59	6/1841 (0.3%)	2.03	51/2500 (2.0%)
1	2U	1.63	11/1841 (0.6%)	1.91	44/2500 (1.8%)
1	2V	1.59	7/1841 (0.4%)	1.98	45/2500 (1.8%)
1	2W	1.66	11/1841 (0.6%)	1.92	40/2500 (1.6%)
1	2X	1.66	11/1841 (0.6%)	2.13	44/2500 (1.8%)
1	2Y	1.68	14/1841 (0.8%)	2.09	45/2500 (1.8%)
1	2Z	1.67	18/1841 (1.0%)	1.95	44/2500 (1.8%)
1	2a	1.60	6/1841 (0.3%)	2.02	46/2500 (1.8%)
1	2b	1.67	11/1841 (0.6%)	1.92	33/2500 (1.3%)
1	2c	1.58	10/1841 (0.5%)	2.01	54/2500 (2.2%)
1	2d	1.62	10/1841 (0.5%)	1.91	28/2500 (1.1%)
1	2e	1.64	14/1841 (0.8%)	1.97	47/2500 (1.9%)
1	2f	1.64	12/1841 (0.7%)	1.97	34/2500 (1.4%)
1	2g	1.63	10/1841 (0.5%)	2.04	41/2500 (1.6%)
1	2h	1.58	7/1841 (0.4%)	1.99	43/2500 (1.7%)
1	2i	1.60	6/1841 (0.3%)	2.14	49/2500 (2.0%)
1	2j	1.63	9/1841 (0.5%)	2.10	51/2500 (2.0%)
1	2k	1.60	9/1841 (0.5%)	2.00	47/2500 (1.9%)
1	2l	1.61	10/1841 (0.5%)	2.12	53/2500 (2.1%)
1	2m	1.63	16/1841 (0.9%)	1.97	39/2500 (1.6%)
1	2n	1.63	9/1841 (0.5%)	2.07	44/2500 (1.8%)
1	2o	1.62	9/1841 (0.5%)	2.04	55/2500 (2.2%)
1	2p	1.66	8/1841 (0.4%)	2.09	47/2500 (1.9%)
1	2q	1.68	13/1841 (0.7%)	1.97	32/2500 (1.3%)
1	2r	1.63	11/1841 (0.6%)	2.07	43/2500 (1.7%)
1	2s	1.65	13/1841 (0.7%)	2.14	50/2500 (2.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	2t	1.66	15/1841 (0.8%)	1.95	46/2500 (1.8%)
1	2u	1.62	10/1841 (0.5%)	2.01	37/2500 (1.5%)
1	2v	1.58	6/1841 (0.3%)	2.01	44/2500 (1.8%)
1	2w	1.65	6/1841 (0.3%)	2.04	55/2500 (2.2%)
1	2x	1.66	8/1841 (0.4%)	1.91	49/2500 (2.0%)
1	2y	1.68	14/1841 (0.8%)	2.03	50/2500 (2.0%)
1	2z	1.65	11/1841 (0.6%)	1.95	44/2500 (1.8%)
1	3	1.67	7/1841 (0.4%)	2.00	45/2500 (1.8%)
1	30	1.63	7/1841 (0.4%)	1.92	40/2500 (1.6%)
1	31	1.65	15/1841 (0.8%)	1.98	43/2500 (1.7%)
1	32	1.63	7/1841 (0.4%)	2.09	53/2500 (2.1%)
1	33	1.59	6/1841 (0.3%)	2.05	51/2500 (2.0%)
1	34	1.60	7/1841 (0.4%)	2.00	42/2500 (1.7%)
1	35	1.62	13/1841 (0.7%)	2.12	52/2500 (2.1%)
1	36	1.59	10/1841 (0.5%)	2.02	44/2500 (1.8%)
1	37	1.58	3/1841 (0.2%)	1.95	40/2500 (1.6%)
1	38	1.65	10/1841 (0.5%)	2.08	45/2500 (1.8%)
1	39	1.63	18/1841 (1.0%)	1.96	42/2500 (1.7%)
1	3A	1.65	14/1841 (0.8%)	1.99	39/2500 (1.6%)
1	3B	1.65	9/1841 (0.5%)	2.02	47/2500 (1.9%)
1	3C	1.64	8/1841 (0.4%)	2.02	51/2500 (2.0%)
1	3D	1.69	13/1841 (0.7%)	1.98	38/2500 (1.5%)
1	3E	1.62	9/1841 (0.5%)	2.11	44/2500 (1.8%)
1	3F	1.67	6/1841 (0.3%)	2.02	58/2500 (2.3%)
1	3G	1.68	15/1841 (0.8%)	1.93	54/2500 (2.2%)
1	3H	1.64	10/1841 (0.5%)	2.05	50/2500 (2.0%)
1	3I	1.60	7/1841 (0.4%)	2.14	49/2500 (2.0%)
1	3J	1.61	11/1841 (0.6%)	1.99	48/2500 (1.9%)
1	3K	1.64	8/1841 (0.4%)	2.04	44/2500 (1.8%)
1	3L	1.66	14/1841 (0.8%)	2.13	58/2500 (2.3%)
1	3M	1.63	12/1841 (0.7%)	2.02	47/2500 (1.9%)
1	3N	1.64	10/1841 (0.5%)	2.01	46/2500 (1.8%)
1	3O	1.70	18/1841 (1.0%)	1.98	48/2500 (1.9%)
1	3P	1.64	8/1841 (0.4%)	2.05	47/2500 (1.9%)
1	3Q	1.62	12/1841 (0.7%)	1.99	42/2500 (1.7%)
1	3R	1.57	5/1841 (0.3%)	2.09	52/2500 (2.1%)
1	3S	1.66	12/1841 (0.7%)	1.95	33/2500 (1.3%)
1	3T	1.60	15/1841 (0.8%)	2.05	37/2500 (1.5%)
1	3U	1.64	8/1841 (0.4%)	2.07	39/2500 (1.6%)
1	3V	1.67	15/1841 (0.8%)	1.90	39/2500 (1.6%)
1	3W	1.65	9/1841 (0.5%)	2.05	55/2500 (2.2%)
1	3X	1.66	14/1841 (0.8%)	2.02	53/2500 (2.1%)
1	3Y	1.62	11/1841 (0.6%)	1.94	39/2500 (1.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	3Z	1.67	12/1841 (0.7%)	2.05	50/2500 (2.0%)
1	3a	1.61	11/1841 (0.6%)	2.02	44/2500 (1.8%)
1	3b	1.61	11/1841 (0.6%)	1.93	44/2500 (1.8%)
1	3c	1.64	8/1841 (0.4%)	2.02	42/2500 (1.7%)
1	3d	1.66	16/1841 (0.9%)	2.02	44/2500 (1.8%)
1	3e	1.65	17/1841 (0.9%)	1.98	52/2500 (2.1%)
1	3f	1.60	11/1841 (0.6%)	2.10	51/2500 (2.0%)
1	3g	1.62	11/1841 (0.6%)	2.09	43/2500 (1.7%)
1	3h	1.63	11/1841 (0.6%)	1.95	38/2500 (1.5%)
1	3i	1.60	7/1841 (0.4%)	1.94	37/2500 (1.5%)
1	3j	1.62	10/1841 (0.5%)	1.95	44/2500 (1.8%)
1	3k	1.61	8/1841 (0.4%)	1.98	47/2500 (1.9%)
1	3l	1.67	14/1841 (0.8%)	2.00	47/2500 (1.9%)
1	3m	1.65	9/1841 (0.5%)	1.93	42/2500 (1.7%)
1	3n	1.62	10/1841 (0.5%)	2.01	38/2500 (1.5%)
1	3o	1.67	17/1841 (0.9%)	2.14	47/2500 (1.9%)
1	3p	1.63	9/1841 (0.5%)	2.17	54/2500 (2.2%)
1	3q	1.64	11/1841 (0.6%)	1.96	44/2500 (1.8%)
1	3r	1.60	4/1841 (0.2%)	1.94	33/2500 (1.3%)
1	3s	1.61	11/1841 (0.6%)	2.11	37/2500 (1.5%)
1	3t	1.63	10/1841 (0.5%)	1.89	33/2500 (1.3%)
1	3u	1.66	15/1841 (0.8%)	2.03	40/2500 (1.6%)
1	3v	1.66	8/1841 (0.4%)	1.98	52/2500 (2.1%)
1	3w	1.58	6/1841 (0.3%)	1.98	40/2500 (1.6%)
1	3x	1.63	8/1841 (0.4%)	2.01	40/2500 (1.6%)
1	3y	1.59	9/1841 (0.5%)	2.02	53/2500 (2.1%)
1	3z	1.65	11/1841 (0.6%)	2.09	47/2500 (1.9%)
1	4	1.61	7/1841 (0.4%)	1.94	37/2500 (1.5%)
1	40	1.63	11/1841 (0.6%)	2.00	41/2500 (1.6%)
1	41	1.59	10/1841 (0.5%)	2.07	39/2500 (1.6%)
1	42	1.61	5/1841 (0.3%)	1.99	40/2500 (1.6%)
1	43	1.69	11/1841 (0.6%)	1.97	43/2500 (1.7%)
1	44	1.62	11/1841 (0.6%)	2.01	47/2500 (1.9%)
1	45	1.55	4/1841 (0.2%)	2.02	48/2500 (1.9%)
1	46	1.64	12/1841 (0.7%)	1.98	44/2500 (1.8%)
1	47	1.65	10/1841 (0.5%)	2.10	36/2500 (1.4%)
1	48	1.66	13/1841 (0.7%)	2.08	41/2500 (1.6%)
1	49	1.62	8/1841 (0.4%)	2.06	52/2500 (2.1%)
1	4A	1.55	7/1841 (0.4%)	2.09	44/2500 (1.8%)
1	4B	1.56	5/1841 (0.3%)	1.98	41/2500 (1.6%)
1	4C	1.60	3/1841 (0.2%)	1.95	39/2500 (1.6%)
1	4D	1.65	15/1841 (0.8%)	1.93	36/2500 (1.4%)
1	4E	1.64	11/1841 (0.6%)	2.11	49/2500 (2.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	4F	1.63	9/1841 (0.5%)	1.96	48/2500 (1.9%)
1	4G	1.65	14/1841 (0.8%)	1.93	41/2500 (1.6%)
1	4H	1.63	9/1841 (0.5%)	2.05	38/2500 (1.5%)
1	4I	1.59	7/1841 (0.4%)	2.00	38/2500 (1.5%)
1	4J	1.65	9/1841 (0.5%)	2.02	67/2500 (2.7%)
1	4K	1.64	14/1841 (0.8%)	1.98	40/2500 (1.6%)
1	4L	1.60	13/1841 (0.7%)	1.99	36/2500 (1.4%)
1	4M	1.63	11/1841 (0.6%)	2.03	49/2500 (2.0%)
1	4N	1.59	9/1841 (0.5%)	2.05	46/2500 (1.8%)
1	4O	1.60	8/1841 (0.4%)	2.04	47/2500 (1.9%)
1	4P	1.60	7/1841 (0.4%)	2.02	45/2500 (1.8%)
1	4Q	1.63	14/1841 (0.8%)	1.99	43/2500 (1.7%)
1	4R	1.65	12/1841 (0.7%)	1.88	40/2500 (1.6%)
1	4S	1.68	16/1841 (0.9%)	2.03	39/2500 (1.6%)
1	4T	1.61	12/1841 (0.7%)	2.00	37/2500 (1.5%)
1	4U	1.58	9/1841 (0.5%)	1.99	49/2500 (2.0%)
1	4V	1.58	9/1841 (0.5%)	1.97	44/2500 (1.8%)
1	4W	1.62	8/1841 (0.4%)	1.96	42/2500 (1.7%)
1	4X	1.66	8/1841 (0.4%)	2.01	42/2500 (1.7%)
1	4Y	1.61	9/1841 (0.5%)	2.03	48/2500 (1.9%)
1	4Z	1.62	9/1841 (0.5%)	2.12	53/2500 (2.1%)
1	4a	1.62	9/1841 (0.5%)	2.02	46/2500 (1.8%)
1	4b	1.61	11/1841 (0.6%)	2.05	61/2500 (2.4%)
1	4c	1.63	10/1841 (0.5%)	1.98	43/2500 (1.7%)
1	4d	1.64	11/1841 (0.6%)	2.19	48/2500 (1.9%)
1	4e	1.63	10/1841 (0.5%)	1.97	38/2500 (1.5%)
1	4f	1.65	7/1841 (0.4%)	2.00	37/2500 (1.5%)
1	4g	1.56	7/1841 (0.4%)	1.96	42/2500 (1.7%)
1	4h	1.64	14/1841 (0.8%)	2.04	55/2500 (2.2%)
1	4i	1.60	2/1841 (0.1%)	2.06	51/2500 (2.0%)
1	4j	1.65	8/1841 (0.4%)	1.99	42/2500 (1.7%)
1	4k	1.64	13/1841 (0.7%)	1.97	47/2500 (1.9%)
1	4l	1.62	7/1841 (0.4%)	2.11	46/2500 (1.8%)
1	4m	1.64	13/1841 (0.7%)	1.99	43/2500 (1.7%)
1	4n	1.62	7/1841 (0.4%)	2.04	50/2500 (2.0%)
1	4o	1.67	14/1841 (0.8%)	2.08	40/2500 (1.6%)
1	4p	1.56	7/1841 (0.4%)	1.92	43/2500 (1.7%)
1	4q	1.68	14/1841 (0.8%)	2.13	42/2500 (1.7%)
1	4r	1.67	9/1841 (0.5%)	2.04	45/2500 (1.8%)
1	4s	1.62	5/1841 (0.3%)	1.94	43/2500 (1.7%)
1	4t	1.62	12/1841 (0.7%)	2.02	43/2500 (1.7%)
1	4u	1.63	12/1841 (0.7%)	2.11	47/2500 (1.9%)
1	4v	1.66	10/1841 (0.5%)	2.11	45/2500 (1.8%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	4w	1.65	6/1841 (0.3%)	2.08	54/2500 (2.2%)
1	4x	1.62	15/1841 (0.8%)	2.03	46/2500 (1.8%)
1	4y	1.63	10/1841 (0.5%)	1.92	33/2500 (1.3%)
1	4z	1.59	7/1841 (0.4%)	1.97	49/2500 (2.0%)
1	5	1.64	12/1841 (0.7%)	2.02	44/2500 (1.8%)
1	50	1.63	15/1841 (0.8%)	1.94	36/2500 (1.4%)
1	51	1.63	9/1841 (0.5%)	2.01	42/2500 (1.7%)
1	52	1.63	9/1841 (0.5%)	2.19	42/2500 (1.7%)
1	53	1.66	9/1841 (0.5%)	2.09	44/2500 (1.8%)
1	54	1.68	14/1841 (0.8%)	2.06	48/2500 (1.9%)
1	55	1.63	9/1841 (0.5%)	1.95	45/2500 (1.8%)
1	56	1.67	12/1841 (0.7%)	1.85	36/2500 (1.4%)
1	57	1.64	14/1841 (0.8%)	2.06	48/2500 (1.9%)
1	58	1.68	15/1841 (0.8%)	2.06	49/2500 (2.0%)
1	59	1.65	13/1841 (0.7%)	2.07	39/2500 (1.6%)
1	5A	1.62	11/1841 (0.6%)	2.07	50/2500 (2.0%)
1	5B	1.59	4/1841 (0.2%)	2.01	38/2500 (1.5%)
1	5C	1.64	11/1841 (0.6%)	2.13	47/2500 (1.9%)
1	5D	1.64	12/1841 (0.7%)	2.06	50/2500 (2.0%)
1	5E	1.62	8/1841 (0.4%)	2.13	49/2500 (2.0%)
1	5F	1.61	9/1841 (0.5%)	1.90	31/2500 (1.2%)
1	5G	1.65	12/1841 (0.7%)	2.00	41/2500 (1.6%)
1	5H	1.64	12/1841 (0.7%)	1.98	47/2500 (1.9%)
1	5I	1.64	8/1841 (0.4%)	2.13	50/2500 (2.0%)
1	5J	1.61	10/1841 (0.5%)	2.03	42/2500 (1.7%)
1	5K	1.62	9/1841 (0.5%)	1.97	39/2500 (1.6%)
1	5L	1.66	10/1841 (0.5%)	1.99	52/2500 (2.1%)
1	5M	1.58	6/1841 (0.3%)	2.12	49/2500 (2.0%)
1	5N	1.58	9/1841 (0.5%)	2.00	42/2500 (1.7%)
1	5O	1.62	6/1841 (0.3%)	2.00	41/2500 (1.6%)
1	5P	1.67	11/1841 (0.6%)	2.02	35/2500 (1.4%)
1	5Q	1.60	8/1841 (0.4%)	2.06	50/2500 (2.0%)
1	5R	1.61	9/1841 (0.5%)	1.95	46/2500 (1.8%)
1	5S	1.61	7/1841 (0.4%)	2.04	45/2500 (1.8%)
1	5T	1.67	10/1841 (0.5%)	2.07	38/2500 (1.5%)
1	5U	1.63	9/1841 (0.5%)	1.90	33/2500 (1.3%)
1	5V	1.62	10/1841 (0.5%)	2.05	51/2500 (2.0%)
1	5W	1.66	12/1841 (0.7%)	1.93	41/2500 (1.6%)
1	5X	1.56	6/1841 (0.3%)	2.09	58/2500 (2.3%)
1	5Y	1.63	11/1841 (0.6%)	2.01	46/2500 (1.8%)
1	5Z	1.66	12/1841 (0.7%)	1.97	47/2500 (1.9%)
1	5a	1.64	9/1841 (0.5%)	1.95	41/2500 (1.6%)
1	5b	1.62	10/1841 (0.5%)	1.95	31/2500 (1.2%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	5c	1.67	13/1841 (0.7%)	2.01	49/2500 (2.0%)
1	5d	1.67	3/1841 (0.2%)	2.10	44/2500 (1.8%)
1	5e	1.57	6/1841 (0.3%)	1.96	39/2500 (1.6%)
1	5f	1.67	10/1841 (0.5%)	1.96	39/2500 (1.6%)
1	5g	1.63	6/1841 (0.3%)	2.11	49/2500 (2.0%)
1	5h	1.62	7/1841 (0.4%)	1.97	43/2500 (1.7%)
1	5i	1.59	8/1841 (0.4%)	2.13	51/2500 (2.0%)
1	5j	1.60	11/1841 (0.6%)	1.91	36/2500 (1.4%)
1	5k	1.64	12/1841 (0.7%)	1.95	38/2500 (1.5%)
1	5l	1.66	10/1841 (0.5%)	2.00	44/2500 (1.8%)
1	5m	1.62	11/1841 (0.6%)	2.09	48/2500 (1.9%)
1	5n	1.63	7/1841 (0.4%)	2.12	51/2500 (2.0%)
1	5o	1.62	9/1841 (0.5%)	1.99	38/2500 (1.5%)
1	5p	1.67	15/1841 (0.8%)	1.91	39/2500 (1.6%)
1	5q	1.63	8/1841 (0.4%)	2.12	59/2500 (2.4%)
1	5r	1.60	9/1841 (0.5%)	2.05	40/2500 (1.6%)
1	5s	1.61	10/1841 (0.5%)	2.03	38/2500 (1.5%)
1	5t	1.66	12/1841 (0.7%)	2.03	46/2500 (1.8%)
1	5u	1.59	13/1841 (0.7%)	2.15	53/2500 (2.1%)
1	5v	1.63	10/1841 (0.5%)	1.89	33/2500 (1.3%)
1	5w	1.62	11/1841 (0.6%)	2.06	41/2500 (1.6%)
1	5x	1.68	15/1841 (0.8%)	2.12	49/2500 (2.0%)
1	5y	1.61	10/1841 (0.5%)	2.08	56/2500 (2.2%)
1	5z	1.63	6/1841 (0.3%)	1.97	40/2500 (1.6%)
1	6	1.69	13/1841 (0.7%)	2.00	36/2500 (1.4%)
1	60	1.64	7/1841 (0.4%)	1.95	47/2500 (1.9%)
1	61	1.55	5/1841 (0.3%)	1.93	38/2500 (1.5%)
1	62	1.63	10/1841 (0.5%)	1.94	34/2500 (1.4%)
1	63	1.65	12/1841 (0.7%)	2.10	40/2500 (1.6%)
1	64	1.61	9/1841 (0.5%)	2.03	33/2500 (1.3%)
1	65	1.66	14/1841 (0.8%)	2.05	43/2500 (1.7%)
1	66	1.60	10/1841 (0.5%)	2.03	47/2500 (1.9%)
1	67	1.59	7/1841 (0.4%)	1.98	53/2500 (2.1%)
1	68	1.63	11/1841 (0.6%)	1.99	44/2500 (1.8%)
1	69	1.59	7/1841 (0.4%)	1.98	40/2500 (1.6%)
1	6A	1.64	14/1841 (0.8%)	2.08	53/2500 (2.1%)
1	6B	1.59	7/1841 (0.4%)	2.05	44/2500 (1.8%)
1	6C	1.62	10/1841 (0.5%)	2.04	57/2500 (2.3%)
1	6D	1.64	9/1841 (0.5%)	2.07	44/2500 (1.8%)
1	6E	1.58	5/1841 (0.3%)	2.02	44/2500 (1.8%)
1	6F	1.66	4/1841 (0.2%)	2.05	33/2500 (1.3%)
1	6G	1.58	6/1841 (0.3%)	1.99	41/2500 (1.6%)
1	6H	1.67	13/1841 (0.7%)	1.98	37/2500 (1.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	6I	1.61	17/1841 (0.9%)	2.04	46/2500 (1.8%)
1	6J	1.63	12/1841 (0.7%)	2.03	39/2500 (1.6%)
1	6K	1.57	6/1841 (0.3%)	2.07	39/2500 (1.6%)
1	6L	1.63	10/1841 (0.5%)	1.98	40/2500 (1.6%)
1	6M	1.64	10/1841 (0.5%)	2.02	44/2500 (1.8%)
1	6N	1.61	10/1841 (0.5%)	1.98	39/2500 (1.6%)
1	6O	1.63	15/1841 (0.8%)	1.81	26/2500 (1.0%)
1	6P	1.68	13/1841 (0.7%)	2.03	43/2500 (1.7%)
1	6Q	1.61	14/1841 (0.8%)	1.88	35/2500 (1.4%)
1	6R	1.63	7/1841 (0.4%)	2.04	51/2500 (2.0%)
1	6S	1.60	10/1841 (0.5%)	1.99	38/2500 (1.5%)
1	6T	1.65	20/1841 (1.1%)	1.93	37/2500 (1.5%)
1	6U	1.63	10/1841 (0.5%)	1.91	33/2500 (1.3%)
1	6V	1.63	8/1841 (0.4%)	1.95	41/2500 (1.6%)
1	6W	1.66	9/1841 (0.5%)	2.06	43/2500 (1.7%)
1	6X	1.62	6/1841 (0.3%)	1.91	36/2500 (1.4%)
1	6Y	1.65	9/1841 (0.5%)	1.96	38/2500 (1.5%)
1	6Z	1.58	9/1841 (0.5%)	2.00	45/2500 (1.8%)
1	6a	1.63	11/1841 (0.6%)	2.13	50/2500 (2.0%)
1	6b	1.59	8/1841 (0.4%)	1.91	41/2500 (1.6%)
1	6c	1.62	7/1841 (0.4%)	1.91	41/2500 (1.6%)
1	6d	1.62	9/1841 (0.5%)	2.06	41/2500 (1.6%)
1	6e	1.64	7/1841 (0.4%)	1.97	43/2500 (1.7%)
1	6f	1.62	12/1841 (0.7%)	2.04	53/2500 (2.1%)
1	6g	1.60	9/1841 (0.5%)	2.17	51/2500 (2.0%)
1	6h	1.67	11/1841 (0.6%)	2.12	49/2500 (2.0%)
1	6i	1.59	10/1841 (0.5%)	2.01	42/2500 (1.7%)
1	6j	1.67	13/1841 (0.7%)	2.05	52/2500 (2.1%)
1	6k	1.66	14/1841 (0.8%)	2.00	44/2500 (1.8%)
1	6l	1.64	3/1841 (0.2%)	2.04	55/2500 (2.2%)
1	6m	1.66	10/1841 (0.5%)	1.98	38/2500 (1.5%)
1	6n	1.62	11/1841 (0.6%)	2.04	60/2500 (2.4%)
1	6o	1.65	12/1841 (0.7%)	1.99	42/2500 (1.7%)
1	6p	1.66	6/1841 (0.3%)	2.04	43/2500 (1.7%)
1	6q	1.60	5/1841 (0.3%)	1.99	43/2500 (1.7%)
1	6r	1.60	7/1841 (0.4%)	1.95	39/2500 (1.6%)
1	6s	1.64	13/1841 (0.7%)	2.02	41/2500 (1.6%)
1	6t	1.66	15/1841 (0.8%)	2.01	46/2500 (1.8%)
1	6u	1.65	10/1841 (0.5%)	1.94	40/2500 (1.6%)
1	6v	1.63	8/1841 (0.4%)	1.95	45/2500 (1.8%)
1	6w	1.62	10/1841 (0.5%)	1.98	43/2500 (1.7%)
1	6x	1.58	6/1841 (0.3%)	1.90	41/2500 (1.6%)
1	6y	1.60	11/1841 (0.6%)	1.96	41/2500 (1.6%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	6z	1.64	11/1841 (0.6%)	2.02	49/2500 (2.0%)
1	7	1.65	9/1841 (0.5%)	2.12	46/2500 (1.8%)
1	70	1.66	11/1841 (0.6%)	1.94	40/2500 (1.6%)
1	71	1.62	14/1841 (0.8%)	2.07	39/2500 (1.6%)
1	72	1.62	5/1841 (0.3%)	2.08	54/2500 (2.2%)
1	73	1.65	9/1841 (0.5%)	2.16	48/2500 (1.9%)
1	74	1.64	10/1841 (0.5%)	1.97	48/2500 (1.9%)
1	75	1.58	6/1841 (0.3%)	2.08	51/2500 (2.0%)
1	76	1.61	16/1841 (0.9%)	1.93	41/2500 (1.6%)
1	77	1.66	8/1841 (0.4%)	2.07	51/2500 (2.0%)
1	78	1.60	10/1841 (0.5%)	2.02	46/2500 (1.8%)
1	79	1.68	13/1841 (0.7%)	1.91	50/2500 (2.0%)
1	7A	1.63	12/1841 (0.7%)	1.94	36/2500 (1.4%)
1	7B	1.61	10/1841 (0.5%)	2.05	53/2500 (2.1%)
1	7C	1.59	5/1841 (0.3%)	2.00	50/2500 (2.0%)
1	7D	1.65	8/1841 (0.4%)	2.01	38/2500 (1.5%)
1	7E	1.62	10/1841 (0.5%)	2.08	56/2500 (2.2%)
1	7F	1.58	9/1841 (0.5%)	2.01	41/2500 (1.6%)
1	7G	1.63	8/1841 (0.4%)	2.07	46/2500 (1.8%)
1	7H	1.64	15/1841 (0.8%)	2.03	52/2500 (2.1%)
1	7I	1.65	12/1841 (0.7%)	1.99	45/2500 (1.8%)
1	7J	1.61	6/1841 (0.3%)	1.99	43/2500 (1.7%)
1	7K	1.66	13/1841 (0.7%)	1.98	41/2500 (1.6%)
1	7L	1.63	9/1841 (0.5%)	2.01	42/2500 (1.7%)
1	7M	1.69	10/1841 (0.5%)	2.08	47/2500 (1.9%)
1	7N	1.71	19/1841 (1.0%)	2.03	51/2500 (2.0%)
1	7O	1.60	5/1841 (0.3%)	1.96	38/2500 (1.5%)
1	7P	1.68	10/1841 (0.5%)	1.99	54/2500 (2.2%)
1	7Q	1.63	6/1841 (0.3%)	1.96	44/2500 (1.8%)
1	7R	1.66	17/1841 (0.9%)	2.09	53/2500 (2.1%)
1	7S	1.60	12/1841 (0.7%)	2.09	49/2500 (2.0%)
1	7T	1.65	11/1841 (0.6%)	1.89	30/2500 (1.2%)
1	7U	1.60	11/1841 (0.6%)	1.92	35/2500 (1.4%)
1	7V	1.63	9/1841 (0.5%)	1.97	45/2500 (1.8%)
1	7W	1.67	15/1841 (0.8%)	1.93	47/2500 (1.9%)
1	7X	1.65	10/1841 (0.5%)	1.94	46/2500 (1.8%)
1	7Y	1.58	5/1841 (0.3%)	2.05	43/2500 (1.7%)
1	7Z	1.62	5/1841 (0.3%)	1.94	45/2500 (1.8%)
1	7a	1.63	14/1841 (0.8%)	1.92	42/2500 (1.7%)
1	7b	1.65	11/1841 (0.6%)	2.12	56/2500 (2.2%)
1	7c	1.58	6/1841 (0.3%)	1.96	37/2500 (1.5%)
1	7d	1.65	9/1841 (0.5%)	2.03	39/2500 (1.6%)
1	7e	1.60	2/1841 (0.1%)	2.04	40/2500 (1.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	7f	1.58	10/1841 (0.5%)	2.02	40/2500 (1.6%)
1	7g	1.64	9/1841 (0.5%)	2.10	37/2500 (1.5%)
1	7h	1.59	9/1841 (0.5%)	1.95	44/2500 (1.8%)
1	7i	1.62	8/1841 (0.4%)	1.95	44/2500 (1.8%)
1	7j	1.56	9/1841 (0.5%)	2.03	44/2500 (1.8%)
1	7k	1.65	14/1841 (0.8%)	1.95	43/2500 (1.7%)
1	7l	1.58	13/1841 (0.7%)	2.01	50/2500 (2.0%)
1	7m	1.61	11/1841 (0.6%)	2.04	51/2500 (2.0%)
1	7n	1.59	8/1841 (0.4%)	2.06	44/2500 (1.8%)
1	7o	1.62	4/1841 (0.2%)	2.00	38/2500 (1.5%)
1	7p	1.59	10/1841 (0.5%)	1.97	36/2500 (1.4%)
1	7q	1.61	8/1841 (0.4%)	2.07	48/2500 (1.9%)
1	7r	1.57	9/1841 (0.5%)	1.95	41/2500 (1.6%)
1	7s	1.63	8/1841 (0.4%)	2.01	42/2500 (1.7%)
1	7t	1.59	8/1841 (0.4%)	2.00	52/2500 (2.1%)
1	7u	1.64	10/1841 (0.5%)	2.02	48/2500 (1.9%)
1	7v	1.63	12/1841 (0.7%)	2.06	43/2500 (1.7%)
1	7w	1.64	9/1841 (0.5%)	2.06	44/2500 (1.8%)
1	7x	1.62	8/1841 (0.4%)	2.01	54/2500 (2.2%)
1	7y	1.65	12/1841 (0.7%)	1.95	44/2500 (1.8%)
1	7z	1.65	10/1841 (0.5%)	1.97	40/2500 (1.6%)
1	8	1.61	8/1841 (0.4%)	2.02	49/2500 (2.0%)
1	80	1.60	10/1841 (0.5%)	1.97	34/2500 (1.4%)
1	81	1.59	10/1841 (0.5%)	2.05	52/2500 (2.1%)
1	82	1.59	9/1841 (0.5%)	1.95	46/2500 (1.8%)
1	83	1.61	10/1841 (0.5%)	2.05	46/2500 (1.8%)
1	84	1.66	9/1841 (0.5%)	2.02	42/2500 (1.7%)
1	85	1.67	12/1841 (0.7%)	2.01	45/2500 (1.8%)
1	86	1.59	5/1841 (0.3%)	2.00	45/2500 (1.8%)
1	87	1.59	11/1841 (0.6%)	1.99	48/2500 (1.9%)
1	88	1.63	7/1841 (0.4%)	2.07	41/2500 (1.6%)
1	89	1.59	15/1841 (0.8%)	1.99	43/2500 (1.7%)
1	8A	1.61	9/1841 (0.5%)	2.03	48/2500 (1.9%)
1	8B	1.59	10/1841 (0.5%)	2.09	48/2500 (1.9%)
1	8C	1.64	14/1841 (0.8%)	2.05	53/2500 (2.1%)
1	8D	1.64	13/1841 (0.7%)	2.05	43/2500 (1.7%)
1	8E	1.61	9/1841 (0.5%)	1.98	50/2500 (2.0%)
1	8F	1.65	14/1841 (0.8%)	1.98	44/2500 (1.8%)
1	8G	1.64	8/1841 (0.4%)	2.00	49/2500 (2.0%)
1	8H	1.59	8/1841 (0.4%)	2.01	45/2500 (1.8%)
1	8I	1.64	7/1841 (0.4%)	1.95	42/2500 (1.7%)
1	8J	1.62	11/1841 (0.6%)	1.87	33/2500 (1.3%)
1	8K	1.62	12/1841 (0.7%)	2.09	52/2500 (2.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	8L	1.65	11/1841 (0.6%)	1.97	41/2500 (1.6%)
1	8M	1.69	15/1841 (0.8%)	1.94	35/2500 (1.4%)
1	8N	1.67	12/1841 (0.7%)	2.01	57/2500 (2.3%)
1	8O	1.66	12/1841 (0.7%)	2.03	52/2500 (2.1%)
1	8P	1.69	14/1841 (0.8%)	2.03	50/2500 (2.0%)
1	8Q	1.66	11/1841 (0.6%)	2.01	52/2500 (2.1%)
1	8R	1.68	14/1841 (0.8%)	2.09	44/2500 (1.8%)
1	8S	1.59	11/1841 (0.6%)	1.95	40/2500 (1.6%)
1	8T	1.61	10/1841 (0.5%)	2.03	46/2500 (1.8%)
1	8U	1.62	14/1841 (0.8%)	2.03	44/2500 (1.8%)
1	8V	1.68	18/1841 (1.0%)	1.96	39/2500 (1.6%)
1	8W	1.62	11/1841 (0.6%)	2.10	51/2500 (2.0%)
1	8X	1.65	8/1841 (0.4%)	2.05	54/2500 (2.2%)
1	8Y	1.64	12/1841 (0.7%)	1.98	33/2500 (1.3%)
1	8Z	1.60	8/1841 (0.4%)	1.93	36/2500 (1.4%)
1	8a	1.69	14/1841 (0.8%)	2.01	42/2500 (1.7%)
1	8b	1.68	7/1841 (0.4%)	2.04	36/2500 (1.4%)
1	8c	1.58	10/1841 (0.5%)	2.05	43/2500 (1.7%)
1	8d	1.64	14/1841 (0.8%)	2.04	44/2500 (1.8%)
1	8e	1.63	9/1841 (0.5%)	2.02	52/2500 (2.1%)
1	8f	1.63	11/1841 (0.6%)	1.96	42/2500 (1.7%)
1	8g	1.63	9/1841 (0.5%)	2.03	43/2500 (1.7%)
1	8h	1.62	9/1841 (0.5%)	2.06	45/2500 (1.8%)
1	8i	1.65	8/1841 (0.4%)	1.97	48/2500 (1.9%)
1	8j	1.64	8/1841 (0.4%)	1.97	43/2500 (1.7%)
1	8k	1.64	10/1841 (0.5%)	2.06	45/2500 (1.8%)
1	8l	1.62	12/1841 (0.7%)	2.08	48/2500 (1.9%)
1	8m	1.60	9/1841 (0.5%)	2.07	55/2500 (2.2%)
1	8n	1.65	13/1841 (0.7%)	2.09	57/2500 (2.3%)
1	8o	1.64	9/1841 (0.5%)	1.94	43/2500 (1.7%)
1	8p	1.61	9/1841 (0.5%)	2.04	49/2500 (2.0%)
1	8q	1.59	6/1841 (0.3%)	2.09	54/2500 (2.2%)
1	8r	1.57	3/1841 (0.2%)	2.02	44/2500 (1.8%)
1	8s	1.64	15/1841 (0.8%)	1.98	34/2500 (1.4%)
1	8t	1.65	14/1841 (0.8%)	2.05	54/2500 (2.2%)
1	8u	1.64	9/1841 (0.5%)	1.94	41/2500 (1.6%)
1	8v	1.59	7/1841 (0.4%)	2.04	41/2500 (1.6%)
1	8w	1.61	12/1841 (0.7%)	2.05	47/2500 (1.9%)
1	8x	1.61	12/1841 (0.7%)	2.04	42/2500 (1.7%)
1	8y	1.69	17/1841 (0.9%)	2.00	41/2500 (1.6%)
1	8z	1.64	10/1841 (0.5%)	2.04	36/2500 (1.4%)
1	9	1.67	11/1841 (0.6%)	1.98	44/2500 (1.8%)
1	90	1.67	16/1841 (0.9%)	1.98	39/2500 (1.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	91	1.60	7/1841 (0.4%)	1.96	39/2500 (1.6%)
1	92	1.61	6/1841 (0.3%)	2.00	42/2500 (1.7%)
1	93	1.66	11/1841 (0.6%)	2.05	52/2500 (2.1%)
1	94	1.61	9/1841 (0.5%)	1.98	54/2500 (2.2%)
1	95	1.62	11/1841 (0.6%)	2.18	54/2500 (2.2%)
1	96	1.65	6/1841 (0.3%)	2.08	51/2500 (2.0%)
1	97	1.62	11/1841 (0.6%)	1.96	44/2500 (1.8%)
1	98	1.65	12/1841 (0.7%)	2.04	40/2500 (1.6%)
1	99	1.68	13/1841 (0.7%)	1.97	45/2500 (1.8%)
1	9A	1.55	8/1841 (0.4%)	1.86	32/2500 (1.3%)
1	9B	1.63	11/1841 (0.6%)	2.04	50/2500 (2.0%)
1	9C	1.65	11/1841 (0.6%)	2.00	36/2500 (1.4%)
1	9D	1.60	16/1841 (0.9%)	1.96	41/2500 (1.6%)
1	9E	1.62	10/1841 (0.5%)	1.90	34/2500 (1.4%)
1	9F	1.66	11/1841 (0.6%)	2.04	45/2500 (1.8%)
1	9G	1.62	11/1841 (0.6%)	1.98	52/2500 (2.1%)
1	9H	1.66	9/1841 (0.5%)	2.07	50/2500 (2.0%)
1	9I	1.69	11/1841 (0.6%)	2.00	39/2500 (1.6%)
1	9J	1.60	9/1841 (0.5%)	1.98	32/2500 (1.3%)
1	9K	1.61	15/1841 (0.8%)	2.01	51/2500 (2.0%)
1	9L	1.65	15/1841 (0.8%)	1.93	34/2500 (1.4%)
1	9M	1.62	12/1841 (0.7%)	1.96	45/2500 (1.8%)
1	9N	1.68	19/1841 (1.0%)	2.04	53/2500 (2.1%)
1	9O	1.63	9/1841 (0.5%)	2.05	44/2500 (1.8%)
1	9P	1.63	8/1841 (0.4%)	1.95	42/2500 (1.7%)
1	9Q	1.68	11/1841 (0.6%)	1.94	33/2500 (1.3%)
1	9R	1.60	7/1841 (0.4%)	1.99	42/2500 (1.7%)
1	9S	1.65	7/1841 (0.4%)	2.07	45/2500 (1.8%)
1	9T	1.65	15/1841 (0.8%)	1.95	35/2500 (1.4%)
1	9U	1.68	7/1841 (0.4%)	2.10	56/2500 (2.2%)
1	9V	1.62	4/1841 (0.2%)	2.03	42/2500 (1.7%)
1	9W	1.66	15/1841 (0.8%)	2.04	49/2500 (2.0%)
1	9X	1.61	8/1841 (0.4%)	1.97	45/2500 (1.8%)
1	9Y	1.60	9/1841 (0.5%)	1.95	43/2500 (1.7%)
1	9Z	1.64	10/1841 (0.5%)	2.04	38/2500 (1.5%)
1	9a	1.61	8/1841 (0.4%)	2.07	50/2500 (2.0%)
1	9b	1.66	16/1841 (0.9%)	1.89	31/2500 (1.2%)
1	9c	1.61	8/1841 (0.4%)	2.07	46/2500 (1.8%)
1	9d	1.62	9/1841 (0.5%)	1.97	37/2500 (1.5%)
1	9e	1.64	7/1841 (0.4%)	1.99	44/2500 (1.8%)
1	9f	1.60	6/1841 (0.3%)	1.91	35/2500 (1.4%)
1	9g	1.64	10/1841 (0.5%)	2.02	45/2500 (1.8%)
1	9h	1.65	12/1841 (0.7%)	2.01	41/2500 (1.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	9i	1.65	10/1841 (0.5%)	1.88	38/2500 (1.5%)
1	9j	1.63	8/1841 (0.4%)	1.98	32/2500 (1.3%)
1	9k	1.69	13/1841 (0.7%)	2.17	49/2500 (2.0%)
1	9l	1.62	9/1841 (0.5%)	2.05	45/2500 (1.8%)
1	9m	1.61	7/1841 (0.4%)	2.06	50/2500 (2.0%)
1	9n	1.63	8/1841 (0.4%)	1.93	44/2500 (1.8%)
1	9o	1.65	6/1841 (0.3%)	1.96	57/2500 (2.3%)
1	9p	1.65	13/1841 (0.7%)	2.02	51/2500 (2.0%)
1	9q	1.60	10/1841 (0.5%)	2.00	42/2500 (1.7%)
1	9r	1.63	12/1841 (0.7%)	2.00	44/2500 (1.8%)
1	9s	1.67	14/1841 (0.8%)	2.04	50/2500 (2.0%)
1	9t	1.67	15/1841 (0.8%)	2.00	47/2500 (1.9%)
1	9u	1.63	17/1841 (0.9%)	2.01	46/2500 (1.8%)
1	9v	1.64	10/1841 (0.5%)	2.00	41/2500 (1.6%)
1	9w	1.62	8/1841 (0.4%)	2.02	50/2500 (2.0%)
1	9x	1.65	8/1841 (0.4%)	1.99	42/2500 (1.7%)
1	9y	1.59	11/1841 (0.6%)	2.08	45/2500 (1.8%)
1	9z	1.65	11/1841 (0.6%)	2.06	48/2500 (1.9%)
1	A	1.60	8/1841 (0.4%)	1.99	49/2500 (2.0%)
1	B	1.62	10/1841 (0.5%)	2.08	47/2500 (1.9%)
1	C	1.60	11/1841 (0.6%)	2.01	52/2500 (2.1%)
1	D	1.63	13/1841 (0.7%)	1.99	43/2500 (1.7%)
1	E	1.64	10/1841 (0.5%)	1.92	36/2500 (1.4%)
1	F	1.66	10/1841 (0.5%)	1.98	35/2500 (1.4%)
1	G	1.60	8/1841 (0.4%)	1.95	43/2500 (1.7%)
1	H	1.61	18/1841 (1.0%)	2.00	50/2500 (2.0%)
1	I	1.58	8/1841 (0.4%)	1.97	49/2500 (2.0%)
1	J	1.64	12/1841 (0.7%)	2.00	43/2500 (1.7%)
1	K	1.57	5/1841 (0.3%)	1.99	51/2500 (2.0%)
1	L	1.61	7/1841 (0.4%)	1.98	40/2500 (1.6%)
1	M	1.66	11/1841 (0.6%)	2.08	42/2500 (1.7%)
1	N	1.59	8/1841 (0.4%)	1.94	46/2500 (1.8%)
1	O	1.63	9/1841 (0.5%)	1.96	52/2500 (2.1%)
1	P	1.64	11/1841 (0.6%)	2.05	45/2500 (1.8%)
1	Q	1.65	12/1841 (0.7%)	2.04	48/2500 (1.9%)
1	R	1.67	15/1841 (0.8%)	1.99	35/2500 (1.4%)
1	S	1.63	14/1841 (0.8%)	2.01	40/2500 (1.6%)
1	T	1.67	16/1841 (0.9%)	1.99	47/2500 (1.9%)
1	U	1.60	7/1841 (0.4%)	1.94	38/2500 (1.5%)
1	V	1.63	12/1841 (0.7%)	2.00	44/2500 (1.8%)
1	W	1.62	8/1841 (0.4%)	2.08	40/2500 (1.6%)
1	X	1.65	15/1841 (0.8%)	1.96	38/2500 (1.5%)
1	Y	1.64	12/1841 (0.7%)	2.11	52/2500 (2.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	Z	1.62	9/1841 (0.5%)	2.04	45/2500 (1.8%)
1	a	1.61	9/1841 (0.5%)	2.04	40/2500 (1.6%)
1	a0	1.60	8/1841 (0.4%)	1.94	45/2500 (1.8%)
1	a1	1.62	9/1841 (0.5%)	2.03	42/2500 (1.7%)
1	a2	1.63	13/1841 (0.7%)	2.04	51/2500 (2.0%)
1	a3	1.68	14/1841 (0.8%)	2.00	44/2500 (1.8%)
1	a4	1.61	9/1841 (0.5%)	2.07	44/2500 (1.8%)
1	a5	1.63	13/1841 (0.7%)	1.99	40/2500 (1.6%)
1	a6	1.59	7/1841 (0.4%)	1.90	43/2500 (1.7%)
1	a7	1.63	11/1841 (0.6%)	2.02	52/2500 (2.1%)
1	a8	1.65	9/1841 (0.5%)	1.93	43/2500 (1.7%)
1	a9	1.65	12/1841 (0.7%)	1.97	51/2500 (2.0%)
1	aA	1.62	9/1841 (0.5%)	2.13	45/2500 (1.8%)
1	aB	1.64	10/1841 (0.5%)	2.07	43/2500 (1.7%)
1	aC	1.65	7/1841 (0.4%)	1.97	45/2500 (1.8%)
1	aD	1.68	14/1841 (0.8%)	1.95	42/2500 (1.7%)
1	aE	1.66	10/1841 (0.5%)	1.99	42/2500 (1.7%)
1	aF	1.63	11/1841 (0.6%)	1.93	41/2500 (1.6%)
1	aG	1.66	12/1841 (0.7%)	1.95	43/2500 (1.7%)
1	aH	1.58	12/1841 (0.7%)	2.00	37/2500 (1.5%)
1	aI	1.64	9/1841 (0.5%)	2.03	52/2500 (2.1%)
1	aJ	1.62	11/1841 (0.6%)	1.99	38/2500 (1.5%)
1	aK	1.61	6/1841 (0.3%)	2.07	46/2500 (1.8%)
1	aL	1.62	13/1841 (0.7%)	2.03	49/2500 (2.0%)
1	aM	1.63	17/1841 (0.9%)	2.00	50/2500 (2.0%)
1	aN	1.62	11/1841 (0.6%)	2.03	46/2500 (1.8%)
1	aO	1.67	7/1841 (0.4%)	2.07	54/2500 (2.2%)
1	aP	1.64	11/1841 (0.6%)	2.10	55/2500 (2.2%)
1	aQ	1.61	8/1841 (0.4%)	2.04	50/2500 (2.0%)
1	aR	1.63	11/1841 (0.6%)	2.04	43/2500 (1.7%)
1	aS	1.67	15/1841 (0.8%)	1.97	40/2500 (1.6%)
1	aT	1.66	7/1841 (0.4%)	1.96	44/2500 (1.8%)
1	aU	1.61	10/1841 (0.5%)	2.06	49/2500 (2.0%)
1	aV	1.67	7/1841 (0.4%)	2.03	49/2500 (2.0%)
1	aW	1.64	10/1841 (0.5%)	2.04	36/2500 (1.4%)
1	aX	1.65	14/1841 (0.8%)	1.99	44/2500 (1.8%)
1	aY	1.60	16/1841 (0.9%)	2.15	48/2500 (1.9%)
1	aZ	1.62	10/1841 (0.5%)	2.00	47/2500 (1.9%)
1	aa	1.67	11/1841 (0.6%)	1.94	34/2500 (1.4%)
1	ab	1.63	5/1841 (0.3%)	2.04	49/2500 (2.0%)
1	ac	1.63	13/1841 (0.7%)	1.93	44/2500 (1.8%)
1	ad	1.63	8/1841 (0.4%)	2.04	46/2500 (1.8%)
1	ae	1.62	7/1841 (0.4%)	1.99	46/2500 (1.8%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	af	1.64	12/1841 (0.7%)	2.08	42/2500 (1.7%)
1	ag	1.61	7/1841 (0.4%)	2.03	40/2500 (1.6%)
1	ah	1.69	14/1841 (0.8%)	2.13	53/2500 (2.1%)
1	ai	1.58	9/1841 (0.5%)	2.01	39/2500 (1.6%)
1	aj	1.68	13/1841 (0.7%)	1.97	47/2500 (1.9%)
1	ak	1.64	12/1841 (0.7%)	2.14	55/2500 (2.2%)
1	al	1.66	10/1841 (0.5%)	2.07	52/2500 (2.1%)
1	am	1.65	12/1841 (0.7%)	2.14	46/2500 (1.8%)
1	an	1.64	3/1841 (0.2%)	1.92	46/2500 (1.8%)
1	ao	1.64	16/1841 (0.9%)	1.88	41/2500 (1.6%)
1	ap	1.62	5/1841 (0.3%)	2.05	48/2500 (1.9%)
1	aq	1.63	10/1841 (0.5%)	2.02	41/2500 (1.6%)
1	ar	1.66	10/1841 (0.5%)	1.94	36/2500 (1.4%)
1	as	1.64	11/1841 (0.6%)	1.94	42/2500 (1.7%)
1	at	1.62	8/1841 (0.4%)	1.94	38/2500 (1.5%)
1	au	1.68	16/1841 (0.9%)	2.04	46/2500 (1.8%)
1	av	1.62	10/1841 (0.5%)	2.09	47/2500 (1.9%)
1	aw	1.63	9/1841 (0.5%)	2.05	49/2500 (2.0%)
1	ax	1.65	9/1841 (0.5%)	1.99	46/2500 (1.8%)
1	ay	1.63	11/1841 (0.6%)	2.00	33/2500 (1.3%)
1	az	1.65	10/1841 (0.5%)	2.12	51/2500 (2.0%)
1	b	1.59	5/1841 (0.3%)	2.05	47/2500 (1.9%)
1	b0	1.62	9/1841 (0.5%)	2.07	46/2500 (1.8%)
1	b1	1.60	6/1841 (0.3%)	1.98	45/2500 (1.8%)
1	b2	1.62	16/1841 (0.9%)	1.97	35/2500 (1.4%)
1	b3	1.64	14/1841 (0.8%)	1.99	46/2500 (1.8%)
1	b4	1.60	12/1841 (0.7%)	2.05	37/2500 (1.5%)
1	b5	1.63	8/1841 (0.4%)	1.94	47/2500 (1.9%)
1	b6	1.65	8/1841 (0.4%)	2.02	49/2500 (2.0%)
1	b7	1.66	11/1841 (0.6%)	1.90	25/2500 (1.0%)
1	b8	1.65	14/1841 (0.8%)	2.01	36/2500 (1.4%)
1	b9	1.67	10/1841 (0.5%)	1.96	44/2500 (1.8%)
1	bA	1.65	17/1841 (0.9%)	2.04	40/2500 (1.6%)
1	bB	1.63	16/1841 (0.9%)	2.03	44/2500 (1.8%)
1	bC	1.63	13/1841 (0.7%)	2.10	50/2500 (2.0%)
1	bD	1.62	13/1841 (0.7%)	1.96	37/2500 (1.5%)
1	bE	1.63	8/1841 (0.4%)	2.02	47/2500 (1.9%)
1	bF	1.63	12/1841 (0.7%)	1.98	49/2500 (2.0%)
1	bG	1.63	5/1841 (0.3%)	2.03	41/2500 (1.6%)
1	bH	1.64	10/1841 (0.5%)	2.01	50/2500 (2.0%)
1	bI	1.64	13/1841 (0.7%)	1.96	44/2500 (1.8%)
1	bJ	1.63	9/1841 (0.5%)	2.03	45/2500 (1.8%)
1	bK	1.61	10/1841 (0.5%)	1.98	48/2500 (1.9%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	bL	1.60	6/1841 (0.3%)	2.04	44/2500 (1.8%)
1	bM	1.69	14/1841 (0.8%)	1.97	31/2500 (1.2%)
1	bN	1.63	5/1841 (0.3%)	1.95	36/2500 (1.4%)
1	bO	1.68	17/1841 (0.9%)	2.05	50/2500 (2.0%)
1	bP	1.62	12/1841 (0.7%)	2.13	50/2500 (2.0%)
1	bQ	1.66	14/1841 (0.8%)	1.94	39/2500 (1.6%)
1	bR	1.66	12/1841 (0.7%)	2.03	45/2500 (1.8%)
1	bS	1.60	9/1841 (0.5%)	1.96	41/2500 (1.6%)
1	bT	1.65	11/1841 (0.6%)	2.04	45/2500 (1.8%)
1	bU	1.63	9/1841 (0.5%)	2.01	45/2500 (1.8%)
1	bV	1.62	9/1841 (0.5%)	1.94	42/2500 (1.7%)
1	bW	1.60	14/1841 (0.8%)	2.13	52/2500 (2.1%)
1	bX	1.64	9/1841 (0.5%)	1.97	44/2500 (1.8%)
1	bY	1.65	11/1841 (0.6%)	2.00	59/2500 (2.4%)
1	bZ	1.61	10/1841 (0.5%)	2.14	53/2500 (2.1%)
1	ba	1.67	5/1841 (0.3%)	2.04	43/2500 (1.7%)
1	bb	1.61	8/1841 (0.4%)	1.97	54/2500 (2.2%)
1	bc	1.63	9/1841 (0.5%)	1.99	44/2500 (1.8%)
1	bd	1.64	9/1841 (0.5%)	1.92	37/2500 (1.5%)
1	be	1.60	9/1841 (0.5%)	2.07	47/2500 (1.9%)
1	bf	1.59	10/1841 (0.5%)	2.05	49/2500 (2.0%)
1	bg	1.66	12/1841 (0.7%)	1.98	45/2500 (1.8%)
1	bh	1.64	12/1841 (0.7%)	1.93	41/2500 (1.6%)
1	bi	1.65	11/1841 (0.6%)	2.05	48/2500 (1.9%)
1	bj	1.64	8/1841 (0.4%)	1.90	31/2500 (1.2%)
1	bk	1.67	11/1841 (0.6%)	2.00	44/2500 (1.8%)
1	bl	1.62	7/1841 (0.4%)	2.09	47/2500 (1.9%)
1	bm	1.64	5/1841 (0.3%)	1.94	40/2500 (1.6%)
1	bn	1.66	9/1841 (0.5%)	1.91	33/2500 (1.3%)
1	bo	1.62	10/1841 (0.5%)	1.99	48/2500 (1.9%)
1	bp	1.66	14/1841 (0.8%)	2.01	48/2500 (1.9%)
1	bq	1.61	11/1841 (0.6%)	1.99	46/2500 (1.8%)
1	br	1.61	15/1841 (0.8%)	2.09	56/2500 (2.2%)
1	bs	1.66	13/1841 (0.7%)	1.93	43/2500 (1.7%)
1	bt	1.64	12/1841 (0.7%)	2.06	52/2500 (2.1%)
1	bu	1.70	16/1841 (0.9%)	1.95	48/2500 (1.9%)
1	bv	1.59	9/1841 (0.5%)	2.10	54/2500 (2.2%)
1	bw	1.65	9/1841 (0.5%)	1.97	47/2500 (1.9%)
1	bx	1.68	10/1841 (0.5%)	2.01	51/2500 (2.0%)
1	by	1.59	10/1841 (0.5%)	2.02	46/2500 (1.8%)
1	bz	1.65	16/1841 (0.9%)	1.98	40/2500 (1.6%)
1	c	1.62	10/1841 (0.5%)	1.99	46/2500 (1.8%)
1	c0	1.61	8/1841 (0.4%)	1.99	42/2500 (1.7%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	c1	1.62	12/1841 (0.7%)	2.00	47/2500 (1.9%)
1	c2	1.71	8/1841 (0.4%)	2.09	50/2500 (2.0%)
1	c3	1.64	10/1841 (0.5%)	2.00	44/2500 (1.8%)
1	c4	1.64	17/1841 (0.9%)	1.96	49/2500 (2.0%)
1	c5	1.66	8/1841 (0.4%)	2.11	53/2500 (2.1%)
1	c6	1.61	7/1841 (0.4%)	2.01	41/2500 (1.6%)
1	c7	1.67	14/1841 (0.8%)	1.88	36/2500 (1.4%)
1	c8	1.65	11/1841 (0.6%)	2.08	43/2500 (1.7%)
1	c9	1.68	11/1841 (0.6%)	2.00	52/2500 (2.1%)
1	cA	1.60	15/1841 (0.8%)	2.00	40/2500 (1.6%)
1	cB	1.61	10/1841 (0.5%)	2.08	56/2500 (2.2%)
1	cC	1.65	6/1841 (0.3%)	2.02	54/2500 (2.2%)
1	cD	1.59	12/1841 (0.7%)	2.12	57/2500 (2.3%)
1	cE	1.62	5/1841 (0.3%)	2.01	49/2500 (2.0%)
1	cF	1.62	10/1841 (0.5%)	2.00	46/2500 (1.8%)
1	cG	1.61	8/1841 (0.4%)	2.01	57/2500 (2.3%)
1	cH	1.61	11/1841 (0.6%)	2.10	58/2500 (2.3%)
1	cI	1.63	14/1841 (0.8%)	1.94	38/2500 (1.5%)
1	cJ	1.61	10/1841 (0.5%)	1.91	38/2500 (1.5%)
1	cK	1.72	15/1841 (0.8%)	2.12	50/2500 (2.0%)
1	cL	1.59	5/1841 (0.3%)	2.00	48/2500 (1.9%)
1	cM	1.68	15/1841 (0.8%)	1.99	39/2500 (1.6%)
1	cN	1.61	11/1841 (0.6%)	1.98	40/2500 (1.6%)
1	cO	1.60	7/1841 (0.4%)	1.97	39/2500 (1.6%)
1	cP	1.62	10/1841 (0.5%)	2.02	43/2500 (1.7%)
1	cQ	1.57	1/1841 (0.1%)	2.12	43/2500 (1.7%)
1	cR	1.66	11/1841 (0.6%)	2.07	53/2500 (2.1%)
1	cS	1.62	12/1841 (0.7%)	2.05	44/2500 (1.8%)
1	cT	1.69	15/1841 (0.8%)	1.96	35/2500 (1.4%)
1	cU	1.64	6/1841 (0.3%)	2.02	45/2500 (1.8%)
1	cV	1.62	6/1841 (0.3%)	2.06	44/2500 (1.8%)
1	cW	1.60	10/1841 (0.5%)	2.07	57/2500 (2.3%)
1	cX	1.58	9/1841 (0.5%)	1.96	42/2500 (1.7%)
1	cY	1.60	12/1841 (0.7%)	1.94	34/2500 (1.4%)
1	cZ	1.66	8/1841 (0.4%)	2.12	47/2500 (1.9%)
1	ca	1.65	11/1841 (0.6%)	2.06	49/2500 (2.0%)
1	cb	1.63	11/1841 (0.6%)	1.95	43/2500 (1.7%)
1	cc	1.66	15/1841 (0.8%)	1.92	40/2500 (1.6%)
1	cd	1.63	9/1841 (0.5%)	2.10	53/2500 (2.1%)
1	ce	1.66	11/1841 (0.6%)	2.04	43/2500 (1.7%)
1	cf	1.64	8/1841 (0.4%)	2.04	61/2500 (2.4%)
1	cg	1.60	7/1841 (0.4%)	2.03	37/2500 (1.5%)
1	ch	1.62	8/1841 (0.4%)	1.98	34/2500 (1.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	ci	1.63	13/1841 (0.7%)	2.12	49/2500 (2.0%)
1	cj	1.60	8/1841 (0.4%)	2.08	39/2500 (1.6%)
1	ck	1.68	14/1841 (0.8%)	1.94	50/2500 (2.0%)
1	cl	1.68	17/1841 (0.9%)	2.01	44/2500 (1.8%)
1	cm	1.59	9/1841 (0.5%)	1.99	51/2500 (2.0%)
1	cn	1.63	9/1841 (0.5%)	2.03	53/2500 (2.1%)
1	co	1.64	10/1841 (0.5%)	1.96	44/2500 (1.8%)
1	cp	1.60	15/1841 (0.8%)	2.02	51/2500 (2.0%)
1	cq	1.57	6/1841 (0.3%)	2.00	56/2500 (2.2%)
1	cr	1.62	7/1841 (0.4%)	1.98	48/2500 (1.9%)
1	cs	1.62	10/1841 (0.5%)	1.98	38/2500 (1.5%)
1	ct	1.65	10/1841 (0.5%)	2.03	51/2500 (2.0%)
1	cu	1.64	8/1841 (0.4%)	1.97	27/2500 (1.1%)
1	cv	1.60	12/1841 (0.7%)	2.08	51/2500 (2.0%)
1	cw	1.64	12/1841 (0.7%)	1.95	39/2500 (1.6%)
1	cx	1.60	9/1841 (0.5%)	1.96	49/2500 (2.0%)
1	cy	1.67	16/1841 (0.9%)	1.99	49/2500 (2.0%)
1	cz	1.59	7/1841 (0.4%)	1.96	39/2500 (1.6%)
1	d	1.64	7/1841 (0.4%)	1.90	37/2500 (1.5%)
1	d0	1.63	9/1841 (0.5%)	1.94	48/2500 (1.9%)
1	d1	1.64	10/1841 (0.5%)	1.95	46/2500 (1.8%)
1	d2	1.62	11/1841 (0.6%)	2.00	45/2500 (1.8%)
1	d3	1.62	11/1841 (0.6%)	1.98	41/2500 (1.6%)
1	d4	1.65	9/1841 (0.5%)	2.05	55/2500 (2.2%)
1	d5	1.60	12/1841 (0.7%)	1.91	37/2500 (1.5%)
1	d6	1.62	13/1841 (0.7%)	1.98	39/2500 (1.6%)
1	d7	1.60	10/1841 (0.5%)	2.02	48/2500 (1.9%)
1	d8	1.63	8/1841 (0.4%)	1.90	40/2500 (1.6%)
1	d9	1.60	9/1841 (0.5%)	1.97	41/2500 (1.6%)
1	dA	1.64	13/1841 (0.7%)	2.08	50/2500 (2.0%)
1	dB	1.63	8/1841 (0.4%)	2.03	54/2500 (2.2%)
1	dC	1.64	17/1841 (0.9%)	2.05	57/2500 (2.3%)
1	dD	1.66	13/1841 (0.7%)	2.06	57/2500 (2.3%)
1	dE	1.61	5/1841 (0.3%)	1.99	39/2500 (1.6%)
1	dF	1.67	15/1841 (0.8%)	2.02	40/2500 (1.6%)
1	dG	1.67	17/1841 (0.9%)	2.01	37/2500 (1.5%)
1	dH	1.65	11/1841 (0.6%)	1.97	42/2500 (1.7%)
1	dI	1.56	8/1841 (0.4%)	2.06	56/2500 (2.2%)
1	dJ	1.60	11/1841 (0.6%)	1.94	38/2500 (1.5%)
1	dK	1.63	16/1841 (0.9%)	1.91	31/2500 (1.2%)
1	dL	1.65	13/1841 (0.7%)	2.02	36/2500 (1.4%)
1	dM	1.66	15/1841 (0.8%)	2.10	38/2500 (1.5%)
1	dN	1.58	6/1841 (0.3%)	1.93	29/2500 (1.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	dO	1.65	17/1841 (0.9%)	1.92	28/2500 (1.1%)
1	dP	1.61	9/1841 (0.5%)	1.97	51/2500 (2.0%)
1	dQ	1.65	11/1841 (0.6%)	2.03	43/2500 (1.7%)
1	dR	1.61	7/1841 (0.4%)	1.92	34/2500 (1.4%)
1	dS	1.58	7/1841 (0.4%)	1.93	36/2500 (1.4%)
1	dT	1.65	16/1841 (0.9%)	2.00	42/2500 (1.7%)
1	dU	1.64	8/1841 (0.4%)	1.99	47/2500 (1.9%)
1	dV	1.56	7/1841 (0.4%)	1.96	47/2500 (1.9%)
1	dW	1.64	11/1841 (0.6%)	2.04	51/2500 (2.0%)
1	dX	1.65	12/1841 (0.7%)	1.97	42/2500 (1.7%)
1	dY	1.65	8/1841 (0.4%)	1.99	46/2500 (1.8%)
1	dZ	1.64	11/1841 (0.6%)	1.93	49/2500 (2.0%)
1	da	1.65	13/1841 (0.7%)	1.93	34/2500 (1.4%)
1	db	1.66	11/1841 (0.6%)	2.01	49/2500 (2.0%)
1	dc	1.63	14/1841 (0.8%)	2.03	52/2500 (2.1%)
1	dd	1.64	11/1841 (0.6%)	2.06	50/2500 (2.0%)
1	de	1.63	8/1841 (0.4%)	1.95	32/2500 (1.3%)
1	df	1.65	12/1841 (0.7%)	1.95	33/2500 (1.3%)
1	dg	1.60	12/1841 (0.7%)	2.05	47/2500 (1.9%)
1	dh	1.60	9/1841 (0.5%)	1.94	41/2500 (1.6%)
1	di	1.64	8/1841 (0.4%)	2.05	46/2500 (1.8%)
1	dj	1.66	15/1841 (0.8%)	1.97	37/2500 (1.5%)
1	dk	1.65	16/1841 (0.9%)	2.06	44/2500 (1.8%)
1	dl	1.59	12/1841 (0.7%)	2.04	42/2500 (1.7%)
1	dm	1.64	14/1841 (0.8%)	1.93	39/2500 (1.6%)
1	dn	1.67	13/1841 (0.7%)	2.06	47/2500 (1.9%)
1	do	1.69	12/1841 (0.7%)	1.98	57/2500 (2.3%)
1	dp	1.63	10/1841 (0.5%)	2.04	42/2500 (1.7%)
1	dq	1.61	9/1841 (0.5%)	2.01	44/2500 (1.8%)
1	dr	1.58	7/1841 (0.4%)	2.02	42/2500 (1.7%)
1	ds	1.61	14/1841 (0.8%)	2.11	47/2500 (1.9%)
1	dt	1.62	12/1841 (0.7%)	1.93	38/2500 (1.5%)
1	du	1.58	10/1841 (0.5%)	2.00	42/2500 (1.7%)
1	dv	1.65	6/1841 (0.3%)	2.11	47/2500 (1.9%)
1	dw	1.66	13/1841 (0.7%)	2.07	44/2500 (1.8%)
1	dx	1.67	12/1841 (0.7%)	2.05	48/2500 (1.9%)
1	dy	1.64	7/1841 (0.4%)	2.14	46/2500 (1.8%)
1	dz	1.64	10/1841 (0.5%)	1.99	46/2500 (1.8%)
1	e	1.67	13/1841 (0.7%)	1.96	42/2500 (1.7%)
1	e0	1.61	13/1841 (0.7%)	2.02	52/2500 (2.1%)
1	e1	1.65	16/1841 (0.9%)	1.99	44/2500 (1.8%)
1	e2	1.63	7/1841 (0.4%)	2.11	46/2500 (1.8%)
1	e3	1.60	9/1841 (0.5%)	2.07	53/2500 (2.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	e4	1.57	7/1841 (0.4%)	2.04	54/2500 (2.2%)
1	e5	1.64	14/1841 (0.8%)	2.01	42/2500 (1.7%)
1	e6	1.63	13/1841 (0.7%)	1.98	43/2500 (1.7%)
1	e7	1.63	13/1841 (0.7%)	2.00	29/2500 (1.2%)
1	e8	1.62	5/1841 (0.3%)	2.03	41/2500 (1.6%)
1	e9	1.62	8/1841 (0.4%)	1.97	47/2500 (1.9%)
1	eA	1.64	14/1841 (0.8%)	1.94	40/2500 (1.6%)
1	eB	1.62	5/1841 (0.3%)	2.09	50/2500 (2.0%)
1	eC	1.64	8/1841 (0.4%)	2.01	47/2500 (1.9%)
1	eD	1.65	10/1841 (0.5%)	2.00	50/2500 (2.0%)
1	eE	1.65	13/1841 (0.7%)	1.98	40/2500 (1.6%)
1	eF	1.64	10/1841 (0.5%)	2.09	41/2500 (1.6%)
1	eG	1.60	7/1841 (0.4%)	1.94	36/2500 (1.4%)
1	eH	1.63	16/1841 (0.9%)	2.03	39/2500 (1.6%)
1	eI	1.66	12/1841 (0.7%)	1.99	43/2500 (1.7%)
1	eJ	1.61	10/1841 (0.5%)	2.01	45/2500 (1.8%)
1	eK	1.67	14/1841 (0.8%)	1.90	46/2500 (1.8%)
1	eL	1.73	14/1841 (0.8%)	1.98	45/2500 (1.8%)
1	eM	1.68	10/1841 (0.5%)	2.10	55/2500 (2.2%)
1	eN	1.60	7/1841 (0.4%)	1.96	40/2500 (1.6%)
1	eO	1.62	6/1841 (0.3%)	1.95	39/2500 (1.6%)
1	eP	1.63	10/1841 (0.5%)	2.02	40/2500 (1.6%)
1	eQ	1.60	15/1841 (0.8%)	2.00	56/2500 (2.2%)
1	eR	1.66	13/1841 (0.7%)	2.02	54/2500 (2.2%)
1	eS	1.62	14/1841 (0.8%)	2.02	40/2500 (1.6%)
1	eT	1.65	7/1841 (0.4%)	1.96	48/2500 (1.9%)
1	eU	1.62	9/1841 (0.5%)	2.07	45/2500 (1.8%)
1	eV	1.64	13/1841 (0.7%)	1.96	31/2500 (1.2%)
1	eW	1.57	5/1841 (0.3%)	2.06	45/2500 (1.8%)
1	eX	1.64	14/1841 (0.8%)	2.02	47/2500 (1.9%)
1	eY	1.60	9/1841 (0.5%)	2.02	43/2500 (1.7%)
1	eZ	1.66	11/1841 (0.6%)	2.00	45/2500 (1.8%)
1	ea	1.60	9/1841 (0.5%)	2.00	46/2500 (1.8%)
1	eb	1.64	10/1841 (0.5%)	2.06	50/2500 (2.0%)
1	ec	1.61	8/1841 (0.4%)	2.01	40/2500 (1.6%)
1	ed	1.61	3/1841 (0.2%)	2.01	48/2500 (1.9%)
1	ee	1.60	8/1841 (0.4%)	2.15	46/2500 (1.8%)
1	ef	1.64	9/1841 (0.5%)	2.06	34/2500 (1.4%)
1	eg	1.61	12/1841 (0.7%)	2.05	49/2500 (2.0%)
1	eh	1.60	10/1841 (0.5%)	1.98	43/2500 (1.7%)
1	ei	1.58	11/1841 (0.6%)	2.14	51/2500 (2.0%)
1	ej	1.61	8/1841 (0.4%)	2.01	43/2500 (1.7%)
1	ek	1.63	13/1841 (0.7%)	1.95	33/2500 (1.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	el	1.63	7/1841 (0.4%)	2.04	46/2500 (1.8%)
1	em	1.69	20/1841 (1.1%)	1.99	44/2500 (1.8%)
1	en	1.61	3/1841 (0.2%)	2.02	46/2500 (1.8%)
1	eo	1.67	13/1841 (0.7%)	1.96	43/2500 (1.7%)
1	ep	1.64	8/1841 (0.4%)	1.99	50/2500 (2.0%)
1	eq	1.60	11/1841 (0.6%)	2.03	45/2500 (1.8%)
1	er	1.61	11/1841 (0.6%)	2.02	47/2500 (1.9%)
1	es	1.67	12/1841 (0.7%)	2.02	38/2500 (1.5%)
1	et	1.61	10/1841 (0.5%)	1.96	41/2500 (1.6%)
1	eu	1.66	14/1841 (0.8%)	2.04	40/2500 (1.6%)
1	ev	1.64	7/1841 (0.4%)	2.04	49/2500 (2.0%)
1	ew	1.61	13/1841 (0.7%)	2.00	41/2500 (1.6%)
1	ex	1.60	3/1841 (0.2%)	1.94	34/2500 (1.4%)
1	ey	1.66	11/1841 (0.6%)	2.06	48/2500 (1.9%)
1	ez	1.60	7/1841 (0.4%)	1.96	42/2500 (1.7%)
1	f	1.63	10/1841 (0.5%)	1.96	45/2500 (1.8%)
1	f0	1.64	14/1841 (0.8%)	1.90	36/2500 (1.4%)
1	f1	1.65	12/1841 (0.7%)	1.98	48/2500 (1.9%)
1	f2	1.61	6/1841 (0.3%)	1.93	32/2500 (1.3%)
1	f3	1.67	13/1841 (0.7%)	2.00	47/2500 (1.9%)
1	f4	1.68	15/1841 (0.8%)	1.97	41/2500 (1.6%)
1	f5	1.59	6/1841 (0.3%)	2.27	52/2500 (2.1%)
1	f6	1.69	16/1841 (0.9%)	1.91	33/2500 (1.3%)
1	f7	1.67	13/1841 (0.7%)	2.05	49/2500 (2.0%)
1	f8	1.65	12/1841 (0.7%)	1.98	51/2500 (2.0%)
1	f9	1.63	8/1841 (0.4%)	2.00	43/2500 (1.7%)
1	fA	1.62	8/1841 (0.4%)	1.93	40/2500 (1.6%)
1	fB	1.65	9/1841 (0.5%)	2.08	49/2500 (2.0%)
1	fC	1.67	8/1841 (0.4%)	2.09	42/2500 (1.7%)
1	fD	1.68	14/1841 (0.8%)	1.96	34/2500 (1.4%)
1	fE	1.67	12/1841 (0.7%)	1.92	37/2500 (1.5%)
1	fF	1.63	7/1841 (0.4%)	2.02	48/2500 (1.9%)
1	fG	1.64	11/1841 (0.6%)	2.04	43/2500 (1.7%)
1	fH	1.60	13/1841 (0.7%)	1.95	36/2500 (1.4%)
1	fI	1.68	16/1841 (0.9%)	2.08	52/2500 (2.1%)
1	fJ	1.62	13/1841 (0.7%)	1.97	46/2500 (1.8%)
1	fK	1.57	5/1841 (0.3%)	2.08	49/2500 (2.0%)
1	fL	1.62	10/1841 (0.5%)	1.97	39/2500 (1.6%)
1	fM	1.64	15/1841 (0.8%)	1.98	49/2500 (2.0%)
1	fN	1.64	7/1841 (0.4%)	1.97	45/2500 (1.8%)
1	fO	1.65	12/1841 (0.7%)	2.06	42/2500 (1.7%)
1	fP	1.58	5/1841 (0.3%)	2.09	53/2500 (2.1%)
1	fQ	1.56	8/1841 (0.4%)	2.07	48/2500 (1.9%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	fR	1.65	7/1841 (0.4%)	2.00	55/2500 (2.2%)
1	fS	1.59	3/1841 (0.2%)	1.93	44/2500 (1.8%)
1	fT	1.63	16/1841 (0.9%)	1.99	42/2500 (1.7%)
1	fU	1.61	10/1841 (0.5%)	1.92	40/2500 (1.6%)
1	fV	1.62	10/1841 (0.5%)	2.06	39/2500 (1.6%)
1	fW	1.64	12/1841 (0.7%)	2.01	42/2500 (1.7%)
1	fX	1.60	10/1841 (0.5%)	2.00	43/2500 (1.7%)
1	fY	1.64	9/1841 (0.5%)	1.94	34/2500 (1.4%)
1	fZ	1.68	16/1841 (0.9%)	1.99	44/2500 (1.8%)
1	fa	1.62	11/1841 (0.6%)	2.02	52/2500 (2.1%)
1	fb	1.59	12/1841 (0.7%)	1.87	34/2500 (1.4%)
1	fc	1.66	7/1841 (0.4%)	2.03	41/2500 (1.6%)
1	fd	1.64	9/1841 (0.5%)	1.99	39/2500 (1.6%)
1	fe	1.65	13/1841 (0.7%)	1.97	47/2500 (1.9%)
1	ff	1.66	8/1841 (0.4%)	2.07	45/2500 (1.8%)
1	fg	1.61	7/1841 (0.4%)	2.01	52/2500 (2.1%)
1	fh	1.64	8/1841 (0.4%)	1.97	43/2500 (1.7%)
1	fi	1.58	8/1841 (0.4%)	1.99	52/2500 (2.1%)
1	fj	1.62	7/1841 (0.4%)	1.96	43/2500 (1.7%)
1	fk	1.59	7/1841 (0.4%)	2.10	40/2500 (1.6%)
1	fl	1.67	12/1841 (0.7%)	2.02	47/2500 (1.9%)
1	fm	1.65	10/1841 (0.5%)	2.11	42/2500 (1.7%)
1	fn	1.66	16/1841 (0.9%)	2.04	42/2500 (1.7%)
1	fo	1.64	9/1841 (0.5%)	2.12	46/2500 (1.8%)
1	fp	1.62	7/1841 (0.4%)	2.01	58/2500 (2.3%)
1	fq	1.61	8/1841 (0.4%)	2.07	53/2500 (2.1%)
1	fr	1.59	12/1841 (0.7%)	1.98	37/2500 (1.5%)
1	fs	1.66	16/1841 (0.9%)	1.98	41/2500 (1.6%)
1	ft	1.60	9/1841 (0.5%)	2.05	39/2500 (1.6%)
1	fu	1.63	15/1841 (0.8%)	2.01	35/2500 (1.4%)
1	fv	1.65	4/1841 (0.2%)	1.94	43/2500 (1.7%)
1	fw	1.60	4/1841 (0.2%)	2.05	43/2500 (1.7%)
1	fx	1.57	7/1841 (0.4%)	1.93	31/2500 (1.2%)
1	fy	1.62	15/1841 (0.8%)	2.03	44/2500 (1.8%)
1	fz	1.61	6/1841 (0.3%)	2.04	54/2500 (2.2%)
1	g	1.65	9/1841 (0.5%)	1.94	40/2500 (1.6%)
1	g0	1.64	8/1841 (0.4%)	1.96	40/2500 (1.6%)
1	g1	1.64	14/1841 (0.8%)	2.03	42/2500 (1.7%)
1	g2	1.65	11/1841 (0.6%)	2.01	46/2500 (1.8%)
1	g3	1.65	10/1841 (0.5%)	2.01	47/2500 (1.9%)
1	g4	1.63	12/1841 (0.7%)	2.00	44/2500 (1.8%)
1	g5	1.65	11/1841 (0.6%)	2.04	49/2500 (2.0%)
1	g6	1.65	8/1841 (0.4%)	1.93	30/2500 (1.2%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	g7	1.71	13/1841 (0.7%)	2.05	40/2500 (1.6%)
1	g8	1.63	6/1841 (0.3%)	1.93	43/2500 (1.7%)
1	g9	1.65	11/1841 (0.6%)	2.04	55/2500 (2.2%)
1	gA	1.61	11/1841 (0.6%)	1.97	44/2500 (1.8%)
1	gB	1.61	2/1841 (0.1%)	2.07	44/2500 (1.8%)
1	gC	1.70	15/1841 (0.8%)	2.06	61/2500 (2.4%)
1	gD	1.63	8/1841 (0.4%)	2.07	50/2500 (2.0%)
1	gE	1.59	7/1841 (0.4%)	1.92	45/2500 (1.8%)
1	gF	1.65	7/1841 (0.4%)	2.01	40/2500 (1.6%)
1	gG	1.60	8/1841 (0.4%)	2.10	50/2500 (2.0%)
1	gH	1.69	13/1841 (0.7%)	1.96	44/2500 (1.8%)
1	gI	1.62	11/1841 (0.6%)	2.02	49/2500 (2.0%)
1	gJ	1.66	10/1841 (0.5%)	1.95	41/2500 (1.6%)
1	gK	1.66	13/1841 (0.7%)	1.98	41/2500 (1.6%)
1	gL	1.64	10/1841 (0.5%)	2.04	47/2500 (1.9%)
1	gM	1.65	8/1841 (0.4%)	2.01	49/2500 (2.0%)
1	gN	1.65	11/1841 (0.6%)	1.98	42/2500 (1.7%)
1	gO	1.66	11/1841 (0.6%)	2.01	43/2500 (1.7%)
1	gP	1.63	9/1841 (0.5%)	2.04	43/2500 (1.7%)
1	gQ	1.61	10/1841 (0.5%)	2.00	47/2500 (1.9%)
1	gR	1.55	5/1841 (0.3%)	1.98	46/2500 (1.8%)
1	gS	1.62	8/1841 (0.4%)	1.97	40/2500 (1.6%)
1	gT	1.64	16/1841 (0.9%)	2.04	44/2500 (1.8%)
1	gU	1.63	8/1841 (0.4%)	2.03	42/2500 (1.7%)
1	gV	1.67	9/1841 (0.5%)	2.02	41/2500 (1.6%)
1	gW	1.61	12/1841 (0.7%)	2.02	54/2500 (2.2%)
1	gX	1.64	13/1841 (0.7%)	2.09	48/2500 (1.9%)
1	gY	1.63	9/1841 (0.5%)	1.97	42/2500 (1.7%)
1	gZ	1.61	9/1841 (0.5%)	1.91	34/2500 (1.4%)
1	ga	1.59	8/1841 (0.4%)	2.06	49/2500 (2.0%)
1	gb	1.64	16/1841 (0.9%)	2.09	43/2500 (1.7%)
1	gc	1.66	10/1841 (0.5%)	1.91	34/2500 (1.4%)
1	gd	1.62	11/1841 (0.6%)	2.21	57/2500 (2.3%)
1	ge	1.58	4/1841 (0.2%)	2.02	38/2500 (1.5%)
1	gf	1.59	8/1841 (0.4%)	2.01	45/2500 (1.8%)
1	gg	1.68	17/1841 (0.9%)	2.08	55/2500 (2.2%)
1	gh	1.67	13/1841 (0.7%)	2.04	48/2500 (1.9%)
1	gi	1.62	13/1841 (0.7%)	2.14	60/2500 (2.4%)
1	gj	1.66	11/1841 (0.6%)	2.05	49/2500 (2.0%)
1	gk	1.60	8/1841 (0.4%)	2.04	49/2500 (2.0%)
1	gl	1.65	11/1841 (0.6%)	1.95	38/2500 (1.5%)
1	gm	1.62	7/1841 (0.4%)	2.02	46/2500 (1.8%)
1	gn	1.62	7/1841 (0.4%)	2.14	50/2500 (2.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	go	1.61	10/1841 (0.5%)	2.09	41/2500 (1.6%)
1	gp	1.68	17/1841 (0.9%)	1.92	46/2500 (1.8%)
1	gq	1.61	6/1841 (0.3%)	1.97	46/2500 (1.8%)
1	gr	1.61	11/1841 (0.6%)	1.99	48/2500 (1.9%)
1	gs	1.62	7/1841 (0.4%)	2.13	45/2500 (1.8%)
1	gt	1.67	13/1841 (0.7%)	2.05	47/2500 (1.9%)
1	gu	1.62	5/1841 (0.3%)	2.02	44/2500 (1.8%)
1	gv	1.61	8/1841 (0.4%)	2.02	42/2500 (1.7%)
1	gw	1.62	13/1841 (0.7%)	2.00	39/2500 (1.6%)
1	gx	1.64	12/1841 (0.7%)	1.97	46/2500 (1.8%)
1	gy	1.61	12/1841 (0.7%)	2.00	43/2500 (1.7%)
1	gz	1.66	15/1841 (0.8%)	2.07	45/2500 (1.8%)
1	h	1.63	11/1841 (0.6%)	1.96	35/2500 (1.4%)
1	h0	1.61	10/1841 (0.5%)	1.95	50/2500 (2.0%)
1	h1	1.61	10/1841 (0.5%)	1.99	45/2500 (1.8%)
1	h2	1.63	9/1841 (0.5%)	2.01	46/2500 (1.8%)
1	h3	1.62	11/1841 (0.6%)	2.00	58/2500 (2.3%)
1	h4	1.65	12/1841 (0.7%)	1.93	33/2500 (1.3%)
1	h5	1.66	9/1841 (0.5%)	1.97	43/2500 (1.7%)
1	h6	1.59	5/1841 (0.3%)	1.92	43/2500 (1.7%)
1	h7	1.64	10/1841 (0.5%)	2.02	51/2500 (2.0%)
1	h8	1.59	9/1841 (0.5%)	1.95	41/2500 (1.6%)
1	h9	1.67	13/1841 (0.7%)	1.99	48/2500 (1.9%)
1	hA	1.60	13/1841 (0.7%)	2.07	44/2500 (1.8%)
1	hB	1.63	10/1841 (0.5%)	1.93	36/2500 (1.4%)
1	hC	1.65	8/1841 (0.4%)	1.99	44/2500 (1.8%)
1	hD	1.66	12/1841 (0.7%)	2.11	48/2500 (1.9%)
1	hE	1.62	6/1841 (0.3%)	1.97	35/2500 (1.4%)
1	hF	1.65	13/1841 (0.7%)	2.03	43/2500 (1.7%)
1	hG	1.65	12/1841 (0.7%)	2.02	49/2500 (2.0%)
1	hH	1.57	6/1841 (0.3%)	2.04	43/2500 (1.7%)
1	hI	1.63	9/1841 (0.5%)	1.96	43/2500 (1.7%)
1	hJ	1.67	18/1841 (1.0%)	2.02	46/2500 (1.8%)
1	hK	1.64	10/1841 (0.5%)	2.08	47/2500 (1.9%)
1	hL	1.63	11/1841 (0.6%)	1.94	44/2500 (1.8%)
1	hM	1.62	5/1841 (0.3%)	2.22	46/2500 (1.8%)
1	hN	1.64	14/1841 (0.8%)	2.02	42/2500 (1.7%)
1	hO	1.62	10/1841 (0.5%)	1.97	38/2500 (1.5%)
1	hP	1.60	9/1841 (0.5%)	1.94	41/2500 (1.6%)
1	hQ	1.63	12/1841 (0.7%)	2.11	57/2500 (2.3%)
1	hR	1.73	22/1841 (1.2%)	1.91	45/2500 (1.8%)
1	hS	1.63	8/1841 (0.4%)	1.93	45/2500 (1.8%)
1	hT	1.61	9/1841 (0.5%)	1.95	45/2500 (1.8%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	hU	1.63	13/1841 (0.7%)	1.96	40/2500 (1.6%)
1	hV	1.58	13/1841 (0.7%)	2.00	52/2500 (2.1%)
1	hW	1.64	9/1841 (0.5%)	2.02	49/2500 (2.0%)
1	hX	1.60	12/1841 (0.7%)	2.06	43/2500 (1.7%)
1	hY	1.61	10/1841 (0.5%)	2.04	42/2500 (1.7%)
1	hZ	1.62	9/1841 (0.5%)	2.07	50/2500 (2.0%)
1	ha	1.64	4/1841 (0.2%)	1.94	45/2500 (1.8%)
1	hb	1.66	14/1841 (0.8%)	1.93	44/2500 (1.8%)
1	hc	1.62	11/1841 (0.6%)	2.03	49/2500 (2.0%)
1	hd	1.62	9/1841 (0.5%)	1.97	44/2500 (1.8%)
1	he	1.60	13/1841 (0.7%)	1.96	41/2500 (1.6%)
1	hf	1.66	16/1841 (0.9%)	2.04	57/2500 (2.3%)
1	hg	1.62	11/1841 (0.6%)	2.10	54/2500 (2.2%)
1	hh	1.69	13/1841 (0.7%)	1.95	37/2500 (1.5%)
1	hi	1.66	11/1841 (0.6%)	2.07	54/2500 (2.2%)
1	hj	1.61	6/1841 (0.3%)	1.96	46/2500 (1.8%)
1	hk	1.65	12/1841 (0.7%)	1.98	41/2500 (1.6%)
1	hl	1.67	10/1841 (0.5%)	2.03	42/2500 (1.7%)
1	hm	1.63	11/1841 (0.6%)	2.08	44/2500 (1.8%)
1	hn	1.60	12/1841 (0.7%)	2.02	39/2500 (1.6%)
1	ho	1.61	9/1841 (0.5%)	2.05	40/2500 (1.6%)
1	hp	1.63	14/1841 (0.8%)	2.07	50/2500 (2.0%)
1	hq	1.64	11/1841 (0.6%)	2.02	42/2500 (1.7%)
1	hr	1.63	4/1841 (0.2%)	2.05	56/2500 (2.2%)
1	hs	1.68	12/1841 (0.7%)	2.08	50/2500 (2.0%)
1	ht	1.59	10/1841 (0.5%)	1.94	38/2500 (1.5%)
1	hu	1.65	12/1841 (0.7%)	2.05	44/2500 (1.8%)
1	hv	1.65	10/1841 (0.5%)	1.97	46/2500 (1.8%)
1	hw	1.57	6/1841 (0.3%)	2.11	47/2500 (1.9%)
1	hx	1.61	8/1841 (0.4%)	1.99	40/2500 (1.6%)
1	hy	1.61	7/1841 (0.4%)	2.06	52/2500 (2.1%)
1	hz	1.62	12/1841 (0.7%)	2.04	51/2500 (2.0%)
1	i	1.66	12/1841 (0.7%)	1.97	37/2500 (1.5%)
1	i0	1.67	13/1841 (0.7%)	2.09	37/2500 (1.5%)
1	i1	1.59	11/1841 (0.6%)	1.99	52/2500 (2.1%)
1	i2	1.64	7/1841 (0.4%)	1.96	42/2500 (1.7%)
1	i3	1.65	8/1841 (0.4%)	1.94	33/2500 (1.3%)
1	i4	1.65	15/1841 (0.8%)	1.95	46/2500 (1.8%)
1	i5	1.66	16/1841 (0.9%)	1.99	48/2500 (1.9%)
1	i6	1.64	12/1841 (0.7%)	2.08	46/2500 (1.8%)
1	i7	1.61	7/1841 (0.4%)	2.04	50/2500 (2.0%)
1	i8	1.61	7/1841 (0.4%)	2.00	42/2500 (1.7%)
1	i9	1.64	13/1841 (0.7%)	2.07	58/2500 (2.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	iA	1.63	8/1841 (0.4%)	2.03	50/2500 (2.0%)
1	iB	1.60	10/1841 (0.5%)	1.97	40/2500 (1.6%)
1	iC	1.58	6/1841 (0.3%)	2.02	48/2500 (1.9%)
1	iD	1.60	11/1841 (0.6%)	1.97	39/2500 (1.6%)
1	iE	1.64	13/1841 (0.7%)	1.97	45/2500 (1.8%)
1	iF	1.67	14/1841 (0.8%)	1.99	48/2500 (1.9%)
1	iG	1.63	12/1841 (0.7%)	2.03	55/2500 (2.2%)
1	iH	1.68	14/1841 (0.8%)	2.10	48/2500 (1.9%)
1	iI	1.64	13/1841 (0.7%)	1.98	45/2500 (1.8%)
1	iJ	1.62	9/1841 (0.5%)	1.98	46/2500 (1.8%)
1	iK	1.63	11/1841 (0.6%)	2.04	48/2500 (1.9%)
1	iL	1.64	12/1841 (0.7%)	2.02	48/2500 (1.9%)
1	iM	1.65	11/1841 (0.6%)	2.16	46/2500 (1.8%)
1	iN	1.62	8/1841 (0.4%)	2.06	57/2500 (2.3%)
1	iO	1.63	8/1841 (0.4%)	2.05	44/2500 (1.8%)
1	iP	1.68	14/1841 (0.8%)	1.95	38/2500 (1.5%)
1	iQ	1.62	13/1841 (0.7%)	2.02	46/2500 (1.8%)
1	iR	1.59	13/1841 (0.7%)	2.11	53/2500 (2.1%)
1	iS	1.65	10/1841 (0.5%)	1.98	45/2500 (1.8%)
1	iT	1.68	12/1841 (0.7%)	2.08	55/2500 (2.2%)
1	iU	1.58	11/1841 (0.6%)	2.03	37/2500 (1.5%)
1	iV	1.63	10/1841 (0.5%)	1.92	42/2500 (1.7%)
1	iW	1.61	9/1841 (0.5%)	2.05	45/2500 (1.8%)
1	iX	1.65	13/1841 (0.7%)	2.00	45/2500 (1.8%)
1	iY	1.58	6/1841 (0.3%)	1.94	45/2500 (1.8%)
1	iZ	1.63	10/1841 (0.5%)	1.93	46/2500 (1.8%)
1	ia	1.60	9/1841 (0.5%)	2.09	49/2500 (2.0%)
1	ib	1.60	13/1841 (0.7%)	1.97	41/2500 (1.6%)
1	ic	1.63	16/1841 (0.9%)	2.02	49/2500 (2.0%)
1	id	1.60	8/1841 (0.4%)	1.94	43/2500 (1.7%)
1	ie	1.64	9/1841 (0.5%)	2.04	49/2500 (2.0%)
1	if	1.61	7/1841 (0.4%)	2.03	46/2500 (1.8%)
1	ig	1.66	14/1841 (0.8%)	2.11	43/2500 (1.7%)
1	ih	1.64	14/1841 (0.8%)	2.00	42/2500 (1.7%)
1	ii	1.63	9/1841 (0.5%)	2.00	49/2500 (2.0%)
1	ij	1.65	8/1841 (0.4%)	2.00	48/2500 (1.9%)
1	ik	1.66	14/1841 (0.8%)	1.96	48/2500 (1.9%)
1	il	1.59	6/1841 (0.3%)	2.04	54/2500 (2.2%)
1	im	1.64	12/1841 (0.7%)	2.02	43/2500 (1.7%)
1	in	1.63	8/1841 (0.4%)	1.97	49/2500 (2.0%)
1	io	1.68	13/1841 (0.7%)	2.11	59/2500 (2.4%)
1	ip	1.62	10/1841 (0.5%)	1.95	44/2500 (1.8%)
1	iq	1.66	9/1841 (0.5%)	1.89	44/2500 (1.8%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	ir	1.61	9/1841 (0.5%)	1.95	42/2500 (1.7%)
1	is	1.57	7/1841 (0.4%)	1.93	41/2500 (1.6%)
1	it	1.69	14/1841 (0.8%)	2.15	51/2500 (2.0%)
1	iu	1.65	8/1841 (0.4%)	2.06	47/2500 (1.9%)
1	iv	1.62	11/1841 (0.6%)	2.00	50/2500 (2.0%)
1	iw	1.59	10/1841 (0.5%)	1.98	44/2500 (1.8%)
1	ix	1.63	12/1841 (0.7%)	2.03	47/2500 (1.9%)
1	iy	1.58	8/1841 (0.4%)	2.02	39/2500 (1.6%)
1	iz	1.62	11/1841 (0.6%)	2.12	54/2500 (2.2%)
1	j	1.63	7/1841 (0.4%)	2.02	34/2500 (1.4%)
1	j0	1.65	11/1841 (0.6%)	2.11	46/2500 (1.8%)
1	j1	1.68	15/1841 (0.8%)	2.09	59/2500 (2.4%)
1	j2	1.65	7/1841 (0.4%)	2.10	35/2500 (1.4%)
1	j3	1.63	4/1841 (0.2%)	1.94	38/2500 (1.5%)
1	j4	1.61	5/1841 (0.3%)	2.06	49/2500 (2.0%)
1	j5	1.61	12/1841 (0.7%)	1.98	42/2500 (1.7%)
1	j6	1.64	10/1841 (0.5%)	1.90	37/2500 (1.5%)
1	j7	1.65	13/1841 (0.7%)	2.03	51/2500 (2.0%)
1	j8	1.66	11/1841 (0.6%)	2.01	41/2500 (1.6%)
1	j9	1.63	12/1841 (0.7%)	1.96	49/2500 (2.0%)
1	jA	1.69	14/1841 (0.8%)	1.98	37/2500 (1.5%)
1	jB	1.69	21/1841 (1.1%)	2.06	42/2500 (1.7%)
1	jC	1.64	14/1841 (0.8%)	2.03	46/2500 (1.8%)
1	jD	1.65	13/1841 (0.7%)	2.02	42/2500 (1.7%)
1	jE	1.63	10/1841 (0.5%)	2.09	36/2500 (1.4%)
1	jF	1.70	13/1841 (0.7%)	2.03	44/2500 (1.8%)
1	jG	1.60	9/1841 (0.5%)	1.97	45/2500 (1.8%)
1	jH	1.64	8/1841 (0.4%)	1.94	33/2500 (1.3%)
1	jI	1.61	8/1841 (0.4%)	2.07	49/2500 (2.0%)
1	jJ	1.62	6/1841 (0.3%)	2.05	38/2500 (1.5%)
1	jK	1.58	6/1841 (0.3%)	1.97	45/2500 (1.8%)
1	jL	1.63	8/1841 (0.4%)	2.00	38/2500 (1.5%)
1	jM	1.64	15/1841 (0.8%)	1.97	39/2500 (1.6%)
1	jN	1.65	12/1841 (0.7%)	2.04	47/2500 (1.9%)
1	jO	1.60	11/1841 (0.6%)	2.08	51/2500 (2.0%)
1	jP	1.61	12/1841 (0.7%)	2.04	52/2500 (2.1%)
1	jQ	1.64	15/1841 (0.8%)	1.98	46/2500 (1.8%)
1	jR	1.67	10/1841 (0.5%)	2.04	56/2500 (2.2%)
1	jS	1.62	9/1841 (0.5%)	1.97	37/2500 (1.5%)
1	jT	1.59	10/1841 (0.5%)	2.04	47/2500 (1.9%)
1	jU	1.61	7/1841 (0.4%)	2.14	62/2500 (2.5%)
1	jV	1.62	8/1841 (0.4%)	2.01	47/2500 (1.9%)
1	jW	1.66	13/1841 (0.7%)	1.97	40/2500 (1.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	jX	1.59	7/1841 (0.4%)	2.01	50/2500 (2.0%)
1	jY	1.61	6/1841 (0.3%)	2.00	43/2500 (1.7%)
1	jZ	1.69	14/1841 (0.8%)	2.01	49/2500 (2.0%)
1	ja	1.67	14/1841 (0.8%)	1.95	35/2500 (1.4%)
1	jb	1.70	12/1841 (0.7%)	1.99	49/2500 (2.0%)
1	jc	1.64	13/1841 (0.7%)	1.99	36/2500 (1.4%)
1	jd	1.65	11/1841 (0.6%)	2.02	36/2500 (1.4%)
1	je	1.64	14/1841 (0.8%)	1.98	59/2500 (2.4%)
1	jf	1.66	13/1841 (0.7%)	2.06	38/2500 (1.5%)
1	jg	1.64	11/1841 (0.6%)	1.96	46/2500 (1.8%)
1	jh	1.65	12/1841 (0.7%)	1.97	39/2500 (1.6%)
1	ji	1.73	19/1841 (1.0%)	1.98	36/2500 (1.4%)
1	jj	1.66	10/1841 (0.5%)	2.03	56/2500 (2.2%)
1	jk	1.62	6/1841 (0.3%)	2.10	45/2500 (1.8%)
1	jl	1.63	9/1841 (0.5%)	2.00	47/2500 (1.9%)
1	jm	1.64	13/1841 (0.7%)	2.00	37/2500 (1.5%)
1	jn	1.62	10/1841 (0.5%)	1.97	44/2500 (1.8%)
1	jo	1.62	12/1841 (0.7%)	2.02	42/2500 (1.7%)
1	jp	1.58	9/1841 (0.5%)	1.94	43/2500 (1.7%)
1	jq	1.61	7/1841 (0.4%)	1.99	43/2500 (1.7%)
1	jr	1.65	7/1841 (0.4%)	2.08	50/2500 (2.0%)
1	js	1.68	15/1841 (0.8%)	2.11	46/2500 (1.8%)
1	jt	1.65	14/1841 (0.8%)	2.01	48/2500 (1.9%)
1	ju	1.61	12/1841 (0.7%)	1.94	38/2500 (1.5%)
1	jv	1.65	13/1841 (0.7%)	1.98	41/2500 (1.6%)
1	jw	1.63	8/1841 (0.4%)	1.93	41/2500 (1.6%)
1	jx	1.68	14/1841 (0.8%)	2.02	44/2500 (1.8%)
1	jy	1.64	11/1841 (0.6%)	2.02	46/2500 (1.8%)
1	jz	1.67	12/1841 (0.7%)	2.02	40/2500 (1.6%)
1	k	1.65	10/1841 (0.5%)	1.97	47/2500 (1.9%)
1	k0	1.61	13/1841 (0.7%)	1.96	42/2500 (1.7%)
1	k1	1.60	8/1841 (0.4%)	2.12	56/2500 (2.2%)
1	k2	1.62	7/1841 (0.4%)	2.05	49/2500 (2.0%)
1	k3	1.69	17/1841 (0.9%)	2.02	44/2500 (1.8%)
1	k4	1.65	9/1841 (0.5%)	2.07	44/2500 (1.8%)
1	k5	1.63	11/1841 (0.6%)	2.01	44/2500 (1.8%)
1	k6	1.59	7/1841 (0.4%)	2.05	48/2500 (1.9%)
1	k7	1.65	12/1841 (0.7%)	2.00	50/2500 (2.0%)
1	k8	1.62	6/1841 (0.3%)	1.98	51/2500 (2.0%)
1	k9	1.67	9/1841 (0.5%)	1.97	40/2500 (1.6%)
1	kA	1.64	10/1841 (0.5%)	2.02	50/2500 (2.0%)
1	kB	1.62	10/1841 (0.5%)	1.97	44/2500 (1.8%)
1	kC	1.65	16/1841 (0.9%)	1.92	39/2500 (1.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	kD	1.61	15/1841 (0.8%)	2.04	44/2500 (1.8%)
1	kE	1.65	12/1841 (0.7%)	1.96	45/2500 (1.8%)
1	kF	1.62	9/1841 (0.5%)	2.11	49/2500 (2.0%)
1	kG	1.61	7/1841 (0.4%)	2.01	43/2500 (1.7%)
1	kH	1.66	11/1841 (0.6%)	1.93	42/2500 (1.7%)
1	kI	1.60	5/1841 (0.3%)	2.00	49/2500 (2.0%)
1	kJ	1.67	18/1841 (1.0%)	1.93	38/2500 (1.5%)
1	kK	1.59	7/1841 (0.4%)	1.91	38/2500 (1.5%)
1	kL	1.66	11/1841 (0.6%)	1.96	52/2500 (2.1%)
1	kM	1.60	10/1841 (0.5%)	1.96	35/2500 (1.4%)
1	kN	1.62	10/1841 (0.5%)	2.00	45/2500 (1.8%)
1	kO	1.61	9/1841 (0.5%)	1.95	40/2500 (1.6%)
1	kP	1.62	7/1841 (0.4%)	2.00	41/2500 (1.6%)
1	kQ	1.65	14/1841 (0.8%)	1.95	39/2500 (1.6%)
1	kR	1.65	7/1841 (0.4%)	1.98	40/2500 (1.6%)
1	kS	1.64	11/1841 (0.6%)	2.00	45/2500 (1.8%)
1	kT	1.56	12/1841 (0.7%)	2.01	47/2500 (1.9%)
1	kU	1.66	14/1841 (0.8%)	1.90	39/2500 (1.6%)
1	kV	1.65	11/1841 (0.6%)	2.10	46/2500 (1.8%)
1	kW	1.67	18/1841 (1.0%)	2.09	41/2500 (1.6%)
1	kX	1.64	13/1841 (0.7%)	1.99	51/2500 (2.0%)
1	kY	1.61	7/1841 (0.4%)	1.99	35/2500 (1.4%)
1	kZ	1.64	13/1841 (0.7%)	1.98	47/2500 (1.9%)
1	ka	1.64	9/1841 (0.5%)	1.98	49/2500 (2.0%)
1	kb	1.63	9/1841 (0.5%)	2.15	55/2500 (2.2%)
1	kc	1.62	9/1841 (0.5%)	1.97	46/2500 (1.8%)
1	kd	1.64	7/1841 (0.4%)	2.08	48/2500 (1.9%)
1	ke	1.58	5/1841 (0.3%)	2.05	41/2500 (1.6%)
1	kf	1.62	8/1841 (0.4%)	2.10	46/2500 (1.8%)
1	kg	1.64	12/1841 (0.7%)	2.05	54/2500 (2.2%)
1	kh	1.65	11/1841 (0.6%)	2.03	47/2500 (1.9%)
1	ki	1.61	8/1841 (0.4%)	2.04	51/2500 (2.0%)
1	kj	1.63	6/1841 (0.3%)	2.00	44/2500 (1.8%)
1	kk	1.64	11/1841 (0.6%)	2.05	46/2500 (1.8%)
1	kl	1.65	12/1841 (0.7%)	2.01	37/2500 (1.5%)
1	km	1.60	6/1841 (0.3%)	2.05	46/2500 (1.8%)
1	kn	1.62	12/1841 (0.7%)	2.06	46/2500 (1.8%)
1	ko	1.61	10/1841 (0.5%)	1.96	37/2500 (1.5%)
1	kp	1.65	12/1841 (0.7%)	1.93	42/2500 (1.7%)
1	kq	1.62	11/1841 (0.6%)	1.97	36/2500 (1.4%)
1	kr	1.69	11/1841 (0.6%)	2.17	63/2500 (2.5%)
1	ks	1.67	12/1841 (0.7%)	1.96	35/2500 (1.4%)
1	kt	1.68	12/1841 (0.7%)	1.95	52/2500 (2.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	ku	1.60	9/1841 (0.5%)	2.03	42/2500 (1.7%)
1	kv	1.66	13/1841 (0.7%)	2.11	55/2500 (2.2%)
1	kw	1.58	10/1841 (0.5%)	1.96	42/2500 (1.7%)
1	kx	1.63	10/1841 (0.5%)	1.95	45/2500 (1.8%)
1	ky	1.64	14/1841 (0.8%)	1.98	46/2500 (1.8%)
1	kz	1.62	15/1841 (0.8%)	2.05	43/2500 (1.7%)
1	l	1.67	8/1841 (0.4%)	2.16	41/2500 (1.6%)
1	l0	1.69	19/1841 (1.0%)	2.21	53/2500 (2.1%)
1	l1	1.61	7/1841 (0.4%)	1.97	41/2500 (1.6%)
1	l2	1.61	7/1841 (0.4%)	1.89	34/2500 (1.4%)
1	l3	1.68	12/1841 (0.7%)	1.96	41/2500 (1.6%)
1	l4	1.64	11/1841 (0.6%)	2.07	50/2500 (2.0%)
1	l5	1.55	3/1841 (0.2%)	2.00	40/2500 (1.6%)
1	l6	1.57	6/1841 (0.3%)	1.98	46/2500 (1.8%)
1	l7	1.61	4/1841 (0.2%)	2.22	51/2500 (2.0%)
1	l8	1.58	3/1841 (0.2%)	1.94	36/2500 (1.4%)
1	l9	1.66	13/1841 (0.7%)	2.04	45/2500 (1.8%)
1	lA	1.64	9/1841 (0.5%)	2.14	57/2500 (2.3%)
1	lB	1.64	11/1841 (0.6%)	2.18	45/2500 (1.8%)
1	lC	1.63	10/1841 (0.5%)	2.00	50/2500 (2.0%)
1	lD	1.56	6/1841 (0.3%)	2.05	46/2500 (1.8%)
1	lE	1.62	10/1841 (0.5%)	2.13	44/2500 (1.8%)
1	lF	1.68	11/1841 (0.6%)	2.02	48/2500 (1.9%)
1	lG	1.66	7/1841 (0.4%)	1.88	32/2500 (1.3%)
1	lH	1.65	9/1841 (0.5%)	2.00	45/2500 (1.8%)
1	lI	1.66	9/1841 (0.5%)	2.10	55/2500 (2.2%)
1	lJ	1.66	12/1841 (0.7%)	2.06	41/2500 (1.6%)
1	lK	1.67	10/1841 (0.5%)	1.97	45/2500 (1.8%)
1	lL	1.65	10/1841 (0.5%)	2.04	43/2500 (1.7%)
1	lM	1.62	10/1841 (0.5%)	2.08	51/2500 (2.0%)
1	lN	1.61	9/1841 (0.5%)	1.98	40/2500 (1.6%)
1	lO	1.60	6/1841 (0.3%)	2.03	53/2500 (2.1%)
1	lP	1.66	14/1841 (0.8%)	1.90	40/2500 (1.6%)
1	lQ	1.68	17/1841 (0.9%)	2.08	45/2500 (1.8%)
1	lR	1.64	13/1841 (0.7%)	2.03	48/2500 (1.9%)
1	la	1.61	4/1841 (0.2%)	1.89	40/2500 (1.6%)
1	lb	1.64	7/1841 (0.4%)	2.01	50/2500 (2.0%)
1	lc	1.66	15/1841 (0.8%)	1.97	41/2500 (1.6%)
1	ld	1.60	4/1841 (0.2%)	2.12	45/2500 (1.8%)
1	le	1.62	13/1841 (0.7%)	1.93	39/2500 (1.6%)
1	lf	1.68	17/1841 (0.9%)	2.00	39/2500 (1.6%)
1	lg	1.70	20/1841 (1.1%)	1.92	43/2500 (1.7%)
1	lh	1.66	17/1841 (0.9%)	2.03	48/2500 (1.9%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	li	1.58	7/1841 (0.4%)	1.95	42/2500 (1.7%)
1	lj	1.63	7/1841 (0.4%)	1.99	43/2500 (1.7%)
1	lk	1.63	15/1841 (0.8%)	2.05	46/2500 (1.8%)
1	ll	1.60	3/1841 (0.2%)	2.03	51/2500 (2.0%)
1	lm	1.55	5/1841 (0.3%)	2.03	47/2500 (1.9%)
1	ln	1.57	10/1841 (0.5%)	2.04	47/2500 (1.9%)
1	lo	1.59	6/1841 (0.3%)	2.03	41/2500 (1.6%)
1	lp	1.62	7/1841 (0.4%)	1.94	43/2500 (1.7%)
1	lq	1.61	10/1841 (0.5%)	2.01	37/2500 (1.5%)
1	lr	1.65	9/1841 (0.5%)	1.98	44/2500 (1.8%)
1	ls	1.67	12/1841 (0.7%)	1.98	46/2500 (1.8%)
1	lt	1.61	5/1841 (0.3%)	2.02	39/2500 (1.6%)
1	lu	1.69	13/1841 (0.7%)	1.96	43/2500 (1.7%)
1	lv	1.65	10/1841 (0.5%)	1.97	47/2500 (1.9%)
1	lw	1.63	19/1841 (1.0%)	2.06	48/2500 (1.9%)
1	lx	1.61	8/1841 (0.4%)	1.89	34/2500 (1.4%)
1	ly	1.64	6/1841 (0.3%)	1.96	40/2500 (1.6%)
1	lz	1.61	11/1841 (0.6%)	2.02	45/2500 (1.8%)
1	m	1.63	6/1841 (0.3%)	1.98	49/2500 (2.0%)
1	n	1.58	6/1841 (0.3%)	2.03	44/2500 (1.8%)
1	o	1.65	7/1841 (0.4%)	1.98	49/2500 (2.0%)
1	p	1.64	12/1841 (0.7%)	2.01	47/2500 (1.9%)
1	q	1.62	10/1841 (0.5%)	1.93	39/2500 (1.6%)
1	r	1.66	12/1841 (0.7%)	1.96	42/2500 (1.7%)
1	s	1.64	10/1841 (0.5%)	1.94	36/2500 (1.4%)
1	t	1.63	11/1841 (0.6%)	2.00	45/2500 (1.8%)
1	u	1.65	10/1841 (0.5%)	2.15	52/2500 (2.1%)
1	v	1.61	9/1841 (0.5%)	1.99	45/2500 (1.8%)
1	w	1.63	8/1841 (0.4%)	1.96	46/2500 (1.8%)
1	x	1.60	12/1841 (0.7%)	2.01	44/2500 (1.8%)
1	y	1.65	10/1841 (0.5%)	2.06	41/2500 (1.6%)
1	z	1.63	11/1841 (0.6%)	2.11	51/2500 (2.0%)
All	All	1.63	14053/2496396 (0.6%)	2.01	60301/3390000 (1.8%)

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	0	0	5
1	1	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	10	0	3
1	11	0	4
1	12	0	7
1	13	0	8
1	14	0	11
1	15	0	5
1	16	0	4
1	17	0	6
1	18	0	3
1	19	0	3
1	1A	0	4
1	1B	0	6
1	1C	0	5
1	1D	0	5
1	1E	0	3
1	1F	0	8
1	1G	0	5
1	1H	0	6
1	1I	0	4
1	1J	0	4
1	1K	0	9
1	1L	0	3
1	1M	0	9
1	1N	0	4
1	1O	0	2
1	1P	0	5
1	1Q	0	4
1	1R	0	6
1	1S	0	8
1	1T	0	9
1	1U	0	4
1	1V	0	7
1	1W	0	7
1	1X	0	7
1	1Y	0	4
1	1Z	0	2
1	1a	0	3
1	1b	0	6
1	1c	0	6
1	1d	0	6
1	1e	0	3
1	1f	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	1g	0	5
1	1h	0	10
1	1i	0	6
1	1j	0	5
1	1k	0	3
1	1l	0	5
1	1m	0	7
1	1n	0	2
1	1o	0	12
1	1p	0	1
1	1q	0	6
1	1r	0	8
1	1s	0	3
1	1t	0	4
1	1u	0	2
1	1v	0	4
1	1w	0	7
1	1x	0	5
1	1y	0	7
1	1z	0	6
1	2	0	3
1	20	0	4
1	21	0	8
1	22	0	6
1	23	0	8
1	24	0	5
1	25	0	4
1	26	0	9
1	27	0	1
1	28	0	6
1	29	0	7
1	2A	0	6
1	2B	0	5
1	2C	0	5
1	2D	0	10
1	2E	0	6
1	2F	0	4
1	2G	0	10
1	2H	0	5
1	2I	0	6
1	2J	0	6
1	2K	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	2L	0	3
1	2M	0	4
1	2N	0	8
1	2O	0	2
1	2P	0	3
1	2Q	0	7
1	2R	0	5
1	2S	0	3
1	2T	0	7
1	2U	0	11
1	2V	0	4
1	2W	0	7
1	2X	0	2
1	2Y	0	4
1	2Z	0	6
1	2a	0	4
1	2b	0	3
1	2c	0	5
1	2d	0	8
1	2e	0	3
1	2f	0	6
1	2g	0	7
1	2h	0	9
1	2i	0	4
1	2j	0	7
1	2k	0	3
1	2l	0	8
1	2m	0	6
1	2n	0	5
1	2o	0	9
1	2p	0	6
1	2q	0	8
1	2r	0	5
1	2s	0	6
1	2t	0	8
1	2u	0	2
1	2v	0	7
1	2w	0	3
1	2x	0	3
1	2y	0	5
1	2z	0	8
1	3	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	30	0	3
1	31	0	4
1	32	0	4
1	33	0	5
1	34	0	4
1	35	0	10
1	36	0	2
1	37	0	7
1	38	0	8
1	39	0	3
1	3A	0	4
1	3B	0	9
1	3C	0	1
1	3D	0	5
1	3E	0	2
1	3F	0	4
1	3G	0	5
1	3H	0	5
1	3I	0	4
1	3J	0	3
1	3K	0	1
1	3L	0	5
1	3M	0	6
1	3N	0	7
1	3O	0	6
1	3P	0	5
1	3Q	0	8
1	3R	0	5
1	3S	0	9
1	3T	0	8
1	3U	0	8
1	3V	0	4
1	3W	0	9
1	3X	0	6
1	3Y	0	6
1	3Z	0	7
1	3a	0	8
1	3b	0	7
1	3c	0	5
1	3d	0	10
1	3e	0	7
1	3f	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	3g	0	4
1	3h	0	5
1	3i	0	7
1	3j	0	3
1	3k	0	7
1	3l	0	6
1	3m	0	5
1	3n	0	4
1	3o	0	4
1	3p	0	7
1	3q	0	5
1	3r	0	9
1	3s	0	9
1	3t	0	9
1	3u	0	5
1	3v	0	5
1	3w	0	7
1	3x	0	2
1	3y	0	6
1	3z	0	8
1	4	0	8
1	40	0	4
1	41	0	4
1	42	0	9
1	43	0	3
1	44	0	5
1	45	0	3
1	46	0	7
1	47	0	8
1	48	0	3
1	49	0	5
1	4A	0	8
1	4B	0	4
1	4C	0	5
1	4D	0	5
1	4E	0	8
1	4F	0	7
1	4G	0	4
1	4H	0	1
1	4I	0	7
1	4J	0	6
1	4K	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	4L	0	7
1	4M	0	4
1	4N	0	5
1	4O	0	4
1	4P	0	4
1	4Q	0	3
1	4R	0	7
1	4S	0	7
1	4T	0	2
1	4U	0	6
1	4V	0	2
1	4W	0	3
1	4X	0	5
1	4Y	0	10
1	4Z	0	3
1	4a	0	8
1	4b	0	5
1	4c	0	7
1	4d	0	6
1	4e	0	7
1	4f	0	4
1	4g	0	7
1	4h	0	3
1	4i	0	4
1	4j	0	6
1	4k	0	5
1	4l	0	5
1	4m	0	7
1	4n	0	3
1	4o	0	10
1	4p	0	6
1	4q	0	6
1	4r	0	7
1	4s	0	5
1	4t	0	3
1	4u	0	5
1	4v	0	3
1	4w	0	8
1	4x	0	4
1	4y	0	6
1	4z	0	6
1	5	0	13

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	50	0	5
1	51	0	3
1	52	0	2
1	53	0	2
1	54	0	3
1	55	0	8
1	56	0	8
1	57	0	5
1	58	0	5
1	59	0	5
1	5A	0	11
1	5B	0	3
1	5C	0	3
1	5D	0	6
1	5E	0	6
1	5F	0	7
1	5G	0	4
1	5H	0	6
1	5I	0	4
1	5J	0	7
1	5K	0	2
1	5L	0	4
1	5M	0	5
1	5N	0	2
1	5O	0	6
1	5P	0	8
1	5Q	0	8
1	5R	0	5
1	5S	0	4
1	5T	0	8
1	5U	0	7
1	5V	0	3
1	5W	0	6
1	5X	0	5
1	5Y	0	1
1	5Z	0	4
1	5a	0	6
1	5b	0	6
1	5c	0	5
1	5d	0	5
1	5e	0	1
1	5f	0	6

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	5g	0	6
1	5h	0	4
1	5i	0	4
1	5j	0	1
1	5k	0	6
1	5l	0	7
1	5m	0	6
1	5n	0	4
1	5o	0	7
1	5p	0	5
1	5q	0	3
1	5r	0	5
1	5s	0	7
1	5t	0	6
1	5u	0	4
1	5v	0	6
1	5w	0	5
1	5x	0	6
1	5y	0	7
1	5z	0	4
1	6	0	5
1	60	0	3
1	61	0	2
1	62	0	6
1	63	0	5
1	64	0	6
1	65	0	9
1	66	0	2
1	67	0	5
1	68	0	7
1	69	0	4
1	6A	0	2
1	6B	0	7
1	6C	0	9
1	6D	0	4
1	6E	0	4
1	6F	0	4
1	6G	0	2
1	6H	0	5
1	6I	0	6
1	6J	0	4
1	6K	0	7

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	6L	0	4
1	6M	0	6
1	6N	0	7
1	6O	0	8
1	6P	0	10
1	6Q	0	4
1	6R	0	5
1	6S	0	4
1	6T	0	10
1	6U	0	7
1	6V	0	3
1	6W	0	6
1	6X	0	5
1	6Y	0	7
1	6Z	0	9
1	6a	0	4
1	6b	0	6
1	6c	0	2
1	6d	0	5
1	6e	0	4
1	6f	0	6
1	6g	0	6
1	6h	0	3
1	6i	0	5
1	6j	0	6
1	6k	0	2
1	6l	0	8
1	6m	0	4
1	6n	0	3
1	6o	0	6
1	6p	0	5
1	6q	0	5
1	6r	0	3
1	6s	0	6
1	6t	0	4
1	6u	0	7
1	6v	0	6
1	6w	0	6
1	6x	0	6
1	6y	0	2
1	6z	0	2
1	7	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	70	0	5
1	71	0	7
1	72	0	4
1	73	0	3
1	74	0	3
1	75	0	9
1	76	0	4
1	77	0	12
1	78	0	4
1	79	0	6
1	7A	0	4
1	7B	0	4
1	7C	0	7
1	7D	0	8
1	7E	0	3
1	7F	0	2
1	7G	0	7
1	7H	0	10
1	7I	0	8
1	7J	0	7
1	7K	0	5
1	7L	0	10
1	7M	0	8
1	7N	0	4
1	7O	0	4
1	7P	0	6
1	7Q	0	3
1	7R	0	3
1	7S	0	2
1	7T	0	5
1	7U	0	5
1	7V	0	4
1	7W	0	6
1	7X	0	5
1	7Y	0	5
1	7Z	0	7
1	7a	0	4
1	7b	0	4
1	7c	0	13
1	7d	0	6
1	7e	0	7
1	7f	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	7g	0	6
1	7h	0	8
1	7i	0	7
1	7j	0	7
1	7k	0	8
1	7l	0	8
1	7m	0	4
1	7n	0	7
1	7o	0	4
1	7p	0	3
1	7q	0	6
1	7r	0	8
1	7s	0	8
1	7t	0	5
1	7u	0	3
1	7v	0	2
1	7w	0	6
1	7x	0	5
1	7y	0	3
1	7z	0	7
1	8	0	9
1	80	0	8
1	81	0	5
1	82	0	6
1	83	0	4
1	84	0	6
1	85	0	3
1	86	0	5
1	87	0	8
1	88	0	9
1	89	0	5
1	8A	0	7
1	8B	0	9
1	8C	0	5
1	8D	0	3
1	8E	0	6
1	8F	0	9
1	8G	0	7
1	8H	0	4
1	8I	0	3
1	8J	0	4
1	8K	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	8L	0	4
1	8M	0	4
1	8N	0	4
1	8O	0	4
1	8P	0	5
1	8Q	0	5
1	8R	0	7
1	8S	0	7
1	8T	0	3
1	8U	0	7
1	8V	0	4
1	8W	0	5
1	8X	0	10
1	8Y	0	5
1	8Z	0	2
1	8a	0	5
1	8b	0	3
1	8c	0	6
1	8d	0	7
1	8e	0	4
1	8f	0	5
1	8g	0	6
1	8h	0	3
1	8i	0	7
1	8j	0	4
1	8k	0	6
1	8l	0	9
1	8m	0	6
1	8n	0	3
1	8o	0	3
1	8p	0	7
1	8q	0	5
1	8r	0	5
1	8s	0	6
1	8t	0	7
1	8u	0	3
1	8v	0	10
1	8w	0	2
1	8x	0	4
1	8y	0	2
1	8z	0	5
1	9	0	6

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	90	0	7
1	91	0	2
1	92	0	8
1	93	0	4
1	94	0	5
1	95	0	4
1	96	0	4
1	97	0	5
1	98	0	6
1	99	0	3
1	9A	0	4
1	9B	0	8
1	9C	0	5
1	9D	0	6
1	9E	0	5
1	9F	0	4
1	9G	0	7
1	9H	0	5
1	9I	0	6
1	9J	0	2
1	9K	0	5
1	9L	0	4
1	9M	0	6
1	9N	0	5
1	9O	0	10
1	9P	0	6
1	9Q	0	4
1	9R	0	2
1	9S	0	5
1	9T	0	8
1	9U	0	5
1	9V	0	3
1	9W	0	6
1	9X	0	8
1	9Y	0	10
1	9Z	0	4
1	9a	0	6
1	9b	0	6
1	9c	0	6
1	9d	0	11
1	9e	0	7
1	9f	0	10

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	9g	0	8
1	9h	0	8
1	9i	0	6
1	9j	0	7
1	9k	0	3
1	9l	0	6
1	9m	0	4
1	9n	0	9
1	9o	0	7
1	9p	0	9
1	9q	0	7
1	9r	0	6
1	9s	0	6
1	9t	0	9
1	9u	0	5
1	9v	0	7
1	9w	0	3
1	9x	0	3
1	9y	0	4
1	9z	0	3
1	A	0	9
1	B	0	2
1	C	0	5
1	D	0	10
1	E	0	2
1	F	0	6
1	G	0	6
1	H	0	3
1	I	0	4
1	J	0	4
1	K	0	6
1	L	0	8
1	M	0	9
1	N	0	10
1	O	0	9
1	P	0	7
1	Q	0	3
1	R	0	8
1	S	0	3
1	T	0	4
1	U	0	4
1	V	0	7

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	W	0	3
1	X	0	2
1	Y	0	2
1	Z	0	2
1	a	0	7
1	a0	0	9
1	a1	0	4
1	a2	0	3
1	a3	0	4
1	a4	0	8
1	a5	0	5
1	a6	0	6
1	a7	0	5
1	a8	0	3
1	a9	0	6
1	aA	0	5
1	aB	0	4
1	aC	0	6
1	aD	0	5
1	aE	0	5
1	aF	0	6
1	aG	0	5
1	aH	0	3
1	aI	0	2
1	aJ	0	3
1	aK	0	9
1	aL	0	5
1	aM	0	5
1	aN	0	3
1	aO	0	9
1	aP	0	7
1	aQ	0	4
1	aR	0	5
1	aS	0	7
1	aT	0	2
1	aU	0	8
1	aV	0	8
1	aW	0	5
1	aX	0	8
1	aY	0	7
1	aZ	0	10
1	aa	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	ab	0	7
1	ac	0	8
1	ad	0	6
1	ae	0	7
1	af	0	5
1	ag	0	7
1	ah	0	4
1	ai	0	7
1	aj	0	5
1	ak	0	1
1	al	0	5
1	am	0	6
1	an	0	3
1	ao	0	7
1	ap	0	8
1	aq	0	5
1	ar	0	3
1	as	0	5
1	at	0	5
1	au	0	6
1	av	0	8
1	aw	0	6
1	ax	0	10
1	ay	0	3
1	az	0	7
1	b	0	6
1	b0	0	4
1	b1	0	9
1	b2	0	6
1	b3	0	10
1	b4	0	7
1	b5	0	7
1	b6	0	8
1	b7	0	4
1	b8	0	3
1	b9	0	3
1	bA	0	4
1	bB	0	8
1	bC	0	7
1	bD	0	4
1	bE	0	12
1	bF	0	7

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	bG	0	4
1	bH	0	6
1	bI	0	6
1	bJ	0	6
1	bK	0	5
1	bL	0	5
1	bM	0	5
1	bN	0	6
1	bO	0	2
1	bP	0	3
1	bQ	0	3
1	bR	0	13
1	bS	0	5
1	bT	0	6
1	bU	0	5
1	bV	0	6
1	bW	0	9
1	bX	0	3
1	bY	0	5
1	bZ	0	7
1	ba	0	7
1	bb	0	6
1	bc	0	6
1	bd	0	2
1	be	0	3
1	bf	0	8
1	bg	0	6
1	bh	0	4
1	bi	0	7
1	bj	0	5
1	bk	0	6
1	bl	0	4
1	bm	0	10
1	bn	0	6
1	bo	0	6
1	bp	0	3
1	bq	0	8
1	br	0	8
1	bs	0	6
1	bt	0	3
1	bu	0	2
1	bv	0	6

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	bw	0	5
1	bx	0	9
1	by	0	5
1	bz	0	7
1	c	0	7
1	c0	0	7
1	c1	0	4
1	c2	0	5
1	c3	0	6
1	c4	0	8
1	c5	0	4
1	c6	0	1
1	c7	0	6
1	c8	0	4
1	c9	0	4
1	cA	0	5
1	cB	0	7
1	cC	0	5
1	cD	0	4
1	cE	0	4
1	cF	0	2
1	cG	0	3
1	cH	0	7
1	cI	0	4
1	cJ	0	5
1	cK	0	4
1	cL	0	5
1	cM	0	4
1	cN	0	5
1	cO	0	6
1	cP	0	2
1	cQ	0	9
1	cR	0	3
1	cS	0	4
1	cT	0	11
1	cU	0	8
1	cV	0	5
1	cW	0	9
1	cX	0	5
1	cY	0	4
1	cZ	0	5
1	ca	0	8

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	cb	0	6
1	cc	0	7
1	cd	0	3
1	ce	0	2
1	cf	0	2
1	cg	0	8
1	ch	0	4
1	ci	0	6
1	cj	0	8
1	ck	0	6
1	cl	0	2
1	cm	0	5
1	cn	0	8
1	co	0	3
1	cp	0	8
1	cq	0	6
1	cr	0	6
1	cs	0	9
1	ct	0	6
1	cu	0	7
1	cv	0	7
1	cw	0	4
1	cx	0	5
1	cy	0	4
1	cz	0	4
1	d	0	5
1	d0	0	5
1	d1	0	4
1	d2	0	7
1	d3	0	4
1	d4	0	7
1	d5	0	5
1	d6	0	8
1	d7	0	4
1	d8	0	6
1	d9	0	9
1	dA	0	8
1	dB	0	1
1	dC	0	10
1	dD	0	3
1	dE	0	10
1	dF	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	dG	0	5
1	dH	0	3
1	dI	0	4
1	dJ	0	5
1	dK	0	5
1	dL	0	6
1	dM	0	4
1	dN	0	8
1	dO	0	3
1	dP	0	6
1	dQ	0	9
1	dR	0	5
1	dS	0	6
1	dT	0	5
1	dU	0	7
1	dV	0	5
1	dW	0	8
1	dX	0	5
1	dY	0	6
1	dZ	0	6
1	da	0	5
1	db	0	5
1	dc	0	6
1	dd	0	4
1	de	0	7
1	df	0	8
1	dg	0	7
1	dh	0	4
1	di	0	5
1	dj	0	9
1	dk	0	2
1	dl	0	5
1	dm	0	7
1	dn	0	7
1	do	0	5
1	dp	0	5
1	dq	0	1
1	dr	0	6
1	ds	0	3
1	dt	0	3
1	du	0	5
1	dv	0	6

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	dw	0	7
1	dx	0	8
1	dy	0	2
1	dz	0	7
1	e	0	5
1	e0	0	2
1	e1	0	4
1	e2	0	1
1	e3	0	3
1	e4	0	4
1	e5	0	4
1	e6	0	6
1	e7	0	5
1	e8	0	6
1	e9	0	3
1	eA	0	9
1	eB	0	4
1	eC	0	6
1	eD	0	5
1	eE	0	7
1	eF	0	5
1	eG	0	5
1	eH	0	3
1	eI	0	7
1	eJ	0	4
1	eK	0	6
1	eL	0	4
1	eM	0	6
1	eN	0	7
1	eO	0	3
1	eP	0	10
1	eQ	0	2
1	eR	0	3
1	eS	0	5
1	eT	0	5
1	eU	0	4
1	eV	0	3
1	eW	0	4
1	eX	0	7
1	eY	0	4
1	eZ	0	5
1	ea	0	8

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	eb	0	1
1	ec	0	9
1	ed	0	5
1	ee	0	7
1	ef	0	8
1	eg	0	5
1	eh	0	9
1	ei	0	6
1	ej	0	7
1	ek	0	5
1	el	0	6
1	em	0	6
1	en	0	8
1	eo	0	6
1	ep	0	6
1	eq	0	5
1	er	0	6
1	es	0	4
1	et	0	6
1	eu	0	2
1	ev	0	6
1	ew	0	3
1	ex	0	8
1	ey	0	4
1	ez	0	5
1	f	0	5
1	f1	0	3
1	f2	0	5
1	f3	0	6
1	f4	0	5
1	f5	0	5
1	f6	0	4
1	f7	0	6
1	f8	0	7
1	f9	0	4
1	fA	0	7
1	fB	0	6
1	fC	0	5
1	fD	0	2
1	fE	0	8
1	fF	0	6
1	fG	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	fH	0	5
1	fI	0	4
1	fJ	0	3
1	fK	0	4
1	fL	0	6
1	fM	0	2
1	fN	0	6
1	fO	0	3
1	fP	0	6
1	fQ	0	4
1	fR	0	4
1	fS	0	5
1	fT	0	2
1	fU	0	8
1	fV	0	4
1	fW	0	2
1	fX	0	6
1	fY	0	6
1	fZ	0	7
1	fa	0	5
1	fb	0	6
1	fc	0	5
1	fd	0	4
1	fe	0	7
1	ff	0	6
1	fg	0	3
1	fh	0	8
1	fi	0	5
1	fj	0	4
1	fk	0	7
1	fl	0	3
1	fm	0	4
1	fn	0	6
1	fo	0	6
1	fp	0	4
1	fq	0	9
1	fr	0	2
1	fs	0	10
1	ft	0	6
1	fu	0	7
1	fv	0	6
1	fw	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	fx	0	2
1	fy	0	9
1	fz	0	7
1	g	0	5
1	g0	0	6
1	g1	0	6
1	g2	0	3
1	g3	0	8
1	g4	0	9
1	g5	0	6
1	g6	0	4
1	g7	0	4
1	g8	0	5
1	g9	0	4
1	gA	0	4
1	gB	0	5
1	gC	0	3
1	gD	0	5
1	gE	0	3
1	gF	0	5
1	gG	0	6
1	gH	0	8
1	gI	0	6
1	gJ	0	6
1	gK	0	4
1	gL	0	9
1	gM	0	10
1	gN	0	3
1	gO	0	9
1	gP	0	6
1	gQ	0	1
1	gR	0	5
1	gS	0	8
1	gT	0	5
1	gU	0	8
1	gV	0	3
1	gW	0	6
1	gX	0	10
1	gY	0	5
1	gZ	0	3
1	ga	0	7
1	gb	0	8

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	gc	0	3
1	gd	0	4
1	ge	0	6
1	gf	0	5
1	gg	0	7
1	gh	0	7
1	gi	0	5
1	gj	0	2
1	gk	0	5
1	gl	0	6
1	gm	0	3
1	gn	0	7
1	go	0	7
1	gp	0	7
1	gq	0	7
1	gr	0	7
1	gs	0	7
1	gt	0	5
1	gu	0	4
1	gv	0	5
1	gw	0	6
1	gx	0	4
1	gy	0	5
1	gz	0	3
1	h	0	3
1	h0	0	7
1	h1	0	3
1	h2	0	4
1	h3	0	5
1	h4	0	6
1	h5	0	10
1	h6	0	6
1	h7	0	2
1	h8	0	3
1	h9	0	4
1	hA	0	4
1	hB	0	2
1	hC	0	7
1	hD	0	6
1	hE	0	4
1	hF	0	8
1	hG	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	hH	0	4
1	hI	0	6
1	hJ	0	7
1	hK	0	5
1	hL	0	9
1	hM	0	8
1	hN	0	9
1	hO	0	4
1	hP	0	5
1	hQ	0	4
1	hR	0	6
1	hS	0	5
1	hT	0	5
1	hU	0	9
1	hV	0	9
1	hW	0	9
1	hX	0	4
1	hY	0	9
1	hZ	0	5
1	ha	0	5
1	hb	0	4
1	hc	0	4
1	hd	0	6
1	he	0	8
1	hf	0	4
1	hg	0	4
1	hh	0	4
1	hi	0	3
1	hj	0	6
1	hk	0	3
1	hl	0	2
1	hm	0	6
1	hn	0	7
1	ho	0	8
1	hp	0	11
1	hq	0	8
1	hr	0	6
1	hs	0	8
1	ht	0	5
1	hu	0	3
1	hv	0	7
1	hw	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	hx	0	5
1	hy	0	6
1	hz	0	7
1	i	0	6
1	i0	0	8
1	i1	0	6
1	i2	0	10
1	i3	0	3
1	i4	0	7
1	i5	0	7
1	i6	0	3
1	i7	0	12
1	i8	0	4
1	i9	0	5
1	iA	0	7
1	iB	0	3
1	iC	0	5
1	iD	0	4
1	iE	0	4
1	iF	0	5
1	iG	0	4
1	iH	0	6
1	iI	0	4
1	iJ	0	10
1	iK	0	3
1	iL	0	2
1	iM	0	4
1	iN	0	8
1	iO	0	6
1	iP	0	4
1	iQ	0	3
1	iR	0	7
1	iS	0	8
1	iT	0	5
1	iU	0	1
1	iV	0	7
1	iW	0	5
1	iX	0	4
1	iY	0	7
1	iZ	0	6
1	ia	0	5
1	ib	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	ic	0	3
1	id	0	4
1	ie	0	7
1	if	0	3
1	ig	0	11
1	ih	0	10
1	ii	0	4
1	ij	0	7
1	ik	0	8
1	il	0	7
1	im	0	6
1	in	0	4
1	io	0	4
1	ip	0	6
1	iq	0	4
1	ir	0	6
1	is	0	5
1	it	0	3
1	iu	0	5
1	iv	0	8
1	iw	0	4
1	ix	0	6
1	iy	0	5
1	iz	0	6
1	j	0	2
1	j0	0	6
1	j1	0	3
1	j2	0	7
1	j3	0	6
1	j4	0	3
1	j5	0	8
1	j6	0	6
1	j7	0	2
1	j8	0	5
1	j9	0	9
1	jA	0	7
1	jB	0	6
1	jC	0	7
1	jD	0	7
1	jE	0	4
1	jF	0	8
1	jG	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	jH	0	5
1	jI	0	3
1	jJ	0	7
1	jK	0	7
1	jL	0	6
1	jM	0	5
1	jN	0	4
1	jO	0	8
1	jP	0	6
1	jQ	0	5
1	jR	0	2
1	jS	0	6
1	jT	0	6
1	jU	0	6
1	jV	0	1
1	jW	0	4
1	jX	0	2
1	jY	0	9
1	jZ	0	8
1	ja	0	4
1	jb	0	6
1	jc	0	8
1	jd	0	3
1	je	0	6
1	jf	0	5
1	jg	0	10
1	jh	0	7
1	ji	0	7
1	jj	0	7
1	jk	0	4
1	jl	0	7
1	jm	0	8
1	jn	0	7
1	jo	0	6
1	jp	0	5
1	jq	0	9
1	jr	0	4
1	js	0	7
1	jt	0	8
1	ju	0	7
1	jv	0	2
1	jw	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	jx	0	6
1	jy	0	2
1	jz	0	5
1	k	0	9
1	k0	0	9
1	k1	0	8
1	k2	0	5
1	k3	0	4
1	k4	0	8
1	k5	0	4
1	k6	0	7
1	k7	0	7
1	k8	0	7
1	k9	0	7
1	kA	0	4
1	kB	0	8
1	kC	0	7
1	kD	0	5
1	kE	0	4
1	kF	0	2
1	kG	0	8
1	kH	0	7
1	kI	0	1
1	kJ	0	11
1	kK	0	6
1	kL	0	3
1	kM	0	2
1	kN	0	1
1	kO	0	4
1	kP	0	9
1	kQ	0	5
1	kR	0	8
1	kS	0	4
1	kT	0	5
1	kU	0	8
1	kV	0	5
1	kW	0	8
1	kX	0	6
1	kY	0	5
1	kZ	0	5
1	ka	0	9
1	kb	0	9

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	kc	0	7
1	kd	0	3
1	ke	0	1
1	kf	0	3
1	kg	0	2
1	kh	0	7
1	ki	0	7
1	kj	0	4
1	kk	0	6
1	kl	0	3
1	km	0	4
1	kn	0	6
1	ko	0	10
1	kp	0	6
1	kq	0	4
1	kr	0	7
1	ks	0	4
1	kt	0	6
1	ku	0	6
1	0	9	
1	kw	0	4
1	kx	0	9
1	ky	0	9
1	kz	0	5
1	l	0	5
1	l0	0	10
1	l1	0	4
1	l2	0	5
1	l3	0	6
1	l4	0	3
1	l5	0	5
1	l6	0	2
1	l7	0	8
1	l8	0	8
1	l9	0	4
1	lA	0	4
1	lB	0	7
1	lC	0	5
1	lD	0	3
1	lE	0	4
1	lF	0	7
1	lG	0	6

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	lH	0	11
1	lI	0	5
1	lJ	0	4
1	lK	0	5
1	lL	0	5
1	lM	0	8
1	lN	0	6
1	lO	0	6
1	lP	0	5
1	lQ	0	6
1	lR	0	2
1	la	0	9
1	lb	0	5
1	lc	0	2
1	ld	0	4
1	le	0	5
1	lf	0	10
1	lg	0	1
1	lh	0	5
1	li	0	6
1	lj	0	7
1	lk	0	5
1	ll	0	9
1	ln	0	5
1	lo	0	8
1	lp	0	7
1	lq	0	6
1	lr	0	8
1	ls	0	5
1	lt	0	6
1	lu	0	5
1	lv	0	6
1	lw	0	2
1	lx	0	4
1	ly	0	6
1	lz	0	7
1	m	0	5
1	n	0	9
1	o	0	5
1	p	0	2
1	q	0	6
1	r	0	7

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	s	0	2
1	t	0	6
1	u	0	1
1	v	0	6
1	w	0	5
1	x	0	5
1	y	0	1
1	z	0	6
All	All	0	7415

The worst 5 of 14053 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	gl	33	SER	CA-CB	12.33	1.71	1.52
1	eB	40	PHE	CB-CG	11.07	1.70	1.51
1	fB	130	TYR	CE1-CZ	10.94	1.52	1.38
1	1b	33	SER	CA-CB	10.42	1.68	1.52
1	8o	130	TYR	CG-CD2	10.32	1.52	1.39

The worst 5 of 60301 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	l0	162	ARG	NE-CZ-NH2	-34.90	102.85	120.30
1	2O	143	ARG	NE-CZ-NH1	31.97	136.29	120.30
1	dM	154	ARG	NE-CZ-NH1	31.22	135.91	120.30
1	1I	229	ARG	NE-CZ-NH1	30.75	135.68	120.30
1	M	167	ARG	NE-CZ-NH1	30.63	135.61	120.30

There are no chirality outliers.

5 of 7415 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	g8	130	TYR	Sidechain
1	g8	132	ARG	Sidechain
1	g8	154	ARG	Sidechain
1	g8	18	ARG	Sidechain
1	g8	62	HIS	Sidechain

## 5.2 Too-close contacts

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](#)

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides 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 Tomogram visualisation

This section contains visualisations of the EMDB entry EMD-5639. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

### 6.1 Orthogonal projections

This section was not generated.

### 6.2 Central slices

This section was not generated.

### 6.3 Largest variance slices

This section was not generated.

### 6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

### 6.5 Mask visualisation

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

## 7 Tomogram analysis

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

### 7.1 Map-value distribution

This section was not generated.

## 8 Map-model fit

This section was not generated.