



wwPDB EM Validation Summary Report ⓘ

Mar 31, 2026 – 11:35 AM EDT

PDB ID : 3J3Q / pdb_00003j3q
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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

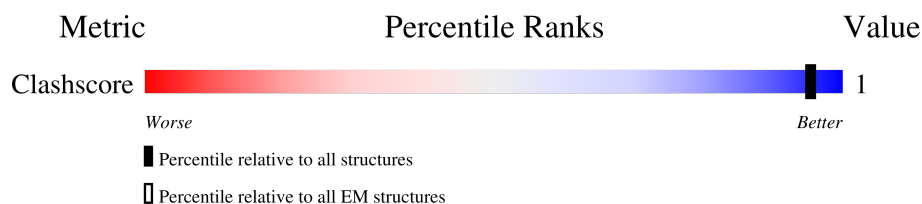
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

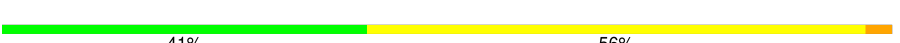
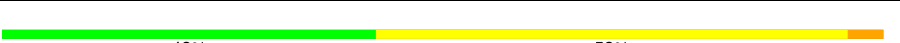
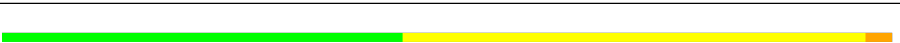
The reported resolution of this entry is unknown.

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



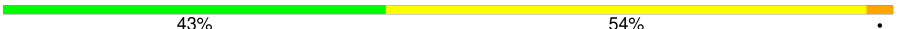
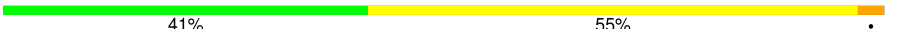
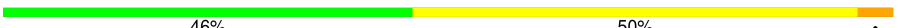
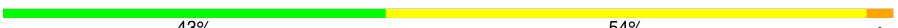
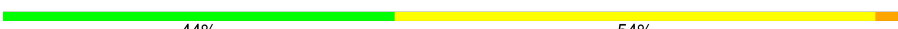
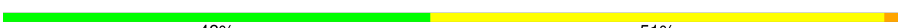
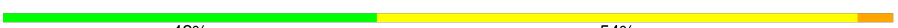
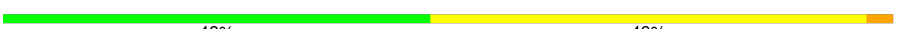
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	0	231	 43% 53% .
1	1	231	 42% 57% .
1	10	231	 44% 53% .
1	11	231	 45% 53% .
1	12	231	 41% 56% .
1	13	231	 43% 52% .
1	14	231	 46% 49% 5% .
1	15	231	 41% 56% .
1	16	231	 51% 46% .
1	17	231	 42% 53% .
1	18	231	 45% 52% .

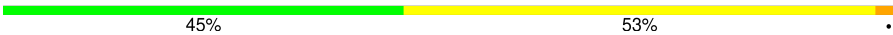
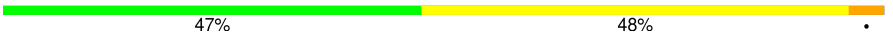
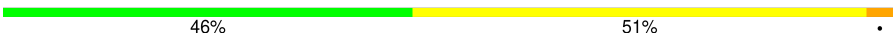
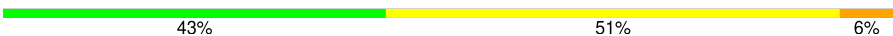
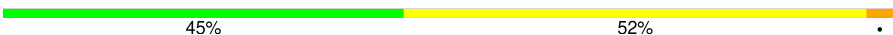
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Mol	Chain	Length	Quality of chain
1	19	231	 45% 54% .
1	1A	231	 43% 54% .
1	1B	231	 50% 47% .
1	1C	231	 41% 55% .
1	1D	231	 51% 47% .
1	1E	231	 51% 45% . .
1	1F	231	 44% 51% 5% .
1	1G	231	 45% 51% .
1	1H	231	 46% 50% .
1	1I	231	 48% 50% .
1	1J	231	 43% 54% .
1	1K	231	 42% 54% .
1	1L	231	 46% 52% .
1	1M	231	 47% 49% .
1	1N	231	 44% 54% .
1	1O	231	 49% 49% .
1	1P	231	 49% 48% .
1	1Q	231	 48% 51% .
1	1R	231	 45% 52% .
1	1S	231	 42% 54% .
1	1T	231	 48% 49% .
1	1U	231	 50% 47% .
1	1V	231	 45% 51% .
1	1W	231	 47% 51% .
1	1X	231	 46% 50% .

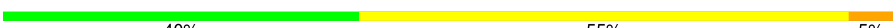
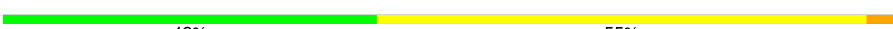
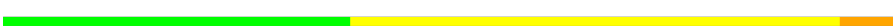
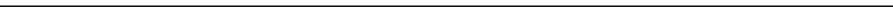
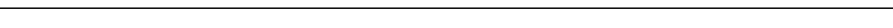
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Mol	Chain	Length	Quality of chain
1	1Y	231	 41%57%.
1	1Z	231	 40%58%.
1	1a	231	 49%49%.
1	1b	231	 45%53%.
1	1c	231	 49%48%.
1	1d	231	 47%48%.
1	1e	231	 48%51%.
1	1f	231	 48%50%.
1	1g	231	 46%51%.
1	1h	231	 43%51%6%.
1	1i	231	 45%52%.
1	1j	231	 50%45%5%.
1	1k	231	 48%50%.
1	1l	231	 44%52%.
1	1m	231	 48%47%6%.
1	1n	231	 45%52%.
1	1o	231	 42%53%5%.
1	1p	231	 52%47%.
1	1q	231	 47%50%.
1	1r	231	 47%49%.
1	1s	231	 44%53%.
1	1t	231	 45%54%.
1	1u	231	 52%45%.
1	1v	231	 48%50%.
1	1w	231	 47%52%.

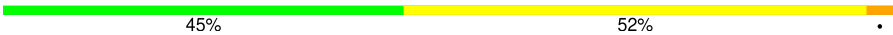
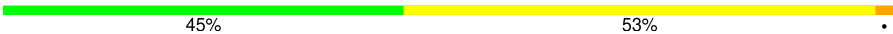
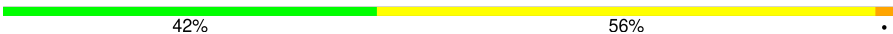
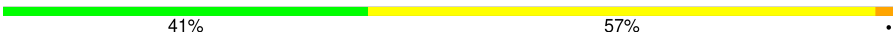
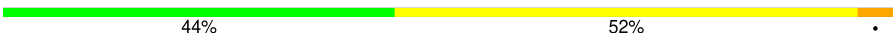
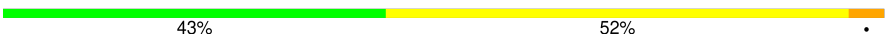
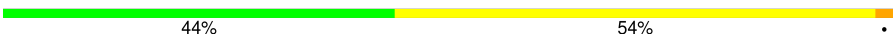
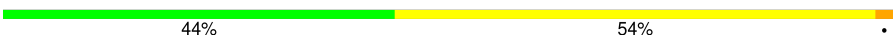
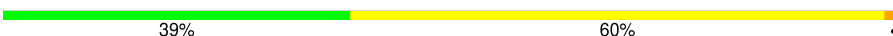
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Mol	Chain	Length	Quality of chain
1	1x	231	
1	1y	231	
1	1z	231	
1	2	231	
1	20	231	
1	21	231	
1	22	231	
1	23	231	
1	24	231	
1	25	231	
1	26	231	
1	27	231	
1	28	231	
1	29	231	
1	2A	231	
1	2B	231	
1	2C	231	
1	2D	231	
1	2E	231	
1	2F	231	
1	2G	231	
1	2H	231	
1	2I	231	
1	2J	231	
1	2K	231	

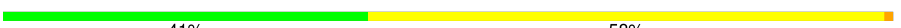
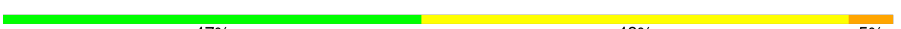
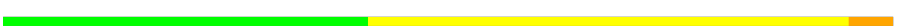
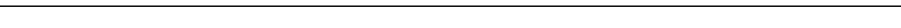
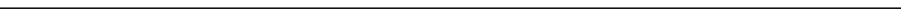
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Mol	Chain	Length	Quality of chain
1	2L	231	
1	2M	231	
1	2N	231	
1	2O	231	
1	2P	231	
1	2Q	231	
1	2R	231	
1	2S	231	
1	2T	231	
1	2U	231	
1	2V	231	
1	2W	231	
1	2X	231	
1	2Y	231	
1	2Z	231	
1	2a	231	
1	2b	231	
1	2c	231	
1	2d	231	
1	2e	231	
1	2f	231	
1	2g	231	
1	2h	231	
1	2i	231	
1	2j	231	

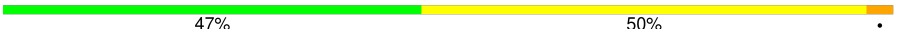
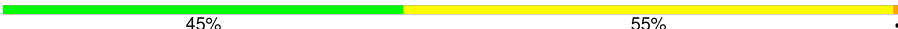
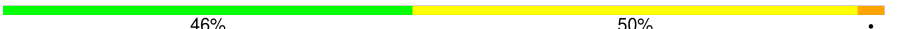
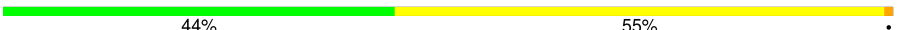
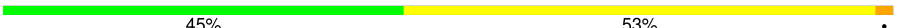
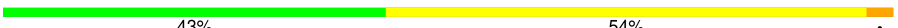
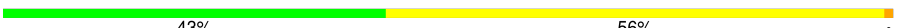
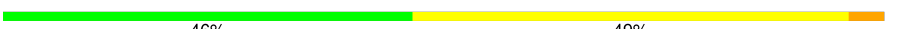
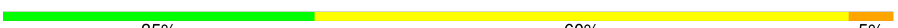
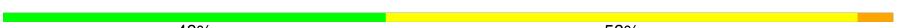
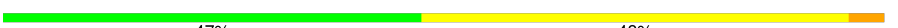
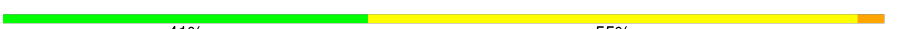
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Mol	Chain	Length	Quality of chain
1	2k	231	 46% 52% .
1	2l	231	 46% 50% .
1	2m	231	 50% 45% 5% .
1	2n	231	 41% 58% .
1	2o	231	 47% 48% 5% .
1	2p	231	 41% 54% 5% .
1	2q	231	 44% 53% .
1	2r	231	 44% 53% .
1	2s	231	 45% 52% .
1	2t	231	 45% 50% .
1	2u	231	 49% 49% .
1	2v	231	 42% 54% .
1	2w	231	 41% 57% .
1	2x	231	 41% 57% .
1	2y	231	 43% 55% .
1	2z	231	 44% 53% .
1	3	231	 45% 52% .
1	30	231	 39% 58% .
1	31	231	 49% 48% .
1	32	231	 43% 53% .
1	33	231	 47% 49% .
1	34	231	 49% 49% .
1	35	231	 49% 47% .
1	36	231	 46% 51% .
1	37	231	 44% 54% .

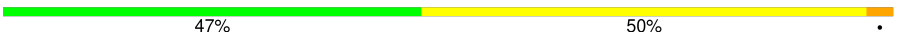
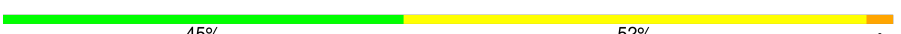
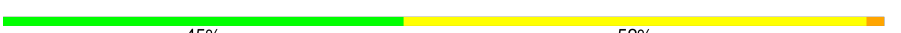
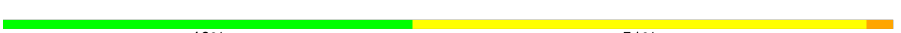
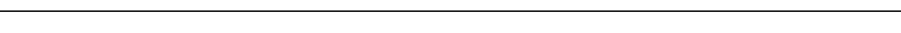
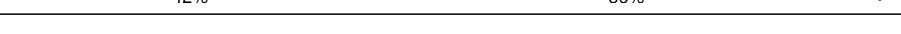
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Mol	Chain	Length	Quality of chain
1	38	231	 47% 52% .
1	39	231	 47% 50% .
1	3A	231	 45% 55% .
1	3B	231	 46% 50% .
1	3C	231	 44% 55% .
1	3D	231	 45% 53% .
1	3E	231	 47% 52% .
1	3F	231	 39% 59% .
1	3G	231	 43% 54% .
1	3H	231	 47% 49% .
1	3I	231	 43% 56% .
1	3J	231	 47% 51% .
1	3K	231	 45% 52% .
1	3L	231	 45% 53% .
1	3M	231	 46% 49% .
1	3N	231	 44% 52% 5% .
1	3O	231	 35% 60% 5% .
1	3P	231	 43% 53% .
1	3Q	231	 43% 54% .
1	3R	231	 47% 48% .
1	3S	231	 41% 55% .
1	3T	231	 46% 52% .
1	3U	231	 47% 49% .
1	3V	231	 45% 51% .
1	3W	231	 43% 53% .

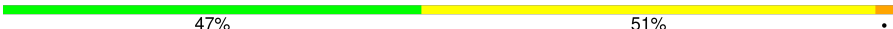
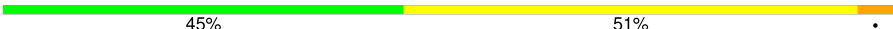
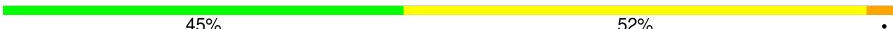
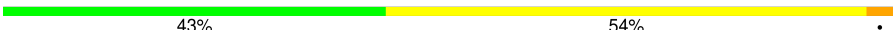
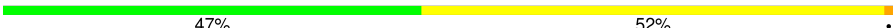
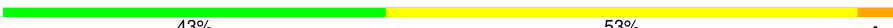
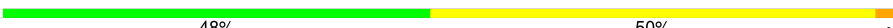
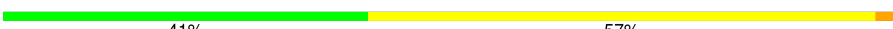
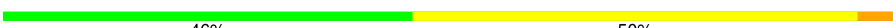
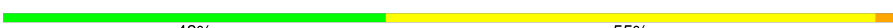
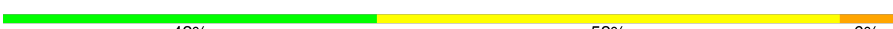
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Mol	Chain	Length	Quality of chain
1	3X	231	
1	3Y	231	
1	3Z	231	
1	3a	231	
1	3b	231	
1	3c	231	
1	3d	231	
1	3e	231	
1	3f	231	
1	3g	231	
1	3h	231	
1	3i	231	
1	3j	231	
1	3k	231	
1	3l	231	
1	3m	231	
1	3n	231	
1	3o	231	
1	3p	231	
1	3q	231	
1	3r	231	
1	3s	231	
1	3t	231	
1	3u	231	
1	3v	231	

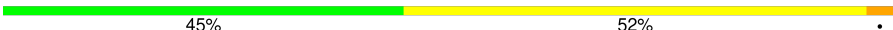
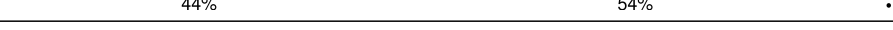
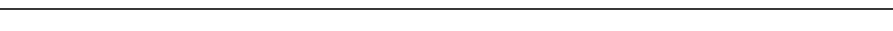
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Mol	Chain	Length	Quality of chain
1	3w	231	 45% 52% .
1	3x	231	 47% 51% .
1	3y	231	 45% 51% .
1	3z	231	 45% 52% .
1	4	231	 43% 54% .
1	40	231	 47% 52% .
1	41	231	 45% 50% .
1	42	231	 42% 52% 5%
1	43	231	 43% 53% .
1	44	231	 44% 53% .
1	45	231	 48% 50% .
1	46	231	 45% 54% .
1	47	231	 46% 51% .
1	48	231	 42% 56% .
1	49	231	 41% 57% .
1	4A	231	 48% 47% 5%
1	4B	231	 46% 50% .
1	4C	231	 54% 43% .
1	4D	231	 43% 54% .
1	4E	231	 43% 55% .
1	4F	231	 42% 52% 6%
1	4G	231	 44% 54% .
1	4H	231	 48% 49% .
1	4I	231	 45% 53% .
1	4J	231	 44% 53% .

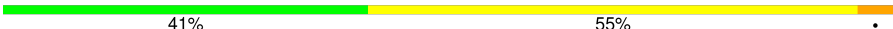
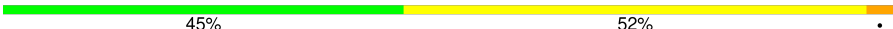
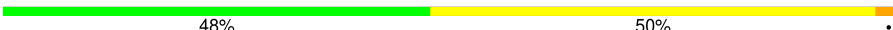
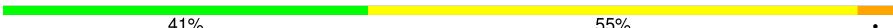
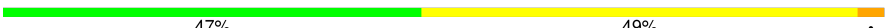
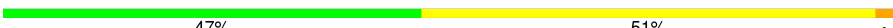
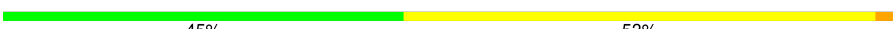
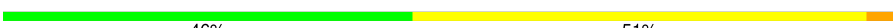
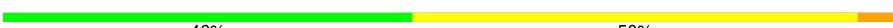
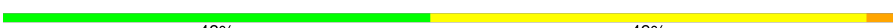
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Mol	Chain	Length	Quality of chain
1	4K	231	 45% 52% .
1	4L	231	 48% 47% 5% .
1	4M	231	 42% 55% .
1	4N	231	 48% 50% .
1	4O	231	 43% 55% .
1	4P	231	 44% 55% .
1	4Q	231	 48% 50% .
1	4R	231	 45% 51% .
1	4S	231	 45% 52% .
1	4T	231	 45% 54% .
1	4U	231	 40% 57% .
1	4V	231	 48% 51% .
1	4W	231	 48% 50% .
1	4X	231	 44% 54% .
1	4Y	231	 45% 51% .
1	4Z	231	 42% 57% .
1	4a	231	 44% 52% .
1	4b	231	 40% 58% .
1	4c	231	 41% 56% .
1	4d	231	 42% 55% .
1	4e	231	 49% 49% .
1	4f	231	 40% 55% 5% .
1	4g	231	 49% 48% .
1	4h	231	 39% 59% .
1	4i	231	 49% 48% .

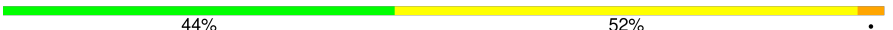
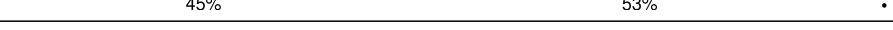
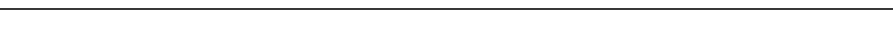
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Mol	Chain	Length	Quality of chain
1	4j	231	
1	4k	231	
1	4l	231	
1	4m	231	
1	4n	231	
1	4o	231	
1	4p	231	
1	4q	231	
1	4r	231	
1	4s	231	
1	4t	231	
1	4u	231	
1	4v	231	
1	4w	231	
1	4x	231	
1	4y	231	
1	4z	231	
1	5	231	
1	50	231	
1	51	231	
1	52	231	
1	53	231	
1	54	231	
1	55	231	
1	56	231	

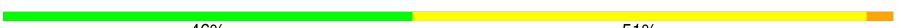
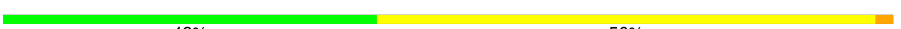
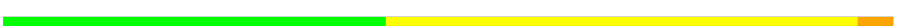
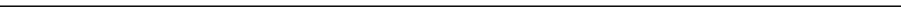
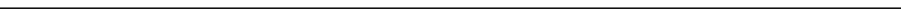
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Mol	Chain	Length	Quality of chain
1	57	231	 44% 52%
1	58	231	 42% 55%
1	59	231	 41% 57%
1	5A	231	 46% 50%
1	5B	231	 46% 52%
1	5C	231	 41% 56%
1	5D	231	 44% 53%
1	5E	231	 43% 54%
1	5F	231	 47% 49%
1	5G	231	 42% 55%
1	5H	231	 51% 47%
1	5I	231	 45% 52%
1	5J	231	 45% 50% 5%
1	5K	231	 45% 53%
1	5L	231	 42% 55%
1	5M	231	 48% 48%
1	5N	231	 50% 48%
1	5O	231	 46% 52%
1	5P	231	 47% 48%
1	5Q	231	 46% 50%
1	5R	231	 44% 53%
1	5S	231	 44% 53%
1	5T	231	 38% 57% 5%
1	5U	231	 47% 50%
1	5V	231	 44% 53%

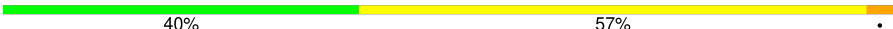
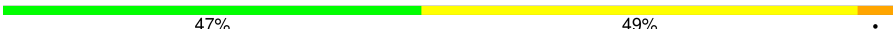
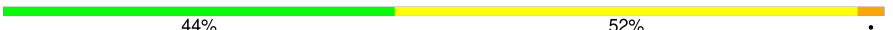
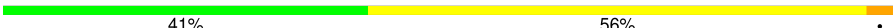
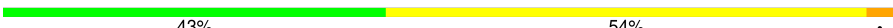
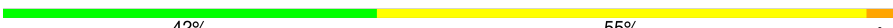
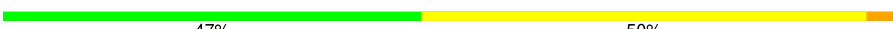
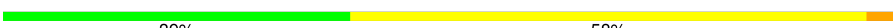
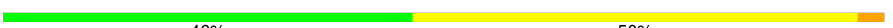
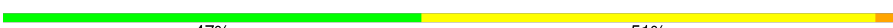
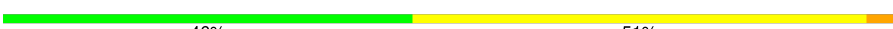
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Mol	Chain	Length	Quality of chain
1	5W	231	 45%50%6%
1	5X	231	 48%50%.
1	5Y	231	 43%56%.
1	5Z	231	 46%51%.
1	5a	231	 42%56%.
1	5b	231	 43%53%.
1	5c	231	 42%54%.
1	5d	231	 45%51%.
1	5e	231	 47%52%
1	5f	231	 38%58%.
1	5g	231	 46%52%.
1	5h	231	 41%58%.
1	5i	231	 47%49%.
1	5j	231	 45%53%.
1	5k	231	 46%50%.
1	5l	231	 42%55%.
1	5m	231	 48%49%.
1	5n	231	 44%54%.
1	5o	231	 46%50%.
1	5p	231	 48%48%.
1	5q	231	 45%54%.
1	5r	231	 46%51%.
1	5s	231	 48%47%.
1	5t	231	 40%57%.
1	5u	231	 45%52%.

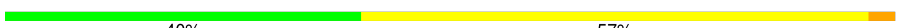
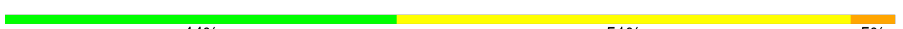
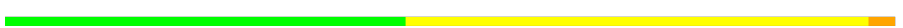
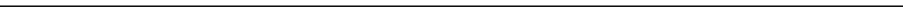
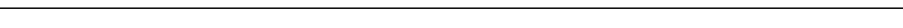
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Mol	Chain	Length	Quality of chain
1	5v	231	 46% 51% .
1	5w	231	 49% 48% .
1	5x	231	 40% 57% .
1	5y	231	 47% 49% .
1	5z	231	 44% 52% .
1	6	231	 41% 56% .
1	60	231	 46% 53% .
1	61	231	 47% 51% .
1	62	231	 43% 54% .
1	63	231	 41% 55% .
1	64	231	 42% 55% .
1	65	231	 44% 52% .
1	66	231	 47% 51% .
1	67	231	 42% 55% .
1	68	231	 47% 50% .
1	69	231	 44% 54% .
1	6A	231	 39% 58% .
1	6B	231	 46% 50% .
1	6C	231	 44% 52% .
1	6D	231	 47% 51% .
1	6E	231	 46% 51% .
1	6F	231	 46% 52% .
1	6G	231	 44% 54% .
1	6H	231	 41% 56% .
1	6I	231	 47% 48% .

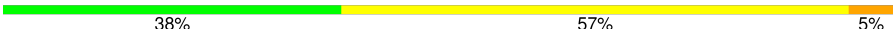
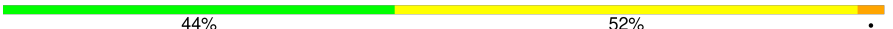
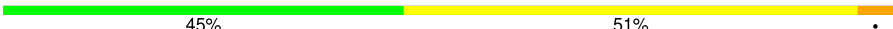
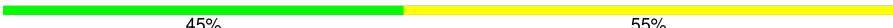
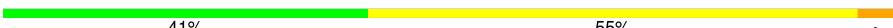
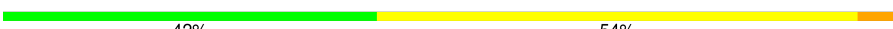
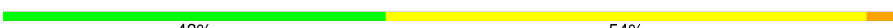
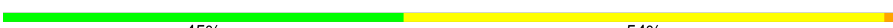
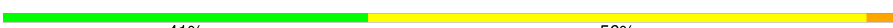
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Mol	Chain	Length	Quality of chain
1	6J	231	 45% 54% .
1	6K	231	 46% 51% .
1	6L	231	 52% 46% .
1	6M	231	 40% 57% .
1	6N	231	 44% 51% 5% .
1	6O	231	 45% 52% .
1	6P	231	 46% 50% .
1	6Q	231	 44% 54% .
1	6R	231	 44% 53% .
1	6S	231	 48% 50% .
1	6T	231	 43% 52% 5% .
1	6U	231	 48% 49% .
1	6V	231	 51% 48% .
1	6W	231	 44% 52% .
1	6X	231	 48% 50% .
1	6Y	231	 46% 50% .
1	6Z	231	 46% 52% .
1	6a	231	 42% 56% .
1	6b	231	 42% 55% .
1	6c	231	 48% 49% .
1	6d	231	 48% 49% .
1	6e	231	 47% 49% .
1	6f	231	 45% 52% .
1	6g	231	 38% 58% .
1	6h	231	 46% 52% .

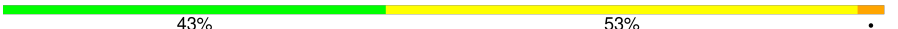
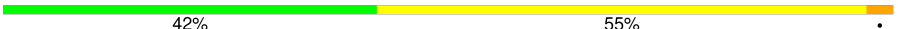
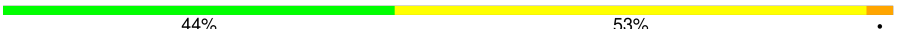
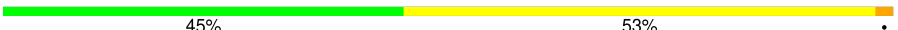
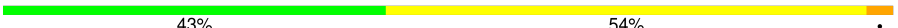
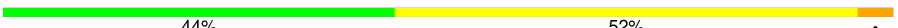
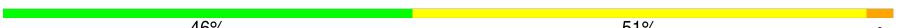
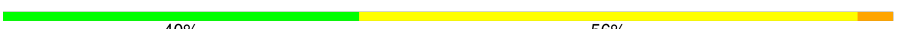
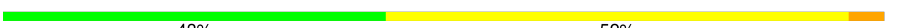
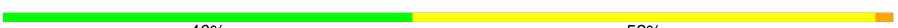
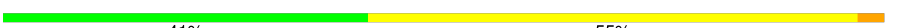
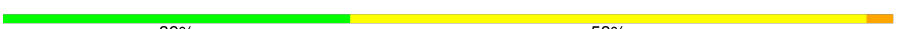
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Mol	Chain	Length	Quality of chain
1	6i	231	
1	6j	231	
1	6k	231	
1	6l	231	
1	6m	231	
1	6n	231	
1	6o	231	
1	6p	231	
1	6q	231	
1	6r	231	
1	6s	231	
1	6t	231	
1	6u	231	
1	6v	231	
1	6w	231	
1	6x	231	
1	6y	231	
1	6z	231	
1	7	231	
1	70	231	
1	71	231	
1	72	231	
1	73	231	
1	74	231	
1	75	231	

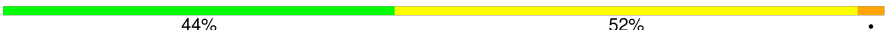
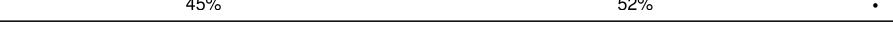
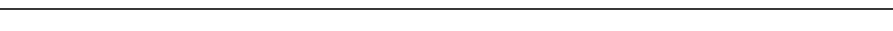
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Mol	Chain	Length	Quality of chain
1	76	231	 51% 48% .
1	77	231	 43% 53% .
1	78	231	 42% 55% .
1	79	231	 44% 53% .
1	7A	231	 45% 53% .
1	7B	231	 43% 54% .
1	7C	231	 42% 55% .
1	7D	231	 42% 54% .
1	7E	231	 44% 52% .
1	7F	231	 48% 51% .
1	7G	231	 46% 51% .
1	7H	231	 42% 55% ..
1	7I	231	 51% 46% .
1	7J	231	 47% 51% .
1	7K	231	 40% 56% .
1	7L	231	 45% 51% .
1	7M	231	 43% 52% .
1	7N	231	 46% 52% .
1	7O	231	 52% 47% .
1	7P	231	 41% 55% .
1	7Q	231	 39% 58% .
1	7R	231	 43% 56% .
1	7S	231	 40% 59% .
1	7T	231	 45% 52% .
1	7U	231	 45% 52% .

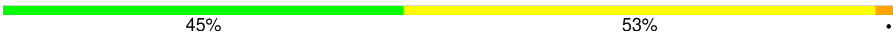
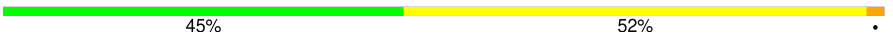
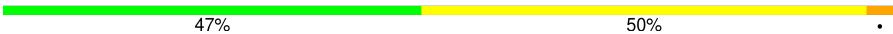
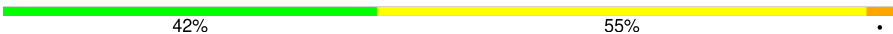
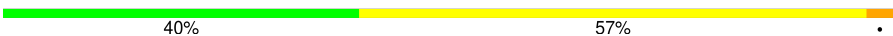
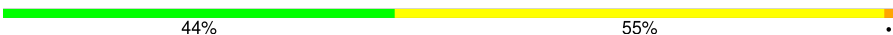
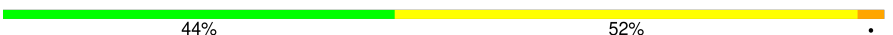
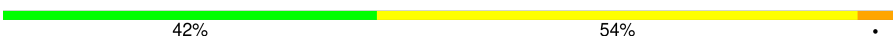
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Mol	Chain	Length	Quality of chain
1	7V	231	
1	7W	231	
1	7X	231	
1	7Y	231	
1	7Z	231	
1	7a	231	
1	7b	231	
1	7c	231	
1	7d	231	
1	7e	231	
1	7f	231	
1	7g	231	
1	7h	231	
1	7i	231	
1	7j	231	
1	7k	231	
1	7l	231	
1	7m	231	
1	7n	231	
1	7o	231	
1	7p	231	
1	7q	231	
1	7r	231	
1	7s	231	
1	7t	231	

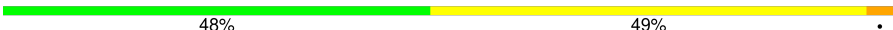
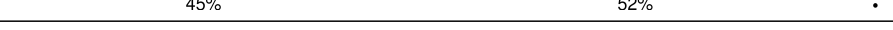
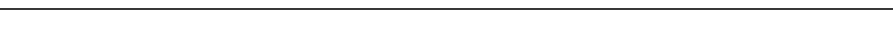
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Mol	Chain	Length	Quality of chain
1	7u	231	
1	7v	231	
1	7w	231	
1	7x	231	
1	7y	231	
1	7z	231	
1	8	231	
1	80	231	
1	81	231	
1	82	231	
1	83	231	
1	84	231	
1	85	231	
1	86	231	
1	87	231	
1	88	231	
1	89	231	
1	8A	231	
1	8B	231	
1	8C	231	
1	8D	231	
1	8E	231	
1	8F	231	
1	8G	231	
1	8H	231	

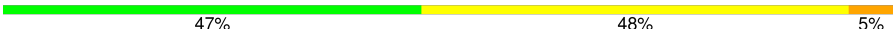
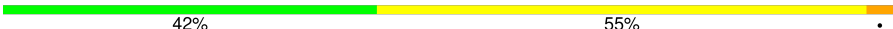
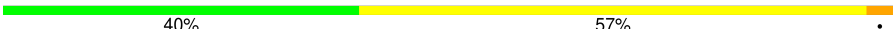
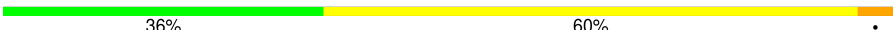
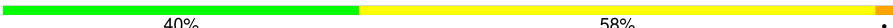
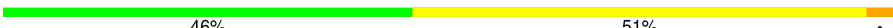
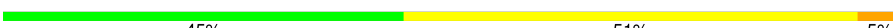
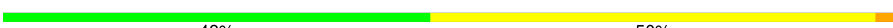
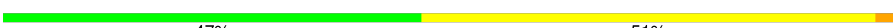
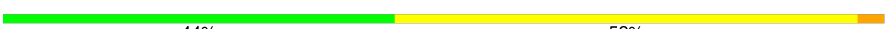
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Mol	Chain	Length	Quality of chain
1	8I	231	 48%49%.
1	8J	231	 43%53%.
1	8K	231	 45%52%.
1	8L	231	 45%52%.
1	8M	231	 42%55%.
1	8N	231	 40%56%.
1	8O	231	 38%60%.
1	8P	231	 39%59%.
1	8Q	231	 48%49%.
1	8R	231	 45%52%.
1	8S	231	 49%48%.
1	8T	231	 48%48%.
1	8U	231	 44%53%..
1	8V	231	 45%52%.
1	8W	231	 47%52%.
1	8X	231	 43%52%5%.
1	8Y	231	 47%49%.
1	8Z	231	 48%49%.
1	8a	231	 41%57%.
1	8b	231	 43%53%.
1	8c	231	 45%52%.
1	8d	231	 46%52%.
1	8e	231	 42%55%.
1	8f	231	 48%48%.
1	8g	231	 48%49%.

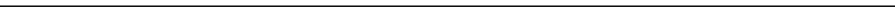
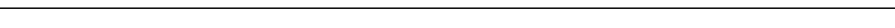
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Mol	Chain	Length	Quality of chain
1	8h	231	 47% 49% .
1	8i	231	 47% 48% 5% .
1	8j	231	 42% 55% .
1	8k	231	 40% 57% .
1	8l	231	 36% 60% .
1	8m	231	 40% 58% .
1	8n	231	 48% 49% .
1	8o	231	 48% 49% .
1	8p	231	 46% 51% .
1	8q	231	 48% 49% .
1	8r	231	 54% 43% .
1	8s	231	 48% 49% .
1	8t	231	 38% 61% .
1	8u	231	 46% 51% .
1	8v	231	 50% 44% 6% .
1	8w	231	 42% 55% .
1	8x	231	 45% 51% 5% .
1	8y	231	 48% 50% .
1	8z	231	 44% 53% .
1	9	231	 47% 51% .
1	90	231	 44% 52% .
1	91	231	 44% 52% .
1	92	231	 43% 54% .
1	93	231	 49% 47% .
1	94	231	 44% 52% .

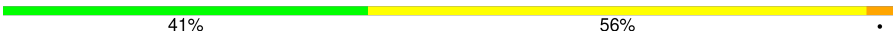
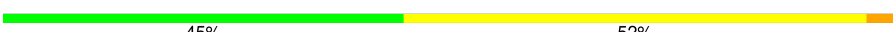
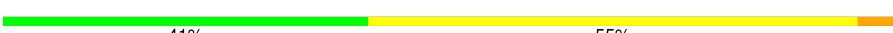
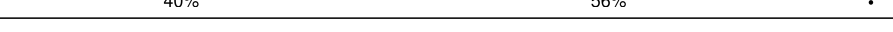
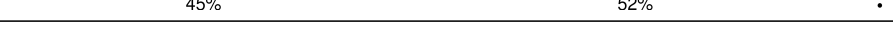
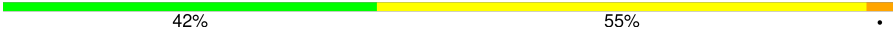
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Mol	Chain	Length	Quality of chain
1	95	231	 46%52%
1	96	231	 40%58%
1	97	231	 47%49%
1	98	231	 49%47%
1	99	231	 49%49%
1	9A	231	 53%45%
1	9B	231	 41%56%
1	9C	231	 48%50%
1	9D	231	 46%51%
1	9E	231	 43%54%
1	9F	231	 48%50%
1	9G	231	 40%58%
1	9H	231	 42%55%
1	9I	231	 44%54%
1	9J	231	 42%55%
1	9K	231	 45%53%
1	9L	231	 48%50%
1	9M	231	 48%50%
1	9N	231	 45%52%
1	9O	231	 42%55%
1	9P	231	 46%51%
1	9Q	231	 51%47%
1	9R	231	 45%53%
1	9S	231	 37%61%
1	9T	231	 45%49%6%

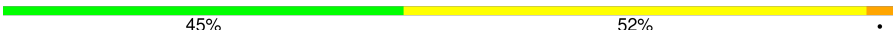
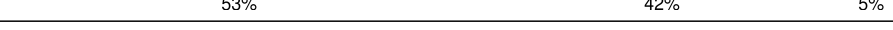
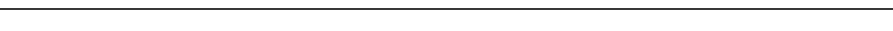
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Mol	Chain	Length	Quality of chain
1	9U	231	
1	9V	231	
1	9W	231	
1	9X	231	
1	9Y	231	
1	9Z	231	
1	9a	231	
1	9b	231	
1	9c	231	
1	9d	231	
1	9e	231	
1	9f	231	
1	9g	231	
1	9h	231	
1	9i	231	
1	9j	231	
1	9k	231	
1	9l	231	
1	9m	231	
1	9n	231	
1	9o	231	
1	9p	231	
1	9q	231	
1	9r	231	
1	9s	231	

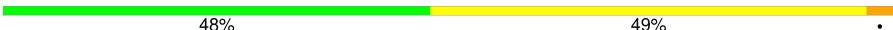
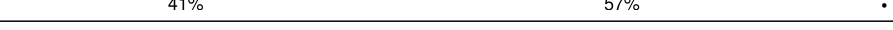
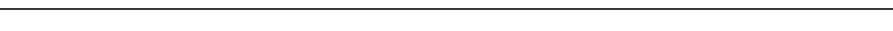
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Mol	Chain	Length	Quality of chain
1	9t	231	
1	9u	231	
1	9v	231	
1	9w	231	
1	9x	231	
1	9y	231	
1	9z	231	
1	A	231	
1	B	231	
1	C	231	
1	D	231	
1	E	231	
1	F	231	
1	G	231	
1	H	231	
1	I	231	
1	J	231	
1	K	231	
1	L	231	
1	M	231	
1	N	231	
1	O	231	
1	P	231	
1	Q	231	
1	R	231	

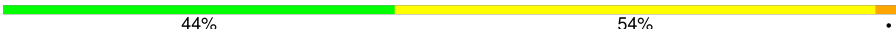
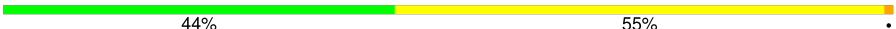
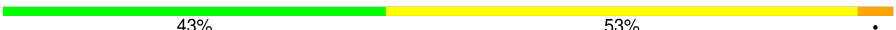
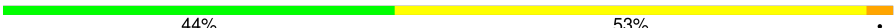
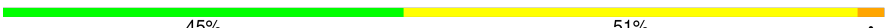
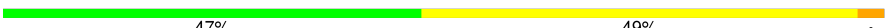
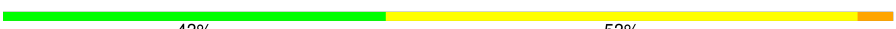
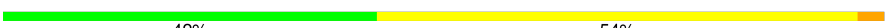
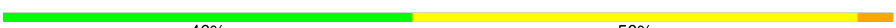
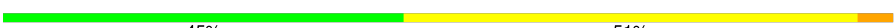
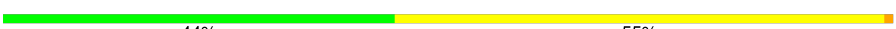
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Mol	Chain	Length	Quality of chain
1	S	231	 48% 49%
1	T	231	 42% 56%
1	U	231	 54% 43%
1	V	231	 39% 57%
1	W	231	 48% 48%
1	X	231	 48% 51%
1	Y	231	 45% 53%
1	Z	231	 40% 58%
1	a	231	 44% 53%
1	a0	231	 44% 52%
1	a1	231	 47% 50%
1	a2	231	 45% 52%
1	a3	231	 44% 54%
1	a4	231	 41% 57%
1	a5	231	 42% 55%
1	a6	231	 52% 44%
1	a7	231	 45% 53%
1	a8	231	 43% 54%
1	a9	231	 42% 52% 5%
1	aA	231	 49% 48%
1	aB	231	 48% 49%
1	aC	231	 47% 50%
1	aD	231	 49% 50%
1	aE	231	 40% 55%
1	aF	231	 42% 55%

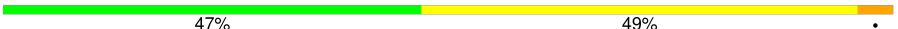
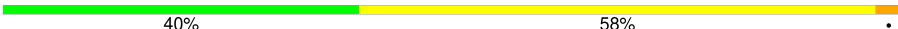
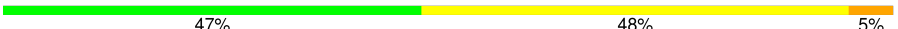
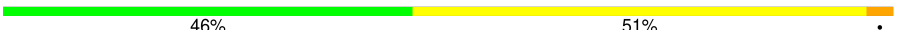
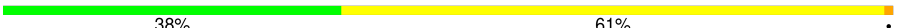
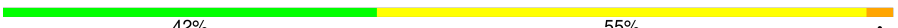
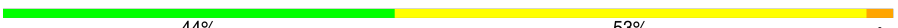
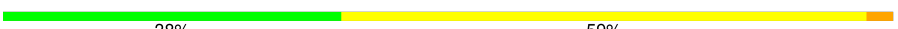
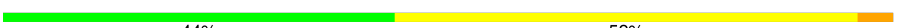
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Mol	Chain	Length	Quality of chain
1	aG	231	 44% 55%
1	aH	231	 44% 54%
1	aI	231	 44% 55%
1	aJ	231	 50% 48%
1	aK	231	 43% 53%
1	aL	231	 44% 53%
1	aM	231	 50% 48%
1	aN	231	 44% 52%
1	aO	231	 45% 51%
1	aP	231	 43% 54%
1	aQ	231	 47% 49%
1	aR	231	 49% 48%
1	aS	231	 49% 48%
1	aT	231	 45% 52%
1	aU	231	 43% 53%
1	aV	231	 45% 52%
1	aW	231	 42% 54%
1	aX	231	 46% 50%
1	aY	231	 47% 49%
1	aZ	231	 45% 51%
1	aa	231	 44% 55%
1	ab	231	 45% 52%
1	ac	231	 50% 46%
1	ad	231	 45% 52%
1	ae	231	 42% 55%

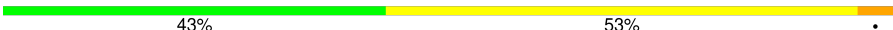
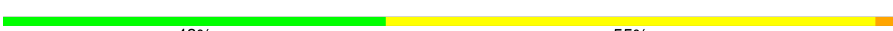
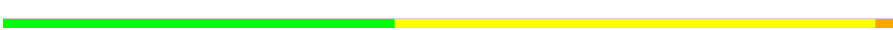
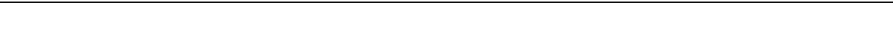
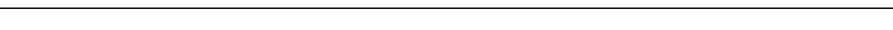
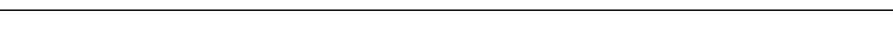
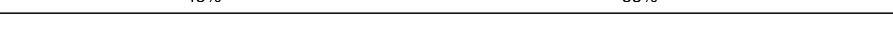
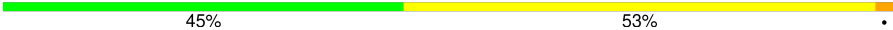
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Mol	Chain	Length	Quality of chain
1	af	231	 51% 47%
1	ag	231	 47% 49%
1	ah	231	 40% 58%
1	ai	231	 47% 48% 5%
1	aj	231	 46% 51%
1	ak	231	 38% 61%
1	al	231	 46% 52%
1	am	231	 52% 46%
1	an	231	 42% 55%
1	ao	231	 45% 52%
1	ap	231	 44% 53%
1	aq	231	 41% 57%
1	ar	231	 46% 51%
1	as	231	 45% 53%
1	at	231	 38% 59%
1	au	231	 44% 52%
1	av	231	 52% 45%
1	aw	231	 44% 52%
1	ax	231	 42% 53%
1	ay	231	 53% 44%
1	az	231	 51% 45%
1	b	231	 46% 52%
1	b0	231	 39% 55% 5%
1	b1	231	 48% 48%
1	b2	231	 45% 49% 5%

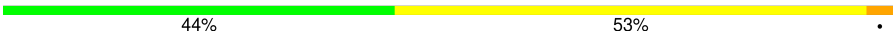
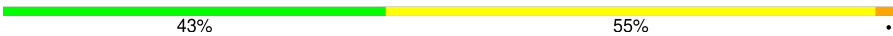
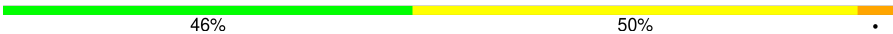
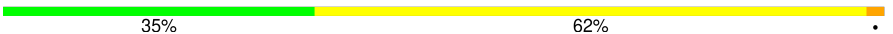
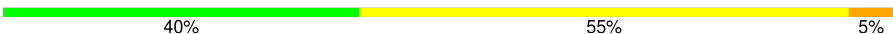
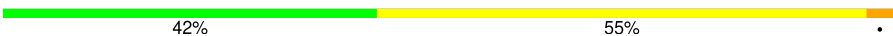
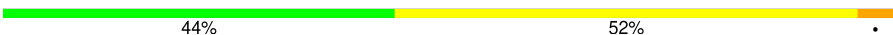
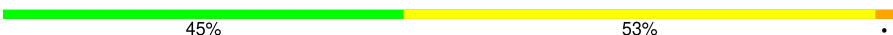
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Mol	Chain	Length	Quality of chain
1	b3	231	 43% 53% .
1	b4	231	 46% 51% .
1	b5	231	 47% 48% .
1	b6	231	 49% 48% .
1	b7	231	 43% 55% .
1	b8	231	 44% 54% .
1	b9	231	 48% 51% .
1	bA	231	 43% 53% .
1	bB	231	 47% 47% 6% .
1	bC	231	 44% 52% .
1	bD	231	 45% 52% .
1	bE	231	 41% 54% 5% .
1	bF	231	 49% 48% .
1	bG	231	 45% 53% .
1	bH	231	 45% 53% .
1	bI	231	 48% 49% .
1	bJ	231	 44% 55% .
1	bK	231	 47% 50% .
1	bL	231	 47% 49% .
1	bM	231	 44% 52% .
1	bN	231	 51% 44% 5% .
1	bO	231	 48% 48% .
1	bP	231	 45% 54% .
1	bQ	231	 45% 53% .
1	bR	231	 43% 52% .

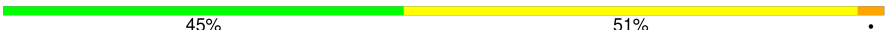
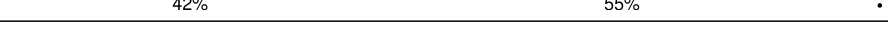
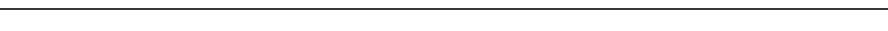
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Mol	Chain	Length	Quality of chain
1	bS	231	 47%50%.
1	bT	231	 42%55%.
1	bU	231	 46%51%.
1	bV	231	 44%53%.
1	bW	231	 43%55%.
1	bX	231	 46%50%.
1	bY	231	 35%62%.
1	bZ	231	 54%44%.
1	ba	231	 40%55%5%.
1	bb	231	 42%55%.
1	bc	231	 44%52%.
1	bd	231	 45%53%.
1	be	231	 49%50%.
1	bf	231	 43%55%..
1	bg	231	 42%55%.
1	bh	231	 43%55%.
1	bi	231	 41%55%.
1	bj	231	 52%47%.
1	bk	231	 45%52%.
1	bl	231	 47%48%5%.
1	bm	231	 41%54%..
1	bn	231	 41%54%5%.
1	bo	231	 44%55%.
1	bp	231	 47%50%.
1	bq	231	 42%55%.

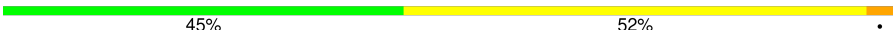
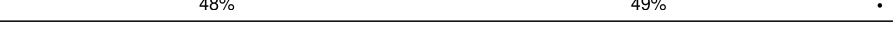
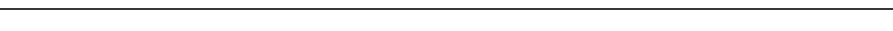
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Mol	Chain	Length	Quality of chain
1	br	231	 45% 51% .
1	bs	231	 49% 47% .
1	bt	231	 51% 46% .
1	bu	231	 42% 55% .
1	bv	231	 45% 51% .
1	bw	231	 41% 54% 5% .
1	bx	231	 43% 51% 6% .
1	by	231	 44% 54% .
1	bz	231	 42% 54% .
1	c	231	 44% 52% .
1	c0	231	 49% 47% .
1	c1	231	 45% 52% .
1	c2	231	 40% 57% .
1	c3	231	 42% 55% .
1	c4	231	 48% 46% 6% .
1	c5	231	 40% 56% .
1	c6	231	 47% 51% .
1	c7	231	 45% 51% .
1	c8	231	 43% 54% .
1	c9	231	 46% 51% .
1	cA	231	 47% 50% .
1	cB	231	 45% 51% .
1	cC	231	 45% 51% .
1	cD	231	 46% 50% .
1	cE	231	 44% 54% .

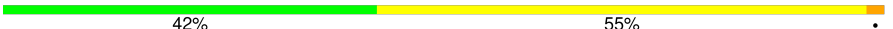
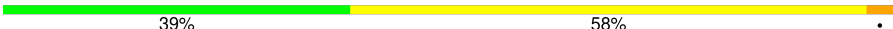
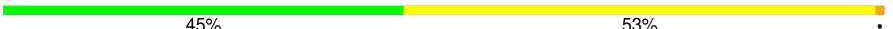
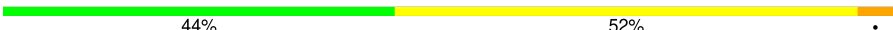
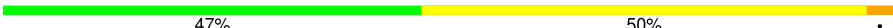
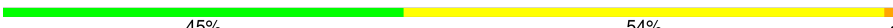
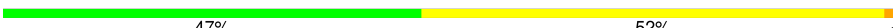
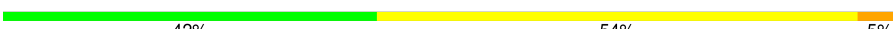
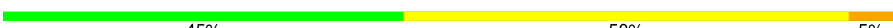
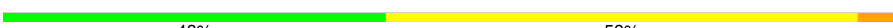
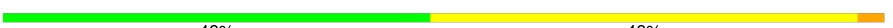
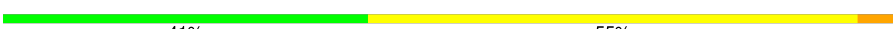
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Mol	Chain	Length	Quality of chain
1	cF	231	
1	cG	231	
1	cH	231	
1	cI	231	
1	cJ	231	
1	cK	231	
1	cL	231	
1	cM	231	
1	cN	231	
1	cO	231	
1	cP	231	
1	cQ	231	
1	cR	231	
1	cS	231	
1	cT	231	
1	cU	231	
1	cV	231	
1	cW	231	
1	cX	231	
1	cY	231	
1	cZ	231	
1	ca	231	
1	cb	231	
1	cc	231	
1	cd	231	

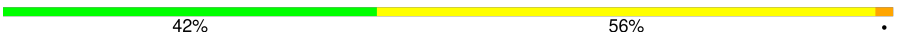
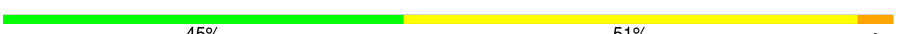
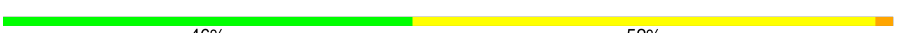
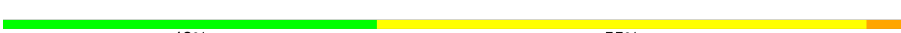
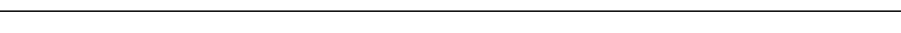
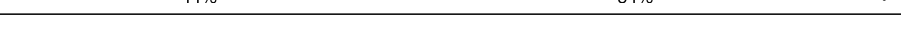
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Mol	Chain	Length	Quality of chain
1	ce	231	
1	cf	231	
1	cg	231	
1	ch	231	
1	ci	231	
1	cj	231	
1	ck	231	
1	cl	231	
1	cm	231	
1	cn	231	
1	co	231	
1	cp	231	
1	cq	231	
1	cr	231	
1	cs	231	
1	ct	231	
1	cu	231	
1	cv	231	
1	cw	231	
1	cx	231	
1	cy	231	
1	cz	231	
1	d	231	
1	d0	231	
1	d1	231	

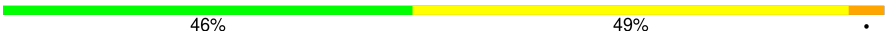
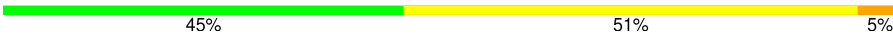
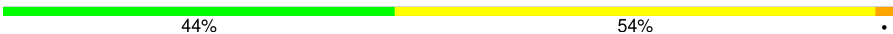
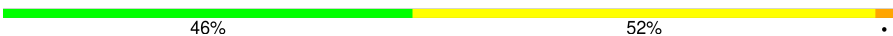
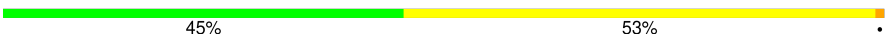
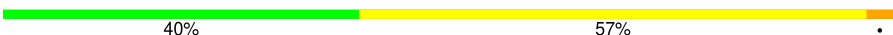
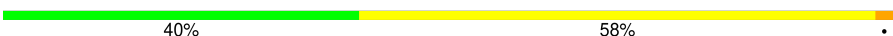
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Mol	Chain	Length	Quality of chain
1	d2	231	 43% 53% .
1	d3	231	 42% 56% .
1	d4	231	 45% 52% .
1	d5	231	 47% 51% .
1	d6	231	 45% 51% .
1	d7	231	 46% 52% .
1	d8	231	 42% 55% .
1	d9	231	 42% 52% 5% .
1	dA	231	 46% 49% . .
1	dB	231	 45% 51% .
1	dC	231	 39% 56% . .
1	dD	231	 47% 52% .
1	dE	231	 49% 47% .
1	dF	231	 43% 54% .
1	dG	231	 44% 54% .
1	dH	231	 48% 51% .
1	dI	231	 48% 50% .
1	dJ	231	 43% 54% .
1	dK	231	 47% 49% .
1	dL	231	 40% 59% .
1	dM	231	 45% 53% .
1	dN	231	 50% 47% .
1	dO	231	 45% 52% .
1	dP	231	 50% 48% .
1	dQ	231	 42% 55% .

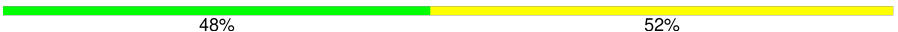
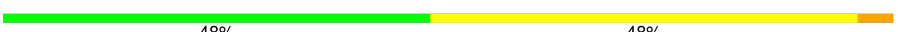
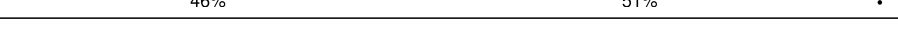
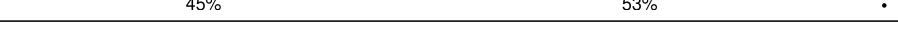
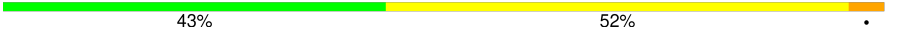
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Mol	Chain	Length	Quality of chain
1	dR	231	
1	dS	231	
1	dT	231	
1	dU	231	
1	dV	231	
1	dW	231	
1	dX	231	
1	dY	231	
1	dZ	231	
1	da	231	
1	db	231	
1	dc	231	
1	dd	231	
1	de	231	
1	df	231	
1	dg	231	
1	dh	231	
1	di	231	
1	dj	231	
1	dk	231	
1	dl	231	
1	dm	231	
1	dn	231	
1	do	231	
1	dp	231	

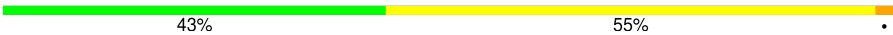
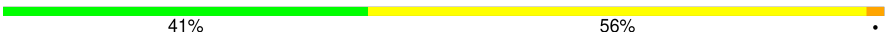
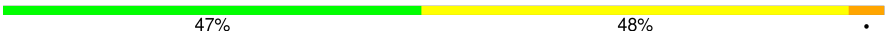
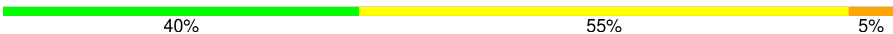
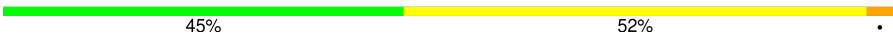
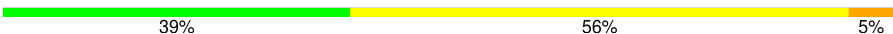
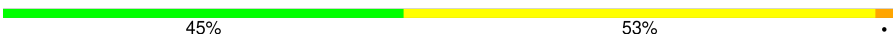
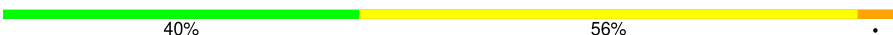
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Mol	Chain	Length	Quality of chain
1	dq	231	 48%52%
1	dr	231	 47%52%. .
1	ds	231	 44%56%
1	dt	231	 48%48%. .
1	du	231	 51%47%. .
1	dv	231	 41%57%. .
1	dw	231	 40%54%6%
1	dx	231	 39%58%. .
1	dy	231	 45%52%. .
1	dz	231	 45%50%5%
1	e	231	 44%52%. .
1	e0	231	 43%54%. .
1	e1	231	 45%53%. .
1	e2	231	 44%55%
1	e3	231	 46%51%.. .
1	e4	231	 46%51%. .
1	e5	231	 45%53%. .
1	e6	231	 47%49%. .
1	e7	231	 48%49%. .
1	e8	231	 39%59%. .
1	e9	231	 51%47%. .
1	eA	231	 44%52%. .
1	eB	231	 43%53%. .
1	eC	231	 43%52%. .
1	eD	231	 48%50%. .

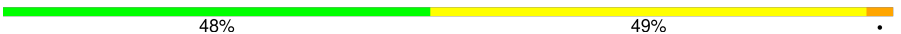
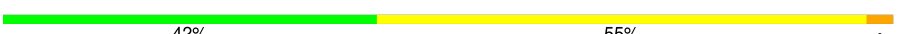
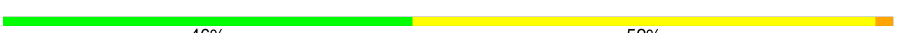
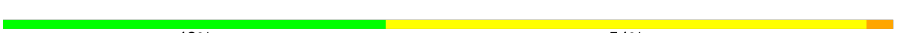
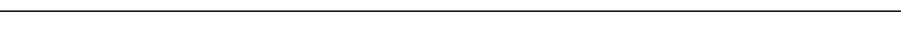
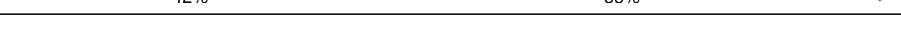
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Mol	Chain	Length	Quality of chain
1	eE	231	
1	eF	231	
1	eG	231	
1	eH	231	
1	eI	231	
1	eJ	231	
1	eK	231	
1	eL	231	
1	eM	231	
1	eN	231	
1	eO	231	
1	eP	231	
1	eQ	231	
1	eR	231	
1	eS	231	
1	eT	231	
1	eU	231	
1	eV	231	
1	eW	231	
1	eX	231	
1	eY	231	
1	eZ	231	
1	ea	231	
1	eb	231	
1	ec	231	

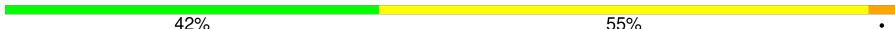
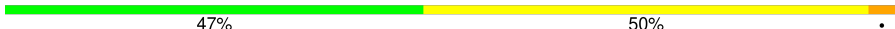
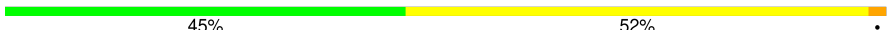
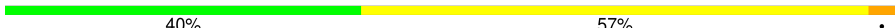
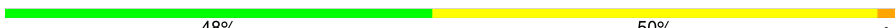
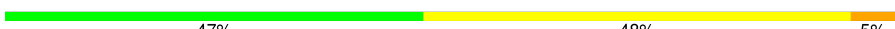
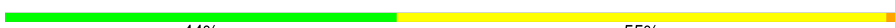
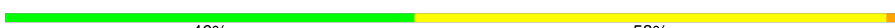
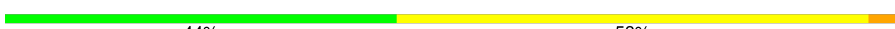
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Mol	Chain	Length	Quality of chain
1	ed	231	 47% 52% .
1	ee	231	 48% 49% .
1	ef	231	 43% 53% .
1	eg	231	 48% 52% .
1	eh	231	 42% 55% .
1	ei	231	 46% 52% .
1	ej	231	 43% 54% .
1	ek	231	 45% 52% .
1	el	231	 46% 50% .
1	em	231	 43% 55% .
1	en	231	 46% 48% 5% .
1	eo	231	 44% 51% 6% .
1	ep	231	 45% 52% .
1	eq	231	 45% 53% .
1	er	231	 42% 55% .
1	es	231	 38% 59% .
1	et	231	 43% 52% 5% .
1	eu	231	 44% 54% .
1	ev	231	 47% 49% .
1	ew	231	 48% 48% .
1	ex	231	 48% 48% .
1	ey	231	 46% 50% .
1	ez	231	 52% 46% .
1	f	231	 45% 51% .
1	f0	231	 48% 51% .

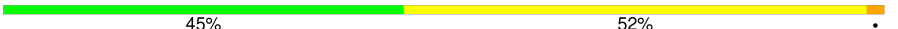
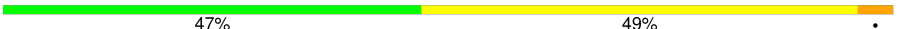
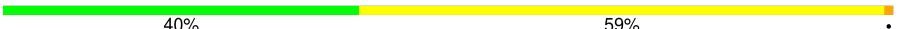
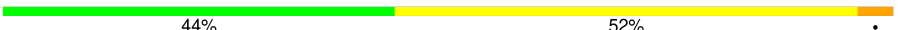
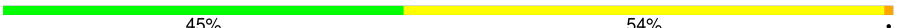
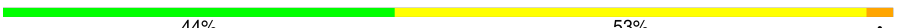
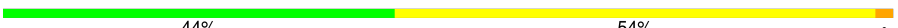
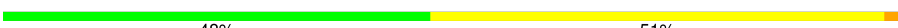
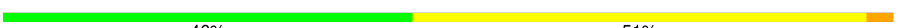
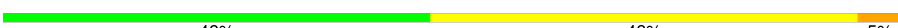
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Mol	Chain	Length	Quality of chain
1	f1	231	 46% 51% .
1	f2	231	 42% 55% .
1	f3	231	 47% 50% .
1	f4	231	 49% 48% .
1	f5	231	 45% 52% .
1	f6	231	 40% 57% .
1	f7	231	 39% 55% 6% .
1	f8	231	 48% 47% 5% .
1	f9	231	 49% 49% .
1	fA	231	 42% 53% 5% .
1	fB	231	 48% 50% .
1	fC	231	 46% 50% .
1	fD	231	 48% 51% .
1	fE	231	 44% 52% .
1	fF	231	 47% 48% 5% .
1	fG	231	 49% 49% .
1	fH	231	 55% 42% .
1	fI	231	 44% 55% .
1	fJ	231	 47% 50% .
1	fK	231	 46% 53% .
1	fL	231	 44% 53% .
1	fM	231	 47% 52% .
1	fN	231	 46% 51% .
1	fO	231	 45% 52% .
1	fP	231	 42% 54% .

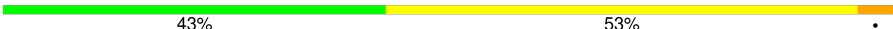
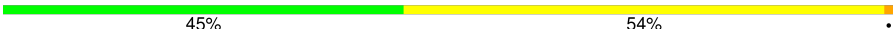
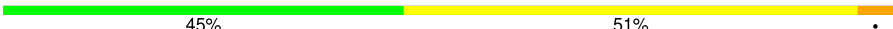
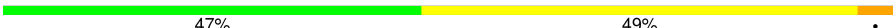
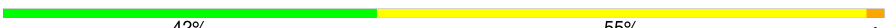
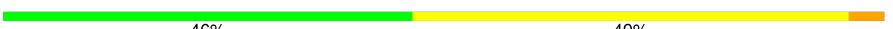
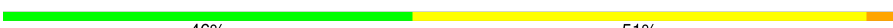
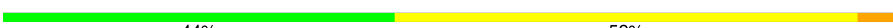
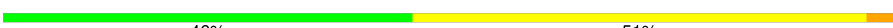
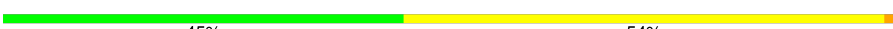
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Mol	Chain	Length	Quality of chain
1	fQ	231	 42%57%
1	fR	231	 45%52%
1	fS	231	 47%49%
1	fT	231	 40%59%
1	fU	231	 44%52%
1	fV	231	 45%54%
1	fW	231	 42%56%
1	fX	231	 53%46%
1	fY	231	 44%53%
1	fZ	231	 44%53%
1	fa	231	 44%54%
1	fb	231	 53%44%
1	fc	231	 42%55%
1	fd	231	 47%50%
1	fe	231	 50%48%
1	ff	231	 45%53%
1	fg	231	 48%51%
1	fh	231	 46%51%
1	fi	231	 42%57%
1	fj	231	 48%48%5%
1	fk	231	 50%45%5%
1	fl	231	 39%59%
1	fm	231	 45%52%
1	fn	231	 43%54%
1	fo	231	 43%54%

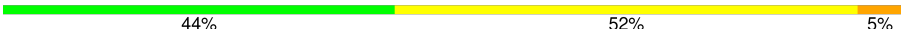
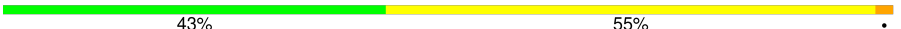
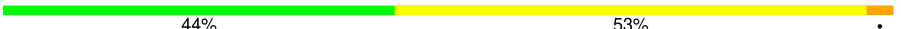
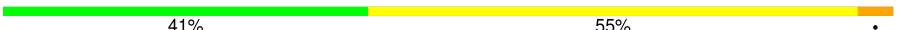
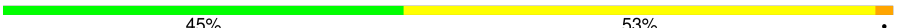
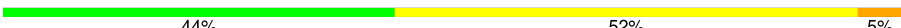
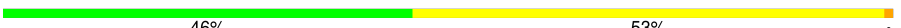
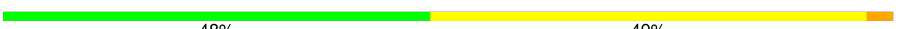
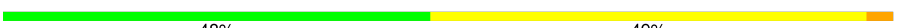
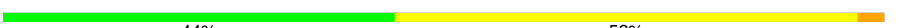
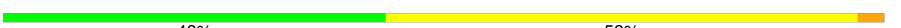
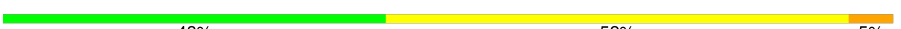
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Mol	Chain	Length	Quality of chain
1	fp	231	 42% 56% .
1	fq	231	 43% 53% .
1	fr	231	 45% 54% .
1	fs	231	 45% 51% .
1	ft	231	 49% 47% .
1	fu	231	 47% 49% .
1	fv	231	 49% 48% .
1	fw	231	 50% 46% .
1	fx	231	 53% 44% .
1	fy	231	 48% 48% .
1	fz	231	 42% 55% .
1	g	231	 39% 58% .
1	g0	231	 46% 50% .
1	g1	231	 47% 50% .
1	g2	231	 46% 49% .
1	g3	231	 45% 50% . .
1	g4	231	 46% 51% .
1	g5	231	 44% 52% .
1	g6	231	 44% 52% .
1	g7	231	 46% 51% .
1	g8	231	 45% 54% .
1	g9	231	 41% 57% .
1	gA	231	 43% 55% .
1	gB	231	 40% 58% .
1	gC	231	 46% 52% .

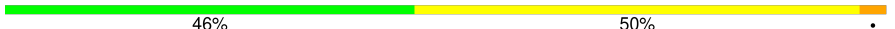
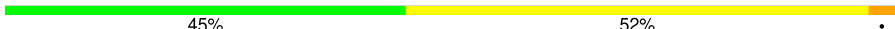
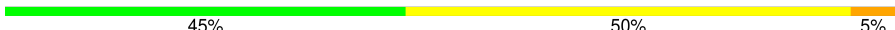
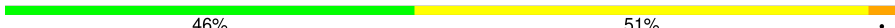
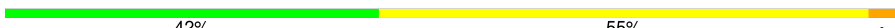
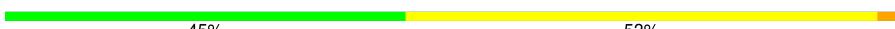
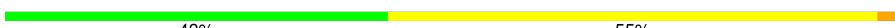
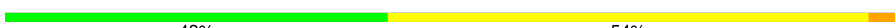
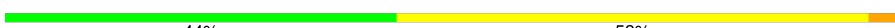
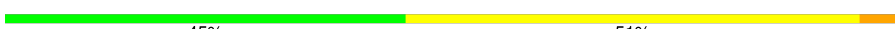
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Mol	Chain	Length	Quality of chain
1	gD	231	 45% 52% .
1	gE	231	 44% 52% 5%
1	gF	231	 43% 55% .
1	gG	231	 44% 53% .
1	gH	231	 41% 55% .
1	gI	231	 45% 53% .
1	gJ	231	 51% 46% .
1	gK	231	 53% 45% .
1	gL	231	 44% 52% 5%
1	gM	231	 42% 54% .
1	gN	231	 46% 53% .
1	gO	231	 41% 55% .
1	gP	231	 48% 48% .
1	gQ	231	 48% 52% .
1	gR	231	 48% 49% .
1	gS	231	 41% 55% .
1	gT	231	 48% 49% .
1	gU	231	 44% 52% .
1	gV	231	 47% 52% .
1	gW	231	 43% 53% .
1	gX	231	 43% 52% 5%
1	gY	231	 49% 47% .
1	gZ	231	 48% 50% .
1	ga	231	 44% 52% .
1	gb	231	 48% 49% .

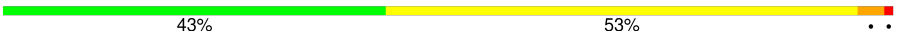
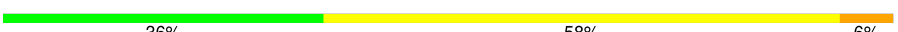
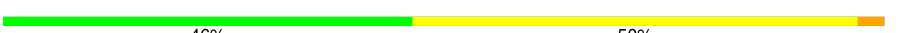
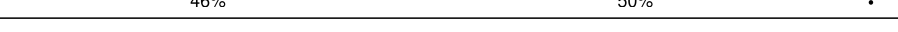
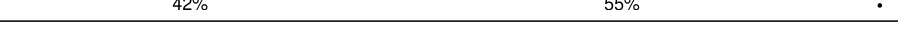
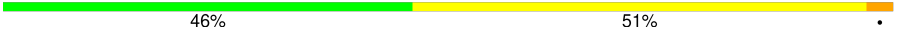
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Mol	Chain	Length	Quality of chain	
1	gc	231		.
1	gd	231		.
1	ge	231		.
1	gf	231		.
1	gg	231		.
1	gh	231		.
1	gi	231		.
1	gj	231		.
1	gk	231		.
1	gl	231		.
1	gm	231		.
1	gn	231		.
1	go	231		.
1	gp	231		.
1	gq	231		.
1	gr	231		.
1	gs	231		.
1	gt	231		.
1	gu	231		.
1	gv	231		.
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1	gx	231		.
1	gy	231		.
1	gz	231		.
1	h	231		.

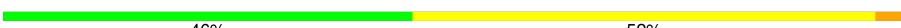
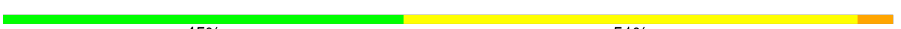
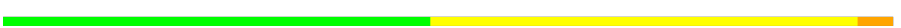
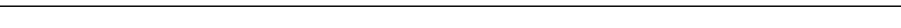
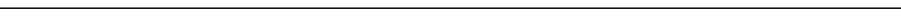
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Mol	Chain	Length	Quality of chain
1	h0	231	 43%53%..
1	h1	231	 40%57%.
1	h2	231	 39%58%.
1	h3	231	 36%58%6%
1	h4	231	 46%50%.
1	h5	231	 42%53%5%
1	h6	231	 44%53%.
1	h7	231	 48%52%.
1	h8	231	 48%50%.
1	h9	231	 41%55%.
1	hA	231	 46%51%.
1	hB	231	 49%50%
1	hC	231	 40%56%.
1	hD	231	 45%50%5%
1	hE	231	 47%51%.
1	hF	231	 46%50%.
1	hG	231	 42%55%.
1	hH	231	 52%46%.
1	hI	231	 44%53%.
1	hJ	231	 47%51%.
1	hK	231	 43%52%5%
1	hL	231	 46%50%..
1	hM	231	 45%48%7%
1	hN	231	 46%51%.
1	hO	231	 48%48%.

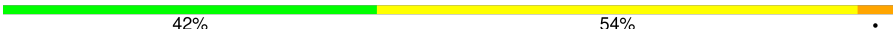
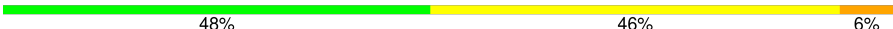
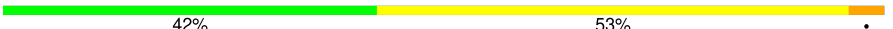
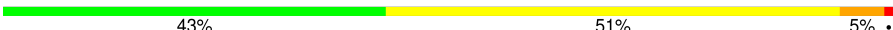
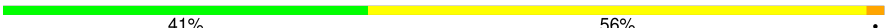
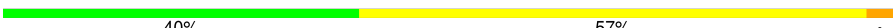
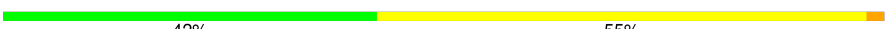
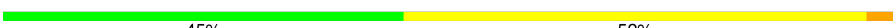
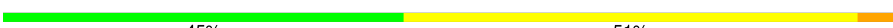
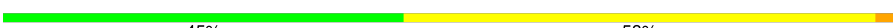
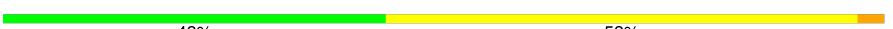
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Mol	Chain	Length	Quality of chain
1	hP	231	 43% 55% .
1	hQ	231	 46% 53% .
1	hR	231	 41% 55% .
1	hS	231	 46% 52% .
1	hT	231	 45% 51% .
1	hU	231	 48% 48% .
1	hV	231	 46% 51% .
1	hW	231	 46% 48% 5% .
1	hX	231	 47% 48% 5% .
1	hY	231	 42% 53% 6% .
1	hZ	231	 42% 54% .
1	ha	231	 43% 54% .
1	hb	231	 50% 46% .
1	hc	231	 46% 50% .
1	hd	231	 52% 45% .
1	he	231	 49% 46% 5% .
1	hf	231	 42% 54% .
1	hg	231	 42% 53% 5% .
1	hh	231	 39% 59% .
1	hi	231	 42% 55% .
1	hj	231	 44% 50% 6% .
1	hk	231	 47% 52% .
1	hl	231	 46% 53% .
1	hm	231	 47% 52% .
1	hn	231	 40% 58% .

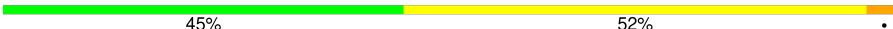
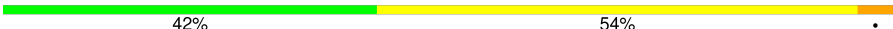
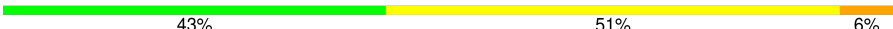
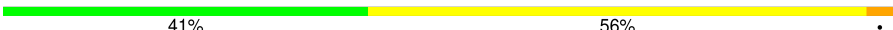
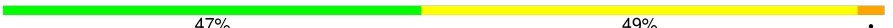
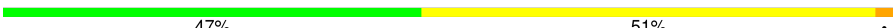
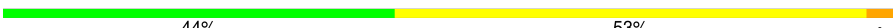
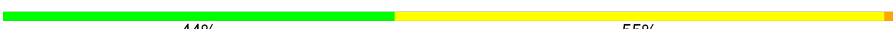
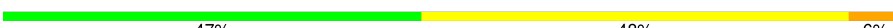
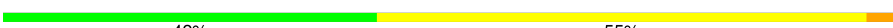
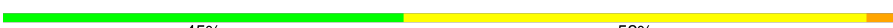
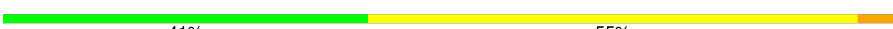
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Mol	Chain	Length	Quality of chain
1	ho	231	 45% 51% .
1	hp	231	 42% 54% .
1	hq	231	 48% 46% 6% .
1	hr	231	 42% 53% .
1	hs	231	 43% 51% 5% .
1	ht	231	 41% 56% .
1	hu	231	 45% 52% .
1	hv	231	 48% 50% .
1	hw	231	 50% 49% .
1	hx	231	 47% 48% 6% .
1	hy	231	 40% 57% .
1	hz	231	 45% 51% .
1	i	231	 45% 52% .
1	i0	231	 45% 52% .
1	i1	231	 42% 55% .
1	i2	231	 48% 46% 6% .
1	i3	231	 45% 52% .
1	i4	231	 45% 51% .
1	i5	231	 46% 51% .
1	i6	231	 45% 53% .
1	i7	231	 43% 53% .
1	i8	231	 41% 57% .
1	i9	231	 40% 57% .
1	iA	231	 48% 49% .
1	iB	231	 48% 51% .

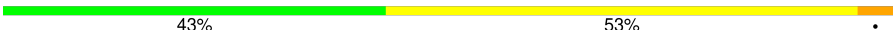
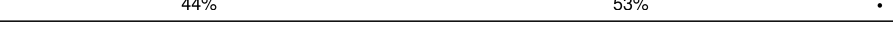
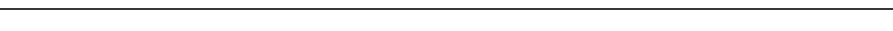
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Mol	Chain	Length	Quality of chain
1	iC	231	 48%49%.
1	iD	231	 45%52%.
1	iE	231	 42%54%.
1	iF	231	 43%51%6%.
1	iG	231	 41%56%.
1	iH	231	 47%49%.
1	iI	231	 48%50%.
1	iJ	231	 43%51%6%.
1	iK	231	 47%51%.
1	iL	231	 46%52%.
1	iM	231	 44%53%.
1	iN	231	 41%55%.
1	iO	231	 48%48%.
1	iP	231	 42%56%.
1	iQ	231	 44%55%.
1	iR	231	 43%53%.
1	iS	231	 47%48%6%.
1	iT	231	 42%55%.
1	iU	231	 45%54%.
1	iV	231	 45%52%.
1	iW	231	 41%55%.
1	iX	231	 40%57%.
1	iY	231	 45%51%..
1	iZ	231	 48%50%.
1	ia	231	 42%55%.

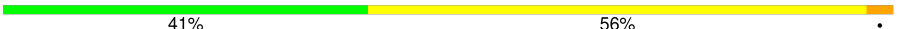
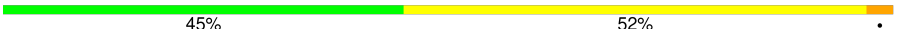
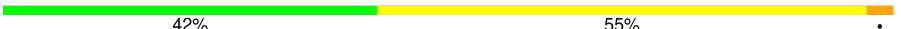
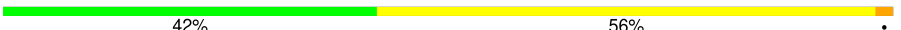
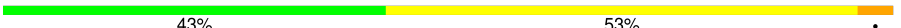
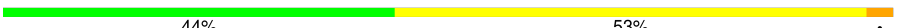
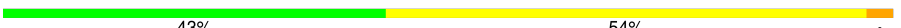
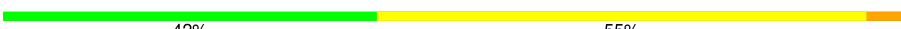
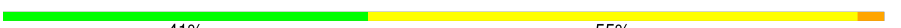
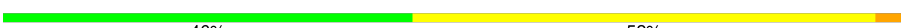
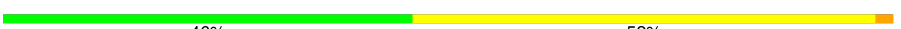
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Mol	Chain	Length	Quality of chain	
1	ib	231		.
1	ic	231		.
1	id	231		.
1	ie	231		.
1	if	231		.
1	ig	231		.
1	ih	231		.
1	ii	231		.
1	ij	231		.
1	ik	231		.
1	il	231		.
1	im	231		.
1	in	231		.
1	io	231		.
1	ip	231		.
1	iq	231		.
1	ir	231		.
1	is	231		.
1	it	231		.
1	iu	231		.
1	iv	231		.
1	iw	231		.
1	ix	231		.
1	iy	231		.
1	iz	231		.

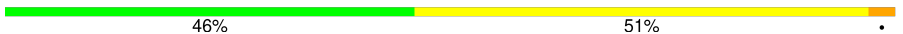
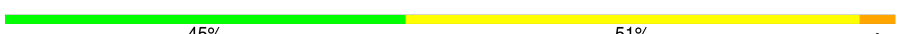
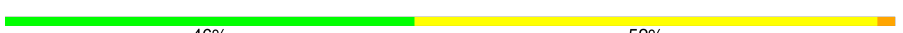
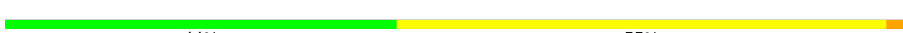
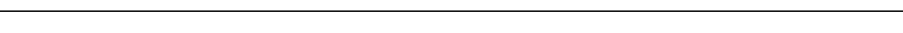
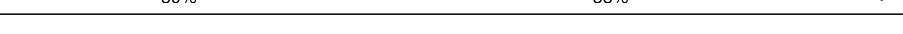
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Mol	Chain	Length	Quality of chain
1	j	231	 45% 54% .
1	j0	231	 41% 56% .
1	j1	231	 45% 52% .
1	j2	231	 42% 55% .
1	j3	231	 42% 56% .
1	j4	231	 43% 53% .
1	j5	231	 43% 53% .
1	j6	231	 44% 52% .
1	j7	231	 44% 53% .
1	j8	231	 45% 52% .
1	j9	231	 43% 54% .
1	jA	231	 53% 44% .
1	jB	231	 42% 51% 6% .
1	jC	231	 45% 52% .
1	jD	231	 42% 55% .
1	jE	231	 41% 55% .
1	jF	231	 41% 55% .
1	jG	231	 49% 47% .
1	jH	231	 51% 46% .
1	jI	231	 46% 52% .
1	jJ	231	 46% 52% .
1	jK	231	 41% 55% .
1	jL	231	 48% 49% .
1	jM	231	 39% 57% .
1	jN	231	 44% 53% .

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Mol	Chain	Length	Quality of chain
1	jO	231	
1	jP	231	
1	jQ	231	
1	jR	231	
1	jS	231	
1	jT	231	
1	jU	231	
1	jV	231	
1	jW	231	
1	jX	231	
1	jY	231	
1	jZ	231	
1	ja	231	
1	jb	231	
1	jc	231	
1	jd	231	
1	je	231	
1	jf	231	
1	jg	231	
1	jh	231	
1	ji	231	
1	jj	231	
1	jk	231	
1	jl	231	
1	jm	231	

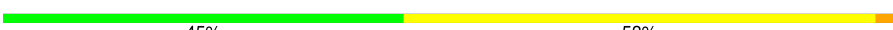
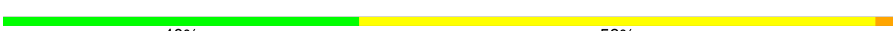
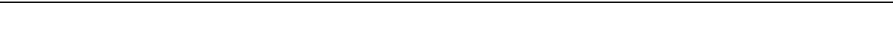
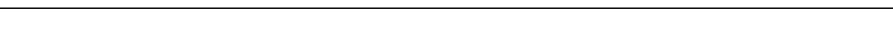
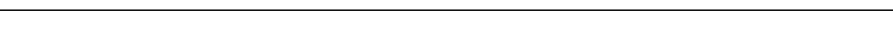
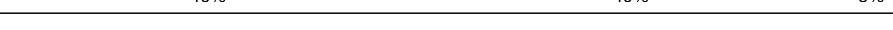
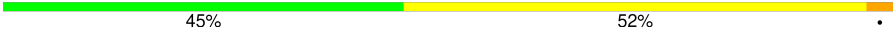
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Mol	Chain	Length	Quality of chain	
1	jn	231	48%	48%
1	jo	231	46%	51%
1	jp	231	40%	56%
1	jq	231	47%	50%
1	jr	231	48%	49%
1	js	231	42%	55%
1	jt	231	41%	56%
1	ju	231	42%	52%
1	jv	231	43%	55%
1	jw	231	45%	51%
1	jx	231	45%	52%
1	jy	231	43%	53%
1	jz	231	45%	52%
1	k	231	40%	57%
1	k0	231	42%	52%
1	k1	231	47%	48%
1	k2	231	45%	53%
1	k3	231	48%	49%
1	k4	231	33%	62%
1	k5	231	51%	45%
1	k6	231	42%	56%
1	k7	231	42%	55%
1	k8	231	51%	46%
1	k9	231	37%	58%
1	kA	231	46%	50%

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Mol	Chain	Length	Quality of chain
1	kB	231	 50% 47% .
1	kC	231	 40% 57% .
1	kD	231	 47% 50% .
1	kE	231	 45% 53% .
1	kF	231	 40% 58% .
1	kG	231	 54% 42% .
1	kH	231	 41% 57% .
1	kI	231	 44% 55% .
1	kJ	231	 44% 52% .
1	kK	231	 48% 49% .
1	kL	231	 44% 54% .
1	kM	231	 48% 50% .
1	kN	231	 43% 55% .
1	kO	231	 46% 49% 5% .
1	kP	231	 44% 53% .
1	kQ	231	 46% 52% .
1	kR	231	 41% 55% .
1	kS	231	 48% 49% .
1	kT	231	 45% 52% .
1	kU	231	 50% 46% .
1	kV	231	 43% 55% ..
1	kW	231	 48% 48% .
1	kX	231	 46% 51% .
1	kY	231	 45% 52% .
1	kZ	231	 46% 52% .

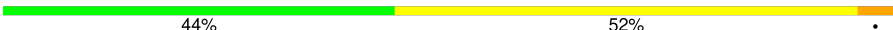
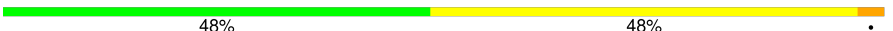
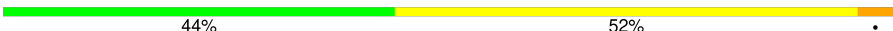
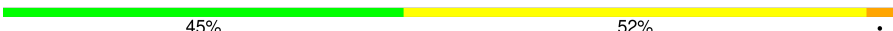
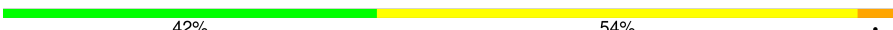
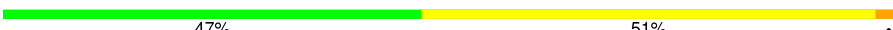
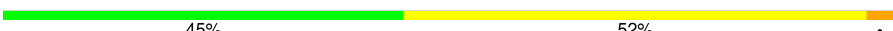
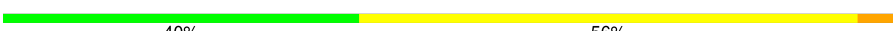
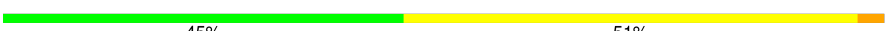
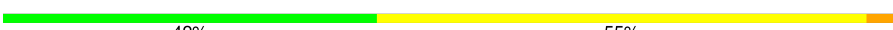
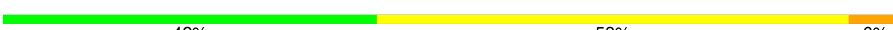
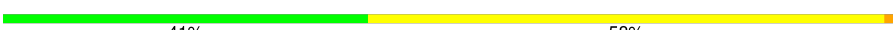
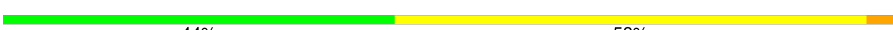
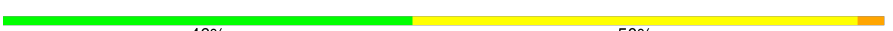
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Mol	Chain	Length	Quality of chain
1	ka	231	44% 52%
1	kb	231	45% 51%
1	kc	231	48% 48%
1	kd	231	46% 51%
1	ke	231	52% 47%
1	kf	231	47% 51%
1	kg	231	43% 56%
1	kh	231	52% 46%
1	ki	231	44% 52%
1	kj	231	49% 50%
1	kk	231	43% 53%
1	kl	231	45% 52%
1	km	231	45% 52%
1	kn	231	49% 47%
1	ko	231	42% 55%
1	kp	231	49% 46%
1	kq	231	47% 50%
1	kr	231	48% 48%
1	ks	231	49% 48%
1	kt	231	45% 52%
1	ku	231	45% 52%
1	kv	231	40% 56%
1	kw	231	49% 47%
1	kx	231	40% 57%
1	ky	231	42% 54%

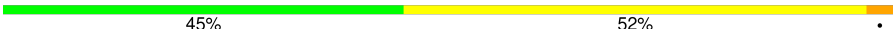
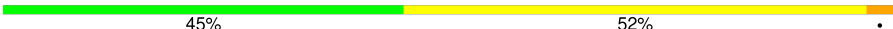
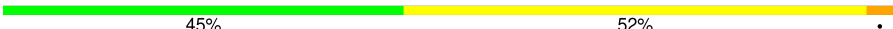
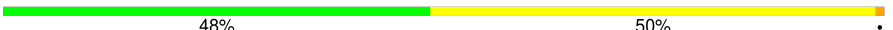
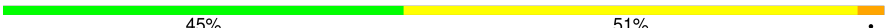
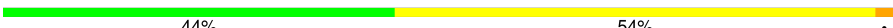
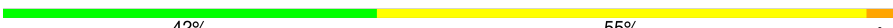
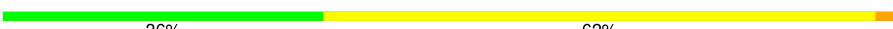
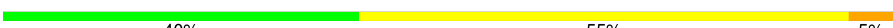
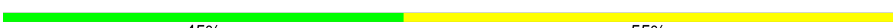
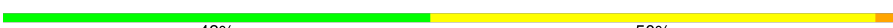
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Mol	Chain	Length	Quality of chain
1	kz	231	 44%52%.
1	l	231	 48%48%.
1	l0	231	 44%52%.
1	l1	231	 45%52%.
1	l2	231	 48%49%.
1	l3	231	 43%51%6%.
1	l4	231	 42%54%.
1	l5	231	 50%48%.
1	l6	231	 47%51%.
1	l7	231	 45%52%.
1	l8	231	 45%52%.
1	l9	231	 42%56%.
1	lA	231	 41%55%.
1	lB	231	 48%50%.
1	lC	231	 40%56%.
1	lD	231	 45%51%.
1	lE	231	 42%55%.
1	lF	231	 42%53%6%.
1	lG	231	 41%58%.
1	lH	231	 44%53%.
1	lI	231	 46%50%.
1	lJ	231	 50%48%.
1	lK	231	 41%56%.
1	lL	231	 42%57%.
1	lM	231	 45%52%.

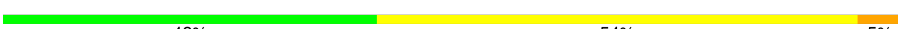
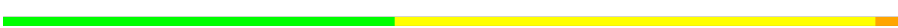
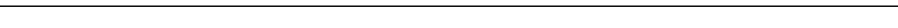
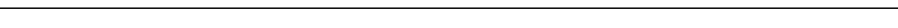
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Mol	Chain	Length	Quality of chain
1	lN	231	 41%53%6%
1	lO	231	 45%52%.
1	lP	231	 45%52%.
1	lQ	231	 45%52%.
1	lR	231	 48%50%.
1	la	231	 45%51%.
1	lb	231	 46%52%.
1	lc	231	 48%50%.
1	ld	231	 44%54%.
1	le	231	 46%51%.
1	lf	231	 42%55%.
1	lg	231	 47%52%.
1	lh	231	 38%58%.
1	li	231	 41%57%.
1	lj	231	 36%62%.
1	lk	231	 49%48%.
1	ll	231	 40%55%5%
1	lm	231	 45%55%.
1	ln	231	 42%53%5%
1	lo	231	 48%50%.
1	lp	231	 51%46%.
1	lq	231	 46%52%.
1	lr	231	 49%47%.
1	ls	231	 45%53%.
1	lt	231	 39%58%.

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Mol	Chain	Length	Quality of chain
1	lu	231	 44% 54% .
1	lv	231	 46% 50% .
1	lw	231	 46% 52% .
1	lx	231	 51% 46% .
1	ly	231	 42% 54% 5% .
1	lz	231	 44% 54% .
1	m	231	 47% 48% .
1	n	231	 52% 45% .
1	o	231	 41% 56% .
1	p	231	 47% 52% .
1	q	231	 49% 48% .
1	r	231	 43% 54% .
1	s	231	 44% 53% .
1	t	231	 48% 47% .
1	u	231	 45% 54% .
1	v	231	 41% 59%
1	w	231	 49% 49% .
1	x	231	 45% 51% .
1	y	231	 42% 56% .
1	z	231	 45% 52% .

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

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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	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	40	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	41	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	42	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	43	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	44	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	45	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	46	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	47	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	48	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	49	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		
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		

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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	C	N	O	S	0	0
			1800	1134	317	336	13		
1	70	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	71	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	72	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	73	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	74	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	75	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	76	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	77	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	78	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	79	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		
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		

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

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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	C	N	O	S	0	0
			1800	1134	317	336	13		
1	81	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	82	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	83	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	84	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	85	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	86	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	87	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	88	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
1	89	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		
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		

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

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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	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	lf	231	Total	C	N	O	S	0	0
			1800	1134	317	336	13		
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	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	lg	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		

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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	1l	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 1800	C 1134	N 317	O 336	S 13	0	0
1	el	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	em	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	en	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	eo	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	ep	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	eq	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	er	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	es	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	et	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	eu	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	ev	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	ew	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	ex	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	ey	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	ez	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	eA	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	eB	231	Total 1800	C 1134	N 317	O 336	S 13	0	0
1	eC	231	Total 1800	C 1134	N 317	O 336	S 13	0	0

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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

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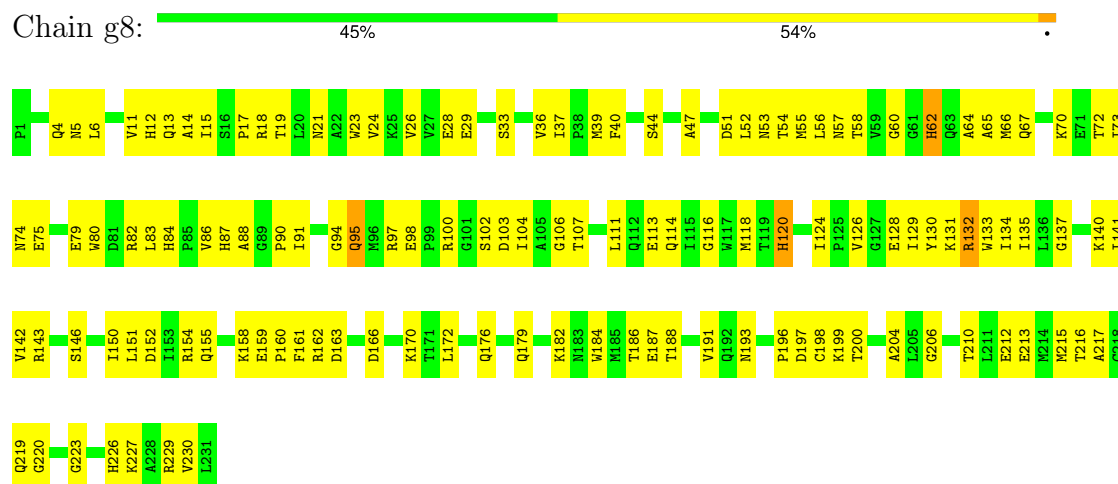
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Chain	Residue	Modelled	Actual	Comment	Reference
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6	92	GLU	ALA	engineered mutation	UNP Q79791
7	92	GLU	ALA	engineered mutation	UNP Q79791
8	92	GLU	ALA	engineered mutation	UNP Q79791
9	92	GLU	ALA	engineered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

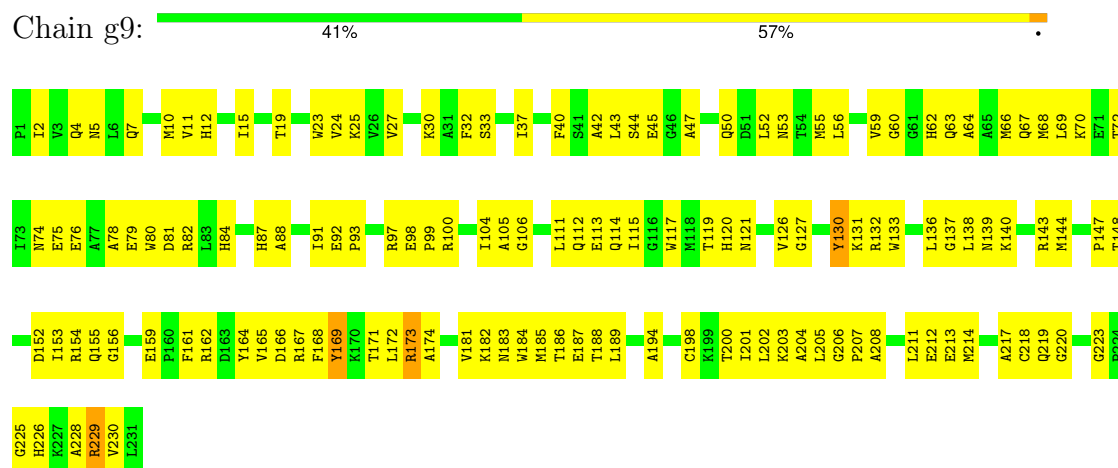
3 Residue-property plots

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.

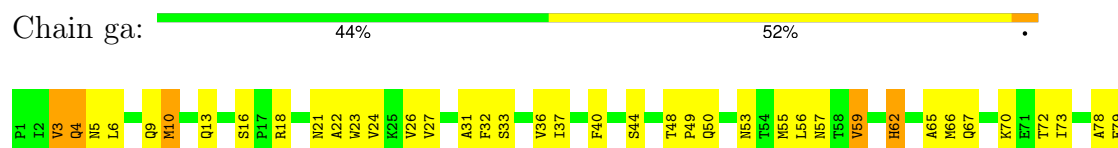
- Molecule 1: capsid protein



- Molecule 1: capsid protein



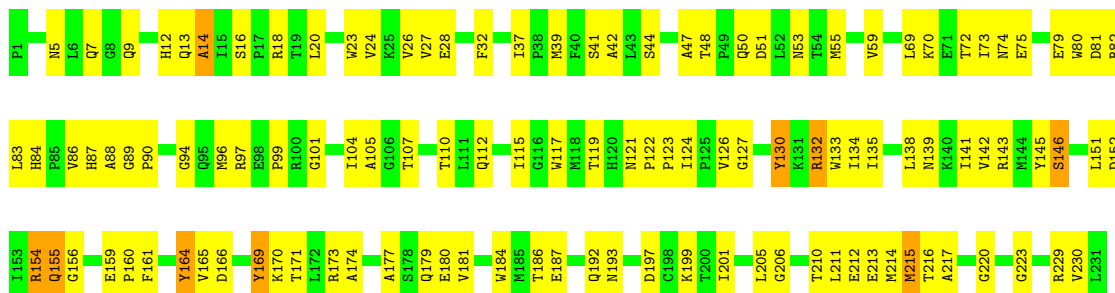
- Molecule 1: capsid protein



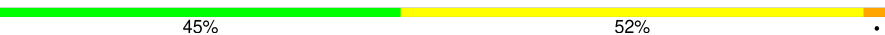
R229
V230
L231

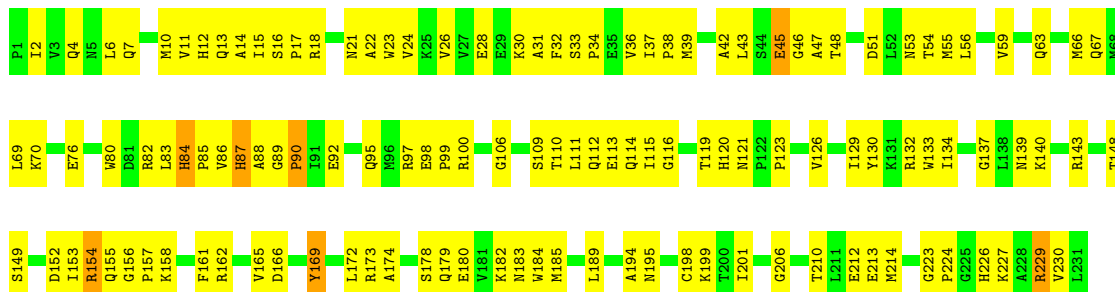
- Molecule 1: capsid protein

Chain ge:  49% 47%

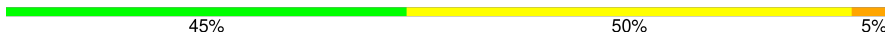


- Molecule 1: capsid protein

Chain gf:  45% 52%

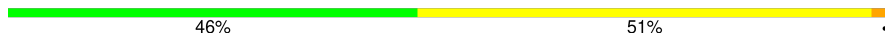


- Molecule 1: capsid protein

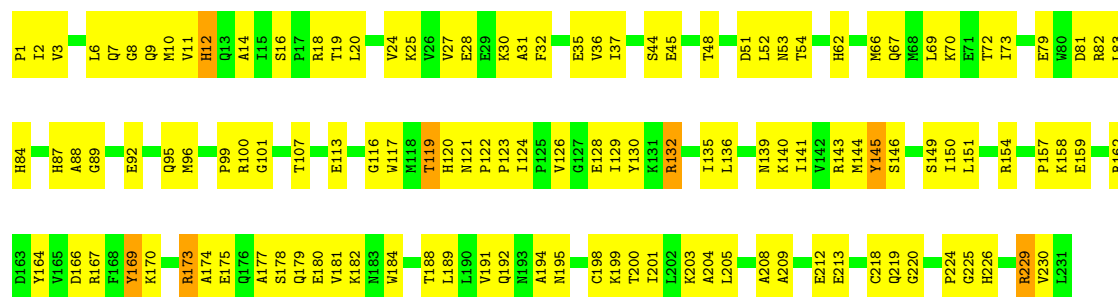
Chain gg:  45% 50% 5%



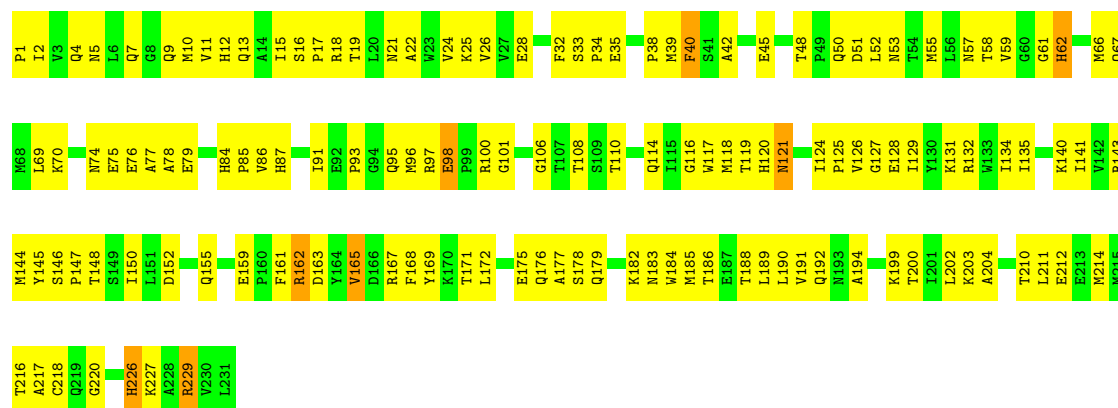
- Molecule 1: capsid protein

Chain gh:  46% 51%

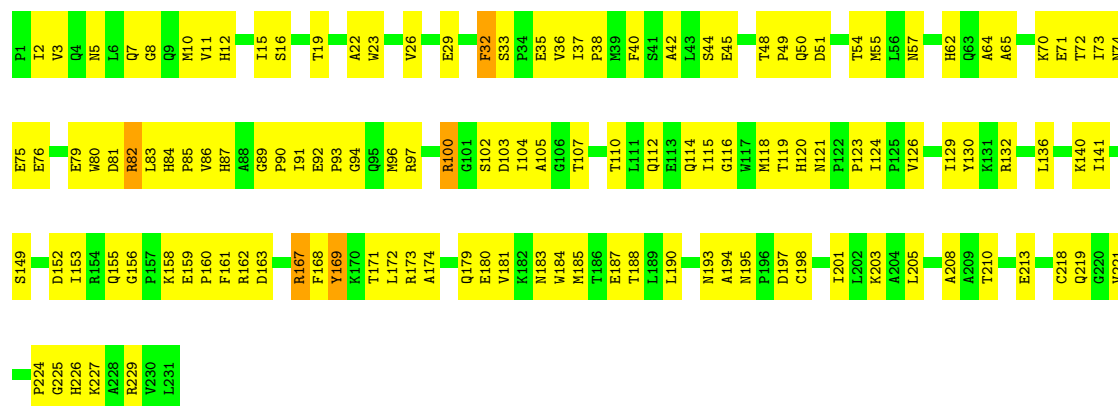




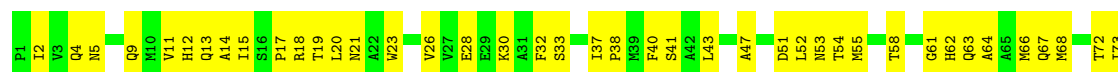
- Molecule 1: capsid protein

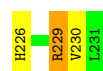


- Molecule 1: capsid protein



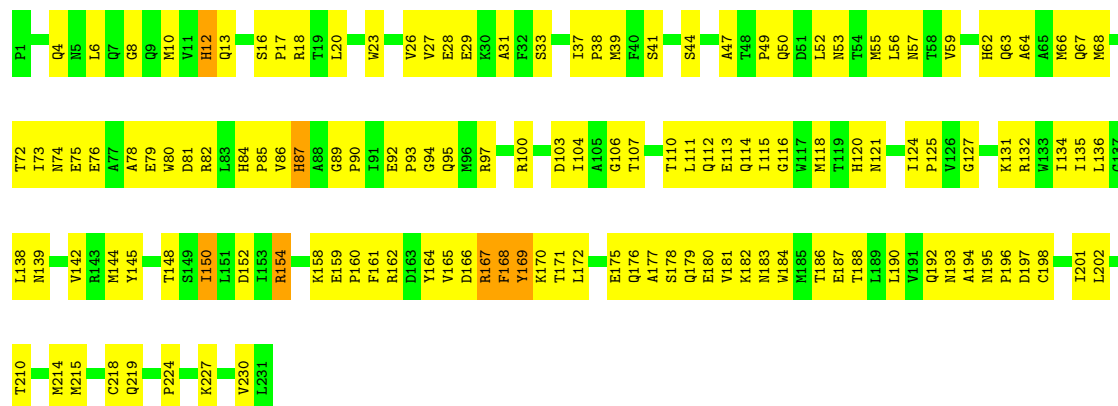
- Molecule 1: capsid protein





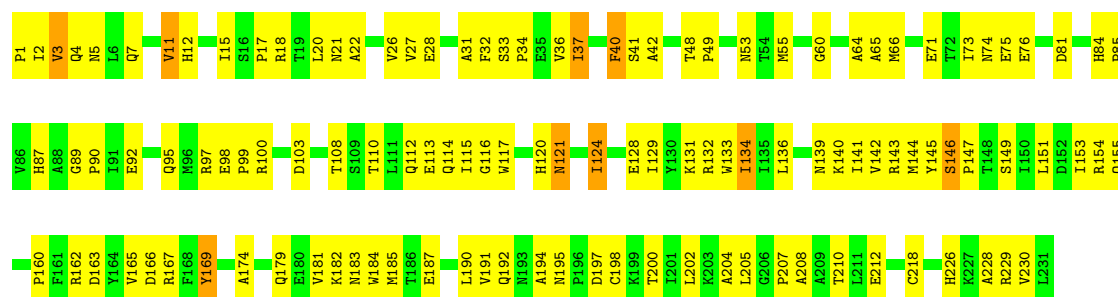
- Molecule 1: capsid protein

Chain gn: 42% 55%



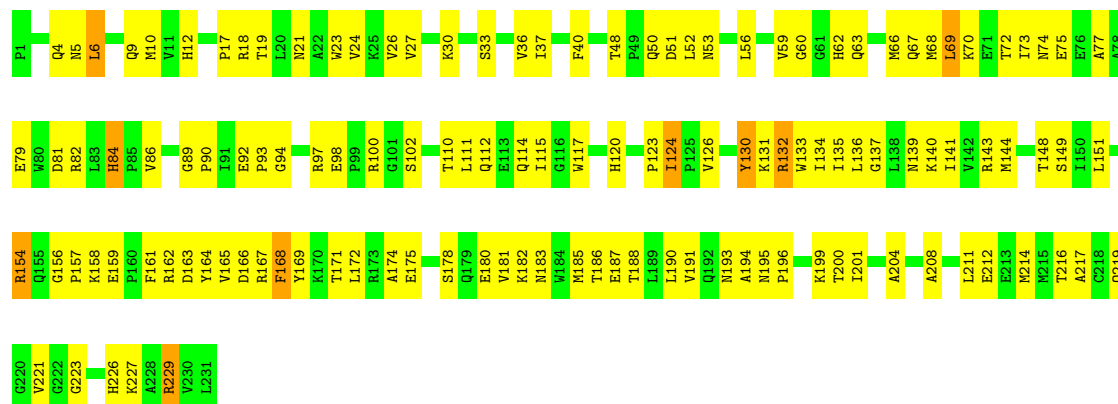
- Molecule 1: capsid protein

Chain go: 48% 48%

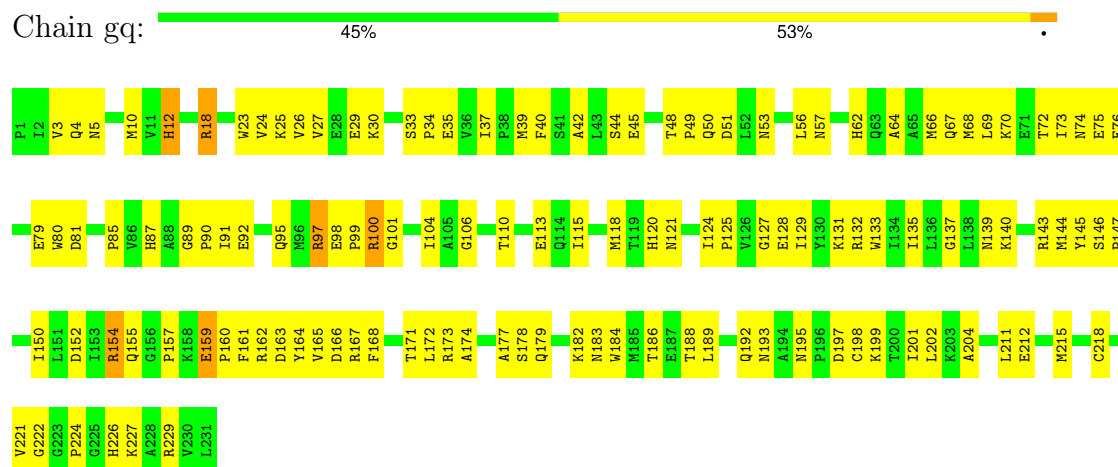


- Molecule 1: capsid protein

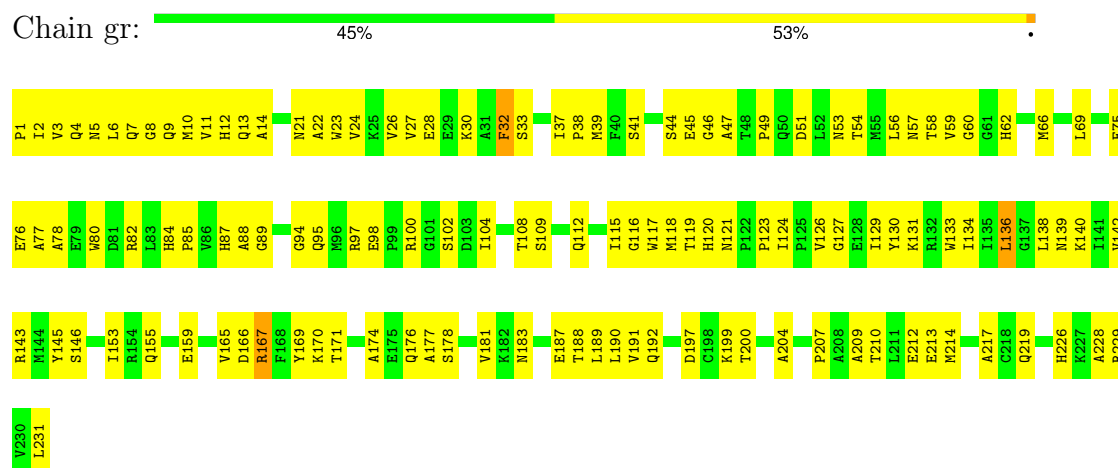
Chain gp: 45% 52%



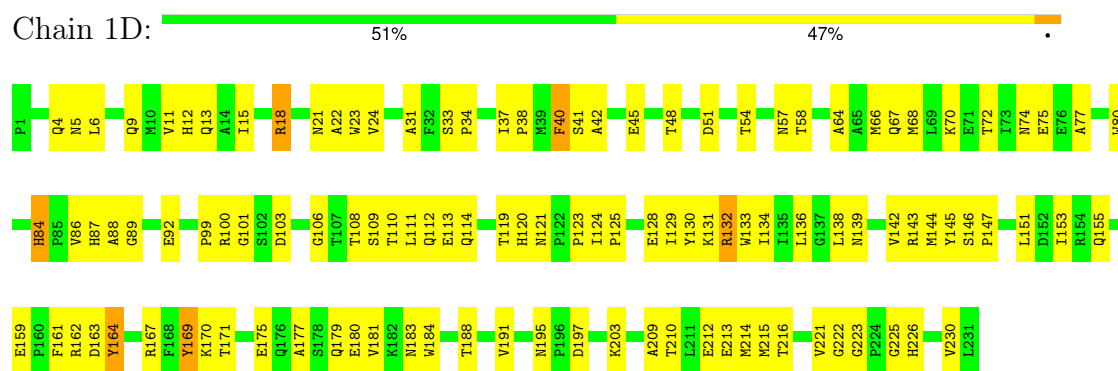
- Molecule 1: capsid protein



- Molecule 1: capsid protein

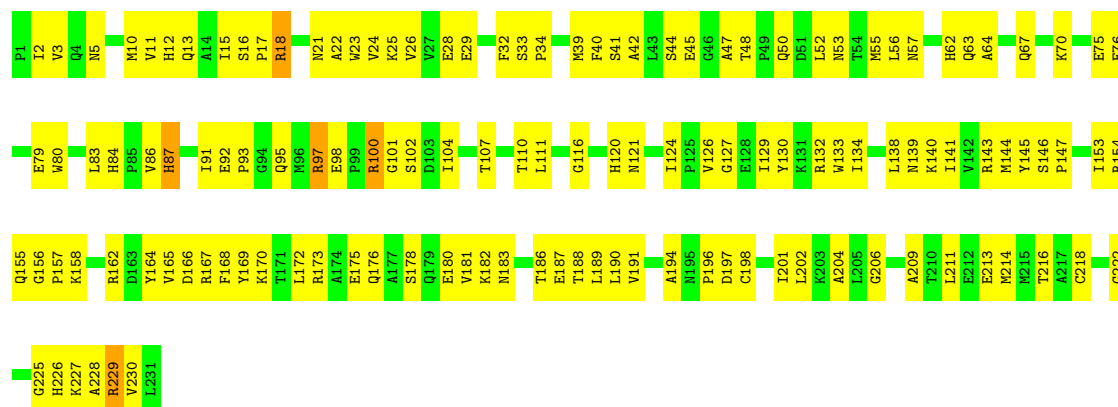


- Molecule 1: capsid protein



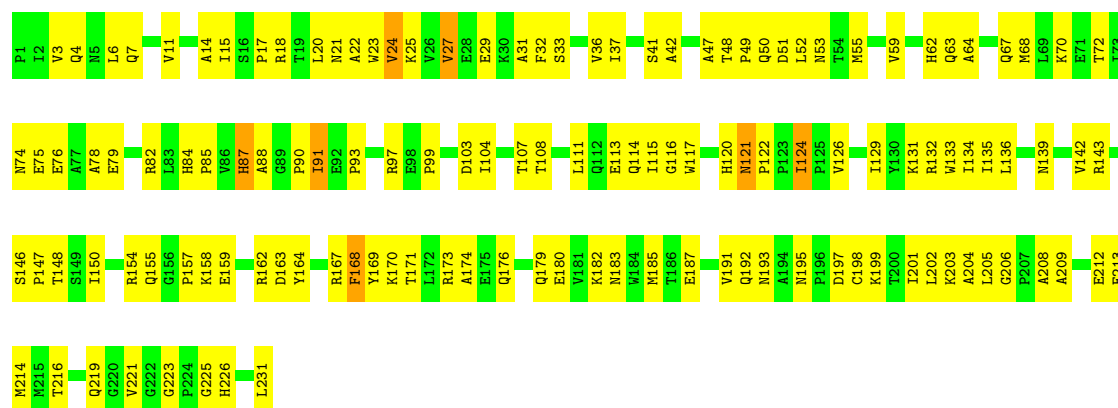
- Molecule 1: capsid protein





• Molecule 1: capsid protein

Chain gt: 43% 54%



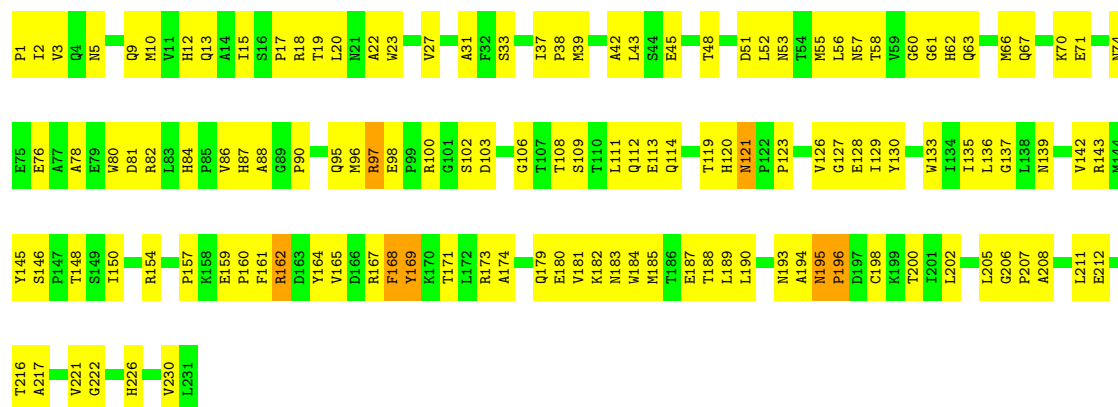
• Molecule 1: capsid protein

Chain gu: 41% 57%

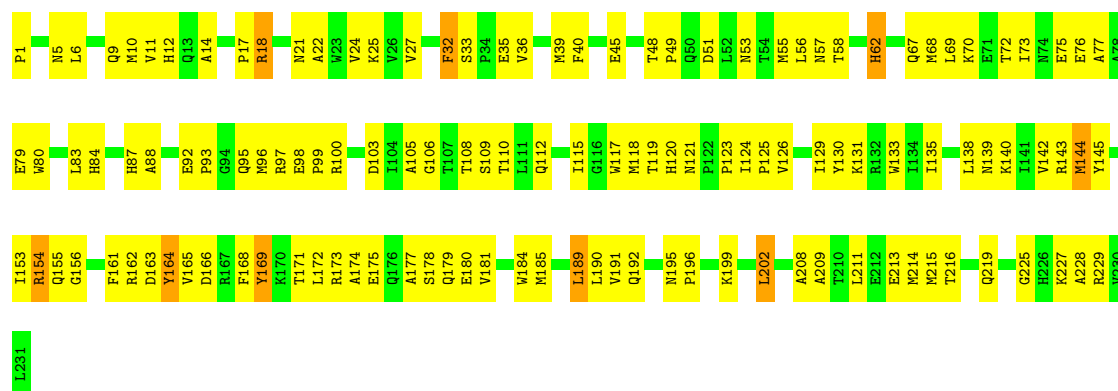


• Molecule 1: capsid protein

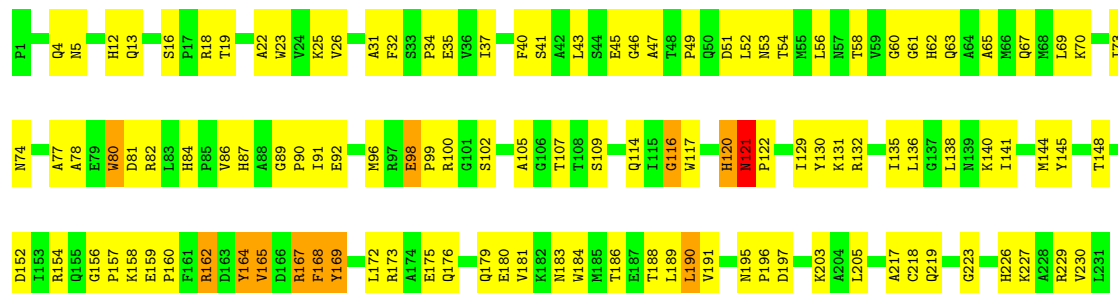
Chain gv: 44% 53%



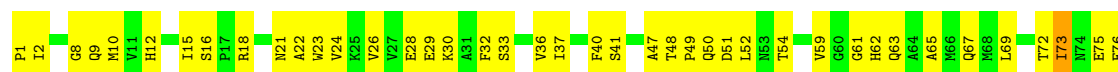
- Molecule 1: capsid protein

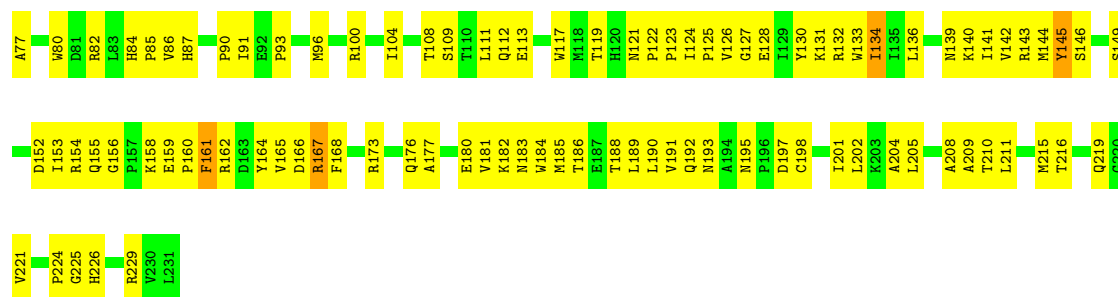


- Molecule 1: capsid protein

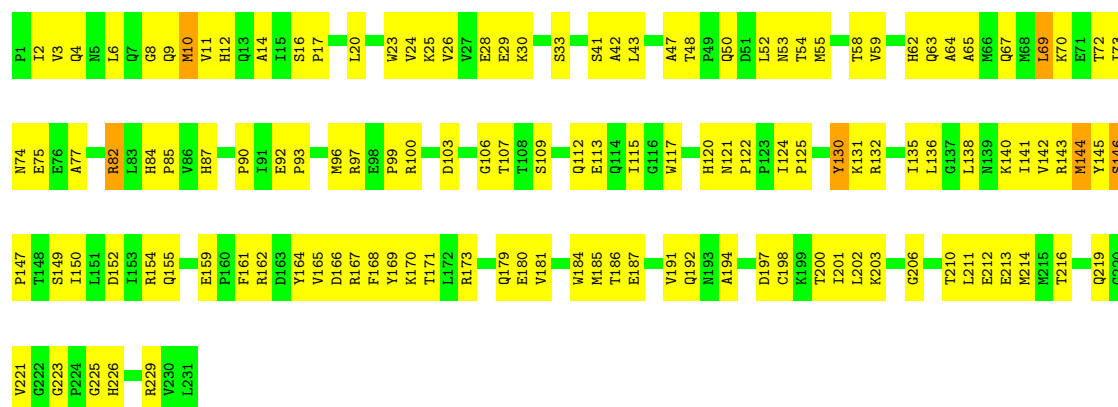


- Molecule 1: capsid protein

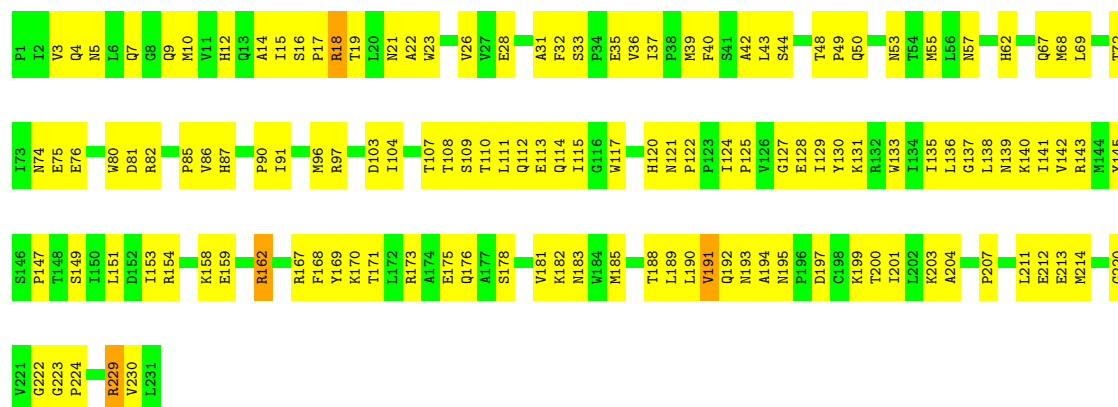




• Molecule 1: capsid protein



• Molecule 1: capsid protein



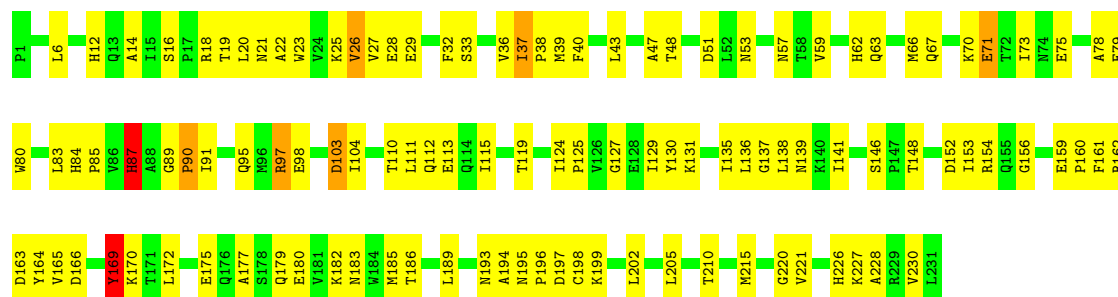
• Molecule 1: capsid protein





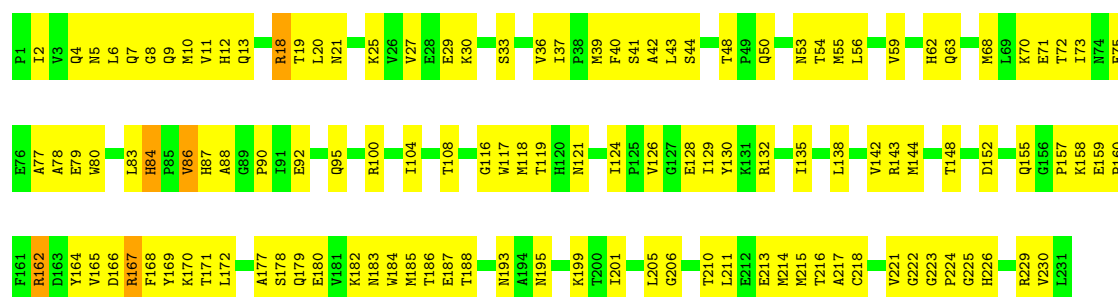
- Molecule 1: capsid protein

Chain 1E: 51% 45%



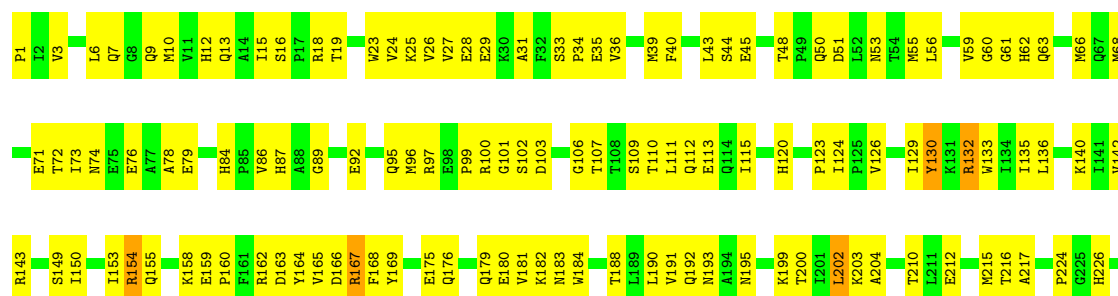
- Molecule 1: capsid protein

Chain gC: 46% 52%



- Molecule 1: capsid protein

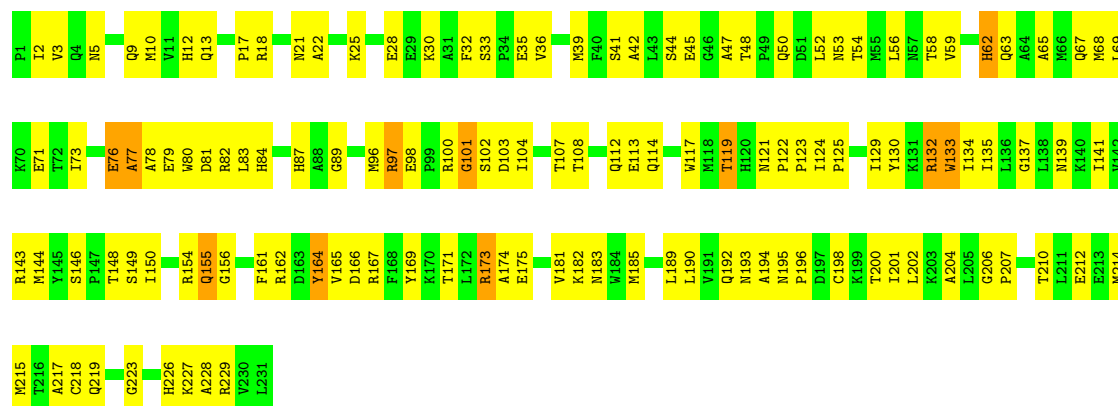
Chain gD: 45% 52%



V230
L231

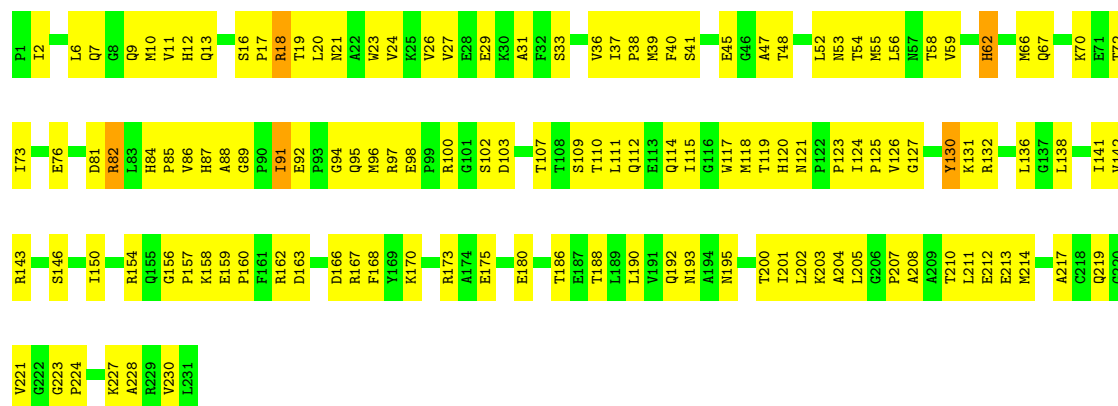
• Molecule 1: capsid protein

Chain gE: 44% 52% 5%



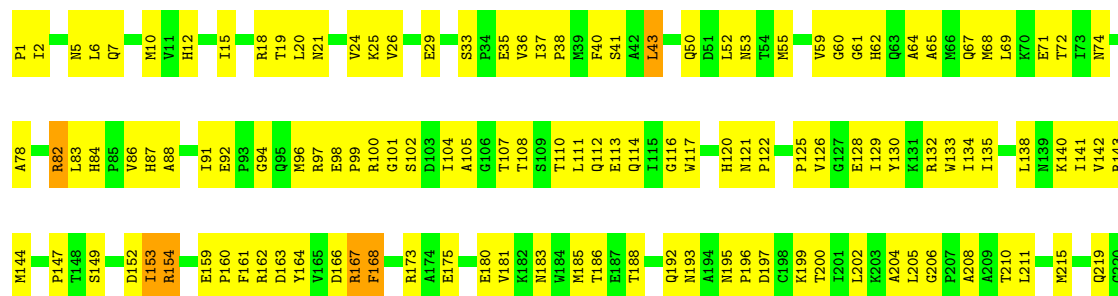
• Molecule 1: capsid protein

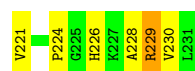
Chain gF: 43% 55%



• Molecule 1: capsid protein

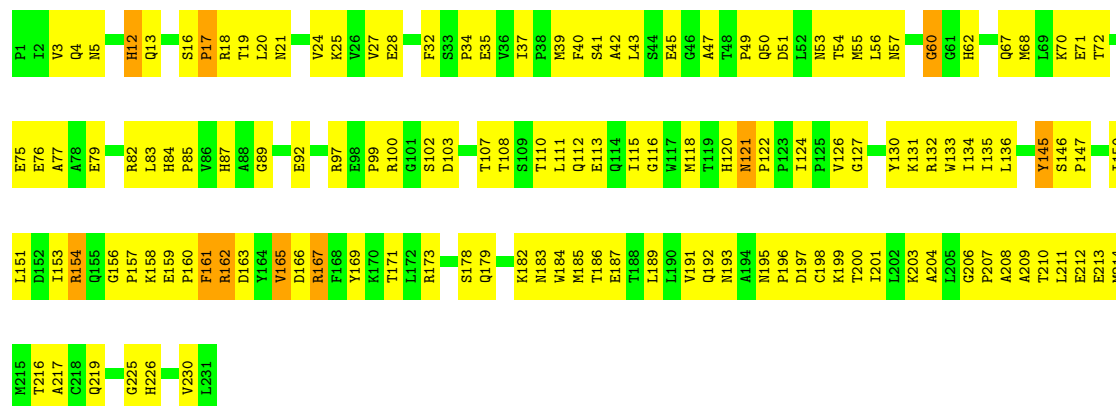
Chain gG: 44% 53%





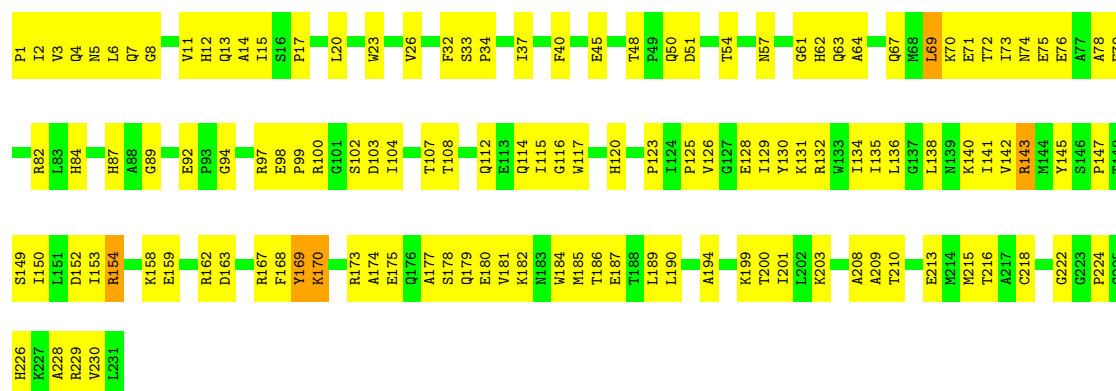
• Molecule 1: capsid protein

Chain gH: 41% 55%



• Molecule 1: capsid protein

Chain gI: 45% 53%



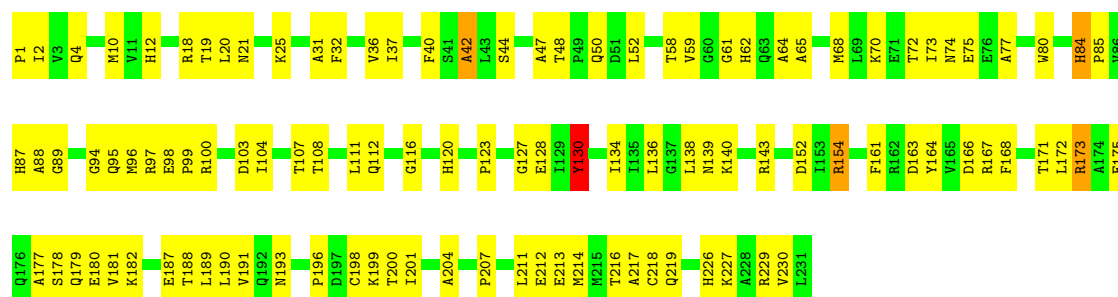
• Molecule 1: capsid protein

Chain gJ: 51% 46%

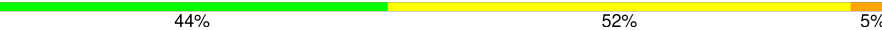


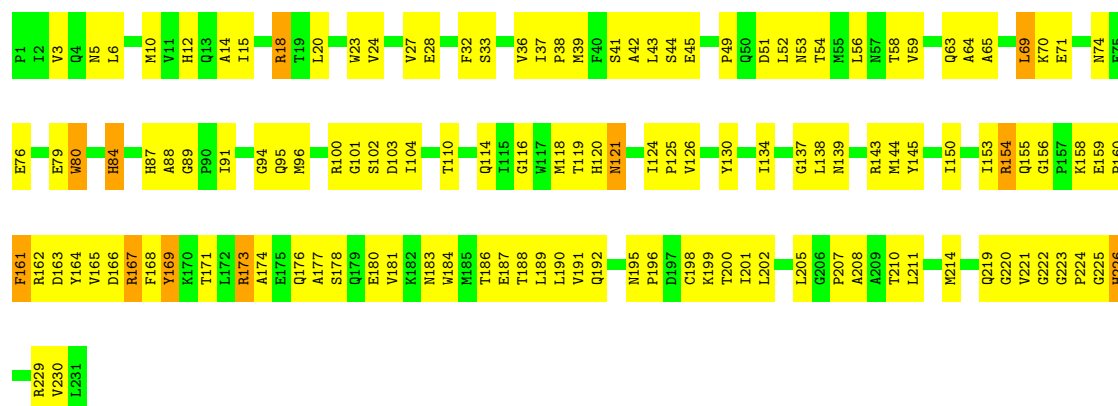
• Molecule 1: capsid protein

Chain gK:  53% 45%

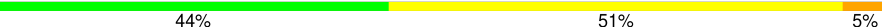


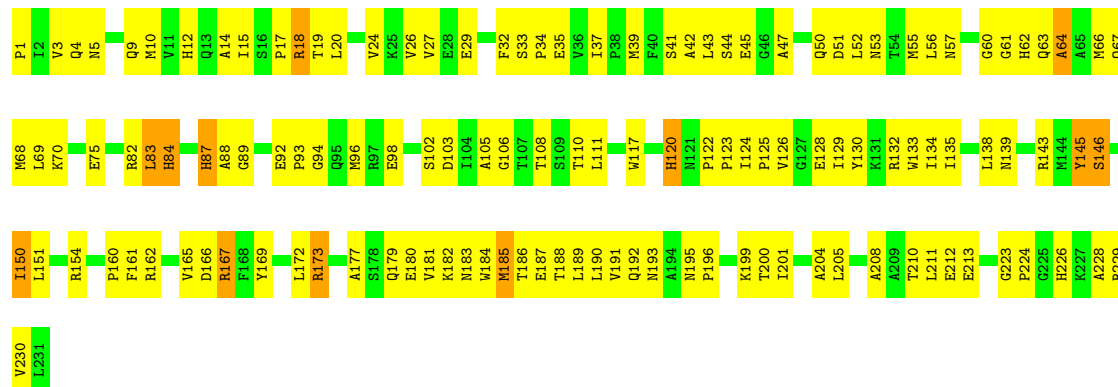
• Molecule 1: capsid protein

Chain gL:  44% 52% 5%

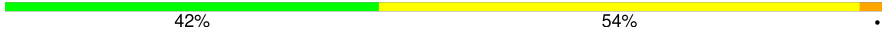


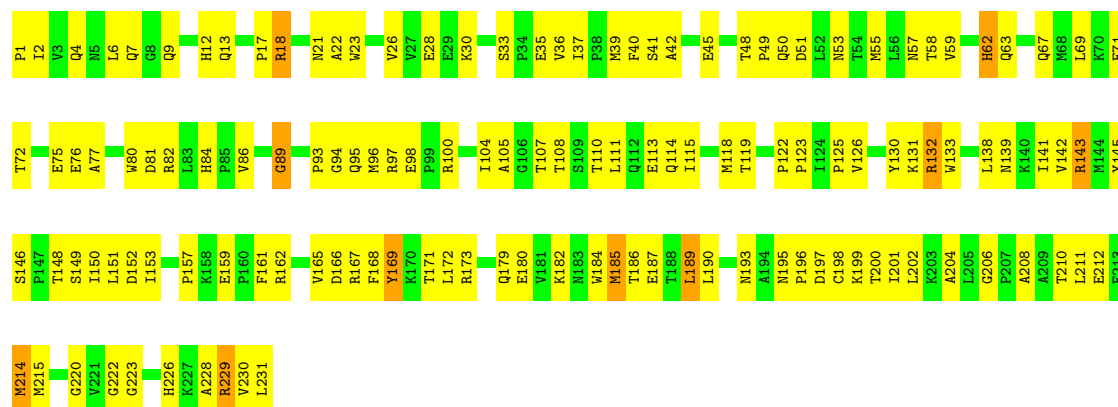
• Molecule 1: capsid protein

Chain 1F:  44% 51% 5%

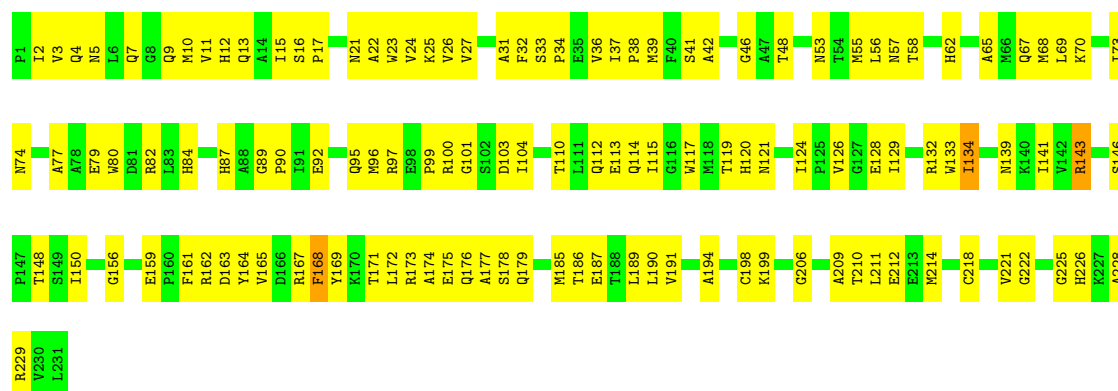


• Molecule 1: capsid protein

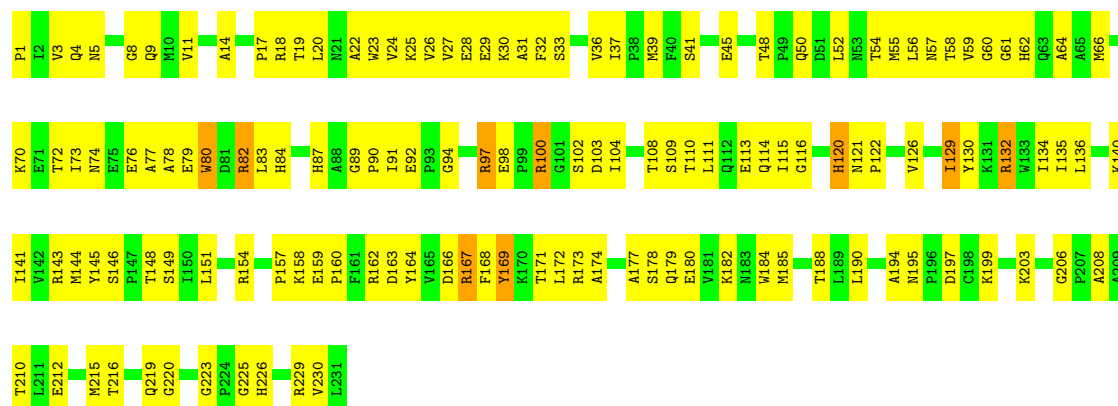
Chain gM:  42% 54%



• Molecule 1: capsid protein



• Molecule 1: capsid protein

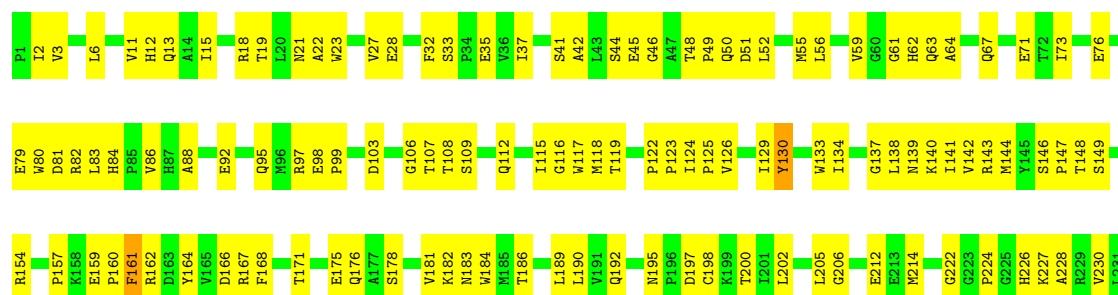


• Molecule 1: capsid protein

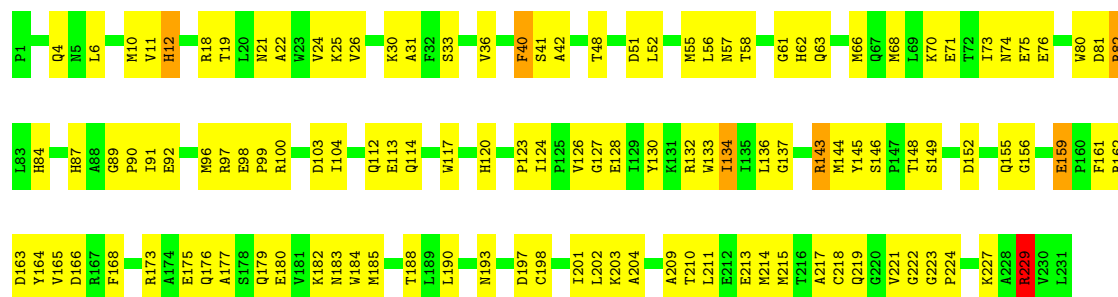




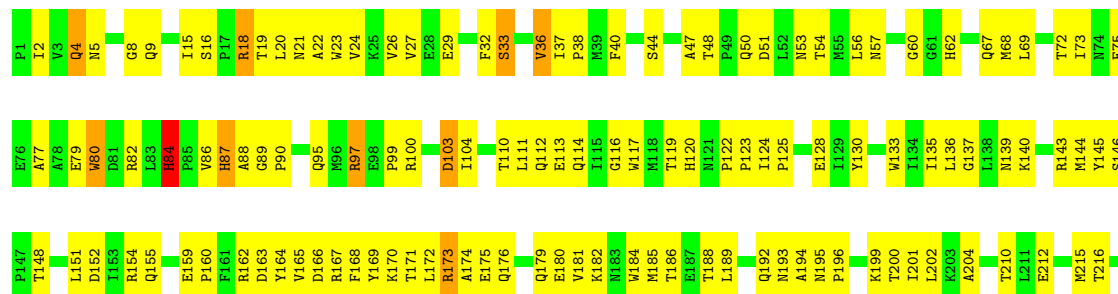
- Molecule 1: capsid protein



- Molecule 1: capsid protein



- Molecule 1: capsid protein



Q219
G220
V221
G222
G223
P224
G225
H226
K227
A228
R229
V230
L231

• Molecule 1: capsid protein

Chain gT: 48% 49%

P1 I2 V3 Q4 N5 L6 Q7 M10 V11 H12 H11 Q13 A14 P17 R18 T19 L20 N21 A22 A22 W23 K25 V26 E29 F32 E35 V36 I37 M39 F40 S41 A42 E45 P49 T54 N57 T58 V59 G60 G61 H62 A65 M66 L69 K70 N74 E79 W80 D81 R82 L83 H84 P85 A88 G89 P90 I91 D153 E92 P93 R100 G101 S102 D103 I104 A105 G106 S109 T110 I111 Q112 I115 W184 M185 W117 M118 T119 H120 N121 P122 P123 A194 N195 P196 D197 Y130 K131 R132 T200 W133 I134 I135 L136 G137 L138 M139 K140 I141 V142 M143 M144 Y145 S146 P147 T148 V230 L231 L151 R154 Q155 K158 E159 P160 R162 D163 Y164 R167 F168 F169 T171 L172 R173 A174 A177 S178 K182 M183 M184 M185 L189 L190 V191 Q192 N193 A194 N195 P196 D197 C198 K199 T200 Q206 A209 E212 E213 M214 M215 C218 P224 V230 L231

• Molecule 1: capsid protein

Chain gU: 44% 52%

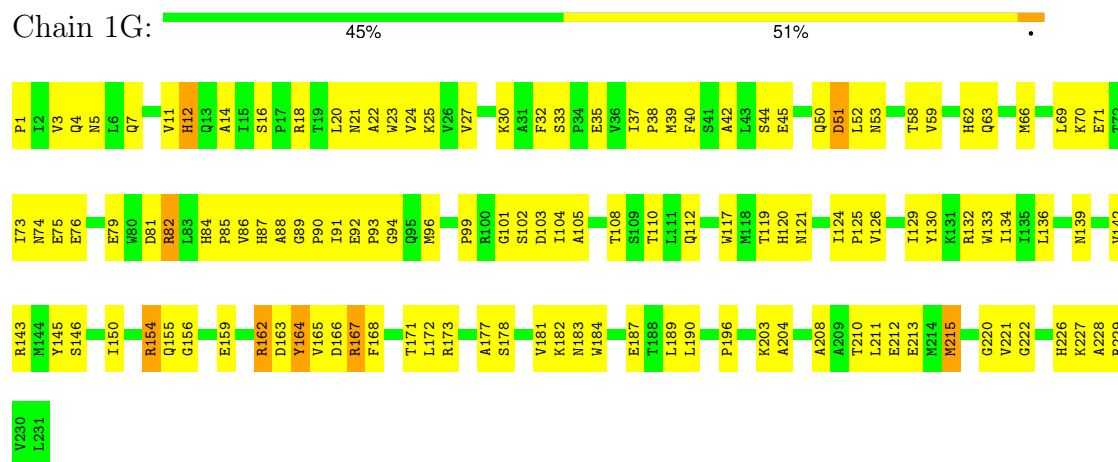
P1 I2 V3 Q4 N5 L6 Q7 G8 G9 M10 R82 L83 H84 A77 A78 W80 E79 H87 A88 G89 Q95 M96 H97 P99 R100 G101 S102 D103 I104 A105 G106 T107 T108 S109 T110 Q114 I115 H120 I124 P125 V126 G127 E128 I129 Y130 K131 R132 L136 G137 K140 I141 V142 S146 P147 I150 I73 N74 E75 E76 A77 A78 W80 E79 H87 A88 G89 Q95 M96 H97 P99 R100 G101 S102 D103 I104 A105 G106 T107 T108 S109 T110 Q114 I115 H120 I124 P125 V126 G127 E128 I129 Y130 K131 R132 L136 G137 K140 I141 V142 S146 P147 I150 R154 Q155 G156 F161 R162 D163 V164 V165 D166 R167 F168 Y169 L172 R173 A174 E175 Q176 S178 Q179 E180 V181 M185 T186 E187 T188 N193 A194 C198 T200 L202 A204 P207 A208 A209 T210 M215 T216 A217 C218 G222 G223 P224 G225 H226 K227 A228 R229 V230 L231

• Molecule 1: capsid protein

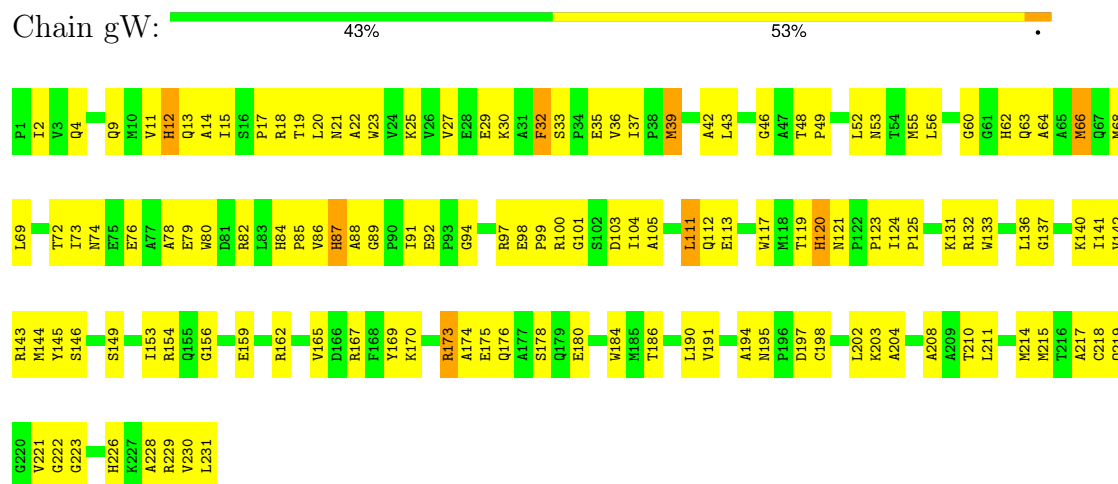
Chain gV: 47% 52%

P1 I2 V3 Q4 N5 L6 Q7 V11 H12 H11 Q13 A14 P17 R18 T19 L20 N21 A22 A22 W23 K25 V26 E29 F32 E35 V36 I37 M39 F40 S41 A42 E45 T48 P49 Q50 D51 M55 L56 N57 T58 V59 G60 G61 H62 Q63 A64 Q67 M68 L69 I73 N74 E75 E76 A77 A78 W80 E79 H87 A88 G89 P90 I91 D153 E92 P93 R100 G101 S102 D103 I104 A105 G106 T107 T108 S109 T110 Q114 I115 H120 I124 P125 V126 G127 E128 I129 Y130 K131 R132 L136 G137 K140 I141 V142 S146 P147 I150 I73 N74 E75 E76 A77 A78 W80 E79 H87 A88 G89 P90 I91 D153 E92 P93 R100 G101 S102 D103 I104 A105 G106 T107 T108 S109 T110 Q114 I115 H120 I124 P125 V126 G127 E128 I129 Y130 K131 R132 L136 G137 K140 I141 V142 S146 P147 I150 R154 Q155 G156 F161 R162 D163 V164 V165 D166 R167 F168 Y169 L172 R173 A174 E175 Q176 S178 Q179 E180 V181 M185 T186 E187 T188 N193 A194 C198 T200 L202 A204 P207 A208 A209 T210 M215 T216 A217 C218 G222 G223 P224 G225 H226 K227 A228 R229 V230 L231

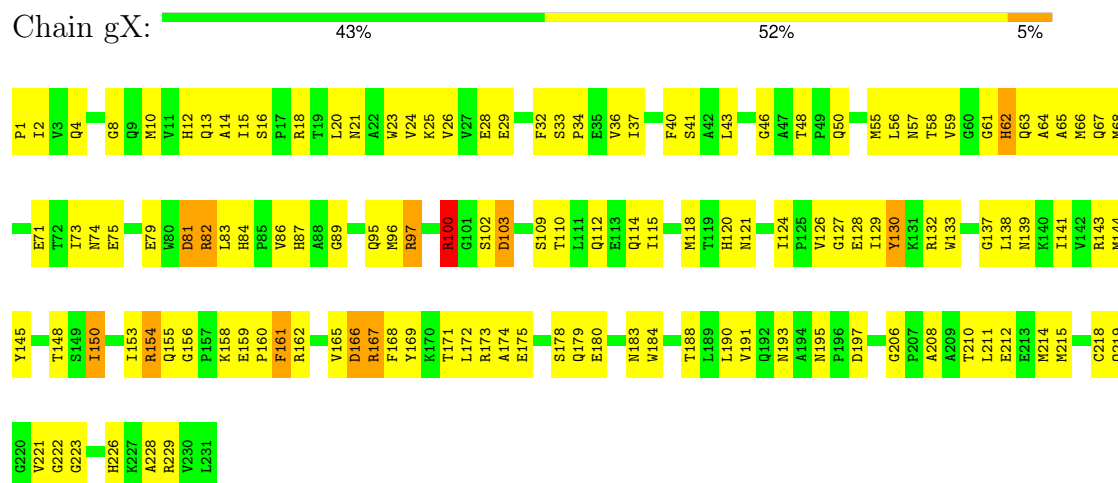
• Molecule 1: capsid protein



- Molecule 1: capsid protein

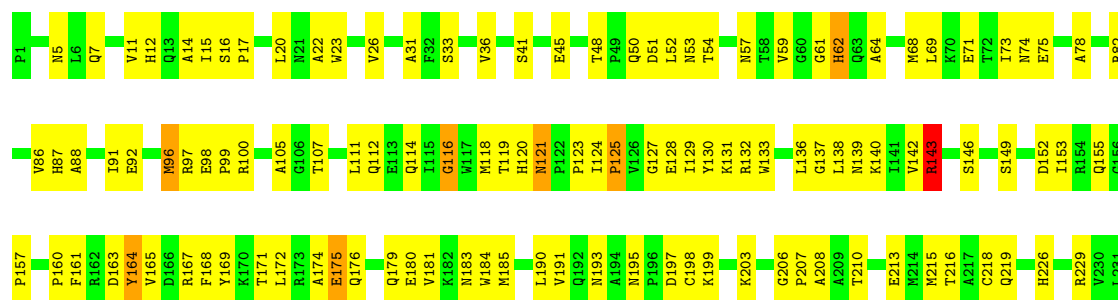


- Molecule 1: capsid protein



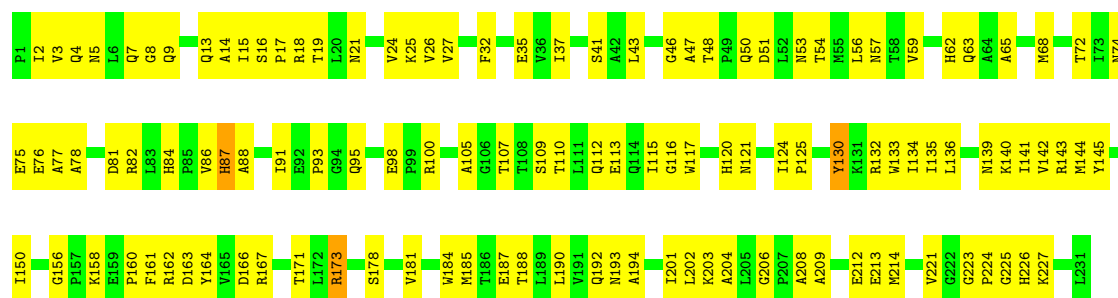
- Molecule 1: capsid protein

Chain gY:  49% 47% .



• Molecule 1: capsid protein

Chain gZ:  48% 50% .



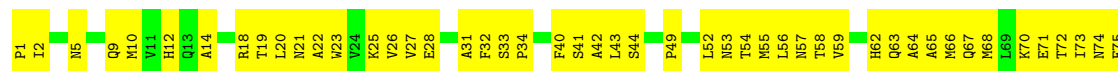
• Molecule 1: capsid protein

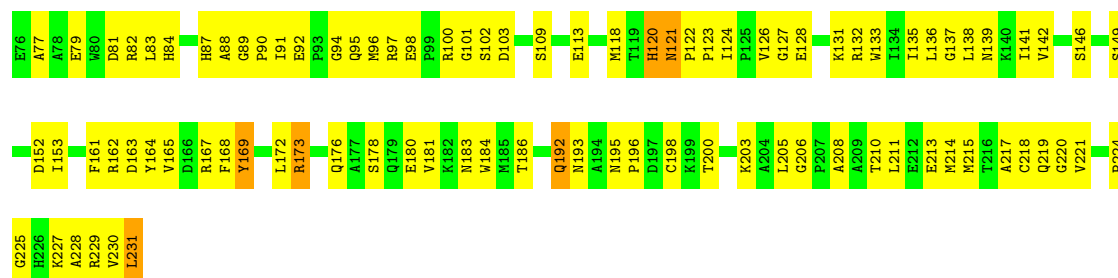
Chain h0:  43% 53% ..



• Molecule 1: capsid protein

Chain h1:  40% 57% .





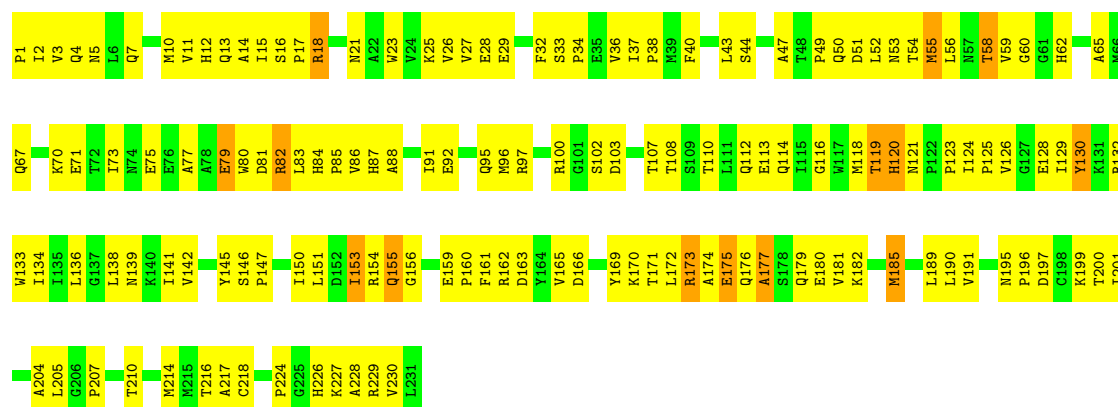
- Molecule 1: capsid protein

Chain h2: 39% 58%



- Molecule 1: capsid protein

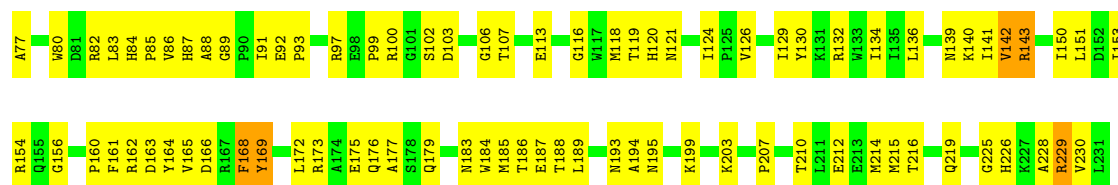
Chain h3: 36% 58% 6%



- Molecule 1: capsid protein

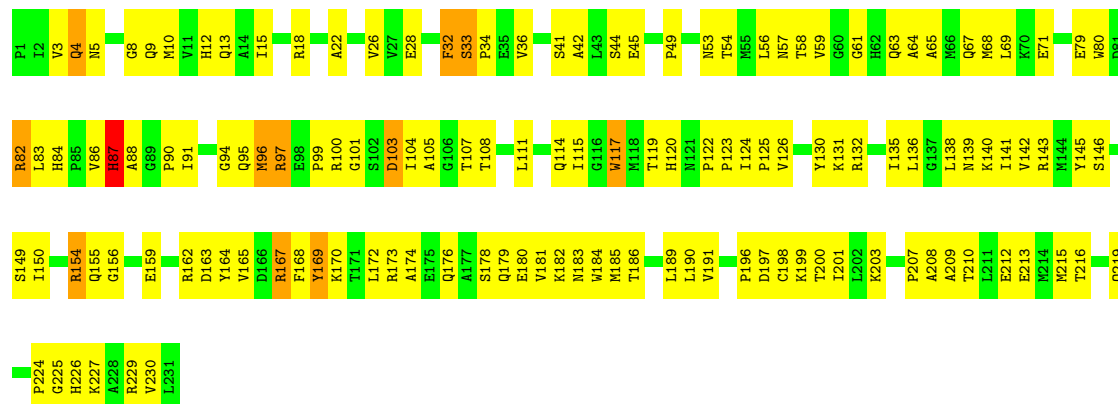
Chain h4: 46% 50%





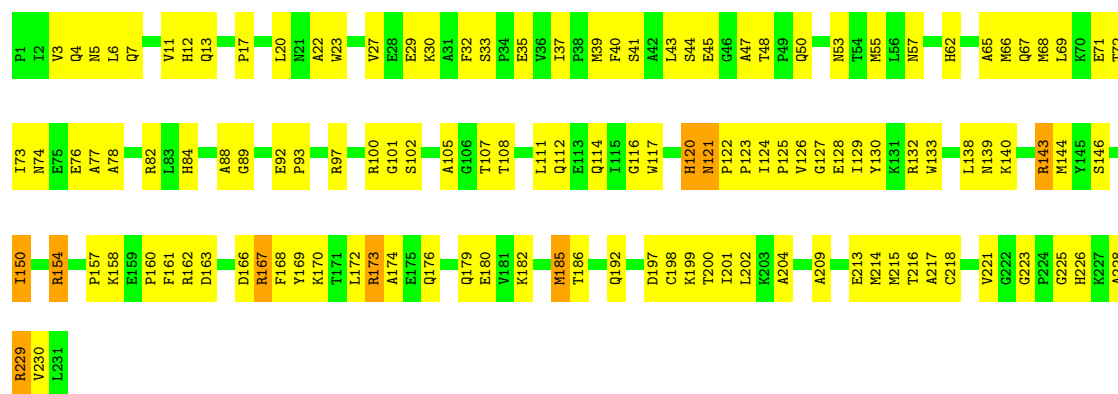
• Molecule 1: capsid protein

Chain h5: 42% 53% 5%



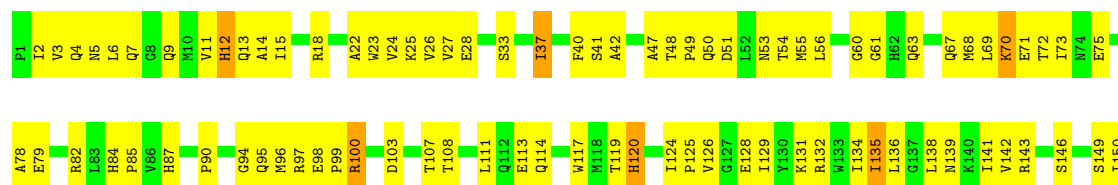
• Molecule 1: capsid protein

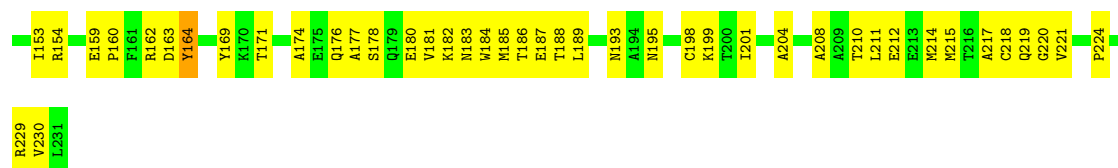
Chain 1H: 46% 50%



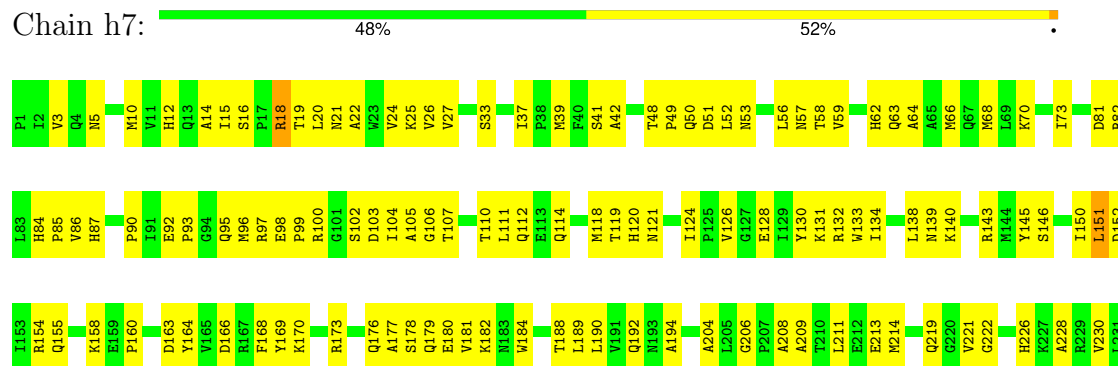
• Molecule 1: capsid protein

Chain h6: 44% 53%

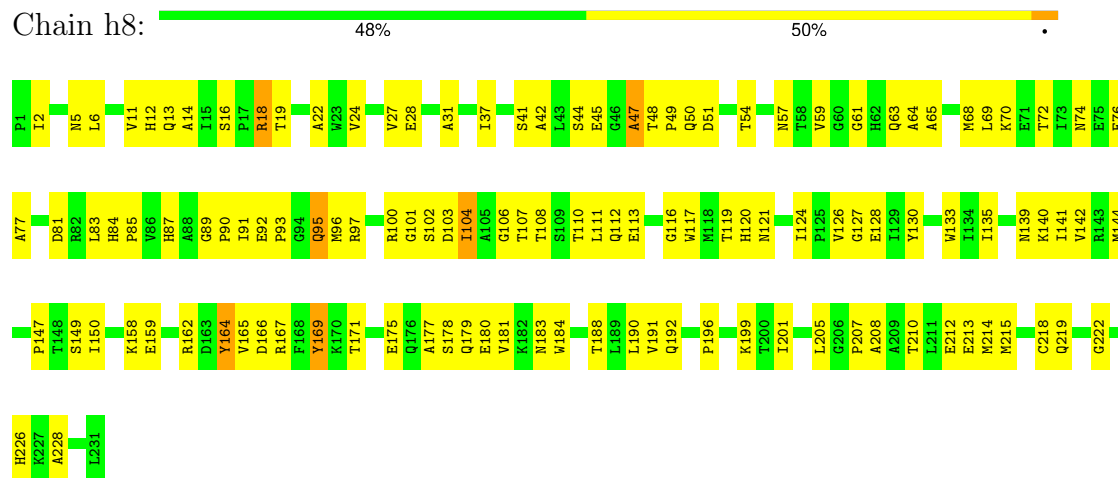




- Molecule 1: capsid protein



- Molecule 1: capsid protein



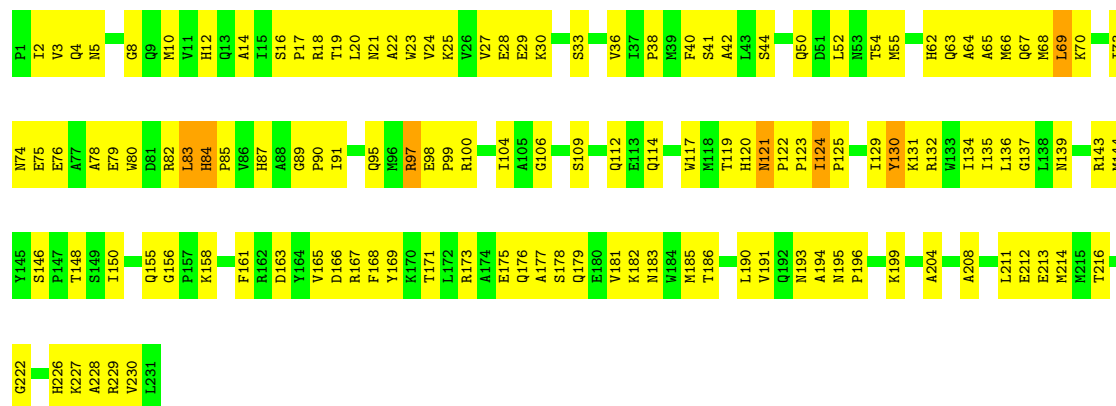
- Molecule 1: capsid protein





- Molecule 1: capsid protein

Chain ha: 43% 54%



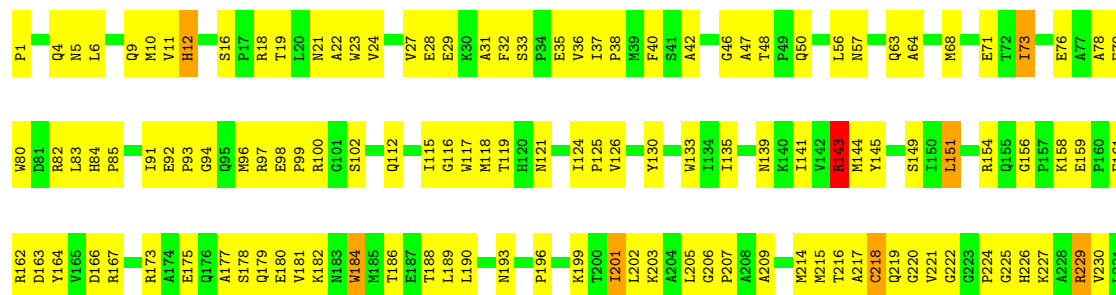
- Molecule 1: capsid protein

Chain hb: 50% 46%



- Molecule 1: capsid protein

Chain hc: 46% 50%



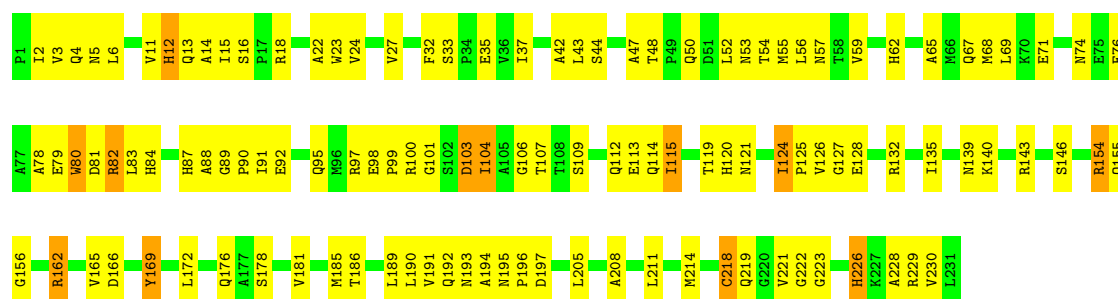
- Molecule 1: capsid protein

Chain hd: 52% 45%



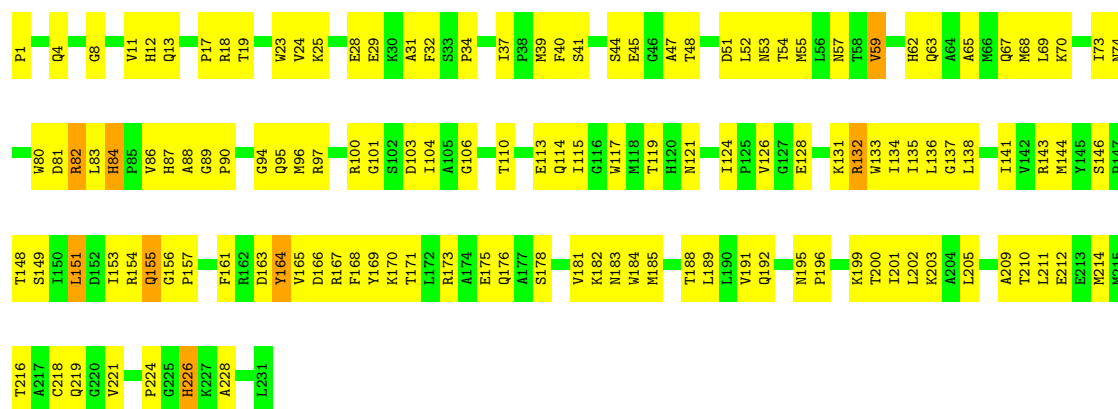
- Molecule 1: capsid protein

Chain he: 49% 46% 5%



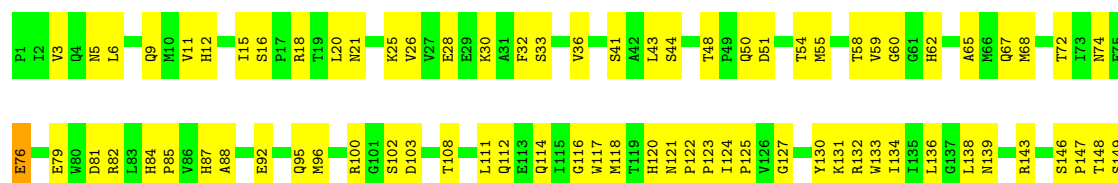
- Molecule 1: capsid protein

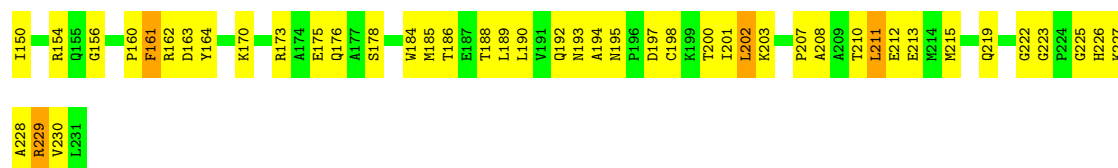
Chain hf: 42% 54% 0%



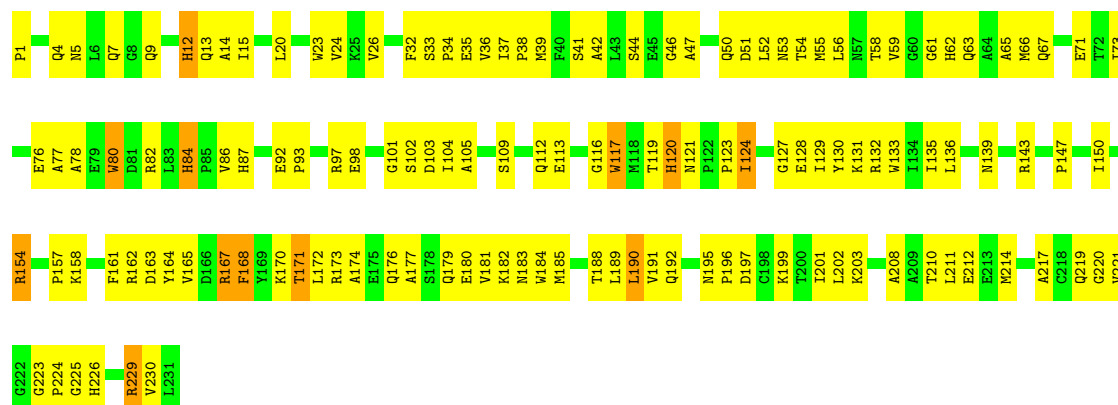
- Molecule 1: capsid protein

Chain 1I: 48% 50% 0%

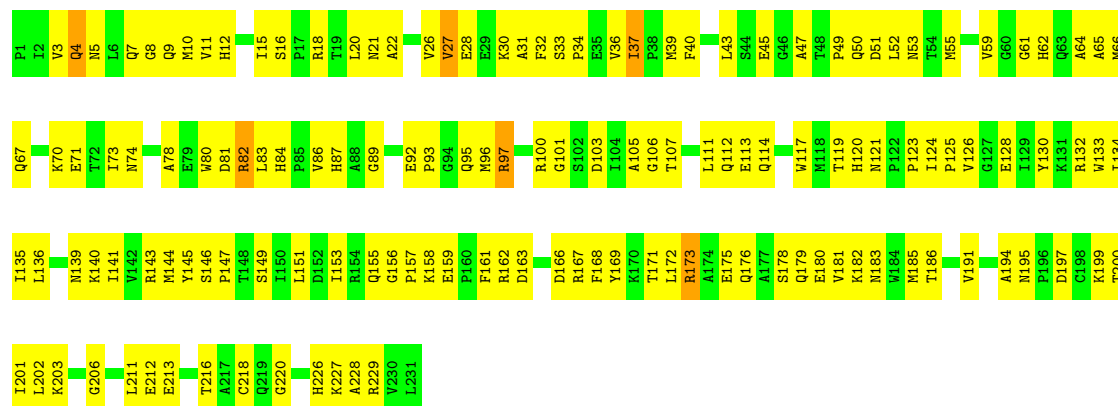




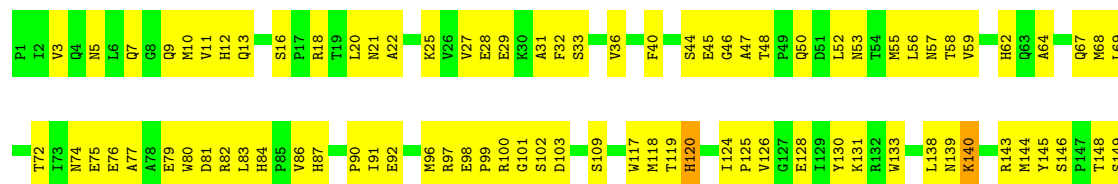
• Molecule 1: capsid protein

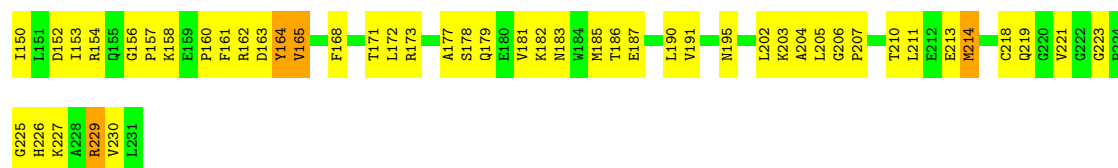


• Molecule 1: capsid protein

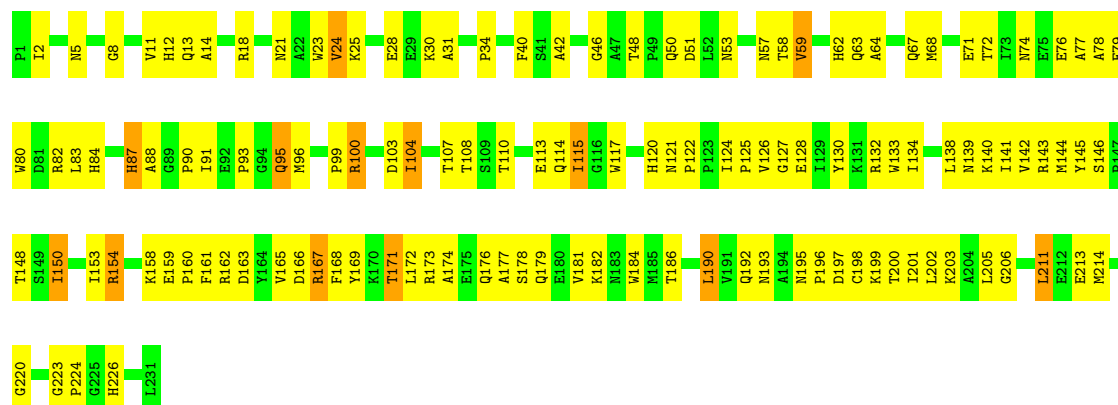


• Molecule 1: capsid protein

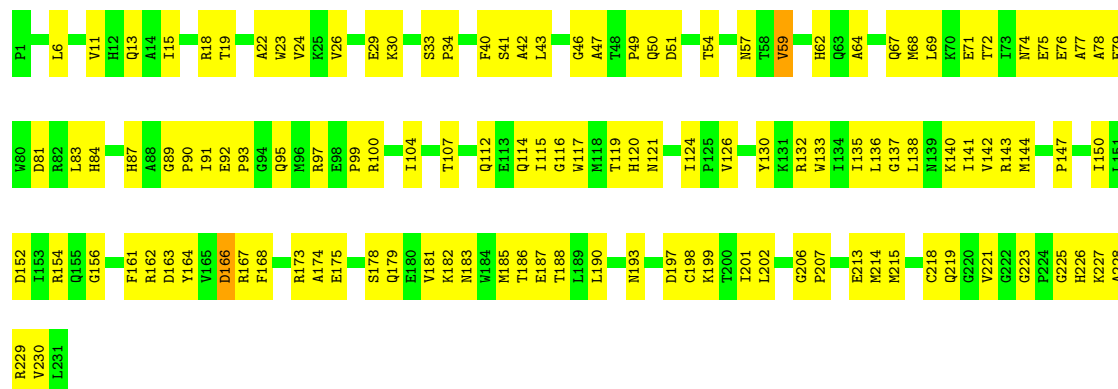




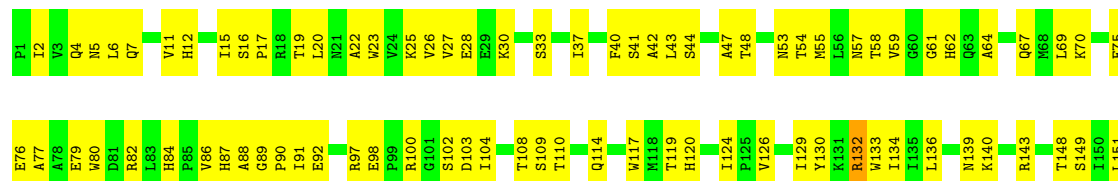
• Molecule 1: capsid protein



• Molecule 1: capsid protein



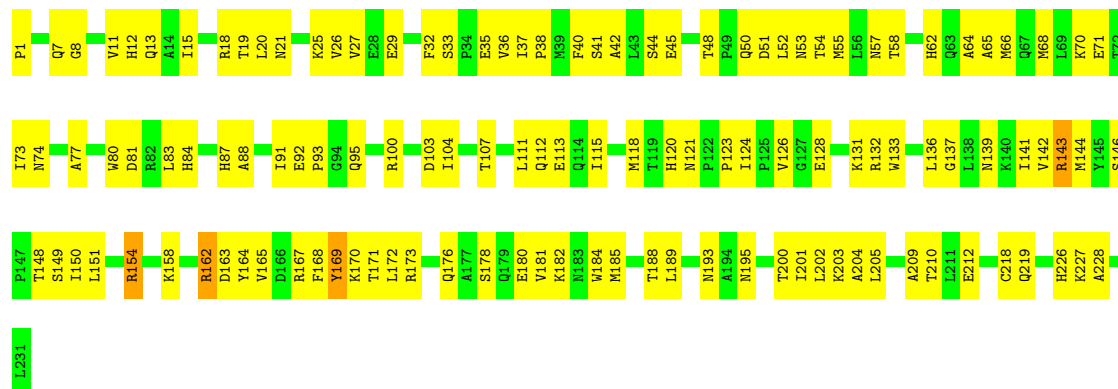
• Molecule 1: capsid protein





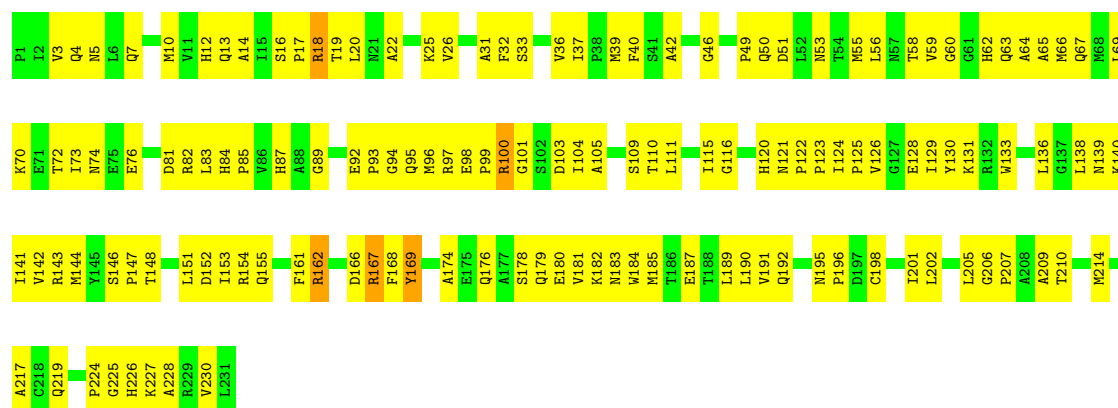
- Molecule 1: capsid protein

Chain hm: 47% 52%



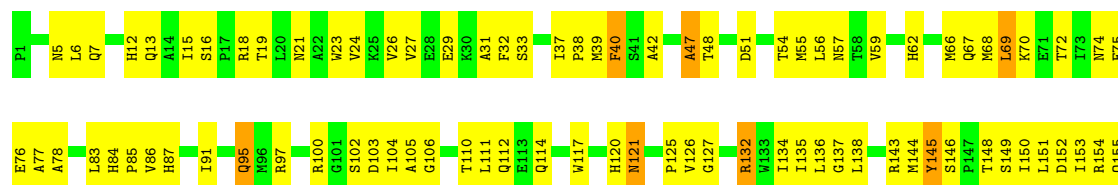
- Molecule 1: capsid protein

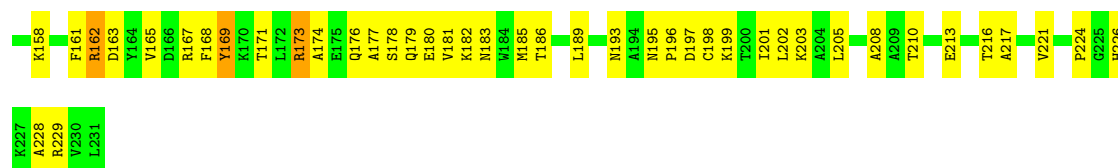
Chain hn: 40% 58%



- Molecule 1: capsid protein

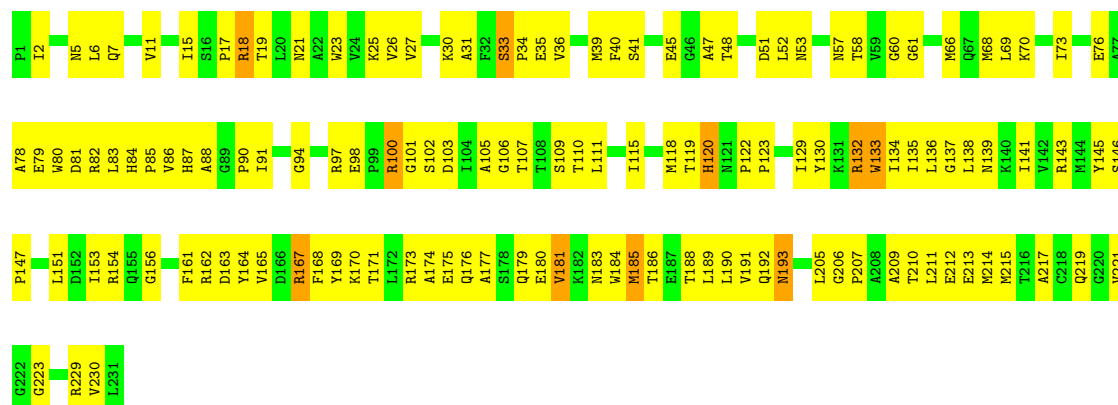
Chain ho: 45% 51%





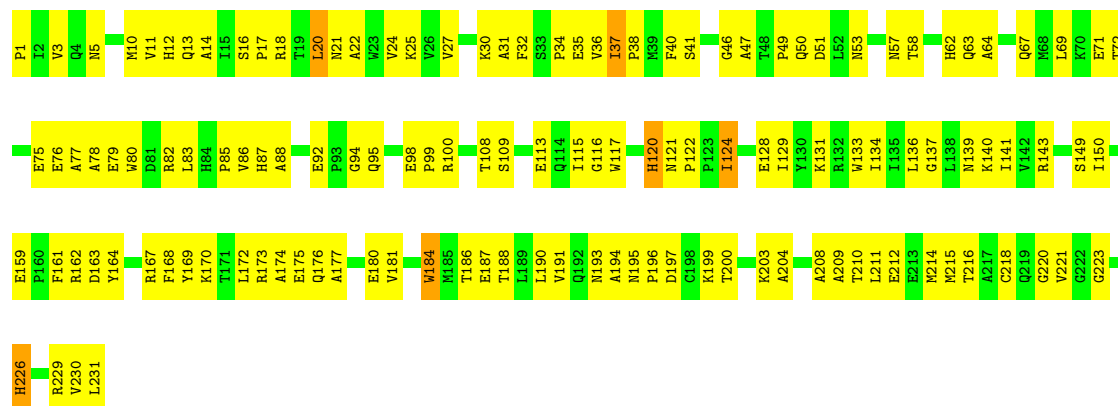
• Molecule 1: capsid protein

Chain hp: 42% 54%



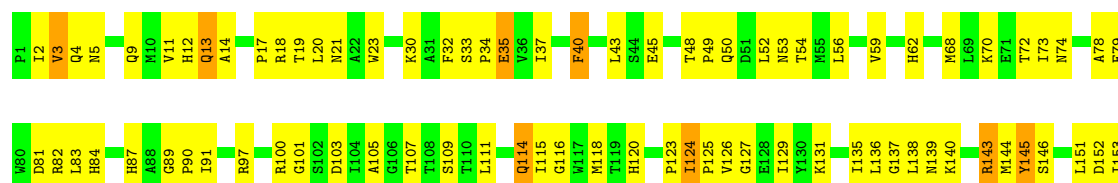
• Molecule 1: capsid protein

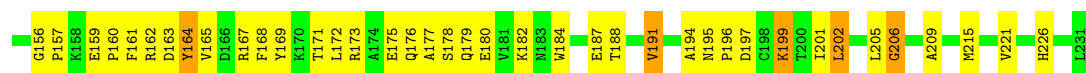
Chain 1J: 43% 54%



• Molecule 1: capsid protein

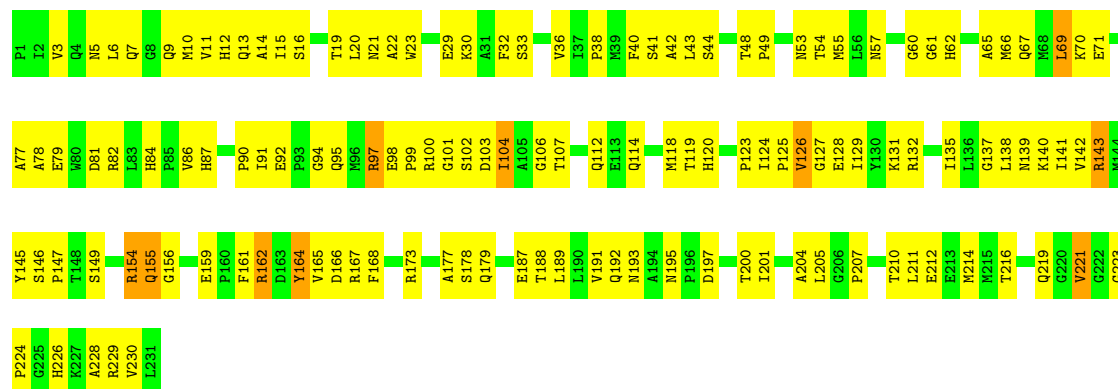
Chain hq: 48% 46% 6%





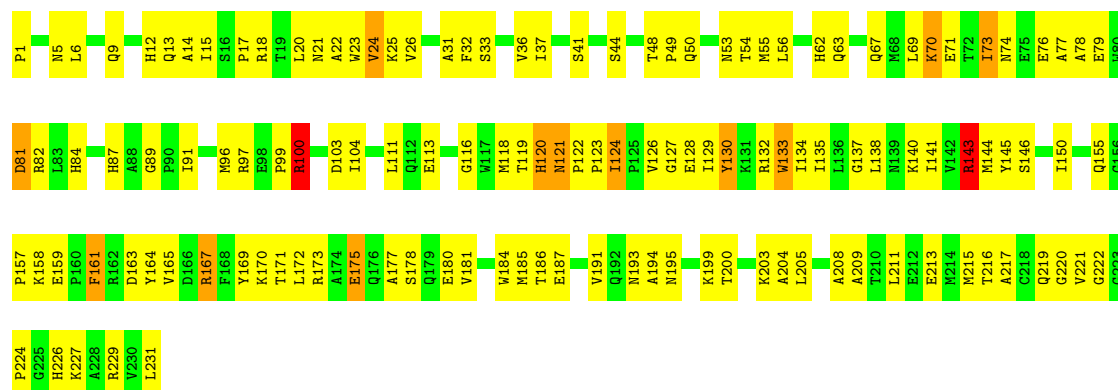
• Molecule 1: capsid protein

Chain hr: •



• Molecule 1: capsid protein

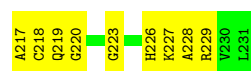
Chain hs: •



• Molecule 1: capsid protein

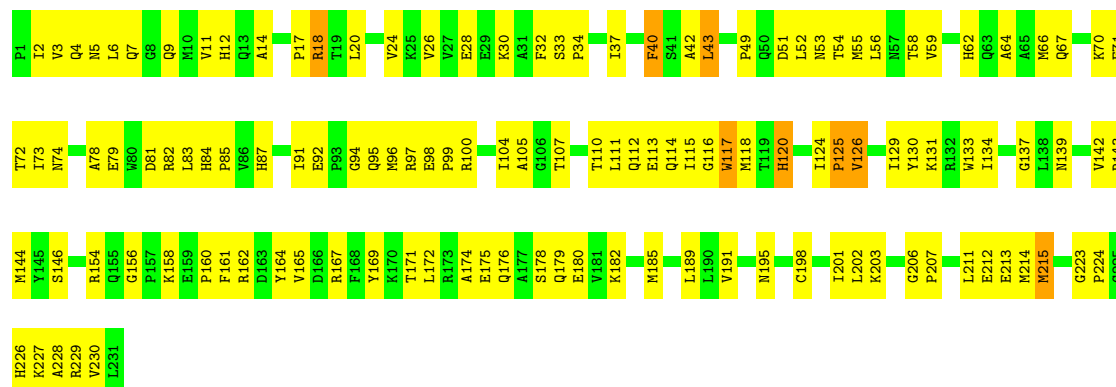
Chain ht: •





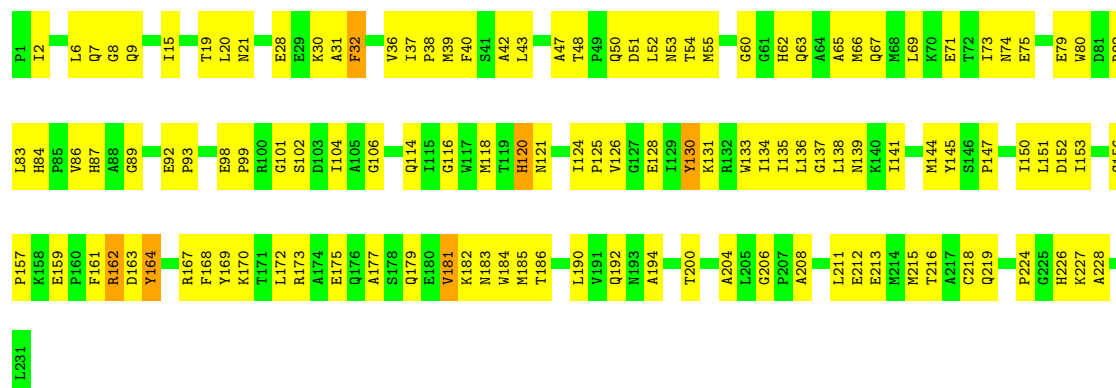
- Molecule 1: capsid protein

Chain hu: 45% 52%



- Molecule 1: capsid protein

Chain hv: 48% 50%

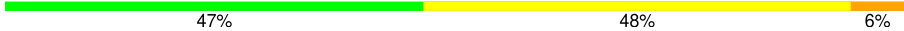


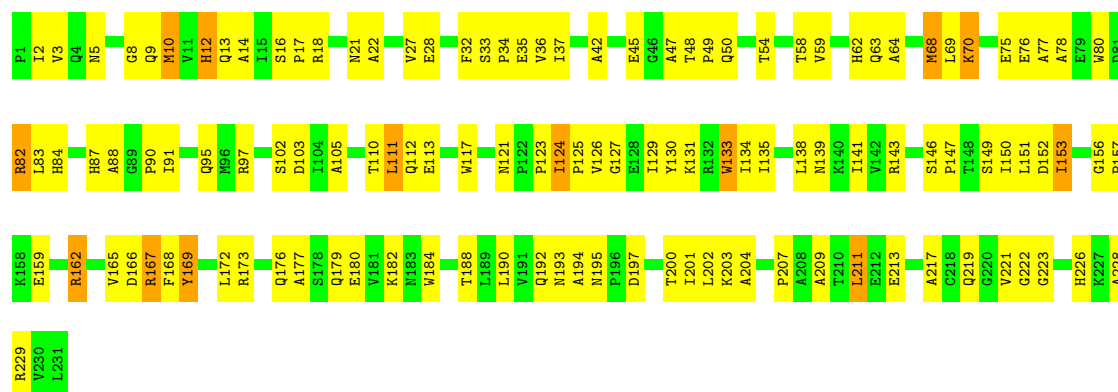
- Molecule 1: capsid protein

Chain hw: 50% 49%

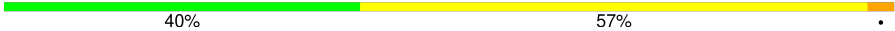


- Molecule 1: capsid protein

Chain hx:  47% 48% 6%

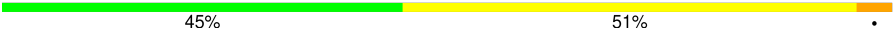


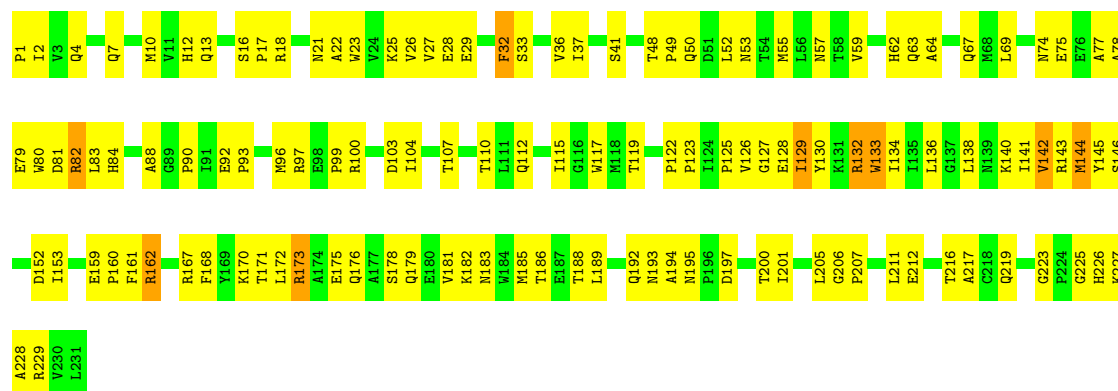
• Molecule 1: capsid protein

Chain hy:  40% 57% .

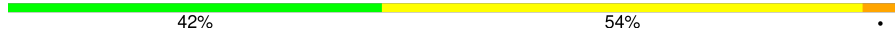


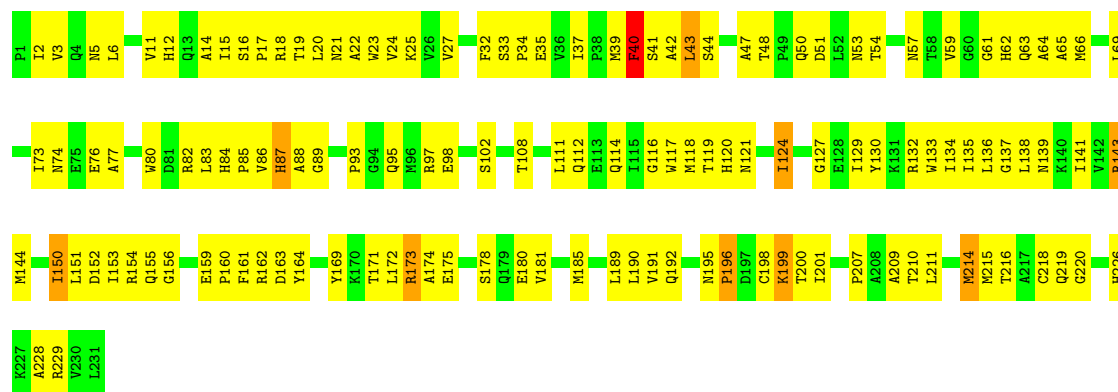
• Molecule 1: capsid protein

Chain hz:  45% 51% .



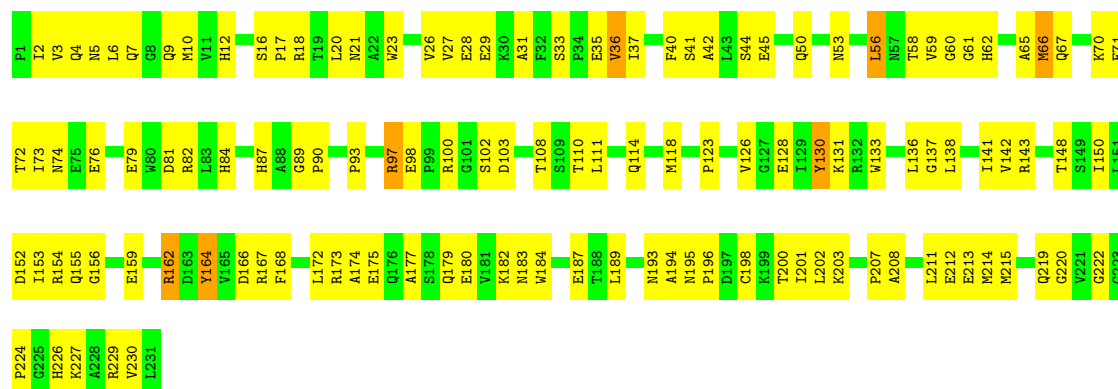
• Molecule 1: capsid protein

Chain 1K:  42% 54% .



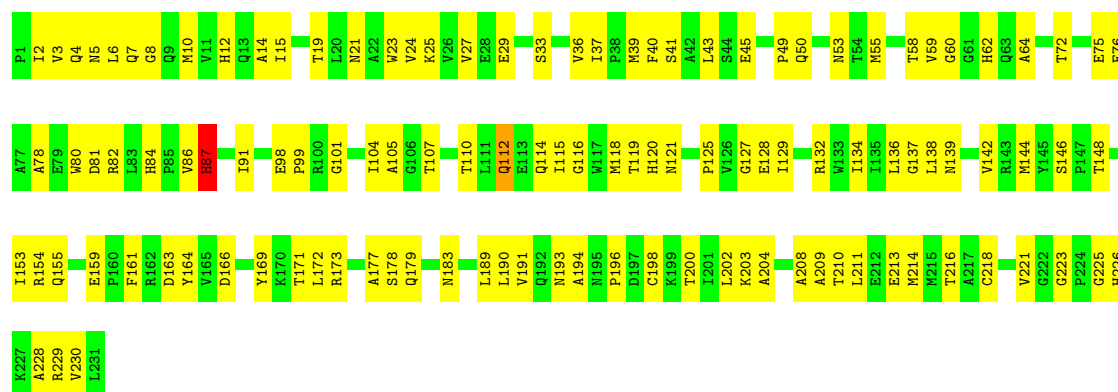
- Molecule 1: capsid protein

Chain hA: 46% 51%



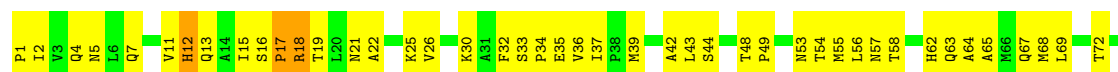
- Molecule 1: capsid protein

Chain hB: 49% 50%



- Molecule 1: capsid protein

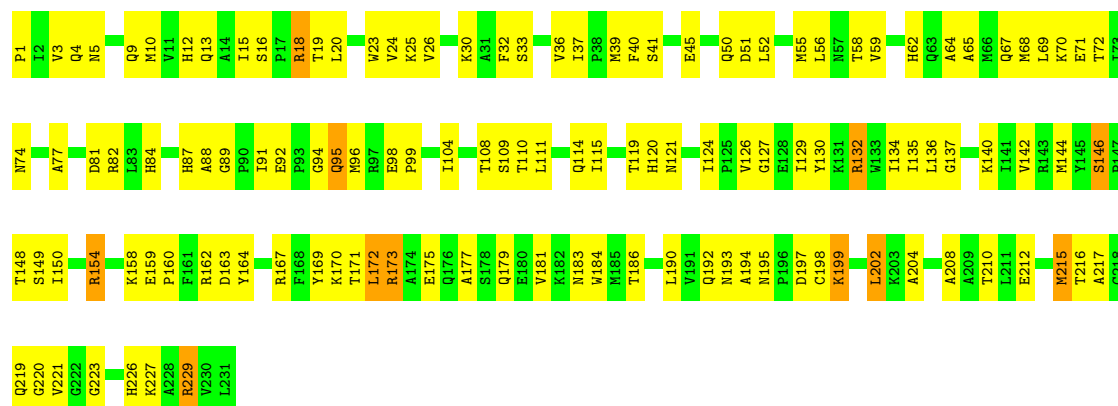
Chain hC: 40% 56%





• Molecule 1: capsid protein

Chain hD: 45% 50% 5%



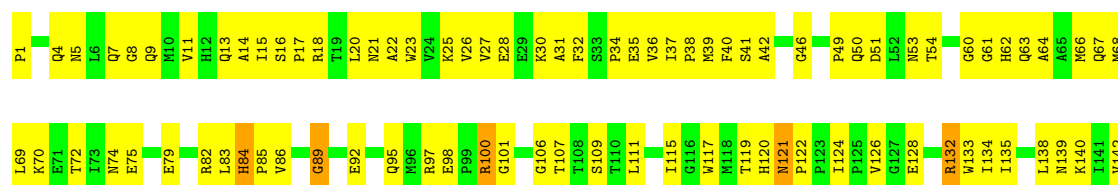
• Molecule 1: capsid protein

Chain hE: 47% 51%



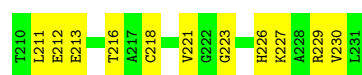
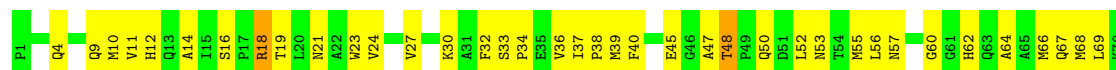
• Molecule 1: capsid protein

Chain hF: 46% 50%

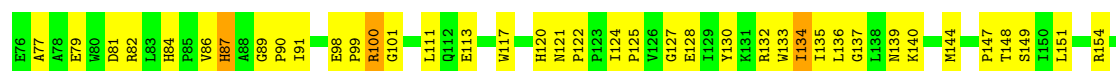
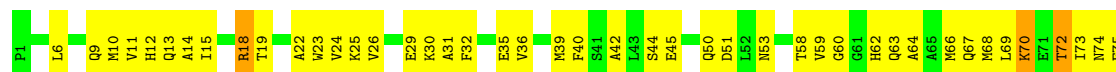




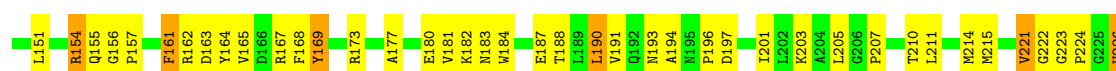
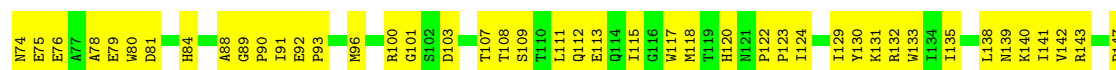
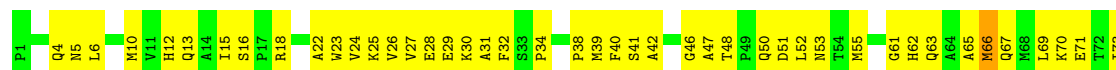
• Molecule 1: capsid protein



• Molecule 1: capsid protein



• Molecule 1: capsid protein



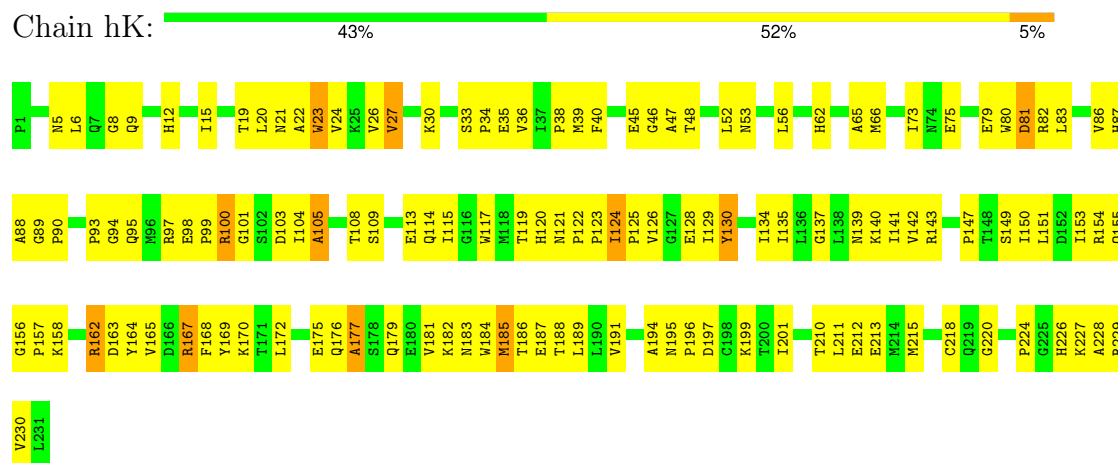
• Molecule 1: capsid protein



• Molecule 1: capsid protein

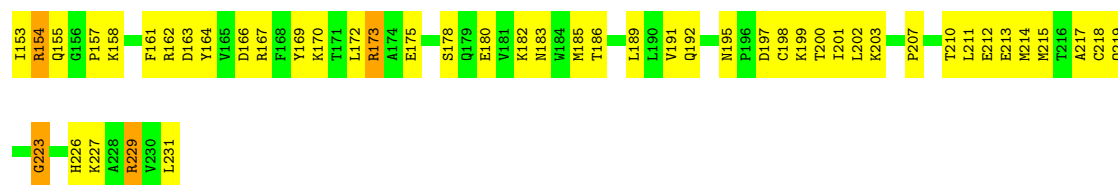


• Molecule 1: capsid protein



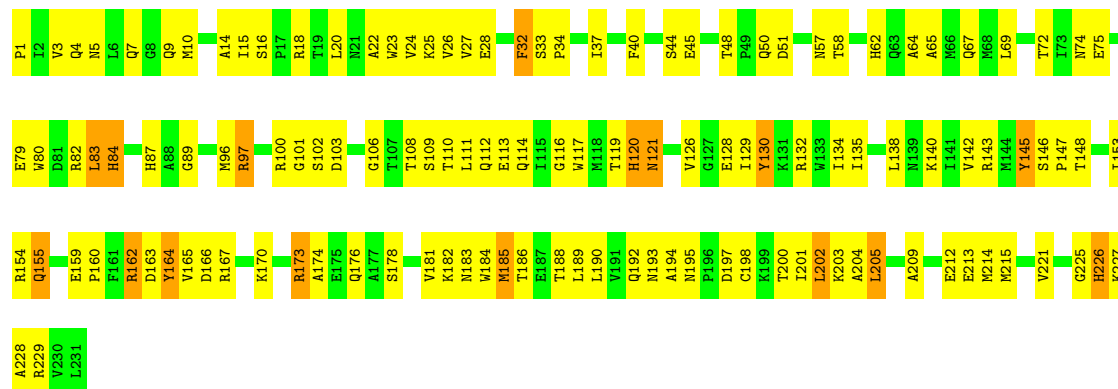
• Molecule 1: capsid protein





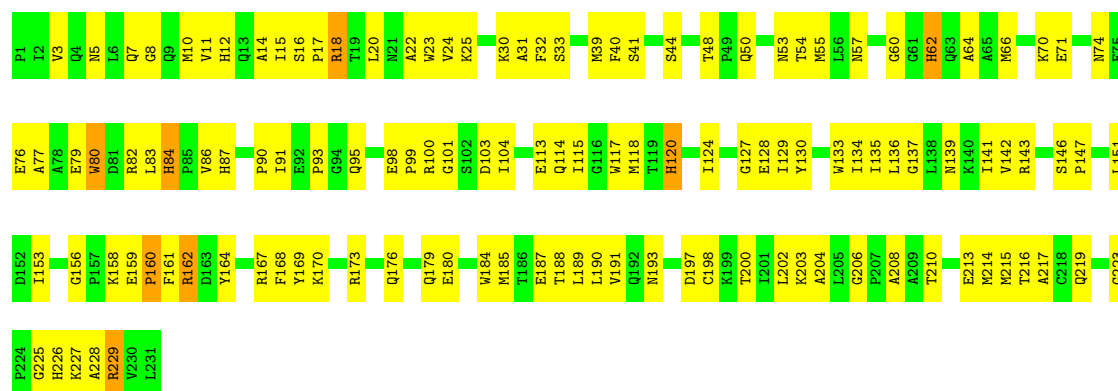
- Molecule 1: capsid protein

Chain hM: 45% 48% 7%



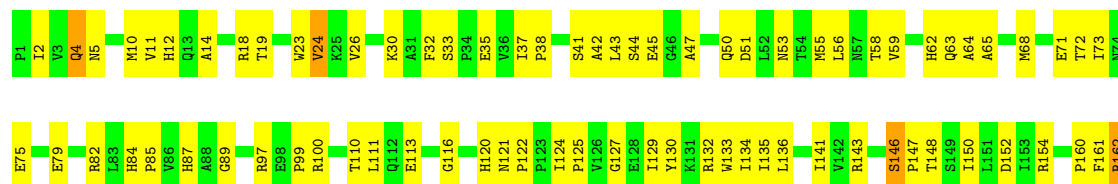
- Molecule 1: capsid protein

Chain hN: 46% 51% 3%



- Molecule 1: capsid protein

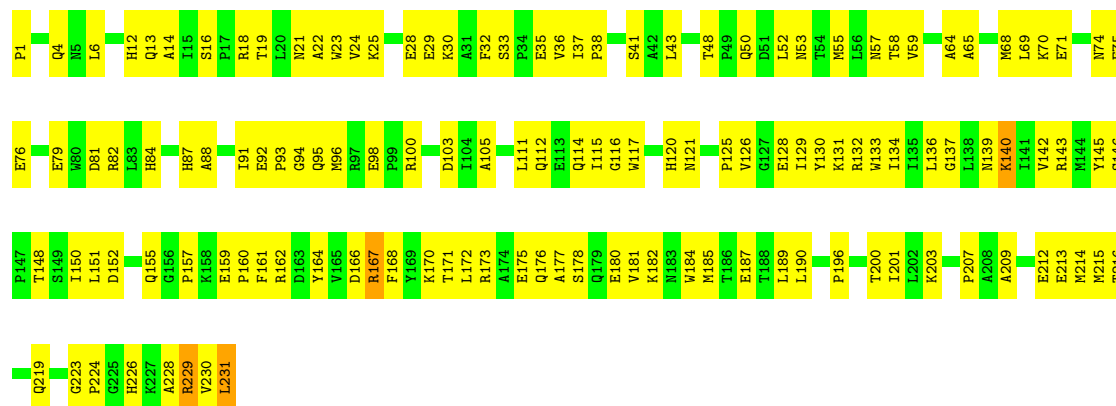
Chain hO: 48% 48% 4%





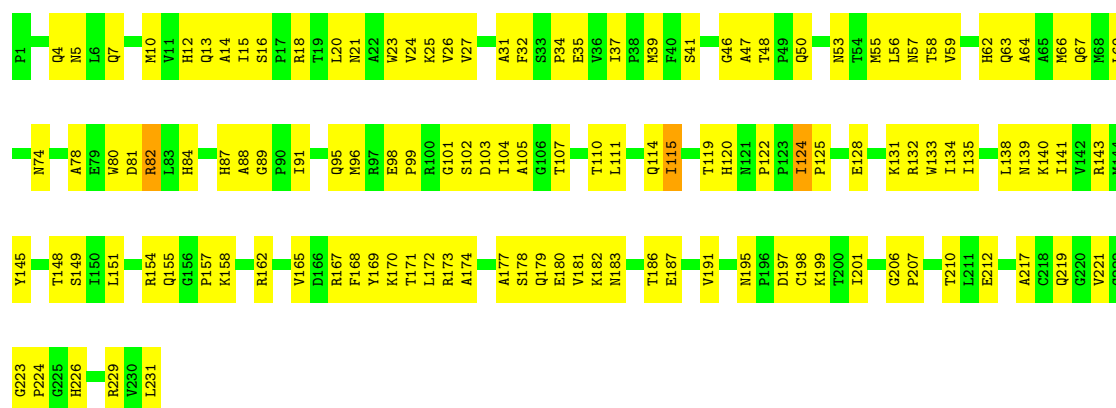
• Molecule 1: capsid protein

Chain hP: 43% 55%



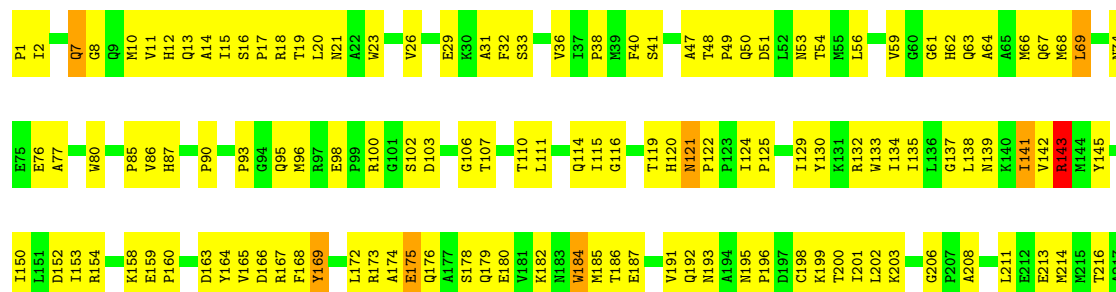
• Molecule 1: capsid protein

Chain hQ: 46% 53%



• Molecule 1: capsid protein

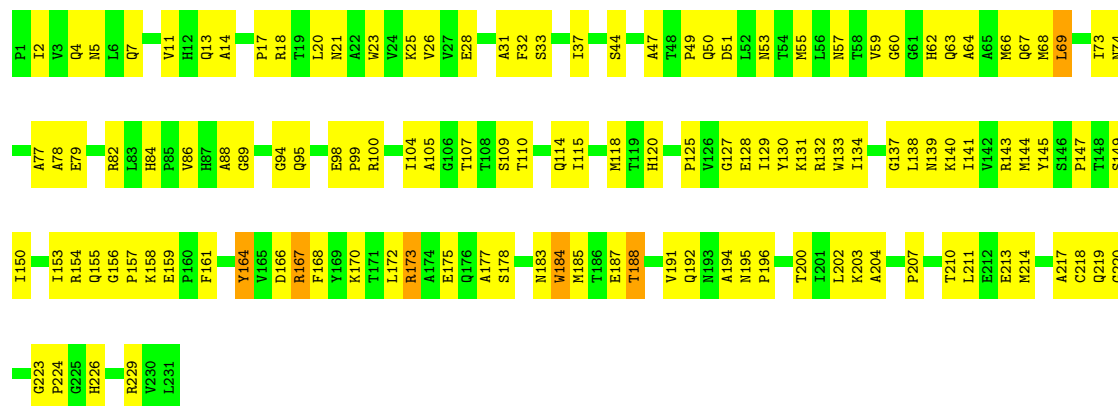
Chain hR: 41% 55%





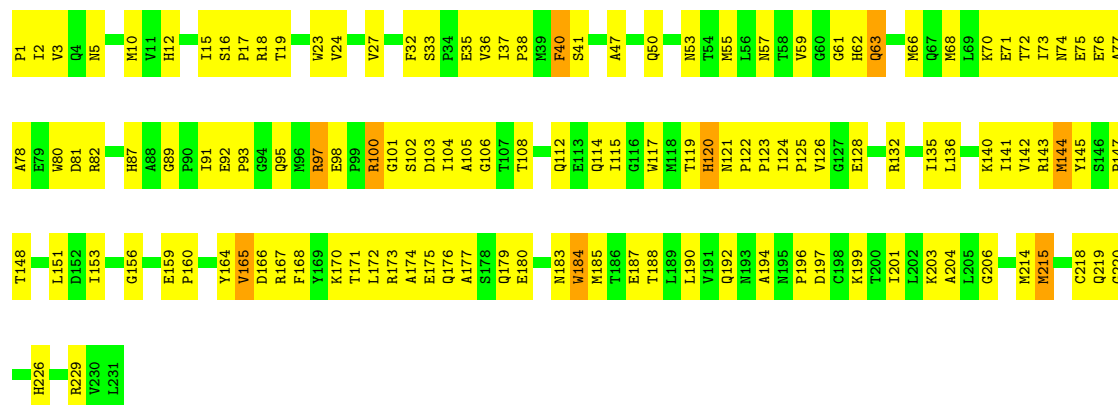
- Molecule 1: capsid protein

Chain hS: 46% 52%



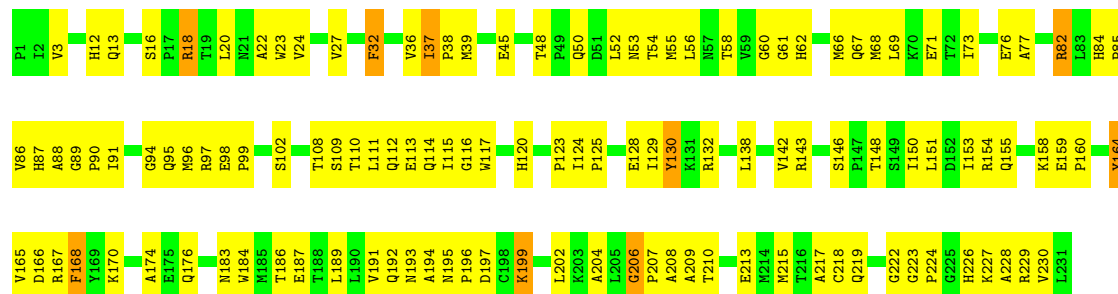
- Molecule 1: capsid protein

Chain hT: 45% 51%



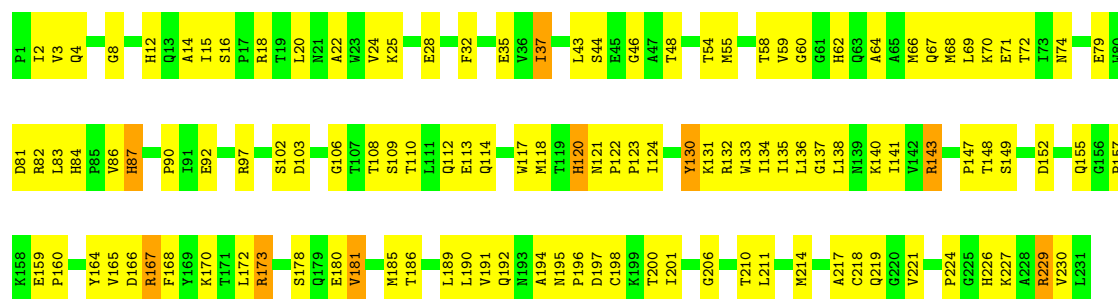
- Molecule 1: capsid protein

Chain 1M: 47% 49%



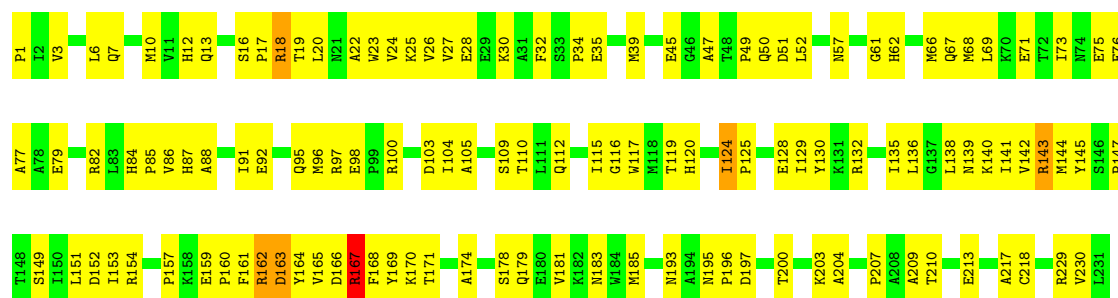
- Molecule 1: capsid protein

Chain hU: 

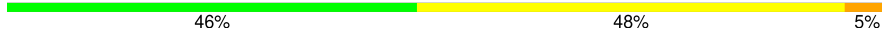


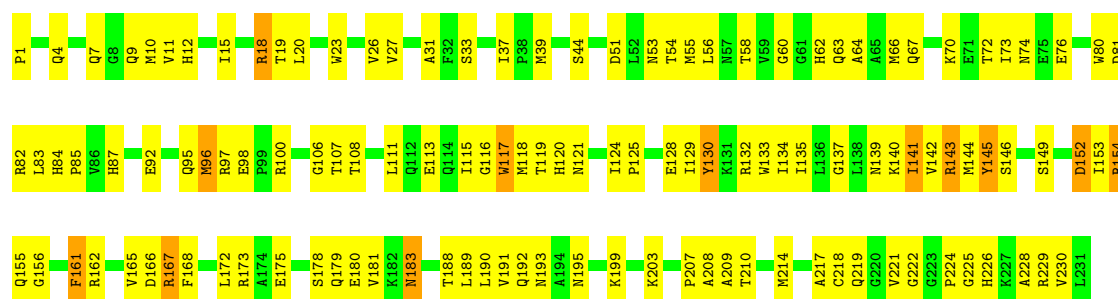
• Molecule 1: capsid protein

Chain hV: 



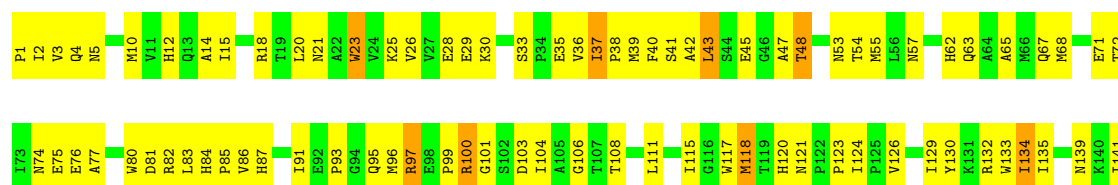
• Molecule 1: capsid protein

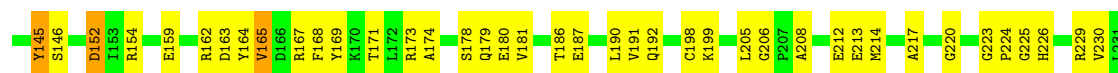
Chain hW: 



• Molecule 1: capsid protein

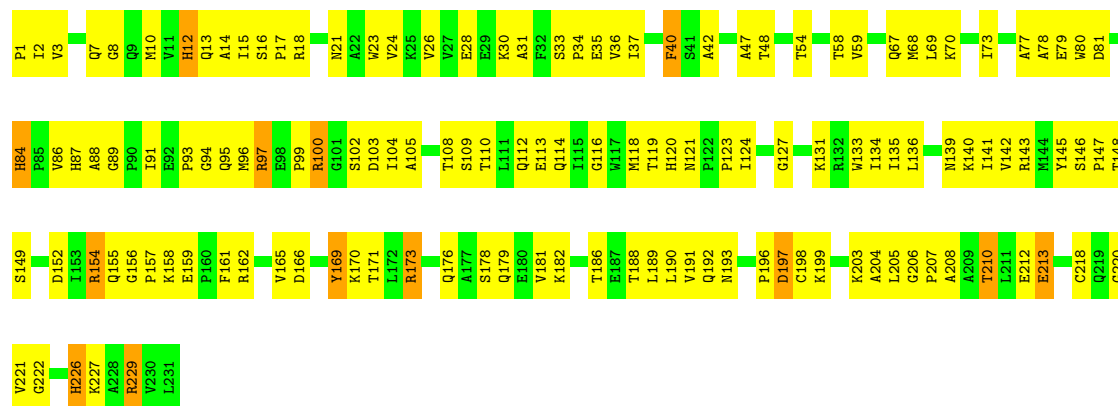
Chain hX: 





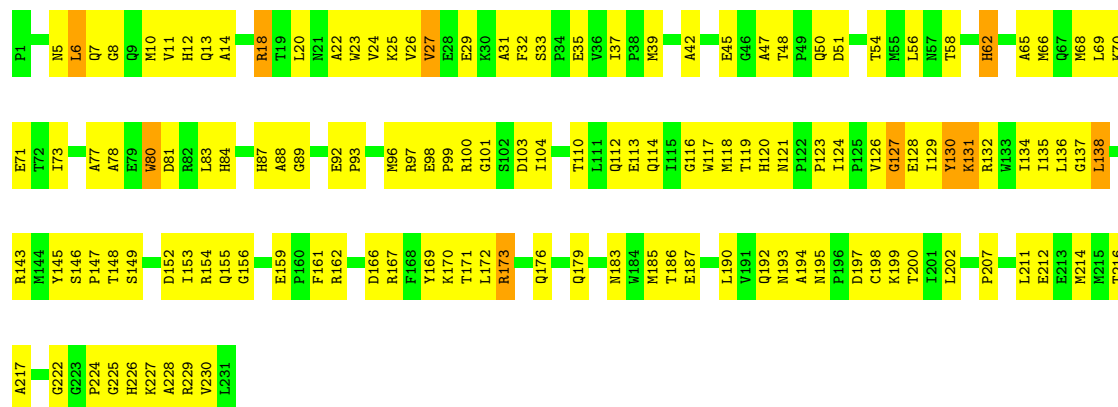
• Molecule 1: capsid protein

Chain hY: 42% 53% 6%



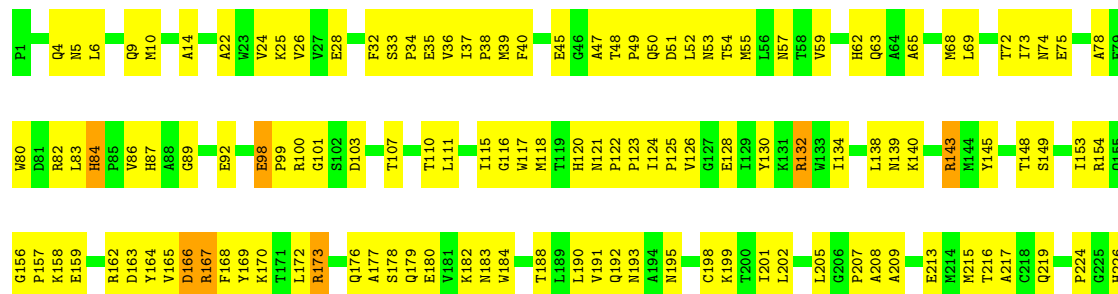
• Molecule 1: capsid protein

Chain hZ: 42% 54% .



• Molecule 1: capsid protein

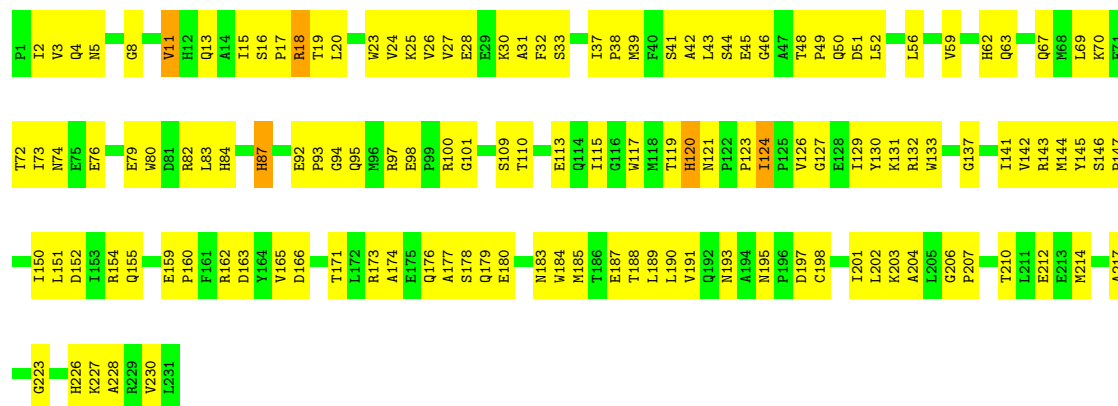
Chain i0: 45% 52% .





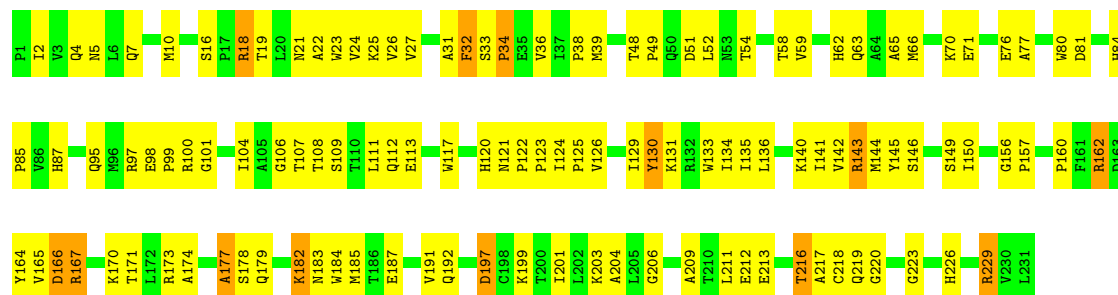
- Molecule 1: capsid protein

Chain i1: 42% 55% .



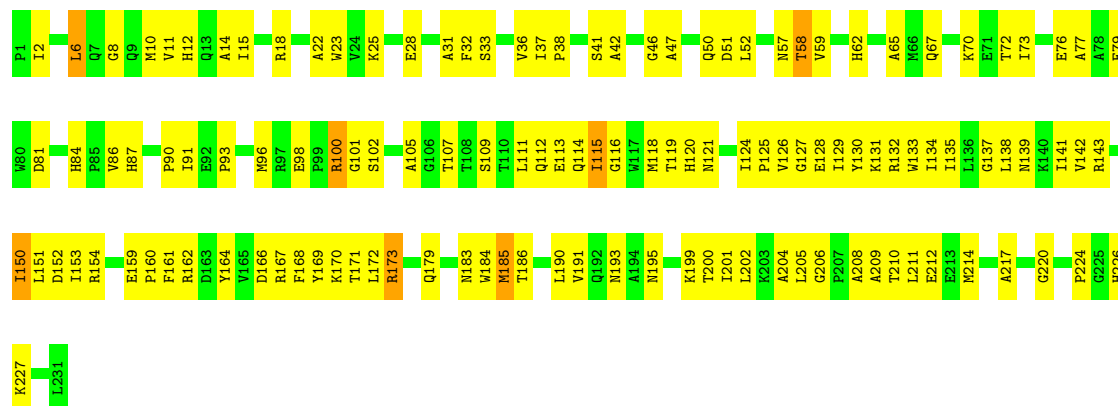
- Molecule 1: capsid protein

Chain i2: 48% 46% 6%

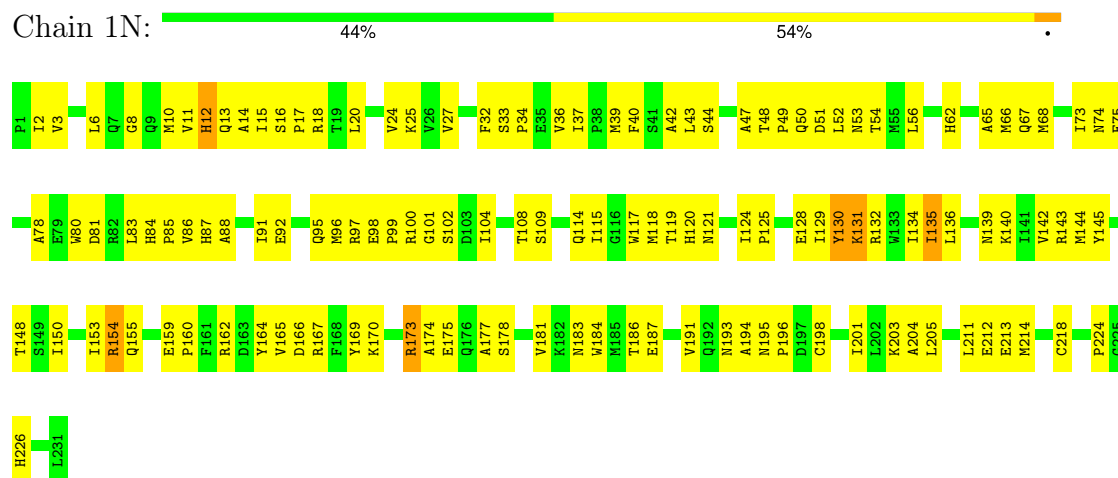


- Molecule 1: capsid protein

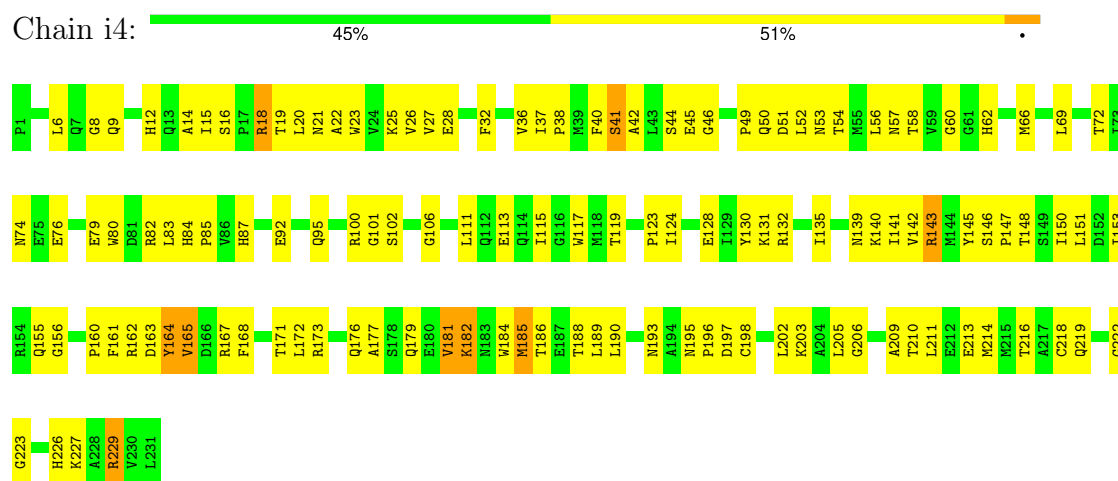
Chain i3: 45% 52% .



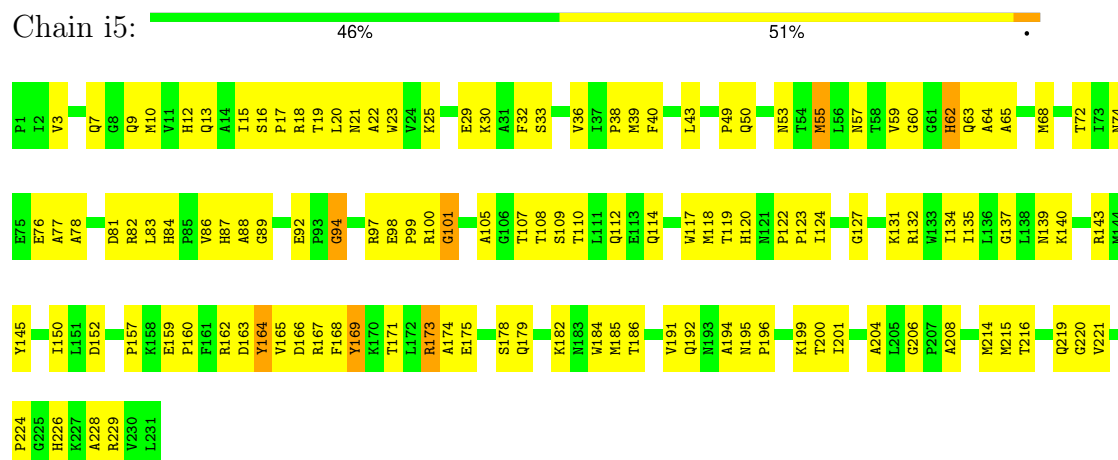
- Molecule 1: capsid protein



- Molecule 1: capsid protein

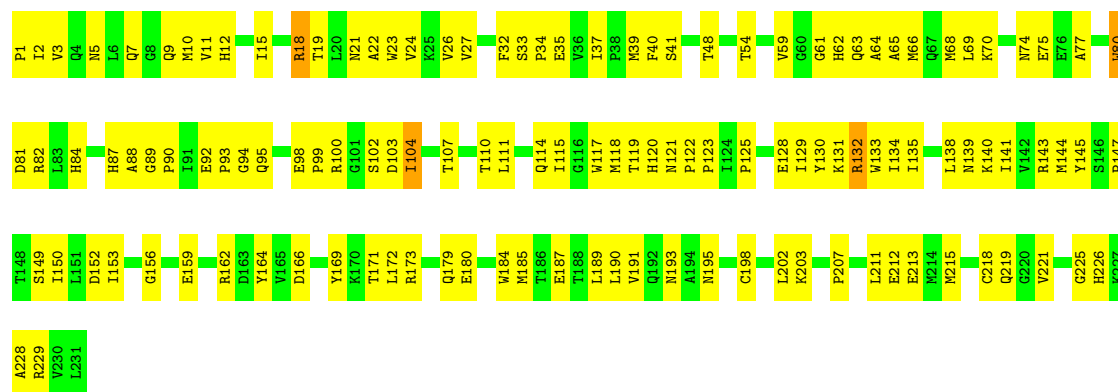


- Molecule 1: capsid protein



- Molecule 1: capsid protein





• Molecule 1: capsid protein

Chain i7: 43% 53%



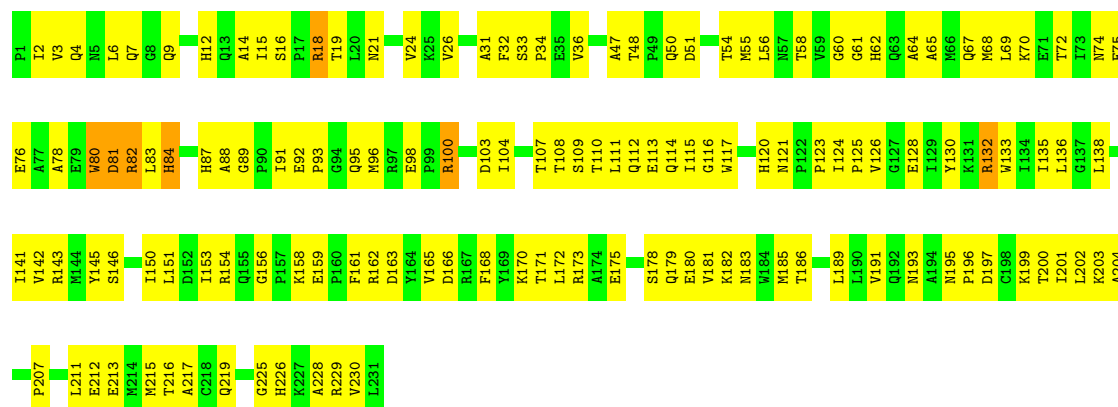
• Molecule 1: capsid protein

Chain i8: 41% 57%

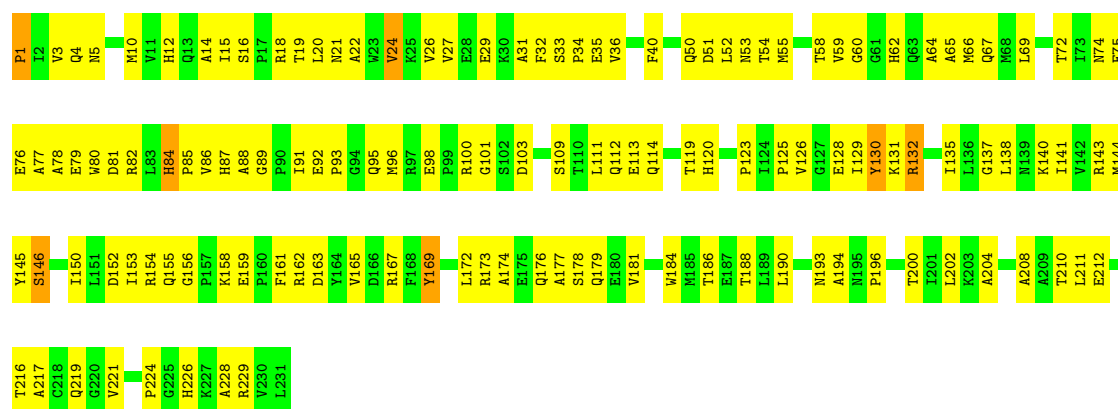


• Molecule 1: capsid protein

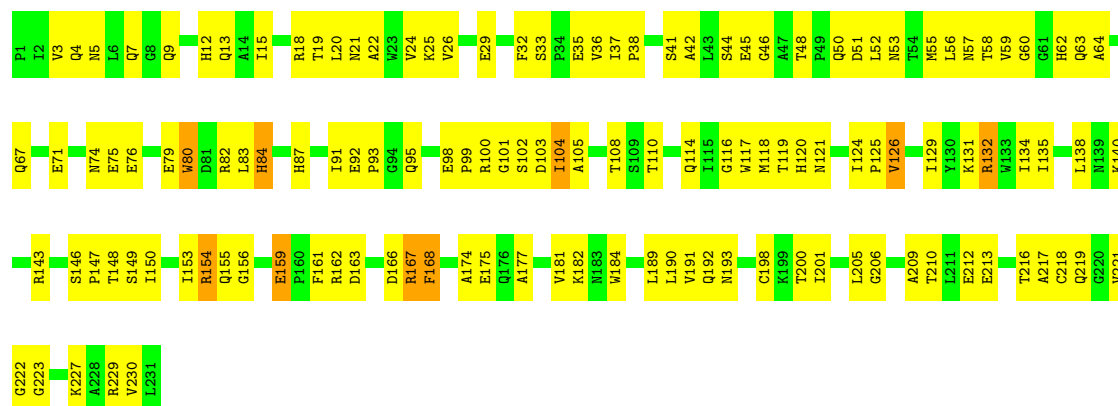
Chain i9: 40% 57%



- Molecule 1: capsid protein

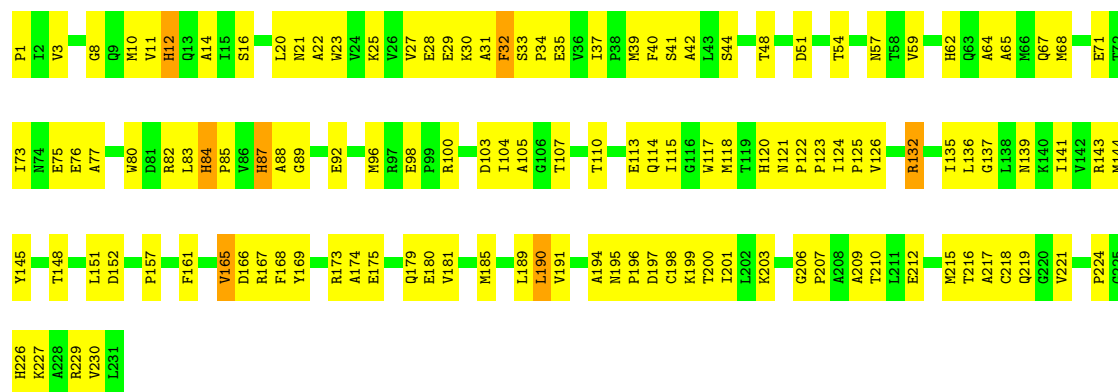


- Molecule 1: capsid protein

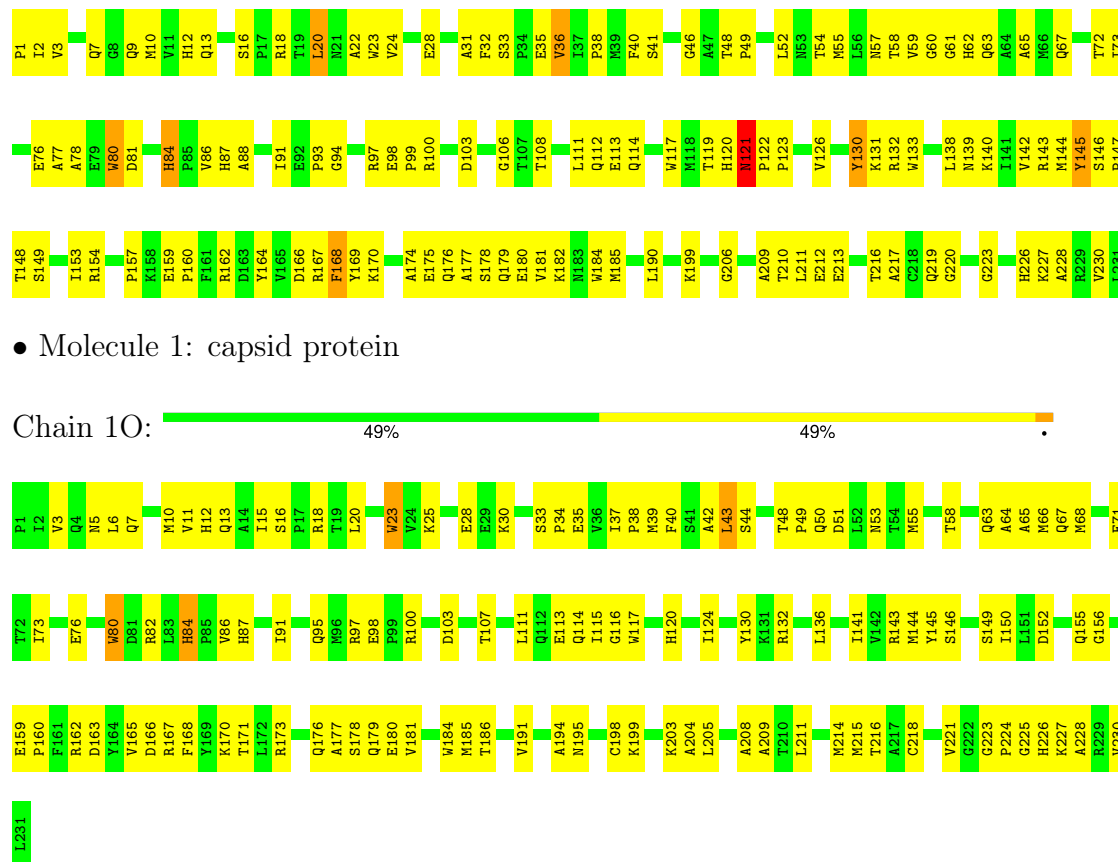


- Molecule 1: capsid protein



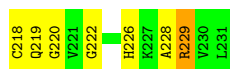


- Molecule 1: capsid protein



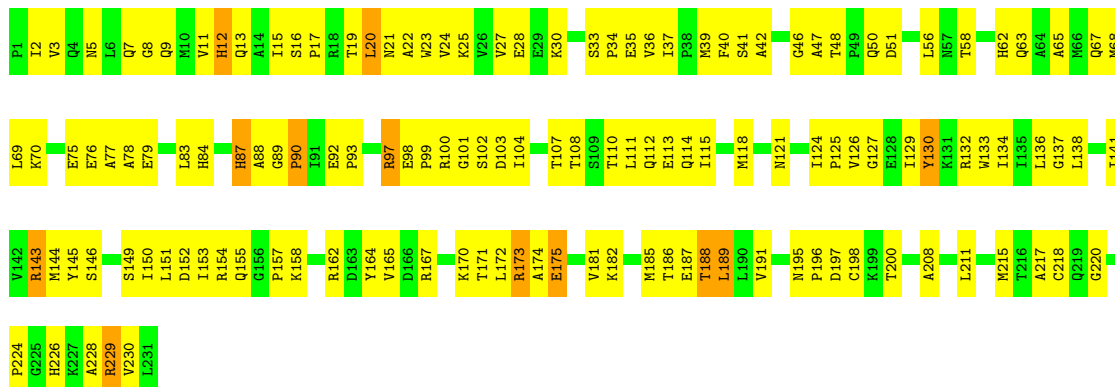
- Molecule 1: capsid protein





• Molecule 1: capsid protein

Chain ii: 41% 54% 5%



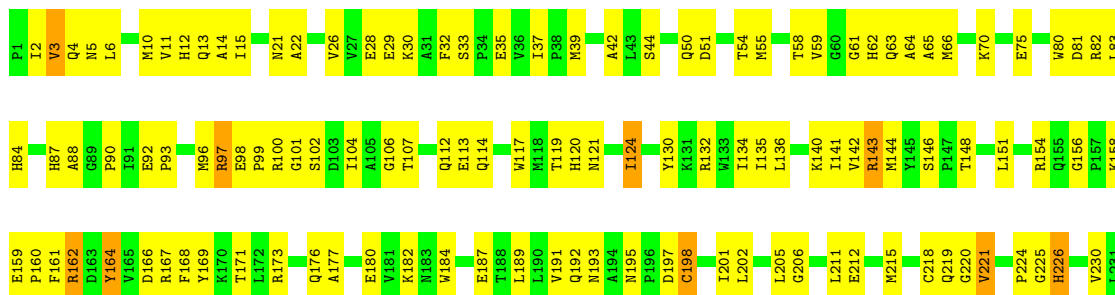
• Molecule 1: capsid protein

Chain ij: 44% 51% 5%

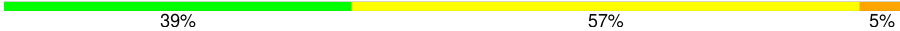


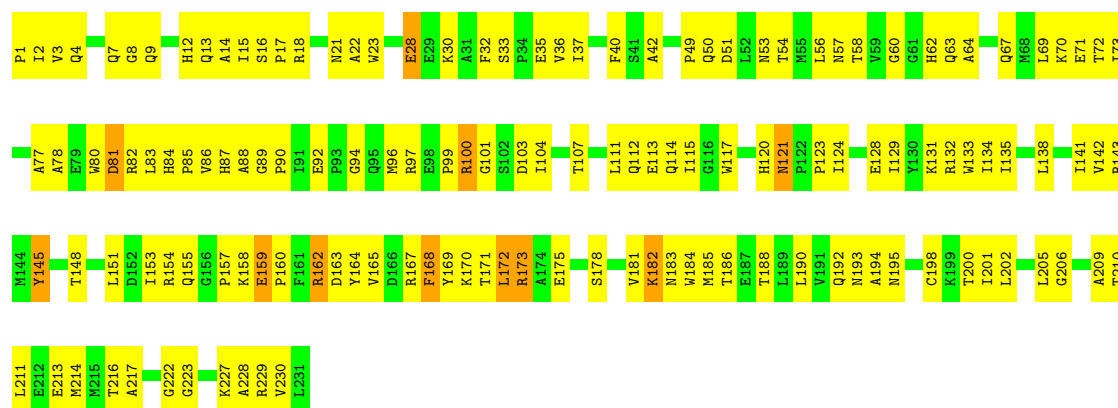
• Molecule 1: capsid protein

Chain ik: 48% 48% 4%

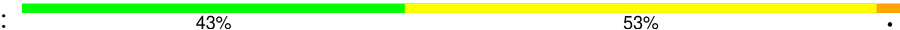


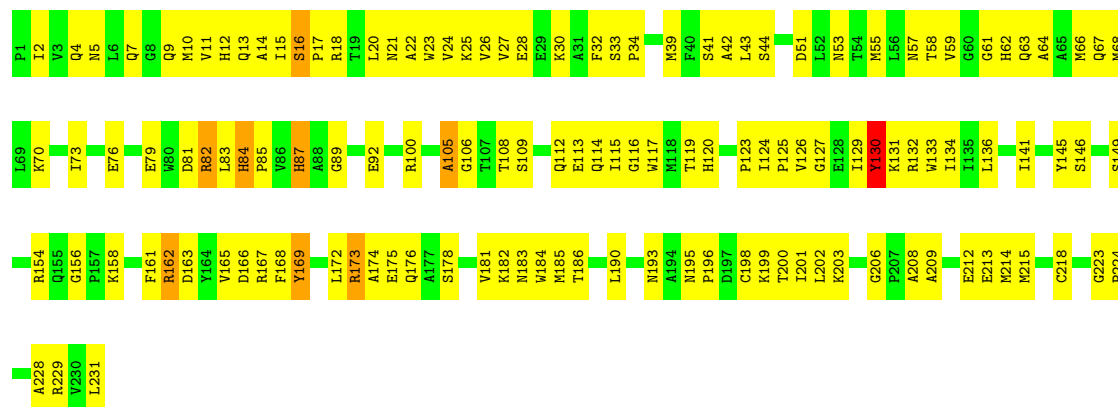
• Molecule 1: capsid protein

Chain il: 

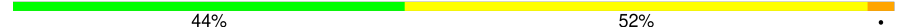


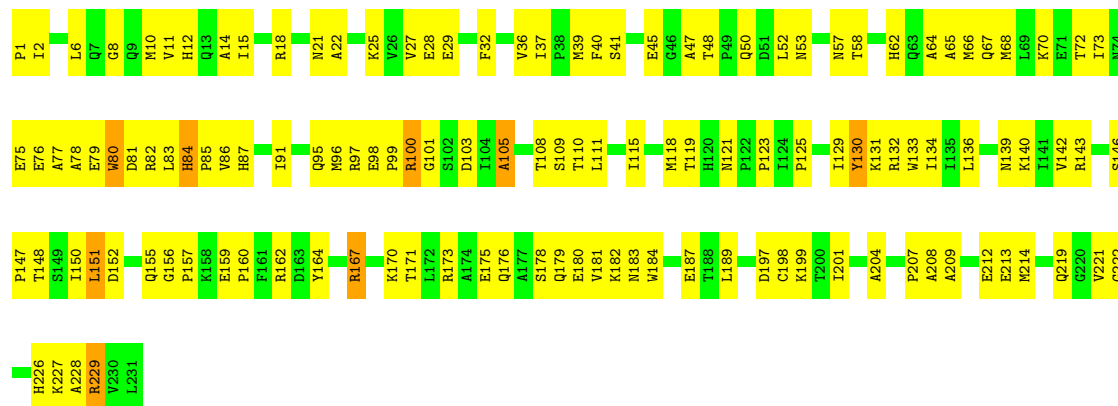
• Molecule 1: capsid protein

Chain im: 



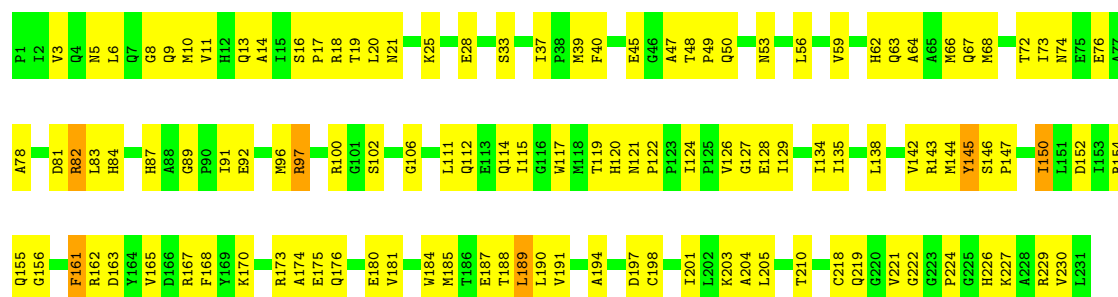
• Molecule 1: capsid protein

Chain in: 



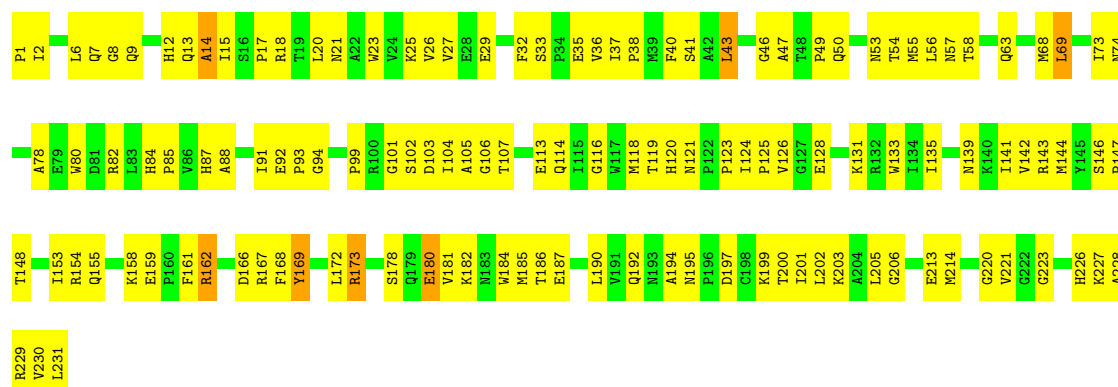
• Molecule 1: capsid protein

Chain 1P: 



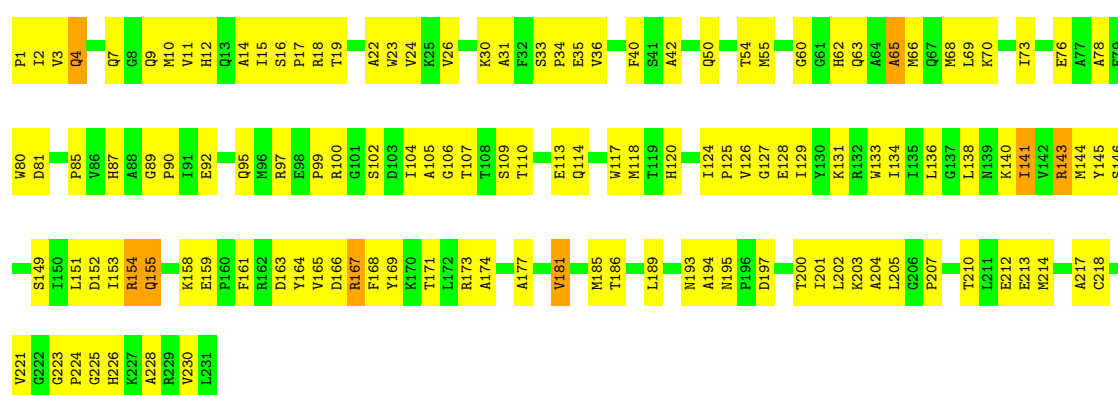
• Molecule 1: capsid protein

Chain io: 



• Molecule 1: capsid protein

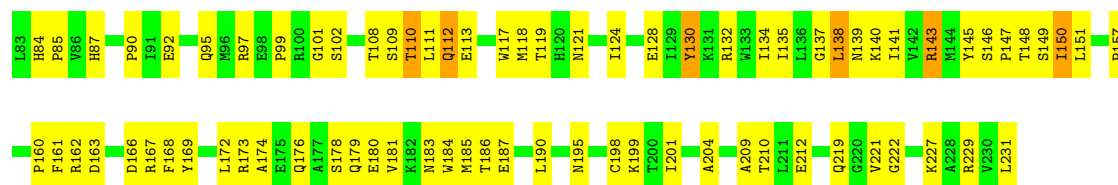
Chain ip: 



• Molecule 1: capsid protein

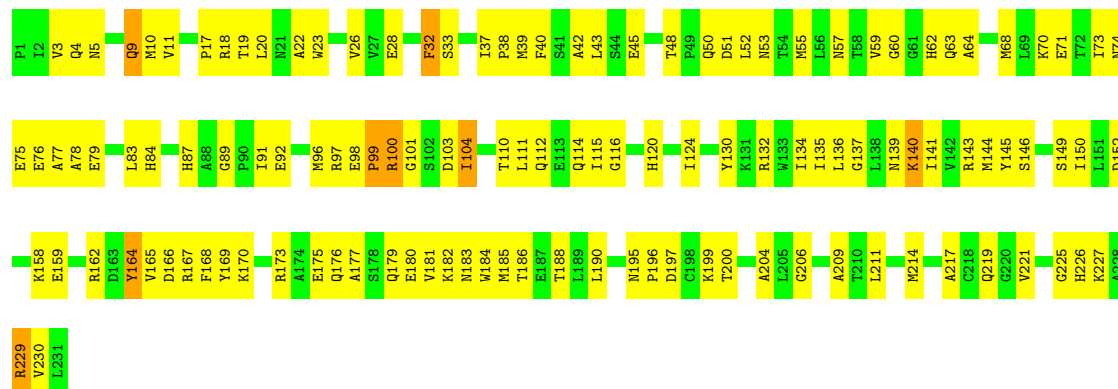
Chain iq: 





• Molecule 1: capsid protein

Chain ir: 46% 51%



• Molecule 1: capsid protein

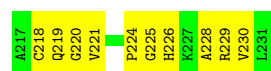
Chain is: 51% 47%



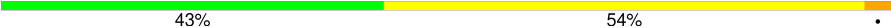
• Molecule 1: capsid protein

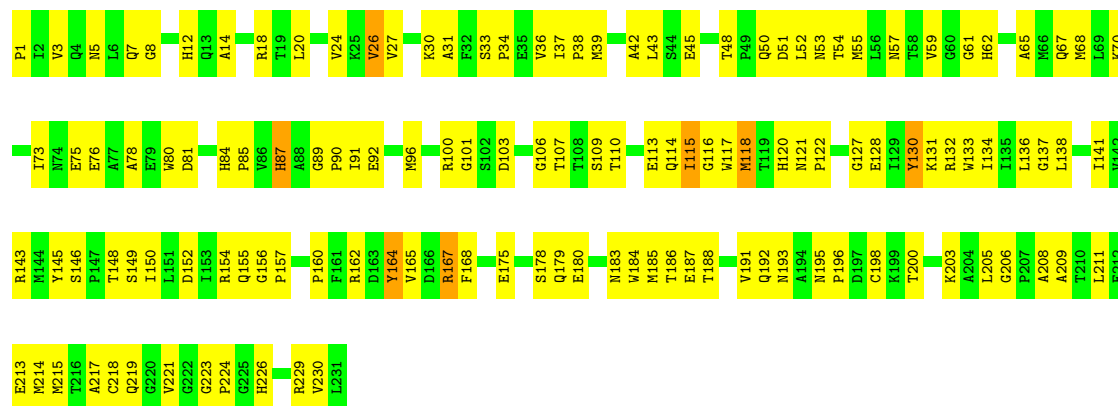
Chain it: 39% 57%



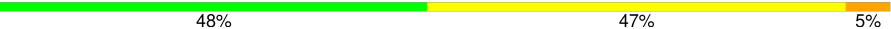


- Molecule 1: capsid protein

Chain iu:  43% 54%



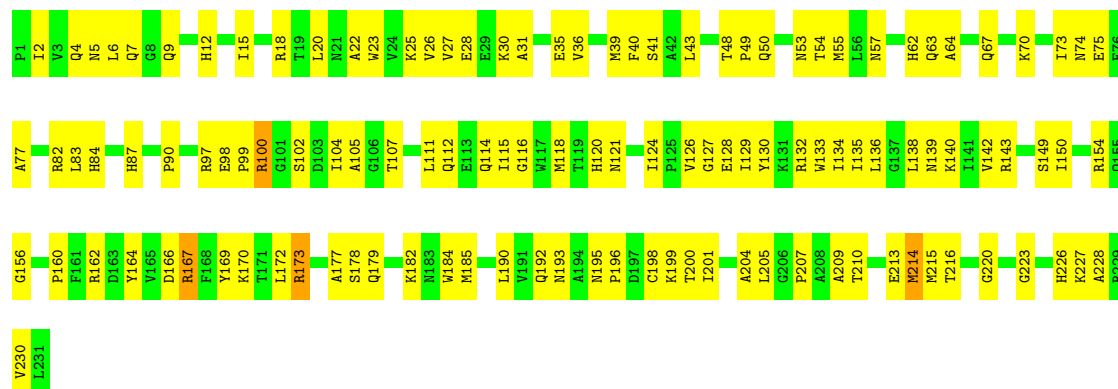
- Molecule 1: capsid protein

Chain iv:  48% 47% 5%

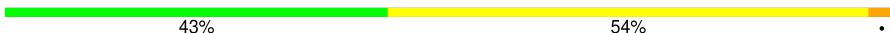


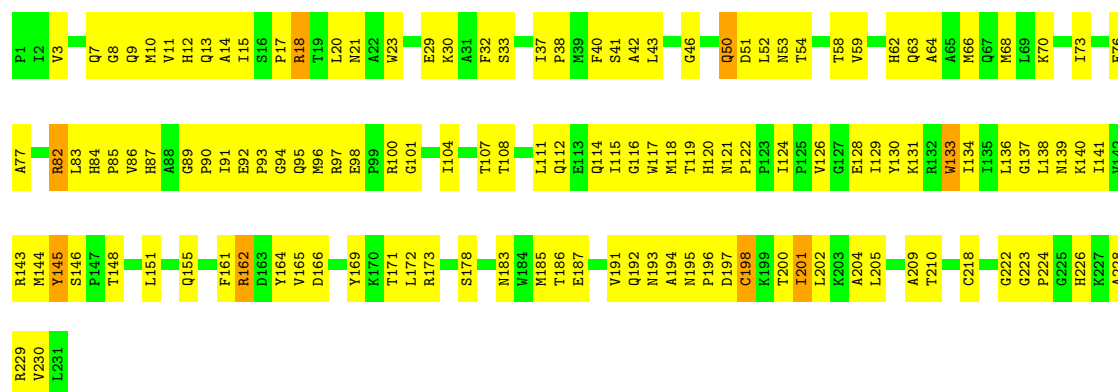
- Molecule 1: capsid protein

Chain iw:  48% 50%



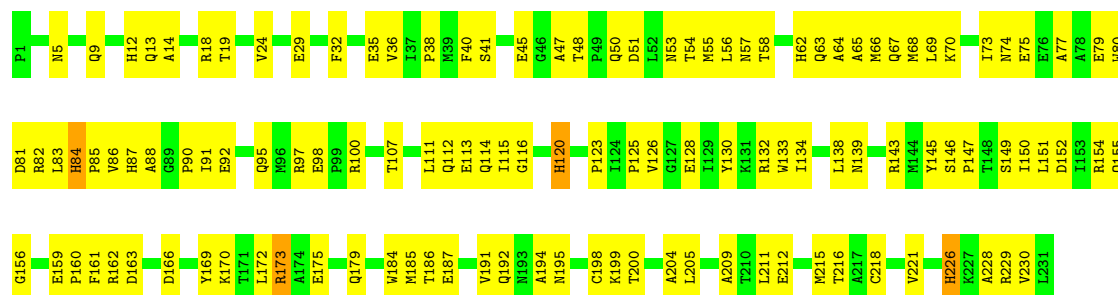
- Molecule 1: capsid protein

Chain ix:  43% 54%

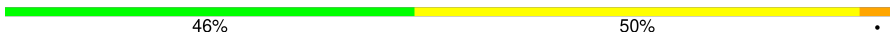


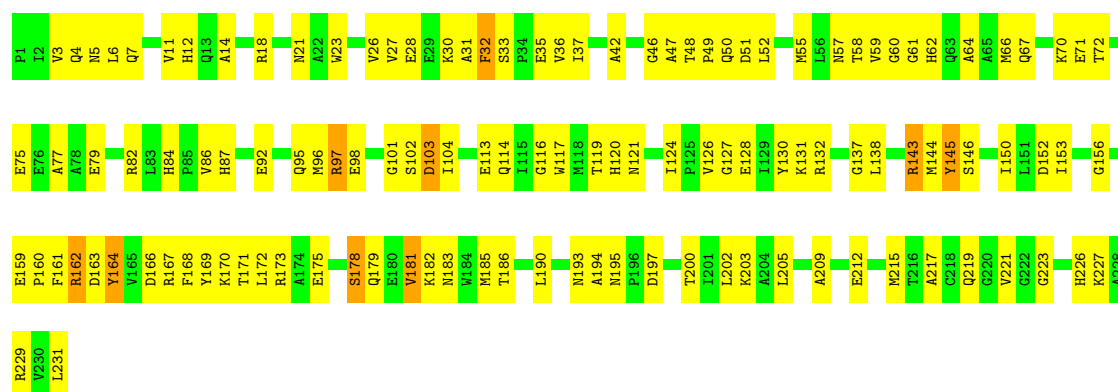
• Molecule 1: capsid protein

Chain 1Q:  48% 51%

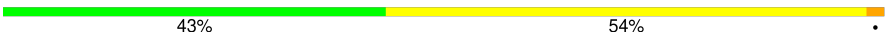


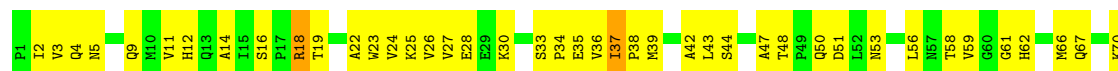
• Molecule 1: capsid protein

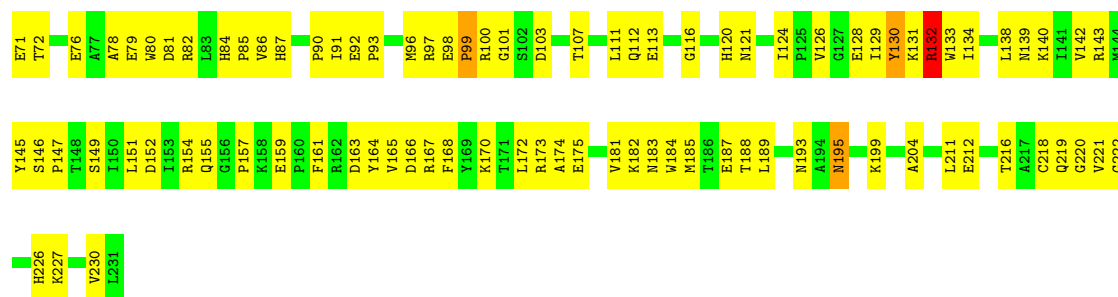
Chain iy:  46% 50%



• Molecule 1: capsid protein

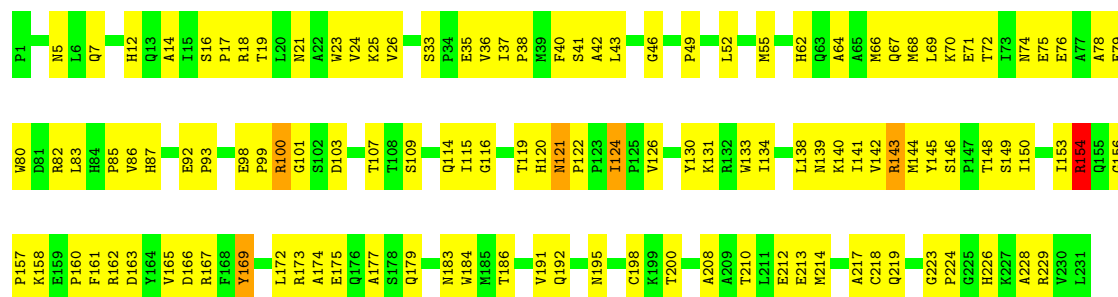
Chain iz:  43% 54%





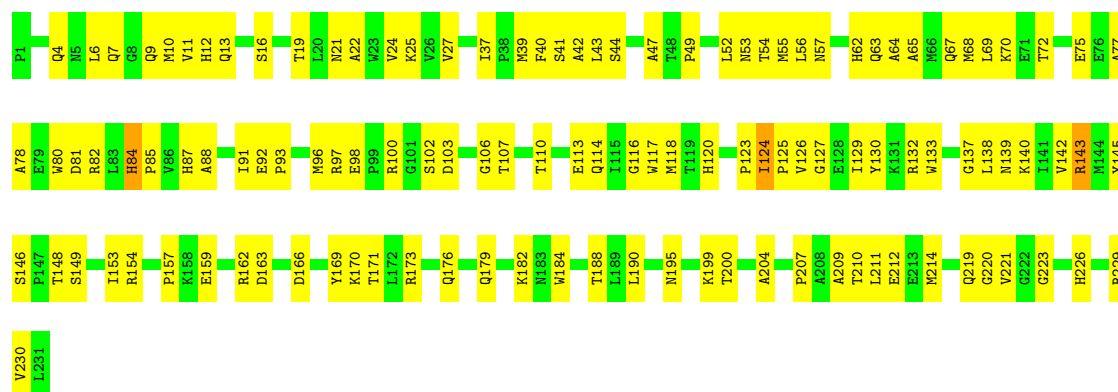
• Molecule 1: capsid protein

Chain iA: 48% 49%



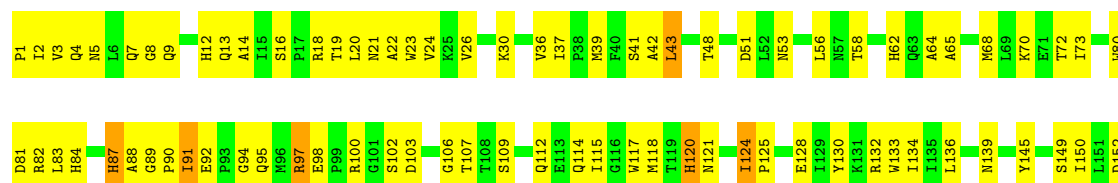
• Molecule 1: capsid protein

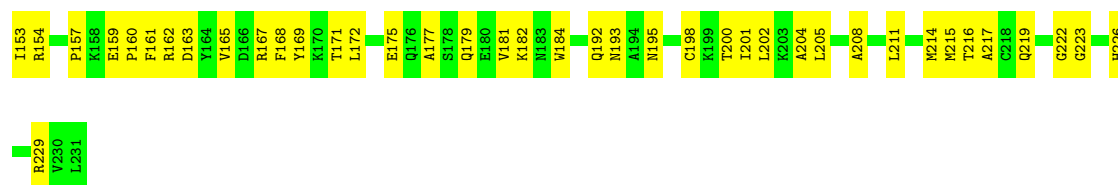
Chain iB: 48% 51%



• Molecule 1: capsid protein

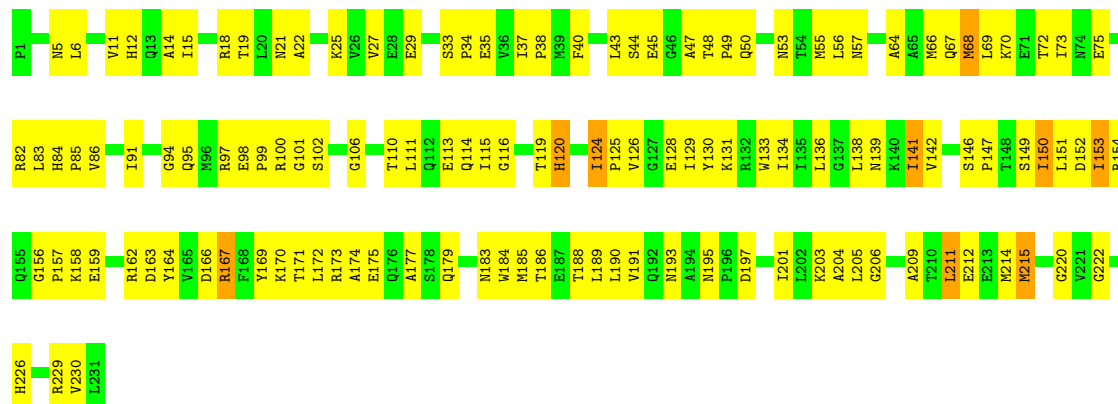
Chain iC: 48% 49%





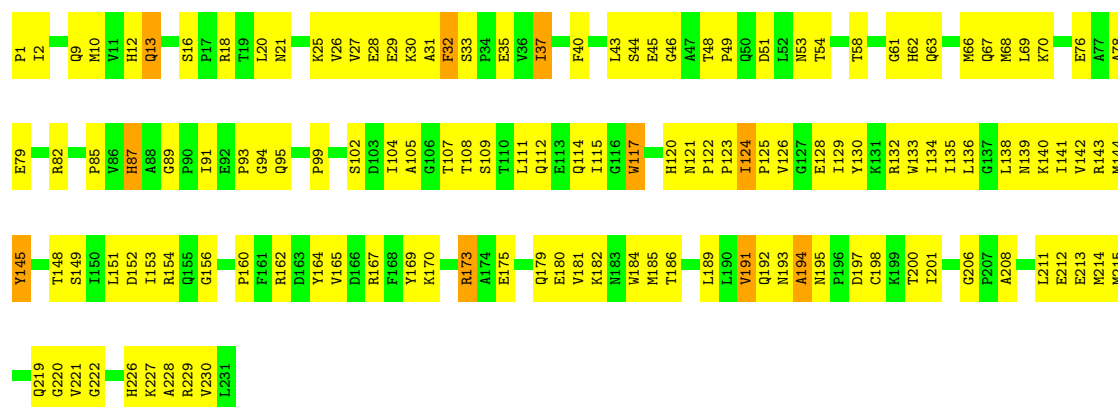
- Molecule 1: capsid protein

Chain iD:



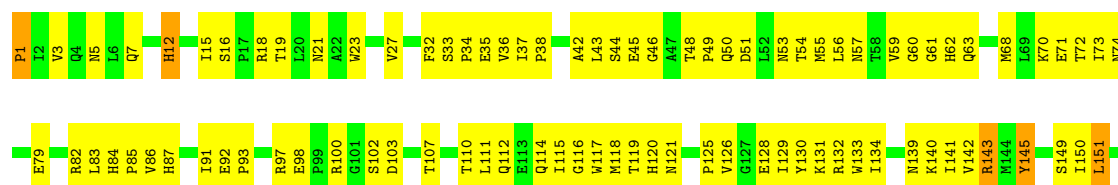
- Molecule 1: capsid protein

Chain iE:



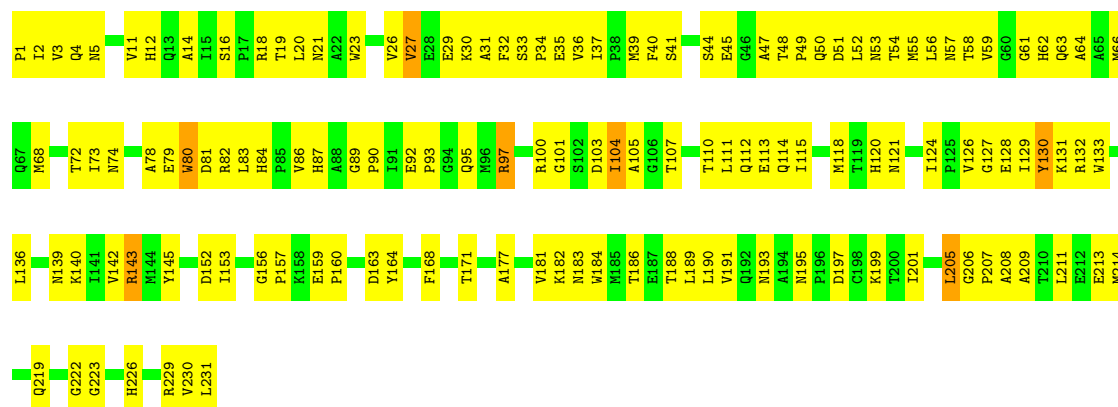
- Molecule 1: capsid protein

Chain iF:

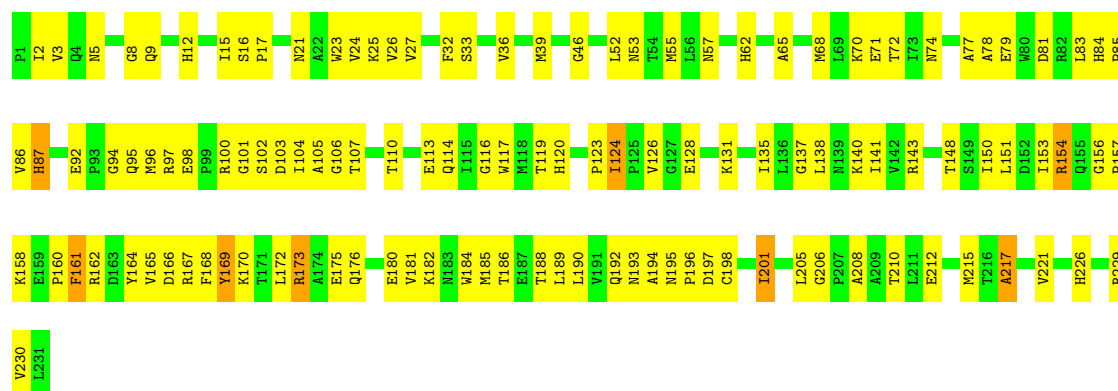




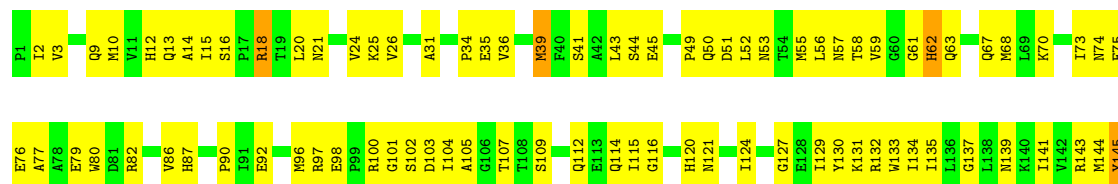
• Molecule 1: capsid protein

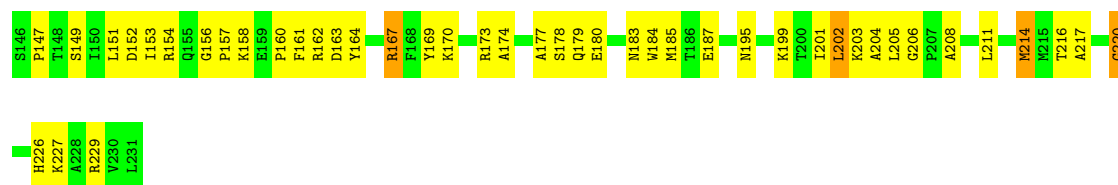


• Molecule 1: capsid protein



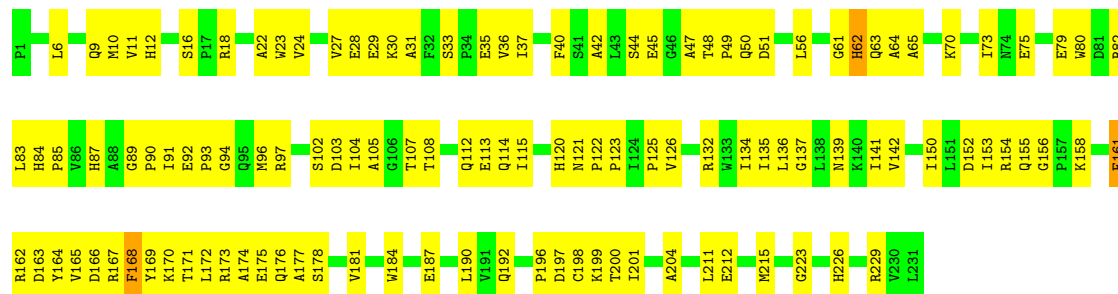
• Molecule 1: capsid protein





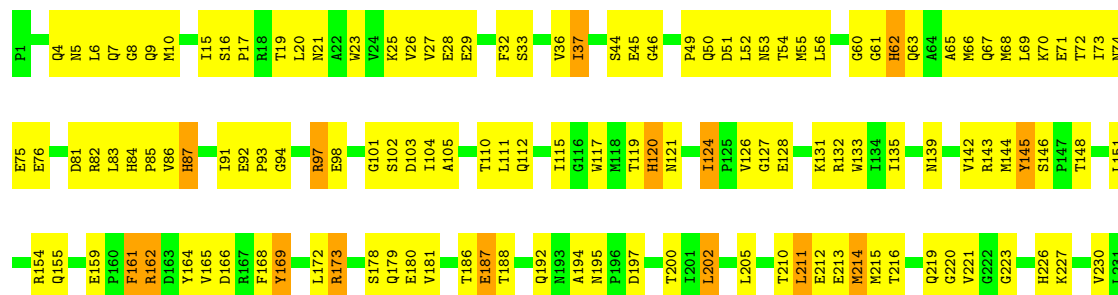
- Molecule 1: capsid protein

Chain iL: 48% 50% .



- Molecule 1: capsid protein

Chain iJ: 43% 51% 6% .



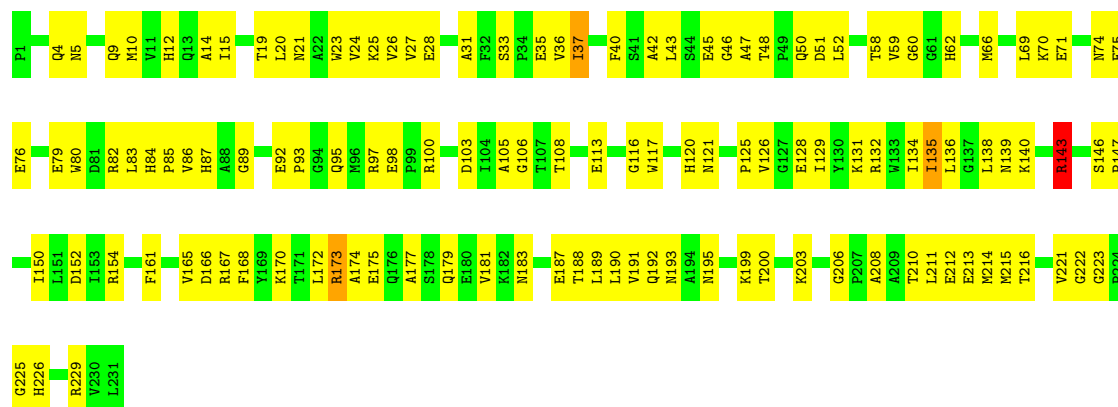
- Molecule 1: capsid protein

Chain iK: 47% 51% .



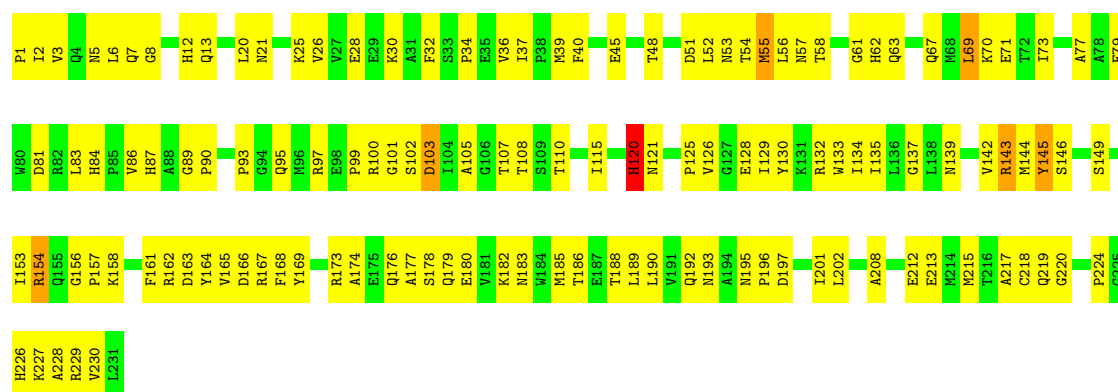
- Molecule 1: capsid protein

Chain iL: 46% 52% .



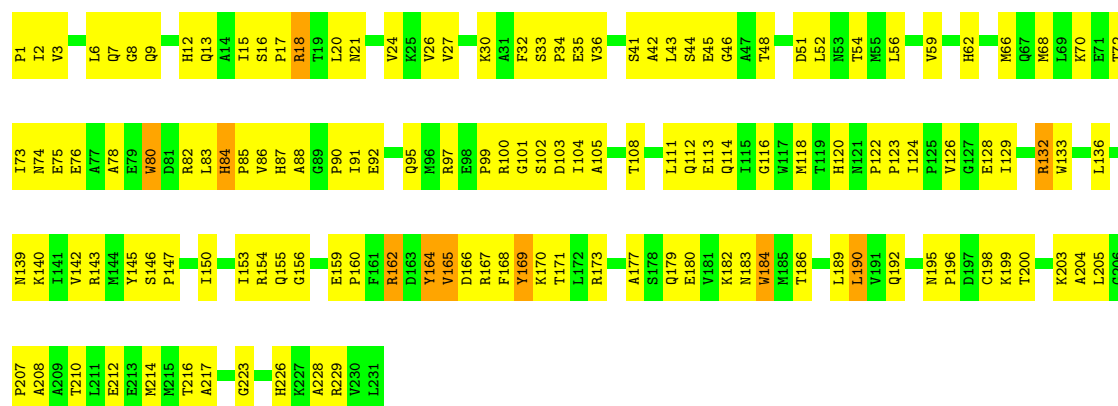
• Molecule 1: capsid protein

Chain iM: 44% 53%



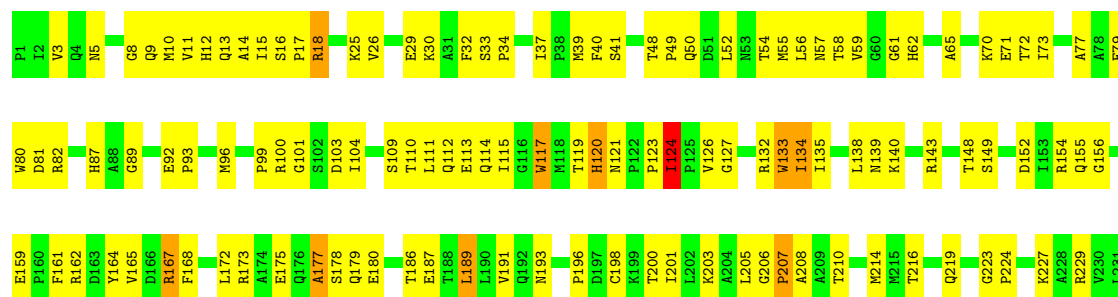
• Molecule 1: capsid protein

Chain iN: 41% 55%



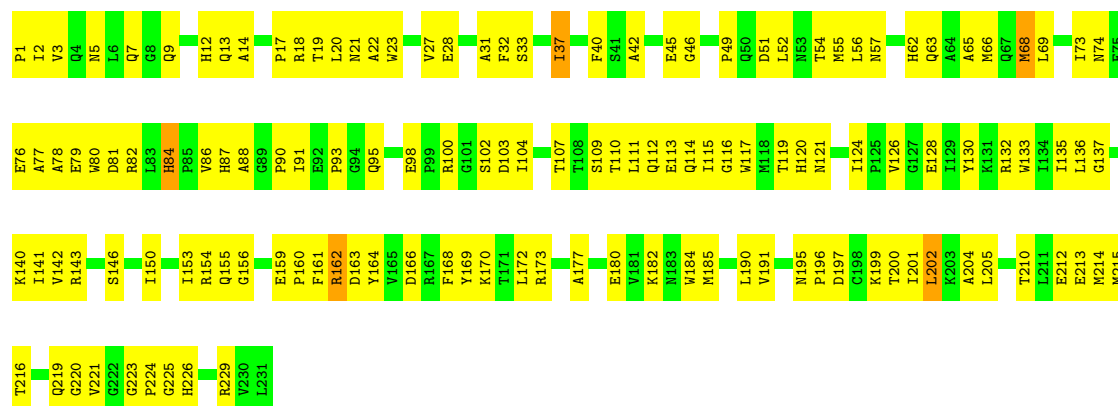
• Molecule 1: capsid protein

Chain iO: 48% 48%



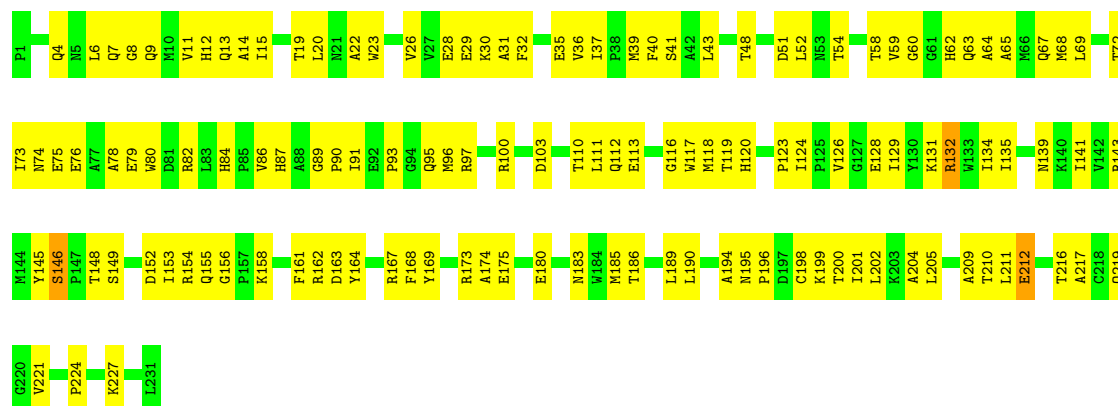
- Molecule 1: capsid protein

Chain iP: .



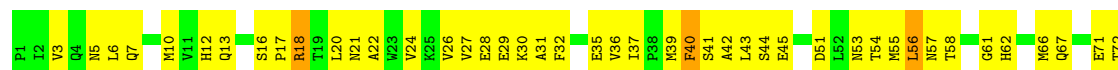
- Molecule 1: capsid protein

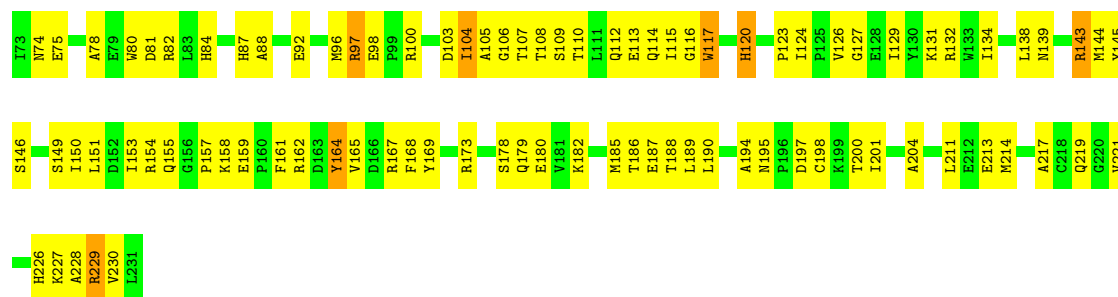
Chain iQ: .



- Molecule 1: capsid protein

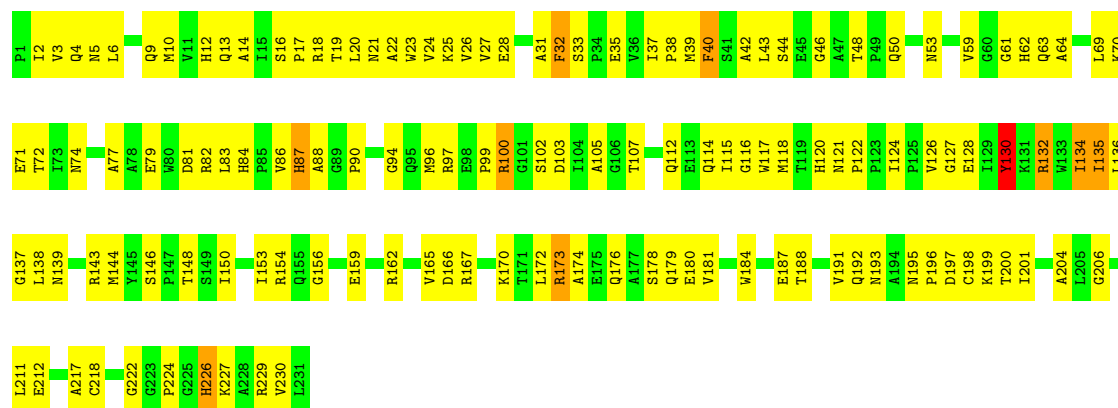
Chain iR: .





• Molecule 1: capsid protein

Chain 1S: 42% 54%



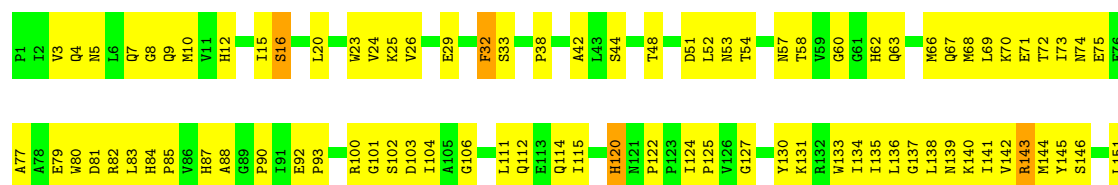
• Molecule 1: capsid protein

Chain iS: 47% 48% 6%



• Molecule 1: capsid protein

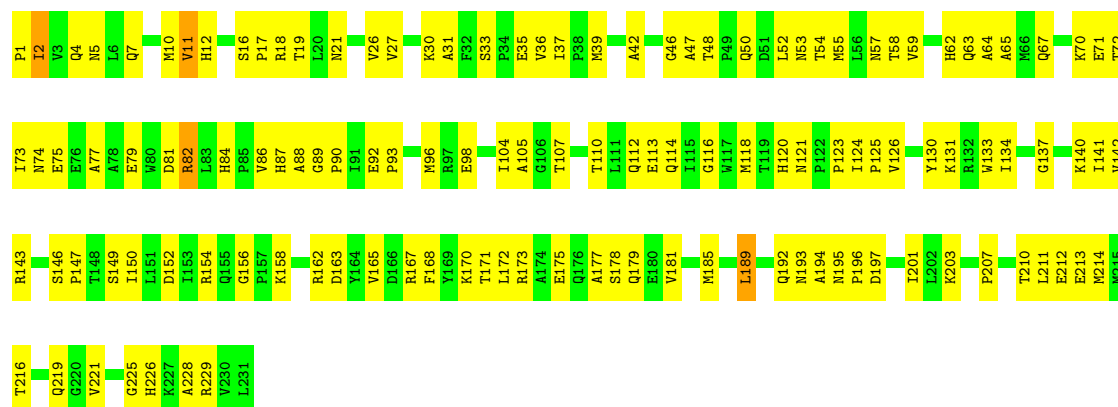
Chain iT: 42% 55%





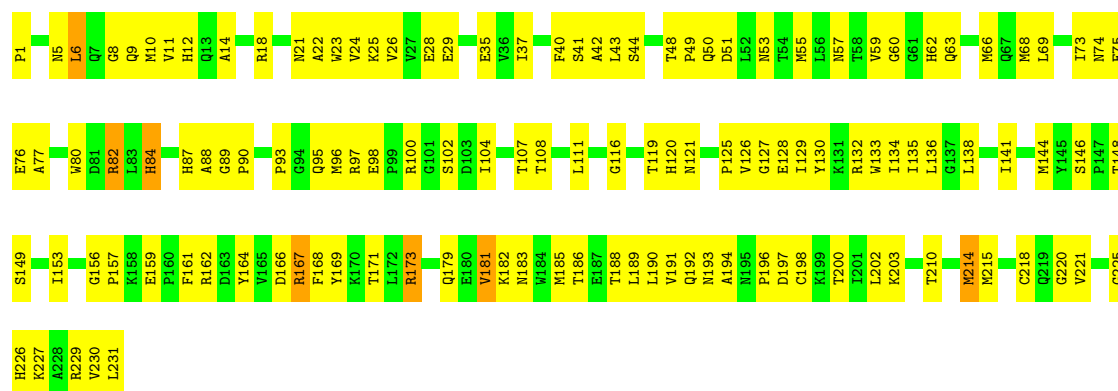
• Molecule 1: capsid protein

Chain iU: 45% 54%



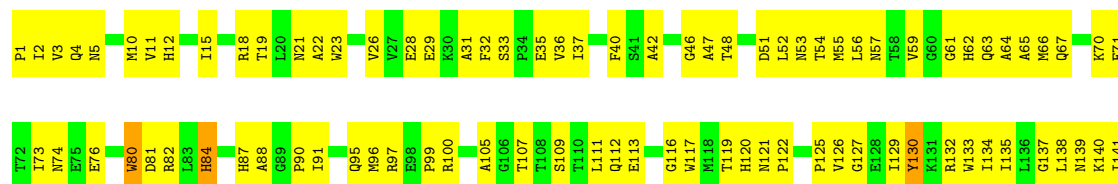
• Molecule 1: capsid protein

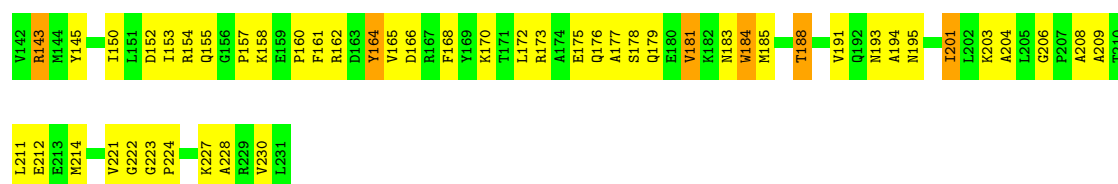
Chain iV: 45% 52%



• Molecule 1: capsid protein

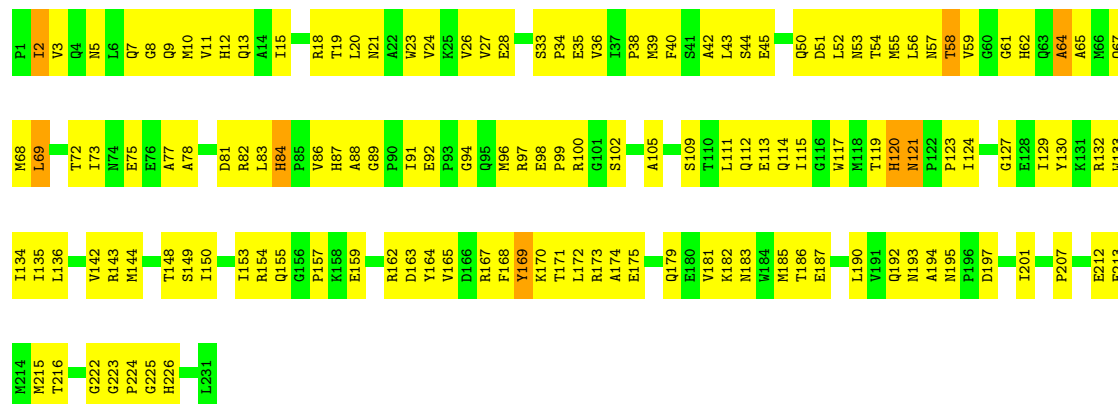
Chain iW: 41% 55%





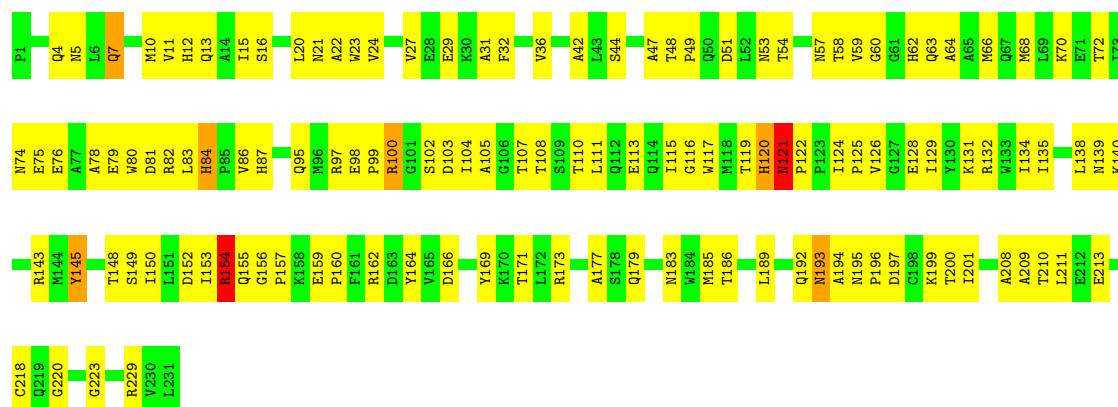
- Molecule 1: capsid protein

Chain iX: 40% 57%



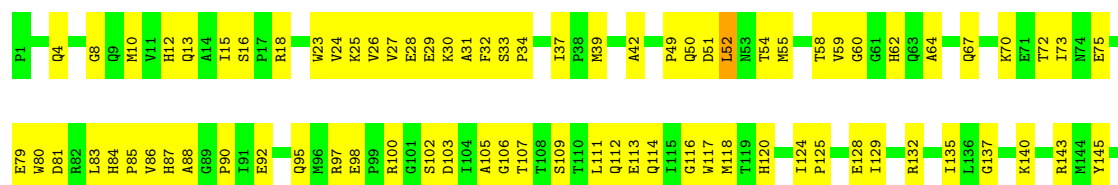
- Molecule 1: capsid protein

Chain iY: 45% 51%



- Molecule 1: capsid protein

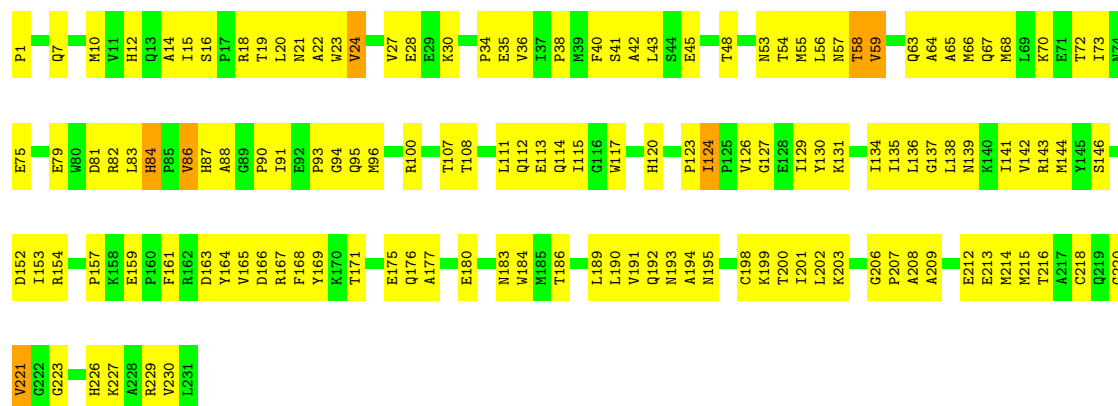
Chain iZ: 48% 50%





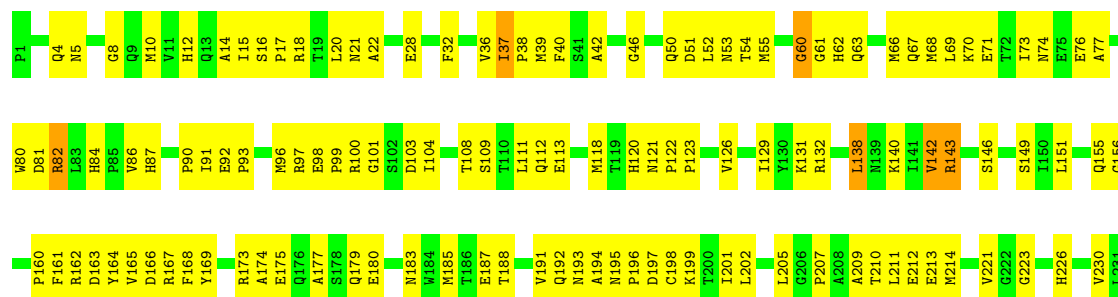
• Molecule 1: capsid protein

Chain j0: 41% 56%



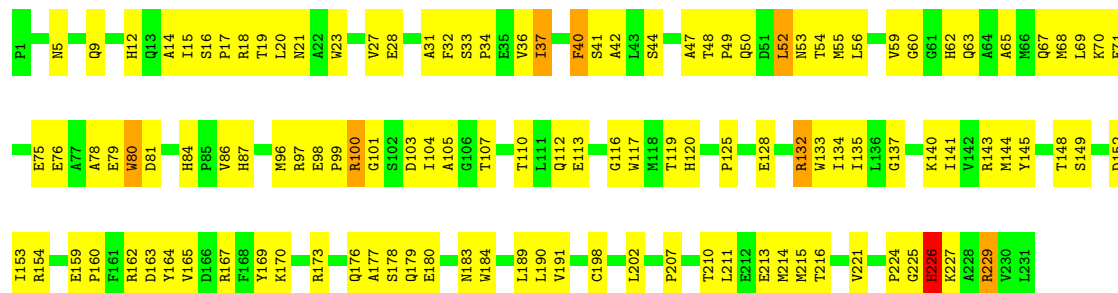
• Molecule 1: capsid protein

Chain j1: 45% 52%

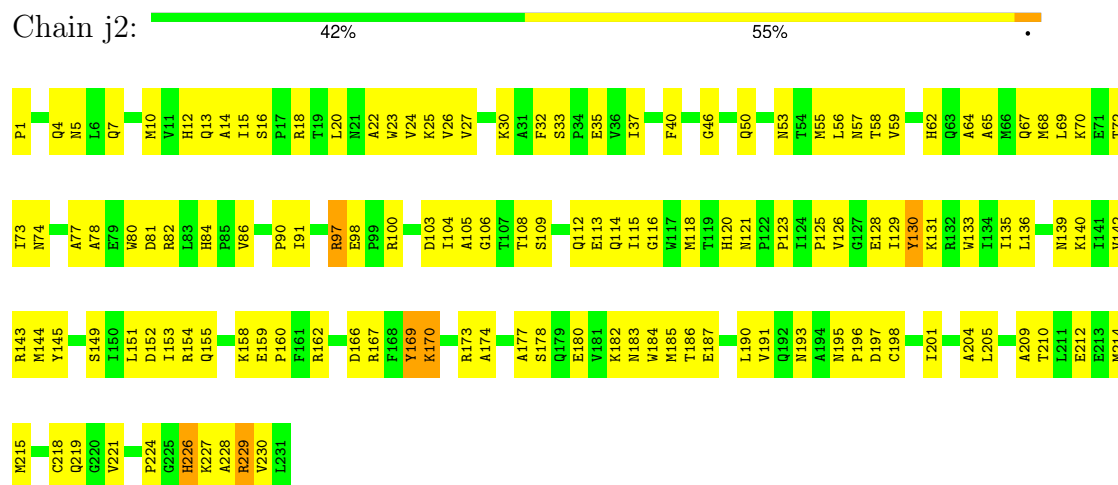


• Molecule 1: capsid protein

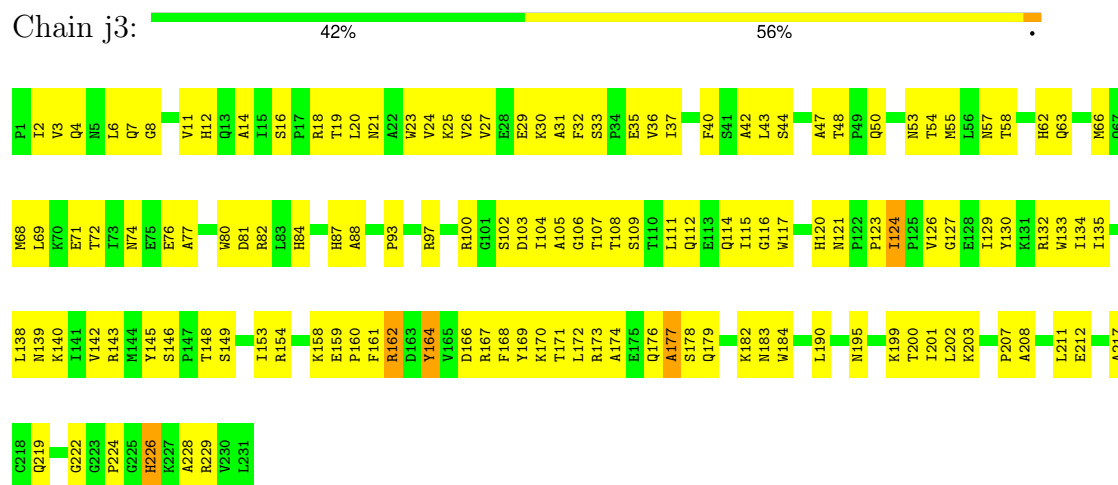
Chain 1T: 48% 49%



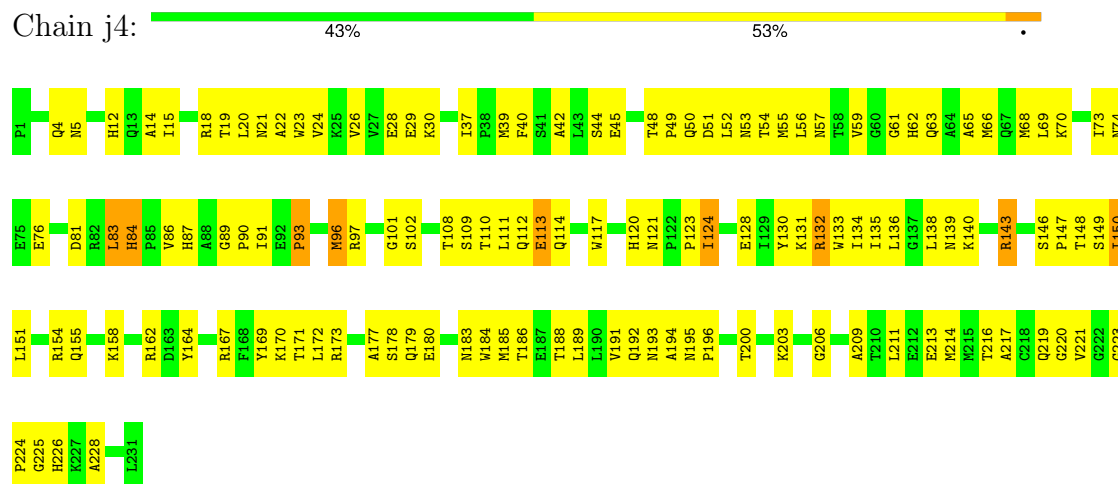
- Molecule 1: capsid protein



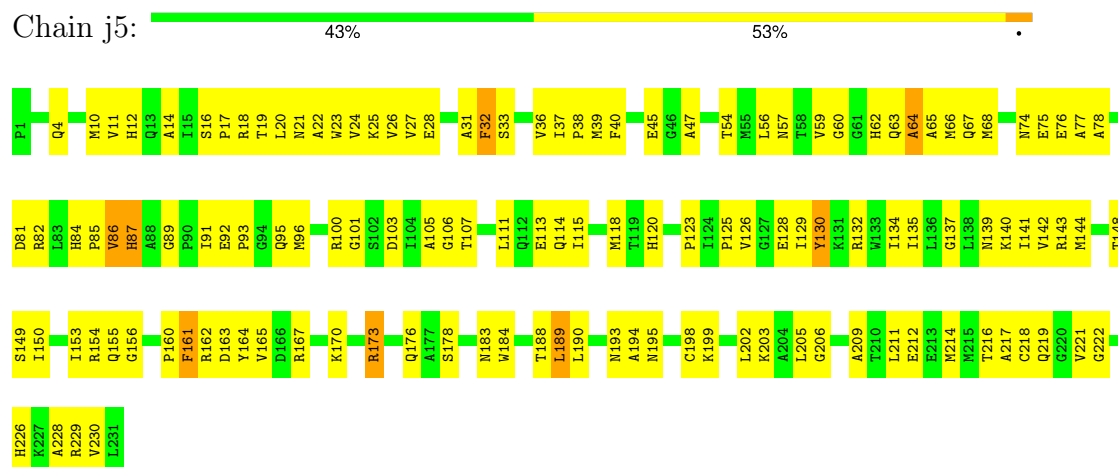
- Molecule 1: capsid protein



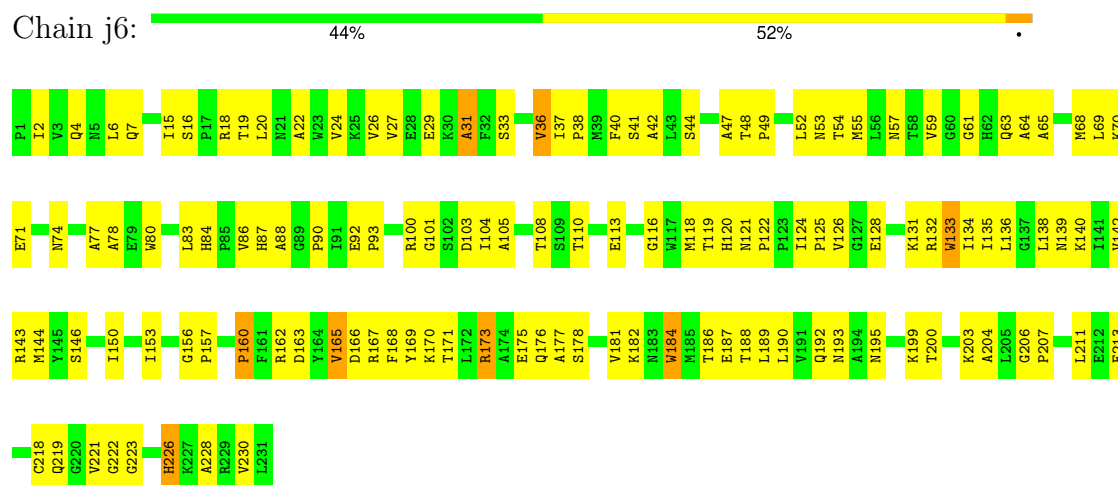
- Molecule 1: capsid protein



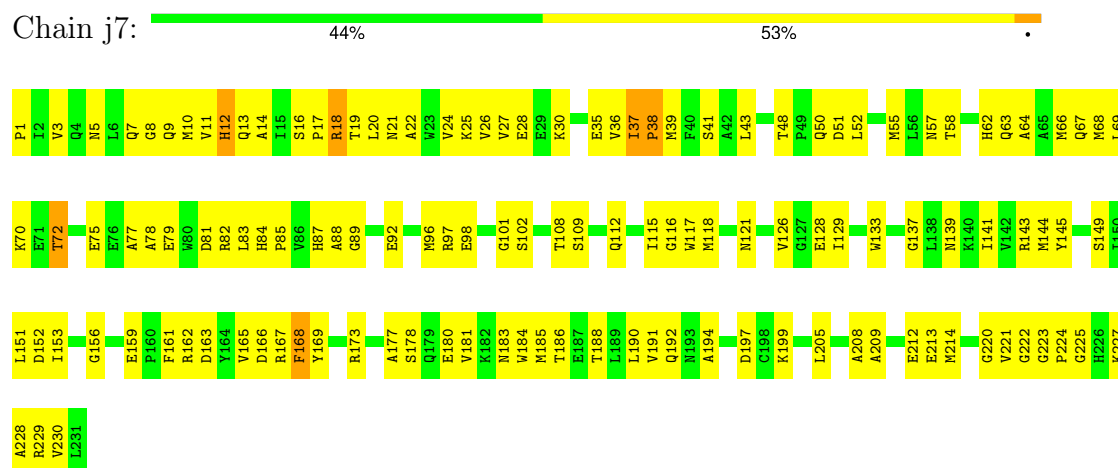
- Molecule 1: capsid protein



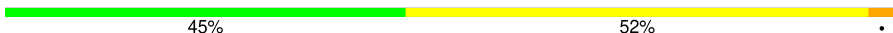
- Molecule 1: capsid protein

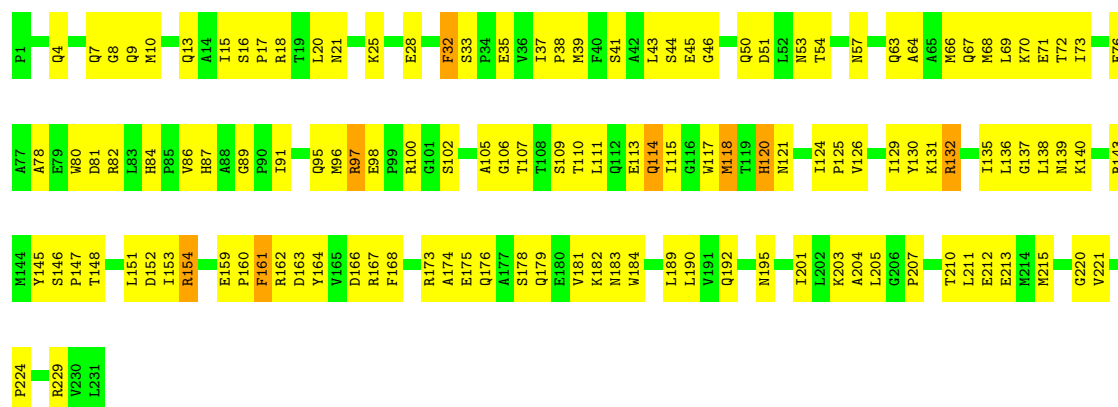


- Molecule 1: capsid protein

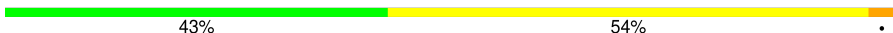


- Molecule 1: capsid protein

Chain j8:  45% 52%



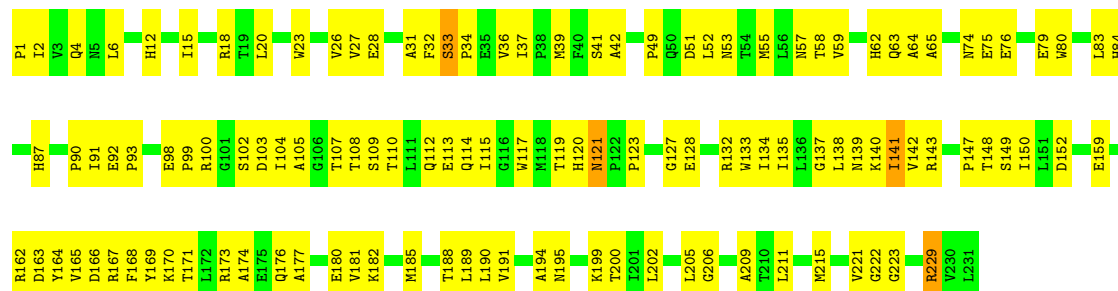
• Molecule 1: capsid protein

Chain j9:  43% 54%

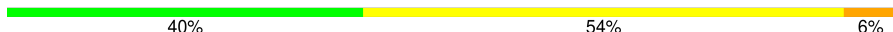


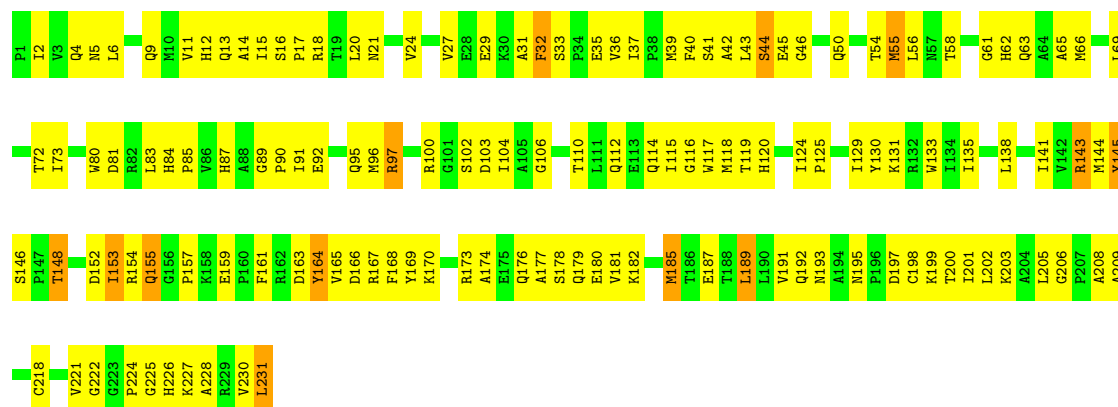
• Molecule 1: capsid protein

Chain ja:  48% 50%



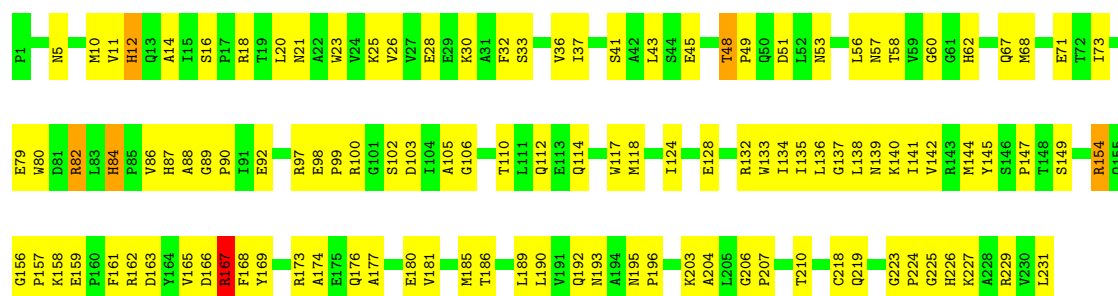
• Molecule 1: capsid protein

Chain jb:  40% 54% 6%



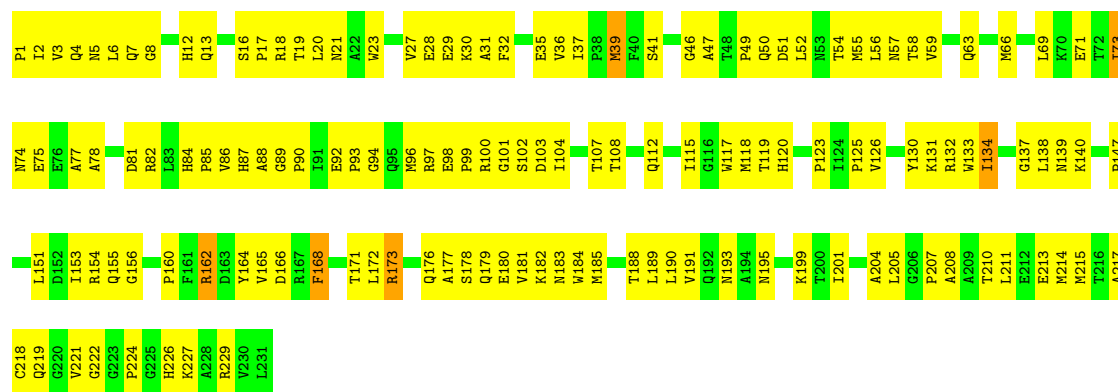
• Molecule 1: capsid protein

Chain 1U: 50% 47%



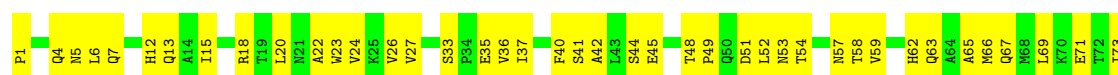
• Molecule 1: capsid protein

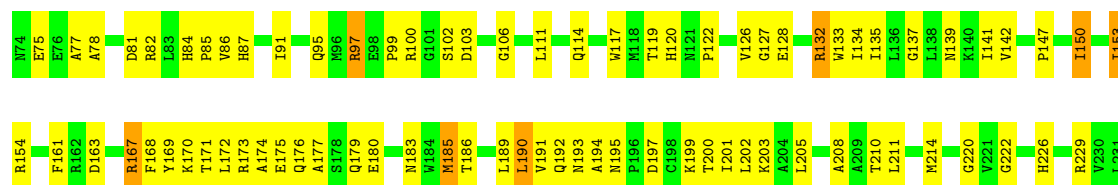
Chain jc: 39% 58%



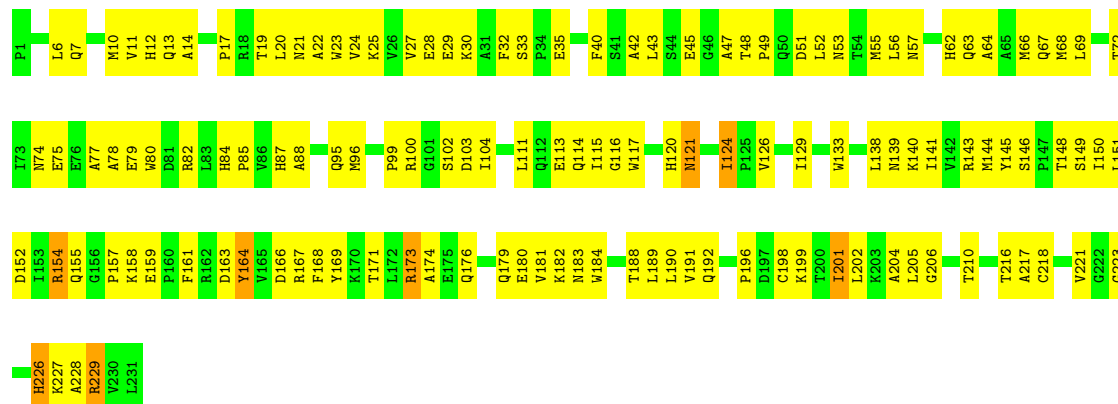
• Molecule 1: capsid protein

Chain jd: 48% 48%

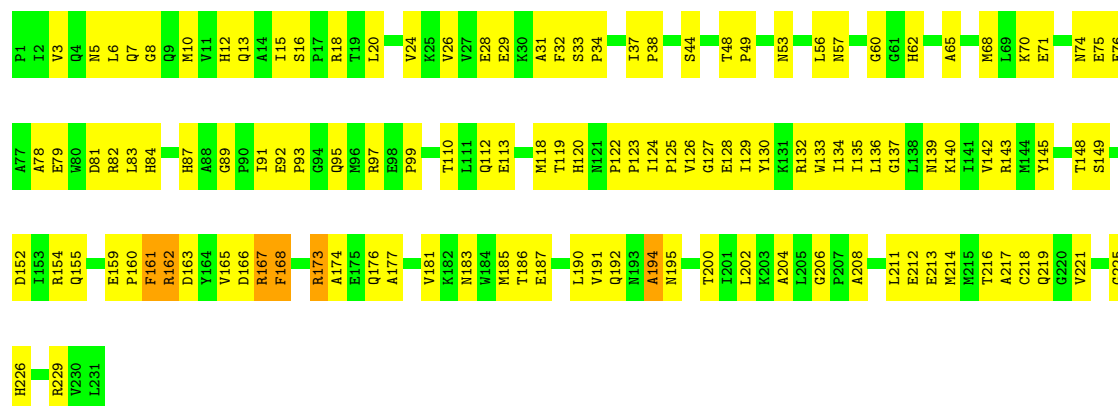




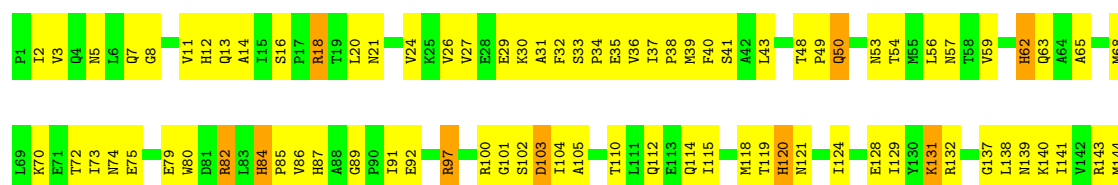
• Molecule 1: capsid protein

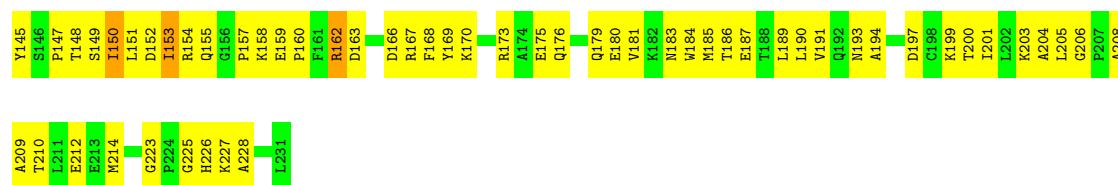


• Molecule 1: capsid protein



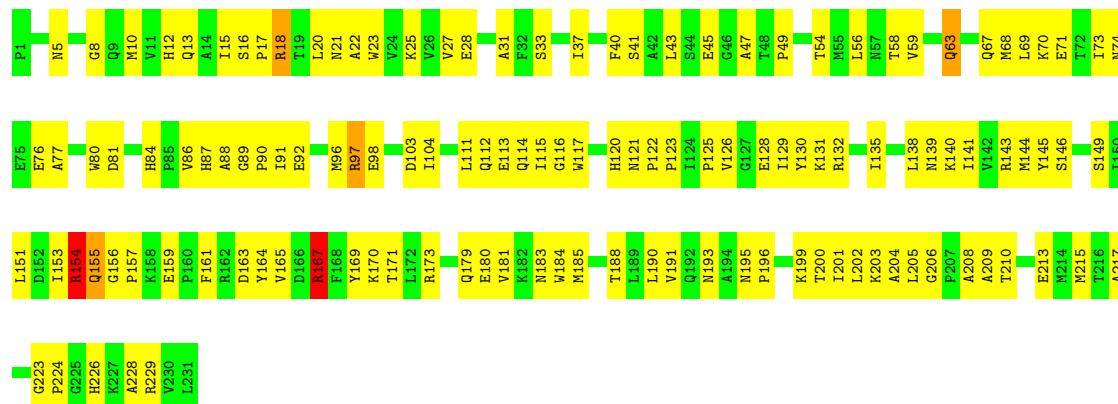
• Molecule 1: capsid protein





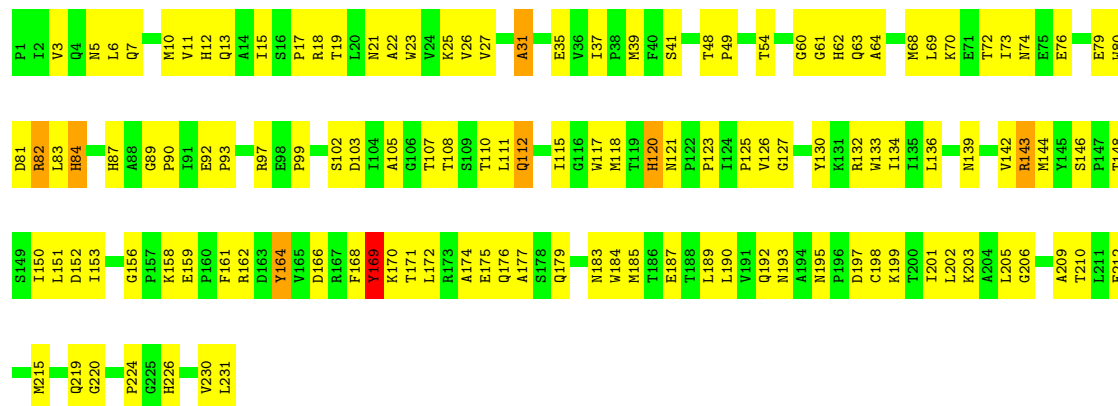
- Molecule 1: capsid protein

Chain jh: 44% 53%



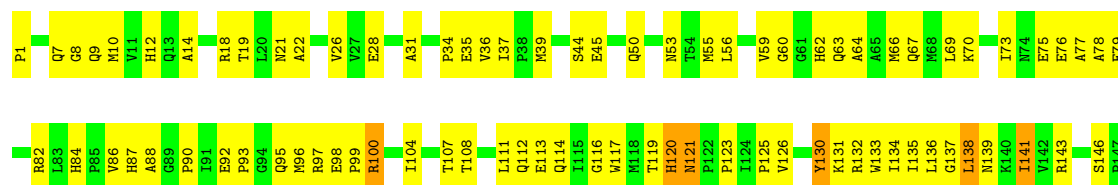
- Molecule 1: capsid protein

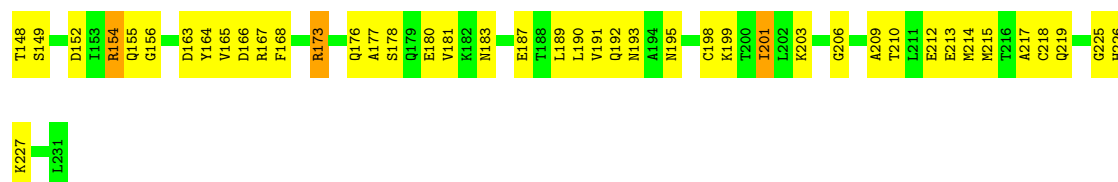
Chain ji: 45% 52%



- Molecule 1: capsid protein

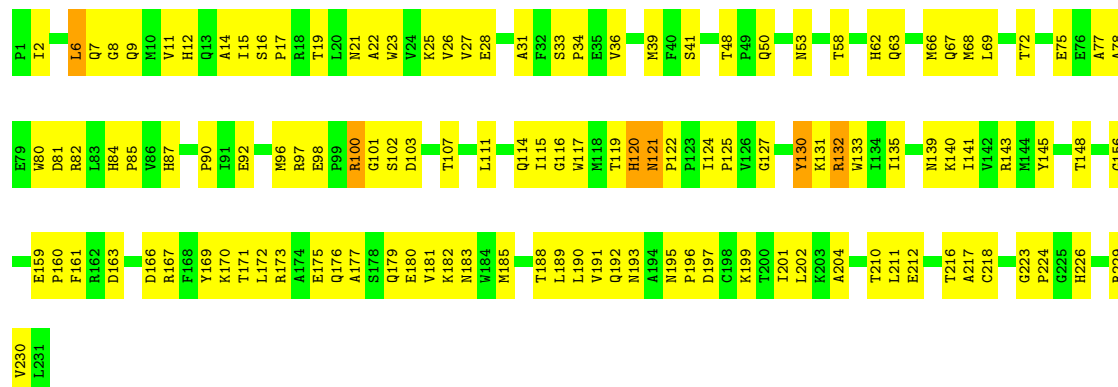
Chain jj: 46% 50%





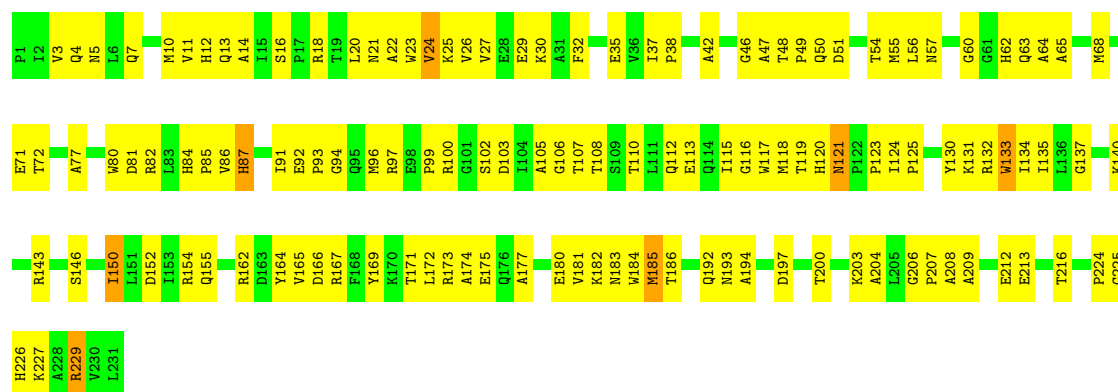
- Molecule 1: capsid protein

Chain jk: 47% 51%



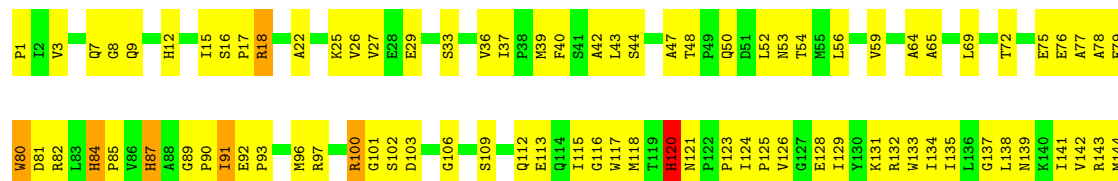
- Molecule 1: capsid protein

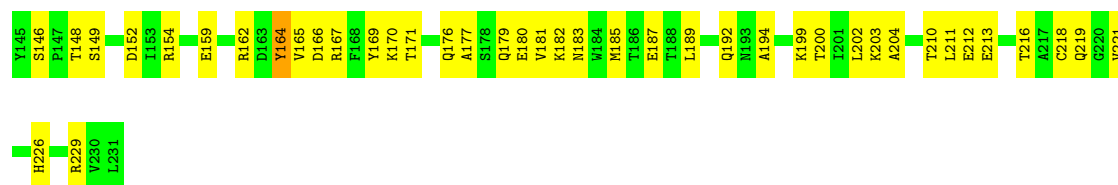
Chain jl: 43% 54%



- Molecule 1: capsid protein

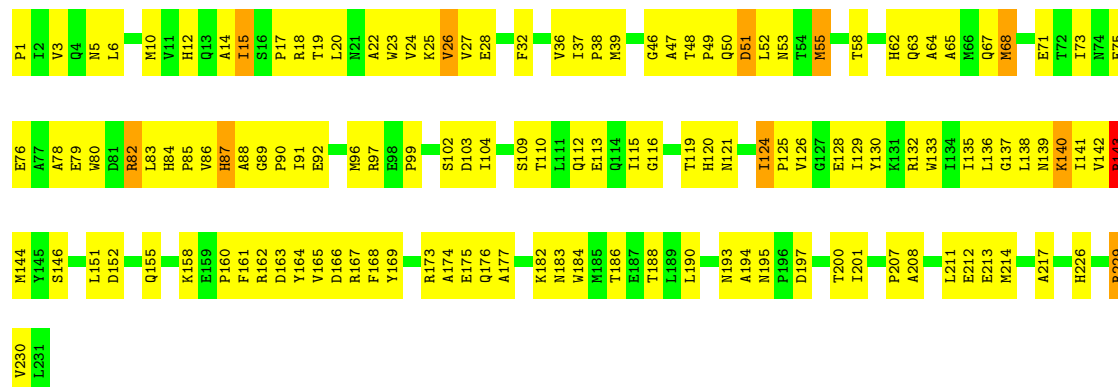
Chain 1V: 45% 51%





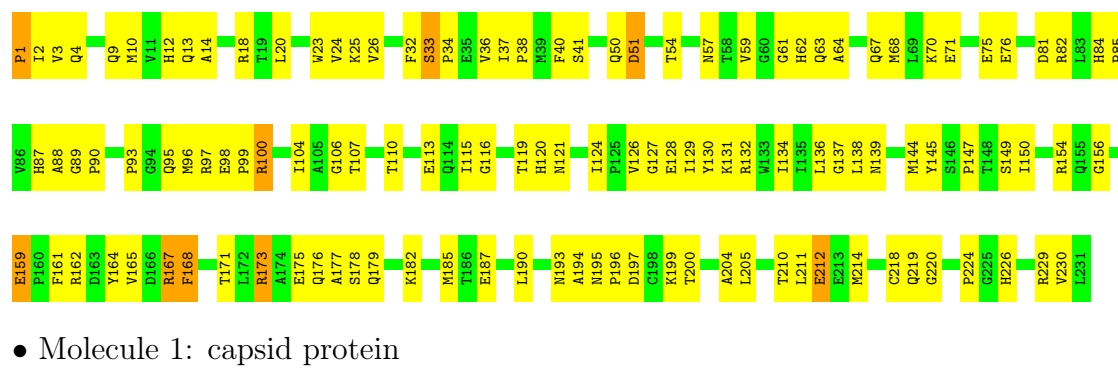
- Molecule 1: capsid protein

Chain jm: 42% 53%



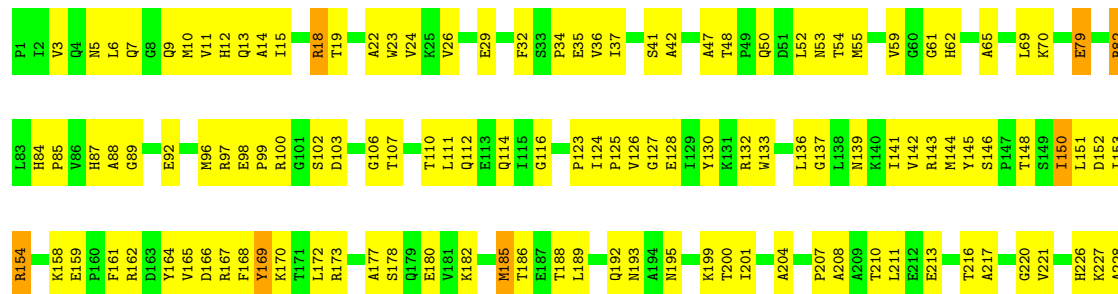
- Molecule 1: capsid protein

Chain jn: 48% 48%



- Molecule 1: capsid protein

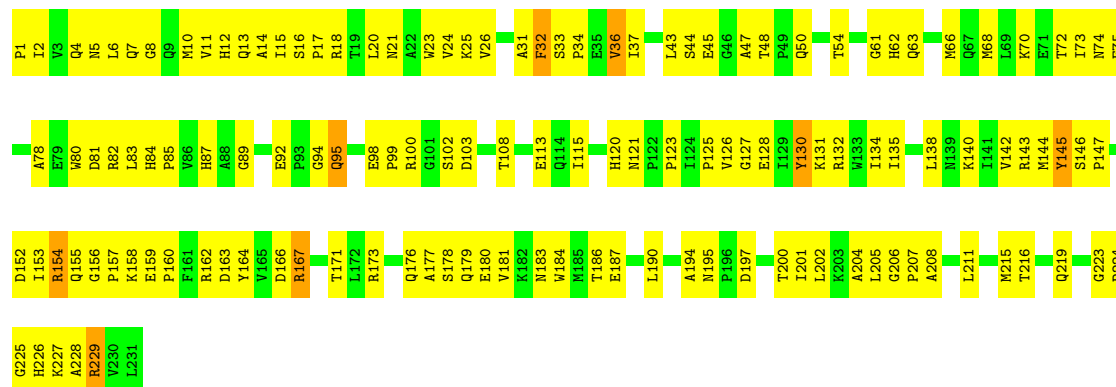
Chain jo: 46% 51%



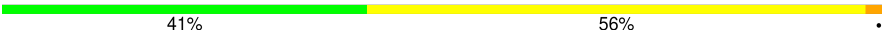
A228
R229
V230
L231

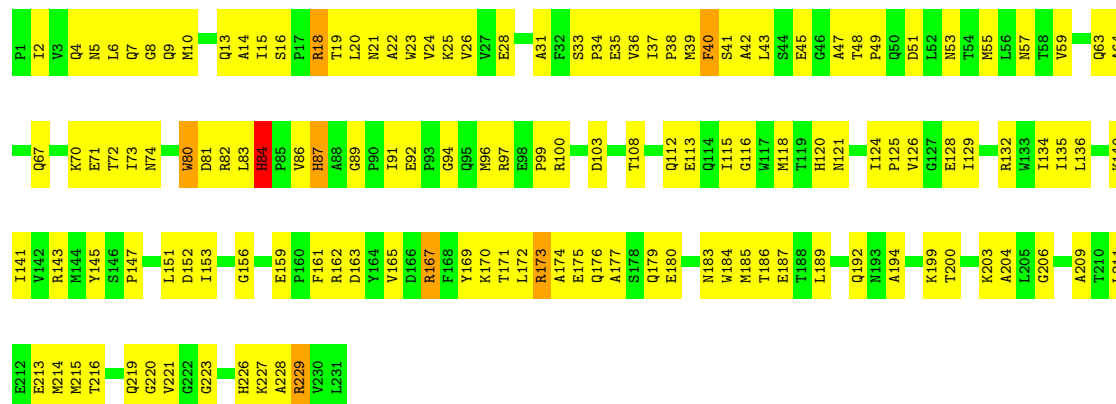
• Molecule 1: capsid protein

Chain js:  42% 55%



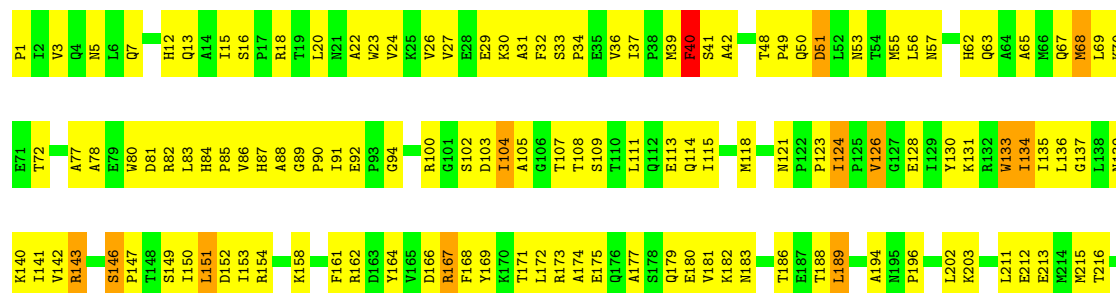
• Molecule 1: capsid protein

Chain jt:  41% 56%



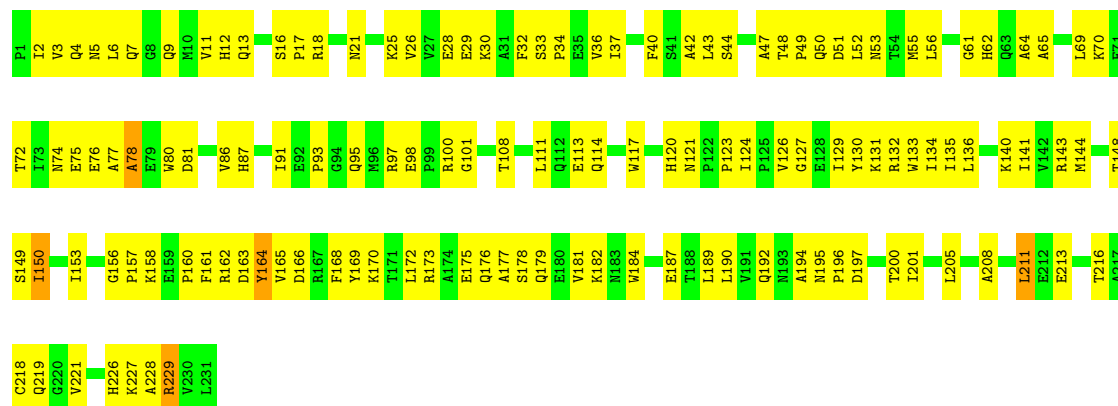
• Molecule 1: capsid protein

Chain ju:  42% 52% 6%

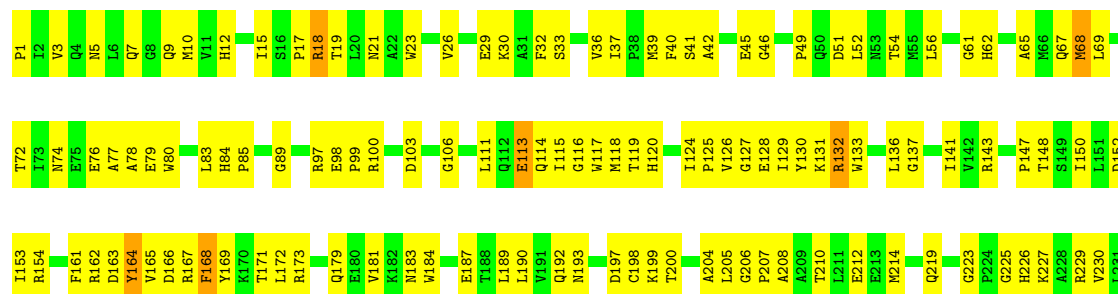




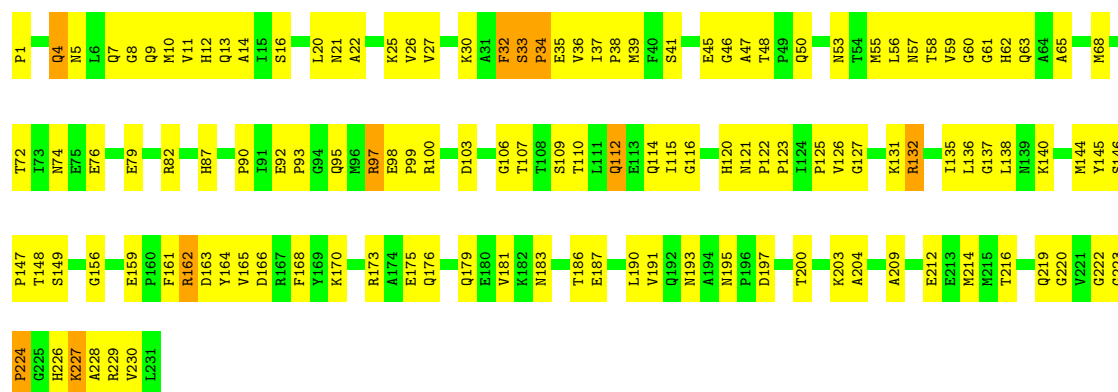
- Molecule 1: capsid protein



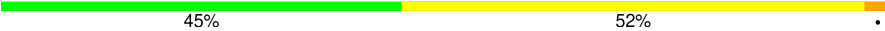
- Molecule 1: capsid protein

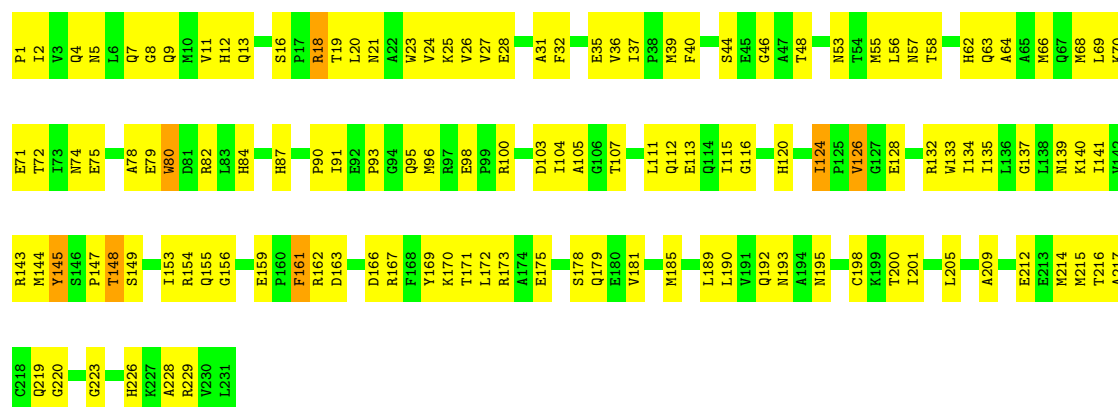


- Molecule 1: capsid protein

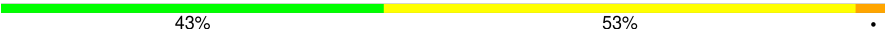


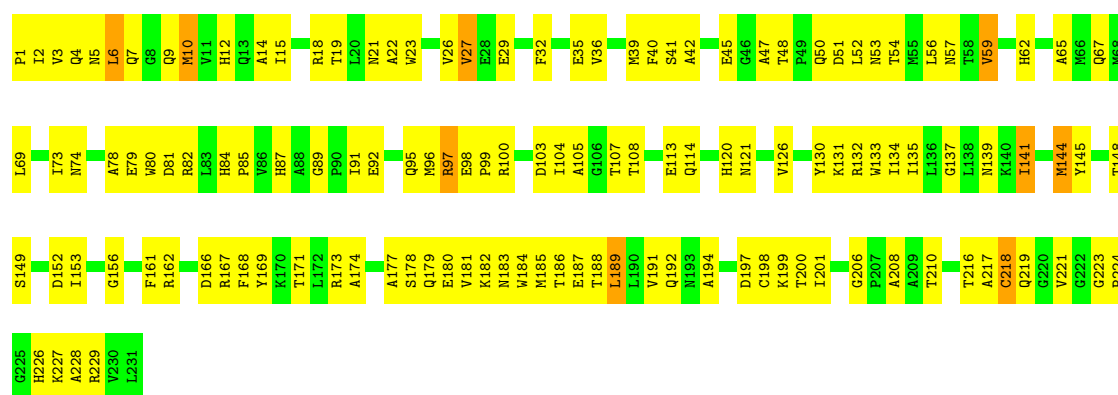
- Molecule 1: capsid protein

Chain jx: 

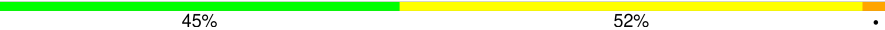


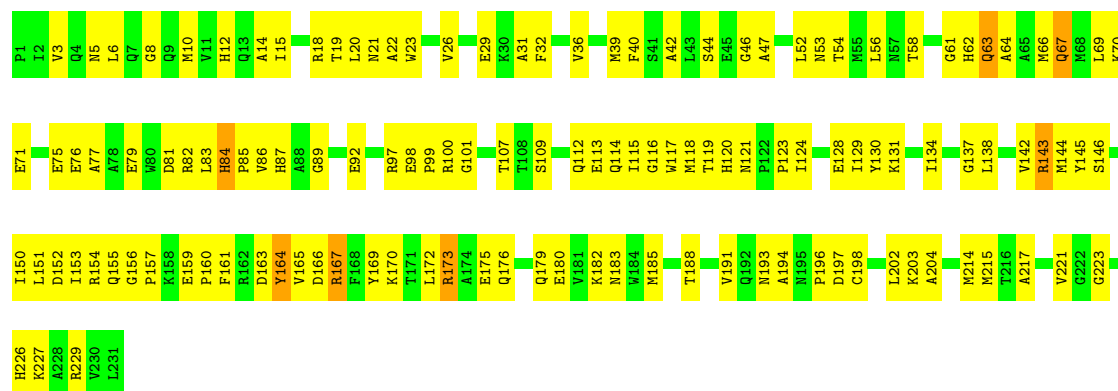
• Molecule 1: capsid protein

Chain jy: 



• Molecule 1: capsid protein

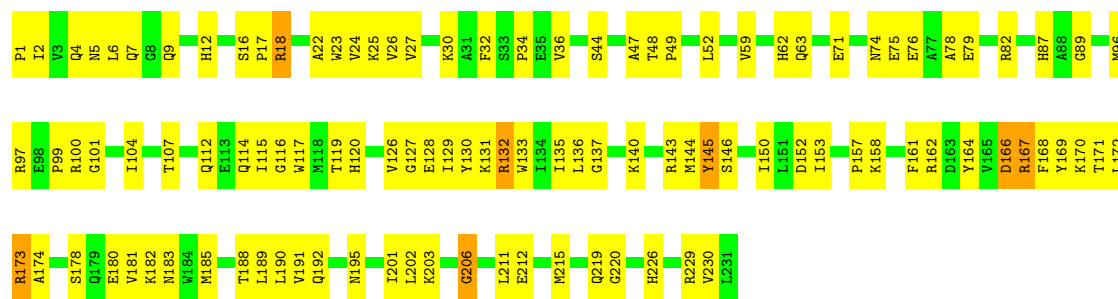
Chain jz: 



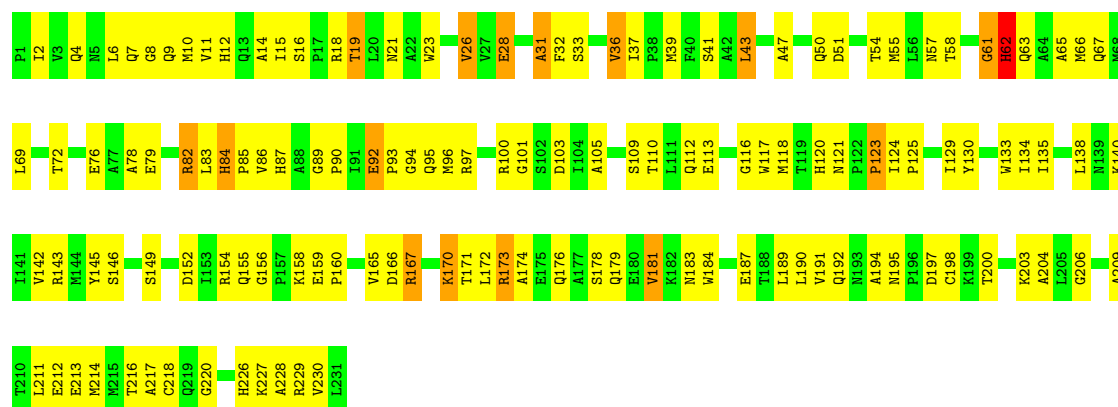
• Molecule 1: capsid protein

Chain ja: 





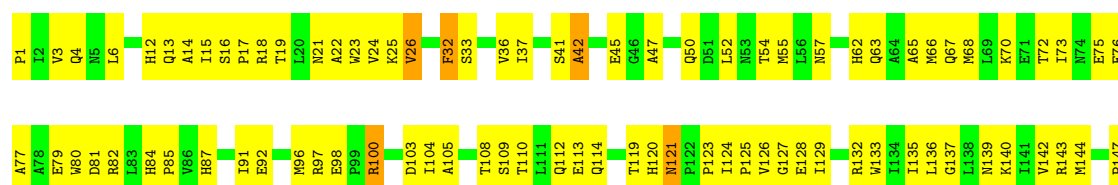
- Molecule 1: capsid protein



- Molecule 1: capsid protein



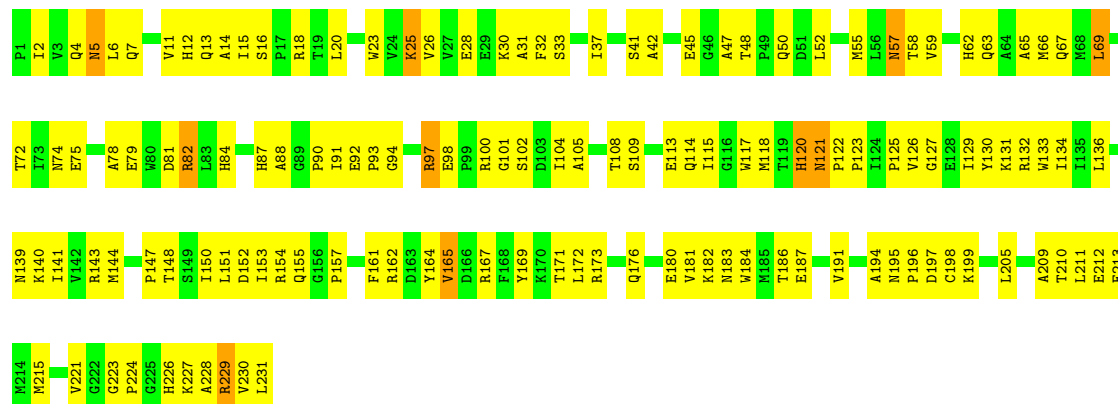
- Molecule 1: capsid protein





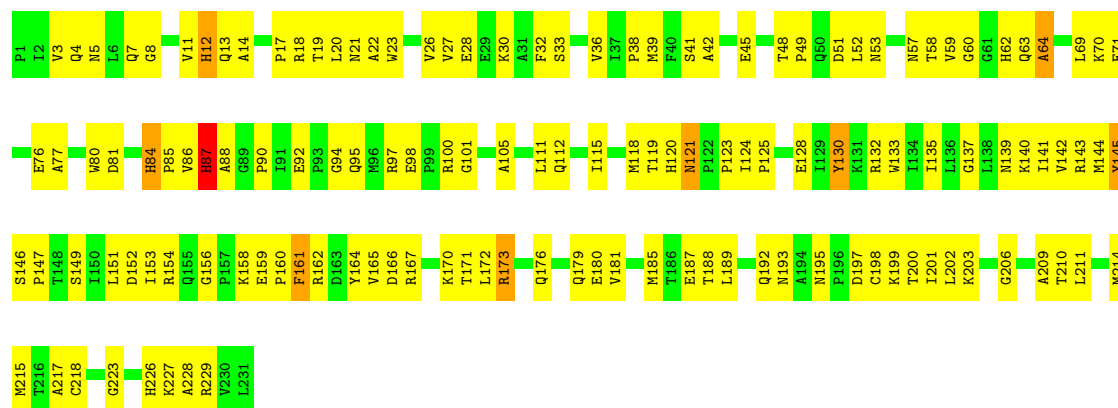
• Molecule 1: capsid protein

Chain jE: 41% 55%



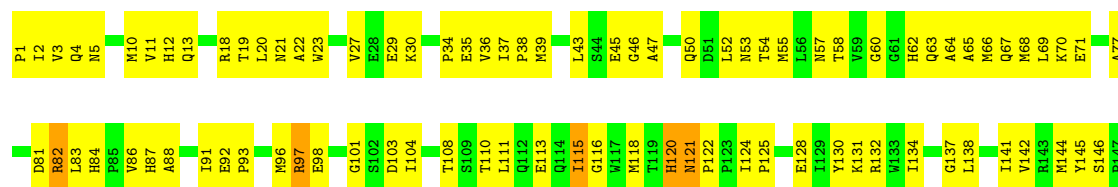
• Molecule 1: capsid protein

Chain jF: 41% 55%



• Molecule 1: capsid protein

Chain 1X: 46% 50%

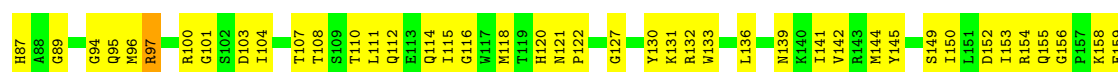




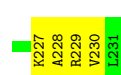
- Molecule 1: capsid protein



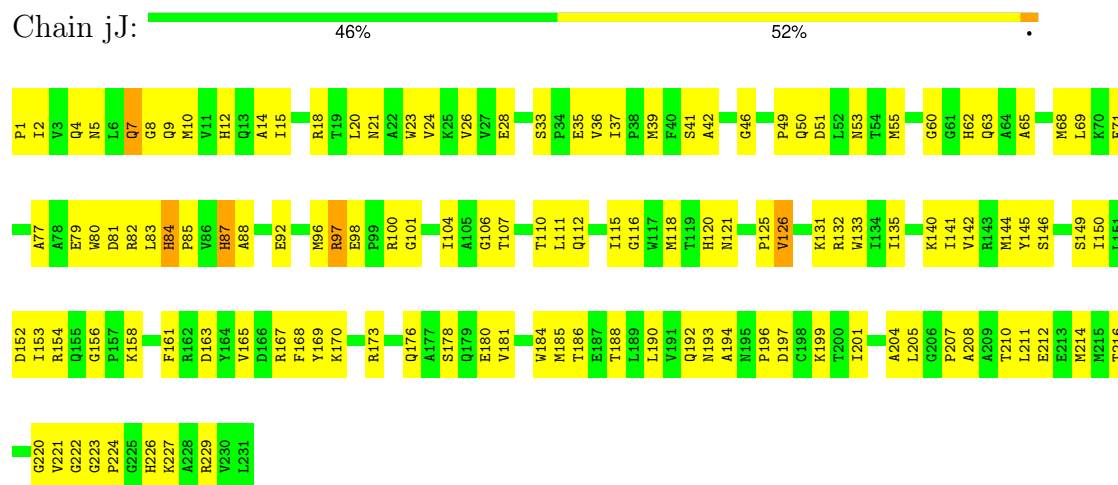
- Molecule 1: capsid protein



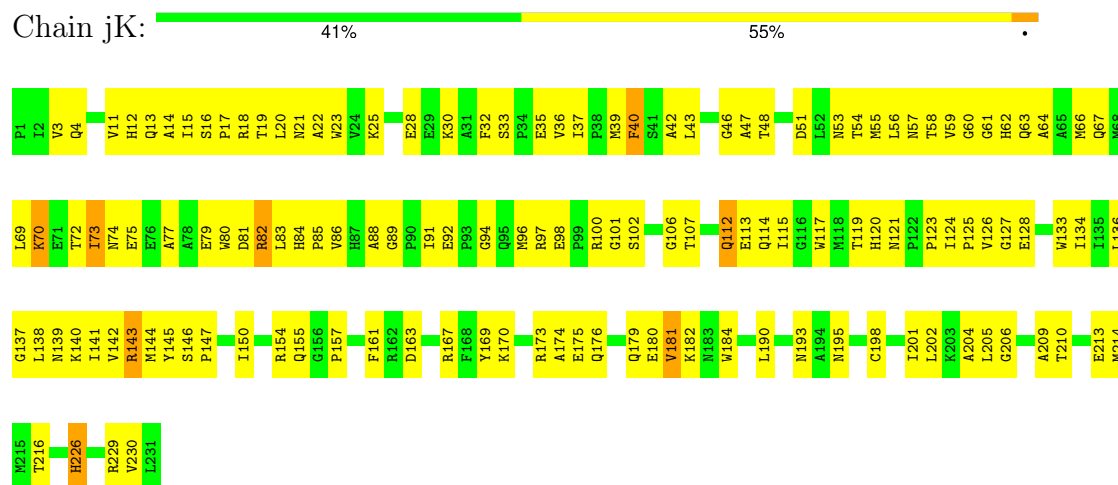
- Molecule 1: capsid protein



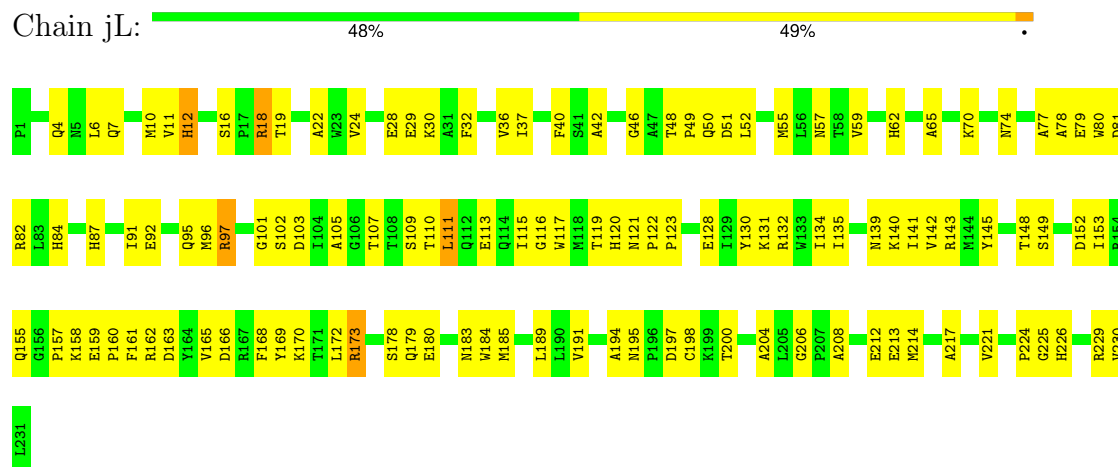
- Molecule 1: capsid protein



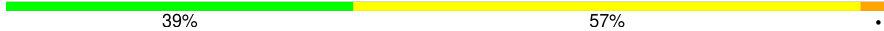
- Molecule 1: capsid protein

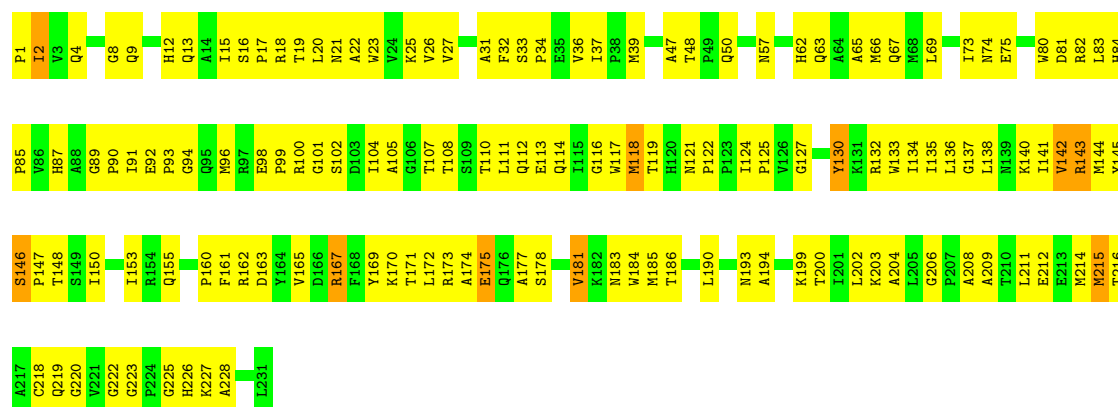


- Molecule 1: capsid protein

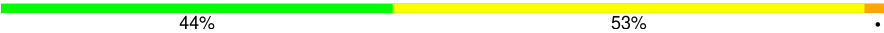


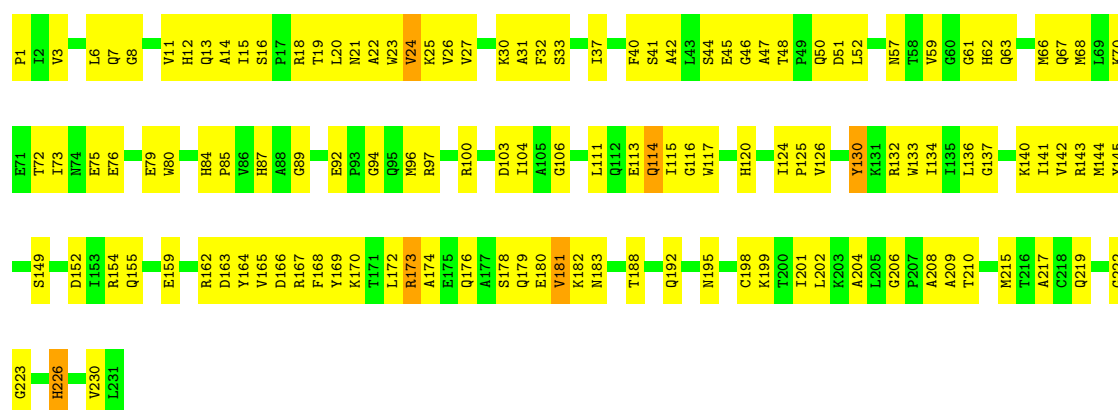
- Molecule 1: capsid protein

Chain jM:  39% 57%

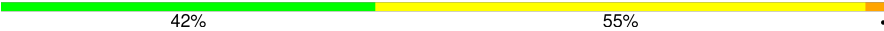


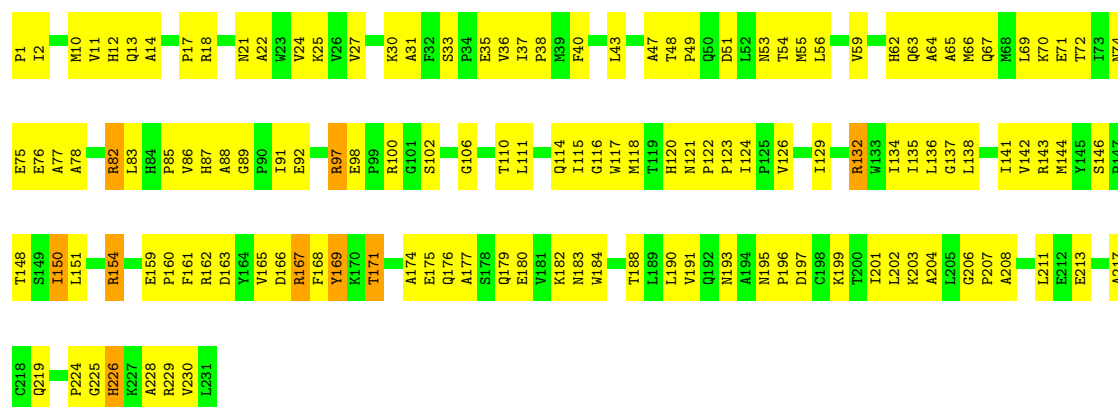
• Molecule 1: capsid protein

Chain jN:  44% 53%

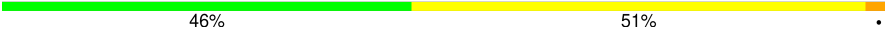


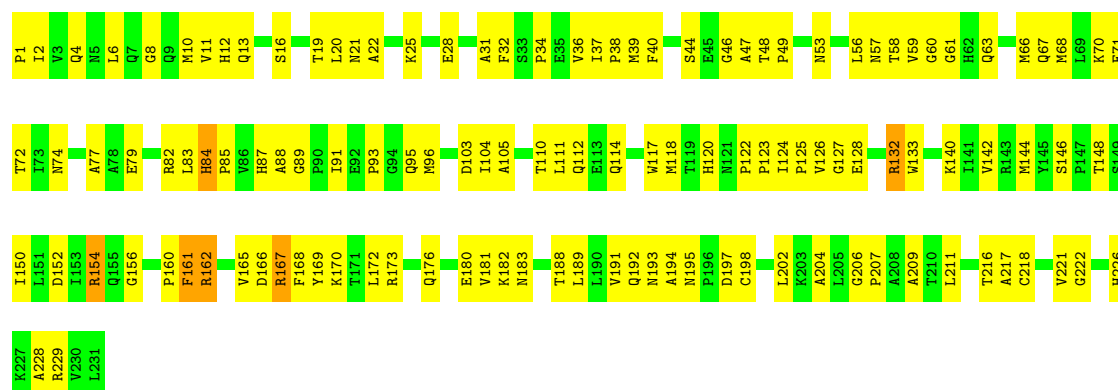
• Molecule 1: capsid protein

Chain jO:  42% 55%

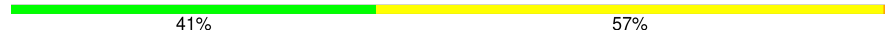


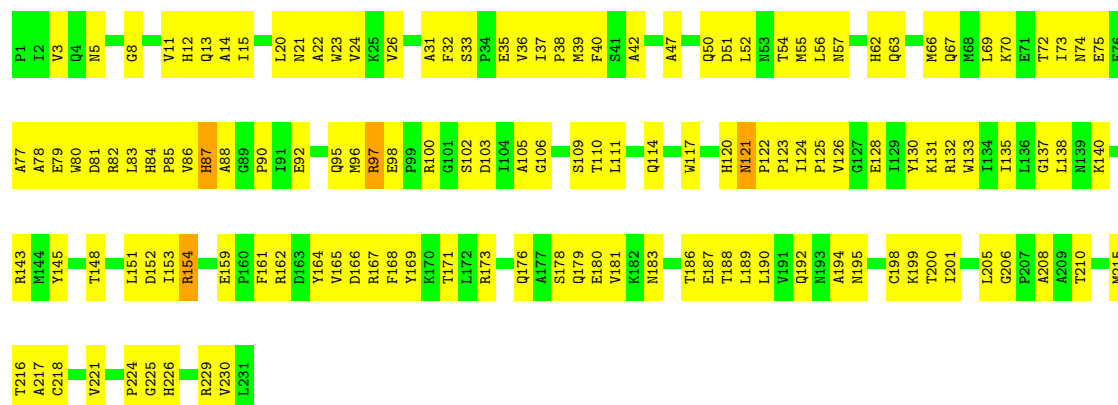
• Molecule 1: capsid protein

Chain jP:  46% 51%

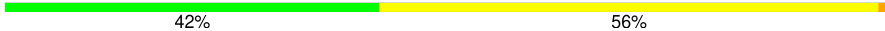


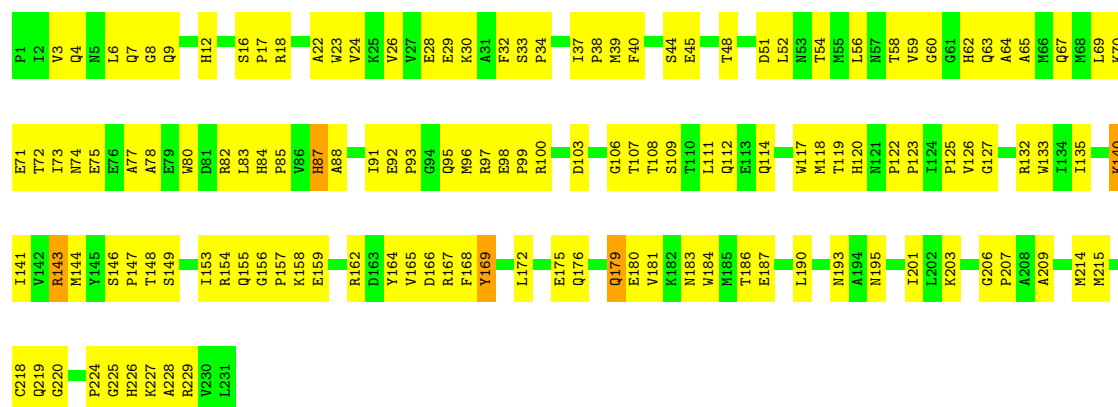
• Molecule 1: capsid protein

Chain 1Y:  41% 57%



• Molecule 1: capsid protein

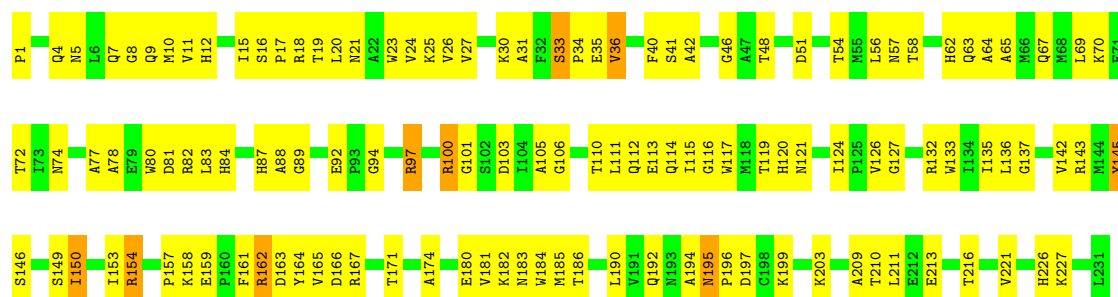
Chain jQ:  42% 56%



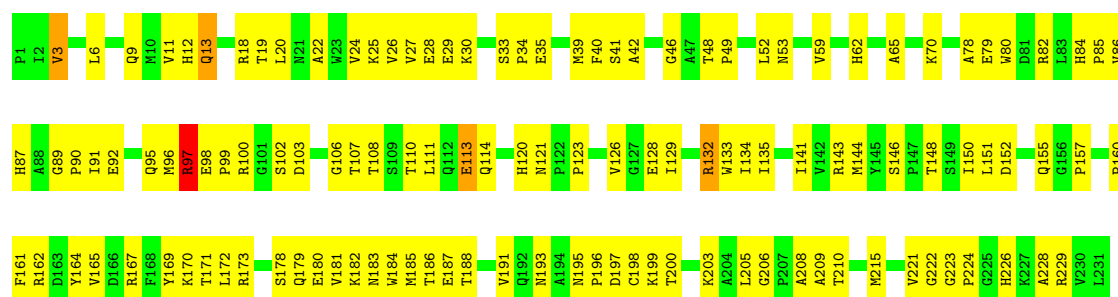
• Molecule 1: capsid protein

Chain jR: 

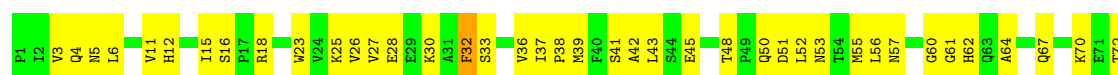
• Molecule 1: capsid protein

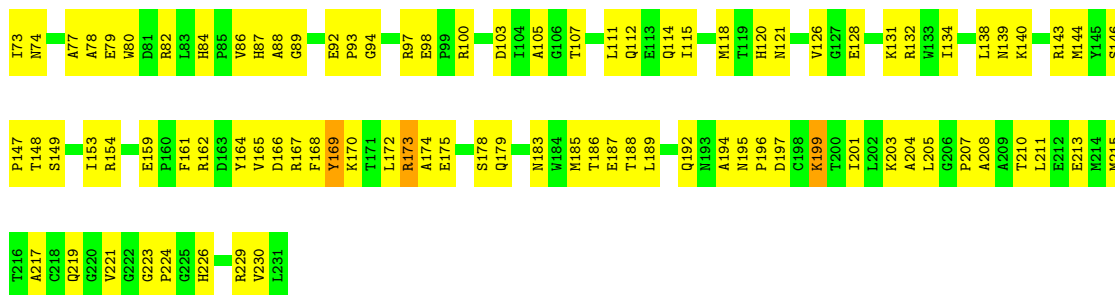
Chain jS: 

• Molecule 1: capsid protein

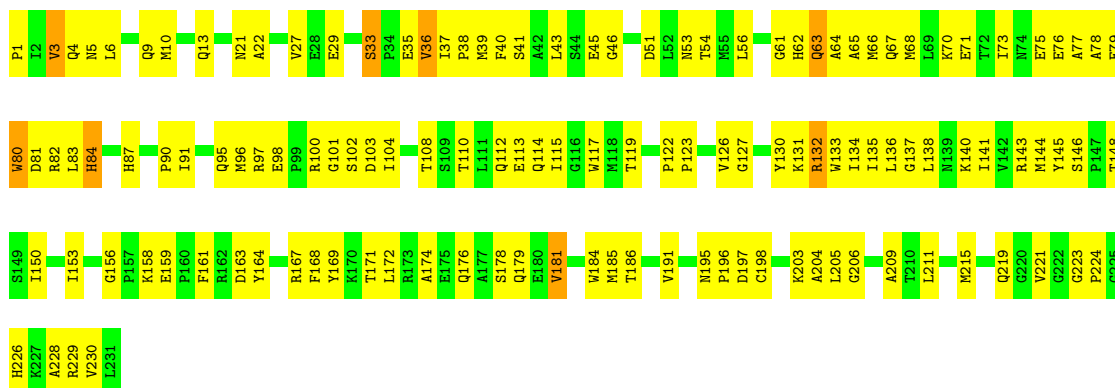
Chain jT: 

• Molecule 1: capsid protein

Chain jU: 



- Molecule 1: capsid protein

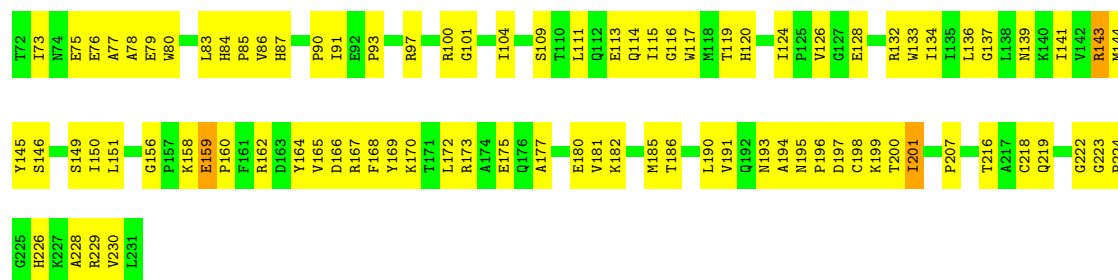


- Molecule 1: capsid protein



- Molecule 1: capsid protein





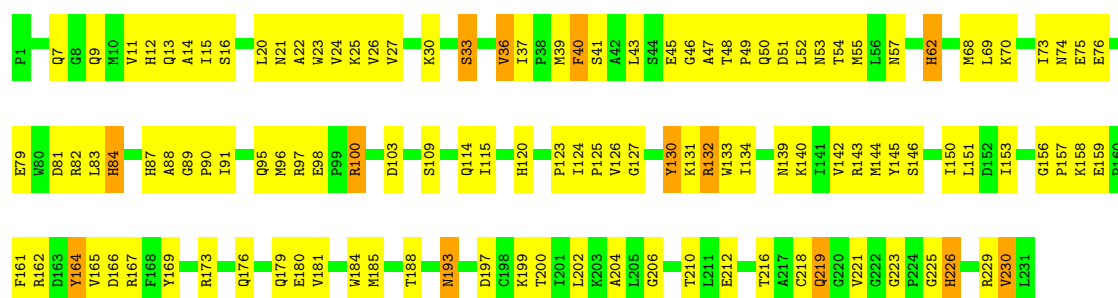
- Molecule 1: capsid protein

Chain jY: 47% 49%



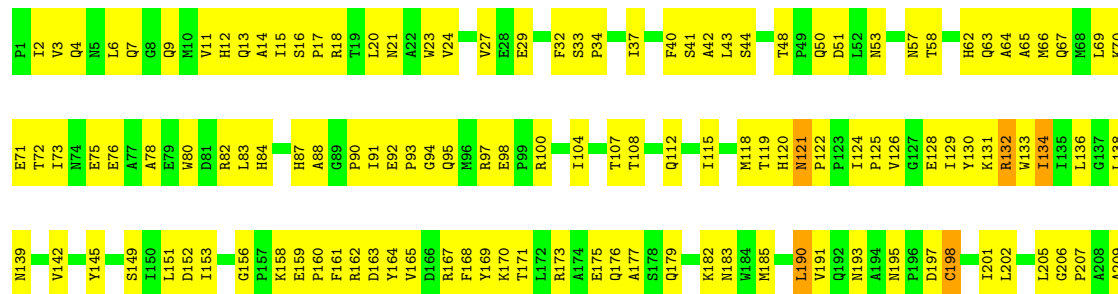
- Molecule 1: capsid protein

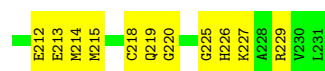
Chain jZ: 48% 47% 6%



- Molecule 1: capsid protein

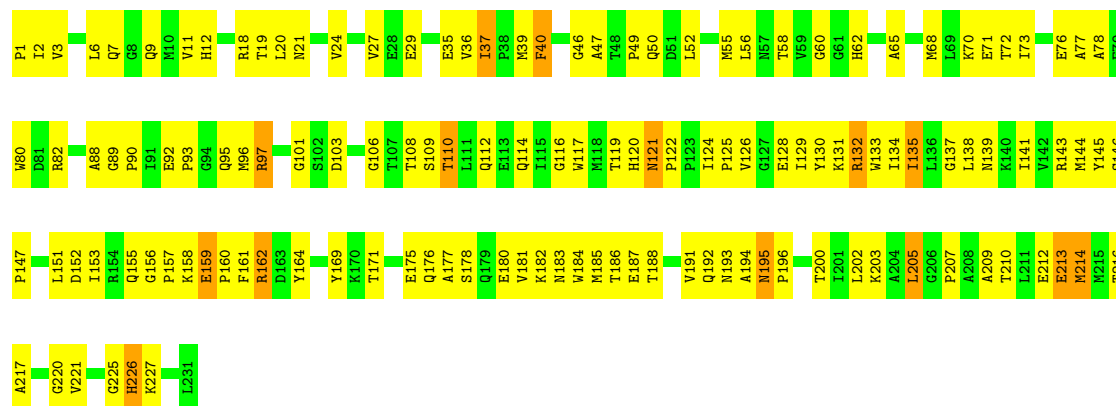
Chain 1Z: 40% 58%





- Molecule 1: capsid protein

Chain k0: 42% 52% 6%



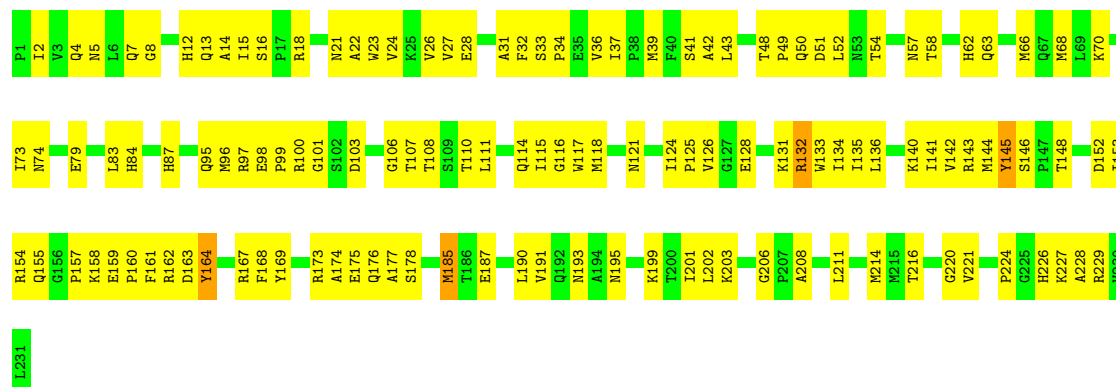
- Molecule 1: capsid protein

Chain k1: 47% 48% 5%



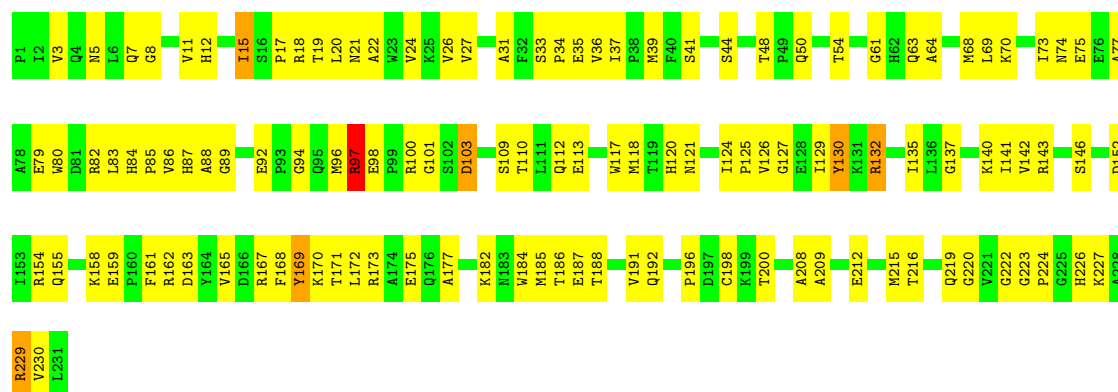
- Molecule 1: capsid protein

Chain k2: 45% 53% 2%

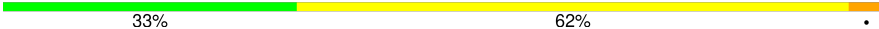


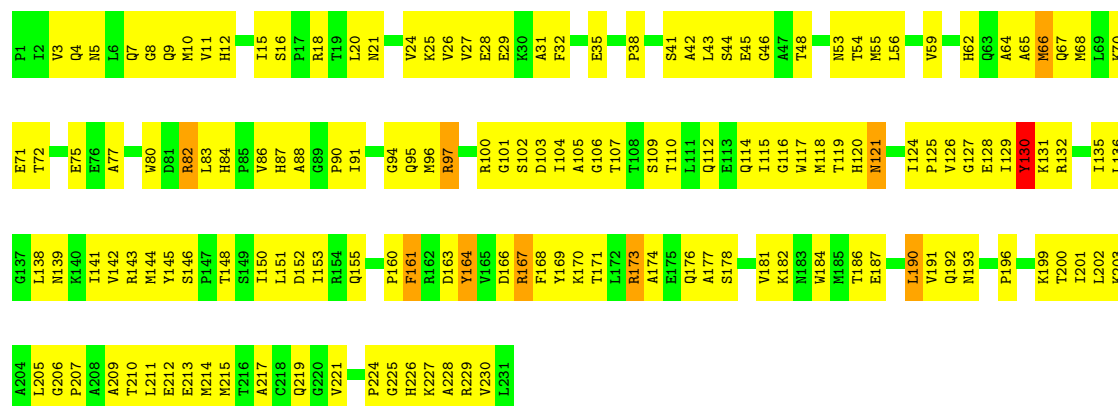
- Molecule 1: capsid protein

Chain k3:  48% 49%



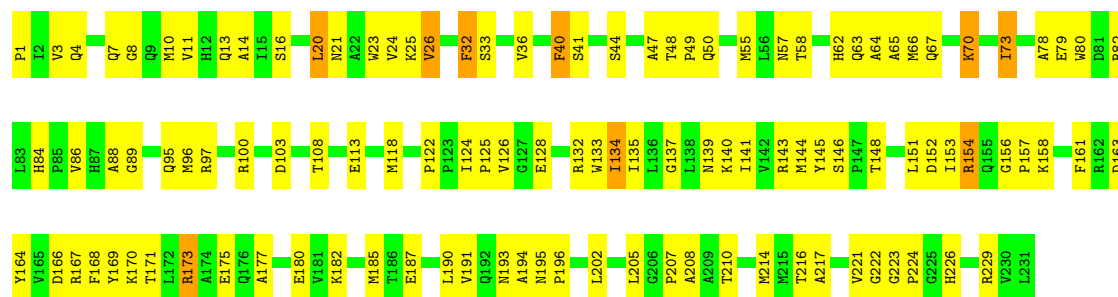
• Molecule 1: capsid protein

Chain k4:  33% 62%



• Molecule 1: capsid protein

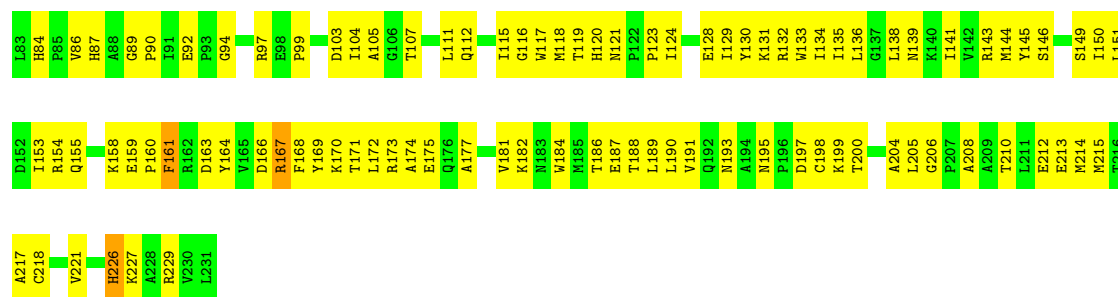
Chain k5:  51% 45%



• Molecule 1: capsid protein

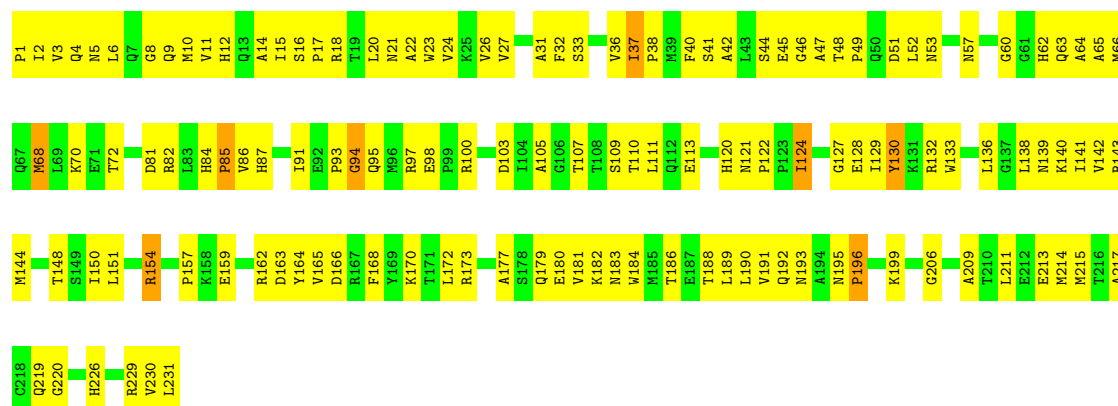
Chain k6:  42% 56%





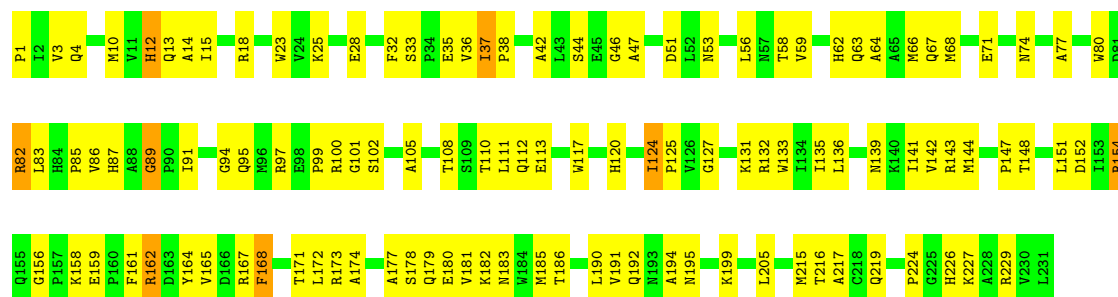
- Molecule 1: capsid protein

Chain k7: 42% 55%



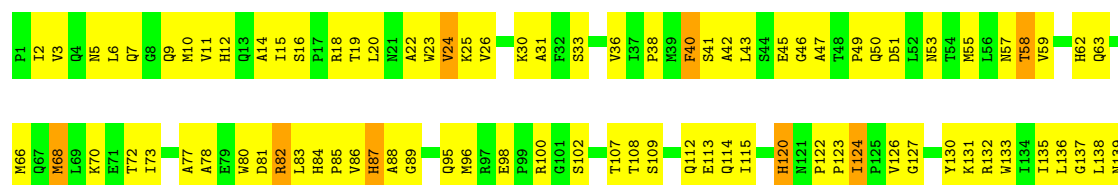
- Molecule 1: capsid protein

Chain k8: 51% 46%



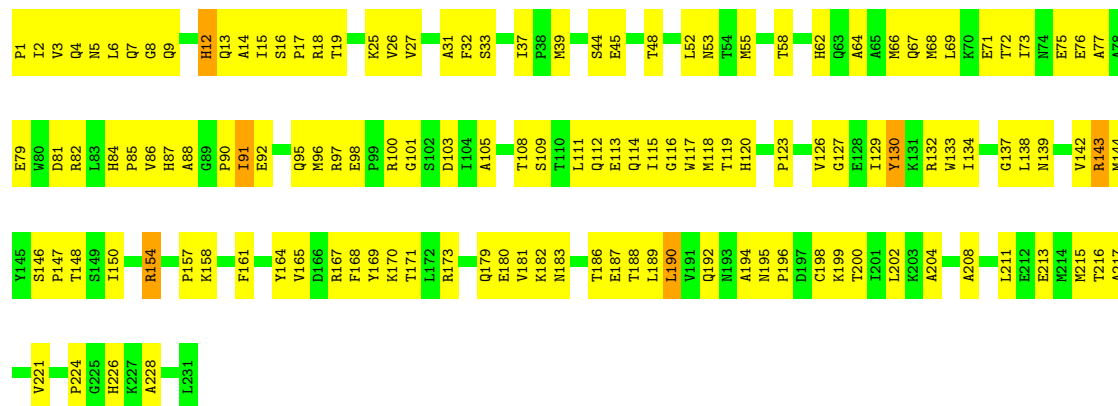
- Molecule 1: capsid protein

Chain k9: 37% 58% 5%

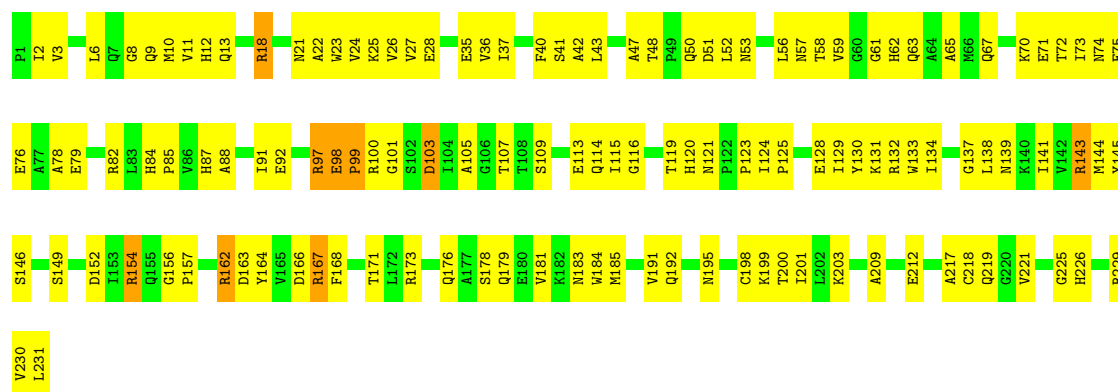




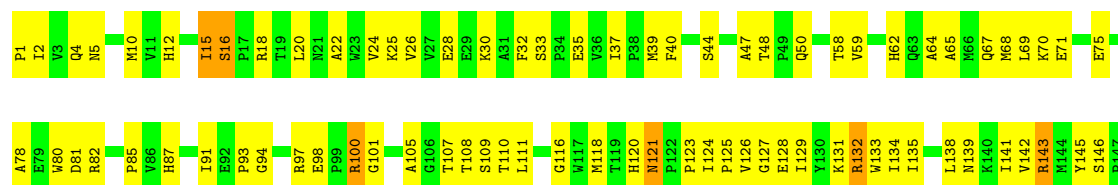
• Molecule 1: capsid protein

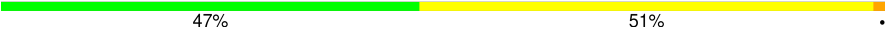


• Molecule 1: capsid protein



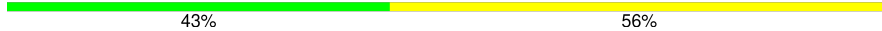
• Molecule 1: capsid protein

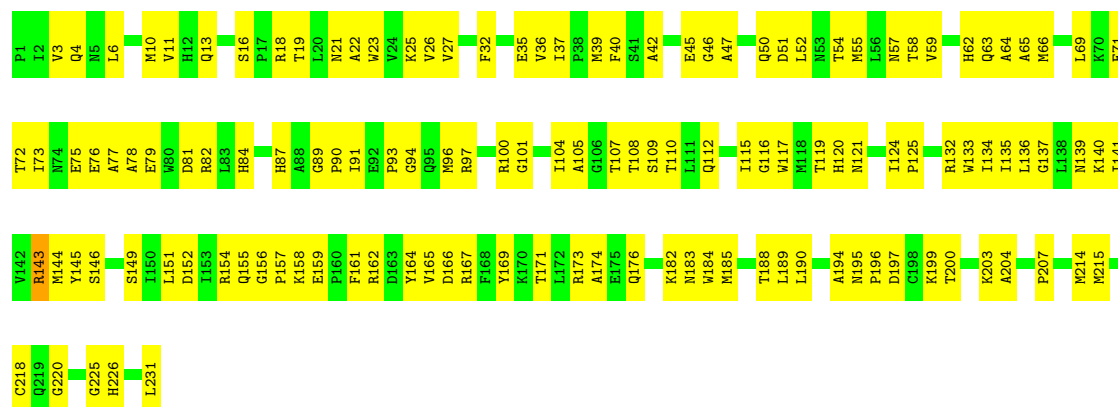


Chain kf: 



• Molecule 1: capsid protein

Chain kg: 

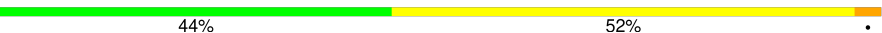


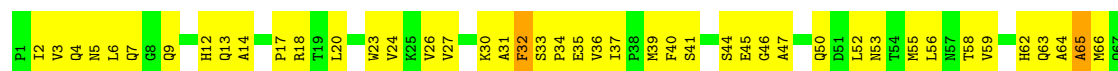
• Molecule 1: capsid protein

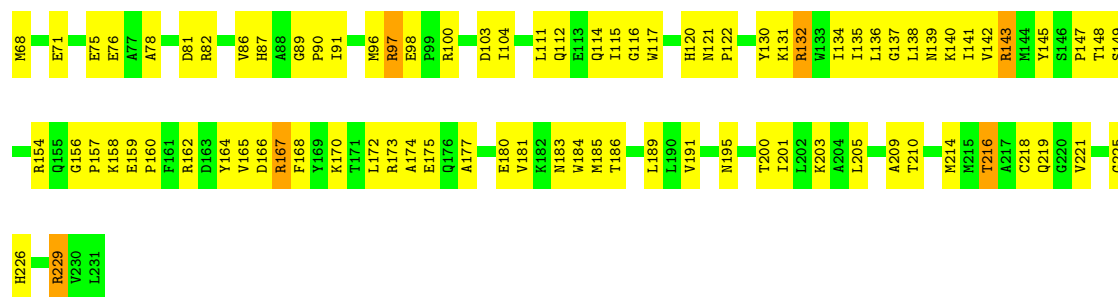
Chain kh: 



• Molecule 1: capsid protein

Chain ki: 

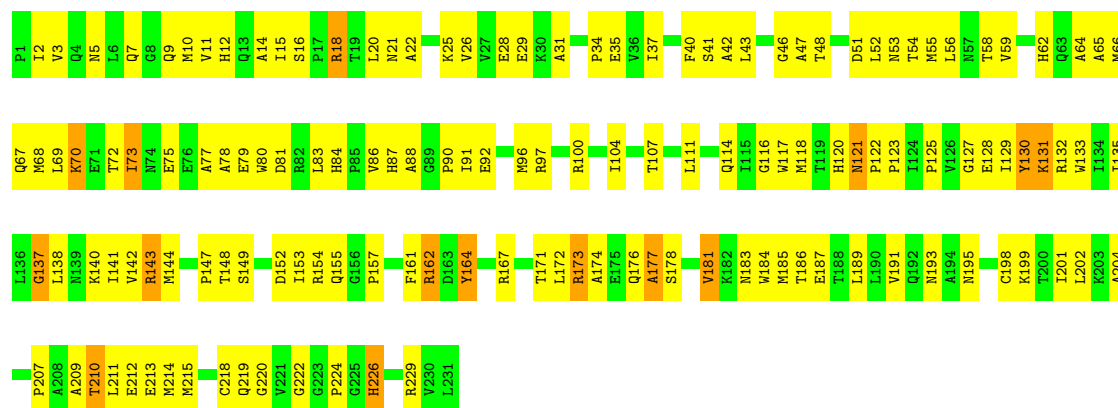




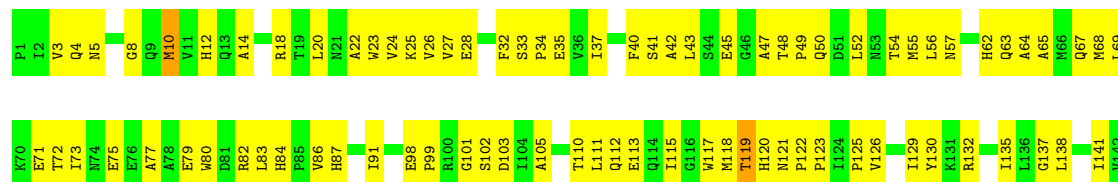
- Molecule 1: capsid protein

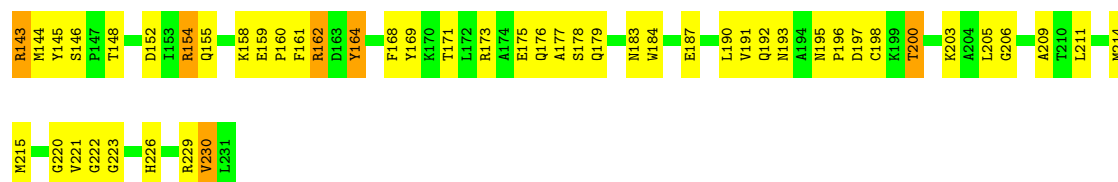


- Molecule 1: capsid protein



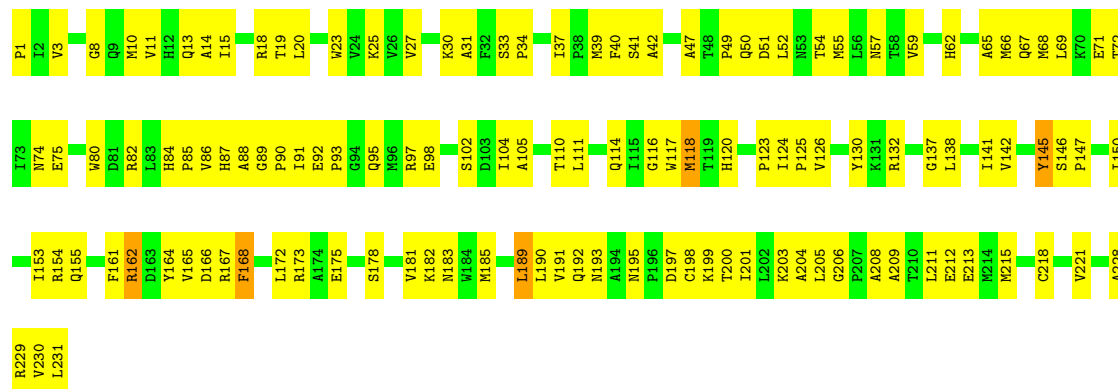
- Molecule 1: capsid protein





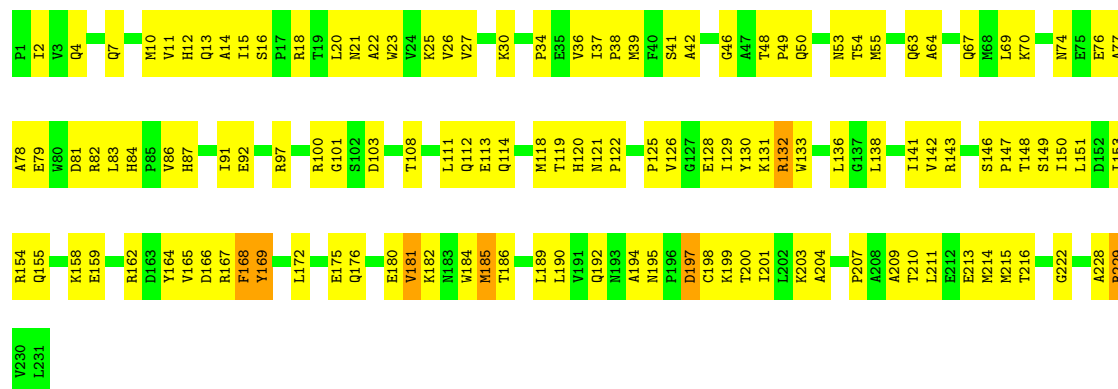
- Molecule 1: capsid protein

Chain kl: 45% 52%



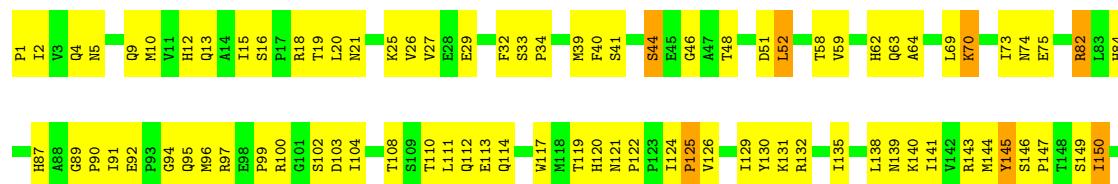
- Molecule 1: capsid protein

Chain km: 45% 52%



- Molecule 1: capsid protein

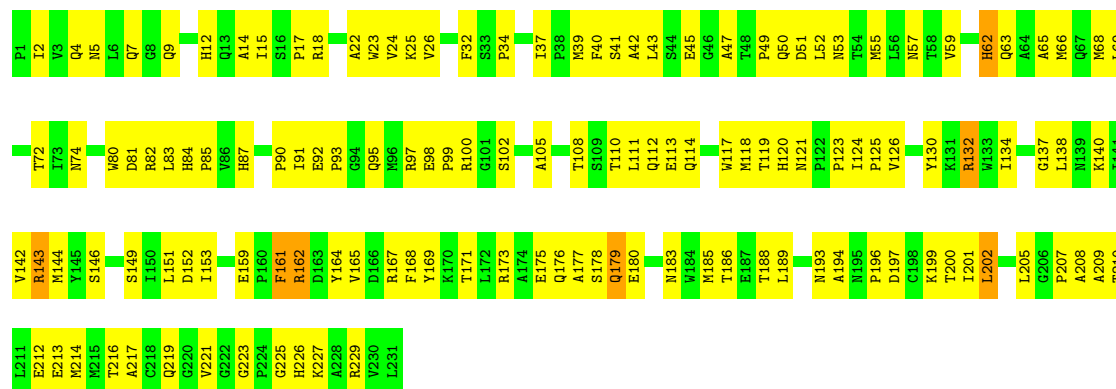
Chain kn: 49% 47%





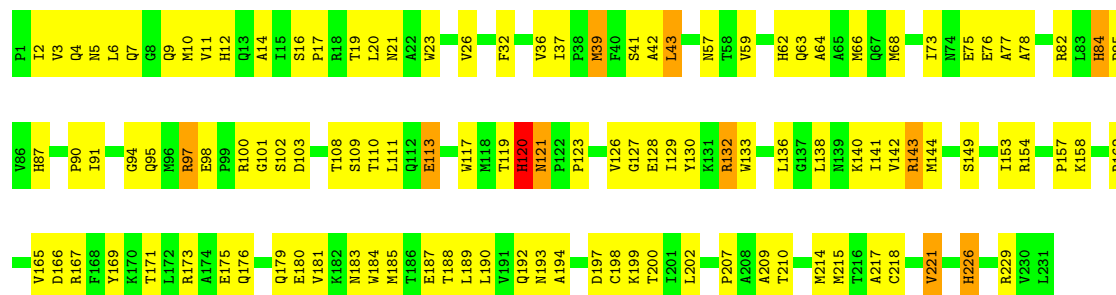
- Molecule 1: capsid protein

Chain ko: 42% 55%



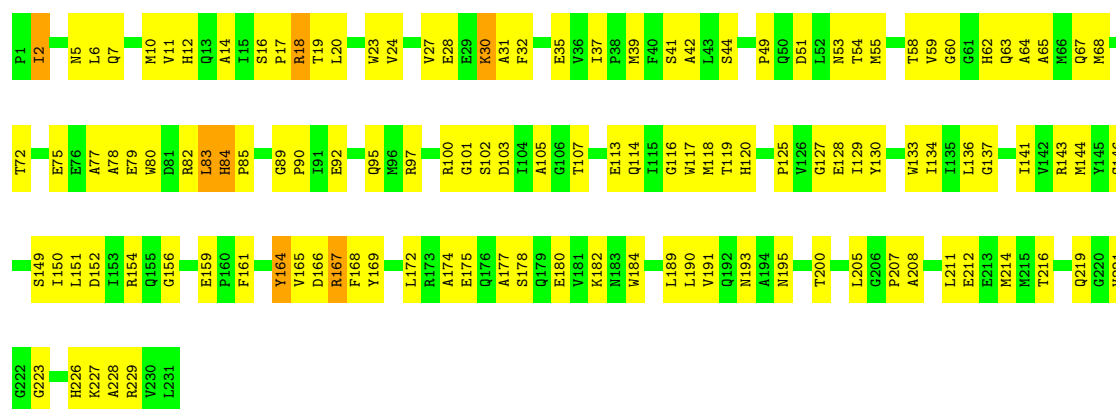
- Molecule 1: capsid protein

Chain kp: 49% 46%



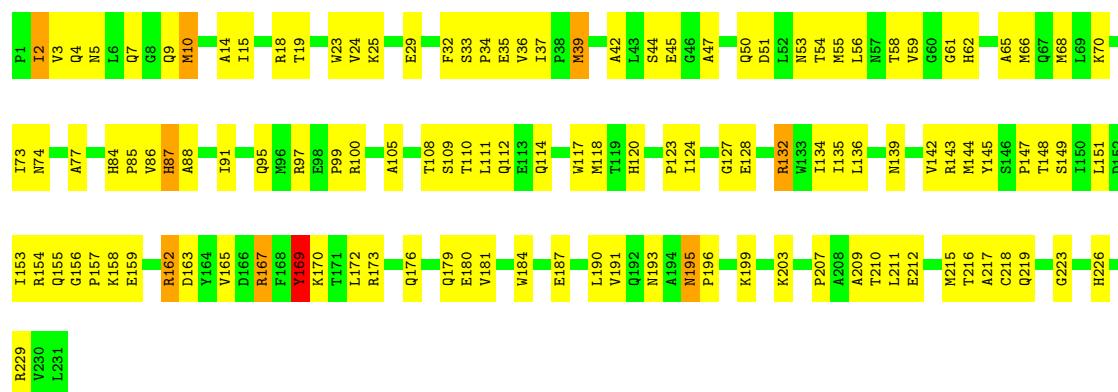
- Molecule 1: capsid protein

Chain kq: 47% 50%



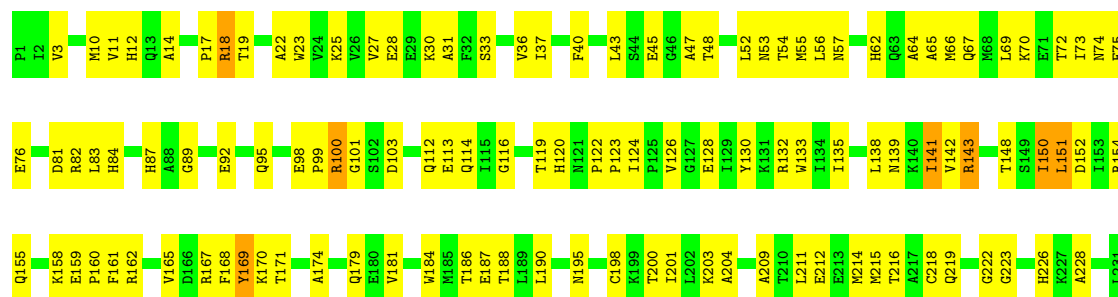
- Molecule 1: capsid protein

Chain kr: 



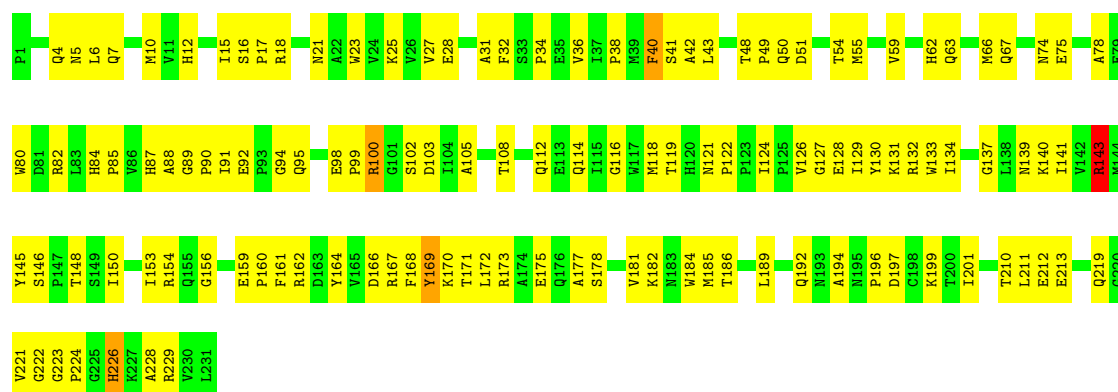
• Molecule 1: capsid protein

Chain ks: 

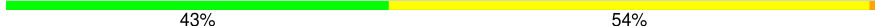


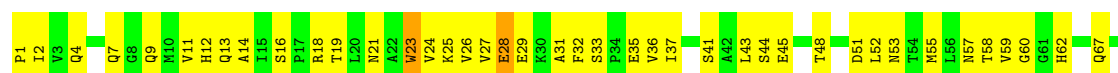
• Molecule 1: capsid protein

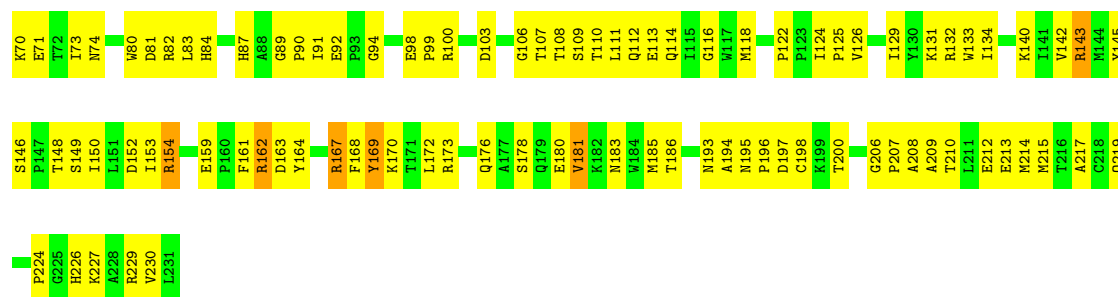
Chain kt: 



• Molecule 1: capsid protein

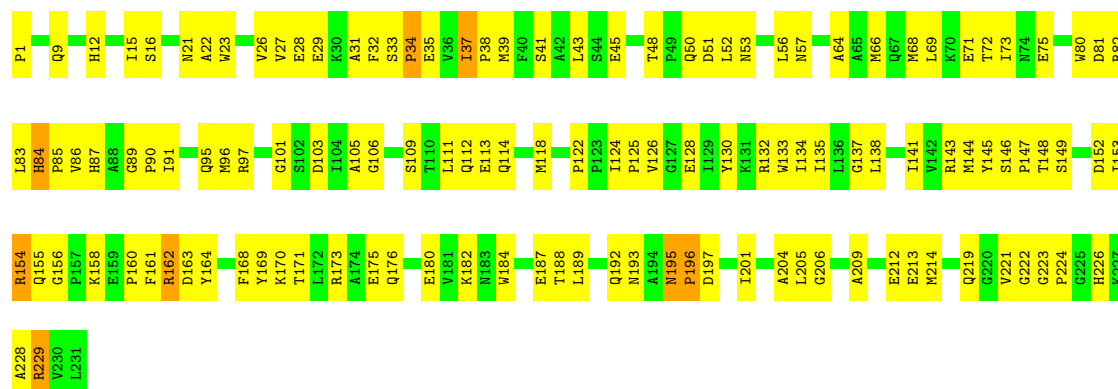
Chain 22: 





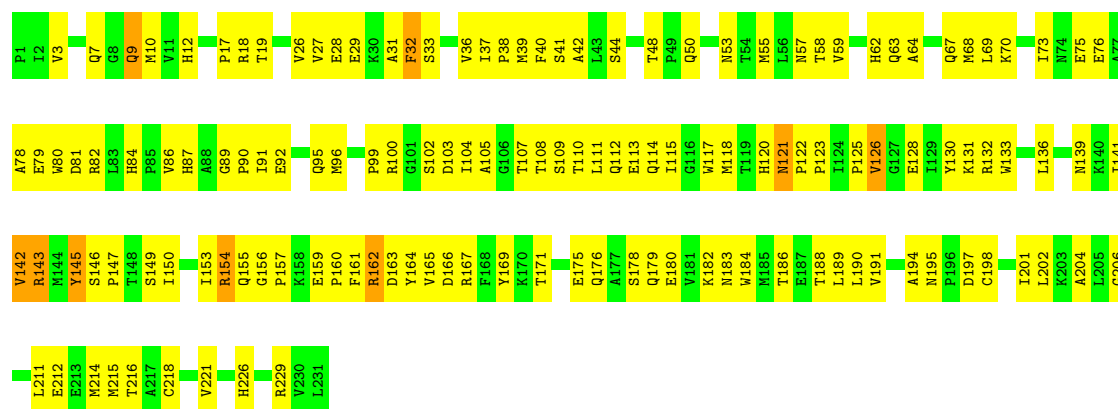
- Molecule 1: capsid protein

Chain ku: 45% 52%



- Molecule 1: capsid protein

Chain kv: 40% 56%



- Molecule 1: capsid protein

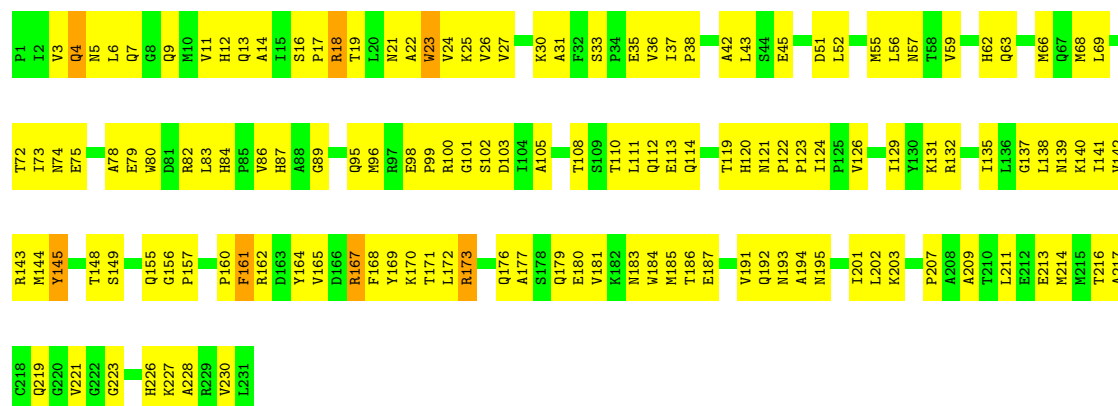
Chain kw: 49% 47%





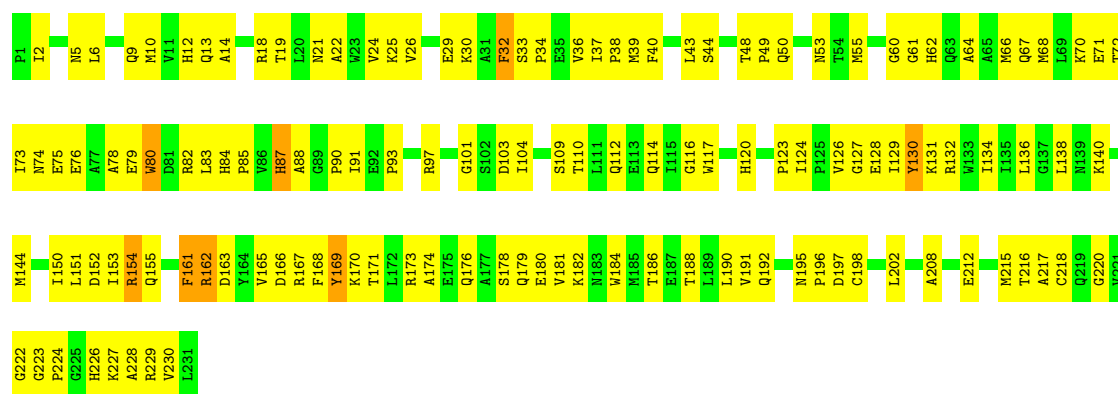
• Molecule 1: capsid protein

Chain kx: 40% 57%



• Molecule 1: capsid protein

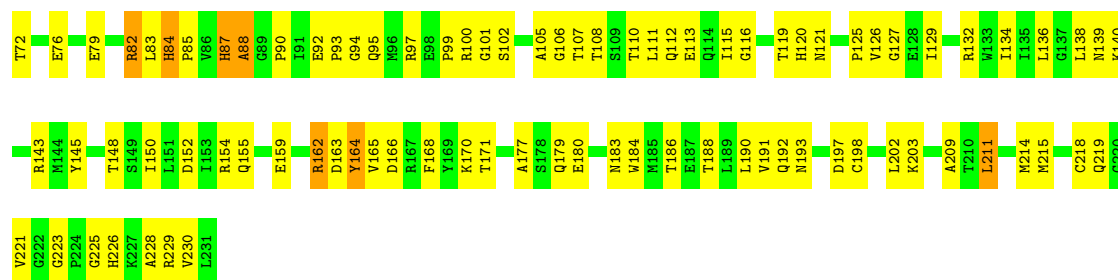
Chain ky: 42% 54%



• Molecule 1: capsid protein

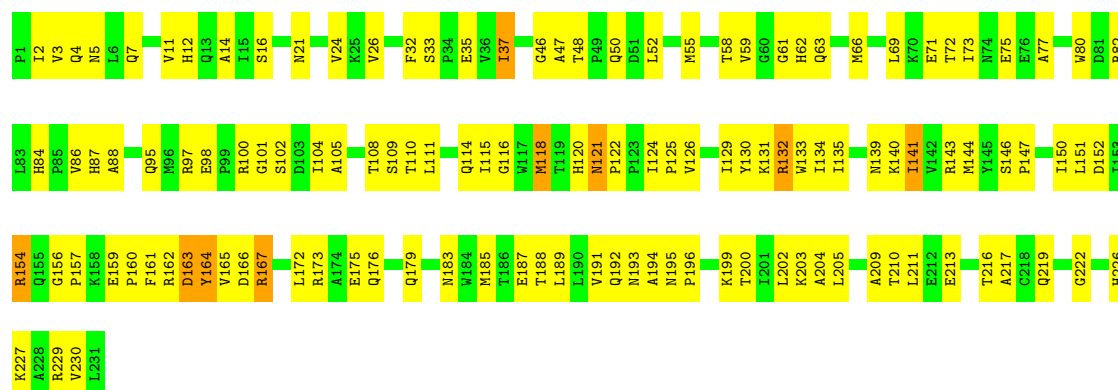
Chain kz: 44% 52%





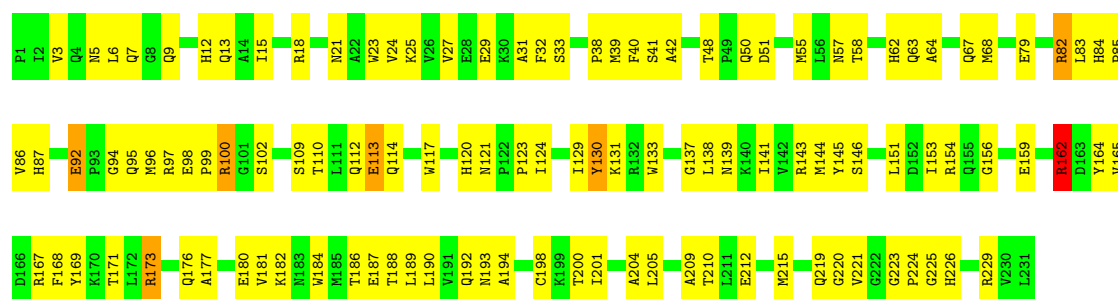
• Molecule 1: capsid protein

Chain kA: 46% 50%



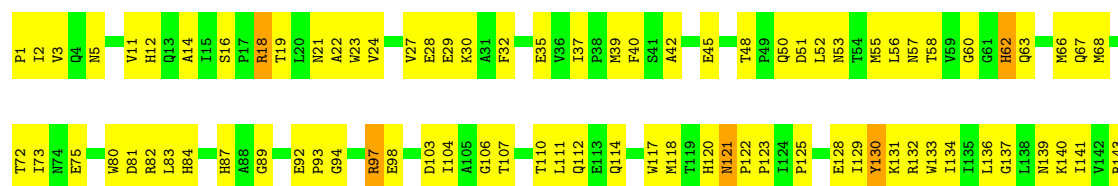
• Molecule 1: capsid protein

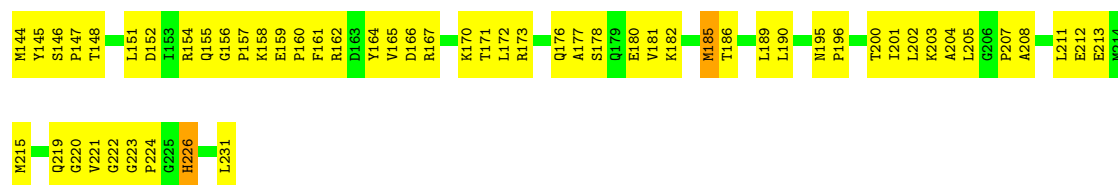
Chain kB: 50% 47%



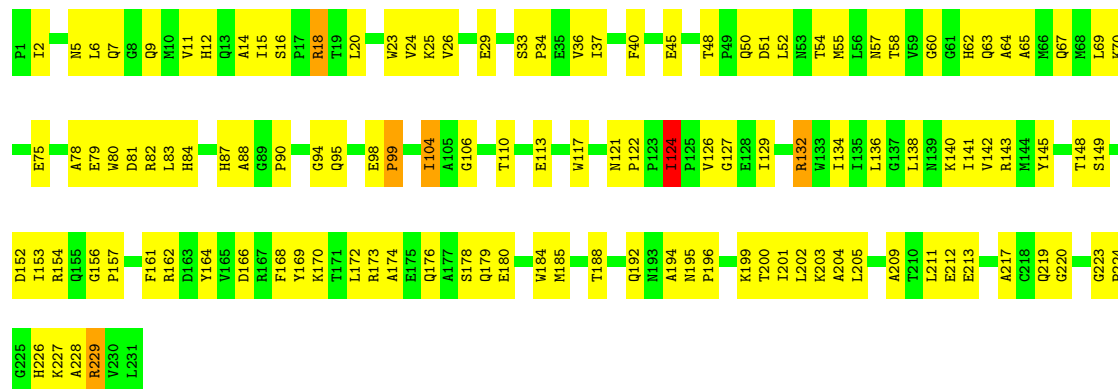
• Molecule 1: capsid protein

Chain kC: 40% 57%

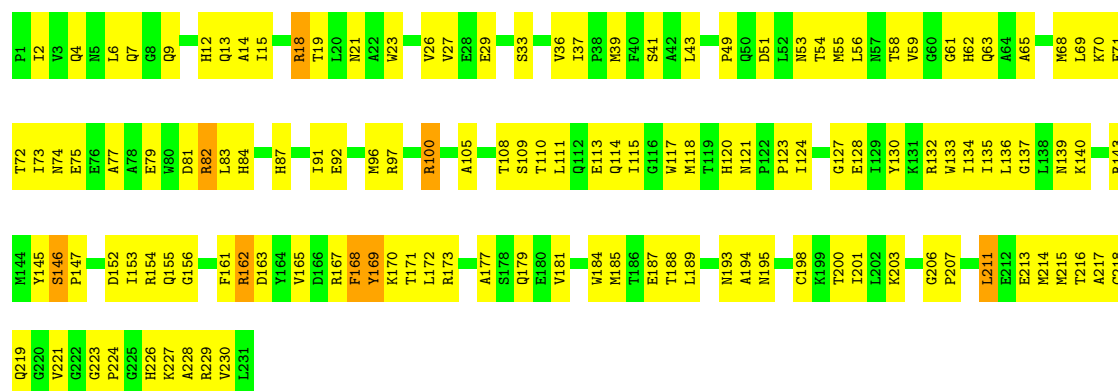




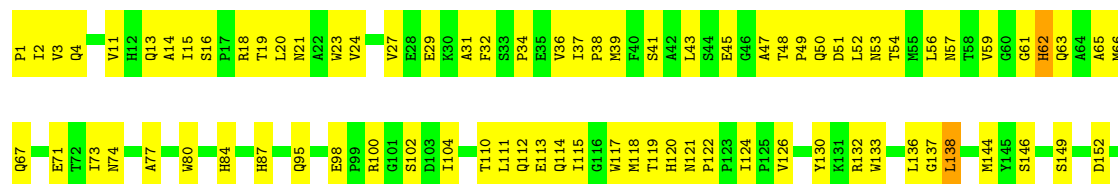
- Molecule 1: capsid protein

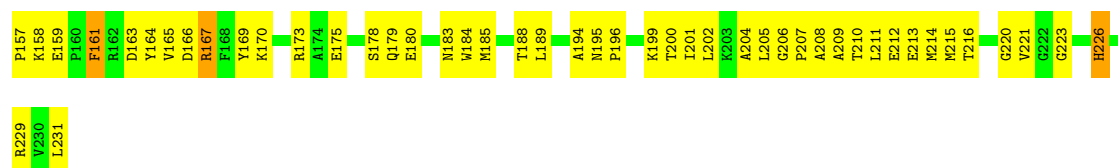


- Molecule 1: capsid protein



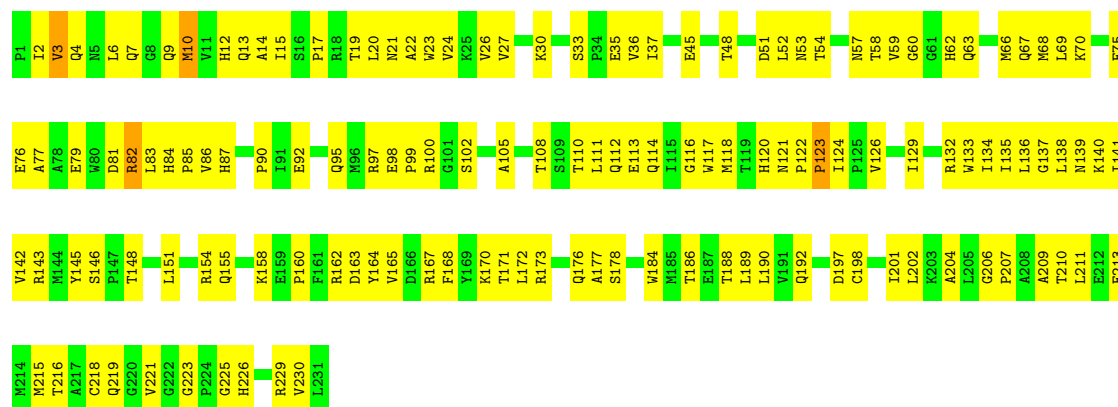
- Molecule 1: capsid protein





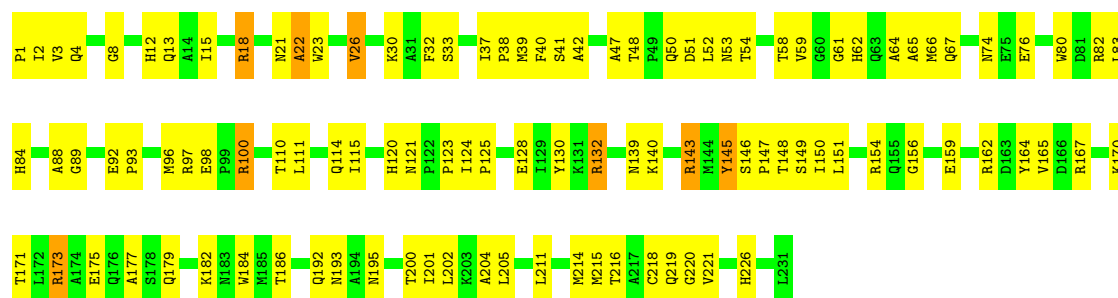
• Molecule 1: capsid protein

Chain kF: 40% 58%



• Molecule 1: capsid protein

Chain kG: 54% 42%



• Molecule 1: capsid protein

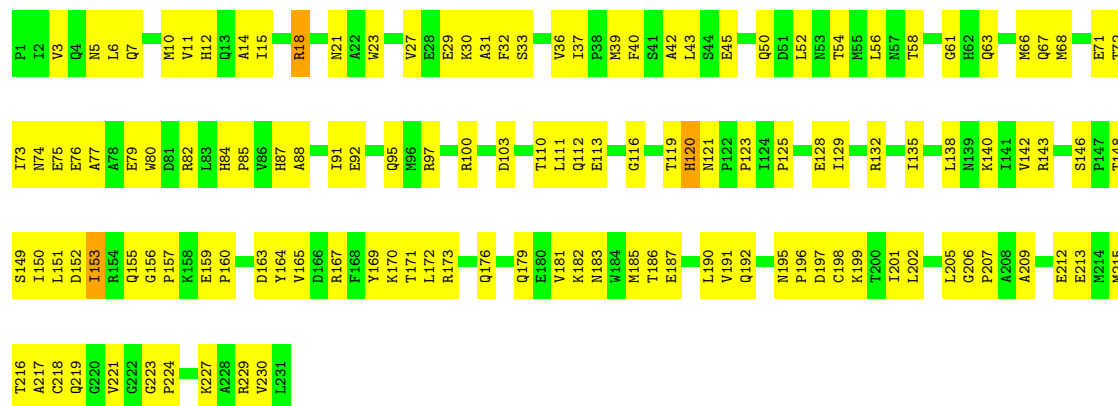
Chain kH: 41% 57%





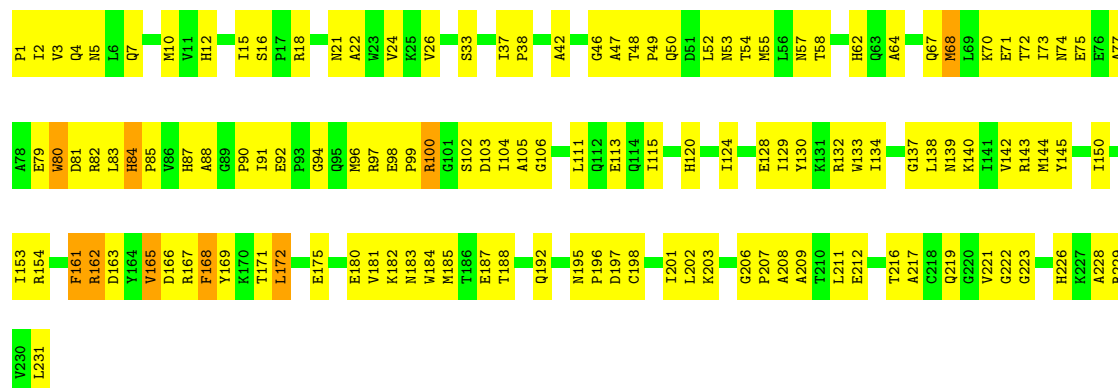
• Molecule 1: capsid protein

Chain kI: 44% 55%



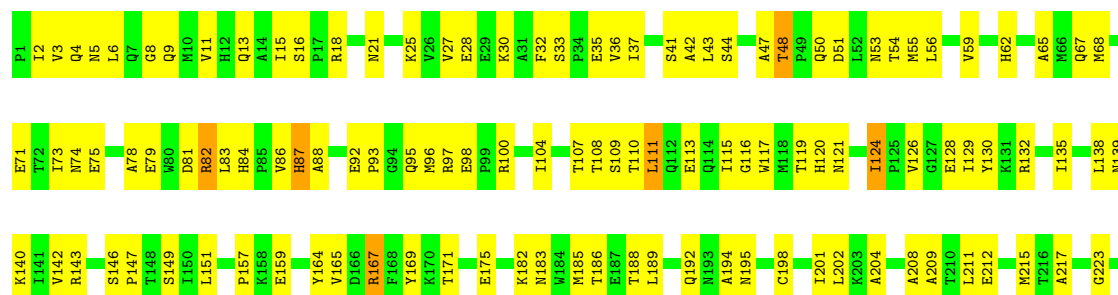
• Molecule 1: capsid protein

Chain kJ: 44% 52%



• Molecule 1: capsid protein

Chain kK: 48% 49%





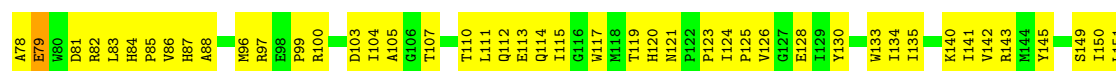
• Molecule 1: capsid protein

Chain kL: 44% 54%



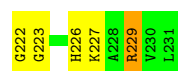
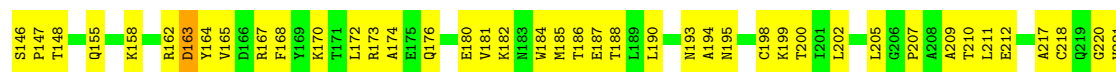
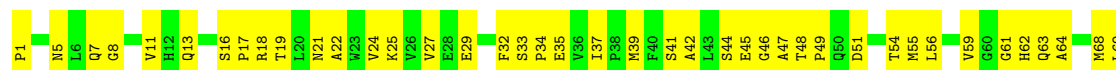
• Molecule 1: capsid protein

Chain kM: 48% 50%

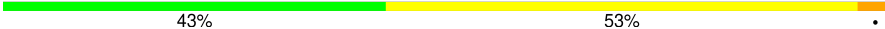


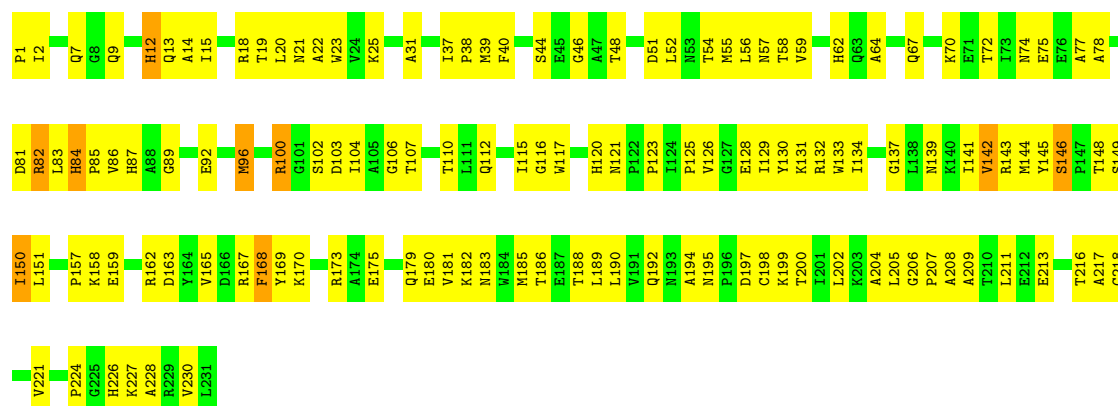
• Molecule 1: capsid protein

Chain kN: 43% 55%

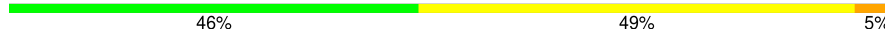


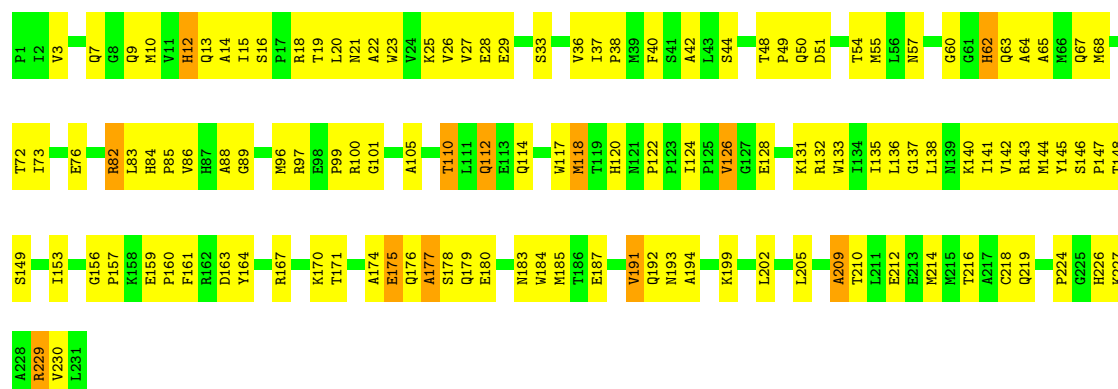
• Molecule 1: capsid protein

Chain 24: 



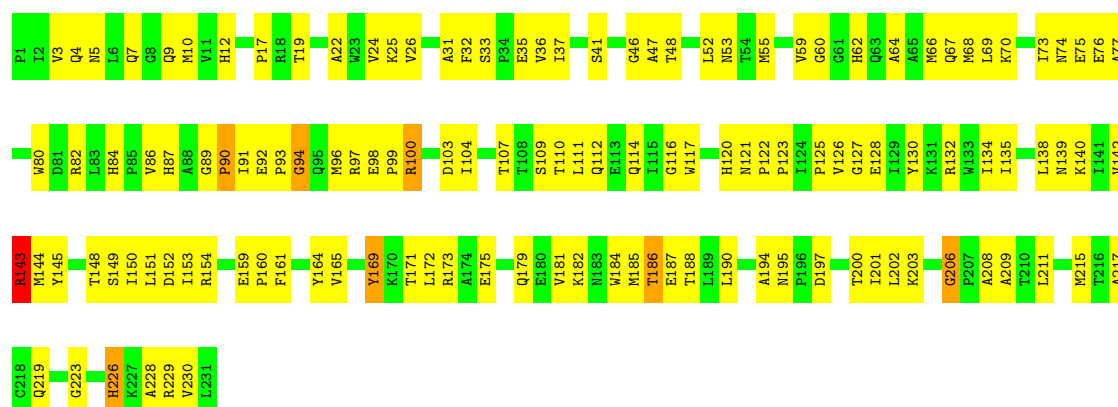
• Molecule 1: capsid protein

Chain kO: 



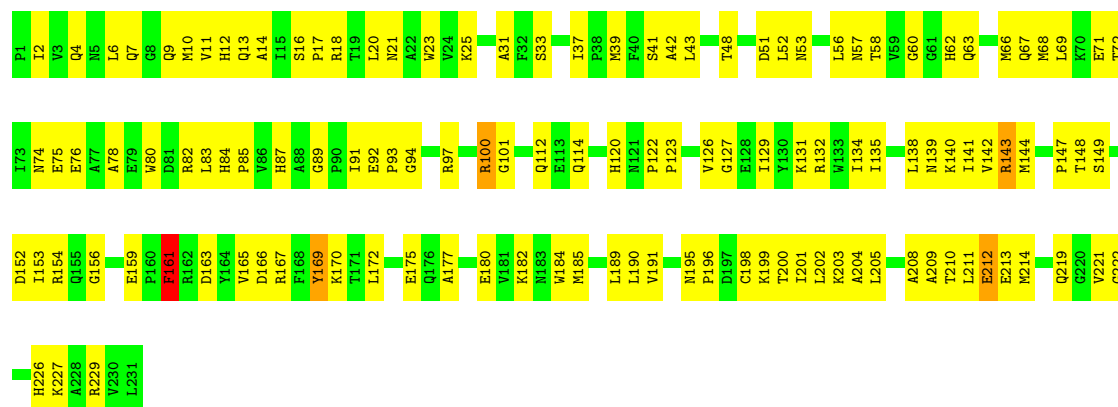
• Molecule 1: capsid protein

Chain kP: 



• Molecule 1: capsid protein

Chain kQ: 



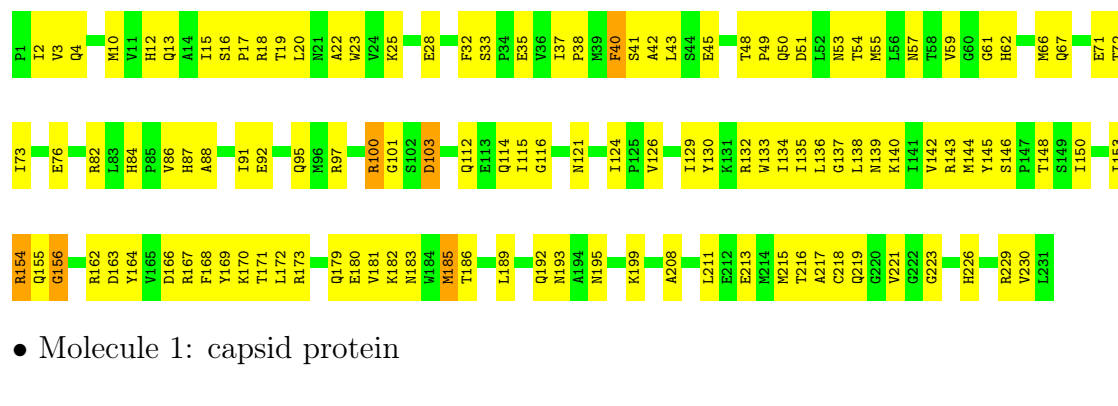
- Molecule 1: capsid protein

Chain kR: 41% 55%



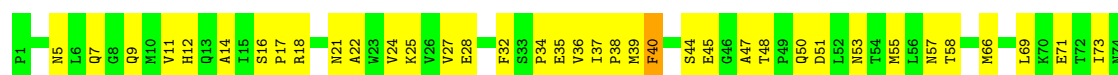
- Molecule 1: capsid protein

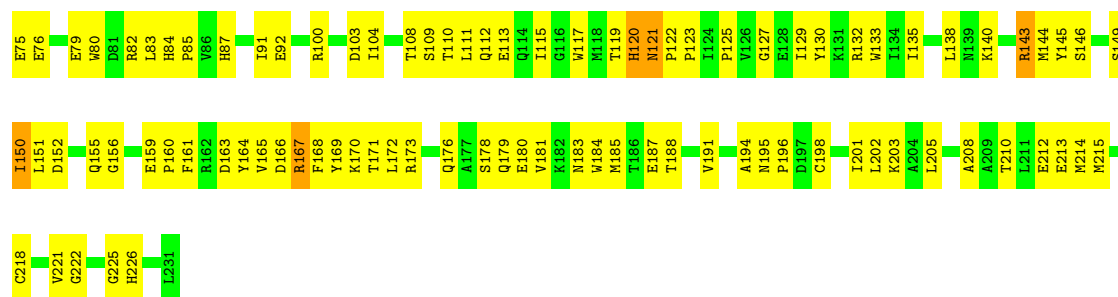
Chain kS: 48% 49%



- Molecule 1: capsid protein

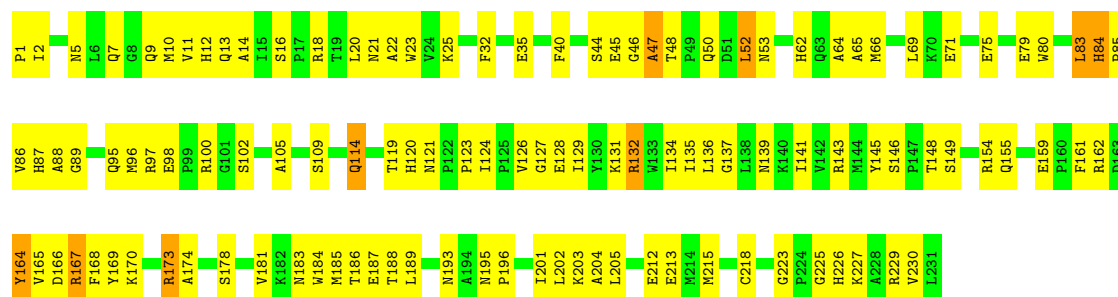
Chain kT: 45% 52%





• Molecule 1: capsid protein

Chain kU: 50% 46%



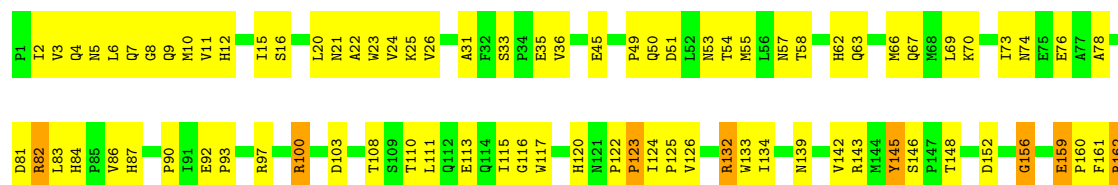
• Molecule 1: capsid protein

Chain kV: 43% 55%



• Molecule 1: capsid protein

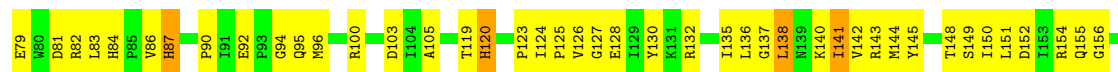
Chain kW: 48% 48%





• Molecule 1: capsid protein

Chain kX: 46% 51%



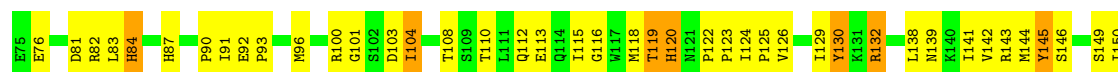
• Molecule 1: capsid protein

Chain 25: 43% 55%



• Molecule 1: capsid protein

Chain kY: 45% 52%

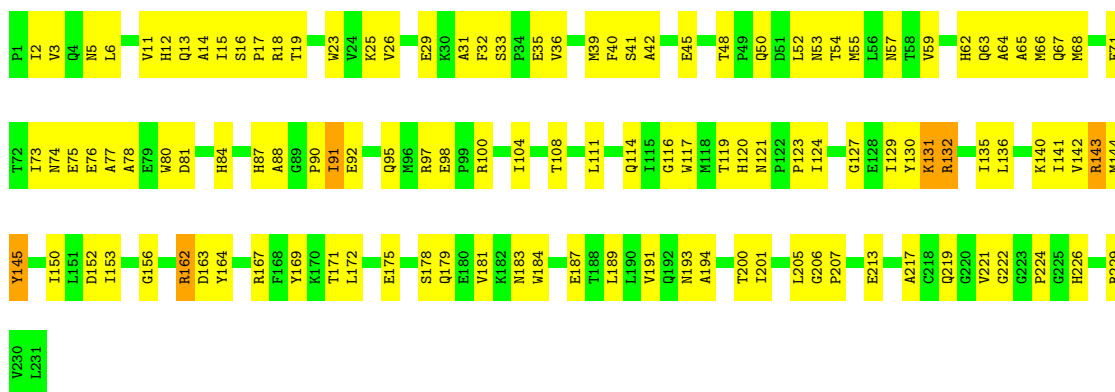


• Molecule 1: capsid protein

R229	P160	W80	P1
V230	F161	D81	I2
L231	R162	H84	N5
	D163	P85	L6
	V164	V86	
	V165	H87	V11
	D166		H12
	R167	P90	Q13
	F168	I91	
	Y169	E92	P17
	K170	P93	R18
	T171	G94	T19
	L172	Q95	L20
	R173	M96	N21
	A174	R97	A22
	E175	E98	W23
	Q176	P99	
	A177	R100	V27
			E28
	V181	D103	E29
	K182		F32
	N183	T110	S33
		L111	P34
	E187	Q112	
	T188	E113	I37
	L189		
	L190	G116	F40
	V191	H117	S41
	Q192	M118	A42
	N193	T119	
	A194	H120	
	N195	N121	G46
	P196		
	D197	G127	P49
	C198	E128	
	K199	T129	L52
	T200	N130	N53
	I201	K131	T54
	L202	R132	M55
			L56
	G206	L136	
	P207	G137	G61
		L138	H62
	T210	N139	Q63
	L211	K140	A64
	E212	T141	A65
	E213	V142	M66
		R143	Q67
	T216	M144	M68
	A217	Y145	L69
	C218	S146	K70
	Q219	P147	E71
		T148	T72
	G222	S149	I73
	G223	I150	N74
		L151	E75
	H226	D152	
	K227		A78
	V228	C155	F70

L211	K140	I73	P1
E212	I141	M74	I2
E213	V142	E75	V3
M214	R143	E76	Q4
M215	M144	A77	N5
	Y145		L6
C218	T148	M80	Q7
Q219		L83	M10
G222	L151	H84	M11
	D152	P85	H12
G225	T153	F86	Q13
H226	R154	H87	A14
			I15
R229	E159	P90	S16
V230	P160	I91	P17
L231	F161		R18
	R162	G94	T19
	D163	Q95	L20
	Y164	M96	N21
	V165	R97	A22
	D166	E98	V23
	R167	P99	V24
	F168	R100	K25
		G101	V26
	T171	S102	V27
	L172	D103	E28
	R173	I104	E29
	A174	A105	K30
		S106	A31
	S178	T107	F32
	Q179	S33	S33
	E180	S109	P34
	V181	T110	E35
	K182	L111	V36
	M183	Q112	I37
	M184	E113	
	M185	Q114	S41
	T186	L115	
	E187	M116	S44
	T188	M117	F45
	L189	M118	G46
	L190	T119	
	V191	H120	D51
	Q192	M121	L52
		P122	M53
	P196	P123	T54
	D197	I124	M55
	C198		L56
	K199	E128	V59
	T200	Y130	
	L201	K131	H62
	L202	R132	Q63
	L205	L133	
	G206	T134	M66
	P207	L135	Q67
	A208	L136	M68
	A209		
	T210	M138	T72

R229	D152	E76	P1
V230	I153	A77	I2
L231	R154		V3
		D81	Q4
	K158	R82	N5
	E159	L83	
	P160	H84	Q9
	F161	P85	M10
	R162	V86	V11
	D163	H87	H11
	V164	A88	Q13
	V165	G89	
	D166	P90	P17
	F168	I91	R18
		E92	T19
		P93	L20
	R173	G94	N21
		Q95	A22
	Q176	M96	W23
	A177	R97	V24
	S178		
		R100	V27
	V181		E28
	K182	D103	E29
	M183		
	V184	G106	F32
	M185	T107	S33
	T186	T108	P34
	E187	S109	F35
	T188		V36
	L189	Q112	I37
	L190	E113	
		Q114	F40
	N195	I115	S41
	P196	G116	A42
	D197	V117	L43
	C198	M118	S44
	K199	T119	E45
		H120	G46
		M121	A47
			T48
	L202	E128	
	K203	I129	D51
	A204	V130	L52
	G205	R131	N53
	P207	R132	L56
	A208	W133	M57
	A209	V134	T58
	T210	I135	V59
	L211	L136	
	E212	G137	Q63
			A64
	M215	L138	A65
	T216	M139	M66
	A217		Q67
	G218	V142	M68
	Q219	R143	
		M144	
	P224		E71
	G225	I150	
	W226	L151	



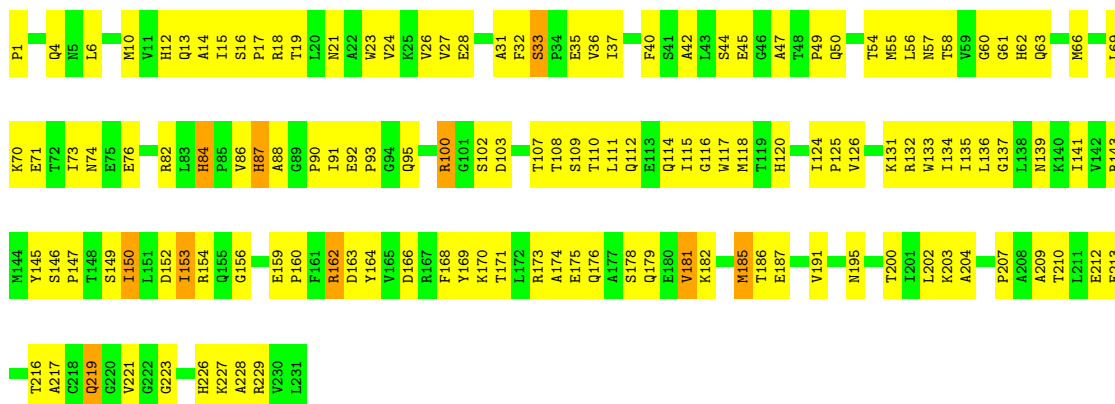
• Molecule 1: capsid protein

Chain 13: 43% 51% 6%



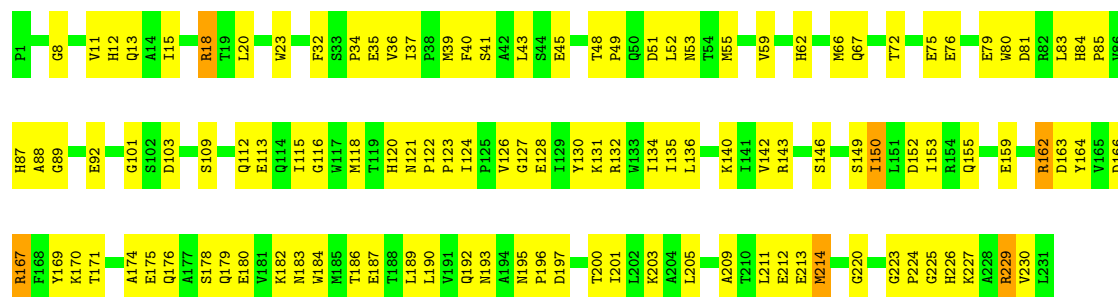
• Molecule 1: capsid protein

Chain 14: 42% 54%



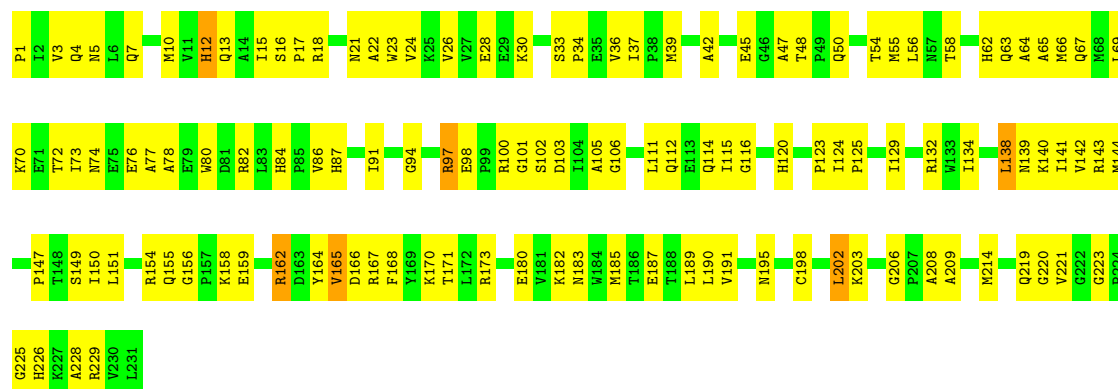
• Molecule 1: capsid protein

Chain 15: 50% 48%



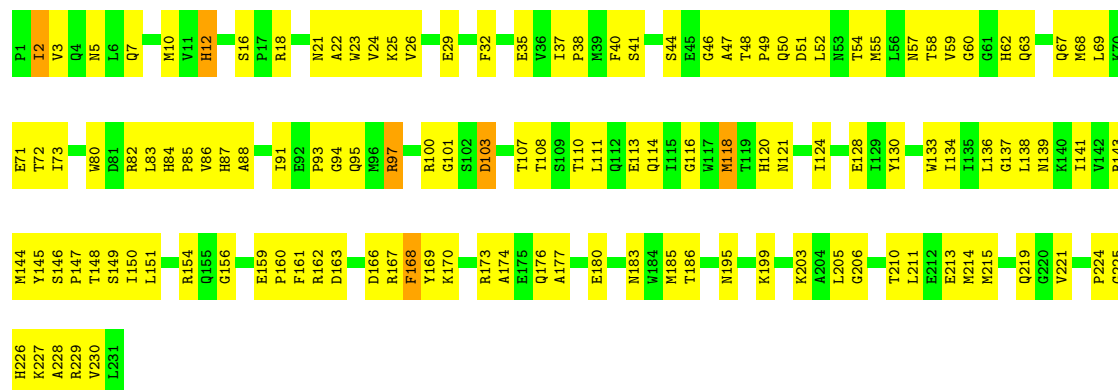
- Molecule 1: capsid protein

Chain 16: 47% 51%



- Molecule 1: capsid protein

Chain 17: 45% 52%



- Molecule 1: capsid protein

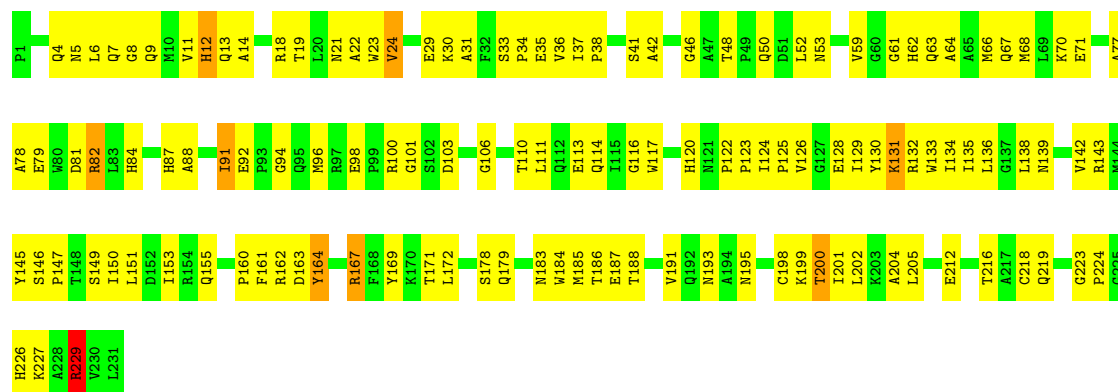
Chain 26: 43% 53%





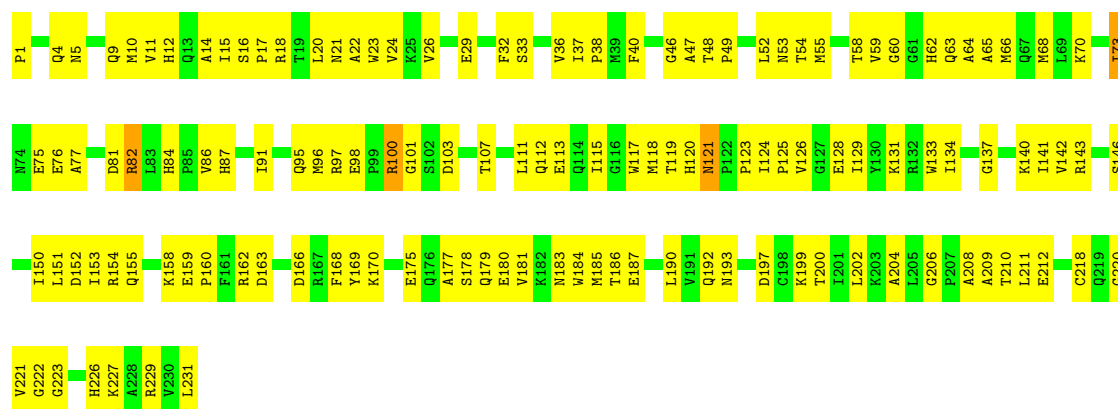
• Molecule 1: capsid protein

Chain l8: 45% 52%



• Molecule 1: capsid protein

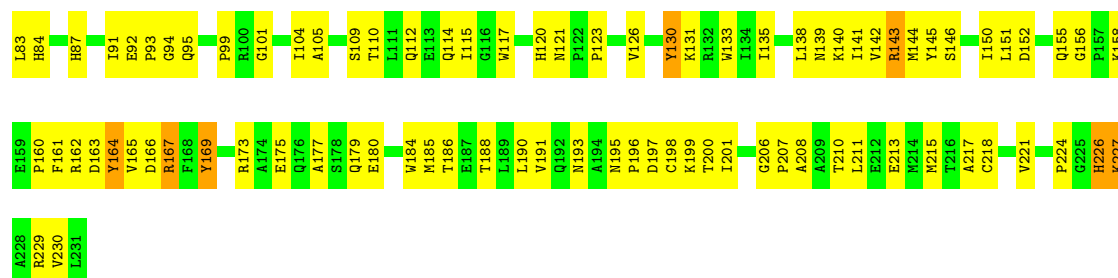
Chain l9: 42% 56%



• Molecule 1: capsid protein

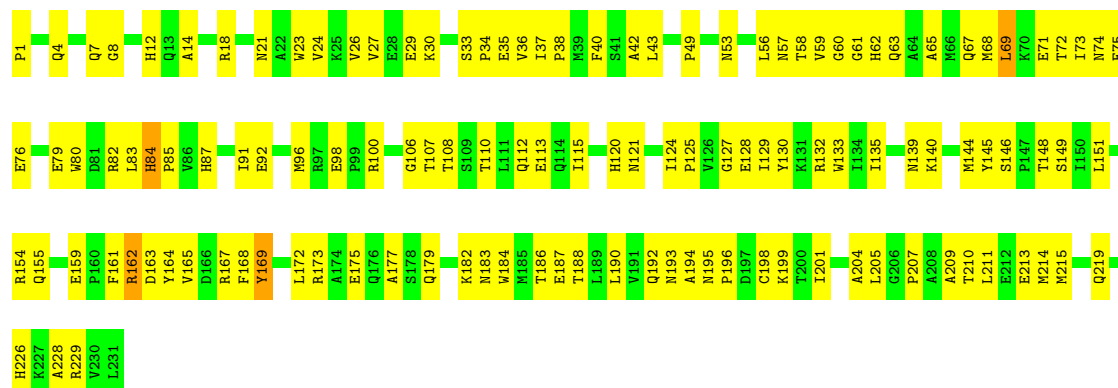
Chain la: 45% 51%





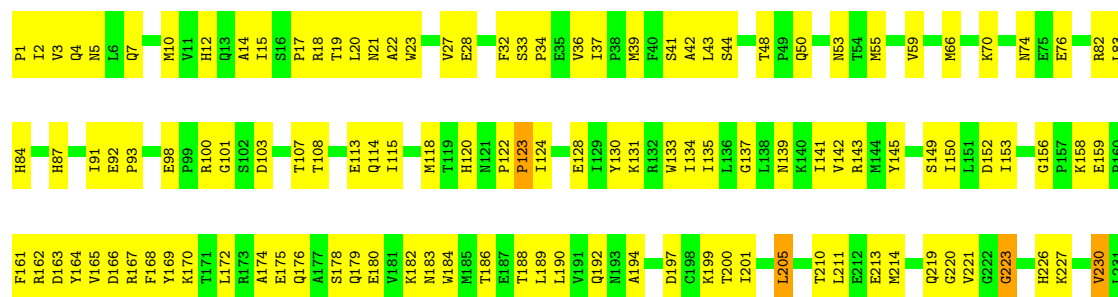
• Molecule 1: capsid protein

Chain lb: 46% 52%



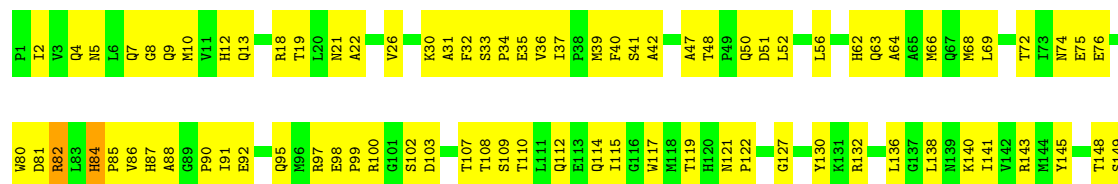
• Molecule 1: capsid protein

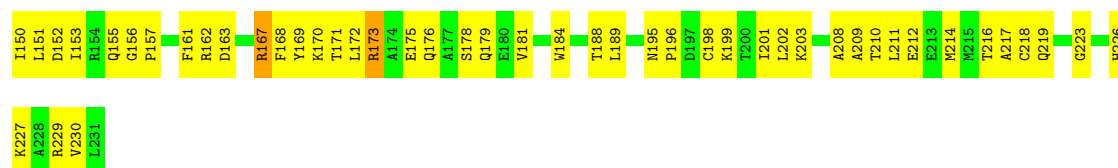
Chain lc: 48% 50%



• Molecule 1: capsid protein

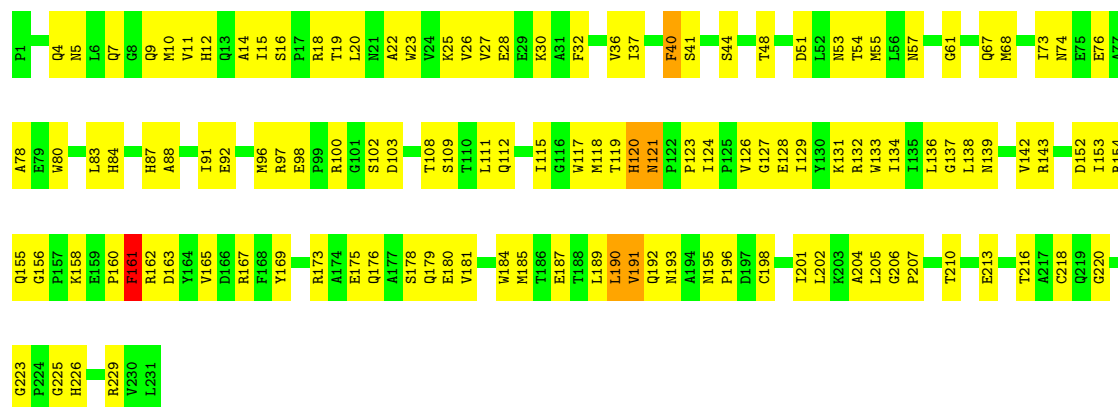
Chain ld: 44% 54%





• Molecule 1: capsid protein

Chain le: 46% 51%



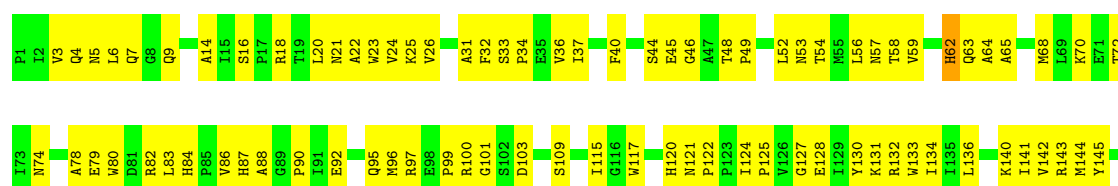
• Molecule 1: capsid protein

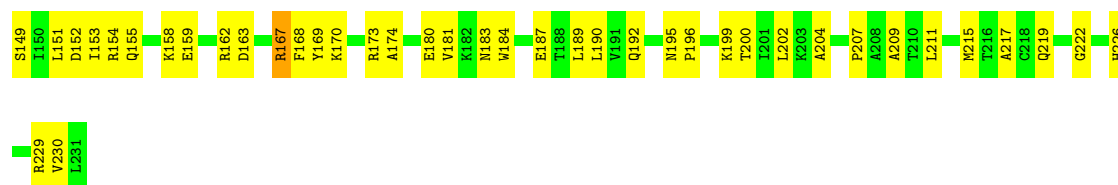
Chain lf: 42% 55%



• Molecule 1: capsid protein

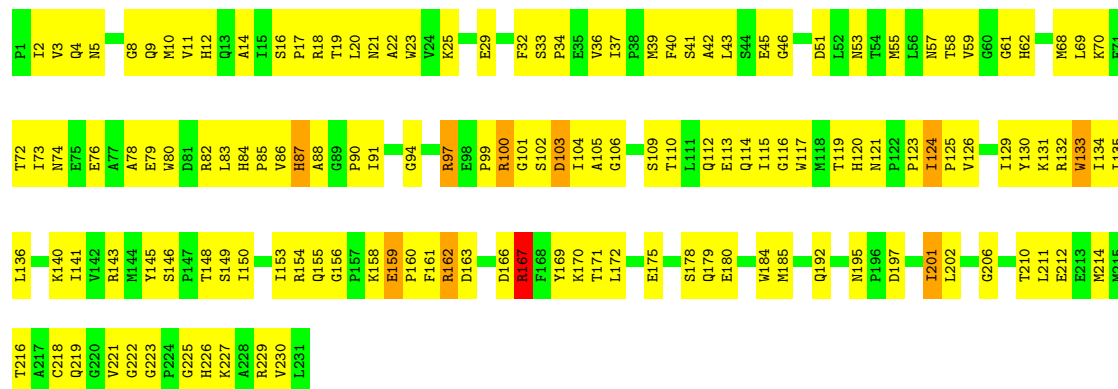
Chain lg: 47% 52%





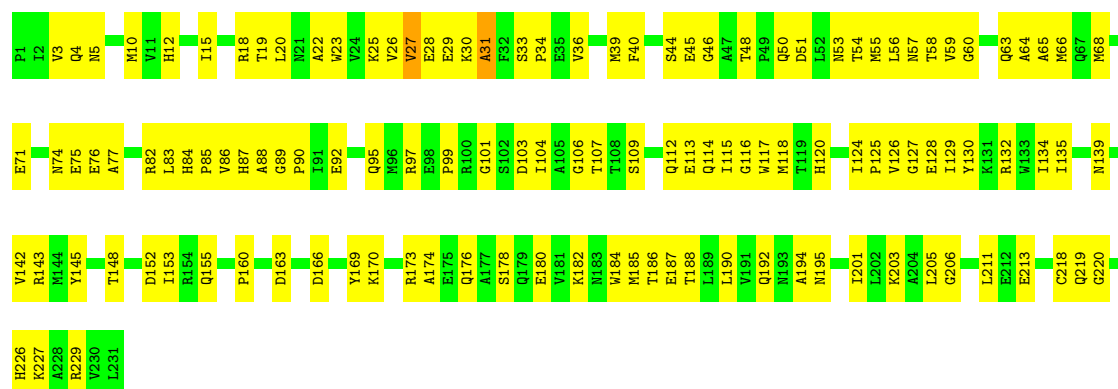
- Molecule 1: capsid protein

Chain lh:



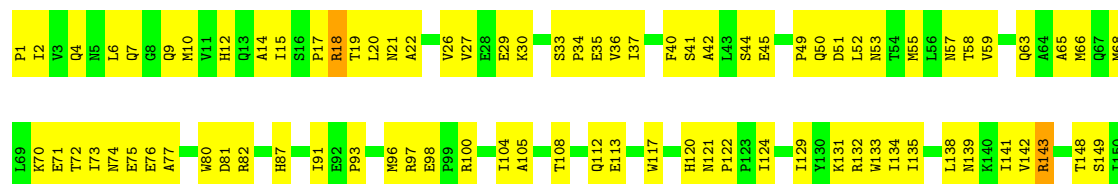
- Molecule 1: capsid protein

Chain 27:



- Molecule 1: capsid protein

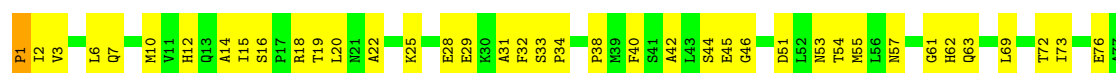
Chain li:





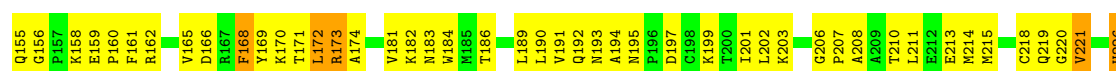
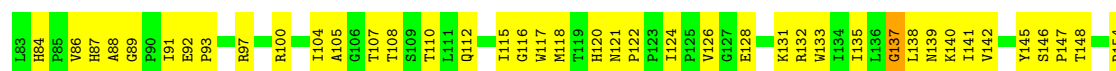
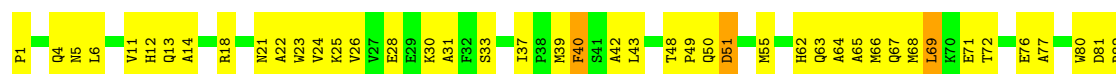
• Molecule 1: capsid protein

Chain lm: 45% 55%



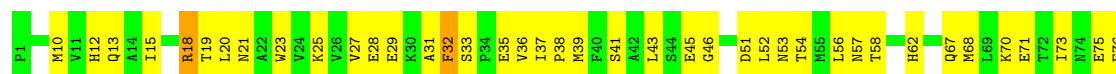
• Molecule 1: capsid protein

Chain ln: 42% 53% 5%



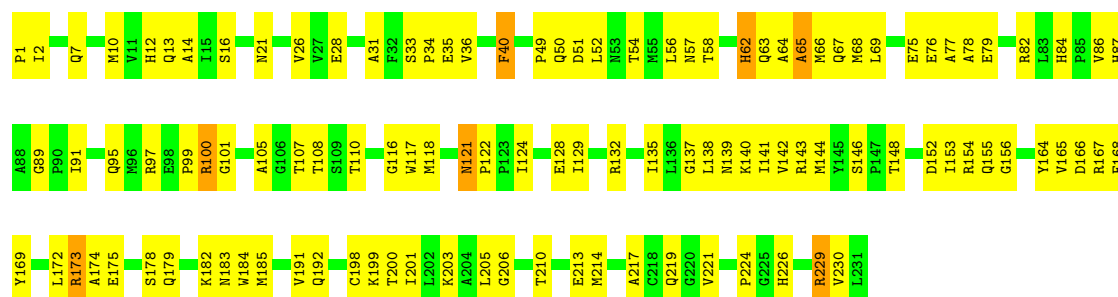
• Molecule 1: capsid protein

Chain lo: 48% 50%

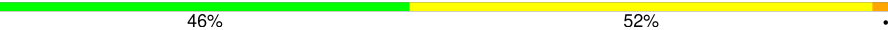


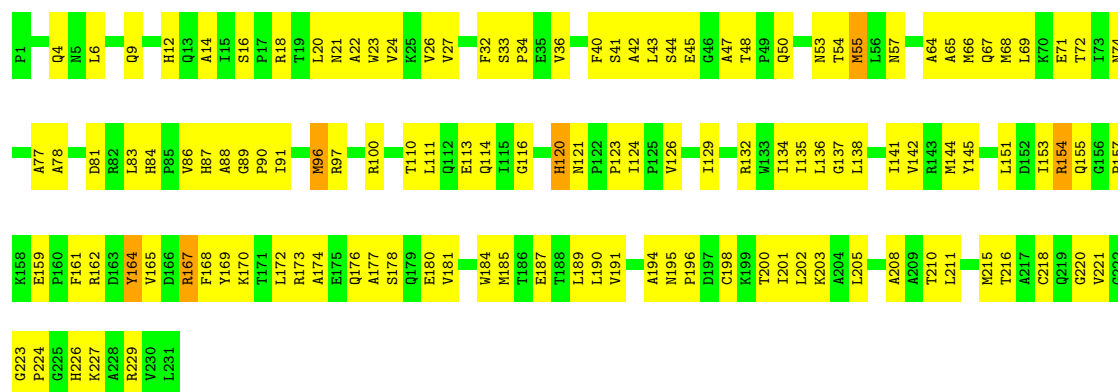
• Molecule 1: capsid protein

Chain lp: 



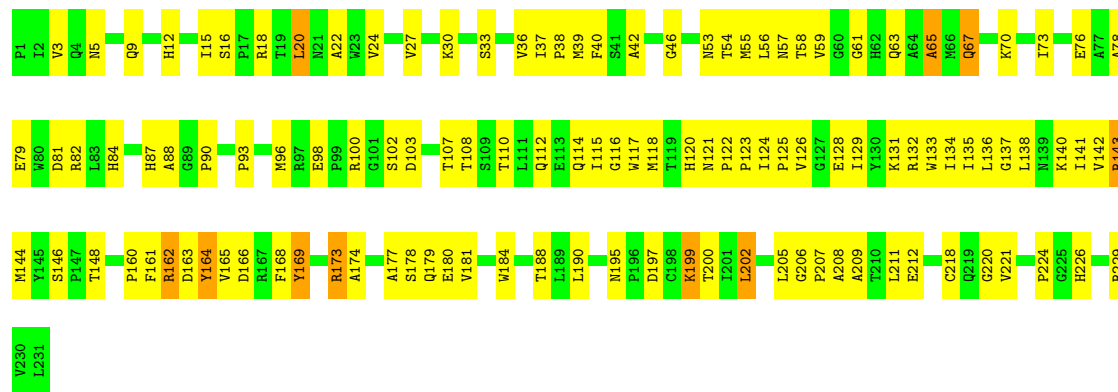
• Molecule 1: capsid protein

Chain lq: 

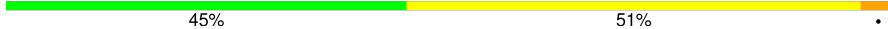


• Molecule 1: capsid protein

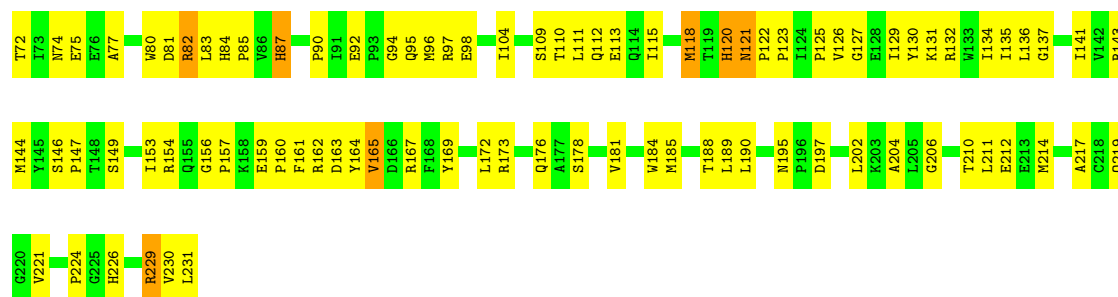
Chain lr: 



• Molecule 1: capsid protein

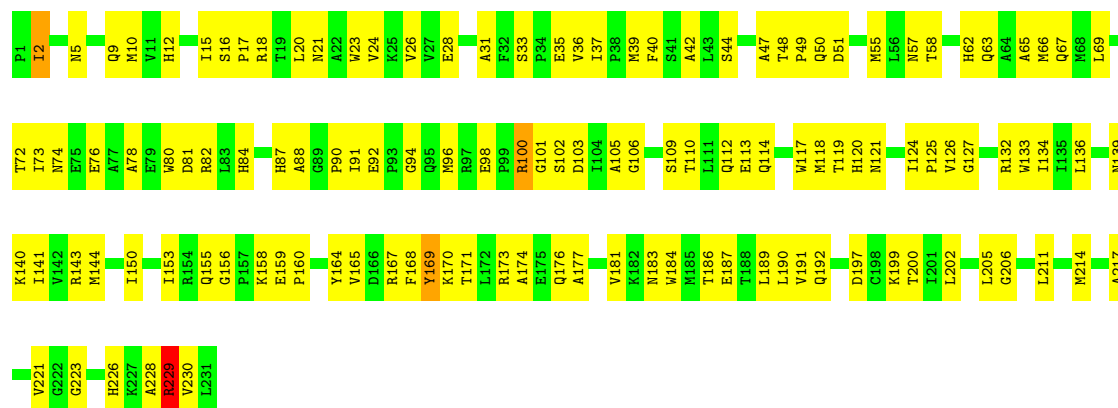
Chain 28: 





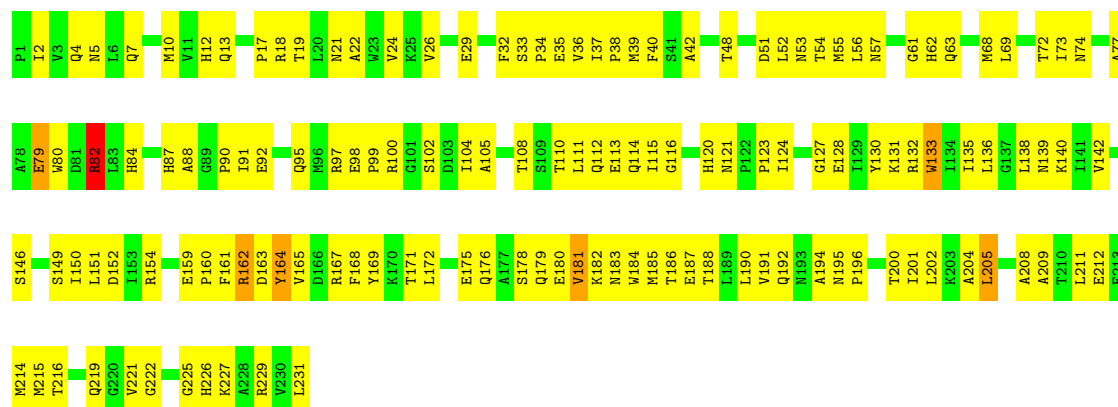
• Molecule 1: capsid protein

Chain ls: 45% 53%



• Molecule 1: capsid protein

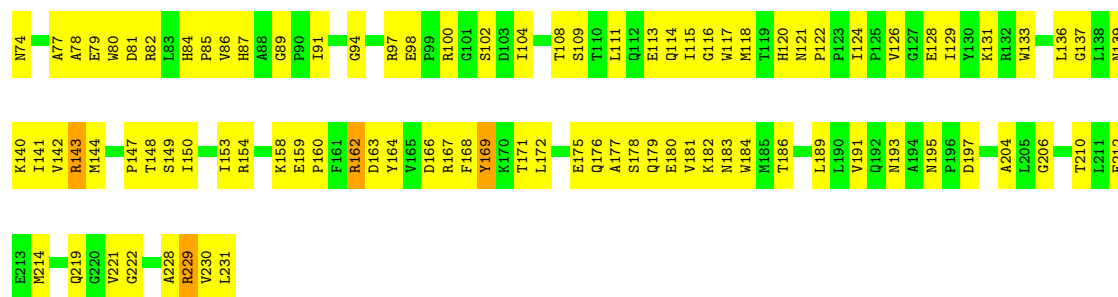
Chain lt: 39% 58%



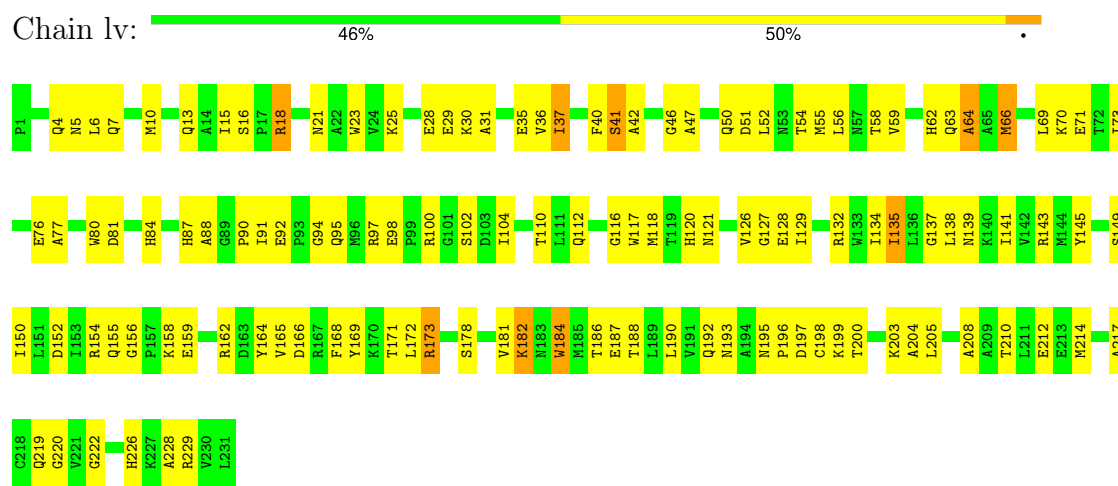
• Molecule 1: capsid protein

Chain lu: 44% 54%

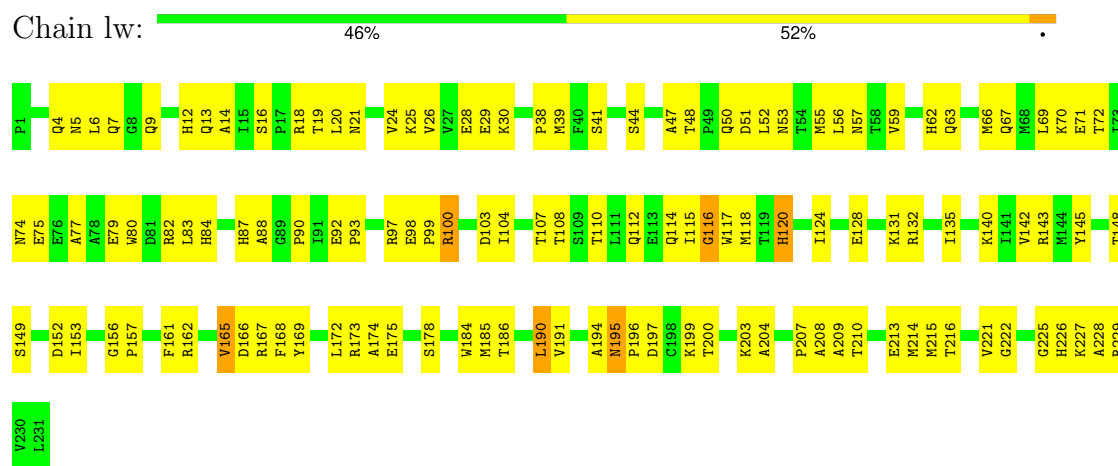




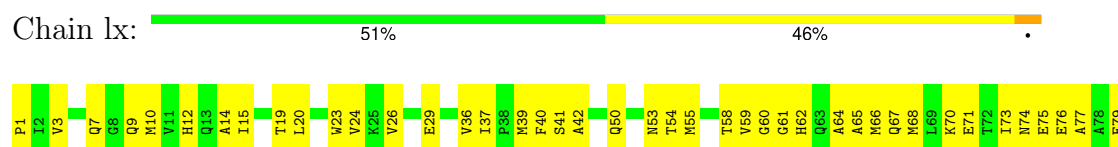
• Molecule 1: capsid protein

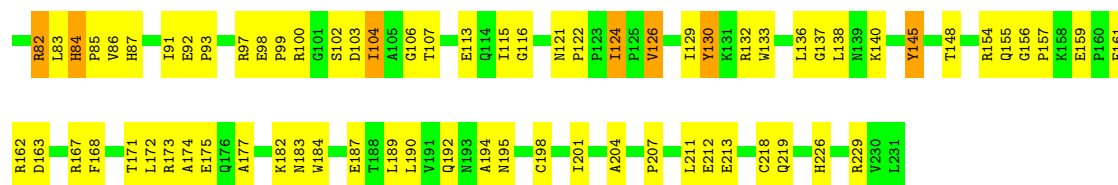


• Molecule 1: capsid protein



• Molecule 1: capsid protein

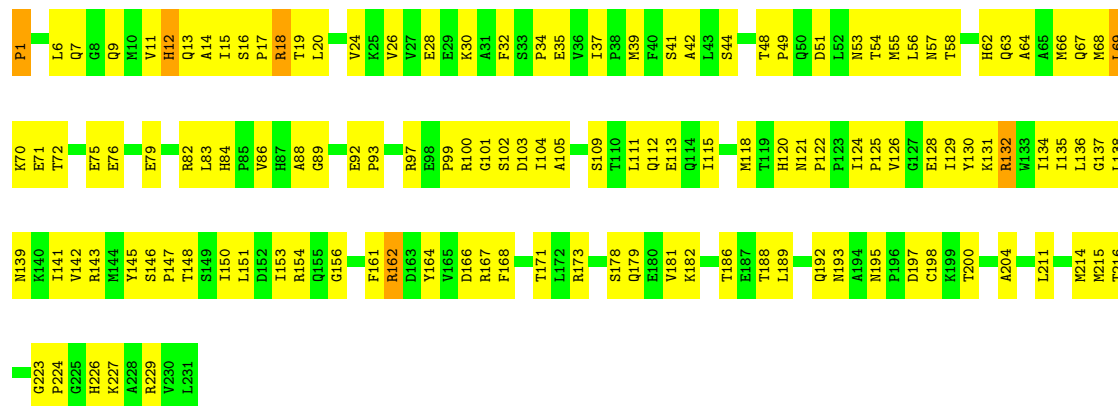




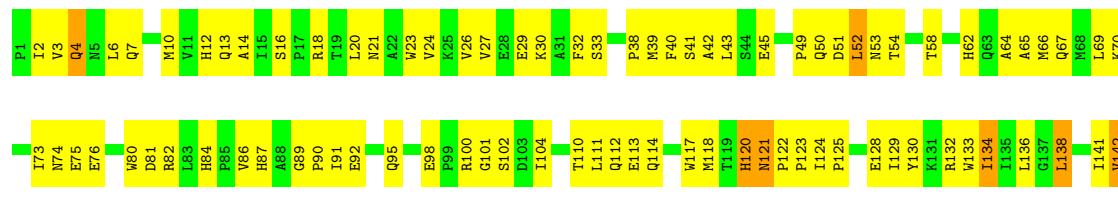
• Molecule 1: capsid protein

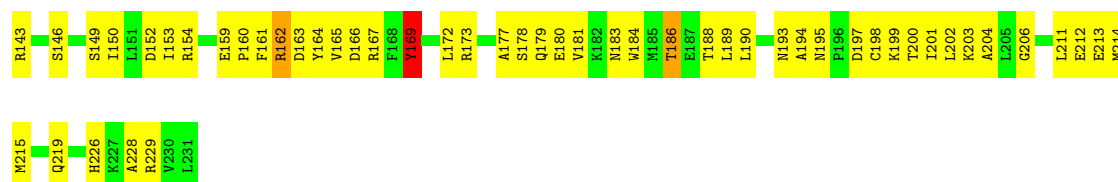


• Molecule 1: capsid protein

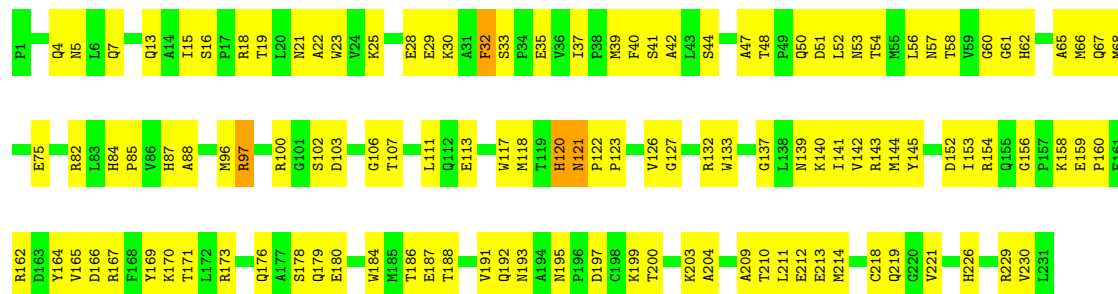


• Molecule 1: capsid protein





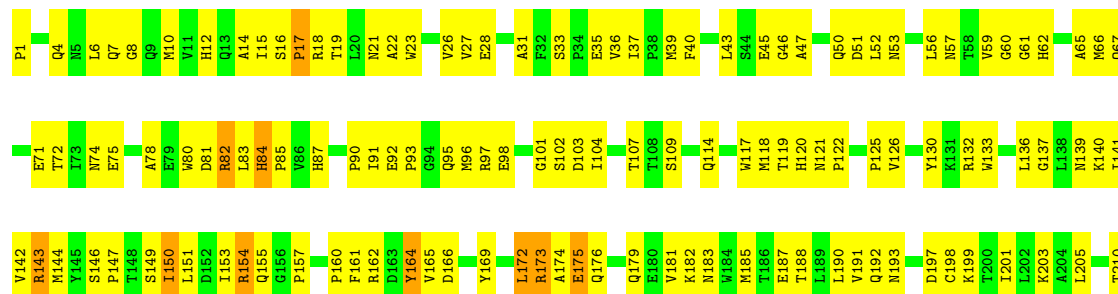
• Molecule 1: capsid protein



• Molecule 1: capsid protein

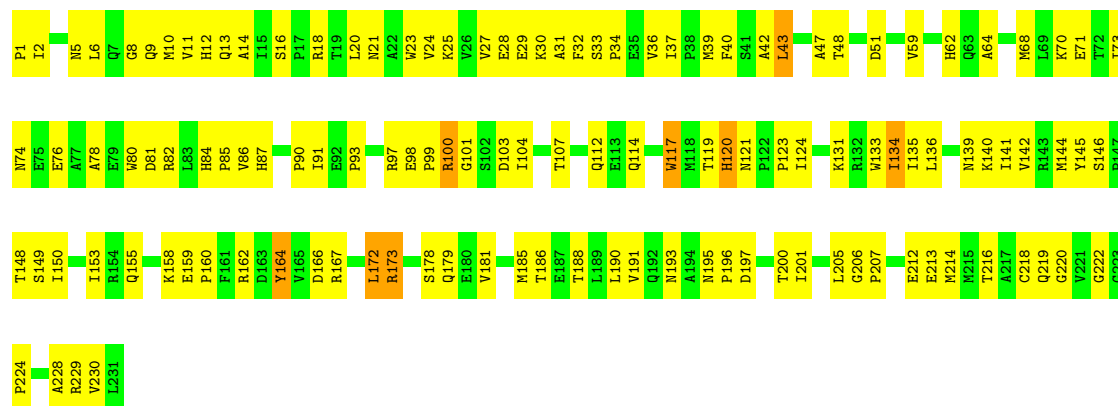


• Molecule 1: capsid protein

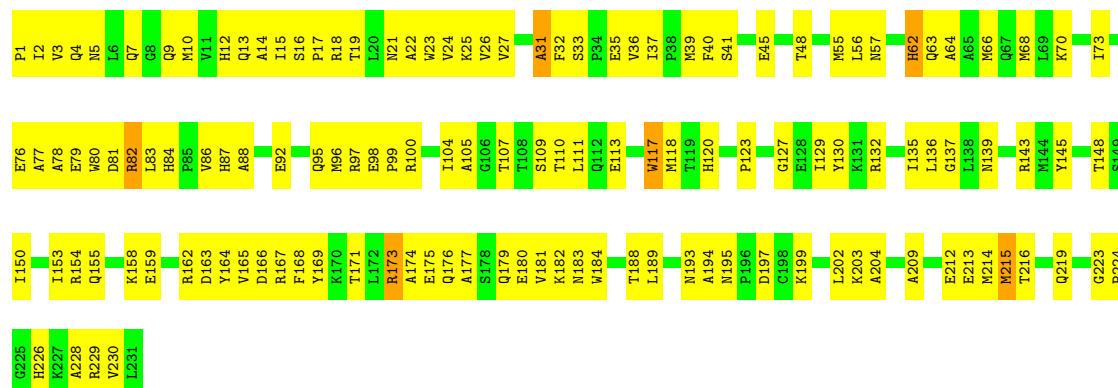




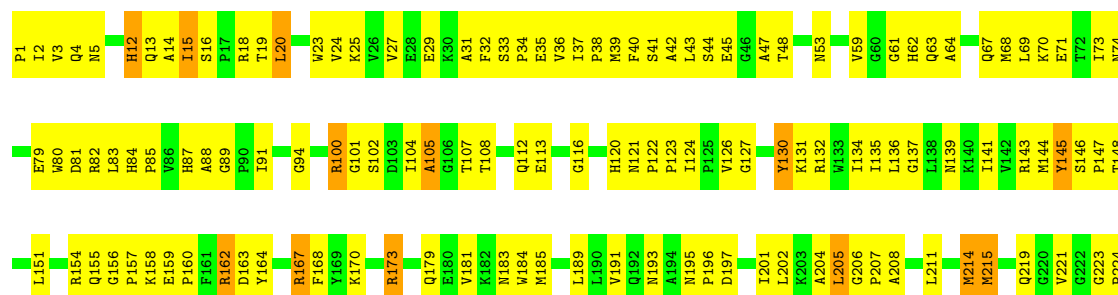
- Molecule 1: capsid protein



- Molecule 1: capsid protein



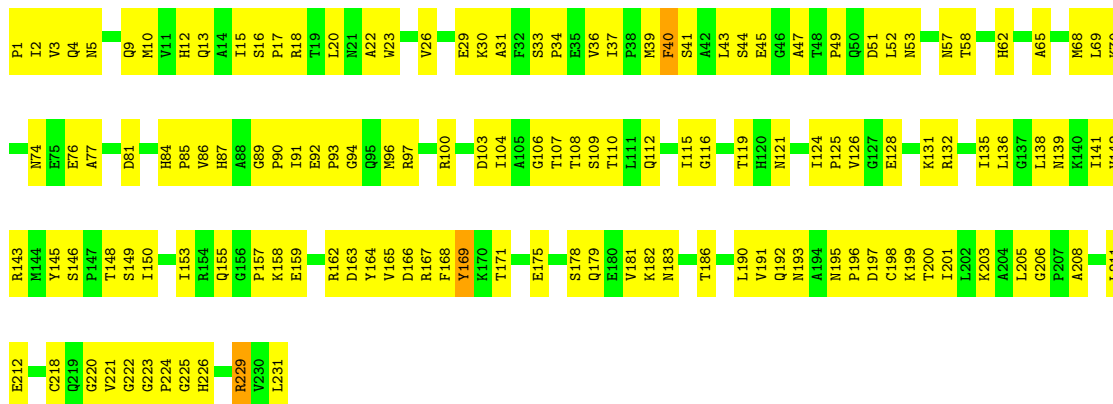
- Molecule 1: capsid protein





• Molecule 1: capsid protein

Chain IG: 41% 58%



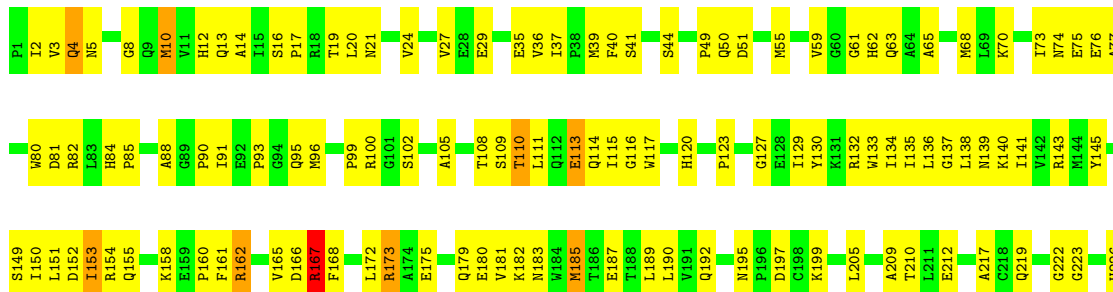
• Molecule 1: capsid protein

Chain IH: 44% 53%



• Molecule 1: capsid protein

Chain II: 46% 50%



K227
A228
R229
V230
L231

• Molecule 1: capsid protein

Chain IJ: 50% 48%

P1 I2 V3 L6 Q7 C8 Q9 M10 H11 H12 H16 P17 P18 T19 V27 E28 F32 S33 P34 P35 E36 V36 I37 P38 M39 N121 A42 E45 G46 A47 T48 P49 Q50 D51 L52 N53 T54 M55 L56 M57 T58 V59 G60 G61 H62 G63 A64 A65 M66 Q67 K70 E71 T72 E76

A77 A78 R82 L83 H84 H87 A88 C89 P90 H12 P91 P92 P93 P94 Q95 Q96 R97 R98 P99 R100 R101 S102 E113 T119 H120 N121 P122 P123 P124 P125 V126 I129 Y130 Q131 R132 W133 I134 I135 L136 L137 L138 M139 G140 I141 V142 V143 M144 Y145 S146 P147 R154 Q155 G156 E159

R162 V165 D166 R167 F168 F169 T171 L172 P173 Q176 A177 S178 Q179 R180 R181 L182 K183 R184 W185 T188 N193 A194 N195 C198 C199 T200 P207 A208 A209 T210 T211 E212 T216 A217 C218 G225 H226 K227 A228 R229 V230 L231

• Molecule 1: capsid protein

Chain IK: 41% 56%

P1 I2 V3 Q4 L6 Q9 M10 H11 H12 H14 A14 H15 H16 P17 S16 P18 R19 T19 R20 N21 A22 W23 V24 V25 K25 E26 V27 E28 E29 E30 K30 A31 F32 V36 I37 P38 M39 F40 S41 A42 L43 S44 T48 P49 Q50 D51 L52 N53 T54 M55 L56 M57 T58 V59 G60 G61 H62 Q63 Q67

M68 L69 K70 E71 T72 T73 N74 A78 E79 W80 D81 H84 P85 V86 H87 A88 G89 P90 E91 E92 Q95 M96 R97 E98 R99 R100 D103 I104 A105 G106 T107 L111 Q112 E113 Q114 I115 G116 W117 H120 N121 P122 P123 I124 T125 V126 G127 E128 I129 R132 W133 I134 L138

N139 K140 I141 M144 Y145 T148 S149 I153 G156 P157 K158 E159 F160 F161 A162 D163 D164 V165 D166 R167 F168 Y169 L172 S178 Q179 E180 V181 K182 M183 W184 M185 T186 E187 T188 A194 N195 P196 T200 I201 L202 K203 A204 L205 G206 P207 A208 A209 T210 W215 C218

Q219 G220 V221 G222 G223 P224 K227 A228 R229 V230 L231

• Molecule 1: capsid protein

Chain IL: 42% 57%

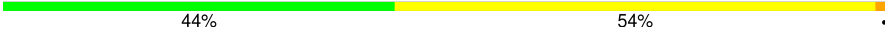
P1 I2 N5 L6 C8 Q9 H12 Q13 H14 A14 S16 P17 R18 N21 A22 W23 V24 K25 E28 E29 K30 A31 F32 S33 V36 I37 P38 M39 F40 S41 S44 E45 P49 M53 M55 L56 M57 T58 V59 G60 G61 H62 Q63 M68 L69 K70 E71 T72 E76

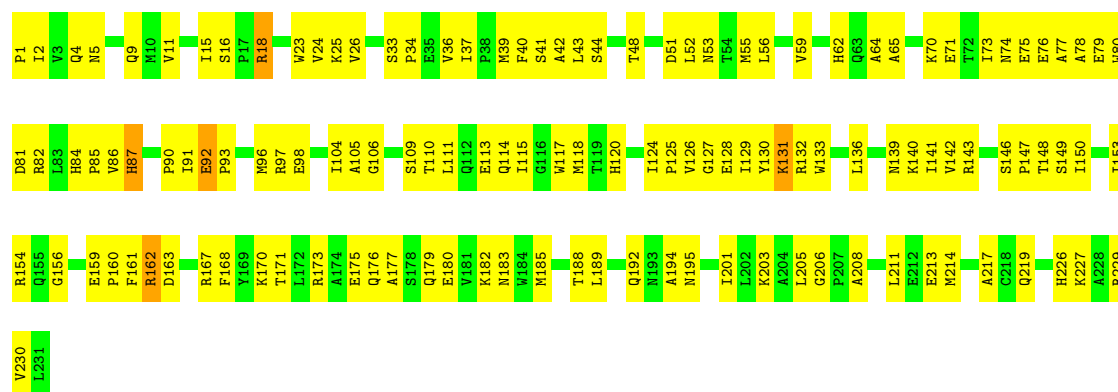
E75 E76 A77 A78 E79 W80 D81 R82 L83 H84 P85 V86 H87 A88 G89 P90 E91 E92 P93 M96 R97 R100 A105 T107 L111 Q114 I115 G116 W117 H120 P123 I124 P125 V126 G127 E128 I129 R130 K131 R132 W133 I134 I135 L136 L137 L138 M139 K140 I141 V142 R143 M144

Y145 T148 S149 I150 G156 P157 K158 E159 F161 R162 D163 Y164 V165 D166 R167 R173 R174 A177 Q179 E180 V181 K182 M183 W184 M185 T186 E187 T188 L189 L190 Y191 Q192 N193 N195 P196 D197 G198 K199 T200 I201 L202 G206 T210 E213 H214 M215 T216 A217 G220

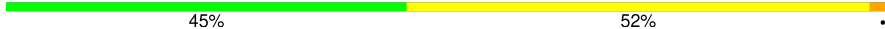
V221 P224 G225 H226 K227 A228 R229 V230 L231

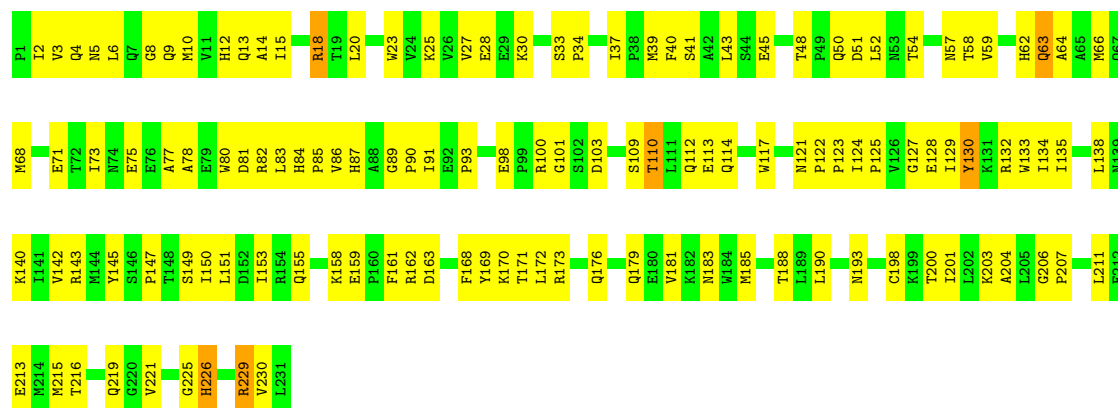
• Molecule 1: capsid protein

Chain 2a: 



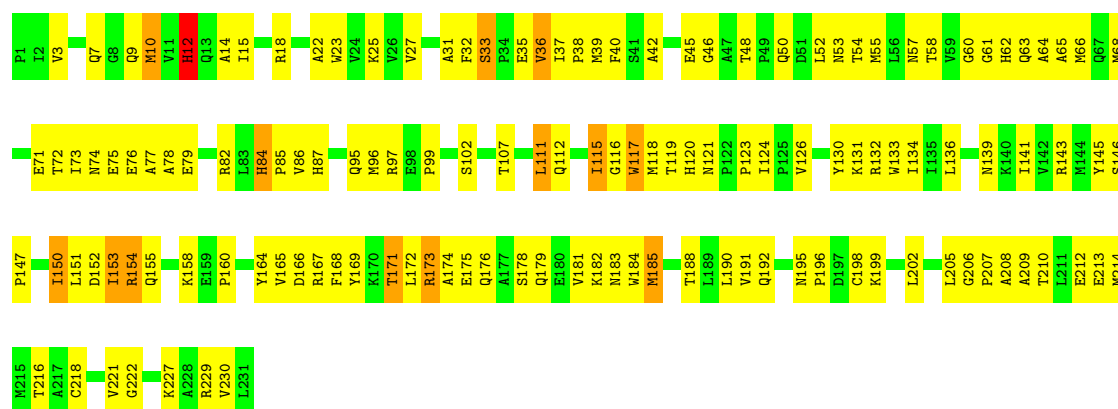
• Molecule 1: capsid protein

Chain 1M: 



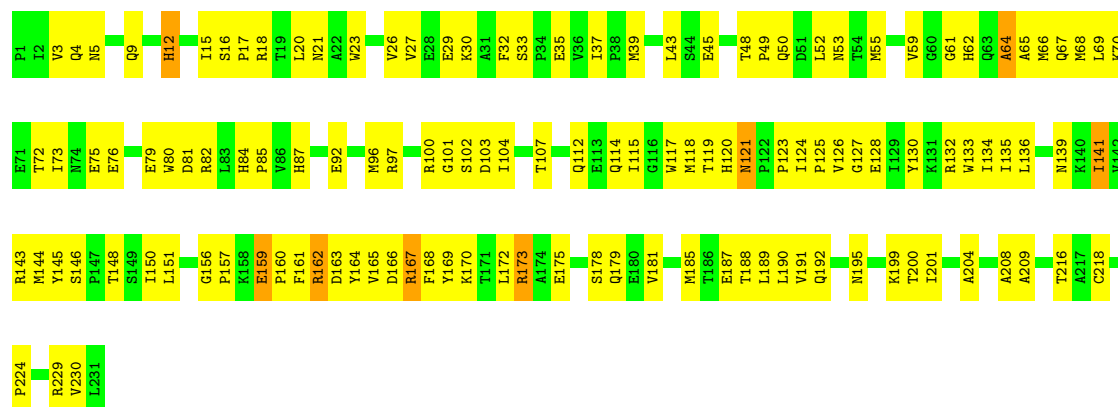
• Molecule 1: capsid protein

Chain 1N: 



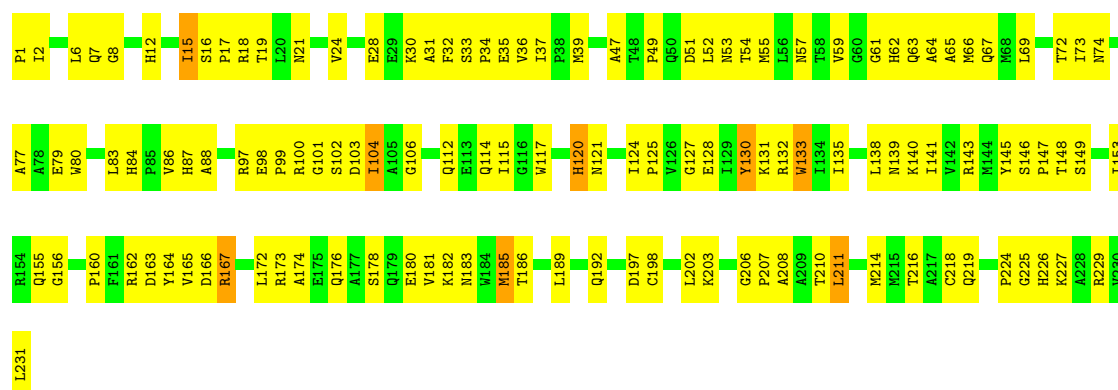
• Molecule 1: capsid protein

Chain 1O: 



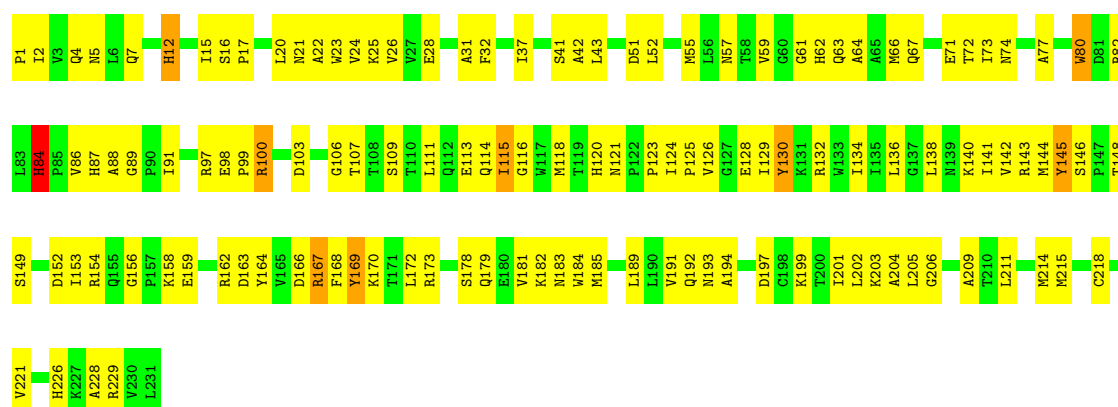
- Molecule 1: capsid protein

Chain IP: 45% 52%



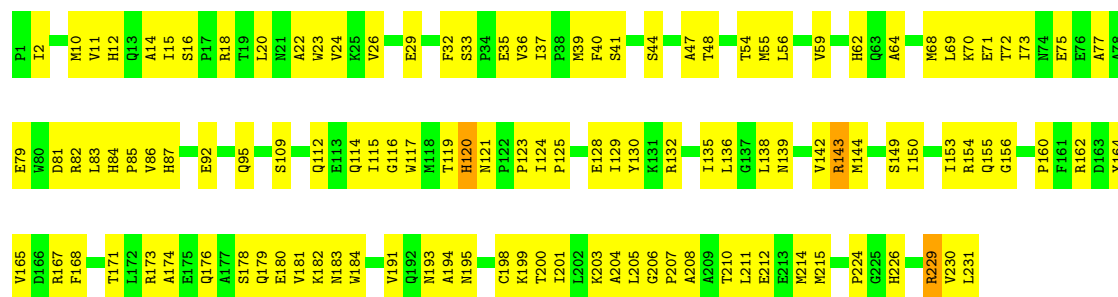
- Molecule 1: capsid protein

Chain IQ: 45% 52%



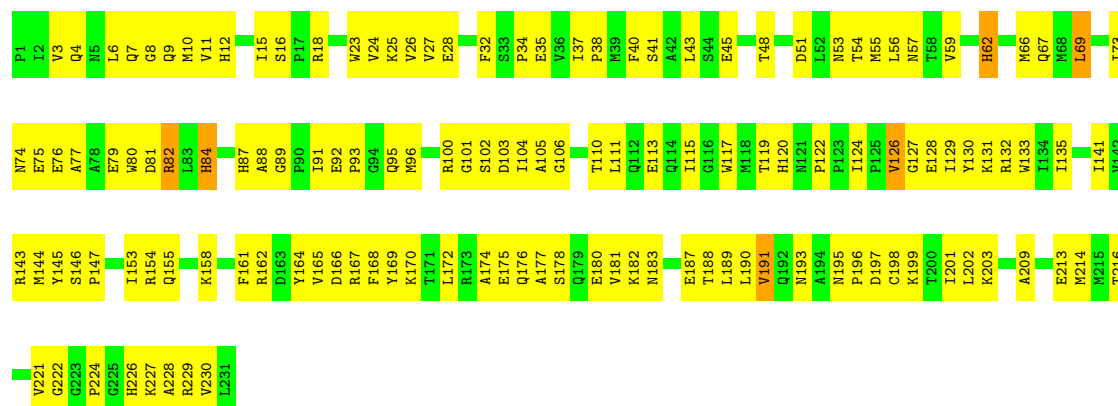
- Molecule 1: capsid protein

Chain IR: 48% 50%



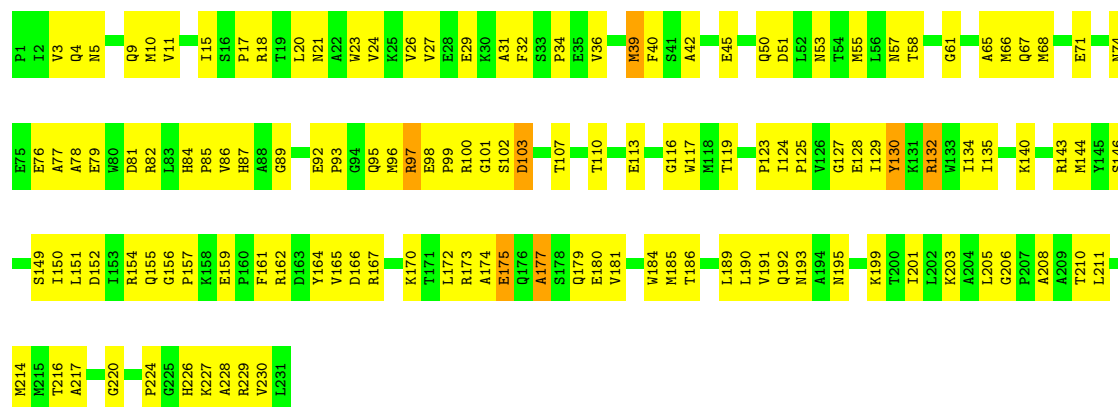
• Molecule 1: capsid protein

Chain 2b: 41% 57%



• Molecule 1: capsid protein

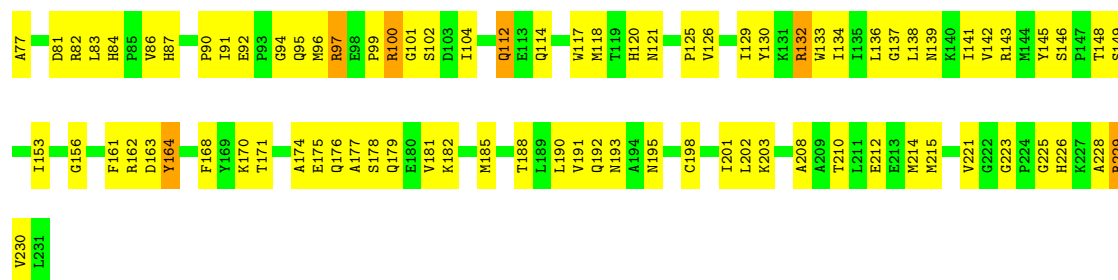
Chain 2c: 44% 53%



• Molecule 1: capsid protein

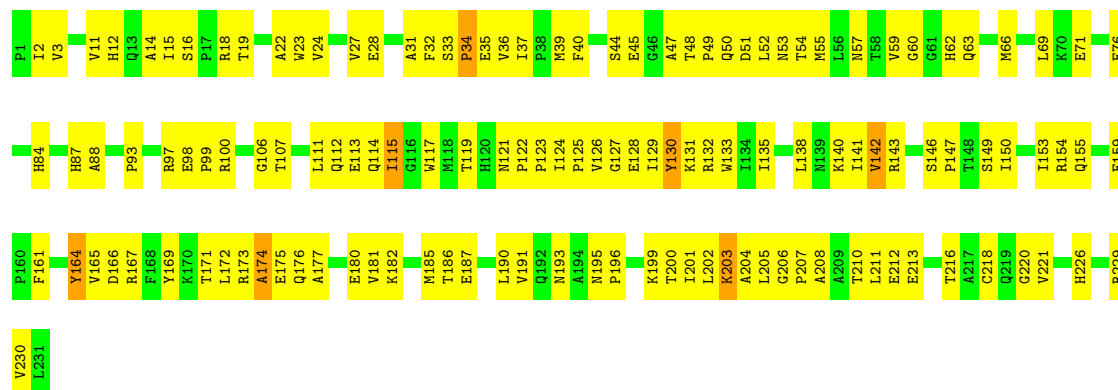
Chain 2d: 46% 51%





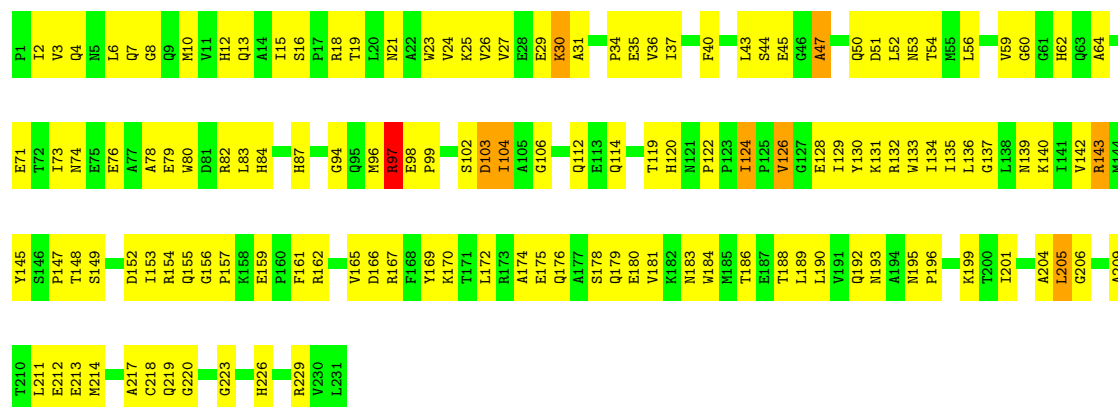
- Molecule 1: capsid protein

Chain 2e: 43% 54%



- Molecule 1: capsid protein

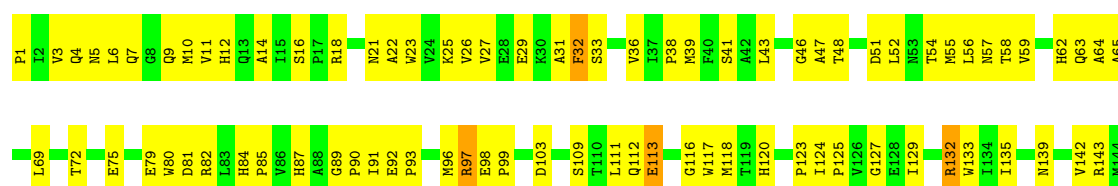
Chain 2f: 42% 55%

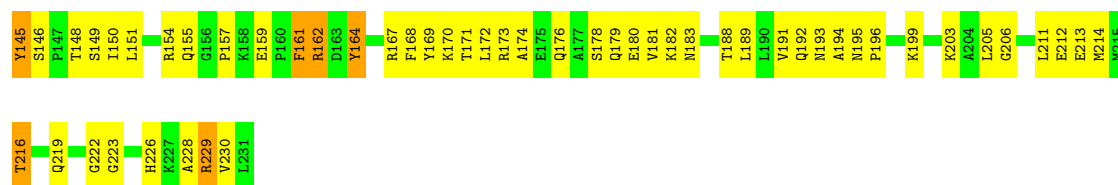


- Molecule 1: capsid protein

Chain 2g: 40% 54% 6%

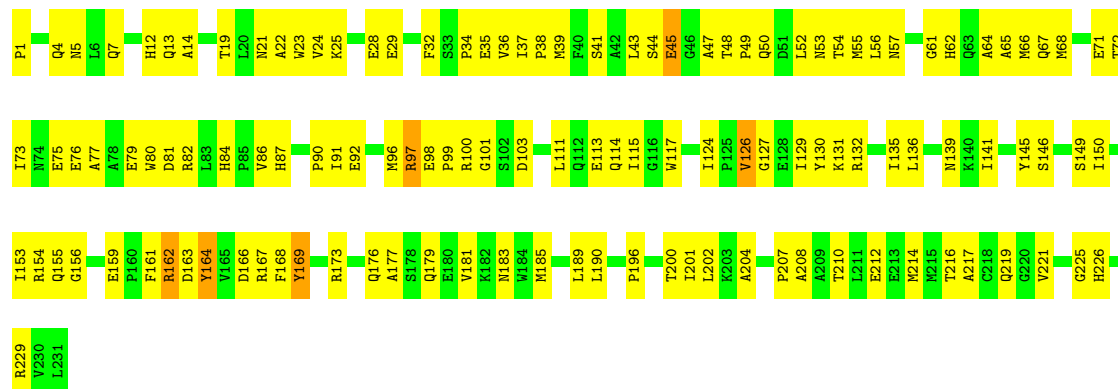






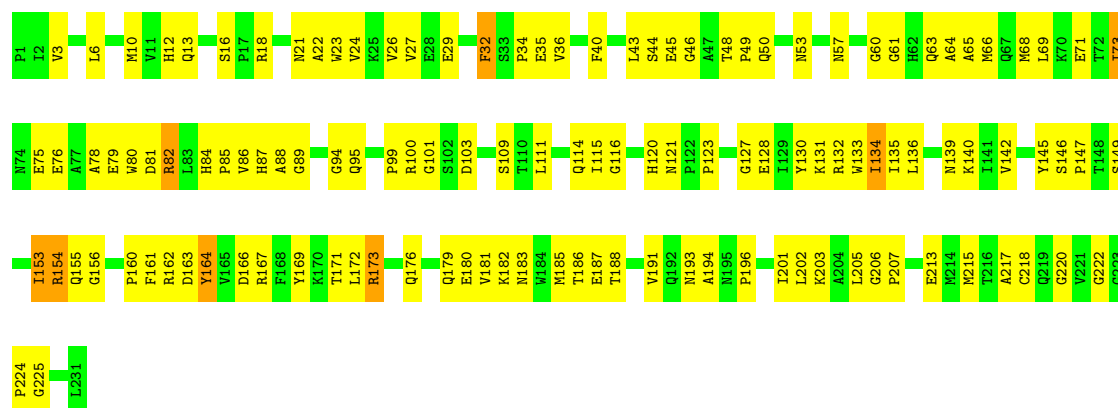
- Molecule 1: capsid protein

Chain 2k:



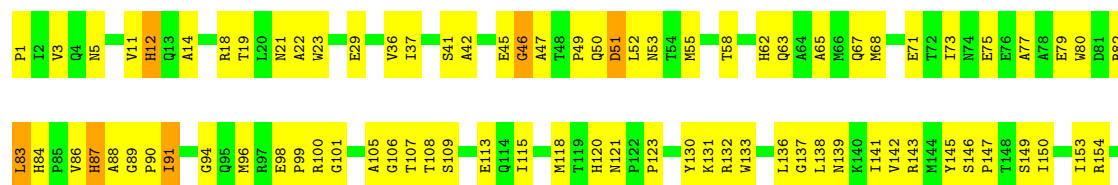
- Molecule 1: capsid protein

Chain 2l:



- Molecule 1: capsid protein

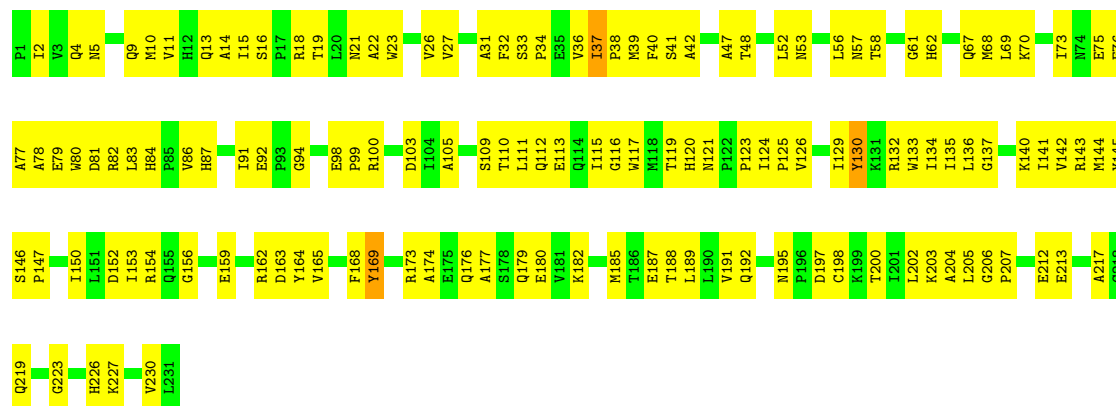
Chain 2m:





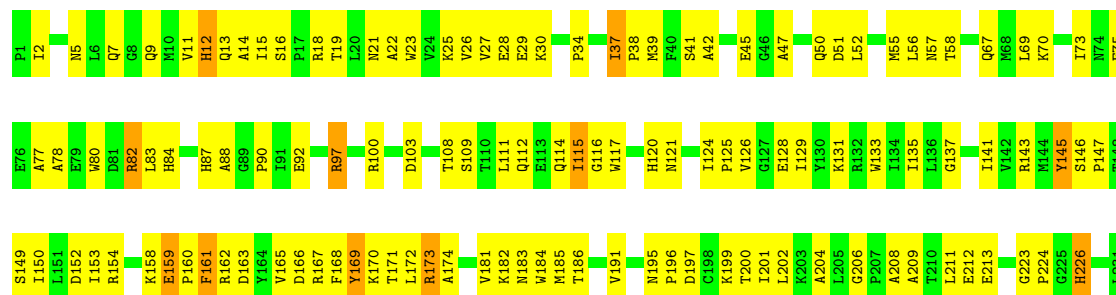
- Molecule 1: capsid protein

Chain 2n: 41% 58%



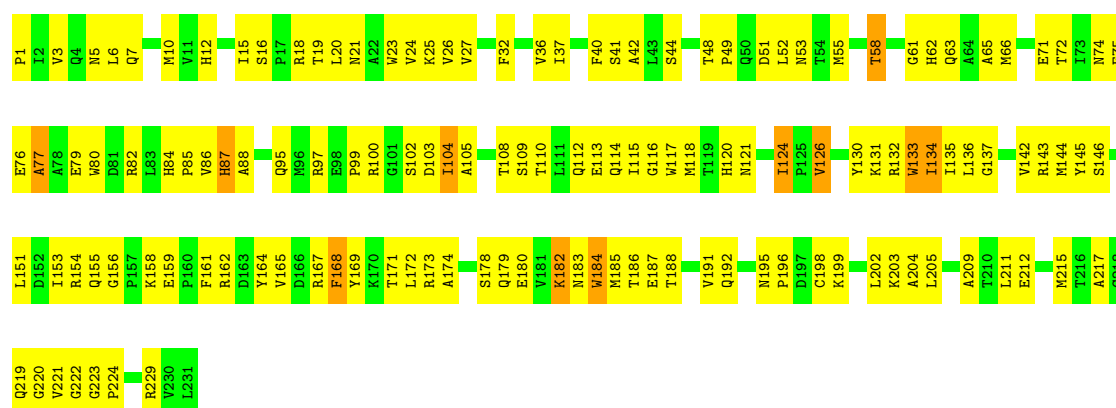
- Molecule 1: capsid protein

Chain 2o: 47% 48% 5%

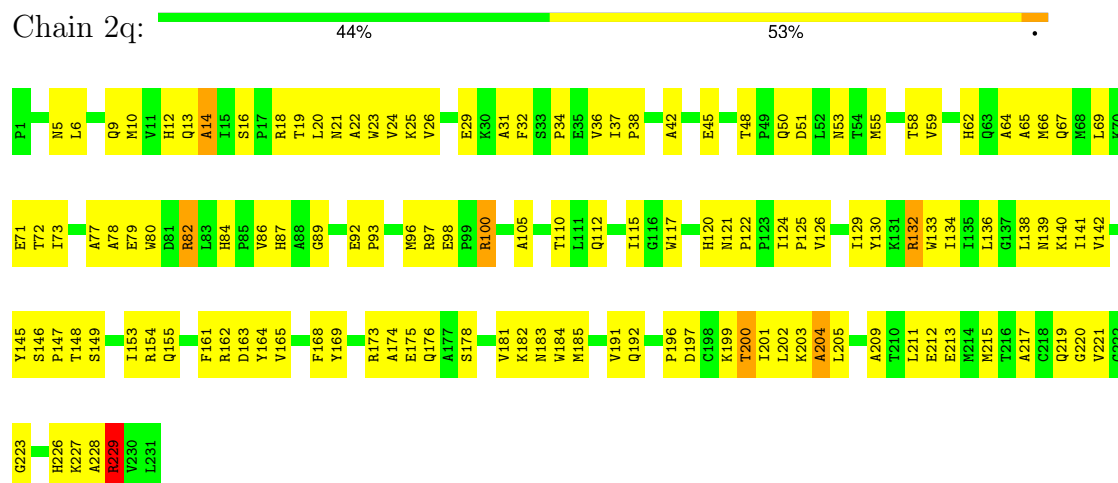


- Molecule 1: capsid protein

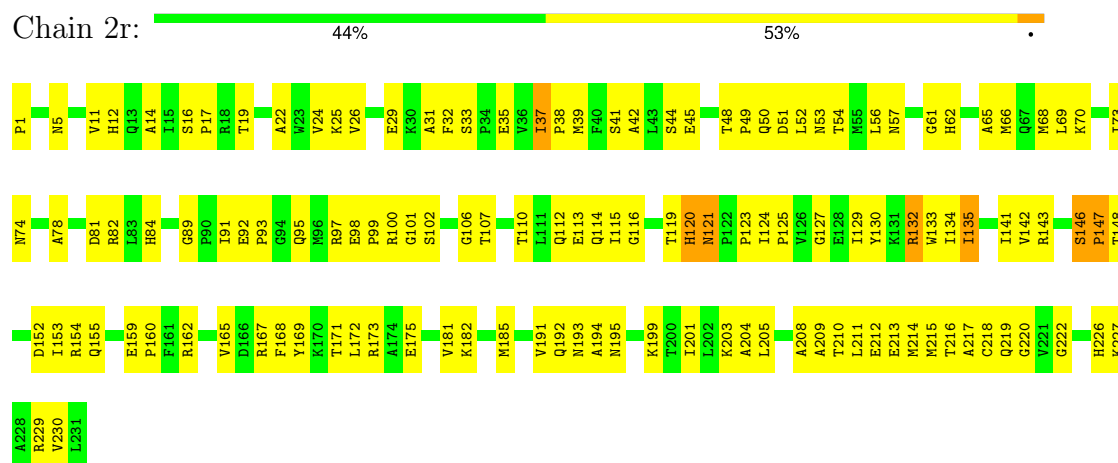
Chain 2p: 41% 54% 5%



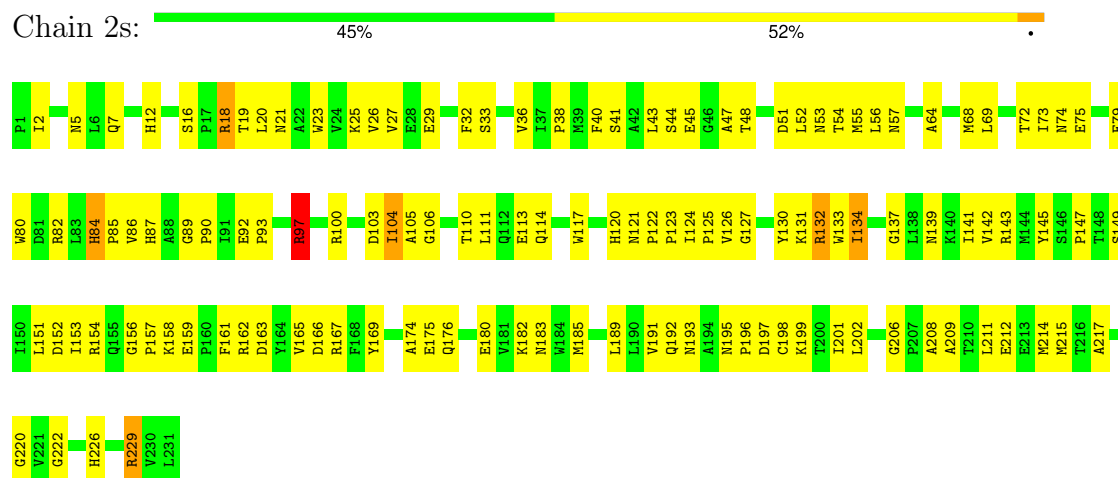
- Molecule 1: capsid protein



- Molecule 1: capsid protein

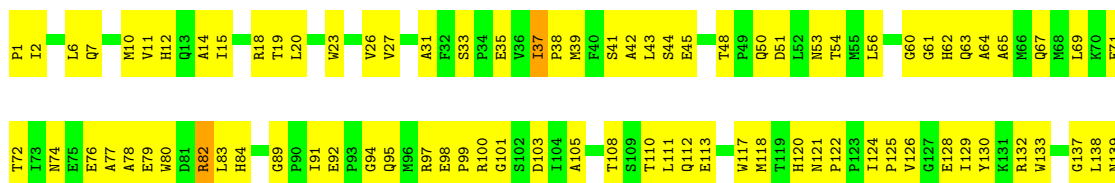


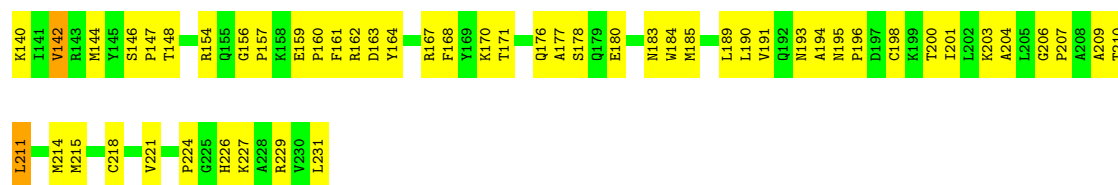
- Molecule 1: capsid protein



- Molecule 1: capsid protein

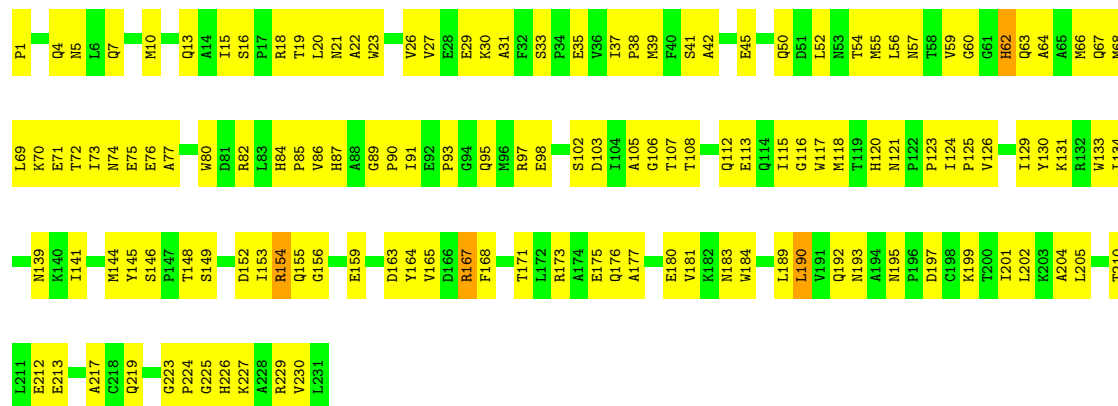






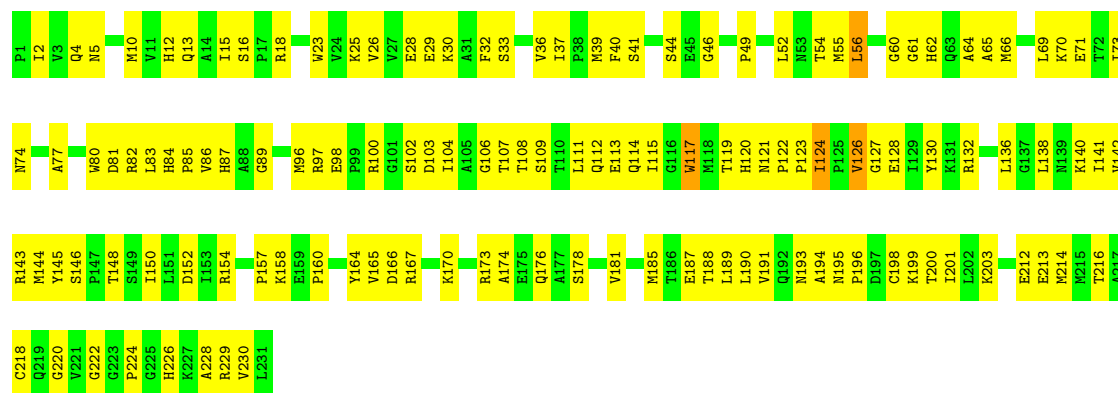
- Molecule 1: capsid protein

Chain 2x: 41% 57%



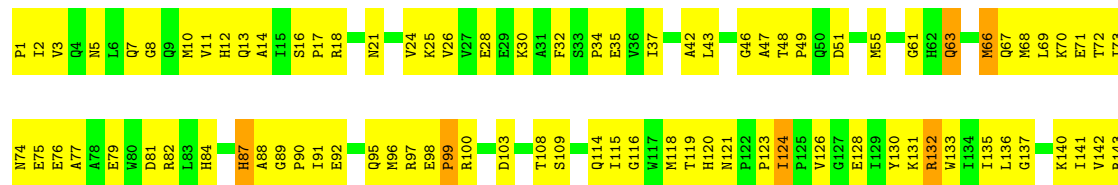
- Molecule 1: capsid protein

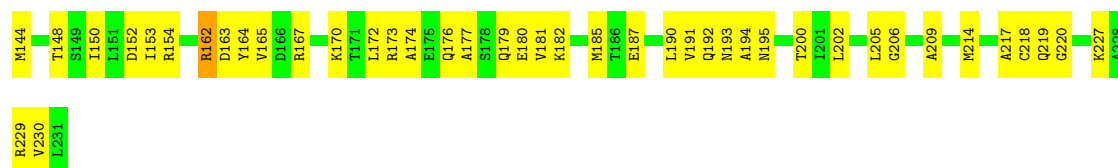
Chain 2y: 43% 55%



- Molecule 1: capsid protein

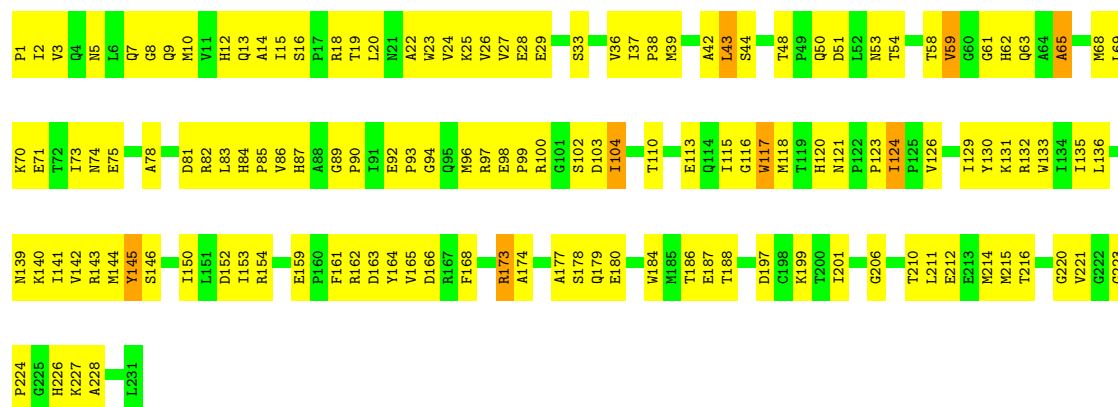
Chain 2z: 44% 53%





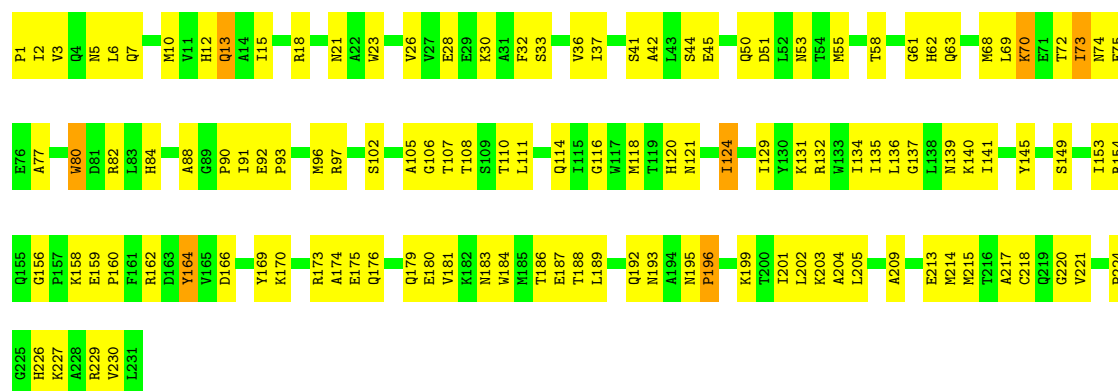
- Molecule 1: capsid protein

Chain 2A: 41% 55%



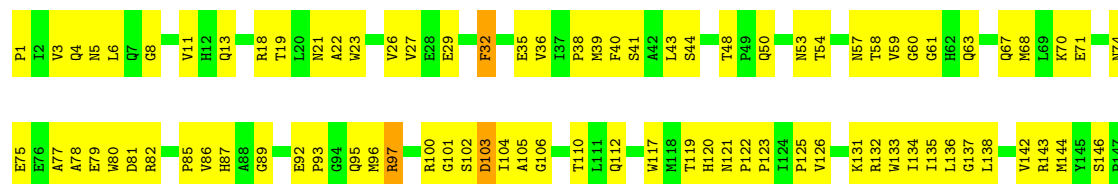
- Molecule 1: capsid protein

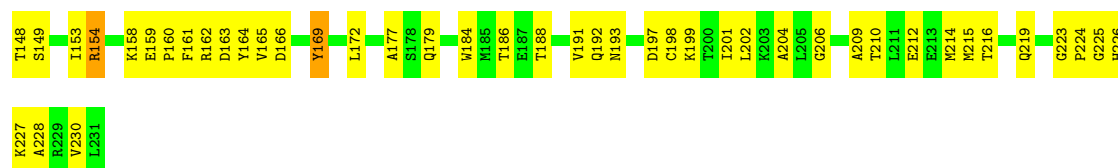
Chain 2B: 47% 50%



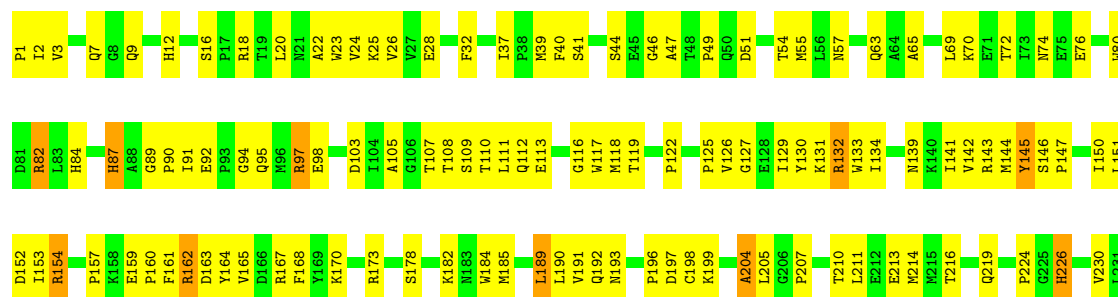
- Molecule 1: capsid protein

Chain 2C: 44% 54%

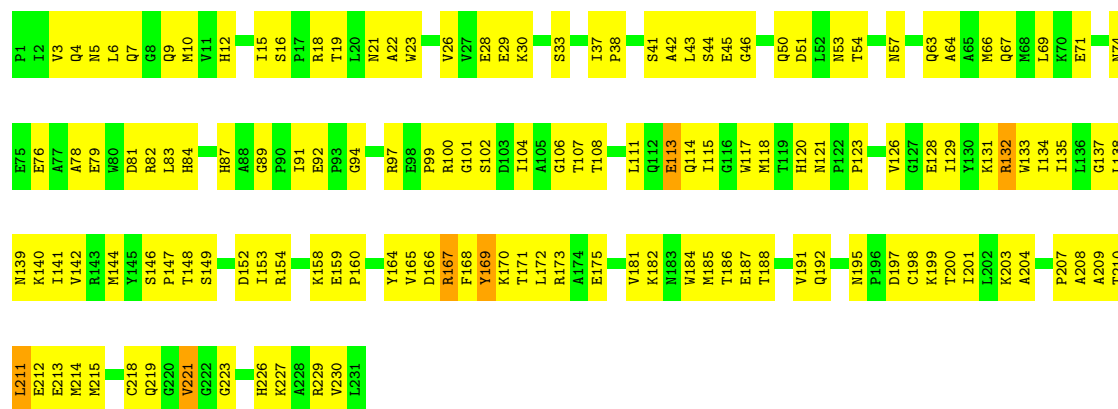




- Molecule 1: capsid protein



- Molecule 1: capsid protein



- Molecule 1: capsid protein



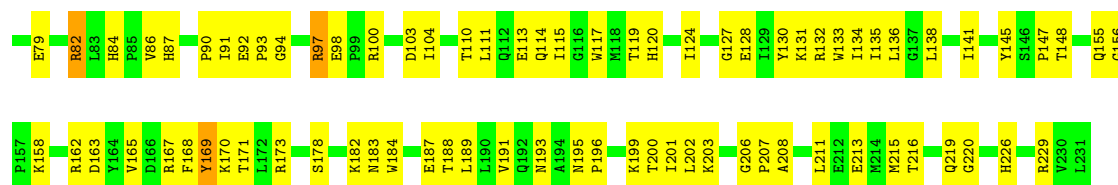
- Molecule 1: capsid protein

G225	H226	K227	A228	R229	V230	L231	E154	T155	E171	T172	A173	R174	L175	H176	V177	E187	T188	E191	T192	E196	T197	A198	R199	L200	H201	V202	E204	T205	G206	P207	A208	E209	T210	L211	E212	E213	M214	T215	A217	C218	Q219	G220	P221	E222	T223	A224	R225	L226	H227	V228	E229	T230	A231	R232	L233	H234	V235	E236	T237	A238	R239	L240	H241	V242	E243	T244	A245	R246	L247	H248	V249	E250	T251	A252	R253	L254	H255	V256	E257	T258	A259	R260	L261	H262	V263	E264	T265	A266	R267	L268	H269	V270	E271	T272	A273	R274	L275	H276	V277	E278	T279	A280	R281	L282	H283	V284	E285	T286	A287	R288	L289	H290	V291	E292	T293	A294	R295	L296	H297	V298	E299	T300	A301	R302	L303	H304	V305	E306	T307	A308	R309	L310	H311	V312	E313	T314	A315	R316	L317	H318	V319	E320	T321	A322	R323	L324	H325	V326	E327	T328	A329	R330	L331	H332	V333	E334	T335	A336	R337	L338	H339	V340	E341	T342	A343	R344	L345	H346	V347	E348	T349	A350	R351	L352	H353	V354	E355	T356	A357	R358	L359	H360	V361	E362	T363	A364	R365	L366	H367	V368	E369	T370	A371	R372	L373	H374	V375	E376	T377	A378	R379	L380	H381	V382	E383	T384	A385	R386	L387	H388	V389	E390	T391	A392	R393	L394	H395	V396	E397	T398	A399	R400	L401	H402	V403	E404	T405	A406	R407	L408	H409	V410	E411	T412	A413	R414	L415	H416	V417	E418	T419	A420	R421	L422	H423	V424	E425	T426	A427	R428	L429	H430	V431	E432	T433	A434	R435	L436	H437	V438	E439	T440	A441	R442	L443	H444	V445	E446	T447	A448	R449	L450	H451	V452	E453	T454	A455	R456	L457	H458	V459	E460	T461	A462	R463	L464	H465	V466	E467	T468	A469	R470	L471	H472	V473	E474	T475	A476	R477	L478	H479	V480	E481	T482	A483	R484	L485	H486	V487	E488	T489	A490	R491	L492	H493	V494	E495	T496	A497	R498	L499	H500	V501	E502	T503	A504	R505	L506	H507	V508	E509	T510	A511	R512	L513	H514	V515	E516	T517	A518	R519	L520	H521	V522	E523	T524	A525	R526	L527	H528	V529	E530	T531	A532	R533	L534	H535	V536	E537	T538	A539	R540	L541	H542	V543	E544	T545	A546	R547	L548	H549	V550	E551	T552	A553	R554	L555	H556	V557	E558	T559	A560	R561	L562	H563	V564	E565	T566	A567	R568	L569	H570	V571	E572	T573	A574	R575	L576	H577	V578	E579	T580	A581	R582	L583	H584	V585	E586	T587	A588	R589	L590	H591	V592	E593	T594	A595	R596	L597	H598	V599	E600	T601	A602	R603	L604	H605	V606	E607	T608	A609	R610	L611	H612	V613	E614	T615	A616	R617	L618	H619	V620	E621	T622	A623	R624	L625	H626	V627	E628	T629	A630	R631	L632	H633	V634	E635	T636	A637	R638	L639	H640	V641	E642	T643	A644	R645	L646	H647	V648	E649	T650	A651	R652	L653	H654	V655	E656	T657	A658	R659	L660	H661	V662	E663	T664	A665	R666	L667	H668	V669	E670	T671	A672	R673	L674	H675	V676	E677	T678	A679	R680	L681	H682	V683	E684	T685	A686	R687	L688	H6

V165	D166	R167	F168	T171	L172	R173	A174	E175	S178	Q179	V181	M182	N183	W184	M185	L186	E187	T188	L189	L190	V191	Q192	N193	A194	R195	F196	D197	C198	K199	T200	I201	L202	L205	A208	A209	T210	L211	L212	E213	M214	M215	V221	H226	C227	A228	R229	V230	L231	V165	D166	R167	F168	T171	L172	R173	A174	E175	S178	Q179	V181	M182	N183	W184	M185	L186	E187	T188	L189	L190	V191	Q192	N193	A194	R195	F196	D197	C198	K199	T200	I201	L202	L205	A208	A209	T210	L211	L212	E213	M214	M215	V221	H226	C227	A228	R229	V230	L231	P185	V86	G89	E92	P93	R97	E98	S102	D103	I104	A105	T108	L111	Q112	E113	Q114	I115	G116	W117	H120	N121	P122	P123	P125	G127	E128	I129	Y130	K131	R132	W133	K140	I141	V142	R143	M144	Y145	S146	P147	D152	I153	R154	E159	P160	R161	D162	F163	P185	V86	G89	E92	P93	R97	E98	S102	D103	I104	A105	T108	L111	Q112	E113	Q114	I115	G116	W117	H120	N121	P122	P123	P125	G127	E128	I129	Y130	K131	R132	W133	K140	I141	V142	R143	M144	Y145	S146	P147	D152	I153	R154	E159	P160	R161	D162	F163
P1	I2	N5	L6	H12	Q13	A14	I15	S16	P17	R18	W23	V24	K25	V26	E28	E29	F32	S33	P34	M39	A42	L43	G46	Q50	D51	L52	M53	T54	M55	L56	N57	T58	V59	H62	M66	Q67	M68	L69	K70	E71	T72	I73	W80	D81	R82	L83	F84	P1	I2	N5	L6	H12	Q13	A14	I15	S16	P17	R18	W23	V24	K25	V26	E28	E29	F32	S33	P34	M39	A42	L43	G46	Q50	D51	L52	M53	T54	M55	L56	N57	T58	V59	H62	M66	Q67	M68	L69	K70	E71	T72	I73	W80	D81	R82	L83	F84																																																																																																

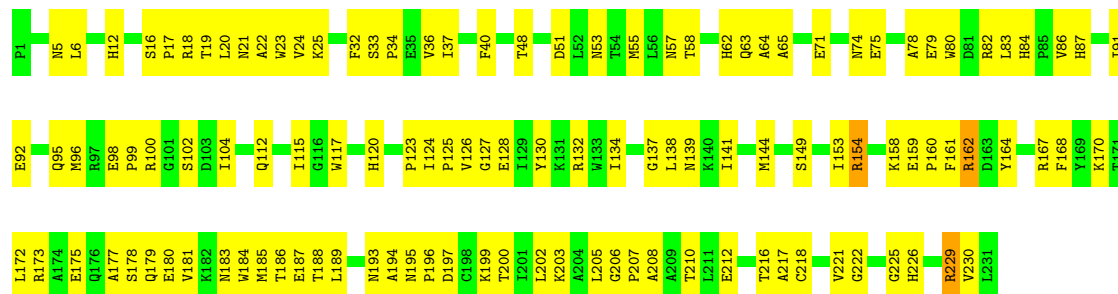
[illegible]

P1	I2	V3	Q4	Q7	G8		H12	Q13	A14	I15	S16	R17	R18	T19	L20	L20	V21	A22	A23	V24	K25	V26	V27		K30	A31	F32	S33	P34	E35	V36	I37	P38	M39	F40	S41	L42	A43	L44		G46	A47	T48	P49	Q50	D51	S52	M53	T54	M55	L56		G62	Q63	A64		K70		E75	



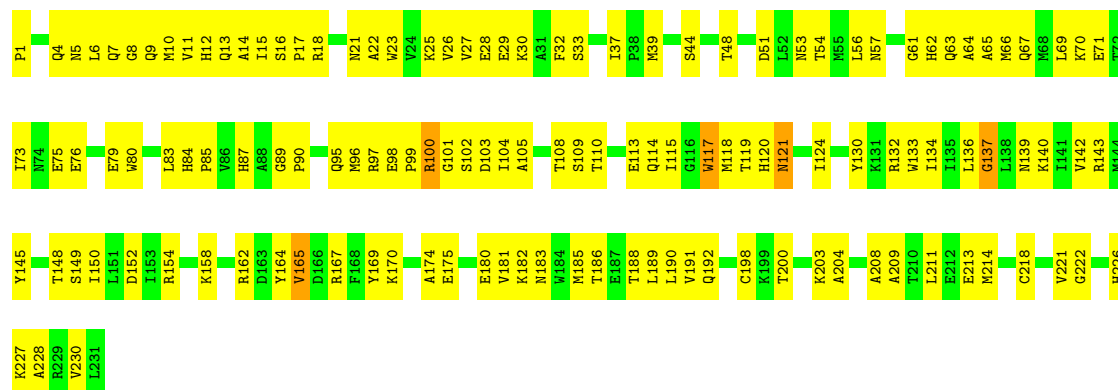
- Molecule 1: capsid protein

Chain 2K: 49% 50%



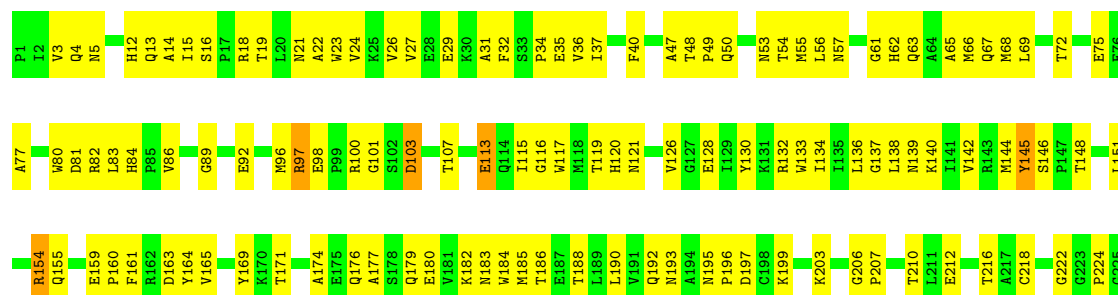
- Molecule 1: capsid protein

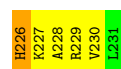
Chain 2L: 43% 55%



- Molecule 1: capsid protein

Chain 2M: 46% 52%

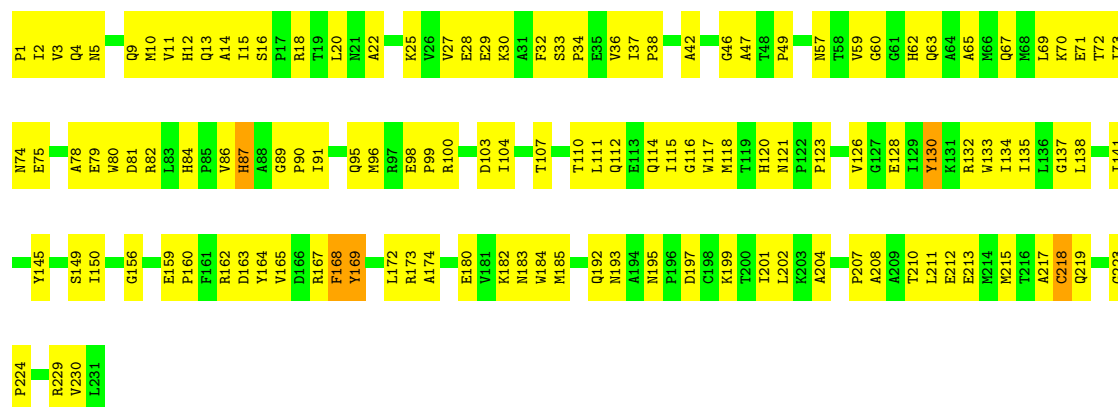




• Molecule 1: capsid protein

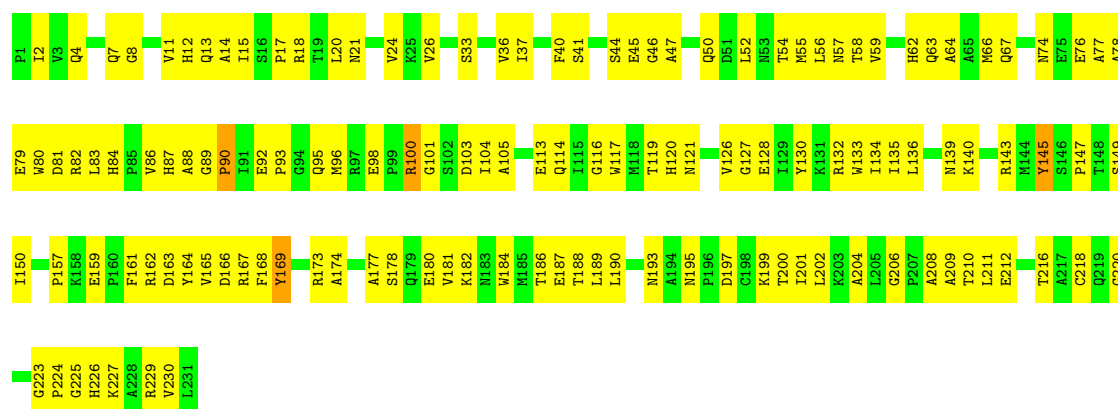
Chain 2N: 47% 48% 5%





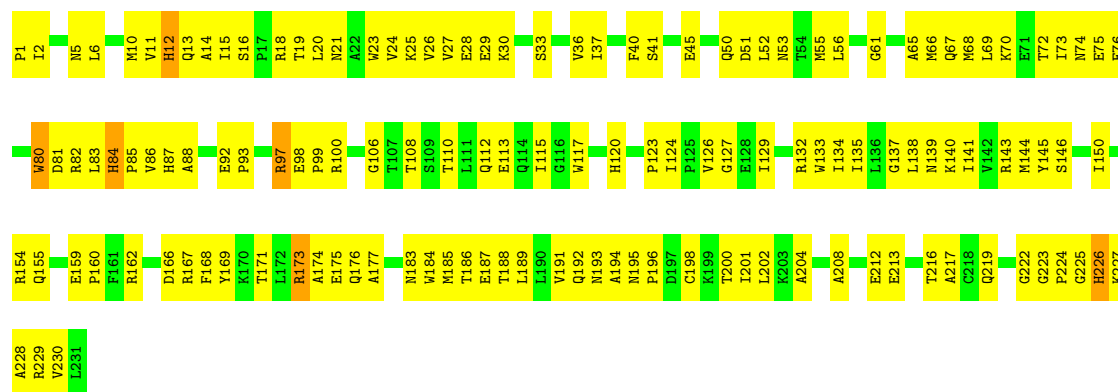
- Molecule 1: capsid protein

Chain 2R: 42% 56%



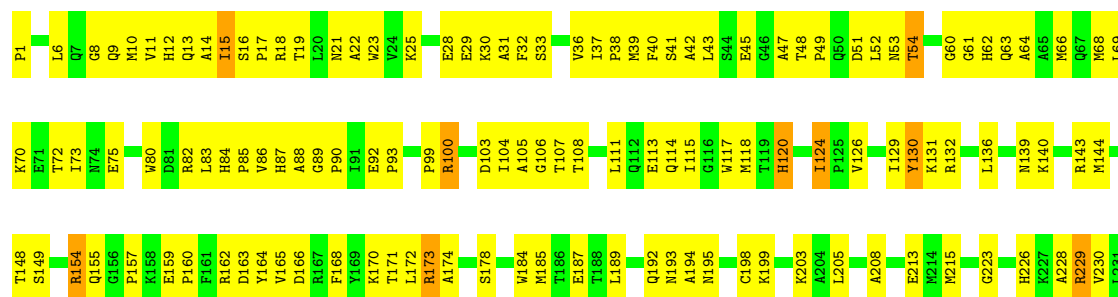
- Molecule 1: capsid protein

Chain 2S: 41% 57%



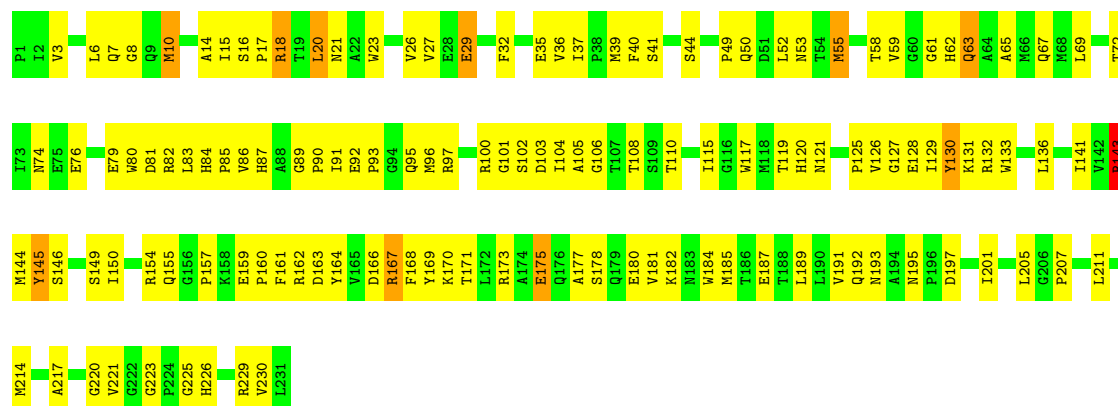
- Molecule 1: capsid protein

Chain 2T: 44% 52%



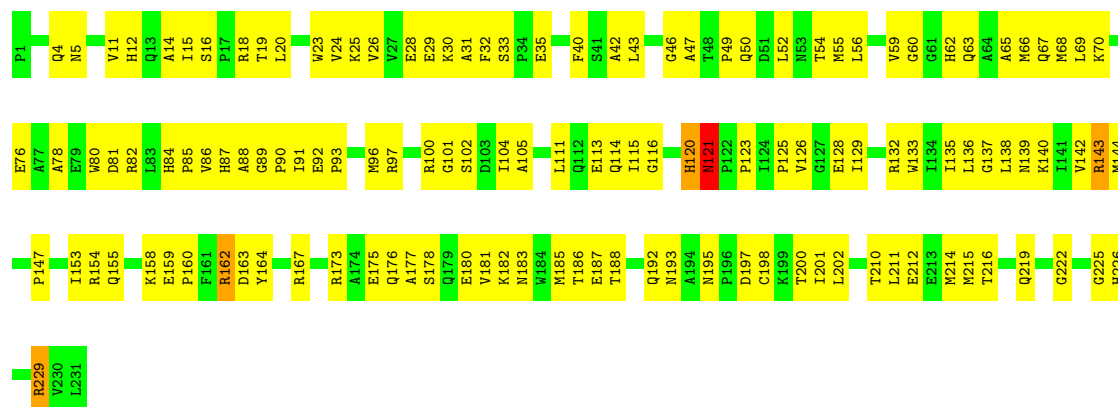
• Molecule 1: capsid protein

Chain 2U: 43% 52%



• Molecule 1: capsid protein

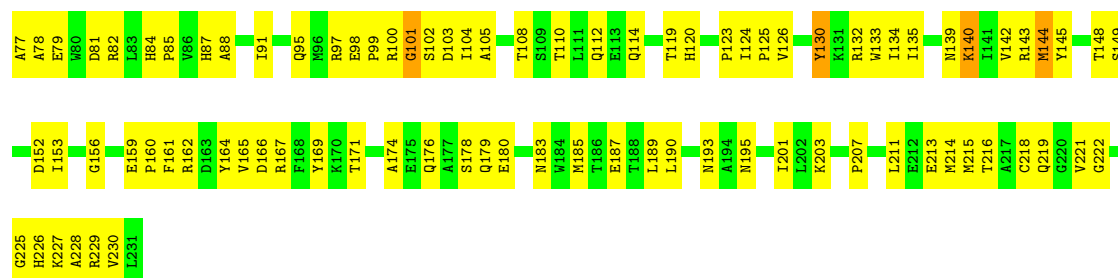
Chain 2V: 44% 54%



• Molecule 1: capsid protein

Chain 2W: 44% 54%





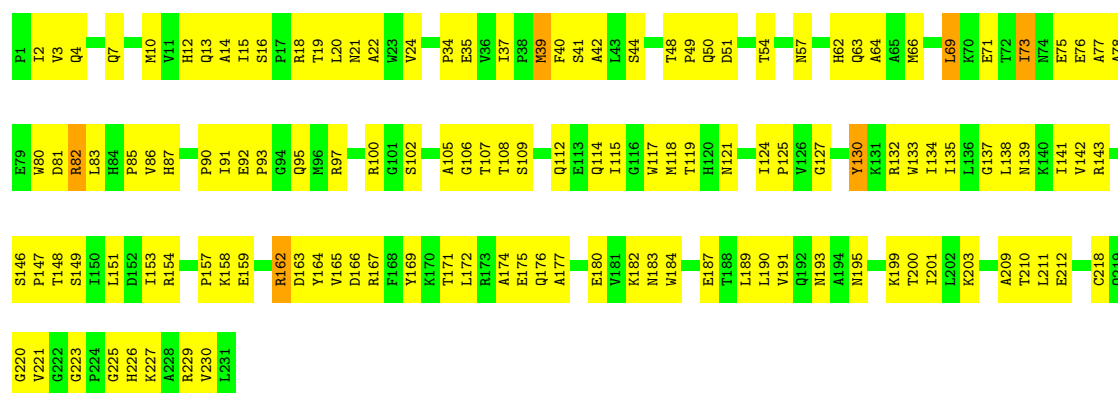
- Molecule 1: capsid protein

Chain 2X: 39% 60%



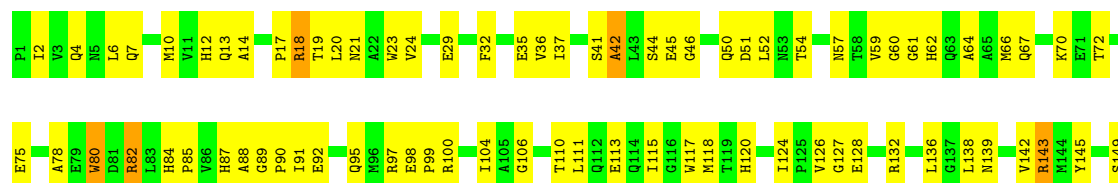
- Molecule 1: capsid protein

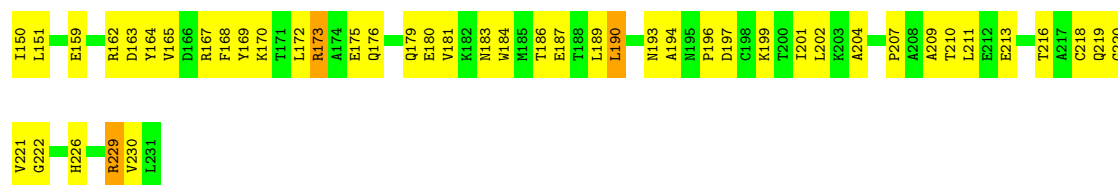
Chain 2Y: 43% 55%



- Molecule 1: capsid protein

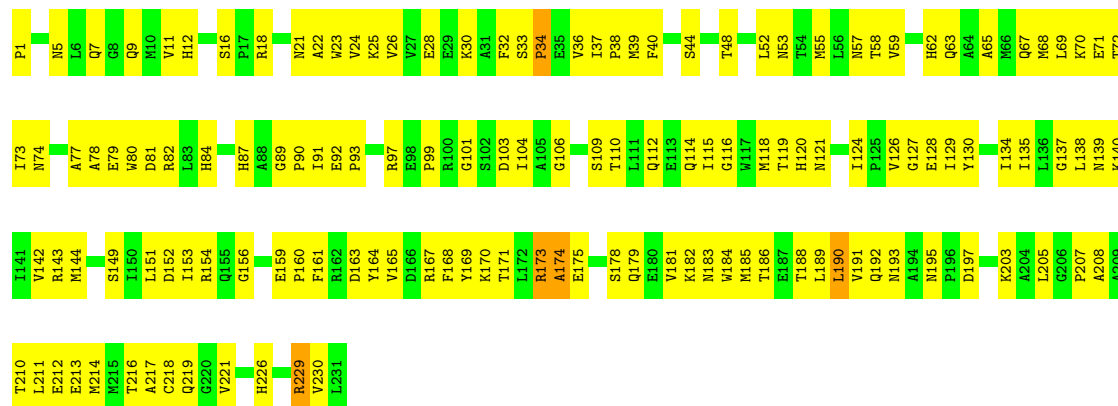
Chain 2Z: 47% 50%





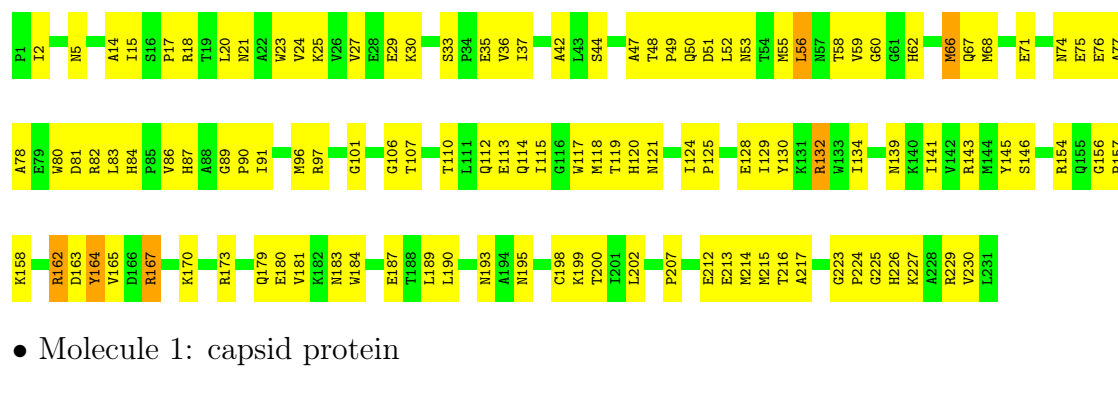
- Molecule 1: capsid protein

Chain 30: 39% 58%



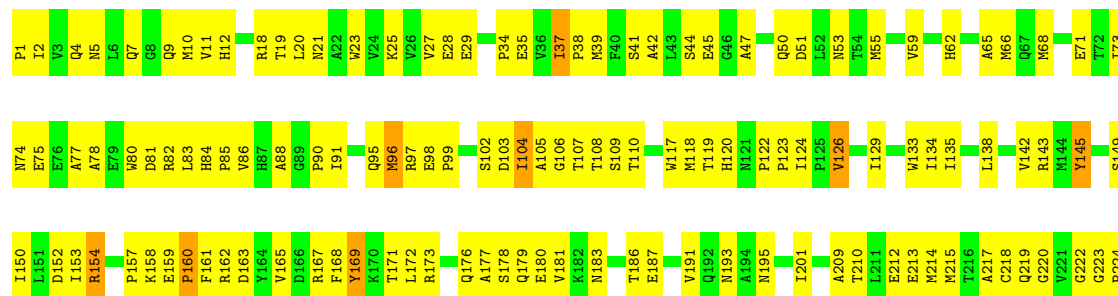
- Molecule 1: capsid protein

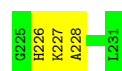
Chain 31: 49% 48%



- Molecule 1: capsid protein

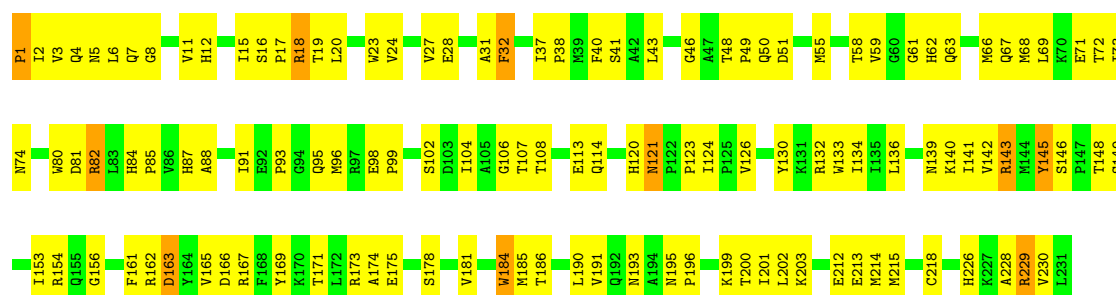
Chain 32: 43% 53%





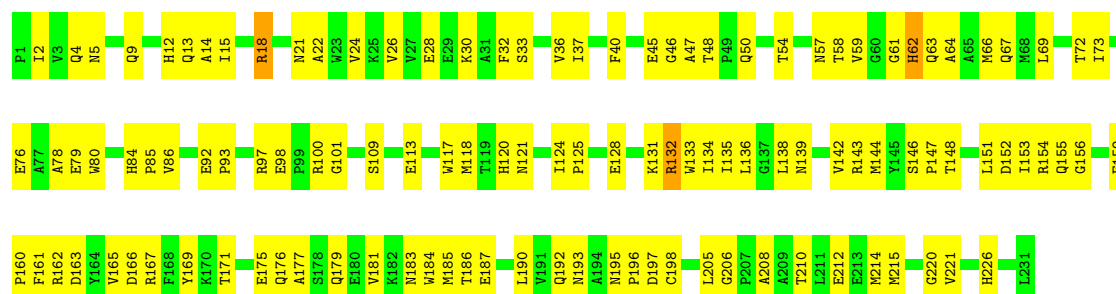
- Molecule 1: capsid protein

Chain 33: 47% 49%



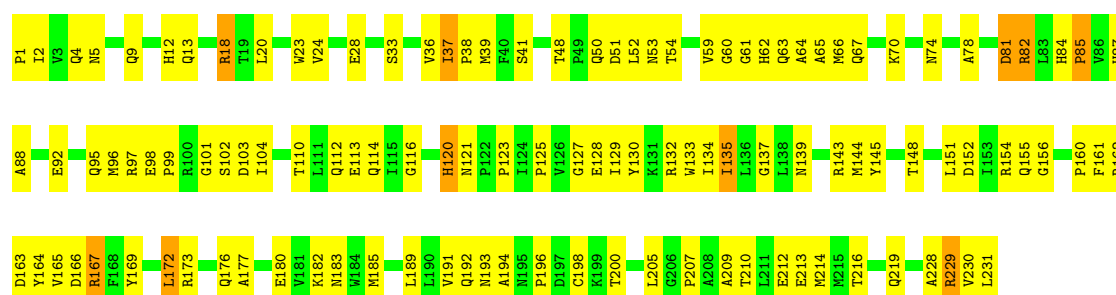
- Molecule 1: capsid protein

Chain 34: 49% 49%



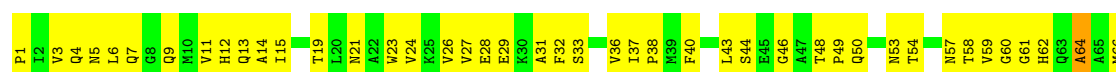
- Molecule 1: capsid protein

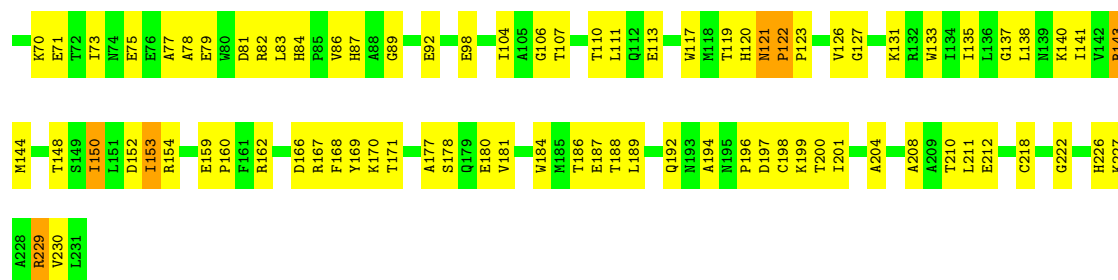
Chain 35: 49% 47%

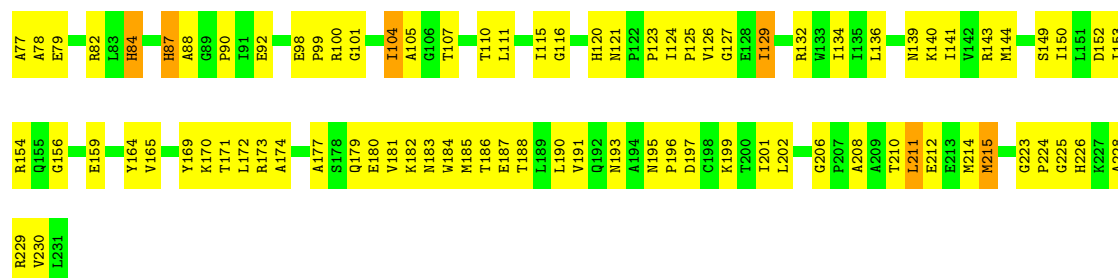


- Molecule 1: capsid protein

Chain 36: 46% 51%

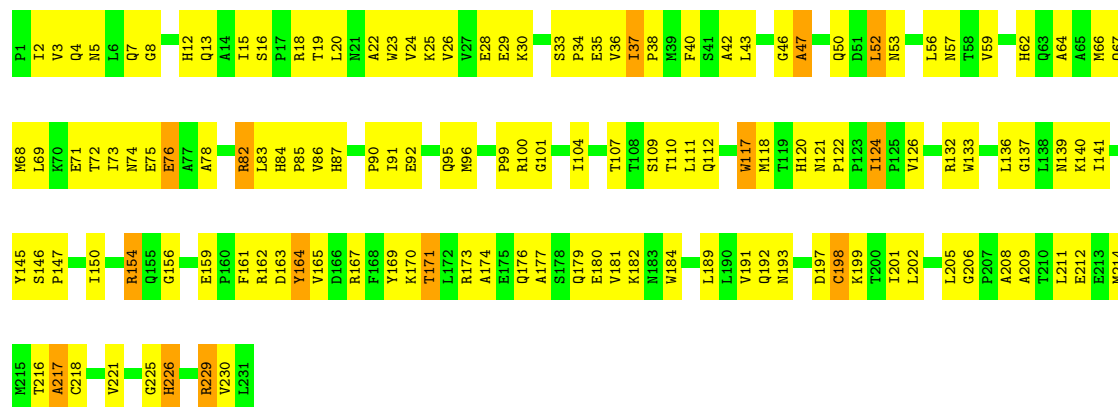






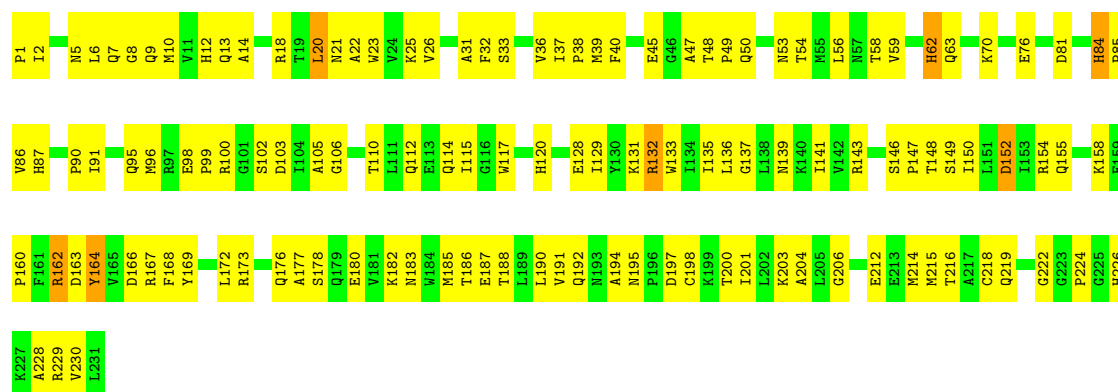
- Molecule 1: capsid protein

Chain 3a: 42% 52% 6%



- Molecule 1: capsid protein

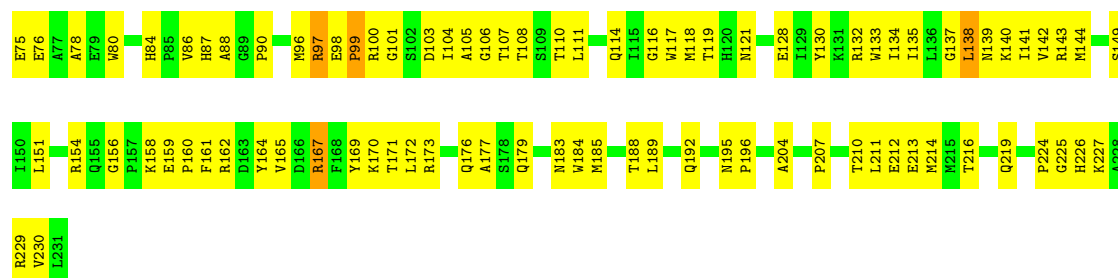
Chain 3b: 45% 52% 6%



- Molecule 1: capsid protein

Chain 3c: 45% 52% 6%





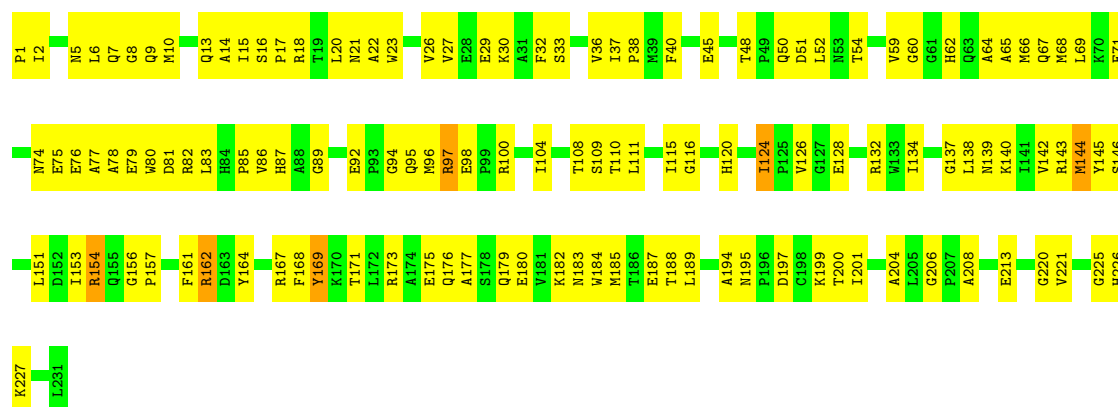
- Molecule 1: capsid protein

Chain 3d: 46% 51%



- Molecule 1: capsid protein

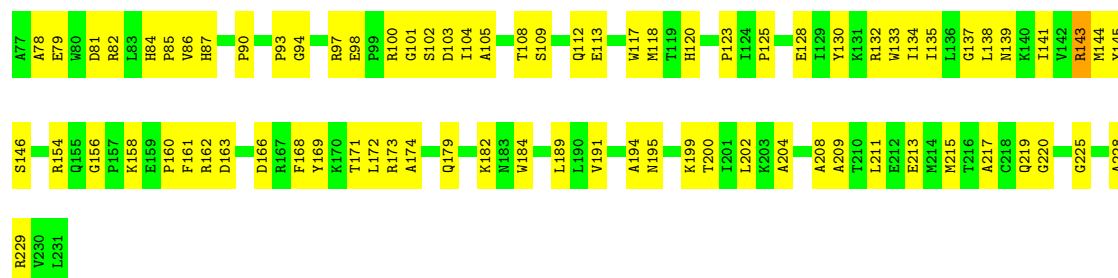
Chain 3e: 45% 52%



- Molecule 1: capsid protein

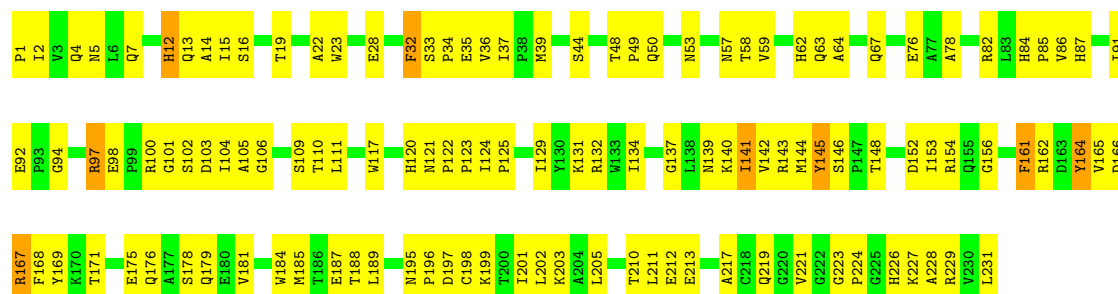
Chain 3f: 49% 50%





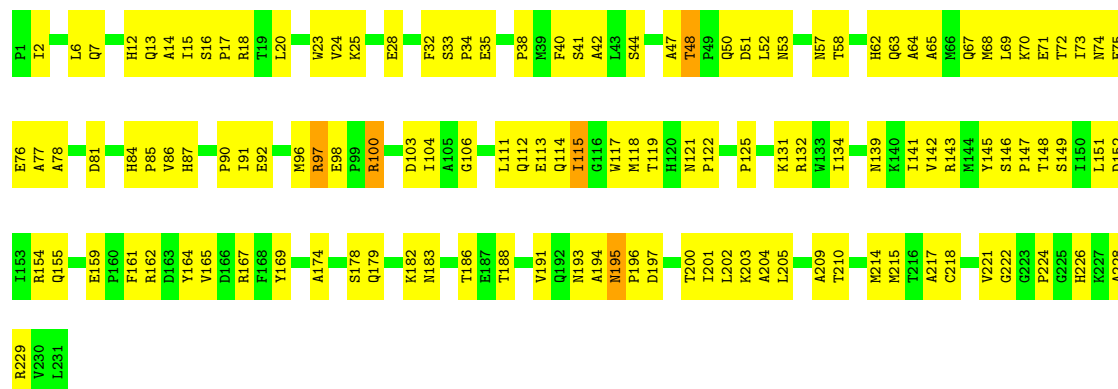
• Molecule 1: capsid protein

Chain 3g: 47% 49%



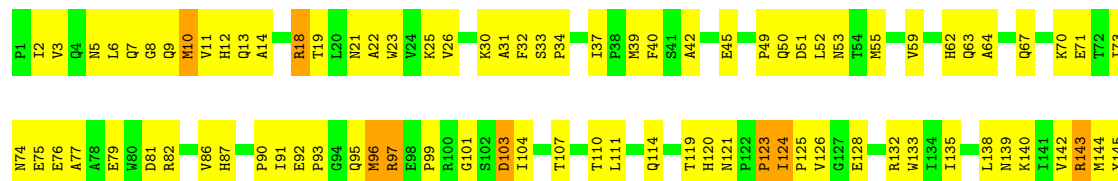
• Molecule 1: capsid protein

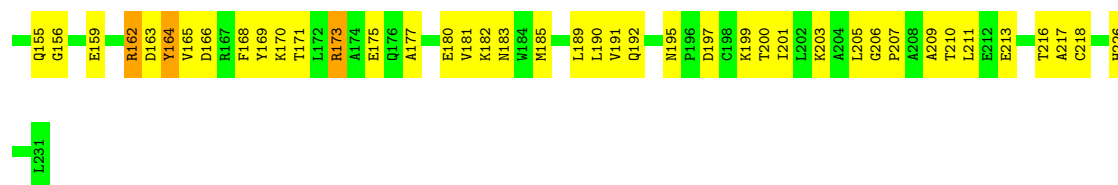
Chain 3h: 45% 53%



• Molecule 1: capsid protein

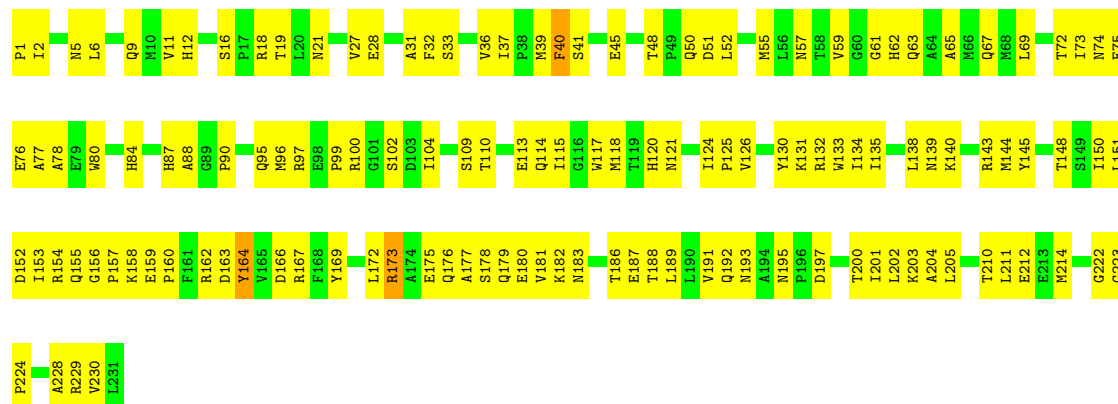
Chain 3i: 45% 50% 5%





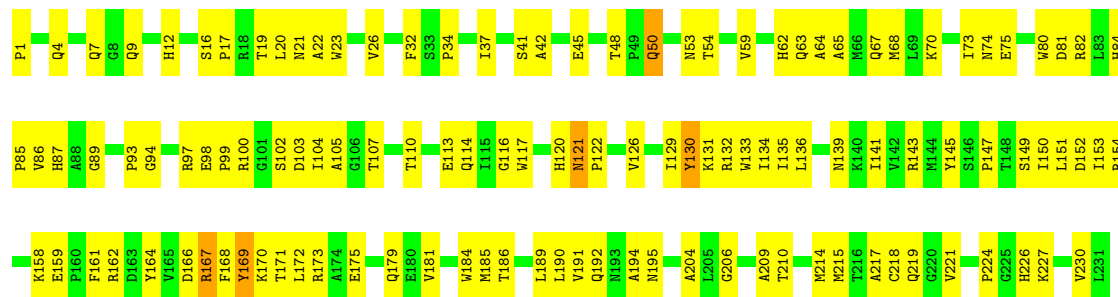
- Molecule 1: capsid protein

Chain 3j: 43% 56%



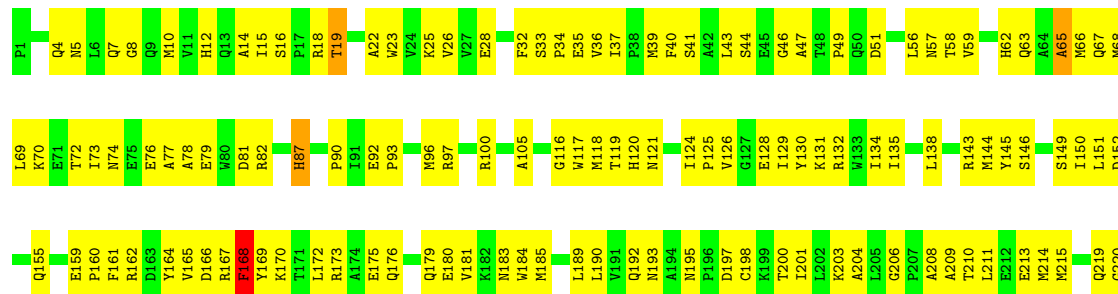
- Molecule 1: capsid protein

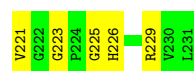
Chain 3k: 48% 50%



- Molecule 1: capsid protein

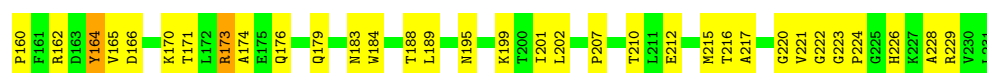
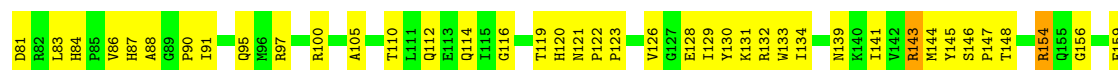
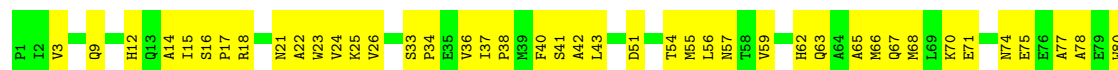
Chain 3l: 42% 56%





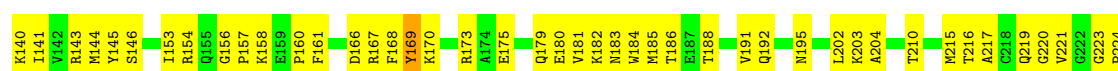
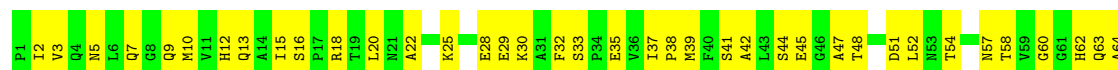
- Molecule 1: capsid protein

Chain 3m: 50% 48%



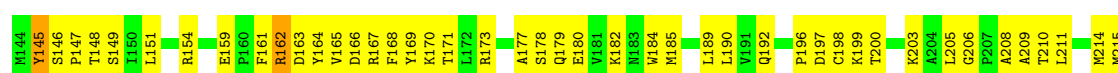
- Molecule 1: capsid protein

Chain 3n: 43% 56%



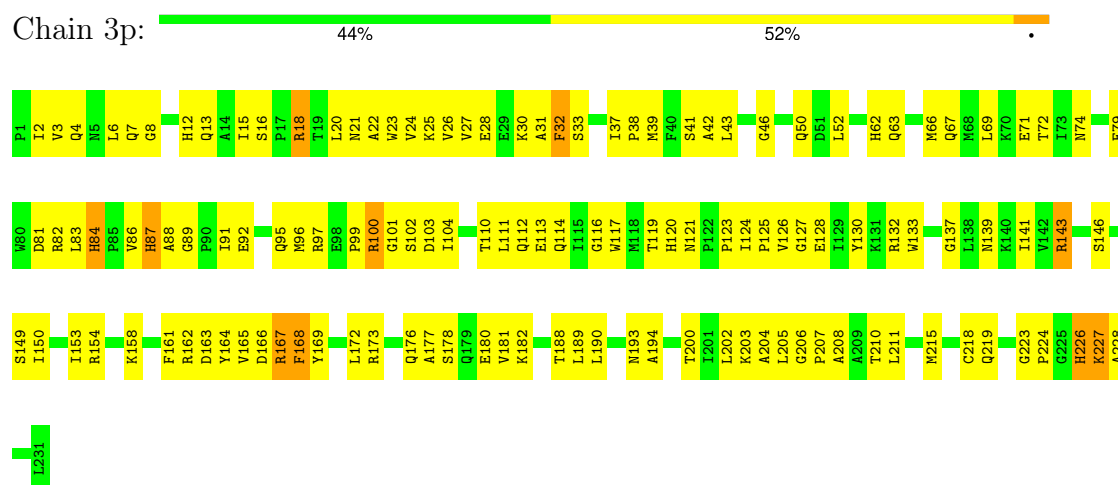
- Molecule 1: capsid protein

Chain 3o: 42% 56%



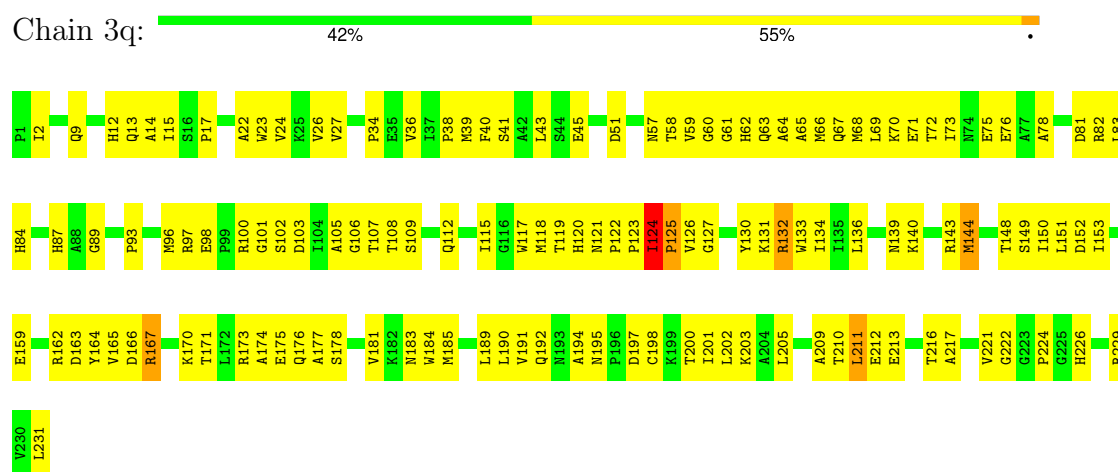
- Molecule 1: capsid protein

Chain 3p:



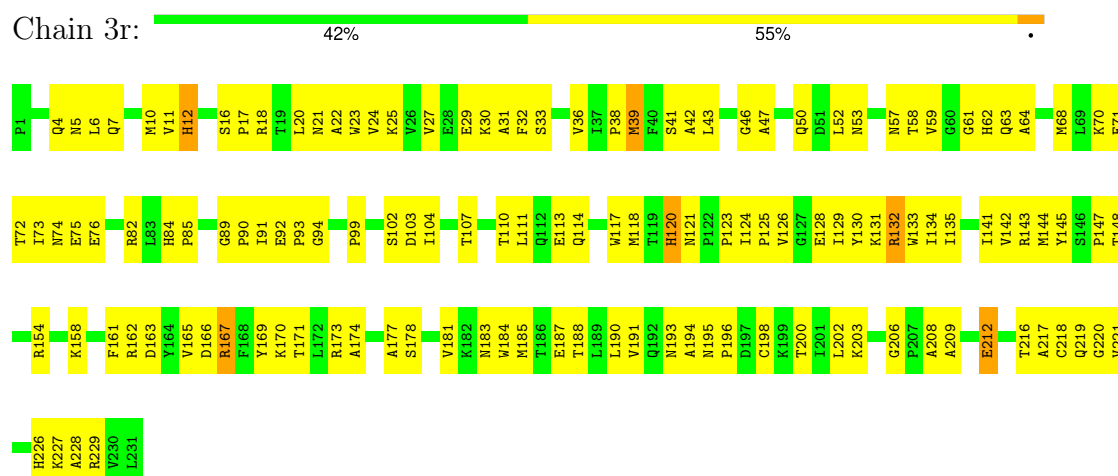
- Molecule 1: capsid protein

Chain 3q:

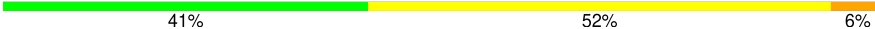


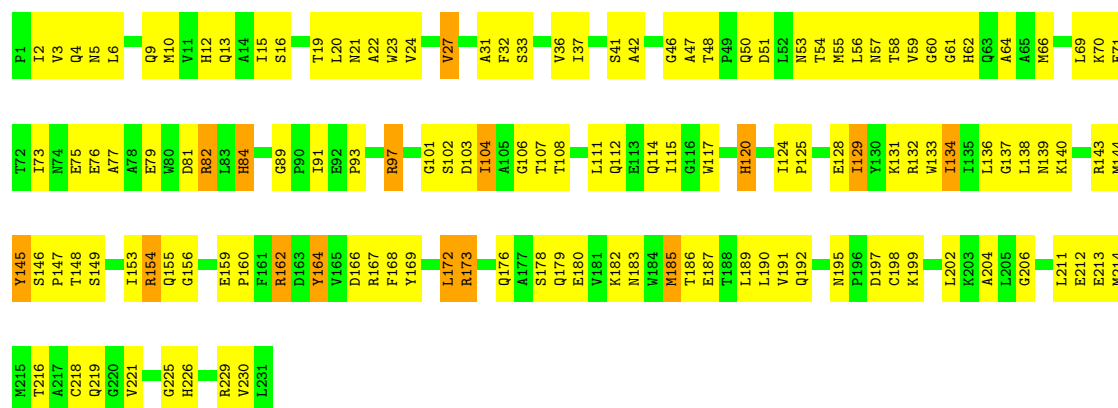
- Molecule 1: capsid protein

Chain 3r:

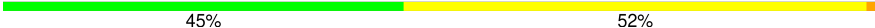


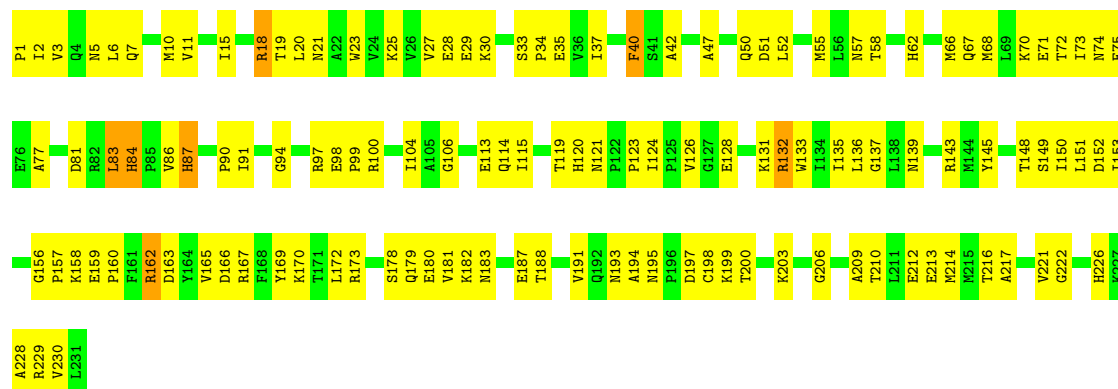
- Molecule 1: capsid protein

Chain 3s: 



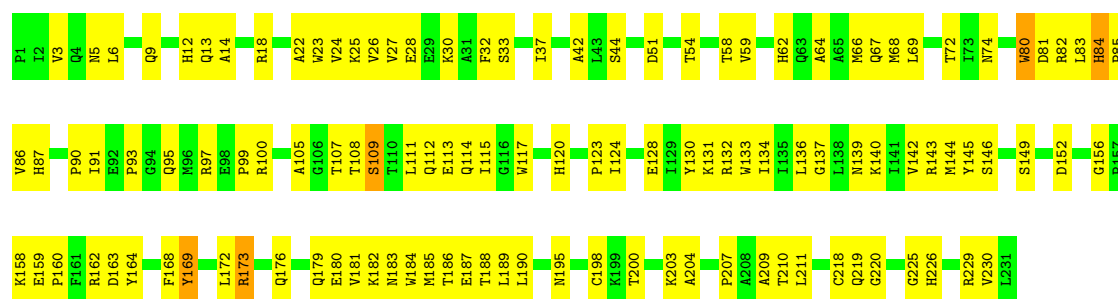
• Molecule 1: capsid protein

Chain 3t: 



• Molecule 1: capsid protein

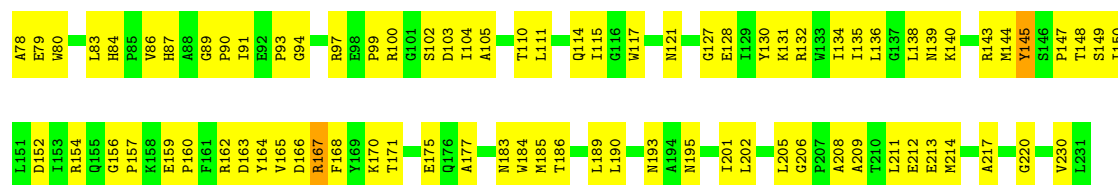
Chain 3u: 



• Molecule 1: capsid protein

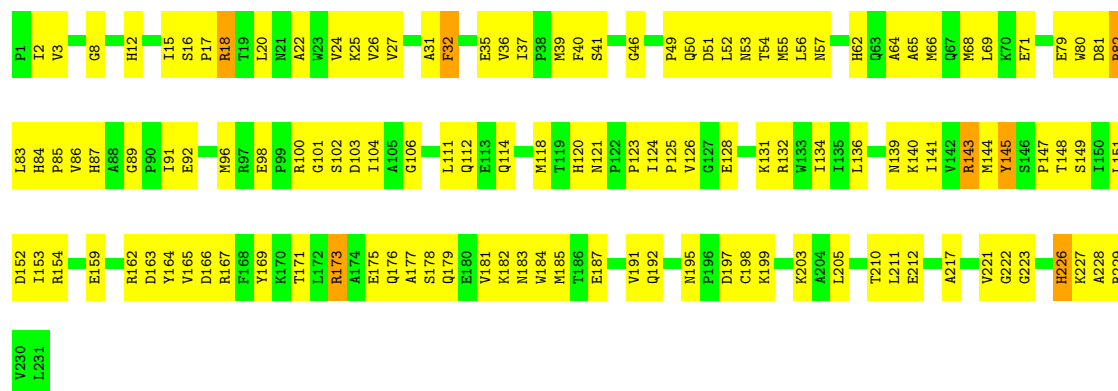
Chain 3v: 





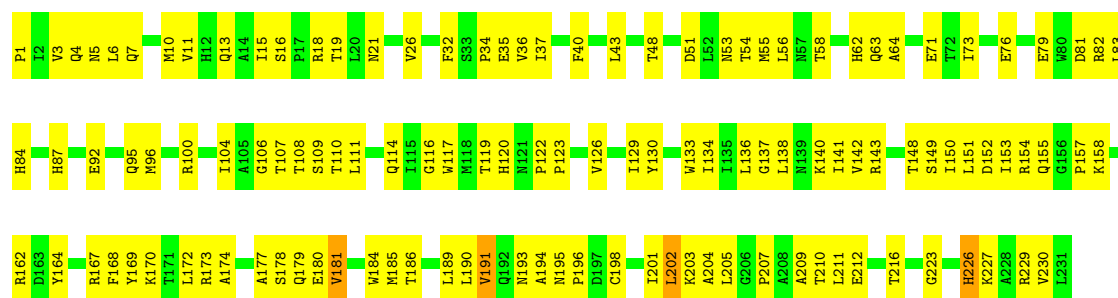
- Molecule 1: capsid protein

Chain 3w: 45% 52%



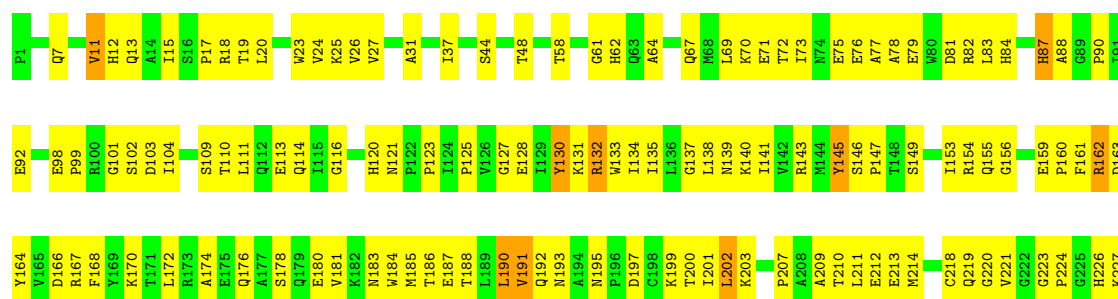
- Molecule 1: capsid protein

Chain 3x: 47% 51%



- Molecule 1: capsid protein

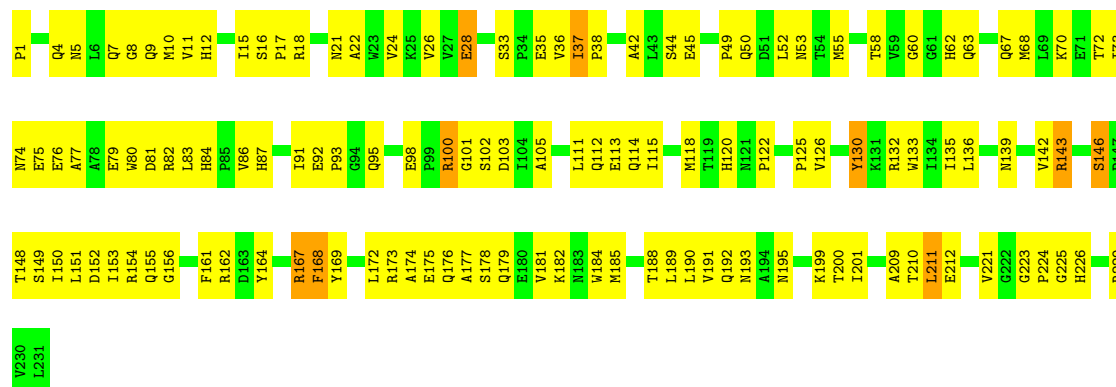
Chain 3y: 45% 51%



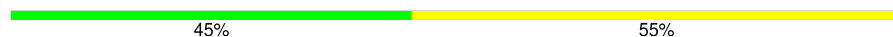


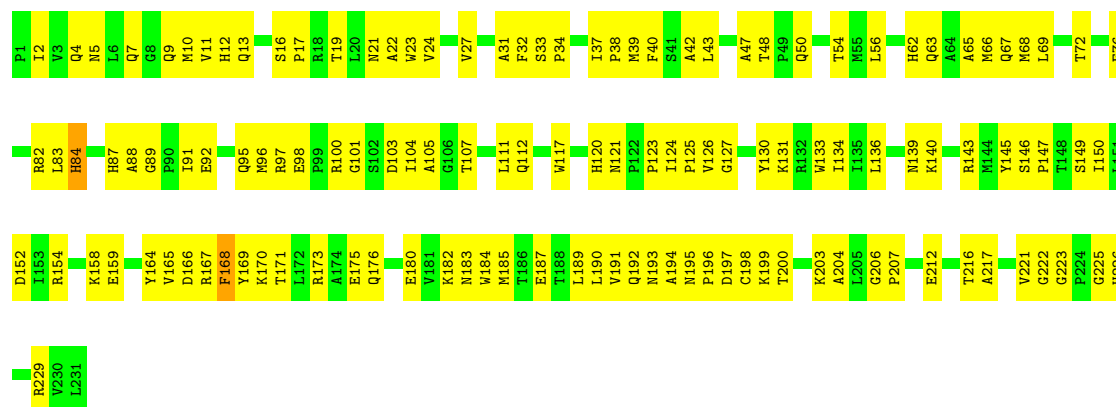
- Molecule 1: capsid protein

Chain 3z: 

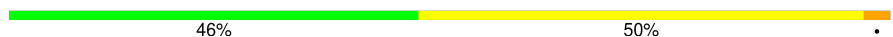


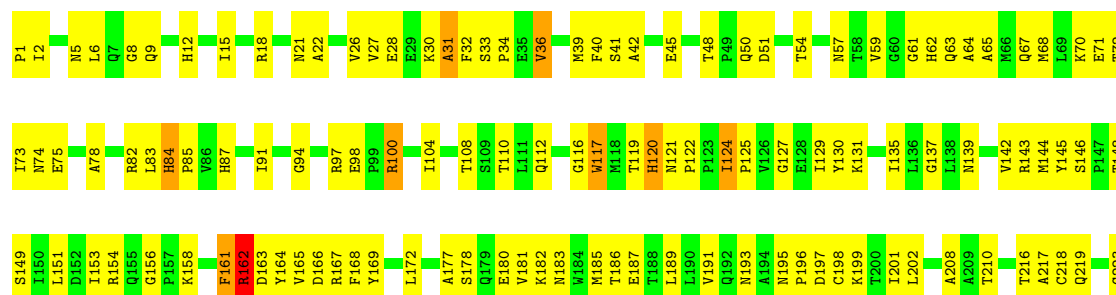
- Molecule 1: capsid protein

Chain 3A: 



- Molecule 1: capsid protein

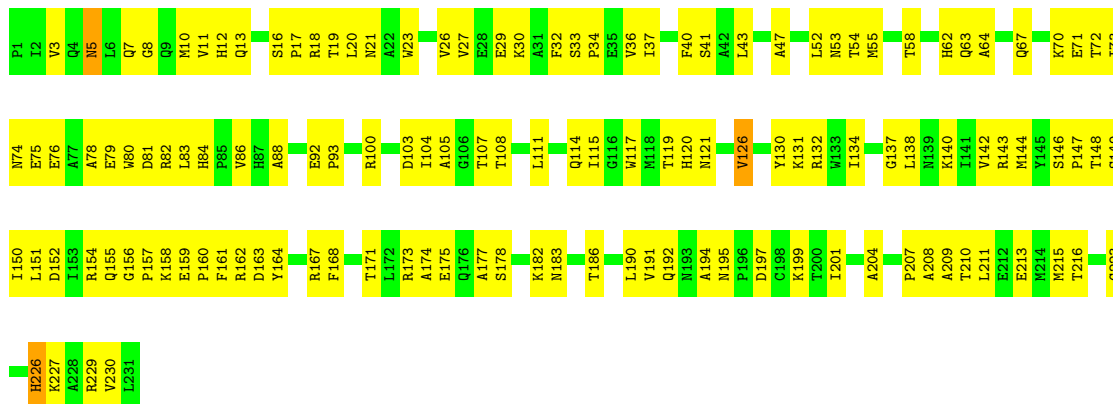
Chain 3B: 



P224
G225
V230
L231

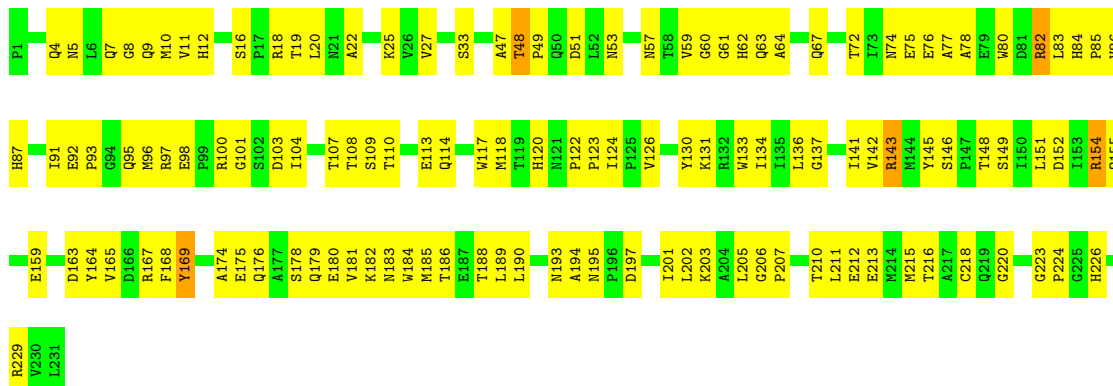
• Molecule 1: capsid protein

Chain 3C: 44% 55%



• Molecule 1: capsid protein

Chain 3D: 45% 53%

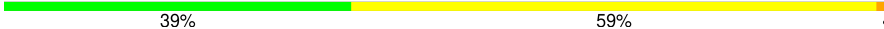


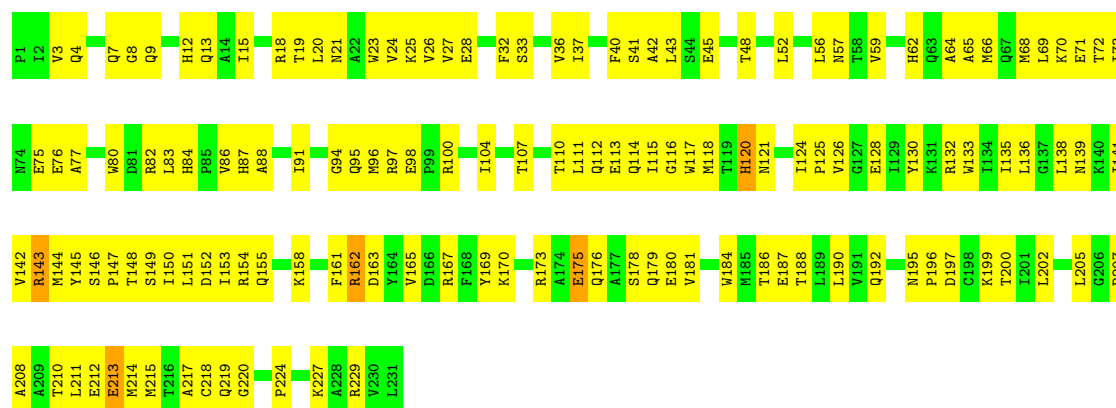
• Molecule 1: capsid protein

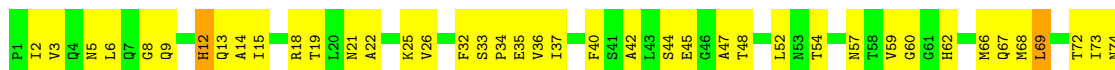
Chain 3E: 47% 52%

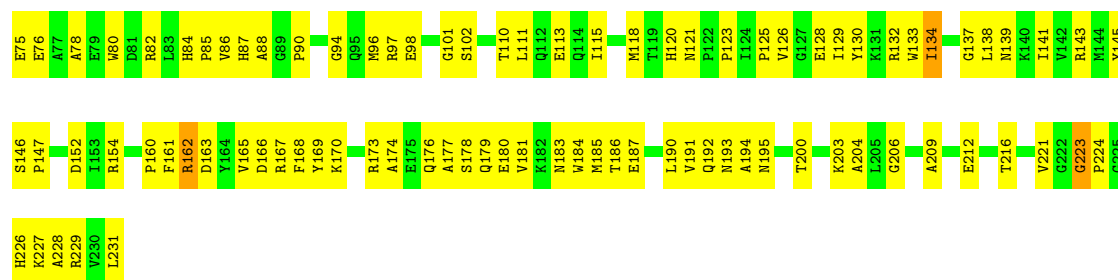


• Molecule 1: capsid protein

Chain 3F:  39% 59%

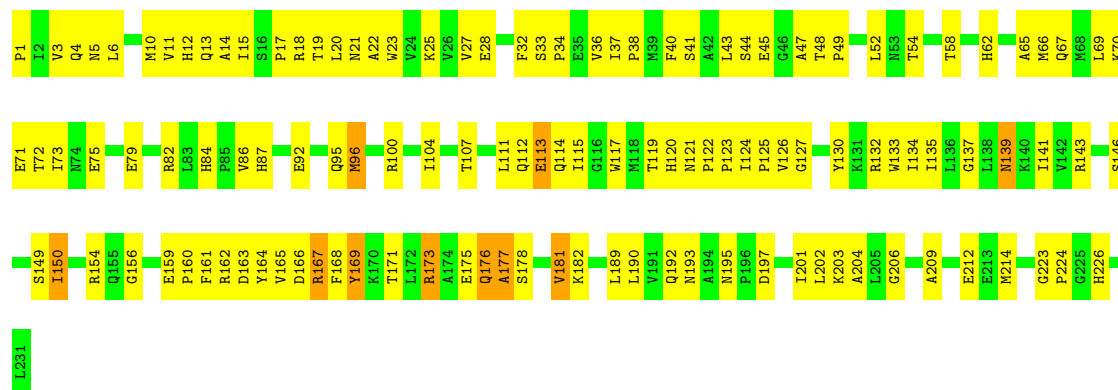






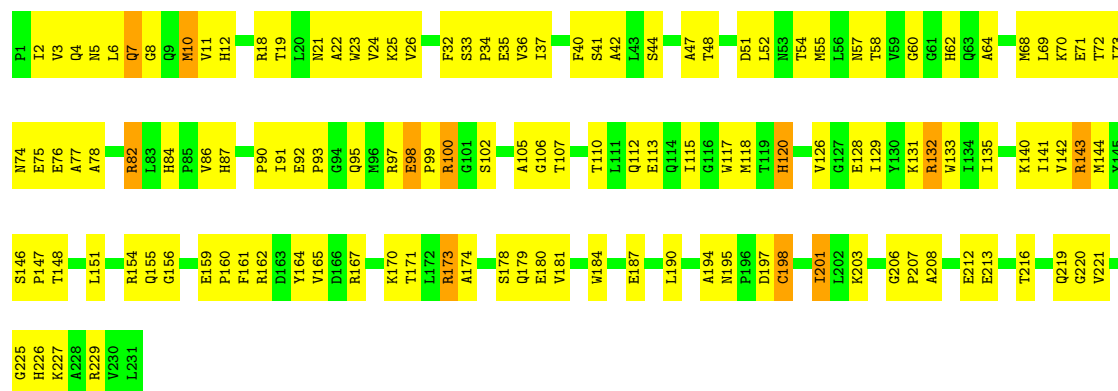
- Molecule 1: capsid protein

Chain 3M: 46% 49%



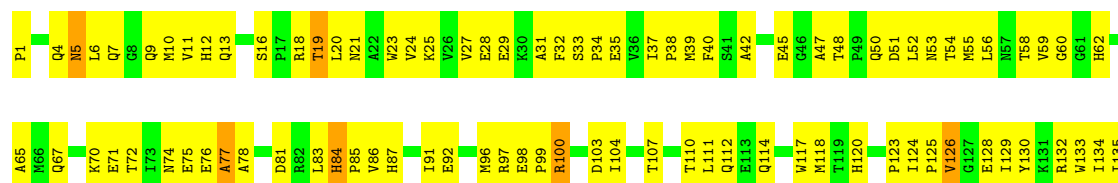
- Molecule 1: capsid protein

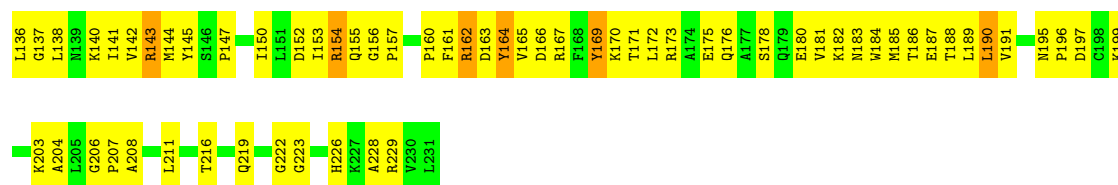
Chain 3N: 44% 52% 5%



- Molecule 1: capsid protein

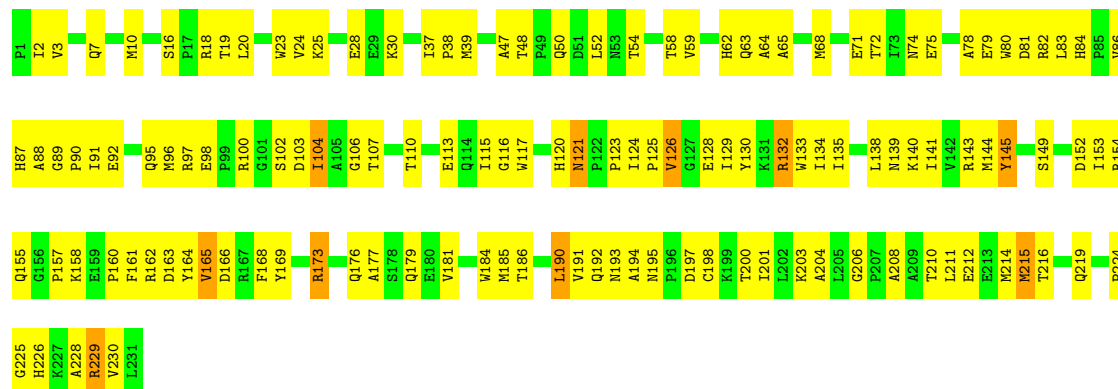
Chain 3O: 35% 60% 5%





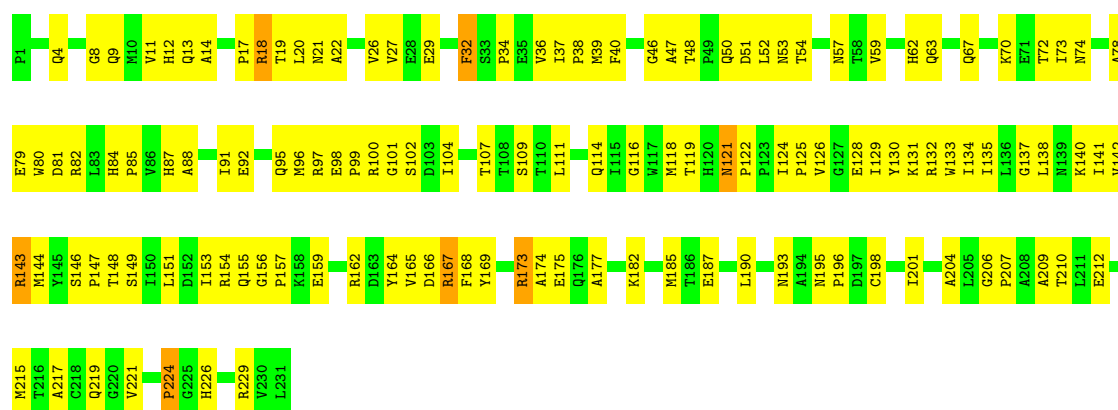
• Molecule 1: capsid protein

Chain 3P: 43% 53%



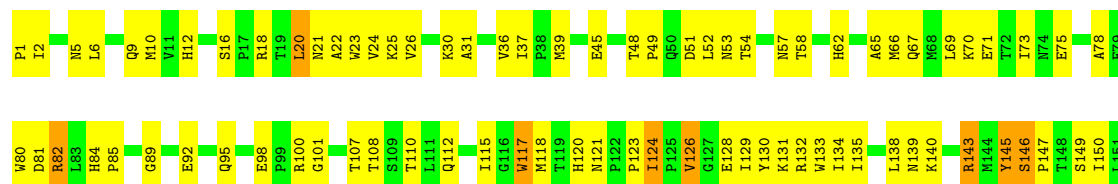
• Molecule 1: capsid protein

Chain 3Q: 43% 54%



• Molecule 1: capsid protein

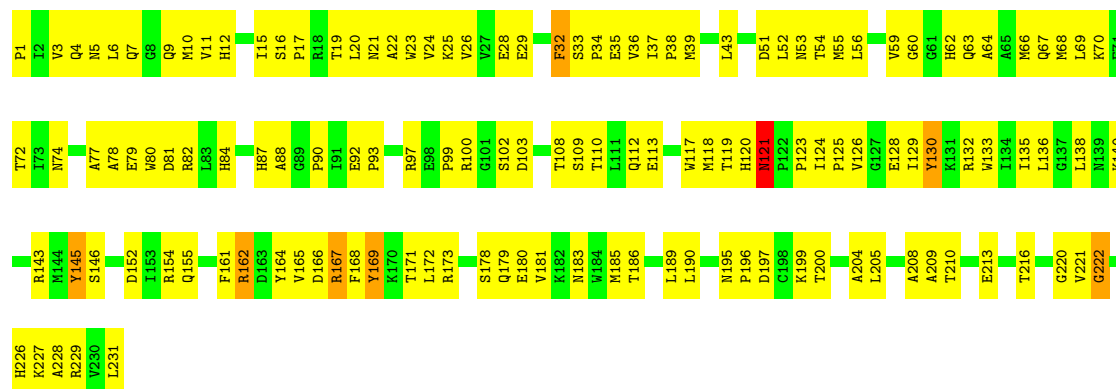
Chain 3R: 47% 48%





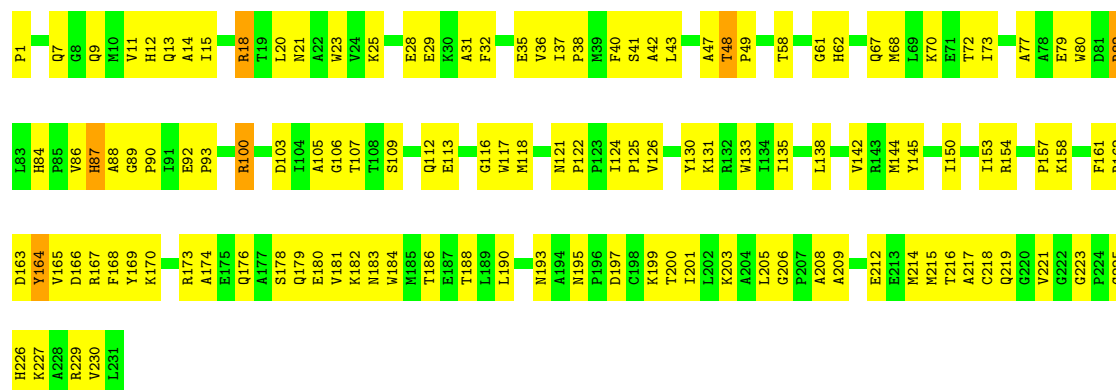
• Molecule 1: capsid protein

Chain 3S: 41% 55%



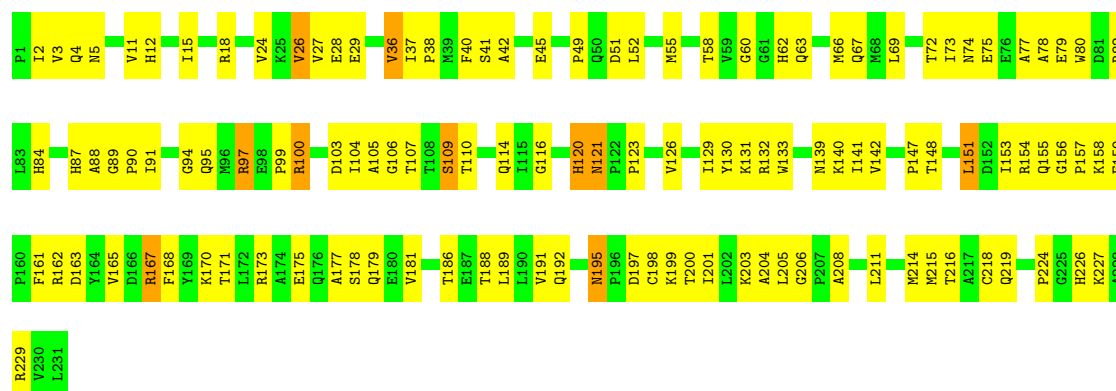
• Molecule 1: capsid protein

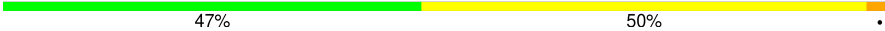
Chain 3T: 46% 52%

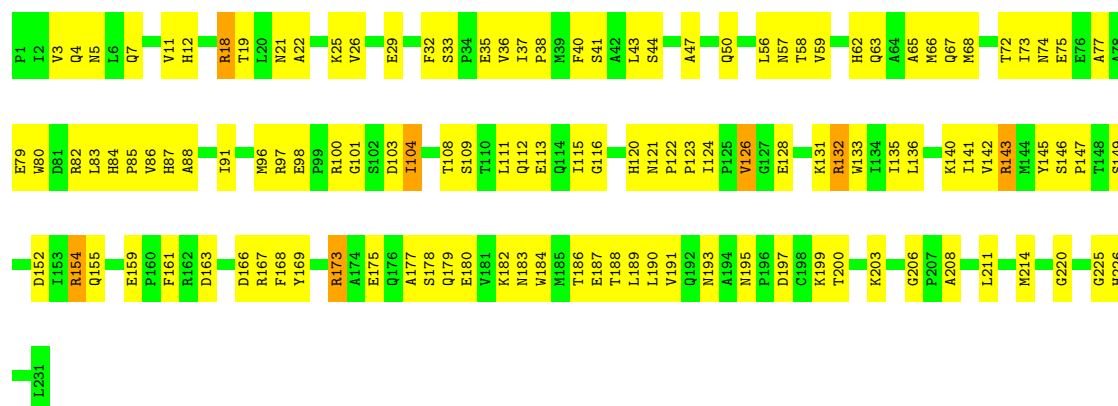


• Molecule 1: capsid protein

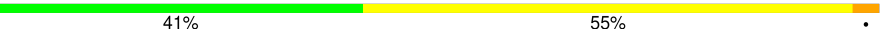
Chain 3U: 47% 49%

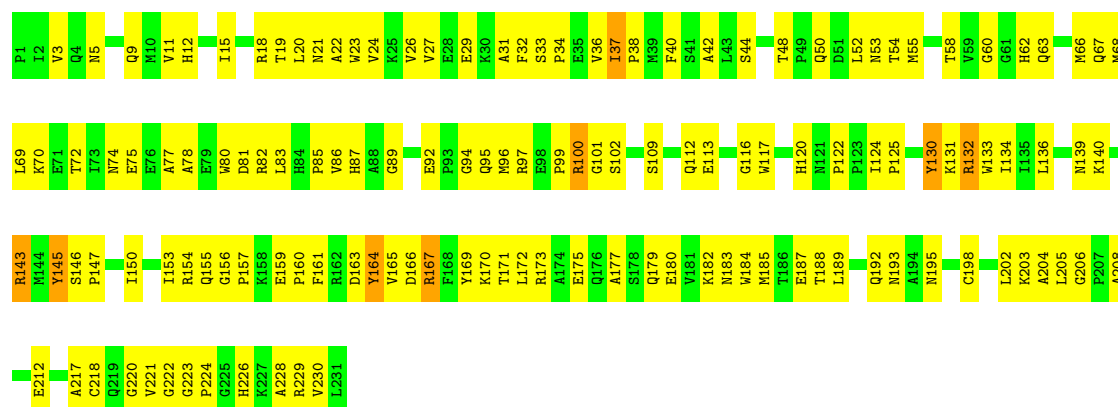


Chain 3Y:  47% 50%

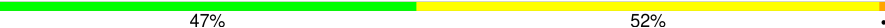


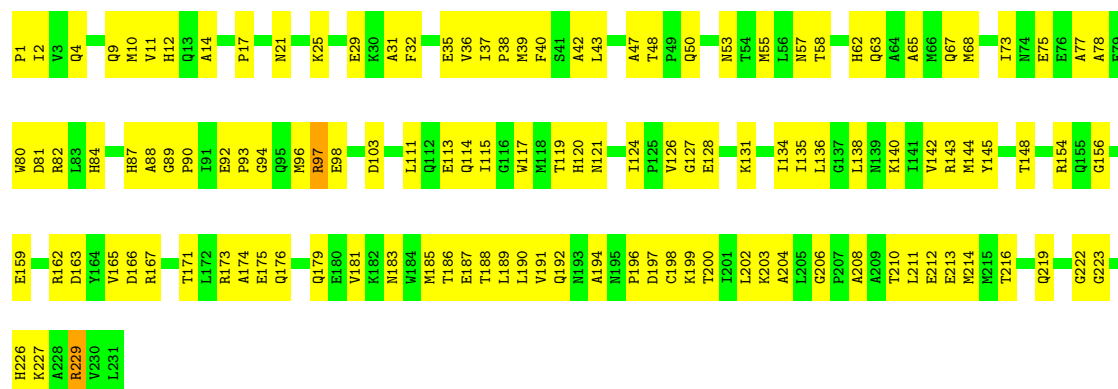
• Molecule 1: capsid protein

Chain 3Z:  41% 55%



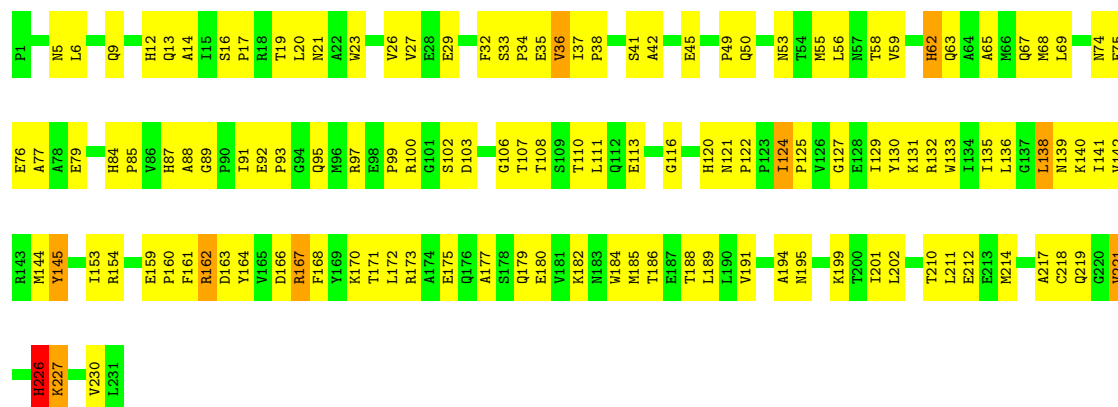
• Molecule 1: capsid protein

Chain 40:  47% 52%



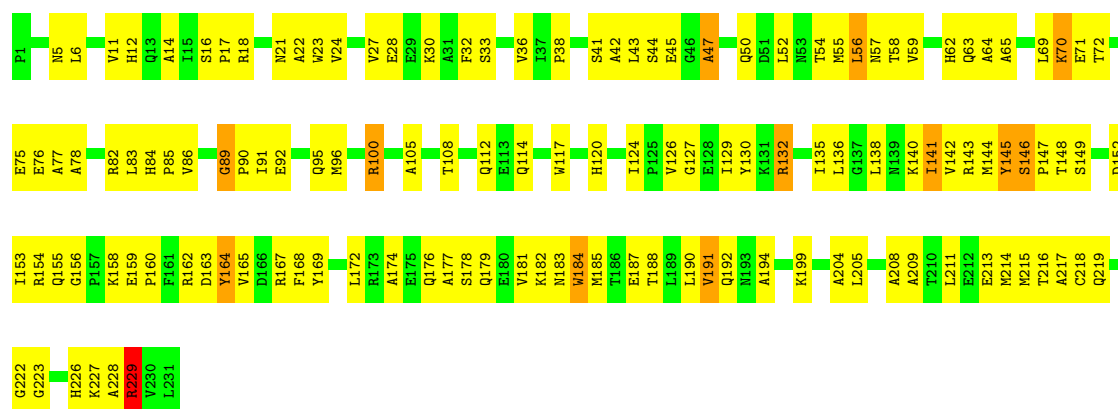
• Molecule 1: capsid protein

Chain 41:  45% 50%



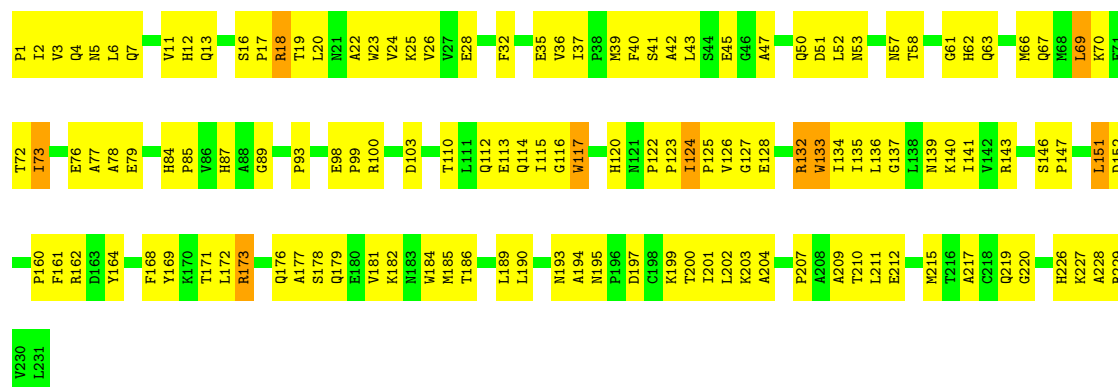
• Molecule 1: capsid protein

Chain 42: 42% 52% 5%



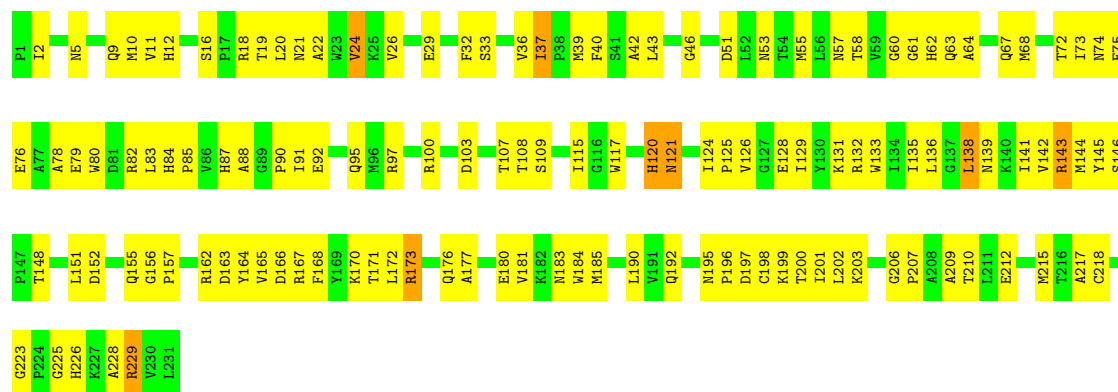
• Molecule 1: capsid protein

Chain 43: 43% 53%



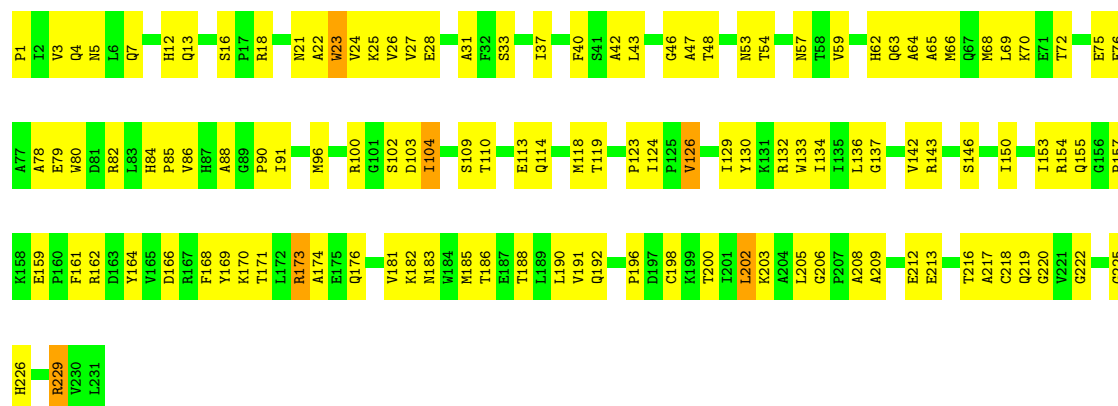
• Molecule 1: capsid protein

Chain 44: 44% 53%



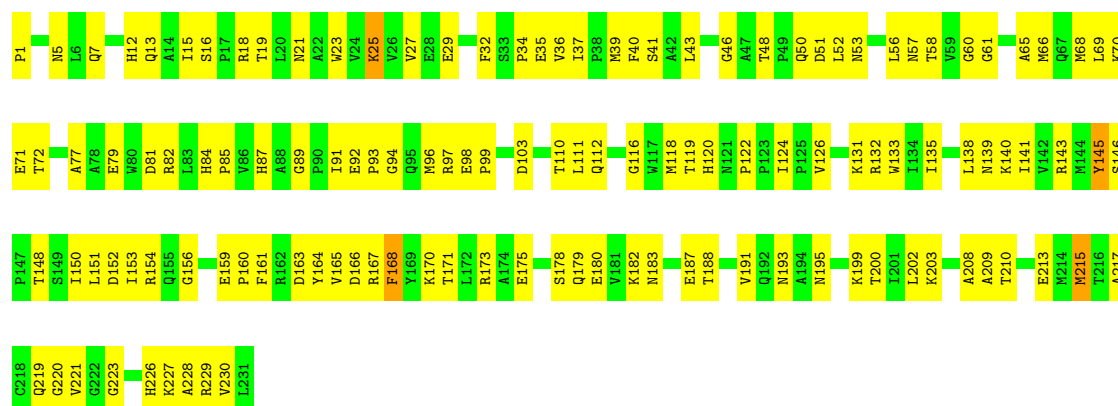
• Molecule 1: capsid protein

Chain 45: 48% 50%



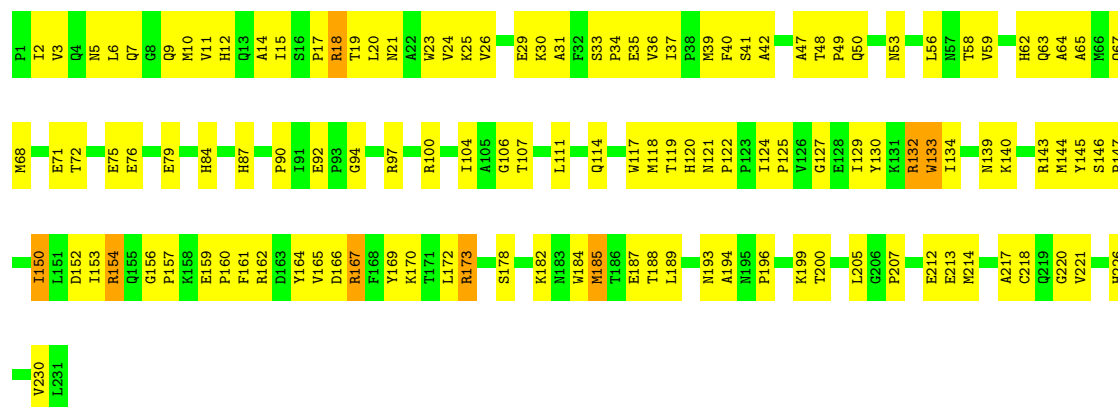
• Molecule 1: capsid protein

Chain 46: 45% 54%



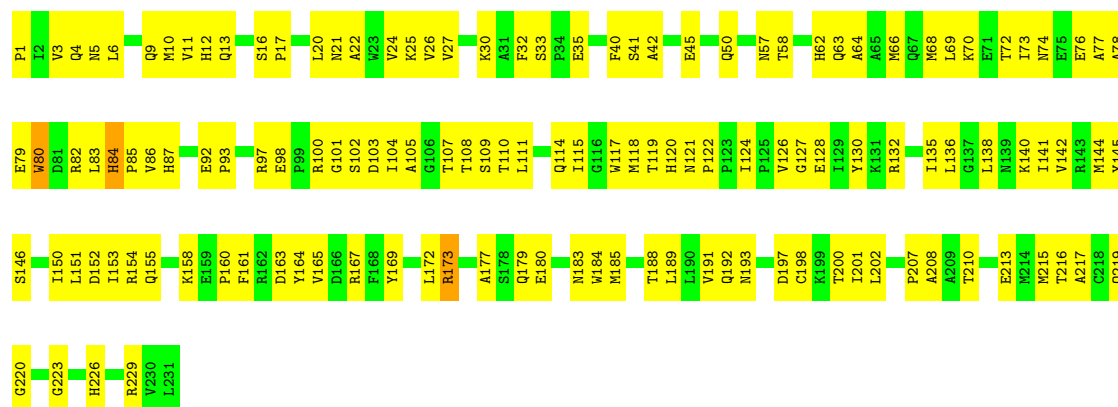
• Molecule 1: capsid protein

Chain 47: 46% 51%



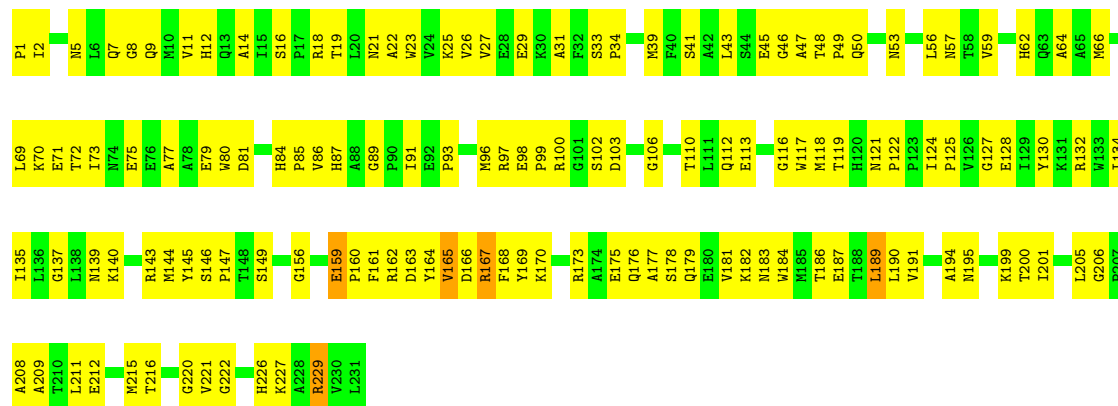
- Molecule 1: capsid protein

Chain 48: 42% 56%



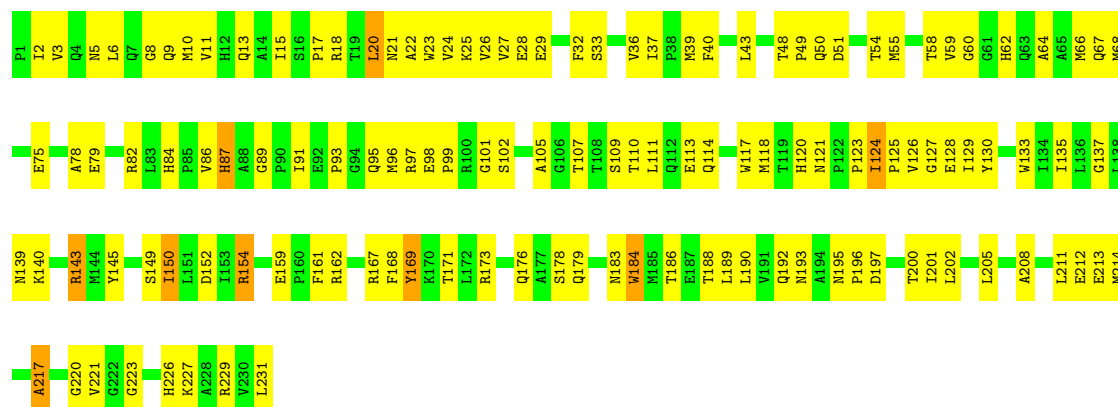
- Molecule 1: capsid protein

Chain 49: 41% 57%



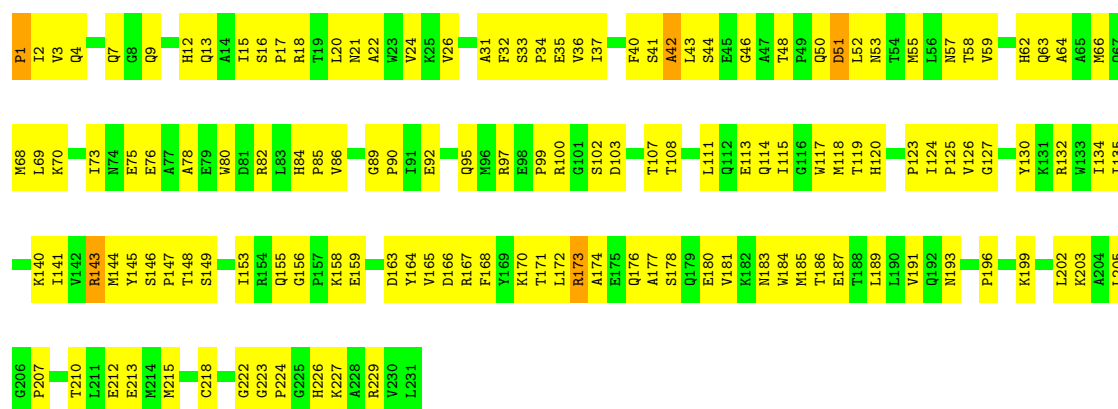
- Molecule 1: capsid protein

Chain 4a: 44% 52%



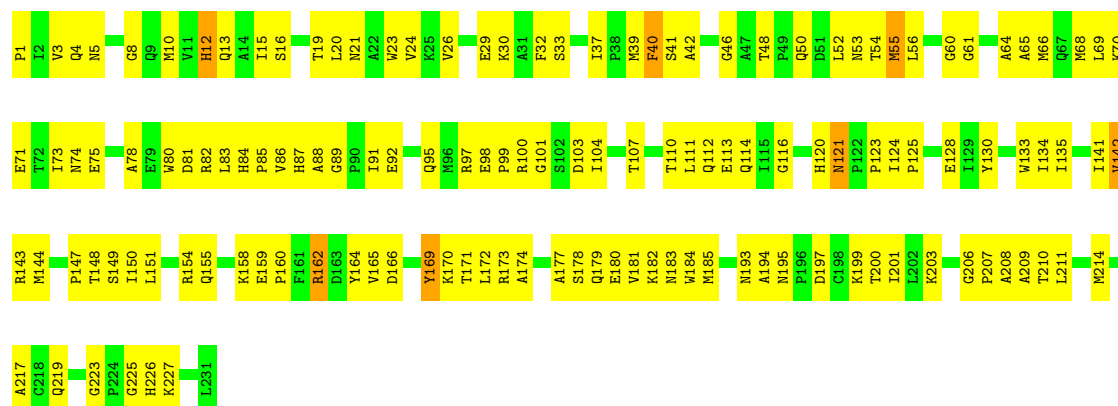
- Molecule 1: capsid protein

Chain 4b: 40% 58%



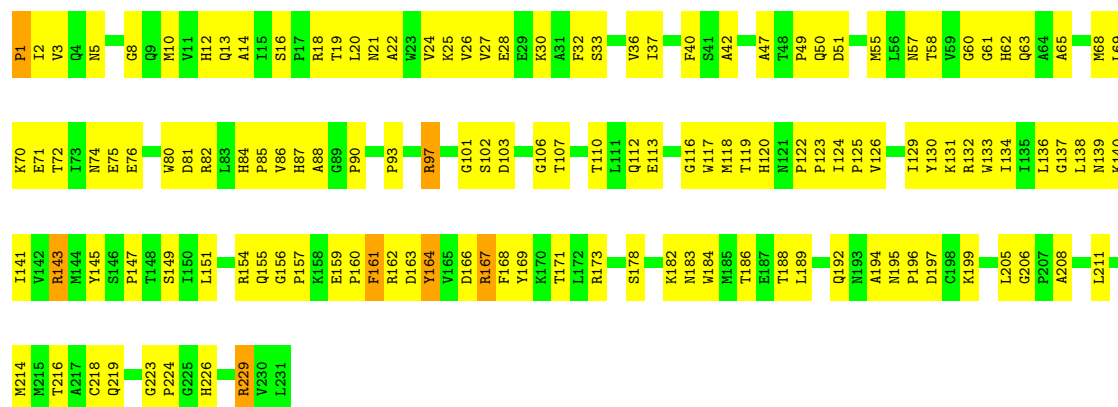
- Molecule 1: capsid protein

Chain 4c: 41% 56%



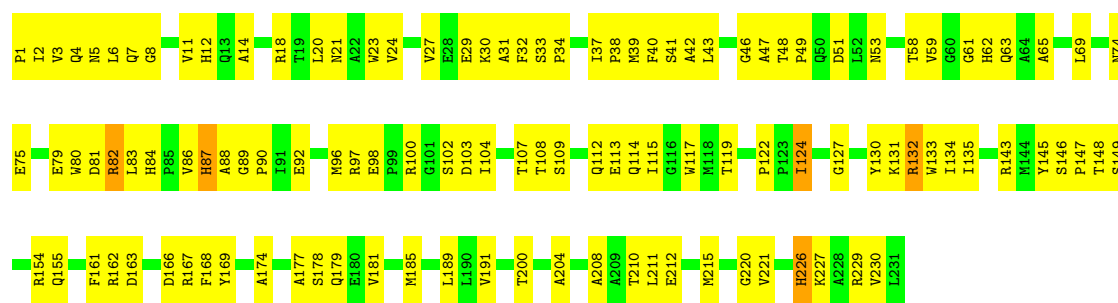
- Molecule 1: capsid protein

Chain 4d: 42% 55%



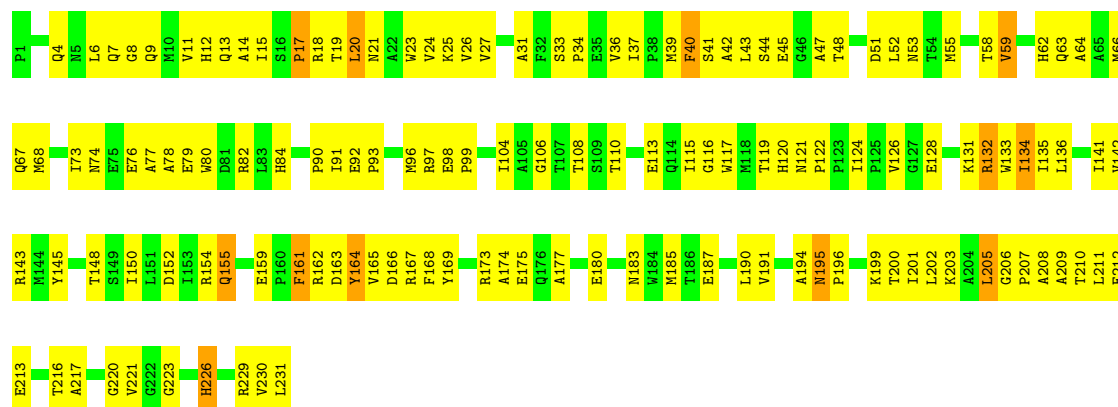
- Molecule 1: capsid protein

Chain 4e: 49% 49%



- Molecule 1: capsid protein

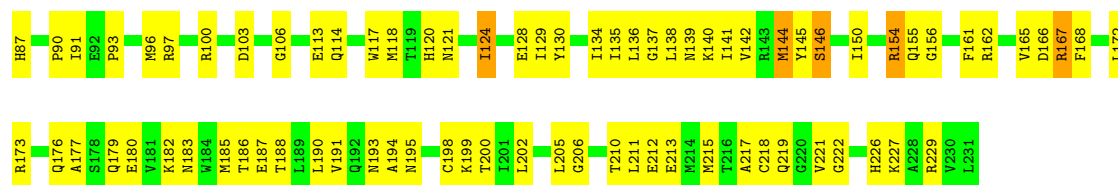
Chain 4f: 40% 55% 5%



- Molecule 1: capsid protein

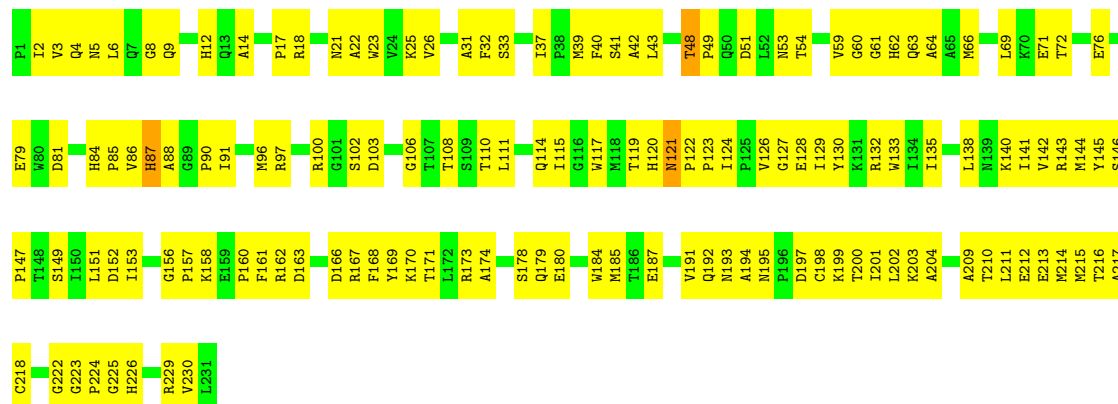
Chain 4g: 49% 48%





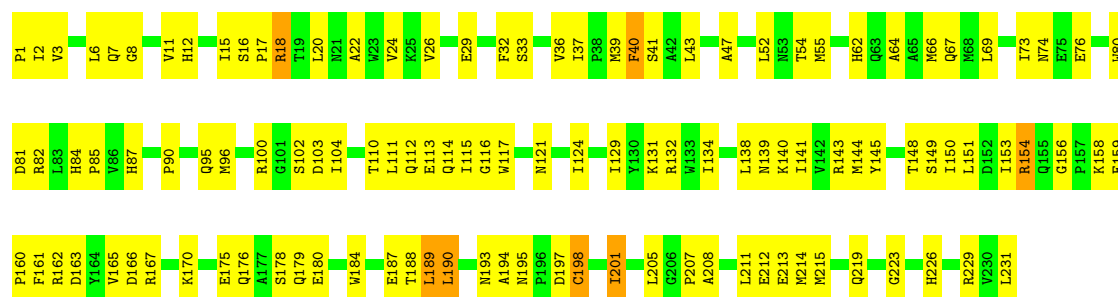
• Molecule 1: capsid protein

Chain 4h: 39% 59%



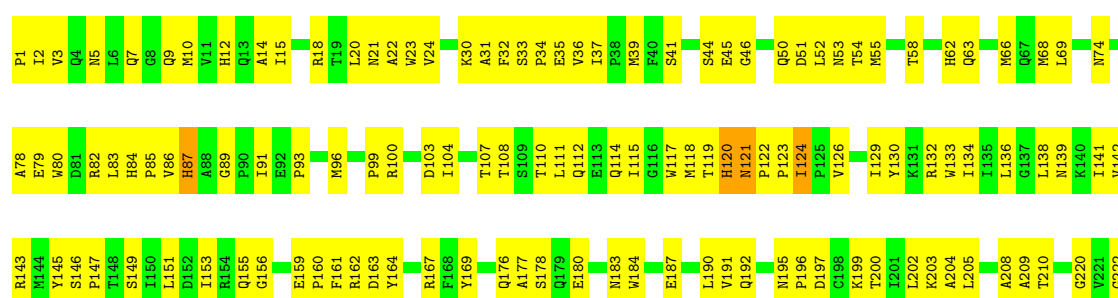
• Molecule 1: capsid protein

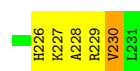
Chain 4i: 49% 48%



• Molecule 1: capsid protein

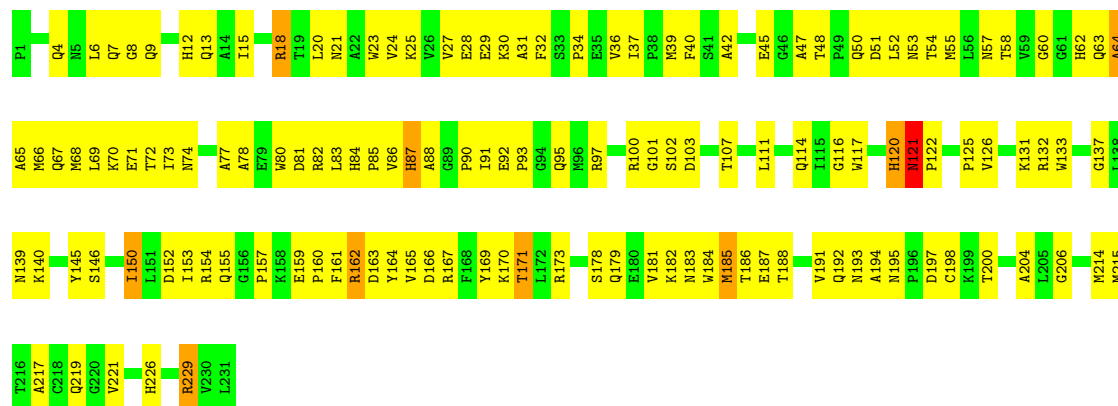
Chain 4j: 43% 55%





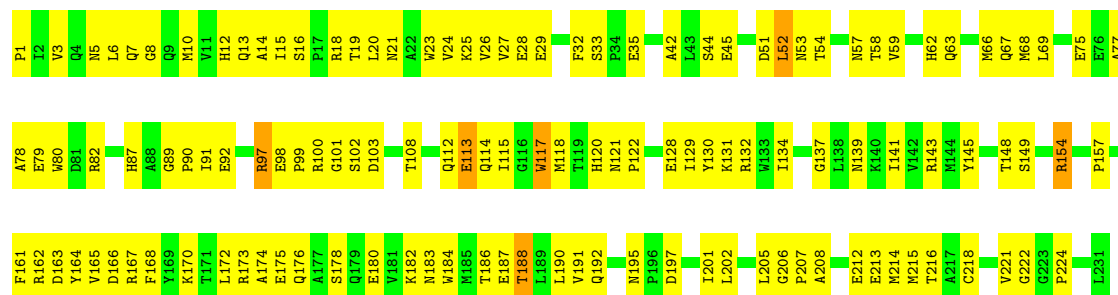
• Molecule 1: capsid protein

Chain 4k: 41% 55%



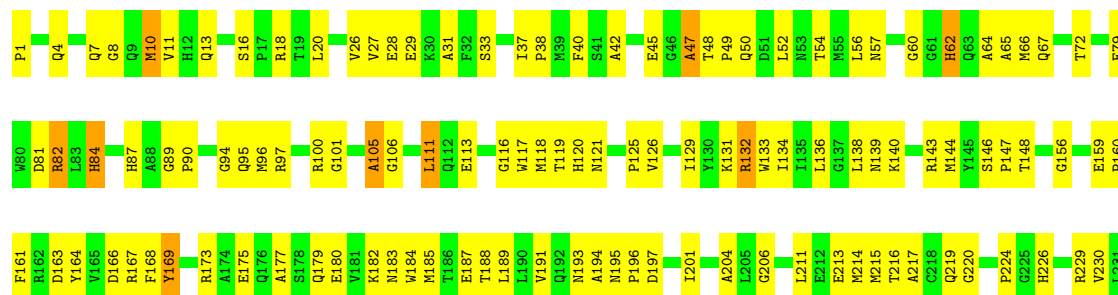
• Molecule 1: capsid protein

Chain 4l: 45% 52%



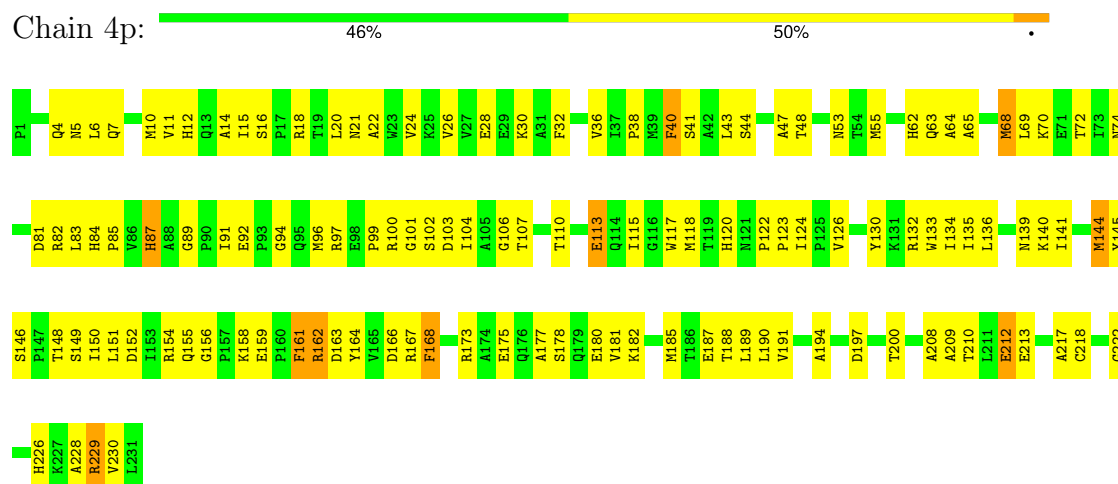
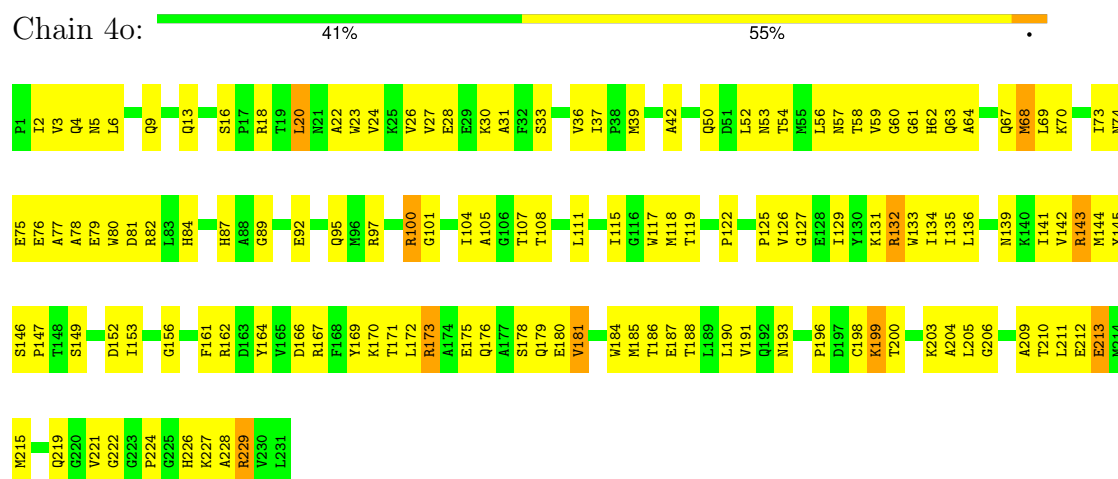
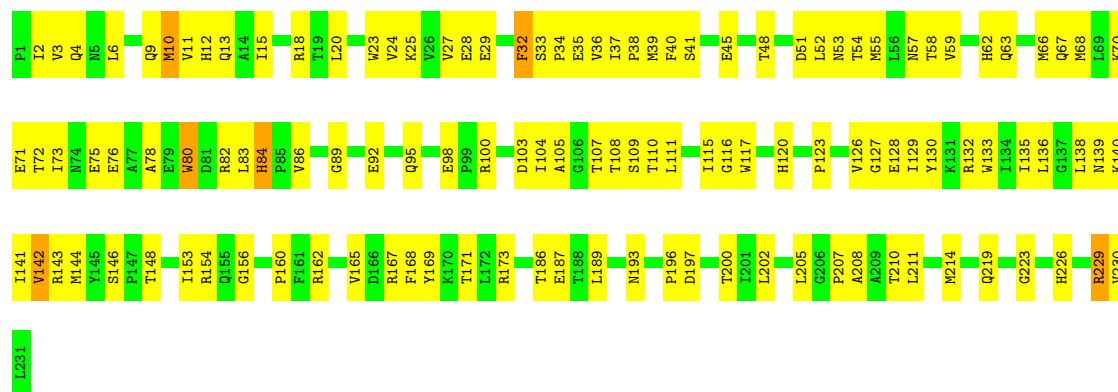
• Molecule 1: capsid protein

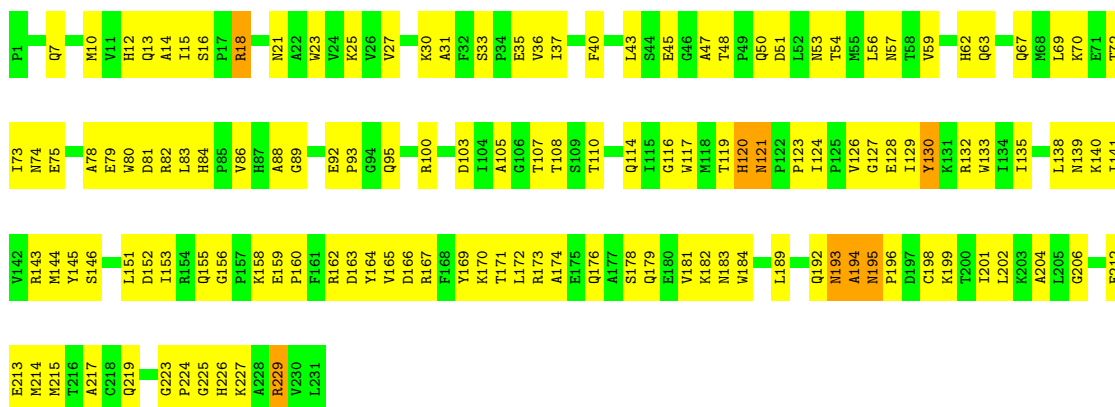
Chain 4m: 49% 47%



• Molecule 1: capsid protein

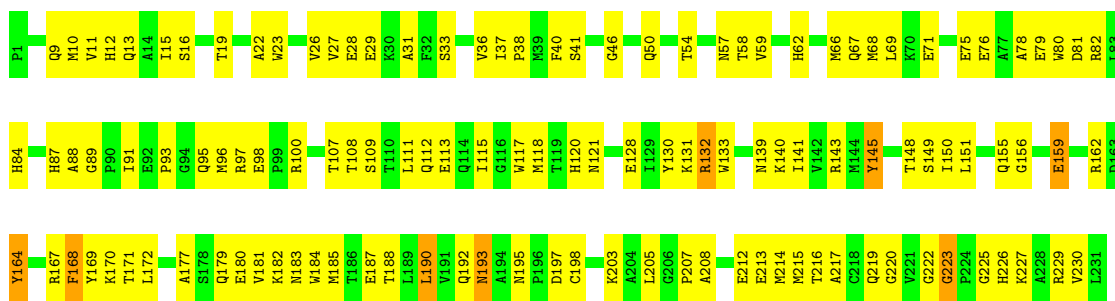
Chain 4n: 48% 50%





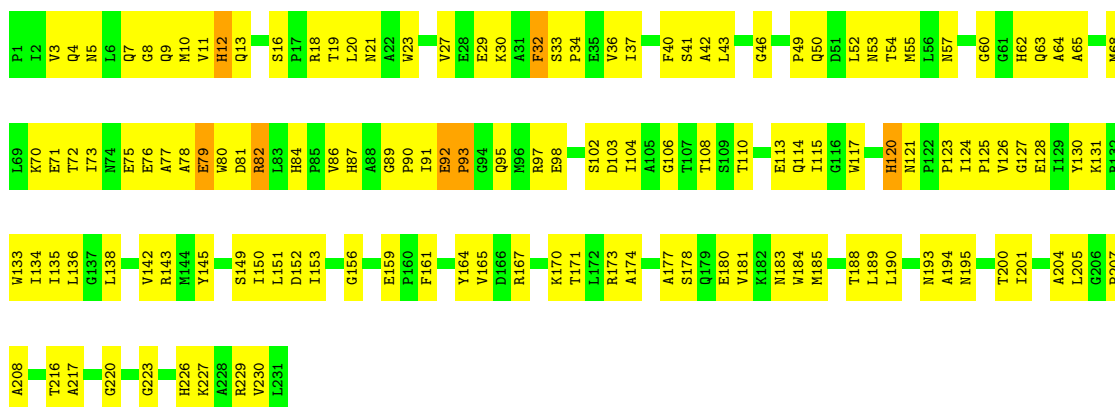
• Molecule 1: capsid protein

Chain 4r: 47% 49%



• Molecule 1: capsid protein

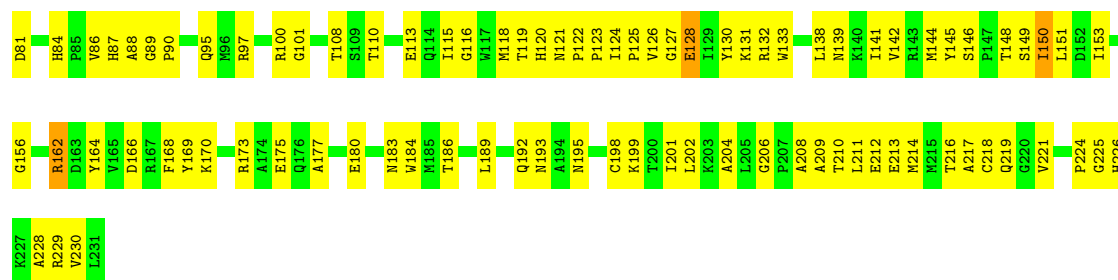
Chain 4s: 42% 55%



• Molecule 1: capsid protein

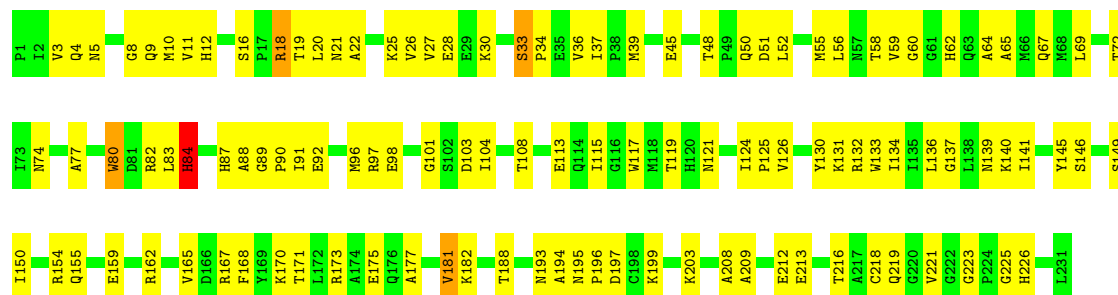
Chain 4t: 47% 51%





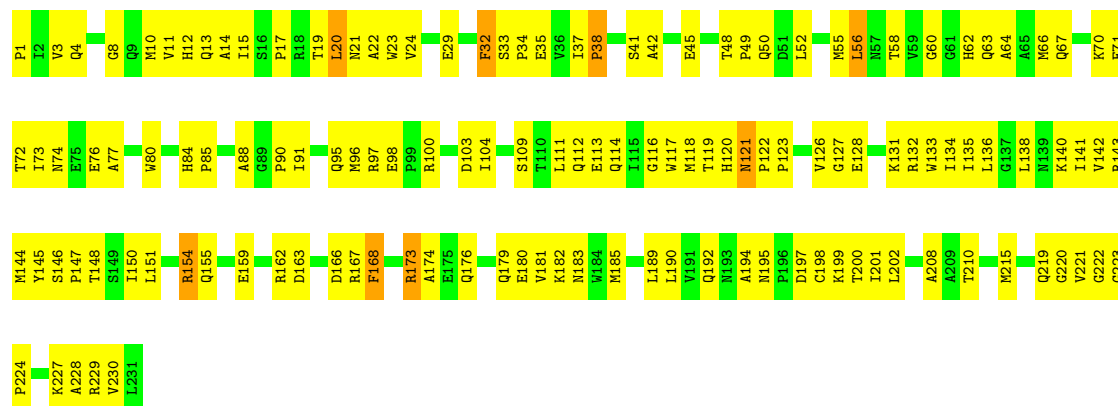
- Molecule 1: capsid protein

Chain 4u: 51% 47%



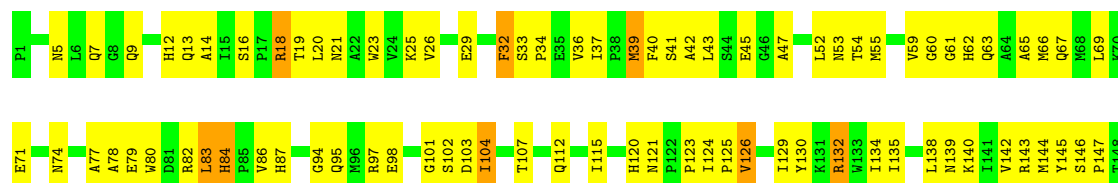
- Molecule 1: capsid protein

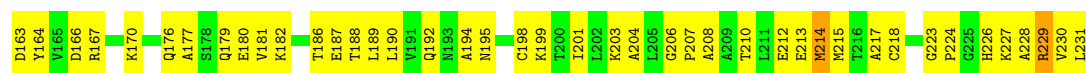
Chain 4v: 42% 55%



- Molecule 1: capsid protein

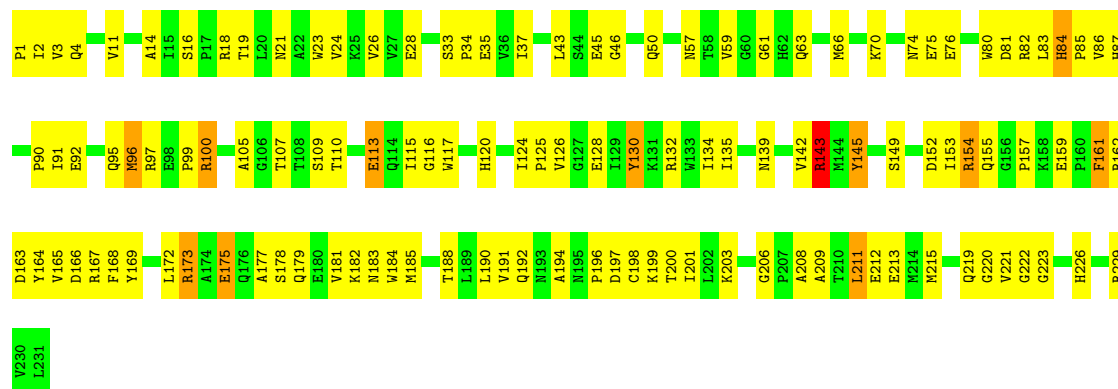
Chain 4w: 45% 50% 5%





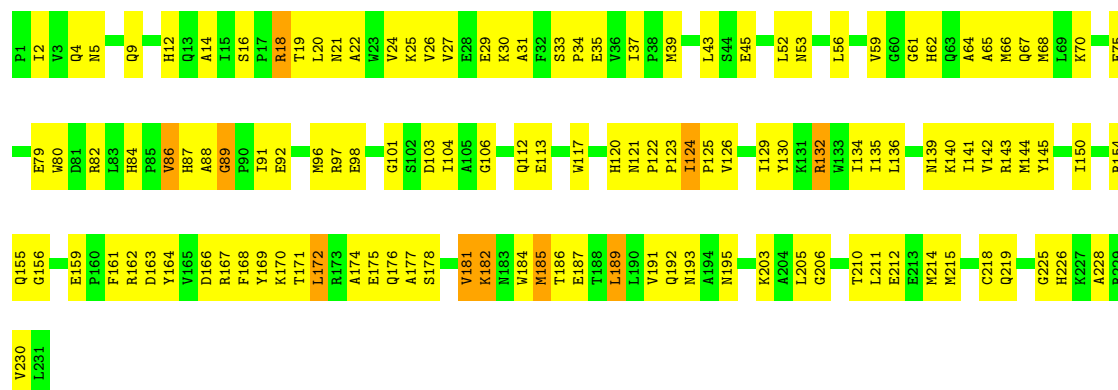
- Molecule 1: capsid protein

Chain 4A: 48% 47% 5%



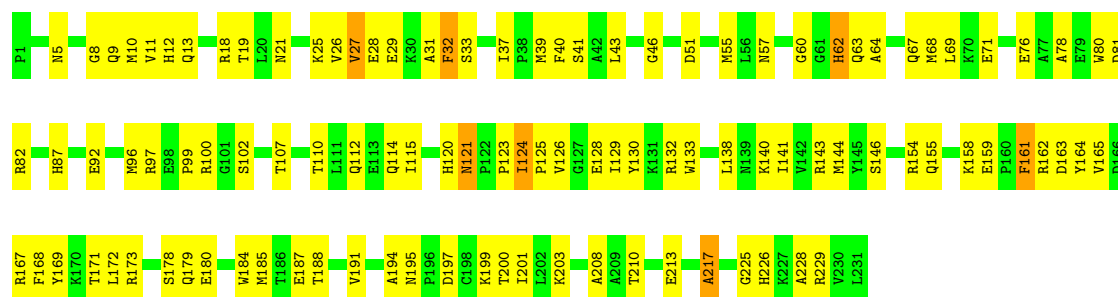
- Molecule 1: capsid protein

Chain 4B: 46% 50% .

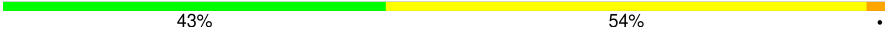


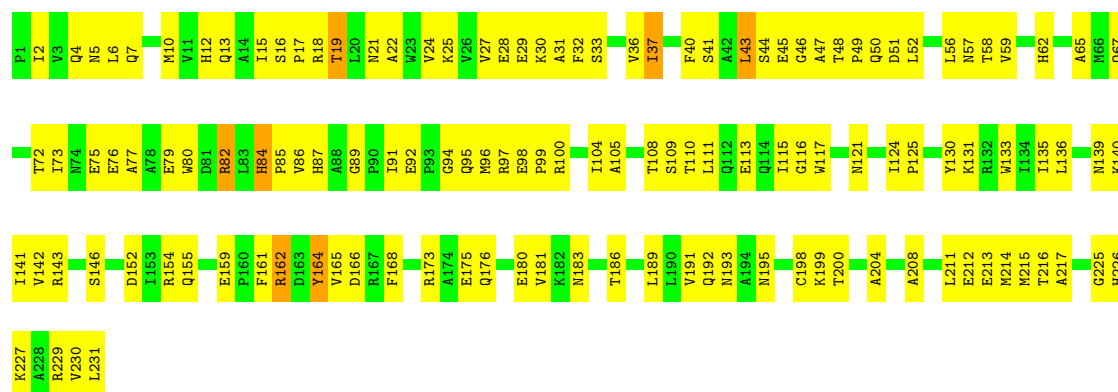
- Molecule 1: capsid protein

Chain 4C: 54% 43% .

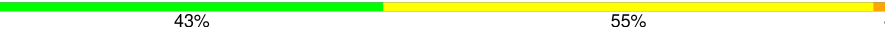


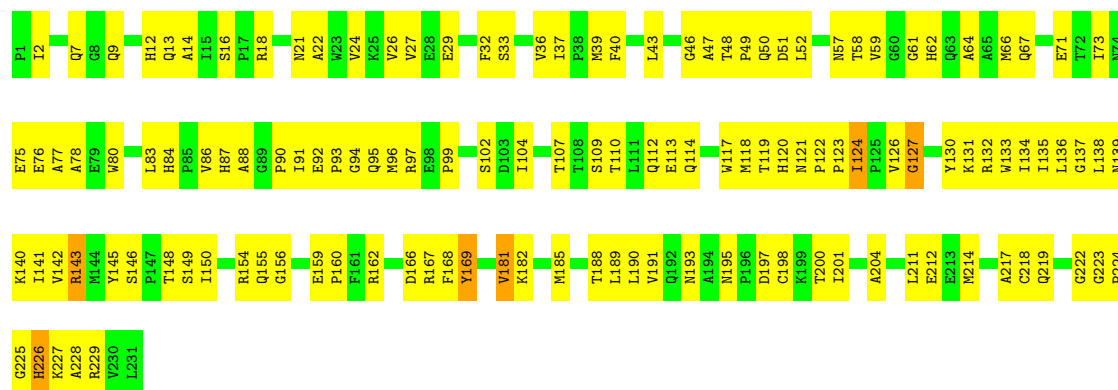
- Molecule 1: capsid protein

Chain 4D: 



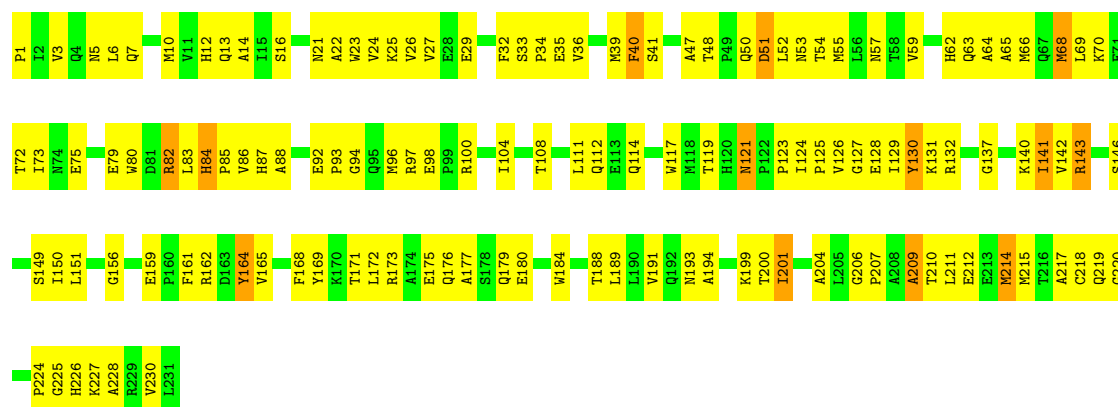
• Molecule 1: capsid protein

Chain 4E: 



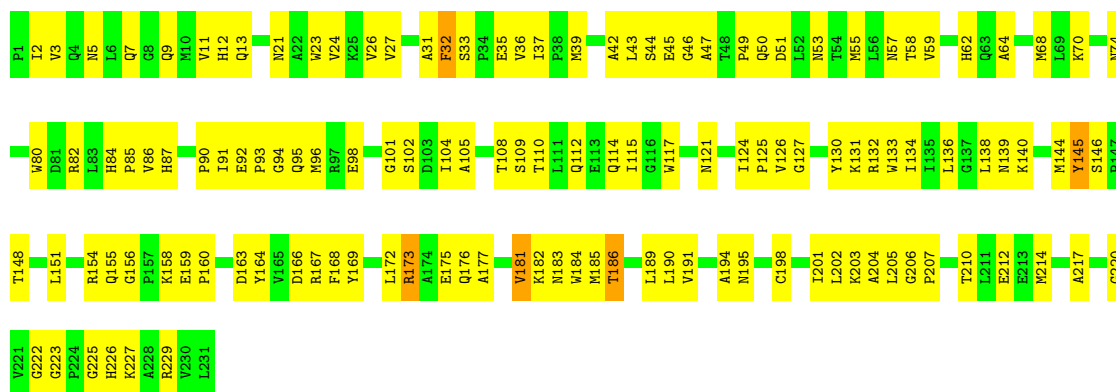
• Molecule 1: capsid protein

Chain 4F: 



• Molecule 1: capsid protein

Chain 4G: 



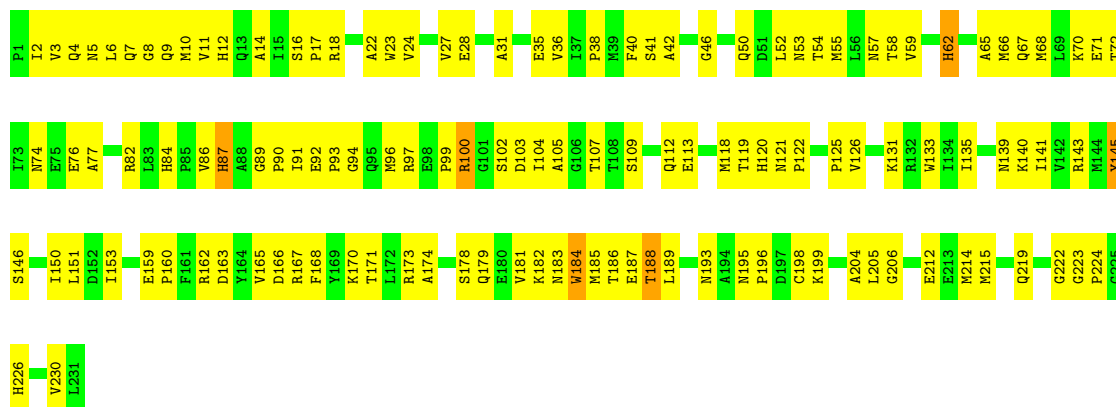
• Molecule 1: capsid protein

Chain 4H: 48% 49%



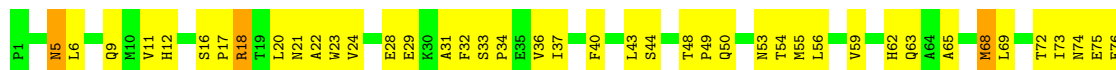
• Molecule 1: capsid protein

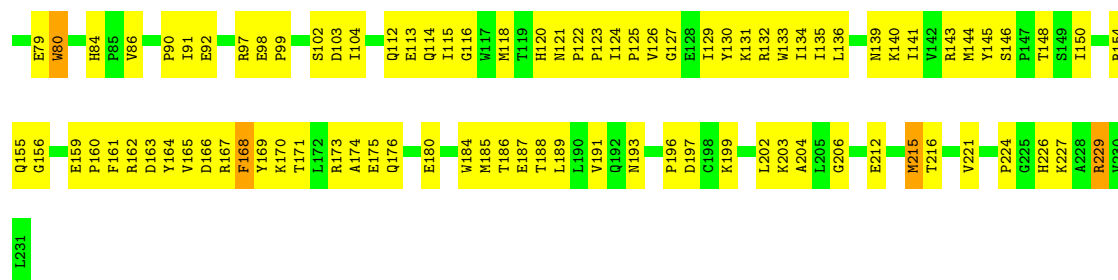
Chain 4I: 45% 53%



• Molecule 1: capsid protein

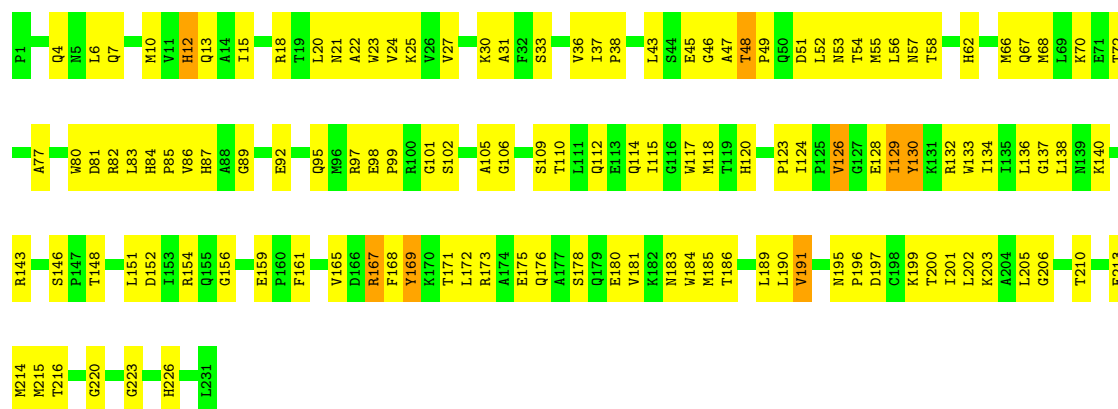
Chain 4J: 44% 53%





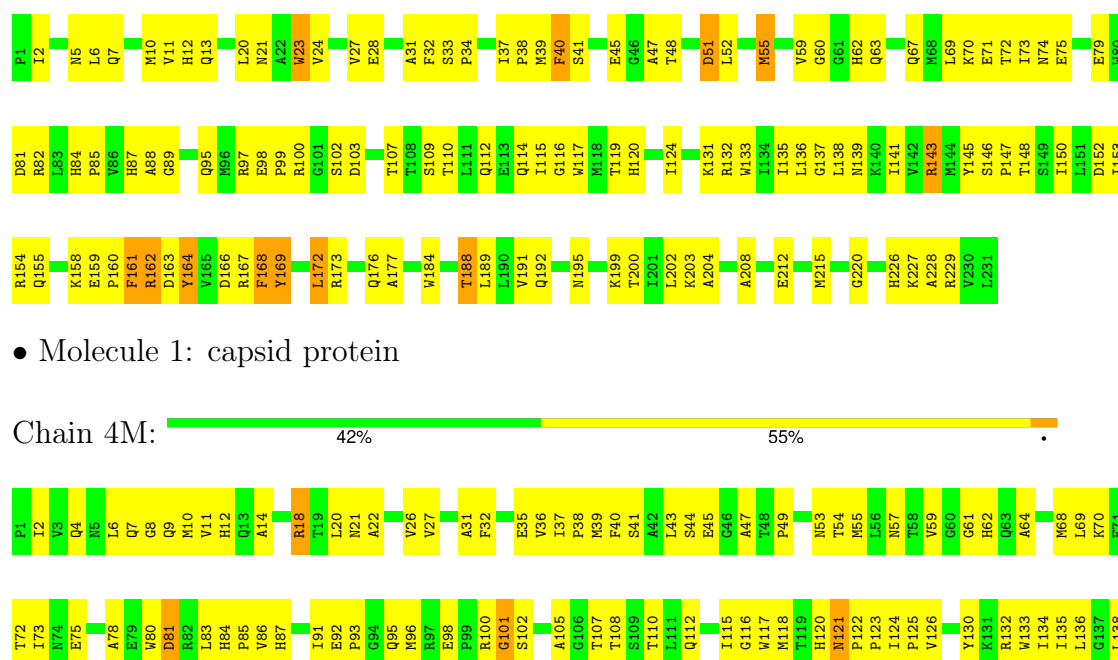
- Molecule 1: capsid protein

Chain 4K: 45% 52%



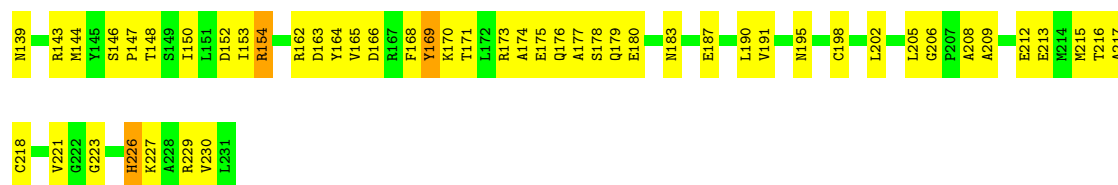
- Molecule 1: capsid protein

Chain 4L: 48% 47% 5%



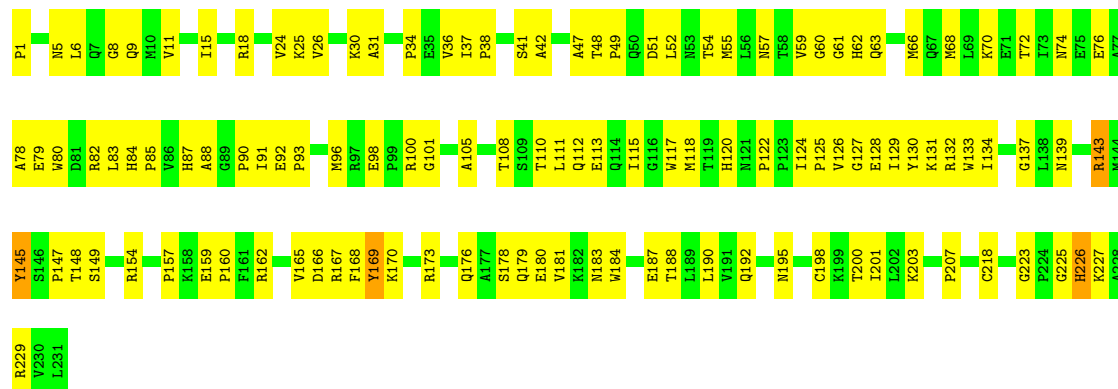
- Molecule 1: capsid protein

Chain 4M: 42% 55%



- Molecule 1: capsid protein

Chain 4N: 48% 50%



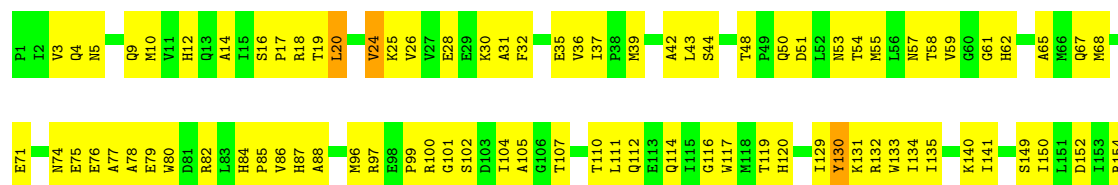
- Molecule 1: capsid protein

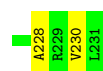
Chain 4O: 43% 55%



- Molecule 1: capsid protein

Chain 4P: 44% 55%





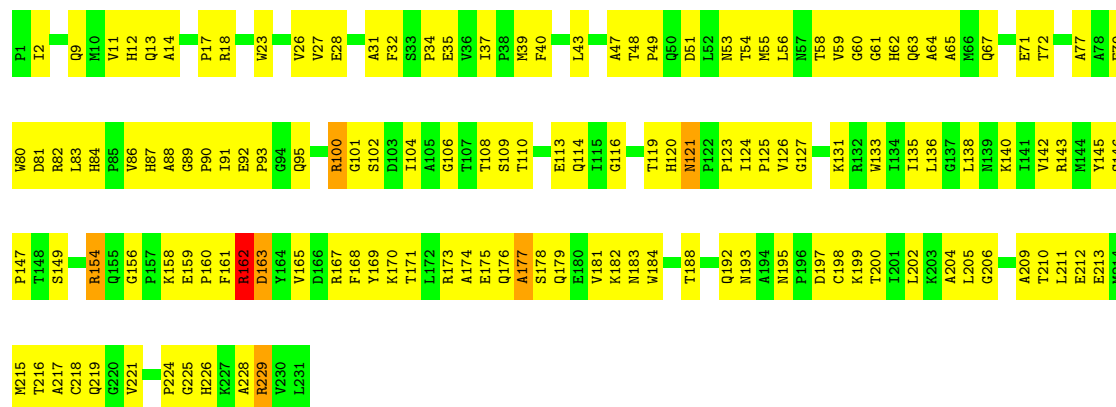
• Molecule 1: capsid protein

Chain 4T: 45% 54%



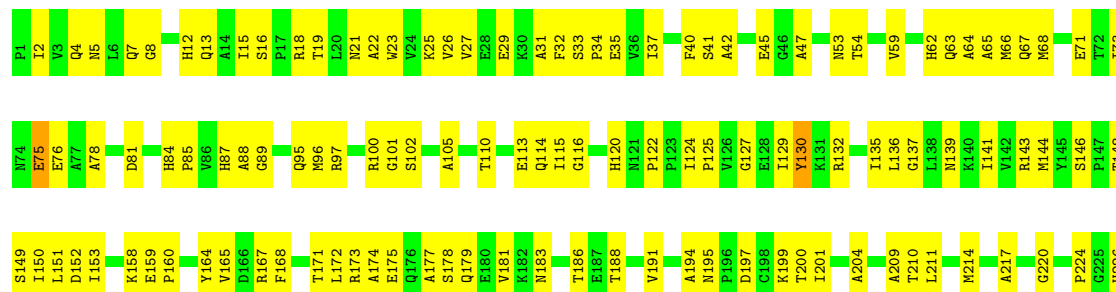
• Molecule 1: capsid protein

Chain 4U: 40% 57%



• Molecule 1: capsid protein

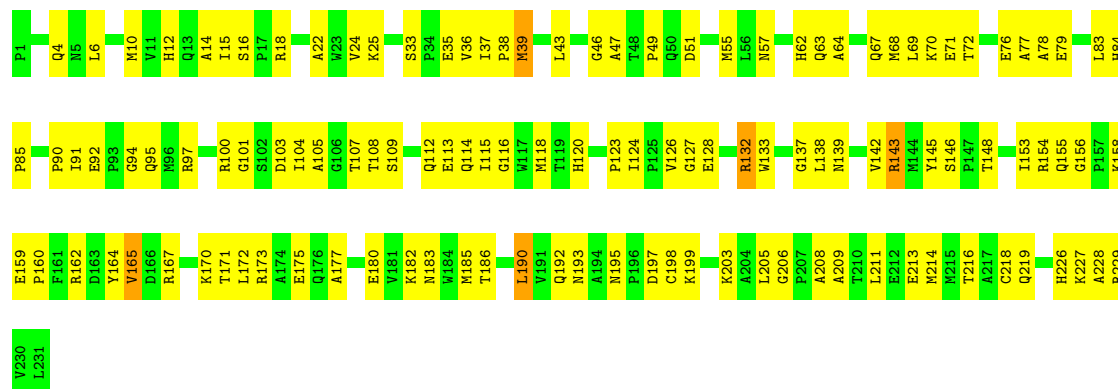
Chain 4V: 48% 51%





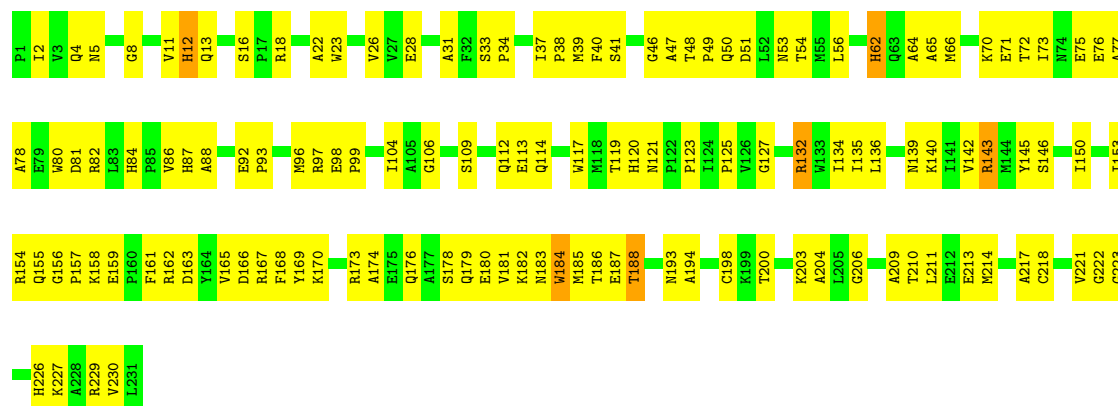
- Molecule 1: capsid protein

Chain 4W: 48% 50%



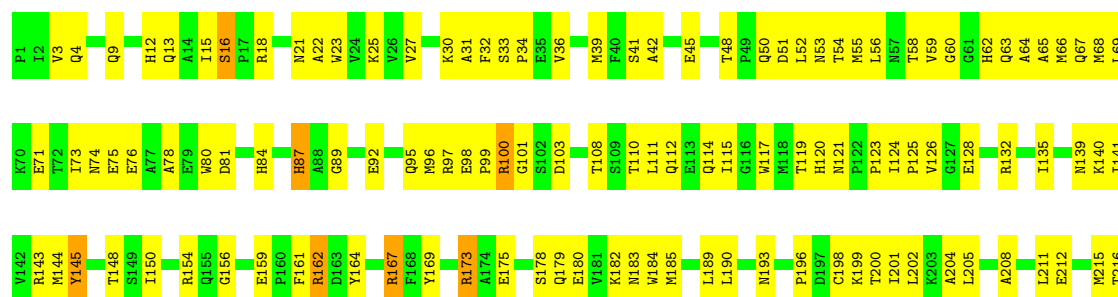
- Molecule 1: capsid protein

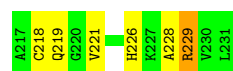
Chain 4X: 44% 54%



- Molecule 1: capsid protein

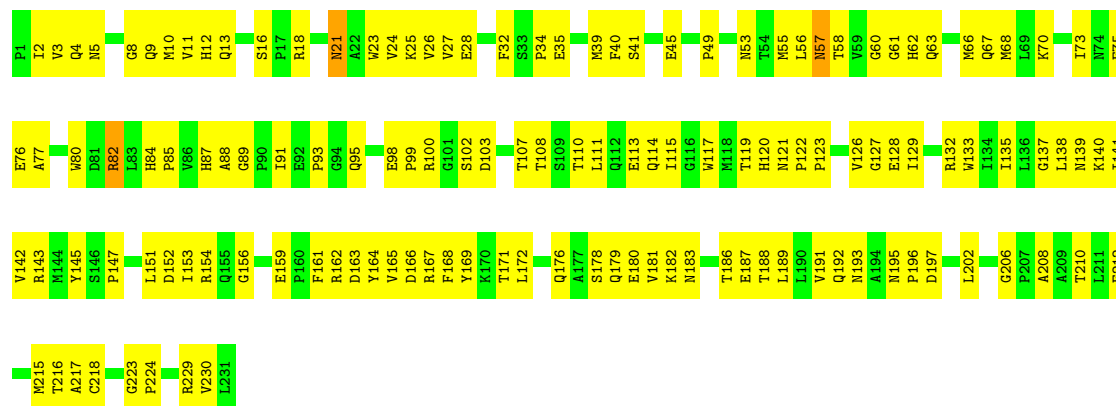
Chain 4Y: 45% 51%





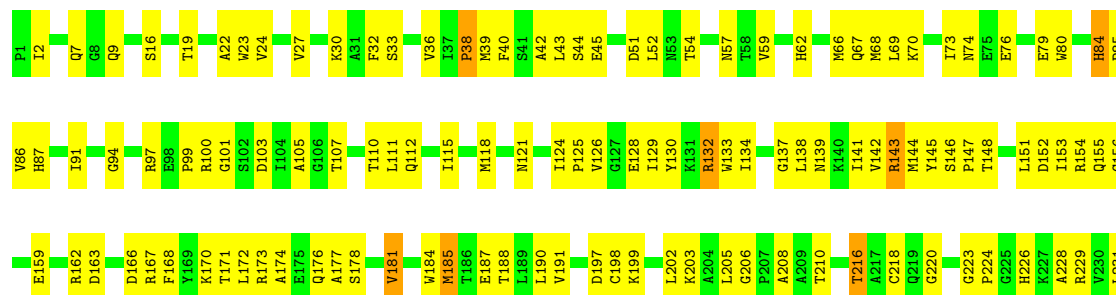
• Molecule 1: capsid protein

Chain 4Z: 42% 57%



• Molecule 1: capsid protein

Chain 50: 48% 49%



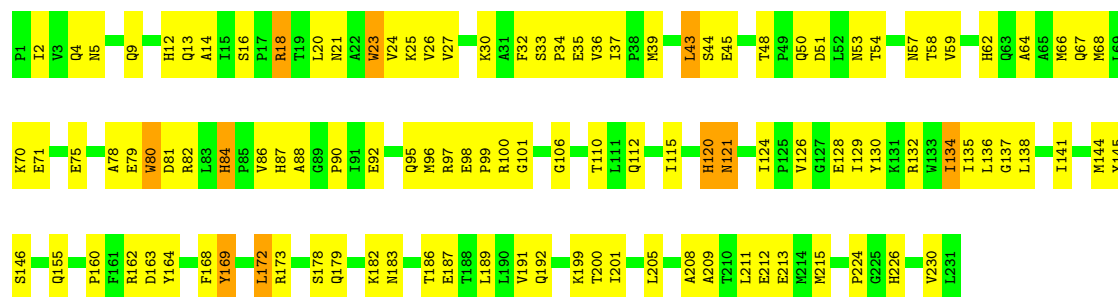
• Molecule 1: capsid protein

Chain 51: 48% 49%



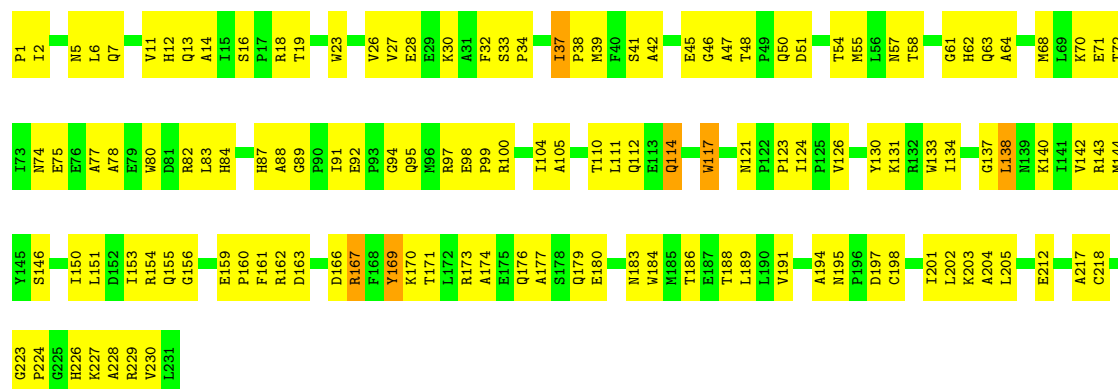
• Molecule 1: capsid protein

Chain 52: 51% 45%



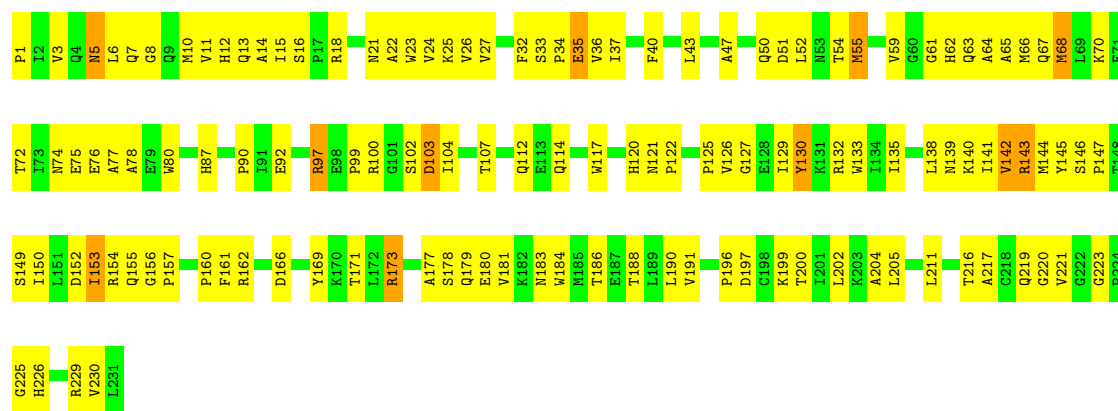
• Molecule 1: capsid protein

Chain 53: 43% 54%



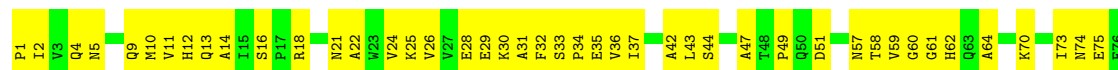
• Molecule 1: capsid protein

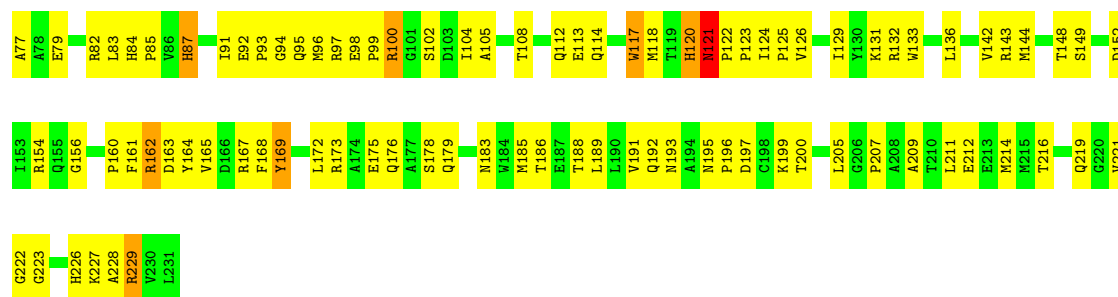
Chain 54: 44% 52% 5%



• Molecule 1: capsid protein

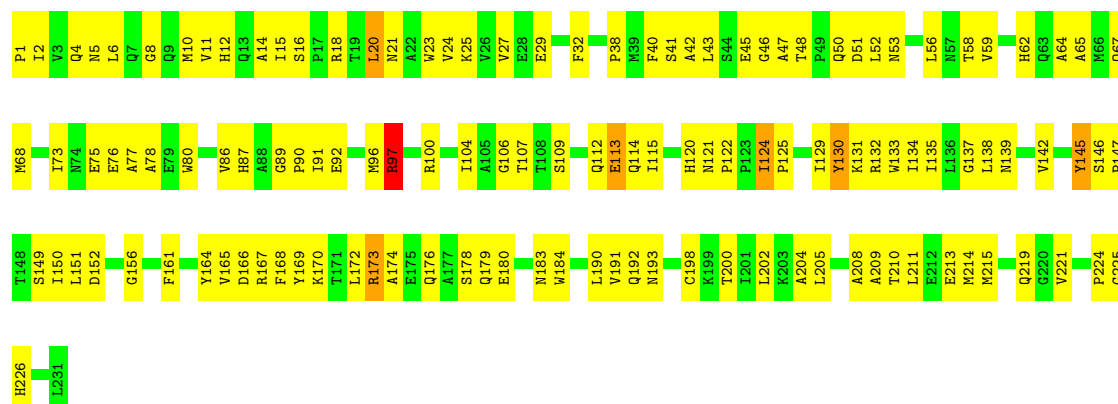
Chain 55: 42% 54%





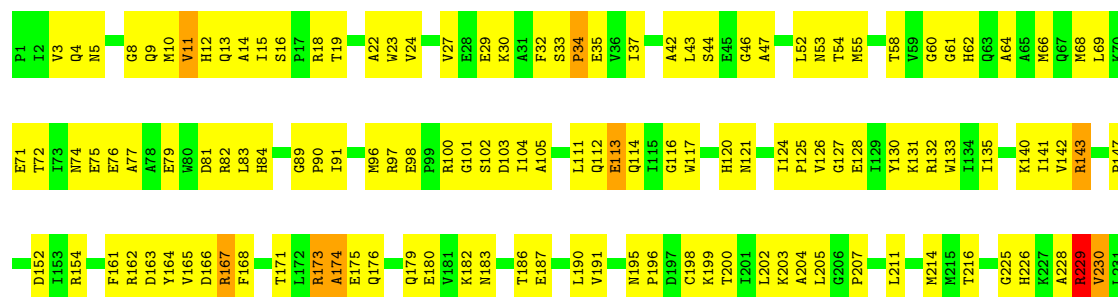
• Molecule 1: capsid protein

Chain 56: 45% 52%



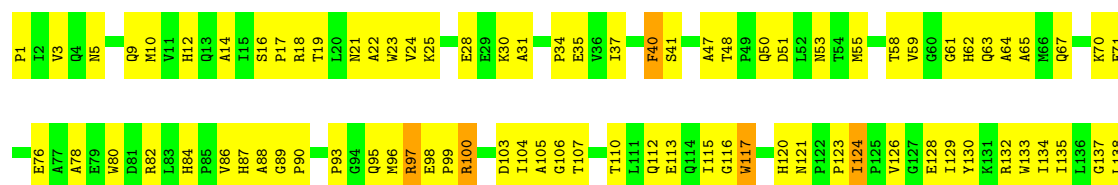
• Molecule 1: capsid protein

Chain 57: 44% 52%



• Molecule 1: capsid protein

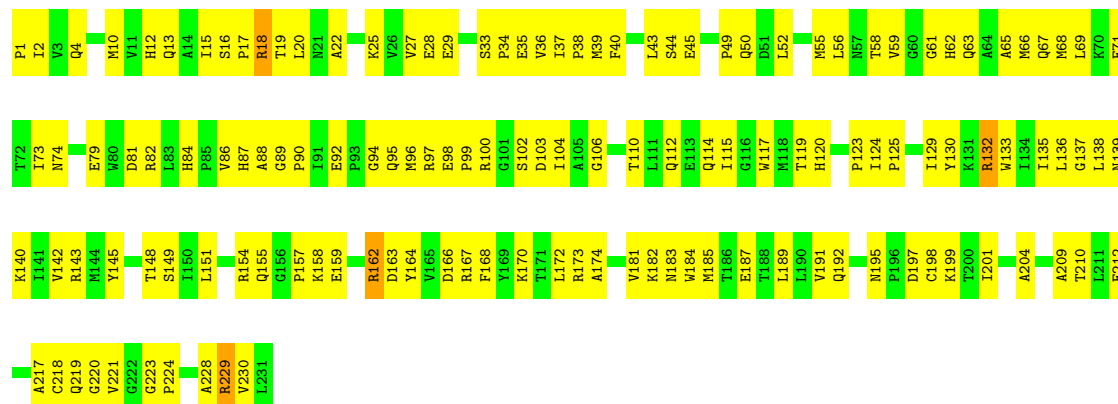
Chain 58: 42% 55%





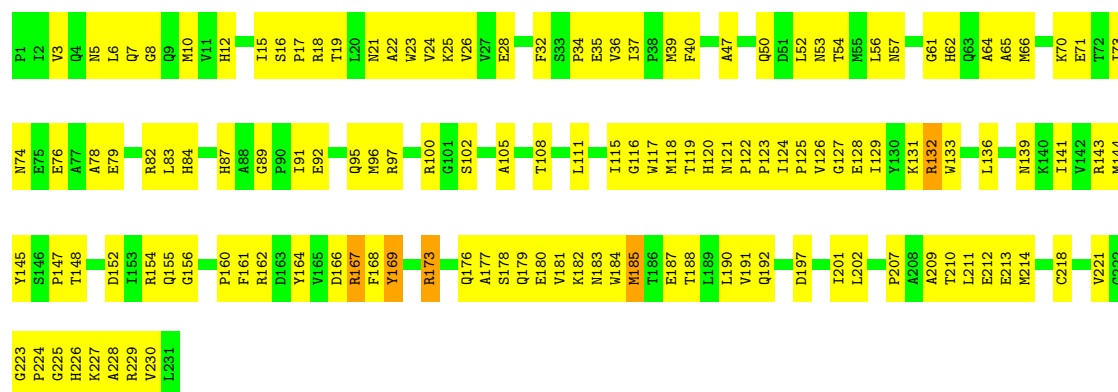
• Molecule 1: capsid protein

Chain 59: 41% 57%



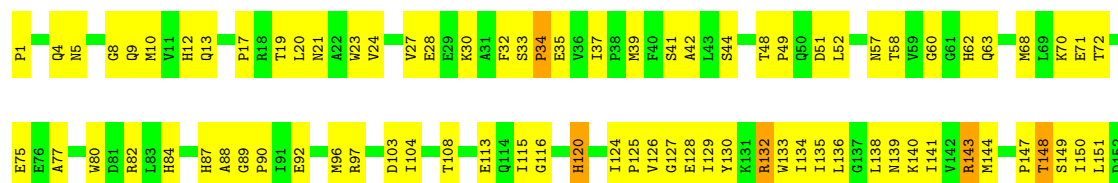
• Molecule 1: capsid protein

Chain 5a: 42% 56%



• Molecule 1: capsid protein

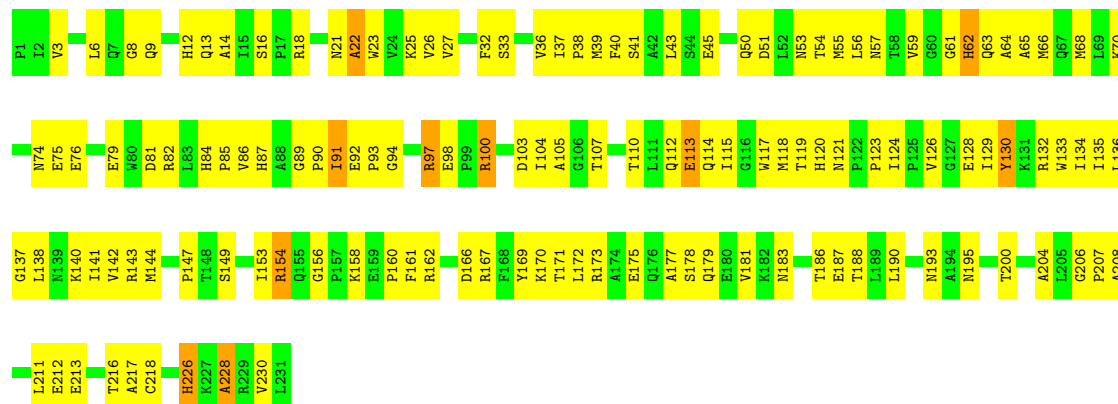
Chain 5b: 43% 53%





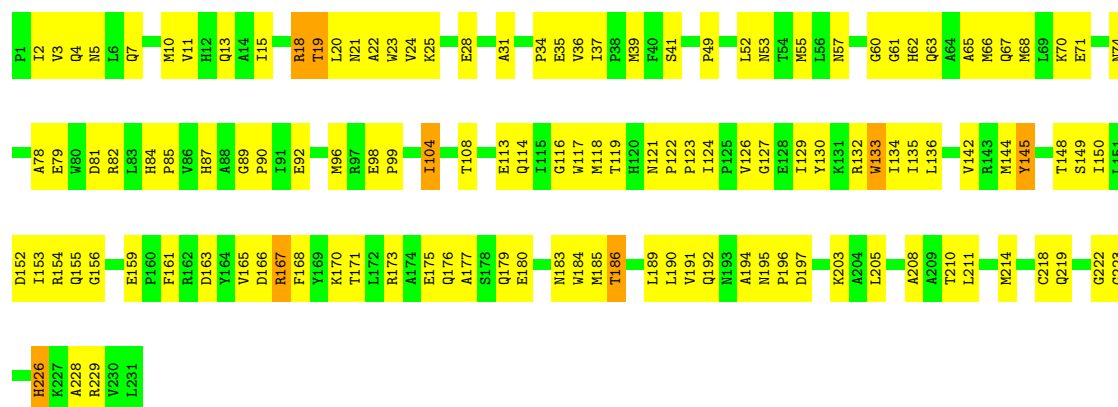
- Molecule 1: capsid protein

Chain 5c: 42% 54%



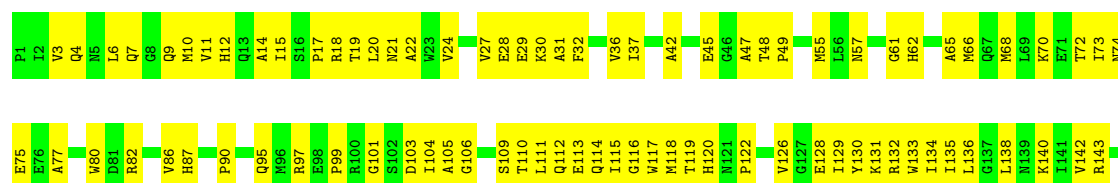
- Molecule 1: capsid protein

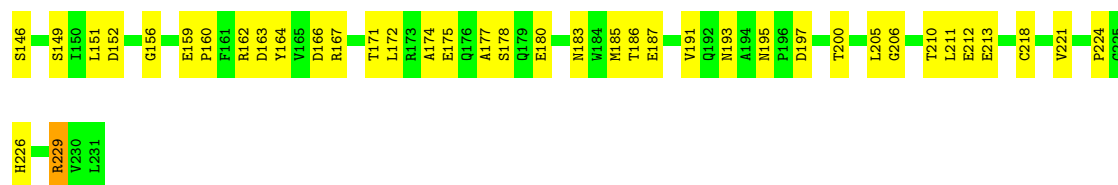
Chain 5d: 45% 51%



- Molecule 1: capsid protein

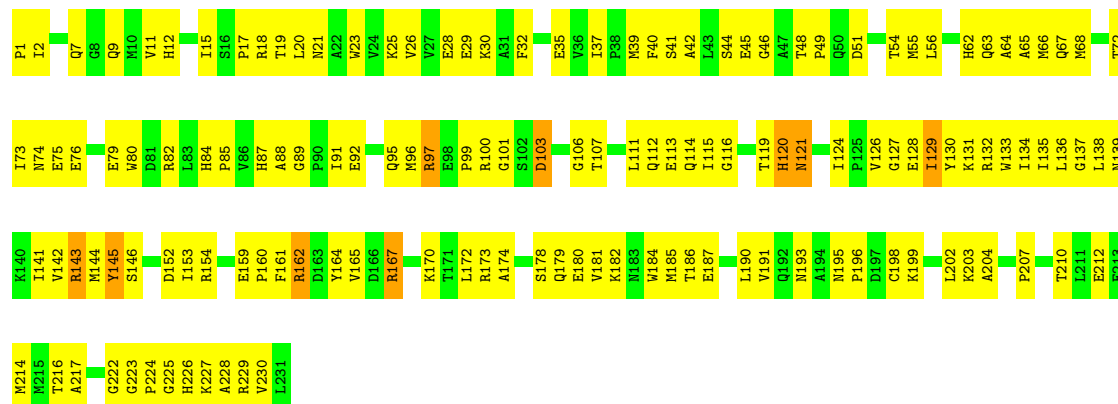
Chain 5e: 47% 52%





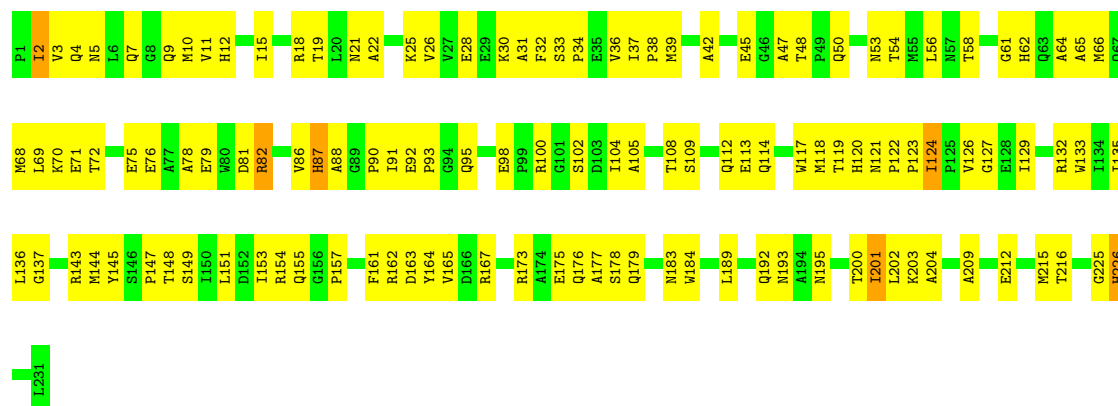
- Molecule 1: capsid protein

Chain 5f:



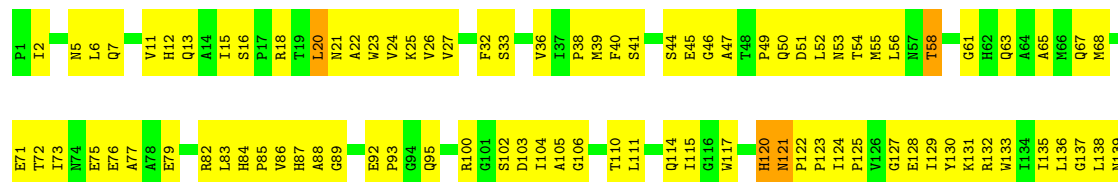
- Molecule 1: capsid protein

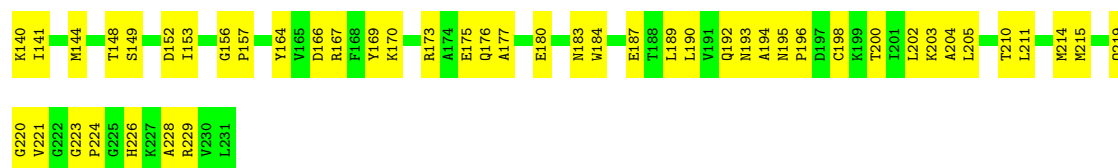
Chain 5g:



- Molecule 1: capsid protein

Chain 5h:

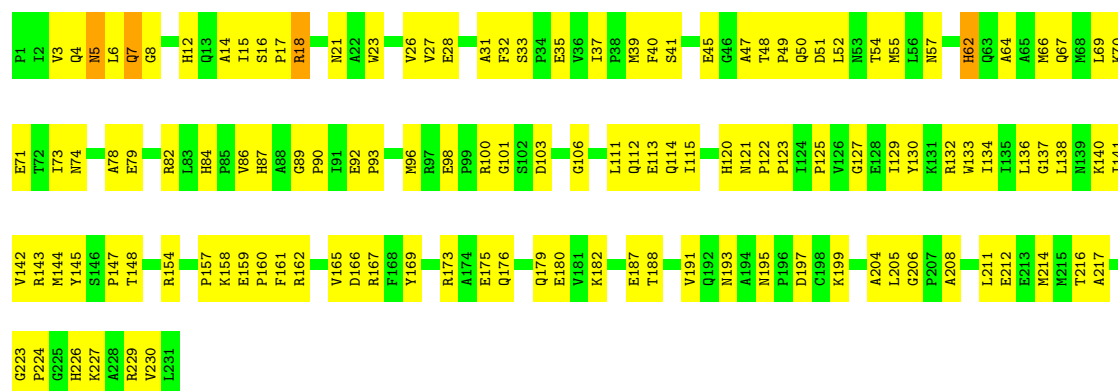




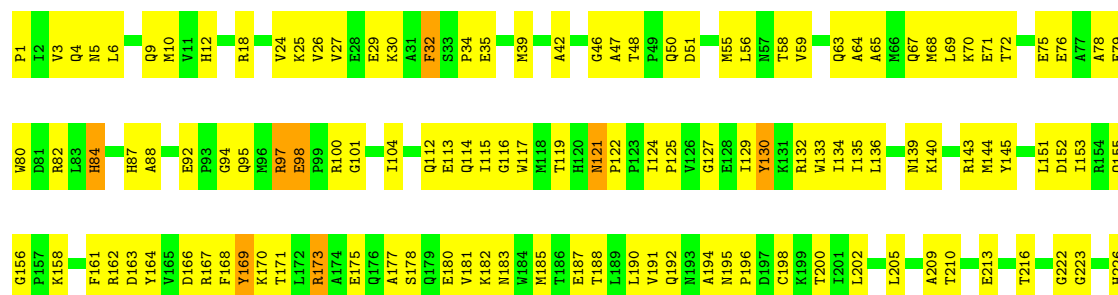
• Molecule 1: capsid protein



• Molecule 1: capsid protein



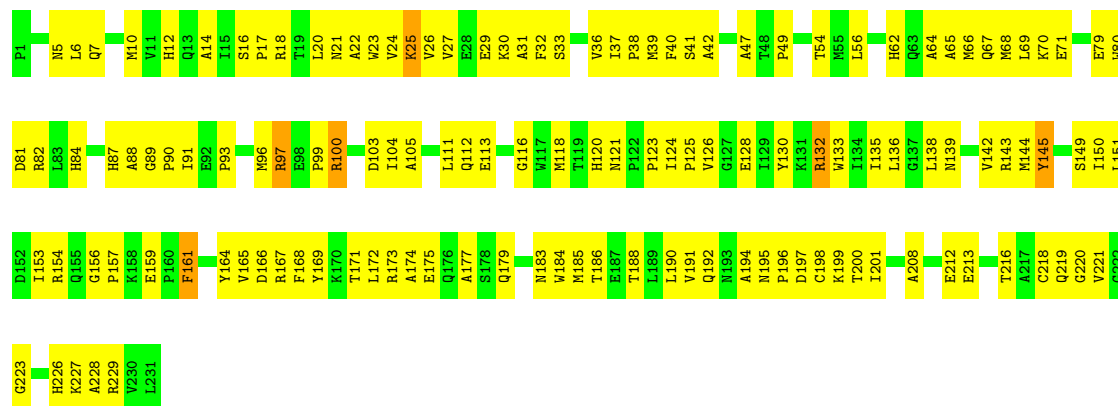
• Molecule 1: capsid protein





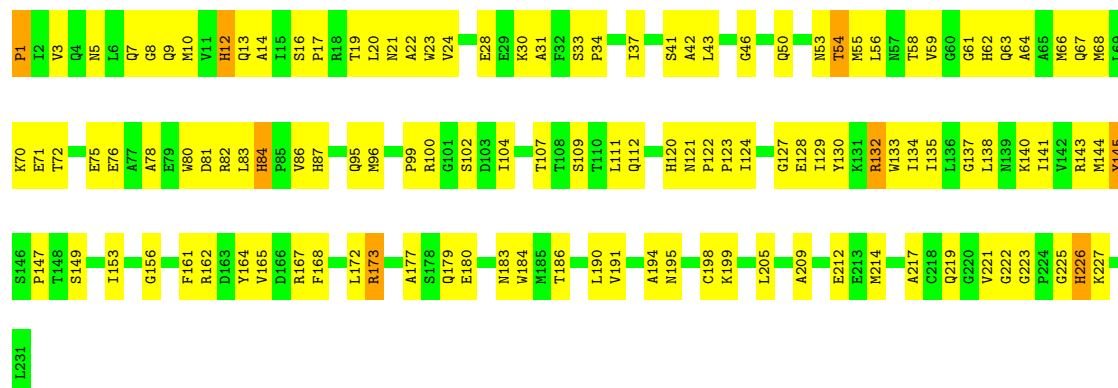
• Molecule 1: capsid protein

Chain 5l:  42% 55%

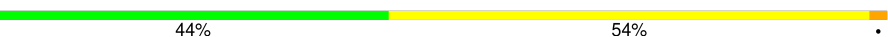


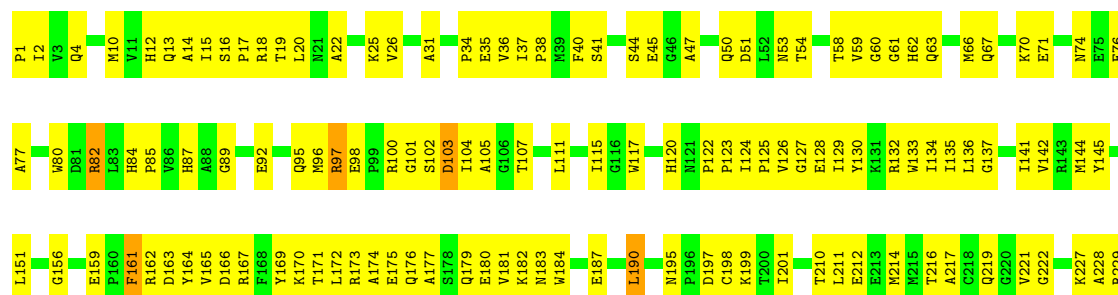
• Molecule 1: capsid protein

Chain 5m:  48% 49%



• Molecule 1: capsid protein

Chain 5n:  44% 54%



V230
L231

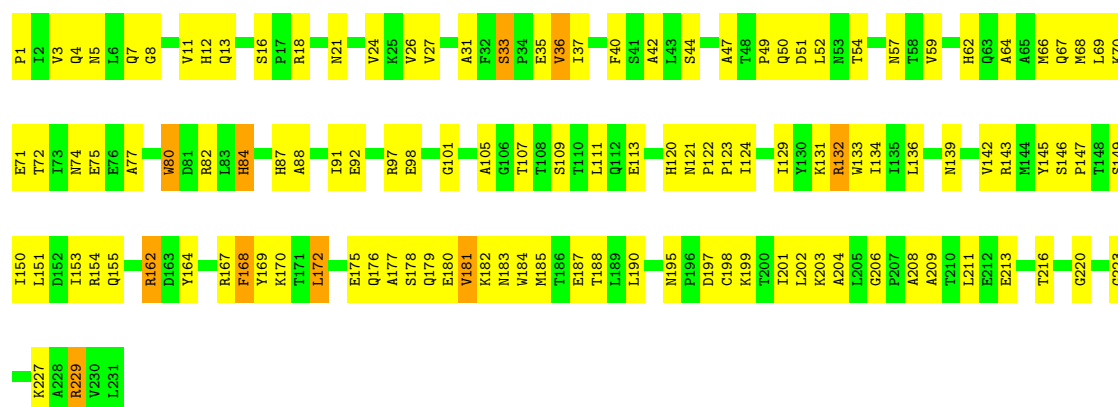
- Molecule 1: capsid protein

Chain 5o: 46% 50%



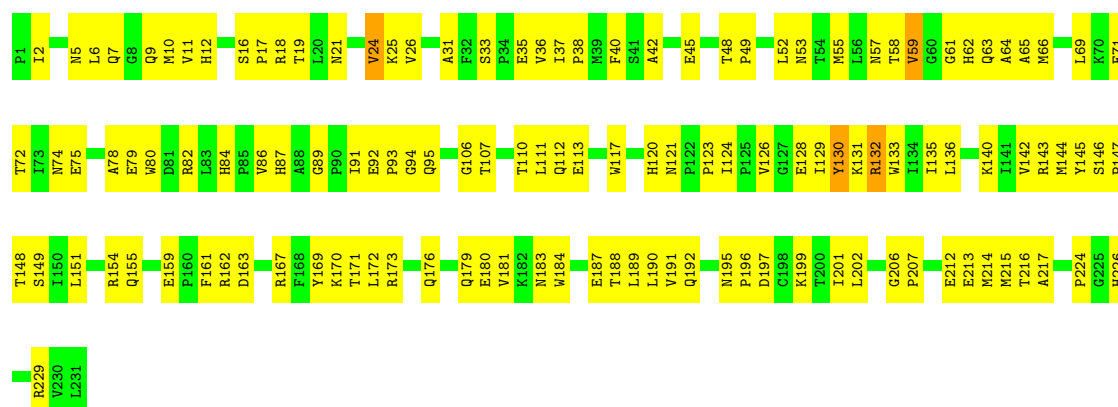
- Molecule 1: capsid protein

Chain 5p: 48% 48%

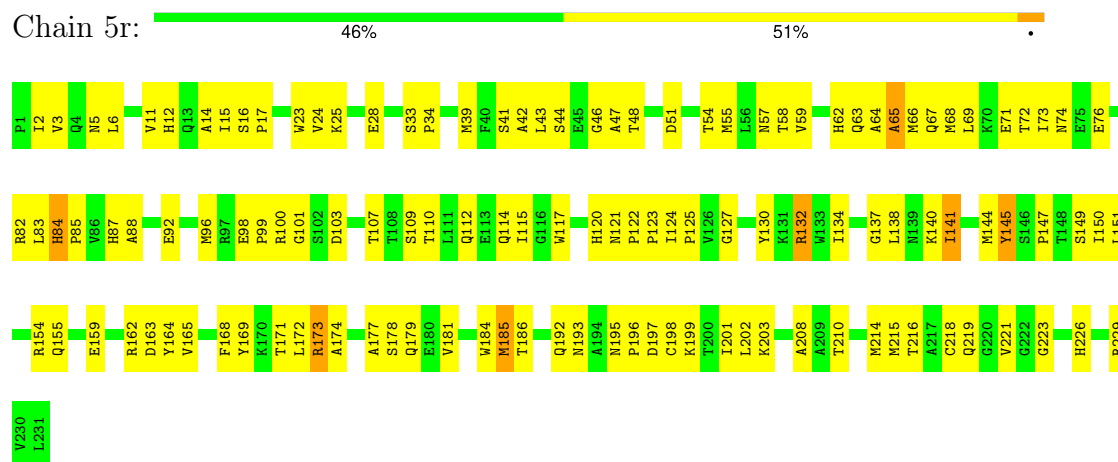


- Molecule 1: capsid protein

Chain 5q: 45% 54%



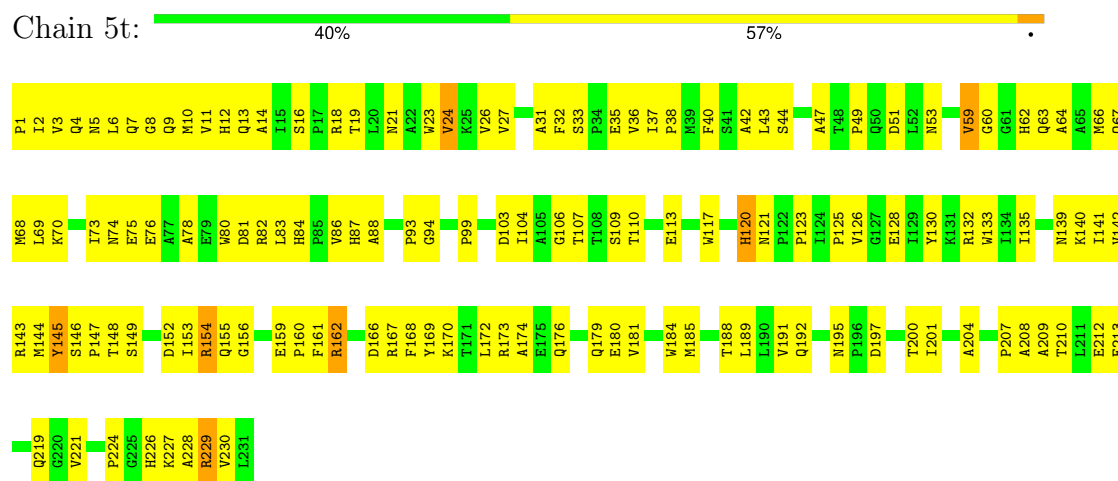
- Molecule 1: capsid protein



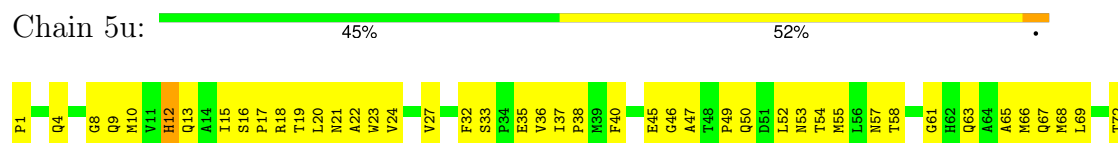
- Molecule 1: capsid protein

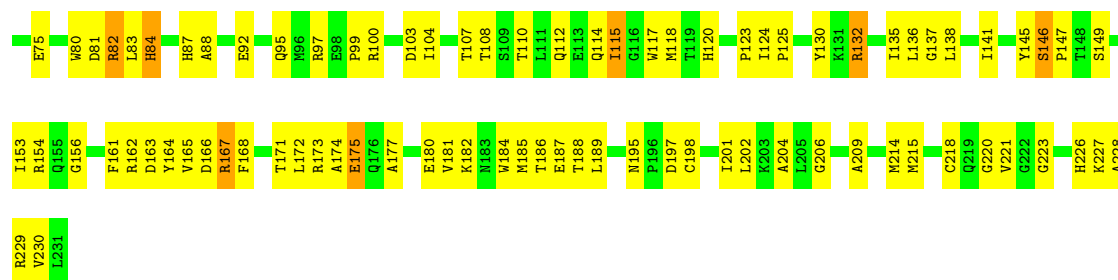


- Molecule 1: capsid protein



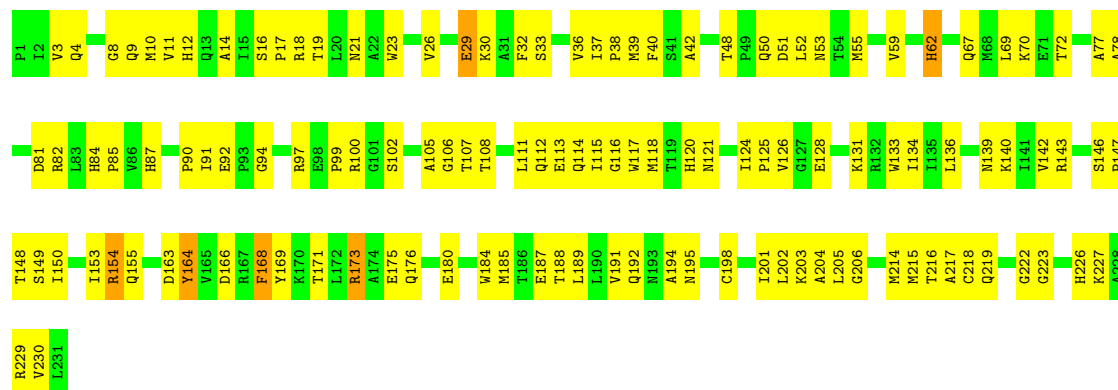
- Molecule 1: capsid protein





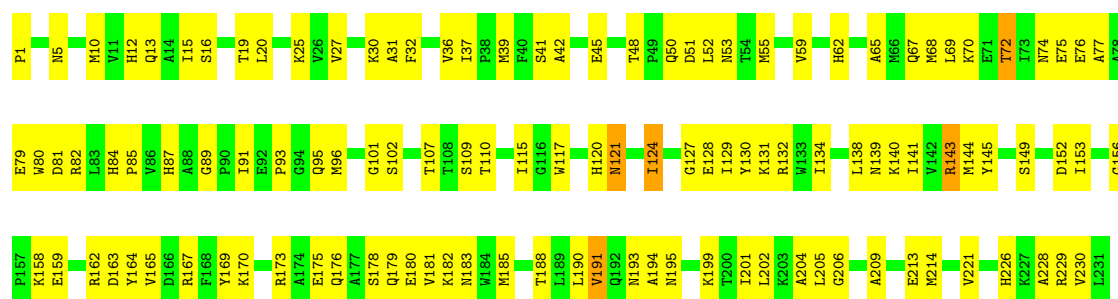
- Molecule 1: capsid protein

Chain 5v: 46% 51%



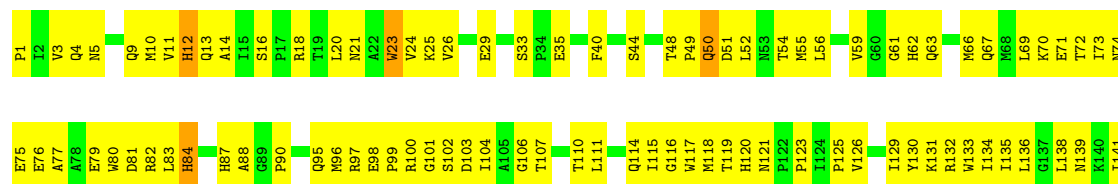
- Molecule 1: capsid protein

Chain 5w: 49% 48%



- Molecule 1: capsid protein

Chain 5x: 40% 57%





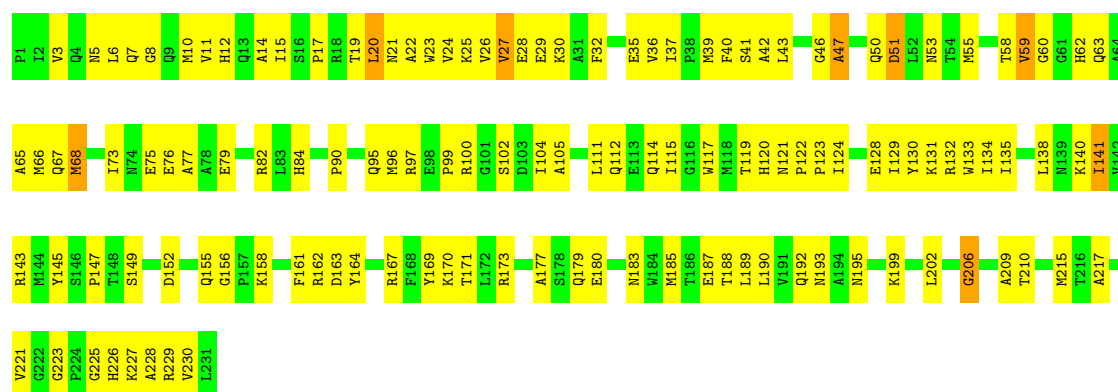
- Molecule 1: capsid protein

Chain 5y: 47% 49%



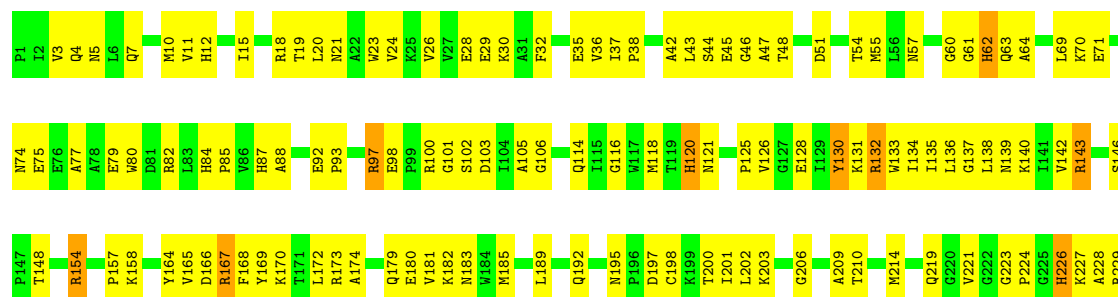
- Molecule 1: capsid protein

Chain 5z: 44% 52%



- Molecule 1: capsid protein

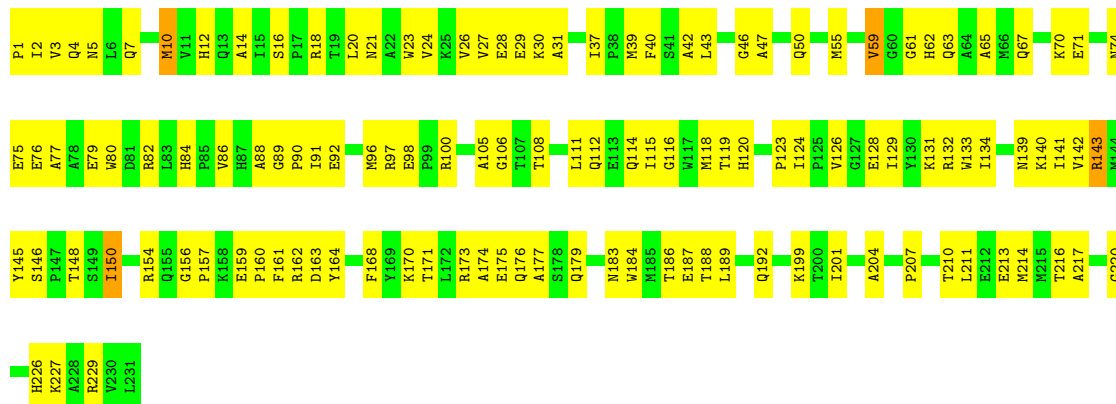
Chain 5A: 46% 50%



V230
L231

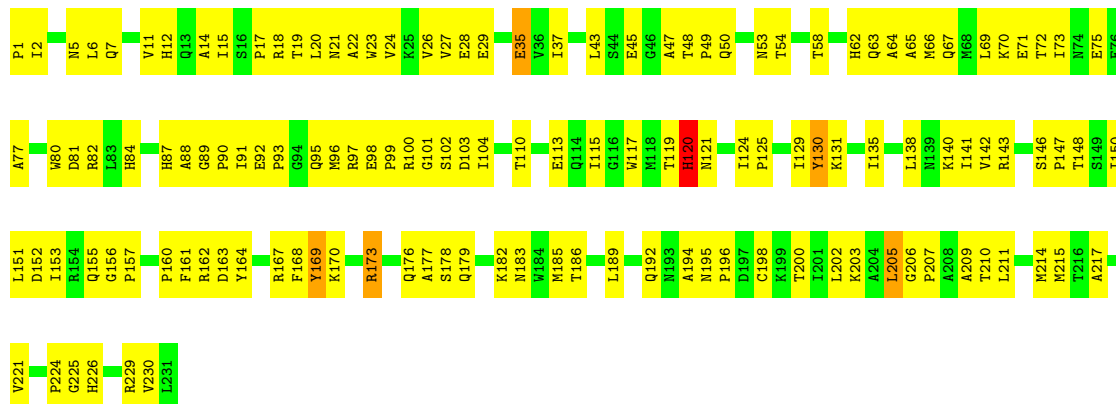
- Molecule 1: capsid protein

Chain 5B: 46% 52%



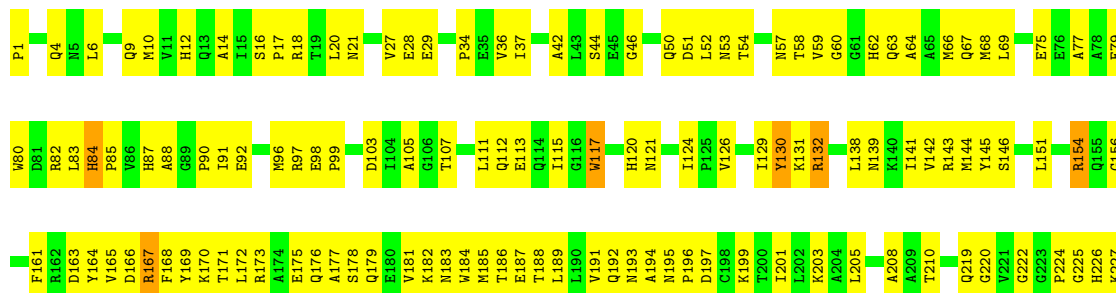
- Molecule 1: capsid protein

Chain 5C: 41% 56%



- Molecule 1: capsid protein

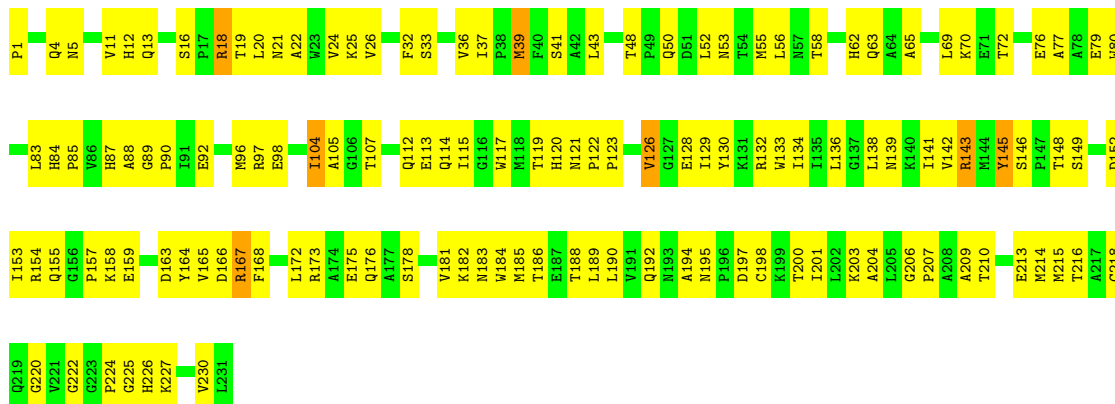
Chain 5D: 44% 53%



A228
R229
V230
L231

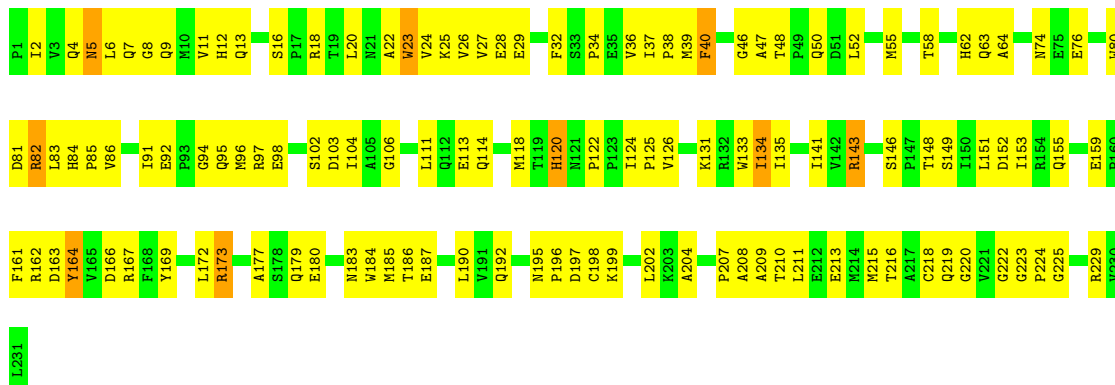
• Molecule 1: capsid protein

Chain 5E: 43% 54%



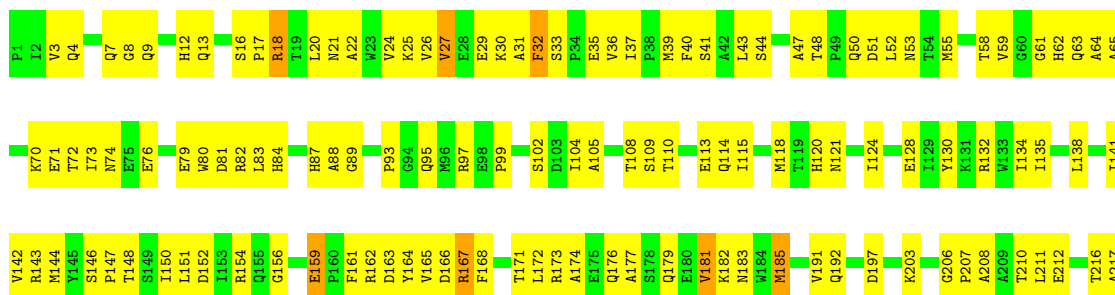
• Molecule 1: capsid protein

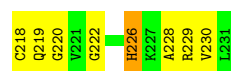
Chain 5F: 47% 49%



• Molecule 1: capsid protein

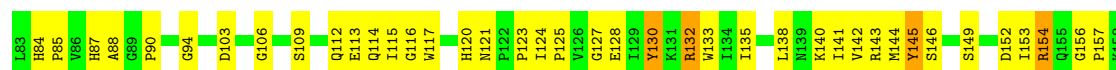
Chain 5G: 42% 55%





• Molecule 1: capsid protein

Chain 5H: 51% 47%



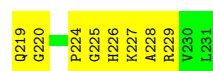
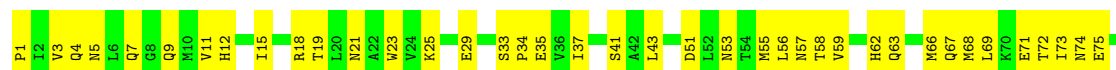
• Molecule 1: capsid protein

Chain 5I: 45% 52%

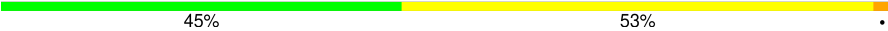


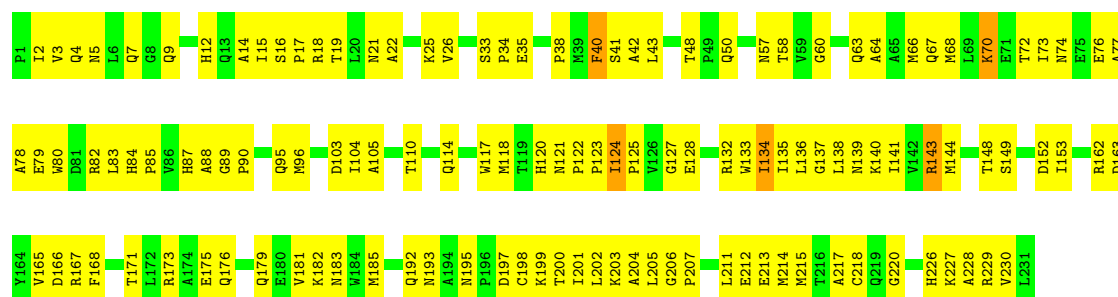
• Molecule 1: capsid protein

Chain 5J: 45% 50% 5%



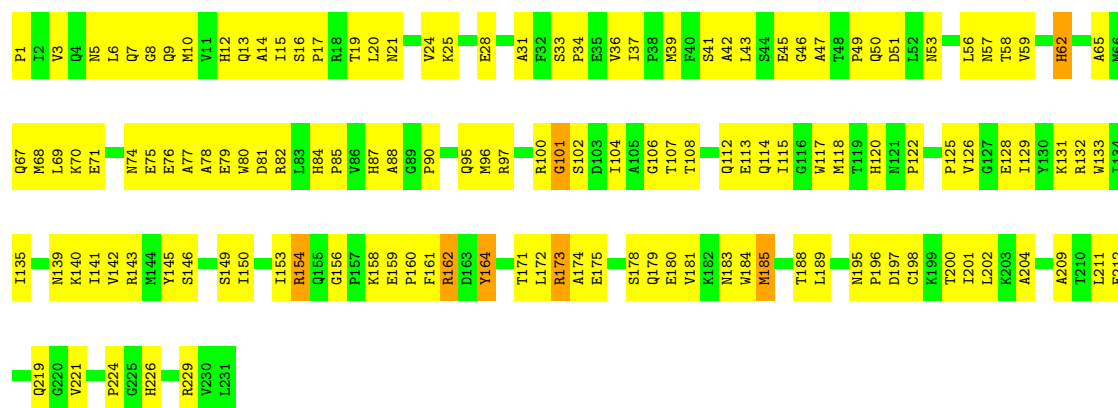
• Molecule 1: capsid protein

Chain 5K:  45% 53%



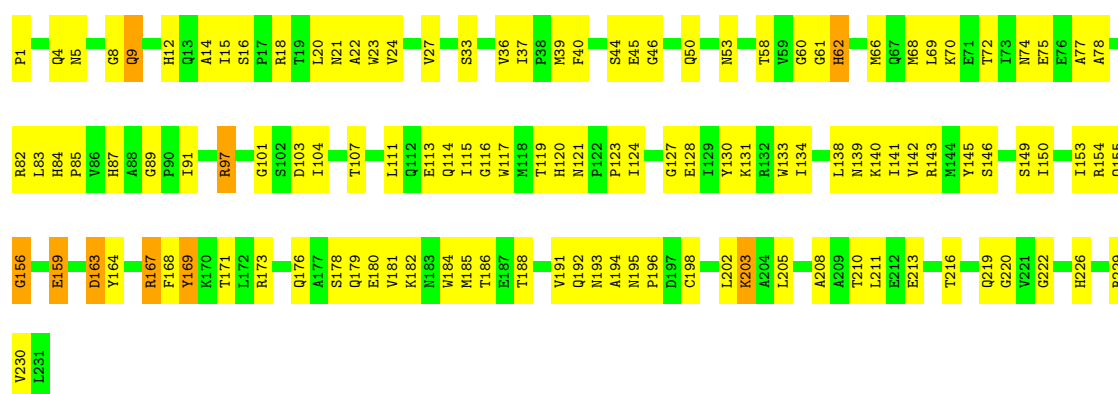
• Molecule 1: capsid protein

Chain 5L:  42% 55%



• Molecule 1: capsid protein

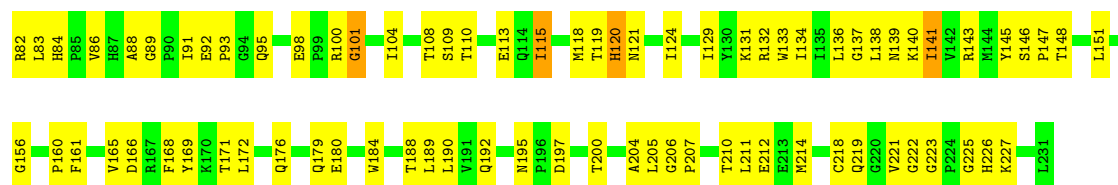
Chain 5M:  48% 48%



• Molecule 1: capsid protein

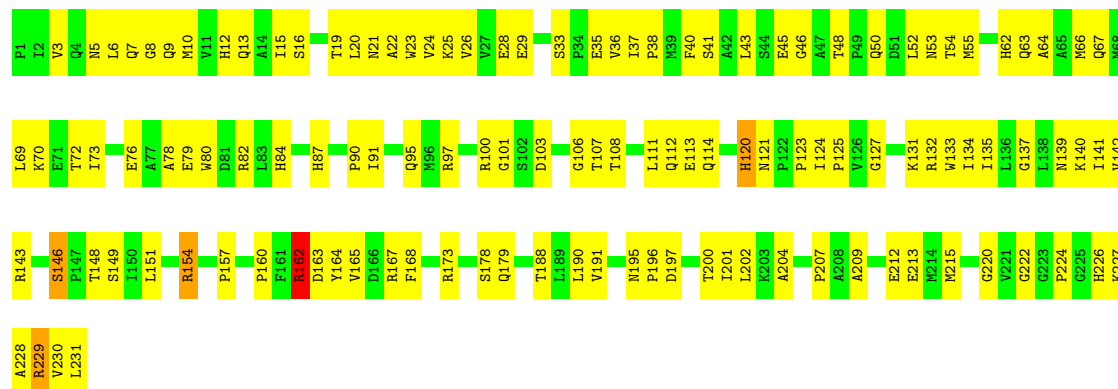
Chain 5N:  50% 48%





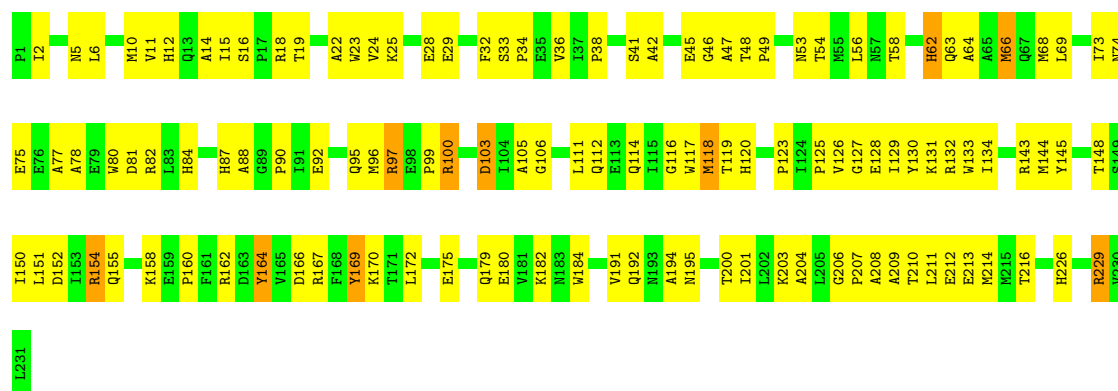
• Molecule 1: capsid protein

Chain 5O: 46% 52%



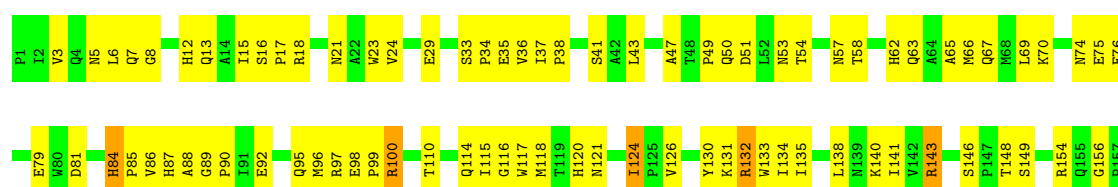
• Molecule 1: capsid protein

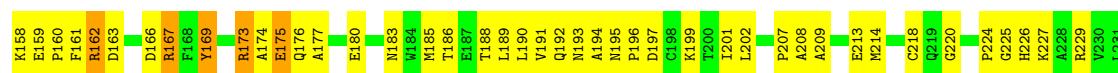
Chain 5P: 47% 48%



• Molecule 1: capsid protein

Chain 5Q: 46% 50%





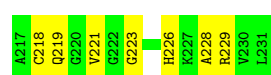
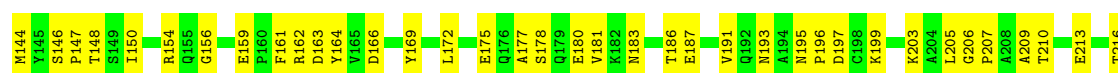
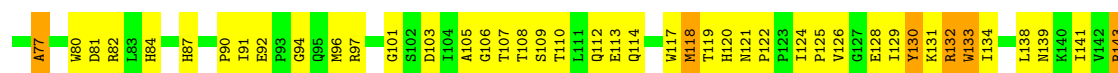
• Molecule 1: capsid protein

Chain 5R: 44% 53%



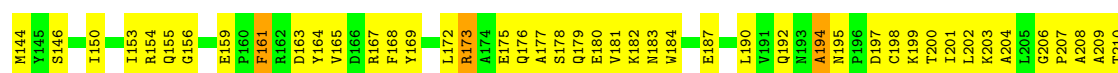
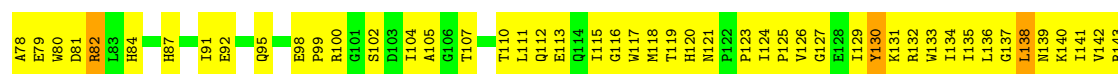
• Molecule 1: capsid protein

Chain 5S: 44% 53%



• Molecule 1: capsid protein

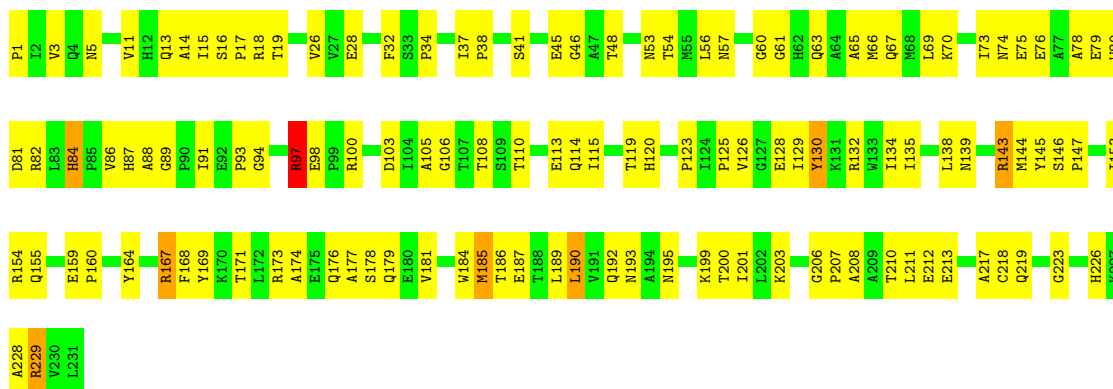
Chain 5T: 38% 57% 5%



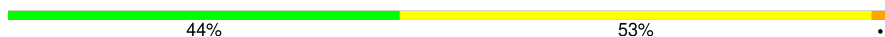


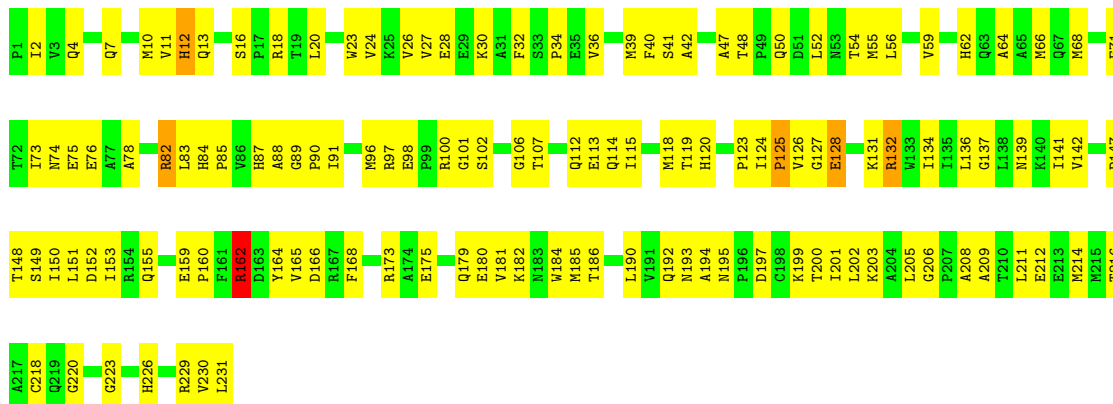
• Molecule 1: capsid protein

Chain 5U:  47% 50%

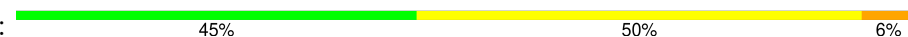


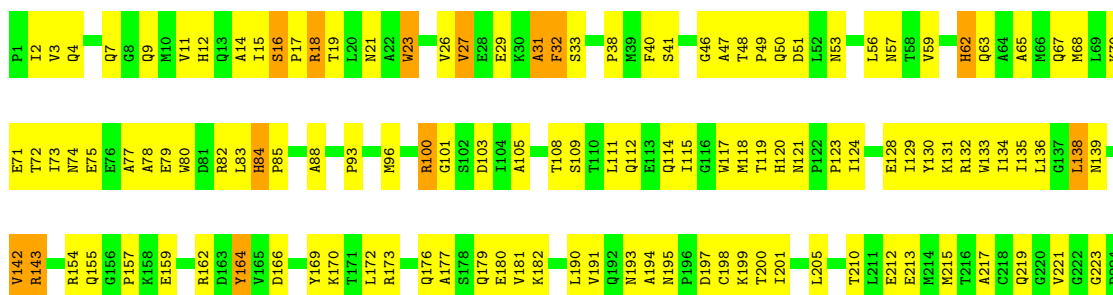
• Molecule 1: capsid protein

Chain 5V:  44% 53%



• Molecule 1: capsid protein

Chain 5W:  45% 50% 6%



G226
H226
K227
A228
R229
V230
L231

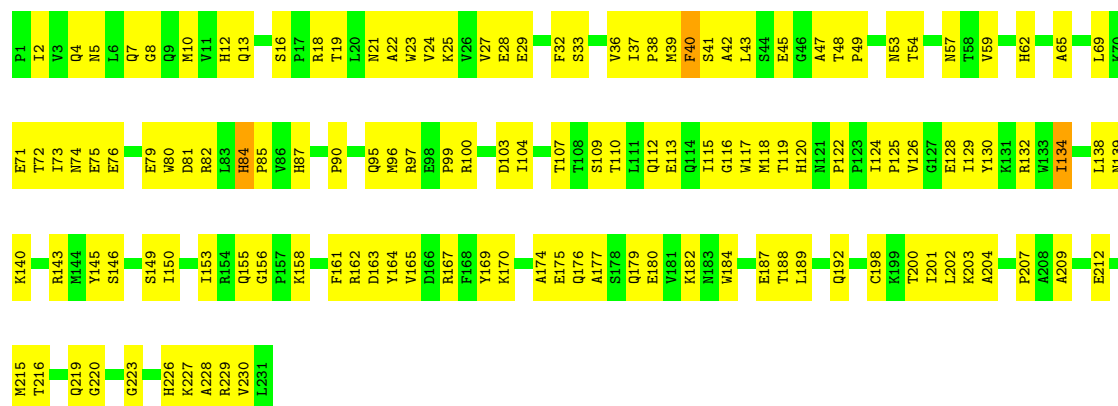
• Molecule 1: capsid protein

Chain 5X: 48% 50%



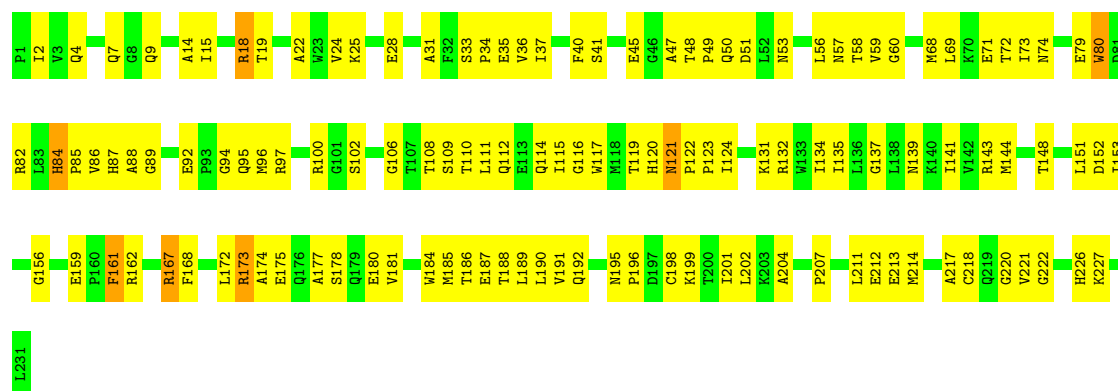
• Molecule 1: capsid protein

Chain 5Y: 43% 56%

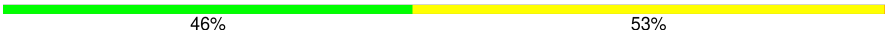
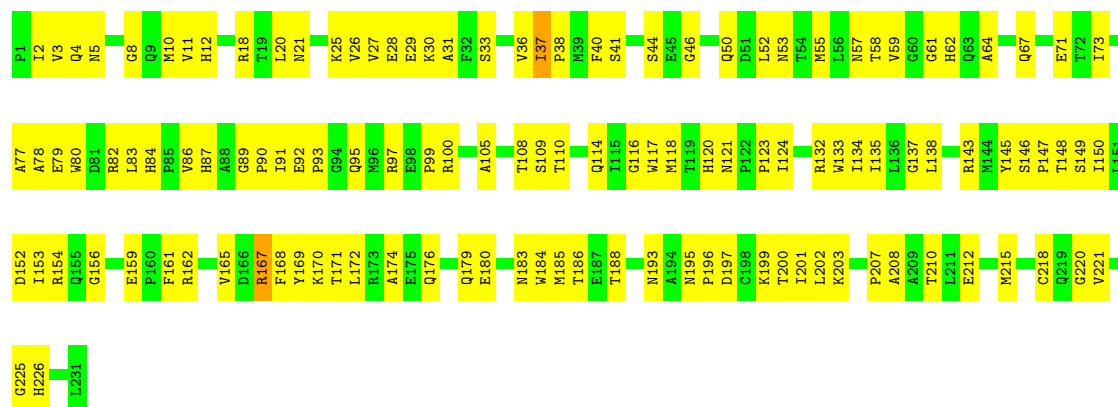


• Molecule 1: capsid protein

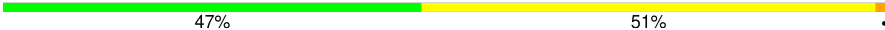
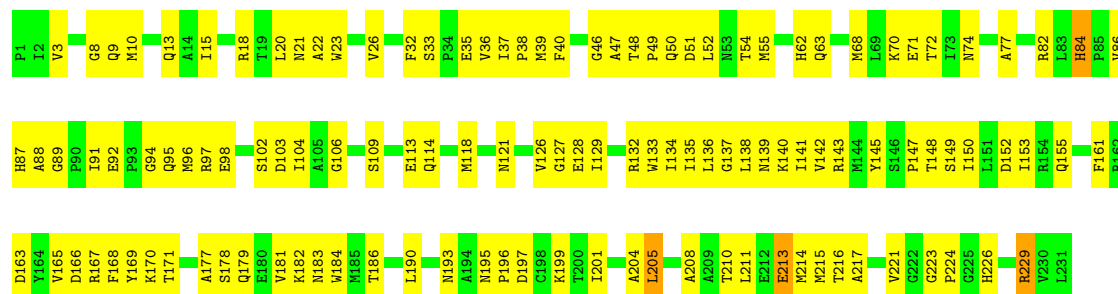
Chain 5Z: 46% 51%



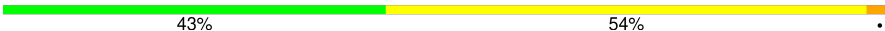
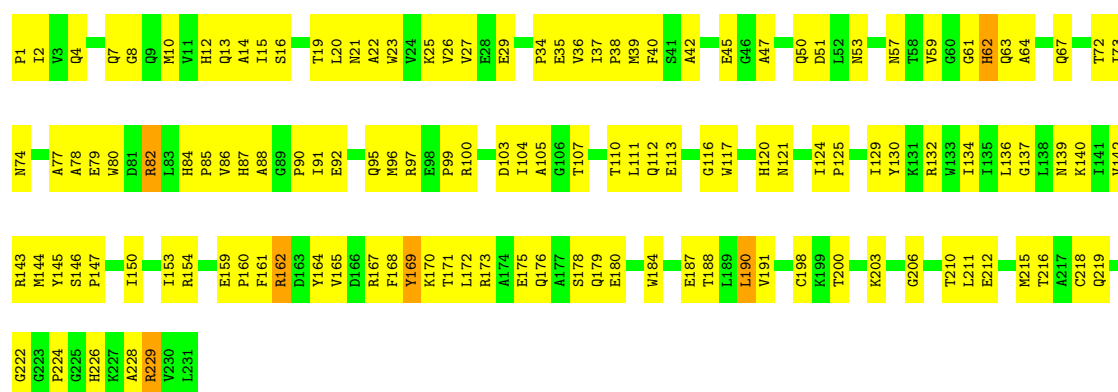
• Molecule 1: capsid protein

Chain 60:  46% 53%

• Molecule 1: capsid protein

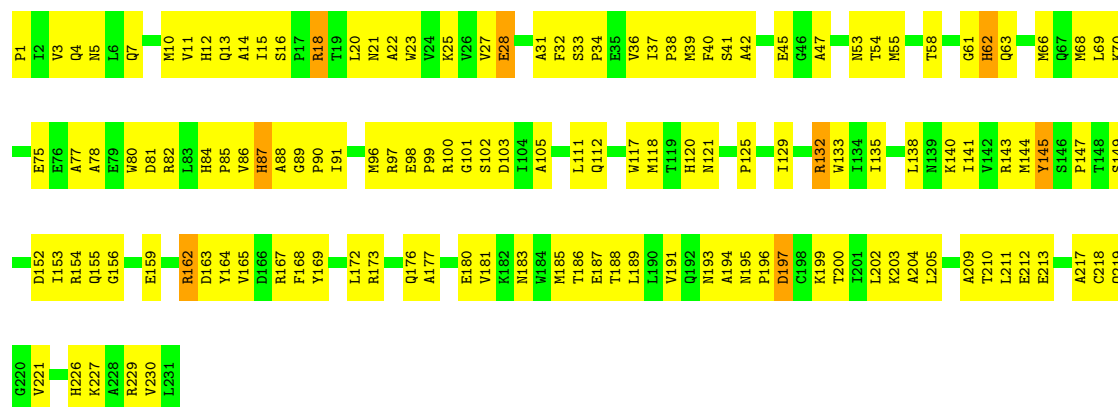
Chain 61:  47% 51%

• Molecule 1: capsid protein

Chain 62:  43% 54%

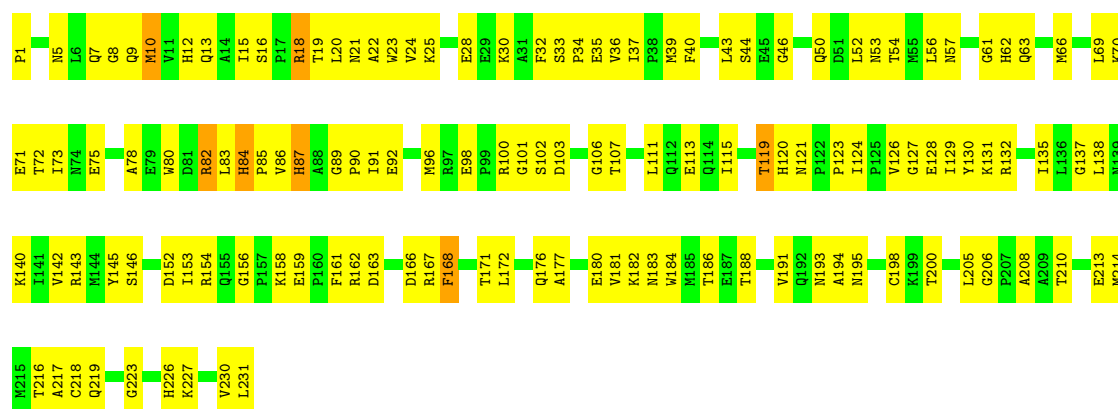
• Molecule 1: capsid protein

Chain 63:  41% 55%



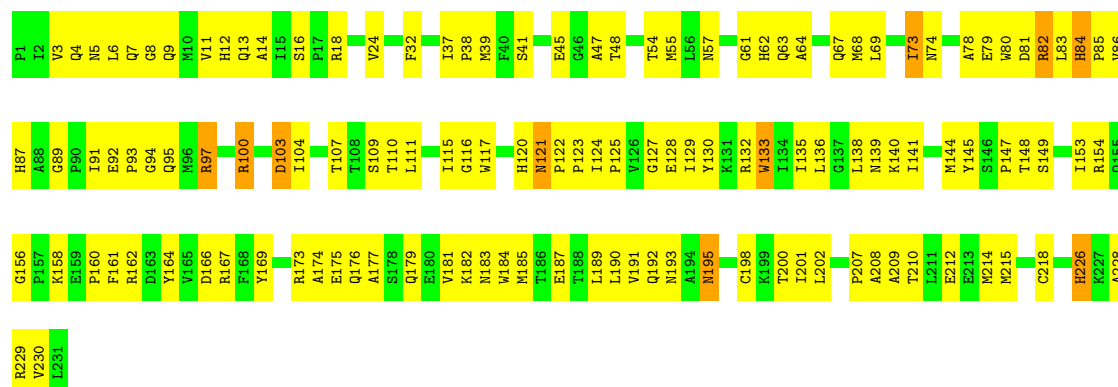
- Molecule 1: capsid protein

Chain 64: 42% 55%



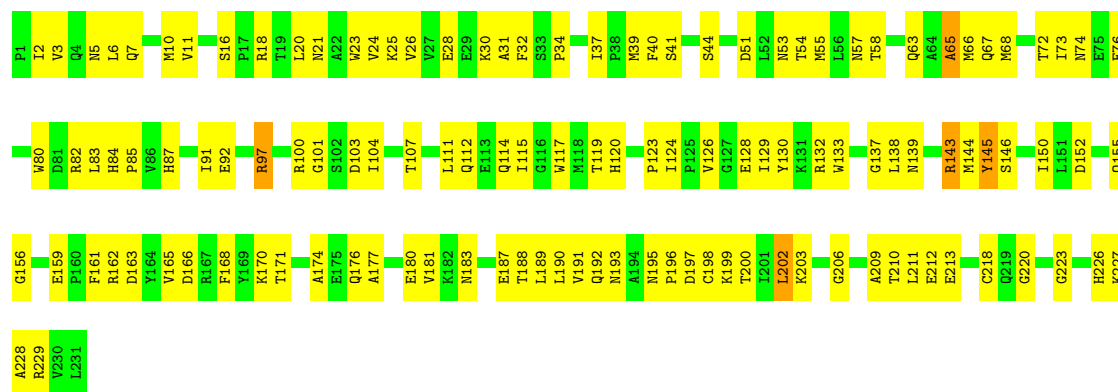
- Molecule 1: capsid protein

Chain 65: 44% 52%



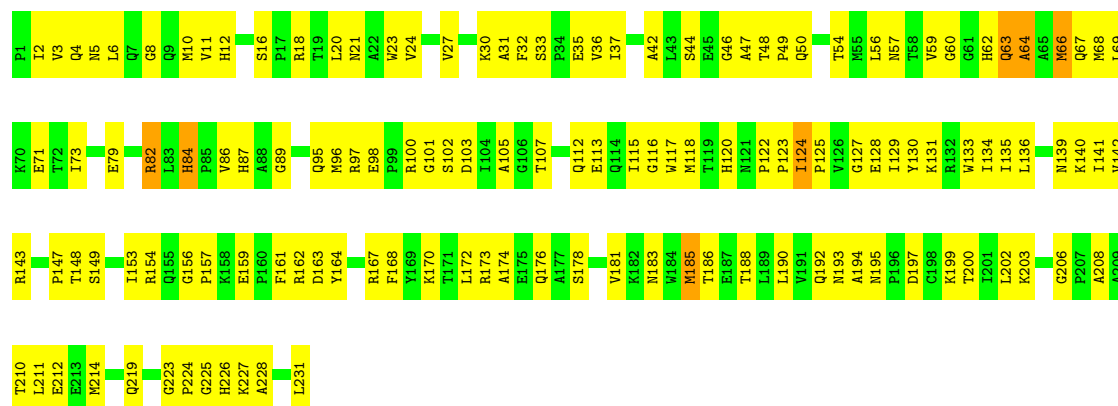
- Molecule 1: capsid protein

Chain 66: 47% 51%



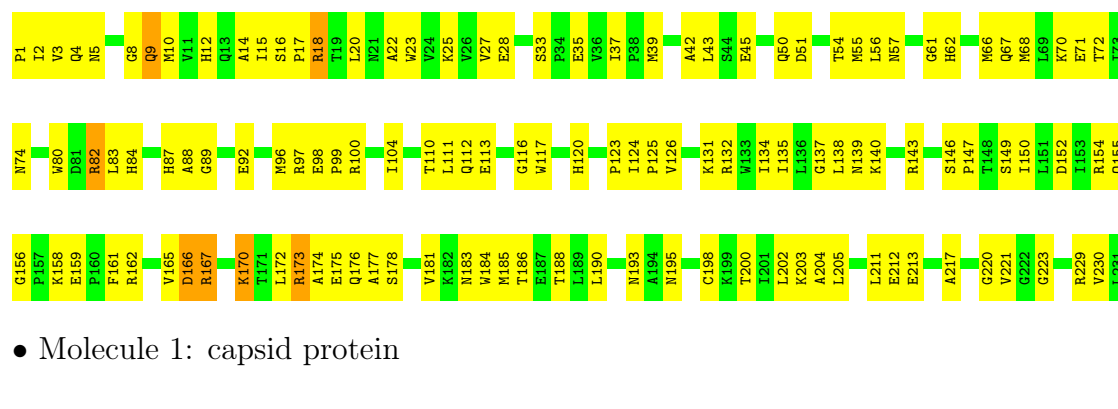
• Molecule 1: capsid protein

Chain 67: 42% 55%



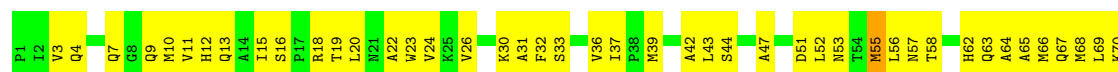
• Molecule 1: capsid protein

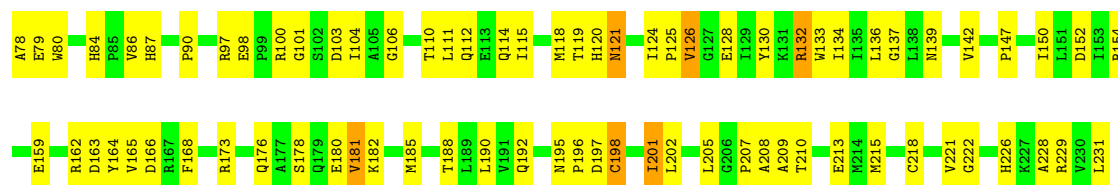
Chain 68: 47% 50%



• Molecule 1: capsid protein

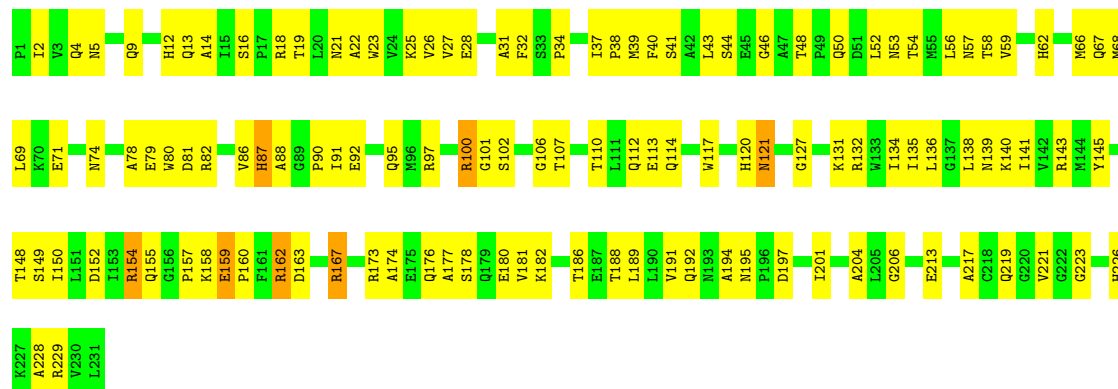
Chain 69: 44% 54%





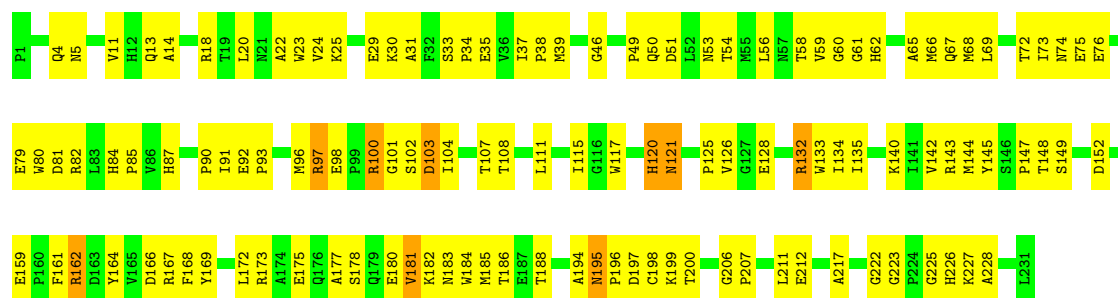
- Molecule 1: capsid protein

Chain 6d: 48% 49%



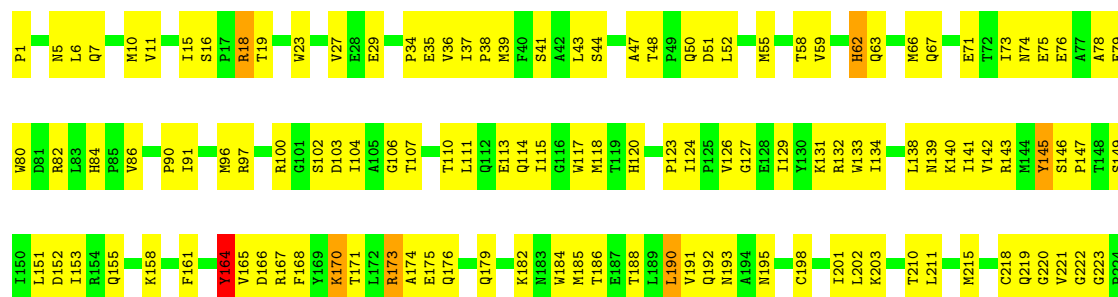
- Molecule 1: capsid protein

Chain 6e: 47% 49%



- Molecule 1: capsid protein

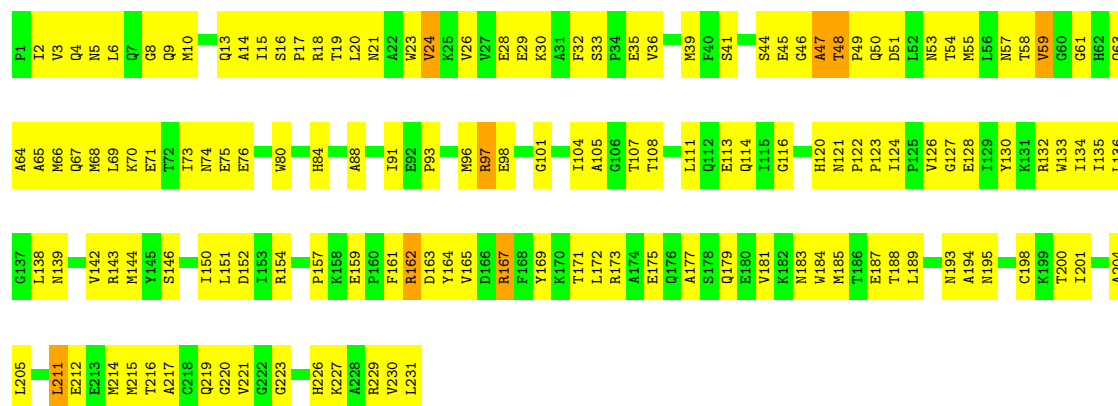
Chain 6f: 45% 52%



G225
H226
K227
A228
R229
V230
L231

• Molecule 1: capsid protein

Chain 6g: 38% 58%



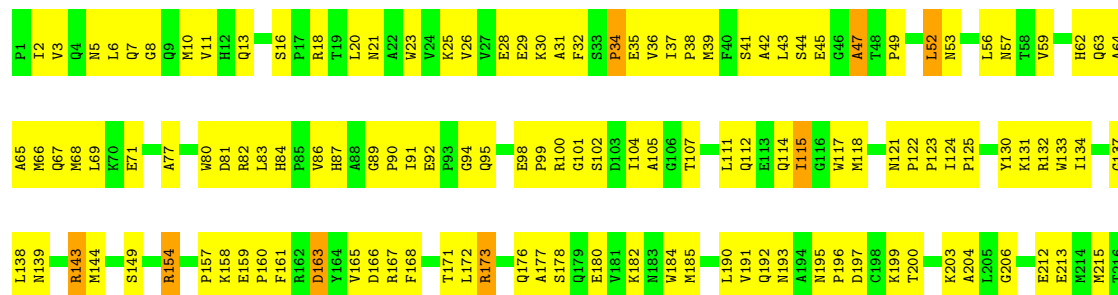
• Molecule 1: capsid protein

Chain 6h: 46% 52%



• Molecule 1: capsid protein

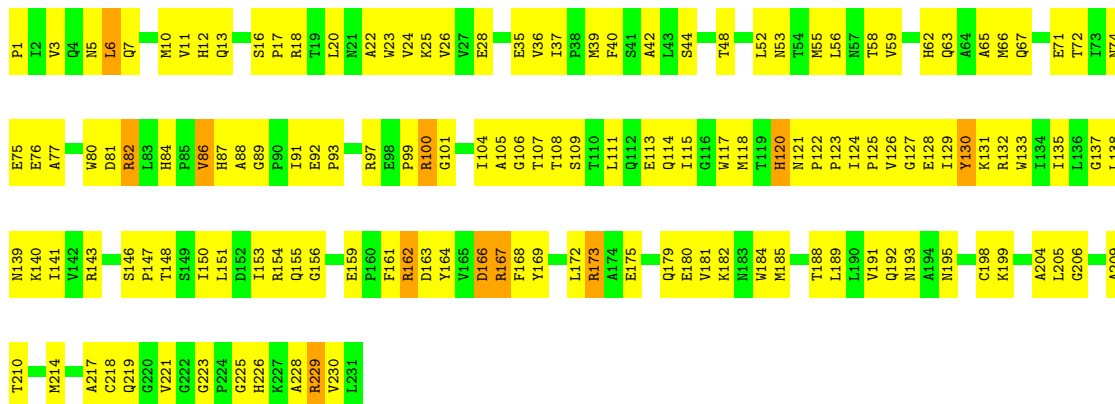
Chain 6i: 41% 55%





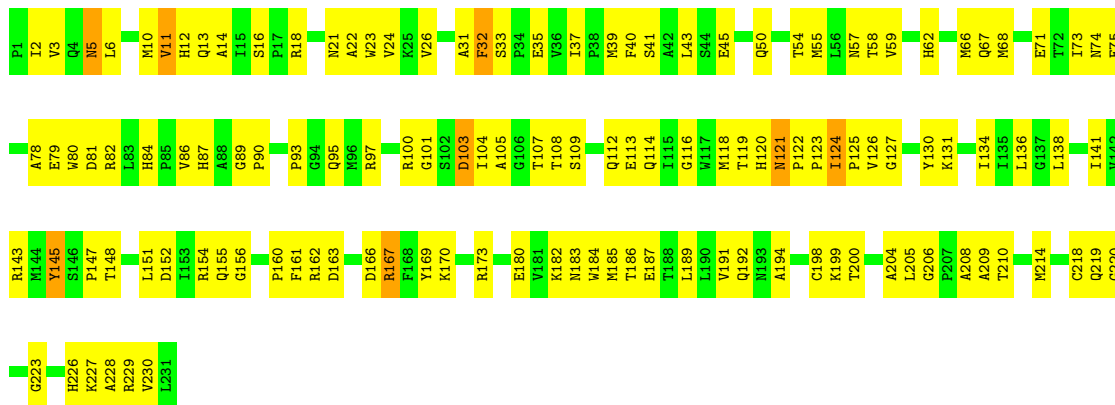
- Molecule 1: capsid protein

Chain 6j: 38% 57% 5%



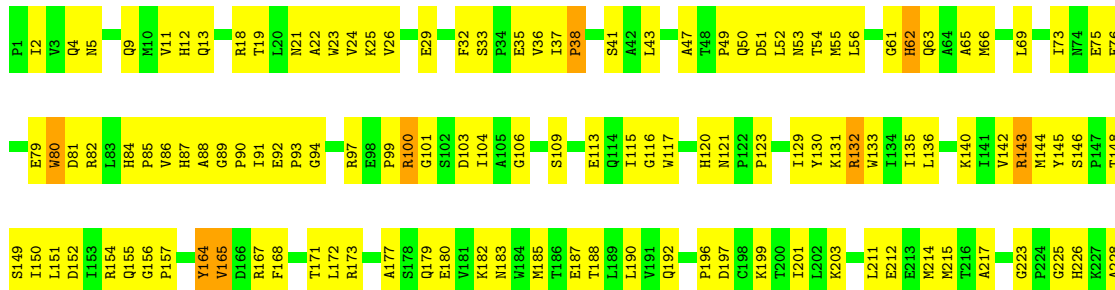
- Molecule 1: capsid protein

Chain 6k: 44% 52% .



- Molecule 1: capsid protein

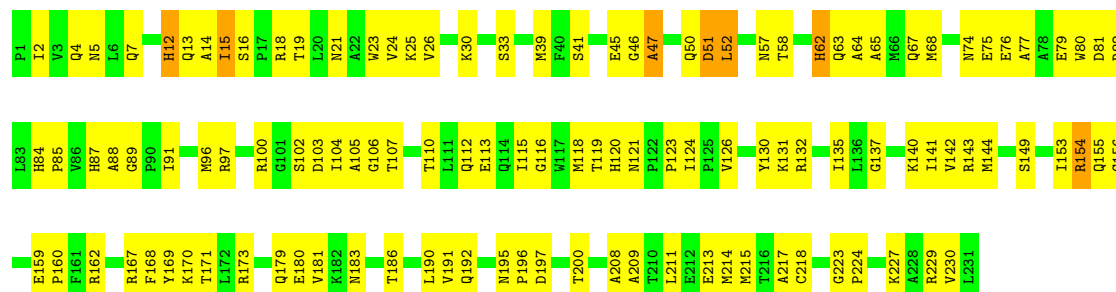
Chain 6l: 45% 51% .





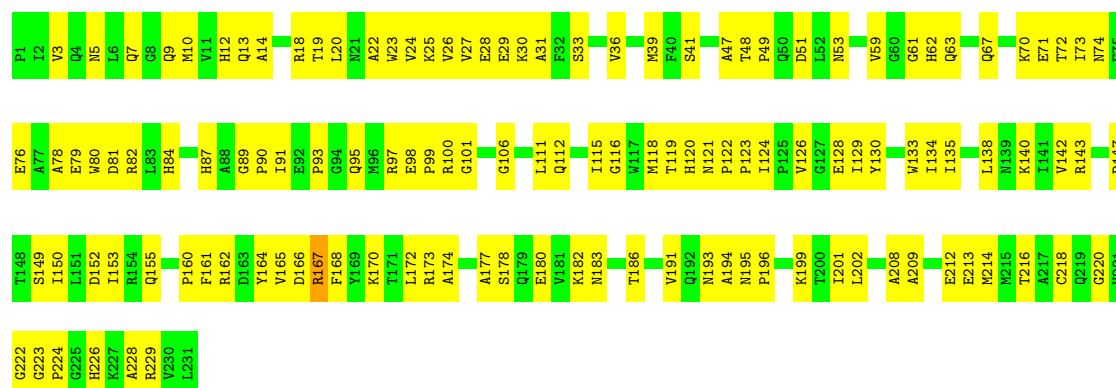
• Molecule 1: capsid protein

Chain 6m: 49% 48%



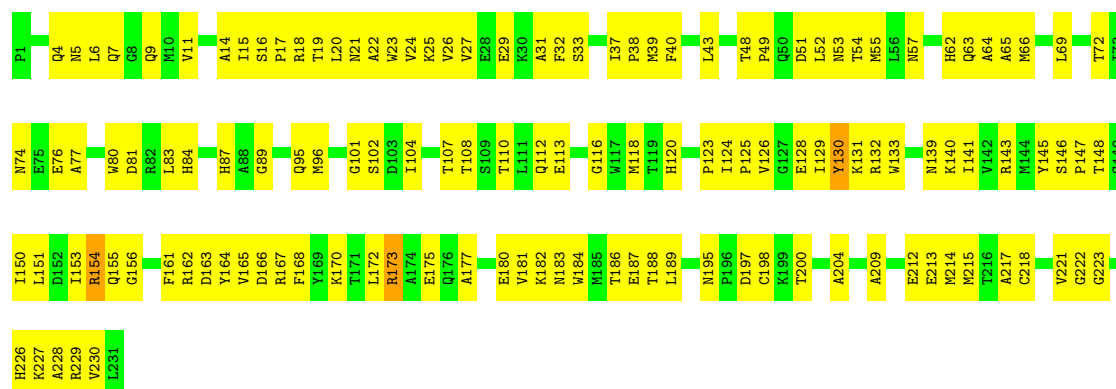
• Molecule 1: capsid protein

Chain 6n: 45% 55%

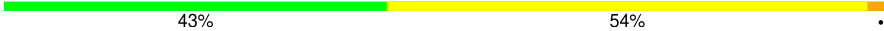


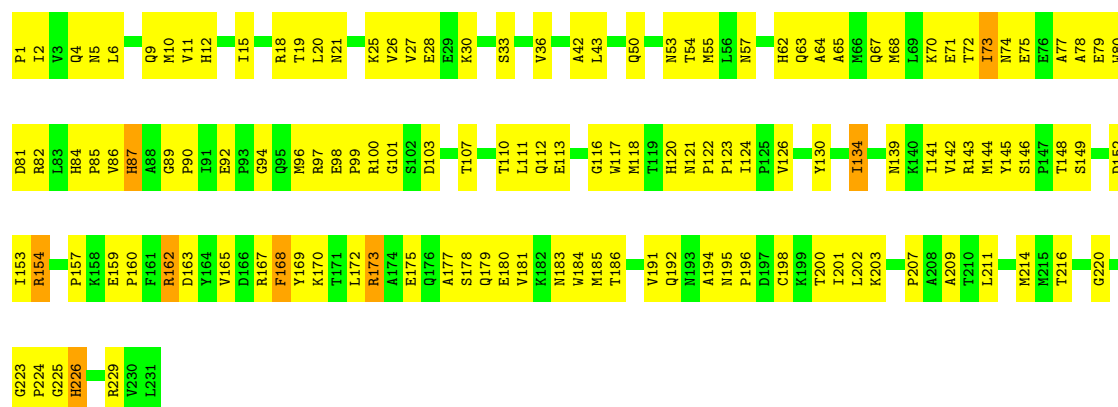
• Molecule 1: capsid protein

Chain 6o: 43% 56%



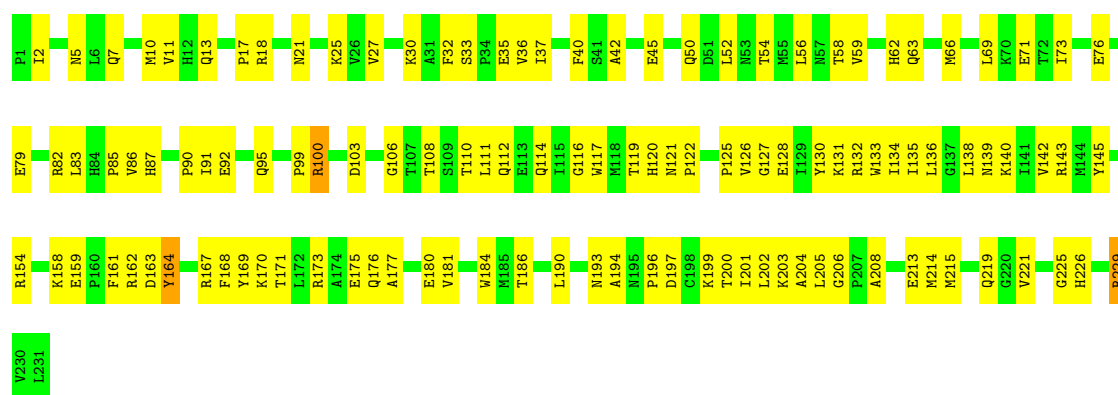
• Molecule 1: capsid protein

Chain 6p:  43% 54%

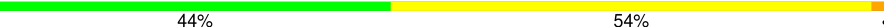


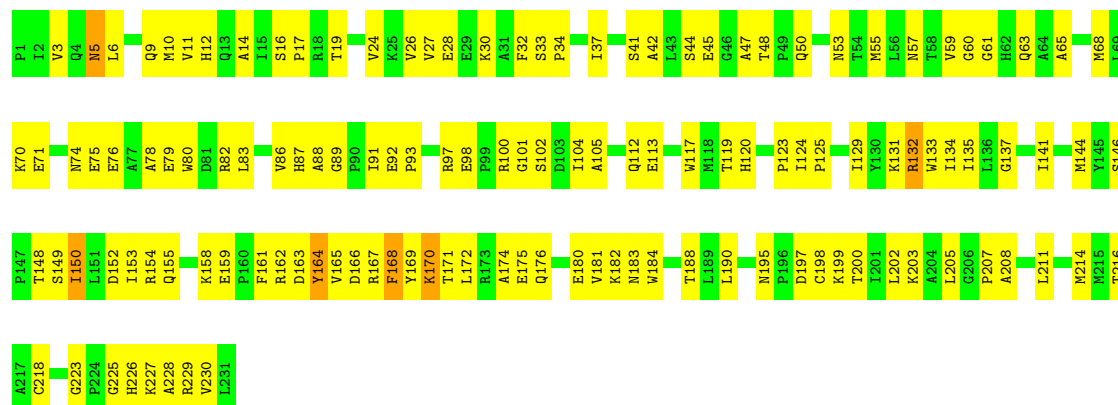
• Molecule 1: capsid protein

Chain 6q:  49% 49%

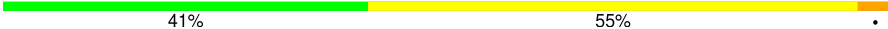


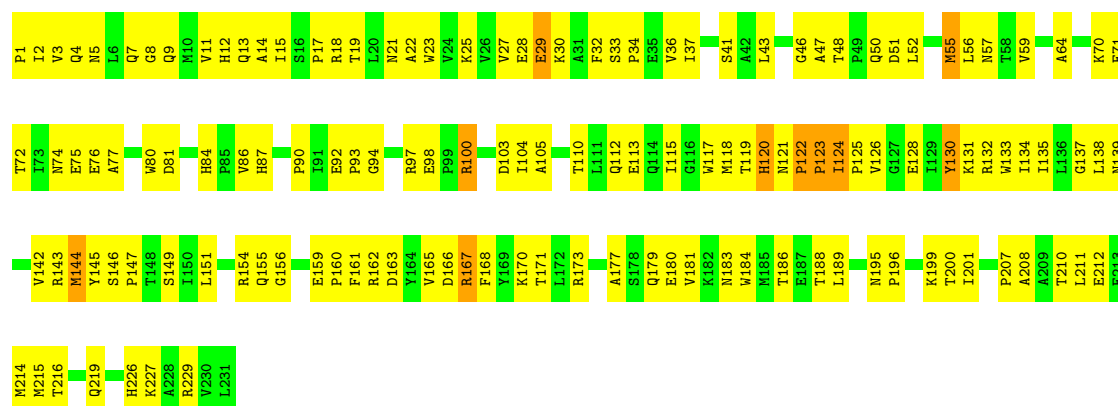
• Molecule 1: capsid protein

Chain 6r:  44% 54%

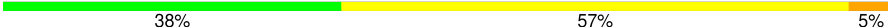


• Molecule 1: capsid protein

Chain 6s: 



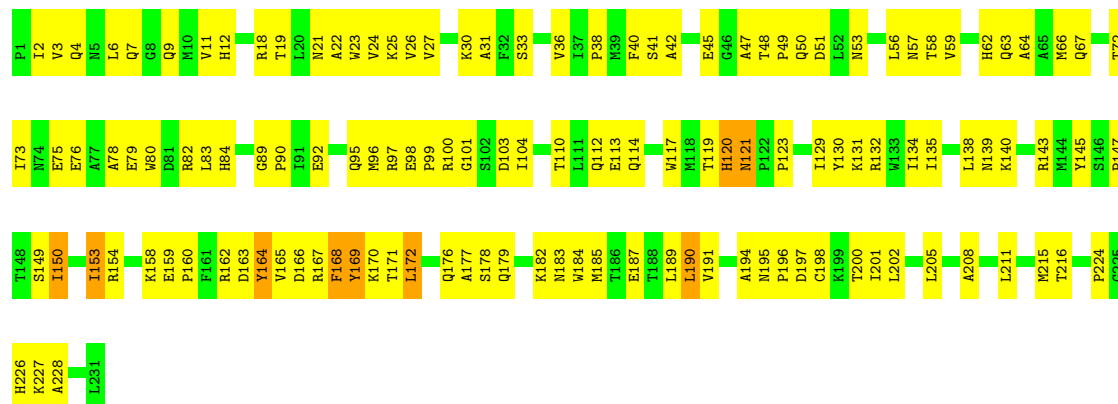
• Molecule 1: capsid protein

Chain 6t: 

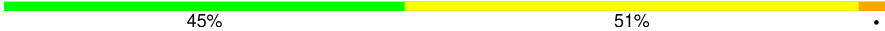


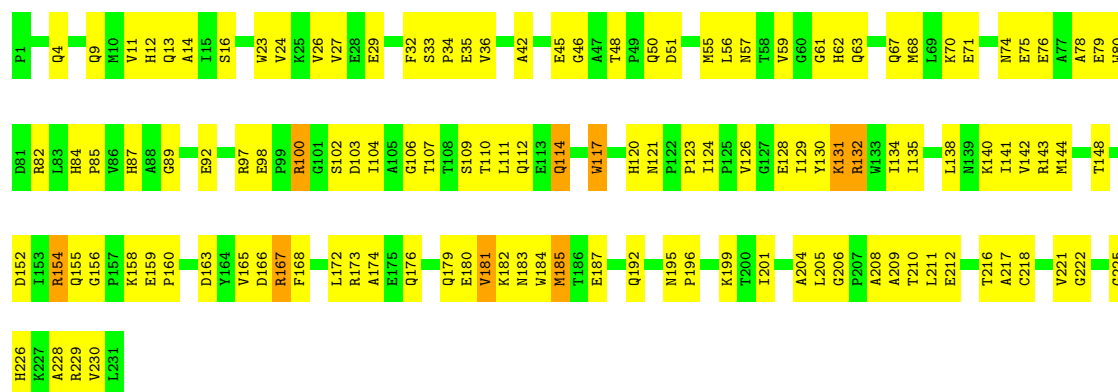
• Molecule 1: capsid protein

Chain 6u: 

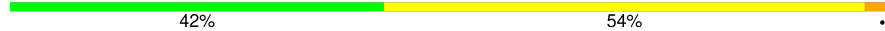


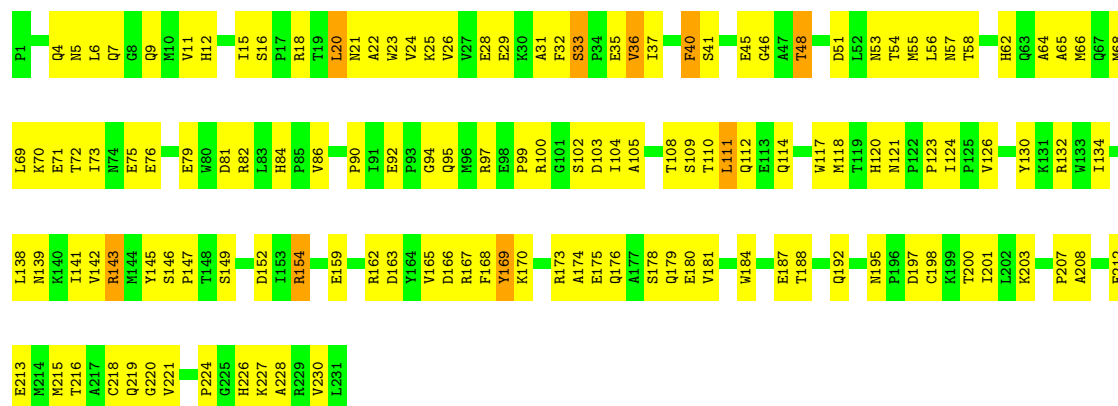
• Molecule 1: capsid protein

Chain 6v: 



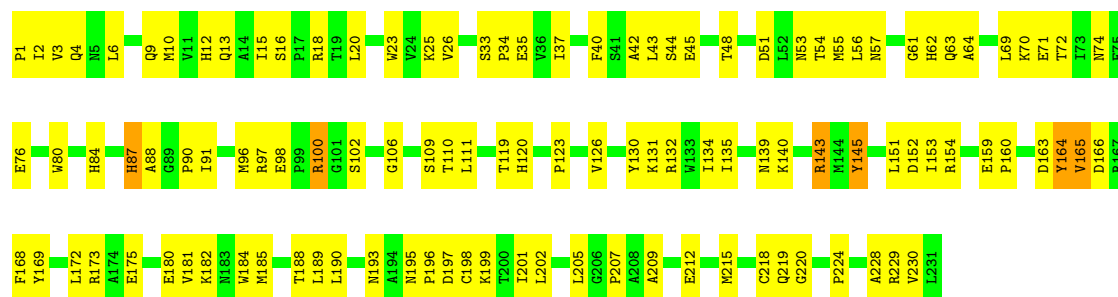
• Molecule 1: capsid protein

Chain 6w: 



• Molecule 1: capsid protein

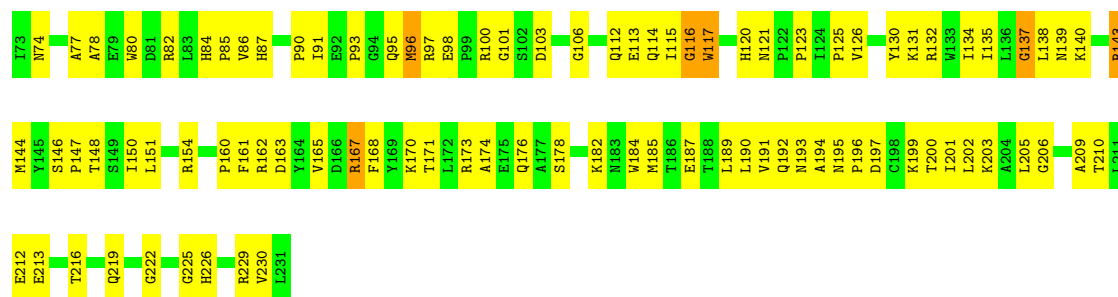
Chain 6x: 



• Molecule 1: capsid protein

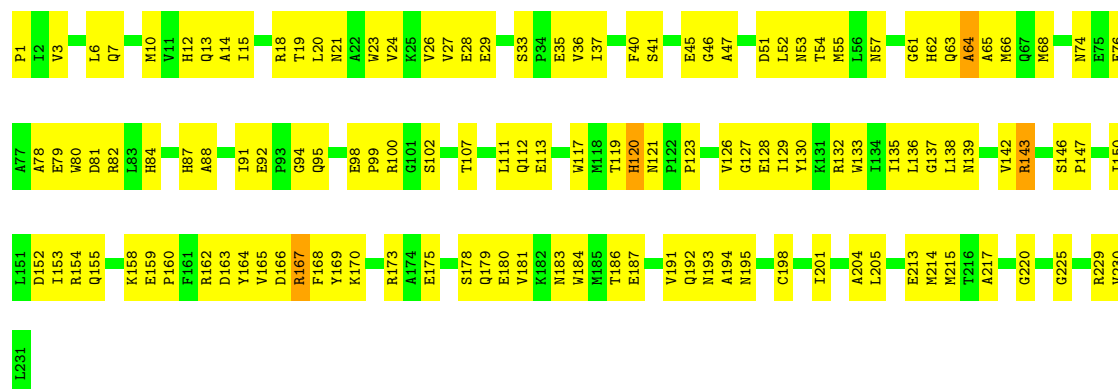
Chain 6y: 





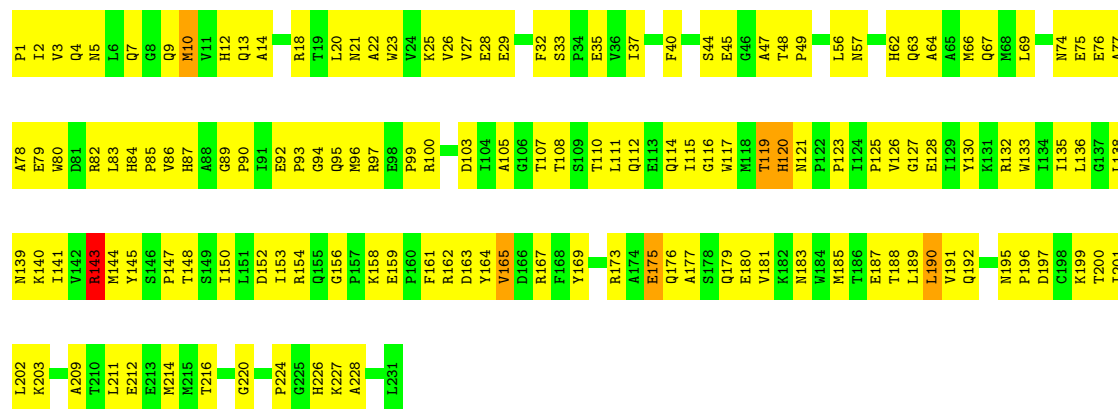
- Molecule 1: capsid protein

Chain 6z: 45% 54%



- Molecule 1: capsid protein

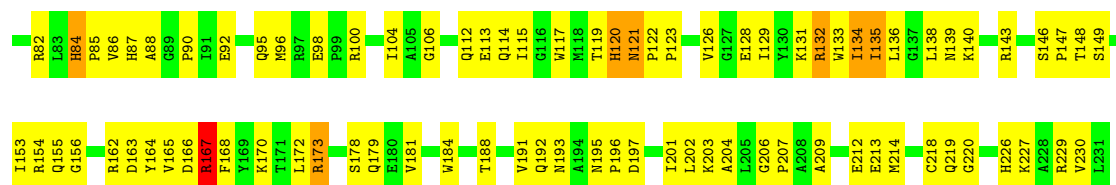
Chain 6A: 39% 58%



- Molecule 1: capsid protein

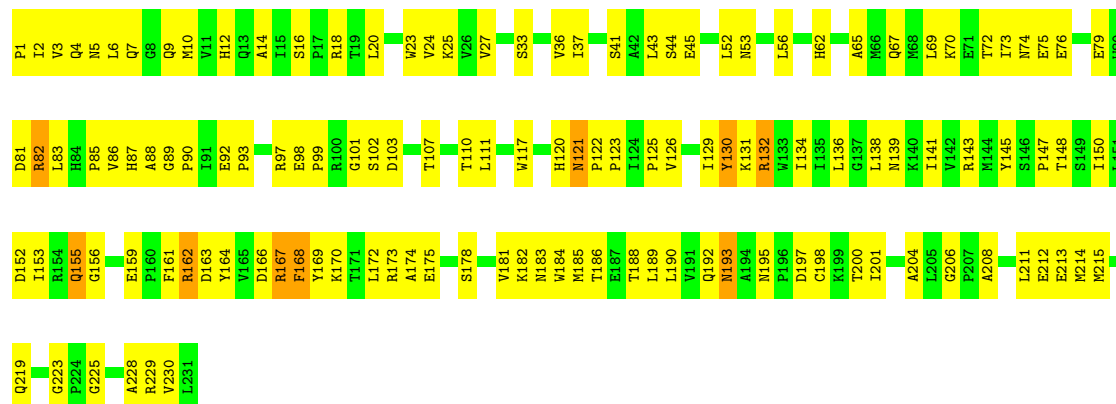
Chain 6B: 46% 50%





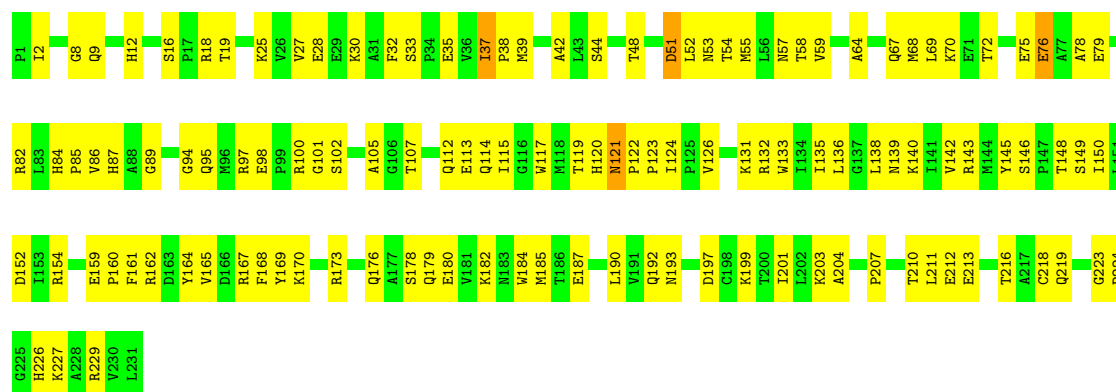
• Molecule 1: capsid protein

Chain 6C: 44% 52%



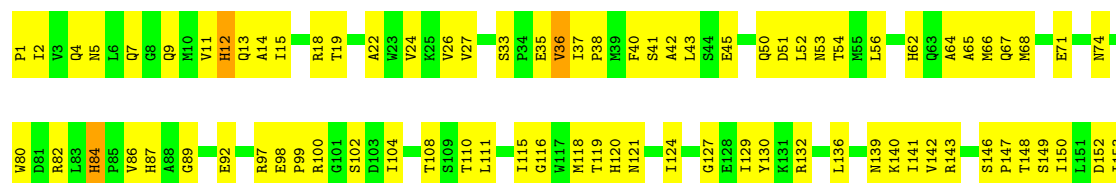
• Molecule 1: capsid protein

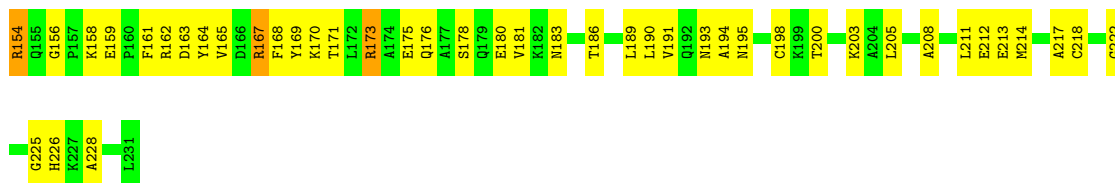
Chain 6D: 47% 51%



• Molecule 1: capsid protein

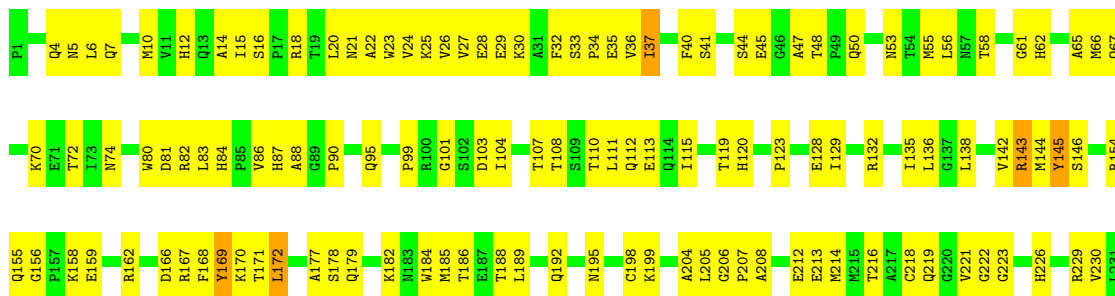
Chain 6E: 46% 51%





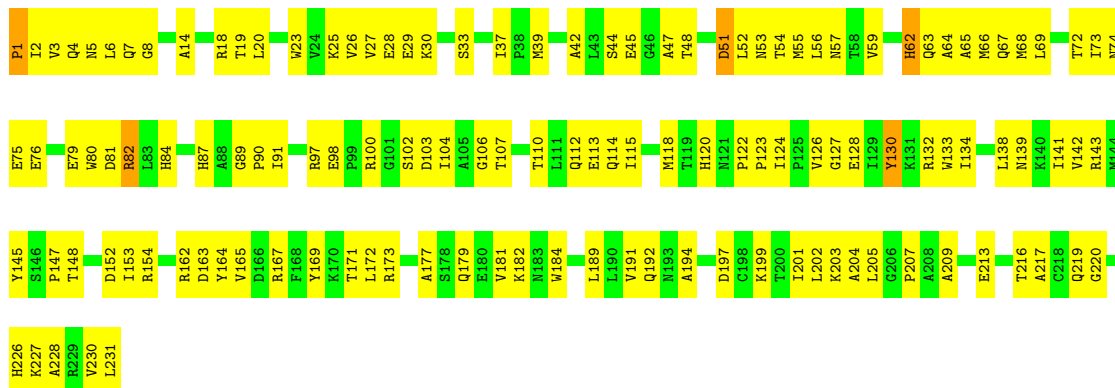
- Molecule 1: capsid protein

Chain 6F: 46% 52%



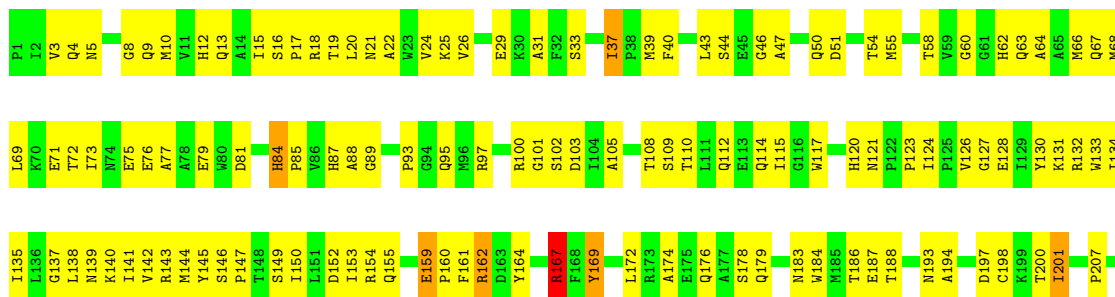
- Molecule 1: capsid protein

Chain 6G: 44% 54%



- Molecule 1: capsid protein

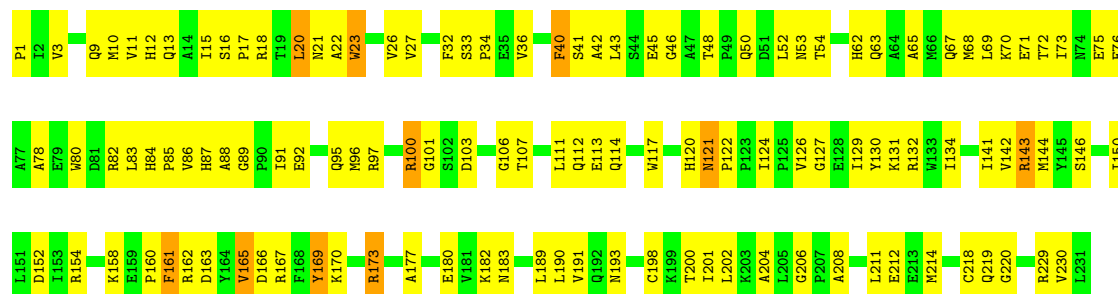
Chain 6H: 41% 56%





- Molecule 1: capsid protein

Chain 6I: 47% 48%



- Molecule 1: capsid protein

Chain 6J: 45% 54%



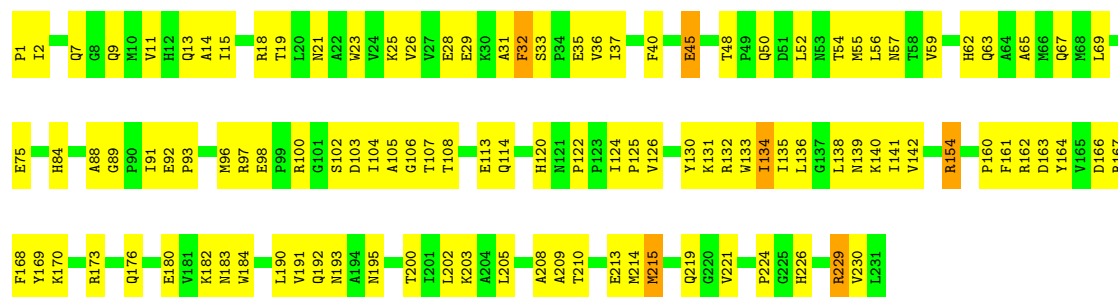
- Molecule 1: capsid protein

Chain 6K: 46% 51%

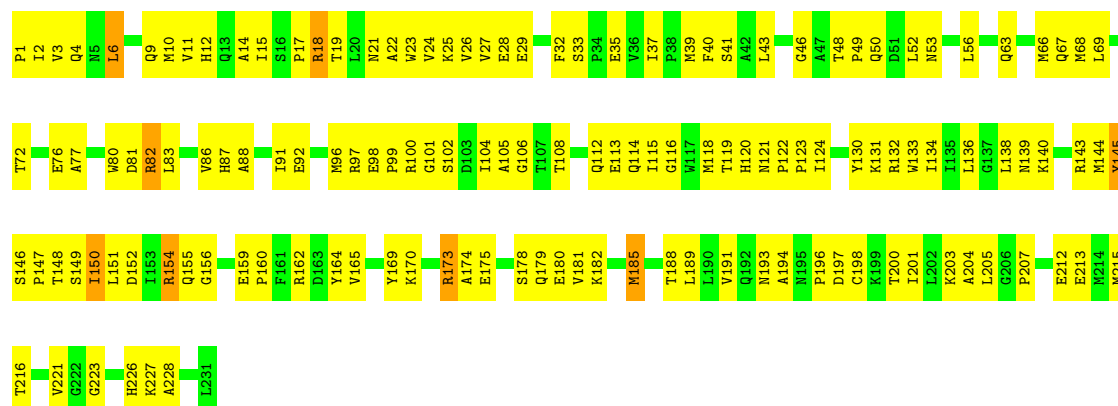


- Molecule 1: capsid protein

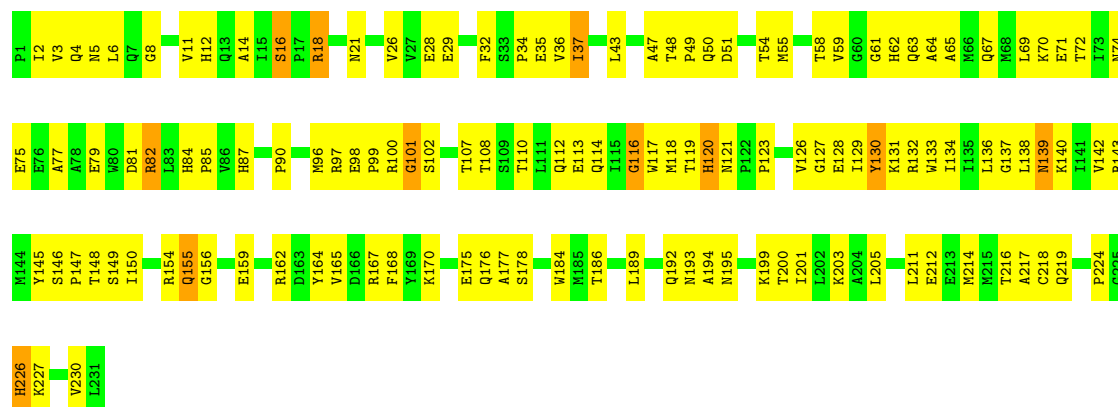
Chain 6L: 52% 46%



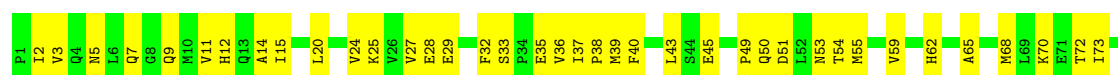
- Molecule 1: capsid protein

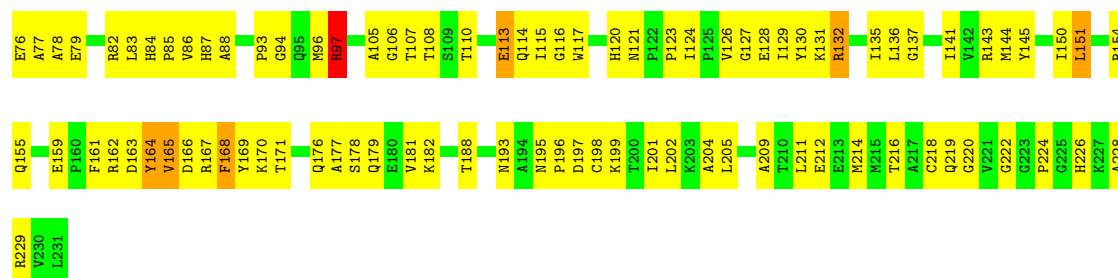


- Molecule 1: capsid protein

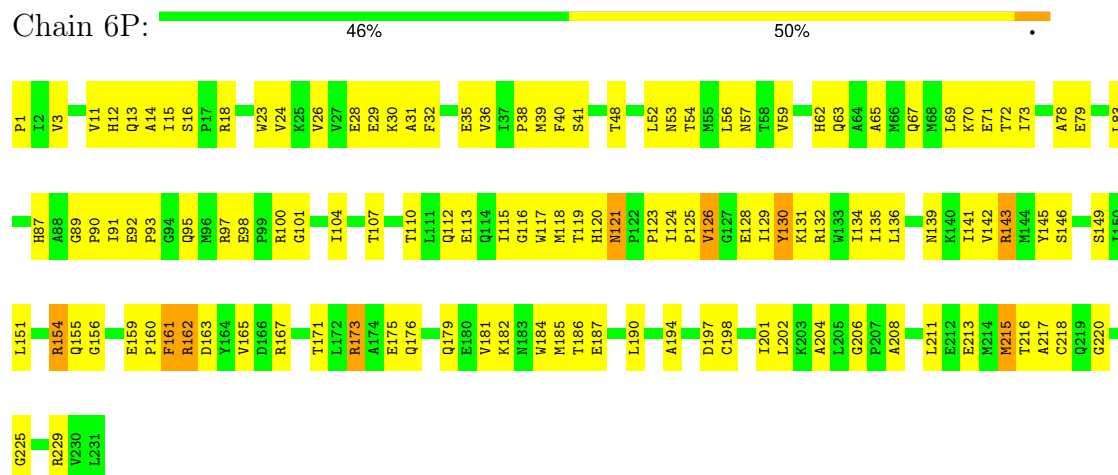


- Molecule 1: capsid protein

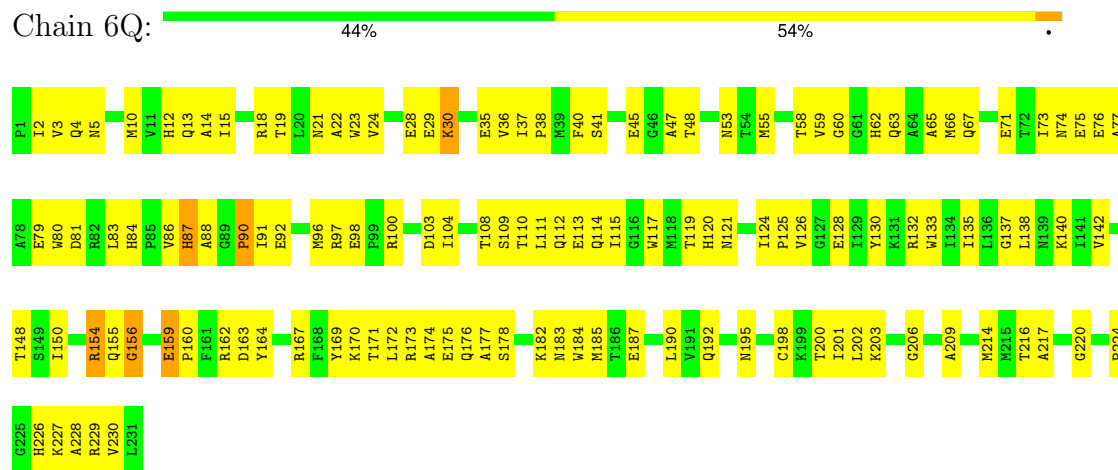




- Molecule 1: capsid protein



- Molecule 1: capsid protein

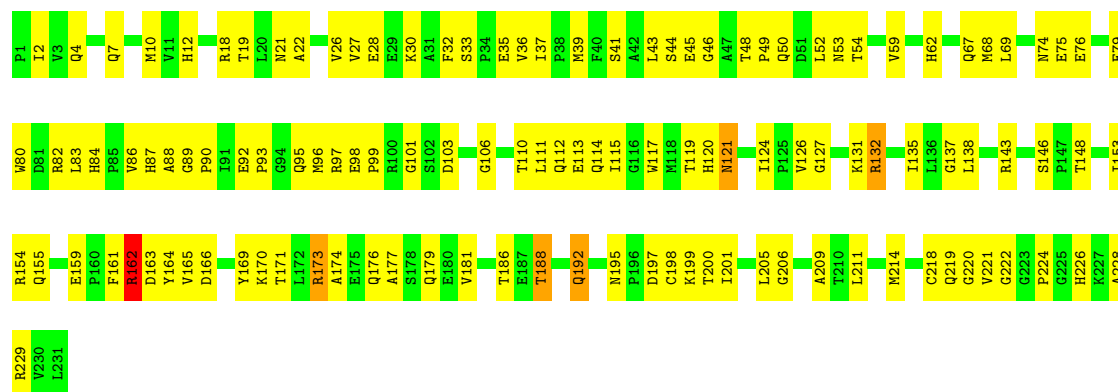


- Molecule 1: capsid protein



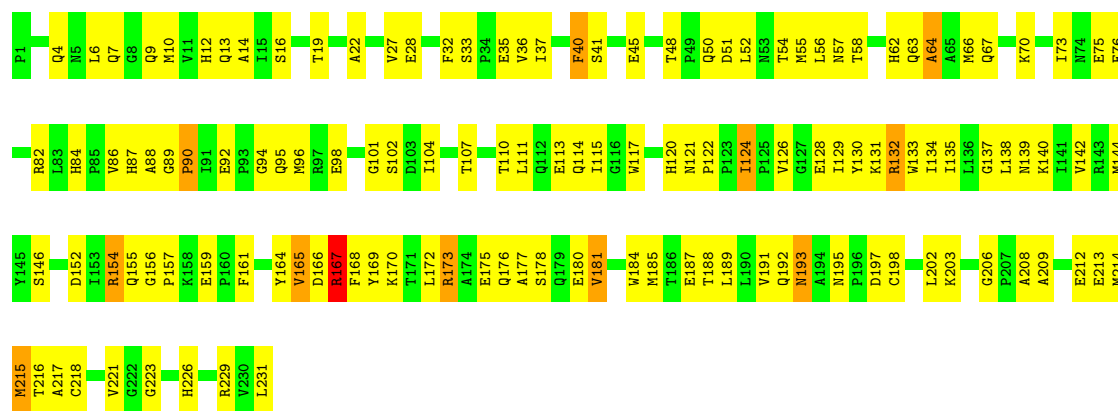
- Molecule 1: capsid protein

Chain 6S: 48% 50%



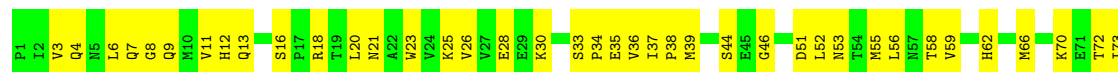
- Molecule 1: capsid protein

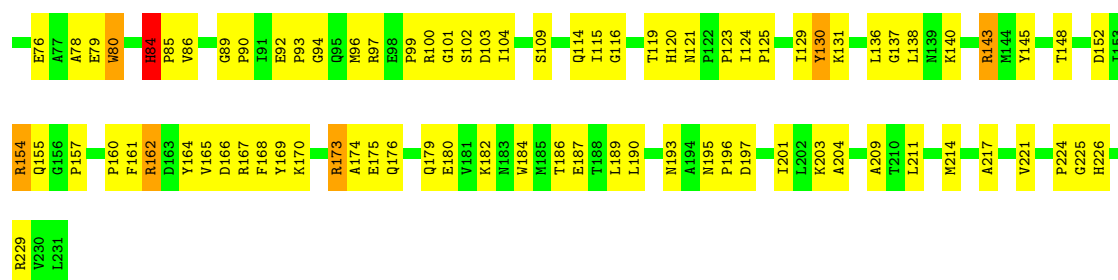
Chain 6T: 43% 52% 5%



- Molecule 1: capsid protein

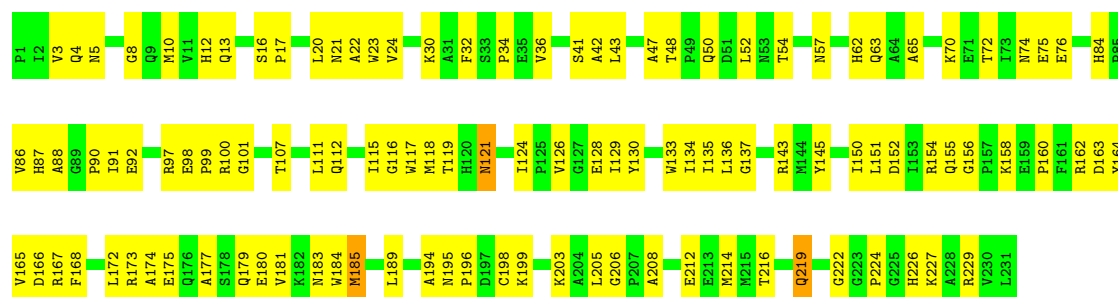
Chain 6U: 48% 49%





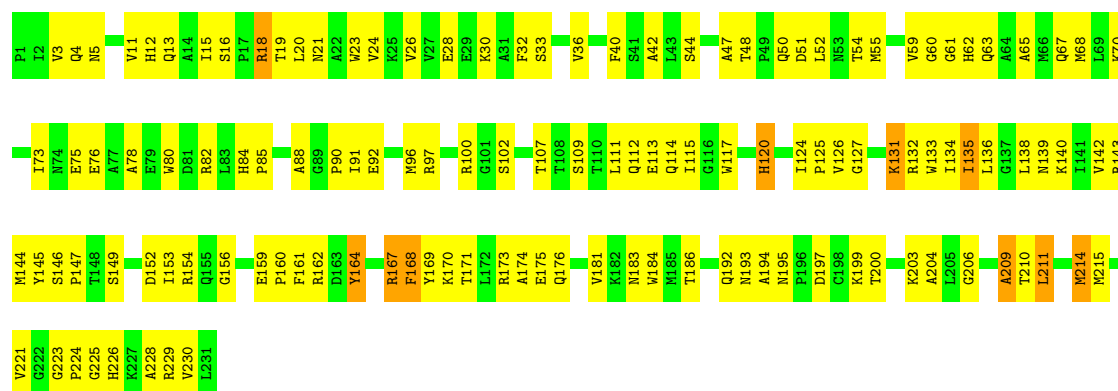
- Molecule 1: capsid protein

Chain 6V: 51% 48%



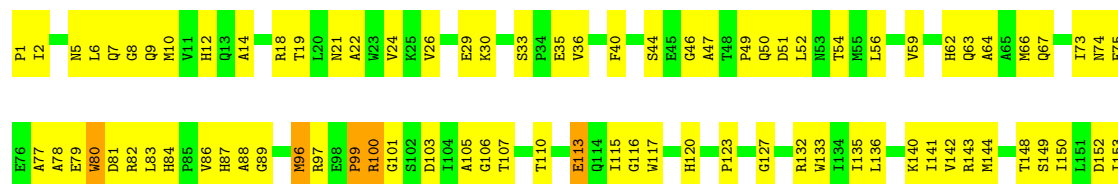
- Molecule 1: capsid protein

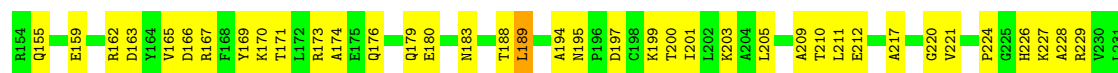
Chain 6W: 44% 52%



- Molecule 1: capsid protein

Chain 6X: 48% 50%





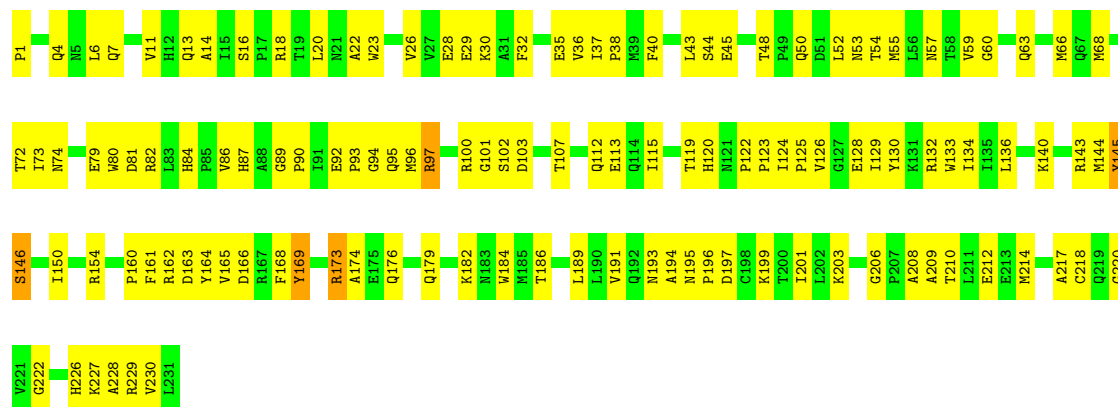
- Molecule 1: capsid protein

Chain 6Y:



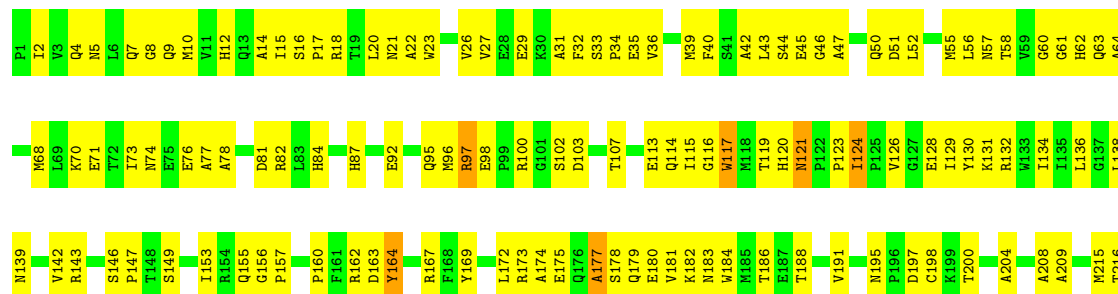
- Molecule 1: capsid protein

Chain 6Z:



- Molecule 1: capsid protein

Chain 70:



A217
C218
Q219
G220
V221

H226
K227
A228
R229
V230
L231

• Molecule 1: capsid protein

Chain 71:  51% 47%

P1
I2
N5
M10
V11
H12
Q13
A14
I15
S16
P17
R18
T19
L20
N21
A22
V23
V24
K25
V26
V27
E28
F32
S33
P34
E35
V36
I37
F38
M39
F40
S41
A42
E45
P49
Q50
T54
N57
T58
A65
K66
Q67
R68
L69
E71
T72
E75
E79

W80
D81
R82
L83
H84
H87
A88
G89
P90
I91
E92
Q95
P96
R97
R100
G101
S102
I104
A105
G106
T107
T108
S109
T110
L111
Q112
E113
Q114
I115
T119
H120
N121
V126
G127
E128
I129
Y130
R131
R132
W133
I134
G137
L138
H139
R143
M144
Y145
T148
I150

L151
D152
I153
R154
Q155
F161
R162
D163
Y164
V165
D166
F167
F168
Y169
R170
R173
A174
E175
Q176
A177
E180
V181
K182
W184
E187
T188
Q192
N195
C198
K199
T200
I201
L202
K203
E212
E213
M214
C218
Q219
G220
V221
G222
G225
A228
R229
V230
L231

• Molecule 1: capsid protein

Chain 72:  45% 51%

P1
I2
V3
L6
Q7
G8
Q9
H10
H11
H12
S16
P17
R18
A22
V26
E28
E29
K30
A31
F32
S33
P34
V36
I37
P38
M39
A42
L43
S44
E45
T48
P49
Q50
D51
L52
N53
T54
M55
L56
V59
G60
G61
H62
Q63
M68
L69
K70
I73
N74

E75
E76
A77
E79
W80
D81
R82
H84
H87
A88
G89
P90
I91
E92
P93
G94
Q95
M96
R97
G101
T104
A105
L111
Q114
I115
W117
H120
N121
T124
P125
V126
G127
E128
Y129
K131
R132
W133
I134
I135
L138
N139
K140
R143
M144
Y145
P147

T148
S149
I150
I153
Q155
K158
E159
P160
F161
R162
D163
Y164
R167
F168
Y169
L172
R173
A174
Q175
Q176
Q179
W184
M185
T188
V191
Q192
N193
N195
D197
T200
I201
A204
L205
G206
A209
T210
L211
E212
E213
T216
A217
C218
Q219
G223

A228
R229
V230
L231

• Molecule 1: capsid protein

Chain 73:  42% 56%

P1
Q4
N5
Q9
M10
V11
H12
A13
I14
S15
P17
R18
T19
A22
V23
V24
K25
V26
V27
S33
P34
E35
V36
I37
P38
M39
F40
S41
A42
L43
S44
E45
P49
Q50
D51
L52
N53
L56
M57
T58
V59
H62
Q63
A64
A65
M66
Q67
M68
T72
E75

E76
A77
W80
D81
R82
L83
H84
P85
H87
A88
P89
I91
E92
P93
Q94
Q95
M96
R97
E98
P99
R100
D103
I104
T108
S109
P109
T110
E113
Q114
L115
G116
W117
M118
T119
H120
N121
I124
P125
V126
G127
E128
I129
Y130
K131
R132
W133
I134
M139
R143
M144
Y145
S146

P147
T148
S149
I150
D152
I153
R154
E159
P160
F161
R162
D163
Y164
V165
F168
Q169
K170
T171
L172
R173
A174
E175
Q176
A177
Q179
K182
M183
W184
T186
E187
L190
V191
N195
C198
K199
T200
I201
L202
K203
A204
L205
G206
P207
A208
A209
T210
L211
M215
T216
Y145
A217

C218
Q219
G220
V221
P224
G225
H226
R229
V230
L231

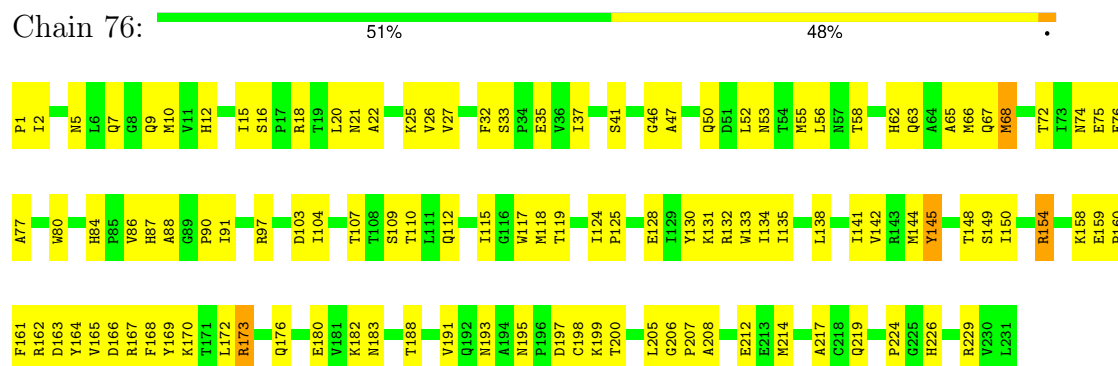
• Molecule 1: capsid protein



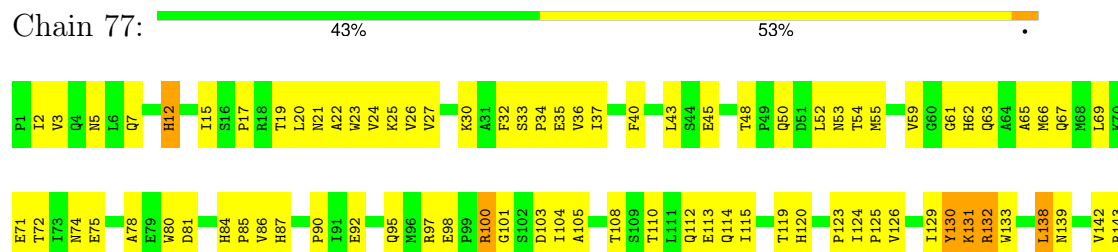
- Molecule 1: capsid protein

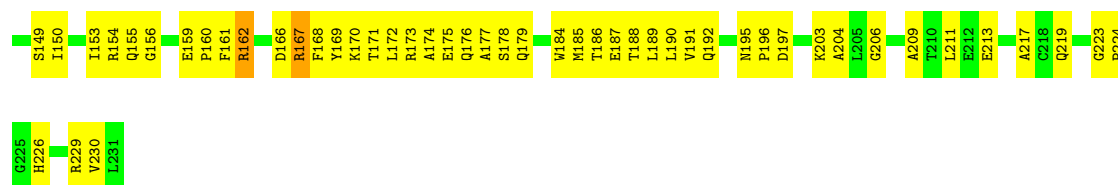


- Molecule 1: capsid protein



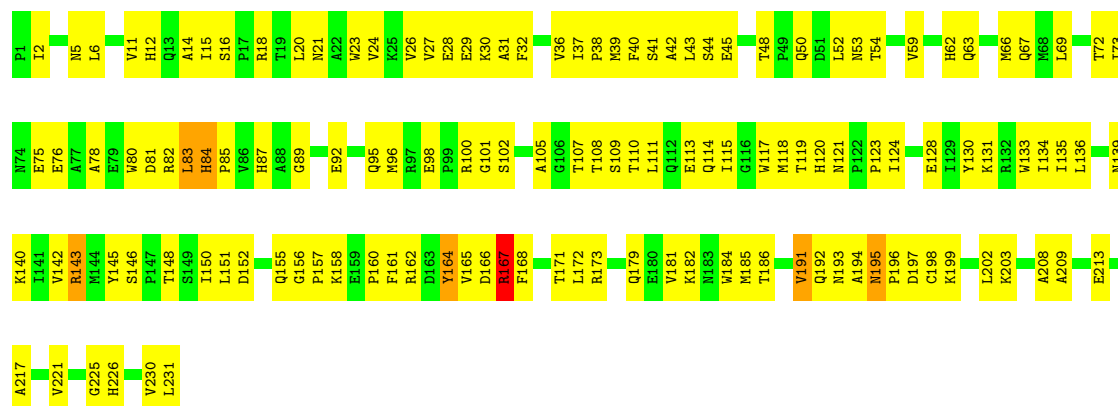
- Molecule 1: capsid protein





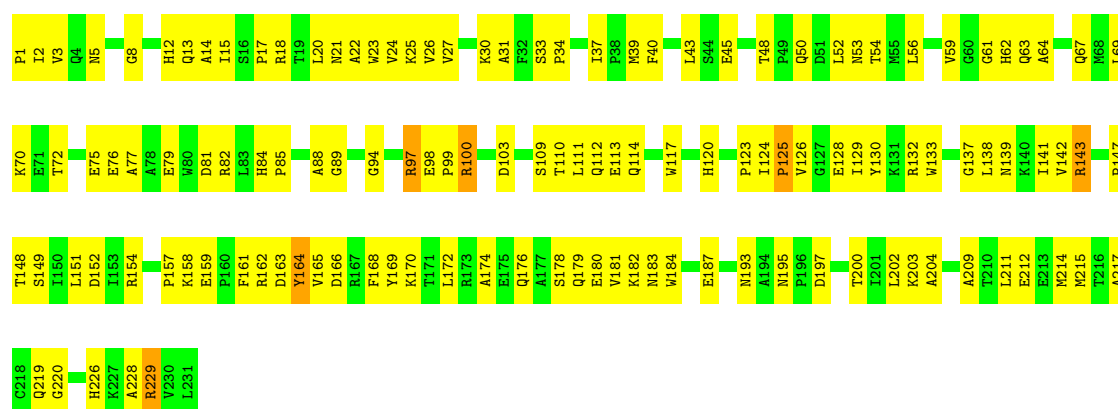
• Molecule 1: capsid protein

Chain 78: 42% 55%



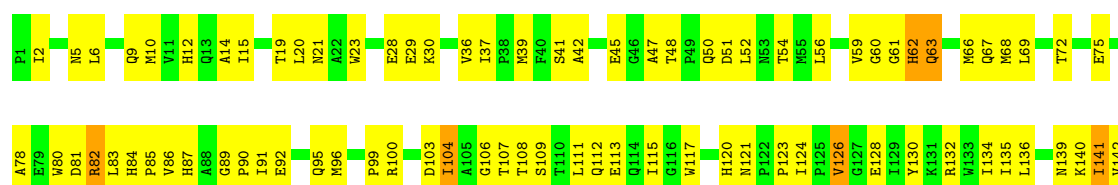
• Molecule 1: capsid protein

Chain 79: 44% 53%



• Molecule 1: capsid protein

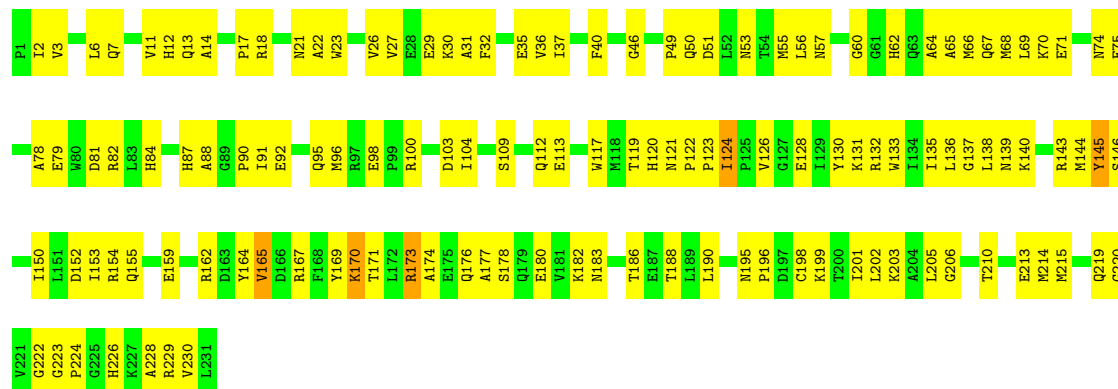
Chain 7a: 44% 52%





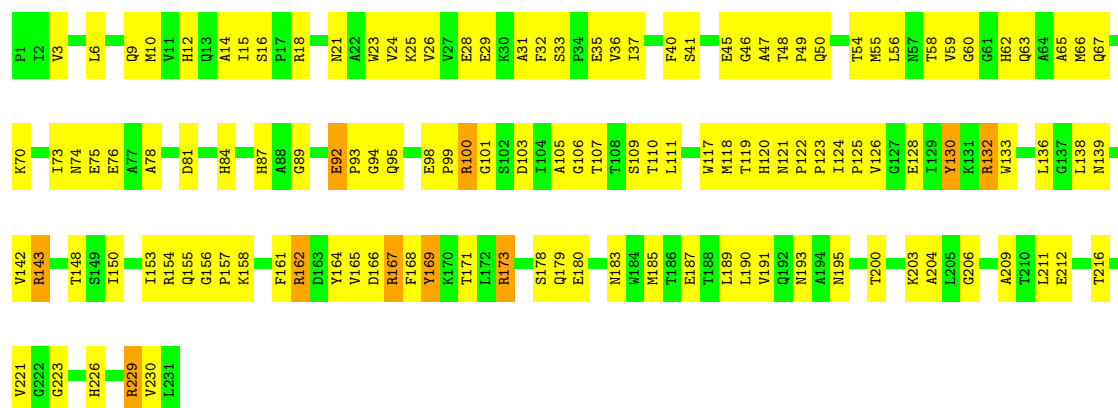
• Molecule 1: capsid protein

Chain 7b: 43% 55%



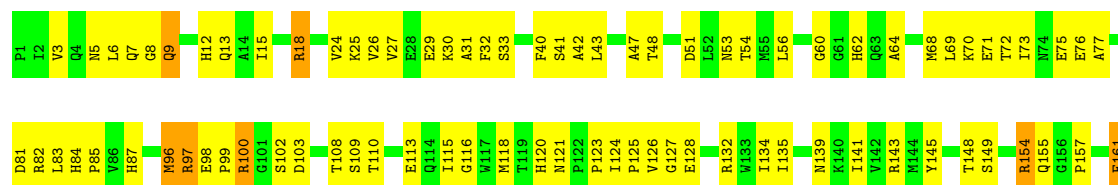
• Molecule 1: capsid protein

Chain 7c: 45% 51%



• Molecule 1: capsid protein

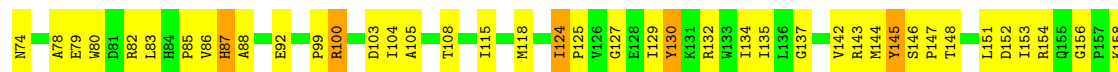
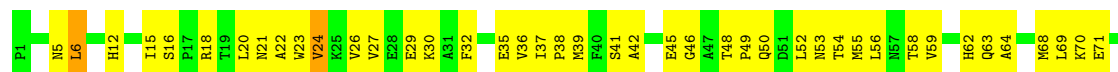
Chain 7d: 48% 48%





- Molecule 1: capsid protein

Chain 7e: 50% 47%



- Molecule 1: capsid protein

Chain 7f: 46% 49% 5%



- Molecule 1: capsid protein

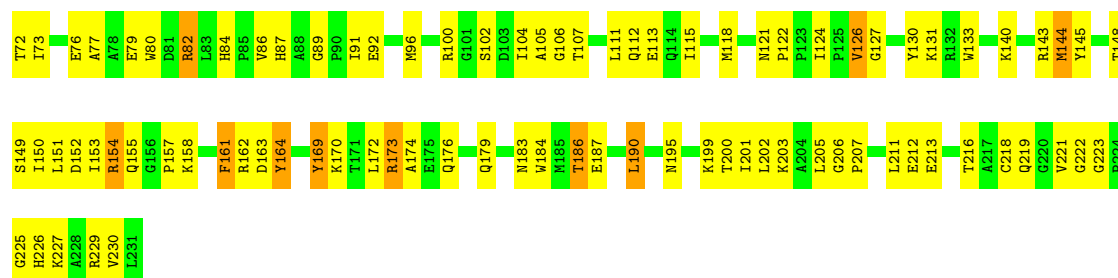
Chain 7g: 47% 52%



- Molecule 1: capsid protein

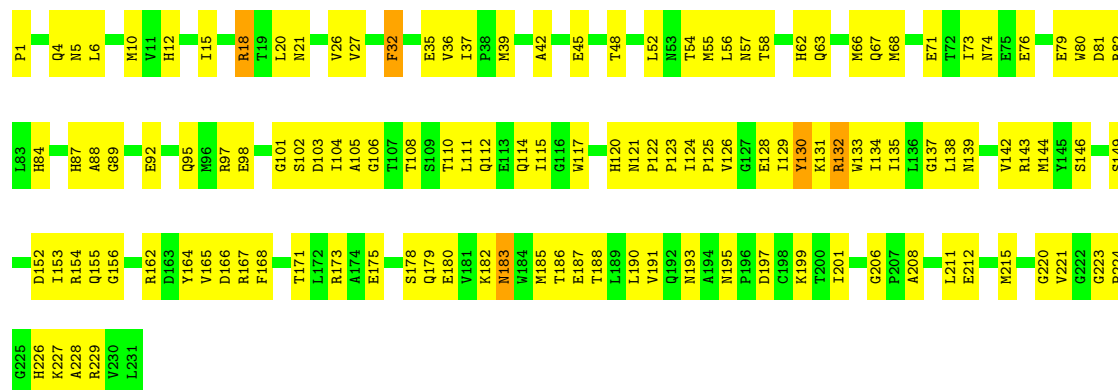
Chain 7h: 46% 48% 6%





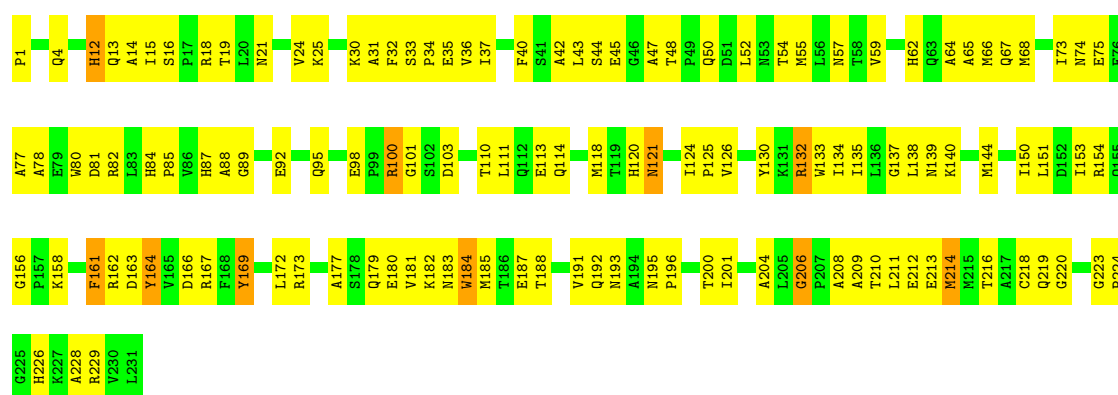
- Molecule 1: capsid protein

Chain 7i: 45% 52%



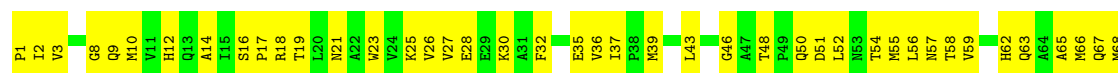
- Molecule 1: capsid protein

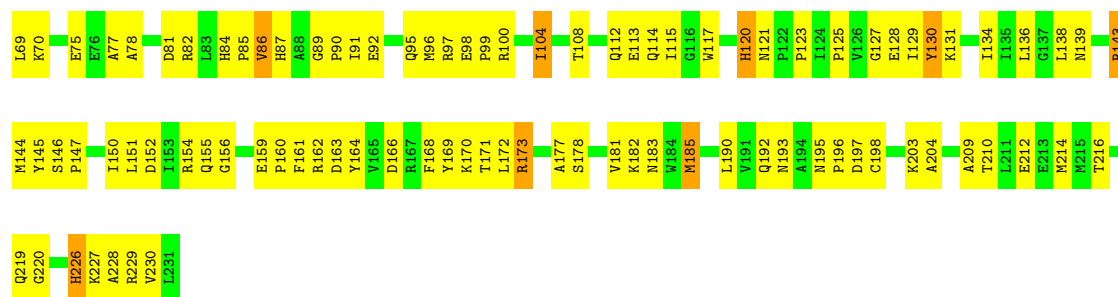
Chain 7j: 45% 51%



- Molecule 1: capsid protein

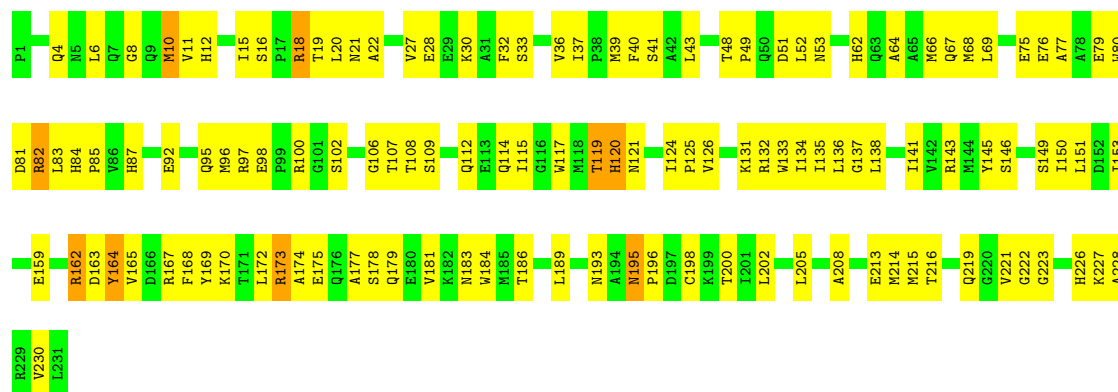
Chain 7k: 42% 55%





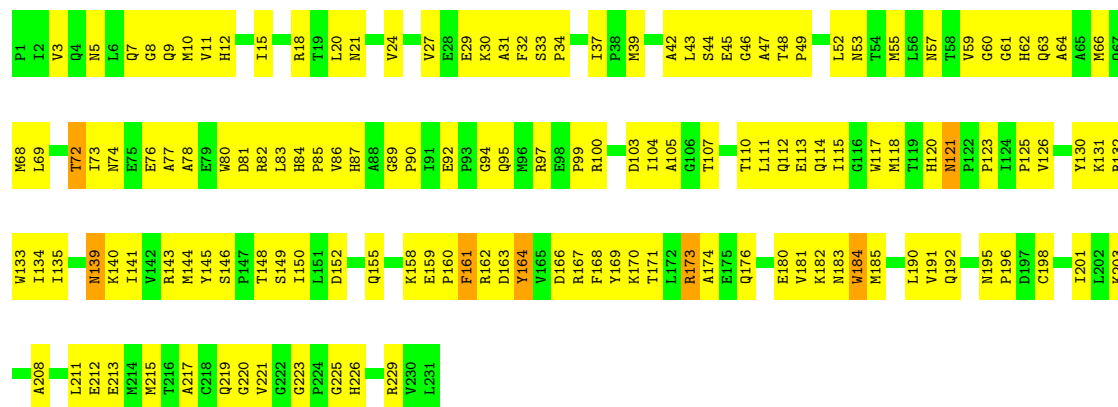
• Molecule 1: capsid protein

Chain 7l: 46% 50%



• Molecule 1: capsid protein

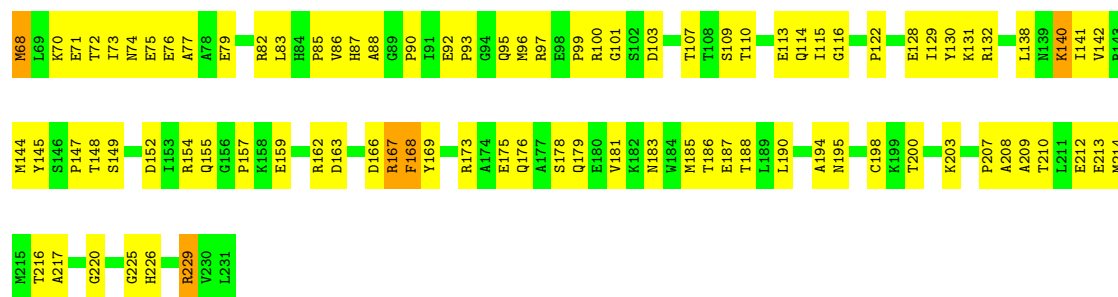
Chain 7m: 38% 59%



• Molecule 1: capsid protein

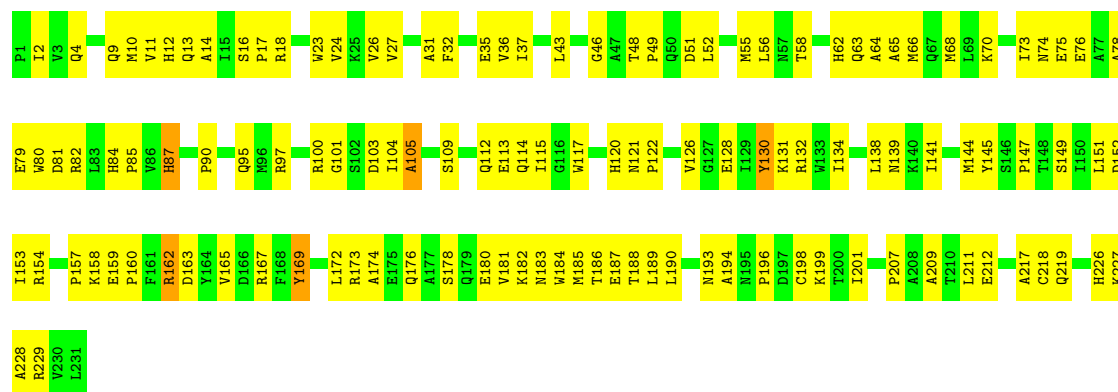
Chain 7n: 43% 54%





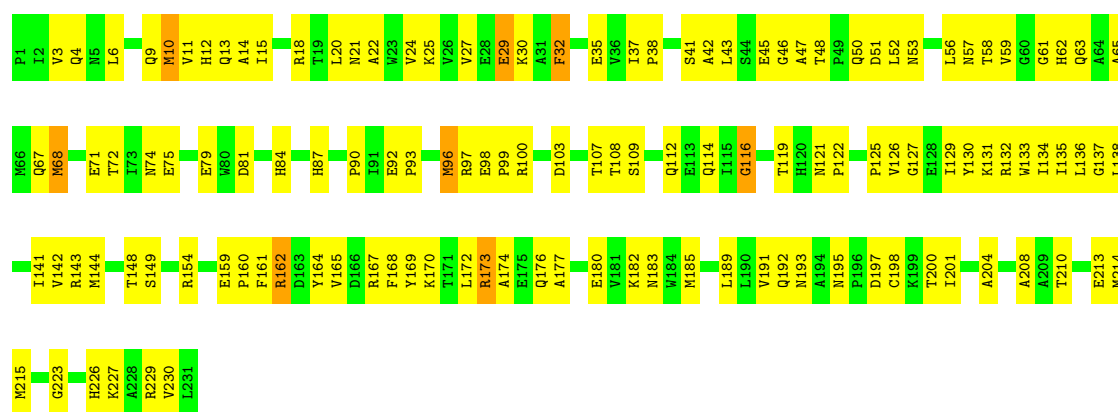
• Molecule 1: capsid protein

Chain 7o: 46% 52%



• Molecule 1: capsid protein

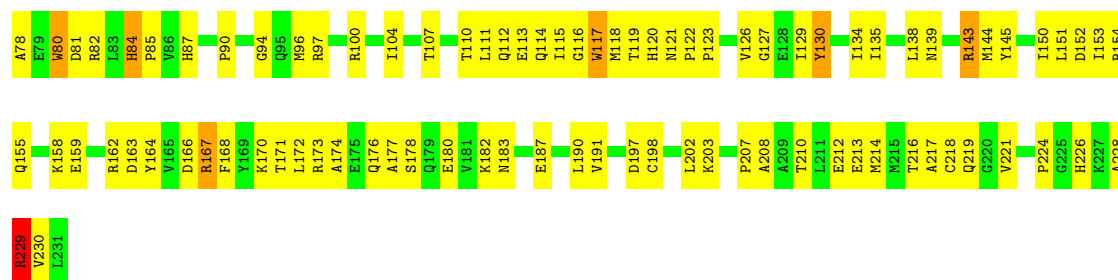
Chain 7p: 44% 52%



• Molecule 1: capsid protein

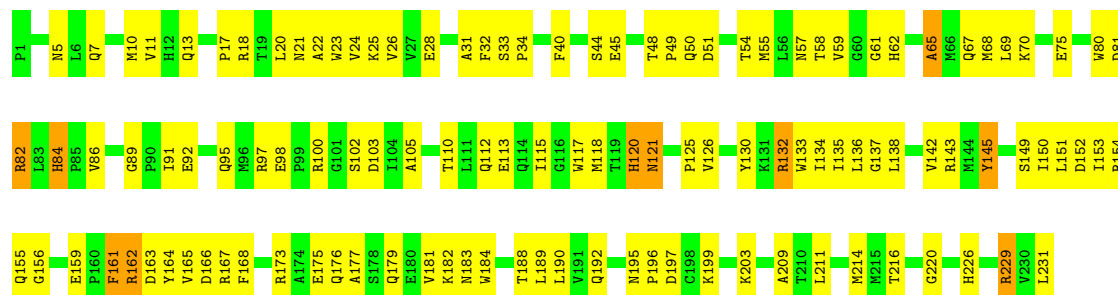
Chain 7q: 44% 53%





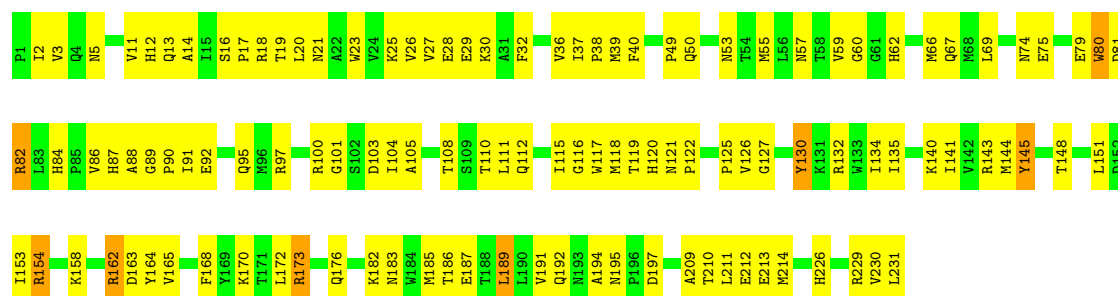
- Molecule 1: capsid protein

Chain 7r: 49% 47%



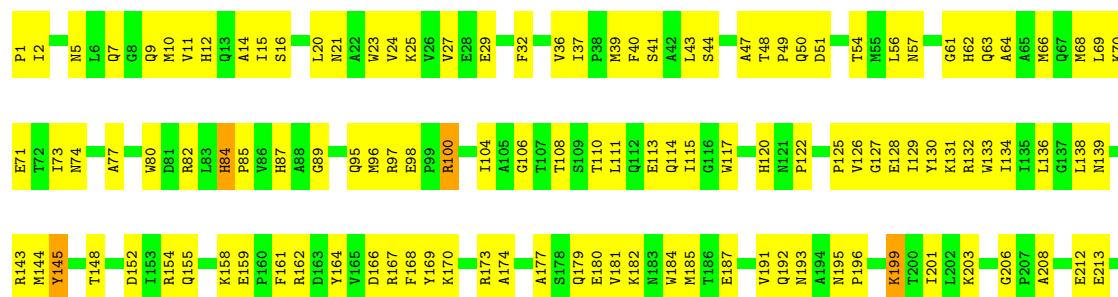
- Molecule 1: capsid protein

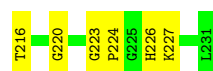
Chain 7s: 49% 47%



- Molecule 1: capsid protein

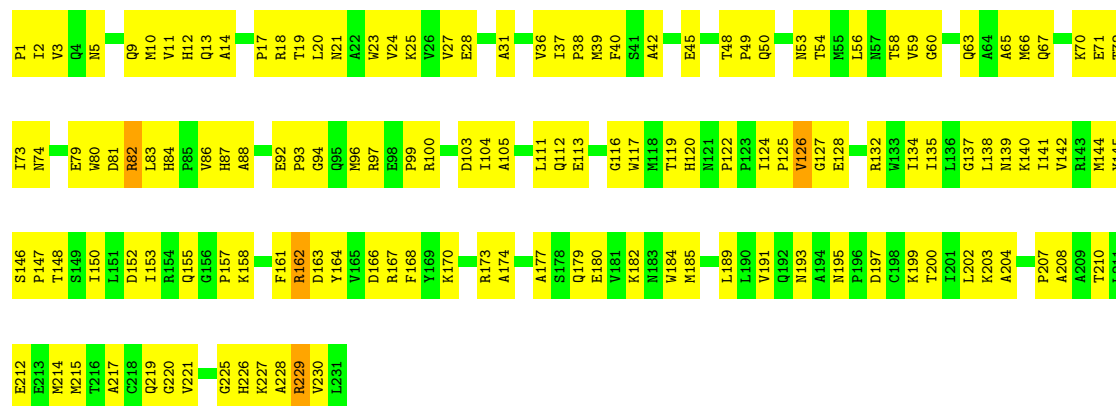
Chain 7t: 45% 53%





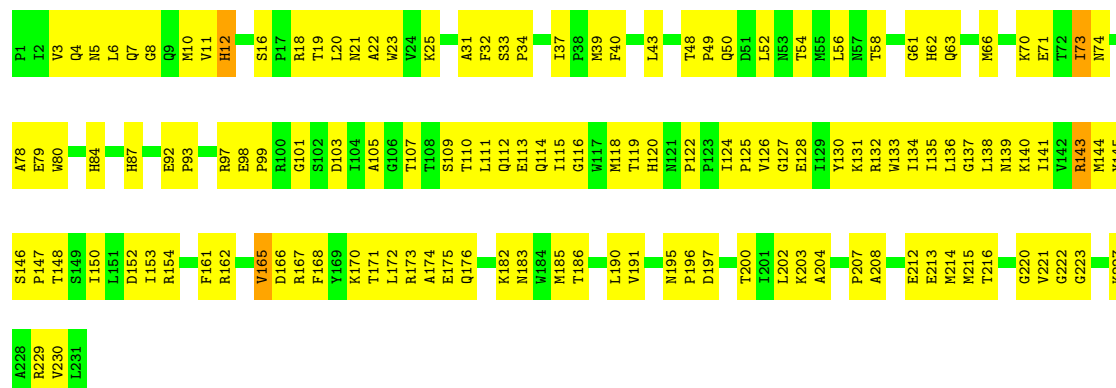
- Molecule 1: capsid protein

Chain 7u: 39% 59%



- Molecule 1: capsid protein

Chain 7v: 42% 56%

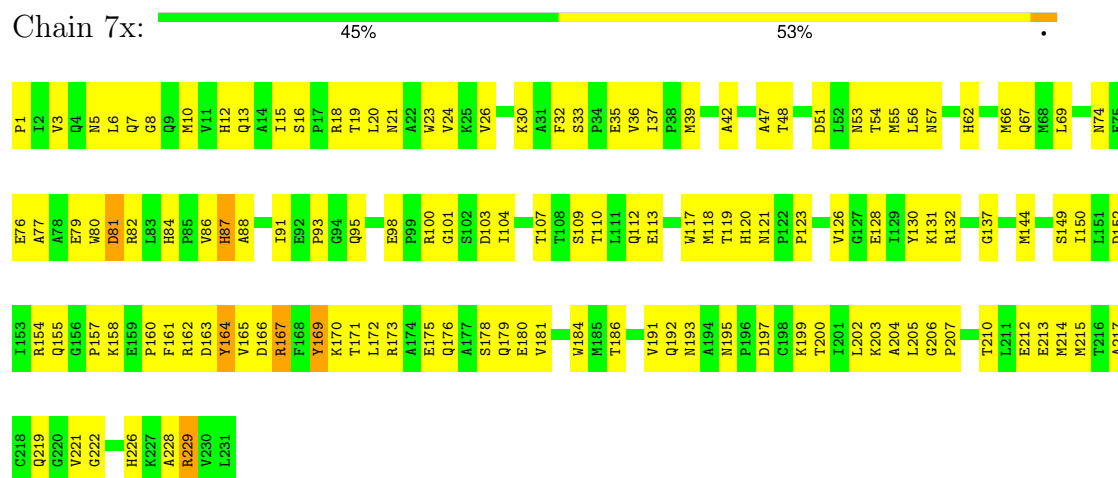


- Molecule 1: capsid protein

Chain 7w: 49% 48%



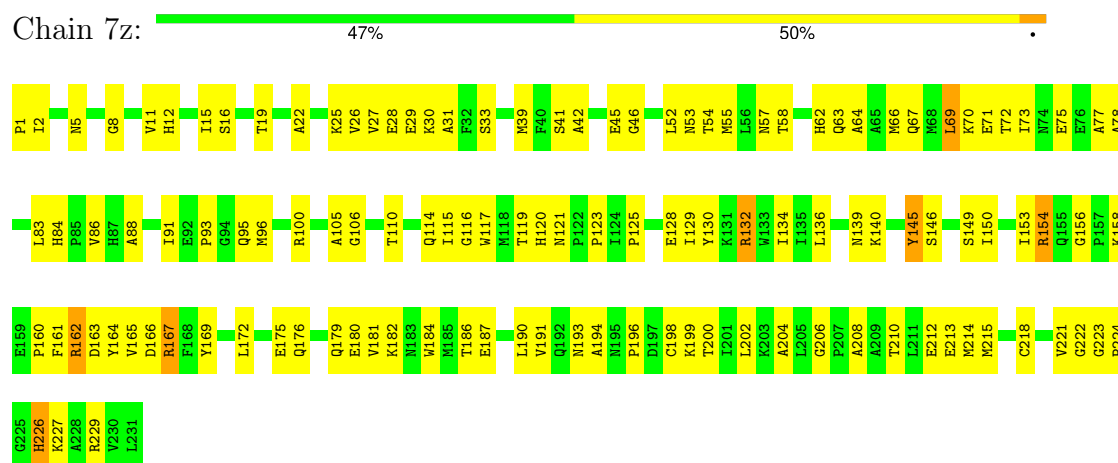
- Molecule 1: capsid protein



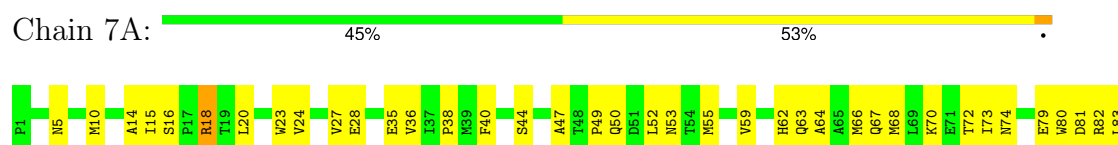
• Molecule 1: capsid protein

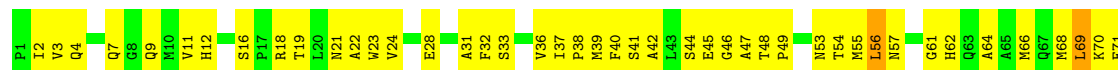


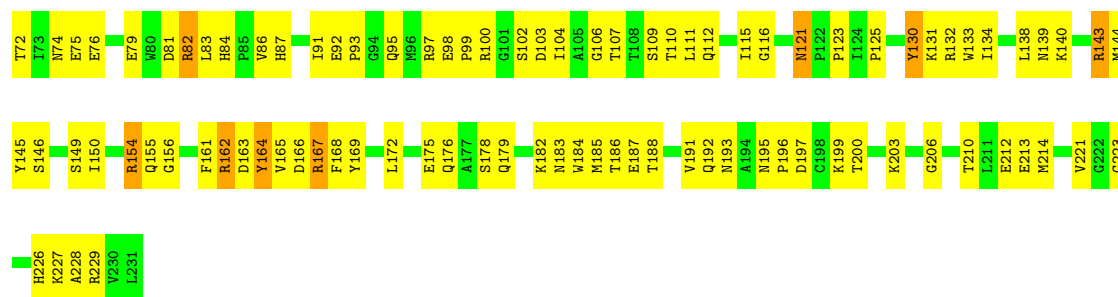
• Molecule 1: capsid protein



• Molecule 1: capsid protein

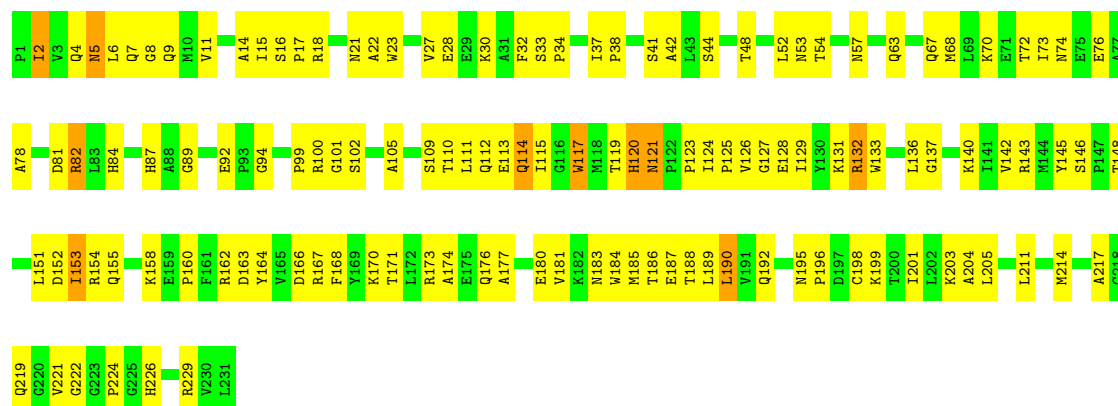






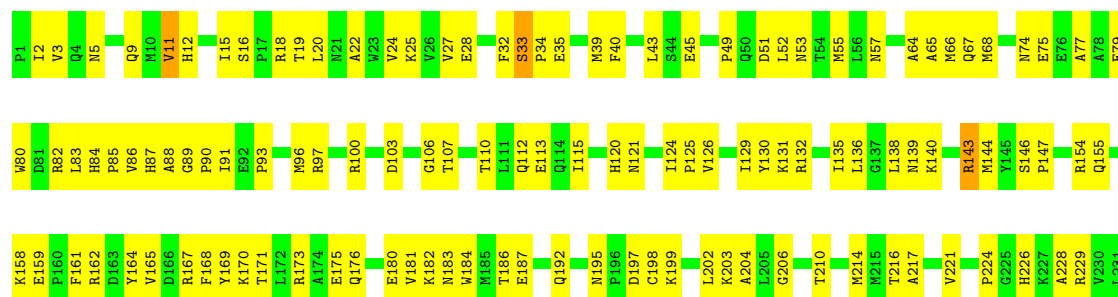
- Molecule 1: capsid protein

Chain 7E: 44% 52%



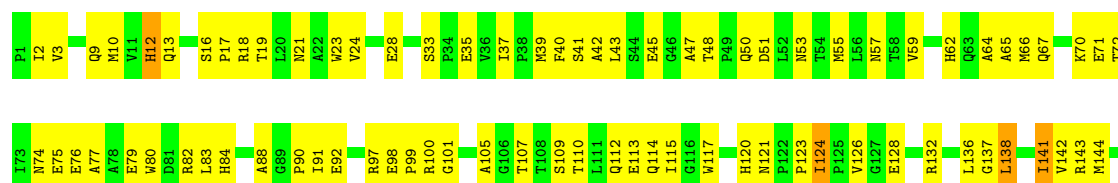
- Molecule 1: capsid protein

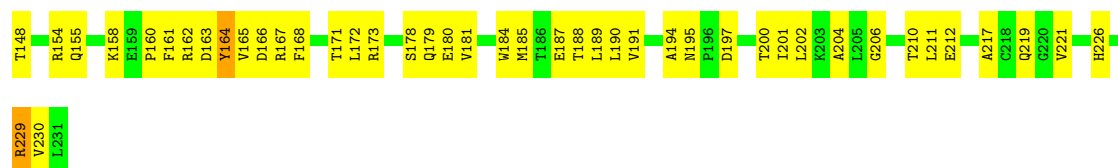
Chain 7F: 48% 51%



- Molecule 1: capsid protein

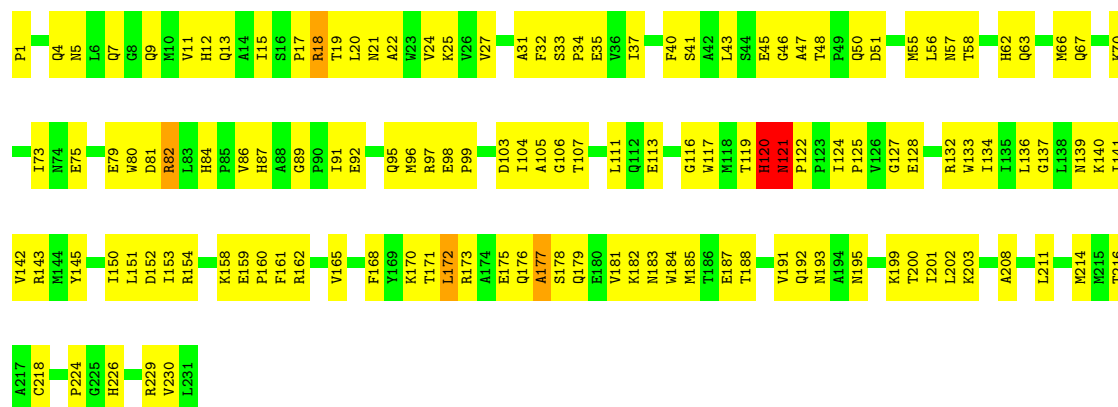
Chain 7G: 46% 51%





- Molecule 1: capsid protein

Chain 7H: 42% 55% ..



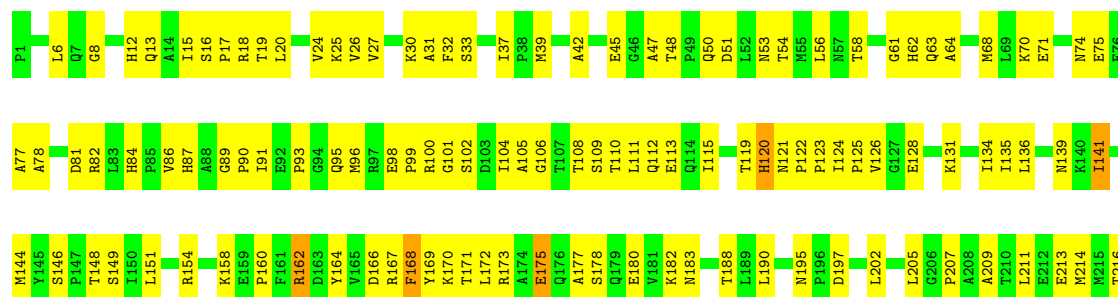
- Molecule 1: capsid protein

Chain 7I: 51% 46% .



- Molecule 1: capsid protein

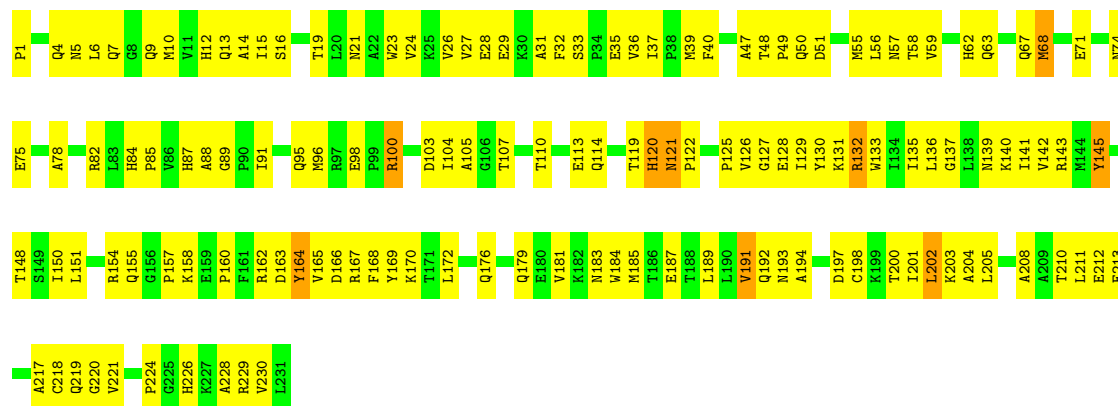
Chain 7J: 47% 51% .





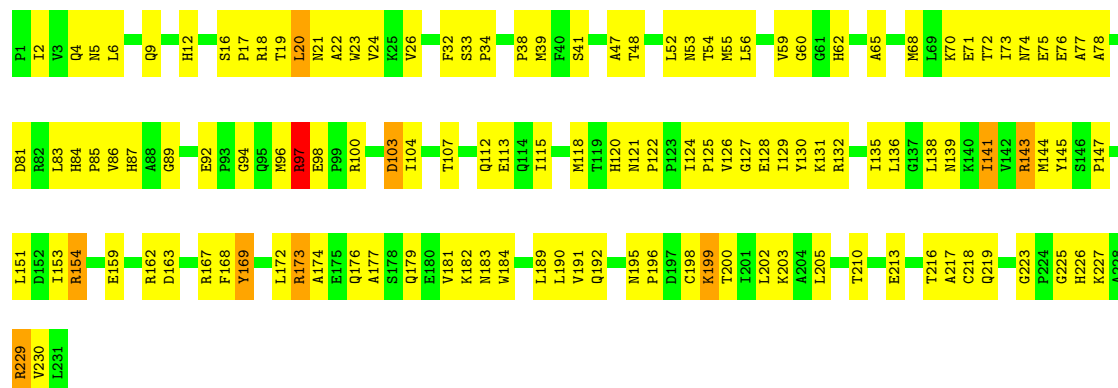
• Molecule 1: capsid protein

Chain 7K: 40% 56%



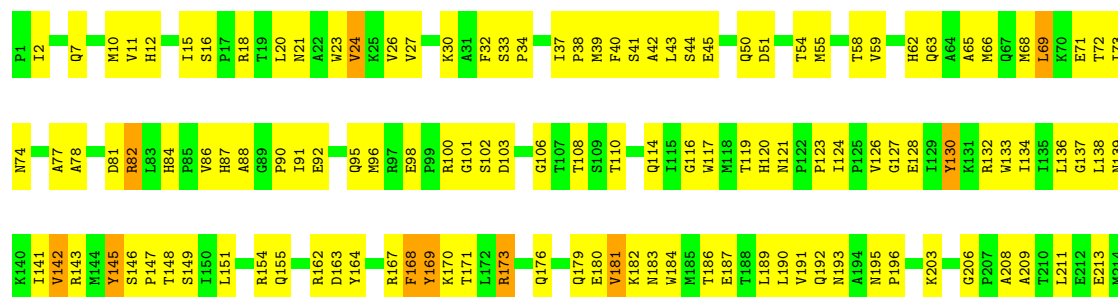
• Molecule 1: capsid protein

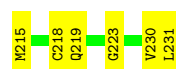
Chain 7L: 45% 51%



• Molecule 1: capsid protein

Chain 7M: 43% 52%





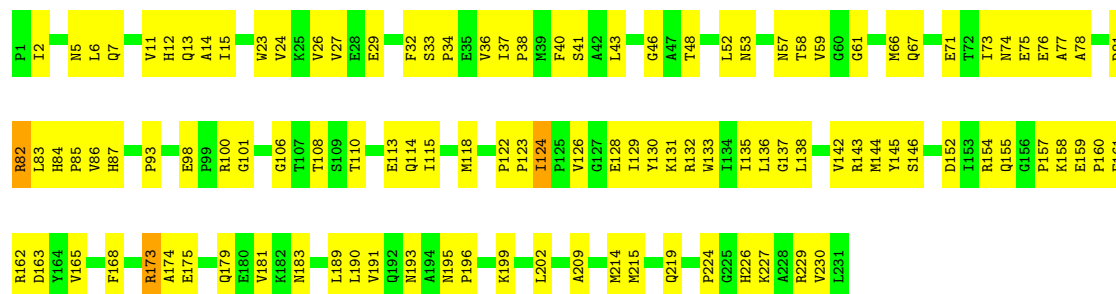
- Molecule 1: capsid protein

Chain 7N: 46% 52%



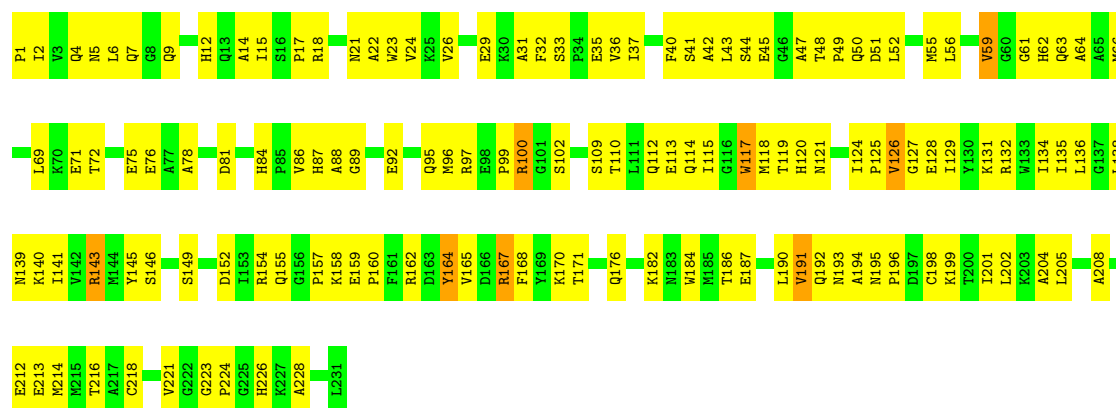
- Molecule 1: capsid protein

Chain 7O: 52% 47%



- Molecule 1: capsid protein

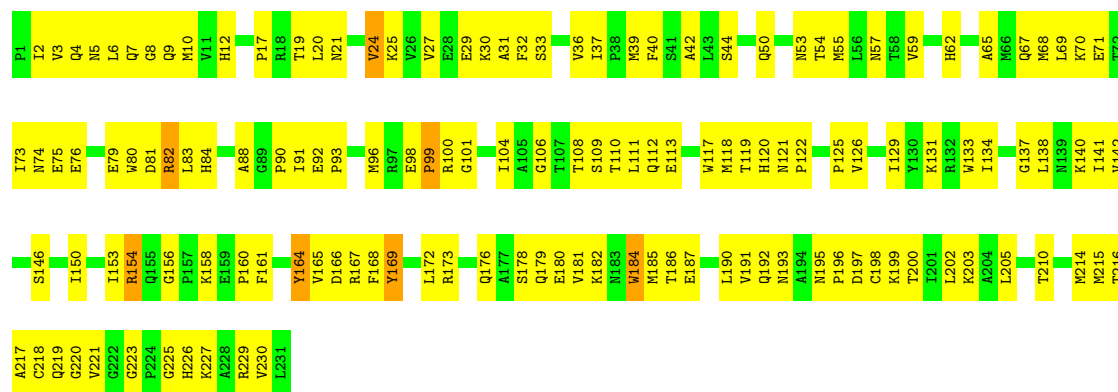
Chain 7P: 41% 55%



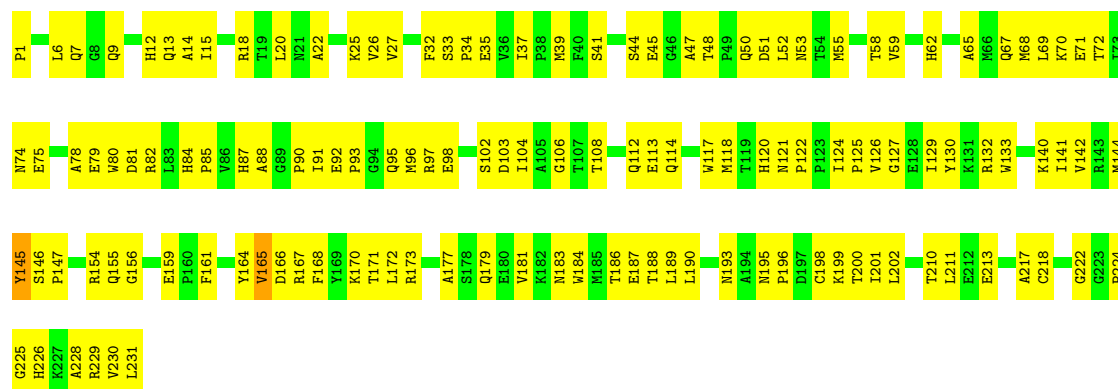
- Molecule 1: capsid protein

Chain 7Q: 39% 58%

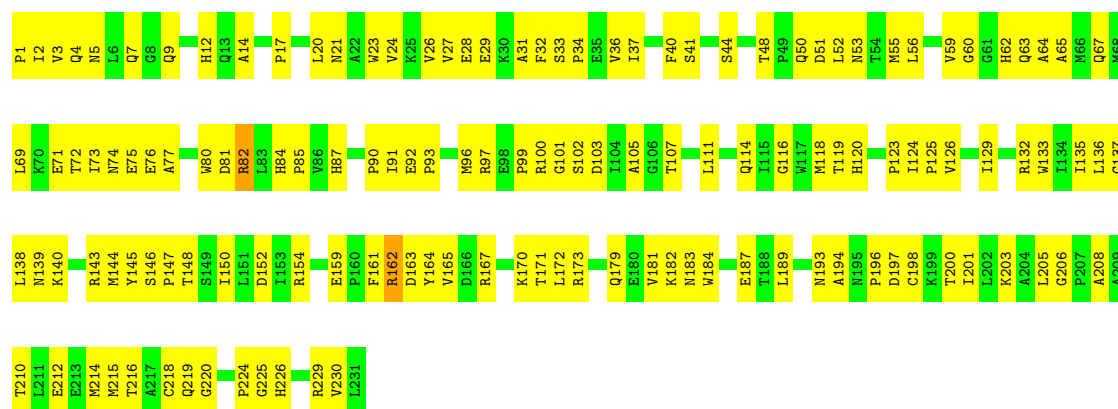




- Molecule 1: capsid protein

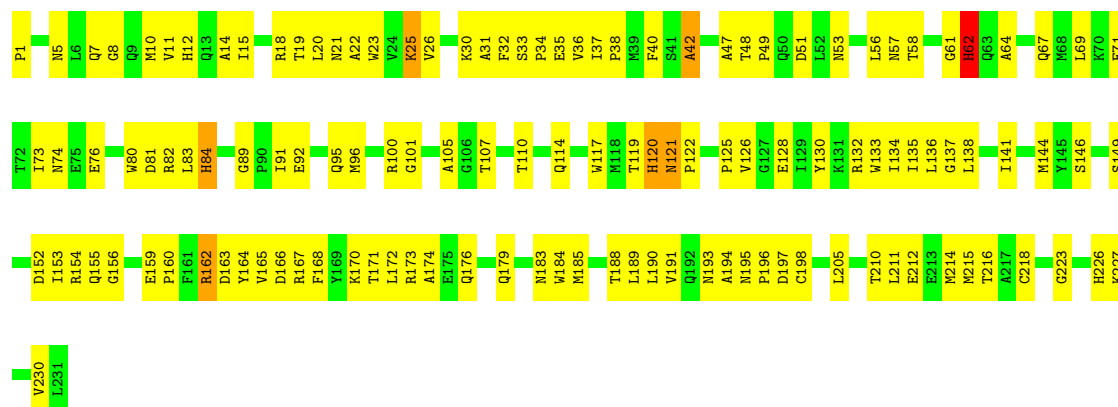


- Molecule 1: capsid protein



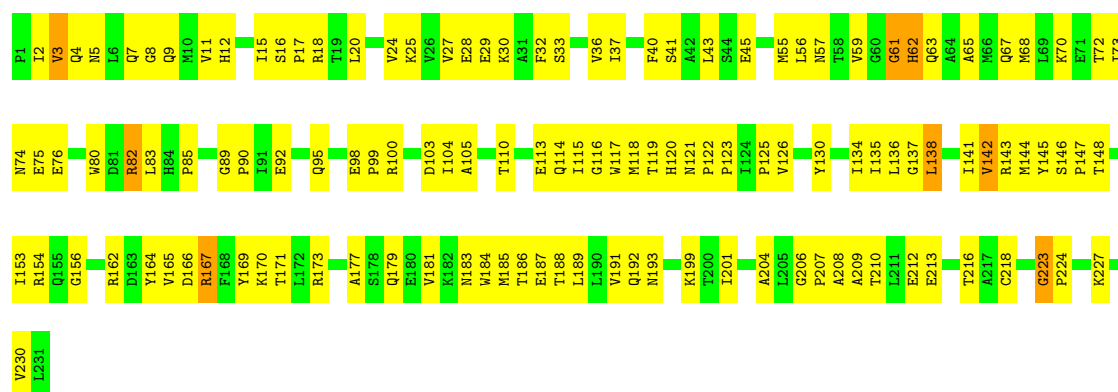
- Molecule 1: capsid protein





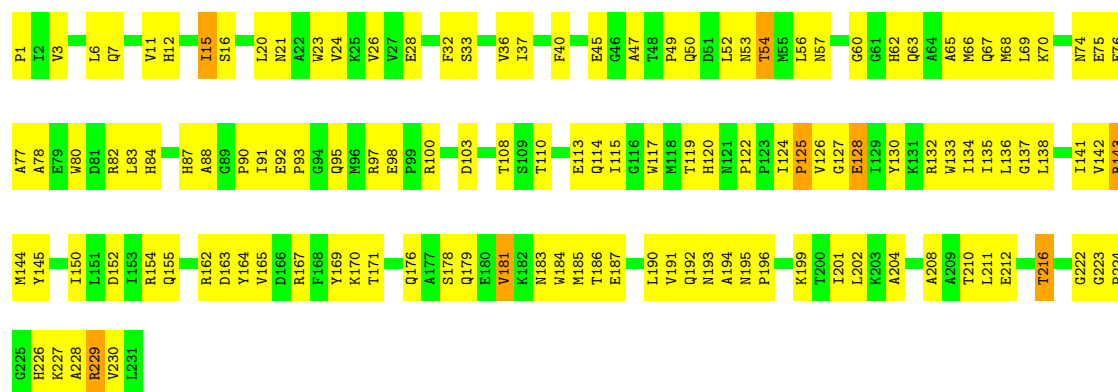
• Molecule 1: capsid protein

Chain 7U: 45% 52%



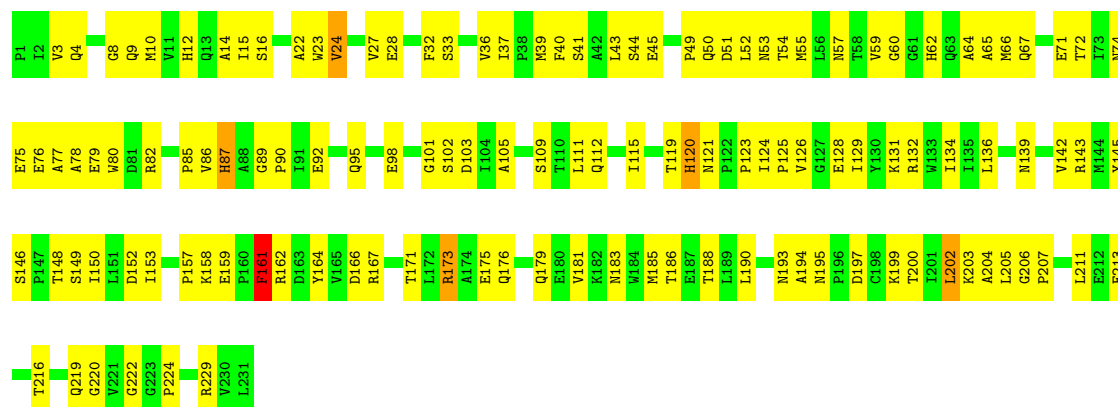
• Molecule 1: capsid protein

Chain 7V: 44% 52%



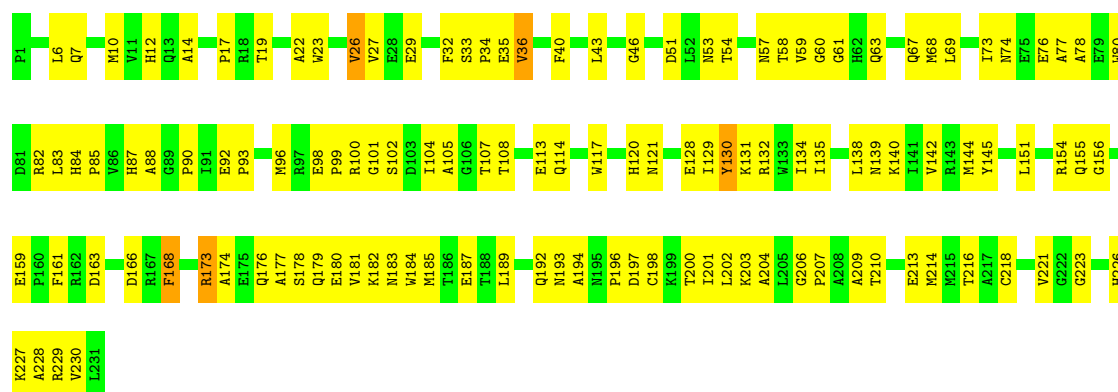
• Molecule 1: capsid protein

Chain 7W: 45% 52%



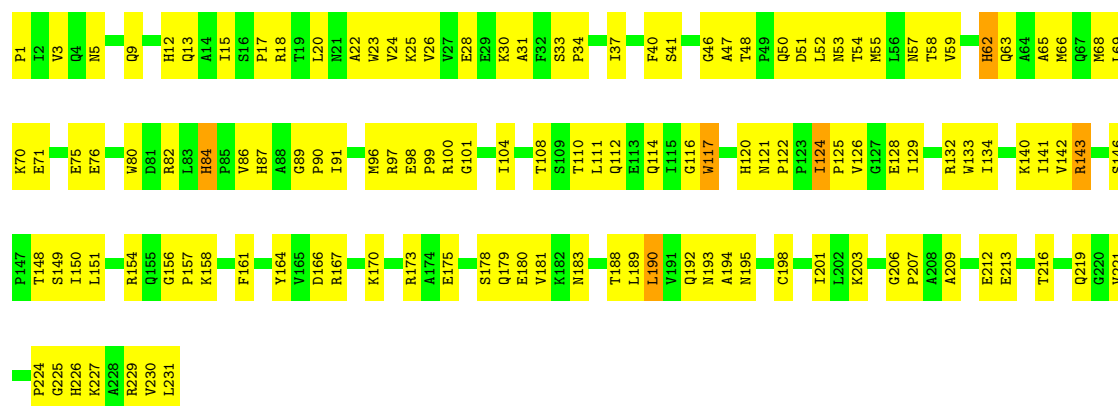
- Molecule 1: capsid protein

Chain 7X: 46% 52%



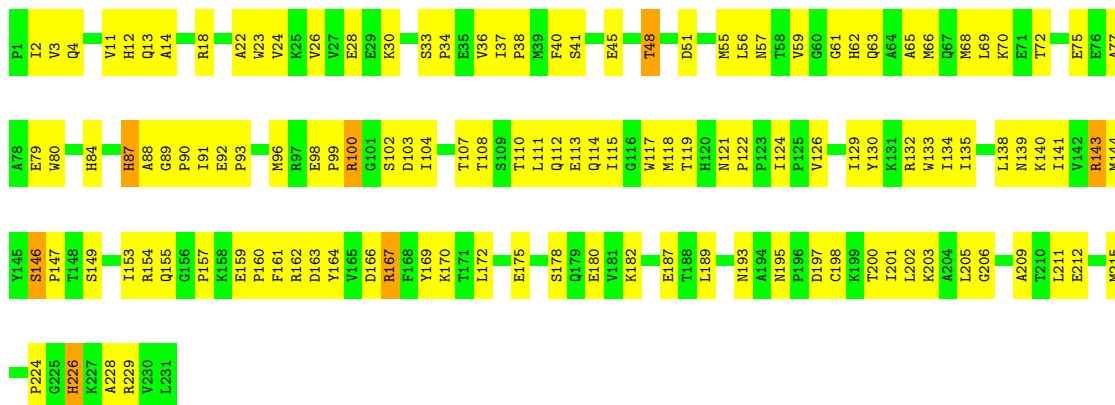
- Molecule 1: capsid protein

Chain 7Y: 45% 53%



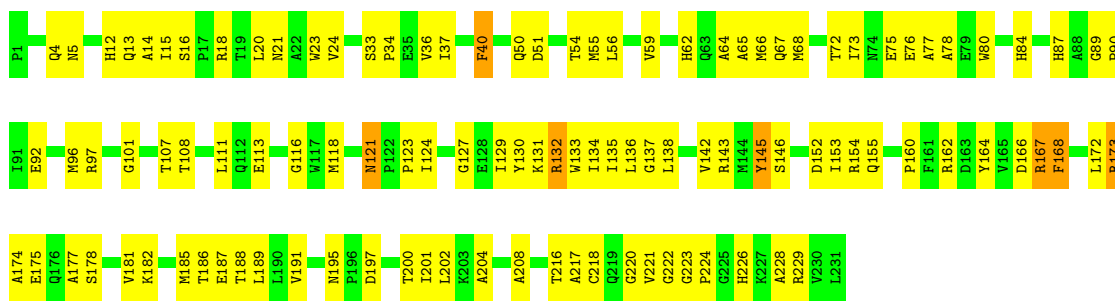
- Molecule 1: capsid protein

Chain 7Z: 46% 51%



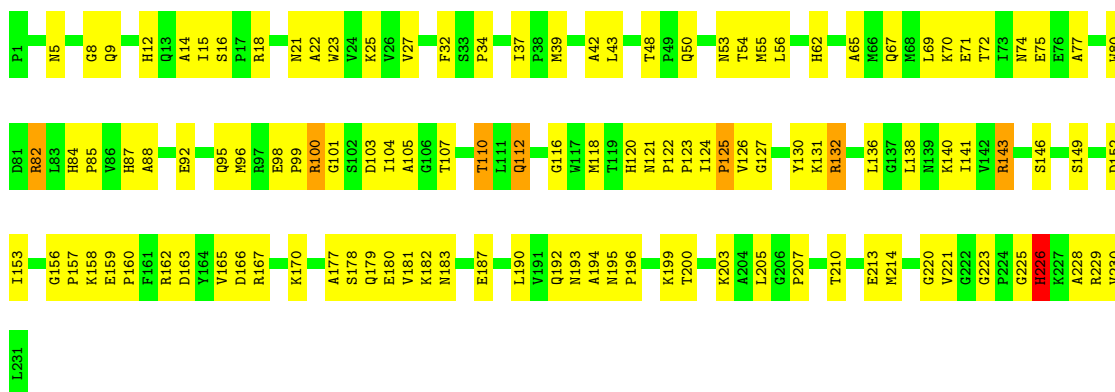
• Molecule 1: capsid protein

Chain 80: 52% 45%



• Molecule 1: capsid protein

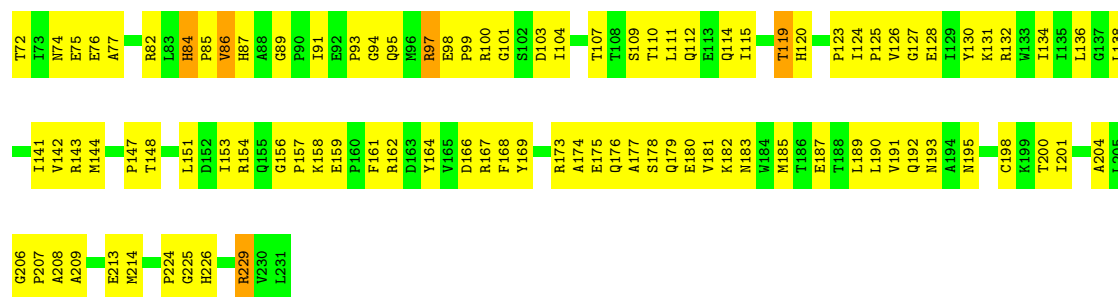
Chain 81: 49% 47%



• Molecule 1: capsid protein

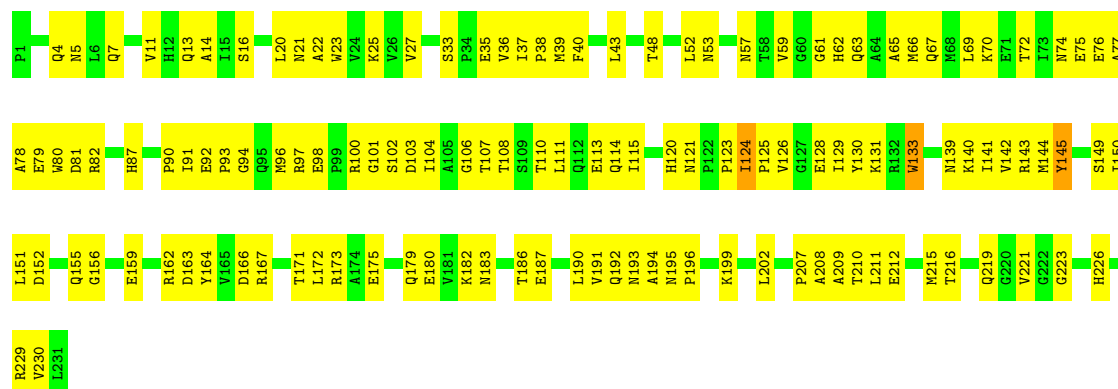
Chain 82: 40% 57%





• Molecule 1: capsid protein

Chain 83: 44% 55%



• Molecule 1: capsid protein

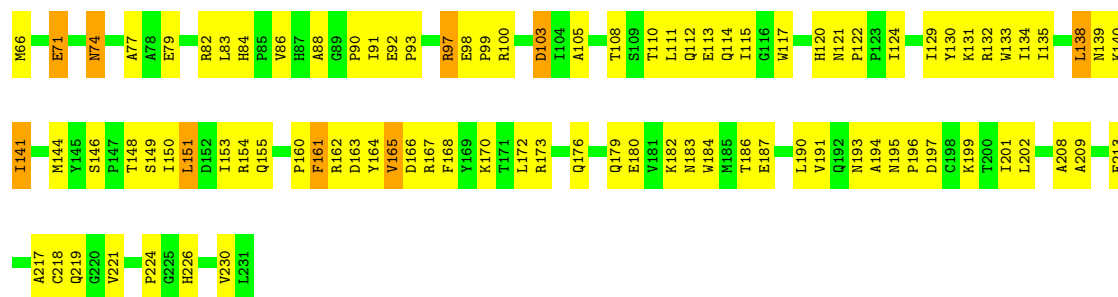
Chain 84: 44% 52%



• Molecule 1: capsid protein

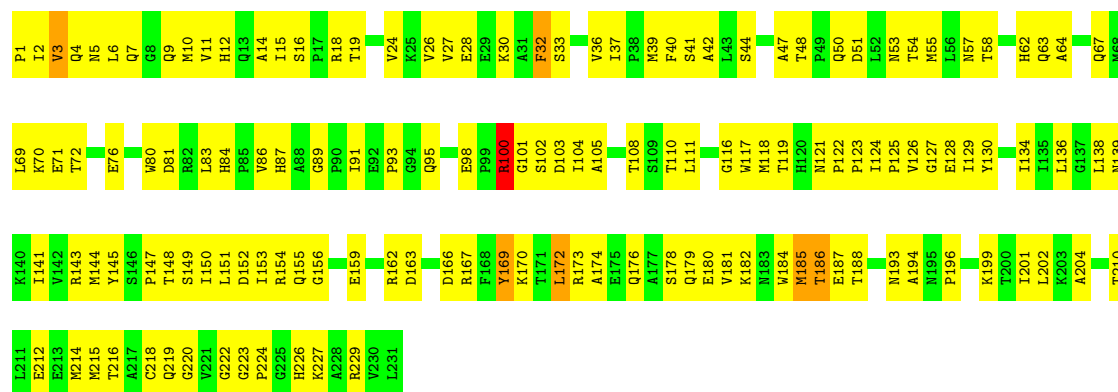
Chain 85: 42% 54%





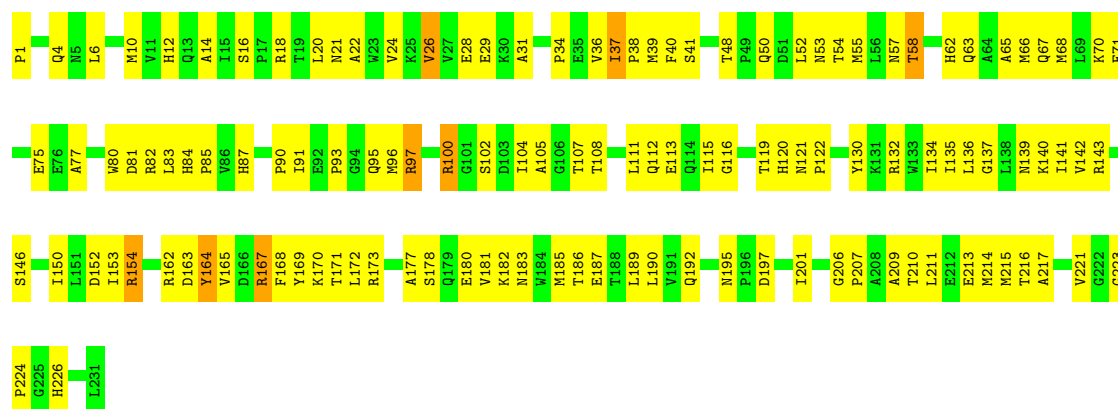
• Molecule 1: capsid protein

Chain 86: 39% 58%



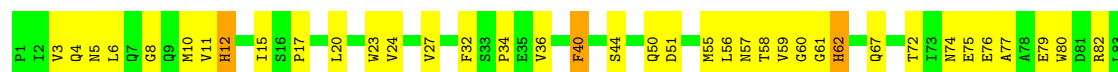
• Molecule 1: capsid protein

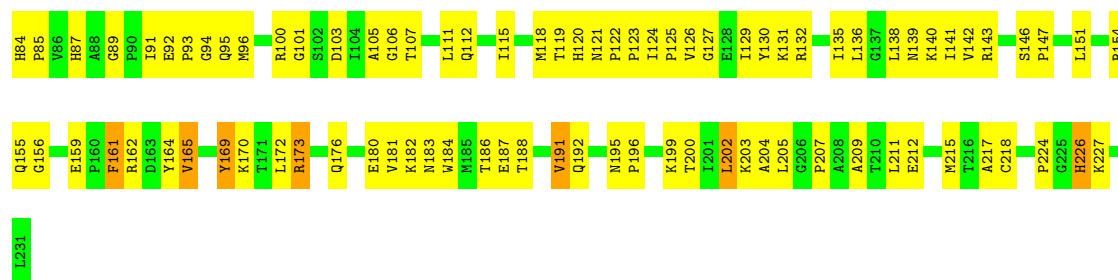
Chain 87: 46% 51%



• Molecule 1: capsid protein

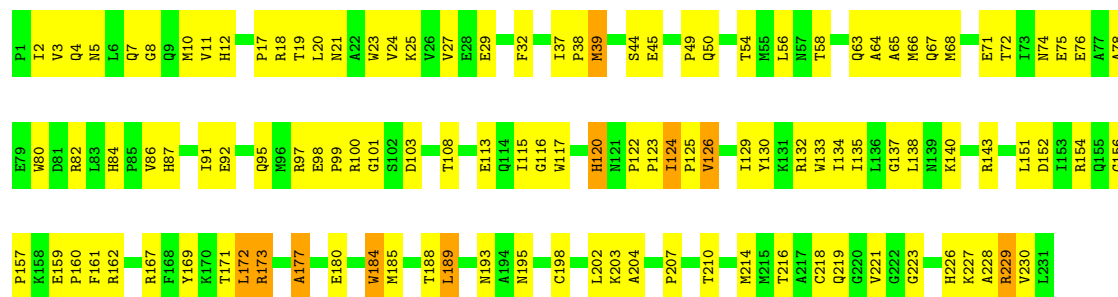
Chain 88: 47% 49%





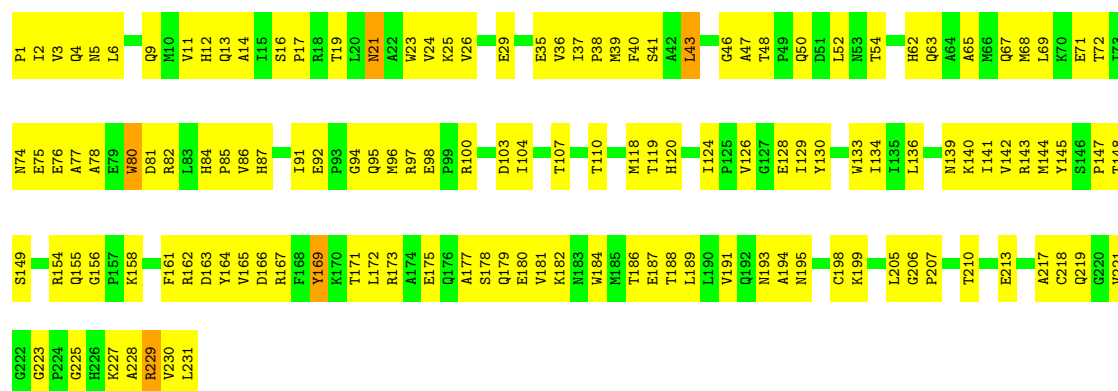
- Molecule 1: capsid protein

Chain 89: 50% 46%



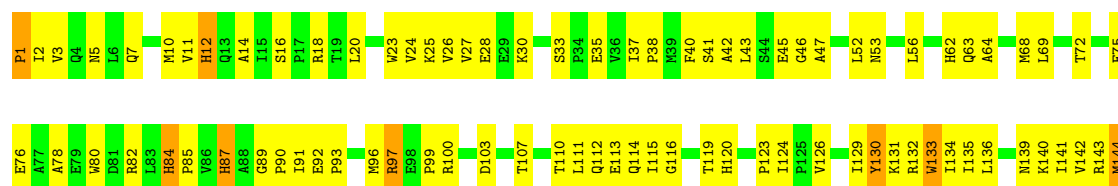
- Molecule 1: capsid protein

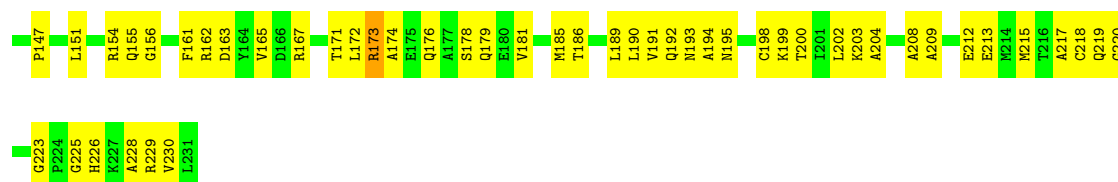
Chain 8a: 41% 57%



- Molecule 1: capsid protein

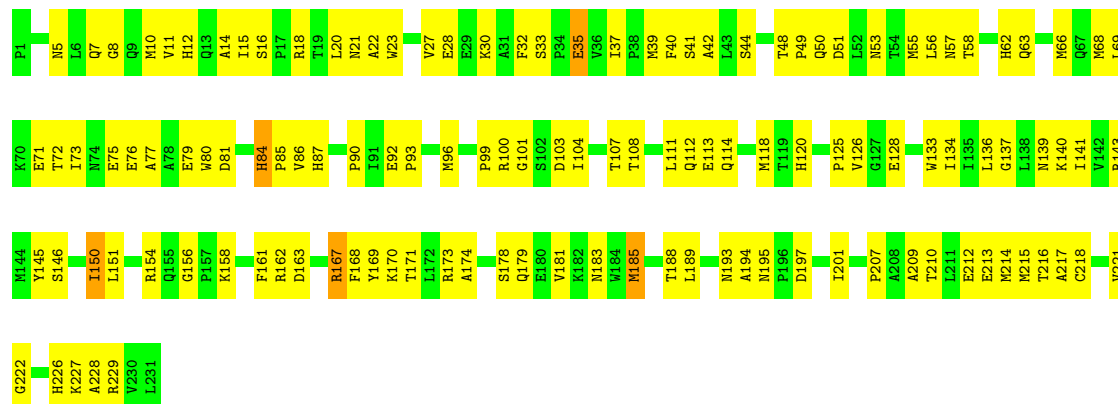
Chain 8b: 43% 53%





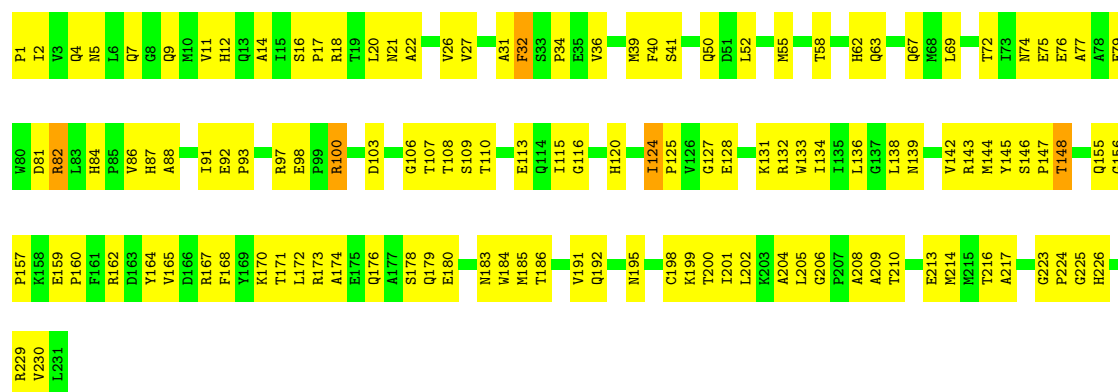
- Molecule 1: capsid protein

Chain 8c: 45% 52%



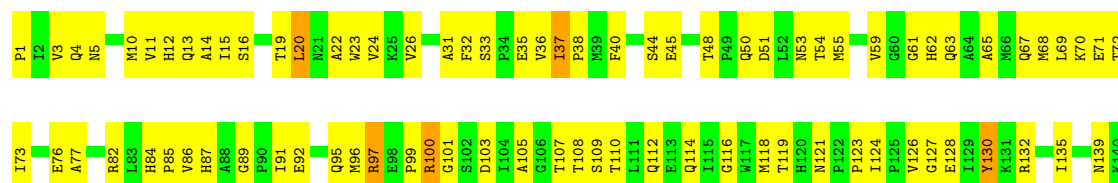
- Molecule 1: capsid protein

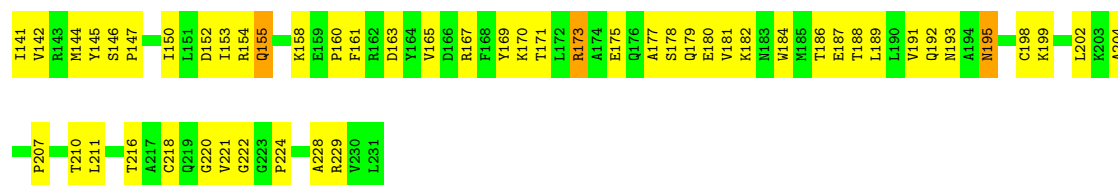
Chain 8d: 46% 52%



- Molecule 1: capsid protein

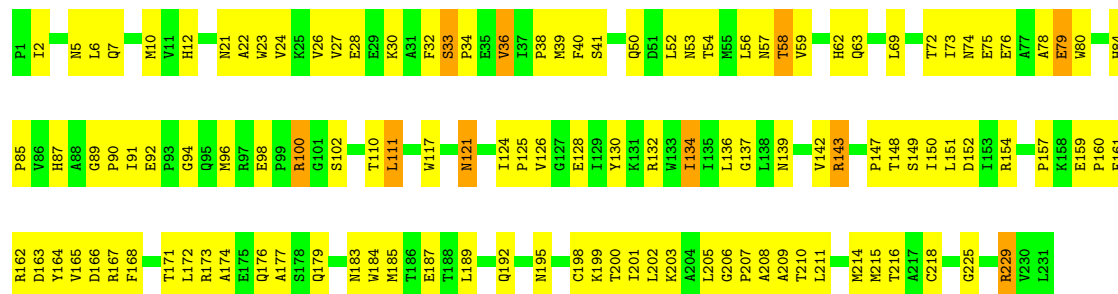
Chain 8e: 42% 55%





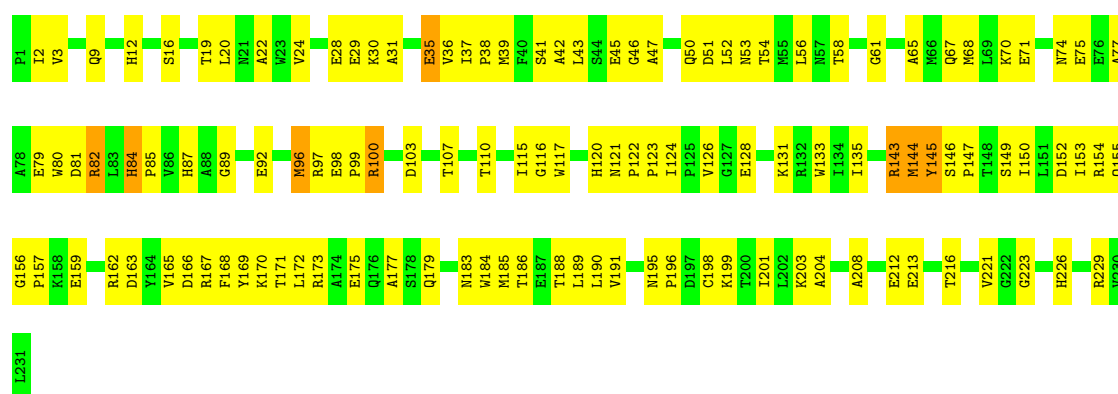
- Molecule 1: capsid protein

Chain 8f: 48% 48%



- Molecule 1: capsid protein

Chain 8g: 48% 49%



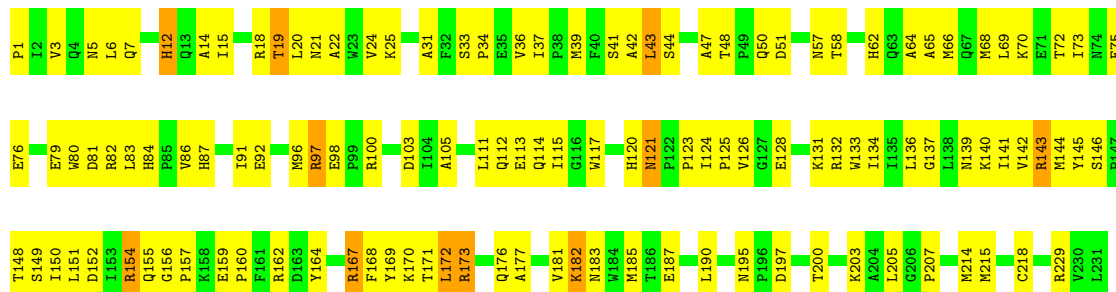
- Molecule 1: capsid protein

Chain 8h: 47% 49%

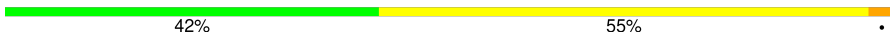
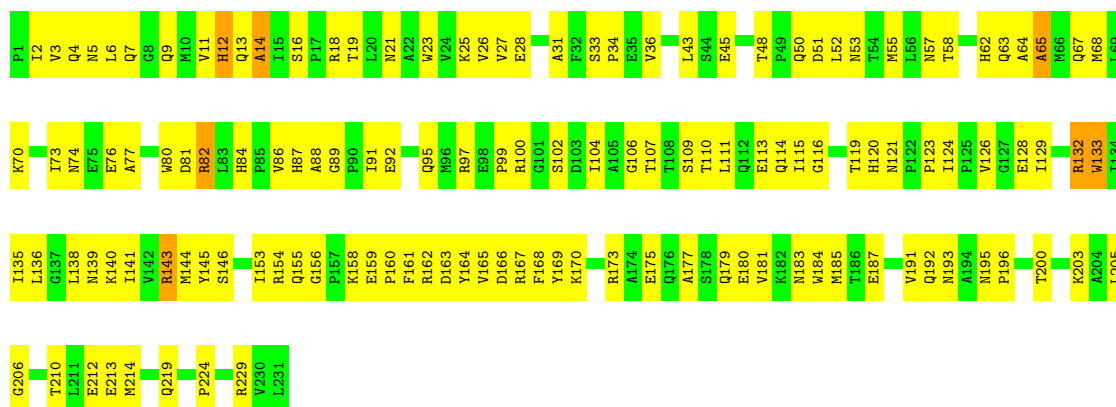


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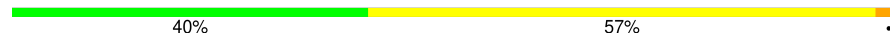
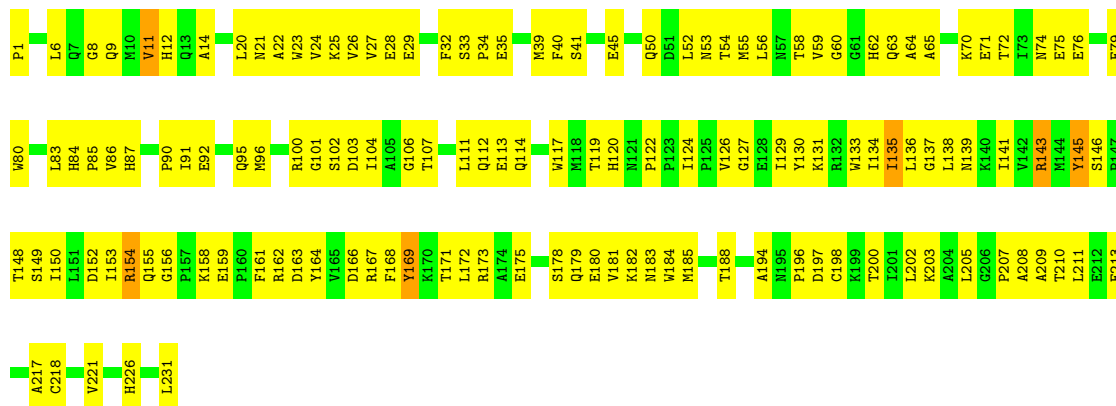
- Molecule 1: capsid protein

Chain 8i:  47% 48% 5%

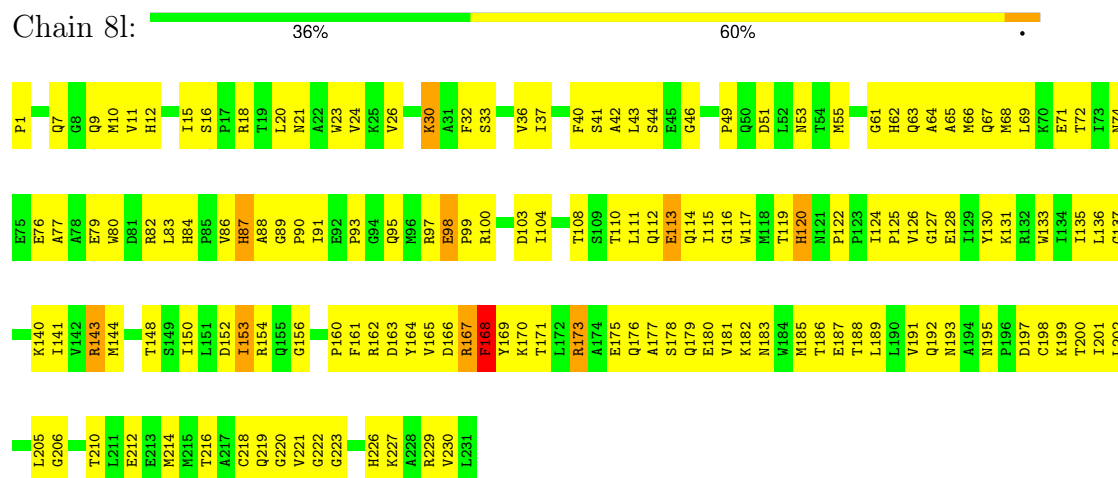
- Molecule 1: capsid protein

Chain 8j:  42% 55% 3%

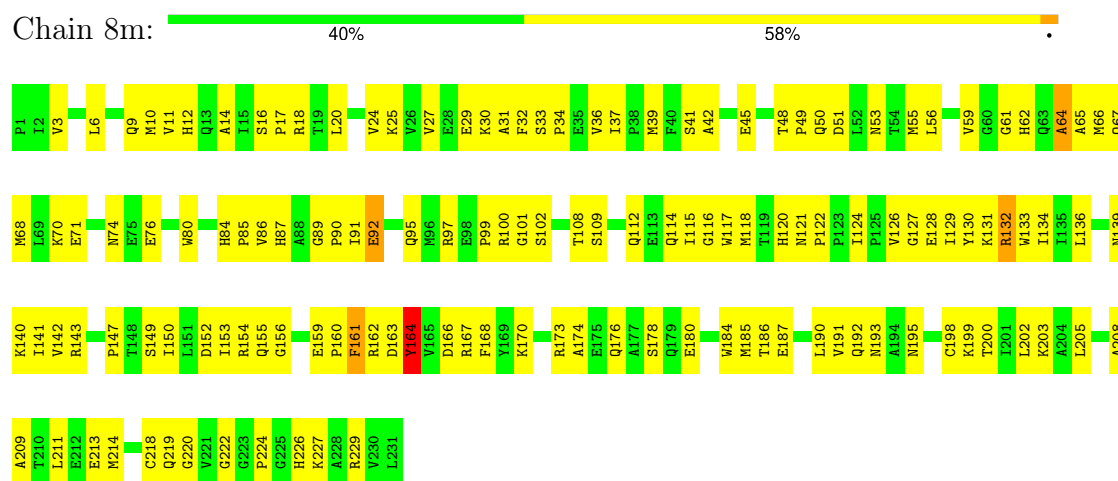
- Molecule 1: capsid protein

Chain 8k:  40% 57% 3%

- Molecule 1: capsid protein



- Molecule 1: capsid protein

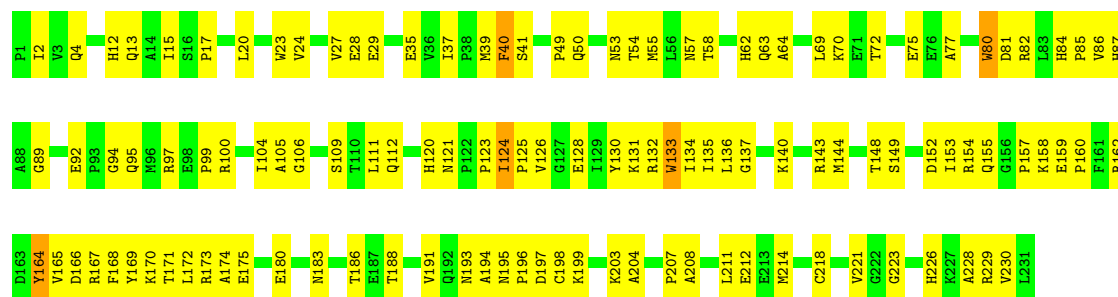


- Molecule 1: capsid protein



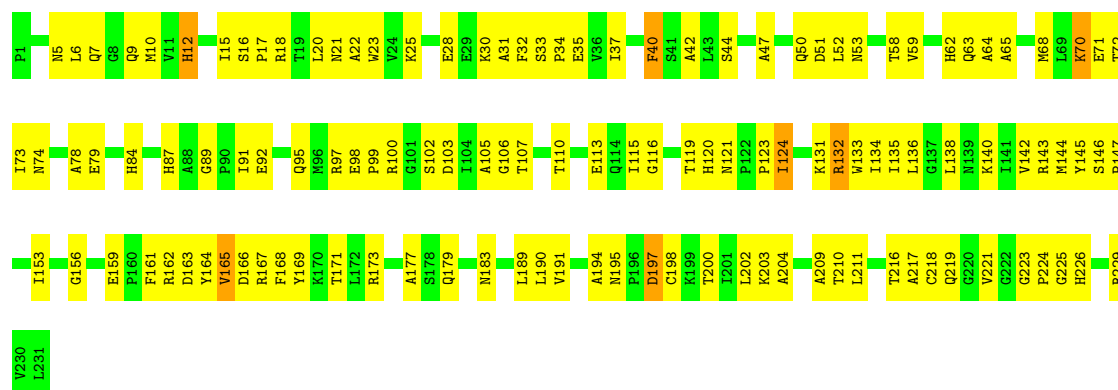
- Molecule 1: capsid protein





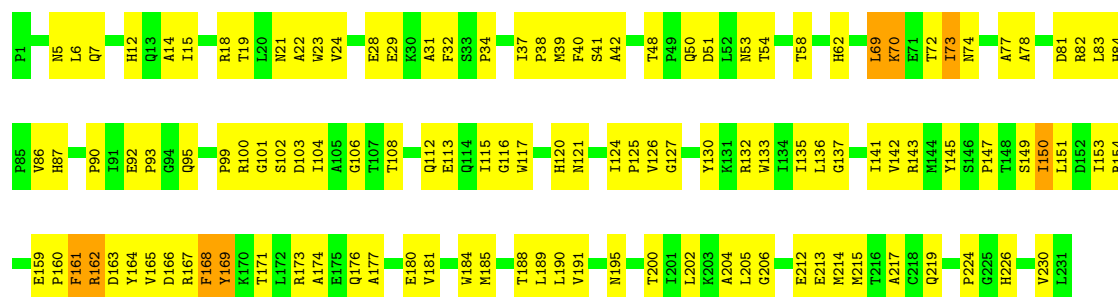
- Molecule 1: capsid protein

Chain 8p:



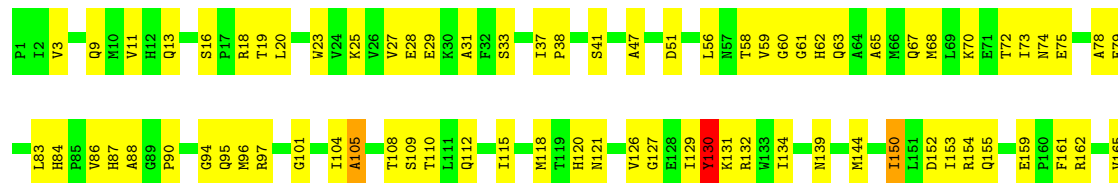
- Molecule 1: capsid protein

Chain 8q:



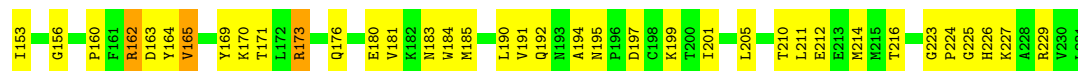
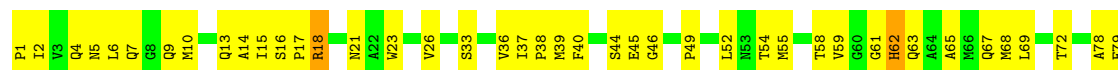
- Molecule 1: capsid protein

Chain 8r:

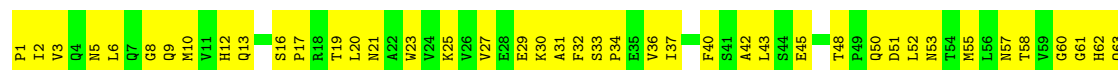
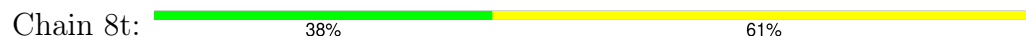




• Molecule 1: capsid protein



• Molecule 1: capsid protein



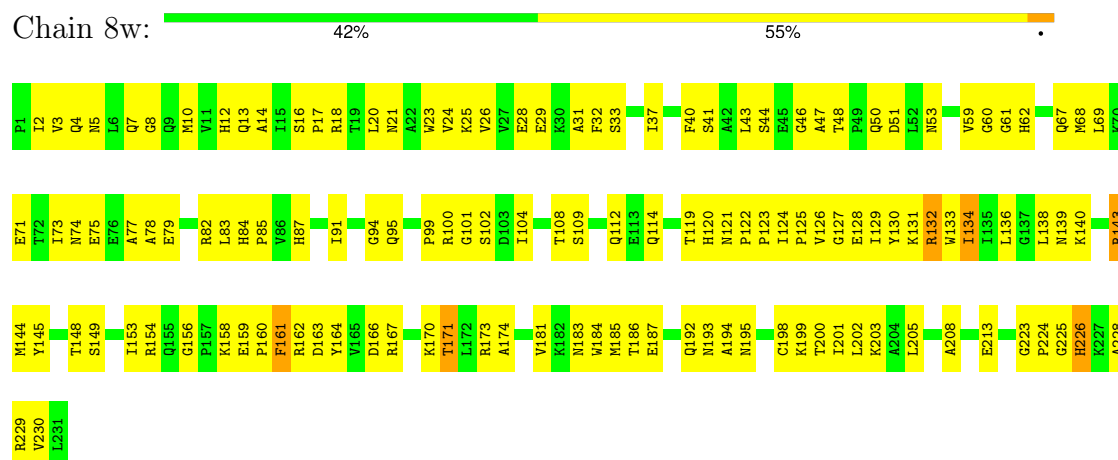
• Molecule 1: capsid protein



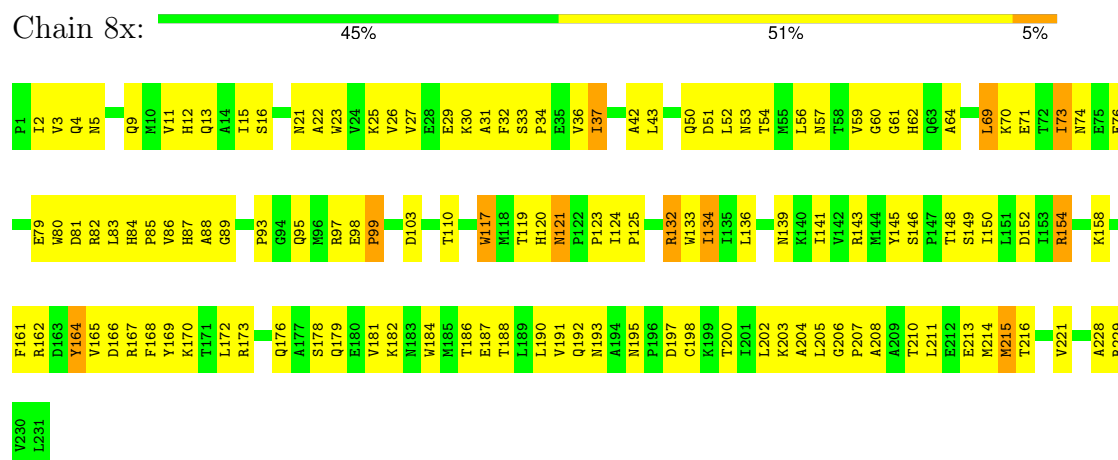
• Molecule 1: capsid protein



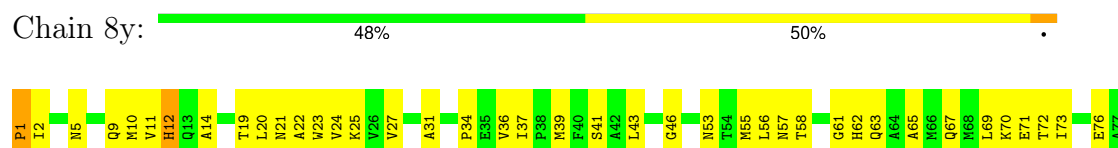
• Molecule 1: capsid protein

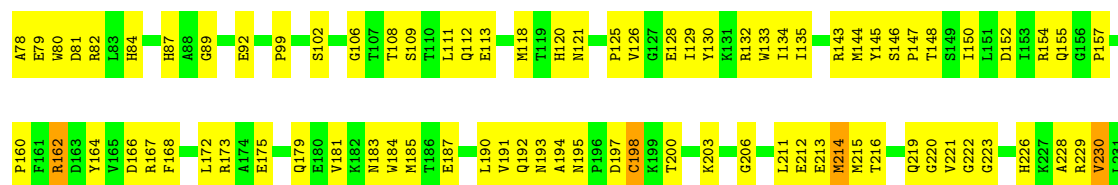


• Molecule 1: capsid protein



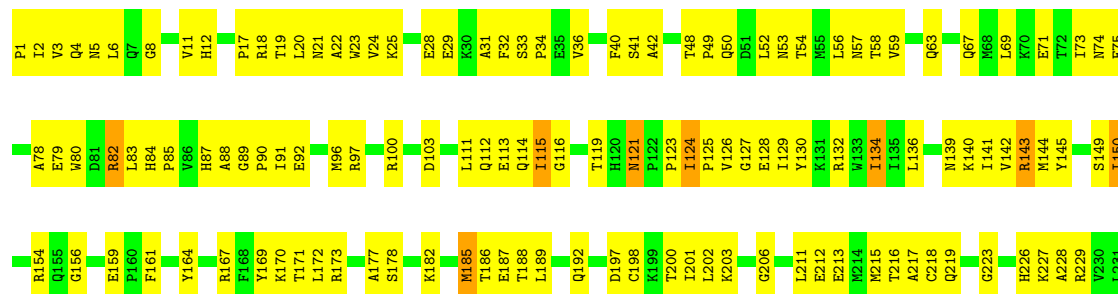
• Molecule 1: capsid protein





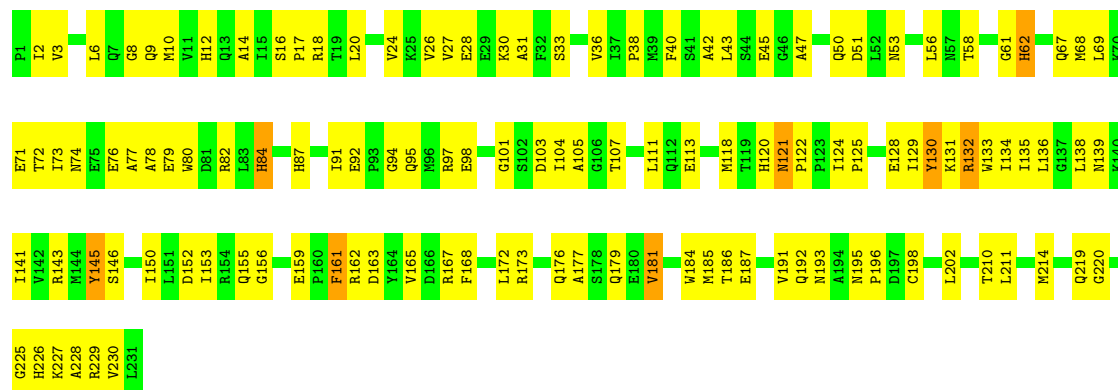
- Molecule 1: capsid protein

Chain 8z:



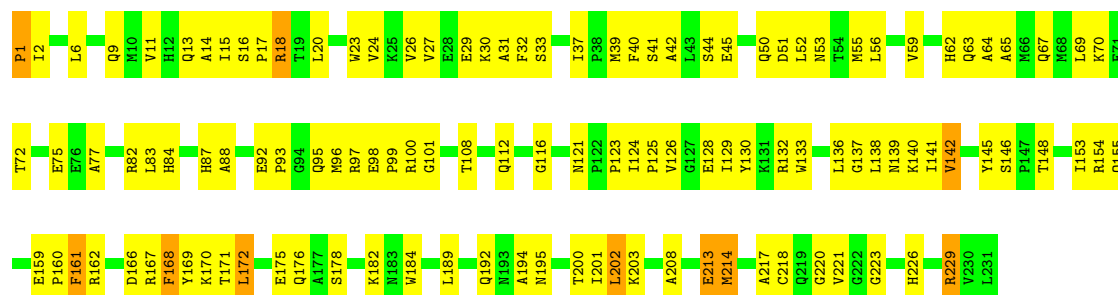
- Molecule 1: capsid protein

Chain 8A:



- Molecule 1: capsid protein

Chain 8B:



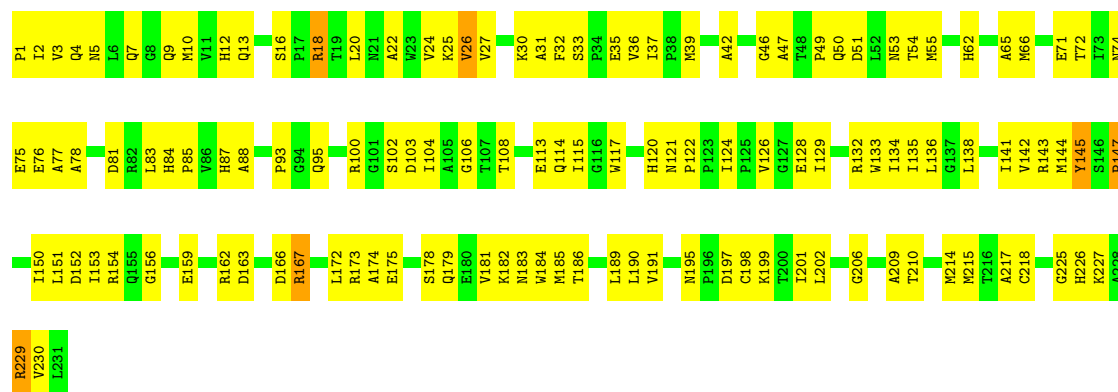
- Molecule 1: capsid protein

[illegible]

V221	G222	G223	F224	G225	H226	K227	A228	R229	V230	L231	L138	K70	P1
G222	G223	F224	G225	H226	K227	A228	R229	V230	L231	L138	K70	P1	I2
G223	F224	G225	H226	K227	A228	R229	V230	L231	L138	K70	P1	V3	Q4
G225	H226	K227	A228	R229	V230	L231	L138	K70	P1	V3	Q4	V75	G8
H226	K227	A228	R229	V230	L231	L138	K70	P1	V3	Q4	V75	G8	Q9
K227	A228	R229	V230	L231	L138	K70	P1	V3	Q4	V75	G8	Q9	M10
A228	R229	V230	L231	L138	K70	P1	V3	Q4	V75	G8	Q9	M10	V11
R229	V230	L231	L138	K70	P1	V3	Q4	V75	G8	Q9	M10	V11	H12
V230	L231	L138	K70	P1	V3	Q4	V75	G8	Q9	M10	V11	H12	I15
L231	L138	K70	P1	V3	Q4	V75	G8	Q9	M10	V11	H12	I15	S16
L138	K70	P1	V3	Q4	V75	G8	Q9	M10	V11	H12	I15	S16	P17
K70	P1	V3	Q4	V75	G8	Q9	M10	V11	H12	I15	S16	P17	R18
P1	V3	Q4	V75	G8	Q9	M10	V11	H12	I15	S16	P17	R18	T19
V3	Q4	V75	G8	Q9	M10	V11	H12	I15	S16	P17	R18	T19	L20
Q4	V75	G8	Q9	M10	V11	H12	I15	S16	P17	R18	T19	L20	N21
V75	G8	Q9	M10	V11	H12	I15	S16	P17	R18	T19	L20	N21	A22
G8	Q9	M10	V11	H12	I15	S16	P17	R18	T19	L20	N21	A22	W23
Q9	M10	V11	H12	I15	S16	P17	R18	T19	L20	N21	A22	W23	V24
M10	V11	H12	I15	S16	P17	R18	T19	L20	N21	A22	W23	V24	K25
V11	H12	I15	S16	P17	R18	T19	L20	N21	A22	W23	V24	K25	V26
H12	I15	S16	P17	R18	T19	L20	N21	A22	W23	V24	K25	V26	V27
I15	S16	P17	R18	T19	L20	N21	A22	W23	V24	K25	V26	V27	E28
S16	P17	R18	T19	L20	N21	A22	W23	V24	K25	V26	V27	E28	F32
P17	R18	T19	L20	N21	A22	W23	V24	K25	V26	V27	E28	F32	S33
R18	T19	L20	N21	A22	W23	V24	K25	V26	V27	E28	F32	S33	P34
T19	L20	N21	A22	W23	V24	K25	V26	V27	E28	F32	S33	P34	V36
L20	N21	A22	W23	V24	K25	V26	V27	E28	F32	S33	P34	V36	I37
N21	A22	W23	V24	K25	V26	V27	E28	F32	S33	P34	V36	I37	P38
A22	W23	V24	K25	V26	V27	E28	F32	S33	P34	V36	I37	P38	M39
W23	V24	K25	V26	V27	E28	F32	S33	P34	V36	I37	P38	M39	F40
V24	K25	V26	V27	E28	F32	S33	P34	V36	I37	P38	M39	F40	S41
K25	V26	V27	E28	F32	S33	P34	V36	I37	P38	M39	F40	S41	A42
V26	V27	E28	F32	S33	P34	V36	I37	P38	M39	F40	S41	A42	L43
V27	E28	F32	S33	P34	V36	I37	P38	M39	F40	S41	A42	L43	S44
E28	F32	S33	P34	V36	I37	P38	M39	F40	S41	A42	L43	S44	Q50
F32	S33	P34	V36	I37	P38	M39	F40	S41	A42	L43	S44	Q50	D51
S33	P34	V36	I37	P38	M39	F40	S41	A42	L43	S44	Q50	D51	T54
P34	V36	I37	P38	M39	F40	S41	A42	L43	S44	Q50	D51	T54	M55
V36	I37	P38	M39	F40	S41	A42	L43	S44	Q50	D51	T54	M55	L56
I37	P38	M39	F40	S41	A42	L43	S44	Q50	D				

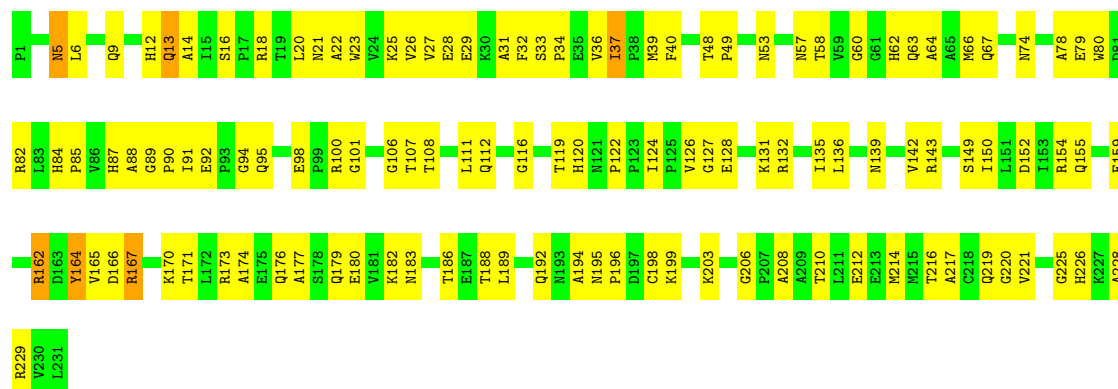
V230	G166	R82	P1
	L231	L83	I3
	E159	H84	V2
		P85	Q5
		V86	N4
	R162	H87	
	D163	A88	Q9
	V165	G89	M10
	D166	P90	V11
	R167	I91	H12
	F168	E92	Q13
	V169		A14
	K170	R97	I15
	T171	R100	P17
	L172		S16
	R173		R18
	A174		
	E176	D103	V23
	Q176	I104	V24
		A105	V24
		G106	K25
	Q179	T107	V26
	E180	T108	V27
	V181	Q112	E28
	K182		E29
	M183		K30
	V184	G116	
	M185	V117	M39
	T186	M118	F40
	E187	T119	S41
	T188	H120	A42
	L189		
	L190	T124	E45
	V191	P125	G46
	Q192	V126	A47
	M193		
	A194	I129	Q50
		V130	
	D197	K131	T54
	C198	R132	M55
	K199	V133	L56
	T200	I134	N57
	I201	I135	
		L136	G61
	A204	G137	H62
	A209	L138	Q63
	T210	N139	A64
	L211		A65
	E212	V142	M66
	E213	R143	Q67
	M214	M144	M68
		V145	
	Q219	T148	T72
	G220	S149	I73
	V221	I150	N74
	G222	L151	E75
	G223	D152	
		I153	A78
	A228	V154	E79
	P230	G155	M80

Chain 8F: 45% 52%



• Molecule 1: capsid protein

Chain 8G: 48% 49%



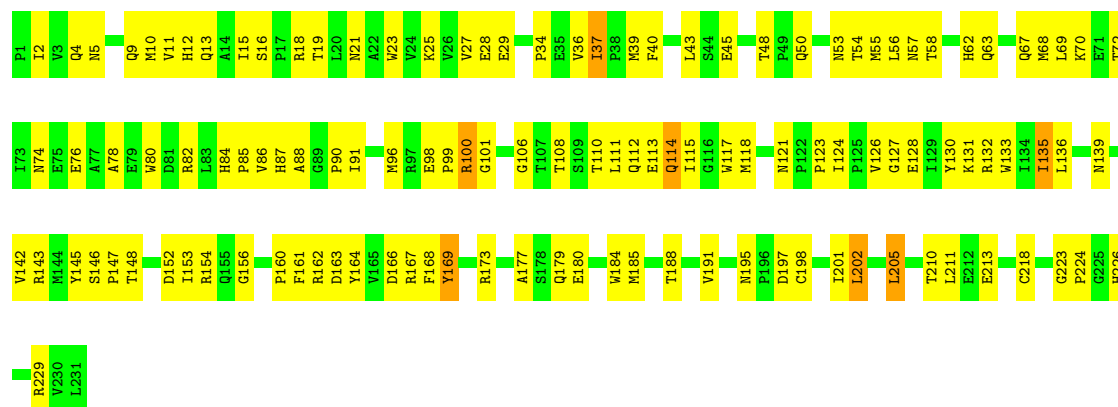
• Molecule 1: capsid protein

Chain 8H: 42% 56%



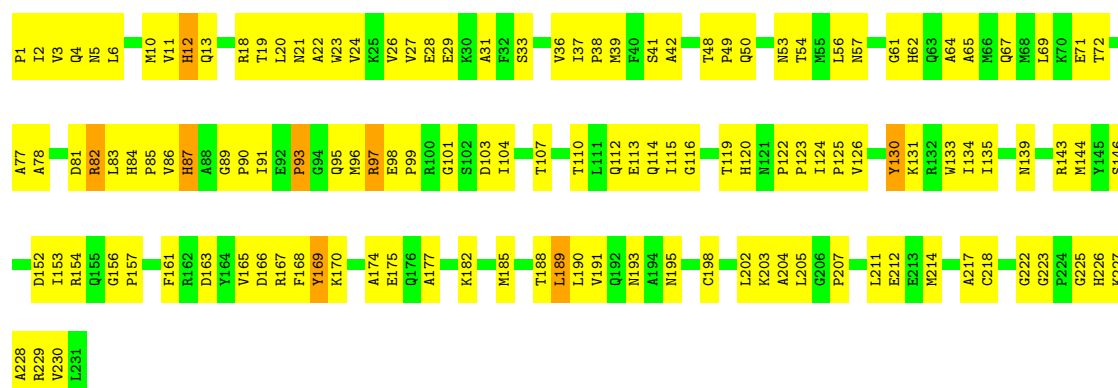
• Molecule 1: capsid protein

Chain 8I: 48% 49%



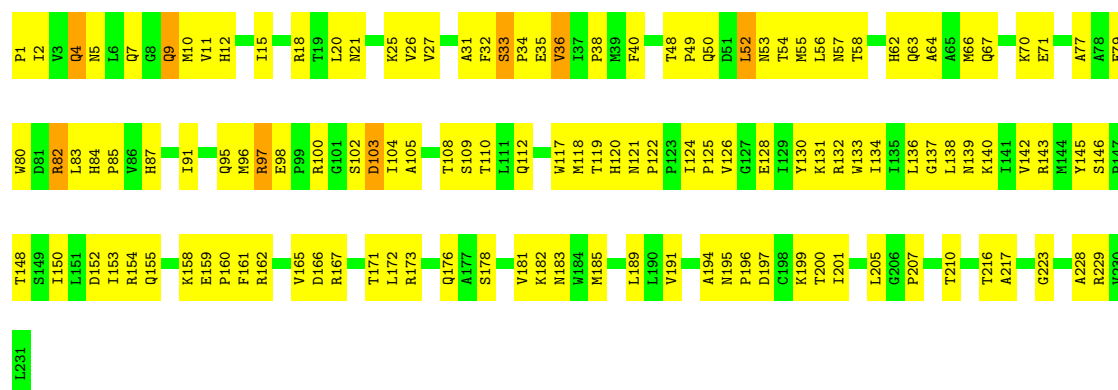
- Molecule 1: capsid protein

Chain 8J: 43% 53%



- Molecule 1: capsid protein

Chain 8K: 45% 52%



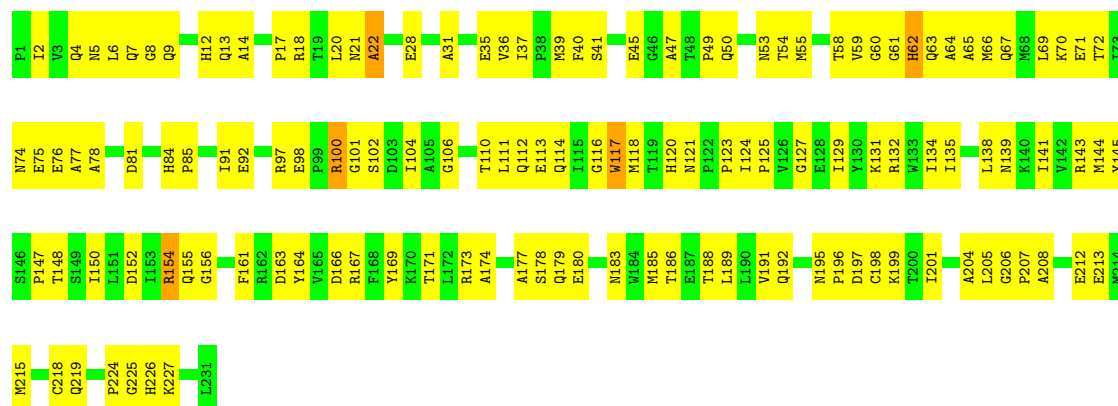
- Molecule 1: capsid protein

Chain 8L: 45% 52%



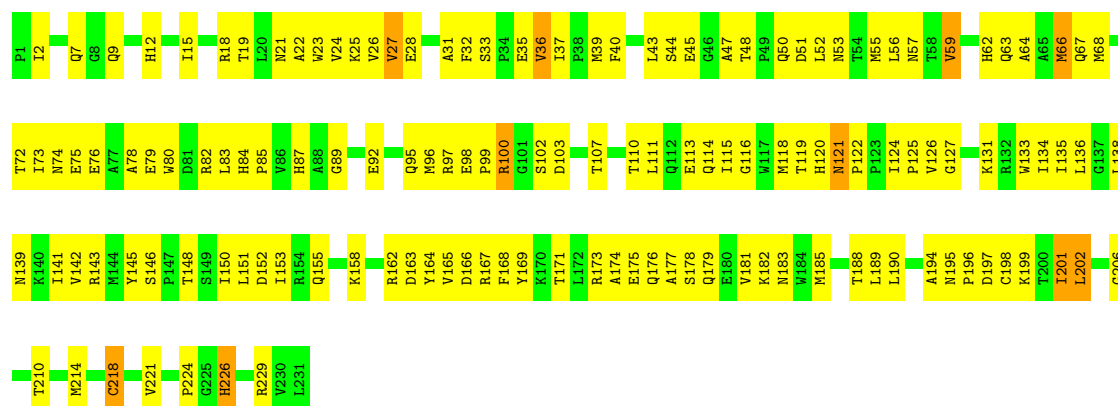
- Molecule 1: capsid protein

Chain 8M: 42% 55%



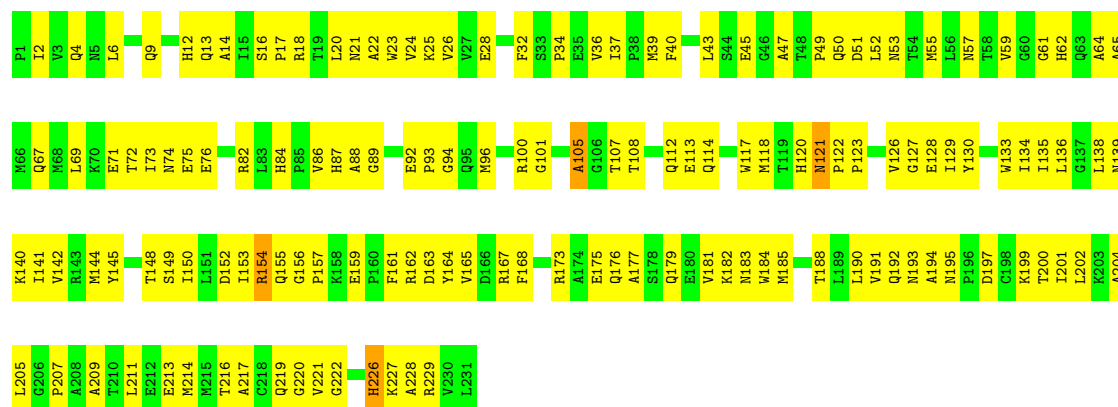
- Molecule 1: capsid protein

Chain 8N: 40% 56%



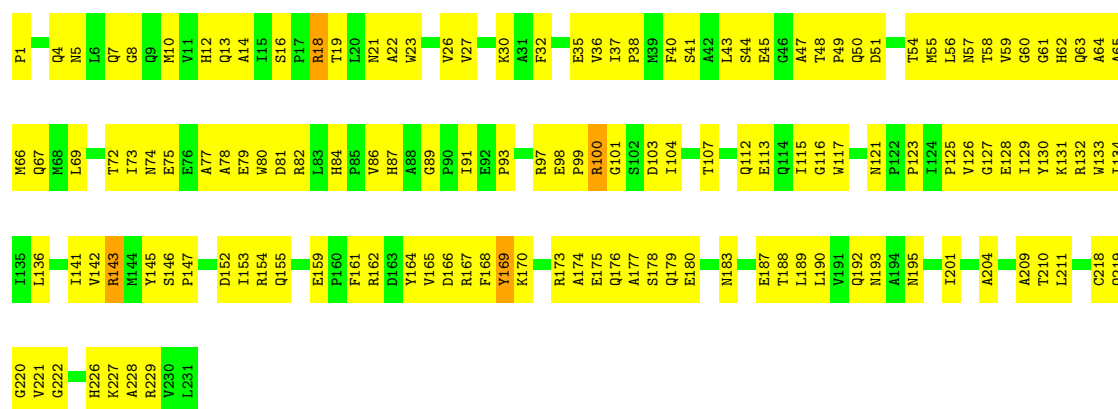
- Molecule 1: capsid protein

Chain 8O: 38% 60%



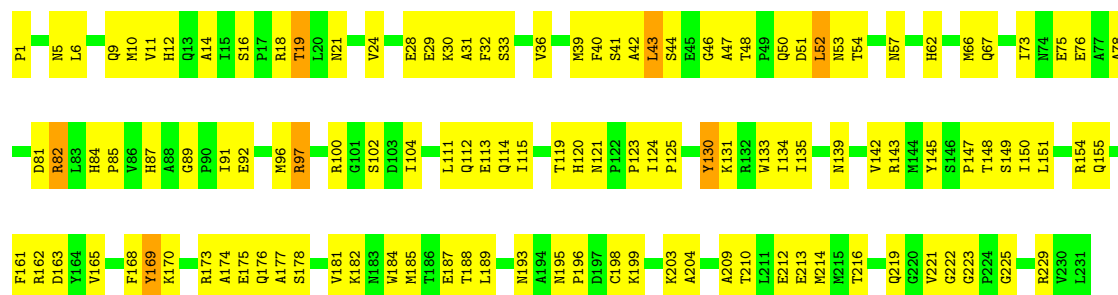
- Molecule 1: capsid protein

Chain 8P: 39% 59%



- Molecule 1: capsid protein

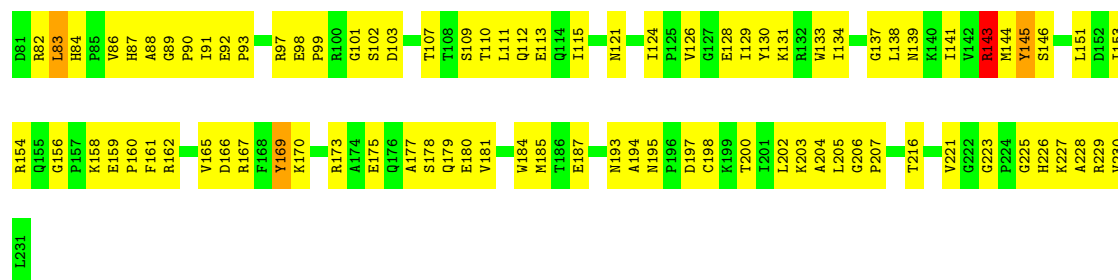
Chain 8Q: 48% 49%



- Molecule 1: capsid protein

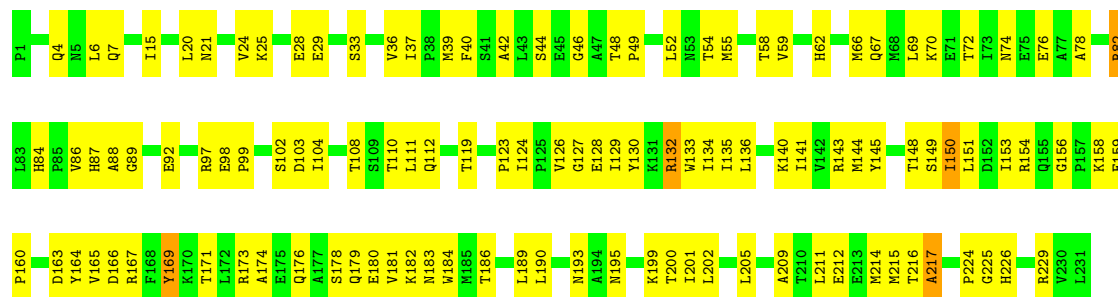
Chain 8R: 45% 52%





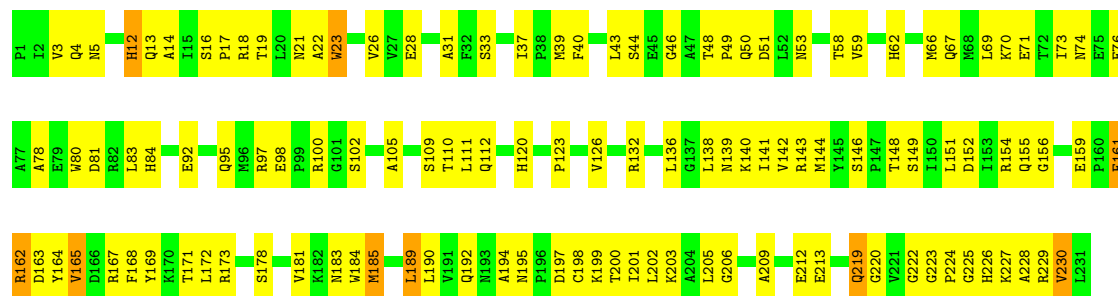
- Molecule 1: capsid protein

Chain 8S: 49% 48%



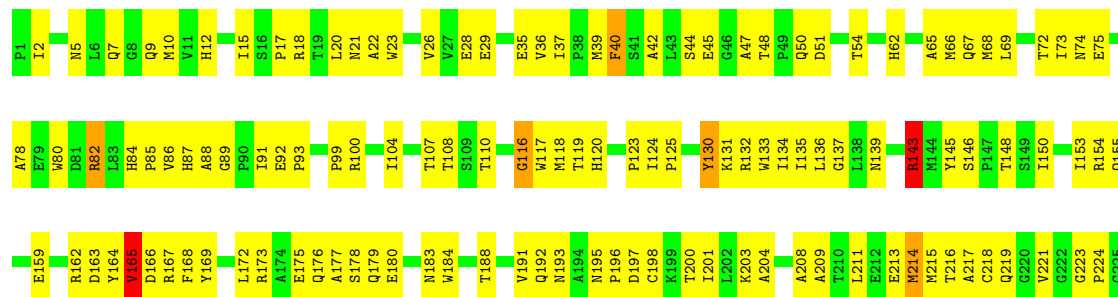
- Molecule 1: capsid protein

Chain 8T: 48% 48%



- Molecule 1: capsid protein

Chain 8U: 44% 53%



H226
V230
L231

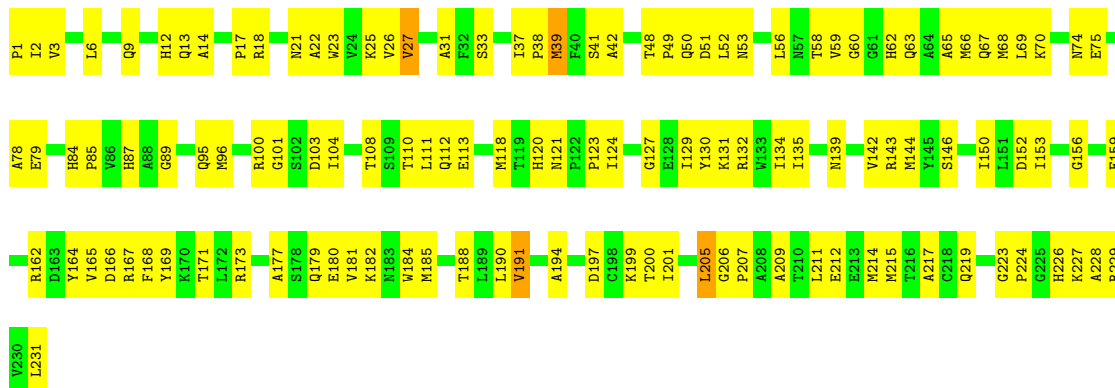
- Molecule 1: capsid protein

Chain 8V:  45% 52%

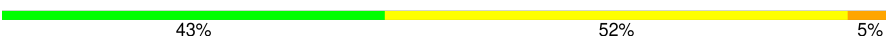


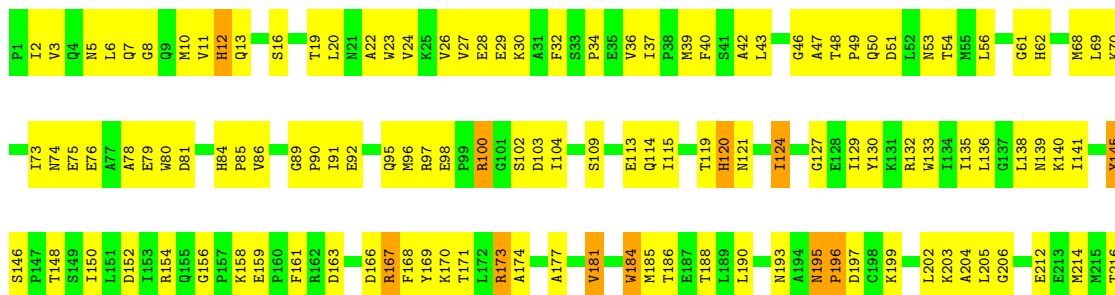
- Molecule 1: capsid protein

Chain 8W:  47% 52%



- Molecule 1: capsid protein

Chain 8X:  43% 52% 5%



A217
C218
Q219
G220
V221
G222
P224
G225
H226
K227
A228
R229
V230
L231

• Molecule 1: capsid protein

Chain 8Y: 47% 49%

P1 Q4 N5 L6 V221 G222 P224 G225 H226 K227 A228 R229 V230 L231

L83 H84 P85 V86 H87 F161 A162 D163 D166 F167 F168 Y169 T170 L171 L172 A177 S178 Q179 F180 V181 E187 T188 L189 L190 W191 Q192 N193 A194 N195 P196 D197 C198 X199 T200 L201 L202 K203 A204 L205 Y129 Y130 W133 I134 A64 A65 M66 Q67 M68 L69 K70 E71 T72 I73 A77 W80

L83 H84 P85 V86 H87 F161 A162 D163 D166 F167 F168 Y169 T170 L171 L172 A177 S178 Q179 F180 V181 E187 T188 L189 L190 W191 Q192 N193 A194 N195 P196 D197 C198 X199 T200 L201 L202 K203 A204 L205 Y129 Y130 W133 I134 A64 A65 M66 Q67 M68 L69 K70 E71 T72 I73 A77 W80

L231

• Molecule 1: capsid protein

Chain 8Z: 48% 49%

P1 N5 L6 V221 G222 P224 G225 H226 K227 A228 R229 V230 L231

H87 G89 P90 I91 E92 M96 R97 E98 P99 R100 G101 S102 D103 T107 T108 S109 T110 L111 Q112 E113 Q114 T115 L116 G117 W117 L118 C119 H120 W121 P122 P123 V126 G127 E128 I129 Y130 K131 R132 W133 L138 N139 K140 I141 S146 T153 R154 Q155 Q156 E159 P160 D163

H87 G89 P90 I91 E92 M96 R97 E98 P99 R100 G101 S102 D103 T107 T108 S109 T110 L111 Q112 E113 Q114 T115 L116 G117 W117 L118 C119 H120 W121 P122 P123 V126 G127 E128 I129 Y130 K131 R132 W133 L138 N139 K140 I141 S146 T153 R154 Q155 Q156 E159 P160 D163

Y164 V165 D166 F167 F168 Y169 K170 R173 A174 Q179 E180 M183 P17 T186 E187 T188 L189 L190 Q192 N193 A194 N195 P196 D197 C198 X199 T200 L201 L202 K203 A204 A209 T210 L211 E212 E213 M214 M215 T216 A217 C218 Q219 G220 G223 P224 R229 V230 L231

• Molecule 1: capsid protein

Chain 90: 44% 52%

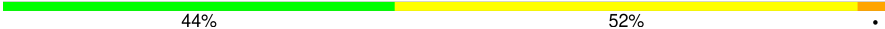
P1 I2 V3 Q4 Q7 M10 V11 H12 Q13 A14 I15 S16 P17 R18 V24 K25 V26 V27 E28 E29 K30 A31 F32 S33 P34 E35 V36 I37 F40 S41 E45 G46 A47 T48 D51 L52 M53 T54 M55 L56 V59 H62 Q63 A64 A65 M66 Q67 M68 L69 K70 E71 T72

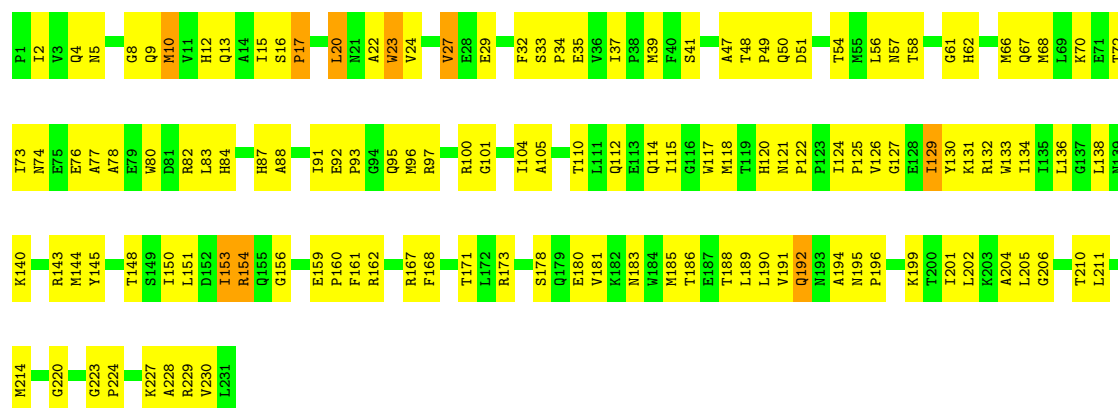
E76 A77 G78 E79 H80 D81 R82 L83 H84 P85 V86 H87 A88 G89 P90 E92 P93 M96 E97 E98 P99 R100 G101 S102 D103 T108 T109 I115 T119 H120 M121 I124 P125 V126 G127 E128 I129 Y130 W133 I134 I135 L136 N139 K140 V141 V142 R143 Q144 Y145 S146 P147 T148

S149 I150 R154 G155 Q156 P157 K158 E159 P160 F161 R162 H163 Y164 R167 F168 Y169 K170 T171 E175 Q176 A177 S178 Q179 F180 V181 E182 N183 W184 M185 T186 T188 L189 L190 V191 Q192 N193 A194 N195 P196 D197 T200 T201 L202 G206 A209 T210 L211 E212 E213 M214 M215 T216

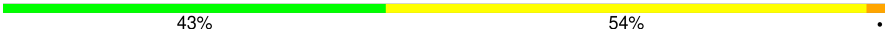
V221 G222 G223 H226 K227 A228 R229 V230 L231

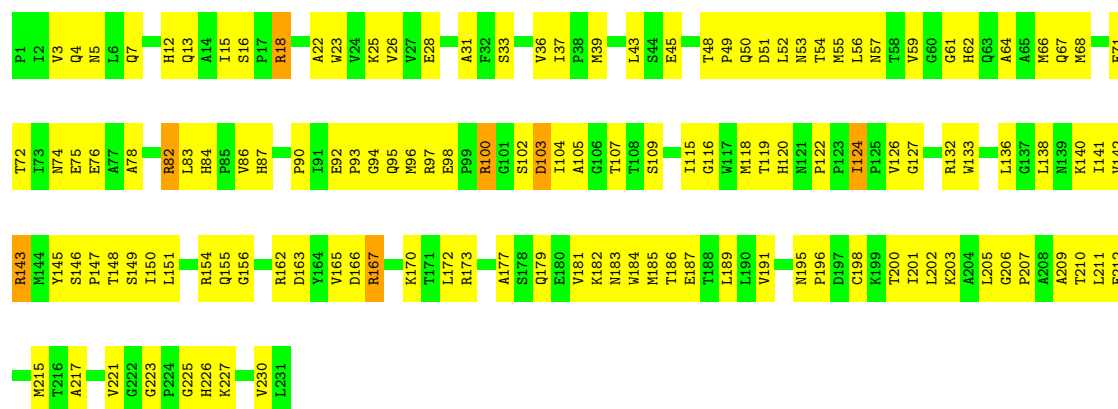
• Molecule 1: capsid protein

Chain 91:  44% 52%



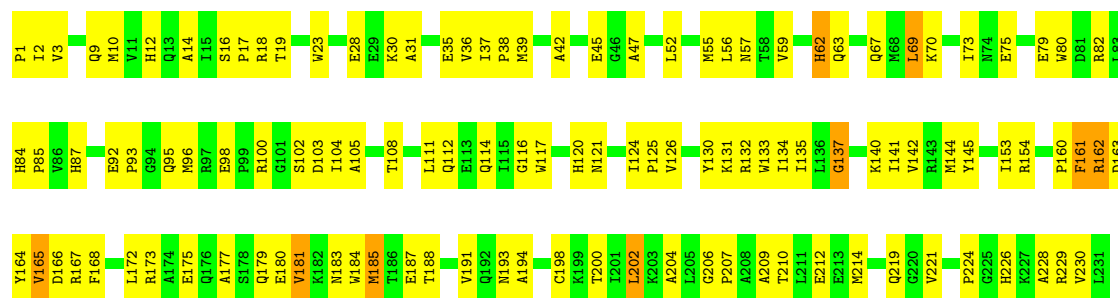
• Molecule 1: capsid protein

Chain 92:  43% 54%



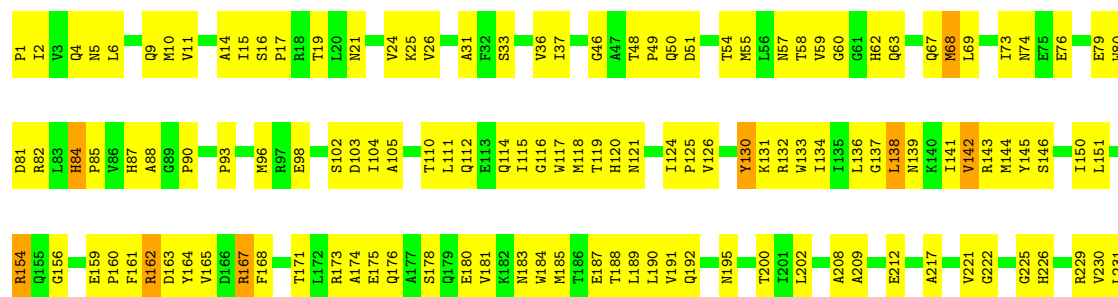
• Molecule 1: capsid protein

Chain 93:  49% 47%



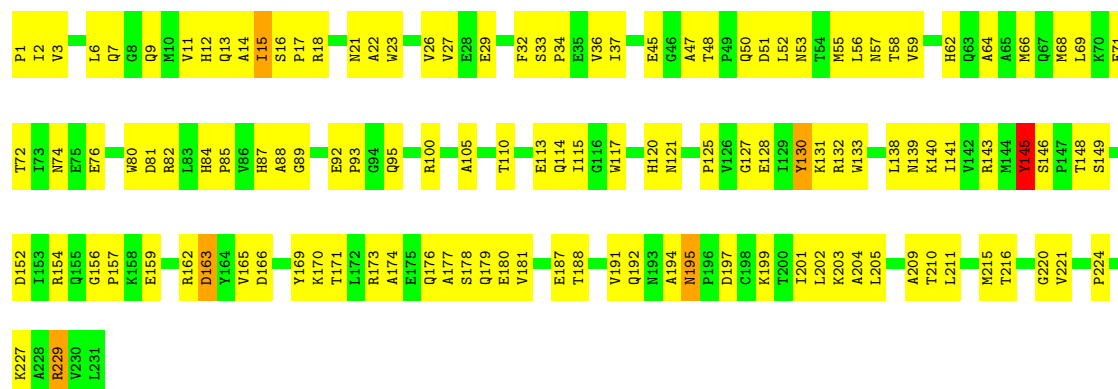
• Molecule 1: capsid protein

Chain 94:  44% 52%



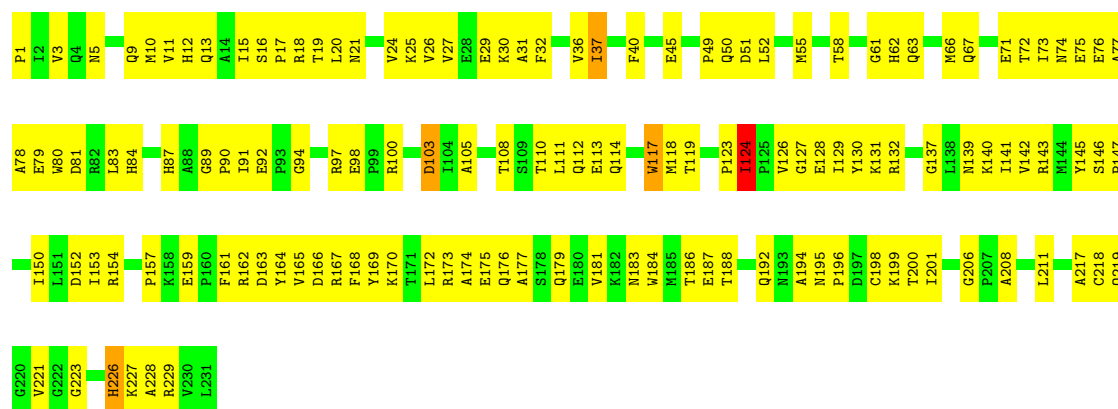
• Molecule 1: capsid protein

Chain 95: 46% 52%



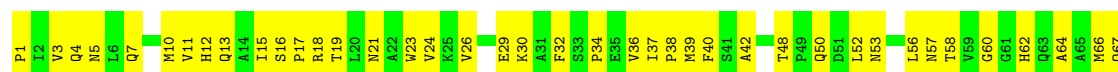
• Molecule 1: capsid protein

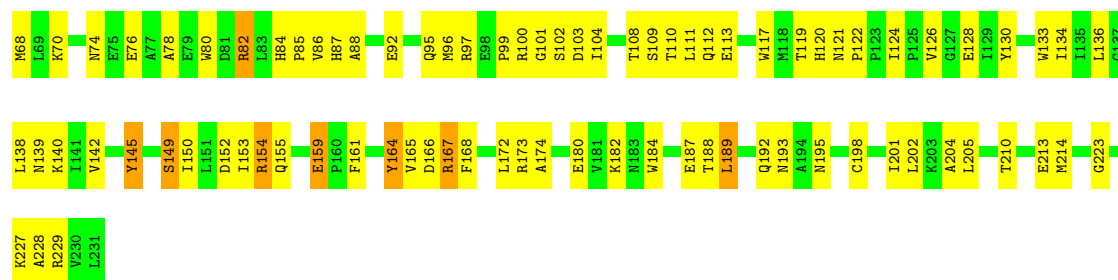
Chain 96: 40% 58%



• Molecule 1: capsid protein

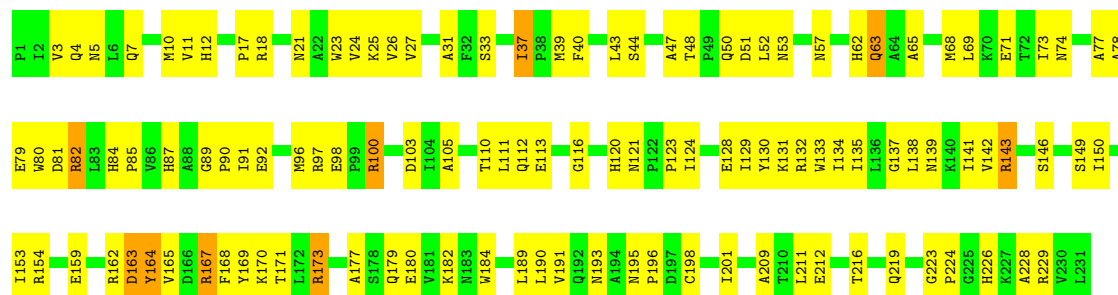
Chain 97: 47% 49%





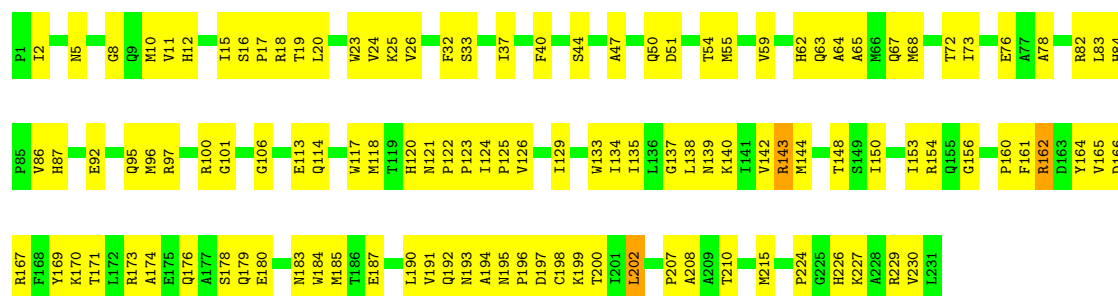
- Molecule 1: capsid protein

Chain 98: 49% 47%



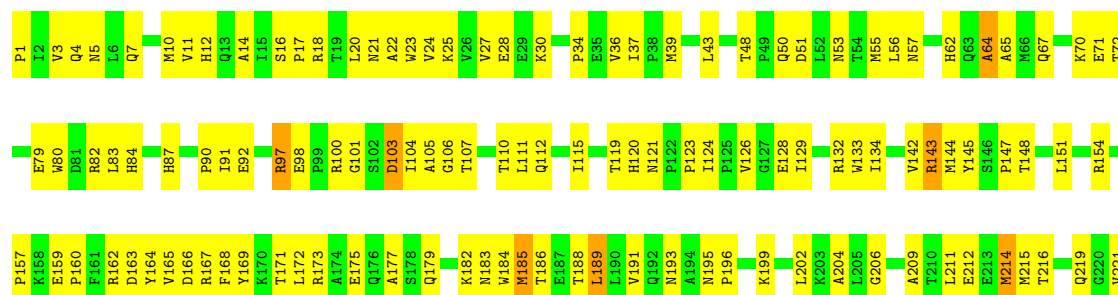
- Molecule 1: capsid protein

Chain 99: 49% 49%



- Molecule 1: capsid protein

Chain 9a: 45% 52%



G222
G223
P224
G225
H226
K227
A228
R229
V230
L231

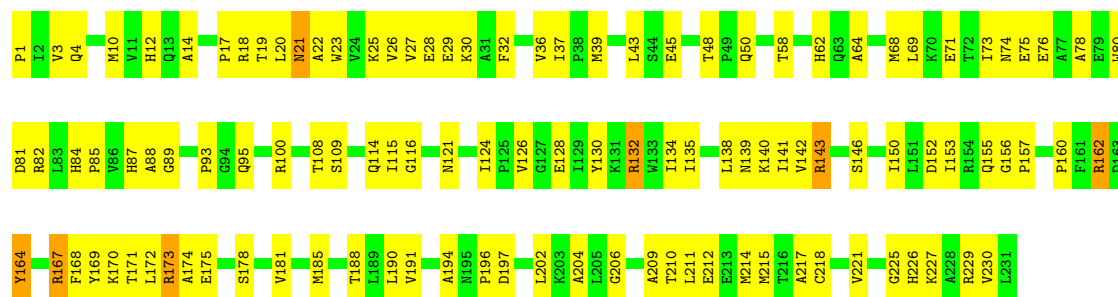
• Molecule 1: capsid protein

Chain 9b: 45% 53%



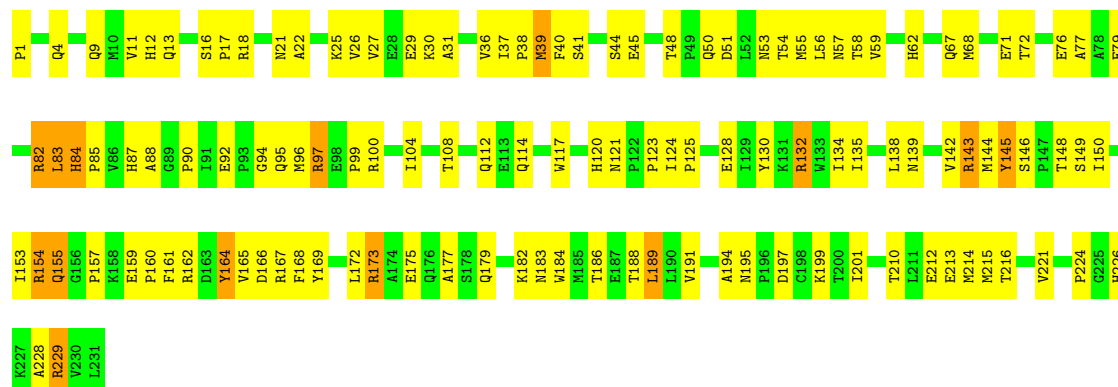
• Molecule 1: capsid protein

Chain 9c: 51% 46%

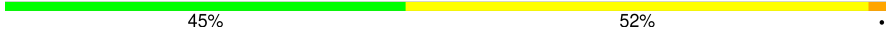


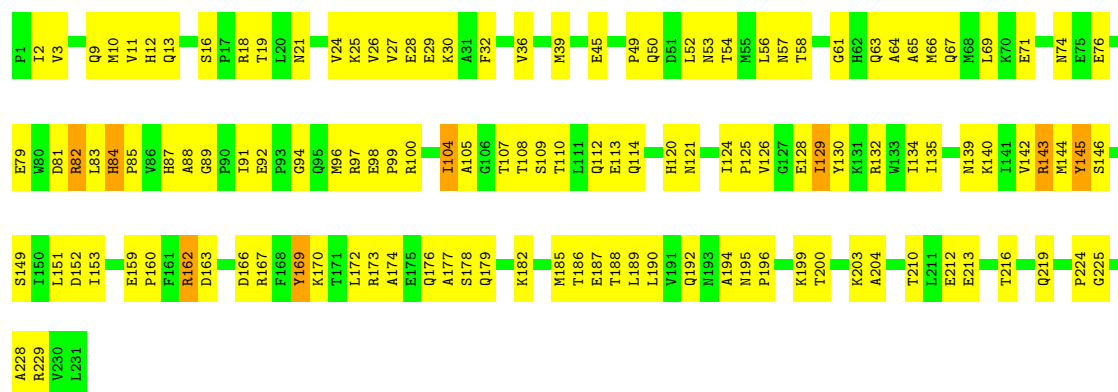
• Molecule 1: capsid protein

Chain 9d: 46% 48% 6%

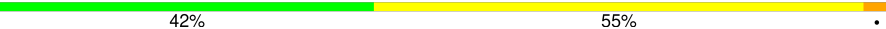


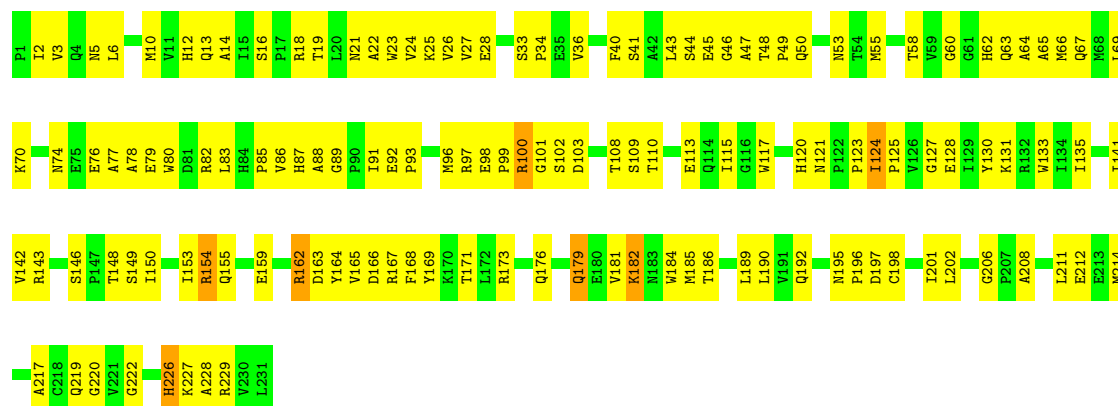
• Molecule 1: capsid protein

Chain 9e:  45% 52%



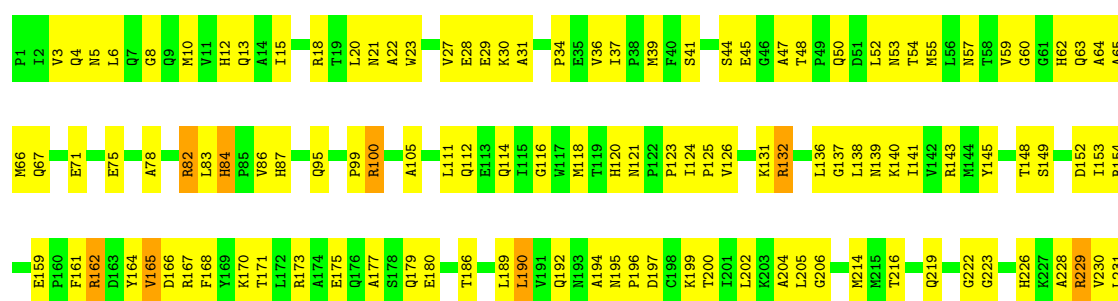
• Molecule 1: capsid protein

Chain 9f:  42% 55%



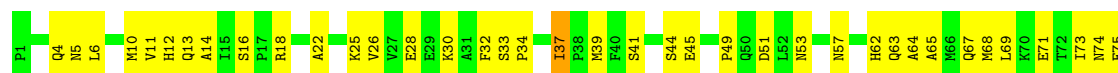
• Molecule 1: capsid protein

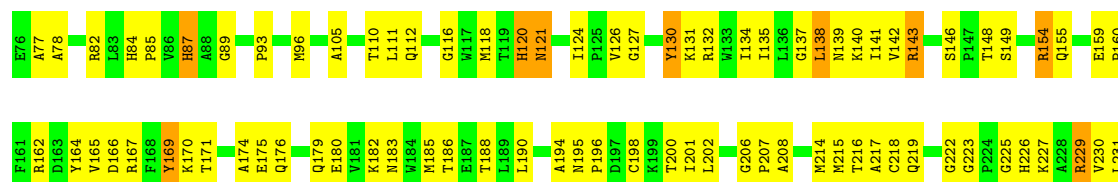
Chain 9g:  48% 48%



• Molecule 1: capsid protein

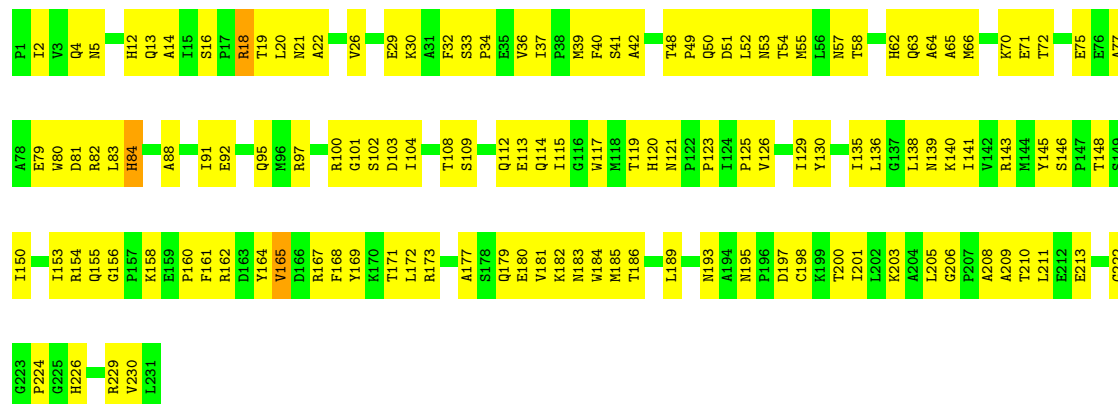
Chain 9h:  48% 48%





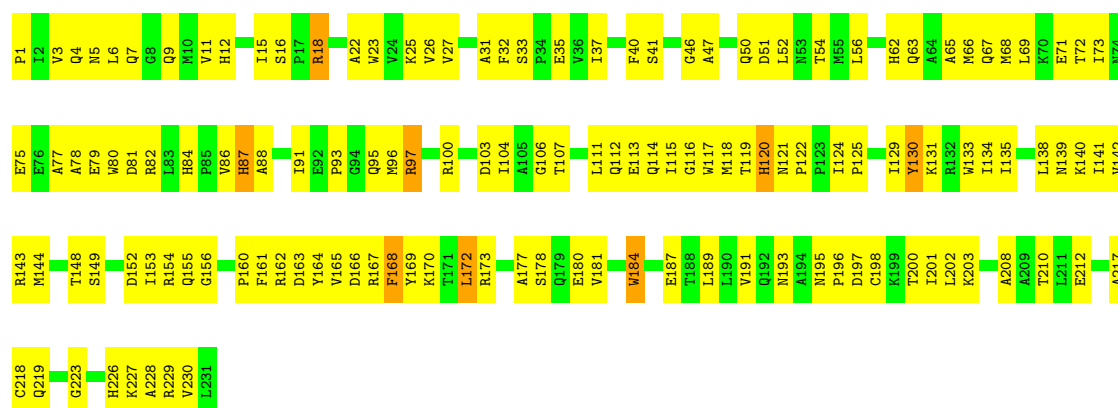
• Molecule 1: capsid protein

Chain 9i: 43% 55%



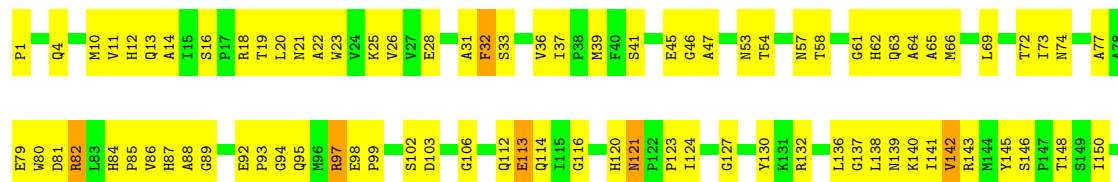
• Molecule 1: capsid protein

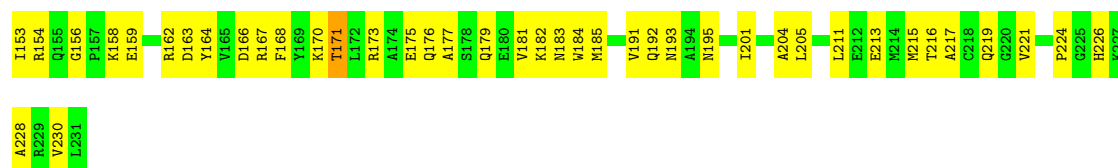
Chain 9j: 40% 56%



• Molecule 1: capsid protein

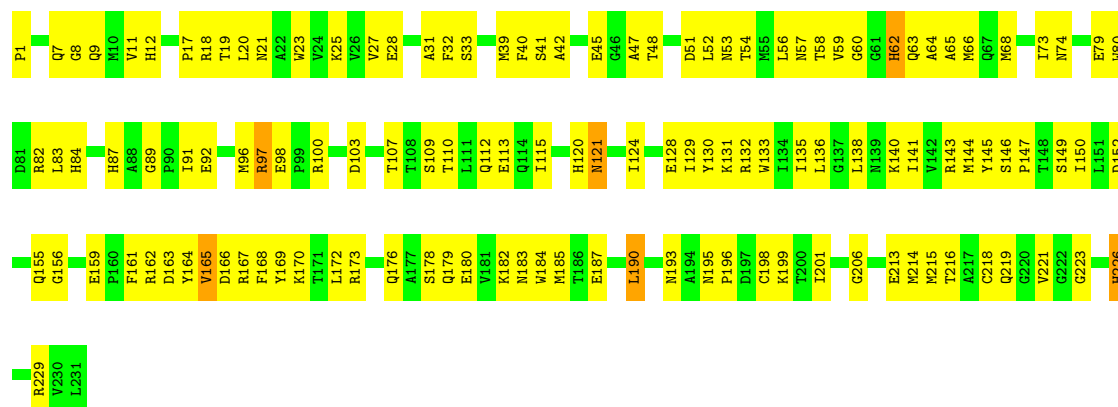
Chain 9k: 45% 52%





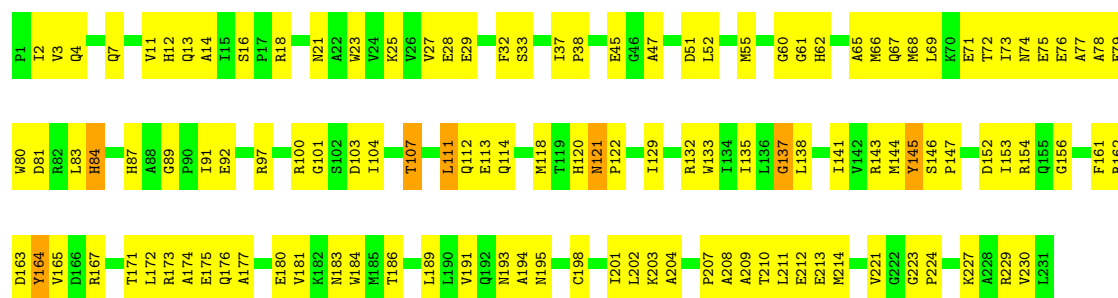
- Molecule 1: capsid protein

Chain 9l: 45% 52%



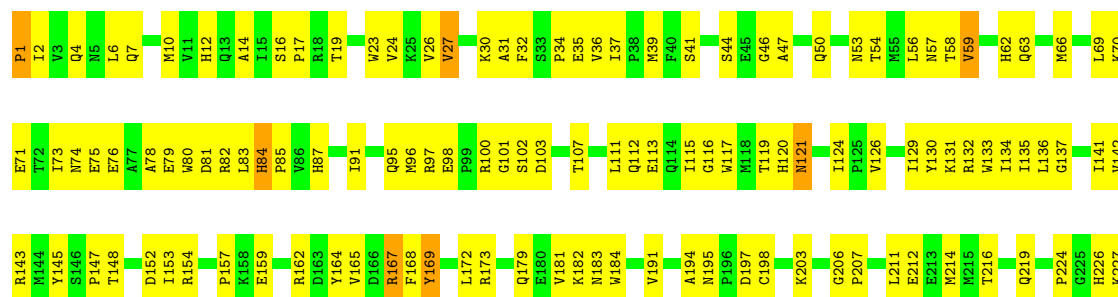
- Molecule 1: capsid protein

Chain 9m: 47% 50%



- Molecule 1: capsid protein

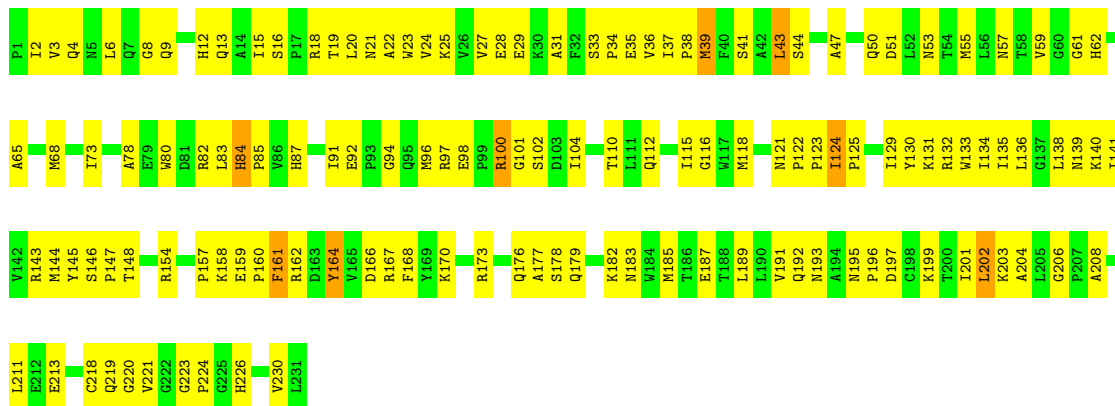
Chain 9n: 46% 51%



K227
A228
R229
V230
L231

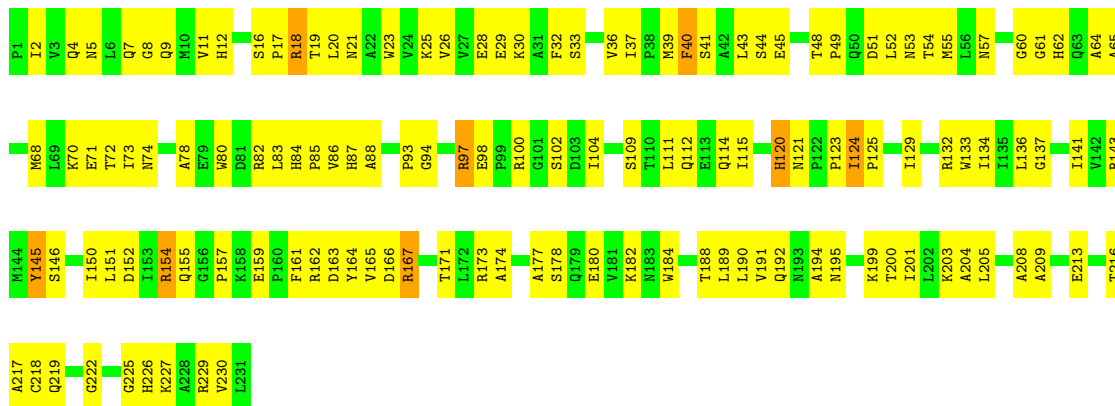
• Molecule 1: capsid protein

Chain 9r: 42% 55%



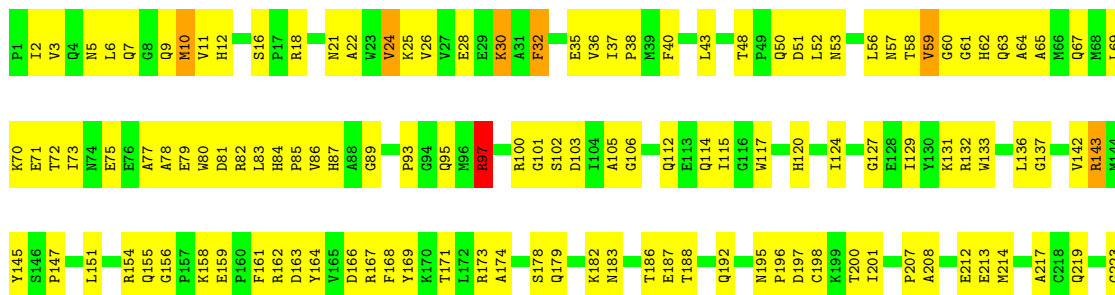
• Molecule 1: capsid protein

Chain 9s: 42% 54%



• Molecule 1: capsid protein

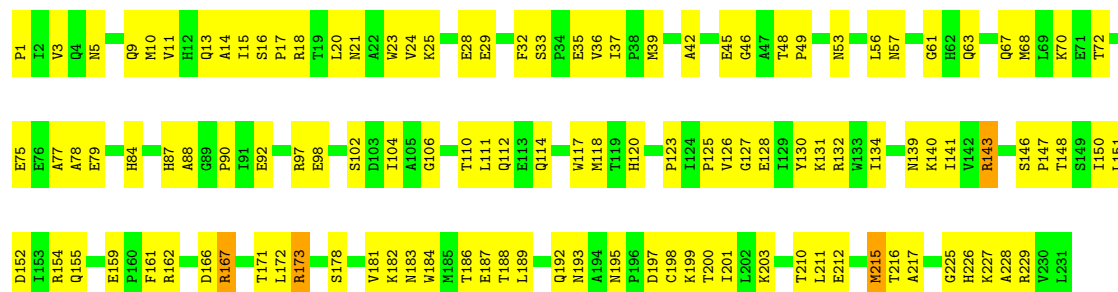
Chain 9t: 45% 52%





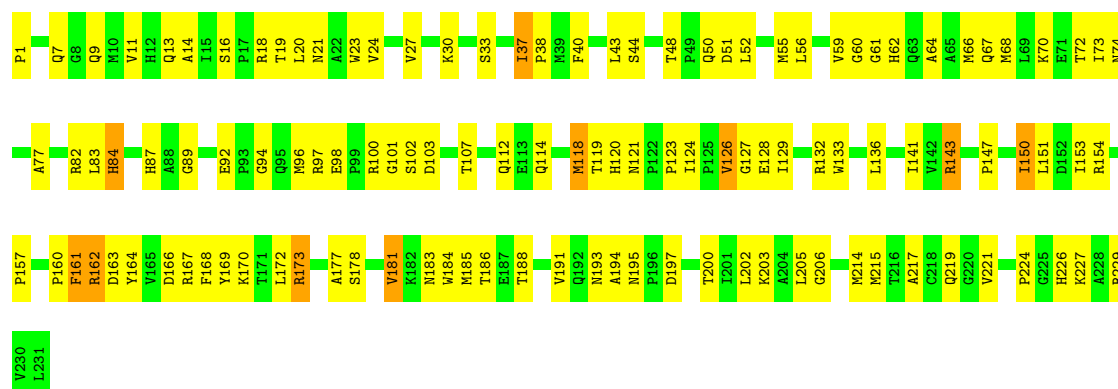
• Molecule 1: capsid protein

Chain 9u: 49% 49%



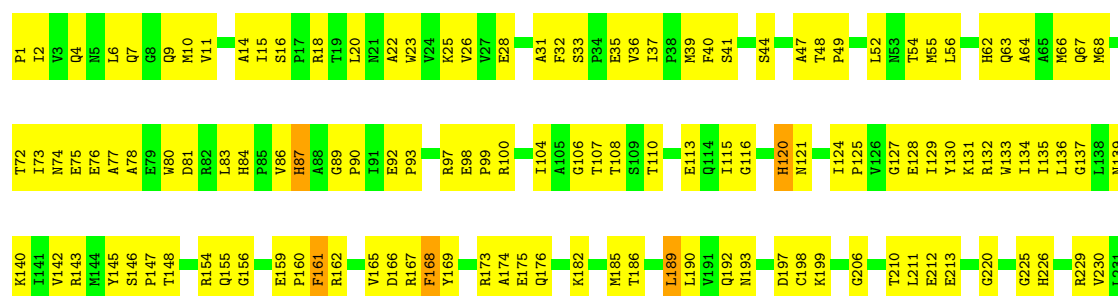
• Molecule 1: capsid protein

Chain 9v: 49% 46%



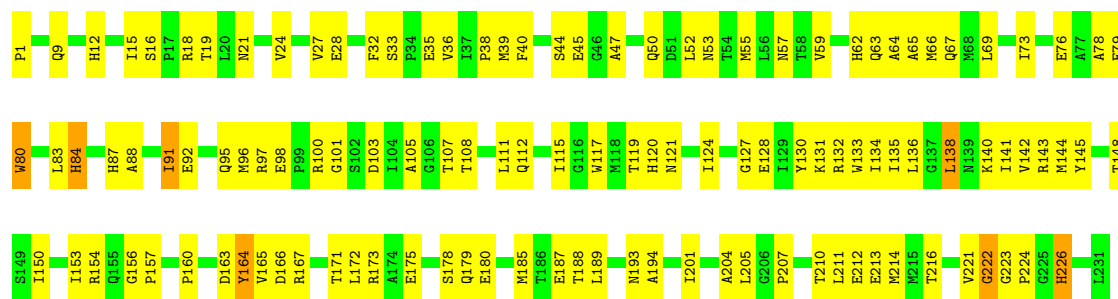
• Molecule 1: capsid protein

Chain 9w: 44% 54%

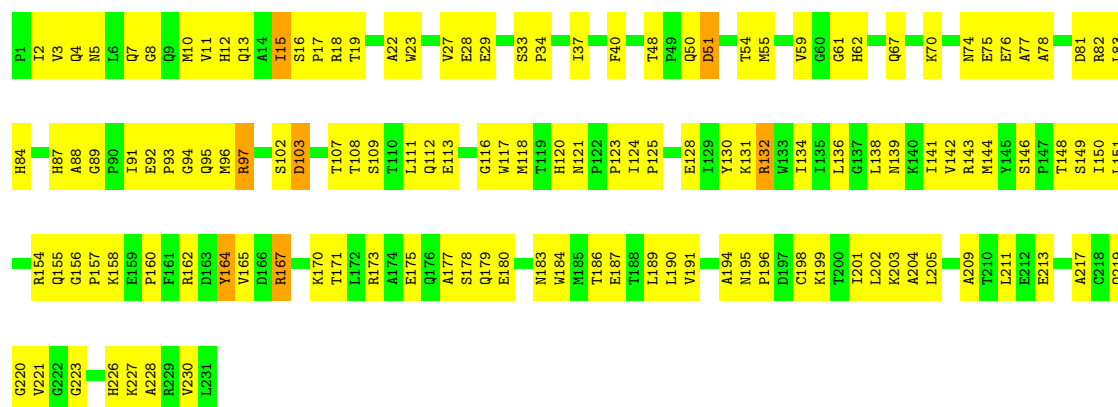


• Molecule 1: capsid protein

Chain 9x: 48% 48%



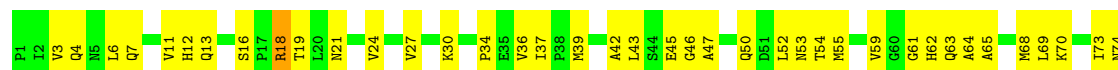
• Molecule 1: capsid protein

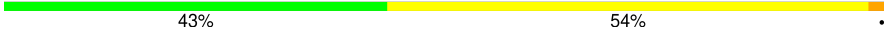


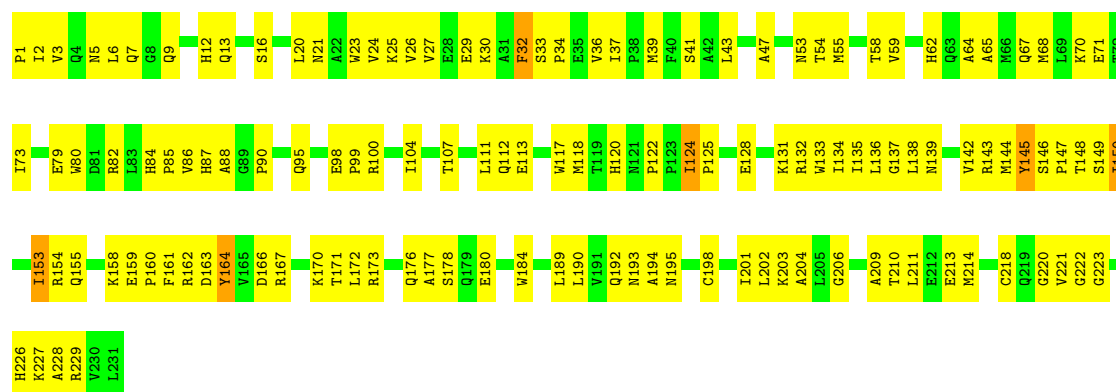
• Molecule 1: capsid protein



• Molecule 1: capsid protein

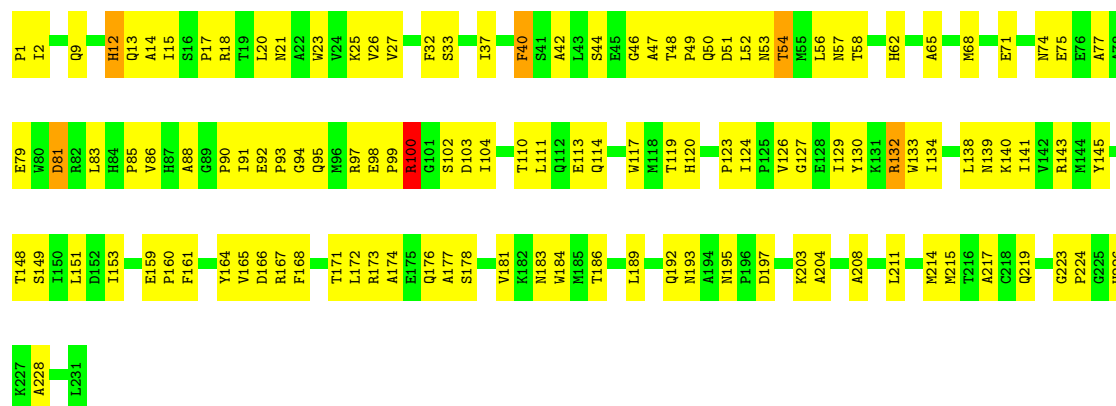


Chain 9E:  43% 54%



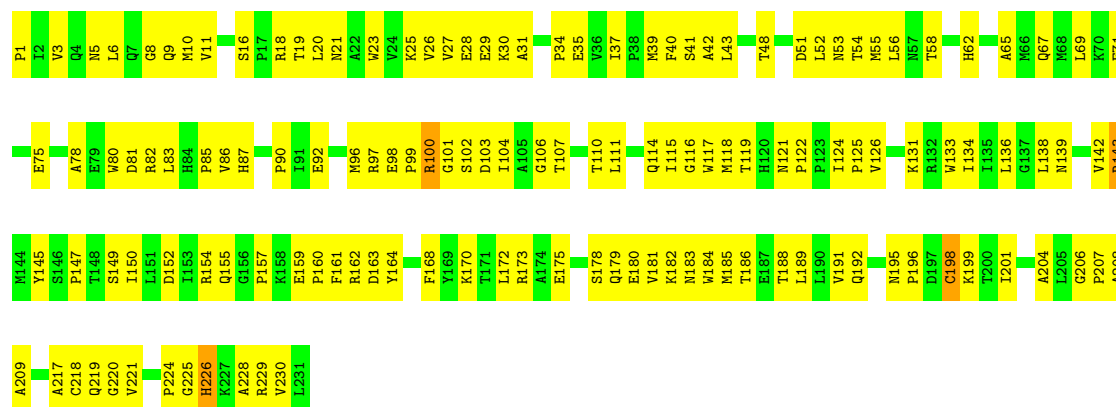
• Molecule 1: capsid protein

Chain 9F:  48% 50%

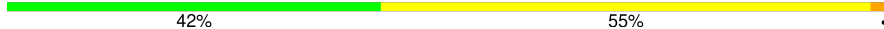


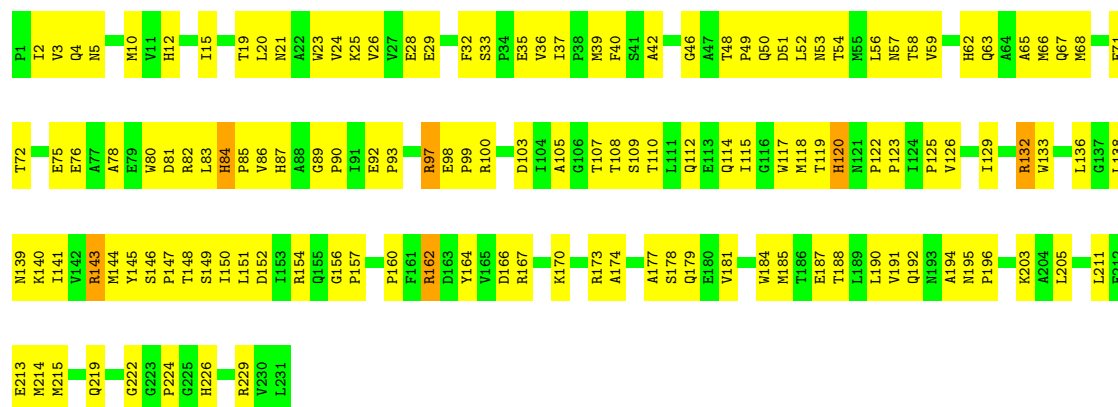
• Molecule 1: capsid protein

Chain 9G:  40% 58%



• Molecule 1: capsid protein

Chain 9H:  42% 55%



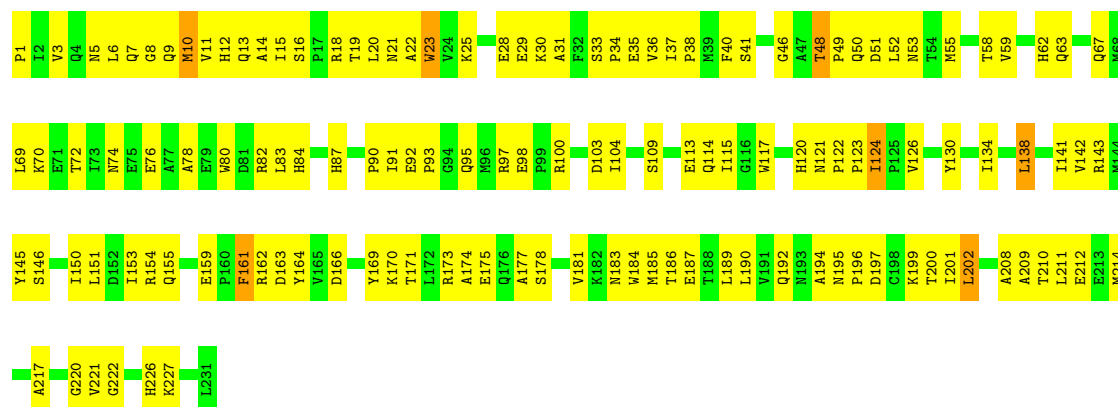
• Molecule 1: capsid protein

Chain 9I: 44% 54%



• Molecule 1: capsid protein

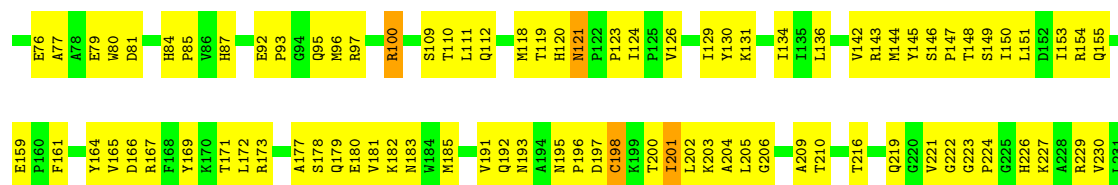
Chain 9J: 42% 55%



• Molecule 1: capsid protein

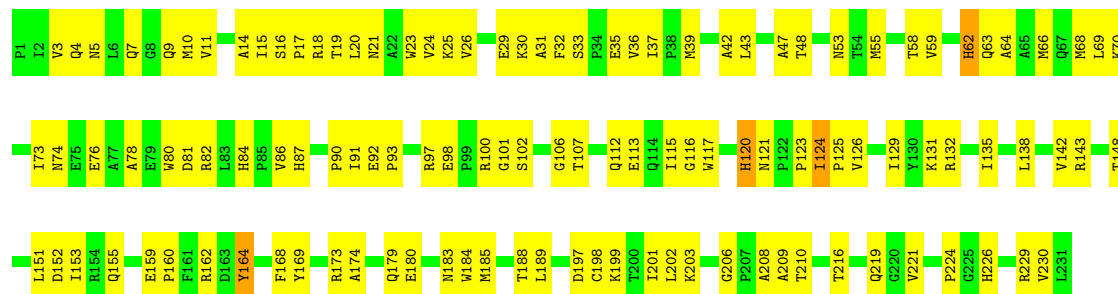
Chain 9K: 45% 53%





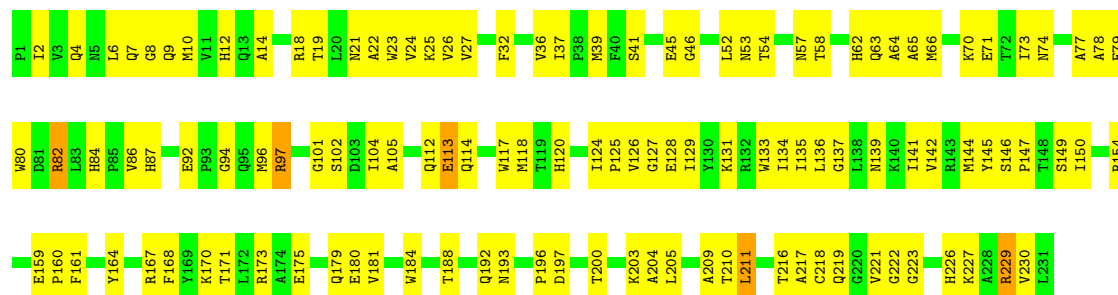
- Molecule 1: capsid protein

Chain 9L: 48% 50%



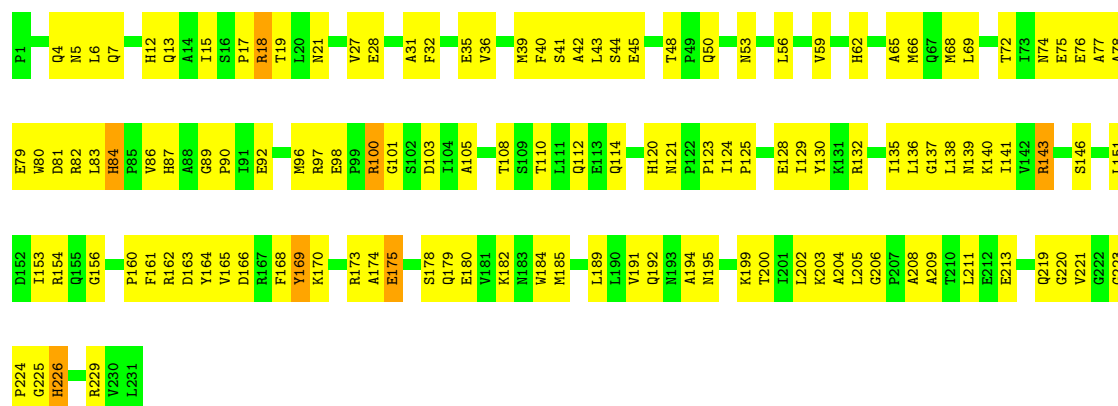
- Molecule 1: capsid protein

Chain 9M: 48% 50%

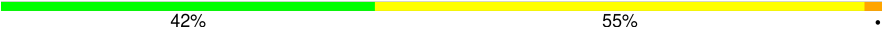


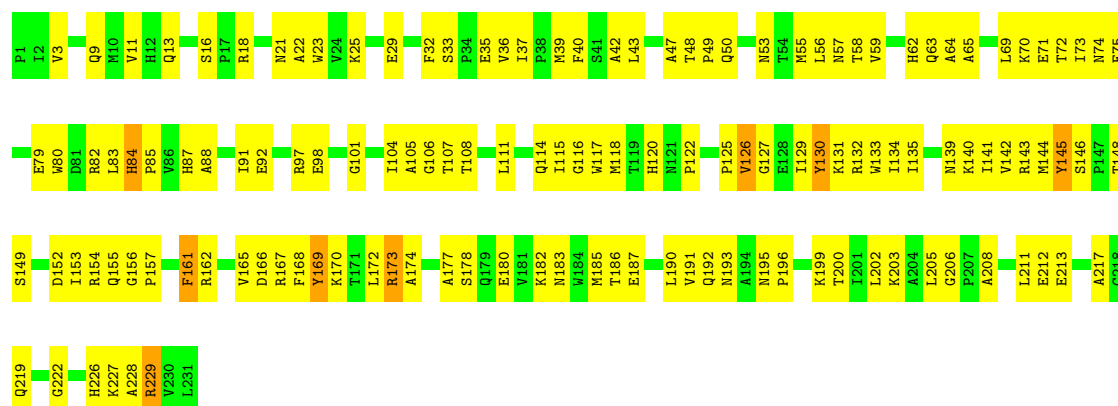
- Molecule 1: capsid protein

Chain 9N: 45% 52%

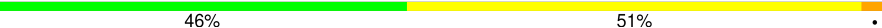


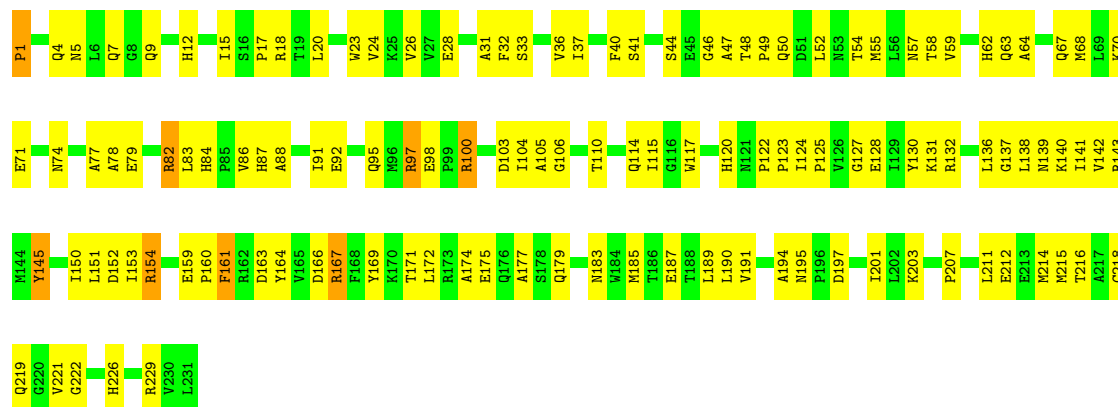
- Molecule 1: capsid protein

Chain 9O:  42% 55%



• Molecule 1: capsid protein

Chain 9P:  46% 51%



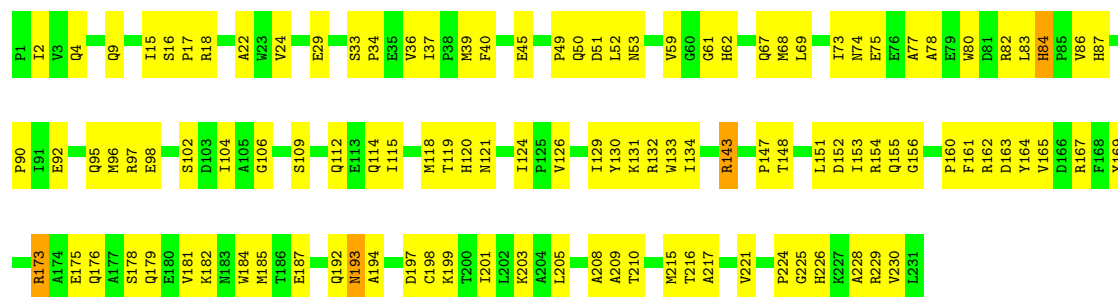
• Molecule 1: capsid protein

Chain Y:  45% 53%



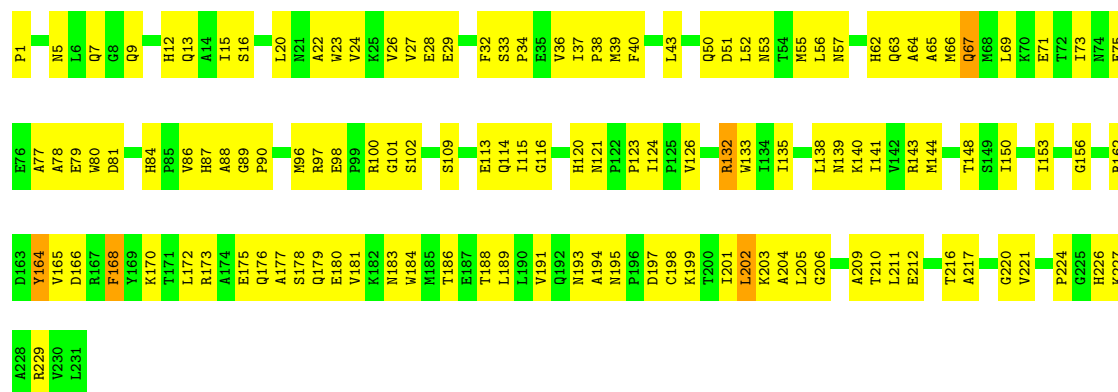
• Molecule 1: capsid protein

Chain 9Q:  51% 47%



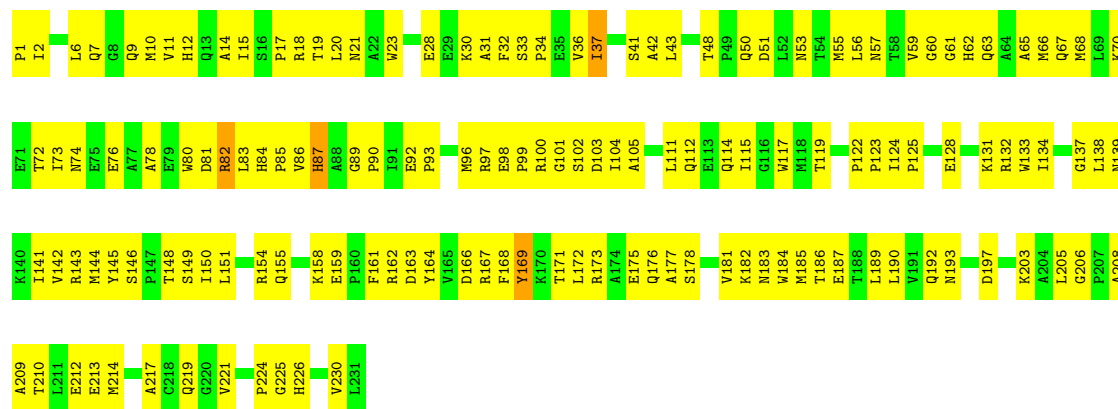
• Molecule 1: capsid protein

Chain 9R: 45% 53%



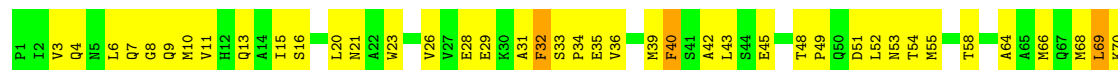
• Molecule 1: capsid protein

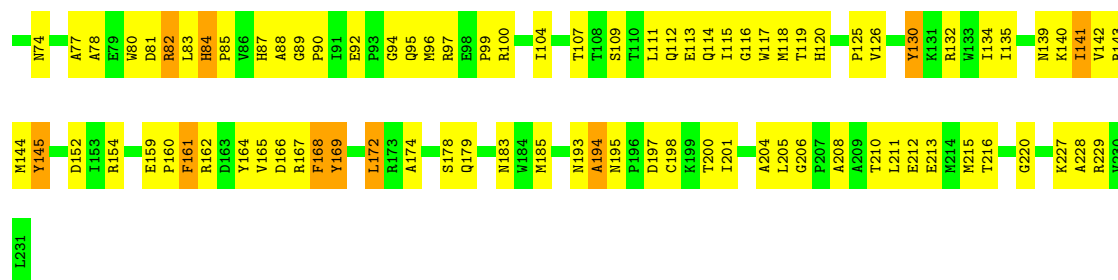
Chain 9S: 37% 61%



• Molecule 1: capsid protein

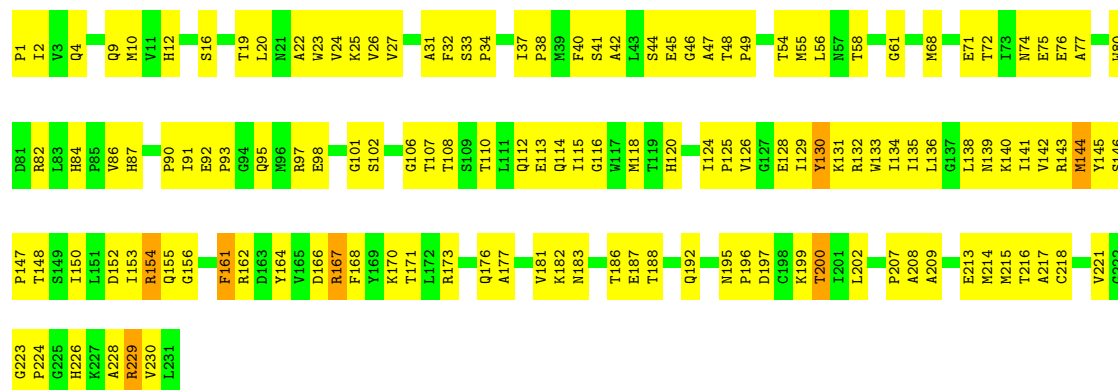
Chain 9T: 45% 49% 6%





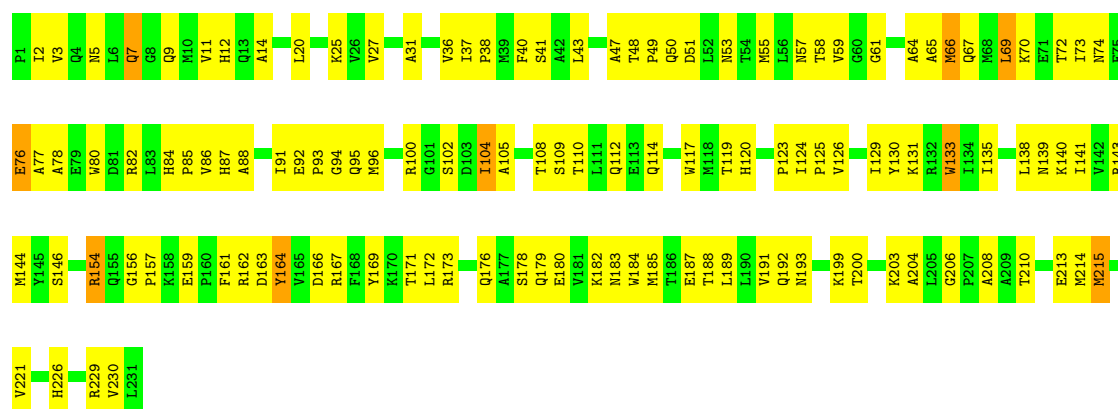
- Molecule 1: capsid protein

Chain 9U: 41% 56%



- Molecule 1: capsid protein

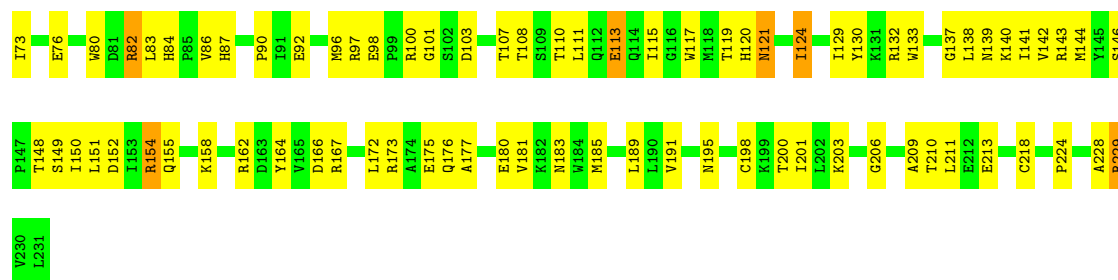
Chain 9V: 46% 50%



- Molecule 1: capsid protein

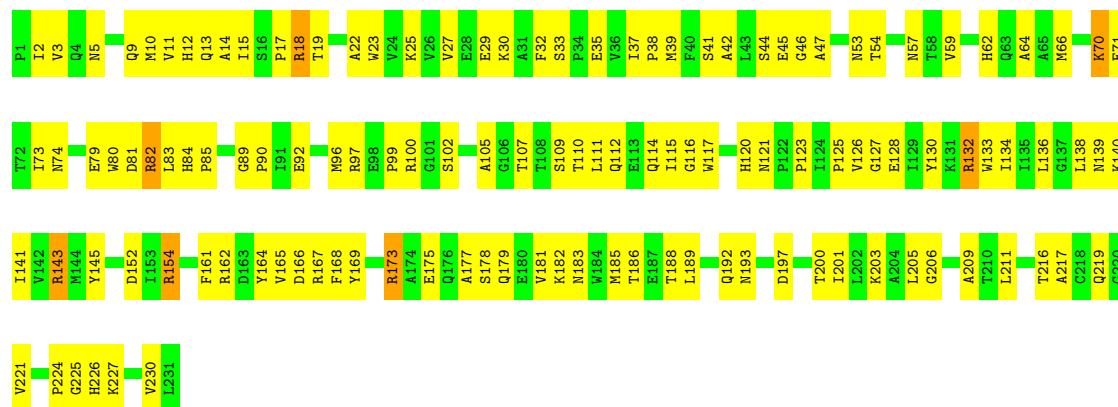
Chain 9W: 49% 47%





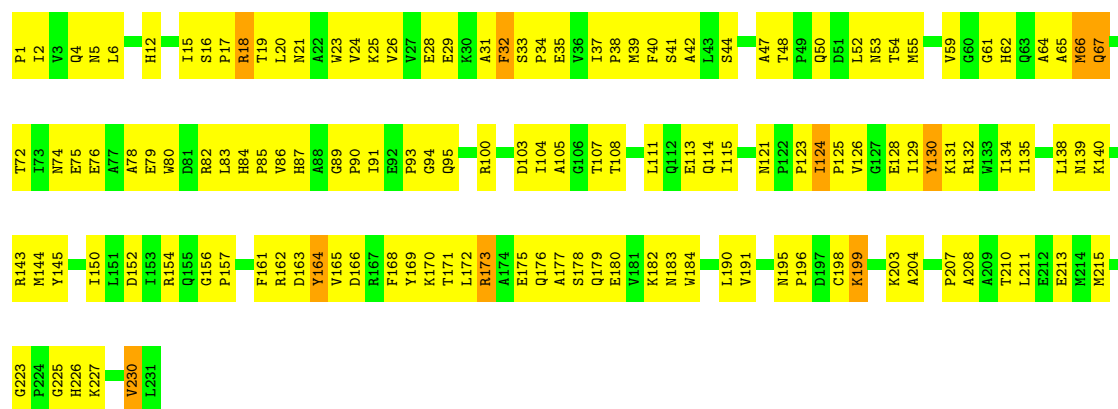
- Molecule 1: capsid protein

Chain 9X: 45% 52%



- Molecule 1: capsid protein

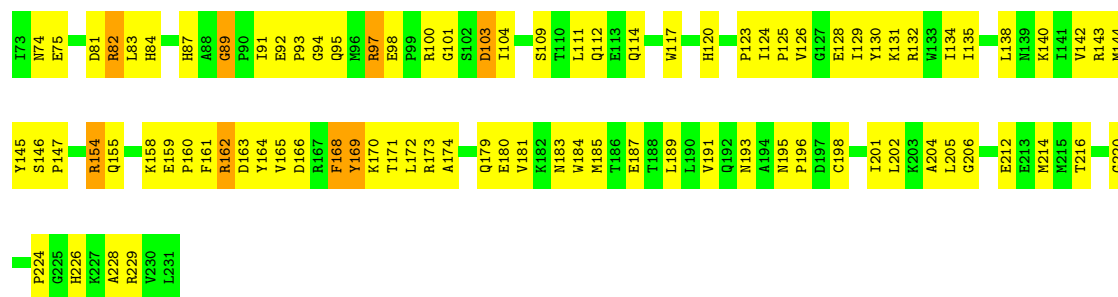
Chain 9Y: 41% 55%



- Molecule 1: capsid protein

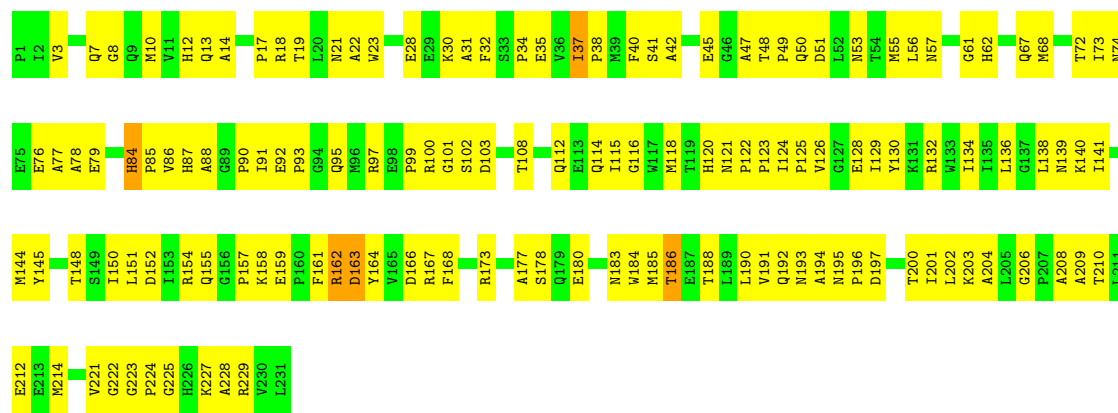
Chain 9Z: 43% 54%





• Molecule 1: capsid protein

Chain Z: 40% 58%



• Molecule 1: capsid protein

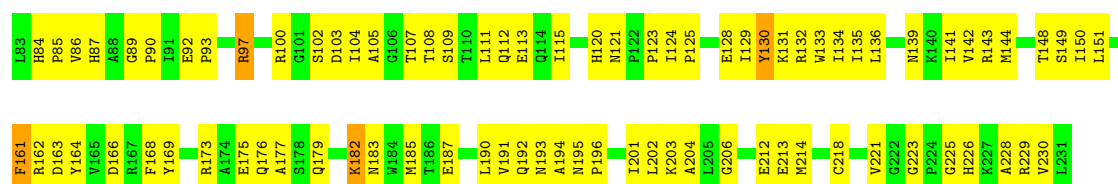
Chain a0: 44% 52%



• Molecule 1: capsid protein

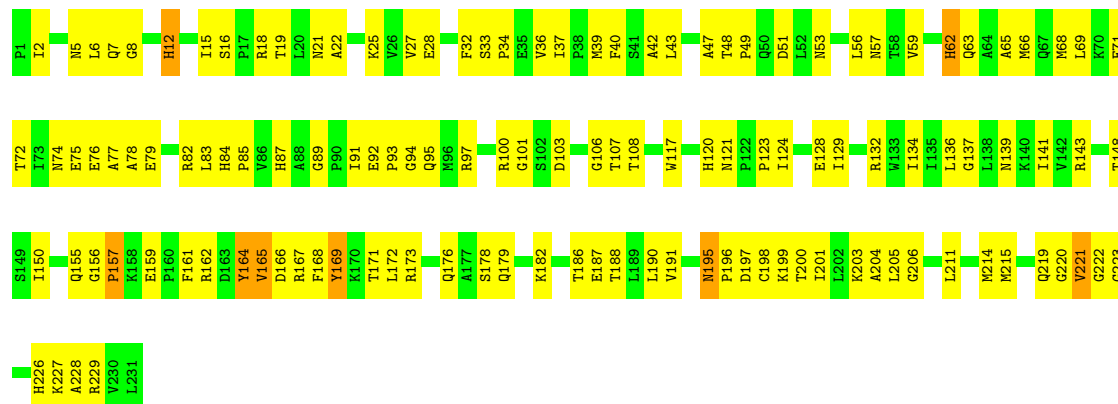
Chain a1: 47% 50%





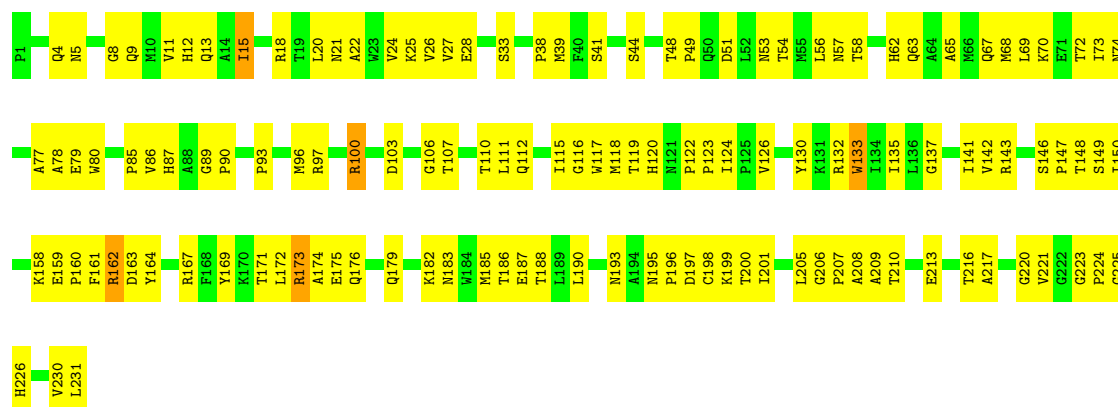
- Molecule 1: capsid protein

Chain a2: 45% 52%



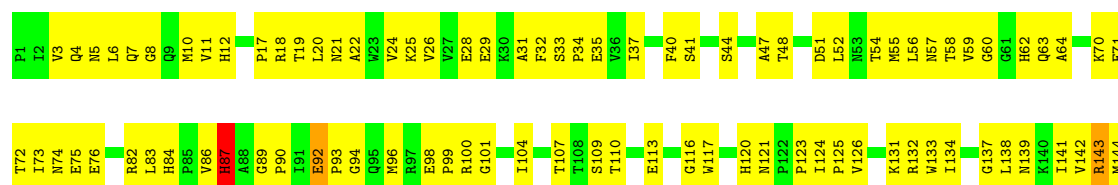
- Molecule 1: capsid protein

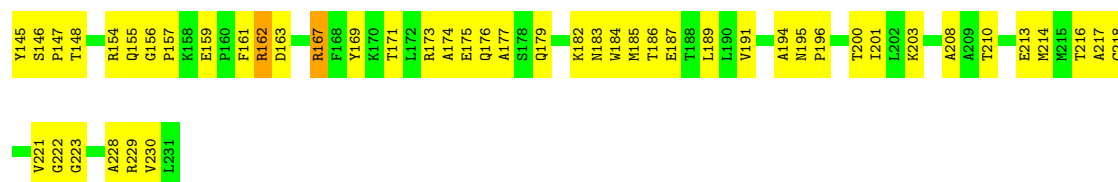
Chain a3: 44% 54%



- Molecule 1: capsid protein

Chain a4: 41% 57%





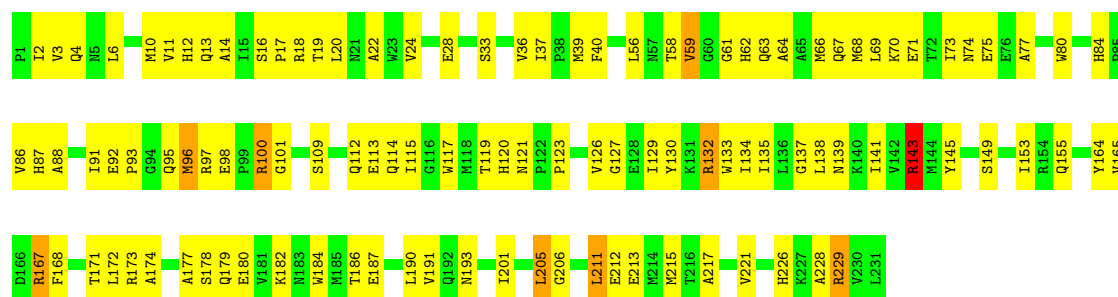
- Molecule 1: capsid protein

Chain a5: 42% 55%



- Molecule 1: capsid protein

Chain a6: 52% 44%

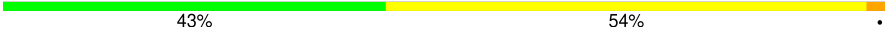


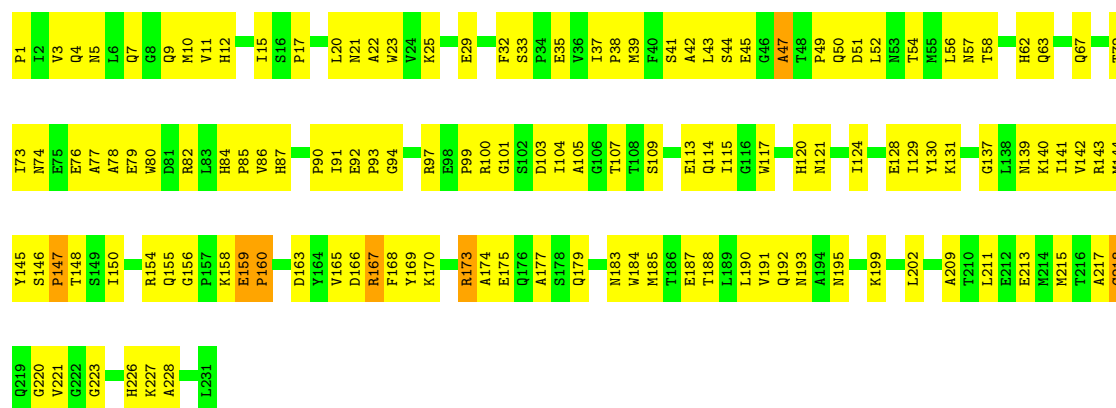
- Molecule 1: capsid protein

Chain a7: 45% 53%

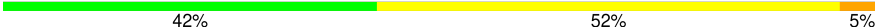


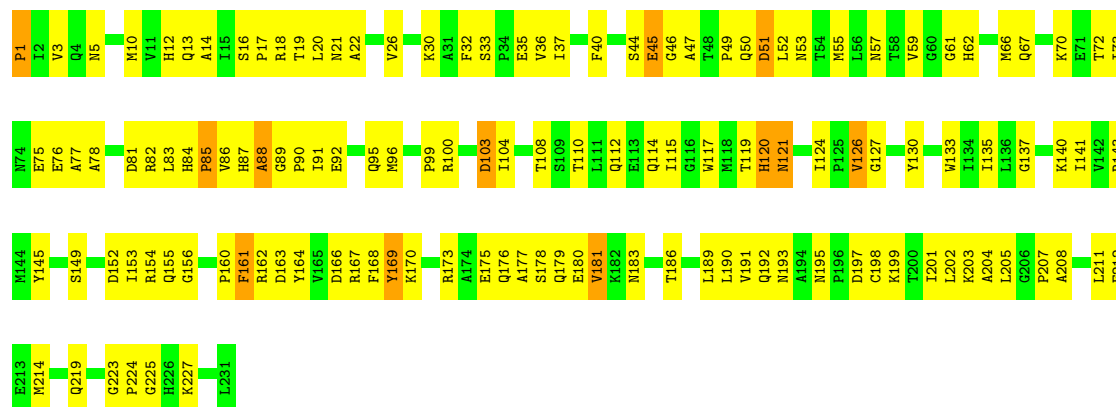
- Molecule 1: capsid protein

Chain a8:  43% 54%

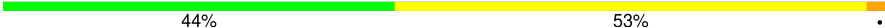


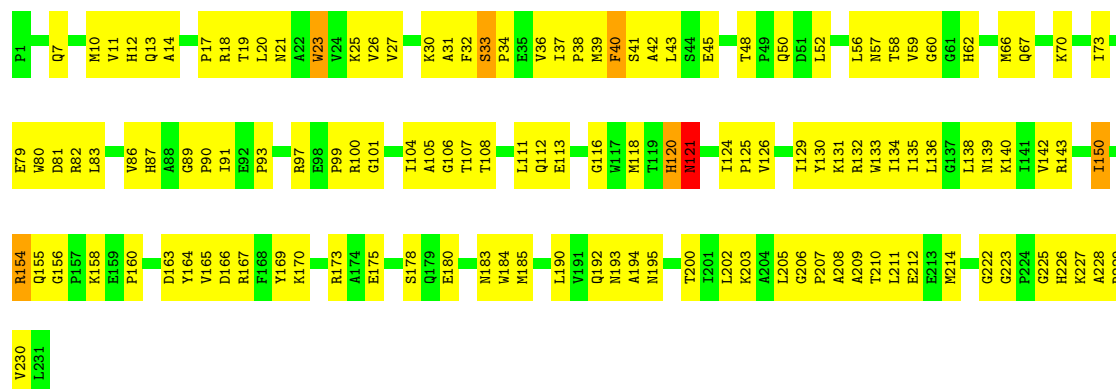
• Molecule 1: capsid protein

Chain a9:  42% 52% 5%



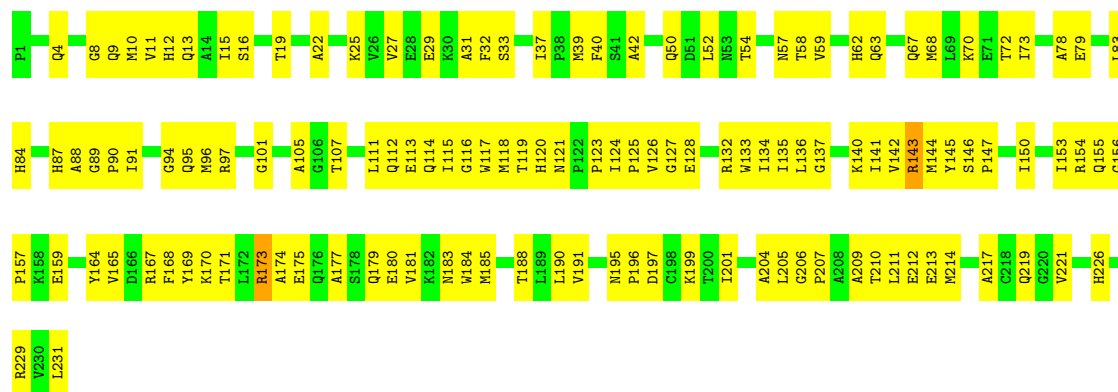
• Molecule 1: capsid protein

Chain 10:  44% 53%



• Molecule 1: capsid protein

Chain aa:  44% 55%



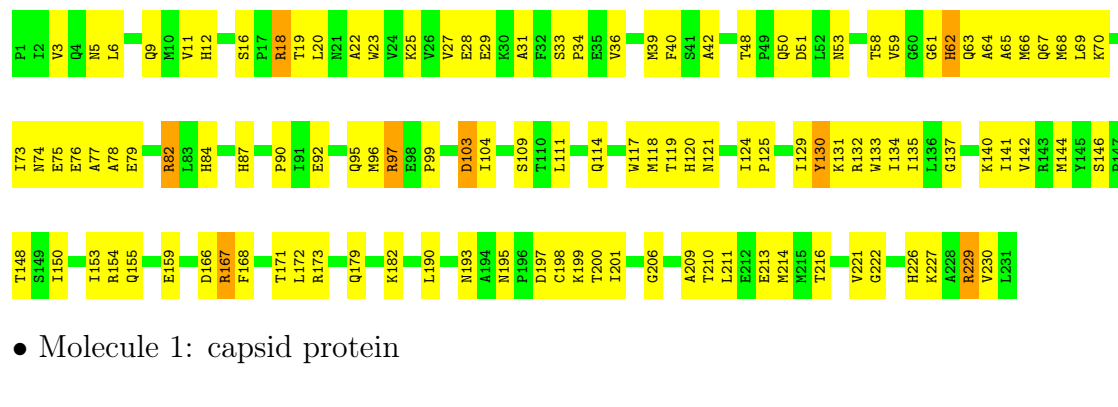
- Molecule 1: capsid protein

Chain ab: 45% 52%



- Molecule 1: capsid protein

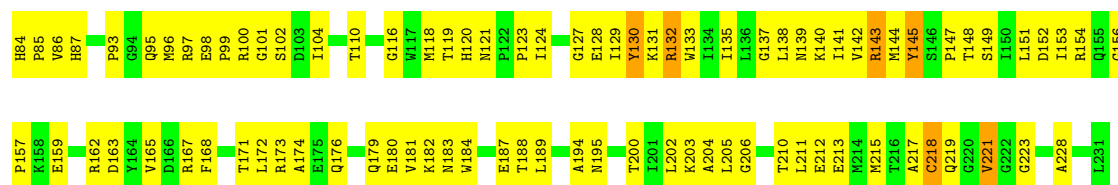
Chain ac: 50% 46%



- Molecule 1: capsid protein

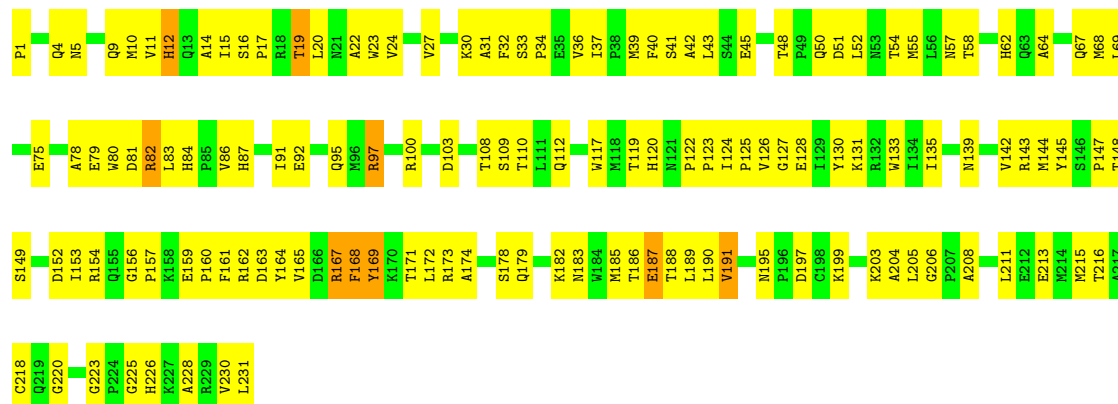
Chain ad: 45% 52%





• Molecule 1: capsid protein

Chain ae: 42% 55%



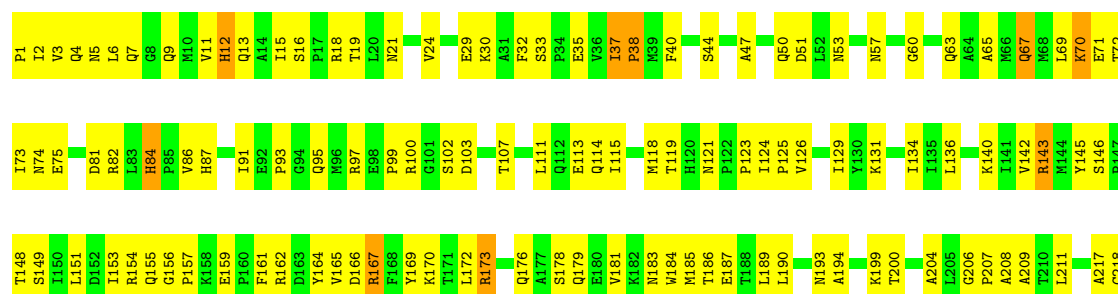
• Molecule 1: capsid protein

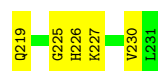
Chain af: 51% 47%



• Molecule 1: capsid protein

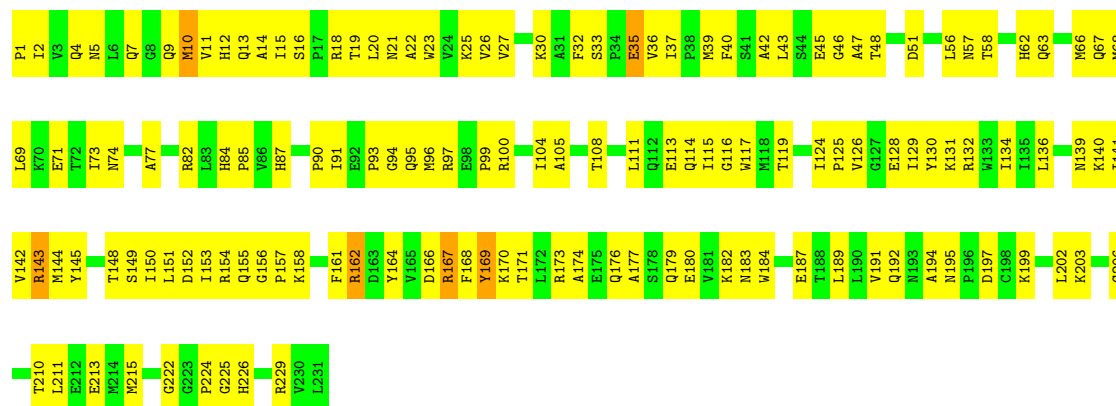
Chain ag: 47% 49%





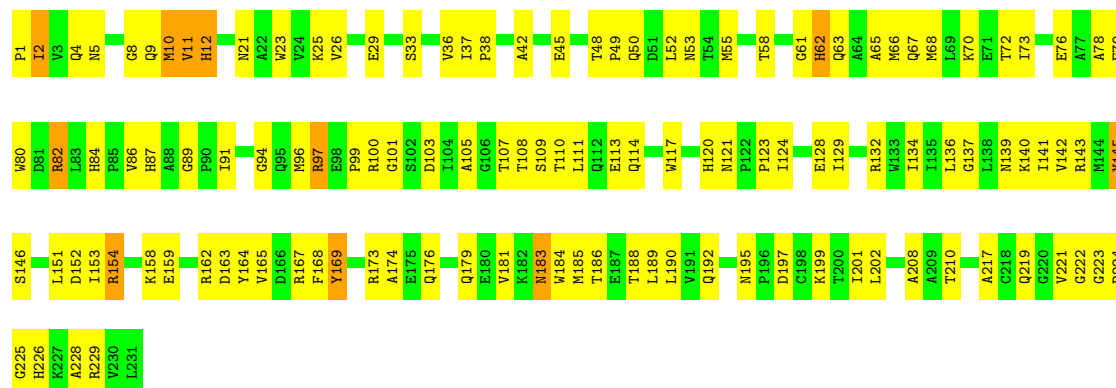
• Molecule 1: capsid protein

Chain ah: 40% 58%



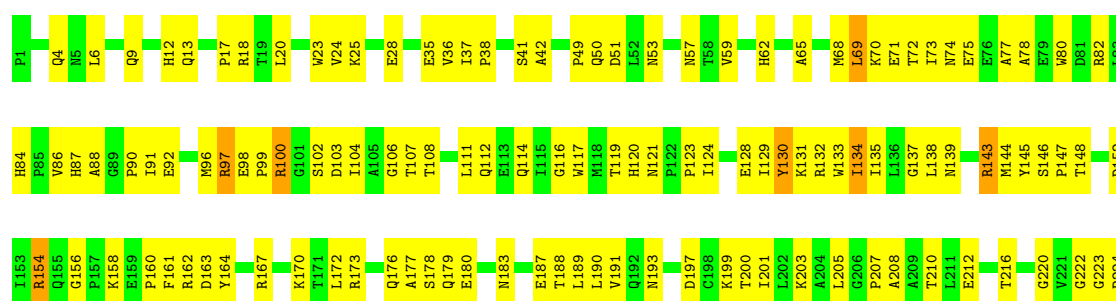
• Molecule 1: capsid protein

Chain ai: 47% 48% 5%



• Molecule 1: capsid protein

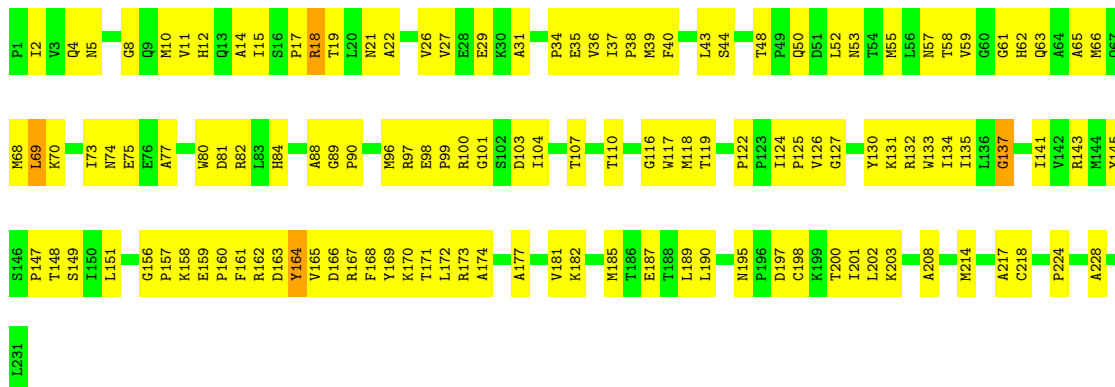
Chain aj: 46% 51%





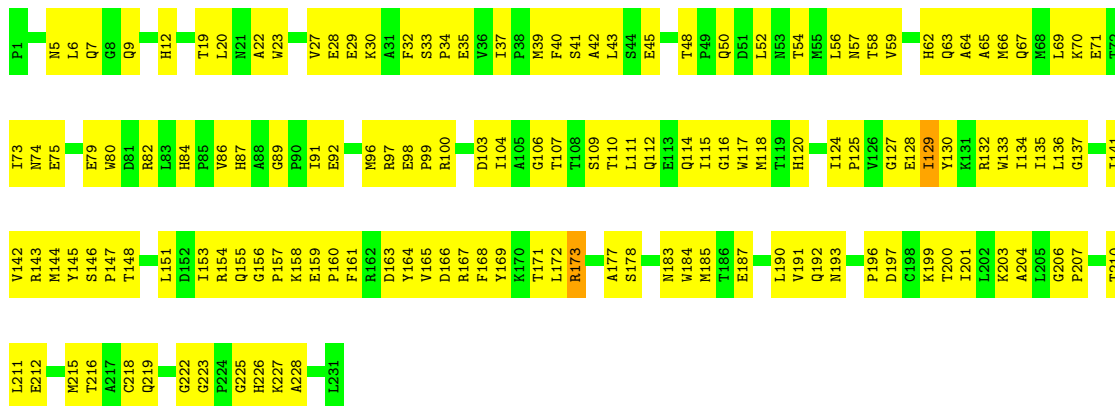
• Molecule 1: capsid protein

Chain 11: 45% 53%



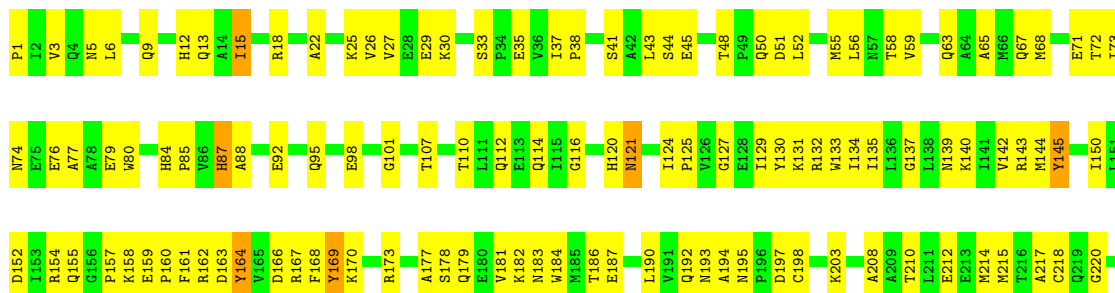
• Molecule 1: capsid protein

Chain ak: 38% 61%



• Molecule 1: capsid protein

Chain al: 46% 52%



G223
P224
G225
H226
K227
A228
R229
V230
L231

• Molecule 1: capsid protein

Chain am:  52% 46%

P1
I2
V3
Q4
N5
Q9
M10
V11
H12
I15
S16
P17
W23
V26
K30
A31
F32
I37
P38
K39
F40
S41
A42
L43
S44
E45
G46
T48
D51
L52
N53
N57
T58
V59
G60
G61
H62
Q63
A64
A65
M66
Q67
K70
A78
E79
W80
R81
R82
L83
H84
H87
E92
P93
G94
Q95
R96
R97
E98
P99
R100
I104
T107
T110
L111
Q112
E113
Q114
I115
G116
V117
M118
T119
H120
N121
P122
S123
I124
V125
V126
R132
L138
M139
K140
I141
V142
R143
M144
P147
T148
S149
D152
I153
R154
Q155
G156
P157
K158
E159
M162
D166
F168
Y169
K170
T171
L172
R173
A174
S178
Q179
E180
M183
W184
T185
T188
L189
E190
V191
Q192
M193
A194
N195
C198
K199
T200
L201
L202
K203
A204
L205
G206
P207
T210
M214
K215
T216
Q219
G220
V221
G225
H226
L231

• Molecule 1: capsid protein

Chain an:  42% 55%

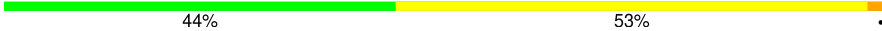
P1
I2
V3
Q4
N5
L6
Q7
G8
Q9
W10
V11
H12
Q13
A14
I15
S16
P17
R18
A22
W23
V24
E29
G30
A31
P34
R39
V36
F40
S41
A42
E45
G46
A47
T48
P49
Q50
D51
L52
N53
T54
M55
L56
T58
V59
G60
G61
H62
Q63
A64
A65
M66
Q67
M68
L69
K70
E71
N74
E76
A77
A78
E79
W80
D81
R82
L83
H84
P85
V86
H87
A88
G89
P90
I91
E92
P93
G94
Q95
M96
R97
E98
G101
S102
D103
T107
T108
S109
I115
G116
T119
H120
I124
P125
V126
I129
Y130
K131
R132
L136
G137
L138
N139
K140
R143
M144
Y145
S146
T148
I153
R154
Q155
G156
P157
P160
F161
R162
D163
V165
D166
R167
F168
Y169
K170
T171
L172
R173
A174
Q176
E175
A177
Q179
E180
V181
M185
T188
L189
N193
A194
N195
P196
D197
C198
T200
K203
A204
L205
G206
P207
A208
A209
T210
L211
E212
M214
M215
T216
A217
Q218
G220
Q219
V221
G222
G223
P224
P225
G225
H226
K227
A228
R229
V230
L231

• Molecule 1: capsid protein

Chain ao:  45% 52%

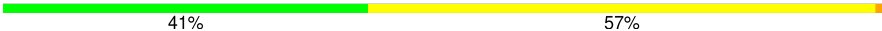
P1
I2
V3
Q4
N5
L6
Q7
G8
Q9
M10
A14
I15
S16
P17
R18
T19
L20
D21
A22
W23
K25
V26
G27
E28
E29
K30
A31
F32
S33
I37
P38
M39
F40
S41
A42
G46
A47
T48
P49
Q50
M53
T54
M55
L56
M57
T58
V59
Q63
Q67
M68
L69
N74
A78
E79
W80
L83
H84
P85
Y86
H87
A88
G89
P90
P93
G94
Q95
M96
R97
E98
P99
E100
G101
Q102
S103
G106
T110
L111
N112
E113
I114
G116
W117
M118
T119
H120
M121
P122
P123
I124
P125
V126
I127
E128
I129
Y130
I134
I135
L136
N139
K140
I141
V142
M143
M144
Y145
T148
S149
I150
E159
P160
F161
R162
D163
Y164
V165
D166
R167
F168
Y169
K170
R173
A174
E175
Q176
A177
S178
G179
E180
K182
N183
W184
M185
L189
G190
V191
A194
N195
P196
D197
C198
K199
T200
I201
L202
A204
L205
G206
P207
T210
L211
E212
E213
M214
M215
T216
A217
G218
Q219
G220
V221
G222
G223
P224
G225
H226
L231

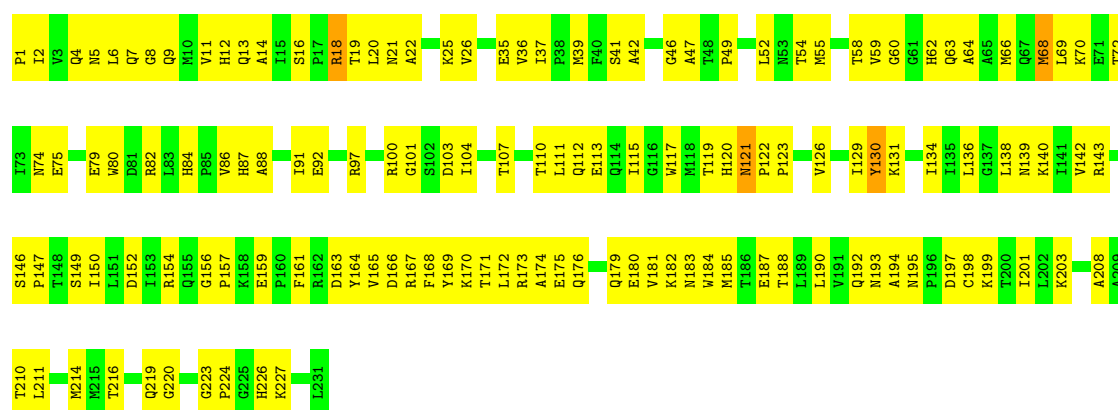
• Molecule 1: capsid protein

Chain ap:  44% 53%

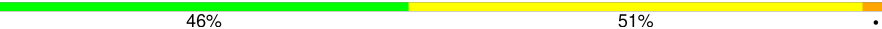


• Molecule 1: capsid protein

Chain aq:  41% 57%

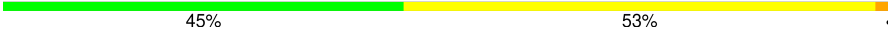


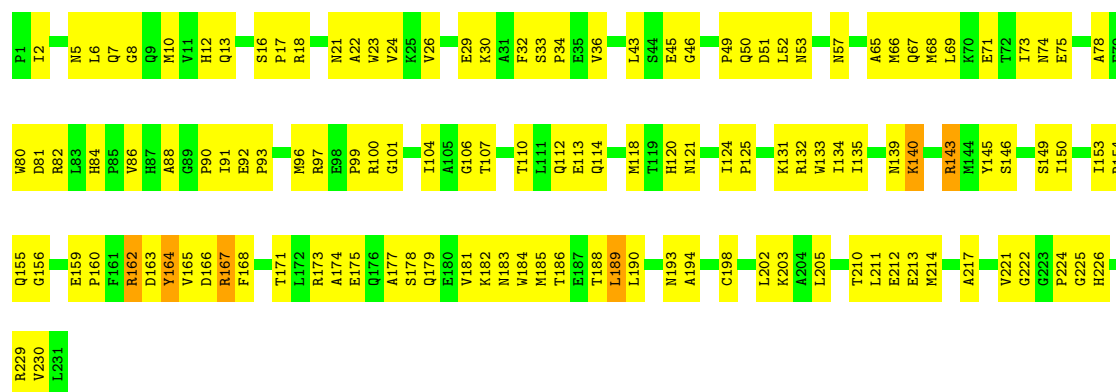
• Molecule 1: capsid protein

Chain ar:  46% 51%

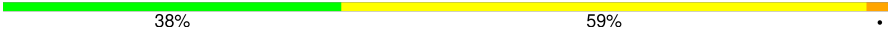


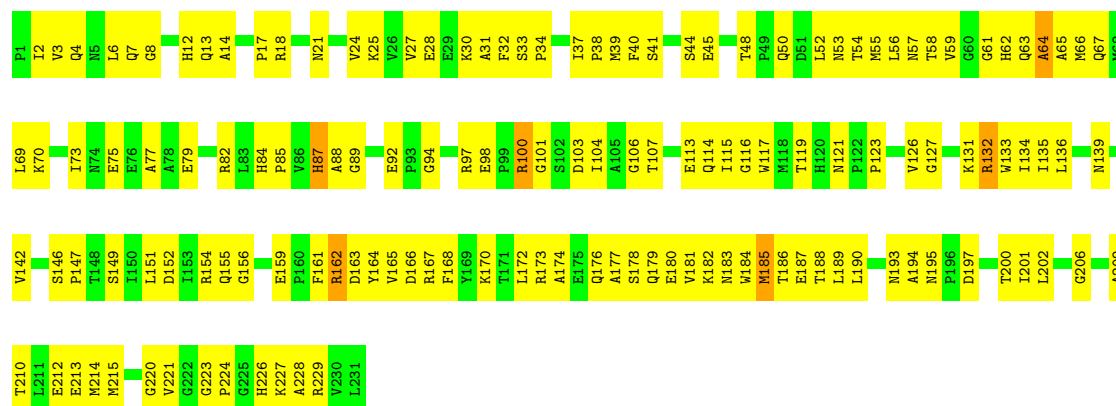
• Molecule 1: capsid protein

Chain as: 



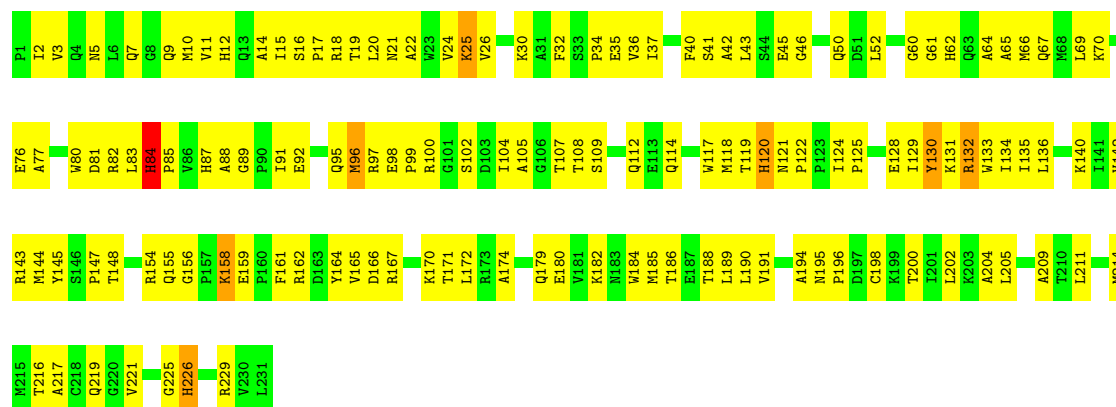
• Molecule 1: capsid protein

Chain at: 



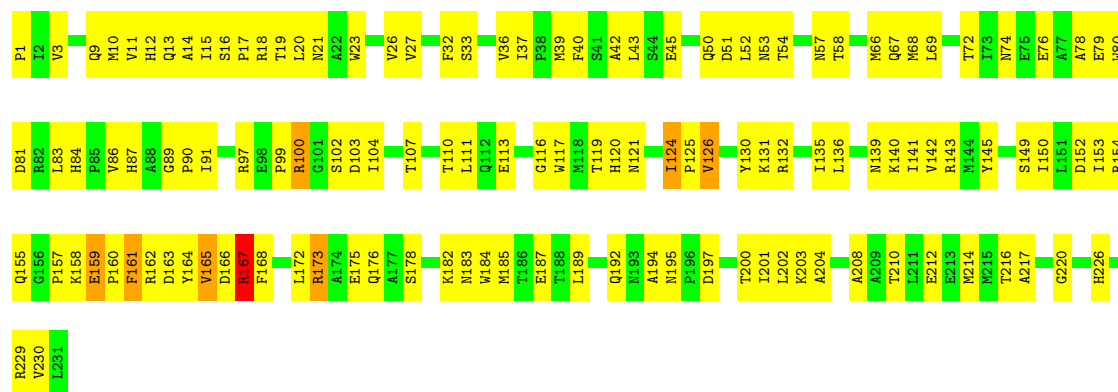
• Molecule 1: capsid protein

Chain 12: 



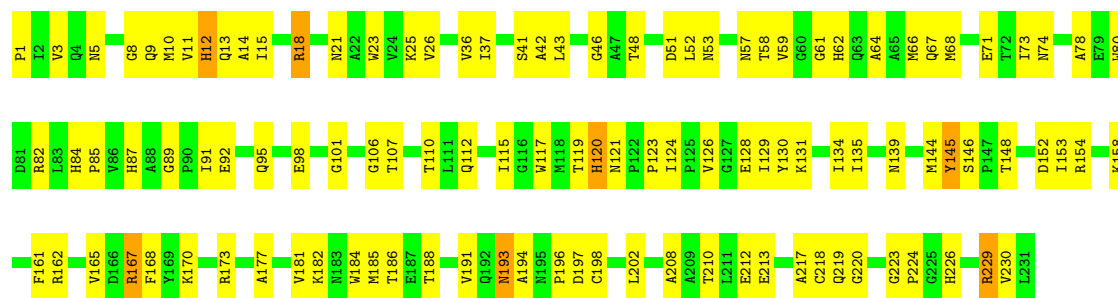
• Molecule 1: capsid protein

Chain au: 



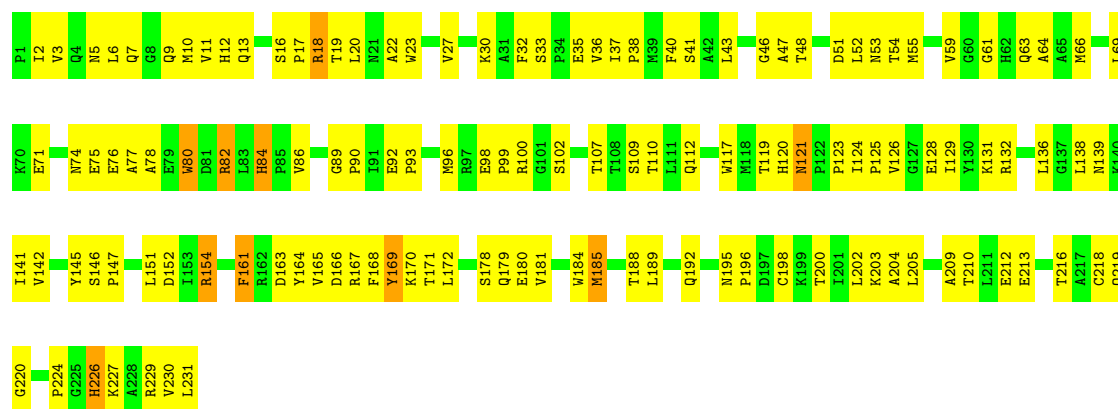
• Molecule 1: capsid protein

Chain av: 52% 45%



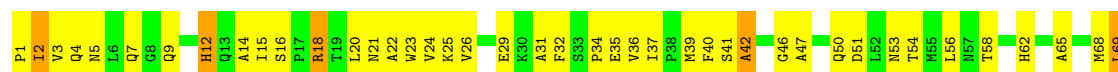
• Molecule 1: capsid protein

Chain aw: 44% 52%

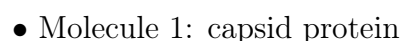


• Molecule 1: capsid protein

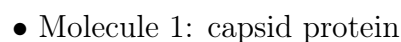
Chain ax: 42% 53%



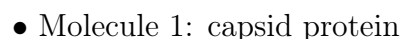
Response	Percentage
Yes, the U.S. is a threat to my country	48%
No, the U.S. is not a threat to my country	49%



Responsibility	Percentage
Current government	47%
Previous government	50%

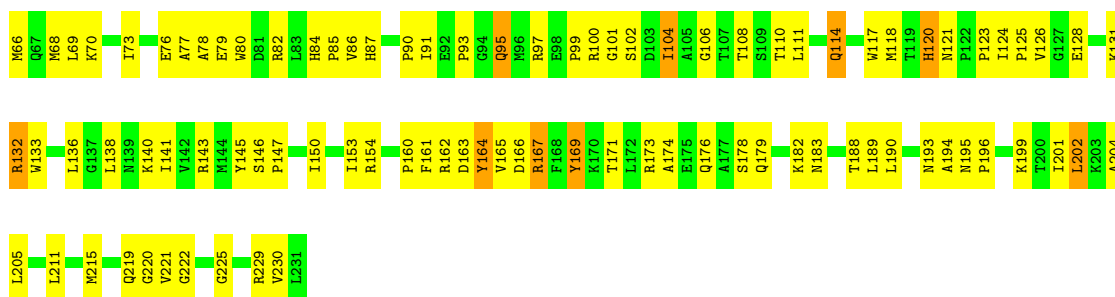


Frequency	Percentage
Often	49%
Not often	50%

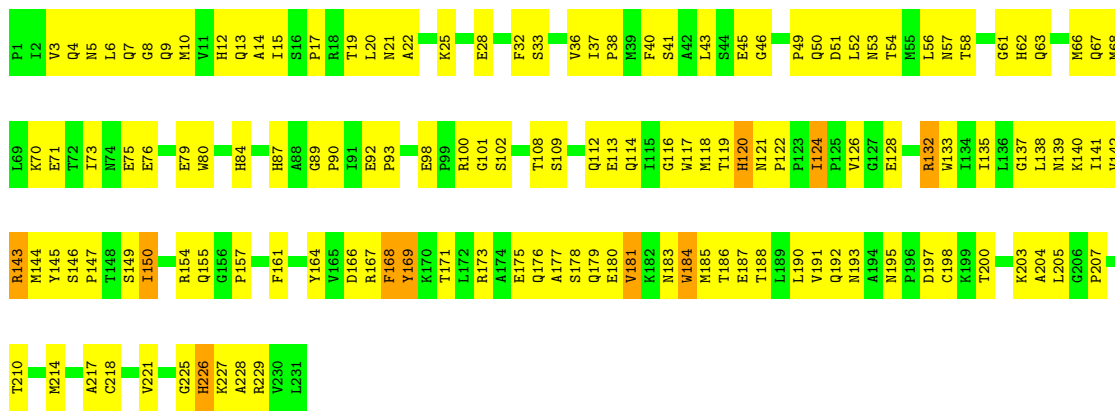


Response	Percentage
Yes, the U.S. is a democracy	43%
No, the U.S. is not a democracy	52%

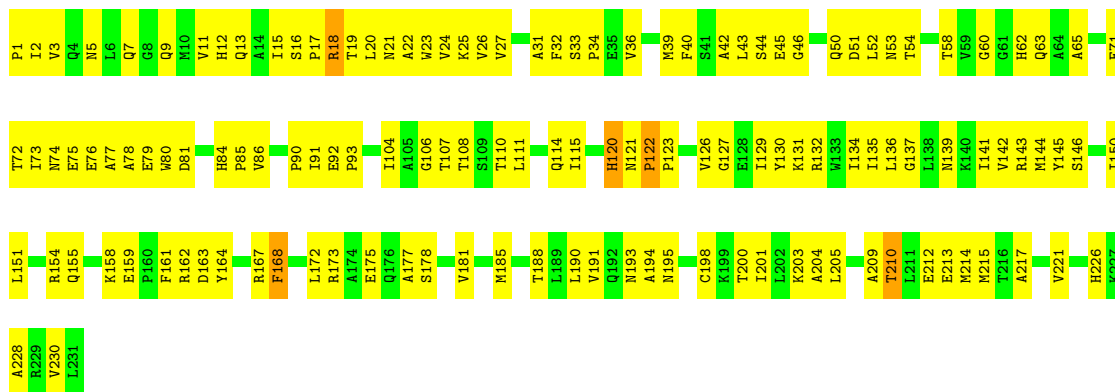




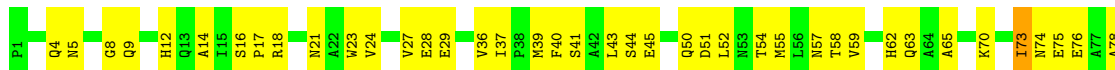
- Molecule 1: capsid protein

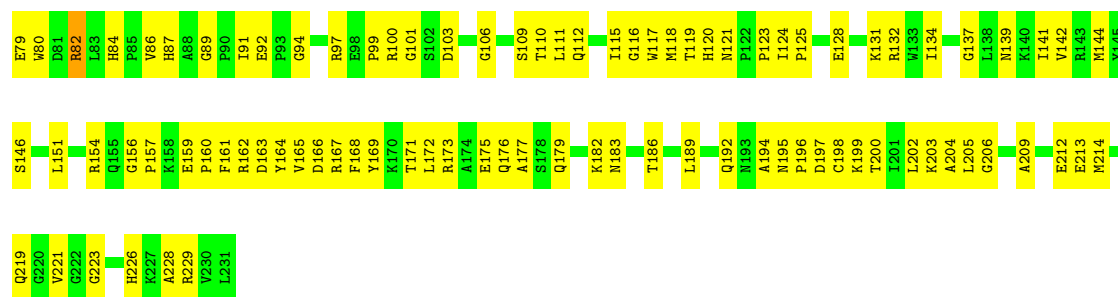


- Molecule 1: capsid protein



- Molecule 1: capsid protein





- Molecule 1: capsid protein

Chain aH: 44% 54%



- Molecule 1: capsid protein

Chain aI: 44% 55%



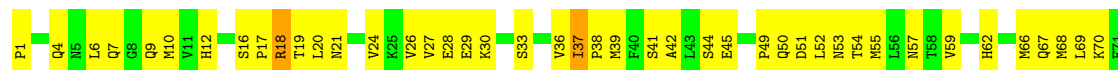
- Molecule 1: capsid protein

Chain aJ: 50% 48%





• Molecule 1: capsid protein

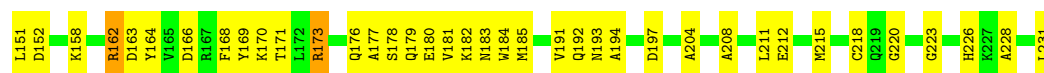


• Molecule 1: capsid protein

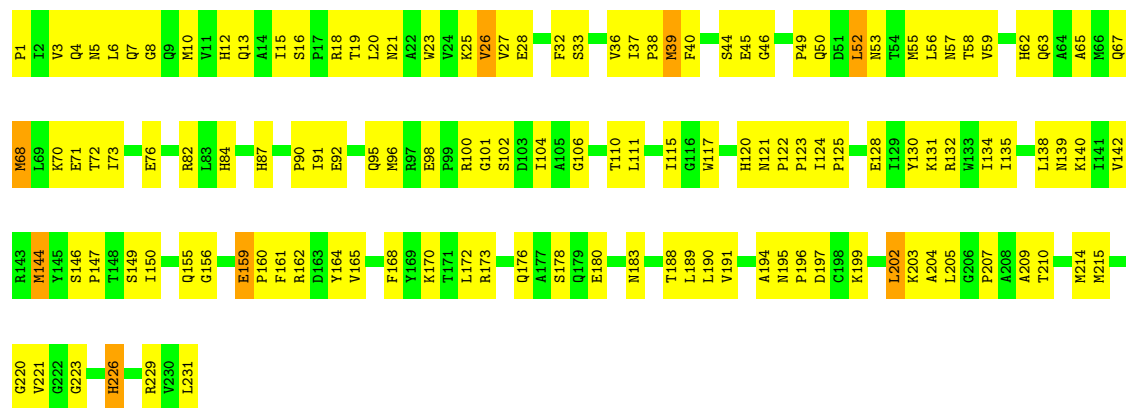


• Molecule 1: capsid protein

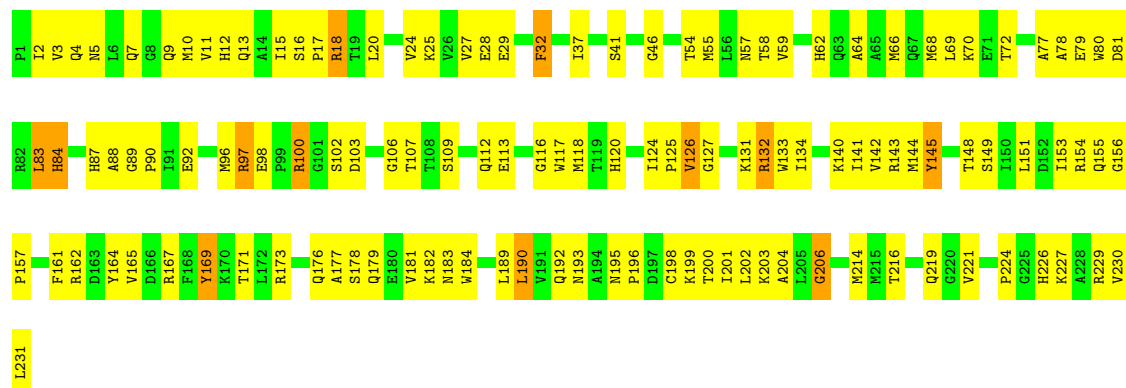




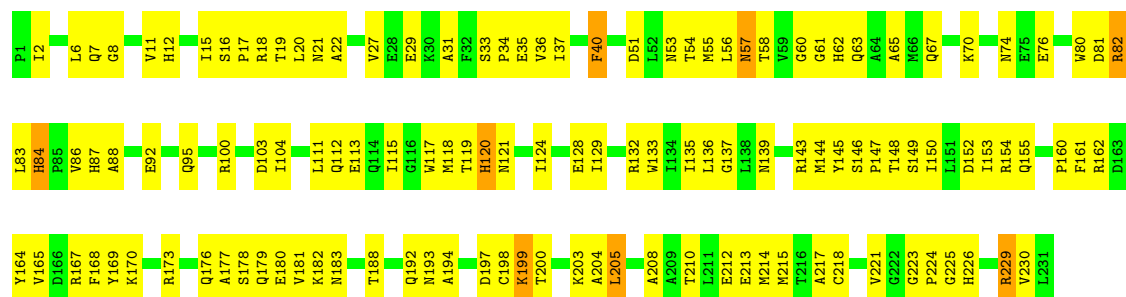
• Molecule 1: capsid protein



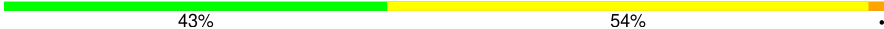
• Molecule 1: capsid protein



• Molecule 1: capsid protein



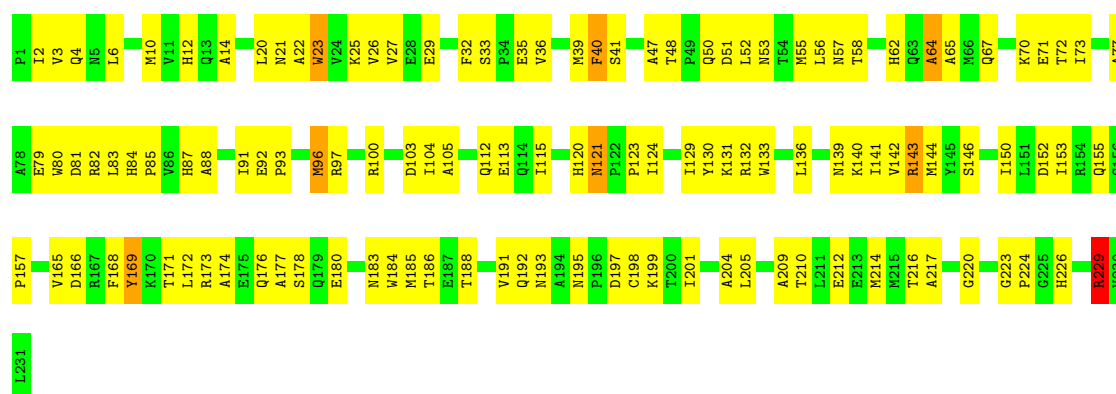
• Molecule 1: capsid protein

Chain aP: 



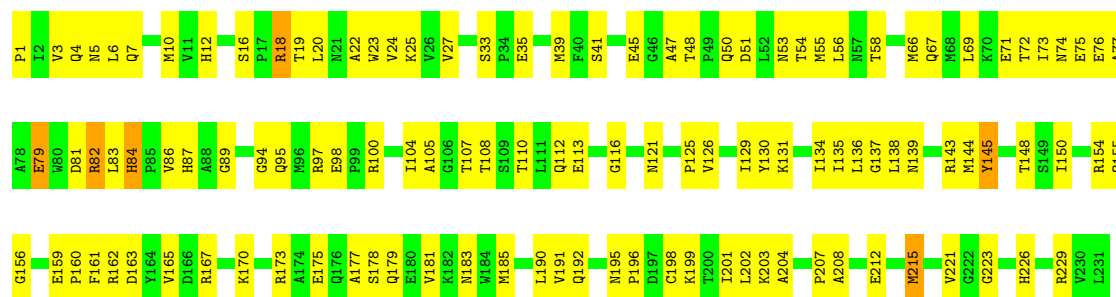
• Molecule 1: capsid protein

Chain aQ: 



• Molecule 1: capsid protein

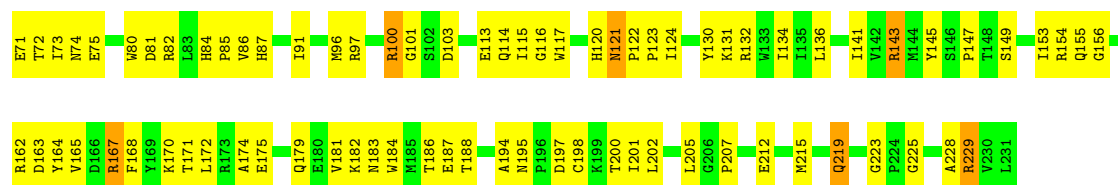
Chain aR: 



• Molecule 1: capsid protein

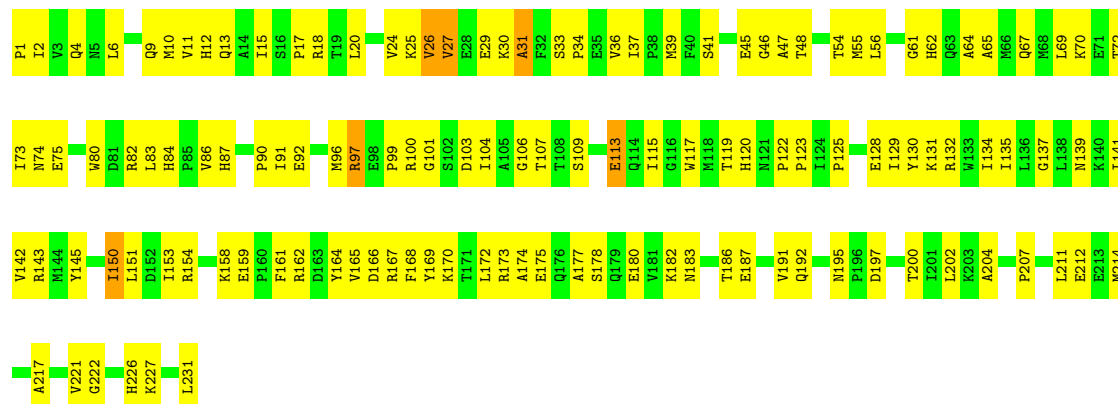
Chain aS: 





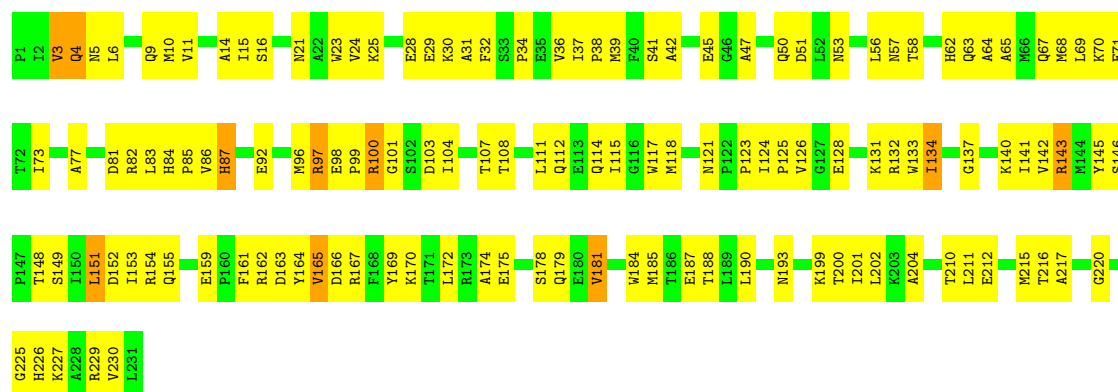
• Molecule 1: capsid protein

Chain aT: 45% 52%



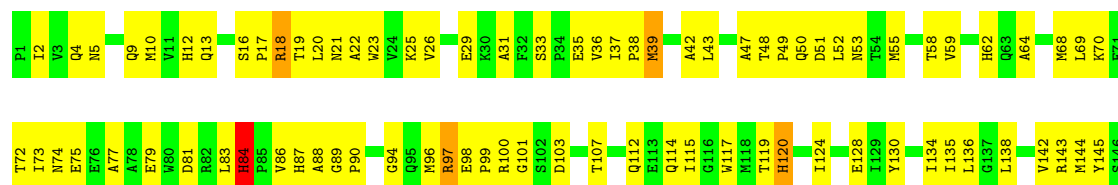
• Molecule 1: capsid protein

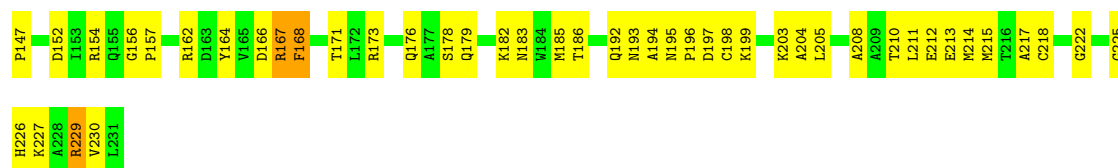
Chain aU: 43% 53%



• Molecule 1: capsid protein

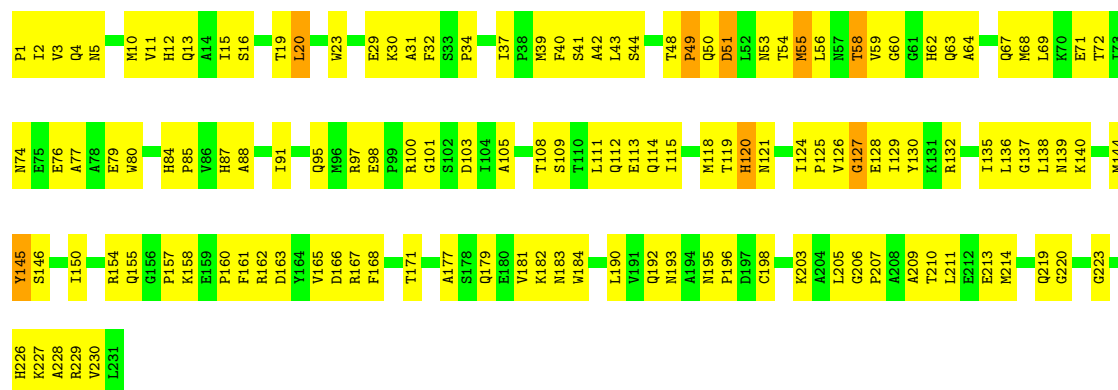
Chain aV: 45% 52%





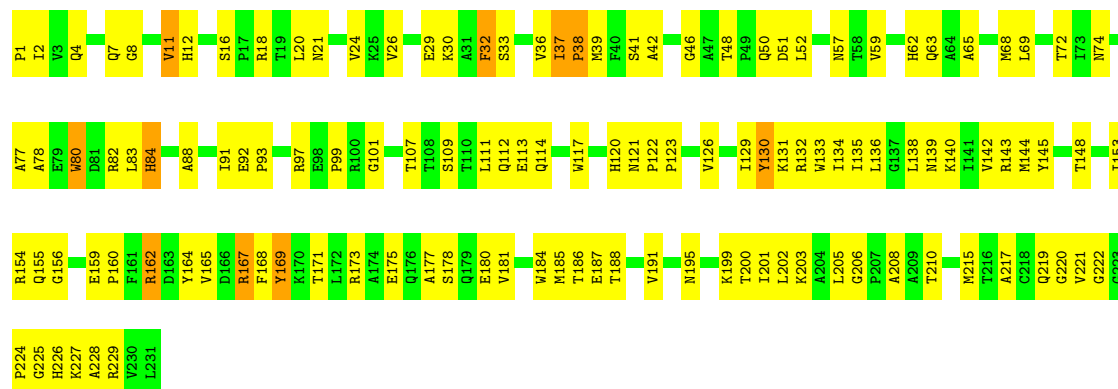
• Molecule 1: capsid protein

Chain aW: 42% 54%



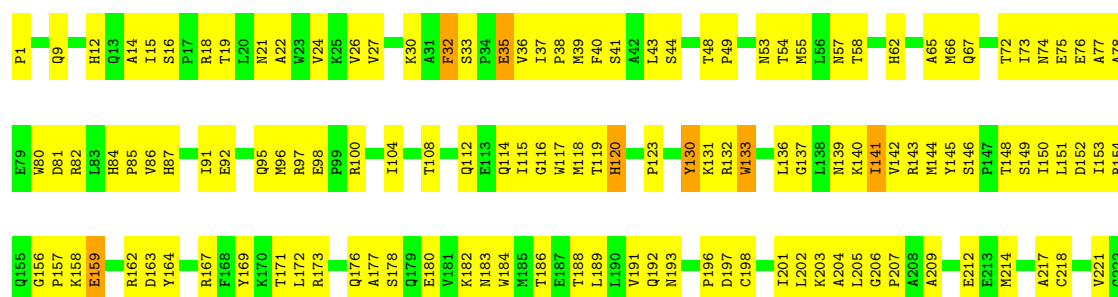
• Molecule 1: capsid protein

Chain aX: 46% 50%



• Molecule 1: capsid protein

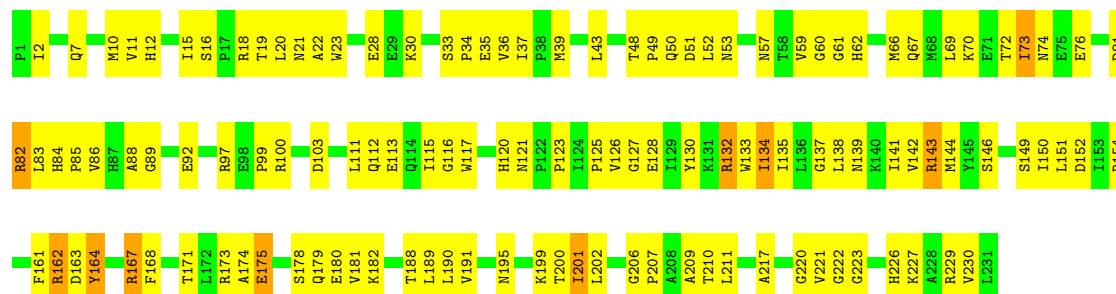
Chain 15: 41% 56%



G223
P224
G225
H226
K227
A228
R229
V230
L231

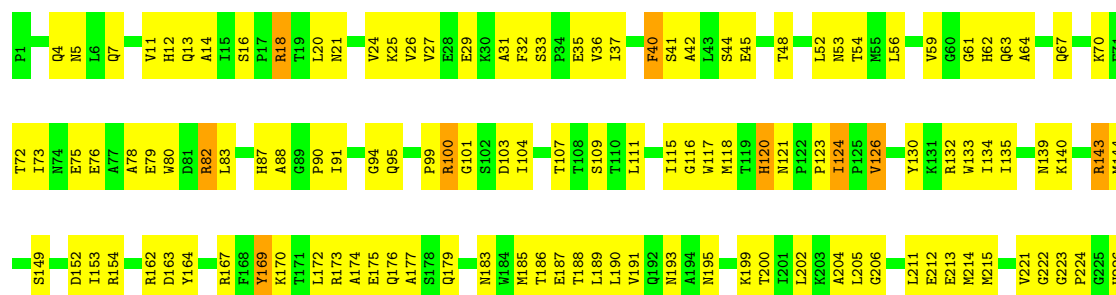
• Molecule 1: capsid protein

Chain aY: 47% 49%



• Molecule 1: capsid protein

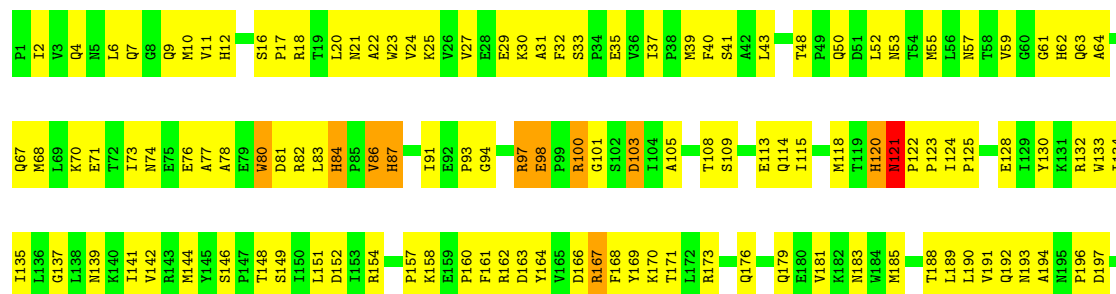
Chain aZ: 45% 51%



K227
A228
R229
V230
L231

• Molecule 1: capsid protein

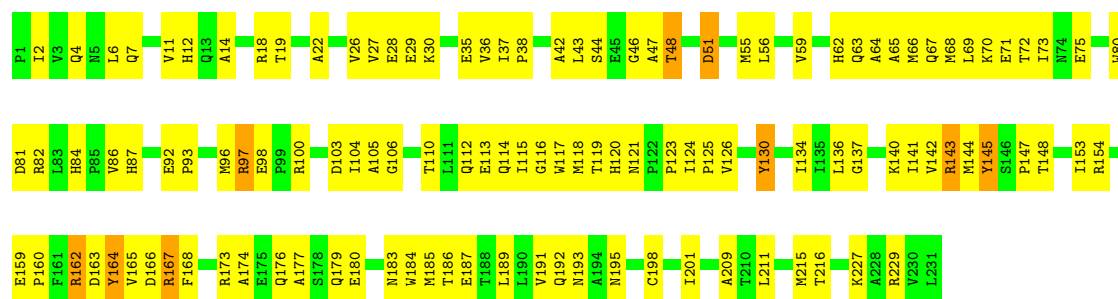
Chain b0: 39% 55% 5%



T200, I201, L202, L205, G206, P207, A208, E212, E213, K214, H215, T216, A217, C218, Q219, D220, V221, G222, G223, G225, H226, K227, A228, R229, V230, L231

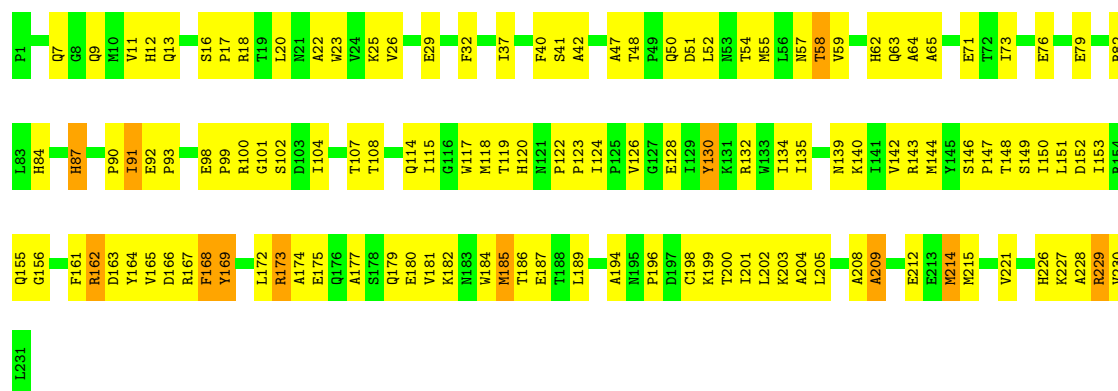
• Molecule 1: capsid protein

Chain b1: 



• Molecule 1: capsid protein

Chain b2: 



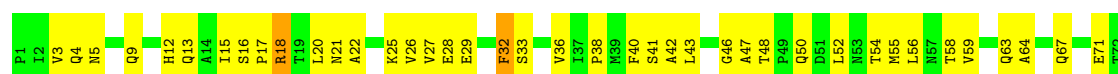
• Molecule 1: capsid protein

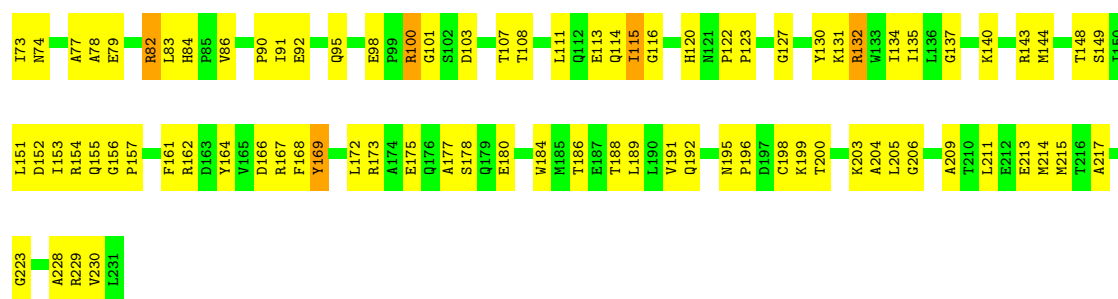
Chain b3: 



• Molecule 1: capsid protein

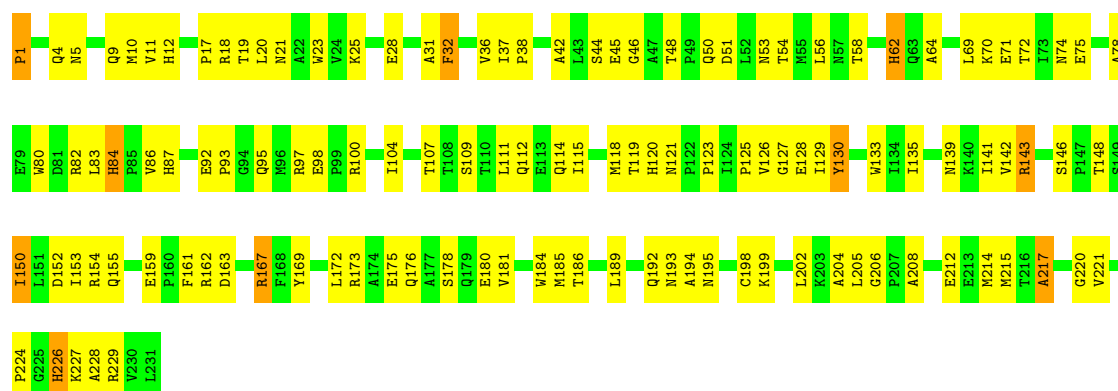
Chain b4: 





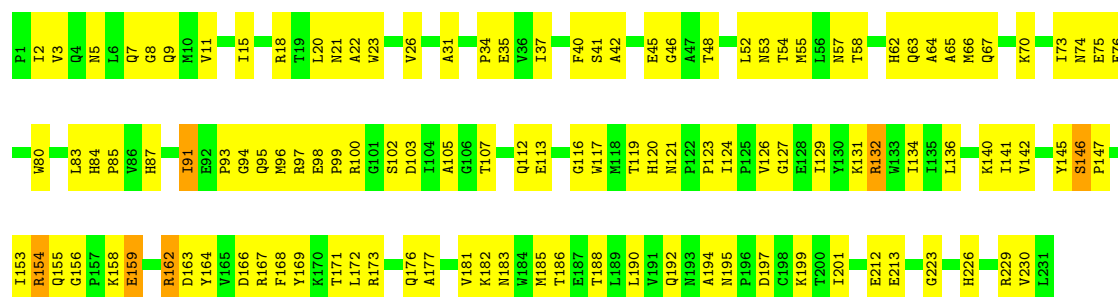
- Molecule 1: capsid protein

Chain b5: 47% 48%



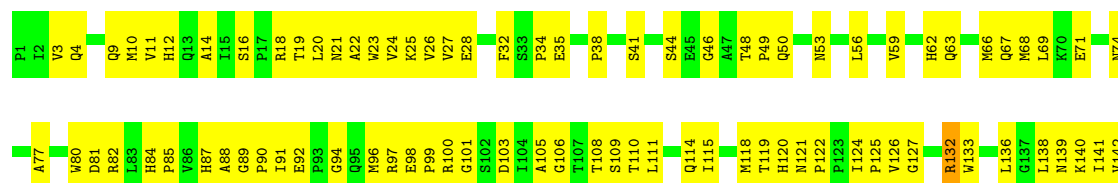
- Molecule 1: capsid protein

Chain b6: 49% 48%



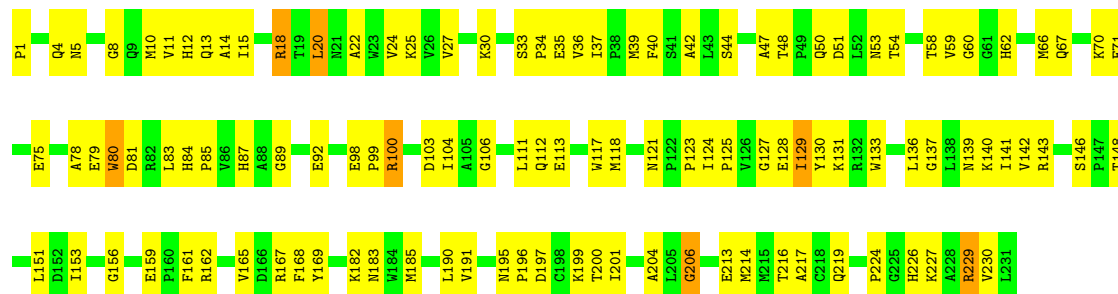
- Molecule 1: capsid protein

Chain b7: 43% 55%

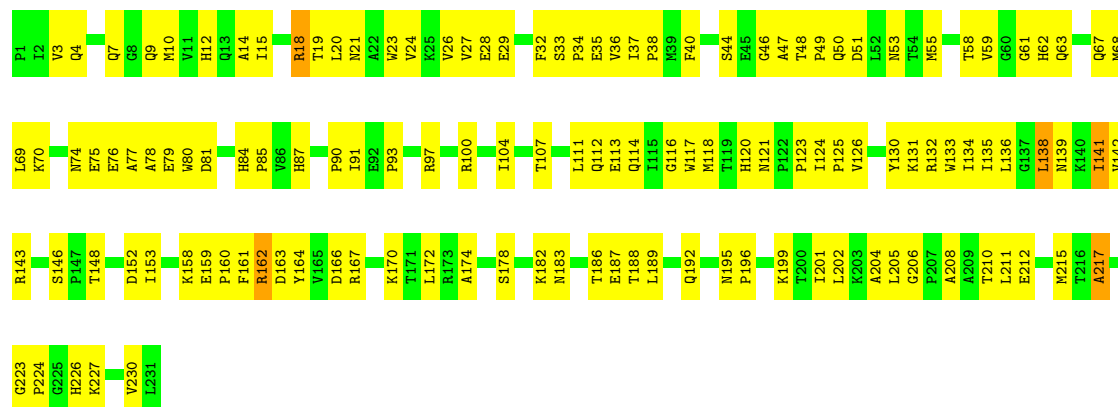




• Molecule 1: capsid protein



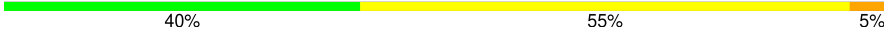
• Molecule 1: capsid protein

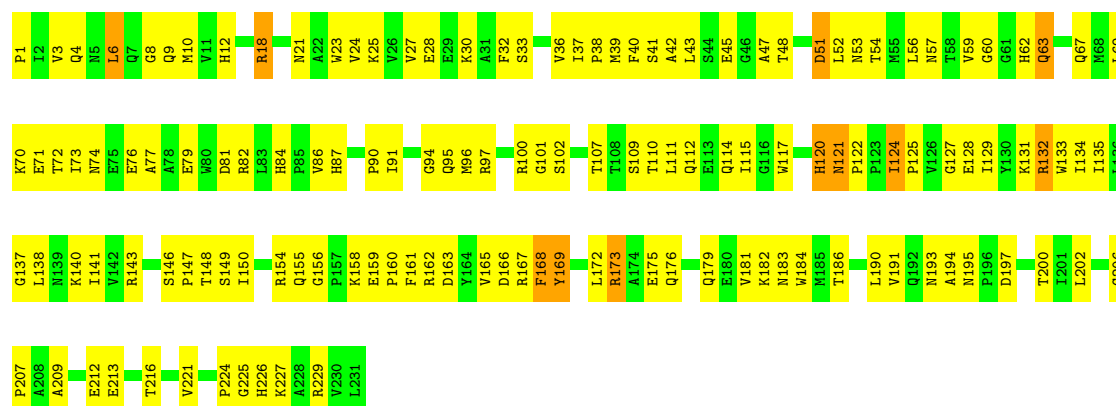


• Molecule 1: capsid protein

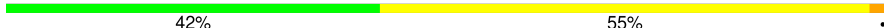


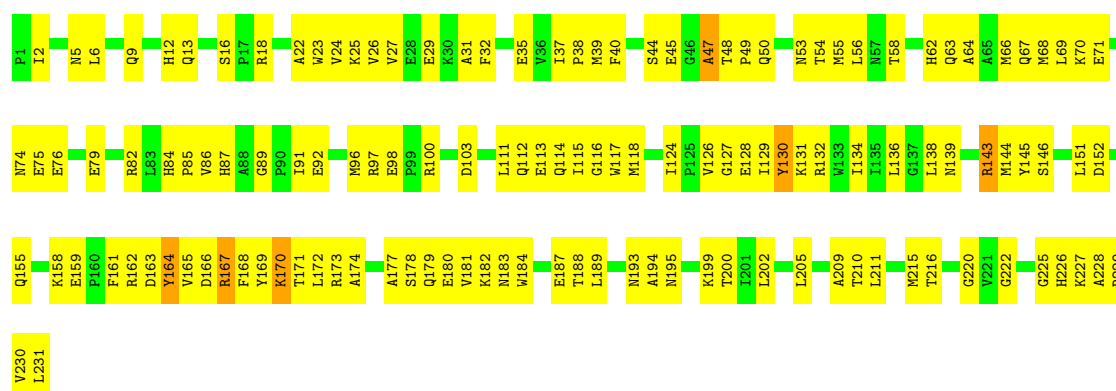
• Molecule 1: capsid protein

Chain ba: 



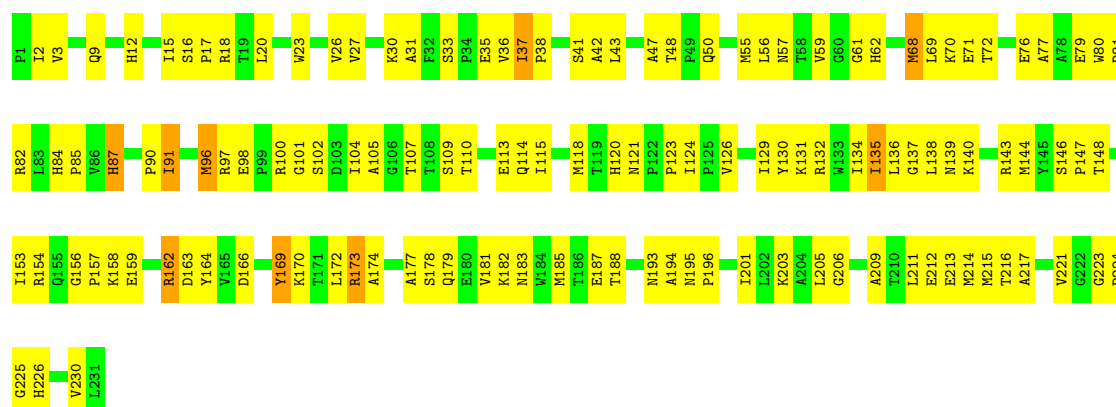
• Molecule 1: capsid protein

Chain bb: 



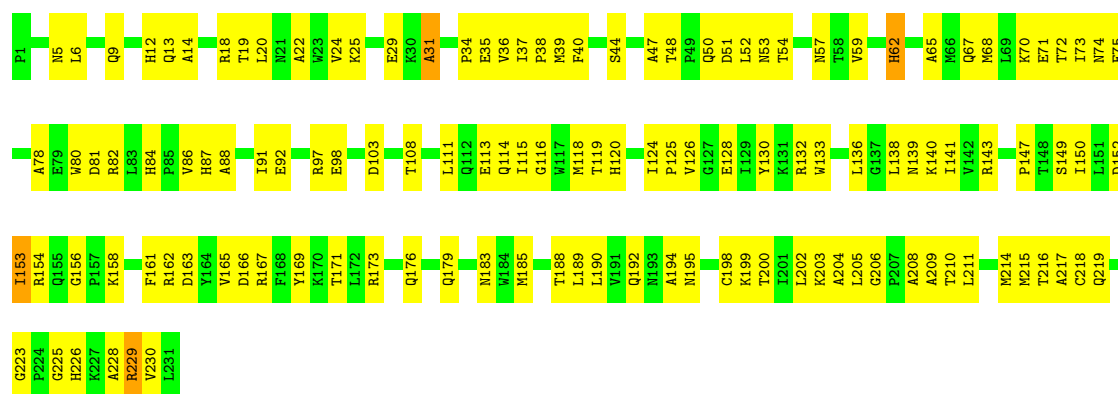
• Molecule 1: capsid protein

Chain bc: 



• Molecule 1: capsid protein

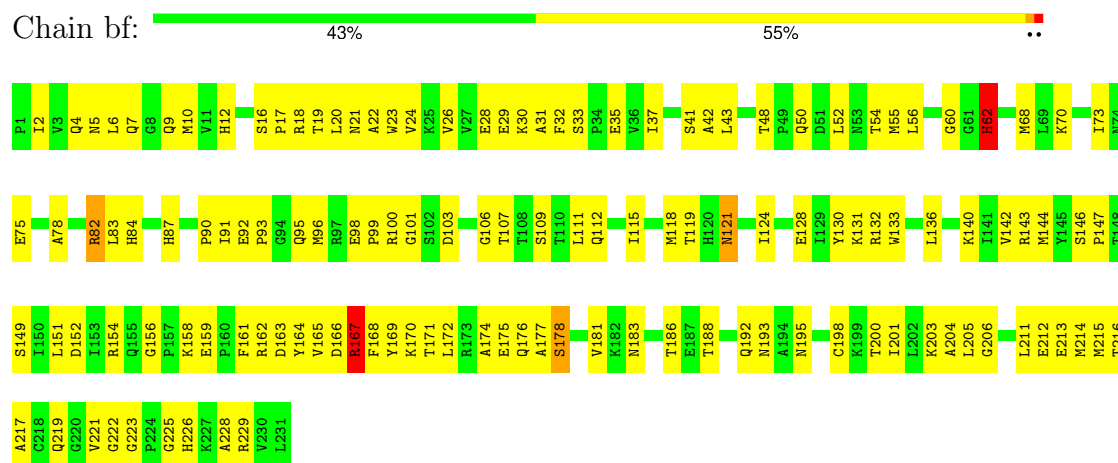
Chain bd: 



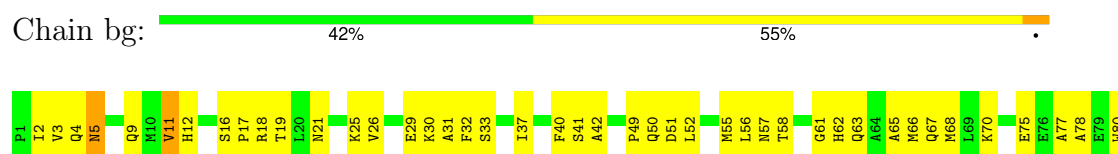
• Molecule 1: capsid protein

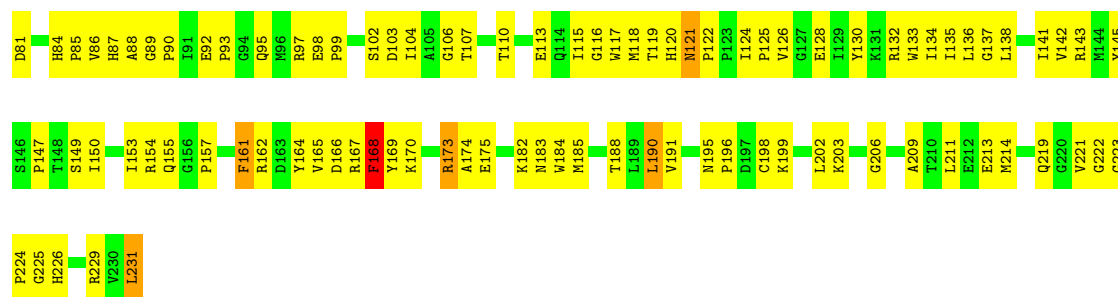


• Molecule 1: capsid protein

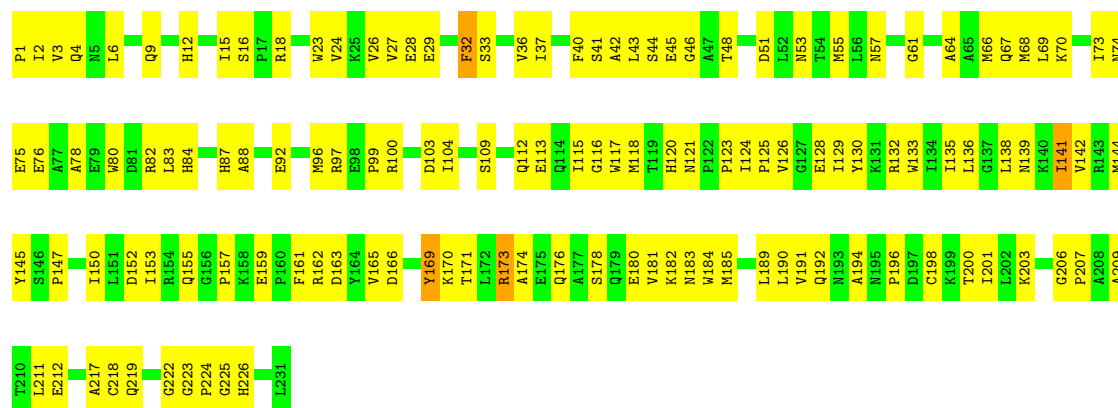


• Molecule 1: capsid protein

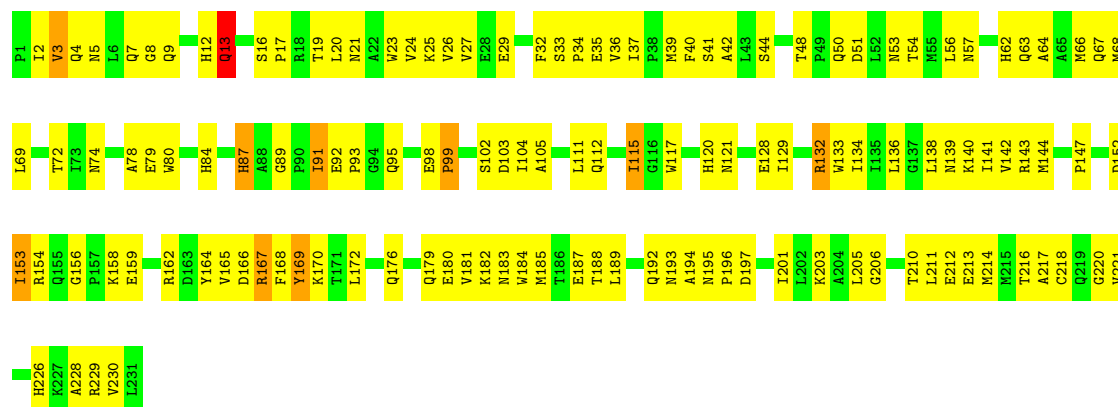




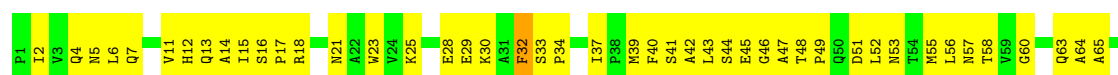
- Molecule 1: capsid protein



- Molecule 1: capsid protein



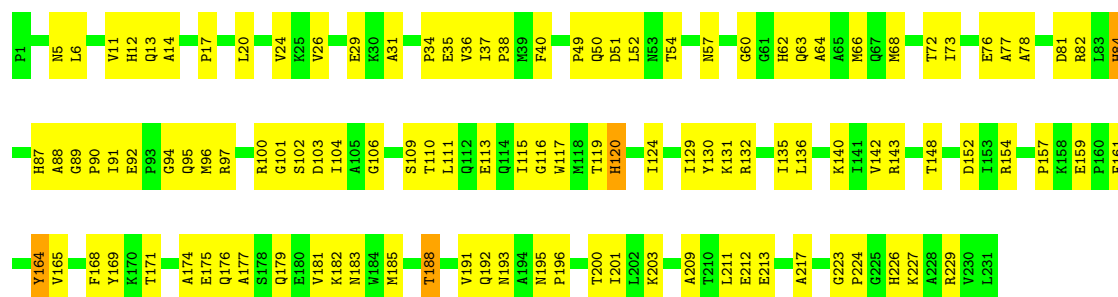
- Molecule 1: capsid protein





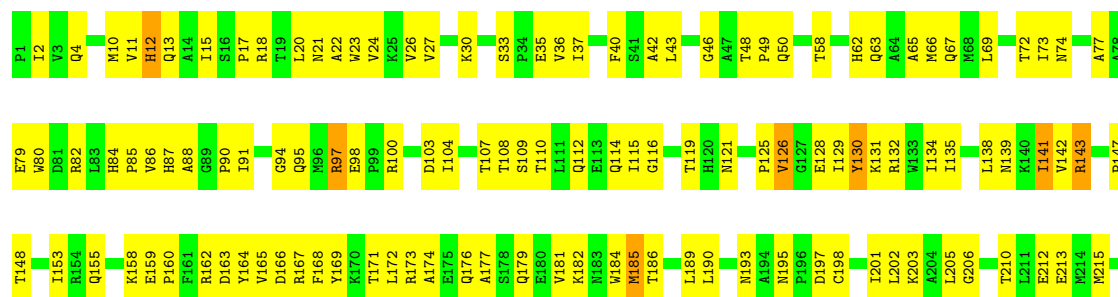
- Molecule 1: capsid protein

Chain bj: 52% 47%



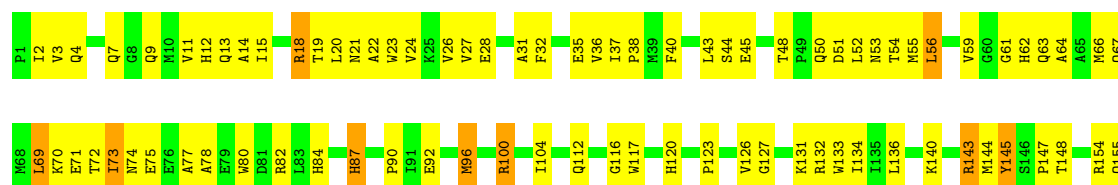
- Molecule 1: capsid protein

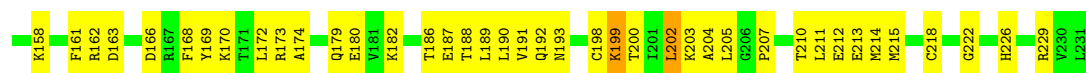
Chain bk: 45% 52%



- Molecule 1: capsid protein

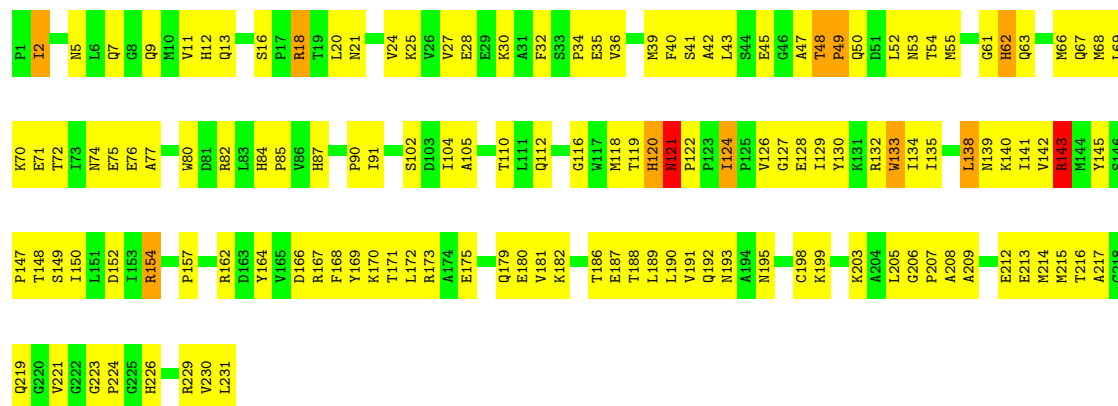
Chain bl: 47% 48% 5%





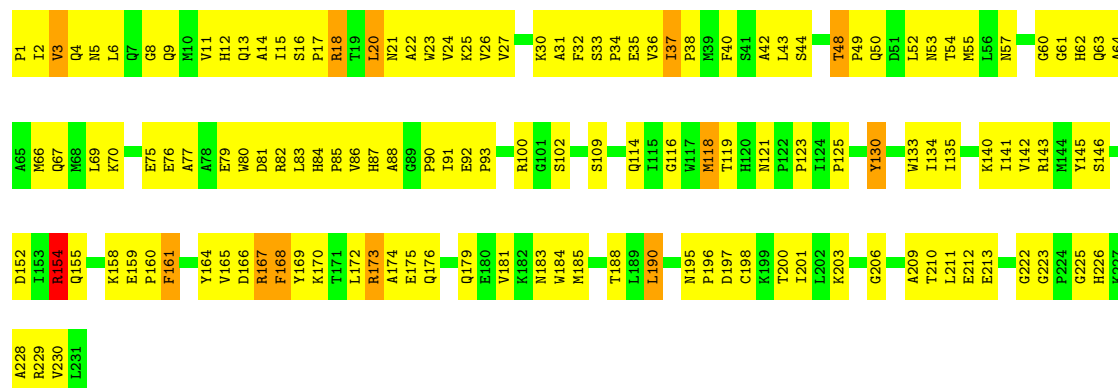
• Molecule 1: capsid protein

Chain bm: 41% 54%



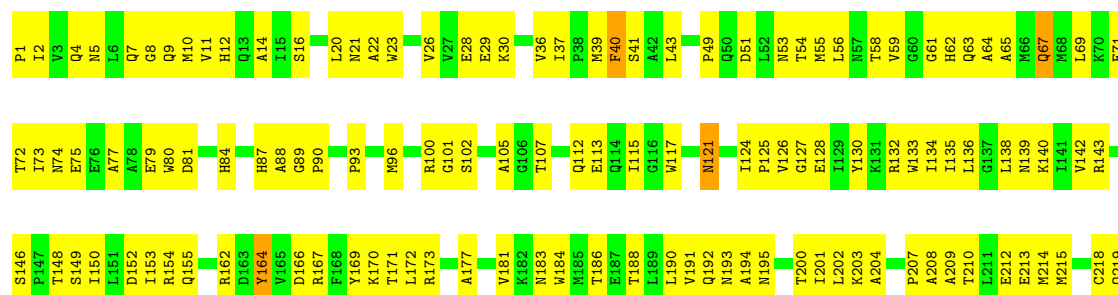
• Molecule 1: capsid protein

Chain bn: 41% 54% 5%



• Molecule 1: capsid protein

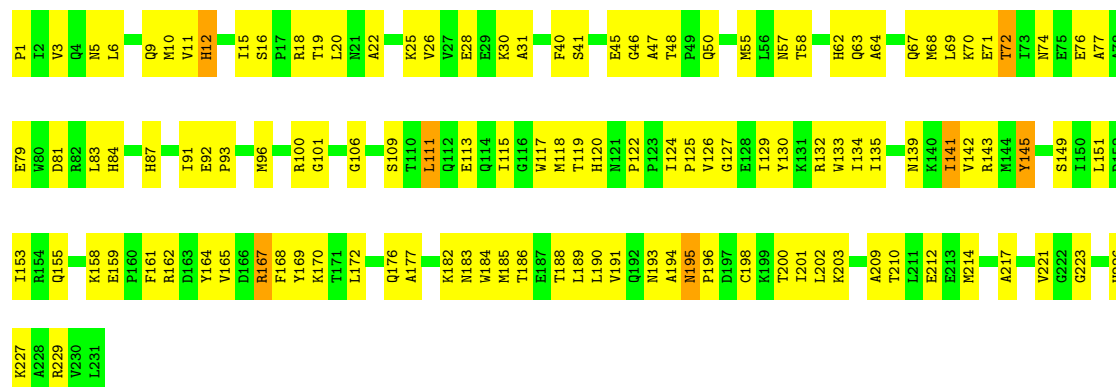
Chain bo: 44% 55%





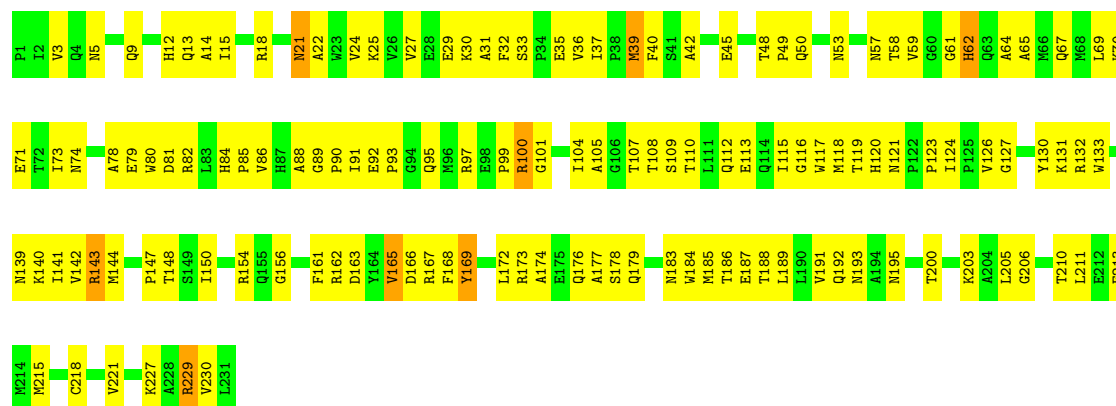
- Molecule 1: capsid protein

Chain bp:  47% 50%



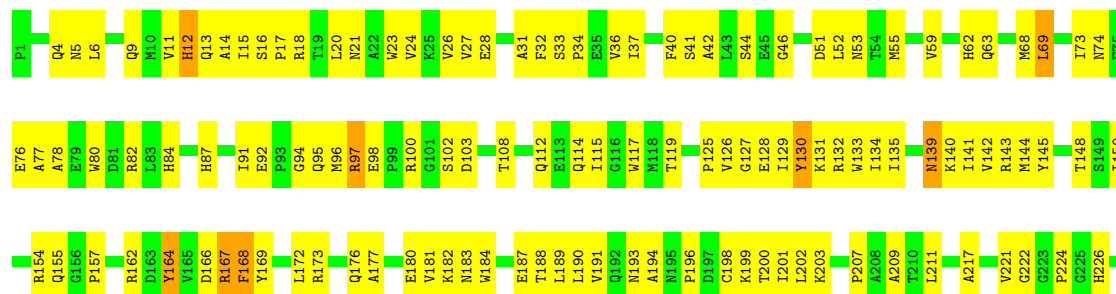
- Molecule 1: capsid protein

Chain bq:  42% 55%

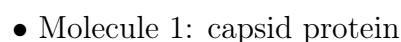


- Molecule 1: capsid protein

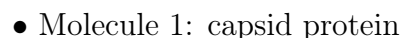
Chain br:  45% 51%



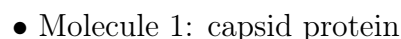
Response	Percentage
Yes, it is a crisis	42%
No, it is not a crisis	55%



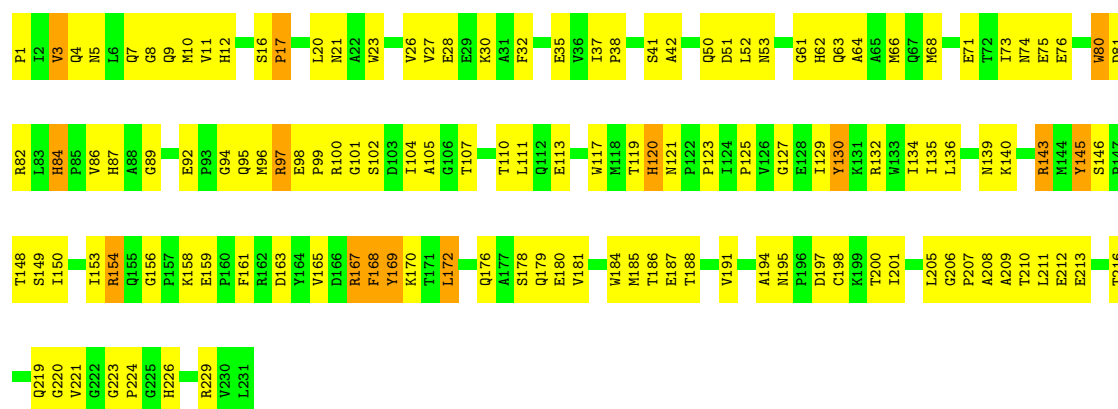
Response	Percentage
Democracy	45%
Dictatorship	51%



Response	Percentage
Yes	41%
No	54%
Don't know	5%

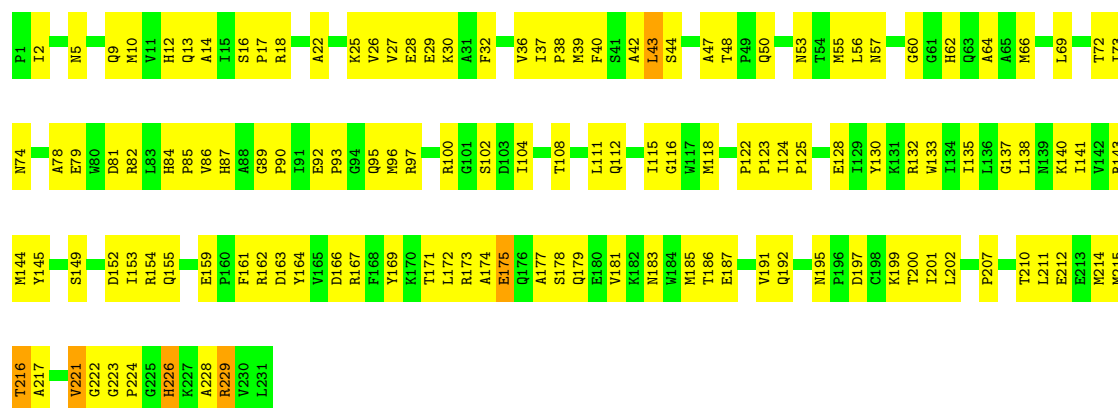


Response	Percentage
U.S. should take more action	43%
U.S. should take less action	51%
U.S. should take the same amount of action	6%



• Molecule 1: capsid protein

Chain by: 44% 54%



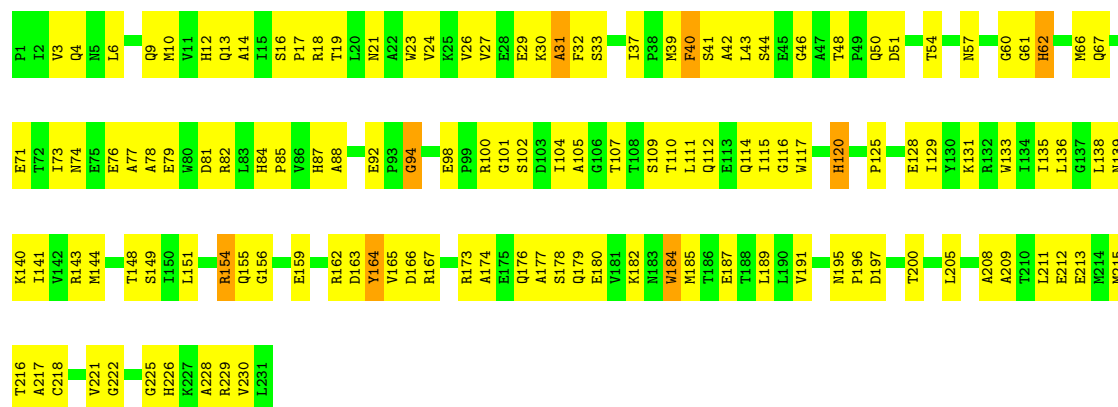
• Molecule 1: capsid protein

Chain bz: 42% 54%



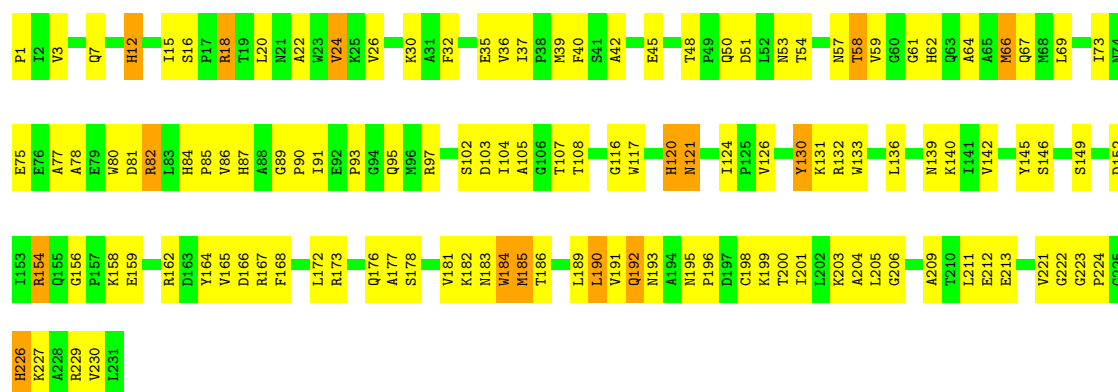
• Molecule 1: capsid protein

Chain ba: 43% 53%



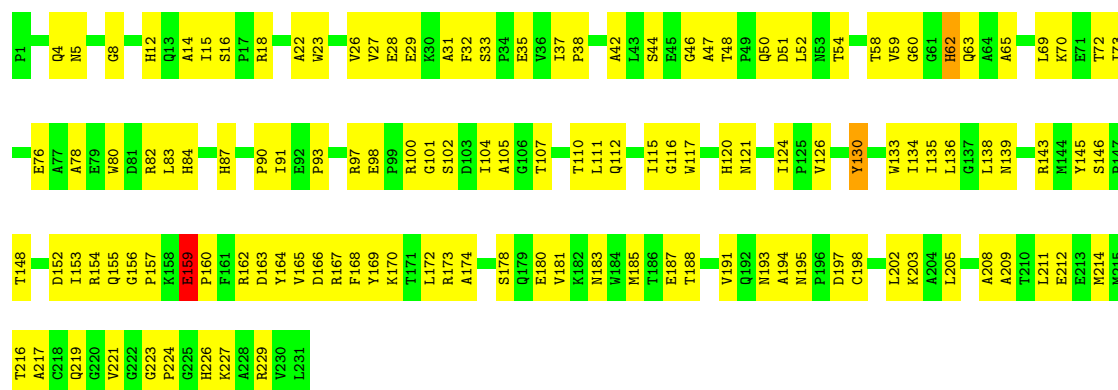
• Molecule 1: capsid protein

Chain bB: 47% 47% 6%



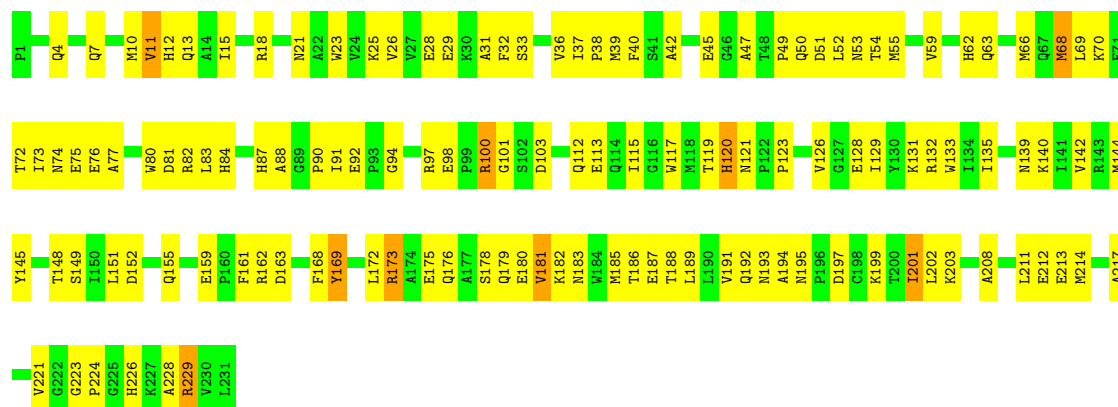
• Molecule 1: capsid protein

Chain 19: 45% 54%

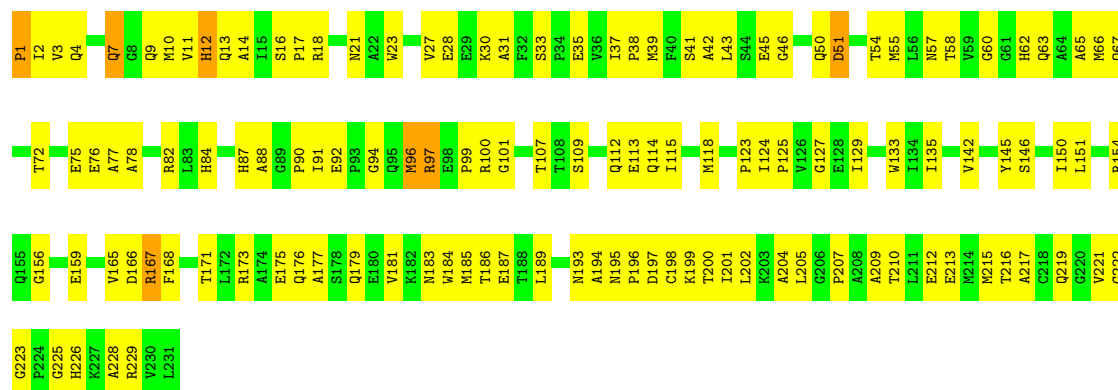


• Molecule 1: capsid protein

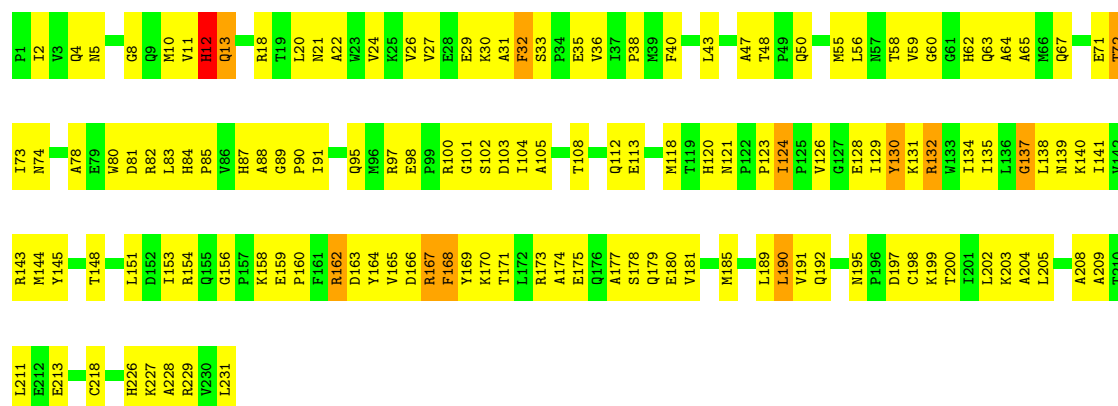
Chain bC: 44% 52%



- Molecule 1: capsid protein



- Molecule 1: capsid protein



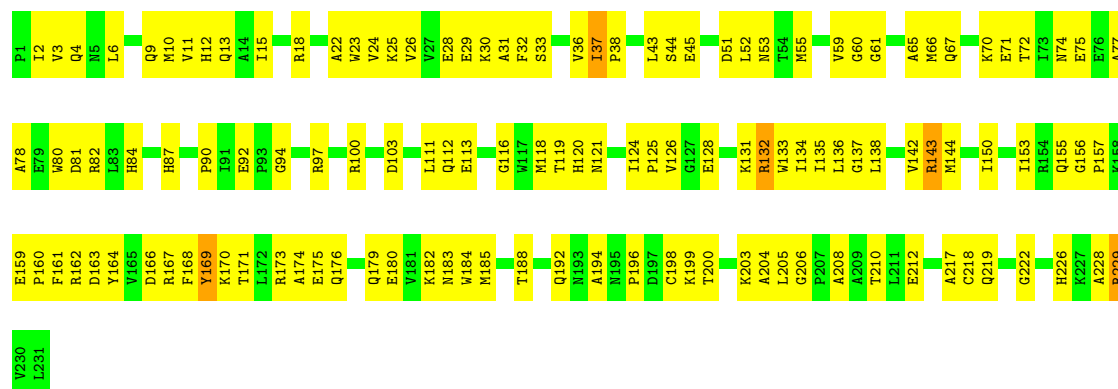
- Molecule 1: capsid protein





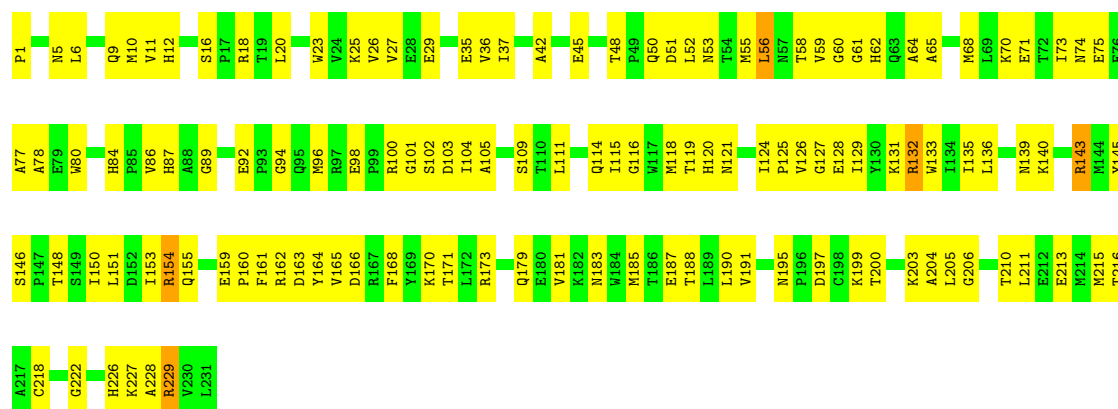
• Molecule 1: capsid protein

Chain bG: 45% 53%



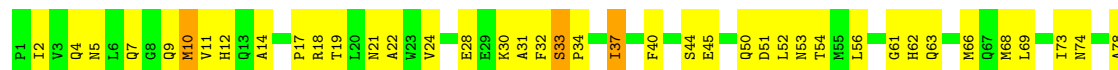
• Molecule 1: capsid protein

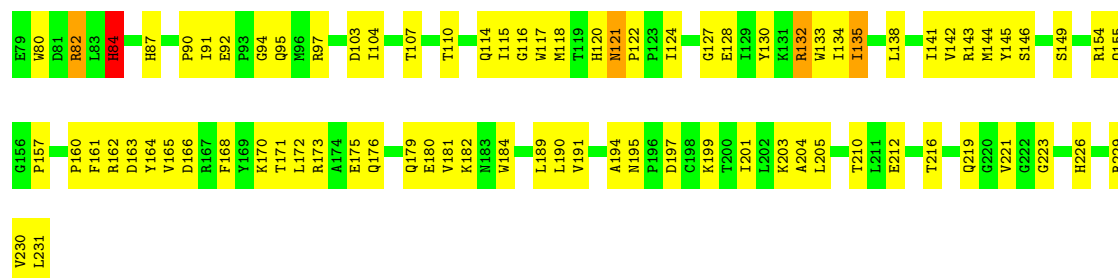
Chain bH: 45% 53%



• Molecule 1: capsid protein

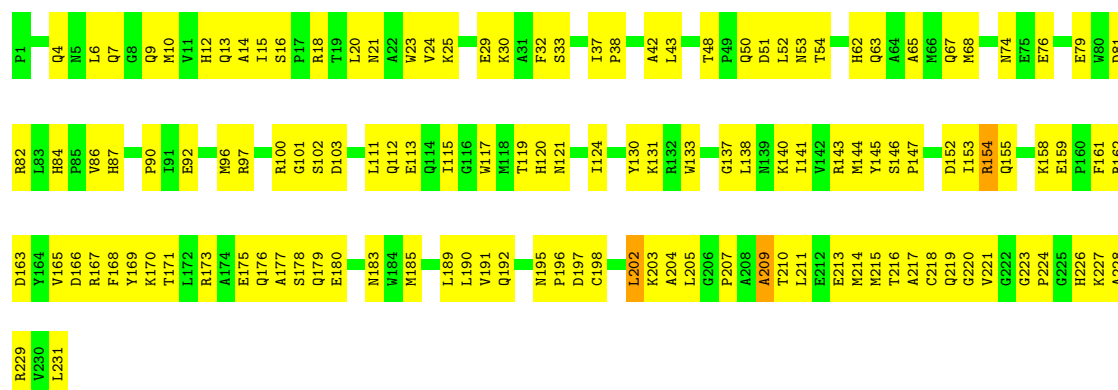
Chain bI: 48% 49%





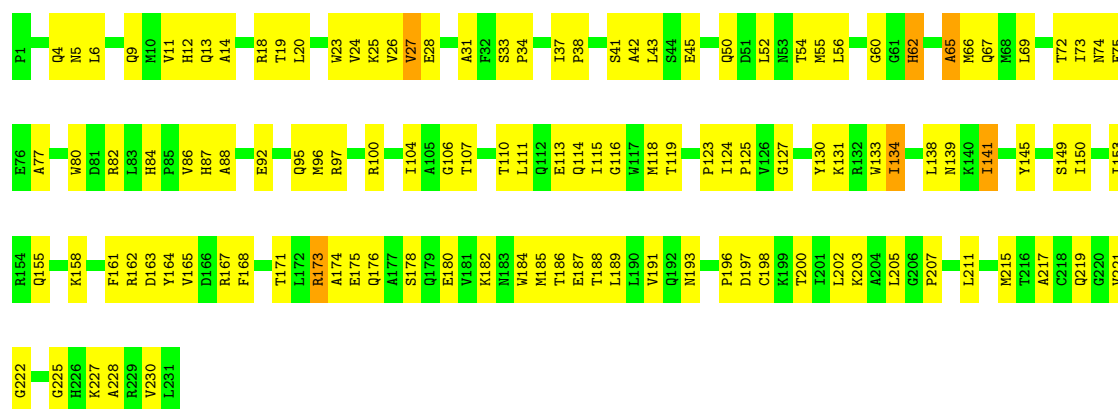
- Molecule 1: capsid protein

Chain bJ: 44% 55%



- Molecule 1: capsid protein

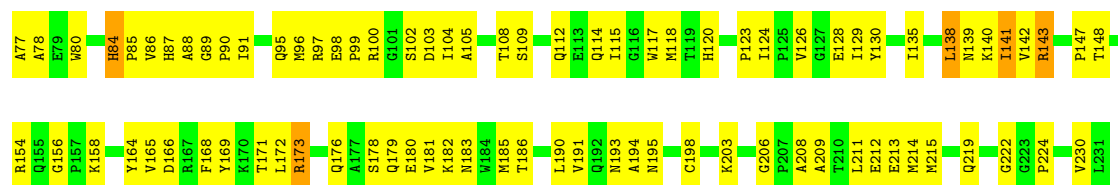
Chain bK: 47% 50%



- Molecule 1: capsid protein

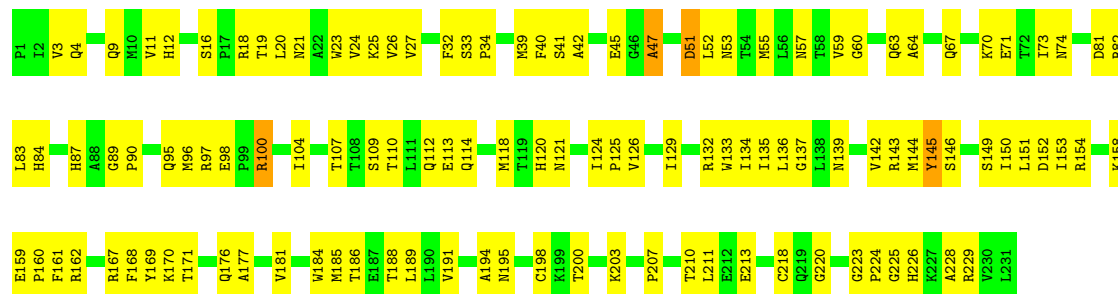
Chain bL: 47% 49%





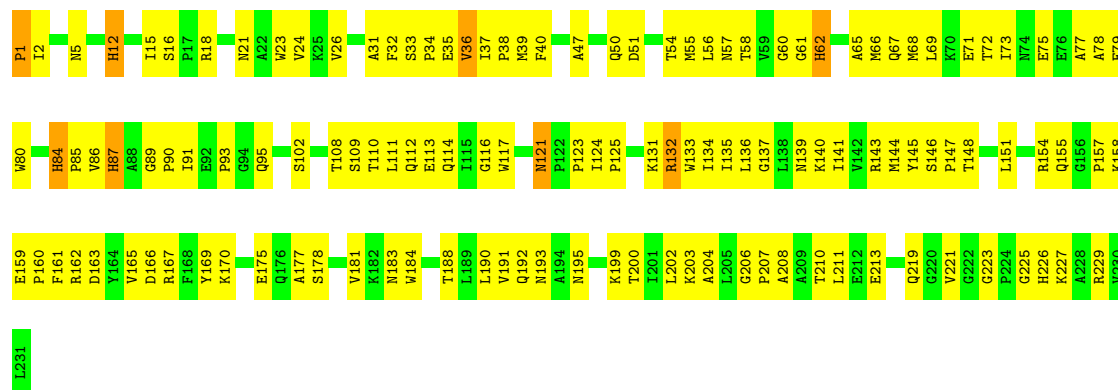
• Molecule 1: capsid protein

Chain 1a: 49% 49%



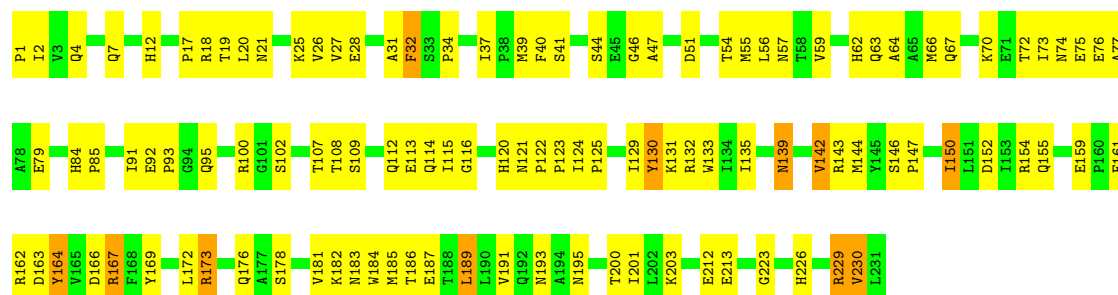
• Molecule 1: capsid protein

Chain 1bM: 44% 52%



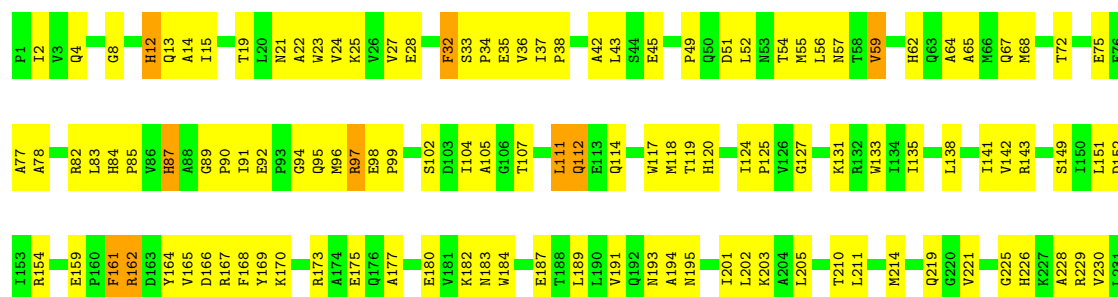
• Molecule 1: capsid protein

Chain 1bN: 51% 44% 5%

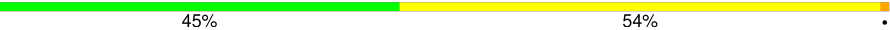


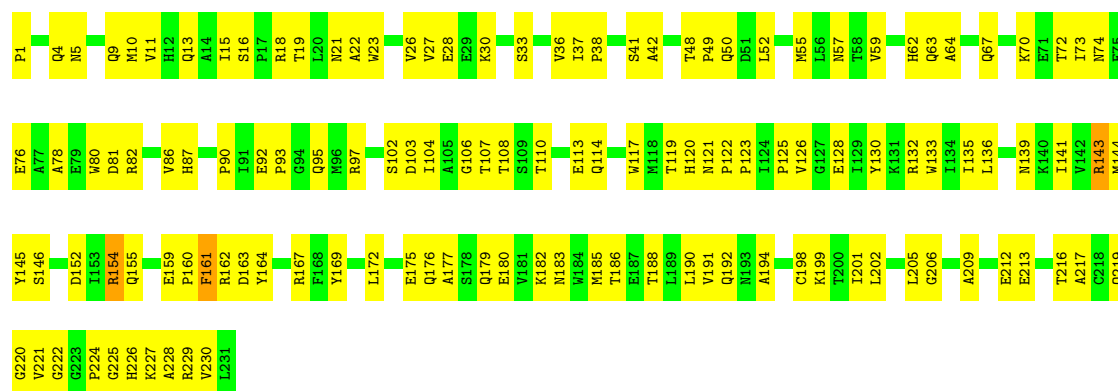
• Molecule 1: capsid protein

Chain bO: 



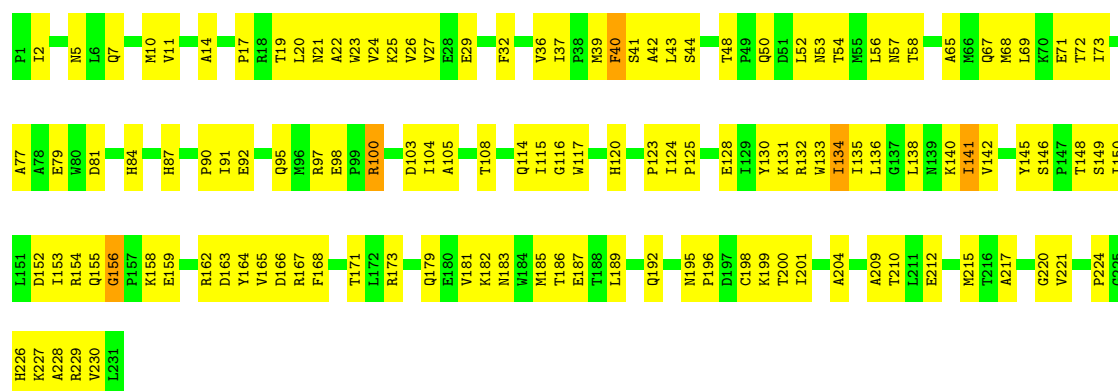
• Molecule 1: capsid protein

Chain bP: 

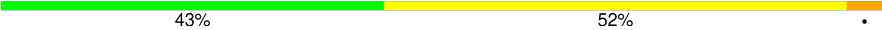


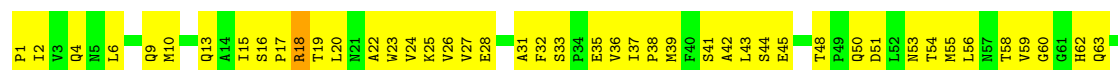
• Molecule 1: capsid protein

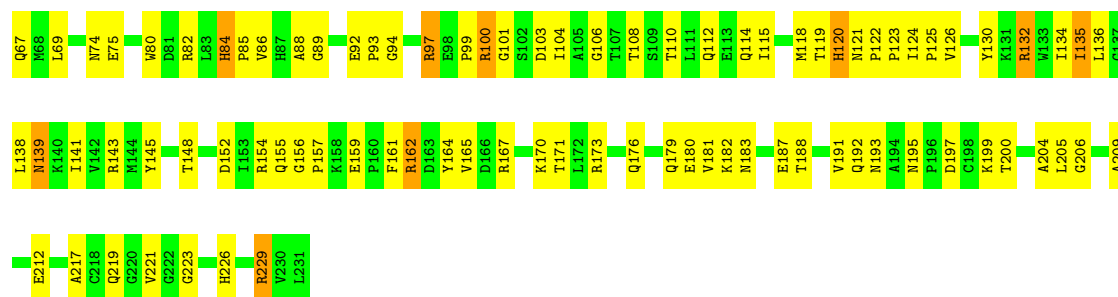
Chain bQ: 



• Molecule 1: capsid protein

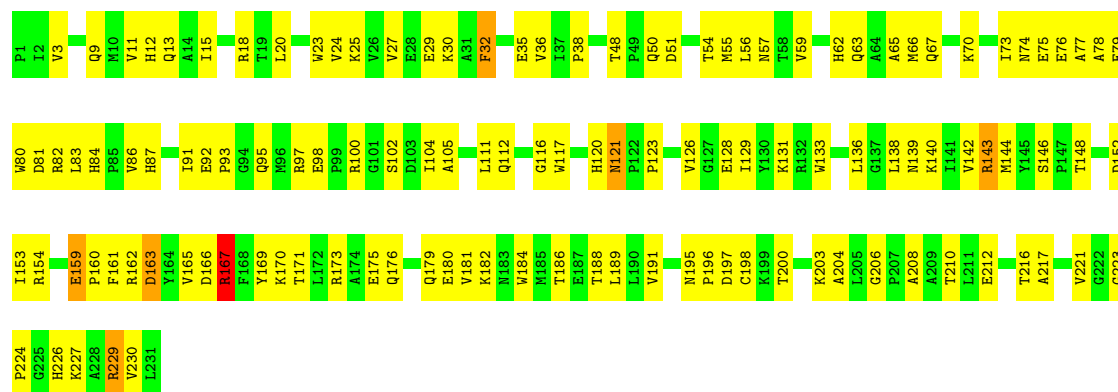
Chain bR: 





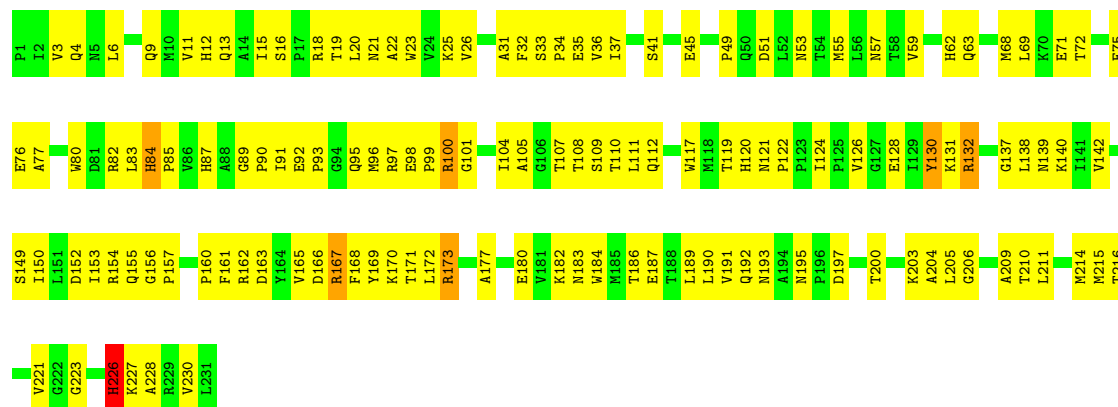
• Molecule 1: capsid protein

Chain bS: 47% 50%



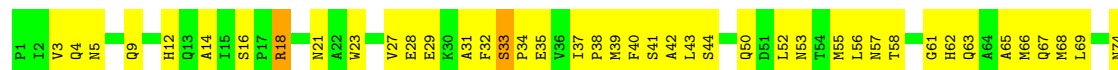
• Molecule 1: capsid protein

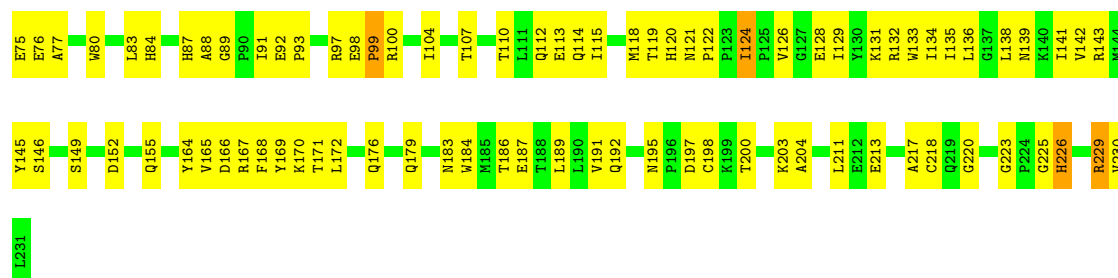
Chain bT: 42% 55%



• Molecule 1: capsid protein

Chain bU: 46% 51%





- Molecule 1: capsid protein

Chain bV: 44% 53%



- Molecule 1: capsid protein

Chain 1b: 45% 53%

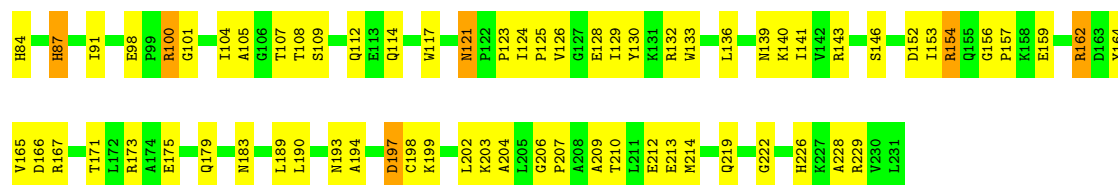


- Molecule 1: capsid protein

Chain bW: 43% 55%

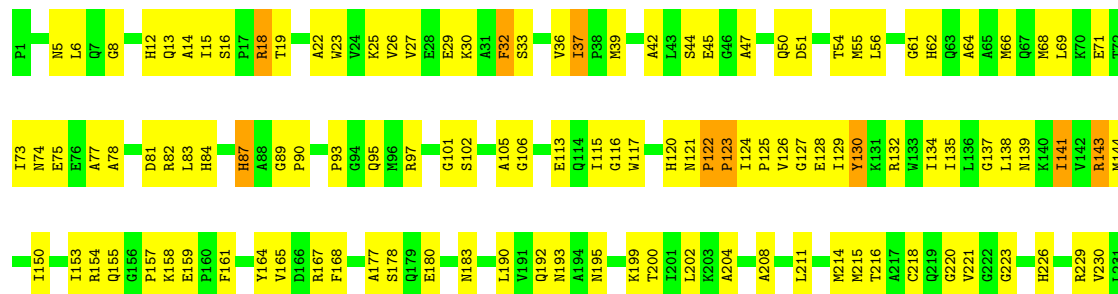






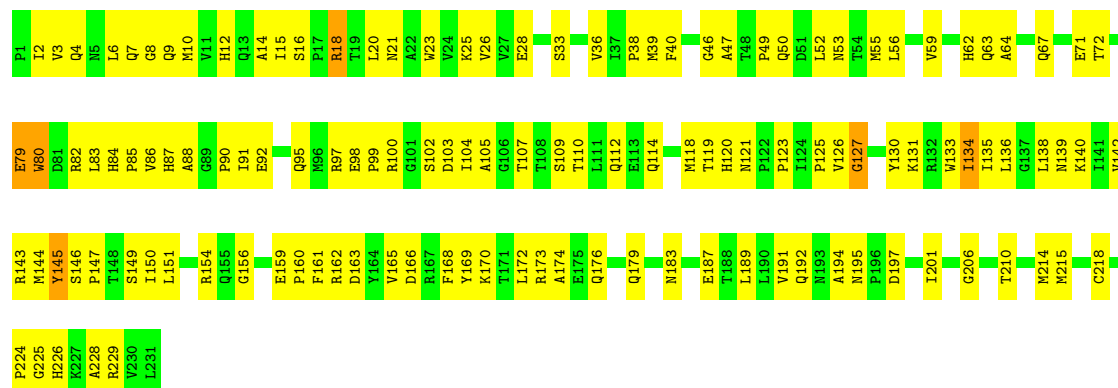
• Molecule 1: capsid protein

Chain c0: 49% 47%



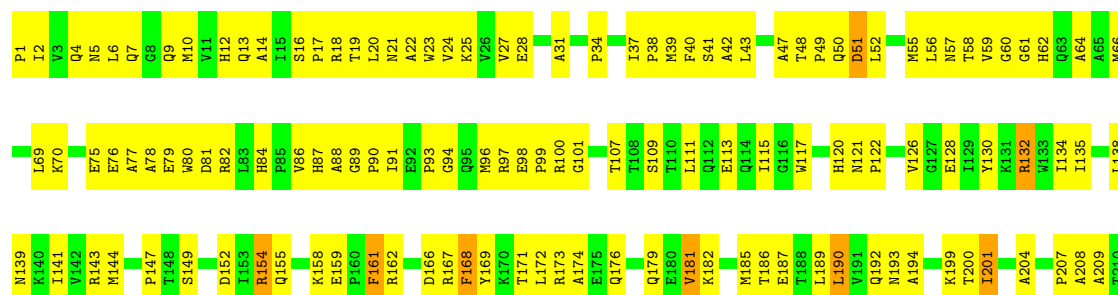
• Molecule 1: capsid protein

Chain c1: 45% 52%

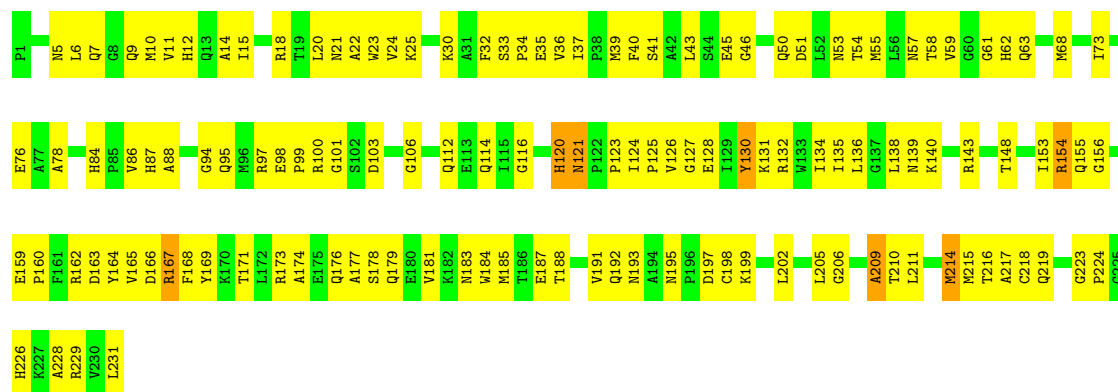


• Molecule 1: capsid protein

Chain c2: 40% 57%

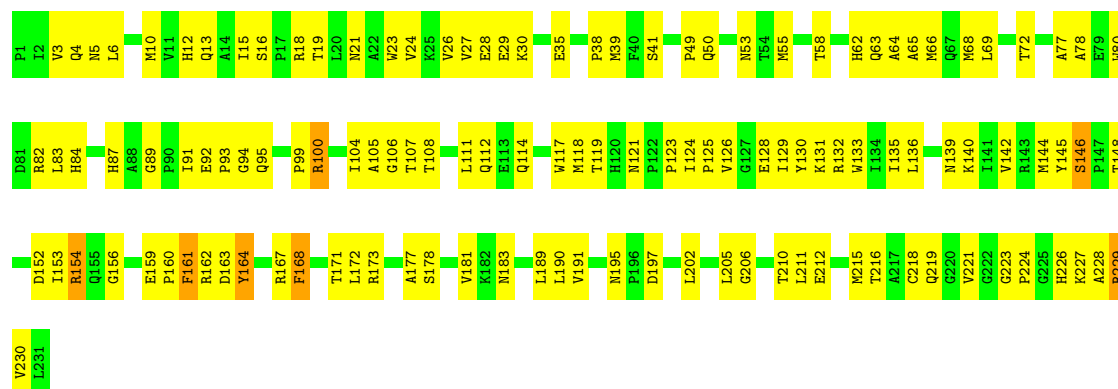






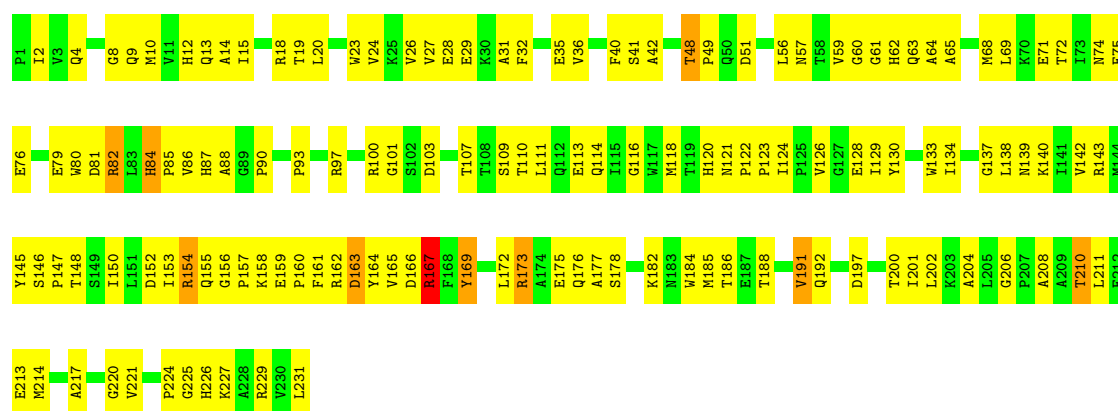
• Molecule 1: capsid protein

Chain c9: 46% 51%



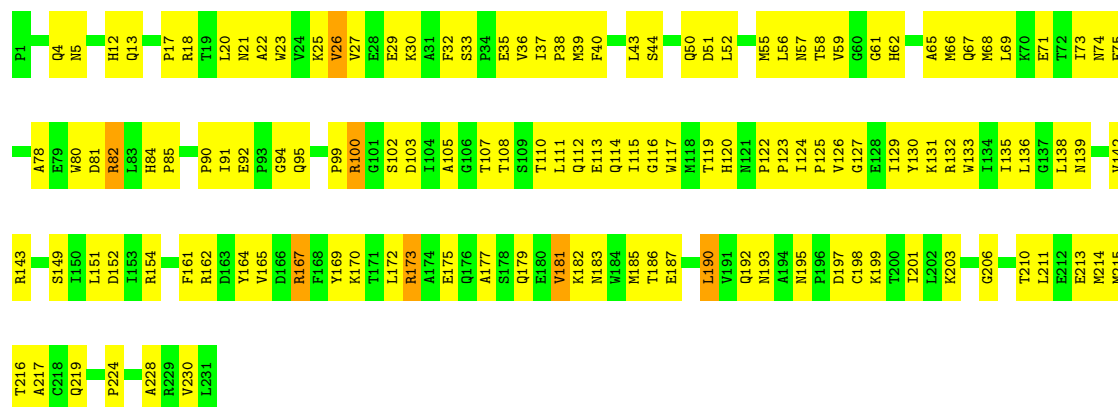
• Molecule 1: capsid protein

Chain ca: 40% 56%



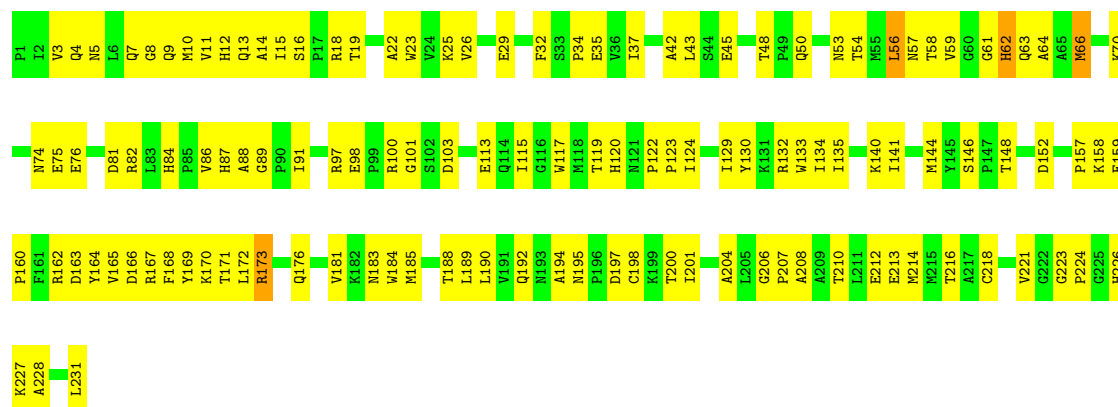
• Molecule 1: capsid protein

Chain cb: 43% 54%



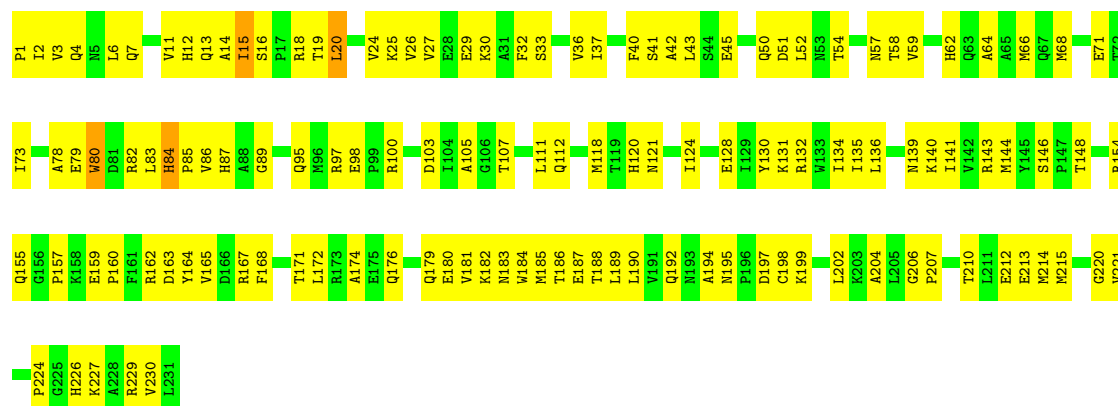
- Molecule 1: capsid protein

Chain cc: 46% 52%



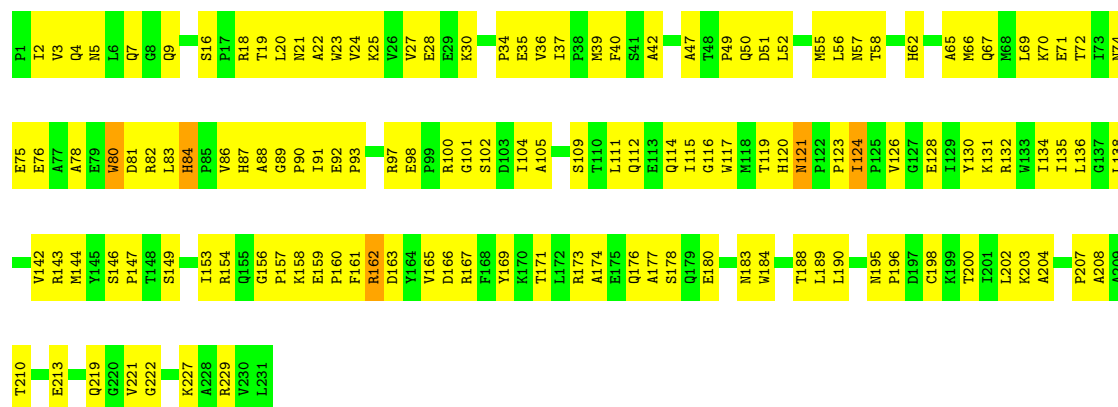
- Molecule 1: capsid protein

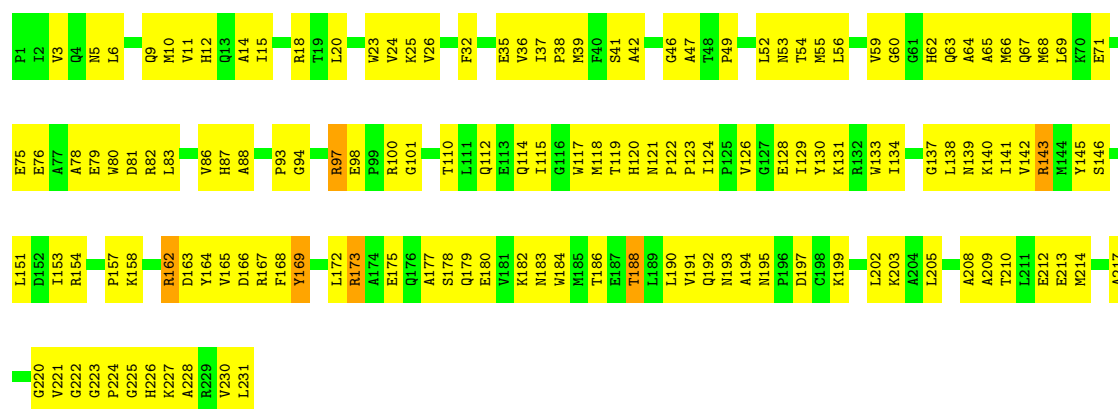
Chain cd: 44% 54%



- Molecule 1: capsid protein

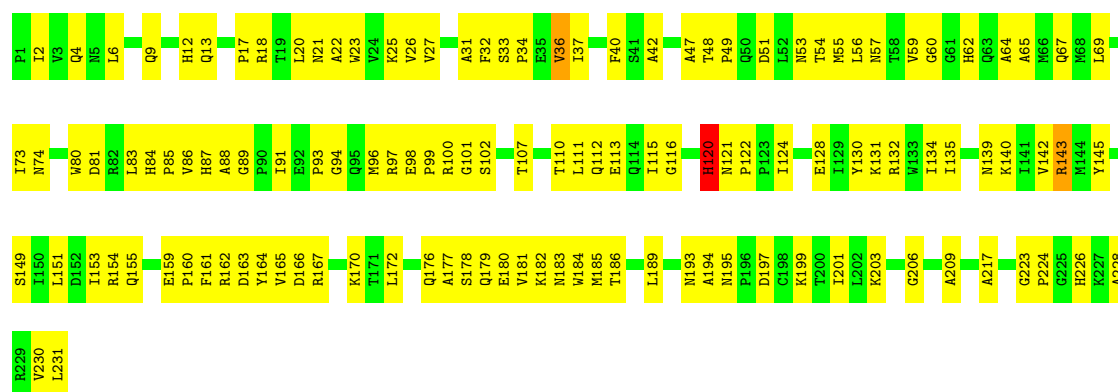
Chain ce: 42% 56%





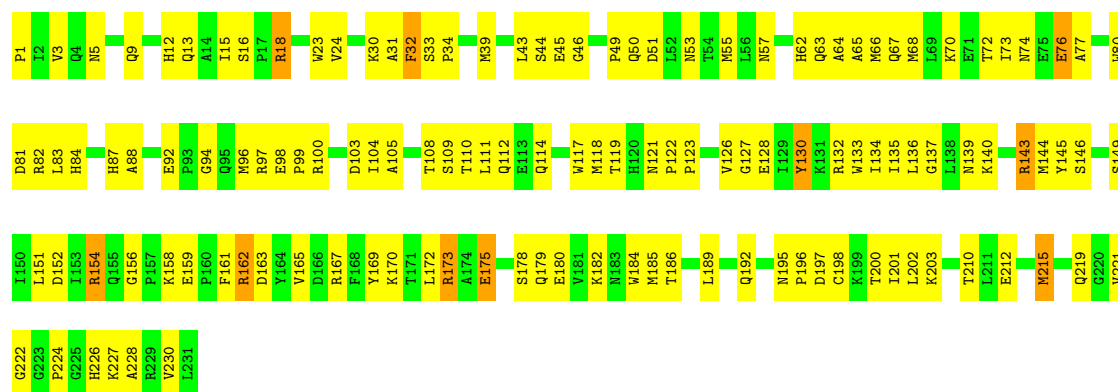
• Molecule 1: capsid protein

Chain ch: 45% 53%



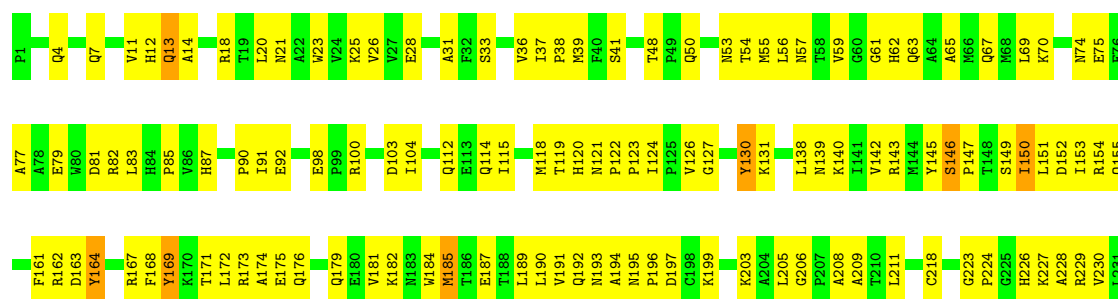
• Molecule 1: capsid protein

Chain ci: 44% 52%



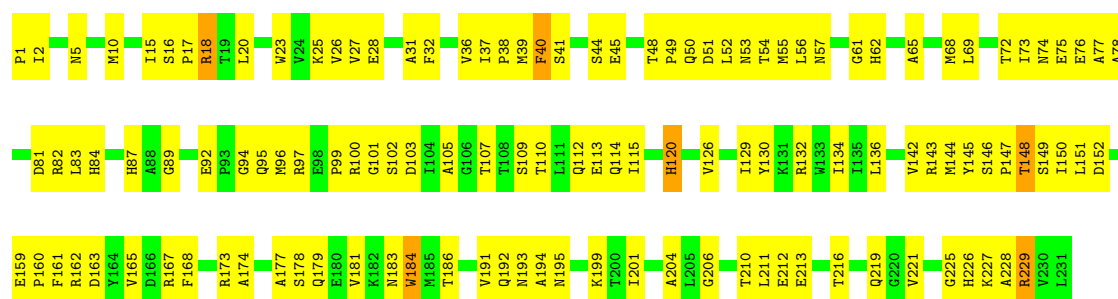
• Molecule 1: capsid protein

Chain cj: 47% 50%



• Molecule 1: capsid protein

Chain ck: 45% 52%



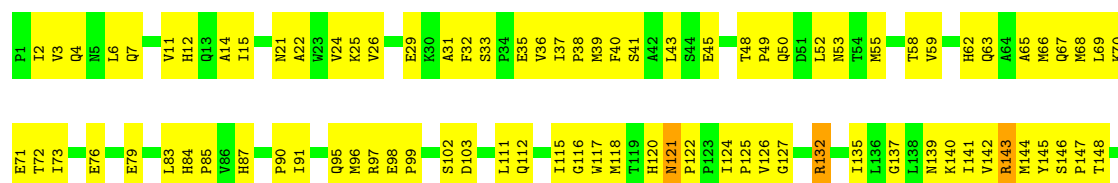
• Molecule 1: capsid protein

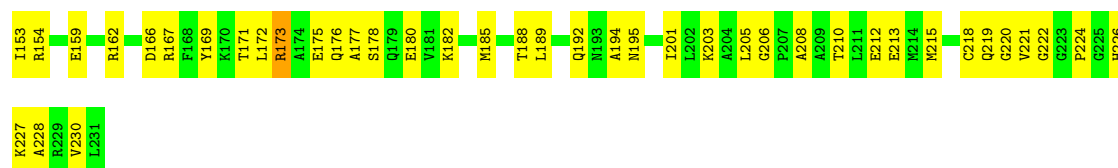
Chain cl: 45% 55%



• Molecule 1: capsid protein

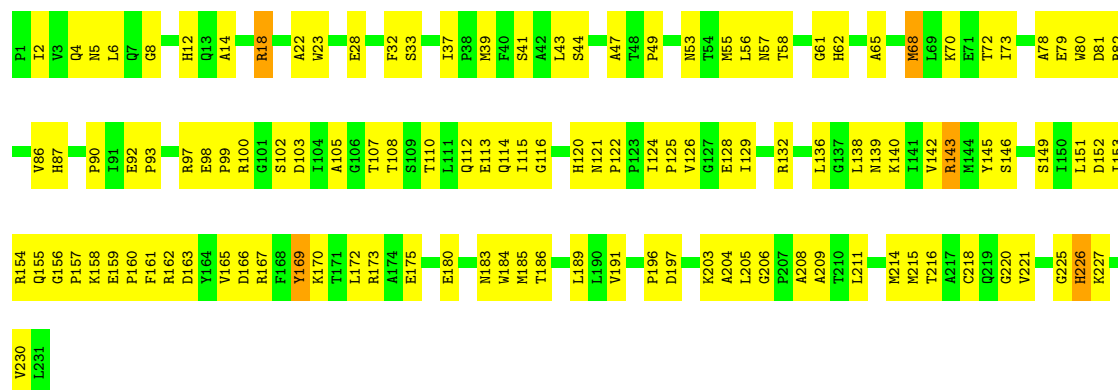
Chain cm: 45% 54%





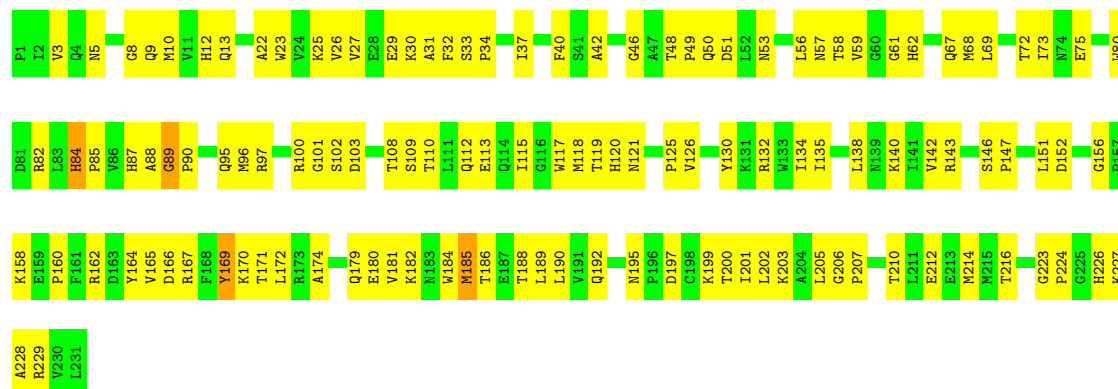
• Molecule 1: capsid protein

Chain cn: 47% 51%



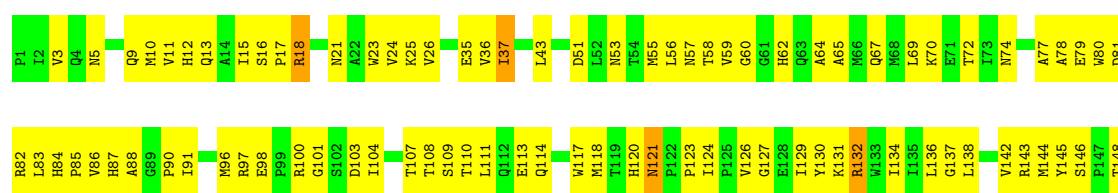
• Molecule 1: capsid protein

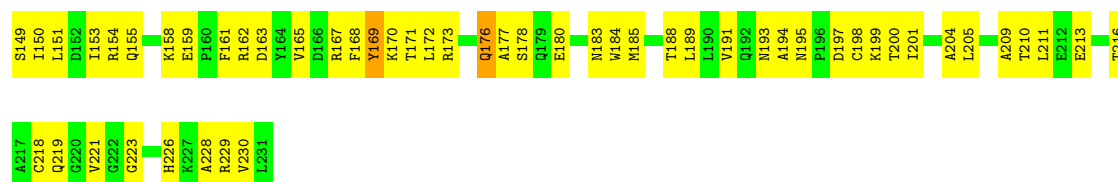
Chain co: 47% 52%



• Molecule 1: capsid protein

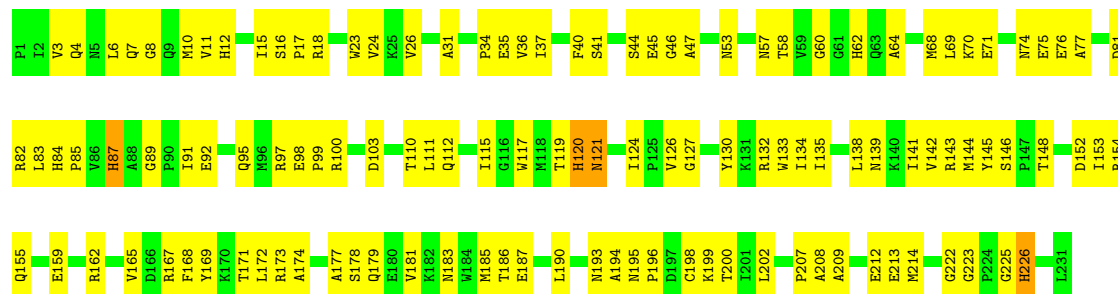
Chain cp: 40% 57%





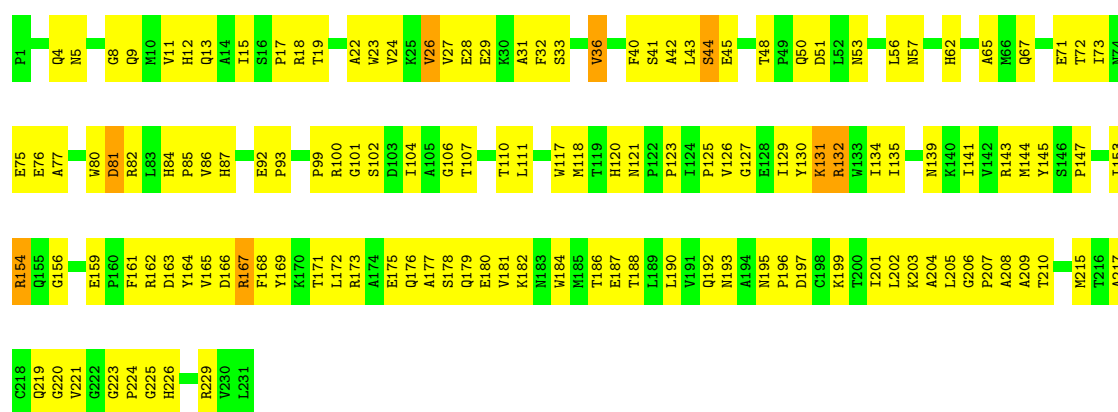
- Molecule 1: capsid protein

Chain 1e: 48% 51%



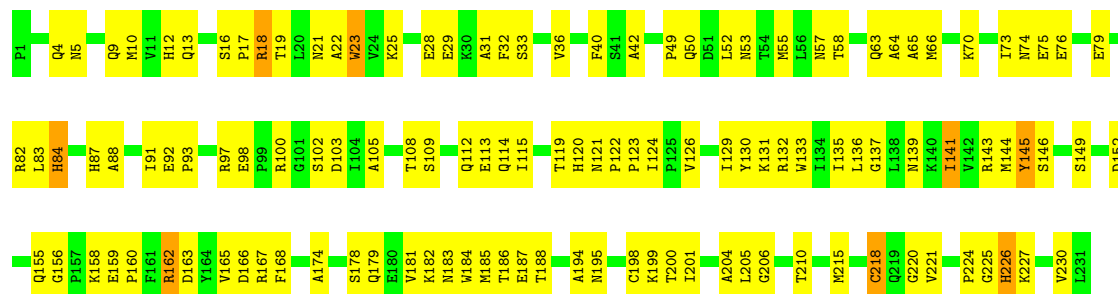
- Molecule 1: capsid protein

Chain cq: 41% 55%

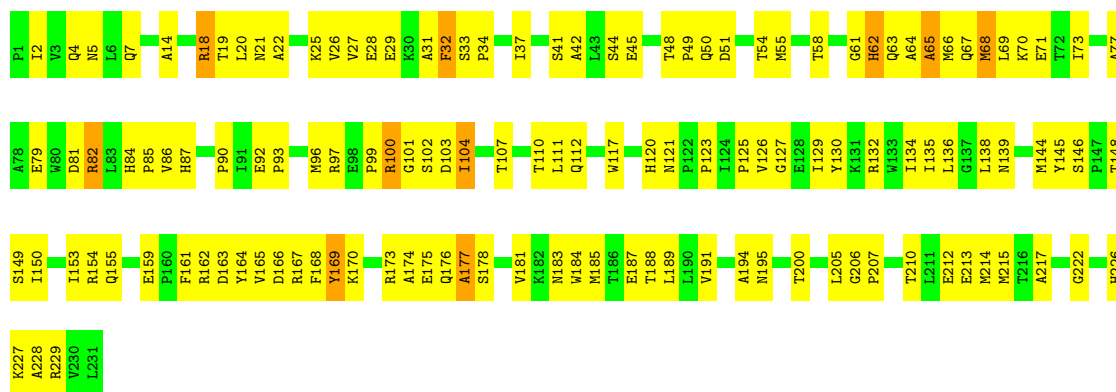


- Molecule 1: capsid protein

Chain cr: 47% 50%

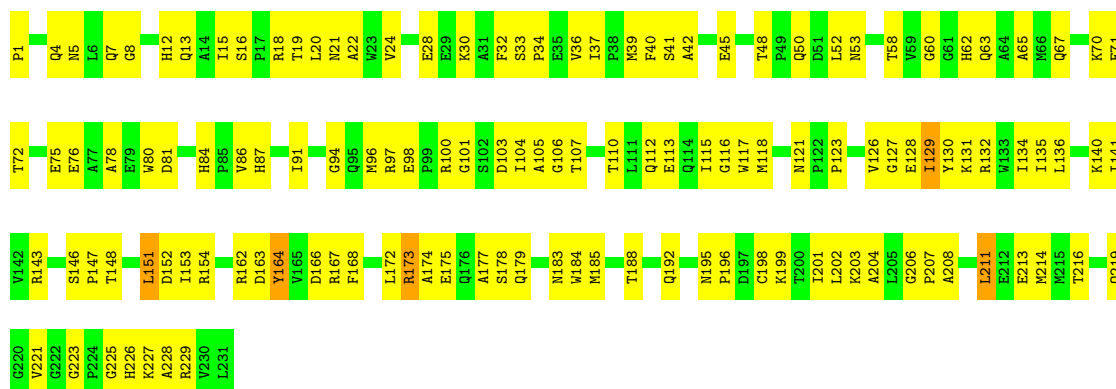


- Molecule 1: capsid protein



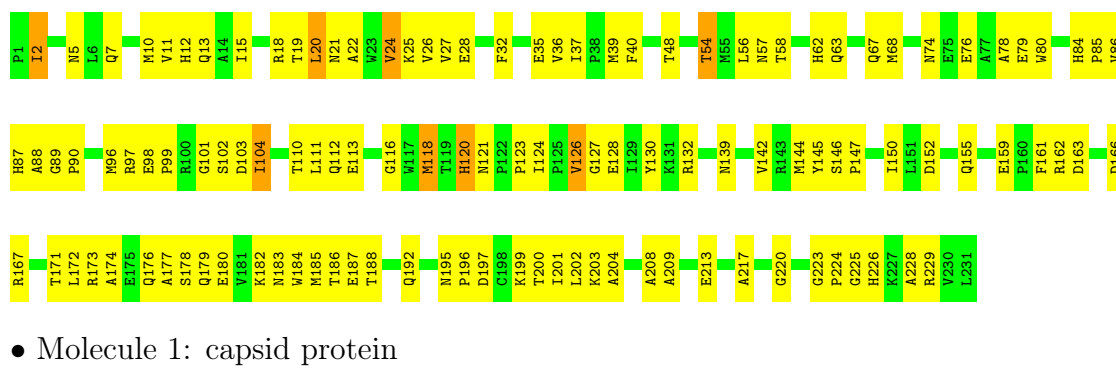
- Molecule 1: capsid protein

Chain cw: 44% 54%



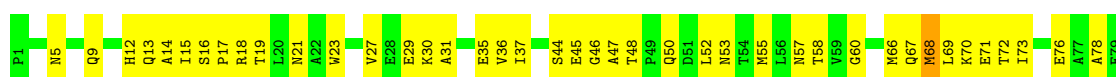
- Molecule 1: capsid protein

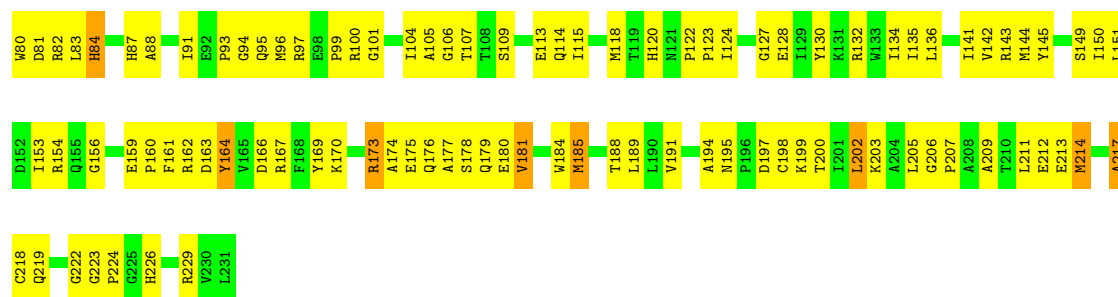
Chain cx: 48% 48%



- Molecule 1: capsid protein

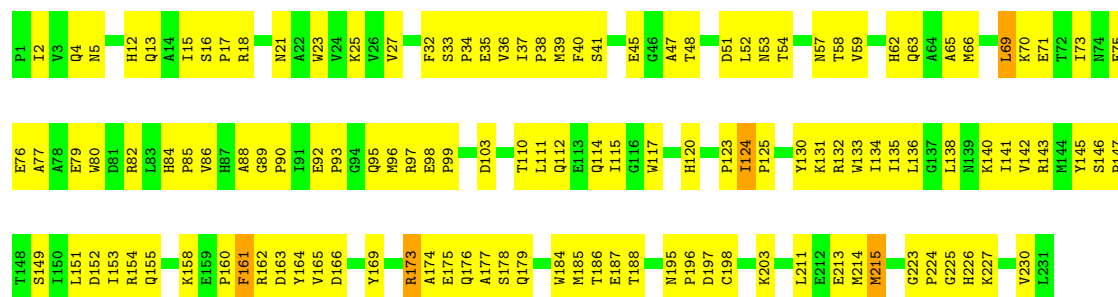
Chain cy: 41% 55%





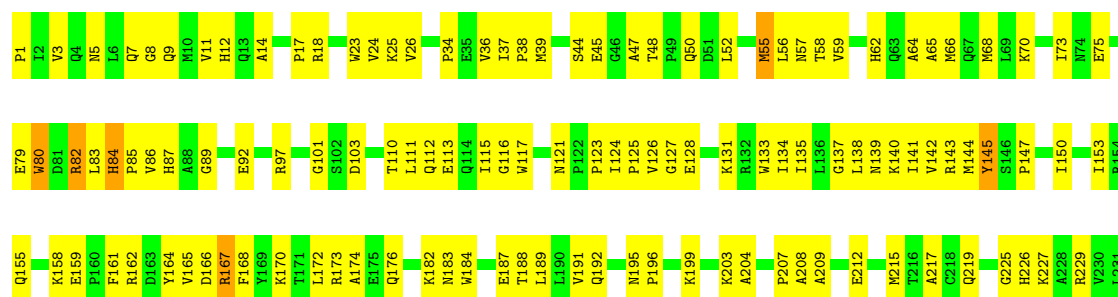
- Molecule 1: capsid protein

Chain cz: 45% 53%



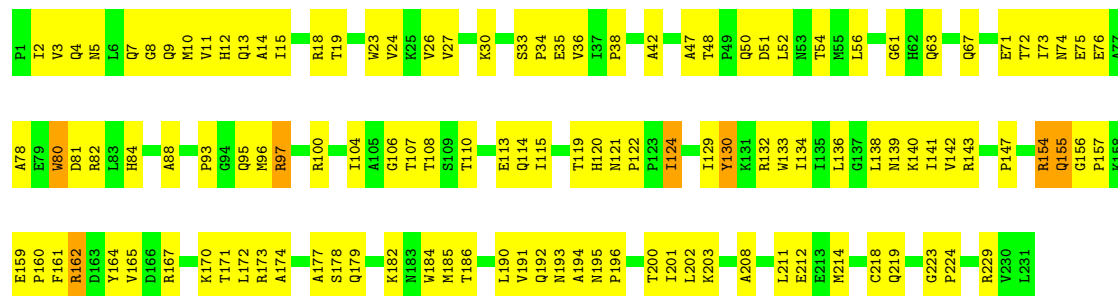
- Molecule 1: capsid protein

Chain 1f: 48% 50%

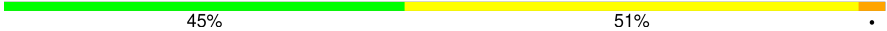


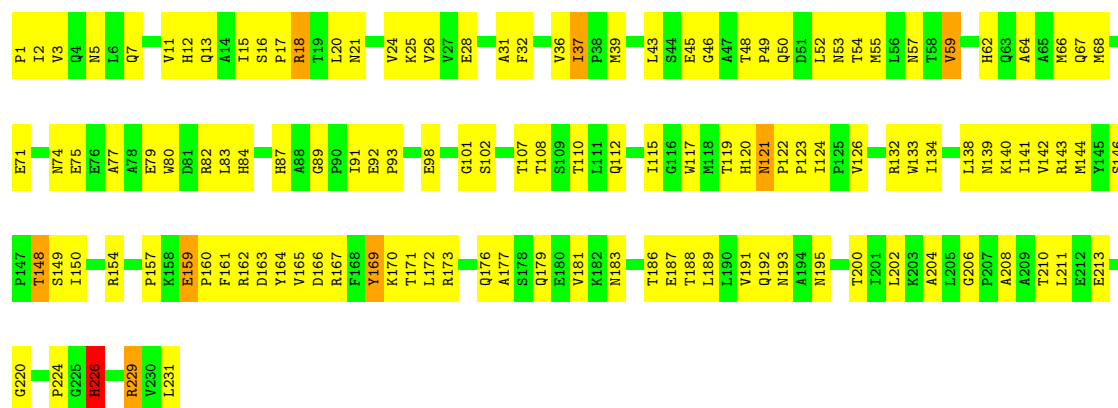
- Molecule 1: capsid protein

Chain cA: 47% 50%

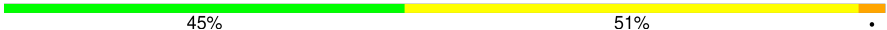


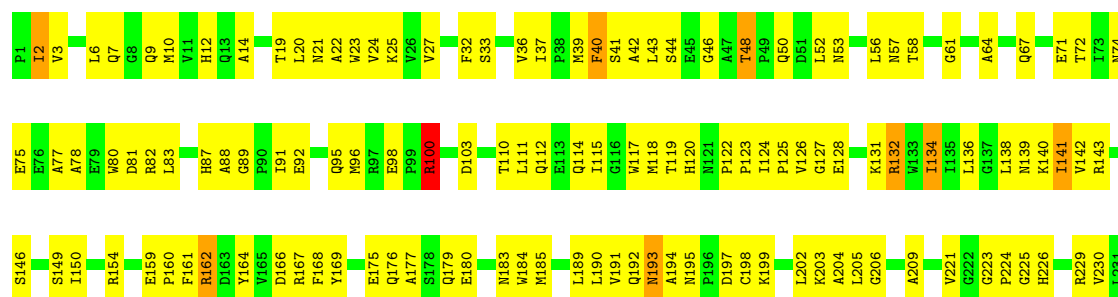
- Molecule 1: capsid protein

Chain cB: 

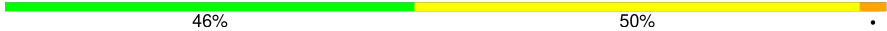


• Molecule 1: capsid protein

Chain cC: 

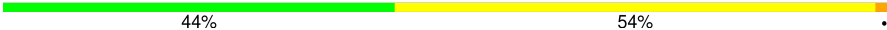


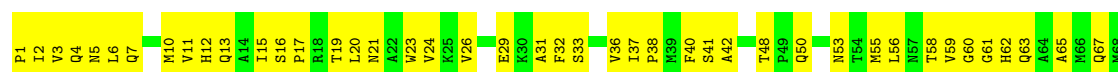
• Molecule 1: capsid protein

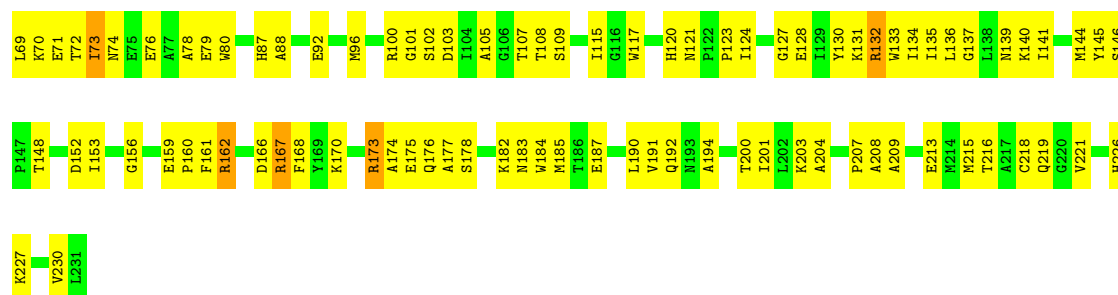
Chain cD: 



• Molecule 1: capsid protein

Chain cE: 

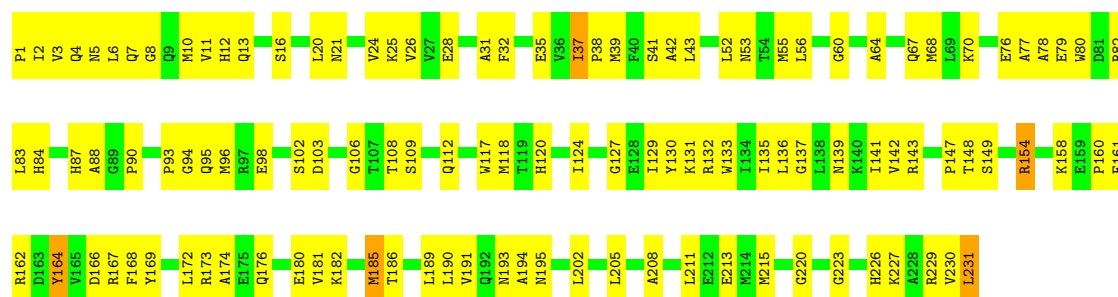




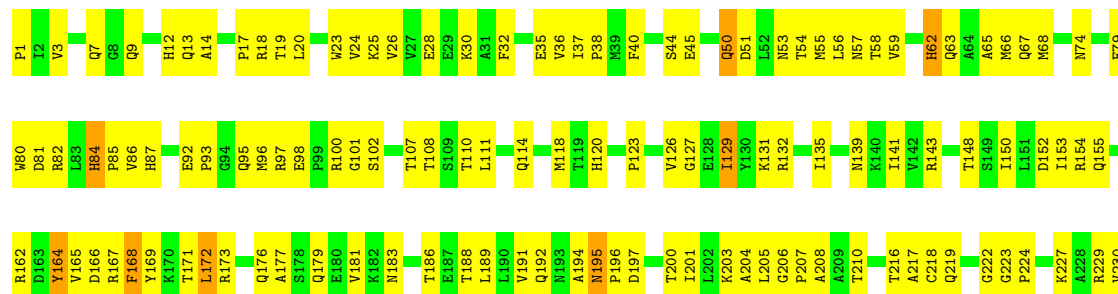
• Molecule 1: capsid protein



• Molecule 1: capsid protein

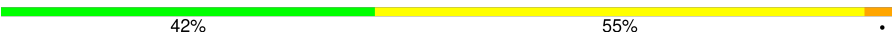
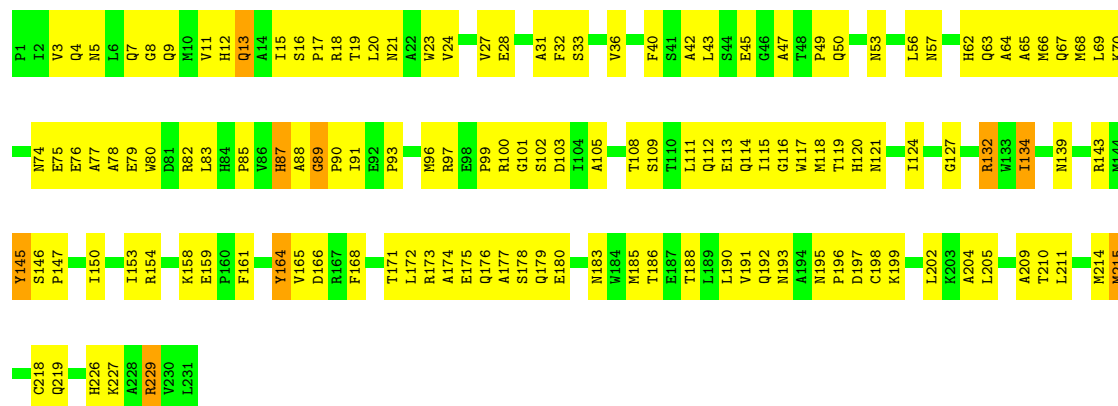


• Molecule 1: capsid protein

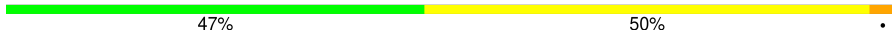
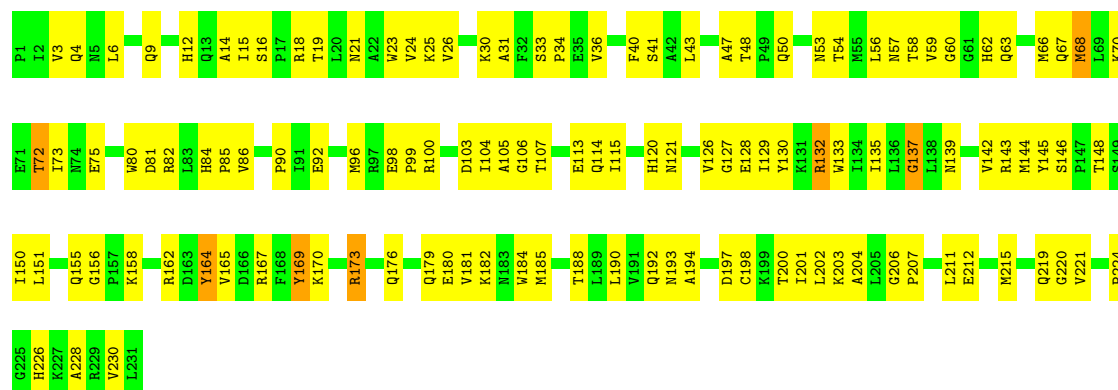


L231

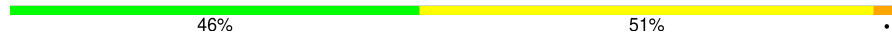
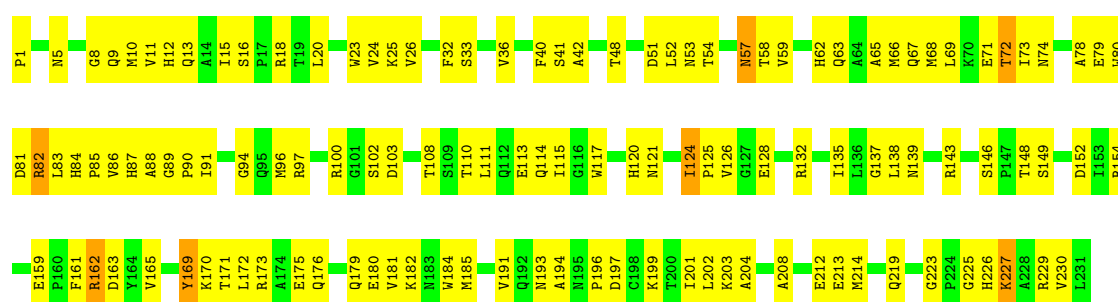
- Molecule 1: capsid protein

Chain cI:  42% 55%

- Molecule 1: capsid protein

Chain cJ:  47% 50%

- Molecule 1: capsid protein

Chain 1g:  46% 51%

- Molecule 1: capsid protein

M215		Y142		E71		P1
	Q219	R143			W72	I2
G220		M144		I73		V3
V221		Y145				
				E76		L6
						Q7
G225		S149				Q8
H226		I150		W80		G9
A227		L151		D81		M10
K228		D152		R82		V11
R229		I153		L83		H12
		R154		H84		Q13
V230		Q155		P85		A14
L231		G156		W86		I15
		P157		A87		
		K158		A88		R18
				G89		T19
		R162		P90		L20
		D163		I91		N21
		Y164		E92		A22
		V165		P93		W23
		D166		G94		V24
		R167		Q95		K25
		F168		M96		V26
		Y169		R97		V27
		K170		E98		
				P99		E28
		R173		R100		E29
				G101		K30
		A177		S102		A31
		V181		D103		F32
				I104		S33
				A105		P34
		W184		G106		E35
		E187		T110		P38
		F188		L111		M39
		L189		Q112		F40
		V190		E113		
		I191		Q114		L43
		Q192		I115		S44
		N193		G116		E45
		A194		W117		G46
		N195				A47
				H120		
		C198		M121		Q50
						D51
		L201		P125		L52
		L202		G126		
		K203		E128		M55
		A204		I129		T58
		L205		Y130		
		G206		K131		H52
		P207		R132		Q63
		A208		W133		A64
		A209		I134		A65
		T210		I135		
		L211				M68
		E212				L69
		E213		L138		K70
		W214				

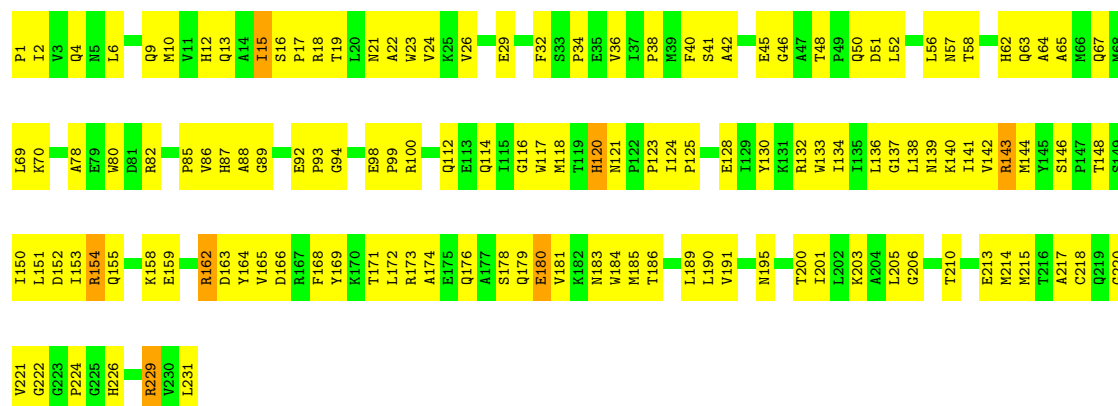
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V230	L231	E159	K70	E71	Q4	P1
		P160	E71	E71	N6	
		F161	T72	T73	N5	
		D163	N74		Q7	
		Y164			G8	
		V165	A77		Q9	
			A78		M10	
		Y169			V11	
		K170	D81		H12	
		T171	R82		Q13	
		L172	L83		A14	
		R173	H84		I15	
		A174	P85		S16	
		E175			P17	
		Q176	A88		R18	
		A177			T19	
		S178	Q95		L20	
		Q179	M96		N21	
		E180	R97		A22	
		V181			V23	
		K182	S102		V24	
			D103			
		T186			V27	
		E187	S109		E28	
					E29	
		L190	Q112		X30	
		V191	I113		A31	
		Q192	Q114		F32	
		N193			S33	
		N195	H120		P34	
					E35	
		C198	P123		V36	
			I124		T37	
			P125		P38	
		T201	V126		M39	
		L202	G127		F40	
		K203			S41	
			Y130		A42	
		P207	K131			
		A208	R132		E45	
		A209				
		T210	I135		T48	
		L211	L136		P49	
		E212	G137		Q50	
		E213	L138		D51	
		M214	N139			
			K140		M55	
					L56	
		C218			N57	
		Q219	R143		T58	
		G220	M144		V59	
		V221	Y145		G60	
		G222	S146		G61	
		G223			H62	
			I150		Q63	
		H226	L151		A64	
		K227	D152		M65	
		A228	T153		A66	
		P229	P154		V67	

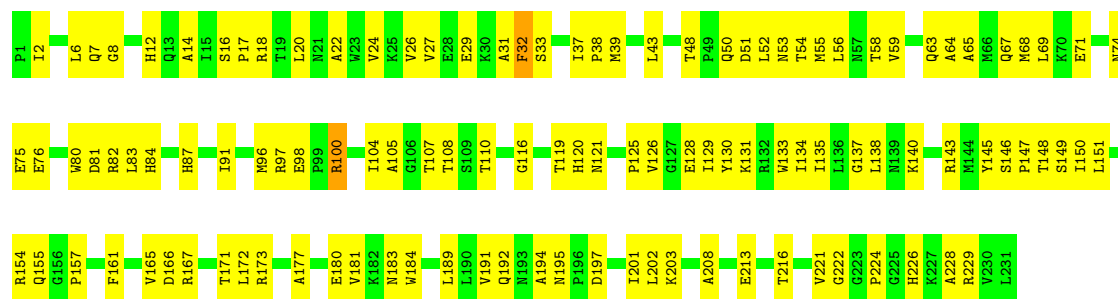
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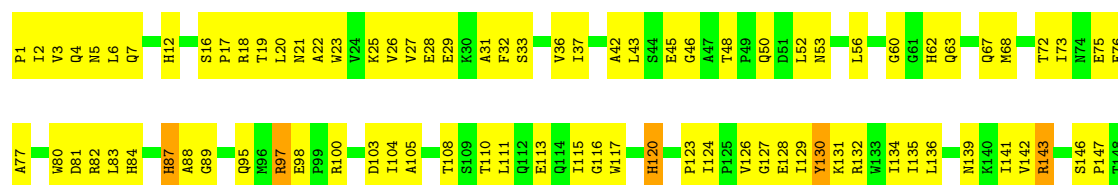
• Molecule 1: capsid protein

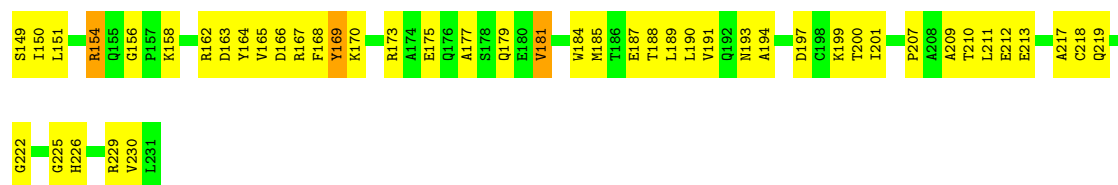


• Molecule 1: capsid protein



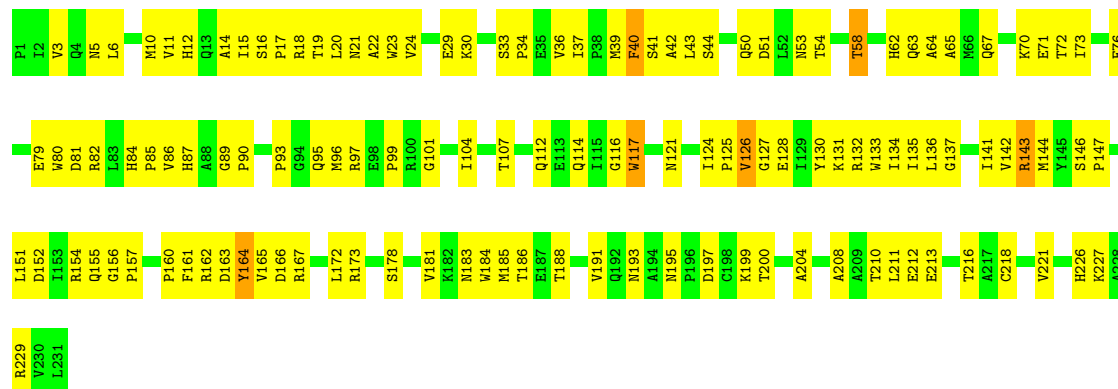
• Molecule 1: capsid protein





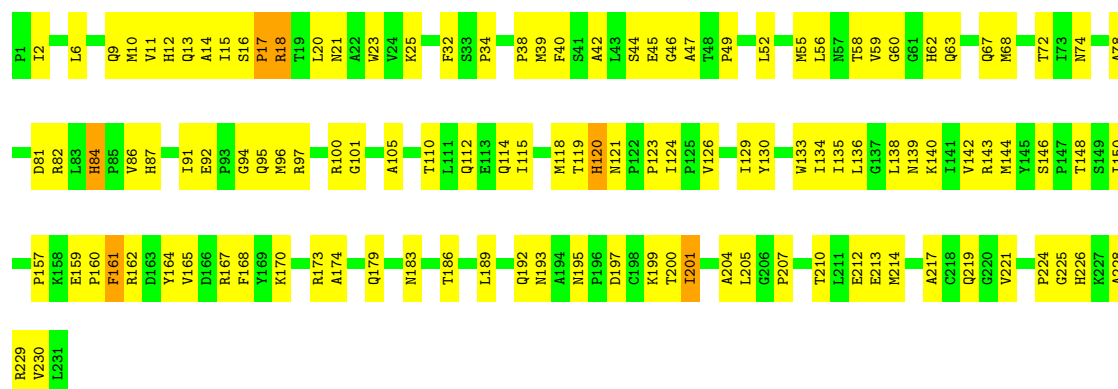
- Molecule 1: capsid protein

Chain cR: 45% 52%



- Molecule 1: capsid protein

Chain cS: 48% 49%



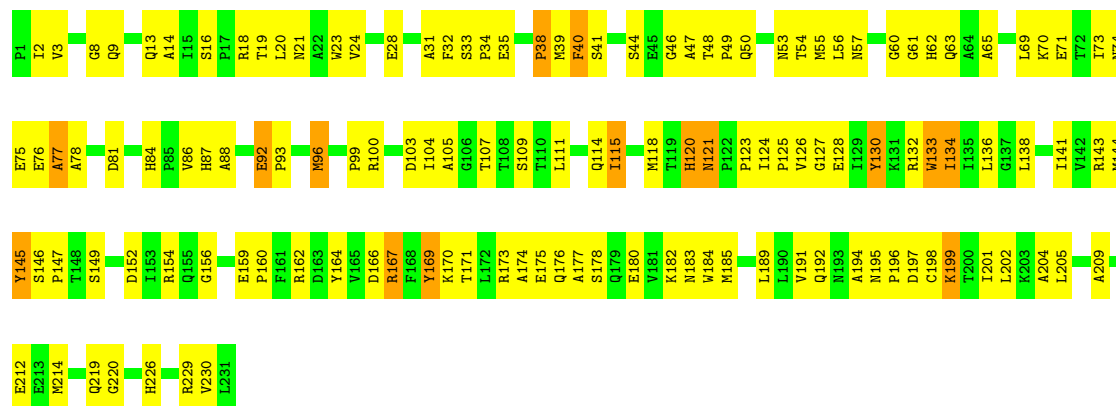
- Molecule 1: capsid protein

Chain cT: 51% 43% 6%

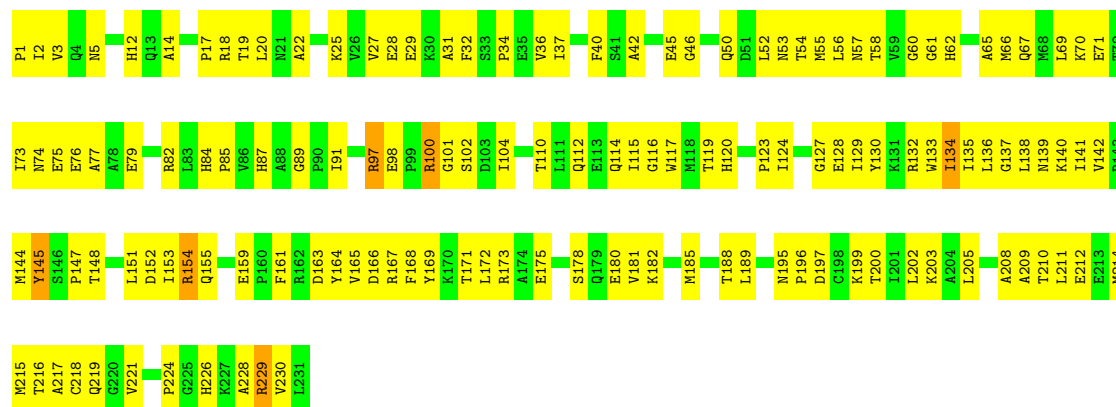




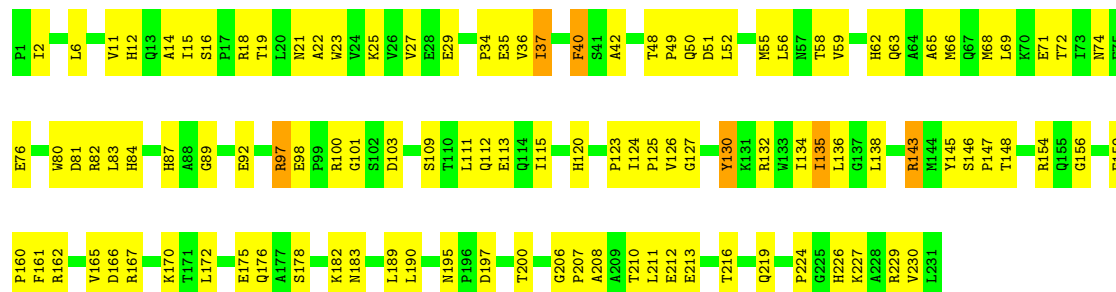
• Molecule 1: capsid protein



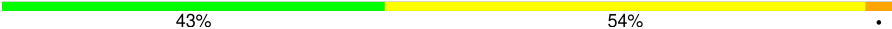
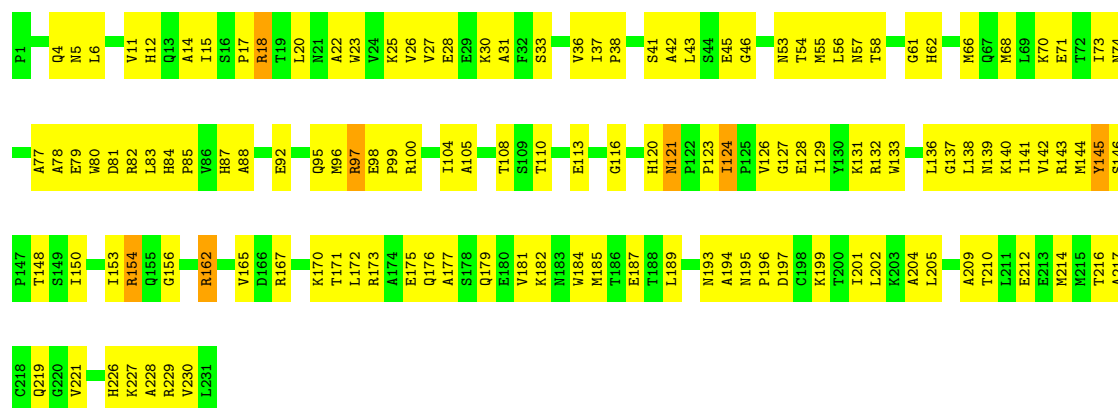
• Molecule 1: capsid protein



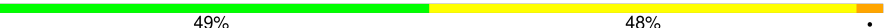
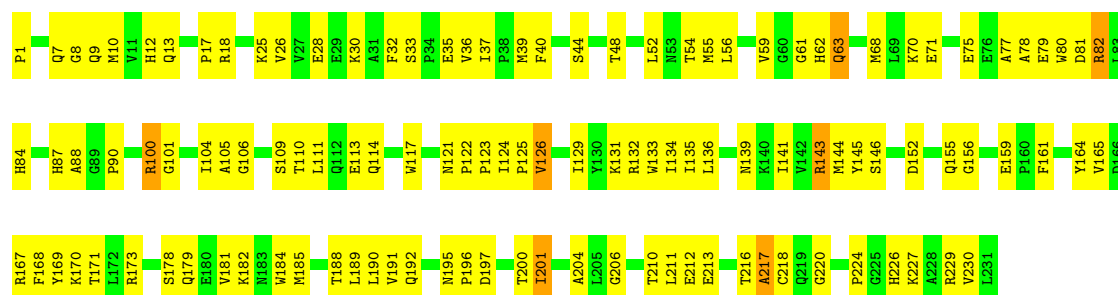
• Molecule 1: capsid protein



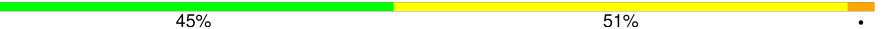
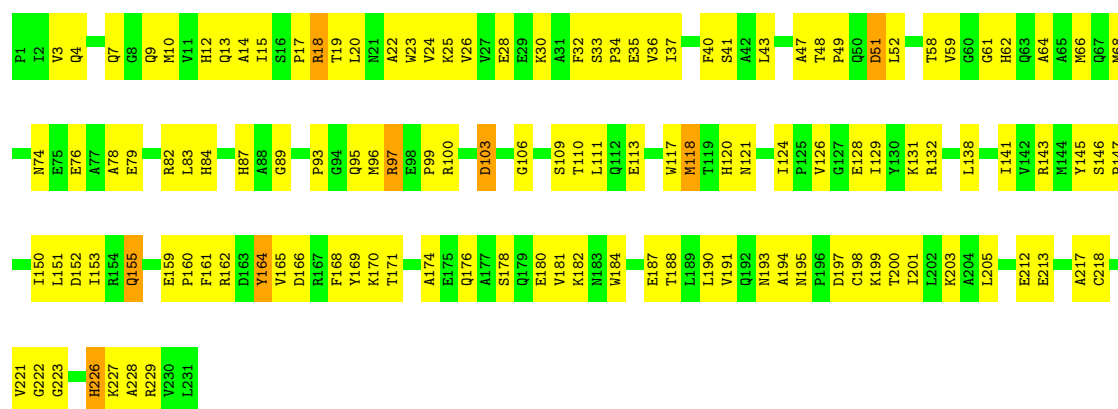
• Molecule 1: capsid protein

Chain cW:  43% 54%

• Molecule 1: capsid protein

Chain cX:  49% 48%

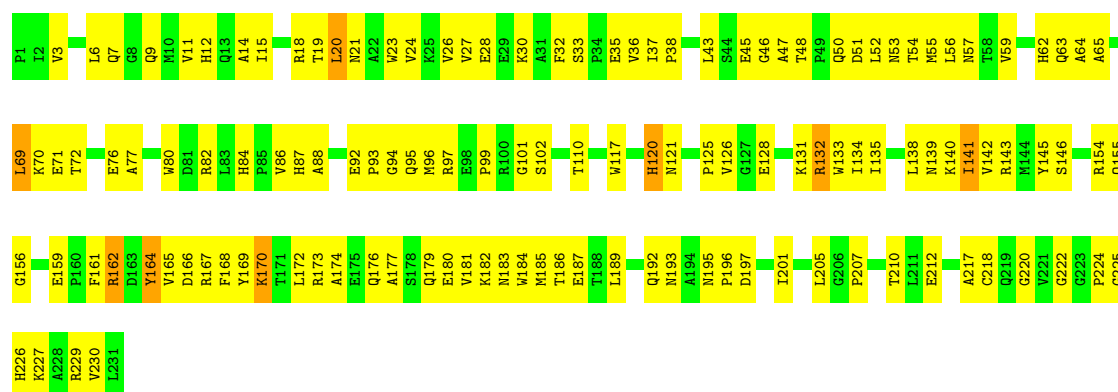
• Molecule 1: capsid protein

Chain cY:  45% 51%

• Molecule 1: capsid protein

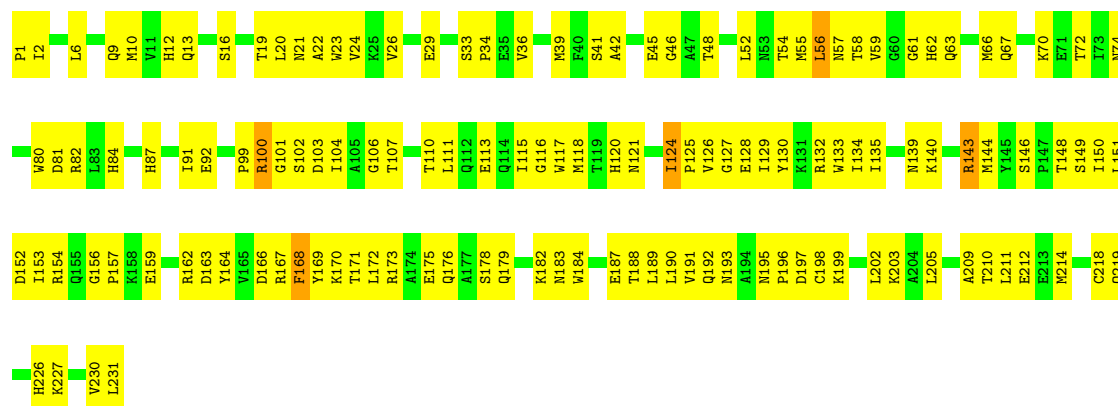
Chain cZ:  44% 53%





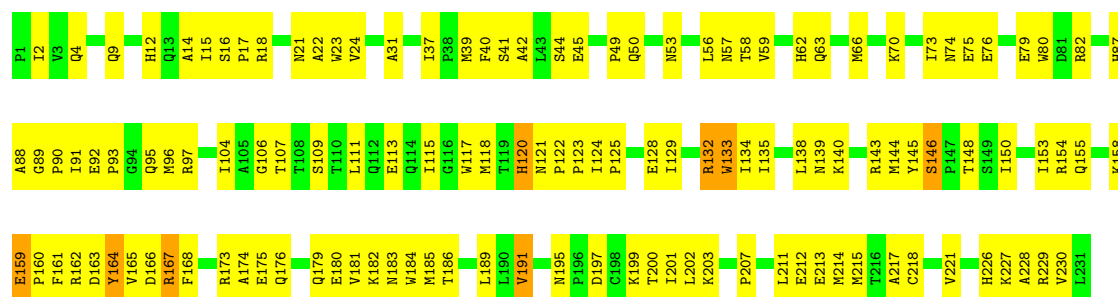
• Molecule 1: capsid protein

Chain d3: .



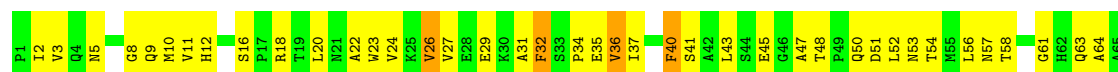
• Molecule 1: capsid protein

Chain 1i: .



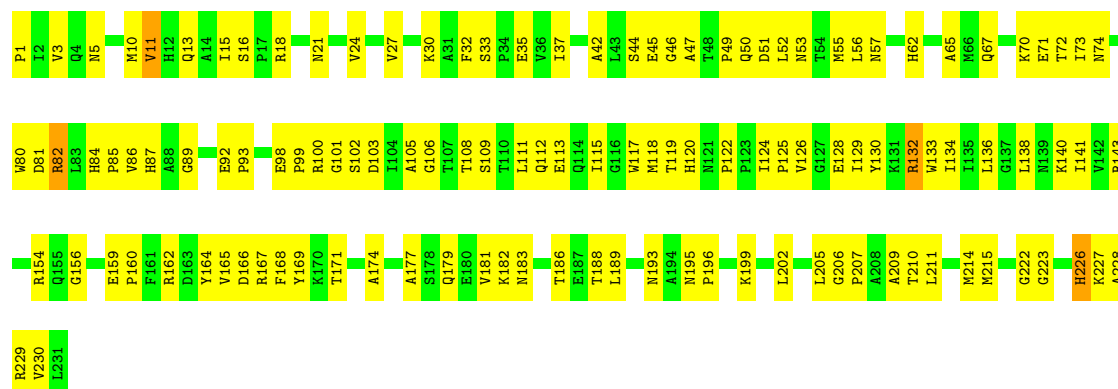
• Molecule 1: capsid protein

Chain d4: .

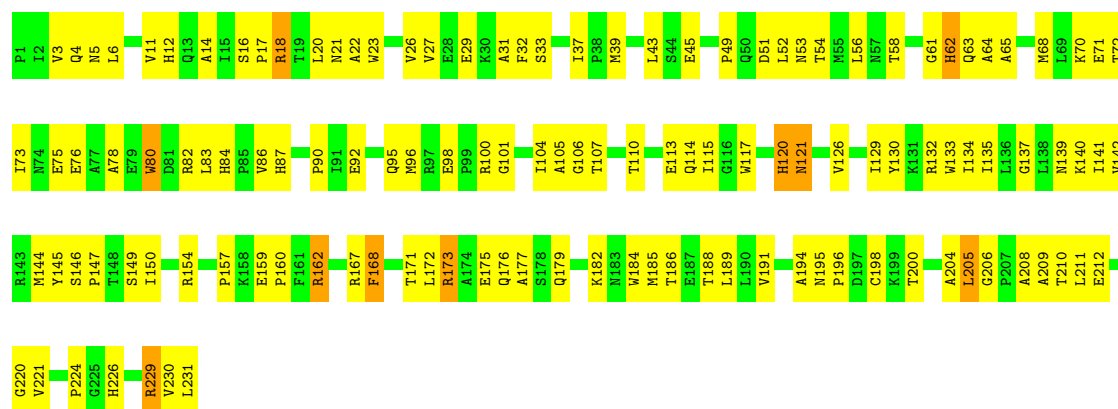




- Molecule 1: capsid protein

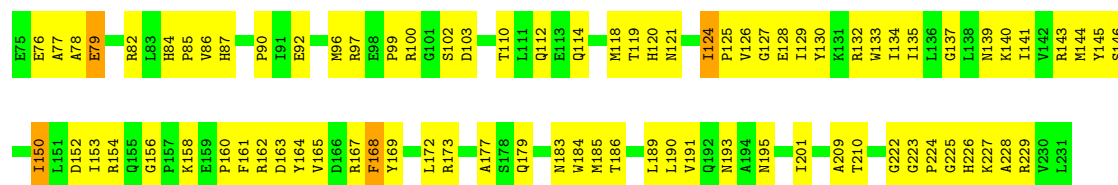


- Molecule 1: capsid protein

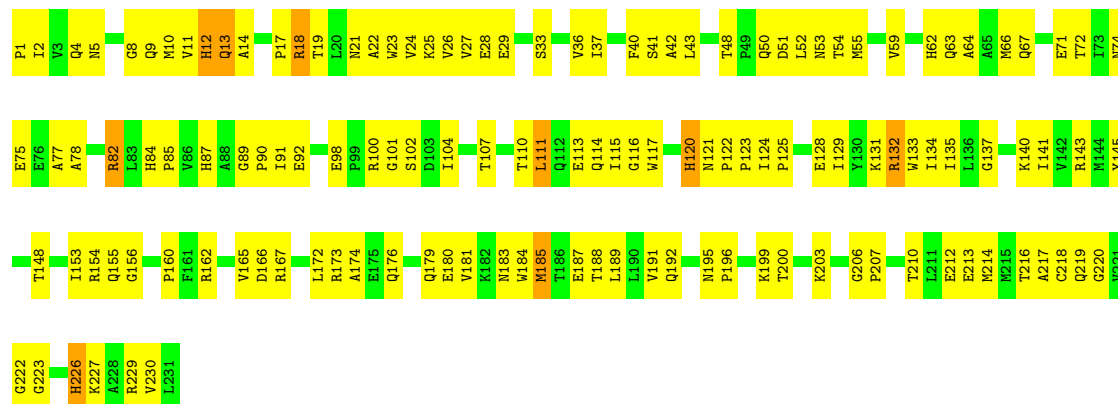


- Molecule 1: capsid protein

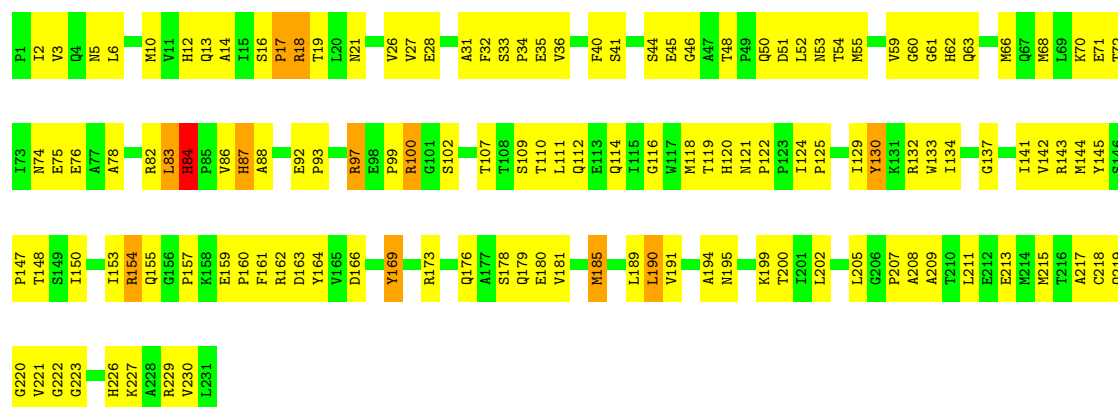




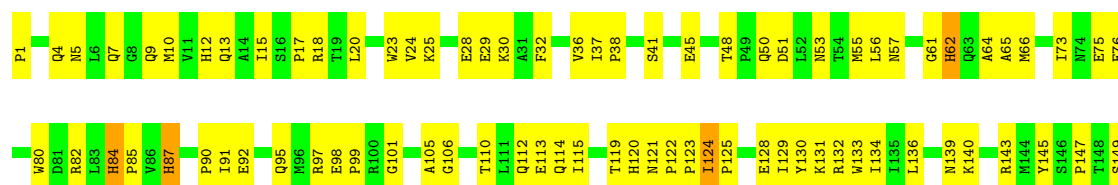
- Molecule 1: capsid protein

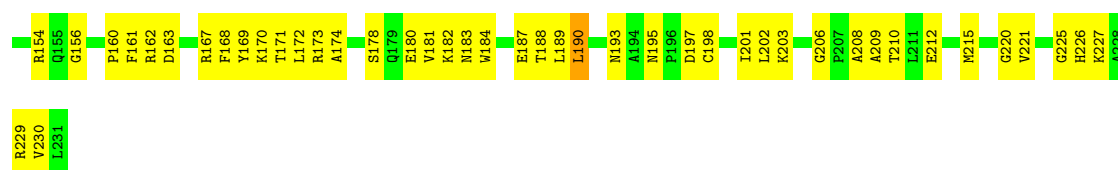


- Molecule 1: capsid protein



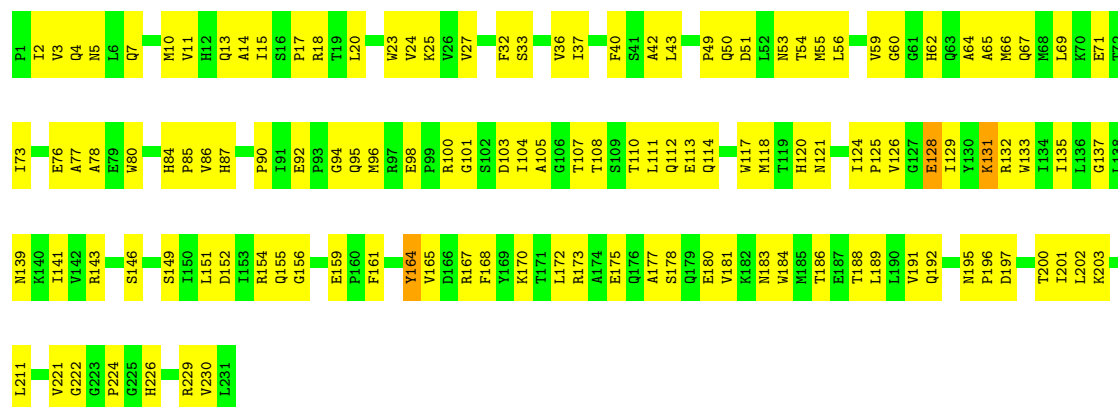
- Molecule 1: capsid protein





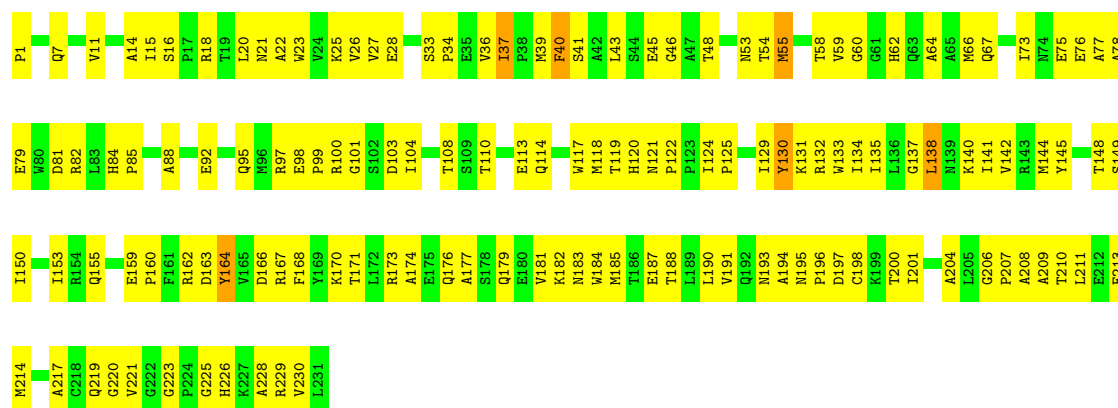
- Molecule 1: capsid protein

Chain db: 45% 53%



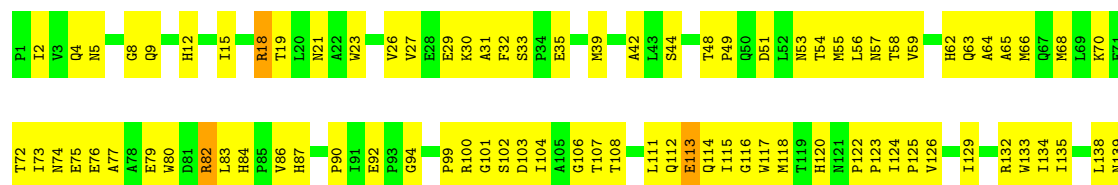
- Molecule 1: capsid protein

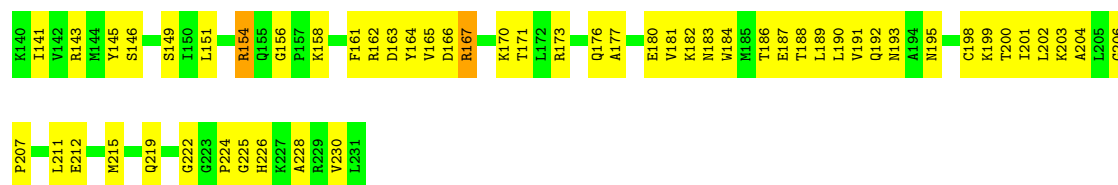
Chain dc: 40% 57%



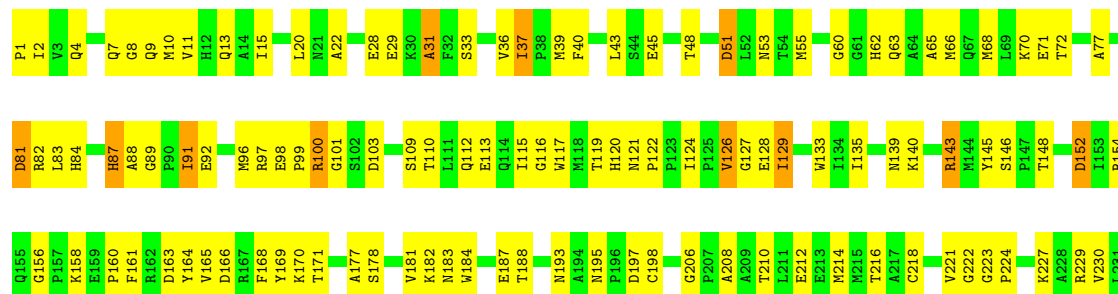
- Molecule 1: capsid protein

Chain dd: 40% 58%

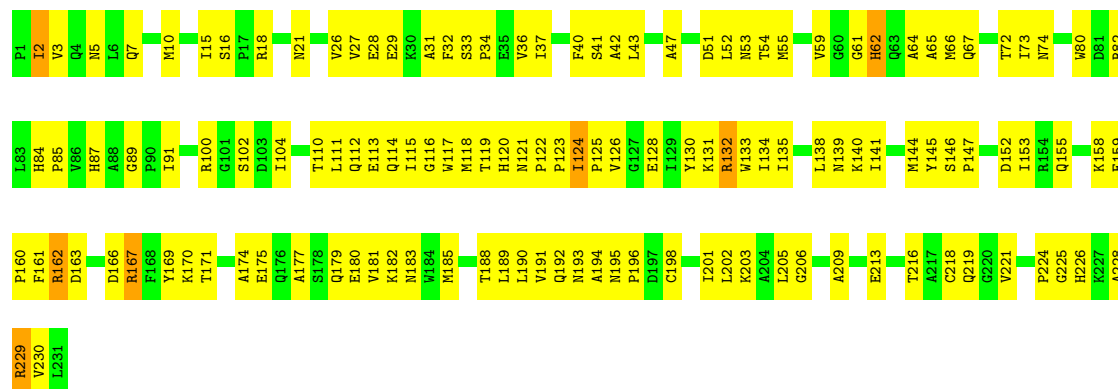




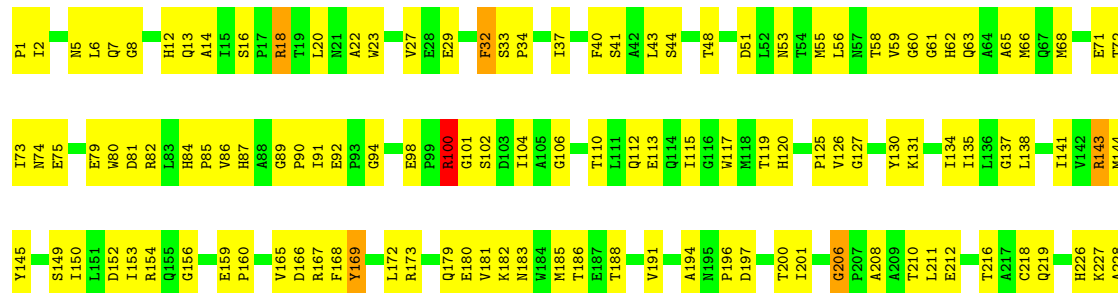
- Molecule 1: capsid protein



- Molecule 1: capsid protein



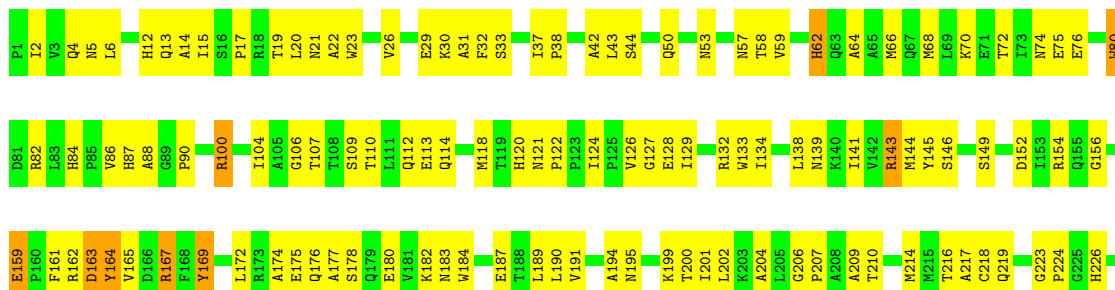
- Molecule 1: capsid protein





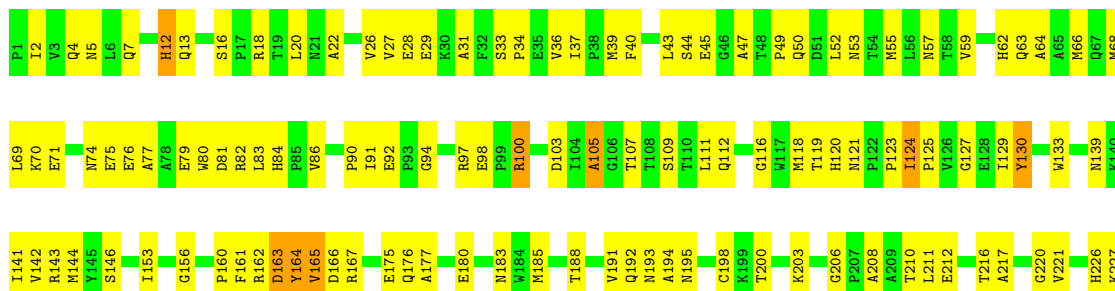
- Molecule 1: capsid protein

Chain dg: 48% 48% .



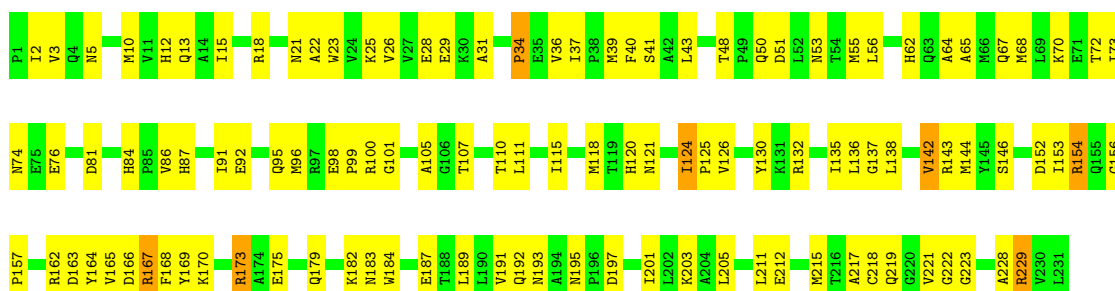
- Molecule 1: capsid protein

Chain dh: 48% 48% .

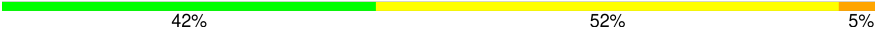


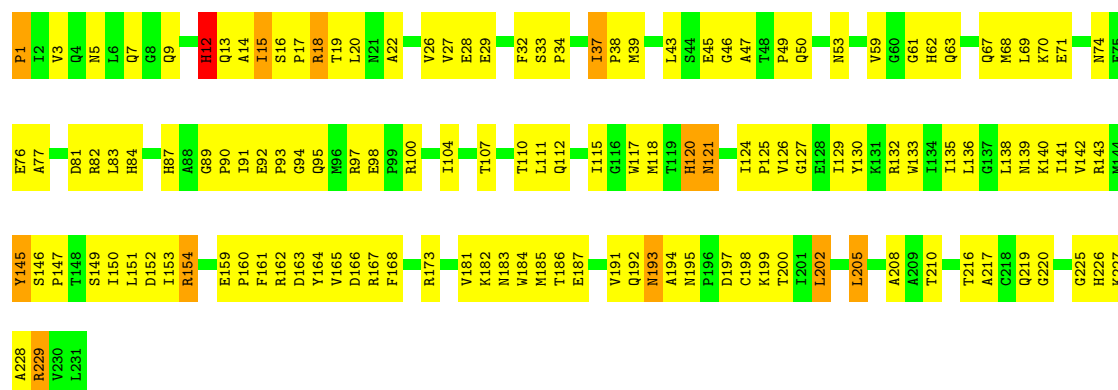
- Molecule 1: capsid protein

Chain di: 51% 46% .

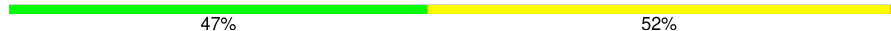


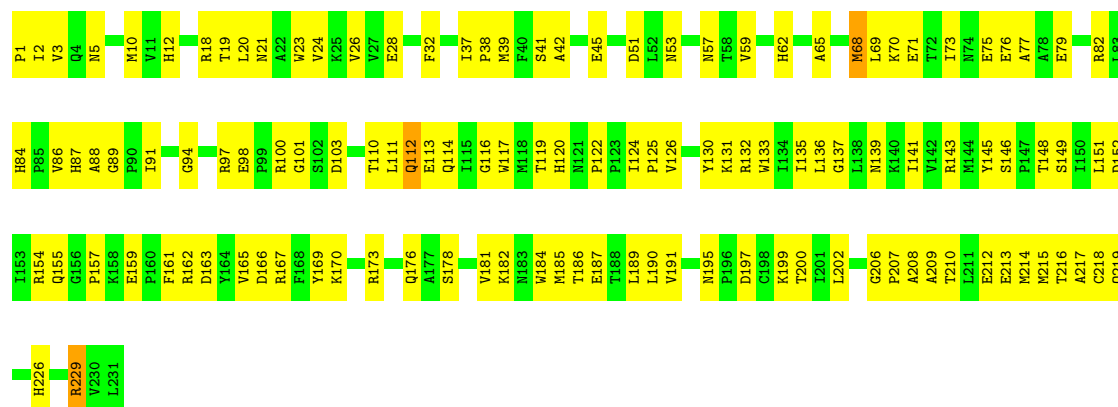
- Molecule 1: capsid protein

Chain dj: 



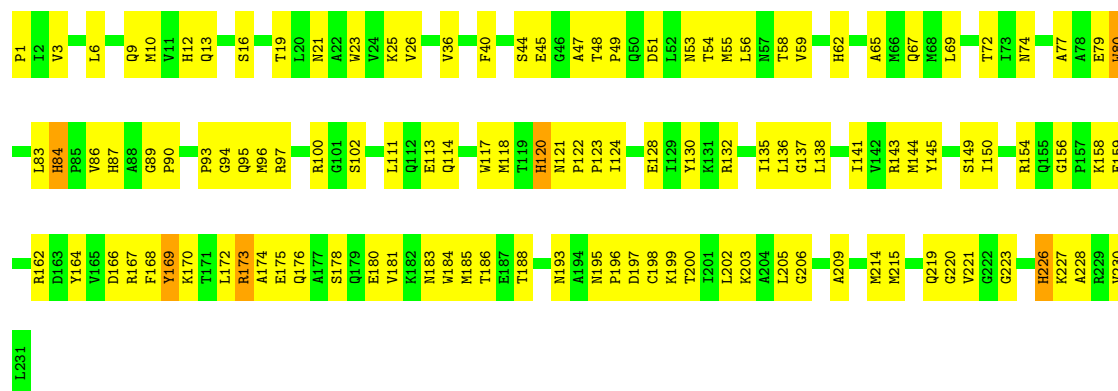
- Molecule 1: capsid protein

Chain dk: 

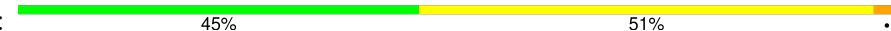


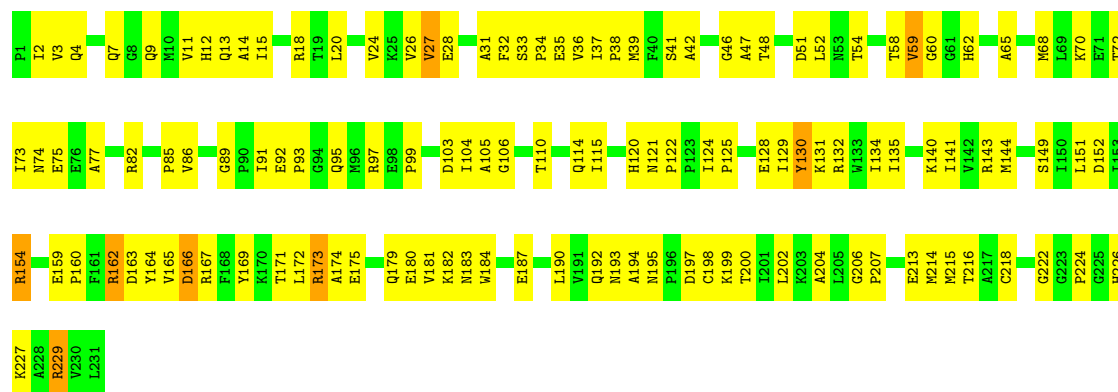
- Molecule 1: capsid protein

Chain dl: 



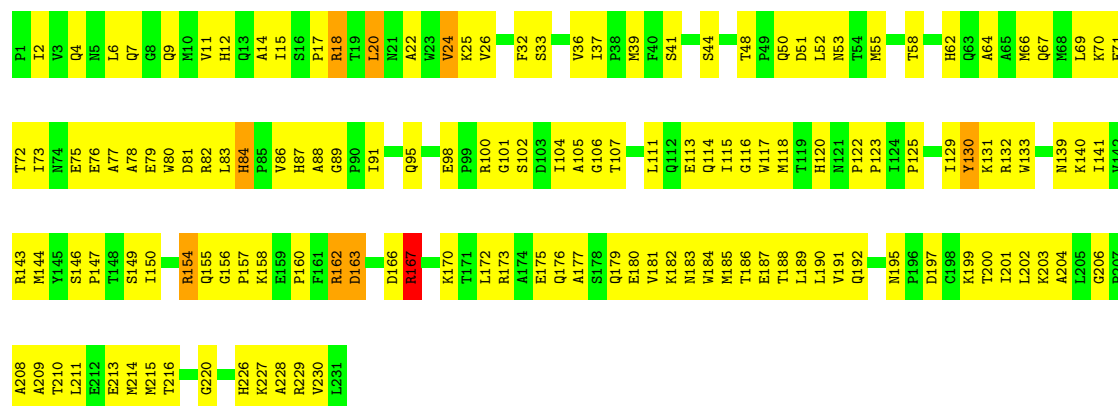
- Molecule 1: capsid protein

Chain dm: 



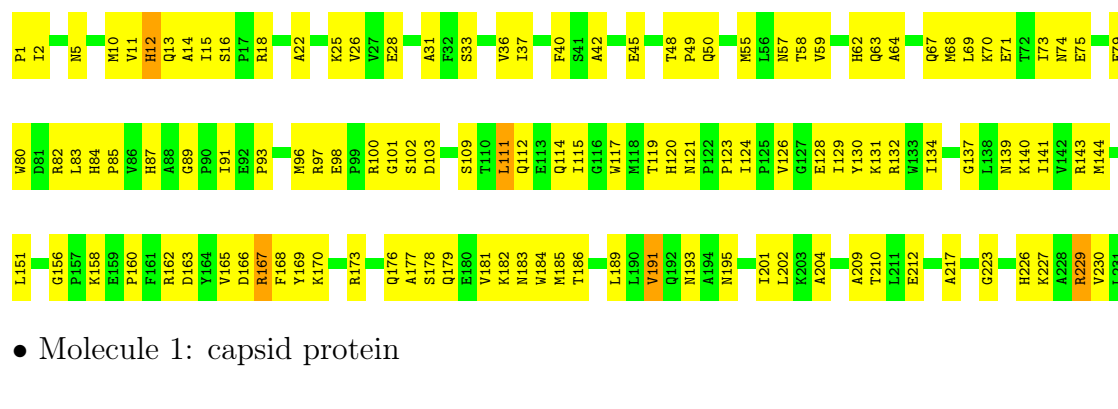
• Molecule 1: capsid protein

Chain dn: 39% 57%



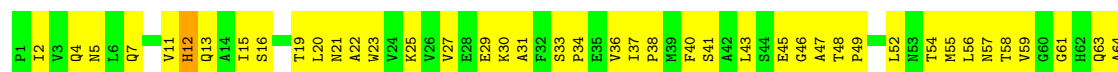
• Molecule 1: capsid protein

Chain 1k: 48% 50%



• Molecule 1: capsid protein

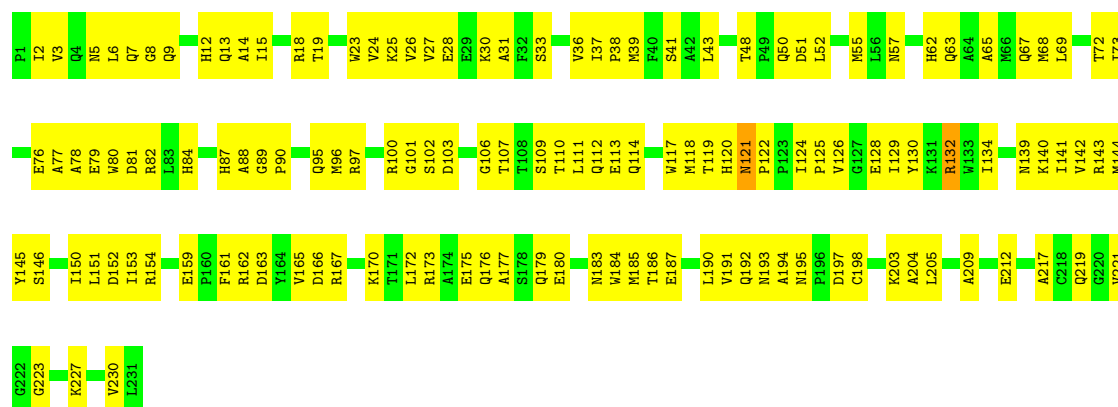
Chain do: 43% 55%





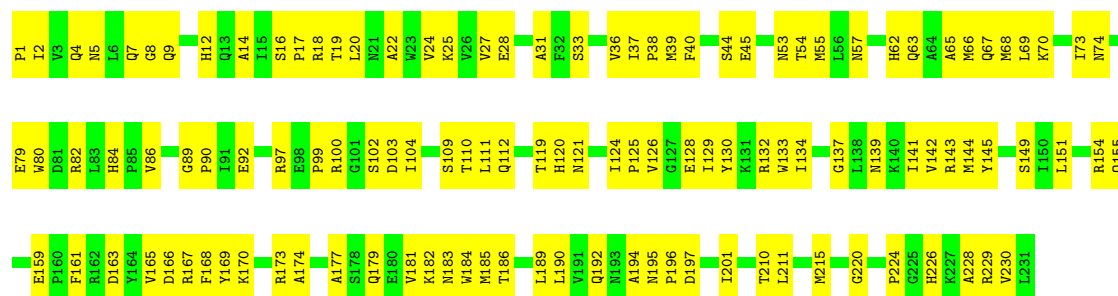
- Molecule 1: capsid protein

Chain dp: 42% 58%



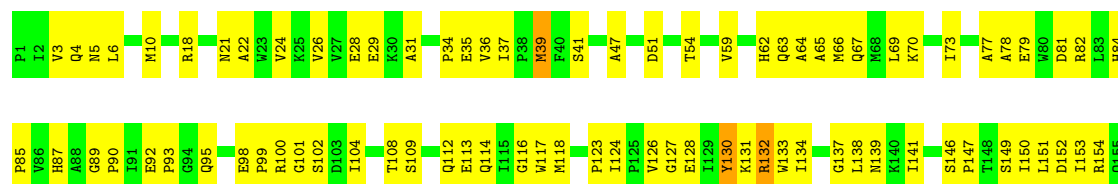
- Molecule 1: capsid protein

Chain dq: 48% 52%



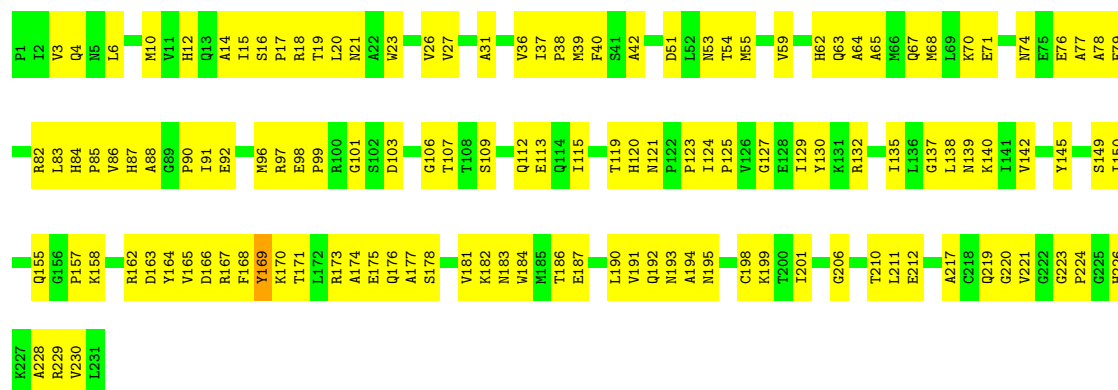
- Molecule 1: capsid protein

Chain dr: 47% 52%

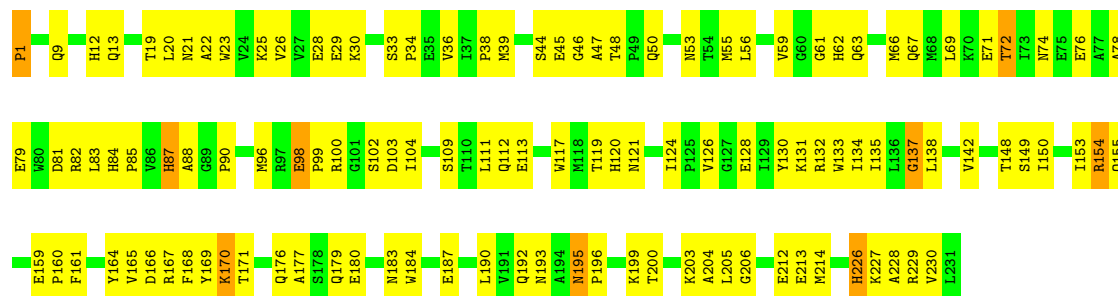




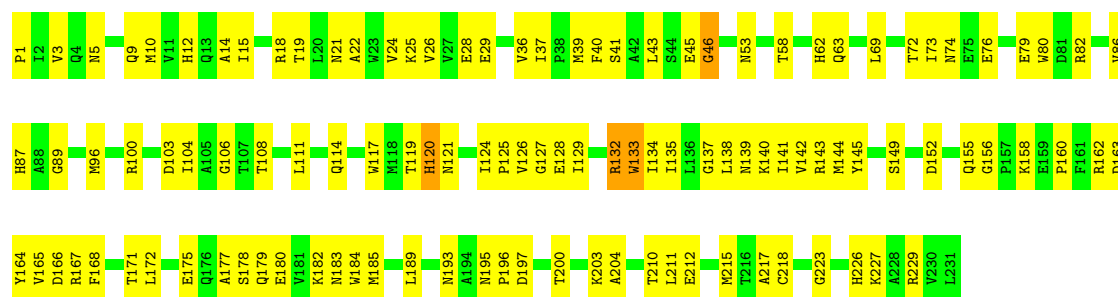
- Molecule 1: capsid protein



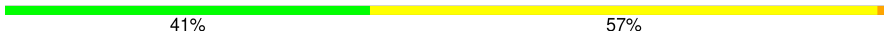
- Molecule 1: capsid protein

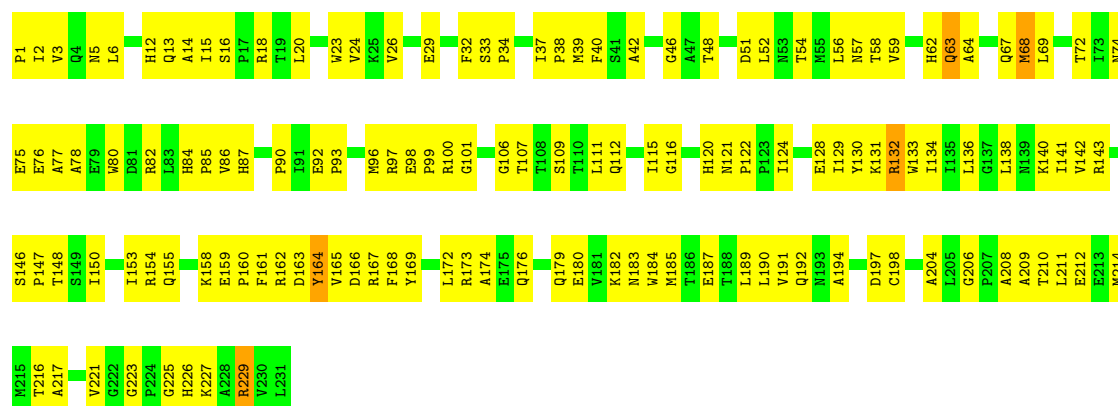


- Molecule 1: capsid protein

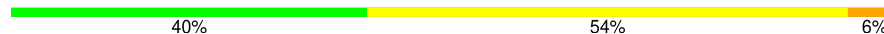


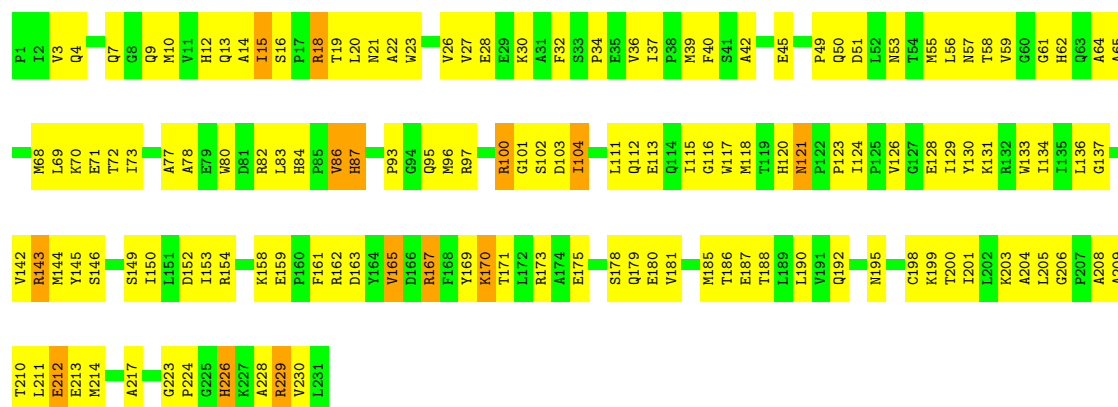
- Molecule 1: capsid protein

Chain dv:  41% 57%

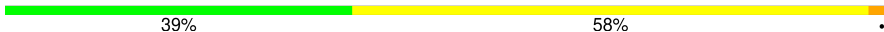


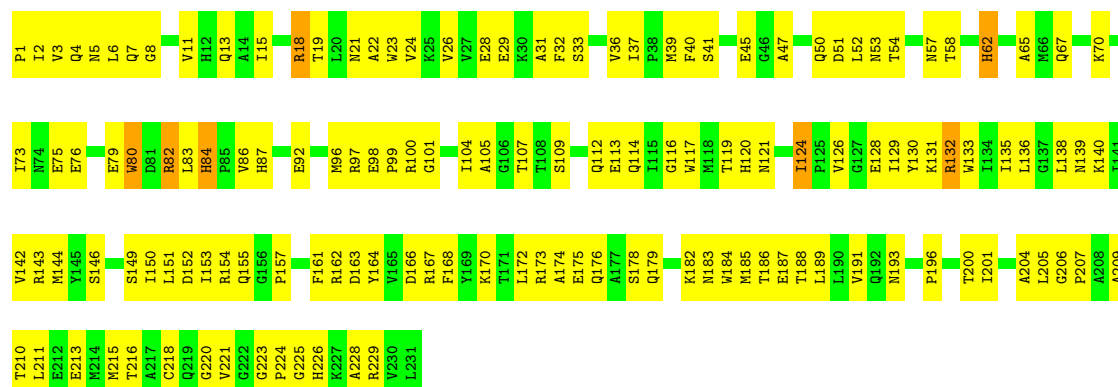
• Molecule 1: capsid protein

Chain dw:  40% 54% 6%

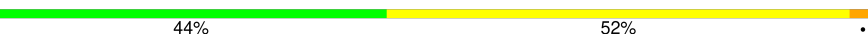


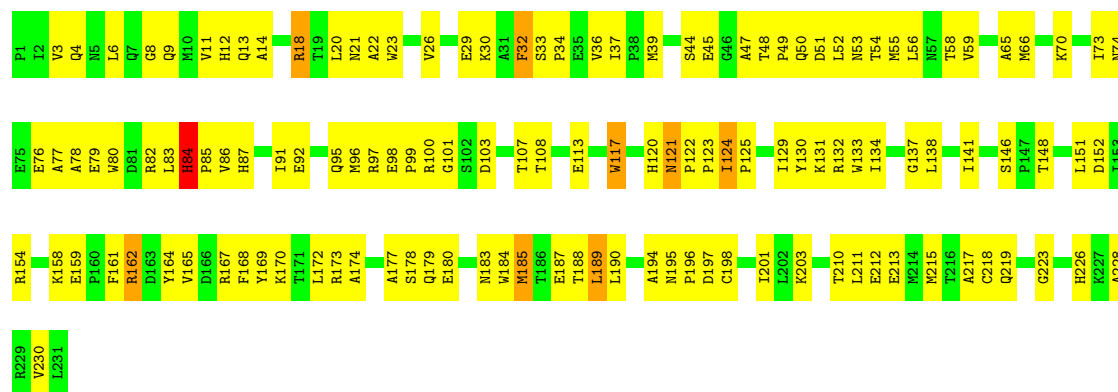
• Molecule 1: capsid protein

Chain dx:  39% 58%

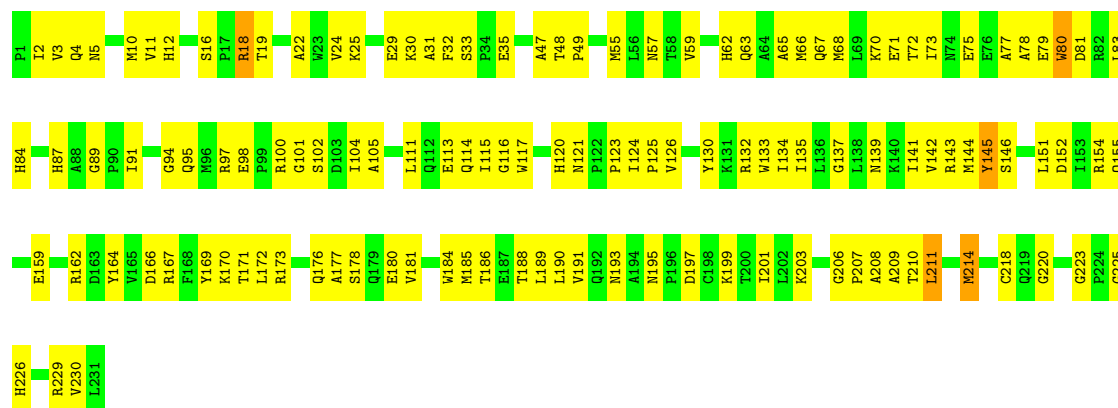


• Molecule 1: capsid protein

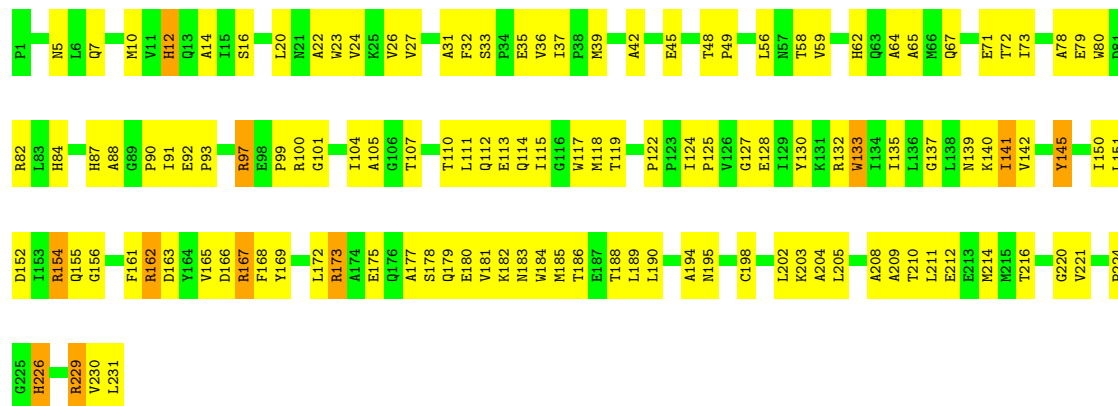
Chain 1l:  44% 52%



- Molecule 1: capsid protein

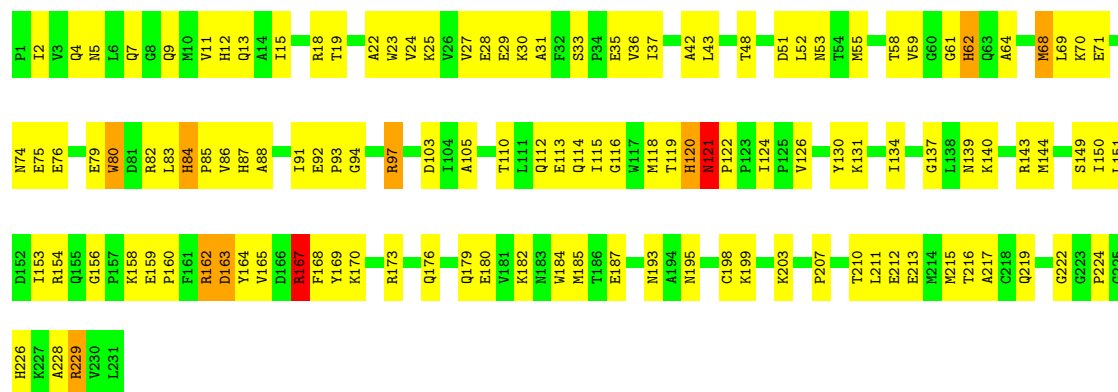


- Molecule 1: capsid protein

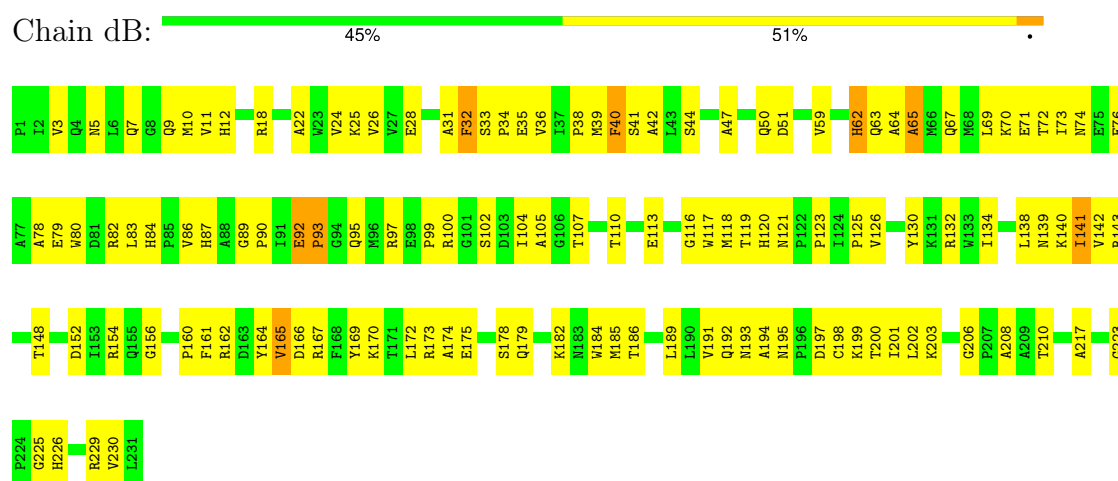


- Molecule 1: capsid protein

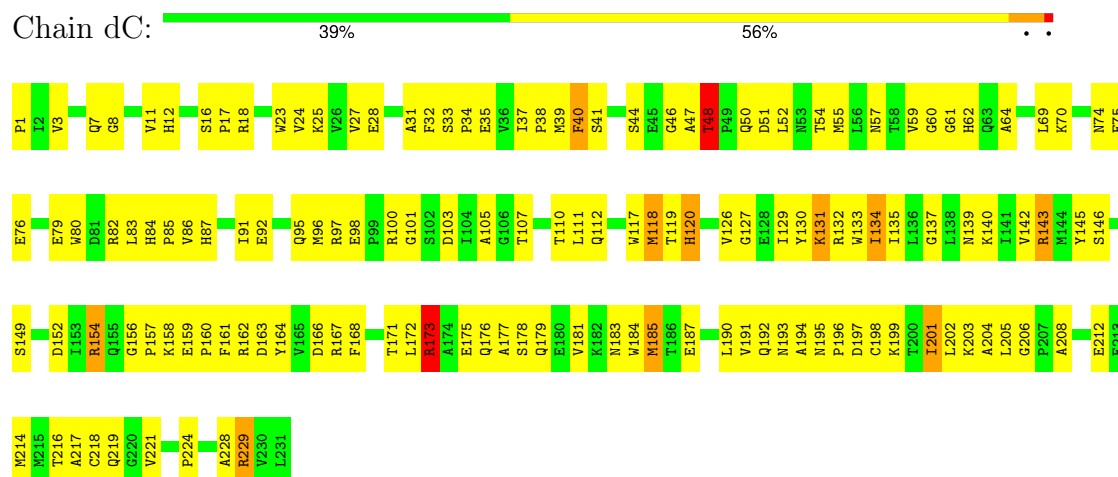




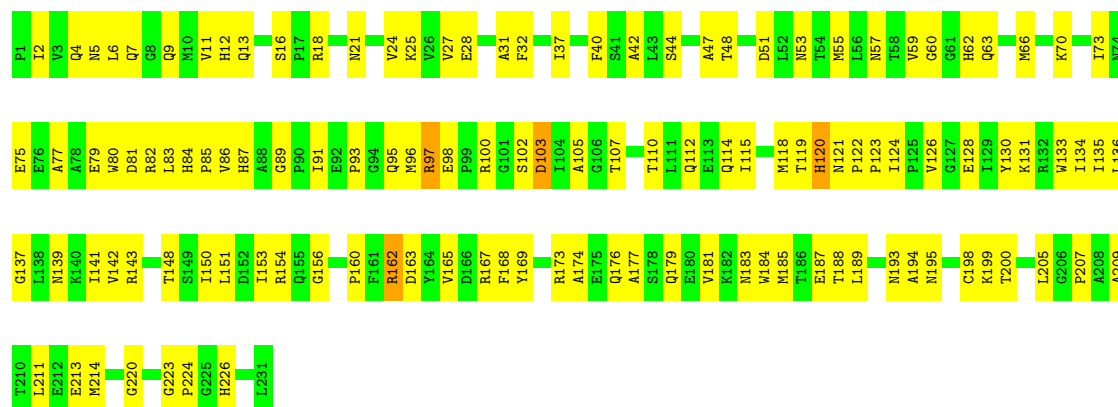
• Molecule 1: capsid protein



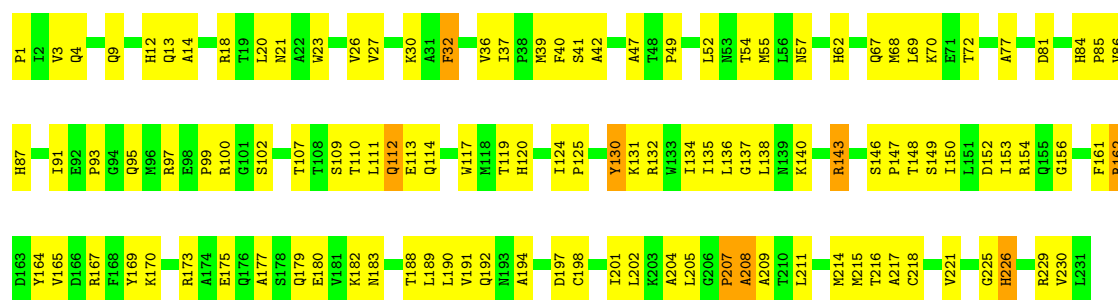
• Molecule 1: capsid protein



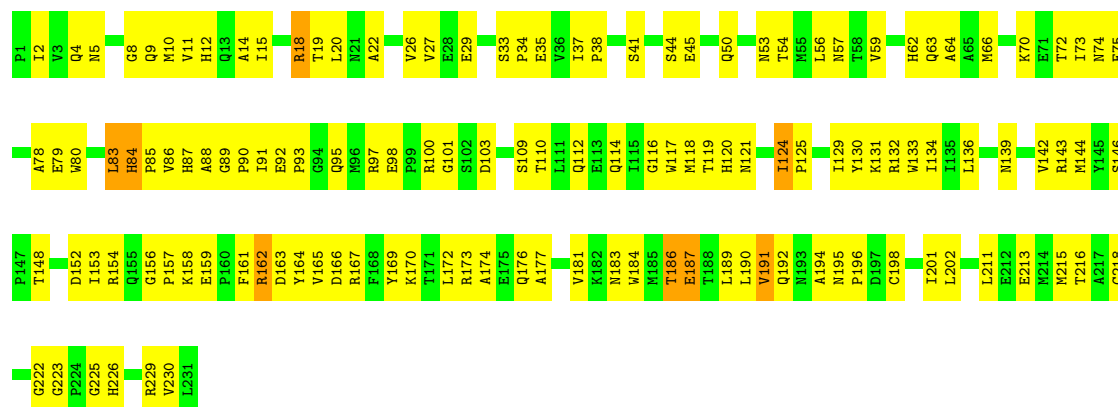
• Molecule 1: capsid protein



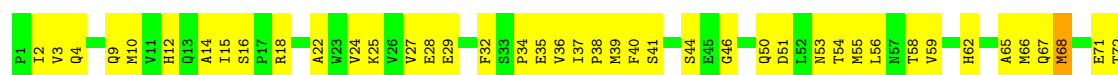
• Molecule 1: capsid protein

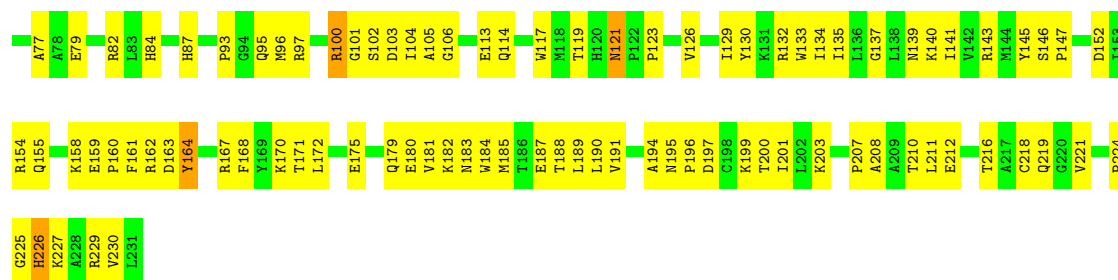


• Molecule 1: capsid protein



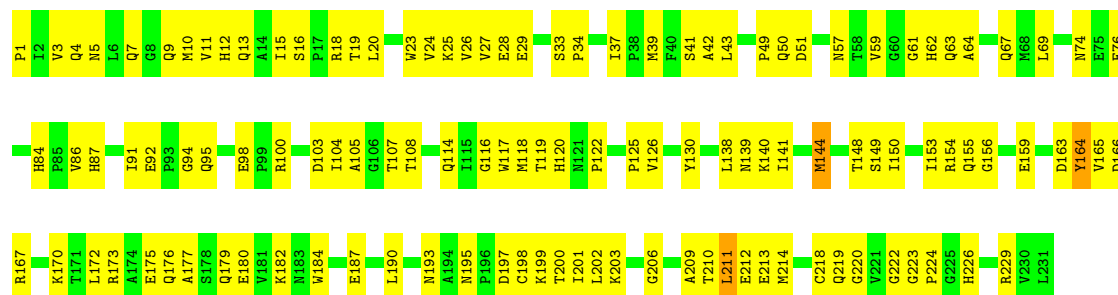
• Molecule 1: capsid protein





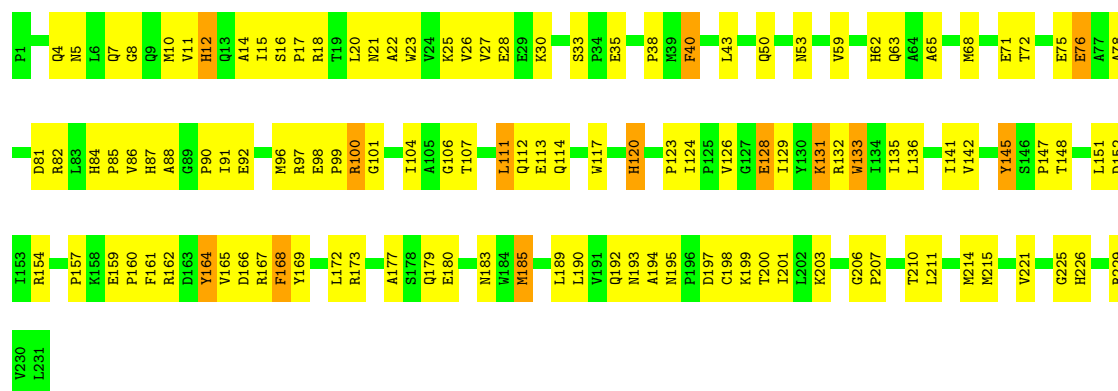
- Molecule 1: capsid protein

Chain dH: 48% 51% .



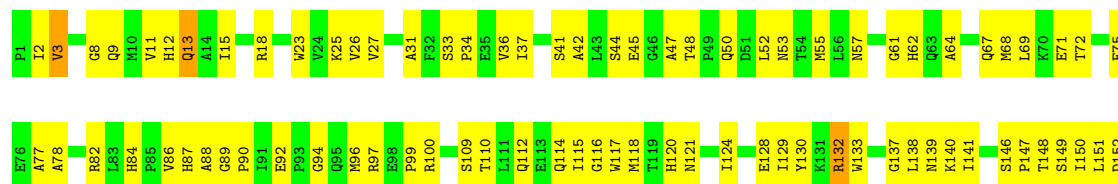
- Molecule 1: capsid protein

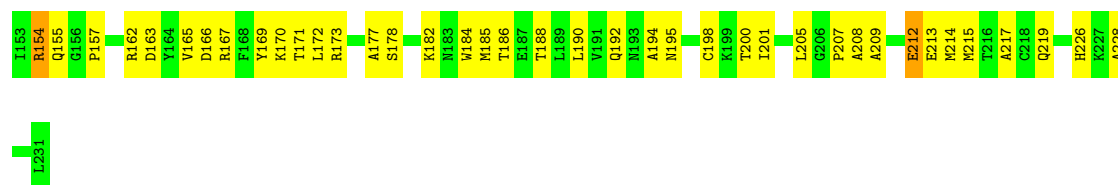
Chain 1m: 48% 47% 6%



- Molecule 1: capsid protein

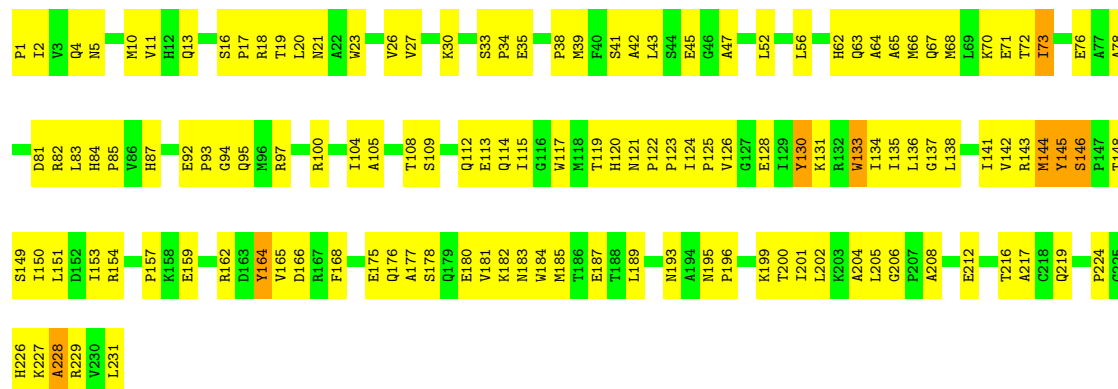
Chain dI: 48% 50% .





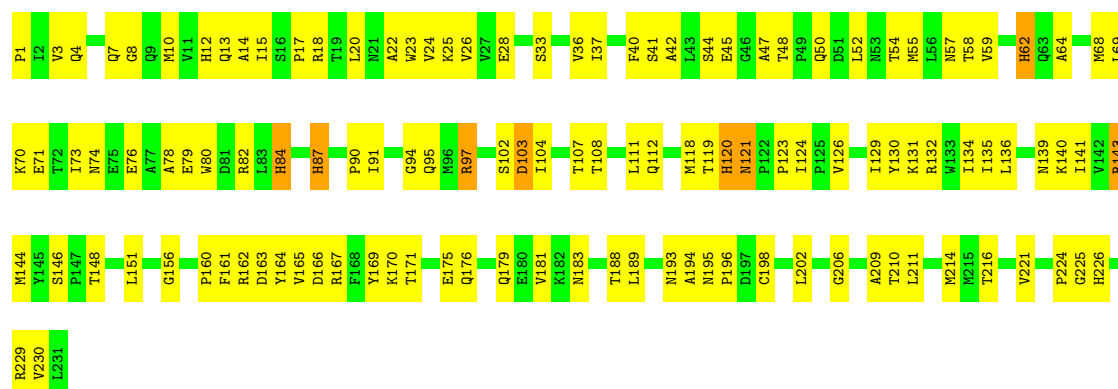
- Molecule 1: capsid protein

Chain dJ: 43% 54%



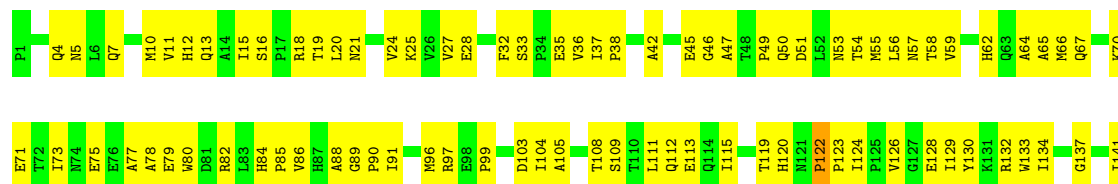
- Molecule 1: capsid protein

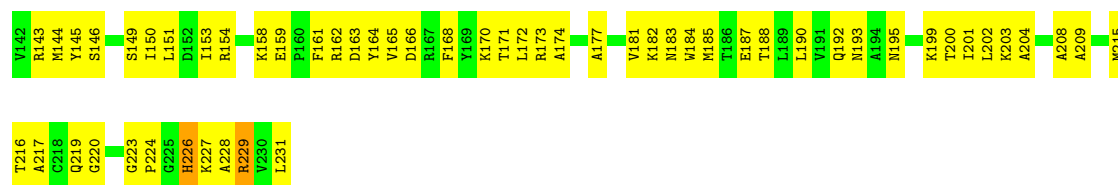
Chain dK: 47% 49%



- Molecule 1: capsid protein

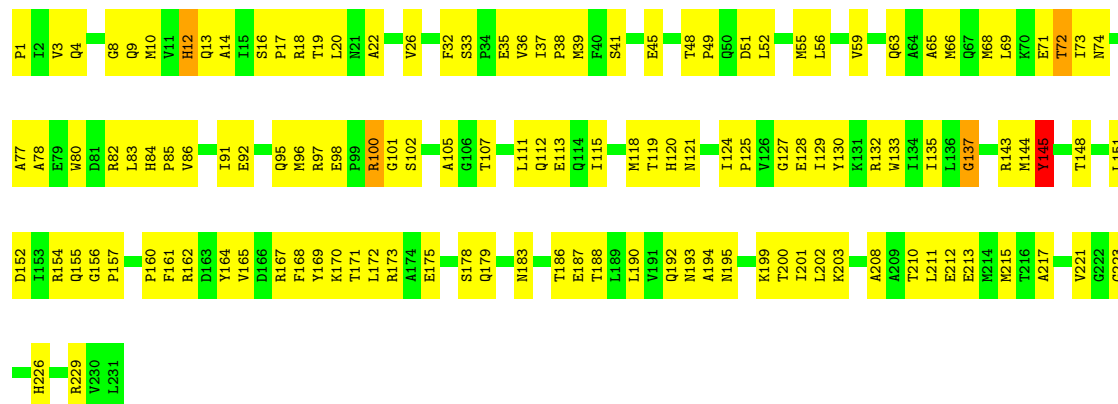
Chain dL: 40% 59%





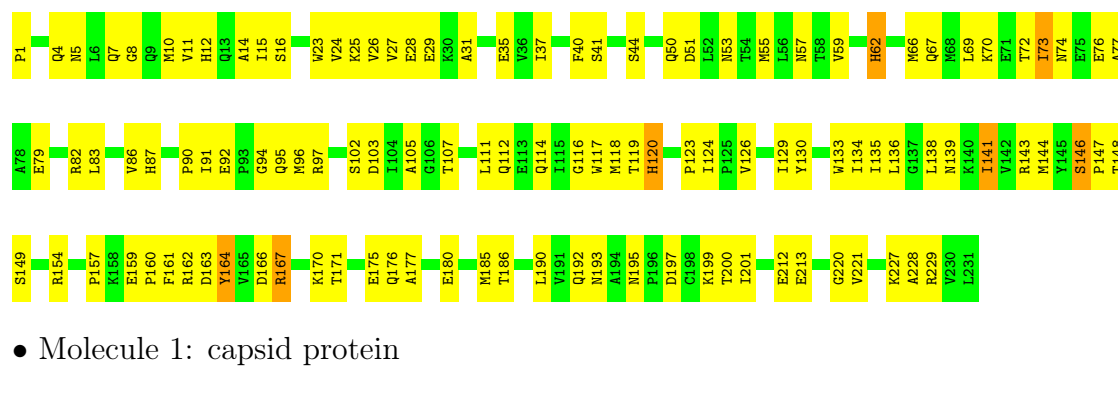
- Molecule 1: capsid protein

Chain dM: 45% 53%



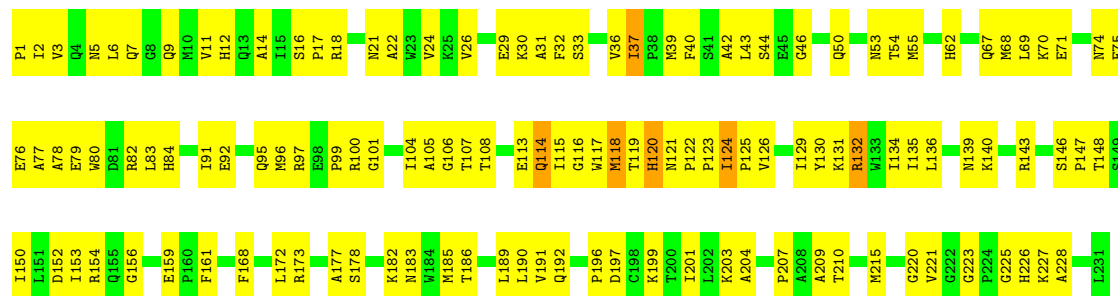
- Molecule 1: capsid protein

Chain dN: 50% 47%



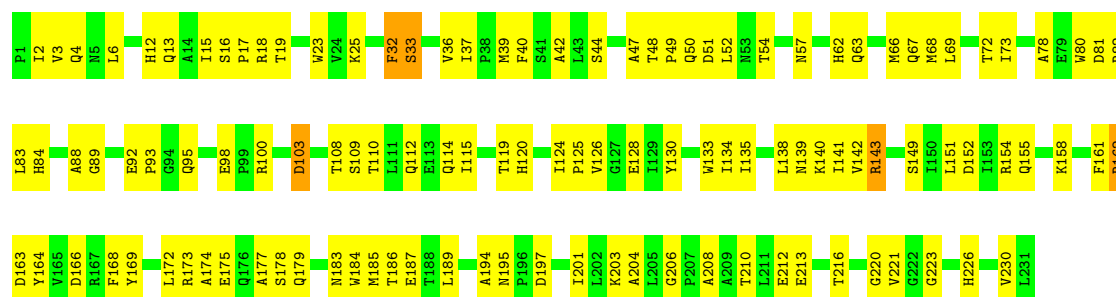
- Molecule 1: capsid protein

Chain dO: 45% 52%

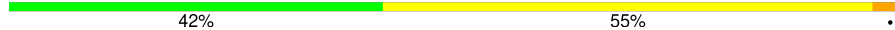


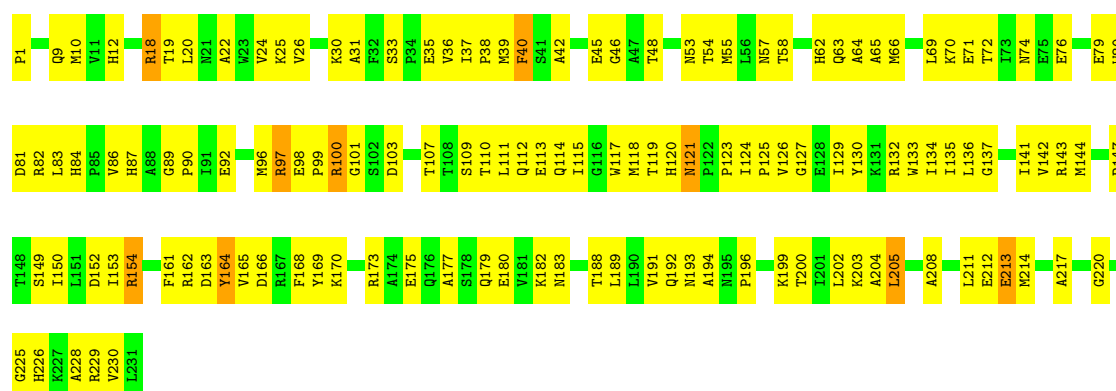
- Molecule 1: capsid protein

Chain dP:  50% 48% .



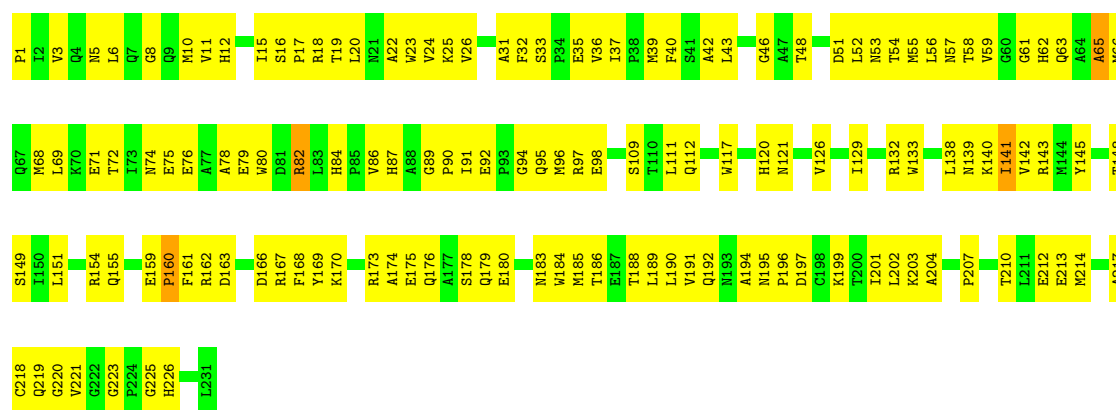
• Molecule 1: capsid protein

Chain dQ:  42% 55% .

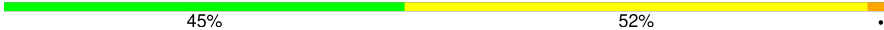


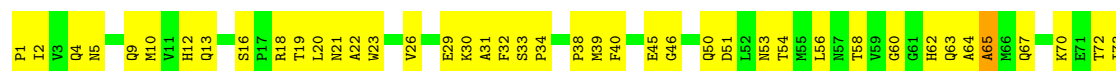
• Molecule 1: capsid protein

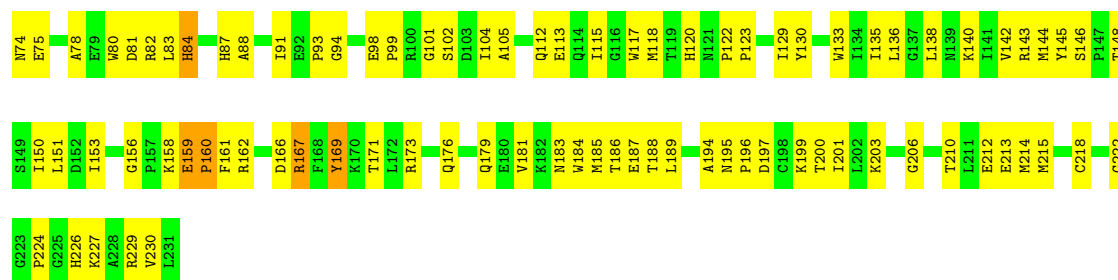
Chain dR:  40% 58% .



• Molecule 1: capsid protein

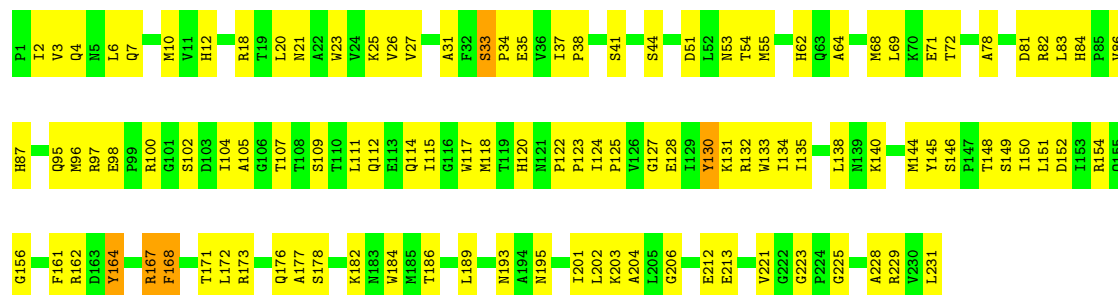
Chain 1n:  45% 52% .





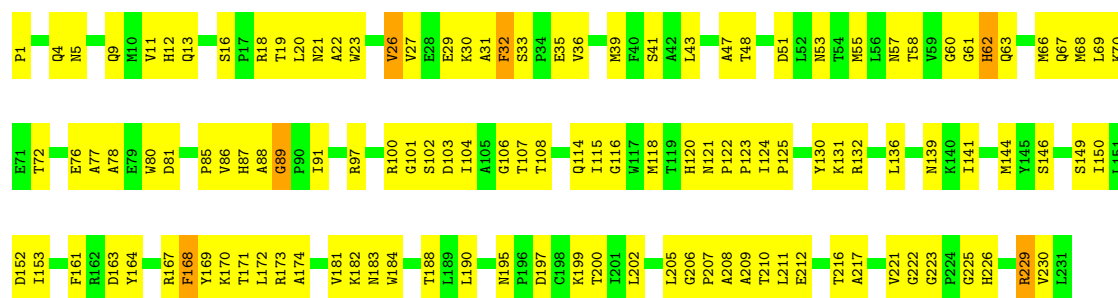
• Molecule 1: capsid protein

Chain dS: 52% 45%



• Molecule 1: capsid protein

Chain dT: 46% 51%



• Molecule 1: capsid protein

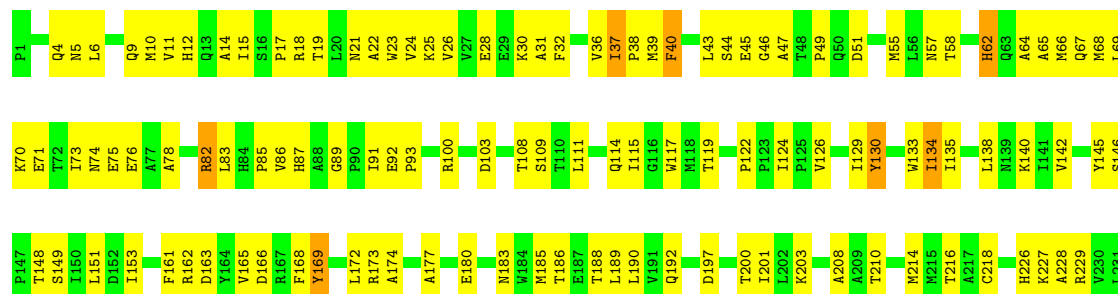
Chain dU: 46% 49%



R229
V230
L231

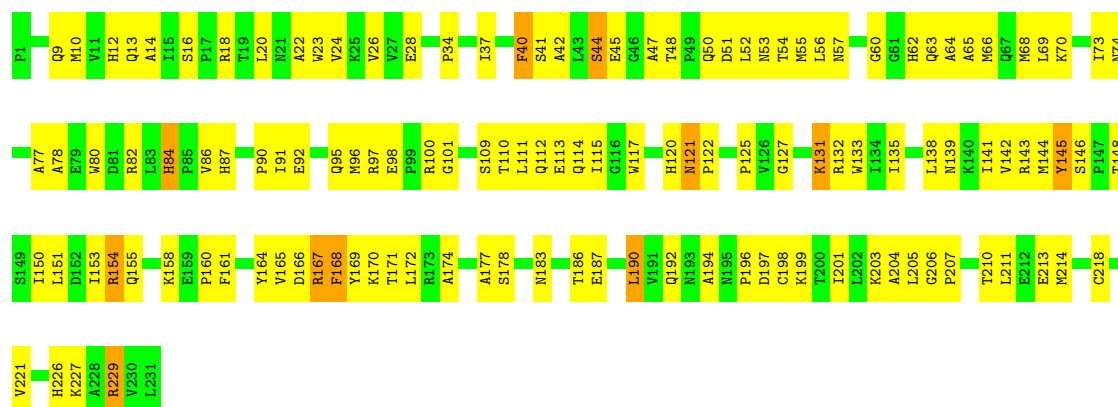
• Molecule 1: capsid protein

Chain dV: 49% 48%



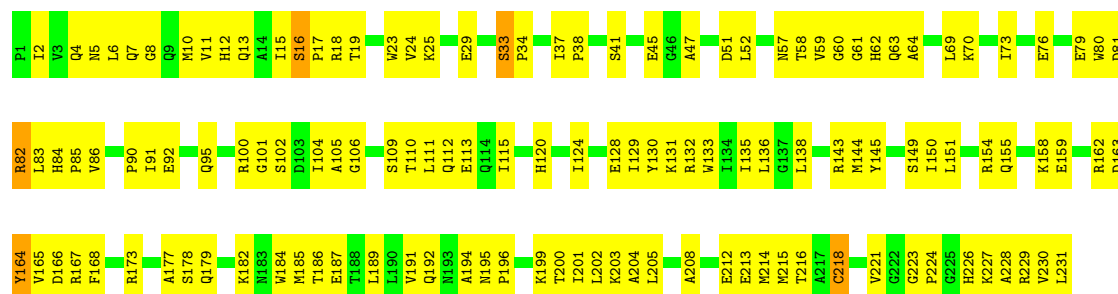
• Molecule 1: capsid protein

Chain dW: 45% 51% 5%



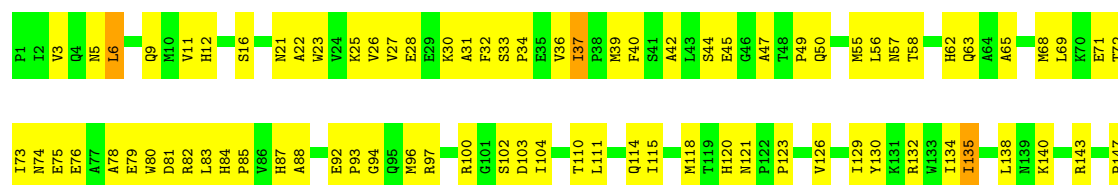
• Molecule 1: capsid protein

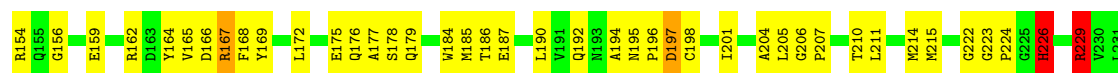
Chain dX: 44% 54%



• Molecule 1: capsid protein

Chain dY: 49% 46%





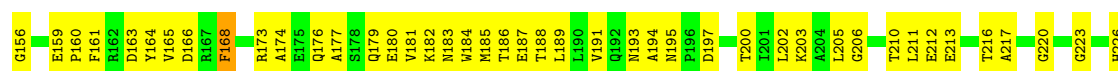
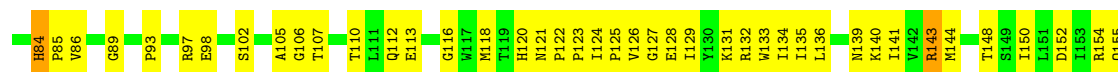
- Molecule 1: capsid protein

Chain e4: 46% 51%



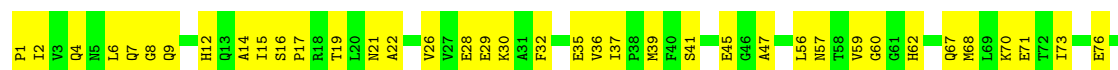
- Molecule 1: capsid protein

Chain e5: 45% 53%



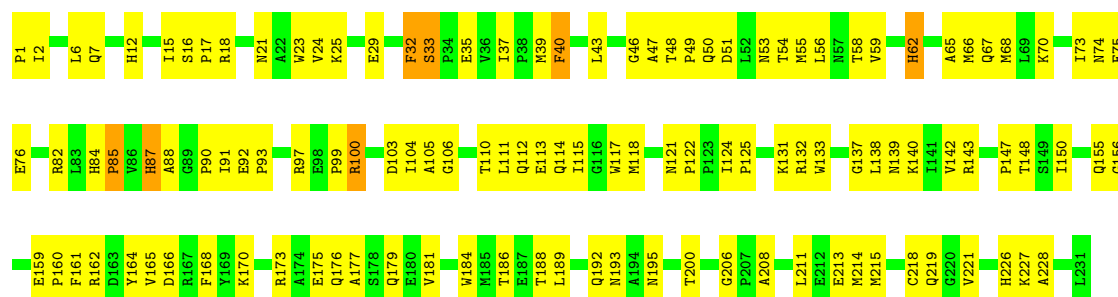
- Molecule 1: capsid protein

Chain e6: 47% 49%



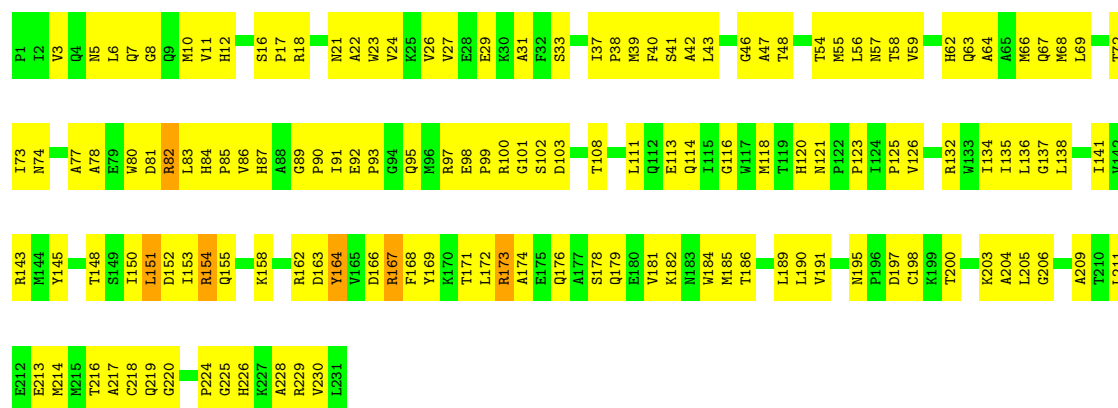
- Molecule 1: capsid protein

Chain e7: 



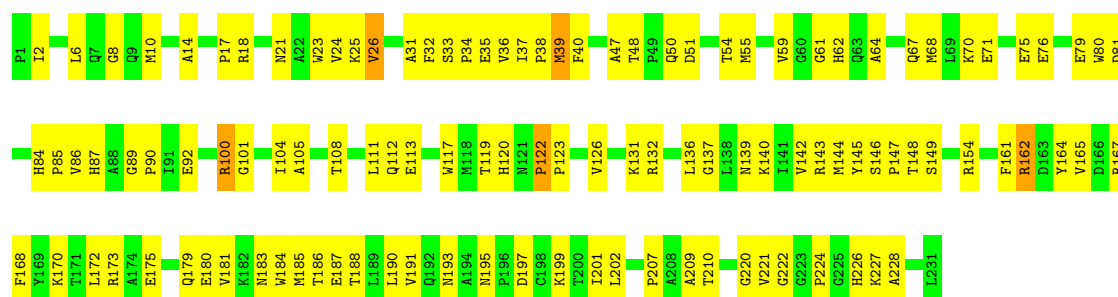
• Molecule 1: capsid protein

Chain e8: 



• Molecule 1: capsid protein

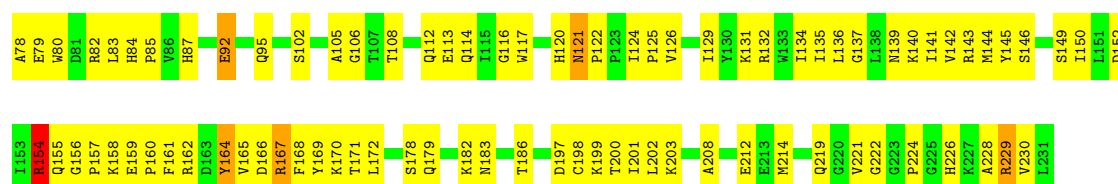
Chain e9: 



• Molecule 1: capsid protein

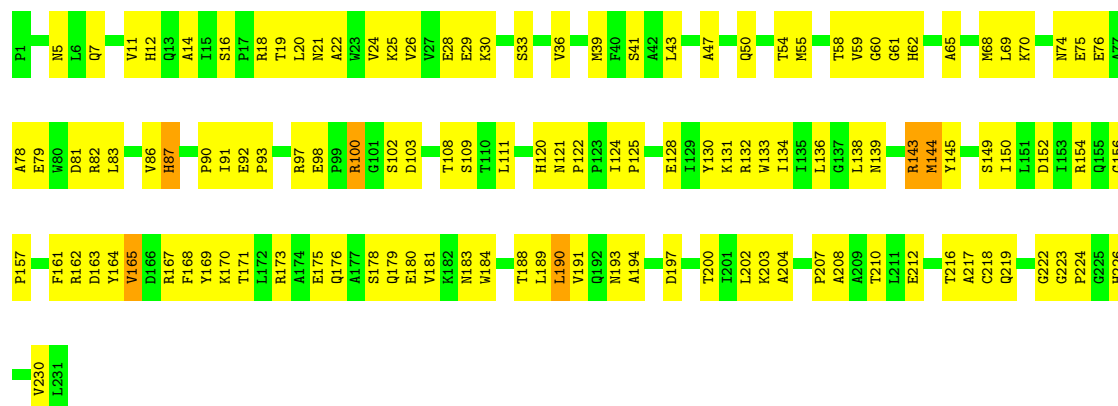
Chain ea: 





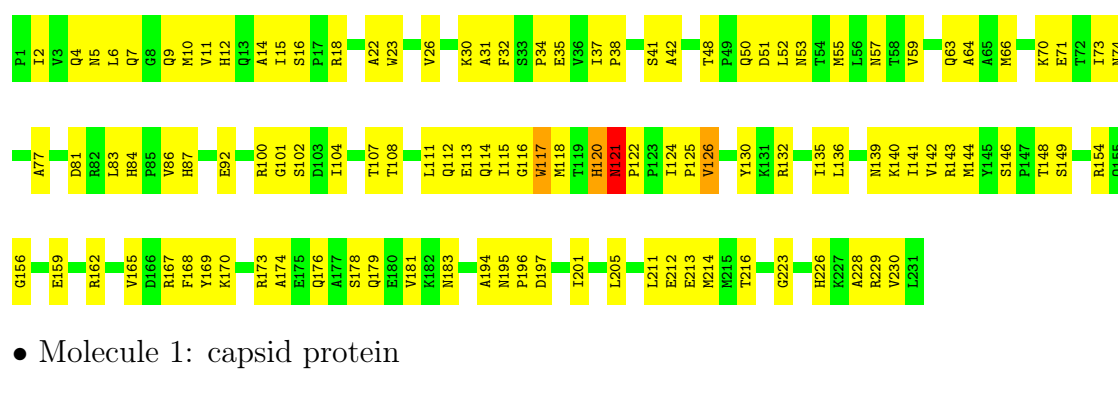
• Molecule 1: capsid protein

Chain eb:



• Molecule 1: capsid protein

Chain 1p:

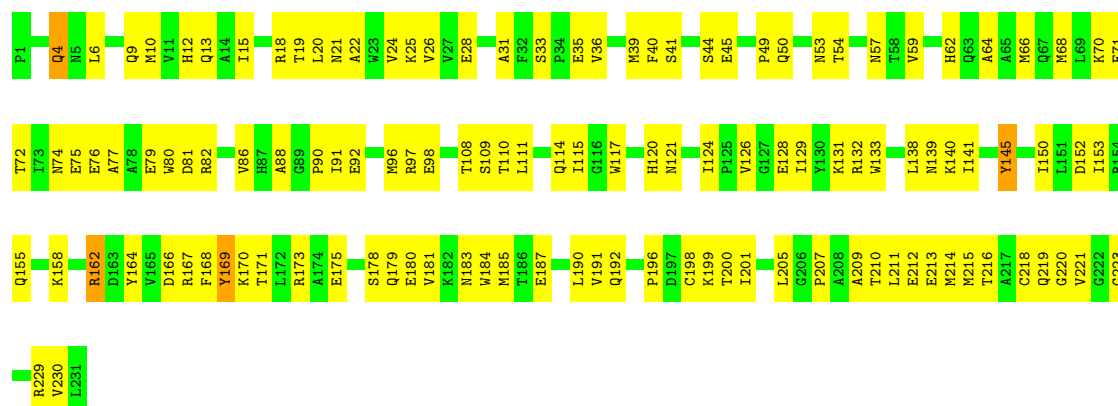


• Molecule 1: capsid protein

Chain ec:



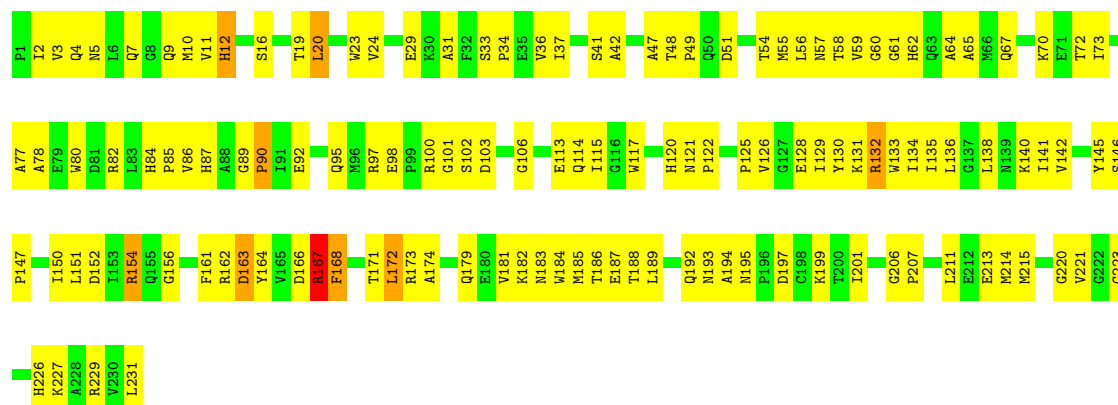
• Molecule 1: capsid protein

Chain ed: 

• Molecule 1: capsid protein

Chain ee: 

• Molecule 1: capsid protein

Chain ef: 

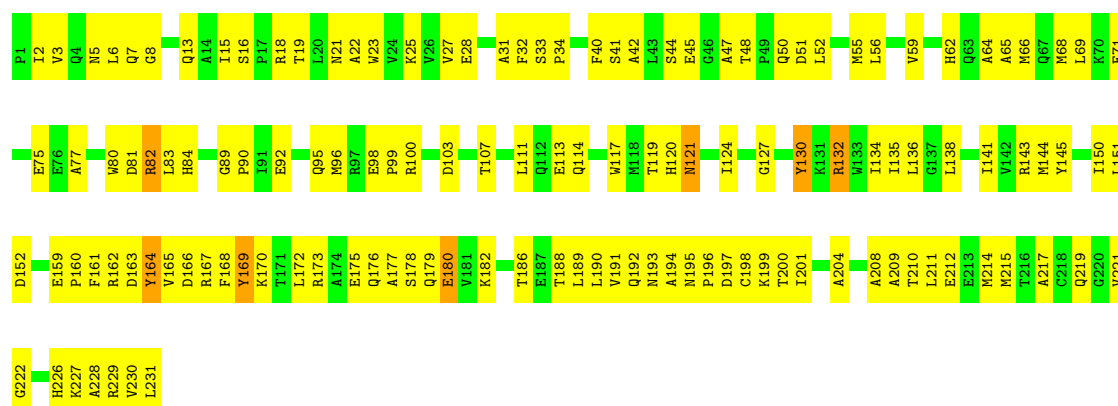
• Molecule 1: capsid protein

Chain eg: 



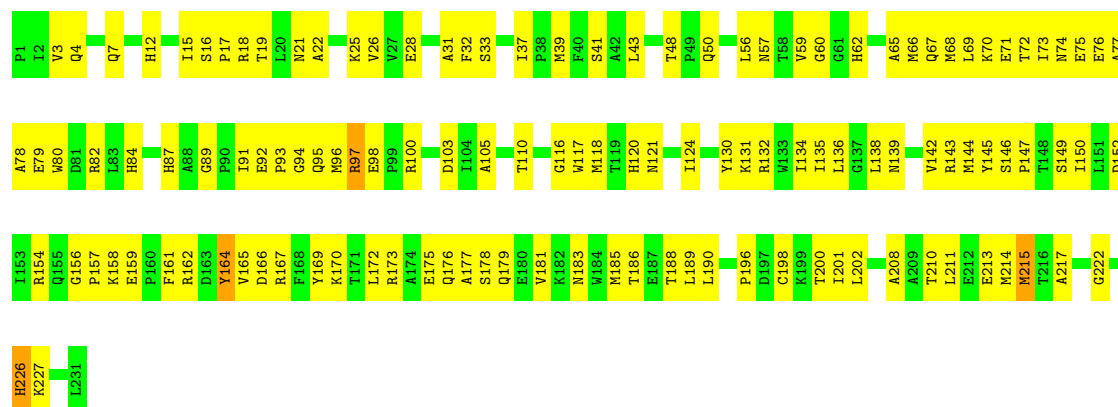
• Molecule 1: capsid protein

Chain eh: 42% 55%



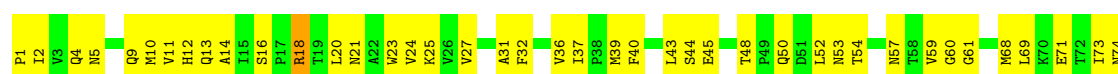
• Molecule 1: capsid protein

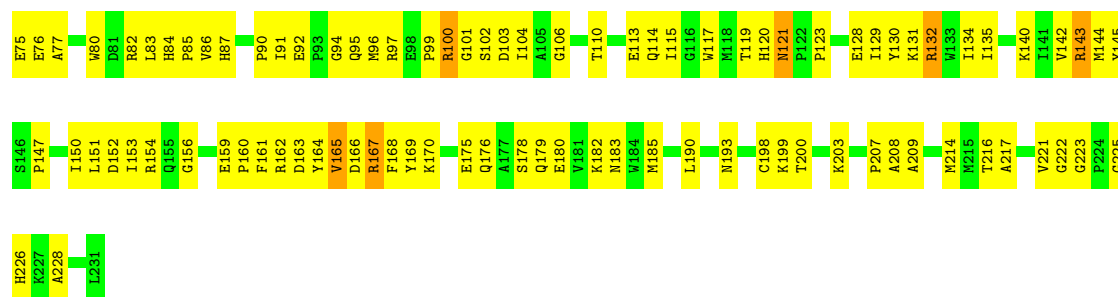
Chain ei: 46% 52%



• Molecule 1: capsid protein

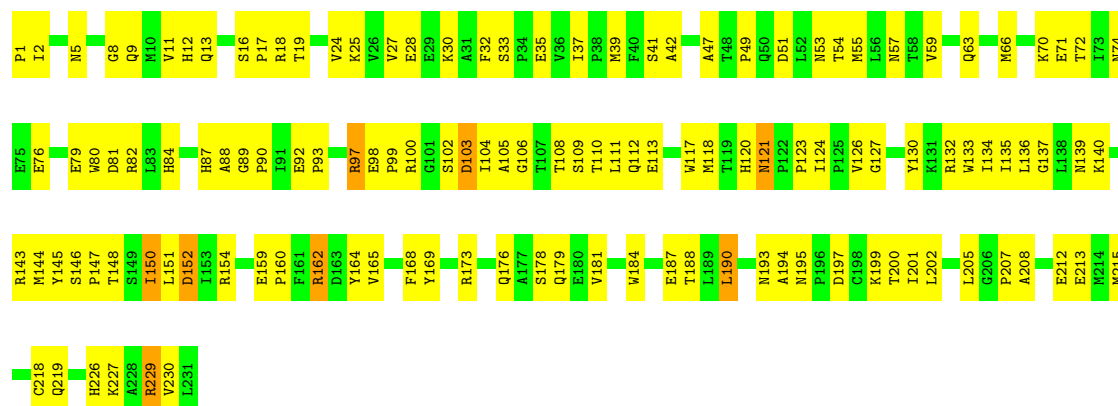
Chain ej: 43% 54%





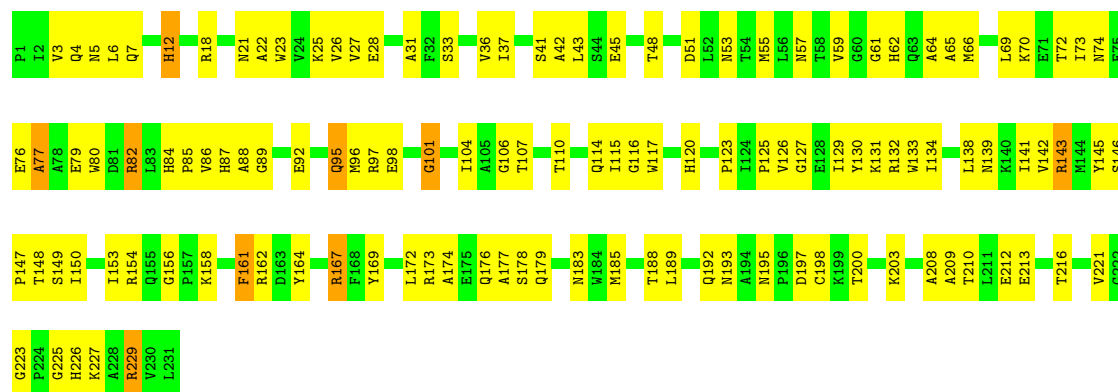
• Molecule 1: capsid protein

Chain ek: 45% 52%



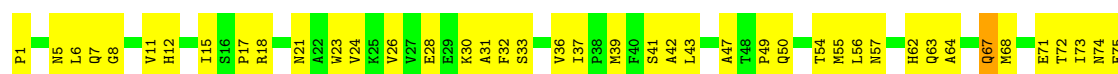
• Molecule 1: capsid protein

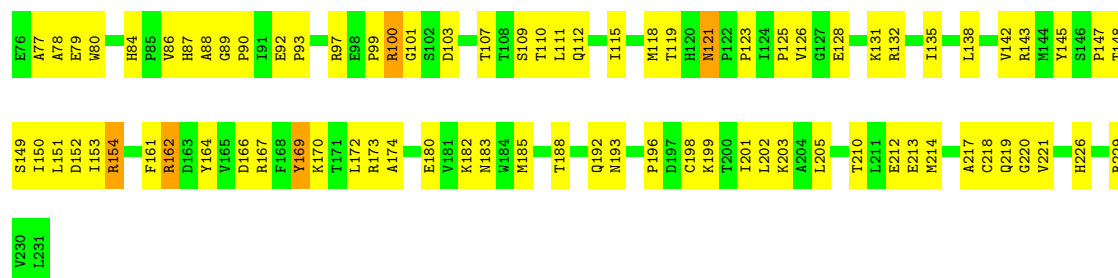
Chain el: 46% 50%



• Molecule 1: capsid protein

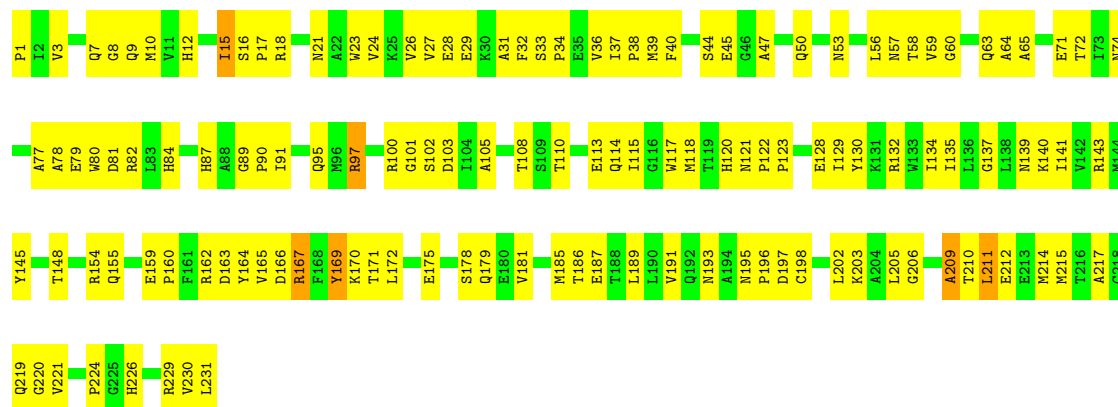
Chain 1q: 47% 50%





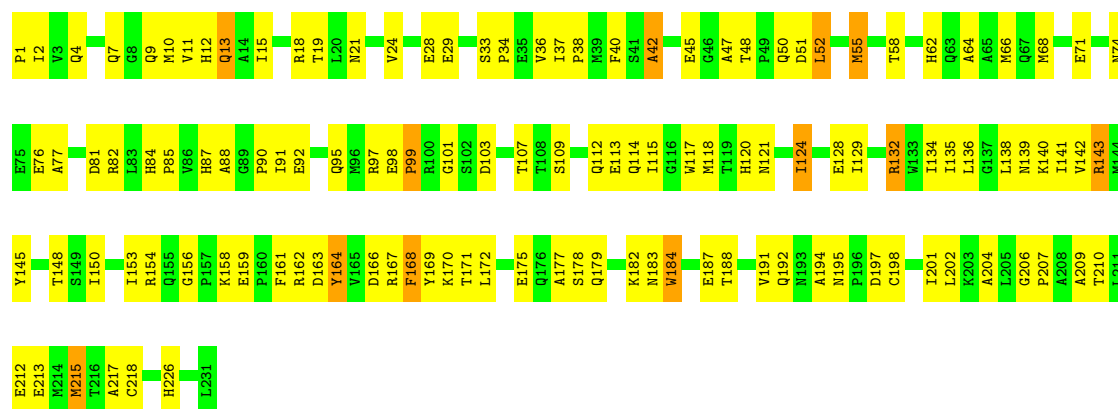
- Molecule 1: capsid protein

Chain em: 43% 55%



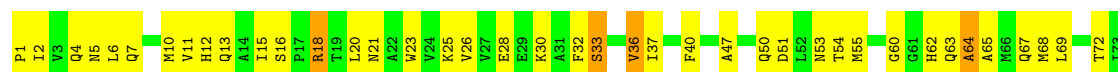
- Molecule 1: capsid protein

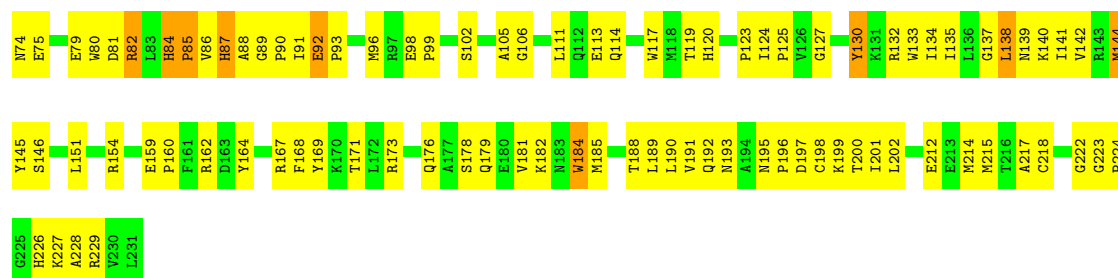
Chain en: 46% 48% 5%



- Molecule 1: capsid protein

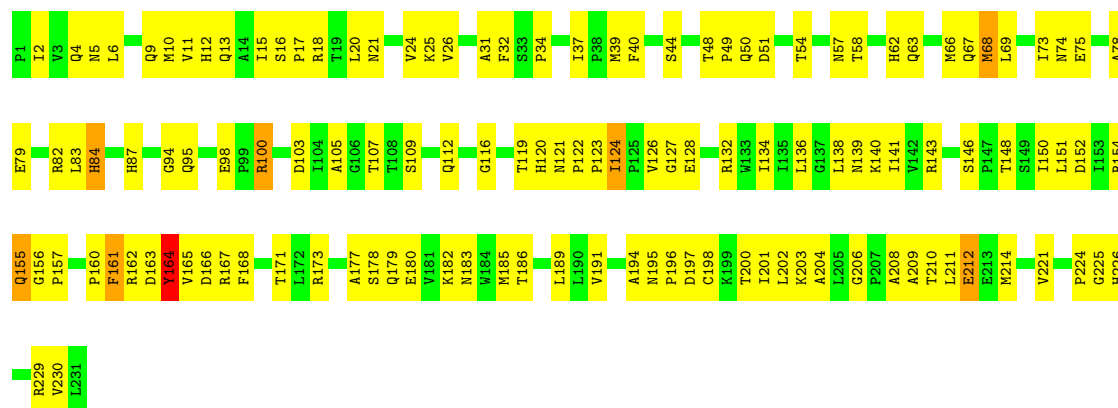
Chain eo: 44% 51% 6%





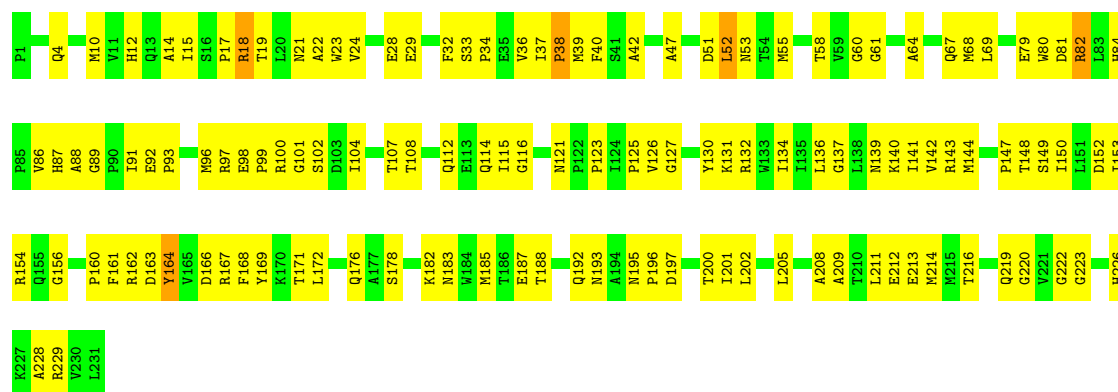
- Molecule 1: capsid protein

Chain ep: 45% 52%



- Molecule 1: capsid protein

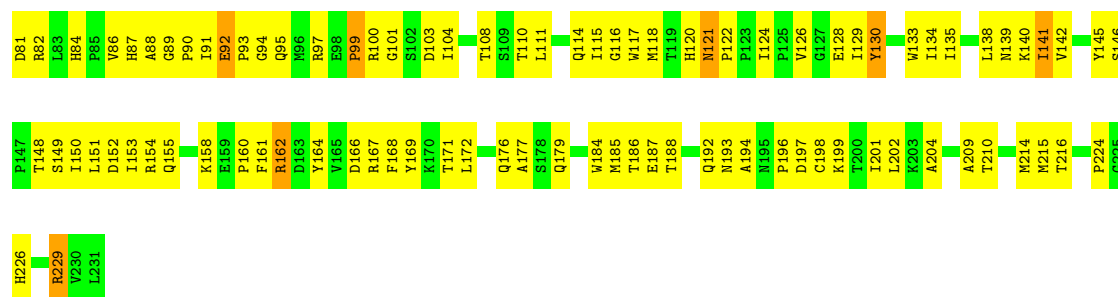
Chain eq: 45% 53%



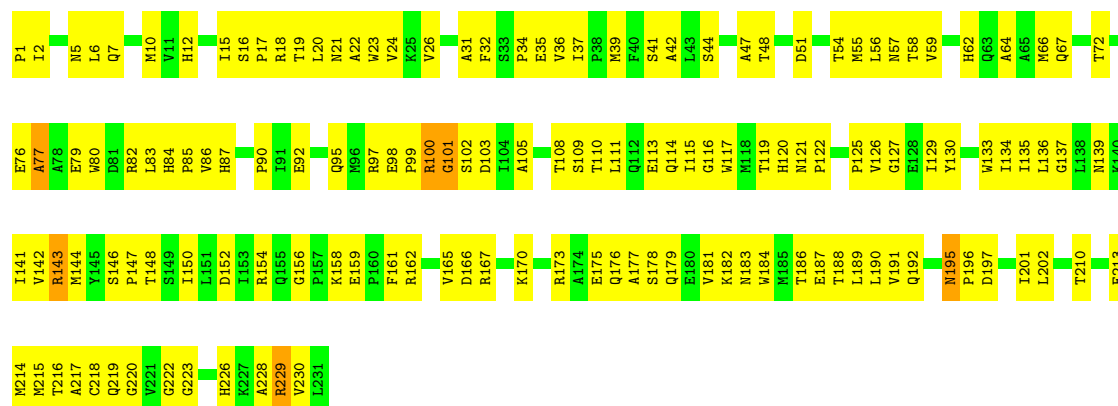
- Molecule 1: capsid protein

Chain er: 42% 55%

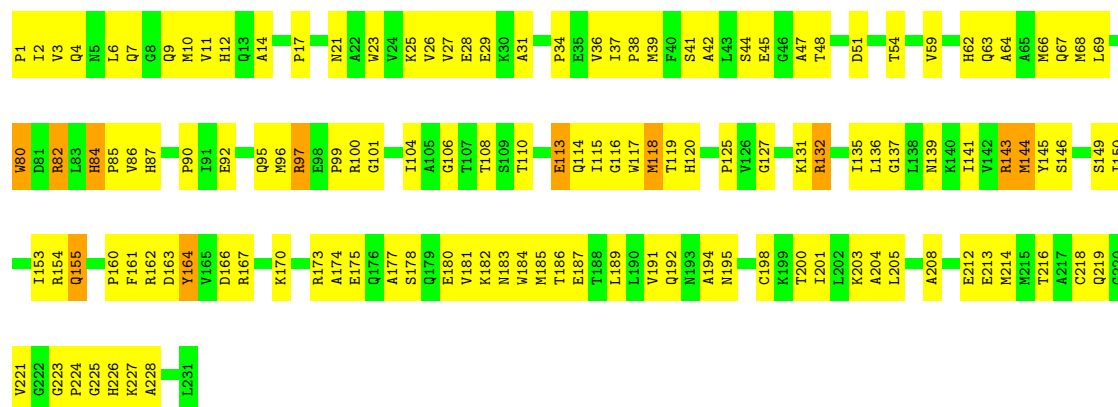




• Molecule 1: capsid protein

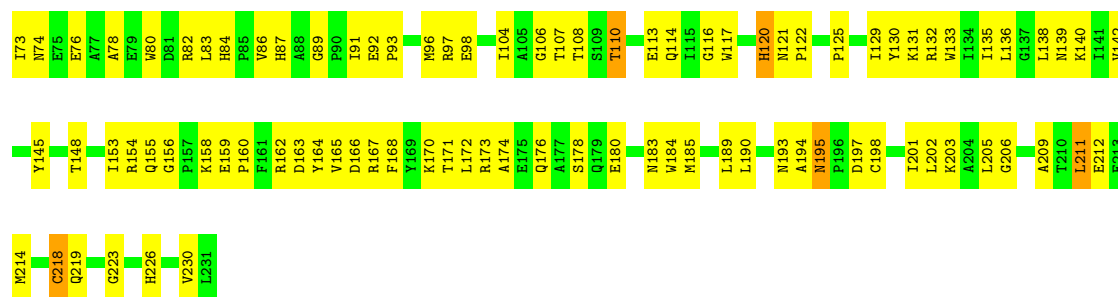


• Molecule 1: capsid protein



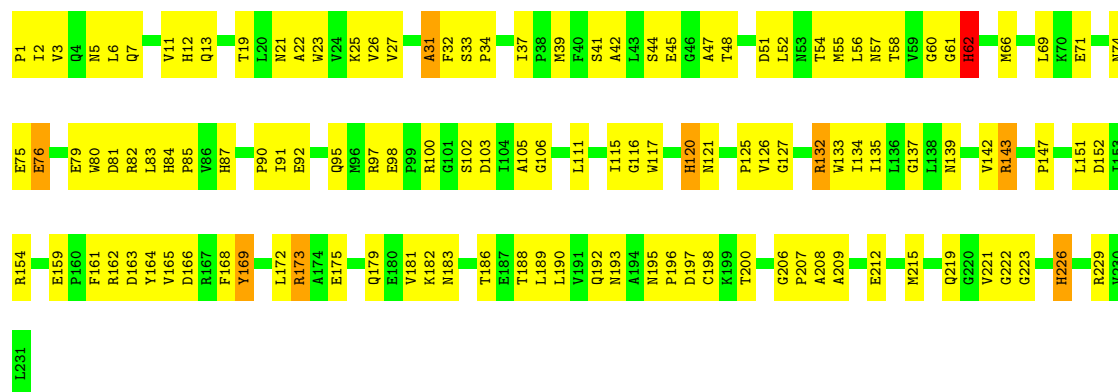
• Molecule 1: capsid protein





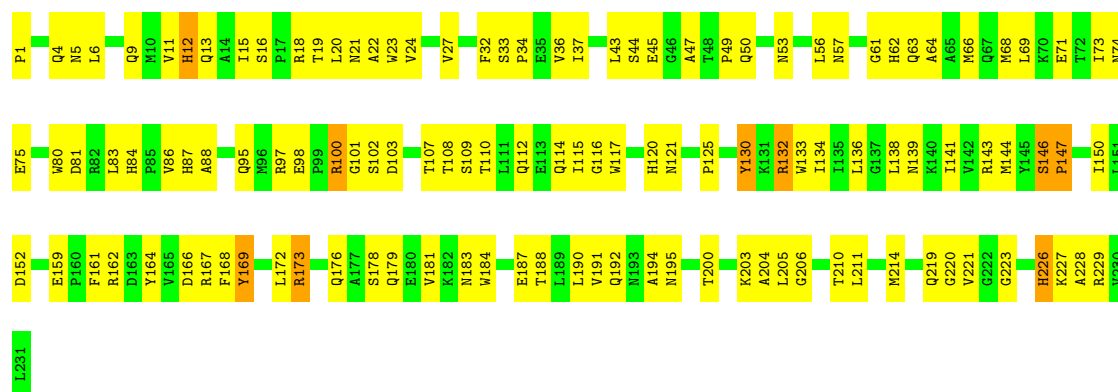
- Molecule 1: capsid protein

Chain ev: 47% 49%



- Molecule 1: capsid protein

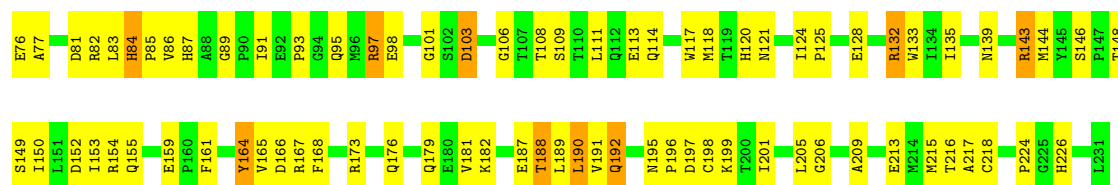
Chain 1r: 47% 49%



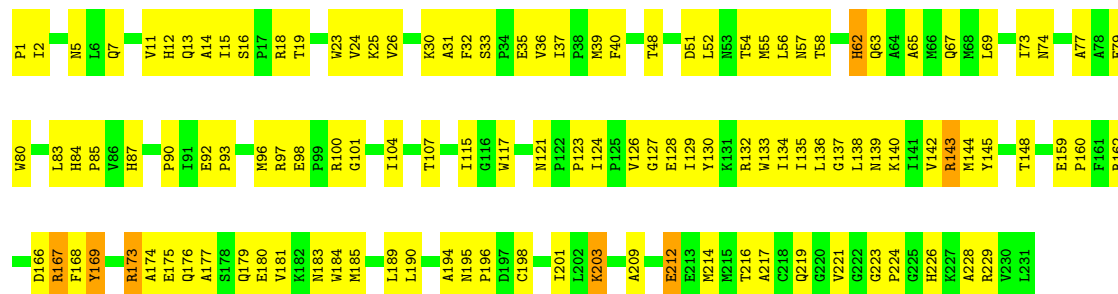
- Molecule 1: capsid protein

Chain ew: 48% 48%

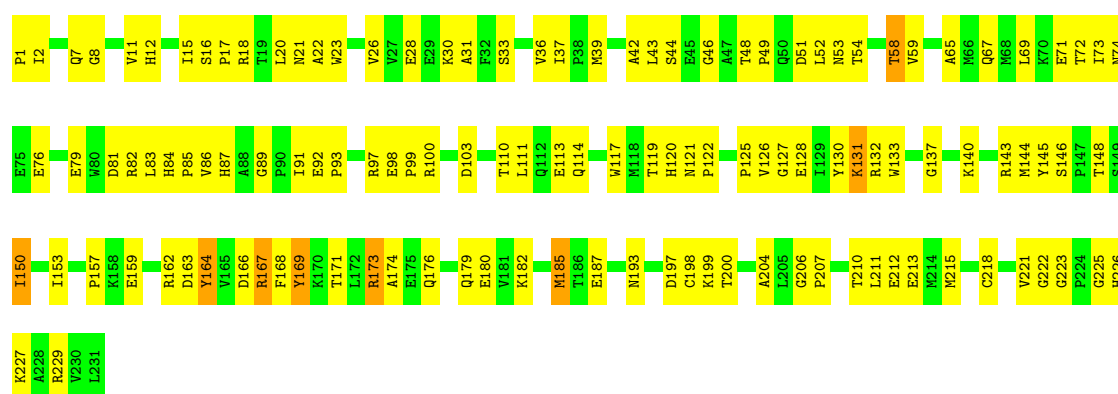




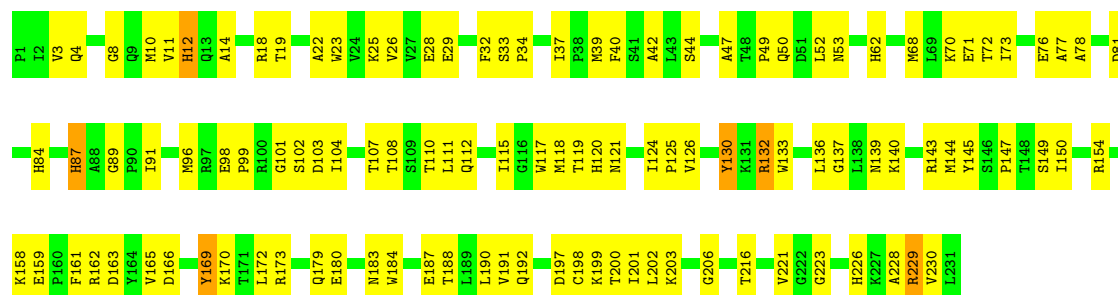
• Molecule 1: capsid protein



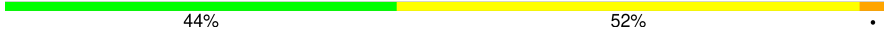
• Molecule 1: capsid protein

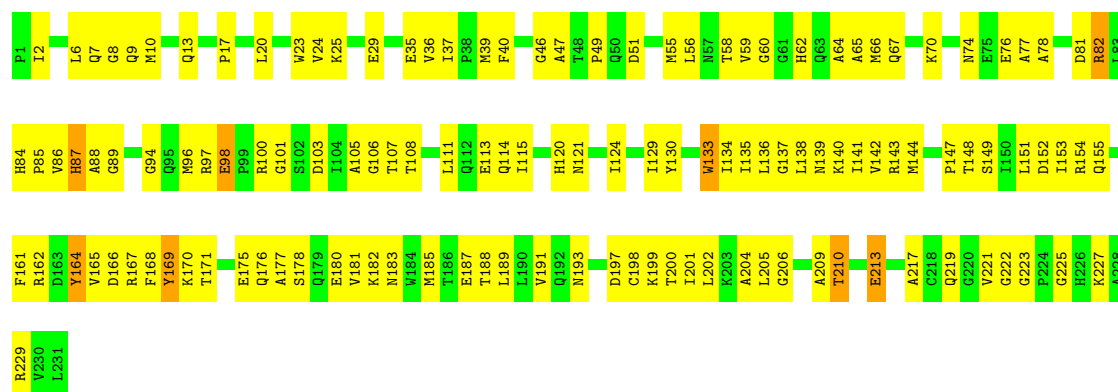


• Molecule 1: capsid protein

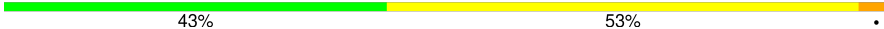


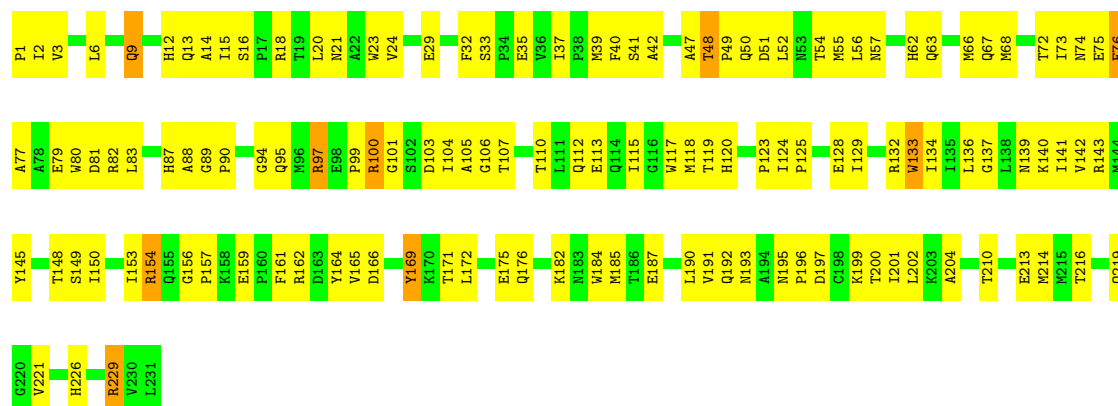
• Molecule 1: capsid protein

Chain eA: 



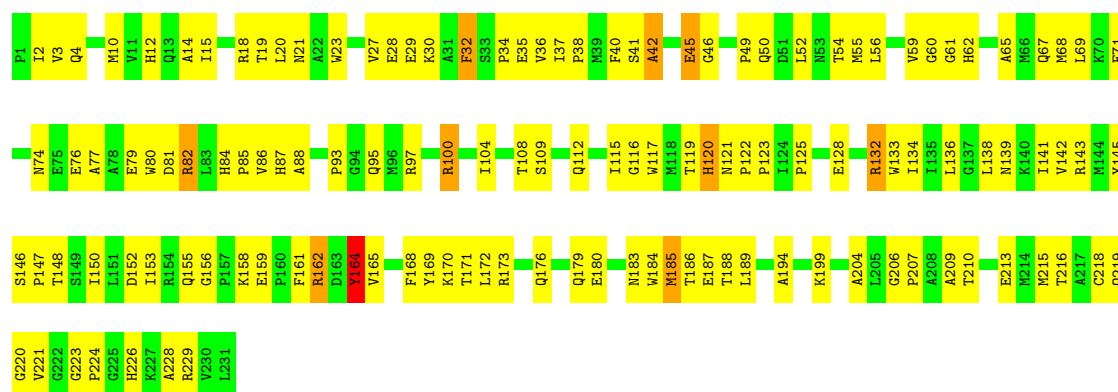
• Molecule 1: capsid protein

Chain eB: 



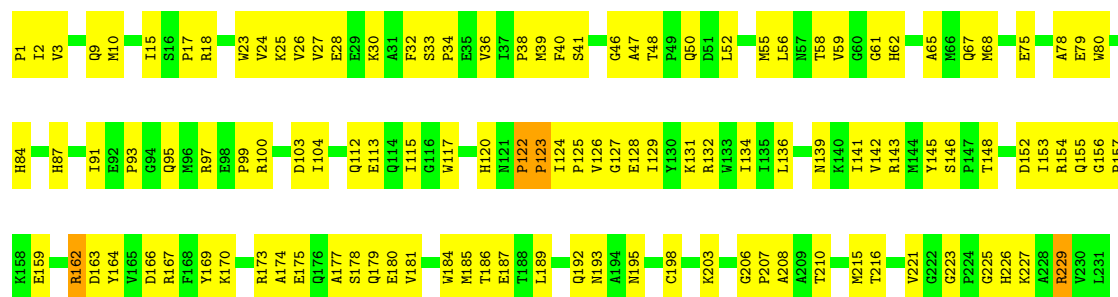
• Molecule 1: capsid protein

Chain eC: 

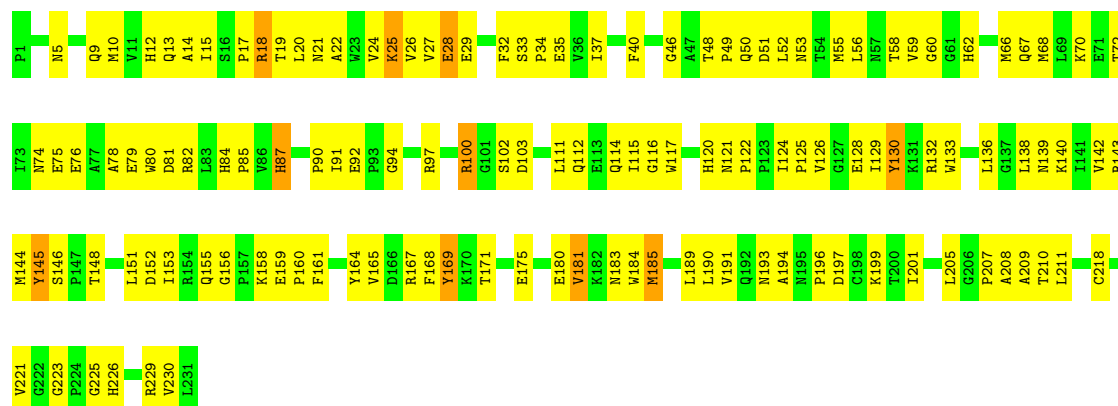


• Molecule 1: capsid protein

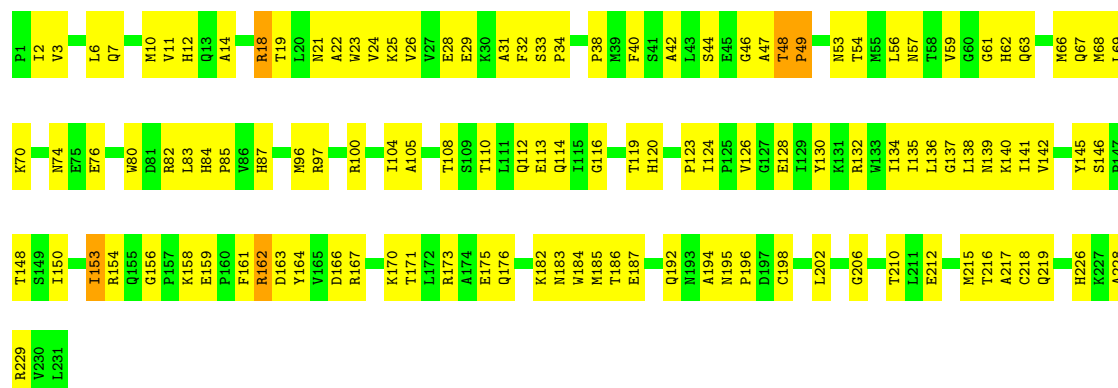
Chain eD: 



• Molecule 1: capsid protein

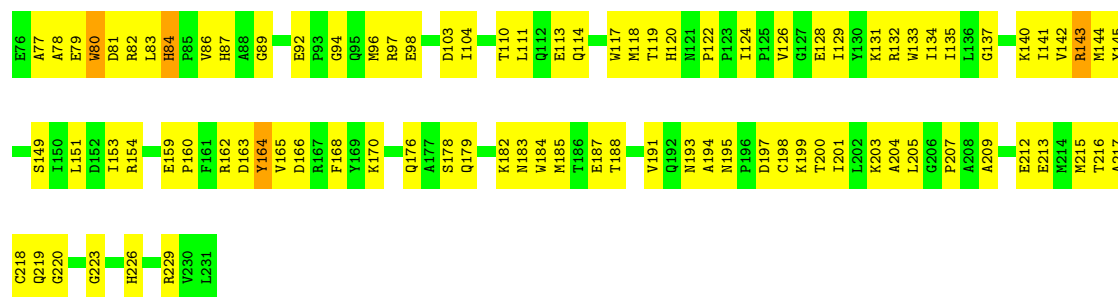


• Molecule 1: capsid protein



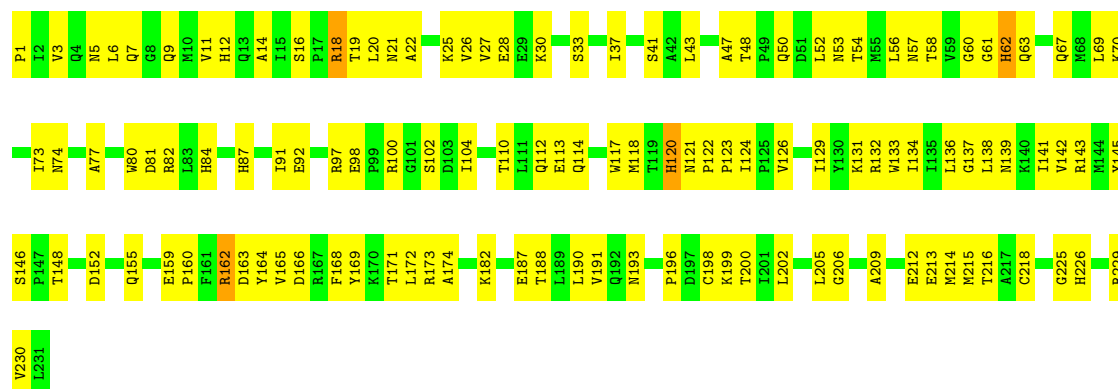
• Molecule 1: capsid protein





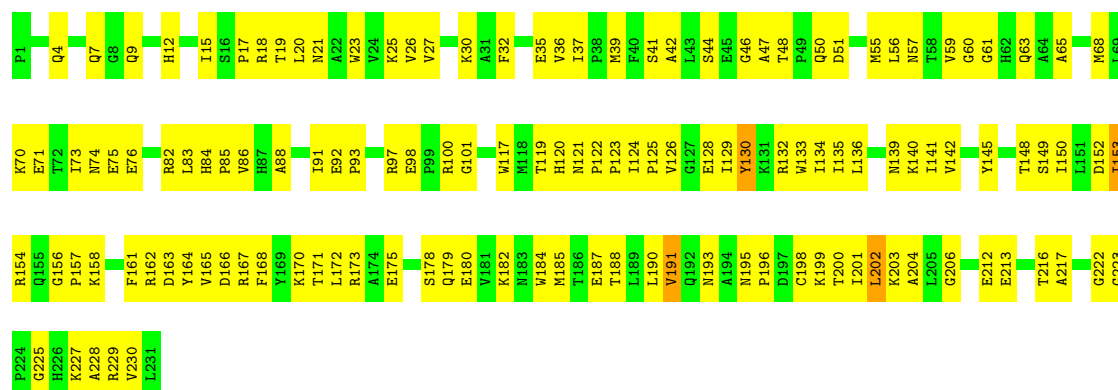
- Molecule 1: capsid protein

Chain eG: 48% 51%



- Molecule 1: capsid protein

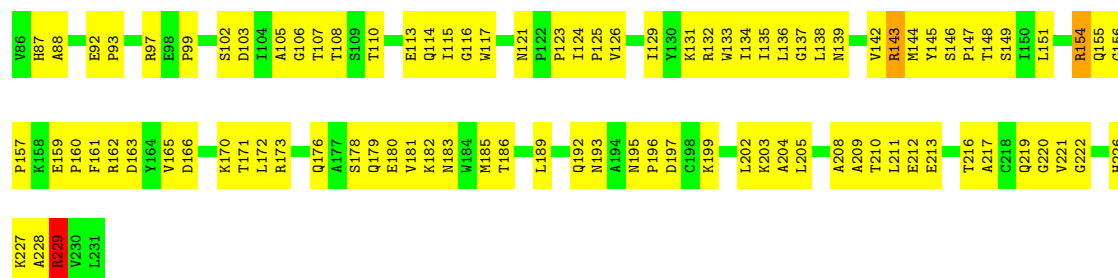
Chain eH: 43% 55%



- Molecule 1: capsid protein

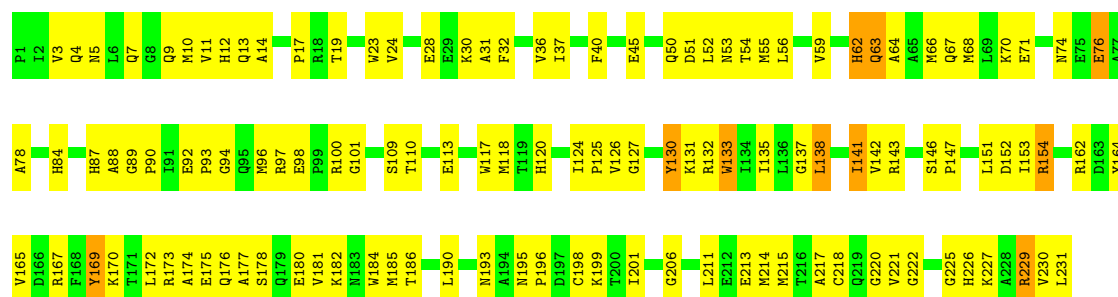
Chain eI: 41% 56%





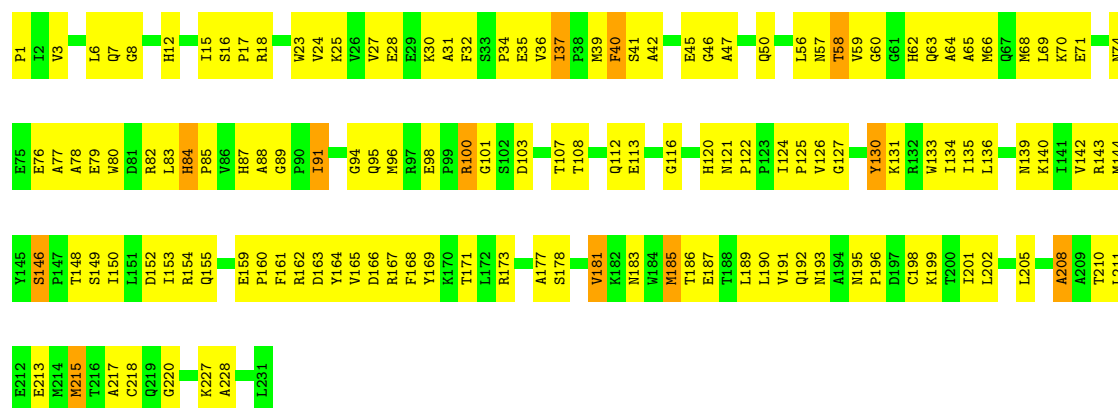
- Molecule 1: capsid protein

Chain eJ: 47% 48%



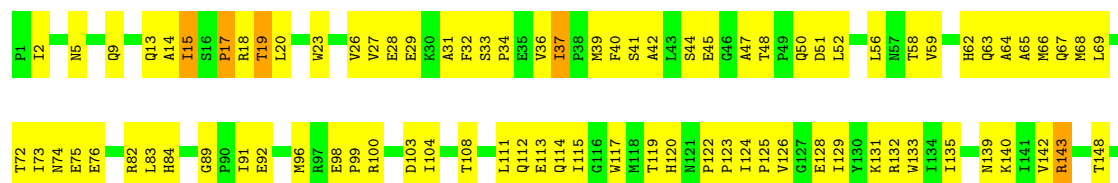
- Molecule 1: capsid protein

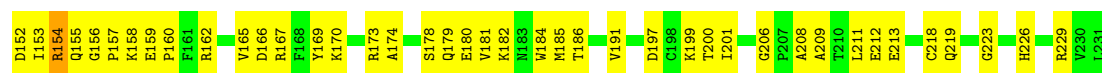
Chain eK: 40% 55% 5%



- Molecule 1: capsid protein

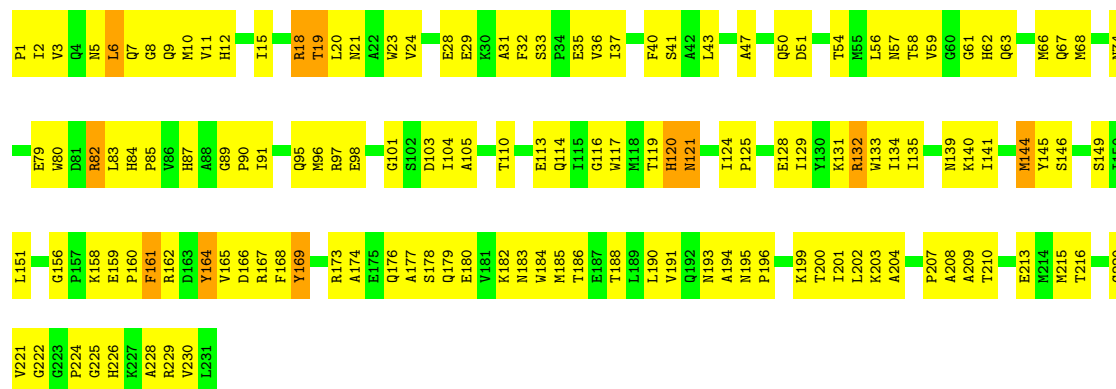
Chain eL: 45% 52%





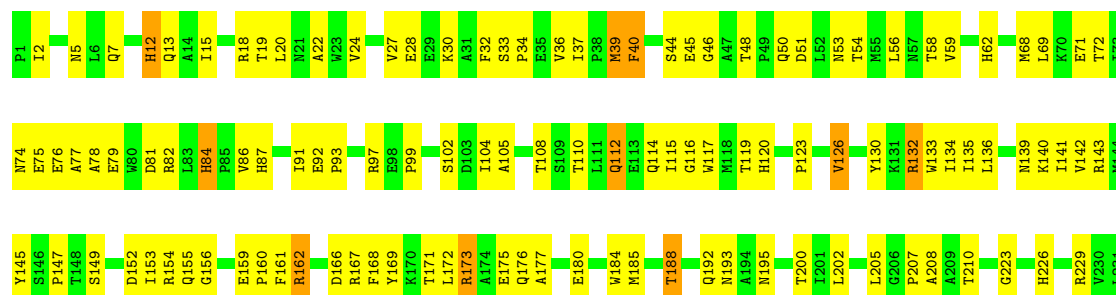
- Molecule 1: capsid protein

Chain eM: 39% 56% 5%



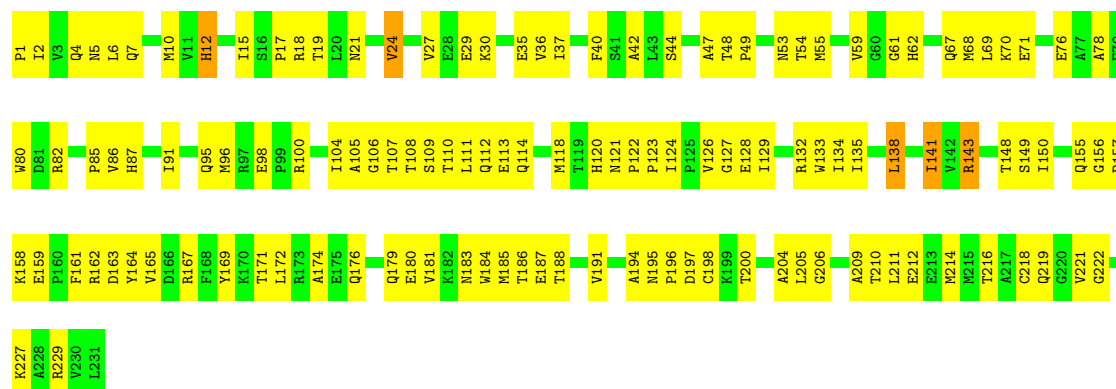
- Molecule 1: capsid protein

Chain eN: 50% 46% 4%

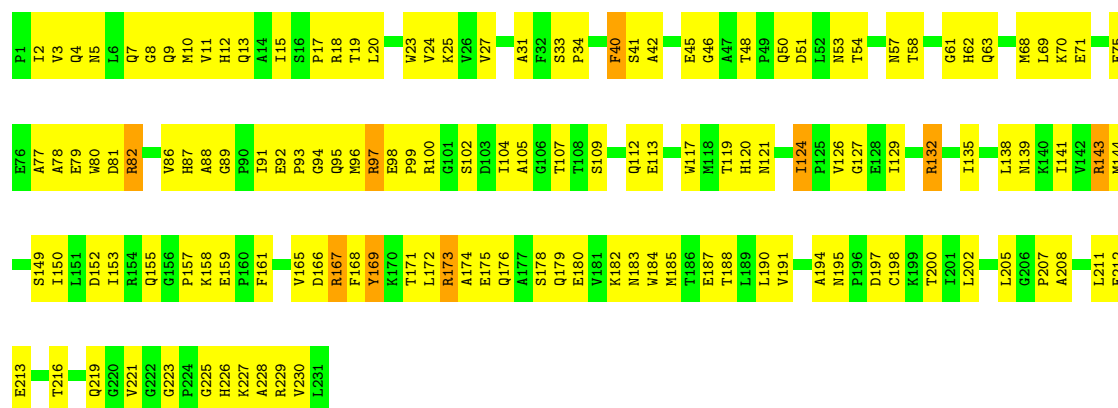


- Molecule 1: capsid protein

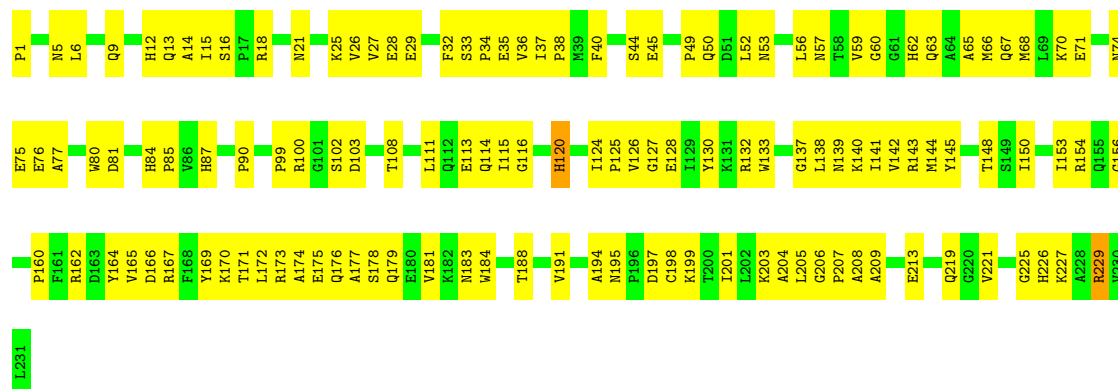
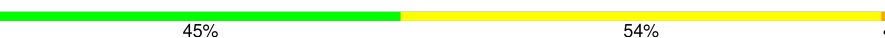
Chain eO: 45% 53% 2%



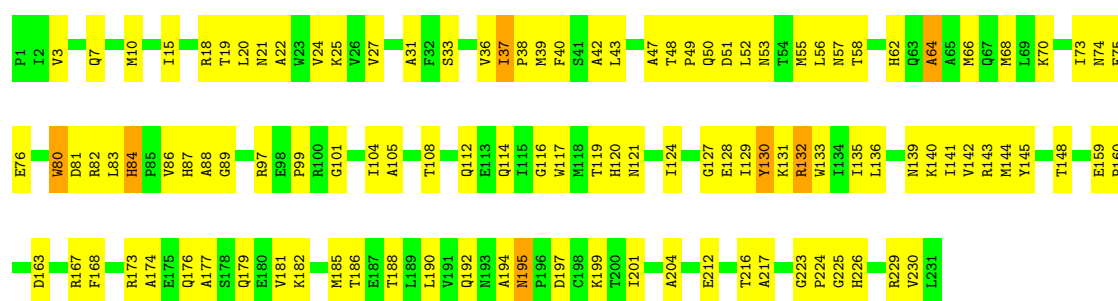
- Molecule 1: capsid protein

Chain eP: 

• Molecule 1: capsid protein

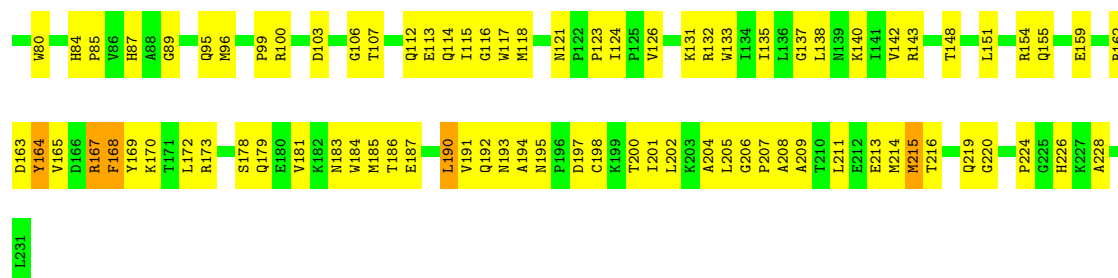
Chain 1t: 

• Molecule 1: capsid protein

Chain eQ: 

• Molecule 1: capsid protein

Chain eR: 



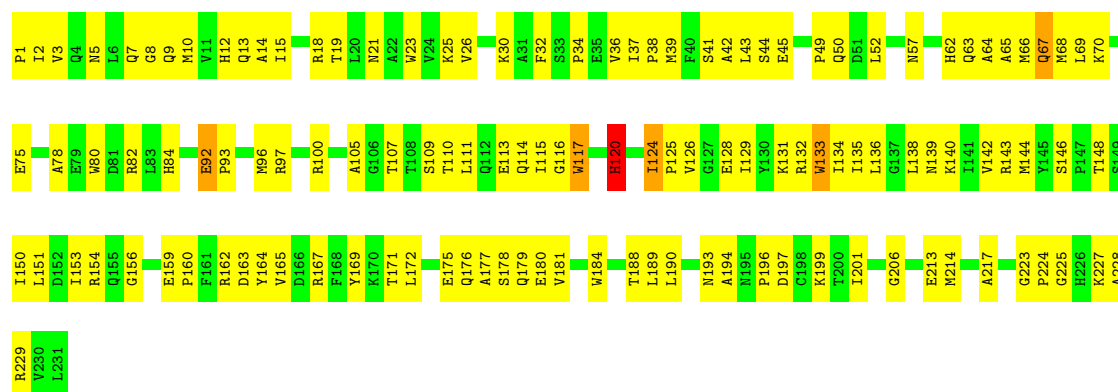
- Molecule 1: capsid protein

Chain eS: 42% 53%



- Molecule 1: capsid protein

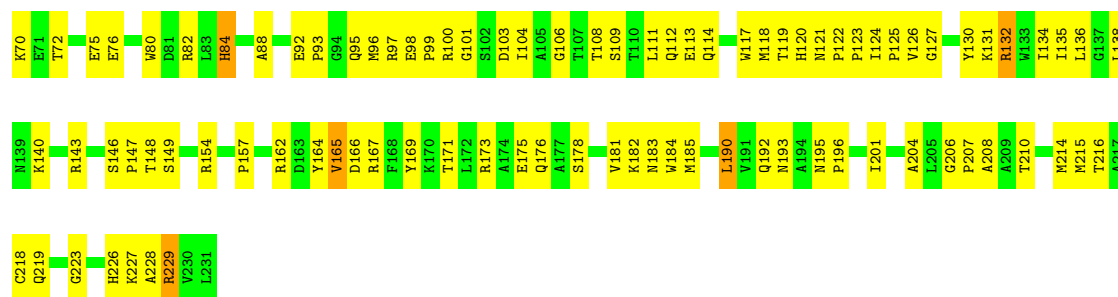
Chain eT: 46% 52%



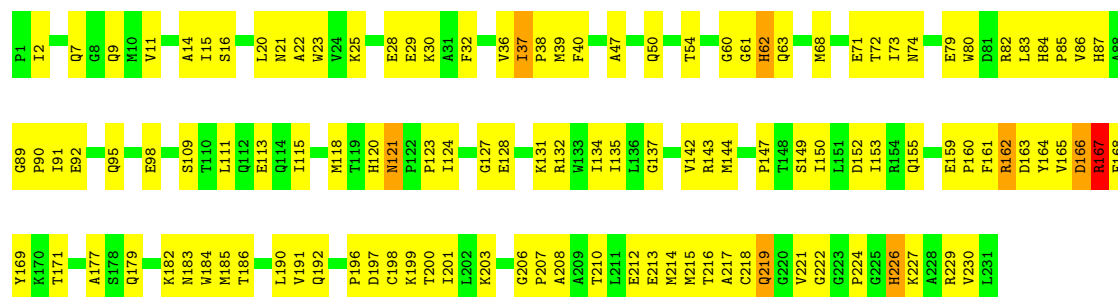
- Molecule 1: capsid protein

Chain eU: 43% 54%

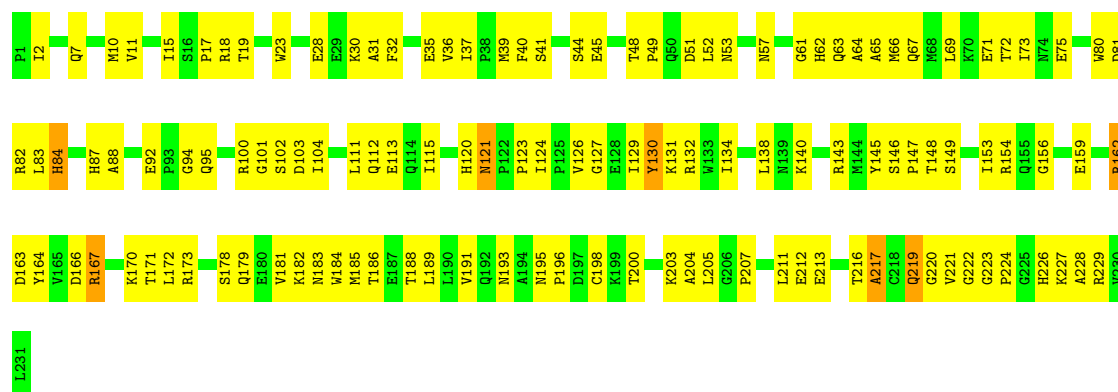




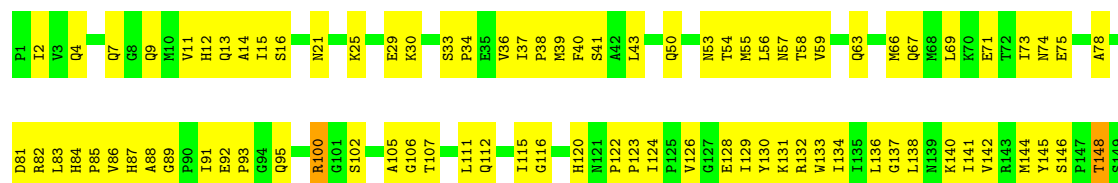
- Molecule 1: capsid protein

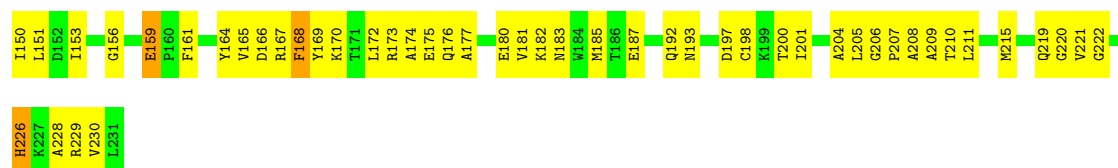


- Molecule 1: capsid protein

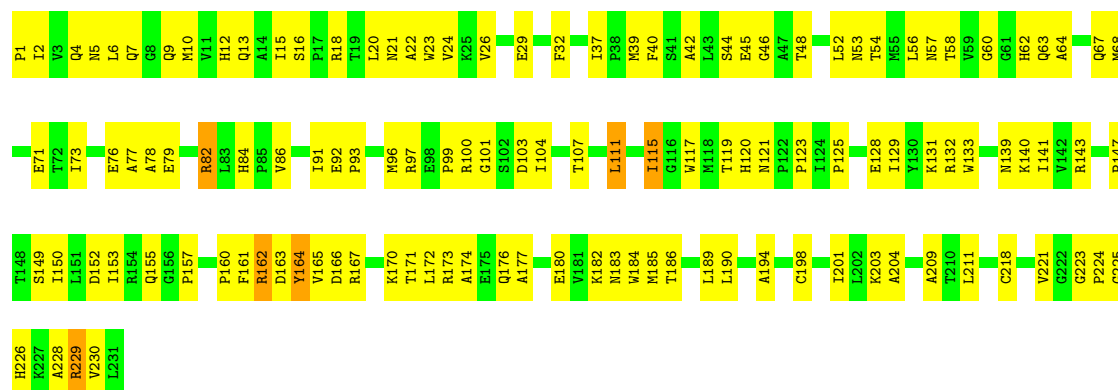


- Molecule 1: capsid protein

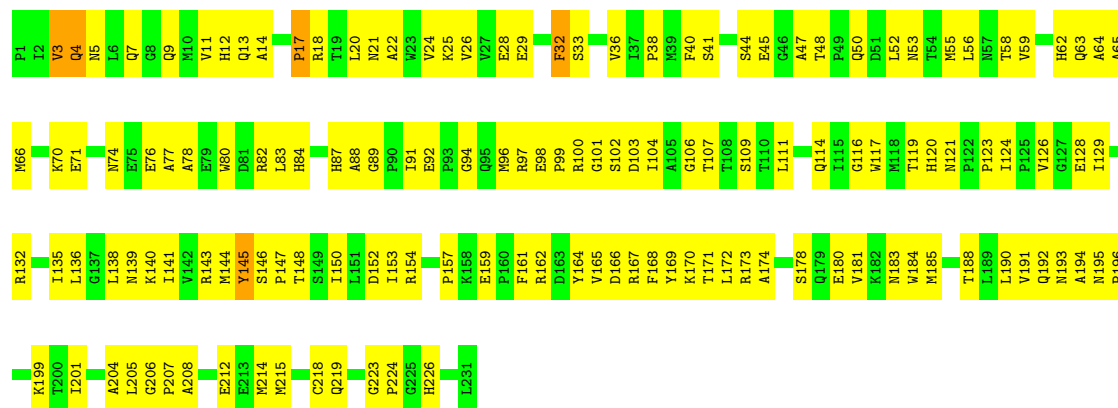




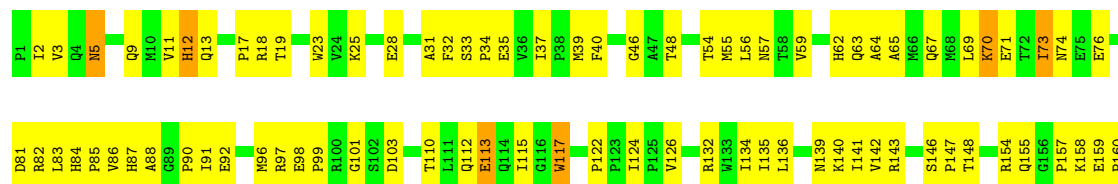
• Molecule 1: capsid protein



• Molecule 1: capsid protein

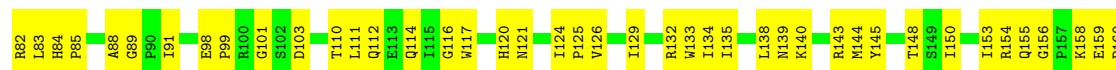
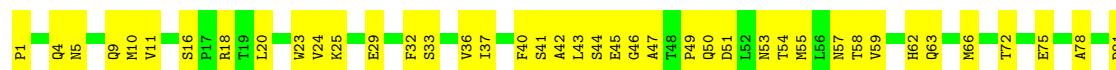


• Molecule 1: capsid protein

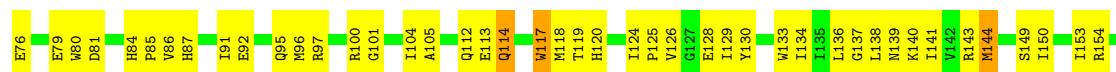
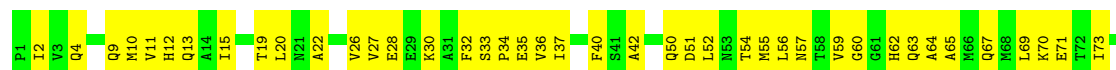




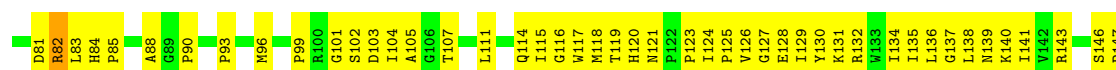
- Molecule 1: capsid protein



- Molecule 1: capsid protein

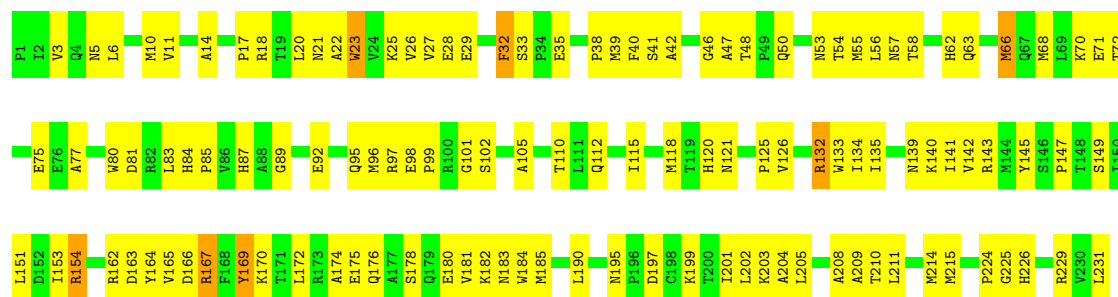


- Molecule 1: capsid protein



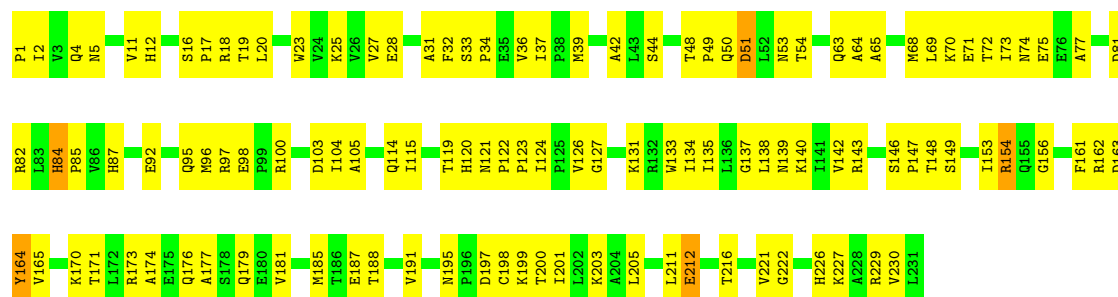
- Molecule 1: capsid protein





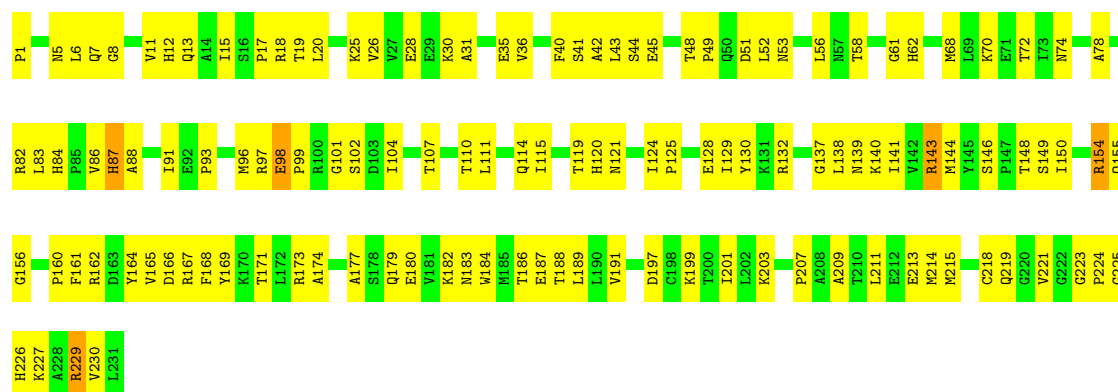
• Molecule 1: capsid protein

Chain f4: 49% 48%



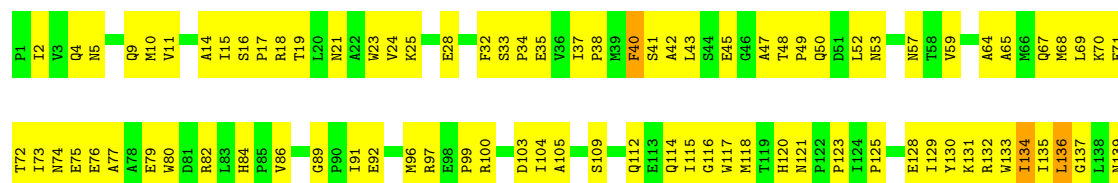
• Molecule 1: capsid protein

Chain f5: 45% 52%



• Molecule 1: capsid protein

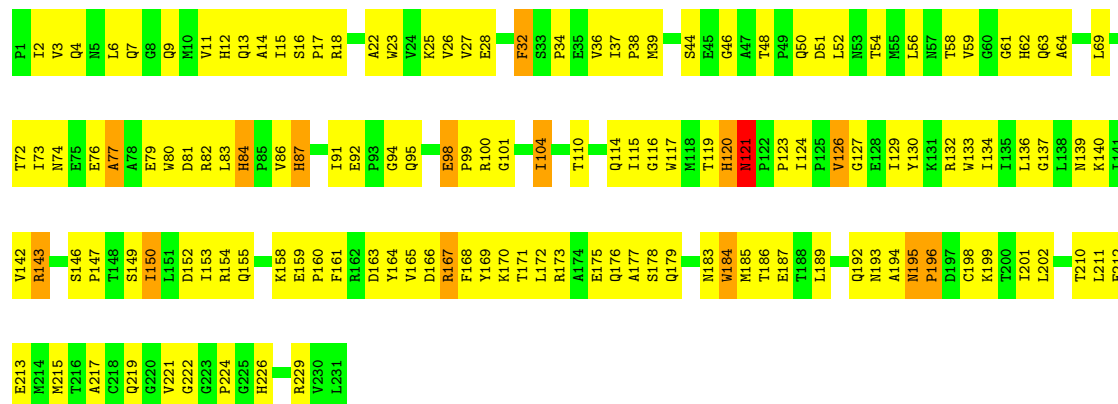
Chain f6: 40% 57%





- Molecule 1: capsid protein

Chain f7: 39% 55% 6%



- Molecule 1: capsid protein

Chain f8: 48% 47% 5%

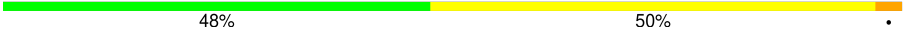


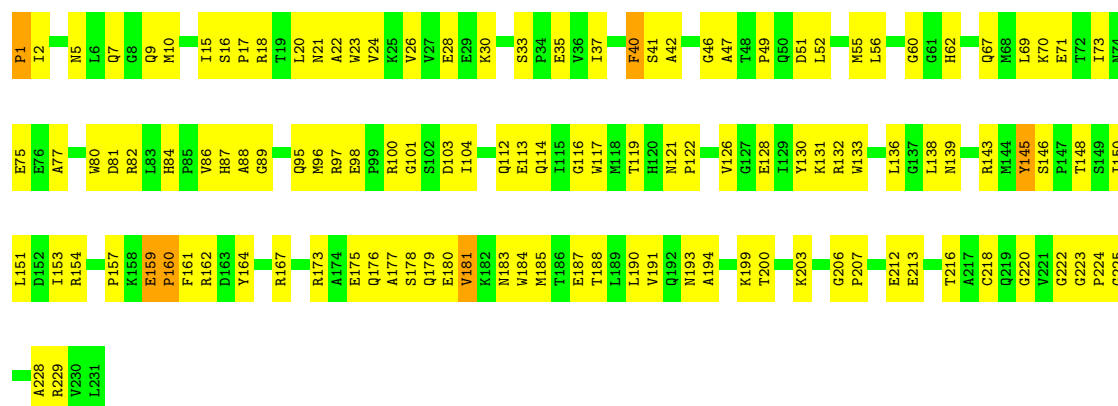
- Molecule 1: capsid protein

Chain f9: 49% 49%

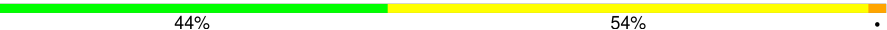


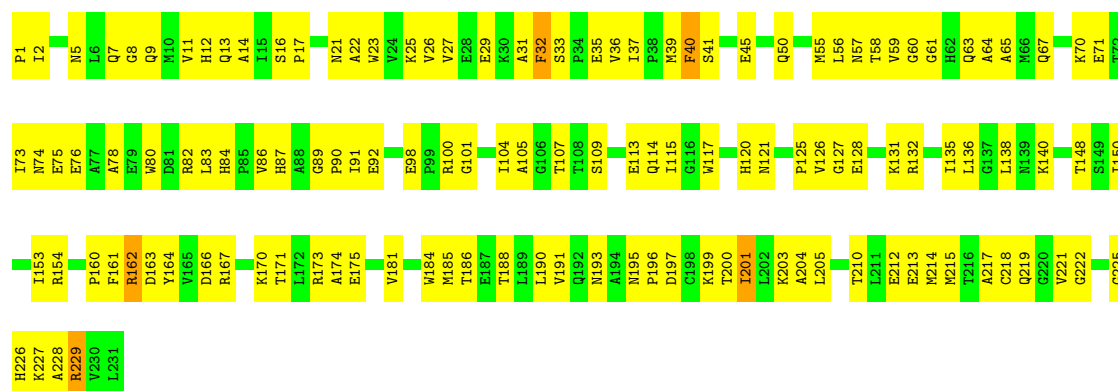
- Molecule 1: capsid protein

Chain 1v:  48% 50%



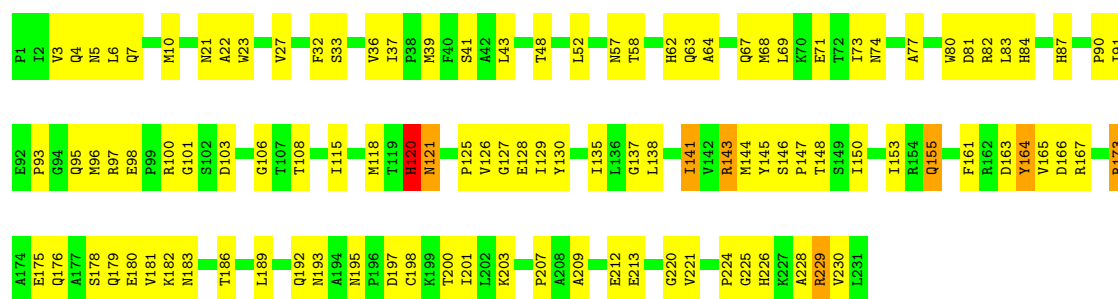
• Molecule 1: capsid protein

Chain fa:  44% 54%



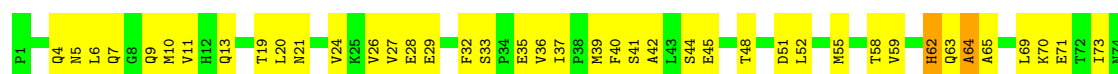
• Molecule 1: capsid protein

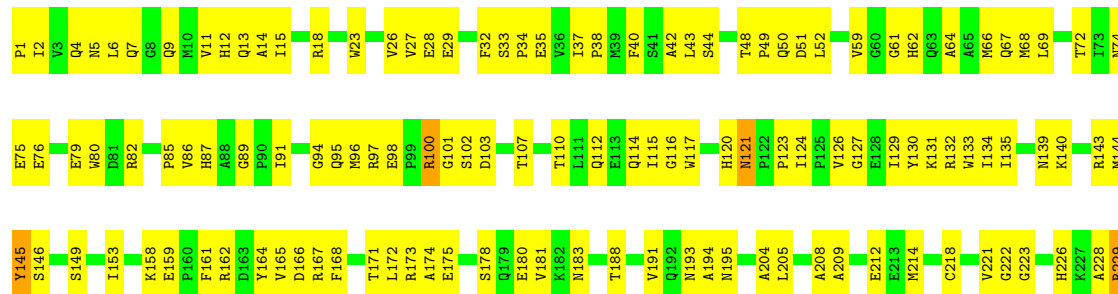
Chain fb:  53% 44%



• Molecule 1: capsid protein

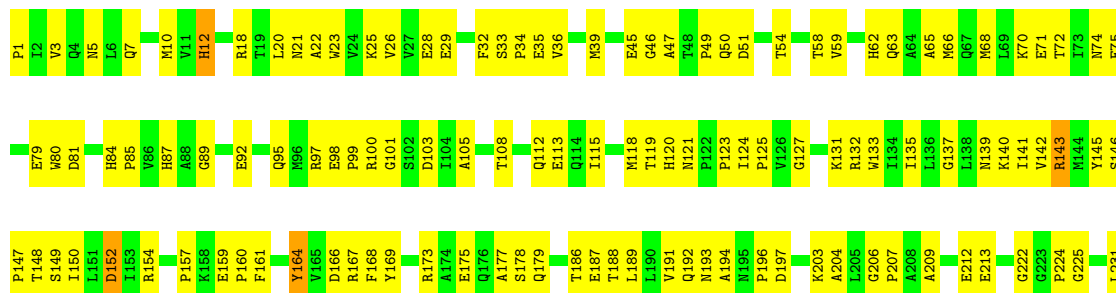
Chain fc:  42% 55%



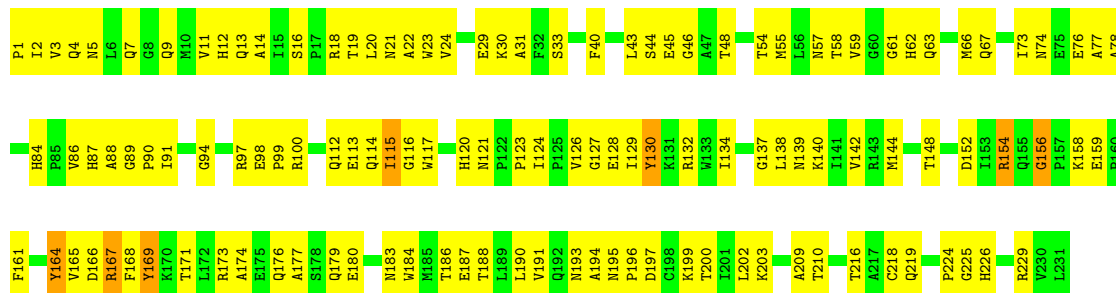


V230
L231

- Molecule 1: capsid protein

Chain fg:  48% 51%

- Molecule 1: capsid protein

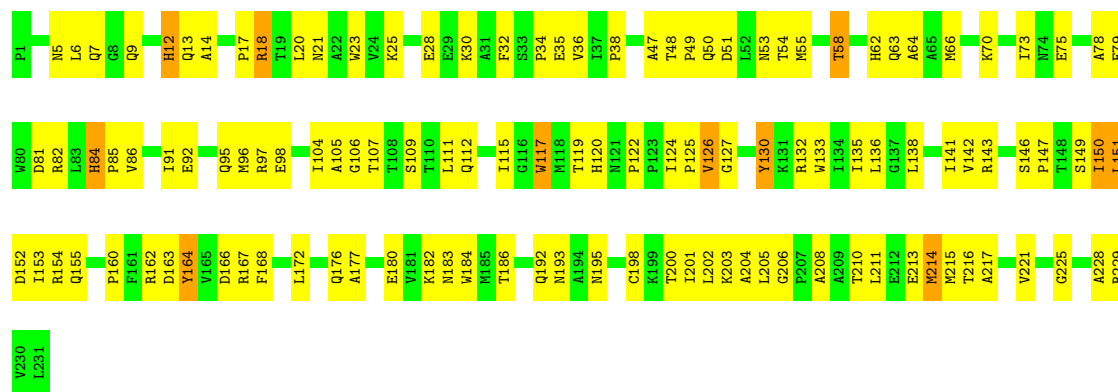
Chain fh:  46% 51%

- Molecule 1: capsid protein

Chain fi:  42% 57%

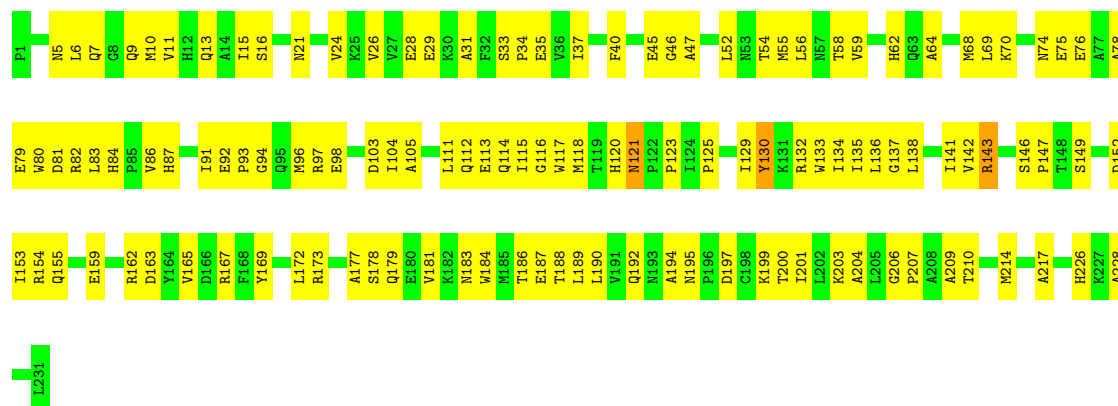
- Molecule 1: capsid protein

Chain fj:  48% 48% 5%



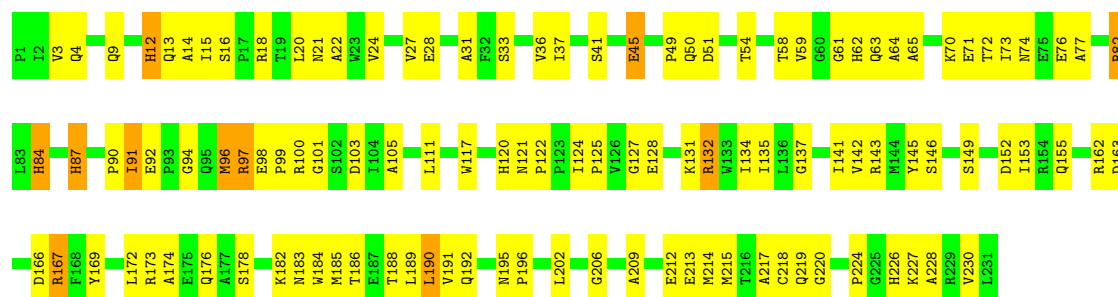
- Molecule 1: capsid protein

Chain 1w: 47% 52%



- Molecule 1: capsid protein

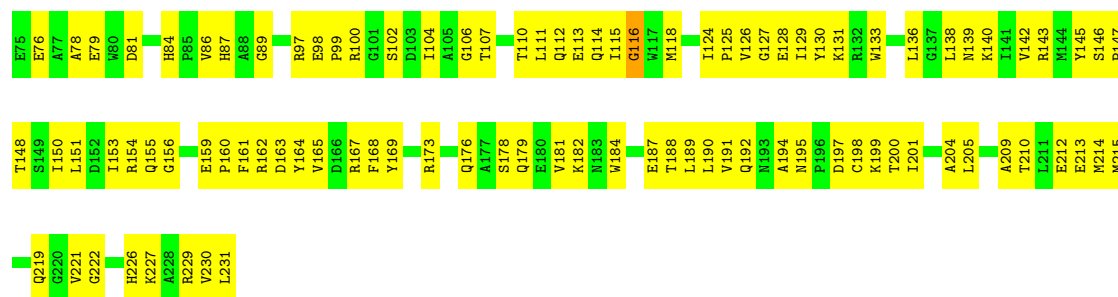
Chain fk: 50% 45% 5%



- Molecule 1: capsid protein

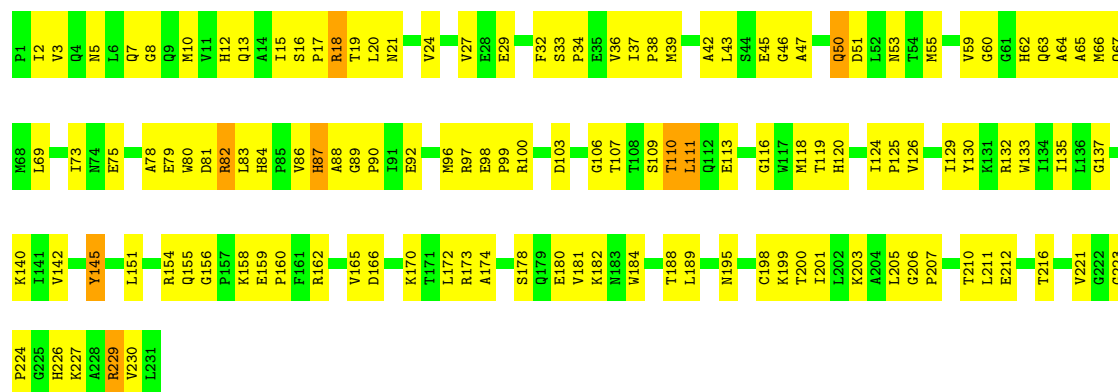
Chain fl: 39% 59%





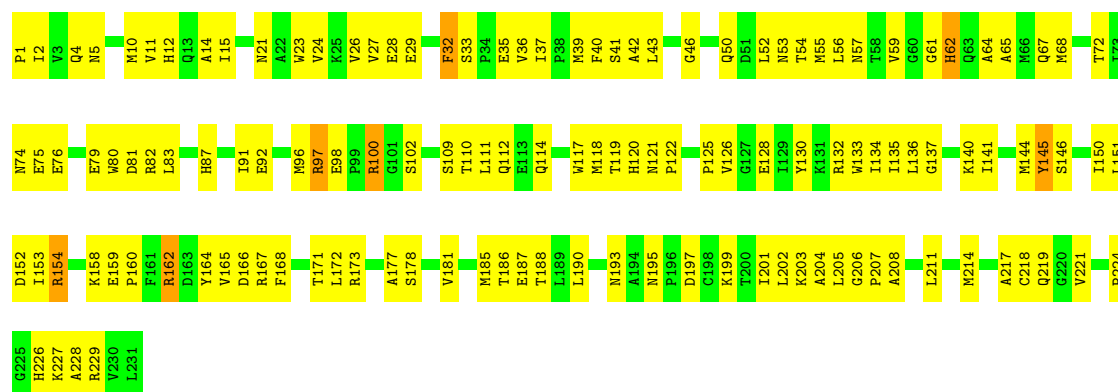
• Molecule 1: capsid protein

Chain fm: 45% 52%



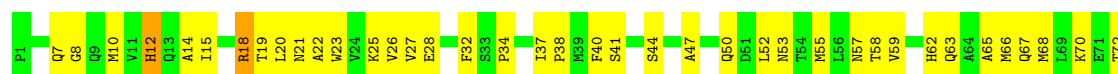
• Molecule 1: capsid protein

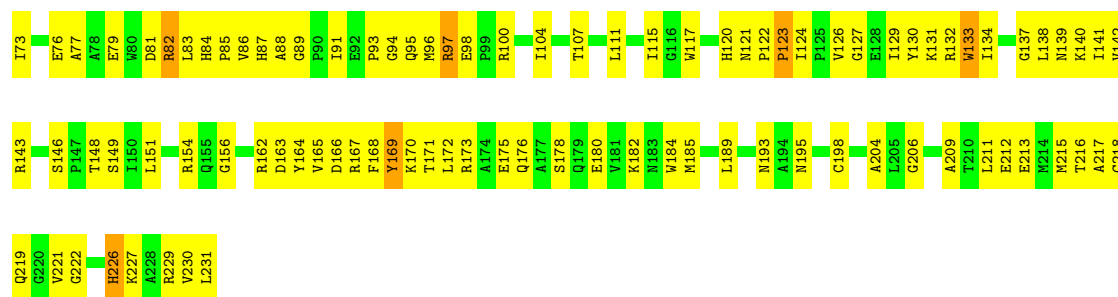
Chain fm: 43% 54%



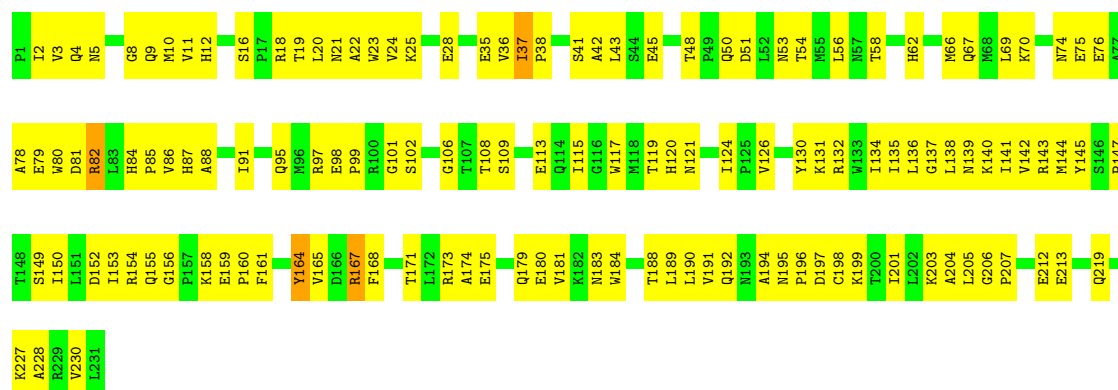
• Molecule 1: capsid protein

Chain fo: 43% 54%

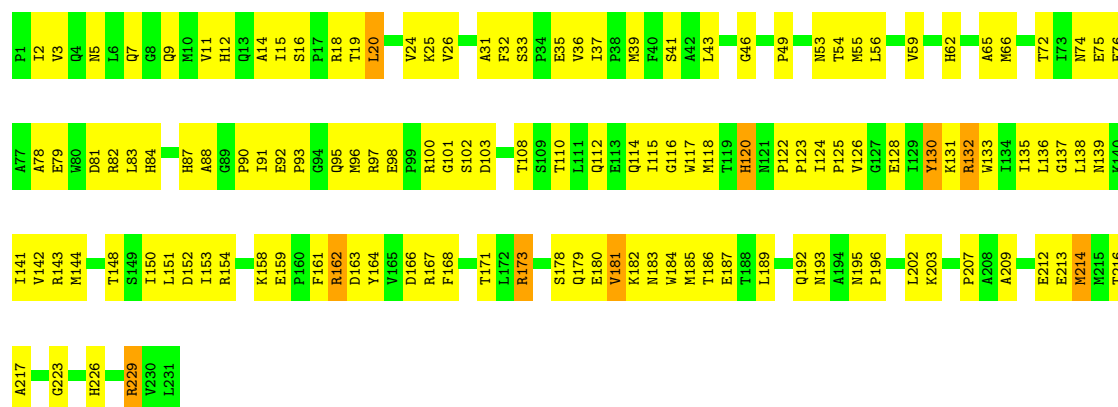




• Molecule 1: capsid protein

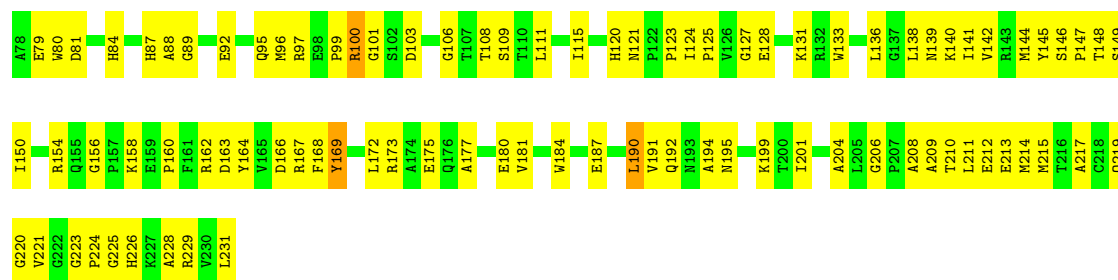


• Molecule 1: capsid protein



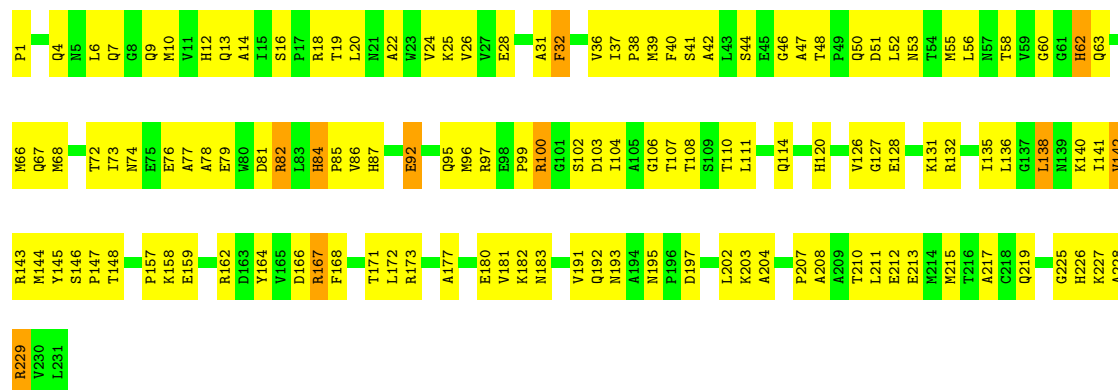
• Molecule 1: capsid protein





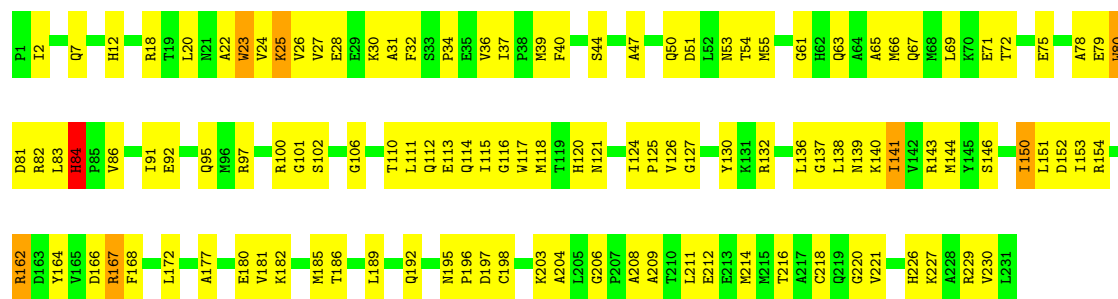
• Molecule 1: capsid protein

Chain fs: 45% 51%



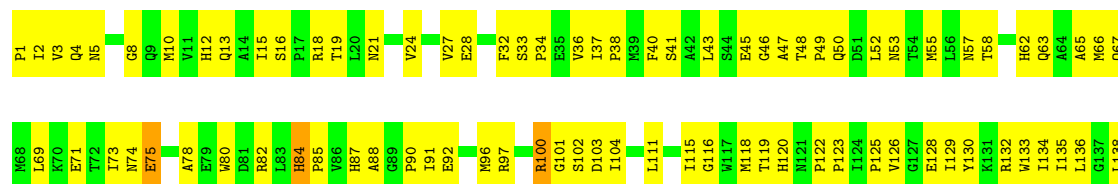
• Molecule 1: capsid protein

Chain ft: 49% 47%



• Molecule 1: capsid protein

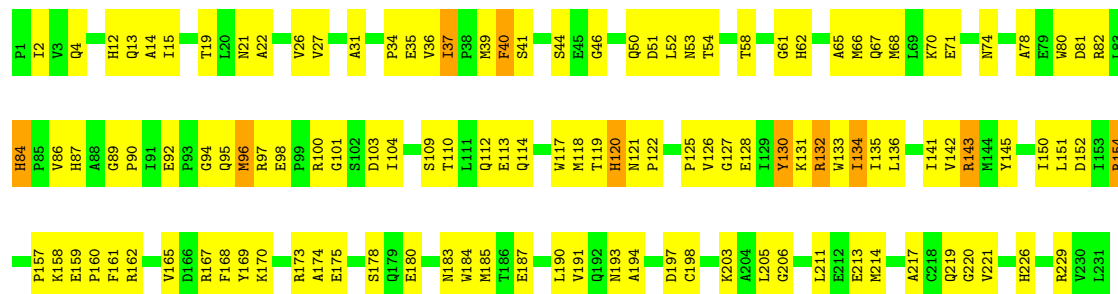
Chain 1x: 41% 57%





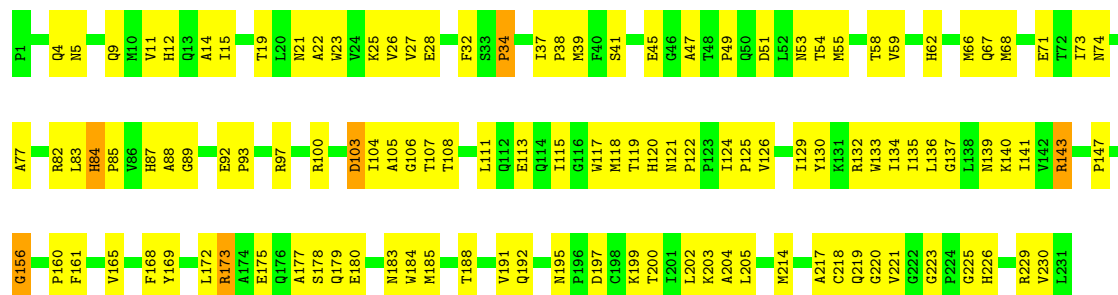
- Molecule 1: capsid protein

Chain fu: 47% 49%



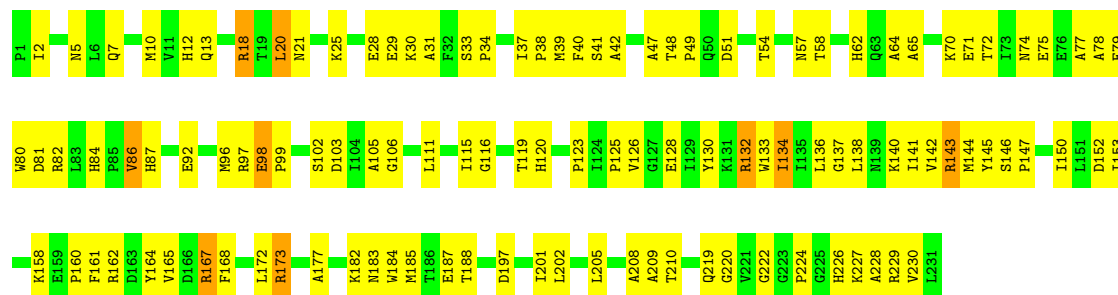
- Molecule 1: capsid protein

Chain fv: 49% 48%



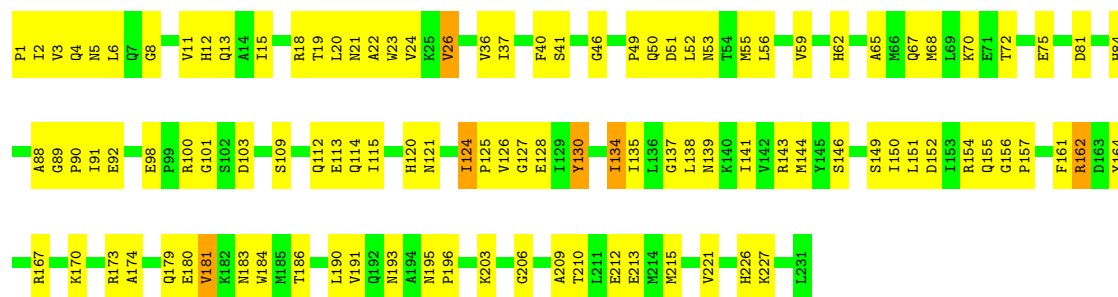
- Molecule 1: capsid protein

Chain fw: 50% 46%

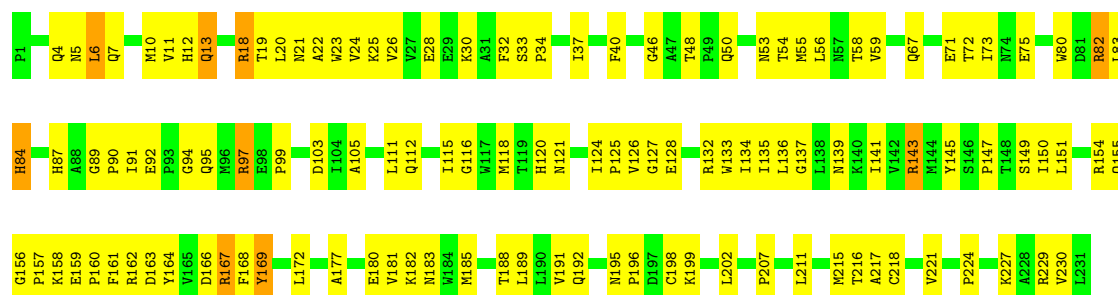


- Molecule 1: capsid protein

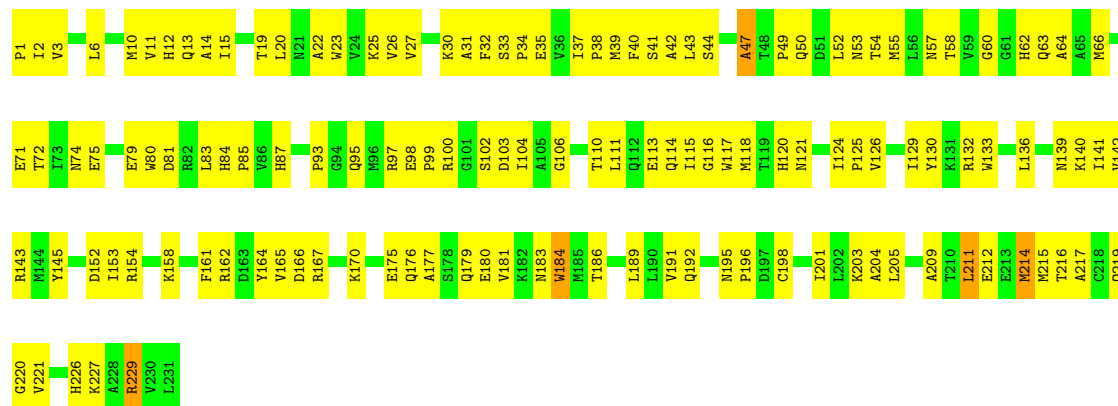
Chain fx: 53% 44%



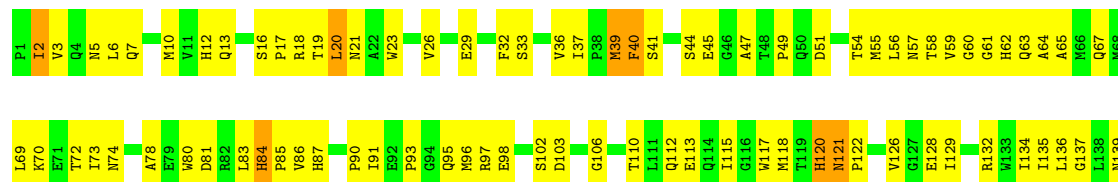
• Molecule 1: capsid protein

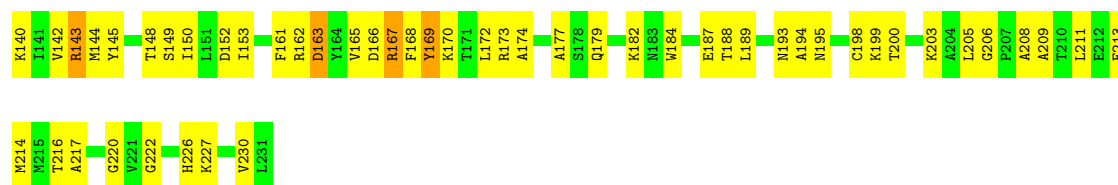


• Molecule 1: capsid protein



• Molecule 1: capsid protein





- Molecule 1: capsid protein

Chain fB: 48% 50%



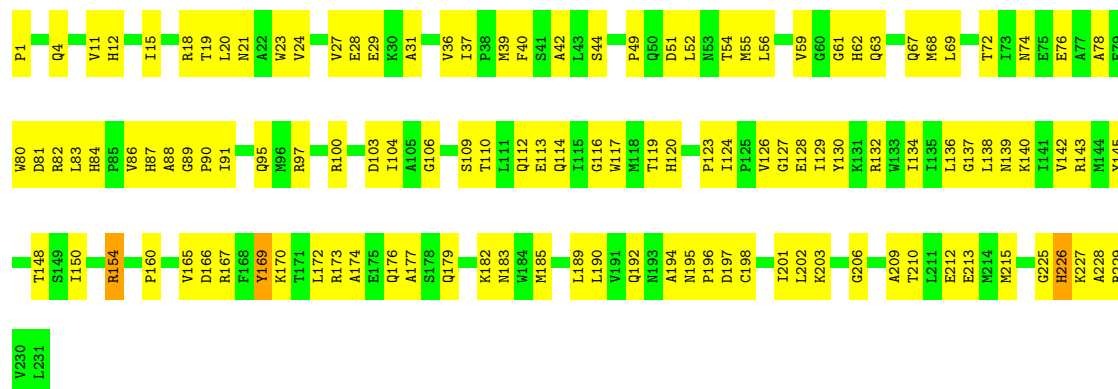
- Molecule 1: capsid protein

Chain fC: 46% 50%



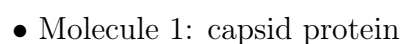
- Molecule 1: capsid protein

Chain fD: 48% 51%

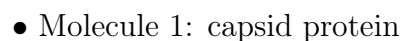


- Molecule 1: capsid protein

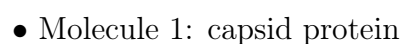
Response	Percentage
Yes, the U.S. is a democracy	42%
No, the U.S. is not a democracy	56%



Response	Percentage
U.S. should take action to reduce greenhouse gas emissions	44%
U.S. should not take action to reduce greenhouse gas emissions	52%

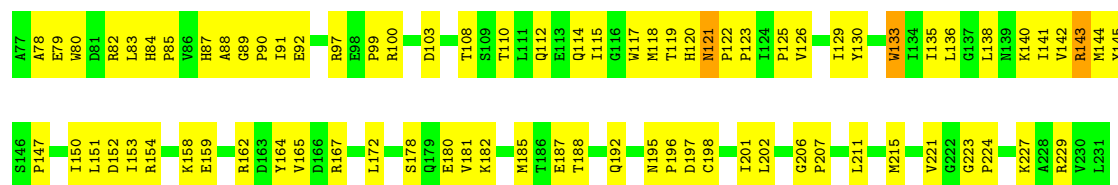


Response	Percentage
Yes, the U.S. is a democracy	47%
No, the U.S. is not a democracy	48%
Don't know	5%

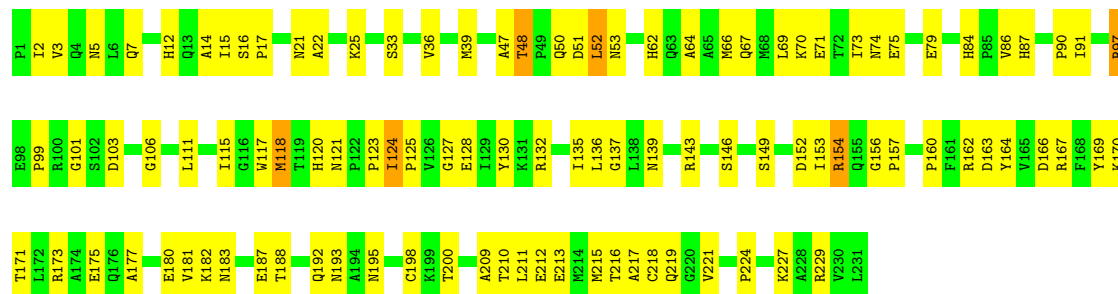


Response	Percentage
Yes, the U.S. is a democracy	49%
No, the U.S. is not a democracy	49%

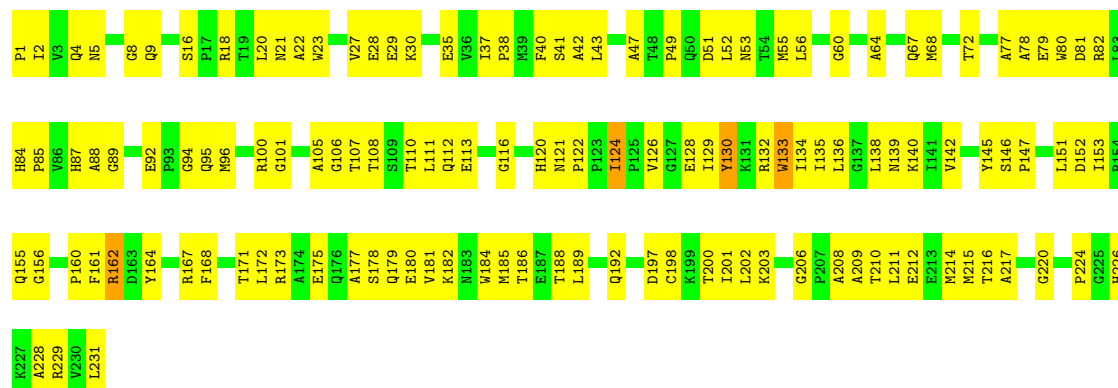




- Molecule 1: capsid protein



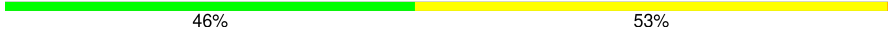
- Molecule 1: capsid protein

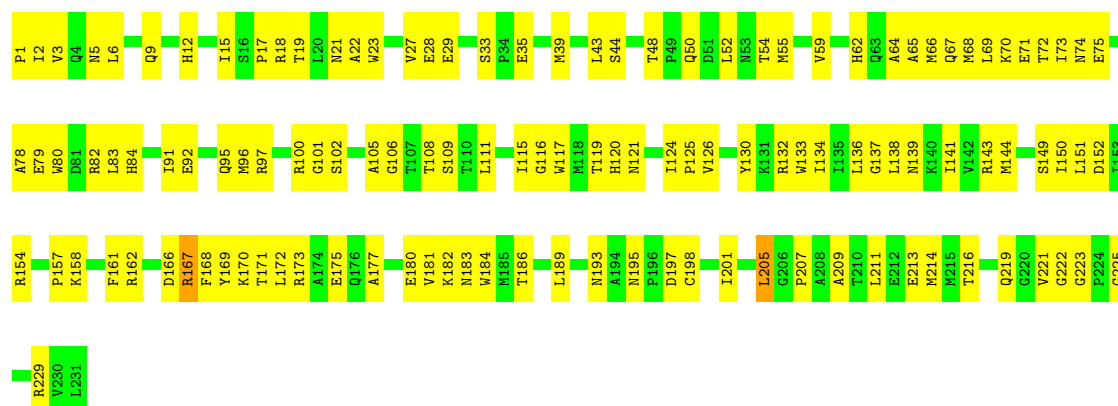


- Molecule 1: capsid protein

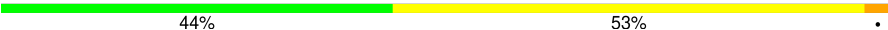


- Molecule 1: capsid protein

Chain fK:  46% 53%



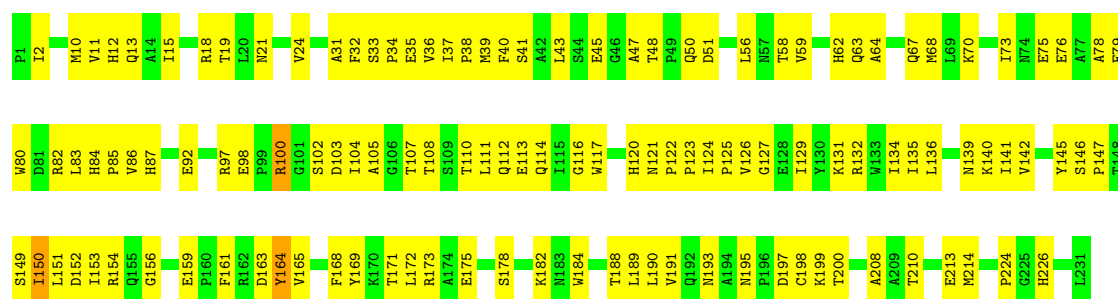
• Molecule 1: capsid protein

Chain fL:  44% 53%



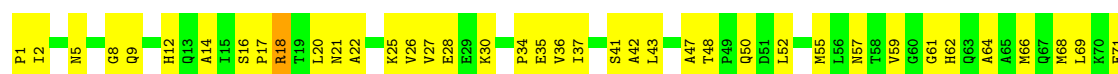
• Molecule 1: capsid protein

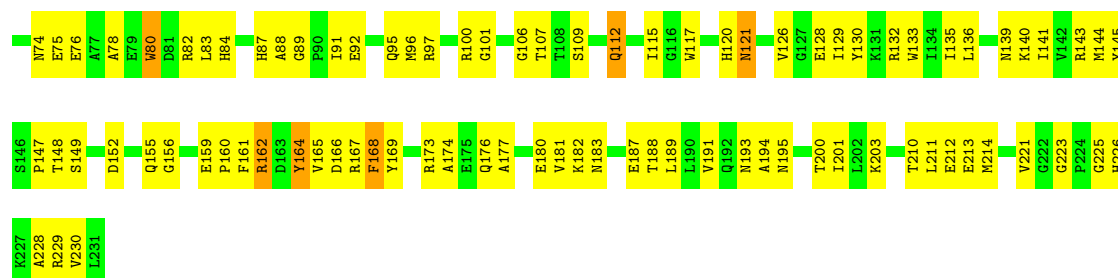
Chain fM:  47% 52%



• Molecule 1: capsid protein

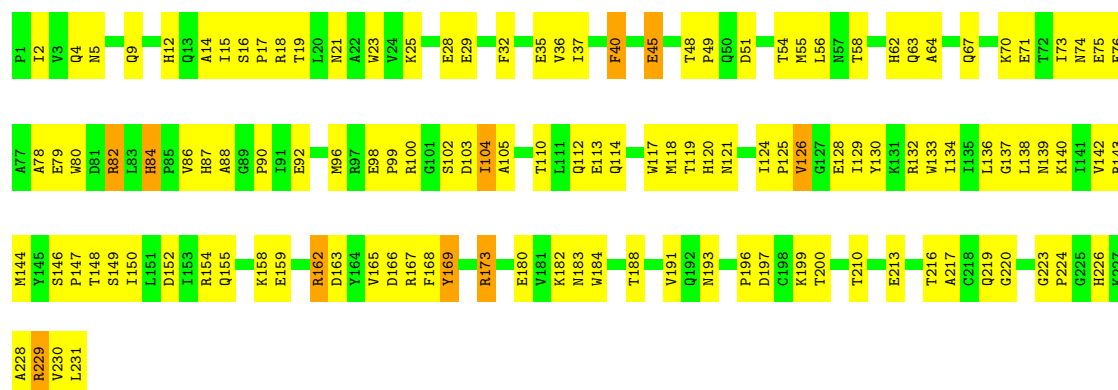
Chain fN:  46% 51%





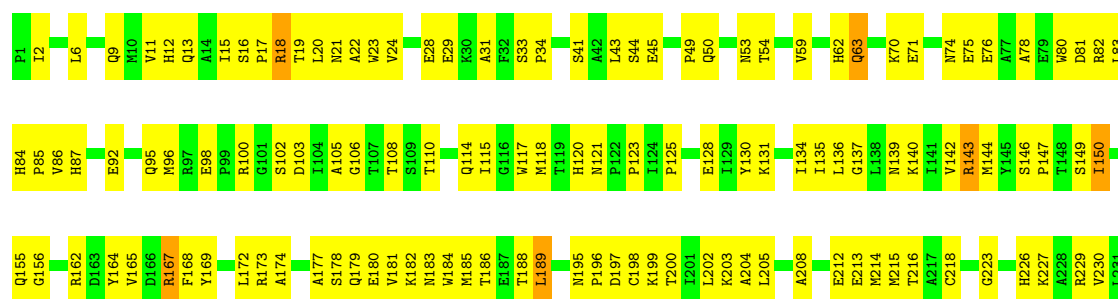
- Molecule 1: capsid protein

Chain 1z: 46% 50%



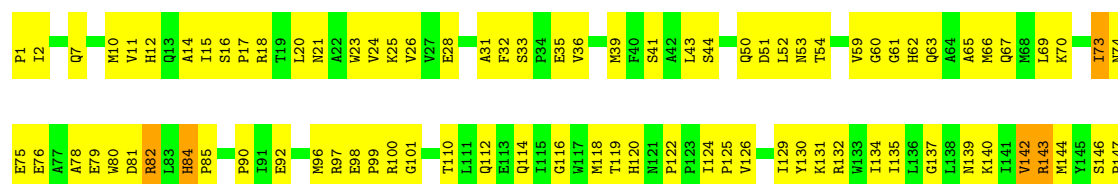
- Molecule 1: capsid protein

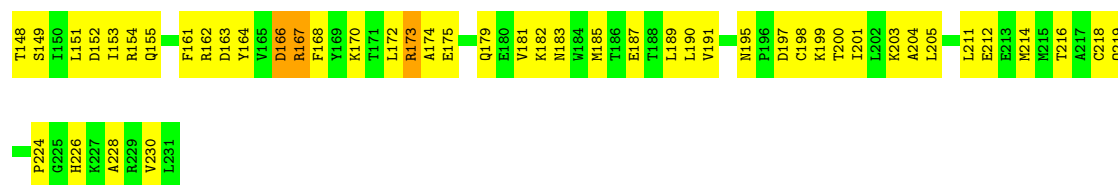
Chain fO: 45% 52%



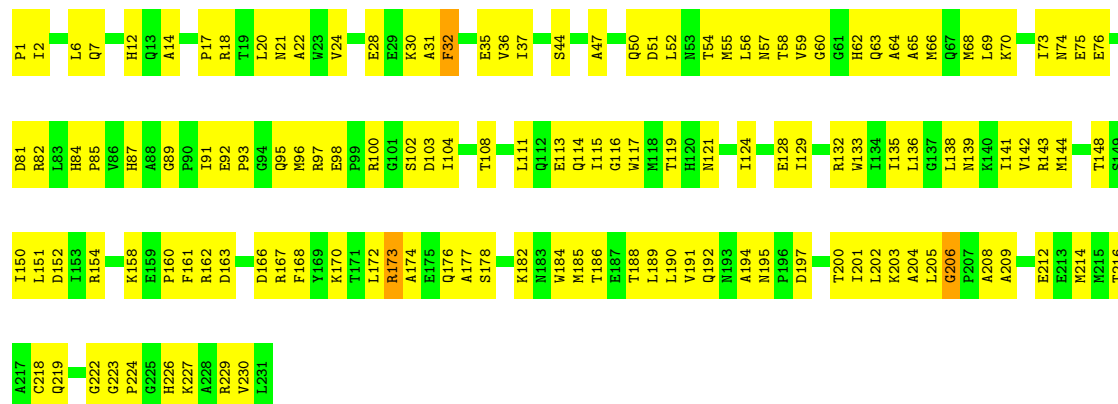
- Molecule 1: capsid protein

Chain fP: 42% 54%

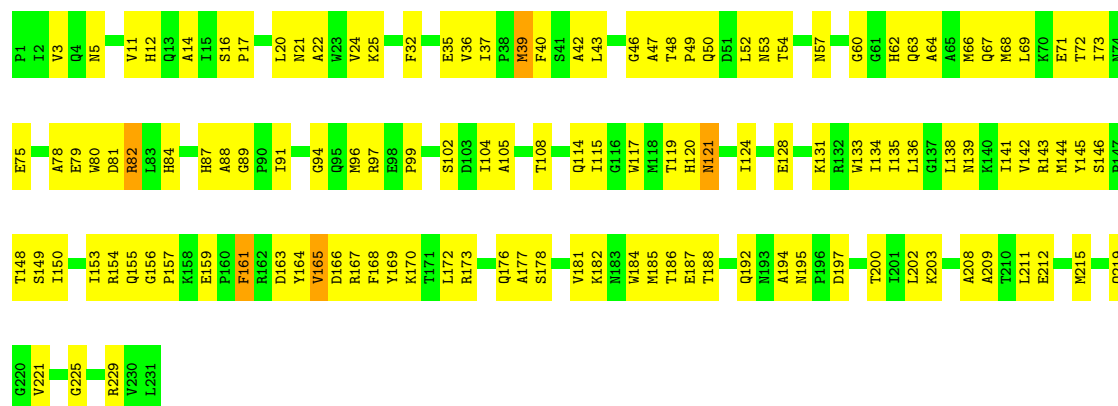




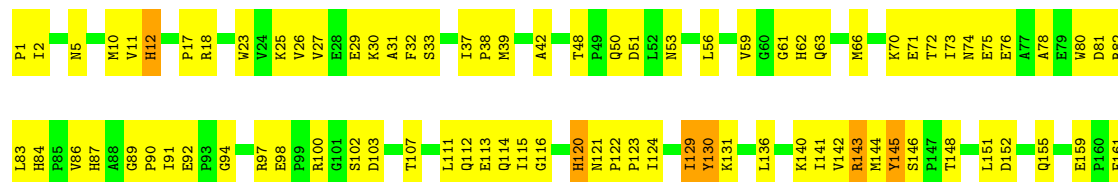
• Molecule 1: capsid protein



• Molecule 1: capsid protein



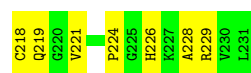
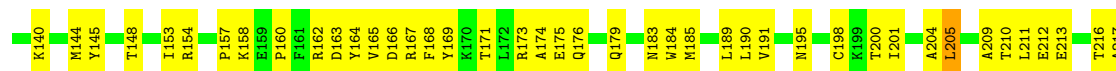
• Molecule 1: capsid protein





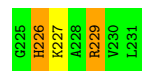
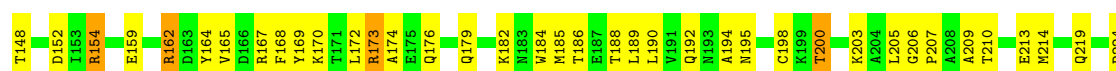
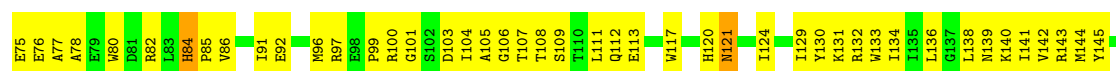
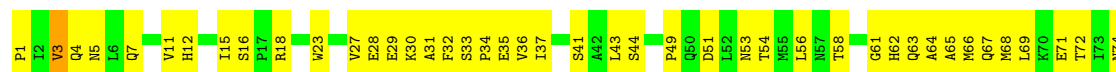
• Molecule 1: capsid protein

Chain fT: 40% 59%



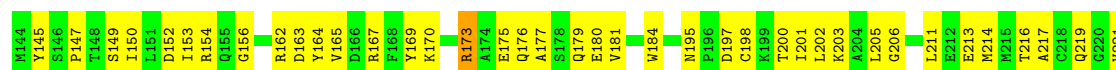
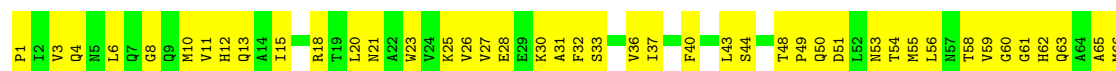
• Molecule 1: capsid protein

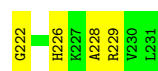
Chain fU: 44% 52%



• Molecule 1: capsid protein

Chain fV: 45% 54%





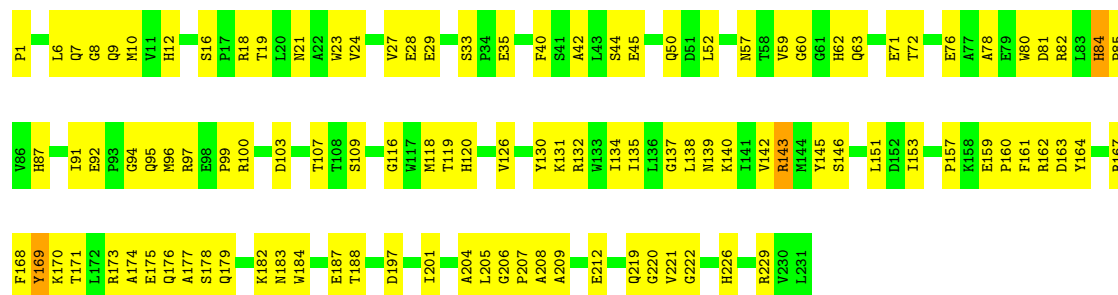
• Molecule 1: capsid protein

Chain fW: 42% 56%



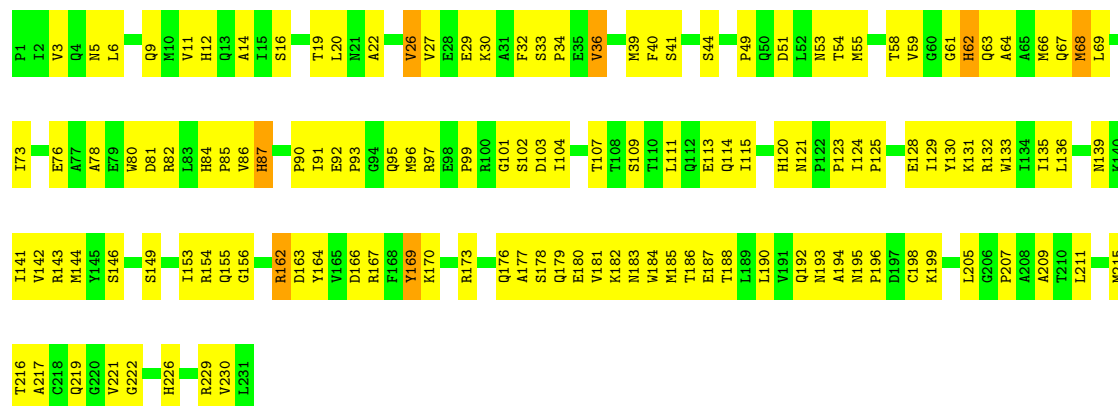
• Molecule 1: capsid protein

Chain fX: 53% 46%



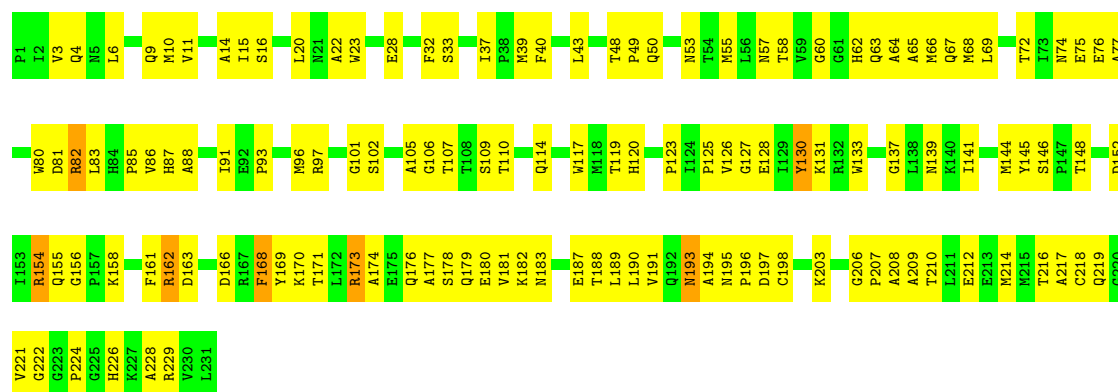
• Molecule 1: capsid protein

Chain 1A: 43% 54%



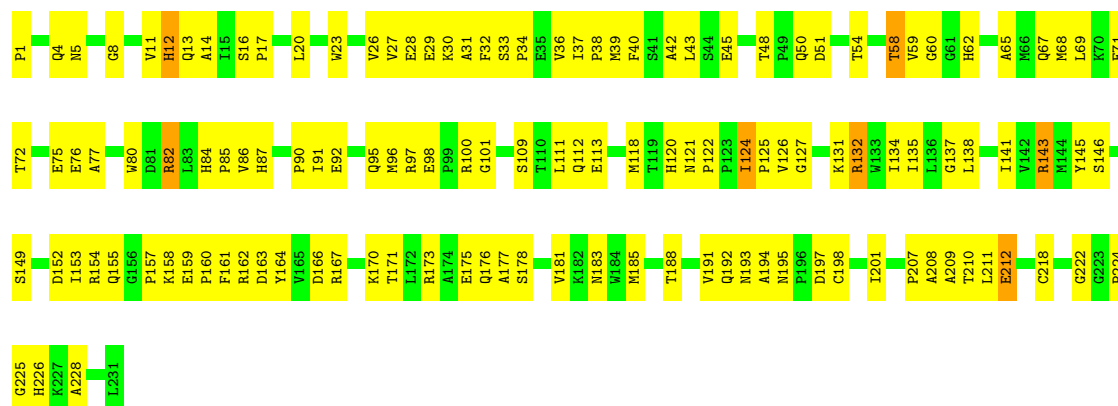
• Molecule 1: capsid protein

Chain fY: 



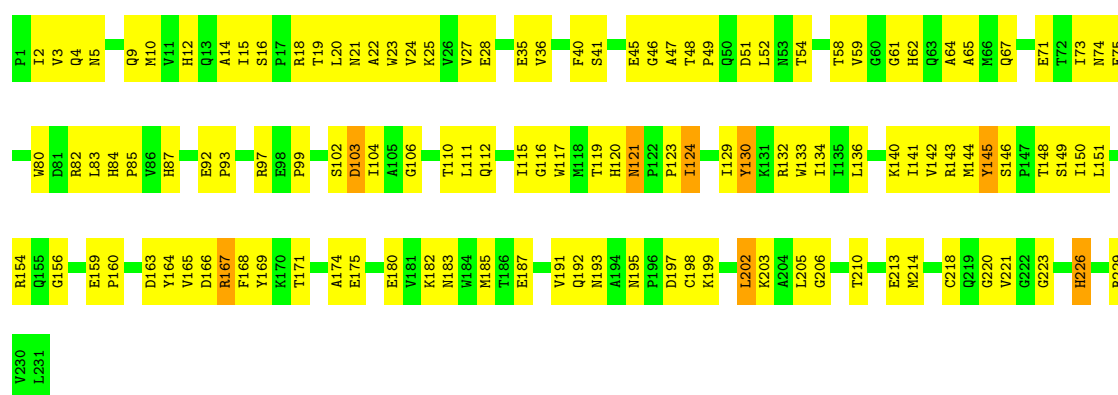
• Molecule 1: capsid protein

Chain fZ: 



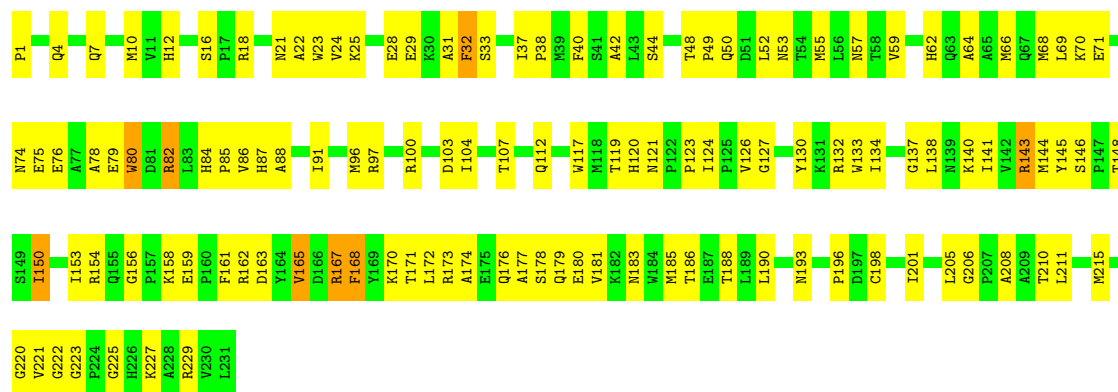
• Molecule 1: capsid protein

Chain g0: 



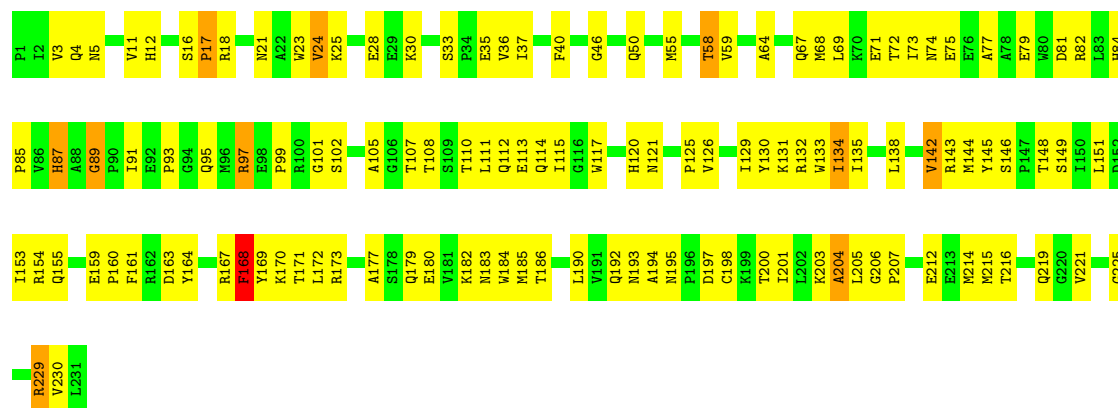
• Molecule 1: capsid protein

Chain g1: 



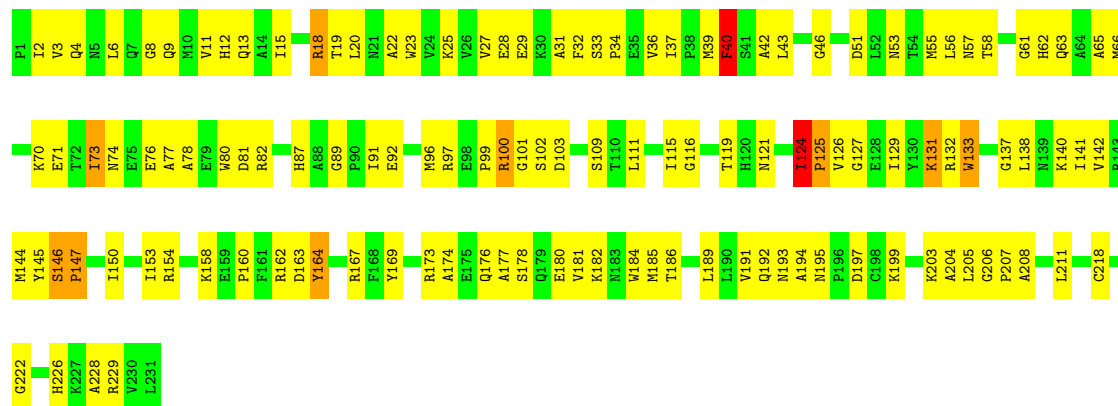
• Molecule 1: capsid protein

Chain g2: 46% 49%



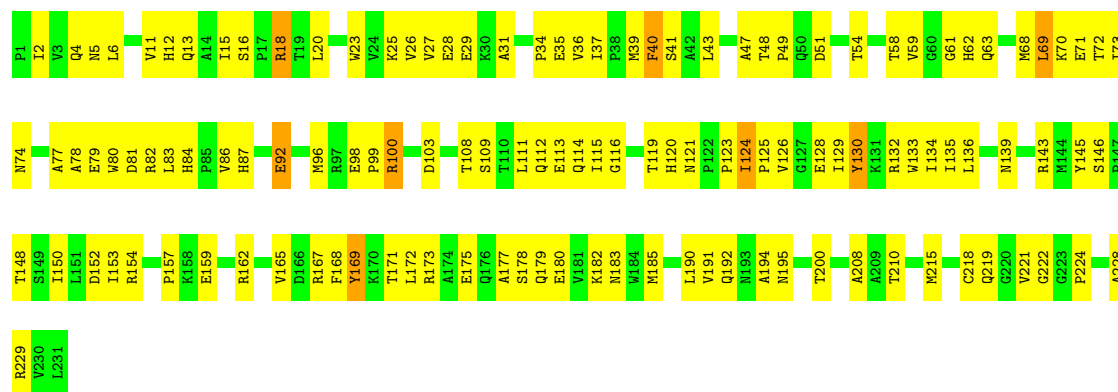
• Molecule 1: capsid protein

Chain g3: 45% 50%

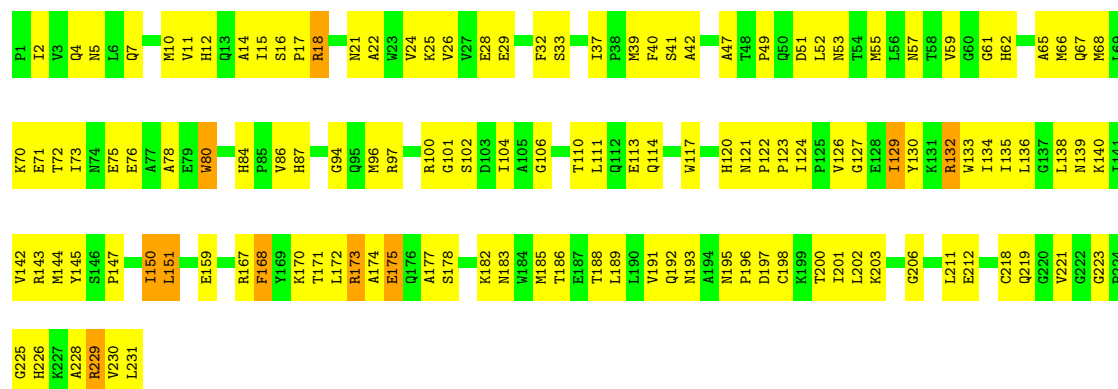


• Molecule 1: capsid protein

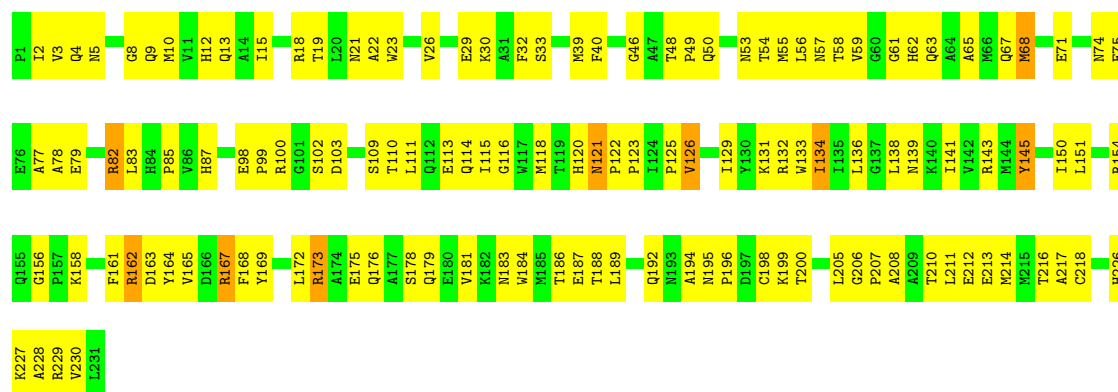
Chain g4: 46% 51%



• Molecule 1: capsid protein

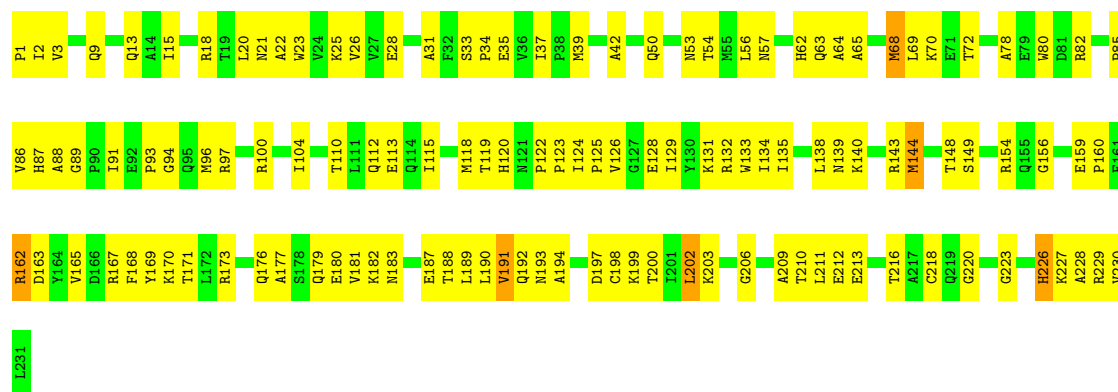


• Molecule 1: capsid protein



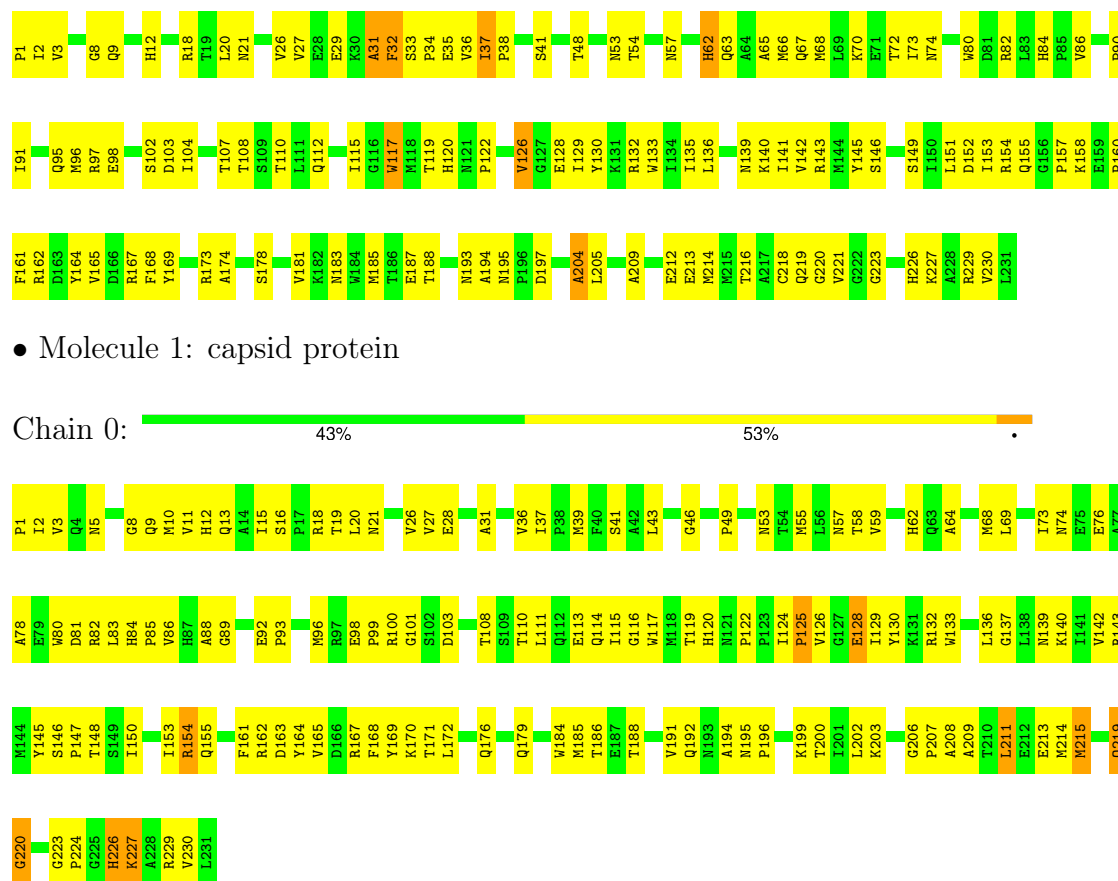
• Molecule 1: capsid protein





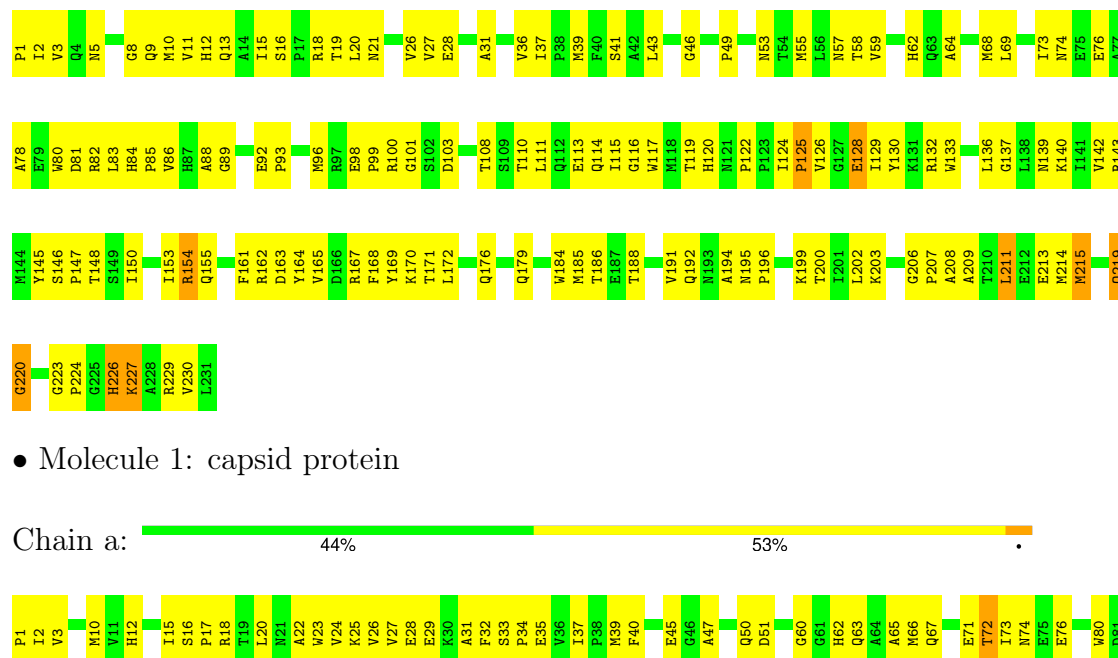
• Molecule 1: capsid protein

Chain 1B: 50% 47%



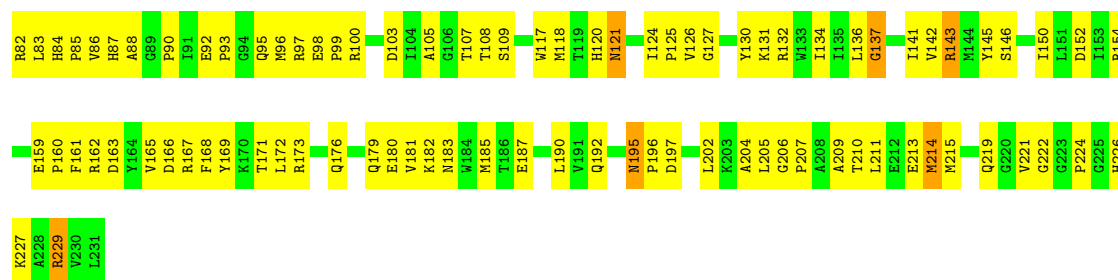
• Molecule 1: capsid protein

Chain 0: 43% 53%

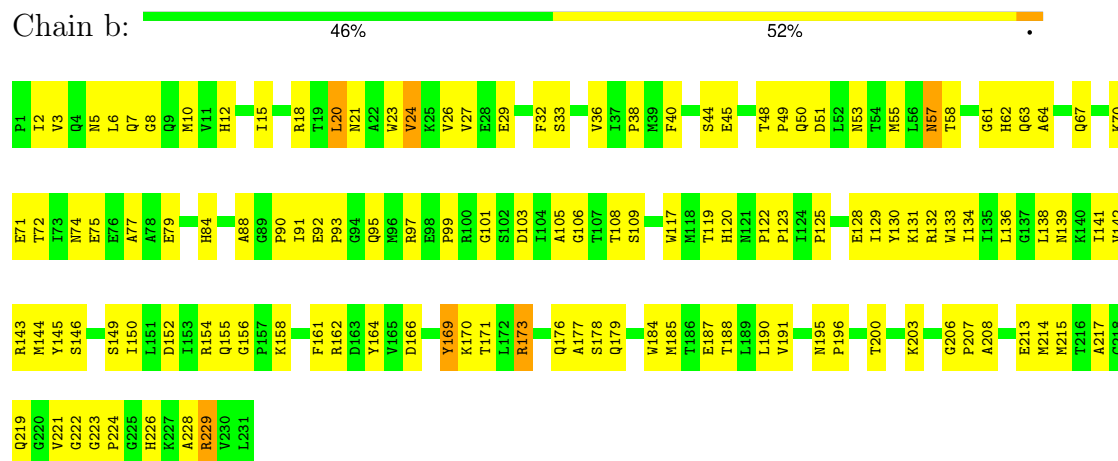


• Molecule 1: capsid protein

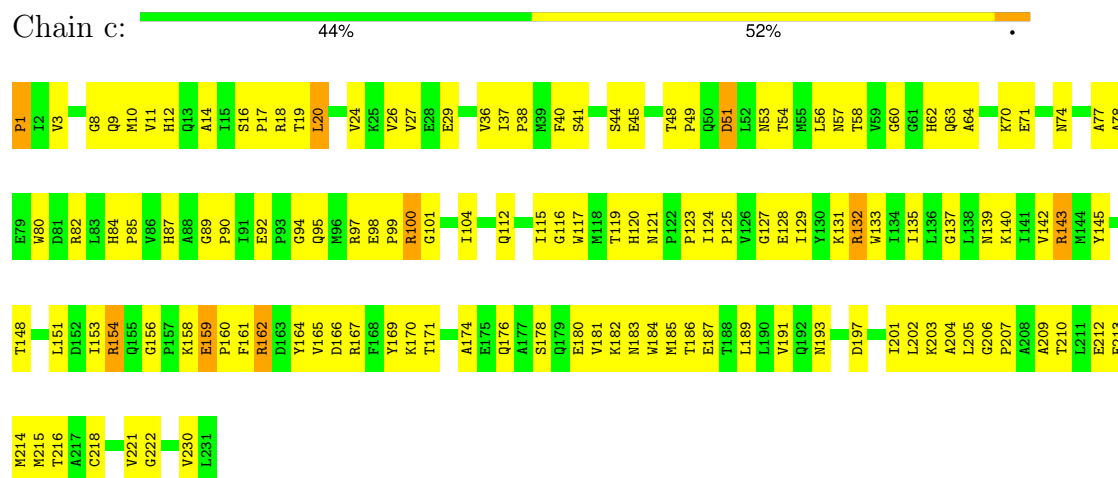
Chain a: 44% 53%



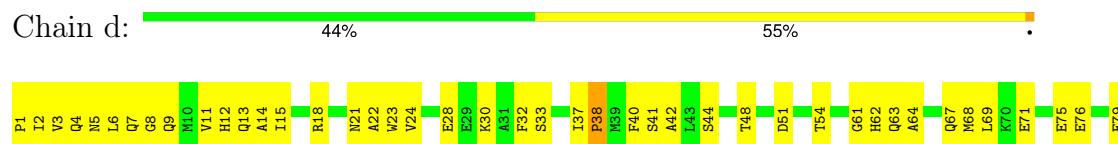
- Molecule 1: capsid protein

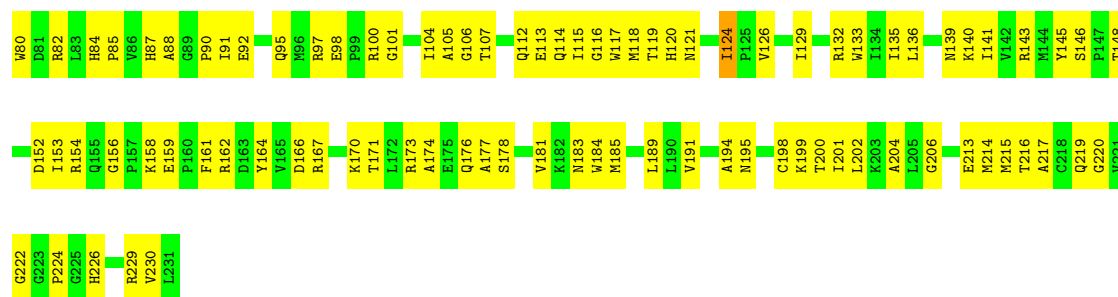


- Molecule 1: capsid protein



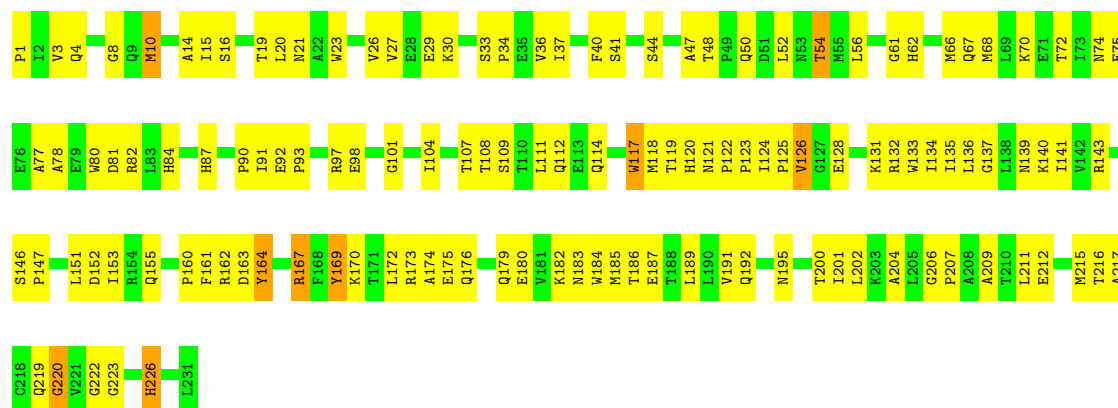
- Molecule 1: capsid protein





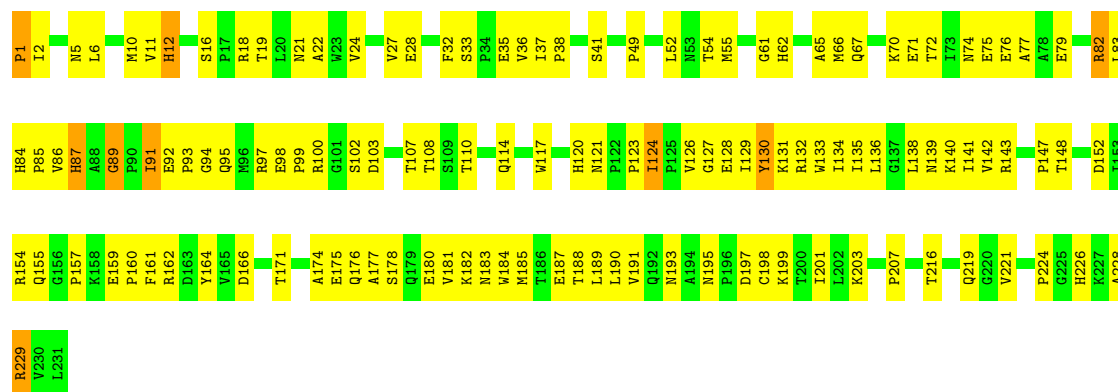
• Molecule 1: capsid protein

Chain e: 44% 52%



• Molecule 1: capsid protein

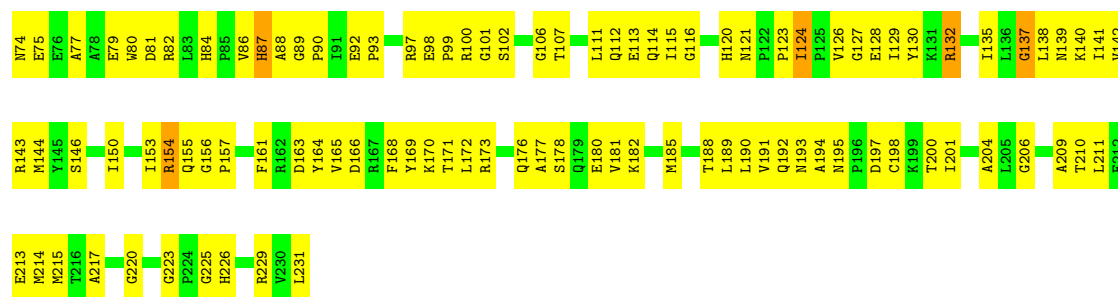
Chain f: 45% 51%



• Molecule 1: capsid protein

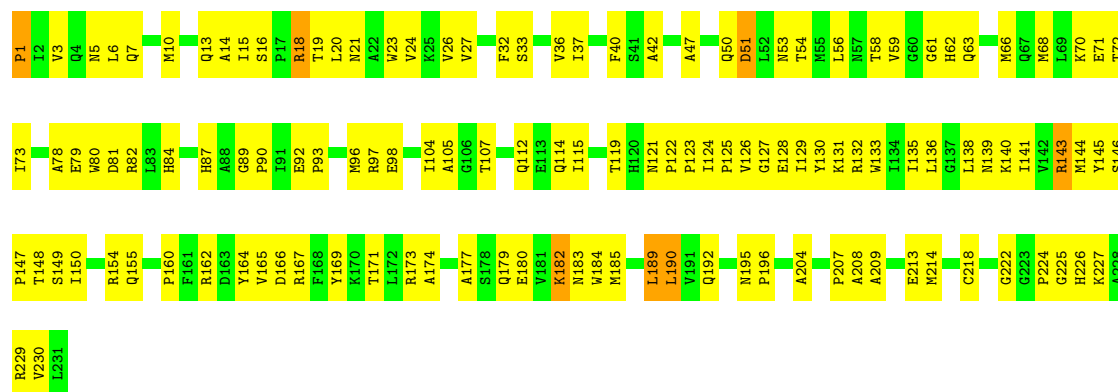
Chain g: 39% 58%





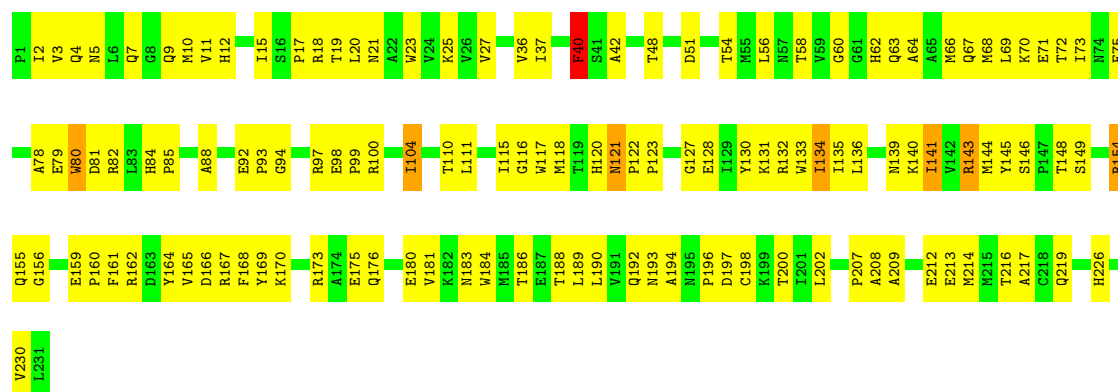
- Molecule 1: capsid protein

Chain h: 45% 52%



- Molecule 1: capsid protein

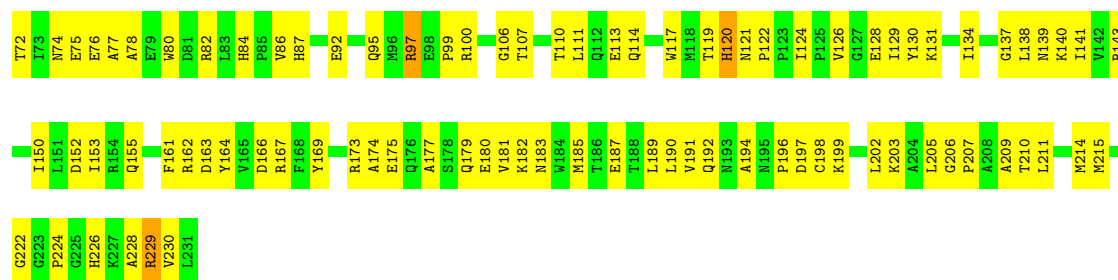
Chain i: 45% 52%



- Molecule 1: capsid protein

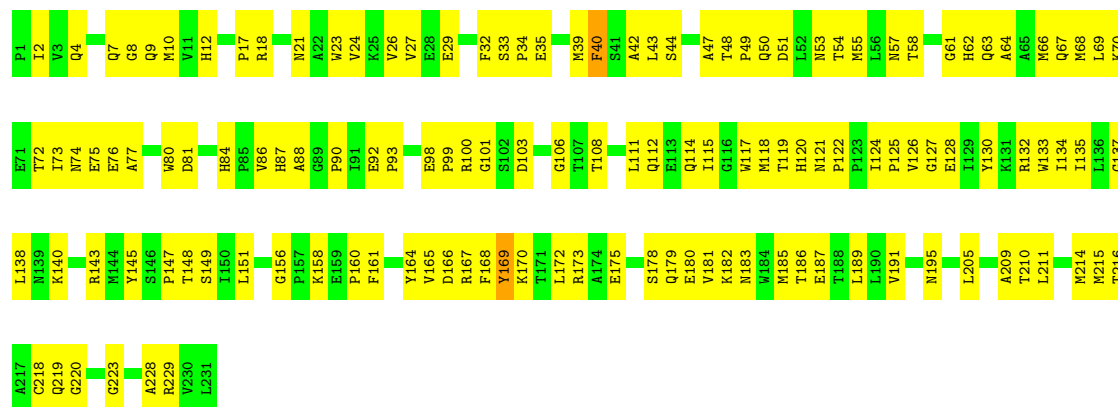
Chain j: 45% 54%





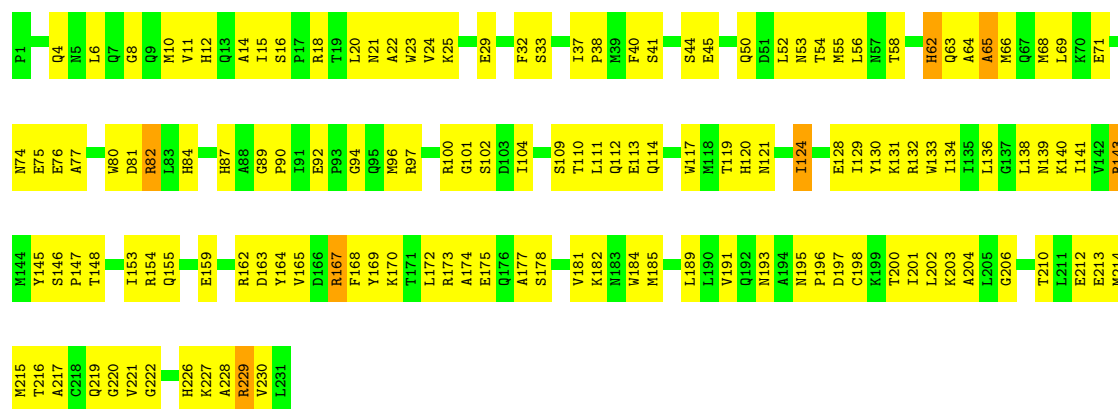
• Molecule 1: capsid protein

Chain 1: 42% 57%



• Molecule 1: capsid protein

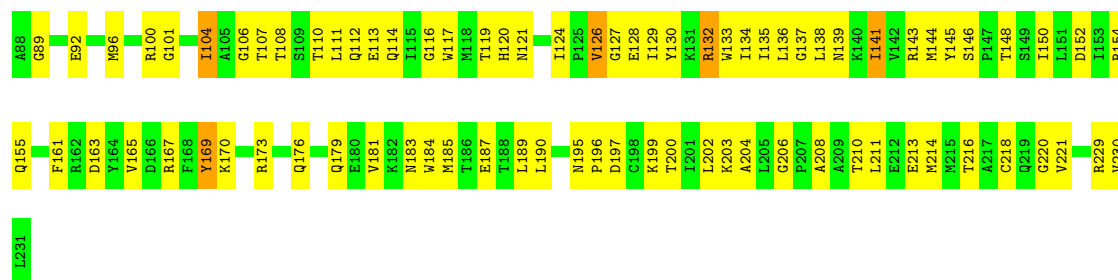
Chain k: 40% 57%



• Molecule 1: capsid protein

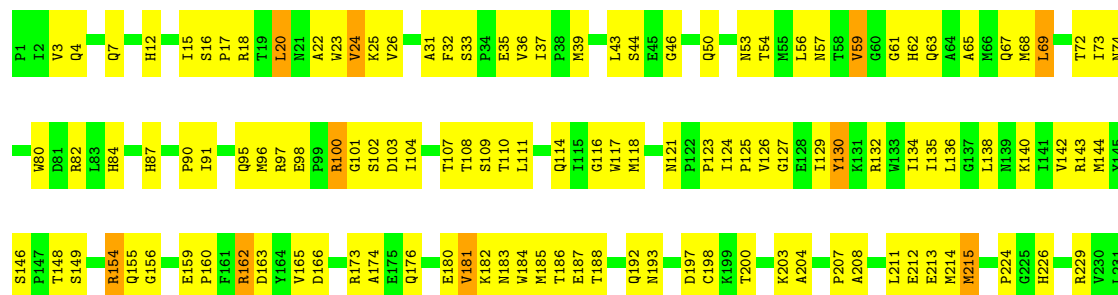
Chain l: 48% 48%





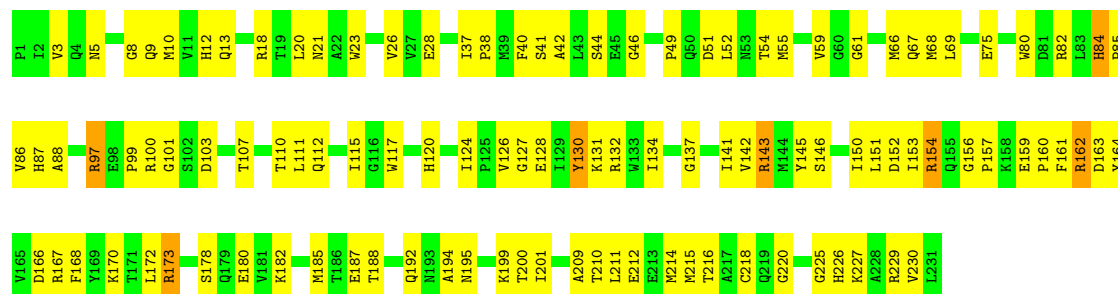
• Molecule 1: capsid protein

Chain m: 47% 48%



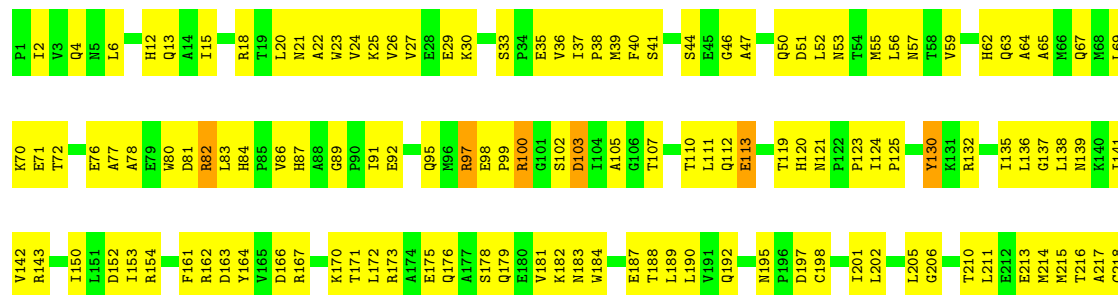
• Molecule 1: capsid protein

Chain n: 52% 45%



• Molecule 1: capsid protein

Chain o: 41% 56%



Q219
G220
V221
G222
G223
P224
H226
K227
A228
R229
V230
L231

• Molecule 1: capsid protein

Chain p:  47% 52%

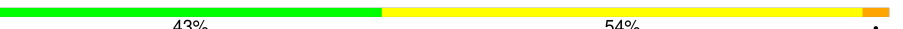
P1
I2
V3
Q4
N5
M10
V11
H12
K227
A228
R229
V230
L231
S16
P17
R18
T19
L20
N21
A22
V23
V24
K25
V26
F32
S33
P34
E35
V36
I37
P38
M39
A47
T48
P49
Q50
D51
L52
M53
M55
L56
M57
T58
V59
G60
G61
H62
Q63
A64
A65
L69
T72
I73
N74
E75
E76
A77
A78
E79
W80
D81
Q82
R83
H84
P85
V86
H87
A88
I91
G94
Q95
M96
N97
P98
P99
R100
G101
S102
D103
I104
Q112
E113
Q114
I115
H120
M121
P122
V126
G127
E128
I129
T130
K131
L132
W133
I134
I135
L136
G137
P138
L139
A208
M139
Q63
K140
T210
L211
E212
M215
R143
M144
P147
T148
S149
I150
E151
L151
D152
I153
R154
Q155
E159
R162
D163
V164
Y164
R167
F168
Y169
K170
R173
A177
S178
E180
V181
K182
M183
W184
M185
L189
L190
V191
Q192
M193
N195
P196
D197
C198
K199
T200
I201
L202
K203
A204
L205
G206
P207
A208
A209
T210
L211
E212
M215
R143
M144
P147
T148
S149
I150
E151
L151

• Molecule 1: capsid protein

Chain q:  49% 48%

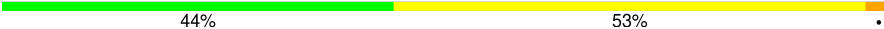
P1
Q4
N5
L6
Q7
G8
H12
I15
S16
P17
R18
T19
L20
N21
A22
K25
V26
V27
A31
F32
S33
P34
E35
V36
I37
P38
A42
L43
N194
S44
V45
G46
A47
D51
T54
M57
T58
V59
H62
Q63
A64
A65
L69
K70
E71
T72
I73
N74
E76
A77
A78
E79
W80
D81
Q82
R83
H84
P85
V86
H87
A88
I91
E92
E98
P99
R100
G101
I104
A105
S109
T110
L111
W117
M118
T119
H120
I124
P125
V126
G127
E128
I129
Y130
K131
R132
W133
L136
G137
L138
M139
K140
T141
V142
R143
M144
S149
D152
Q155
G156
P157
K158
E159
P160
F161
R162
D163
V164
Y165
D166
R167
F168
R173
A174
E175
Q176
A177
E180
N183
W184
T185
M185
T186
E187
T188
L189
L190
V191
Q192
M193
A194
N195
P196
D197
C198
K199
T200
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G206
A209
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L211
M215
T216
Q219
G220
V221
H226
V230
L231

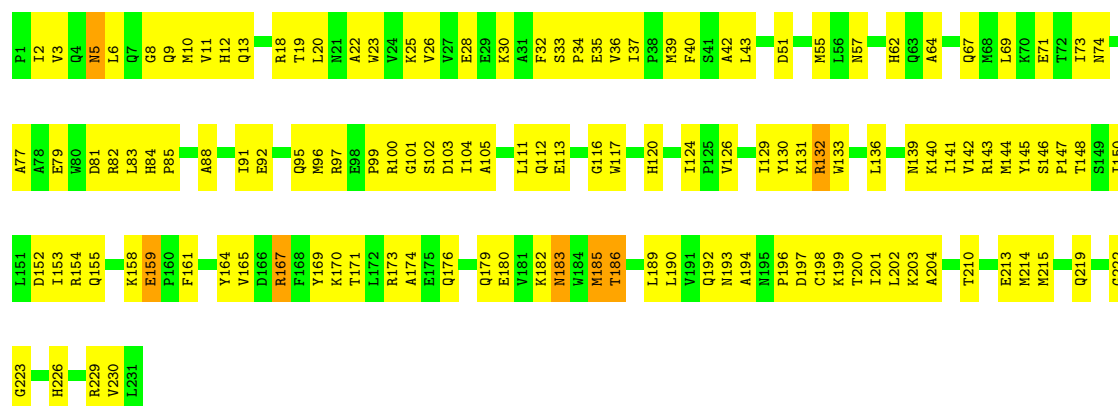
• Molecule 1: capsid protein

Chain r:  43% 54%

P1
I2
V3
Q4
N5
M10
V11
H12
S16
P17
R18
T19
L20
N21
A22
V23
V24
V27
E28
S33
V36
I37
S109
T110
L111
Q112
E113
Q114
W117
M118
T119
H120
P123
V126
G127
E128
I129
Y130
K131
L132
W133
I134
I135
L136
G137
L138
V142
R143
S146
E75
E76
E79
W80
D81
Q82
R83
H84
P85
V86
H87
A88
G89
P90
I91
E92
Q95
N96
E98
G101
S102
D103
T107
T108
S109
T110
L111
Q112
E113
Q114
W117
M118
T119
H120
P123
V126
G127
E128
I129
Y130
K131
L132
W133
I134
I135
L136
G137
L138
V142
R143
S146
P147
I150
L151
R154
P157
K158
E159
P160
F161
Y164
V165
P166
R167
F168
Y169
K170
L171
L172
R173
A174
E175
S178
Q179
E180
V181
K182
M183
W184
E187
T188
L189
L190
N195
D197
C198
K199
T200
I201
G206
P207
A208
A209
T210
L211
E212
M215
R216
C218
Q219
G220
V221
P224
G225
H226
R229
V230
L231

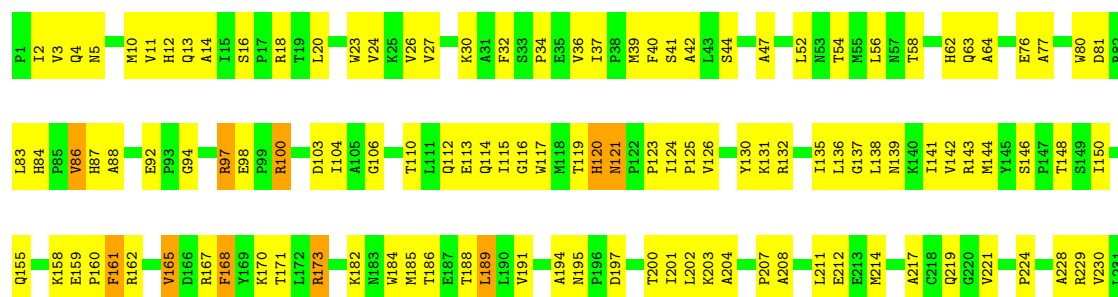
• Molecule 1: capsid protein

Chain s:  44% 53%

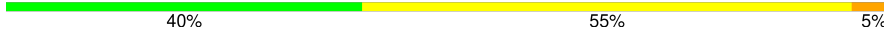


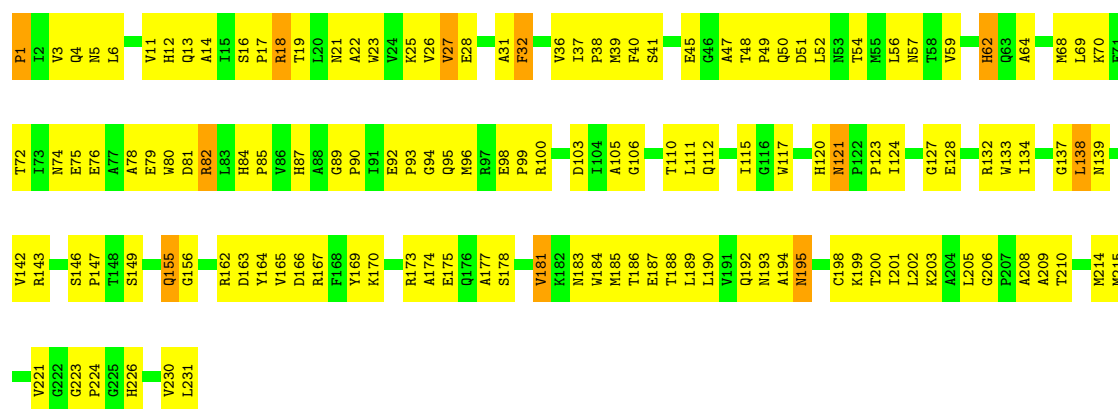
• Molecule 1: capsid protein

Chain t:  48% 47%



• Molecule 1: capsid protein

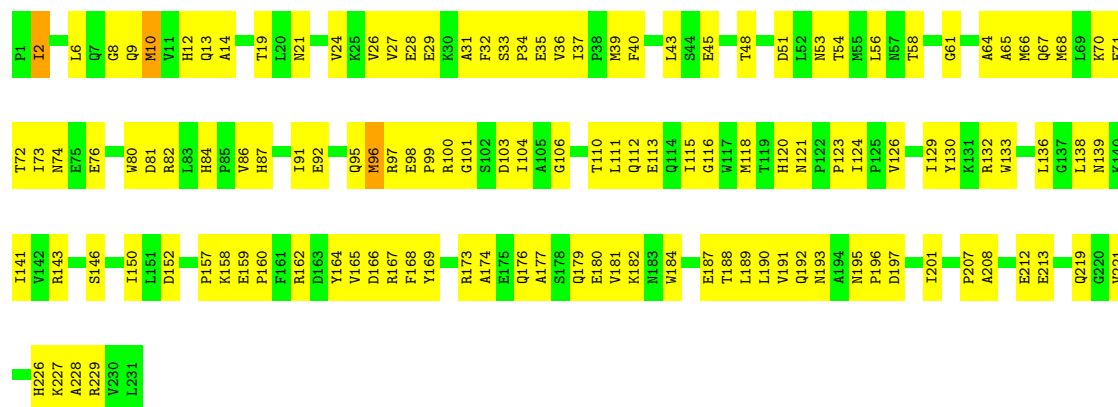
Chain 2:  40% 55% 5%



• Molecule 1: capsid protein

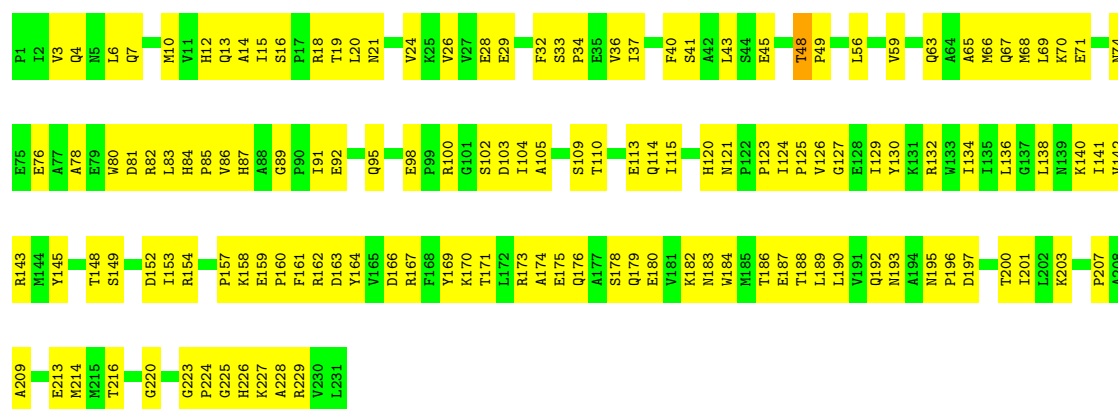
Chain u:  45% 54%





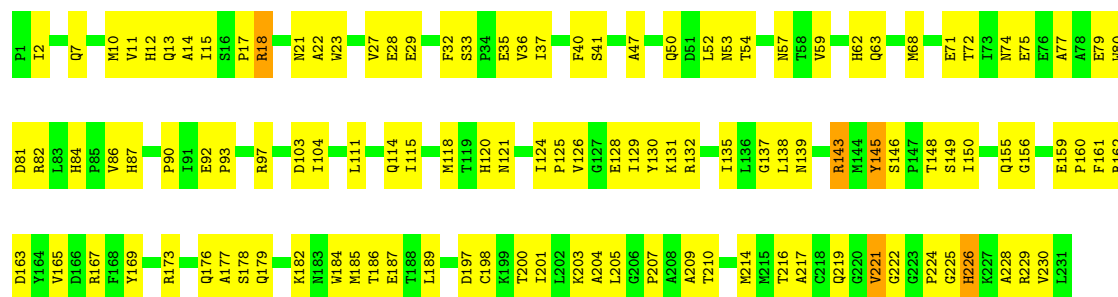
• Molecule 1: capsid protein

Chain v: 41% 59%



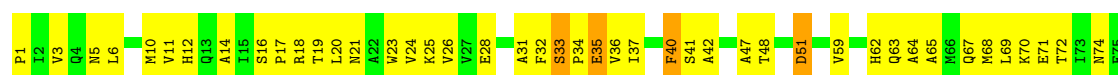
• Molecule 1: capsid protein

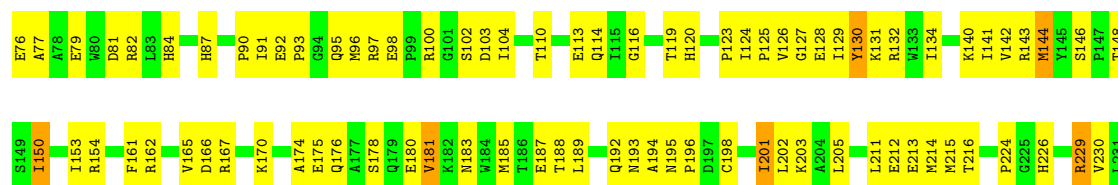
Chain w: 49% 49%



• Molecule 1: capsid protein

Chain x: 45% 51%

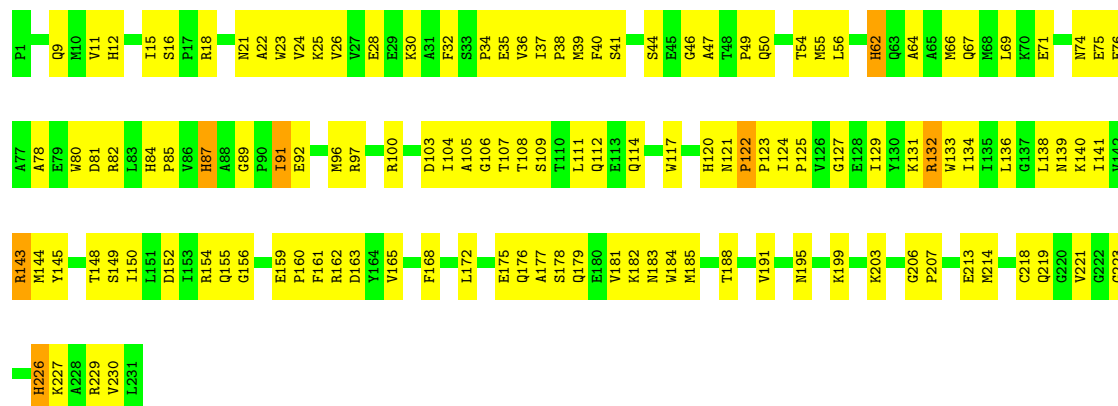




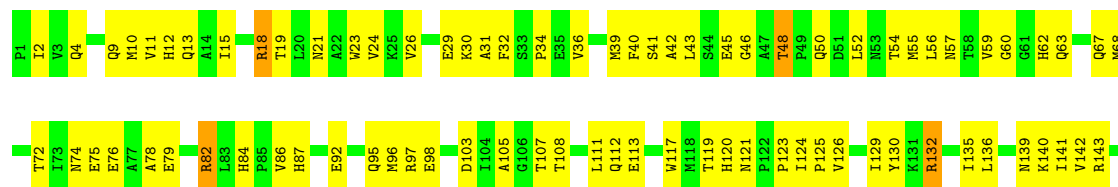
• Molecule 1: capsid protein

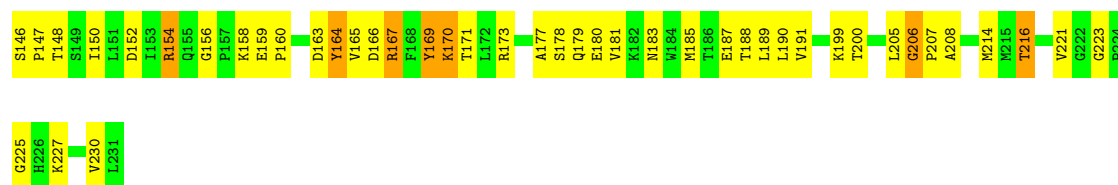


• Molecule 1: capsid protein



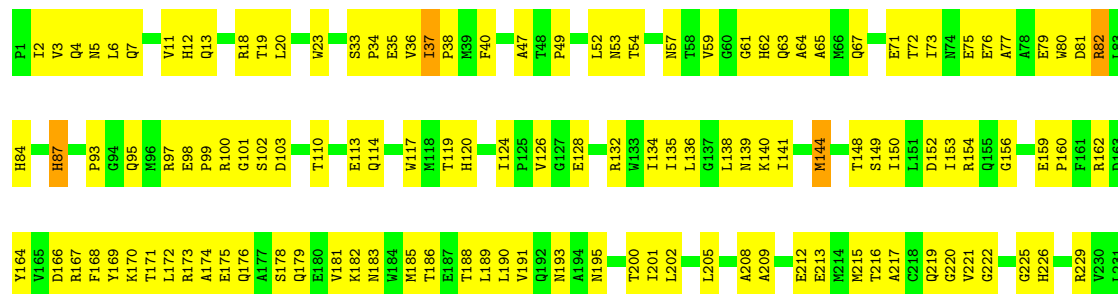
• Molecule 1: capsid protein





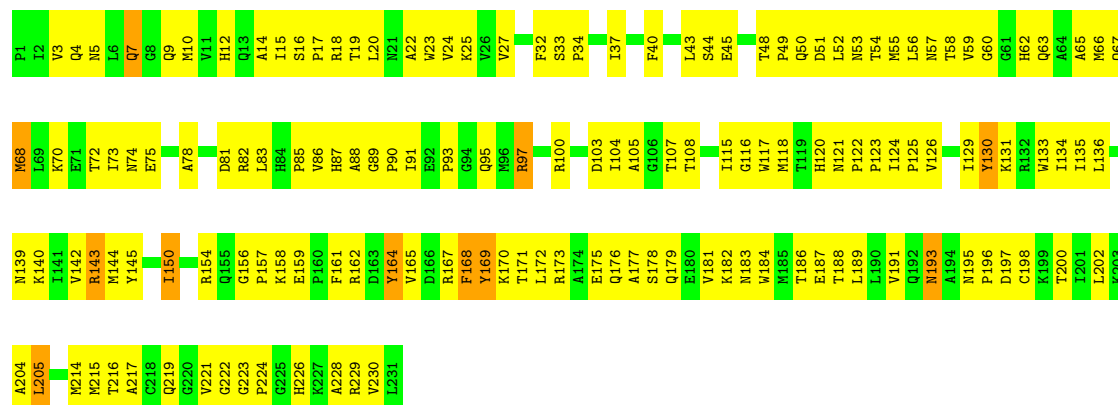
- Molecule 1: capsid protein

Chain B: 46% 52%



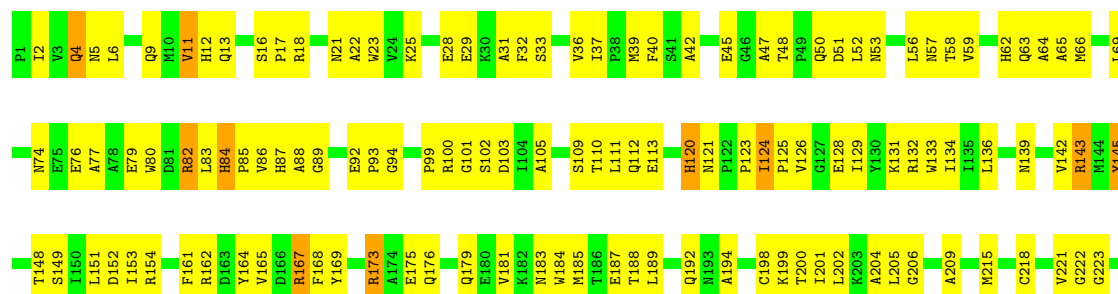
- Molecule 1: capsid protein

Chain C: 36% 59% 5%



- Molecule 1: capsid protein

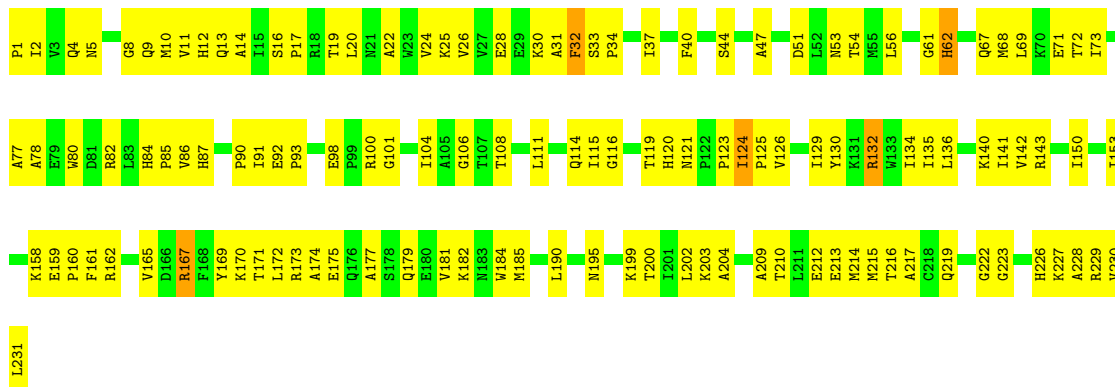
Chain D: 45% 51%





- Molecule 1: capsid protein

Chain 3: 45% 52%



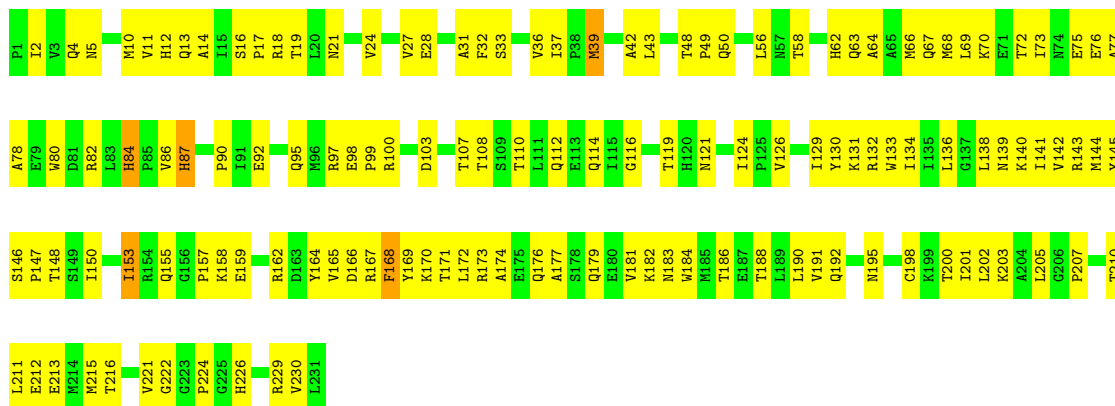
- Molecule 1: capsid protein

Chain E: 46% 52%



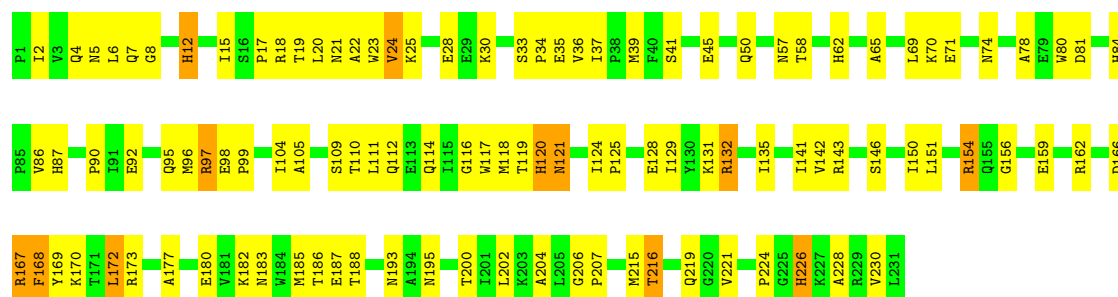
- Molecule 1: capsid protein

Chain F: 42% 56%



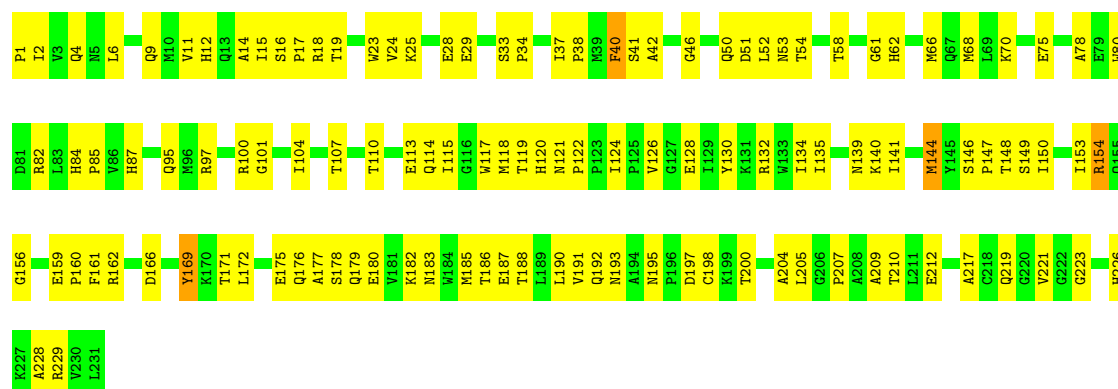
- Molecule 1: capsid protein

Chain G: 



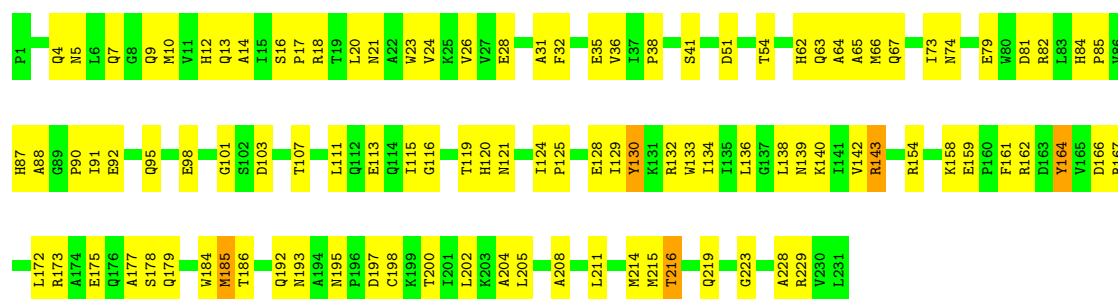
• Molecule 1: capsid protein

Chain H: 



• Molecule 1: capsid protein

Chain I: 



• Molecule 1: capsid protein

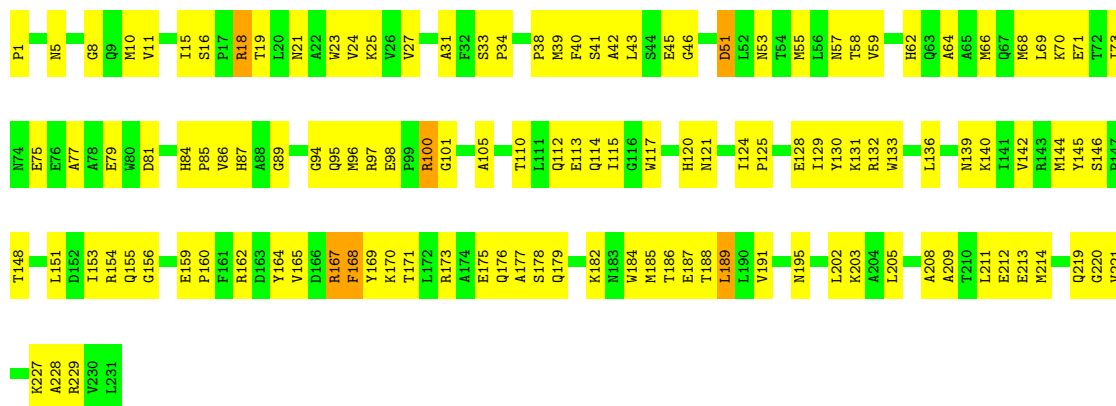
Chain J: 





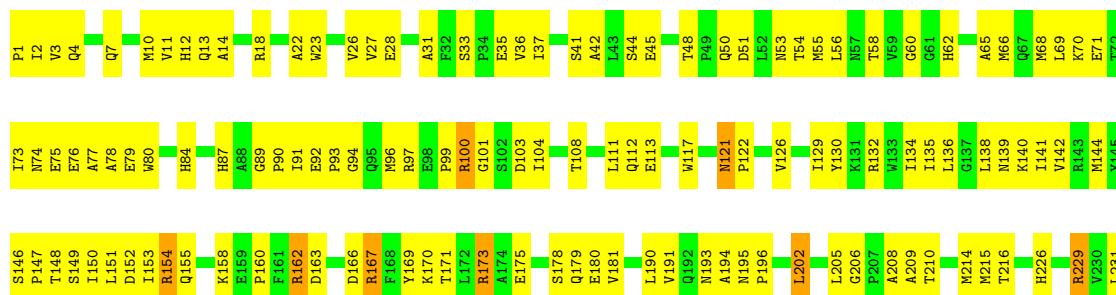
• Molecule 1: capsid protein

Chain K: 46% 52%



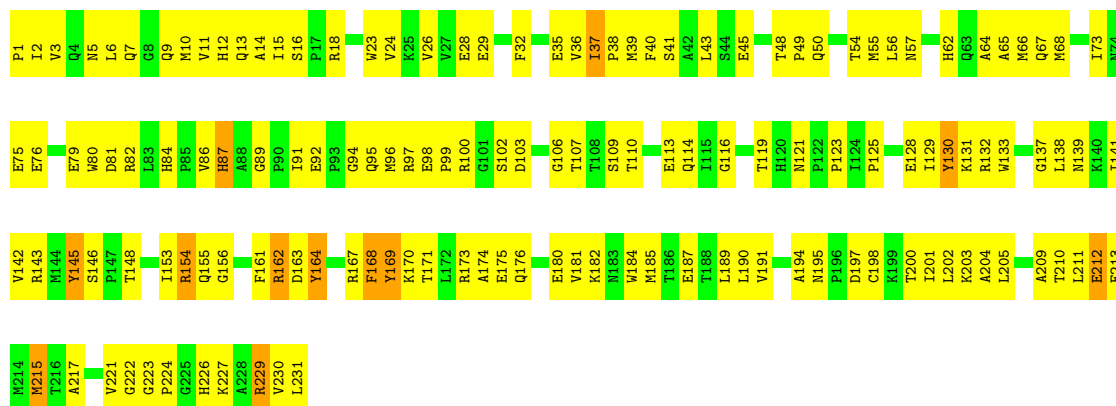
• Molecule 1: capsid protein

Chain L: 45% 52%

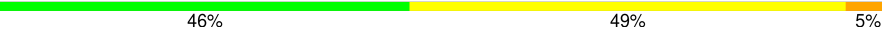


• Molecule 1: capsid protein

Chain M: 38% 57% 5%



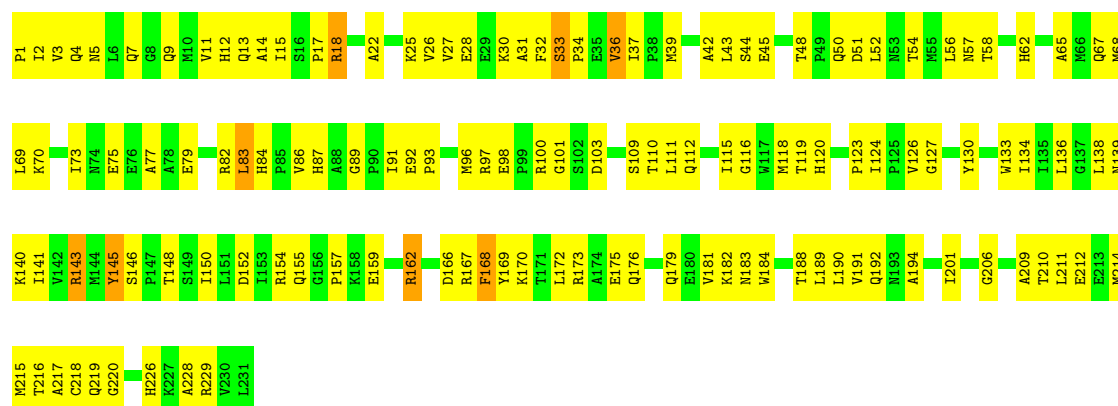
• Molecule 1: capsid protein

Chain N: 

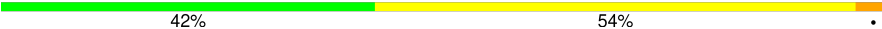


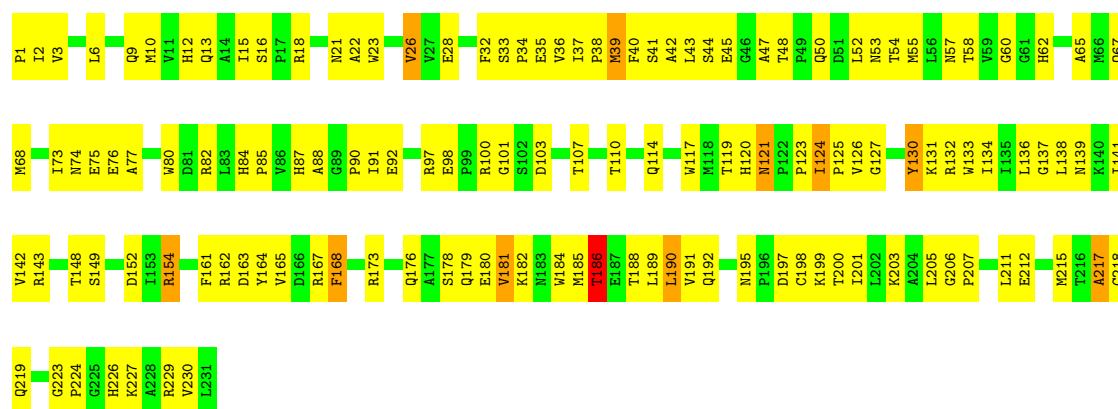
• Molecule 1: capsid protein

Chain 4: 



• Molecule 1: capsid protein

Chain O: 

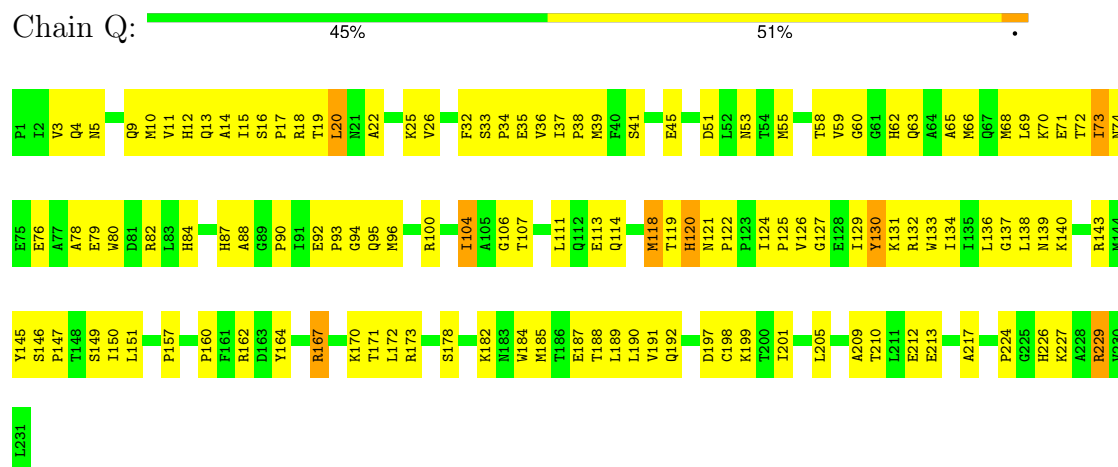


• Molecule 1: capsid protein

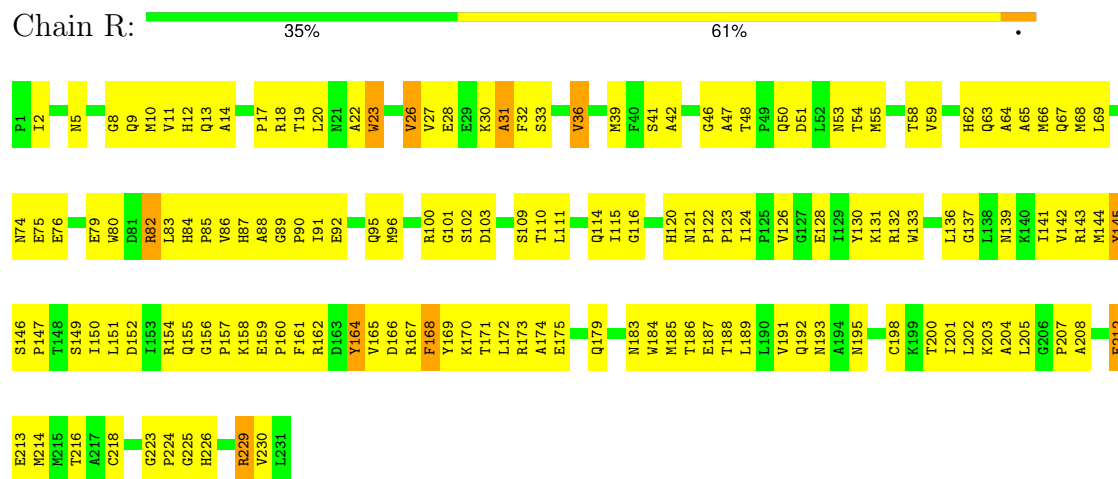
Chain P: 



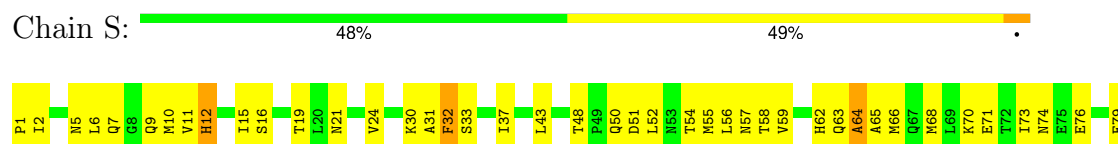
• Molecule 1: capsid protein



• Molecule 1: capsid protein

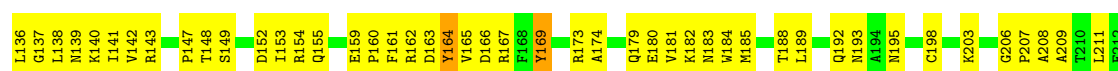


• Molecule 1: capsid protein

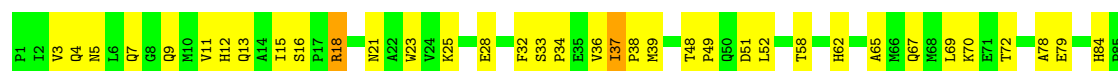




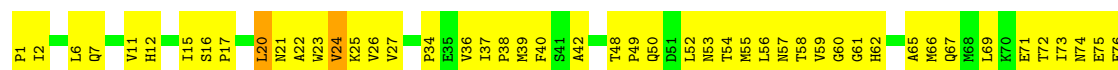
• Molecule 1: capsid protein



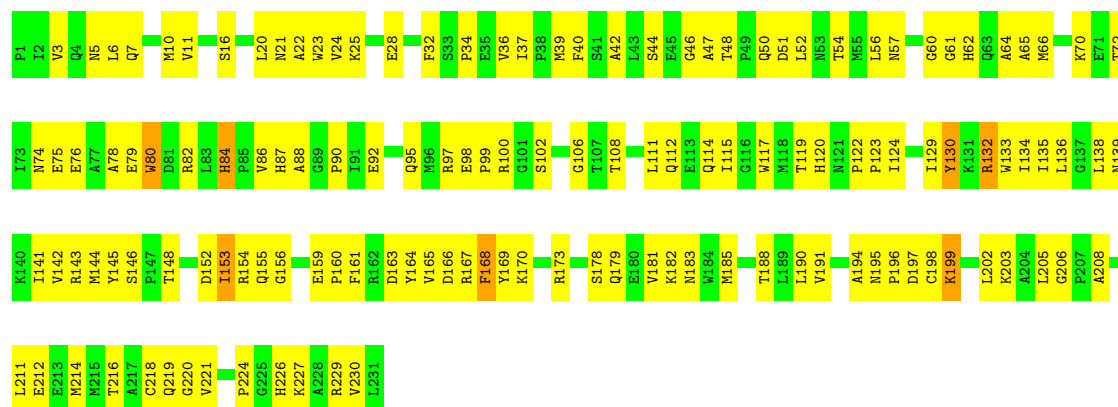
• Molecule 1: capsid protein



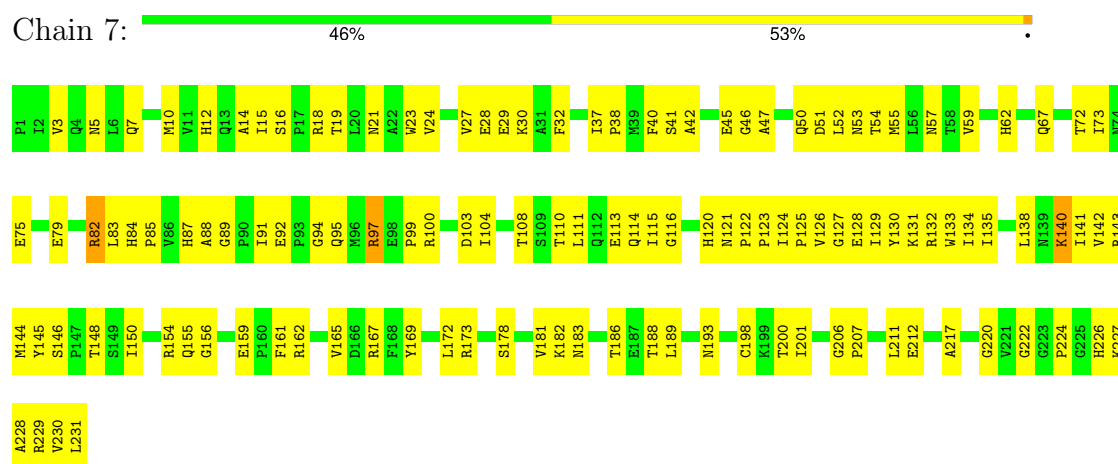
• Molecule 1: capsid protein



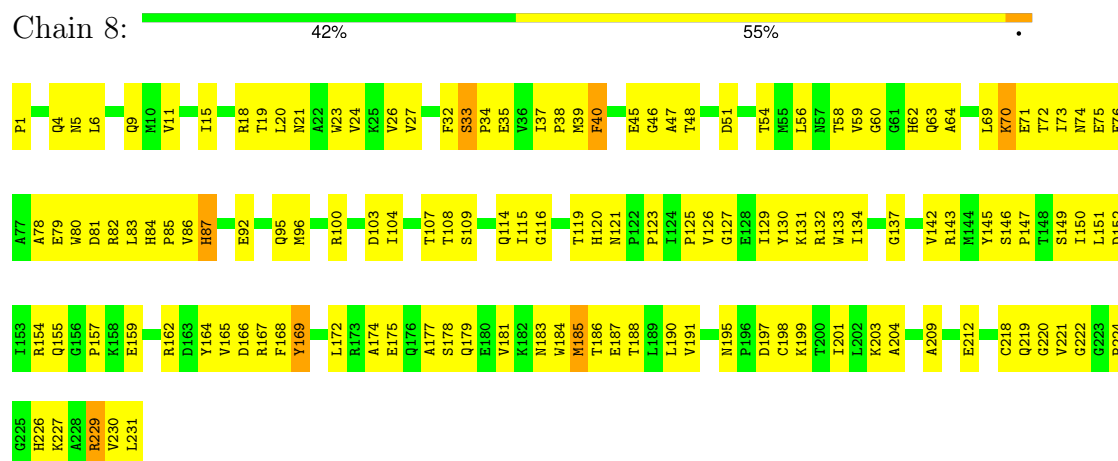




• Molecule 1: capsid protein



• Molecule 1: capsid protein



• Molecule 1: capsid protein

K227	S149	E75	P1
A228	I150	A76	I2
R229	L151	A77	V3
V230	D152	A78	
L231	I153	E79	Q7
		W80	G8
	P157		Q9
	K158	L83	M10
	E159	H84	V11
		P85	H12
	R162	V86	Q13
	D163	H87	A14
	Y164		I15
	D165		
	D166	E92	R18
	P167	P93	T19
	F168	Q95	L20
	Y169	G94	T21
	K170	M96	N21
	T171	R97	A22
	L172	R100	W23
	R173	G101	V24
	A174	S102	V26
	E175	D103	V27
	Q176	I104	E28
	A177	A105	E29
	S178	G106	K30
	Q179	T107	
	E180	T108	S33
	V181	S109	
	K182	T110	V36
	S183	L111	I37
	W184	Q112	P38
	M185	E113	M39
	T186	Q114	F40
	E187		S41
		W117	
	L190	H120	T48
	V191	N121	P49
	N195	P122	Q50
	P196		D51
	D197	P125	L52
		V126	N53
	I201	G127	
		E128	N57
	G206		T58
	P207	K131	V59
		R132	G60
		W133	G61
	T210	H62	
	L211	I134	Q63
	E212	I135	A64
	F213		A65
	M214	L138	M66
	M215		Q67
	T216	V142	M68
		R143	L69
	Q219		
	W226	P147	T73
		T149	N74

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	2.18	61/1841 (3.3%)	2.64	157/2500 (6.3%)
1	1	2.21	57/1841 (3.1%)	2.61	160/2500 (6.4%)
1	10	2.22	58/1841 (3.2%)	2.68	167/2500 (6.7%)
1	11	2.20	63/1841 (3.4%)	2.59	140/2500 (5.6%)
1	12	2.24	71/1841 (3.9%)	2.66	164/2500 (6.6%)
1	13	2.18	60/1841 (3.3%)	2.52	140/2500 (5.6%)
1	14	2.19	60/1841 (3.3%)	2.61	148/2500 (5.9%)
1	15	2.22	61/1841 (3.3%)	2.63	173/2500 (6.9%)
1	16	2.19	52/1841 (2.8%)	2.55	149/2500 (6.0%)
1	17	2.14	61/1841 (3.3%)	2.57	150/2500 (6.0%)
1	18	2.22	57/1841 (3.1%)	2.65	162/2500 (6.5%)
1	19	2.16	58/1841 (3.2%)	2.62	156/2500 (6.2%)
1	1A	2.17	59/1841 (3.2%)	2.60	150/2500 (6.0%)
1	1B	2.25	54/1841 (2.9%)	2.50	128/2500 (5.1%)
1	1C	2.15	60/1841 (3.3%)	2.62	170/2500 (6.8%)
1	1D	2.19	48/1841 (2.6%)	2.53	144/2500 (5.8%)
1	1E	2.13	51/1841 (2.8%)	2.51	131/2500 (5.2%)
1	1F	2.22	62/1841 (3.4%)	2.57	146/2500 (5.8%)
1	1G	2.21	61/1841 (3.3%)	2.55	144/2500 (5.8%)
1	1H	2.16	53/1841 (2.9%)	2.60	158/2500 (6.3%)
1	1I	2.24	69/1841 (3.7%)	2.66	156/2500 (6.2%)
1	1J	2.22	63/1841 (3.4%)	2.57	143/2500 (5.7%)
1	1K	2.21	61/1841 (3.3%)	2.52	134/2500 (5.4%)
1	1L	2.21	68/1841 (3.7%)	2.54	134/2500 (5.4%)
1	1M	2.18	55/1841 (3.0%)	2.65	156/2500 (6.2%)
1	1N	2.21	63/1841 (3.4%)	2.60	172/2500 (6.9%)
1	1O	2.21	59/1841 (3.2%)	2.55	136/2500 (5.4%)
1	1P	2.15	47/1841 (2.6%)	2.57	147/2500 (5.9%)
1	1Q	2.19	53/1841 (2.9%)	2.58	141/2500 (5.6%)
1	1R	2.16	56/1841 (3.0%)	2.58	145/2500 (5.8%)
1	1S	2.24	58/1841 (3.2%)	2.61	167/2500 (6.7%)
1	1T	2.18	54/1841 (2.9%)	2.56	137/2500 (5.5%)
1	1U	2.17	55/1841 (3.0%)	2.56	139/2500 (5.6%)
1	1V	2.24	65/1841 (3.5%)	2.59	147/2500 (5.9%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1W	2.21	61/1841 (3.3%)	2.54	140/2500 (5.6%)
1	1X	2.18	52/1841 (2.8%)	2.55	130/2500 (5.2%)
1	1Y	2.20	64/1841 (3.5%)	2.64	180/2500 (7.2%)
1	1Z	2.19	59/1841 (3.2%)	2.58	158/2500 (6.3%)
1	1a	2.20	46/1841 (2.5%)	2.57	132/2500 (5.3%)
1	1b	2.18	55/1841 (3.0%)	2.56	135/2500 (5.4%)
1	1c	2.23	65/1841 (3.5%)	2.61	136/2500 (5.4%)
1	1d	2.24	59/1841 (3.2%)	2.49	129/2500 (5.2%)
1	1e	2.17	55/1841 (3.0%)	2.67	159/2500 (6.4%)
1	1f	2.13	49/1841 (2.7%)	2.54	133/2500 (5.3%)
1	1g	2.20	60/1841 (3.3%)	2.52	133/2500 (5.3%)
1	1h	2.22	66/1841 (3.6%)	2.59	136/2500 (5.4%)
1	1i	2.19	52/1841 (2.8%)	2.58	162/2500 (6.5%)
1	1j	2.16	50/1841 (2.7%)	2.56	143/2500 (5.7%)
1	1k	2.30	61/1841 (3.3%)	2.56	144/2500 (5.8%)
1	1l	2.26	58/1841 (3.2%)	2.56	155/2500 (6.2%)
1	1m	2.24	58/1841 (3.2%)	2.52	130/2500 (5.2%)
1	1n	2.25	62/1841 (3.4%)	2.58	144/2500 (5.8%)
1	1o	2.29	71/1841 (3.9%)	2.56	140/2500 (5.6%)
1	1p	2.20	58/1841 (3.2%)	2.51	134/2500 (5.4%)
1	1q	2.11	49/1841 (2.7%)	2.56	156/2500 (6.2%)
1	1r	2.17	56/1841 (3.0%)	2.49	124/2500 (5.0%)
1	1s	2.18	61/1841 (3.3%)	2.65	152/2500 (6.1%)
1	1t	2.23	70/1841 (3.8%)	2.55	133/2500 (5.3%)
1	1u	2.18	51/1841 (2.8%)	2.59	125/2500 (5.0%)
1	1v	2.15	56/1841 (3.0%)	2.52	130/2500 (5.2%)
1	1w	2.26	61/1841 (3.3%)	2.54	140/2500 (5.6%)
1	1x	2.23	61/1841 (3.3%)	2.67	163/2500 (6.5%)
1	1y	2.20	56/1841 (3.0%)	2.59	162/2500 (6.5%)
1	1z	2.12	51/1841 (2.8%)	2.62	153/2500 (6.1%)
1	2	2.18	59/1841 (3.2%)	2.55	139/2500 (5.6%)
1	20	2.22	68/1841 (3.7%)	2.56	143/2500 (5.7%)
1	21	2.26	68/1841 (3.7%)	2.64	167/2500 (6.7%)
1	22	2.22	54/1841 (2.9%)	2.60	152/2500 (6.1%)
1	23	2.31	66/1841 (3.6%)	2.63	147/2500 (5.9%)
1	24	2.24	61/1841 (3.3%)	2.62	155/2500 (6.2%)
1	25	2.26	70/1841 (3.8%)	2.61	145/2500 (5.8%)
1	26	2.19	59/1841 (3.2%)	2.54	155/2500 (6.2%)
1	27	2.19	56/1841 (3.0%)	2.58	145/2500 (5.8%)
1	28	2.18	57/1841 (3.1%)	2.62	150/2500 (6.0%)
1	29	2.35	79/1841 (4.3%)	2.62	142/2500 (5.7%)
1	2A	2.24	66/1841 (3.6%)	2.60	150/2500 (6.0%)
1	2B	2.21	64/1841 (3.5%)	2.50	115/2500 (4.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	2C	2.19	52/1841 (2.8%)	2.66	167/2500 (6.7%)
1	2D	2.18	50/1841 (2.7%)	2.56	143/2500 (5.7%)
1	2E	2.20	60/1841 (3.3%)	2.60	171/2500 (6.8%)
1	2F	2.17	52/1841 (2.8%)	2.58	152/2500 (6.1%)
1	2G	2.21	65/1841 (3.5%)	2.65	178/2500 (7.1%)
1	2H	2.21	53/1841 (2.9%)	2.53	141/2500 (5.6%)
1	2I	2.21	58/1841 (3.2%)	2.59	153/2500 (6.1%)
1	2J	2.17	58/1841 (3.2%)	2.59	145/2500 (5.8%)
1	2K	2.18	49/1841 (2.7%)	2.57	141/2500 (5.6%)
1	2L	2.24	62/1841 (3.4%)	2.56	152/2500 (6.1%)
1	2M	2.20	55/1841 (3.0%)	2.63	160/2500 (6.4%)
1	2N	2.19	55/1841 (3.0%)	2.59	151/2500 (6.0%)
1	2O	2.23	55/1841 (3.0%)	2.66	152/2500 (6.1%)
1	2P	2.21	52/1841 (2.8%)	2.58	151/2500 (6.0%)
1	2Q	2.28	74/1841 (4.0%)	2.62	145/2500 (5.8%)
1	2R	2.21	56/1841 (3.0%)	2.60	164/2500 (6.6%)
1	2S	2.29	70/1841 (3.8%)	2.63	172/2500 (6.9%)
1	2T	2.19	48/1841 (2.6%)	2.66	163/2500 (6.5%)
1	2U	2.17	54/1841 (2.9%)	2.57	153/2500 (6.1%)
1	2V	2.18	64/1841 (3.5%)	2.60	154/2500 (6.2%)
1	2W	2.27	59/1841 (3.2%)	2.54	132/2500 (5.3%)
1	2X	2.30	70/1841 (3.8%)	2.65	175/2500 (7.0%)
1	2Y	2.28	73/1841 (4.0%)	2.59	156/2500 (6.2%)
1	2Z	2.23	67/1841 (3.6%)	2.59	153/2500 (6.1%)
1	2a	2.22	62/1841 (3.4%)	2.65	172/2500 (6.9%)
1	2b	2.28	73/1841 (4.0%)	2.64	165/2500 (6.6%)
1	2c	2.17	56/1841 (3.0%)	2.67	166/2500 (6.6%)
1	2d	2.18	54/1841 (2.9%)	2.57	149/2500 (6.0%)
1	2e	2.21	57/1841 (3.1%)	2.59	153/2500 (6.1%)
1	2f	2.19	70/1841 (3.8%)	2.60	160/2500 (6.4%)
1	2g	2.21	63/1841 (3.4%)	2.63	170/2500 (6.8%)
1	2h	2.15	50/1841 (2.7%)	2.57	147/2500 (5.9%)
1	2i	2.16	55/1841 (3.0%)	2.65	156/2500 (6.2%)
1	2j	2.20	53/1841 (2.9%)	2.61	168/2500 (6.7%)
1	2k	2.19	59/1841 (3.2%)	2.56	158/2500 (6.3%)
1	2l	2.17	50/1841 (2.7%)	2.68	171/2500 (6.8%)
1	2m	2.20	51/1841 (2.8%)	2.55	145/2500 (5.8%)
1	2n	2.22	61/1841 (3.3%)	2.56	162/2500 (6.5%)
1	2o	2.17	52/1841 (2.8%)	2.64	157/2500 (6.3%)
1	2p	2.23	60/1841 (3.3%)	2.65	167/2500 (6.7%)
1	2q	2.26	67/1841 (3.6%)	2.57	142/2500 (5.7%)
1	2r	2.16	56/1841 (3.0%)	2.57	167/2500 (6.7%)
1	2s	2.21	60/1841 (3.3%)	2.69	166/2500 (6.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	2t	2.24	58/1841 (3.2%)	2.50	149/2500 (6.0%)
1	2u	2.20	59/1841 (3.2%)	2.58	132/2500 (5.3%)
1	2v	2.18	57/1841 (3.1%)	2.66	175/2500 (7.0%)
1	2w	2.25	64/1841 (3.5%)	2.70	175/2500 (7.0%)
1	2x	2.28	72/1841 (3.9%)	2.51	157/2500 (6.3%)
1	2y	2.25	70/1841 (3.8%)	2.56	126/2500 (5.0%)
1	2z	2.24	64/1841 (3.5%)	2.57	155/2500 (6.2%)
1	3	2.26	58/1841 (3.2%)	2.66	154/2500 (6.2%)
1	30	2.26	72/1841 (3.9%)	2.58	154/2500 (6.2%)
1	31	2.24	65/1841 (3.5%)	2.48	134/2500 (5.4%)
1	32	2.21	57/1841 (3.1%)	2.58	148/2500 (5.9%)
1	33	2.15	51/1841 (2.8%)	2.51	139/2500 (5.6%)
1	34	2.17	51/1841 (2.8%)	2.62	138/2500 (5.5%)
1	35	2.18	60/1841 (3.3%)	2.56	134/2500 (5.4%)
1	36	2.16	56/1841 (3.0%)	2.61	166/2500 (6.6%)
1	37	2.14	51/1841 (2.8%)	2.53	153/2500 (6.1%)
1	38	2.22	50/1841 (2.7%)	2.60	137/2500 (5.5%)
1	39	2.16	53/1841 (2.9%)	2.54	151/2500 (6.0%)
1	3A	2.24	55/1841 (3.0%)	2.56	156/2500 (6.2%)
1	3B	2.24	55/1841 (3.0%)	2.60	153/2500 (6.1%)
1	3C	2.20	53/1841 (2.9%)	2.68	162/2500 (6.5%)
1	3D	2.28	59/1841 (3.2%)	2.50	158/2500 (6.3%)
1	3E	2.19	56/1841 (3.0%)	2.65	147/2500 (5.9%)
1	3F	2.29	67/1841 (3.6%)	2.59	153/2500 (6.1%)
1	3G	2.25	65/1841 (3.5%)	2.55	142/2500 (5.7%)
1	3H	2.18	58/1841 (3.2%)	2.56	139/2500 (5.6%)
1	3I	2.14	60/1841 (3.3%)	2.66	168/2500 (6.7%)
1	3J	2.15	51/1841 (2.8%)	2.62	137/2500 (5.5%)
1	3K	2.26	66/1841 (3.6%)	2.59	145/2500 (5.8%)
1	3L	2.18	56/1841 (3.0%)	2.62	153/2500 (6.1%)
1	3M	2.19	57/1841 (3.1%)	2.58	144/2500 (5.8%)
1	3N	2.21	57/1841 (3.1%)	2.62	170/2500 (6.8%)
1	3O	2.32	81/1841 (4.4%)	2.68	171/2500 (6.8%)
1	3P	2.22	61/1841 (3.3%)	2.60	156/2500 (6.2%)
1	3Q	2.19	63/1841 (3.4%)	2.60	153/2500 (6.1%)
1	3R	2.18	61/1841 (3.3%)	2.60	150/2500 (6.0%)
1	3S	2.24	62/1841 (3.4%)	2.63	173/2500 (6.9%)
1	3T	2.16	53/1841 (2.9%)	2.62	152/2500 (6.1%)
1	3U	2.22	53/1841 (2.9%)	2.64	152/2500 (6.1%)
1	3V	2.27	68/1841 (3.7%)	2.61	143/2500 (5.7%)
1	3W	2.23	57/1841 (3.1%)	2.60	151/2500 (6.0%)
1	3X	2.23	60/1841 (3.3%)	2.59	169/2500 (6.8%)
1	3Y	2.18	53/1841 (2.9%)	2.56	139/2500 (5.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	3Z	2.24	62/1841 (3.4%)	2.62	161/2500 (6.4%)
1	3a	2.18	52/1841 (2.8%)	2.62	157/2500 (6.3%)
1	3b	2.14	43/1841 (2.3%)	2.61	157/2500 (6.3%)
1	3c	2.29	70/1841 (3.8%)	2.62	155/2500 (6.2%)
1	3d	2.18	46/1841 (2.5%)	2.57	165/2500 (6.6%)
1	3e	2.24	56/1841 (3.0%)	2.55	145/2500 (5.8%)
1	3f	2.17	50/1841 (2.7%)	2.57	136/2500 (5.4%)
1	3g	2.16	54/1841 (2.9%)	2.63	163/2500 (6.5%)
1	3h	2.21	54/1841 (2.9%)	2.60	158/2500 (6.3%)
1	3i	2.18	57/1841 (3.1%)	2.54	139/2500 (5.6%)
1	3j	2.21	62/1841 (3.4%)	2.56	152/2500 (6.1%)
1	3k	2.13	45/1841 (2.4%)	2.50	140/2500 (5.6%)
1	3l	2.23	66/1841 (3.6%)	2.59	144/2500 (5.8%)
1	3m	2.23	55/1841 (3.0%)	2.55	132/2500 (5.3%)
1	3n	2.19	59/1841 (3.2%)	2.55	157/2500 (6.3%)
1	3o	2.22	61/1841 (3.3%)	2.68	167/2500 (6.7%)
1	3p	2.21	52/1841 (2.8%)	2.70	177/2500 (7.1%)
1	3q	2.20	66/1841 (3.6%)	2.58	145/2500 (5.8%)
1	3r	2.18	52/1841 (2.8%)	2.59	168/2500 (6.7%)
1	3s	2.21	59/1841 (3.2%)	2.60	168/2500 (6.7%)
1	3t	2.21	58/1841 (3.2%)	2.54	131/2500 (5.2%)
1	3u	2.25	60/1841 (3.3%)	2.54	124/2500 (5.0%)
1	3v	2.24	65/1841 (3.5%)	2.57	124/2500 (5.0%)
1	3w	2.15	54/1841 (2.9%)	2.61	164/2500 (6.6%)
1	3x	2.20	71/1841 (3.9%)	2.52	138/2500 (5.5%)
1	3y	2.14	56/1841 (3.0%)	2.56	140/2500 (5.6%)
1	3z	2.23	54/1841 (2.9%)	2.64	175/2500 (7.0%)
1	4	2.19	62/1841 (3.4%)	2.60	162/2500 (6.5%)
1	40	2.18	50/1841 (2.7%)	2.57	137/2500 (5.5%)
1	41	2.17	57/1841 (3.1%)	2.53	137/2500 (5.5%)
1	42	2.19	57/1841 (3.1%)	2.57	156/2500 (6.2%)
1	43	2.24	64/1841 (3.5%)	2.61	158/2500 (6.3%)
1	44	2.22	68/1841 (3.7%)	2.65	151/2500 (6.0%)
1	45	2.13	51/1841 (2.8%)	2.54	139/2500 (5.6%)
1	46	2.22	58/1841 (3.2%)	2.62	143/2500 (5.7%)
1	47	2.25	65/1841 (3.5%)	2.58	147/2500 (5.9%)
1	48	2.26	66/1841 (3.6%)	2.65	164/2500 (6.6%)
1	49	2.21	63/1841 (3.4%)	2.56	150/2500 (6.0%)
1	4A	2.10	49/1841 (2.7%)	2.54	130/2500 (5.2%)
1	4B	2.11	51/1841 (2.8%)	2.57	163/2500 (6.5%)
1	4C	2.16	42/1841 (2.3%)	2.59	141/2500 (5.6%)
1	4D	2.26	64/1841 (3.5%)	2.49	146/2500 (5.8%)
1	4E	2.17	52/1841 (2.8%)	2.67	160/2500 (6.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	4F	2.19	63/1841 (3.4%)	2.57	148/2500 (5.9%)
1	4G	2.23	66/1841 (3.6%)	2.58	156/2500 (6.2%)
1	4H	2.21	59/1841 (3.2%)	2.56	130/2500 (5.2%)
1	4I	2.15	50/1841 (2.7%)	2.66	166/2500 (6.6%)
1	4J	2.21	54/1841 (2.9%)	2.62	157/2500 (6.3%)
1	4K	2.18	59/1841 (3.2%)	2.65	157/2500 (6.3%)
1	4L	2.17	58/1841 (3.2%)	2.56	147/2500 (5.9%)
1	4M	2.19	60/1841 (3.3%)	2.63	153/2500 (6.1%)
1	4N	2.13	45/1841 (2.4%)	2.62	158/2500 (6.3%)
1	4O	2.19	59/1841 (3.2%)	2.57	143/2500 (5.7%)
1	4P	2.16	52/1841 (2.8%)	2.61	168/2500 (6.7%)
1	4Q	2.16	53/1841 (2.9%)	2.57	149/2500 (6.0%)
1	4R	2.25	63/1841 (3.4%)	2.44	118/2500 (4.7%)
1	4S	2.24	65/1841 (3.5%)	2.56	137/2500 (5.5%)
1	4T	2.22	65/1841 (3.5%)	2.53	144/2500 (5.8%)
1	4U	2.15	52/1841 (2.8%)	2.63	170/2500 (6.8%)
1	4V	2.17	56/1841 (3.0%)	2.55	150/2500 (6.0%)
1	4W	2.18	58/1841 (3.2%)	2.58	145/2500 (5.8%)
1	4X	2.21	58/1841 (3.2%)	2.59	157/2500 (6.3%)
1	4Y	2.13	48/1841 (2.6%)	2.66	160/2500 (6.4%)
1	4Z	2.18	64/1841 (3.5%)	2.71	179/2500 (7.2%)
1	4a	2.19	50/1841 (2.7%)	2.64	172/2500 (6.9%)
1	4b	2.20	72/1841 (3.9%)	2.64	159/2500 (6.4%)
1	4c	2.20	59/1841 (3.2%)	2.64	146/2500 (5.8%)
1	4d	2.19	59/1841 (3.2%)	2.63	164/2500 (6.6%)
1	4e	2.21	56/1841 (3.0%)	2.53	141/2500 (5.6%)
1	4f	2.27	71/1841 (3.9%)	2.59	156/2500 (6.2%)
1	4g	2.13	42/1841 (2.3%)	2.49	139/2500 (5.6%)
1	4h	2.18	63/1841 (3.4%)	2.69	179/2500 (7.2%)
1	4i	2.18	53/1841 (2.9%)	2.62	152/2500 (6.1%)
1	4j	2.21	65/1841 (3.5%)	2.57	149/2500 (6.0%)
1	4k	2.21	66/1841 (3.6%)	2.67	178/2500 (7.1%)
1	4l	2.18	52/1841 (2.8%)	2.56	155/2500 (6.2%)
1	4m	2.17	50/1841 (2.7%)	2.61	139/2500 (5.6%)
1	4n	2.24	63/1841 (3.4%)	2.57	130/2500 (5.2%)
1	4o	2.23	59/1841 (3.2%)	2.58	148/2500 (5.9%)
1	4p	2.11	43/1841 (2.3%)	2.55	146/2500 (5.8%)
1	4q	2.21	67/1841 (3.6%)	2.58	160/2500 (6.4%)
1	4r	2.23	64/1841 (3.5%)	2.58	144/2500 (5.8%)
1	4s	2.22	63/1841 (3.4%)	2.56	152/2500 (6.1%)
1	4t	2.14	55/1841 (3.0%)	2.53	137/2500 (5.5%)
1	4u	2.19	48/1841 (2.6%)	2.59	146/2500 (5.8%)
1	4v	2.21	71/1841 (3.9%)	2.55	143/2500 (5.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	4w	2.20	50/1841 (2.7%)	2.64	149/2500 (6.0%)
1	4x	2.18	62/1841 (3.4%)	2.55	137/2500 (5.5%)
1	4y	2.21	68/1841 (3.7%)	2.63	161/2500 (6.4%)
1	4z	2.15	56/1841 (3.0%)	2.57	138/2500 (5.5%)
1	5	2.23	62/1841 (3.4%)	2.54	136/2500 (5.4%)
1	50	2.19	57/1841 (3.1%)	2.52	141/2500 (5.6%)
1	51	2.19	52/1841 (2.8%)	2.56	150/2500 (6.0%)
1	52	2.23	67/1841 (3.6%)	2.53	125/2500 (5.0%)
1	53	2.24	53/1841 (2.9%)	2.62	165/2500 (6.6%)
1	54	2.27	61/1841 (3.3%)	2.64	168/2500 (6.7%)
1	55	2.22	66/1841 (3.6%)	2.60	152/2500 (6.1%)
1	56	2.26	67/1841 (3.6%)	2.50	124/2500 (5.0%)
1	57	2.21	66/1841 (3.6%)	2.57	152/2500 (6.1%)
1	58	2.25	69/1841 (3.7%)	2.62	147/2500 (5.9%)
1	59	2.25	67/1841 (3.6%)	2.60	164/2500 (6.6%)
1	5A	2.17	51/1841 (2.8%)	2.64	167/2500 (6.7%)
1	5B	2.18	60/1841 (3.3%)	2.60	142/2500 (5.7%)
1	5C	2.26	62/1841 (3.4%)	2.63	167/2500 (6.7%)
1	5D	2.16	54/1841 (2.9%)	2.58	158/2500 (6.3%)
1	5E	2.19	65/1841 (3.5%)	2.61	152/2500 (6.1%)
1	5F	2.20	56/1841 (3.0%)	2.55	137/2500 (5.5%)
1	5G	2.20	60/1841 (3.3%)	2.61	167/2500 (6.7%)
1	5H	2.22	57/1841 (3.1%)	2.60	139/2500 (5.6%)
1	5I	2.21	64/1841 (3.5%)	2.64	153/2500 (6.1%)
1	5J	2.18	51/1841 (2.8%)	2.60	142/2500 (5.7%)
1	5K	2.22	55/1841 (3.0%)	2.60	145/2500 (5.8%)
1	5L	2.24	66/1841 (3.6%)	2.58	171/2500 (6.8%)
1	5M	2.13	48/1841 (2.6%)	2.56	152/2500 (6.1%)
1	5N	2.10	41/1841 (2.2%)	2.64	150/2500 (6.0%)
1	5O	2.20	47/1841 (2.6%)	2.61	157/2500 (6.3%)
1	5P	2.24	61/1841 (3.3%)	2.57	151/2500 (6.0%)
1	5Q	2.15	59/1841 (3.2%)	2.66	169/2500 (6.8%)
1	5R	2.14	53/1841 (2.9%)	2.61	175/2500 (7.0%)
1	5S	2.18	57/1841 (3.1%)	2.64	172/2500 (6.9%)
1	5T	2.25	65/1841 (3.5%)	2.65	161/2500 (6.4%)
1	5U	2.19	61/1841 (3.3%)	2.52	134/2500 (5.4%)
1	5V	2.20	59/1841 (3.2%)	2.66	178/2500 (7.1%)
1	5W	2.27	65/1841 (3.5%)	2.61	145/2500 (5.8%)
1	5X	2.12	41/1841 (2.2%)	2.63	165/2500 (6.6%)
1	5Y	2.26	73/1841 (4.0%)	2.59	147/2500 (5.9%)
1	5Z	2.21	55/1841 (3.0%)	2.58	154/2500 (6.2%)
1	5a	2.22	65/1841 (3.5%)	2.58	148/2500 (5.9%)
1	5b	2.21	74/1841 (4.0%)	2.53	152/2500 (6.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	5c	2.25	66/1841 (3.6%)	2.61	160/2500 (6.4%)
1	5d	2.22	59/1841 (3.2%)	2.59	158/2500 (6.3%)
1	5e	2.12	51/1841 (2.8%)	2.55	140/2500 (5.6%)
1	5f	2.27	72/1841 (3.9%)	2.59	169/2500 (6.8%)
1	5g	2.23	57/1841 (3.1%)	2.56	134/2500 (5.4%)
1	5h	2.22	65/1841 (3.5%)	2.58	149/2500 (6.0%)
1	5i	2.14	53/1841 (2.9%)	2.63	163/2500 (6.5%)
1	5j	2.19	62/1841 (3.4%)	2.58	161/2500 (6.4%)
1	5k	2.24	58/1841 (3.2%)	2.58	147/2500 (5.9%)
1	5l	2.28	70/1841 (3.8%)	2.64	166/2500 (6.6%)
1	5m	2.21	63/1841 (3.4%)	2.58	123/2500 (4.9%)
1	5n	2.22	54/1841 (2.9%)	2.55	141/2500 (5.6%)
1	5o	2.15	54/1841 (2.9%)	2.53	134/2500 (5.4%)
1	5p	2.23	65/1841 (3.5%)	2.52	133/2500 (5.3%)
1	5q	2.17	53/1841 (2.9%)	2.61	167/2500 (6.7%)
1	5r	2.17	46/1841 (2.5%)	2.61	159/2500 (6.4%)
1	5s	2.18	52/1841 (2.8%)	2.63	150/2500 (6.0%)
1	5t	2.28	77/1841 (4.2%)	2.64	150/2500 (6.0%)
1	5u	2.16	56/1841 (3.0%)	2.67	163/2500 (6.5%)
1	5v	2.20	59/1841 (3.2%)	2.56	138/2500 (5.5%)
1	5w	2.21	62/1841 (3.4%)	2.52	134/2500 (5.4%)
1	5x	2.25	66/1841 (3.6%)	2.63	159/2500 (6.4%)
1	5y	2.14	57/1841 (3.1%)	2.65	157/2500 (6.3%)
1	5z	2.26	71/1841 (3.9%)	2.56	146/2500 (5.8%)
1	6	2.26	60/1841 (3.3%)	2.55	152/2500 (6.1%)
1	60	2.22	62/1841 (3.4%)	2.52	140/2500 (5.6%)
1	61	2.14	47/1841 (2.6%)	2.57	162/2500 (6.5%)
1	62	2.19	55/1841 (3.0%)	2.63	176/2500 (7.0%)
1	63	2.24	70/1841 (3.8%)	2.56	145/2500 (5.8%)
1	64	2.22	56/1841 (3.0%)	2.63	166/2500 (6.6%)
1	65	2.23	62/1841 (3.4%)	2.63	151/2500 (6.0%)
1	66	2.16	58/1841 (3.2%)	2.57	140/2500 (5.6%)
1	67	2.20	65/1841 (3.5%)	2.63	167/2500 (6.7%)
1	68	2.20	60/1841 (3.3%)	2.57	146/2500 (5.8%)
1	69	2.16	51/1841 (2.8%)	2.62	158/2500 (6.3%)
1	6A	2.26	63/1841 (3.4%)	2.70	185/2500 (7.4%)
1	6B	2.16	50/1841 (2.7%)	2.65	172/2500 (6.9%)
1	6C	2.16	47/1841 (2.6%)	2.65	147/2500 (5.9%)
1	6D	2.18	47/1841 (2.6%)	2.59	135/2500 (5.4%)
1	6E	2.11	44/1841 (2.4%)	2.66	173/2500 (6.9%)
1	6F	2.24	62/1841 (3.4%)	2.57	144/2500 (5.8%)
1	6G	2.14	50/1841 (2.7%)	2.62	168/2500 (6.7%)
1	6H	2.19	61/1841 (3.3%)	2.57	147/2500 (5.9%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	6I	2.15	48/1841 (2.6%)	2.62	161/2500 (6.4%)
1	6J	2.19	60/1841 (3.3%)	2.60	165/2500 (6.6%)
1	6K	2.14	54/1841 (2.9%)	2.65	150/2500 (6.0%)
1	6L	2.19	43/1841 (2.3%)	2.60	141/2500 (5.6%)
1	6M	2.23	64/1841 (3.5%)	2.61	160/2500 (6.4%)
1	6N	2.17	51/1841 (2.8%)	2.56	139/2500 (5.6%)
1	6O	2.19	57/1841 (3.1%)	2.50	135/2500 (5.4%)
1	6P	2.28	63/1841 (3.4%)	2.59	140/2500 (5.6%)
1	6Q	2.21	65/1841 (3.5%)	2.59	146/2500 (5.8%)
1	6R	2.22	55/1841 (3.0%)	2.64	158/2500 (6.3%)
1	6S	2.16	58/1841 (3.2%)	2.57	153/2500 (6.1%)
1	6T	2.16	55/1841 (3.0%)	2.58	152/2500 (6.1%)
1	6U	2.20	58/1841 (3.2%)	2.55	139/2500 (5.6%)
1	6V	2.17	53/1841 (2.9%)	2.53	123/2500 (4.9%)
1	6W	2.21	64/1841 (3.5%)	2.65	155/2500 (6.2%)
1	6X	2.18	49/1841 (2.7%)	2.57	154/2500 (6.2%)
1	6Y	2.25	62/1841 (3.4%)	2.54	123/2500 (4.9%)
1	6Z	2.12	46/1841 (2.5%)	2.66	167/2500 (6.7%)
1	6a	2.24	64/1841 (3.5%)	2.62	167/2500 (6.7%)
1	6b	2.16	58/1841 (3.2%)	2.59	136/2500 (5.4%)
1	6c	2.20	51/1841 (2.8%)	2.60	147/2500 (5.9%)
1	6d	2.21	61/1841 (3.3%)	2.58	139/2500 (5.6%)
1	6e	2.22	49/1841 (2.7%)	2.61	165/2500 (6.6%)
1	6f	2.20	60/1841 (3.3%)	2.55	139/2500 (5.6%)
1	6g	2.18	61/1841 (3.3%)	2.67	184/2500 (7.4%)
1	6h	2.24	73/1841 (4.0%)	2.64	141/2500 (5.6%)
1	6i	2.17	54/1841 (2.9%)	2.62	159/2500 (6.4%)
1	6j	2.26	71/1841 (3.9%)	2.67	170/2500 (6.8%)
1	6k	2.24	66/1841 (3.6%)	2.60	145/2500 (5.8%)
1	6l	2.23	70/1841 (3.8%)	2.58	146/2500 (5.8%)
1	6m	2.23	56/1841 (3.0%)	2.52	135/2500 (5.4%)
1	6n	2.17	49/1841 (2.7%)	2.65	165/2500 (6.6%)
1	6o	2.22	59/1841 (3.2%)	2.59	146/2500 (5.8%)
1	6p	2.25	62/1841 (3.4%)	2.67	166/2500 (6.6%)
1	6q	2.20	57/1841 (3.1%)	2.53	135/2500 (5.4%)
1	6r	2.20	61/1841 (3.3%)	2.52	144/2500 (5.8%)
1	6s	2.23	62/1841 (3.4%)	2.68	175/2500 (7.0%)
1	6t	2.26	68/1841 (3.7%)	2.62	158/2500 (6.3%)
1	6u	2.25	68/1841 (3.7%)	2.52	136/2500 (5.4%)
1	6v	2.25	62/1841 (3.4%)	2.60	141/2500 (5.6%)
1	6w	2.21	62/1841 (3.4%)	2.61	145/2500 (5.8%)
1	6x	2.16	55/1841 (3.0%)	2.55	140/2500 (5.6%)
1	6y	2.15	55/1841 (3.0%)	2.61	149/2500 (6.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	6z	2.21	54/1841 (2.9%)	2.63	163/2500 (6.5%)
1	7	2.24	69/1841 (3.7%)	2.59	133/2500 (5.3%)
1	70	2.29	68/1841 (3.7%)	2.59	160/2500 (6.4%)
1	71	2.15	54/1841 (2.9%)	2.57	151/2500 (6.0%)
1	72	2.20	59/1841 (3.2%)	2.59	161/2500 (6.4%)
1	73	2.26	71/1841 (3.9%)	2.55	147/2500 (5.9%)
1	74	2.20	52/1841 (2.8%)	2.48	124/2500 (5.0%)
1	75	2.13	55/1841 (3.0%)	2.57	135/2500 (5.4%)
1	76	2.19	63/1841 (3.4%)	2.49	111/2500 (4.4%)
1	77	2.26	66/1841 (3.6%)	2.50	129/2500 (5.2%)
1	78	2.18	59/1841 (3.2%)	2.61	155/2500 (6.2%)
1	79	2.27	65/1841 (3.5%)	2.57	138/2500 (5.5%)
1	7A	2.21	55/1841 (3.0%)	2.57	173/2500 (6.9%)
1	7B	2.19	62/1841 (3.4%)	2.67	156/2500 (6.2%)
1	7C	2.18	56/1841 (3.0%)	2.62	158/2500 (6.3%)
1	7D	2.23	56/1841 (3.0%)	2.64	168/2500 (6.7%)
1	7E	2.25	57/1841 (3.1%)	2.67	182/2500 (7.3%)
1	7F	2.17	57/1841 (3.1%)	2.53	139/2500 (5.6%)
1	7G	2.20	47/1841 (2.6%)	2.56	142/2500 (5.7%)
1	7H	2.21	67/1841 (3.6%)	2.62	164/2500 (6.6%)
1	7I	2.17	51/1841 (2.8%)	2.52	135/2500 (5.4%)
1	7J	2.22	60/1841 (3.3%)	2.59	147/2500 (5.9%)
1	7K	2.25	70/1841 (3.8%)	2.65	164/2500 (6.6%)
1	7L	2.14	45/1841 (2.4%)	2.58	151/2500 (6.0%)
1	7M	2.29	62/1841 (3.4%)	2.64	157/2500 (6.3%)
1	7N	2.32	68/1841 (3.7%)	2.51	135/2500 (5.4%)
1	7O	2.20	61/1841 (3.3%)	2.59	138/2500 (5.5%)
1	7P	2.26	64/1841 (3.5%)	2.58	161/2500 (6.4%)
1	7Q	2.19	55/1841 (3.0%)	2.60	171/2500 (6.8%)
1	7R	2.22	62/1841 (3.4%)	2.61	156/2500 (6.2%)
1	7S	2.19	56/1841 (3.0%)	2.62	161/2500 (6.4%)
1	7T	2.20	54/1841 (2.9%)	2.54	129/2500 (5.2%)
1	7U	2.16	65/1841 (3.5%)	2.57	146/2500 (5.8%)
1	7V	2.24	70/1841 (3.8%)	2.59	144/2500 (5.8%)
1	7W	2.17	50/1841 (2.7%)	2.64	150/2500 (6.0%)
1	7X	2.27	68/1841 (3.7%)	2.49	113/2500 (4.5%)
1	7Y	2.14	50/1841 (2.7%)	2.63	168/2500 (6.7%)
1	7Z	2.19	52/1841 (2.8%)	2.68	171/2500 (6.8%)
1	7a	2.17	54/1841 (2.9%)	2.60	168/2500 (6.7%)
1	7b	2.25	61/1841 (3.3%)	2.63	153/2500 (6.1%)
1	7c	2.14	46/1841 (2.5%)	2.61	171/2500 (6.8%)
1	7d	2.25	51/1841 (2.8%)	2.61	163/2500 (6.5%)
1	7e	2.17	53/1841 (2.9%)	2.60	142/2500 (5.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	7f	2.17	66/1841 (3.6%)	2.54	137/2500 (5.5%)
1	7g	2.20	59/1841 (3.2%)	2.64	158/2500 (6.3%)
1	7h	2.15	44/1841 (2.4%)	2.60	162/2500 (6.5%)
1	7i	2.19	55/1841 (3.0%)	2.57	141/2500 (5.6%)
1	7j	2.17	58/1841 (3.2%)	2.64	166/2500 (6.6%)
1	7k	2.21	68/1841 (3.7%)	2.58	157/2500 (6.3%)
1	7l	2.15	61/1841 (3.3%)	2.66	160/2500 (6.4%)
1	7m	2.22	67/1841 (3.6%)	2.66	177/2500 (7.1%)
1	7n	2.16	47/1841 (2.6%)	2.59	158/2500 (6.3%)
1	7o	2.19	52/1841 (2.8%)	2.61	166/2500 (6.6%)
1	7p	2.13	56/1841 (3.0%)	2.56	152/2500 (6.1%)
1	7q	2.19	59/1841 (3.2%)	2.61	157/2500 (6.3%)
1	7r	2.14	50/1841 (2.7%)	2.59	134/2500 (5.4%)
1	7s	2.20	58/1841 (3.2%)	2.58	138/2500 (5.5%)
1	7t	2.15	54/1841 (2.9%)	2.63	155/2500 (6.2%)
1	7u	2.20	52/1841 (2.8%)	2.68	174/2500 (7.0%)
1	7v	2.23	62/1841 (3.4%)	2.55	134/2500 (5.4%)
1	7w	2.19	60/1841 (3.3%)	2.64	139/2500 (5.6%)
1	7x	2.18	58/1841 (3.2%)	2.59	158/2500 (6.3%)
1	7y	2.23	51/1841 (2.8%)	2.67	164/2500 (6.6%)
1	7z	2.21	54/1841 (2.9%)	2.54	144/2500 (5.8%)
1	8	2.17	62/1841 (3.4%)	2.59	148/2500 (5.9%)
1	80	2.14	52/1841 (2.8%)	2.55	136/2500 (5.4%)
1	81	2.10	47/1841 (2.6%)	2.58	151/2500 (6.0%)
1	82	2.16	54/1841 (2.9%)	2.61	171/2500 (6.8%)
1	83	2.17	61/1841 (3.3%)	2.62	151/2500 (6.0%)
1	84	2.23	62/1841 (3.4%)	2.60	154/2500 (6.2%)
1	85	2.24	64/1841 (3.5%)	2.64	164/2500 (6.6%)
1	86	2.21	62/1841 (3.4%)	2.63	170/2500 (6.8%)
1	87	2.13	54/1841 (2.9%)	2.63	157/2500 (6.3%)
1	88	2.18	62/1841 (3.4%)	2.58	142/2500 (5.7%)
1	89	2.18	50/1841 (2.7%)	2.58	143/2500 (5.7%)
1	8A	2.20	54/1841 (2.9%)	2.62	154/2500 (6.2%)
1	8B	2.13	49/1841 (2.7%)	2.63	154/2500 (6.2%)
1	8C	2.26	68/1841 (3.7%)	2.60	148/2500 (5.9%)
1	8D	2.20	60/1841 (3.3%)	2.66	170/2500 (6.8%)
1	8E	2.18	53/1841 (2.9%)	2.57	156/2500 (6.2%)
1	8F	2.20	60/1841 (3.3%)	2.49	146/2500 (5.8%)
1	8G	2.20	60/1841 (3.3%)	2.57	133/2500 (5.3%)
1	8H	2.20	58/1841 (3.2%)	2.63	169/2500 (6.8%)
1	8I	2.25	65/1841 (3.5%)	2.52	136/2500 (5.4%)
1	8J	2.22	59/1841 (3.2%)	2.55	163/2500 (6.5%)
1	8K	2.20	58/1841 (3.2%)	2.56	143/2500 (5.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	8L	2.19	57/1841 (3.1%)	2.61	144/2500 (5.8%)
1	8M	2.27	64/1841 (3.5%)	2.62	160/2500 (6.4%)
1	8N	2.26	66/1841 (3.6%)	2.65	174/2500 (7.0%)
1	8O	2.25	69/1841 (3.7%)	2.62	159/2500 (6.4%)
1	8P	2.30	76/1841 (4.1%)	2.59	156/2500 (6.2%)
1	8Q	2.27	67/1841 (3.6%)	2.52	132/2500 (5.3%)
1	8R	2.22	61/1841 (3.3%)	2.63	160/2500 (6.4%)
1	8S	2.18	51/1841 (2.8%)	2.54	134/2500 (5.4%)
1	8T	2.20	57/1841 (3.1%)	2.60	145/2500 (5.8%)
1	8U	2.19	56/1841 (3.0%)	2.66	155/2500 (6.2%)
1	8V	2.21	61/1841 (3.3%)	2.56	147/2500 (5.9%)
1	8W	2.18	57/1841 (3.1%)	2.61	142/2500 (5.7%)
1	8X	2.23	62/1841 (3.4%)	2.66	171/2500 (6.8%)
1	8Y	2.23	65/1841 (3.5%)	2.57	141/2500 (5.6%)
1	8Z	2.16	51/1841 (2.8%)	2.56	146/2500 (5.8%)
1	8a	2.26	57/1841 (3.1%)	2.62	162/2500 (6.5%)
1	8b	2.29	68/1841 (3.7%)	2.57	149/2500 (6.0%)
1	8c	2.16	47/1841 (2.6%)	2.54	151/2500 (6.0%)
1	8d	2.18	53/1841 (2.9%)	2.59	155/2500 (6.2%)
1	8e	2.23	66/1841 (3.6%)	2.54	133/2500 (5.3%)
1	8f	2.17	52/1841 (2.8%)	2.55	126/2500 (5.0%)
1	8g	2.22	62/1841 (3.4%)	2.55	139/2500 (5.6%)
1	8h	2.21	58/1841 (3.2%)	2.59	146/2500 (5.8%)
1	8i	2.22	61/1841 (3.3%)	2.59	147/2500 (5.9%)
1	8j	2.22	62/1841 (3.4%)	2.61	161/2500 (6.4%)
1	8k	2.18	57/1841 (3.1%)	2.63	162/2500 (6.5%)
1	8l	2.21	54/1841 (2.9%)	2.65	170/2500 (6.8%)
1	8m	2.17	60/1841 (3.3%)	2.61	162/2500 (6.5%)
1	8n	2.18	55/1841 (3.0%)	2.60	149/2500 (6.0%)
1	8o	2.20	55/1841 (3.0%)	2.61	162/2500 (6.5%)
1	8p	2.13	42/1841 (2.3%)	2.59	152/2500 (6.1%)
1	8q	2.17	59/1841 (3.2%)	2.60	145/2500 (5.8%)
1	8r	2.14	52/1841 (2.8%)	2.52	120/2500 (4.8%)
1	8s	2.20	50/1841 (2.7%)	2.54	123/2500 (4.9%)
1	8t	2.22	71/1841 (3.9%)	2.64	166/2500 (6.6%)
1	8u	2.19	53/1841 (2.9%)	2.51	139/2500 (5.6%)
1	8v	2.19	50/1841 (2.7%)	2.60	140/2500 (5.6%)
1	8w	2.16	58/1841 (3.2%)	2.54	148/2500 (5.9%)
1	8x	2.19	54/1841 (2.9%)	2.59	157/2500 (6.3%)
1	8y	2.24	64/1841 (3.5%)	2.59	136/2500 (5.4%)
1	8z	2.25	67/1841 (3.6%)	2.63	153/2500 (6.1%)
1	9	2.22	57/1841 (3.1%)	2.57	142/2500 (5.7%)
1	90	2.26	59/1841 (3.2%)	2.60	147/2500 (5.9%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	91	2.16	50/1841 (2.7%)	2.64	159/2500 (6.4%)
1	92	2.18	56/1841 (3.0%)	2.61	155/2500 (6.2%)
1	93	2.23	53/1841 (2.9%)	2.62	146/2500 (5.8%)
1	94	2.20	62/1841 (3.4%)	2.64	157/2500 (6.3%)
1	95	2.19	51/1841 (2.8%)	2.68	160/2500 (6.4%)
1	96	2.25	66/1841 (3.6%)	2.68	178/2500 (7.1%)
1	97	2.18	58/1841 (3.2%)	2.54	141/2500 (5.6%)
1	98	2.22	55/1841 (3.0%)	2.63	149/2500 (6.0%)
1	99	2.21	52/1841 (2.8%)	2.51	124/2500 (5.0%)
1	9A	2.07	39/1841 (2.1%)	2.50	138/2500 (5.5%)
1	9B	2.22	61/1841 (3.3%)	2.61	155/2500 (6.2%)
1	9C	2.22	53/1841 (2.9%)	2.58	140/2500 (5.6%)
1	9D	2.14	56/1841 (3.0%)	2.62	139/2500 (5.6%)
1	9E	2.22	63/1841 (3.4%)	2.60	151/2500 (6.0%)
1	9F	2.23	63/1841 (3.4%)	2.55	136/2500 (5.4%)
1	9G	2.17	58/1841 (3.2%)	2.63	171/2500 (6.8%)
1	9H	2.25	69/1841 (3.7%)	2.66	175/2500 (7.0%)
1	9I	2.26	62/1841 (3.4%)	2.54	148/2500 (5.9%)
1	9J	2.16	52/1841 (2.8%)	2.61	158/2500 (6.3%)
1	9K	2.14	49/1841 (2.7%)	2.65	166/2500 (6.6%)
1	9L	2.25	62/1841 (3.4%)	2.54	142/2500 (5.7%)
1	9M	2.17	50/1841 (2.7%)	2.58	139/2500 (5.6%)
1	9N	2.23	51/1841 (2.8%)	2.67	182/2500 (7.3%)
1	9O	2.24	58/1841 (3.2%)	2.64	166/2500 (6.6%)
1	9P	2.22	60/1841 (3.3%)	2.56	161/2500 (6.4%)
1	9Q	2.27	67/1841 (3.6%)	2.52	119/2500 (4.8%)
1	9R	2.20	61/1841 (3.3%)	2.54	148/2500 (5.9%)
1	9S	2.26	79/1841 (4.3%)	2.63	162/2500 (6.5%)
1	9T	2.21	56/1841 (3.0%)	2.54	126/2500 (5.0%)
1	9U	2.26	70/1841 (3.8%)	2.58	157/2500 (6.3%)
1	9V	2.25	56/1841 (3.0%)	2.54	142/2500 (5.7%)
1	9W	2.22	57/1841 (3.1%)	2.57	142/2500 (5.7%)
1	9X	2.18	62/1841 (3.4%)	2.64	157/2500 (6.3%)
1	9Y	2.22	58/1841 (3.2%)	2.60	156/2500 (6.2%)
1	9Z	2.20	63/1841 (3.4%)	2.69	188/2500 (7.5%)
1	9a	2.17	54/1841 (2.9%)	2.60	154/2500 (6.2%)
1	9b	2.19	53/1841 (2.9%)	2.52	146/2500 (5.8%)
1	9c	2.18	51/1841 (2.8%)	2.65	160/2500 (6.4%)
1	9d	2.21	61/1841 (3.3%)	2.65	170/2500 (6.8%)
1	9e	2.24	63/1841 (3.4%)	2.61	154/2500 (6.2%)
1	9f	2.15	55/1841 (3.0%)	2.57	157/2500 (6.3%)
1	9g	2.18	68/1841 (3.7%)	2.58	157/2500 (6.3%)
1	9h	2.21	53/1841 (2.9%)	2.56	142/2500 (5.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	9i	2.23	58/1841 (3.2%)	2.57	173/2500 (6.9%)
1	9j	2.20	59/1841 (3.2%)	2.65	187/2500 (7.5%)
1	9k	2.25	61/1841 (3.3%)	2.64	153/2500 (6.1%)
1	9l	2.17	58/1841 (3.2%)	2.56	144/2500 (5.8%)
1	9m	2.19	63/1841 (3.4%)	2.62	145/2500 (5.8%)
1	9n	2.23	62/1841 (3.4%)	2.53	130/2500 (5.2%)
1	9o	2.22	57/1841 (3.1%)	2.56	150/2500 (6.0%)
1	9p	2.26	60/1841 (3.3%)	2.54	142/2500 (5.7%)
1	9q	2.15	53/1841 (2.9%)	2.60	150/2500 (6.0%)
1	9r	2.17	50/1841 (2.7%)	2.61	164/2500 (6.6%)
1	9s	2.28	75/1841 (4.1%)	2.60	143/2500 (5.7%)
1	9t	2.26	66/1841 (3.6%)	2.63	162/2500 (6.5%)
1	9u	2.18	49/1841 (2.7%)	2.61	156/2500 (6.2%)
1	9v	2.20	57/1841 (3.1%)	2.55	139/2500 (5.6%)
1	9w	2.24	67/1841 (3.6%)	2.59	156/2500 (6.2%)
1	9x	2.21	52/1841 (2.8%)	2.55	138/2500 (5.5%)
1	9y	2.17	51/1841 (2.8%)	2.68	173/2500 (6.9%)
1	9z	2.26	65/1841 (3.5%)	2.58	163/2500 (6.5%)
1	A	2.18	52/1841 (2.8%)	2.59	151/2500 (6.0%)
1	B	2.17	59/1841 (3.2%)	2.55	133/2500 (5.3%)
1	C	2.21	64/1841 (3.5%)	2.70	198/2500 (7.9%)
1	D	2.22	66/1841 (3.6%)	2.53	145/2500 (5.8%)
1	E	2.16	52/1841 (2.8%)	2.52	140/2500 (5.6%)
1	F	2.24	68/1841 (3.7%)	2.55	160/2500 (6.4%)
1	G	2.16	54/1841 (2.9%)	2.53	124/2500 (5.0%)
1	H	2.22	54/1841 (2.9%)	2.62	156/2500 (6.2%)
1	I	2.17	45/1841 (2.4%)	2.49	131/2500 (5.2%)
1	J	2.22	55/1841 (3.0%)	2.50	127/2500 (5.1%)
1	K	2.12	48/1841 (2.6%)	2.56	149/2500 (6.0%)
1	L	2.22	59/1841 (3.2%)	2.47	126/2500 (5.0%)
1	M	2.29	79/1841 (4.3%)	2.61	148/2500 (5.9%)
1	N	2.15	44/1841 (2.4%)	2.68	170/2500 (6.8%)
1	O	2.21	56/1841 (3.0%)	2.70	165/2500 (6.6%)
1	P	2.21	51/1841 (2.8%)	2.62	137/2500 (5.5%)
1	Q	2.21	60/1841 (3.3%)	2.60	146/2500 (5.8%)
1	R	2.29	76/1841 (4.1%)	2.61	153/2500 (6.1%)
1	S	2.25	63/1841 (3.4%)	2.52	133/2500 (5.3%)
1	T	2.24	73/1841 (4.0%)	2.67	156/2500 (6.2%)
1	U	2.14	43/1841 (2.3%)	2.56	131/2500 (5.2%)
1	V	2.25	65/1841 (3.5%)	2.63	170/2500 (6.8%)
1	W	2.17	46/1841 (2.5%)	2.59	154/2500 (6.2%)
1	X	2.20	63/1841 (3.4%)	2.57	138/2500 (5.5%)
1	Y	2.26	66/1841 (3.6%)	2.61	150/2500 (6.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Z	2.25	66/1841 (3.6%)	2.64	160/2500 (6.4%)
1	a	2.14	55/1841 (3.0%)	2.54	139/2500 (5.6%)
1	a0	2.19	55/1841 (3.0%)	2.55	138/2500 (5.5%)
1	a1	2.20	62/1841 (3.4%)	2.64	154/2500 (6.2%)
1	a2	2.18	63/1841 (3.4%)	2.58	151/2500 (6.0%)
1	a3	2.27	71/1841 (3.9%)	2.55	128/2500 (5.1%)
1	a4	2.18	60/1841 (3.3%)	2.60	149/2500 (6.0%)
1	a5	2.21	65/1841 (3.5%)	2.64	155/2500 (6.2%)
1	a6	2.17	43/1841 (2.3%)	2.55	134/2500 (5.4%)
1	a7	2.22	63/1841 (3.4%)	2.57	145/2500 (5.8%)
1	a8	2.24	67/1841 (3.6%)	2.58	149/2500 (6.0%)
1	a9	2.19	54/1841 (2.9%)	2.58	171/2500 (6.8%)
1	aA	2.22	61/1841 (3.3%)	2.58	152/2500 (6.1%)
1	aB	2.23	52/1841 (2.8%)	2.54	142/2500 (5.7%)
1	aC	2.25	60/1841 (3.3%)	2.58	145/2500 (5.8%)
1	aD	2.27	71/1841 (3.9%)	2.56	141/2500 (5.6%)
1	aE	2.24	67/1841 (3.6%)	2.62	157/2500 (6.3%)
1	aF	2.20	59/1841 (3.2%)	2.57	153/2500 (6.1%)
1	aG	2.26	59/1841 (3.2%)	2.57	148/2500 (5.9%)
1	aH	2.16	48/1841 (2.6%)	2.59	156/2500 (6.2%)
1	aI	2.21	64/1841 (3.5%)	2.68	161/2500 (6.4%)
1	aJ	2.19	52/1841 (2.8%)	2.59	132/2500 (5.3%)
1	aK	2.23	56/1841 (3.0%)	2.64	162/2500 (6.5%)
1	aL	2.24	66/1841 (3.6%)	2.65	155/2500 (6.2%)
1	aM	2.17	53/1841 (2.9%)	2.56	141/2500 (5.6%)
1	aN	2.19	60/1841 (3.3%)	2.59	145/2500 (5.8%)
1	aO	2.26	72/1841 (3.9%)	2.57	132/2500 (5.3%)
1	aP	2.19	62/1841 (3.4%)	2.56	141/2500 (5.6%)
1	aQ	2.19	47/1841 (2.6%)	2.62	164/2500 (6.6%)
1	aR	2.16	51/1841 (2.8%)	2.59	145/2500 (5.8%)
1	aS	2.21	47/1841 (2.6%)	2.53	140/2500 (5.6%)
1	aT	2.27	71/1841 (3.9%)	2.60	146/2500 (5.8%)
1	aU	2.14	51/1841 (2.8%)	2.66	171/2500 (6.8%)
1	aV	2.30	58/1841 (3.2%)	2.64	163/2500 (6.5%)
1	aW	2.25	62/1841 (3.4%)	2.67	175/2500 (7.0%)
1	aX	2.27	62/1841 (3.4%)	2.58	160/2500 (6.4%)
1	aY	2.12	47/1841 (2.6%)	2.57	159/2500 (6.4%)
1	aZ	2.19	56/1841 (3.0%)	2.53	147/2500 (5.9%)
1	aa	2.27	65/1841 (3.5%)	2.53	142/2500 (5.7%)
1	ab	2.23	62/1841 (3.4%)	2.68	177/2500 (7.1%)
1	ac	2.17	44/1841 (2.4%)	2.56	146/2500 (5.8%)
1	ad	2.23	64/1841 (3.5%)	2.61	145/2500 (5.8%)
1	ae	2.23	63/1841 (3.4%)	2.65	163/2500 (6.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	af	2.24	57/1841 (3.1%)	2.53	131/2500 (5.2%)
1	ag	2.20	63/1841 (3.4%)	2.55	135/2500 (5.4%)
1	ah	2.26	58/1841 (3.2%)	2.64	165/2500 (6.6%)
1	ai	2.12	55/1841 (3.0%)	2.59	141/2500 (5.6%)
1	aj	2.25	67/1841 (3.6%)	2.59	147/2500 (5.9%)
1	ak	2.20	63/1841 (3.4%)	2.71	187/2500 (7.5%)
1	al	2.17	51/1841 (2.8%)	2.57	137/2500 (5.5%)
1	am	2.22	59/1841 (3.2%)	2.55	131/2500 (5.2%)
1	an	2.26	65/1841 (3.5%)	2.57	155/2500 (6.2%)
1	ao	2.18	59/1841 (3.2%)	2.51	145/2500 (5.8%)
1	ap	2.19	51/1841 (2.8%)	2.61	166/2500 (6.6%)
1	aq	2.19	65/1841 (3.5%)	2.65	169/2500 (6.8%)
1	ar	2.25	68/1841 (3.7%)	2.59	148/2500 (5.9%)
1	as	2.21	55/1841 (3.0%)	2.57	163/2500 (6.5%)
1	at	2.22	63/1841 (3.4%)	2.62	164/2500 (6.6%)
1	au	2.26	55/1841 (3.0%)	2.68	175/2500 (7.0%)
1	av	2.22	54/1841 (2.9%)	2.54	123/2500 (4.9%)
1	aw	2.20	57/1841 (3.1%)	2.63	144/2500 (5.8%)
1	ax	2.23	63/1841 (3.4%)	2.60	160/2500 (6.4%)
1	ay	2.23	63/1841 (3.4%)	2.49	123/2500 (4.9%)
1	az	2.20	61/1841 (3.3%)	2.55	132/2500 (5.3%)
1	b	2.13	41/1841 (2.2%)	2.61	154/2500 (6.2%)
1	b0	2.22	60/1841 (3.3%)	2.67	171/2500 (6.8%)
1	b1	2.21	62/1841 (3.4%)	2.56	134/2500 (5.4%)
1	b2	2.18	49/1841 (2.7%)	2.51	122/2500 (4.9%)
1	b3	2.21	60/1841 (3.3%)	2.60	166/2500 (6.6%)
1	b4	2.17	56/1841 (3.0%)	2.54	139/2500 (5.6%)
1	b5	2.23	60/1841 (3.3%)	2.55	145/2500 (5.8%)
1	b6	2.22	60/1841 (3.3%)	2.52	126/2500 (5.0%)
1	b7	2.24	66/1841 (3.6%)	2.57	152/2500 (6.1%)
1	b8	2.20	62/1841 (3.4%)	2.65	171/2500 (6.8%)
1	b9	2.22	67/1841 (3.6%)	2.56	119/2500 (4.8%)
1	bA	2.22	63/1841 (3.4%)	2.61	163/2500 (6.5%)
1	bB	2.17	51/1841 (2.8%)	2.65	149/2500 (6.0%)
1	bC	2.18	50/1841 (2.7%)	2.63	159/2500 (6.4%)
1	bD	2.18	56/1841 (3.0%)	2.55	149/2500 (6.0%)
1	bE	2.22	68/1841 (3.7%)	2.61	152/2500 (6.1%)
1	bF	2.18	50/1841 (2.7%)	2.57	143/2500 (5.7%)
1	bG	2.20	59/1841 (3.2%)	2.60	155/2500 (6.2%)
1	bH	2.24	68/1841 (3.7%)	2.63	150/2500 (6.0%)
1	bI	2.20	47/1841 (2.6%)	2.52	134/2500 (5.4%)
1	bJ	2.23	65/1841 (3.5%)	2.59	134/2500 (5.4%)
1	bK	2.16	49/1841 (2.7%)	2.56	144/2500 (5.8%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	bL	2.20	56/1841 (3.0%)	2.49	124/2500 (5.0%)
1	bM	2.29	77/1841 (4.2%)	2.57	151/2500 (6.0%)
1	bN	2.22	54/1841 (2.9%)	2.57	145/2500 (5.8%)
1	bO	2.27	59/1841 (3.2%)	2.58	137/2500 (5.5%)
1	bP	2.21	59/1841 (3.2%)	2.61	154/2500 (6.2%)
1	bQ	2.24	55/1841 (3.0%)	2.54	151/2500 (6.0%)
1	bR	2.25	73/1841 (4.0%)	2.62	154/2500 (6.2%)
1	bS	2.19	51/1841 (2.8%)	2.57	148/2500 (5.9%)
1	bT	2.26	68/1841 (3.7%)	2.63	149/2500 (6.0%)
1	bU	2.23	60/1841 (3.3%)	2.55	138/2500 (5.5%)
1	bV	2.21	48/1841 (2.6%)	2.57	154/2500 (6.2%)
1	bW	2.16	60/1841 (3.3%)	2.62	158/2500 (6.3%)
1	bX	2.19	56/1841 (3.0%)	2.56	138/2500 (5.5%)
1	bY	2.23	67/1841 (3.6%)	2.66	181/2500 (7.2%)
1	bZ	2.14	43/1841 (2.3%)	2.57	139/2500 (5.6%)
1	ba	2.27	68/1841 (3.7%)	2.65	164/2500 (6.6%)
1	bb	2.17	57/1841 (3.1%)	2.59	162/2500 (6.5%)
1	bc	2.21	48/1841 (2.6%)	2.62	156/2500 (6.2%)
1	bd	2.23	57/1841 (3.1%)	2.61	161/2500 (6.4%)
1	be	2.15	46/1841 (2.5%)	2.61	156/2500 (6.2%)
1	bf	2.16	49/1841 (2.7%)	2.70	186/2500 (7.4%)
1	bg	2.24	66/1841 (3.6%)	2.59	154/2500 (6.2%)
1	bh	2.25	72/1841 (3.9%)	2.55	140/2500 (5.6%)
1	bi	2.22	56/1841 (3.0%)	2.73	170/2500 (6.8%)
1	bj	2.17	45/1841 (2.4%)	2.55	137/2500 (5.5%)
1	bk	2.25	63/1841 (3.4%)	2.56	140/2500 (5.6%)
1	bl	2.18	56/1841 (3.0%)	2.56	133/2500 (5.3%)
1	bm	2.23	68/1841 (3.7%)	2.57	137/2500 (5.5%)
1	bn	2.26	70/1841 (3.8%)	2.55	142/2500 (5.7%)
1	bo	2.18	55/1841 (3.0%)	2.58	140/2500 (5.6%)
1	bp	2.18	46/1841 (2.5%)	2.60	138/2500 (5.5%)
1	bq	2.20	57/1841 (3.1%)	2.57	148/2500 (5.9%)
1	br	2.19	54/1841 (2.9%)	2.59	158/2500 (6.3%)
1	bs	2.26	67/1841 (3.6%)	2.57	145/2500 (5.8%)
1	bt	2.19	64/1841 (3.5%)	2.48	107/2500 (4.3%)
1	bu	2.28	73/1841 (4.0%)	2.57	143/2500 (5.7%)
1	bv	2.22	62/1841 (3.4%)	2.66	156/2500 (6.2%)
1	bw	2.22	62/1841 (3.4%)	2.61	169/2500 (6.8%)
1	bx	2.26	70/1841 (3.8%)	2.62	163/2500 (6.5%)
1	by	2.14	47/1841 (2.6%)	2.53	143/2500 (5.7%)
1	bz	2.20	67/1841 (3.6%)	2.53	140/2500 (5.6%)
1	c	2.22	61/1841 (3.3%)	2.65	158/2500 (6.3%)
1	c0	2.18	48/1841 (2.6%)	2.53	139/2500 (5.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	c1	2.21	46/1841 (2.5%)	2.60	163/2500 (6.5%)
1	c2	2.31	76/1841 (4.1%)	2.63	168/2500 (6.7%)
1	c3	2.24	69/1841 (3.7%)	2.67	170/2500 (6.8%)
1	c4	2.26	68/1841 (3.7%)	2.51	132/2500 (5.3%)
1	c5	2.28	63/1841 (3.4%)	2.69	175/2500 (7.0%)
1	c6	2.21	52/1841 (2.8%)	2.59	134/2500 (5.4%)
1	c7	2.18	57/1841 (3.1%)	2.59	157/2500 (6.3%)
1	c8	2.21	64/1841 (3.5%)	2.64	168/2500 (6.7%)
1	c9	2.32	68/1841 (3.7%)	2.60	150/2500 (6.0%)
1	cA	2.18	54/1841 (2.9%)	2.59	147/2500 (5.9%)
1	cB	2.19	63/1841 (3.4%)	2.53	146/2500 (5.8%)
1	cC	2.17	50/1841 (2.7%)	2.65	155/2500 (6.2%)
1	cD	2.14	54/1841 (2.9%)	2.64	167/2500 (6.7%)
1	cE	2.18	54/1841 (2.9%)	2.65	165/2500 (6.6%)
1	cF	2.18	61/1841 (3.3%)	2.63	151/2500 (6.0%)
1	cG	2.16	52/1841 (2.8%)	2.54	126/2500 (5.0%)
1	cH	2.15	62/1841 (3.4%)	2.56	136/2500 (5.4%)
1	cI	2.20	56/1841 (3.0%)	2.56	147/2500 (5.9%)
1	cJ	2.17	52/1841 (2.8%)	2.58	156/2500 (6.2%)
1	cK	2.29	72/1841 (3.9%)	2.60	162/2500 (6.5%)
1	cL	2.17	54/1841 (2.9%)	2.55	135/2500 (5.4%)
1	cM	2.26	70/1841 (3.8%)	2.59	152/2500 (6.1%)
1	cN	2.14	52/1841 (2.8%)	2.58	138/2500 (5.5%)
1	cO	2.17	50/1841 (2.7%)	2.69	180/2500 (7.2%)
1	cP	2.20	55/1841 (3.0%)	2.56	141/2500 (5.6%)
1	cQ	2.13	50/1841 (2.7%)	2.67	185/2500 (7.4%)
1	cR	2.21	67/1841 (3.6%)	2.63	165/2500 (6.6%)
1	cS	2.22	64/1841 (3.5%)	2.61	147/2500 (5.9%)
1	cT	2.19	46/1841 (2.5%)	2.57	139/2500 (5.6%)
1	cU	2.19	62/1841 (3.4%)	2.57	157/2500 (6.3%)
1	cV	2.22	62/1841 (3.4%)	2.49	129/2500 (5.2%)
1	cW	2.15	59/1841 (3.2%)	2.67	162/2500 (6.5%)
1	cX	2.18	51/1841 (2.8%)	2.61	161/2500 (6.4%)
1	cY	2.18	63/1841 (3.4%)	2.54	159/2500 (6.4%)
1	cZ	2.25	64/1841 (3.5%)	2.56	140/2500 (5.6%)
1	ca	2.24	59/1841 (3.2%)	2.57	141/2500 (5.6%)
1	cb	2.22	57/1841 (3.1%)	2.55	147/2500 (5.9%)
1	cc	2.20	57/1841 (3.1%)	2.57	148/2500 (5.9%)
1	cd	2.23	60/1841 (3.3%)	2.61	154/2500 (6.2%)
1	ce	2.25	62/1841 (3.4%)	2.62	157/2500 (6.3%)
1	cf	2.24	71/1841 (3.9%)	2.59	141/2500 (5.6%)
1	cg	2.19	61/1841 (3.3%)	2.57	155/2500 (6.2%)
1	ch	2.18	50/1841 (2.7%)	2.57	149/2500 (6.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	ci	2.23	65/1841 (3.5%)	2.63	150/2500 (6.0%)
1	cj	2.18	57/1841 (3.1%)	2.59	143/2500 (5.7%)
1	ck	2.24	64/1841 (3.5%)	2.52	136/2500 (5.4%)
1	cl	2.29	68/1841 (3.7%)	2.62	153/2500 (6.1%)
1	cm	2.19	54/1841 (2.9%)	2.57	143/2500 (5.7%)
1	cn	2.22	65/1841 (3.5%)	2.52	119/2500 (4.8%)
1	co	2.21	59/1841 (3.2%)	2.68	171/2500 (6.8%)
1	cp	2.21	69/1841 (3.7%)	2.57	153/2500 (6.1%)
1	cq	2.15	62/1841 (3.4%)	2.56	158/2500 (6.3%)
1	cr	2.15	49/1841 (2.7%)	2.61	164/2500 (6.6%)
1	cs	2.17	50/1841 (2.7%)	2.65	170/2500 (6.8%)
1	ct	2.26	78/1841 (4.2%)	2.64	144/2500 (5.8%)
1	cu	2.17	49/1841 (2.7%)	2.60	163/2500 (6.5%)
1	cv	2.15	58/1841 (3.2%)	2.59	152/2500 (6.1%)
1	cw	2.18	66/1841 (3.6%)	2.59	148/2500 (5.9%)
1	cx	2.19	59/1841 (3.2%)	2.52	122/2500 (4.9%)
1	cy	2.25	61/1841 (3.3%)	2.64	166/2500 (6.6%)
1	cz	2.17	52/1841 (2.8%)	2.62	168/2500 (6.7%)
1	d	2.20	60/1841 (3.3%)	2.62	149/2500 (6.0%)
1	d0	2.26	72/1841 (3.9%)	2.54	150/2500 (6.0%)
1	d1	2.22	63/1841 (3.4%)	2.56	146/2500 (5.8%)
1	d2	2.17	56/1841 (3.0%)	2.62	155/2500 (6.2%)
1	d3	2.21	62/1841 (3.4%)	2.60	155/2500 (6.2%)
1	d4	2.25	66/1841 (3.6%)	2.61	161/2500 (6.4%)
1	d5	2.18	54/1841 (2.9%)	2.56	144/2500 (5.8%)
1	d6	2.14	48/1841 (2.6%)	2.61	155/2500 (6.2%)
1	d7	2.18	50/1841 (2.7%)	2.64	165/2500 (6.6%)
1	d8	2.20	59/1841 (3.2%)	2.63	166/2500 (6.6%)
1	d9	2.17	64/1841 (3.5%)	2.59	168/2500 (6.7%)
1	dA	2.20	44/1841 (2.4%)	2.62	155/2500 (6.2%)
1	dB	2.16	52/1841 (2.8%)	2.59	139/2500 (5.6%)
1	dC	2.22	62/1841 (3.4%)	2.68	179/2500 (7.2%)
1	dD	2.28	70/1841 (3.8%)	2.58	160/2500 (6.4%)
1	dE	2.20	56/1841 (3.0%)	2.64	151/2500 (6.0%)
1	dF	2.27	73/1841 (4.0%)	2.57	152/2500 (6.1%)
1	dG	2.22	60/1841 (3.3%)	2.65	170/2500 (6.8%)
1	dH	2.19	64/1841 (3.5%)	2.52	131/2500 (5.2%)
1	dI	2.15	51/1841 (2.8%)	2.61	152/2500 (6.1%)
1	dJ	2.18	63/1841 (3.4%)	2.55	148/2500 (5.9%)
1	dK	2.23	50/1841 (2.7%)	2.62	161/2500 (6.4%)
1	dL	2.21	60/1841 (3.3%)	2.63	166/2500 (6.6%)
1	dM	2.24	58/1841 (3.2%)	2.64	159/2500 (6.4%)
1	dN	2.13	54/1841 (2.9%)	2.48	120/2500 (4.8%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	dO	2.26	65/1841 (3.5%)	2.55	141/2500 (5.6%)
1	dP	2.13	43/1841 (2.3%)	2.54	145/2500 (5.8%)
1	dQ	2.29	66/1841 (3.6%)	2.59	163/2500 (6.5%)
1	dR	2.21	68/1841 (3.7%)	2.60	166/2500 (6.6%)
1	dS	2.12	48/1841 (2.6%)	2.52	131/2500 (5.2%)
1	dT	2.19	61/1841 (3.3%)	2.53	139/2500 (5.6%)
1	dU	2.23	58/1841 (3.2%)	2.55	131/2500 (5.2%)
1	dV	2.14	52/1841 (2.8%)	2.55	135/2500 (5.4%)
1	dW	2.27	64/1841 (3.5%)	2.62	162/2500 (6.5%)
1	dX	2.24	72/1841 (3.9%)	2.53	139/2500 (5.6%)
1	dY	2.19	49/1841 (2.7%)	2.55	155/2500 (6.2%)
1	dZ	2.21	58/1841 (3.2%)	2.52	142/2500 (5.7%)
1	da	2.22	61/1841 (3.3%)	2.47	132/2500 (5.3%)
1	db	2.22	53/1841 (2.9%)	2.61	164/2500 (6.6%)
1	dc	2.17	55/1841 (3.0%)	2.68	184/2500 (7.4%)
1	dd	2.19	64/1841 (3.5%)	2.61	162/2500 (6.5%)
1	de	2.20	56/1841 (3.0%)	2.63	154/2500 (6.2%)
1	df	2.24	61/1841 (3.3%)	2.52	130/2500 (5.2%)
1	dg	2.14	49/1841 (2.7%)	2.66	166/2500 (6.6%)
1	dh	2.19	64/1841 (3.5%)	2.54	126/2500 (5.0%)
1	di	2.21	52/1841 (2.8%)	2.57	149/2500 (6.0%)
1	dj	2.24	63/1841 (3.4%)	2.63	148/2500 (5.9%)
1	dk	2.27	59/1841 (3.2%)	2.60	151/2500 (6.0%)
1	dl	2.12	46/1841 (2.5%)	2.59	138/2500 (5.5%)
1	dm	2.20	64/1841 (3.5%)	2.51	126/2500 (5.0%)
1	dn	2.23	74/1841 (4.0%)	2.60	172/2500 (6.9%)
1	do	2.27	68/1841 (3.7%)	2.58	144/2500 (5.8%)
1	dp	2.21	55/1841 (3.0%)	2.58	154/2500 (6.2%)
1	dq	2.21	60/1841 (3.3%)	2.55	141/2500 (5.6%)
1	dr	2.13	52/1841 (2.8%)	2.60	162/2500 (6.5%)
1	ds	2.17	52/1841 (2.8%)	2.64	174/2500 (7.0%)
1	dt	2.20	59/1841 (3.2%)	2.54	118/2500 (4.7%)
1	du	2.17	46/1841 (2.5%)	2.53	127/2500 (5.1%)
1	dv	2.27	72/1841 (3.9%)	2.57	141/2500 (5.6%)
1	dw	2.27	70/1841 (3.8%)	2.68	165/2500 (6.6%)
1	dx	2.28	73/1841 (4.0%)	2.63	170/2500 (6.8%)
1	dy	2.23	63/1841 (3.4%)	2.60	150/2500 (6.0%)
1	dz	2.19	56/1841 (3.0%)	2.53	140/2500 (5.6%)
1	e	2.24	69/1841 (3.7%)	2.55	150/2500 (6.0%)
1	e0	2.18	50/1841 (2.7%)	2.60	161/2500 (6.4%)
1	e1	2.21	57/1841 (3.1%)	2.63	161/2500 (6.4%)
1	e2	2.19	55/1841 (3.0%)	2.60	152/2500 (6.1%)
1	e3	2.13	54/1841 (2.9%)	2.60	146/2500 (5.8%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	e4	2.16	59/1841 (3.2%)	2.57	139/2500 (5.6%)
1	e5	2.22	59/1841 (3.2%)	2.63	152/2500 (6.1%)
1	e6	2.16	50/1841 (2.7%)	2.57	147/2500 (5.9%)
1	e7	2.19	51/1841 (2.8%)	2.57	145/2500 (5.8%)
1	e8	2.19	54/1841 (2.9%)	2.64	168/2500 (6.7%)
1	e9	2.22	52/1841 (2.8%)	2.54	127/2500 (5.1%)
1	eA	2.22	61/1841 (3.3%)	2.54	134/2500 (5.4%)
1	eB	2.18	61/1841 (3.3%)	2.62	151/2500 (6.0%)
1	eC	2.23	67/1841 (3.6%)	2.59	145/2500 (5.8%)
1	eD	2.24	63/1841 (3.4%)	2.54	138/2500 (5.5%)
1	eE	2.22	61/1841 (3.3%)	2.60	151/2500 (6.0%)
1	eF	2.17	46/1841 (2.5%)	2.52	131/2500 (5.2%)
1	eG	2.17	57/1841 (3.1%)	2.50	131/2500 (5.2%)
1	eH	2.18	57/1841 (3.1%)	2.62	161/2500 (6.4%)
1	eI	2.23	64/1841 (3.5%)	2.59	160/2500 (6.4%)
1	eJ	2.21	56/1841 (3.0%)	2.56	151/2500 (6.0%)
1	eK	2.24	66/1841 (3.6%)	2.61	151/2500 (6.0%)
1	eL	2.30	73/1841 (4.0%)	2.61	153/2500 (6.1%)
1	eM	2.29	74/1841 (4.0%)	2.67	155/2500 (6.2%)
1	eN	2.17	50/1841 (2.7%)	2.57	132/2500 (5.3%)
1	eO	2.21	64/1841 (3.5%)	2.55	138/2500 (5.5%)
1	eP	2.18	61/1841 (3.3%)	2.60	166/2500 (6.6%)
1	eQ	2.13	46/1841 (2.5%)	2.55	141/2500 (5.6%)
1	eR	2.24	56/1841 (3.0%)	2.67	154/2500 (6.2%)
1	eS	2.16	49/1841 (2.7%)	2.70	172/2500 (6.9%)
1	eT	2.26	70/1841 (3.8%)	2.57	139/2500 (5.6%)
1	eU	2.16	60/1841 (3.3%)	2.64	166/2500 (6.6%)
1	eV	2.20	55/1841 (3.0%)	2.61	137/2500 (5.5%)
1	eW	2.18	57/1841 (3.1%)	2.56	139/2500 (5.6%)
1	eX	2.20	56/1841 (3.0%)	2.61	158/2500 (6.3%)
1	eY	2.21	65/1841 (3.5%)	2.52	134/2500 (5.4%)
1	eZ	2.24	68/1841 (3.7%)	2.65	165/2500 (6.6%)
1	ea	2.18	63/1841 (3.4%)	2.64	159/2500 (6.4%)
1	eb	2.17	64/1841 (3.5%)	2.62	155/2500 (6.2%)
1	ec	2.18	54/1841 (2.9%)	2.66	150/2500 (6.0%)
1	ed	2.21	56/1841 (3.0%)	2.61	147/2500 (5.9%)
1	ee	2.13	42/1841 (2.3%)	2.61	144/2500 (5.8%)
1	ef	2.26	70/1841 (3.8%)	2.68	168/2500 (6.7%)
1	eg	2.17	53/1841 (2.9%)	2.56	144/2500 (5.8%)
1	eh	2.20	59/1841 (3.2%)	2.54	149/2500 (6.0%)
1	ei	2.14	52/1841 (2.8%)	2.63	151/2500 (6.0%)
1	ej	2.20	61/1841 (3.3%)	2.59	154/2500 (6.2%)
1	ek	2.16	58/1841 (3.2%)	2.61	141/2500 (5.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	el	2.24	67/1841 (3.6%)	2.51	133/2500 (5.3%)
1	em	2.27	67/1841 (3.6%)	2.62	151/2500 (6.0%)
1	en	2.18	67/1841 (3.6%)	2.58	149/2500 (6.0%)
1	eo	2.24	66/1841 (3.6%)	2.60	164/2500 (6.6%)
1	ep	2.21	56/1841 (3.0%)	2.63	152/2500 (6.1%)
1	eq	2.16	58/1841 (3.2%)	2.60	144/2500 (5.8%)
1	er	2.19	61/1841 (3.3%)	2.69	173/2500 (6.9%)
1	es	2.28	78/1841 (4.2%)	2.65	164/2500 (6.6%)
1	et	2.19	55/1841 (3.0%)	2.58	147/2500 (5.9%)
1	eu	2.24	66/1841 (3.6%)	2.52	145/2500 (5.8%)
1	ev	2.26	64/1841 (3.5%)	2.60	152/2500 (6.1%)
1	ew	2.16	54/1841 (2.9%)	2.55	147/2500 (5.9%)
1	ex	2.16	50/1841 (2.7%)	2.55	134/2500 (5.4%)
1	ey	2.18	55/1841 (3.0%)	2.59	148/2500 (5.9%)
1	ez	2.18	47/1841 (2.6%)	2.53	134/2500 (5.4%)
1	f	2.16	51/1841 (2.8%)	2.60	148/2500 (5.9%)
1	f0	2.20	60/1841 (3.3%)	2.54	131/2500 (5.2%)
1	f1	2.21	59/1841 (3.2%)	2.60	158/2500 (6.3%)
1	f2	2.25	64/1841 (3.5%)	2.57	150/2500 (6.0%)
1	f3	2.24	58/1841 (3.2%)	2.59	142/2500 (5.7%)
1	f4	2.26	61/1841 (3.3%)	2.57	137/2500 (5.5%)
1	f5	2.21	65/1841 (3.5%)	2.60	148/2500 (5.9%)
1	f6	2.27	63/1841 (3.4%)	2.57	158/2500 (6.3%)
1	f7	2.28	75/1841 (4.1%)	2.65	172/2500 (6.9%)
1	f8	2.20	64/1841 (3.5%)	2.53	142/2500 (5.7%)
1	f9	2.24	58/1841 (3.2%)	2.63	152/2500 (6.1%)
1	fA	2.23	62/1841 (3.4%)	2.62	161/2500 (6.4%)
1	fB	2.21	51/1841 (2.8%)	2.61	144/2500 (5.8%)
1	fC	2.23	61/1841 (3.3%)	2.66	159/2500 (6.4%)
1	fD	2.31	75/1841 (4.1%)	2.53	122/2500 (4.9%)
1	fE	2.26	64/1841 (3.5%)	2.58	143/2500 (5.7%)
1	fF	2.18	45/1841 (2.4%)	2.59	152/2500 (6.1%)
1	fG	2.22	60/1841 (3.3%)	2.52	145/2500 (5.8%)
1	fH	2.14	51/1841 (2.8%)	2.51	116/2500 (4.6%)
1	fI	2.25	70/1841 (3.8%)	2.56	150/2500 (6.0%)
1	fJ	2.17	52/1841 (2.8%)	2.60	148/2500 (5.9%)
1	fK	2.16	55/1841 (3.0%)	2.56	143/2500 (5.7%)
1	fL	2.23	56/1841 (3.0%)	2.58	142/2500 (5.7%)
1	fM	2.18	61/1841 (3.3%)	2.53	148/2500 (5.9%)
1	fN	2.26	65/1841 (3.5%)	2.54	131/2500 (5.2%)
1	fO	2.19	54/1841 (2.9%)	2.61	156/2500 (6.2%)
1	fP	2.15	54/1841 (2.9%)	2.61	145/2500 (5.8%)
1	fQ	2.13	55/1841 (3.0%)	2.63	165/2500 (6.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	fR	2.25	64/1841 (3.5%)	2.61	160/2500 (6.4%)
1	fS	2.19	65/1841 (3.5%)	2.56	142/2500 (5.7%)
1	fT	2.22	61/1841 (3.3%)	2.58	149/2500 (6.0%)
1	fU	2.23	57/1841 (3.1%)	2.52	134/2500 (5.4%)
1	fV	2.18	53/1841 (2.9%)	2.61	157/2500 (6.3%)
1	fW	2.21	63/1841 (3.4%)	2.63	163/2500 (6.5%)
1	fX	2.14	45/1841 (2.4%)	2.48	123/2500 (4.9%)
1	fY	2.20	61/1841 (3.3%)	2.54	141/2500 (5.6%)
1	fZ	2.30	69/1841 (3.7%)	2.58	133/2500 (5.3%)
1	fa	2.18	56/1841 (3.0%)	2.58	147/2500 (5.9%)
1	fb	2.14	47/1841 (2.6%)	2.51	125/2500 (5.0%)
1	fc	2.32	65/1841 (3.5%)	2.65	169/2500 (6.8%)
1	fd	2.23	63/1841 (3.4%)	2.53	132/2500 (5.3%)
1	fe	2.21	51/1841 (2.8%)	2.61	148/2500 (5.9%)
1	ff	2.27	60/1841 (3.3%)	2.55	151/2500 (6.0%)
1	fg	2.14	51/1841 (2.8%)	2.53	137/2500 (5.5%)
1	fh	2.23	56/1841 (3.0%)	2.51	137/2500 (5.5%)
1	fi	2.16	57/1841 (3.1%)	2.65	163/2500 (6.5%)
1	fj	2.20	60/1841 (3.3%)	2.60	140/2500 (5.6%)
1	fk	2.17	49/1841 (2.7%)	2.52	141/2500 (5.6%)
1	fl	2.24	63/1841 (3.4%)	2.63	168/2500 (6.7%)
1	fm	2.24	59/1841 (3.2%)	2.70	168/2500 (6.7%)
1	fn	2.24	65/1841 (3.5%)	2.66	167/2500 (6.7%)
1	fo	2.21	64/1841 (3.5%)	2.55	145/2500 (5.8%)
1	fp	2.25	70/1841 (3.8%)	2.68	166/2500 (6.6%)
1	fq	2.15	57/1841 (3.1%)	2.66	167/2500 (6.7%)
1	fr	2.21	61/1841 (3.3%)	2.55	150/2500 (6.0%)
1	fs	2.21	61/1841 (3.3%)	2.59	166/2500 (6.6%)
1	ft	2.16	50/1841 (2.7%)	2.61	152/2500 (6.1%)
1	fu	2.19	63/1841 (3.4%)	2.60	143/2500 (5.7%)
1	fv	2.20	56/1841 (3.0%)	2.52	135/2500 (5.4%)
1	fw	2.18	58/1841 (3.2%)	2.58	147/2500 (5.9%)
1	fx	2.12	42/1841 (2.3%)	2.43	118/2500 (4.7%)
1	fy	2.19	67/1841 (3.6%)	2.60	134/2500 (5.4%)
1	fz	2.18	61/1841 (3.3%)	2.62	144/2500 (5.8%)
1	g	2.24	62/1841 (3.4%)	2.63	180/2500 (7.2%)
1	g0	2.23	65/1841 (3.5%)	2.61	165/2500 (6.6%)
1	g1	2.22	63/1841 (3.4%)	2.62	161/2500 (6.4%)
1	g2	2.21	62/1841 (3.4%)	2.65	157/2500 (6.3%)
1	g3	2.23	64/1841 (3.5%)	2.58	149/2500 (6.0%)
1	g4	2.21	55/1841 (3.0%)	2.55	153/2500 (6.1%)
1	g5	2.22	63/1841 (3.4%)	2.59	160/2500 (6.4%)
1	g6	2.19	46/1841 (2.5%)	2.56	164/2500 (6.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	g7	2.32	71/1841 (3.9%)	2.59	149/2500 (6.0%)
1	g8	2.22	56/1841 (3.0%)	2.56	149/2500 (6.0%)
1	g9	2.19	59/1841 (3.2%)	2.60	168/2500 (6.7%)
1	gA	2.20	58/1841 (3.2%)	2.64	170/2500 (6.8%)
1	gB	2.19	68/1841 (3.7%)	2.64	171/2500 (6.8%)
1	gC	2.25	52/1841 (2.8%)	2.68	156/2500 (6.2%)
1	gD	2.23	67/1841 (3.6%)	2.64	146/2500 (5.8%)
1	gE	2.14	42/1841 (2.3%)	2.59	167/2500 (6.7%)
1	gF	2.25	70/1841 (3.8%)	2.66	159/2500 (6.4%)
1	gG	2.15	57/1841 (3.1%)	2.65	167/2500 (6.7%)
1	gH	2.24	70/1841 (3.8%)	2.58	142/2500 (5.7%)
1	gI	2.17	54/1841 (2.9%)	2.60	157/2500 (6.3%)
1	gJ	2.25	64/1841 (3.5%)	2.54	137/2500 (5.5%)
1	gK	2.23	61/1841 (3.3%)	2.53	133/2500 (5.3%)
1	gL	2.21	60/1841 (3.3%)	2.58	145/2500 (5.8%)
1	gM	2.17	51/1841 (2.8%)	2.58	158/2500 (6.3%)
1	gN	2.21	55/1841 (3.0%)	2.54	140/2500 (5.6%)
1	gO	2.24	69/1841 (3.7%)	2.69	179/2500 (7.2%)
1	gP	2.18	49/1841 (2.7%)	2.57	138/2500 (5.5%)
1	gQ	2.16	51/1841 (2.8%)	2.60	149/2500 (6.0%)
1	gR	2.12	49/1841 (2.7%)	2.58	150/2500 (6.0%)
1	gS	2.17	63/1841 (3.4%)	2.47	140/2500 (5.6%)
1	gT	2.19	59/1841 (3.2%)	2.57	132/2500 (5.3%)
1	gU	2.19	55/1841 (3.0%)	2.64	158/2500 (6.3%)
1	gV	2.24	58/1841 (3.2%)	2.60	142/2500 (5.7%)
1	gW	2.13	50/1841 (2.7%)	2.61	161/2500 (6.4%)
1	gX	2.22	74/1841 (4.0%)	2.59	134/2500 (5.4%)
1	gY	2.21	53/1841 (2.9%)	2.47	129/2500 (5.2%)
1	gZ	2.18	48/1841 (2.6%)	2.55	145/2500 (5.8%)
1	ga	2.15	53/1841 (2.9%)	2.65	156/2500 (6.2%)
1	gb	2.21	66/1841 (3.6%)	2.61	146/2500 (5.8%)
1	gc	2.24	64/1841 (3.5%)	2.52	150/2500 (6.0%)
1	gd	2.18	57/1841 (3.1%)	2.60	167/2500 (6.7%)
1	ge	2.15	49/1841 (2.7%)	2.55	136/2500 (5.4%)
1	gf	2.17	59/1841 (3.2%)	2.58	147/2500 (5.9%)
1	gg	2.25	71/1841 (3.9%)	2.60	156/2500 (6.2%)
1	gh	2.23	58/1841 (3.2%)	2.57	138/2500 (5.5%)
1	gi	2.19	61/1841 (3.3%)	2.70	178/2500 (7.1%)
1	gj	2.24	65/1841 (3.5%)	2.64	152/2500 (6.1%)
1	gk	2.17	55/1841 (3.0%)	2.58	147/2500 (5.9%)
1	gl	2.22	59/1841 (3.2%)	2.58	141/2500 (5.6%)
1	gm	2.21	62/1841 (3.4%)	2.55	155/2500 (6.2%)
1	gn	2.17	49/1841 (2.7%)	2.64	163/2500 (6.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	go	2.16	47/1841 (2.6%)	2.62	148/2500 (5.9%)
1	gp	2.26	74/1841 (4.0%)	2.60	170/2500 (6.8%)
1	gq	2.14	52/1841 (2.8%)	2.62	150/2500 (6.0%)
1	gr	2.14	55/1841 (3.0%)	2.62	169/2500 (6.8%)
1	gs	2.21	56/1841 (3.0%)	2.61	152/2500 (6.1%)
1	gt	2.27	64/1841 (3.5%)	2.65	176/2500 (7.0%)
1	gu	2.24	65/1841 (3.5%)	2.55	141/2500 (5.6%)
1	gv	2.18	63/1841 (3.4%)	2.48	139/2500 (5.6%)
1	gw	2.18	57/1841 (3.1%)	2.56	151/2500 (6.0%)
1	gx	2.17	46/1841 (2.5%)	2.56	144/2500 (5.8%)
1	gy	2.22	62/1841 (3.4%)	2.61	166/2500 (6.6%)
1	gz	2.24	62/1841 (3.4%)	2.62	151/2500 (6.0%)
1	h	2.19	55/1841 (3.0%)	2.60	161/2500 (6.4%)
1	h0	2.22	58/1841 (3.2%)	2.63	163/2500 (6.5%)
1	h1	2.18	55/1841 (3.0%)	2.62	154/2500 (6.2%)
1	h2	2.18	55/1841 (3.0%)	2.68	174/2500 (7.0%)
1	h3	2.18	65/1841 (3.5%)	2.62	164/2500 (6.6%)
1	h4	2.20	59/1841 (3.2%)	2.57	152/2500 (6.1%)
1	h5	2.25	63/1841 (3.4%)	2.61	155/2500 (6.2%)
1	h6	2.20	46/1841 (2.5%)	2.59	150/2500 (6.0%)
1	h7	2.20	52/1841 (2.8%)	2.52	133/2500 (5.3%)
1	h8	2.16	57/1841 (3.1%)	2.55	134/2500 (5.4%)
1	h9	2.28	61/1841 (3.3%)	2.58	149/2500 (6.0%)
1	hA	2.12	44/1841 (2.4%)	2.64	165/2500 (6.6%)
1	hB	2.22	51/1841 (2.8%)	2.56	128/2500 (5.1%)
1	hC	2.22	61/1841 (3.3%)	2.59	160/2500 (6.4%)
1	hD	2.28	68/1841 (3.7%)	2.61	149/2500 (6.0%)
1	hE	2.16	53/1841 (2.9%)	2.48	132/2500 (5.3%)
1	hF	2.21	53/1841 (2.9%)	2.64	157/2500 (6.3%)
1	hG	2.26	72/1841 (3.9%)	2.63	168/2500 (6.7%)
1	hH	2.15	45/1841 (2.4%)	2.58	139/2500 (5.6%)
1	hI	2.23	58/1841 (3.2%)	2.57	138/2500 (5.5%)
1	hJ	2.19	62/1841 (3.4%)	2.55	135/2500 (5.4%)
1	hK	2.24	61/1841 (3.3%)	2.52	141/2500 (5.6%)
1	hL	2.20	64/1841 (3.5%)	2.48	123/2500 (4.9%)
1	hM	2.20	53/1841 (2.9%)	2.57	147/2500 (5.9%)
1	hN	2.20	54/1841 (2.9%)	2.58	155/2500 (6.2%)
1	hO	2.16	48/1841 (2.6%)	2.56	145/2500 (5.8%)
1	hP	2.22	66/1841 (3.6%)	2.58	149/2500 (6.0%)
1	hQ	2.23	70/1841 (3.8%)	2.59	159/2500 (6.4%)
1	hR	2.26	71/1841 (3.9%)	2.55	160/2500 (6.4%)
1	hS	2.20	64/1841 (3.5%)	2.55	139/2500 (5.6%)
1	hT	2.21	64/1841 (3.5%)	2.53	138/2500 (5.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	hU	2.20	56/1841 (3.0%)	2.53	135/2500 (5.4%)
1	hV	2.12	54/1841 (2.9%)	2.52	143/2500 (5.7%)
1	hW	2.20	54/1841 (2.9%)	2.59	145/2500 (5.8%)
1	hX	2.16	52/1841 (2.8%)	2.57	135/2500 (5.4%)
1	hY	2.18	60/1841 (3.3%)	2.54	138/2500 (5.5%)
1	hZ	2.25	76/1841 (4.1%)	2.56	138/2500 (5.5%)
1	ha	2.24	62/1841 (3.4%)	2.64	158/2500 (6.3%)
1	hb	2.19	58/1841 (3.2%)	2.53	128/2500 (5.1%)
1	hc	2.19	56/1841 (3.0%)	2.64	153/2500 (6.1%)
1	hd	2.15	48/1841 (2.6%)	2.53	121/2500 (4.8%)
1	he	2.19	57/1841 (3.1%)	2.56	144/2500 (5.8%)
1	hf	2.25	66/1841 (3.6%)	2.59	167/2500 (6.7%)
1	hg	2.21	54/1841 (2.9%)	2.63	170/2500 (6.8%)
1	hh	2.29	71/1841 (3.9%)	2.62	161/2500 (6.4%)
1	hi	2.25	63/1841 (3.4%)	2.56	145/2500 (5.8%)
1	hj	2.18	56/1841 (3.0%)	2.62	153/2500 (6.1%)
1	hk	2.22	60/1841 (3.3%)	2.57	142/2500 (5.7%)
1	hl	2.26	63/1841 (3.4%)	2.61	162/2500 (6.5%)
1	hm	2.22	58/1841 (3.2%)	2.61	150/2500 (6.0%)
1	hn	2.13	57/1841 (3.1%)	2.61	164/2500 (6.6%)
1	ho	2.19	51/1841 (2.8%)	2.66	160/2500 (6.4%)
1	hp	2.17	49/1841 (2.7%)	2.64	167/2500 (6.7%)
1	hq	2.21	62/1841 (3.4%)	2.53	131/2500 (5.2%)
1	hr	2.23	49/1841 (2.7%)	2.64	173/2500 (6.9%)
1	hs	2.26	64/1841 (3.5%)	2.56	138/2500 (5.5%)
1	ht	2.15	59/1841 (3.2%)	2.54	159/2500 (6.4%)
1	hu	2.21	61/1841 (3.3%)	2.57	143/2500 (5.7%)
1	hv	2.20	55/1841 (3.0%)	2.57	147/2500 (5.9%)
1	hw	2.15	48/1841 (2.6%)	2.61	155/2500 (6.2%)
1	hx	2.18	61/1841 (3.3%)	2.53	142/2500 (5.7%)
1	hy	2.19	57/1841 (3.1%)	2.67	171/2500 (6.8%)
1	hz	2.15	48/1841 (2.6%)	2.67	162/2500 (6.5%)
1	i	2.24	62/1841 (3.4%)	2.54	152/2500 (6.1%)
1	i0	2.24	62/1841 (3.4%)	2.66	162/2500 (6.5%)
1	i1	2.21	61/1841 (3.3%)	2.66	163/2500 (6.5%)
1	i2	2.21	47/1841 (2.6%)	2.57	147/2500 (5.9%)
1	i3	2.22	68/1841 (3.7%)	2.53	151/2500 (6.0%)
1	i4	2.23	57/1841 (3.1%)	2.54	132/2500 (5.3%)
1	i5	2.24	61/1841 (3.3%)	2.57	146/2500 (5.8%)
1	i6	2.20	57/1841 (3.1%)	2.64	169/2500 (6.8%)
1	i7	2.17	58/1841 (3.2%)	2.60	152/2500 (6.1%)
1	i8	2.24	75/1841 (4.1%)	2.59	156/2500 (6.2%)
1	i9	2.24	65/1841 (3.5%)	2.57	152/2500 (6.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	iA	2.18	49/1841 (2.7%)	2.68	156/2500 (6.2%)
1	iB	2.13	51/1841 (2.8%)	2.57	144/2500 (5.8%)
1	iC	2.12	45/1841 (2.4%)	2.58	142/2500 (5.7%)
1	iD	2.15	52/1841 (2.8%)	2.57	154/2500 (6.2%)
1	iE	2.20	64/1841 (3.5%)	2.62	153/2500 (6.1%)
1	iF	2.27	71/1841 (3.9%)	2.56	149/2500 (6.0%)
1	iG	2.21	67/1841 (3.6%)	2.57	152/2500 (6.1%)
1	iH	2.26	63/1841 (3.4%)	2.60	156/2500 (6.2%)
1	iI	2.21	57/1841 (3.1%)	2.54	140/2500 (5.6%)
1	iJ	2.21	55/1841 (3.0%)	2.54	138/2500 (5.5%)
1	iK	2.20	63/1841 (3.4%)	2.56	127/2500 (5.1%)
1	iL	2.26	68/1841 (3.7%)	2.62	155/2500 (6.2%)
1	iM	2.26	69/1841 (3.7%)	2.62	146/2500 (5.8%)
1	iN	2.19	56/1841 (3.0%)	2.68	181/2500 (7.2%)
1	iO	2.20	63/1841 (3.4%)	2.50	132/2500 (5.3%)
1	iP	2.28	68/1841 (3.7%)	2.60	172/2500 (6.9%)
1	iQ	2.17	55/1841 (3.0%)	2.61	165/2500 (6.6%)
1	iR	2.19	60/1841 (3.3%)	2.63	168/2500 (6.7%)
1	iS	2.27	68/1841 (3.7%)	2.56	145/2500 (5.8%)
1	iT	2.23	65/1841 (3.5%)	2.62	152/2500 (6.1%)
1	iU	2.14	49/1841 (2.7%)	2.64	160/2500 (6.4%)
1	iV	2.25	65/1841 (3.5%)	2.56	140/2500 (5.6%)
1	iW	2.19	56/1841 (3.0%)	2.65	163/2500 (6.5%)
1	iX	2.25	70/1841 (3.8%)	2.61	161/2500 (6.4%)
1	iY	2.16	59/1841 (3.2%)	2.55	145/2500 (5.8%)
1	iZ	2.18	47/1841 (2.6%)	2.47	130/2500 (5.2%)
1	ia	2.19	63/1841 (3.4%)	2.62	167/2500 (6.7%)
1	ib	2.15	56/1841 (3.0%)	2.68	169/2500 (6.8%)
1	ic	2.20	61/1841 (3.3%)	2.58	148/2500 (5.9%)
1	id	2.14	52/1841 (2.8%)	2.52	125/2500 (5.0%)
1	ie	2.21	55/1841 (3.0%)	2.56	139/2500 (5.6%)
1	if	2.19	55/1841 (3.0%)	2.68	155/2500 (6.2%)
1	ig	2.23	61/1841 (3.3%)	2.68	150/2500 (6.0%)
1	ih	2.22	59/1841 (3.2%)	2.56	158/2500 (6.3%)
1	ii	2.25	77/1841 (4.2%)	2.57	141/2500 (5.6%)
1	ij	2.24	61/1841 (3.3%)	2.59	156/2500 (6.2%)
1	ik	2.20	50/1841 (2.7%)	2.53	142/2500 (5.7%)
1	il	2.17	63/1841 (3.4%)	2.61	160/2500 (6.4%)
1	im	2.21	60/1841 (3.3%)	2.60	138/2500 (5.5%)
1	in	2.21	66/1841 (3.6%)	2.55	153/2500 (6.1%)
1	io	2.30	64/1841 (3.5%)	2.64	152/2500 (6.1%)
1	ip	2.21	68/1841 (3.7%)	2.55	138/2500 (5.5%)
1	iq	2.21	46/1841 (2.5%)	2.56	144/2500 (5.8%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	ir	2.17	59/1841 (3.2%)	2.56	132/2500 (5.3%)
1	is	2.12	51/1841 (2.8%)	2.53	127/2500 (5.1%)
1	it	2.27	64/1841 (3.5%)	2.62	178/2500 (7.1%)
1	iu	2.18	49/1841 (2.7%)	2.65	164/2500 (6.6%)
1	iv	2.20	64/1841 (3.5%)	2.55	138/2500 (5.5%)
1	iw	2.16	57/1841 (3.1%)	2.54	140/2500 (5.6%)
1	ix	2.22	66/1841 (3.6%)	2.50	145/2500 (5.8%)
1	iy	2.18	64/1841 (3.5%)	2.59	145/2500 (5.8%)
1	iz	2.22	64/1841 (3.5%)	2.61	159/2500 (6.4%)
1	j	2.19	52/1841 (2.8%)	2.57	153/2500 (6.1%)
1	j0	2.24	71/1841 (3.9%)	2.61	168/2500 (6.7%)
1	j1	2.25	70/1841 (3.8%)	2.57	144/2500 (5.8%)
1	j2	2.23	66/1841 (3.6%)	2.61	154/2500 (6.2%)
1	j3	2.23	66/1841 (3.6%)	2.56	139/2500 (5.6%)
1	j4	2.20	53/1841 (2.9%)	2.62	151/2500 (6.0%)
1	j5	2.19	53/1841 (2.9%)	2.59	141/2500 (5.6%)
1	j6	2.19	57/1841 (3.1%)	2.60	148/2500 (5.9%)
1	j7	2.21	57/1841 (3.1%)	2.57	142/2500 (5.7%)
1	j8	2.30	65/1841 (3.5%)	2.59	152/2500 (6.1%)
1	j9	2.18	56/1841 (3.0%)	2.63	161/2500 (6.4%)
1	jA	2.20	52/1841 (2.8%)	2.56	138/2500 (5.5%)
1	jB	2.28	60/1841 (3.3%)	2.63	180/2500 (7.2%)
1	jC	2.24	64/1841 (3.5%)	2.62	165/2500 (6.6%)
1	jD	2.21	57/1841 (3.1%)	2.65	162/2500 (6.5%)
1	jE	2.21	60/1841 (3.3%)	2.61	152/2500 (6.1%)
1	jF	2.30	65/1841 (3.5%)	2.56	154/2500 (6.2%)
1	jG	2.16	52/1841 (2.8%)	2.51	118/2500 (4.7%)
1	jH	2.23	60/1841 (3.3%)	2.54	131/2500 (5.2%)
1	jI	2.16	51/1841 (2.8%)	2.62	148/2500 (5.9%)
1	jJ	2.21	54/1841 (2.9%)	2.58	142/2500 (5.7%)
1	jK	2.16	55/1841 (3.0%)	2.58	157/2500 (6.3%)
1	jL	2.20	53/1841 (2.9%)	2.60	145/2500 (5.8%)
1	jM	2.22	66/1841 (3.6%)	2.64	168/2500 (6.7%)
1	jN	2.20	58/1841 (3.2%)	2.61	167/2500 (6.7%)
1	jO	2.22	70/1841 (3.8%)	2.58	152/2500 (6.1%)
1	jP	2.15	53/1841 (2.9%)	2.57	145/2500 (5.8%)
1	jQ	2.21	68/1841 (3.7%)	2.57	142/2500 (5.7%)
1	jR	2.25	67/1841 (3.6%)	2.62	166/2500 (6.6%)
1	jS	2.14	53/1841 (2.9%)	2.59	144/2500 (5.8%)
1	jT	2.16	57/1841 (3.1%)	2.65	175/2500 (7.0%)
1	jU	2.16	53/1841 (2.9%)	2.64	173/2500 (6.9%)
1	jV	2.20	65/1841 (3.5%)	2.58	141/2500 (5.6%)
1	jW	2.21	61/1841 (3.3%)	2.58	160/2500 (6.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	jX	2.16	52/1841 (2.8%)	2.64	163/2500 (6.5%)
1	jY	2.18	58/1841 (3.2%)	2.57	133/2500 (5.3%)
1	jZ	2.26	54/1841 (2.9%)	2.59	156/2500 (6.2%)
1	ja	2.23	64/1841 (3.5%)	2.51	127/2500 (5.1%)
1	jb	2.30	72/1841 (3.9%)	2.57	161/2500 (6.4%)
1	jc	2.18	60/1841 (3.3%)	2.62	164/2500 (6.6%)
1	jd	2.20	58/1841 (3.2%)	2.57	144/2500 (5.8%)
1	je	2.22	62/1841 (3.4%)	2.66	169/2500 (6.8%)
1	jf	2.22	63/1841 (3.4%)	2.56	129/2500 (5.2%)
1	jg	2.25	66/1841 (3.6%)	2.59	145/2500 (5.8%)
1	jh	2.22	63/1841 (3.4%)	2.56	139/2500 (5.6%)
1	ji	2.25	60/1841 (3.3%)	2.64	157/2500 (6.3%)
1	jj	2.22	59/1841 (3.2%)	2.57	142/2500 (5.7%)
1	jk	2.17	52/1841 (2.8%)	2.68	162/2500 (6.5%)
1	jl	2.20	67/1841 (3.6%)	2.59	150/2500 (6.0%)
1	jm	2.25	66/1841 (3.6%)	2.60	161/2500 (6.4%)
1	jn	2.18	49/1841 (2.7%)	2.59	149/2500 (6.0%)
1	jo	2.17	56/1841 (3.0%)	2.52	144/2500 (5.8%)
1	jp	2.15	53/1841 (2.9%)	2.58	168/2500 (6.7%)
1	jq	2.16	51/1841 (2.8%)	2.59	150/2500 (6.0%)
1	jr	2.20	50/1841 (2.7%)	2.55	149/2500 (6.0%)
1	js	2.28	72/1841 (3.9%)	2.64	140/2500 (5.6%)
1	jt	2.22	59/1841 (3.2%)	2.64	170/2500 (6.8%)
1	ju	2.15	51/1841 (2.8%)	2.55	143/2500 (5.7%)
1	jv	2.21	61/1841 (3.3%)	2.62	161/2500 (6.4%)
1	jw	2.22	56/1841 (3.0%)	2.56	147/2500 (5.9%)
1	jx	2.25	71/1841 (3.9%)	2.58	138/2500 (5.5%)
1	jy	2.21	58/1841 (3.2%)	2.61	162/2500 (6.5%)
1	jz	2.21	62/1841 (3.4%)	2.57	153/2500 (6.1%)
1	k	2.25	72/1841 (3.9%)	2.63	162/2500 (6.5%)
1	k0	2.16	66/1841 (3.6%)	2.62	162/2500 (6.5%)
1	k1	2.14	48/1841 (2.6%)	2.59	143/2500 (5.7%)
1	k2	2.16	50/1841 (2.7%)	2.59	145/2500 (5.8%)
1	k3	2.28	72/1841 (3.9%)	2.52	127/2500 (5.1%)
1	k4	2.21	73/1841 (4.0%)	2.61	176/2500 (7.0%)
1	k5	2.19	61/1841 (3.3%)	2.53	125/2500 (5.0%)
1	k6	2.13	50/1841 (2.7%)	2.63	162/2500 (6.5%)
1	k7	2.24	71/1841 (3.9%)	2.67	153/2500 (6.1%)
1	k8	2.20	49/1841 (2.7%)	2.55	139/2500 (5.6%)
1	k9	2.29	73/1841 (4.0%)	2.59	162/2500 (6.5%)
1	kA	2.21	61/1841 (3.3%)	2.55	152/2500 (6.1%)
1	kB	2.19	53/1841 (2.9%)	2.47	118/2500 (4.7%)
1	kC	2.24	70/1841 (3.8%)	2.54	152/2500 (6.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	kD	2.17	47/1841 (2.6%)	2.62	163/2500 (6.5%)
1	kE	2.20	61/1841 (3.3%)	2.57	147/2500 (5.9%)
1	kF	2.23	73/1841 (4.0%)	2.64	171/2500 (6.8%)
1	kG	2.21	48/1841 (2.6%)	2.57	137/2500 (5.5%)
1	kH	2.27	61/1841 (3.3%)	2.59	152/2500 (6.1%)
1	kI	2.17	56/1841 (3.0%)	2.65	159/2500 (6.4%)
1	kJ	2.22	56/1841 (3.0%)	2.60	139/2500 (5.6%)
1	kK	2.21	64/1841 (3.5%)	2.52	122/2500 (4.9%)
1	kL	2.27	69/1841 (3.7%)	2.58	138/2500 (5.5%)
1	kM	2.22	61/1841 (3.3%)	2.61	151/2500 (6.0%)
1	kN	2.18	60/1841 (3.3%)	2.60	157/2500 (6.3%)
1	kO	2.14	48/1841 (2.6%)	2.59	149/2500 (6.0%)
1	kP	2.19	51/1841 (2.8%)	2.58	153/2500 (6.1%)
1	kQ	2.22	58/1841 (3.2%)	2.53	150/2500 (6.0%)
1	kR	2.23	69/1841 (3.7%)	2.58	169/2500 (6.8%)
1	kS	2.17	48/1841 (2.6%)	2.56	136/2500 (5.4%)
1	kT	2.12	45/1841 (2.4%)	2.67	168/2500 (6.7%)
1	kU	2.22	64/1841 (3.5%)	2.54	131/2500 (5.2%)
1	kV	2.22	61/1841 (3.3%)	2.60	151/2500 (6.0%)
1	kW	2.23	64/1841 (3.5%)	2.57	152/2500 (6.1%)
1	kX	2.21	58/1841 (3.2%)	2.58	157/2500 (6.3%)
1	kY	2.19	59/1841 (3.2%)	2.58	154/2500 (6.2%)
1	kZ	2.16	46/1841 (2.5%)	2.57	148/2500 (5.9%)
1	ka	2.23	63/1841 (3.4%)	2.57	143/2500 (5.7%)
1	kb	2.21	62/1841 (3.4%)	2.62	144/2500 (5.8%)
1	kc	2.15	54/1841 (2.9%)	2.48	133/2500 (5.3%)
1	kd	2.19	54/1841 (2.9%)	2.61	150/2500 (6.0%)
1	ke	2.14	51/1841 (2.8%)	2.56	139/2500 (5.6%)
1	kf	2.18	59/1841 (3.2%)	2.64	150/2500 (6.0%)
1	kg	2.24	61/1841 (3.3%)	2.57	157/2500 (6.3%)
1	kh	2.20	60/1841 (3.3%)	2.57	132/2500 (5.3%)
1	ki	2.16	55/1841 (3.0%)	2.61	160/2500 (6.4%)
1	kj	2.20	60/1841 (3.3%)	2.54	135/2500 (5.4%)
1	kk	2.20	53/1841 (2.9%)	2.55	149/2500 (6.0%)
1	kl	2.19	53/1841 (2.9%)	2.60	144/2500 (5.8%)
1	km	2.26	56/1841 (3.0%)	2.59	146/2500 (5.8%)
1	kn	2.17	45/1841 (2.4%)	2.62	157/2500 (6.3%)
1	ko	2.19	65/1841 (3.5%)	2.58	143/2500 (5.7%)
1	kp	2.19	51/1841 (2.8%)	2.52	131/2500 (5.2%)
1	kq	2.20	67/1841 (3.6%)	2.53	139/2500 (5.6%)
1	kr	2.26	63/1841 (3.4%)	2.59	145/2500 (5.8%)
1	ks	2.24	59/1841 (3.2%)	2.49	132/2500 (5.3%)
1	kt	2.30	71/1841 (3.9%)	2.52	145/2500 (5.8%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	ku	2.16	51/1841 (2.8%)	2.58	152/2500 (6.1%)
1	kv	2.22	70/1841 (3.8%)	2.60	155/2500 (6.2%)
1	kw	2.14	54/1841 (2.9%)	2.55	138/2500 (5.5%)
1	kx	2.21	65/1841 (3.5%)	2.55	136/2500 (5.4%)
1	ky	2.21	63/1841 (3.4%)	2.64	160/2500 (6.4%)
1	kz	2.19	57/1841 (3.1%)	2.52	138/2500 (5.5%)
1	l	2.29	64/1841 (3.5%)	2.58	144/2500 (5.8%)
1	l0	2.25	73/1841 (4.0%)	2.61	147/2500 (5.9%)
1	l1	2.17	56/1841 (3.0%)	2.63	167/2500 (6.7%)
1	l2	2.17	51/1841 (2.8%)	2.54	151/2500 (6.0%)
1	l3	2.28	64/1841 (3.5%)	2.58	137/2500 (5.5%)
1	l4	2.19	59/1841 (3.2%)	2.63	166/2500 (6.6%)
1	l5	2.08	39/1841 (2.1%)	2.54	135/2500 (5.4%)
1	l6	2.13	56/1841 (3.0%)	2.57	148/2500 (5.9%)
1	l7	2.20	51/1841 (2.8%)	2.60	142/2500 (5.7%)
1	l8	2.13	45/1841 (2.4%)	2.65	172/2500 (6.9%)
1	l9	2.25	58/1841 (3.2%)	2.59	136/2500 (5.4%)
1	lA	2.26	73/1841 (4.0%)	2.62	154/2500 (6.2%)
1	lB	2.22	64/1841 (3.5%)	2.63	149/2500 (6.0%)
1	lC	2.23	68/1841 (3.7%)	2.69	170/2500 (6.8%)
1	lD	2.13	45/1841 (2.4%)	2.58	156/2500 (6.2%)
1	lE	2.17	55/1841 (3.0%)	2.65	170/2500 (6.8%)
1	lF	2.23	62/1841 (3.4%)	2.59	154/2500 (6.2%)
1	lG	2.20	58/1841 (3.2%)	2.62	159/2500 (6.4%)
1	lH	2.25	71/1841 (3.9%)	2.67	156/2500 (6.2%)
1	lI	2.26	72/1841 (3.9%)	2.56	137/2500 (5.5%)
1	lJ	2.23	60/1841 (3.3%)	2.57	142/2500 (5.7%)
1	lK	2.23	68/1841 (3.7%)	2.54	148/2500 (5.9%)
1	lL	2.18	63/1841 (3.4%)	2.64	172/2500 (6.9%)
1	lM	2.17	51/1841 (2.8%)	2.72	167/2500 (6.7%)
1	lN	2.25	66/1841 (3.6%)	2.59	147/2500 (5.9%)
1	lO	2.16	47/1841 (2.6%)	2.64	172/2500 (6.9%)
1	lP	2.27	80/1841 (4.3%)	2.47	117/2500 (4.7%)
1	lQ	2.22	63/1841 (3.4%)	2.55	141/2500 (5.6%)
1	lR	2.16	58/1841 (3.2%)	2.52	130/2500 (5.2%)
1	la	2.18	53/1841 (2.9%)	2.49	128/2500 (5.1%)
1	lb	2.21	63/1841 (3.4%)	2.60	140/2500 (5.6%)
1	lc	2.23	63/1841 (3.4%)	2.54	136/2500 (5.4%)
1	ld	2.19	61/1841 (3.3%)	2.63	159/2500 (6.4%)
1	le	2.13	44/1841 (2.4%)	2.58	145/2500 (5.8%)
1	lf	2.31	71/1841 (3.9%)	2.63	158/2500 (6.3%)
1	lg	2.27	70/1841 (3.8%)	2.58	150/2500 (6.0%)
1	lh	2.24	82/1841 (4.5%)	2.61	155/2500 (6.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	li	2.19	63/1841 (3.4%)	2.63	165/2500 (6.6%)
1	lj	2.22	61/1841 (3.3%)	2.63	161/2500 (6.4%)
1	lk	2.22	60/1841 (3.3%)	2.59	131/2500 (5.2%)
1	ll	2.22	69/1841 (3.7%)	2.58	155/2500 (6.2%)
1	lm	2.15	59/1841 (3.2%)	2.57	152/2500 (6.1%)
1	ln	2.17	59/1841 (3.2%)	2.61	159/2500 (6.4%)
1	lo	2.18	49/1841 (2.7%)	2.57	141/2500 (5.6%)
1	lp	2.18	53/1841 (2.9%)	2.48	121/2500 (4.8%)
1	lq	2.10	43/1841 (2.3%)	2.62	163/2500 (6.5%)
1	lr	2.22	54/1841 (2.9%)	2.59	146/2500 (5.8%)
1	ls	2.24	54/1841 (2.9%)	2.55	139/2500 (5.6%)
1	lt	2.22	63/1841 (3.4%)	2.60	160/2500 (6.4%)
1	lu	2.25	61/1841 (3.3%)	2.59	156/2500 (6.2%)
1	lv	2.18	62/1841 (3.4%)	2.50	129/2500 (5.2%)
1	lw	2.16	52/1841 (2.8%)	2.64	175/2500 (7.0%)
1	lx	2.17	54/1841 (2.9%)	2.46	113/2500 (4.5%)
1	ly	2.22	59/1841 (3.2%)	2.58	154/2500 (6.2%)
1	lz	2.16	47/1841 (2.6%)	2.63	151/2500 (6.0%)
1	m	2.21	53/1841 (2.9%)	2.56	128/2500 (5.1%)
1	n	2.17	50/1841 (2.7%)	2.53	136/2500 (5.4%)
1	o	2.27	69/1841 (3.7%)	2.61	164/2500 (6.6%)
1	p	2.21	56/1841 (3.0%)	2.65	160/2500 (6.4%)
1	q	2.21	53/1841 (2.9%)	2.64	143/2500 (5.7%)
1	r	2.26	57/1841 (3.1%)	2.57	148/2500 (5.9%)
1	s	2.16	46/1841 (2.5%)	2.58	155/2500 (6.2%)
1	t	2.18	53/1841 (2.9%)	2.61	134/2500 (5.4%)
1	u	2.23	62/1841 (3.4%)	2.60	150/2500 (6.0%)
1	v	2.23	68/1841 (3.7%)	2.60	151/2500 (6.0%)
1	w	2.24	55/1841 (3.0%)	2.51	130/2500 (5.2%)
1	x	2.17	50/1841 (2.7%)	2.58	148/2500 (5.9%)
1	y	2.22	54/1841 (2.9%)	2.65	173/2500 (6.9%)
1	z	2.21	65/1841 (3.5%)	2.62	144/2500 (5.8%)
All	All	2.21	79738/2496396 (3.2%)	2.59	204007/3390000 (6.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	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 79738 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	h6	37	ILE	CA-CB	20.53	1.65	1.54
1	2W	37	ILE	CA-CB	-19.67	1.44	1.54
1	90	37	ILE	CA-CB	-19.09	1.44	1.54
1	aV	37	ILE	CA-CB	-19.00	1.44	1.54
1	5O	37	ILE	CA-CB	-18.67	1.44	1.54

The worst 5 of 204007 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	l0	162	ARG	NE-CZ-NH2	-18.17	102.85	119.20
1	b5	37	ILE	O-C-N	-17.93	108.94	120.42
1	1I	36	VAL	CA-C-N	17.34	131.16	120.24
1	1I	36	VAL	C-N-CA	17.34	131.16	120.24
1	95	33	SER	O-C-N	-17.34	110.61	121.71

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 ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	1800	0	1802	6	0
1	1	1800	0	1802	0	0
1	10	1800	0	1802	5	0
1	11	1800	0	1802	1	0
1	12	1800	0	1802	4	0
1	13	1800	0	1802	6	0
1	14	1800	0	1802	4	0
1	15	1800	0	1802	6	0
1	16	1800	0	1802	4	0
1	17	1800	0	1802	5	0
1	18	1800	0	1802	4	0
1	19	1800	0	1802	2	0
1	1A	1800	0	1802	7	0
1	1B	1800	0	1802	6	0
1	1C	1800	0	1802	2	0
1	1D	1800	0	1802	2	0
1	1E	1800	0	1802	8	0
1	1F	1800	0	1802	6	0
1	1G	1800	0	1802	5	0
1	1H	1800	0	1802	3	0
1	1I	1800	0	1802	4	0
1	1J	1800	0	1802	7	0
1	1K	1800	0	1802	6	0
1	1L	1800	0	1802	2	0
1	1M	1800	0	1802	4	0
1	1N	1800	0	1802	2	0
1	1O	1800	0	1802	5	0
1	1P	1800	0	1802	1	0
1	1Q	1800	0	1802	1	0
1	1R	1800	0	1802	3	0
1	1S	1800	0	1802	3	0
1	1T	1800	0	1802	7	0
1	1U	1800	0	1802	6	0
1	1V	1800	0	1802	5	0
1	1W	1800	0	1802	3	0
1	1X	1800	0	1802	6	0
1	1Y	1800	0	1802	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1Z	1800	0	1802	3	0
1	1a	1800	0	1802	5	0
1	1b	1800	0	1802	5	0
1	1c	1800	0	1802	4	0
1	1d	1800	0	1802	3	0
1	1e	1800	0	1802	2	0
1	1f	1800	0	1802	6	0
1	1g	1800	0	1802	3	0
1	1h	1800	0	1802	9	0
1	1i	1800	0	1802	5	0
1	1j	1800	0	1802	6	0
1	1k	1800	0	1802	3	0
1	1l	1800	0	1802	6	0
1	1m	1800	0	1802	8	0
1	1n	1800	0	1802	5	0
1	1o	1800	0	1802	5	0
1	1p	1800	0	1802	2	0
1	1q	1800	0	1802	2	0
1	1r	1800	0	1802	4	0
1	1s	1800	0	1802	6	0
1	1t	1800	0	1802	1	0
1	1u	1800	0	1802	4	0
1	1v	1800	0	1802	3	0
1	1w	1800	0	1802	1	0
1	1x	1800	0	1802	2	0
1	1y	1800	0	1802	4	0
1	1z	1800	0	1802	5	0
1	2	1800	0	1802	7	0
1	20	1800	0	1802	4	0
1	21	1800	0	1802	7	0
1	22	1800	0	1802	3	0
1	23	1800	0	1802	2	0
1	24	1800	0	1802	5	0
1	25	1800	0	1802	2	0
1	26	1800	0	1802	3	0
1	27	1800	0	1802	1	0
1	28	1800	0	1802	5	0
1	29	1800	0	1802	1	0
1	2A	1800	0	1802	4	0
1	2B	1800	0	1802	7	0
1	2C	1800	0	1802	1	0
1	2D	1800	0	1802	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2E	1800	0	1802	3	0
1	2F	1800	0	1802	1	0
1	2G	1800	0	1802	4	0
1	2H	1800	0	1802	2	0
1	2I	1800	0	1802	3	0
1	2J	1800	0	1802	3	0
1	2K	1800	0	1802	2	0
1	2L	1800	0	1802	4	0
1	2M	1800	0	1802	3	0
1	2N	1800	0	1802	5	0
1	2O	1800	0	1802	5	0
1	2P	1800	0	1802	4	0
1	2Q	1800	0	1802	1	0
1	2R	1800	0	1802	2	0
1	2S	1800	0	1802	7	0
1	2T	1800	0	1802	3	0
1	2U	1800	0	1802	4	0
1	2V	1800	0	1802	4	0
1	2W	1800	0	1802	4	0
1	2X	1800	0	1802	3	0
1	2Y	1800	0	1802	3	0
1	2Z	1800	0	1802	3	0
1	2a	1800	0	1802	2	0
1	2b	1800	0	1802	5	0
1	2c	1800	0	1802	5	0
1	2d	1800	0	1802	6	0
1	2e	1800	0	1802	5	0
1	2f	1800	0	1802	5	0
1	2g	1800	0	1802	7	0
1	2h	1800	0	1802	1	0
1	2i	1800	0	1802	5	0
1	2j	1800	0	1802	5	0
1	2k	1800	0	1802	4	0
1	2l	1800	0	1802	2	0
1	2m	1800	0	1802	8	0
1	2n	1800	0	1802	2	0
1	2o	1800	0	1802	4	0
1	2p	1800	0	1802	12	0
1	2q	1800	0	1802	4	0
1	2r	1800	0	1802	7	0
1	2s	1800	0	1802	4	0
1	2t	1800	0	1802	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2u	1800	0	1802	4	0
1	2v	1800	0	1802	4	0
1	2w	1800	0	1802	2	0
1	2x	1800	0	1802	2	0
1	2y	1800	0	1802	2	0
1	2z	1800	0	1802	4	0
1	3	1800	0	1802	3	0
1	30	1800	0	1802	4	0
1	31	1800	0	1802	2	0
1	32	1800	0	1802	4	0
1	33	1800	0	1802	7	0
1	34	1800	0	1802	2	0
1	35	1800	0	1802	3	0
1	36	1800	0	1802	5	0
1	37	1800	0	1802	2	0
1	38	1800	0	1802	2	0
1	39	1800	0	1802	4	0
1	3A	1800	0	1802	1	0
1	3B	1800	0	1802	4	0
1	3C	1800	0	1802	6	0
1	3D	1800	0	1802	3	0
1	3E	1800	0	1802	1	0
1	3F	1800	0	1802	3	0
1	3G	1800	0	1802	3	0
1	3H	1800	0	1802	6	0
1	3I	1800	0	1802	0	0
1	3J	1800	0	1802	6	0
1	3K	1800	0	1802	6	0
1	3L	1800	0	1802	5	0
1	3M	1800	0	1802	5	0
1	3N	1800	0	1802	4	0
1	3O	1800	0	1802	8	0
1	3P	1800	0	1802	4	0
1	3Q	1800	0	1802	2	0
1	3R	1800	0	1802	6	0
1	3S	1800	0	1802	3	0
1	3T	1800	0	1802	0	0
1	3U	1800	0	1802	4	0
1	3V	1800	0	1802	4	0
1	3W	1800	0	1802	4	0
1	3X	1800	0	1802	8	0
1	3Y	1800	0	1802	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	3Z	1800	0	1802	1	0
1	3a	1800	0	1802	8	0
1	3b	1800	0	1802	4	0
1	3c	1800	0	1802	2	0
1	3d	1800	0	1802	2	0
1	3e	1800	0	1802	3	0
1	3f	1800	0	1802	3	0
1	3g	1800	0	1802	3	0
1	3h	1800	0	1802	3	0
1	3i	1800	0	1802	4	0
1	3j	1800	0	1802	4	0
1	3k	1800	0	1802	4	0
1	3l	1800	0	1802	3	0
1	3m	1800	0	1802	0	0
1	3n	1800	0	1802	1	0
1	3o	1800	0	1802	3	0
1	3p	1800	0	1802	7	0
1	3q	1800	0	1802	7	0
1	3r	1800	0	1802	3	0
1	3s	1800	0	1802	4	0
1	3t	1800	0	1802	3	0
1	3u	1800	0	1802	3	0
1	3v	1800	0	1802	3	0
1	3w	1800	0	1802	2	0
1	3x	1800	0	1802	2	0
1	3y	1800	0	1802	5	0
1	3z	1800	0	1802	6	0
1	4	1800	0	1802	4	0
1	40	1800	0	1802	0	0
1	41	1800	0	1802	6	0
1	42	1800	0	1802	6	0
1	43	1800	0	1802	6	0
1	44	1800	0	1802	4	0
1	45	1800	0	1802	5	0
1	46	1800	0	1802	2	0
1	47	1800	0	1802	2	0
1	48	1800	0	1802	4	0
1	49	1800	0	1802	5	0
1	4A	1800	0	1802	7	0
1	4B	1800	0	1802	8	0
1	4C	1800	0	1802	5	0
1	4D	1800	0	1802	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	4E	1800	0	1802	4	0
1	4F	1800	0	1802	10	0
1	4G	1800	0	1802	4	0
1	4H	1800	0	1802	5	0
1	4I	1800	0	1802	1	0
1	4J	1800	0	1802	5	0
1	4K	1800	0	1802	3	0
1	4L	1800	0	1802	6	0
1	4M	1800	0	1802	5	0
1	4N	1800	0	1802	0	0
1	4O	1800	0	1802	4	0
1	4P	1800	0	1802	1	0
1	4Q	1800	0	1802	2	0
1	4R	1800	0	1802	7	0
1	4S	1800	0	1802	4	0
1	4T	1800	0	1802	0	0
1	4U	1800	0	1802	2	0
1	4V	1800	0	1802	3	0
1	4W	1800	0	1802	3	0
1	4X	1800	0	1802	1	0
1	4Y	1800	0	1802	1	0
1	4Z	1800	0	1802	4	0
1	4a	1800	0	1802	4	0
1	4b	1800	0	1802	3	0
1	4c	1800	0	1802	7	0
1	4d	1800	0	1802	1	0
1	4e	1800	0	1802	1	0
1	4f	1800	0	1802	9	0
1	4g	1800	0	1802	1	0
1	4h	1800	0	1802	1	0
1	4i	1800	0	1802	4	0
1	4j	1800	0	1802	5	0
1	4k	1800	0	1802	7	0
1	4l	1800	0	1802	4	0
1	4m	1800	0	1802	3	0
1	4n	1800	0	1802	4	0
1	4o	1800	0	1802	6	0
1	4p	1800	0	1802	7	0
1	4q	1800	0	1802	4	0
1	4r	1800	0	1802	2	0
1	4s	1800	0	1802	4	0
1	4t	1800	0	1802	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	4u	1800	0	1802	3	0
1	4v	1800	0	1802	6	0
1	4w	1800	0	1802	5	0
1	4x	1800	0	1802	3	0
1	4y	1800	0	1802	4	0
1	4z	1800	0	1802	6	0
1	5	1800	0	1802	0	0
1	50	1800	0	1802	3	0
1	51	1800	0	1802	5	0
1	52	1800	0	1802	6	0
1	53	1800	0	1802	3	0
1	54	1800	0	1802	7	0
1	55	1800	0	1802	7	0
1	56	1800	0	1802	4	0
1	57	1800	0	1802	4	0
1	58	1800	0	1802	4	0
1	59	1800	0	1802	0	0
1	5A	1800	0	1802	0	0
1	5B	1800	0	1802	3	0
1	5C	1800	0	1802	5	0
1	5D	1800	0	1802	2	0
1	5E	1800	0	1802	2	0
1	5F	1800	0	1802	4	0
1	5G	1800	0	1802	3	0
1	5H	1800	0	1802	1	0
1	5I	1800	0	1802	3	0
1	5J	1800	0	1802	5	0
1	5K	1800	0	1802	5	0
1	5L	1800	0	1802	5	0
1	5M	1800	0	1802	3	0
1	5N	1800	0	1802	7	0
1	5O	1800	0	1802	4	0
1	5P	1800	0	1802	4	0
1	5Q	1800	0	1802	2	0
1	5R	1800	0	1802	3	0
1	5S	1800	0	1802	5	0
1	5T	1800	0	1802	7	0
1	5U	1800	0	1802	6	0
1	5V	1800	0	1802	3	0
1	5W	1800	0	1802	7	0
1	5X	1800	0	1802	2	0
1	5Y	1800	0	1802	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	5Z	1800	0	1802	3	0
1	5a	1800	0	1802	3	0
1	5b	1800	0	1802	7	0
1	5c	1800	0	1802	5	0
1	5d	1800	0	1802	5	0
1	5e	1800	0	1802	2	0
1	5f	1800	0	1802	3	0
1	5g	1800	0	1802	5	0
1	5h	1800	0	1802	4	0
1	5i	1800	0	1802	6	0
1	5j	1800	0	1802	5	0
1	5k	1800	0	1802	2	0
1	5l	1800	0	1802	2	0
1	5m	1800	0	1802	4	0
1	5n	1800	0	1802	4	0
1	5o	1800	0	1802	5	0
1	5p	1800	0	1802	5	0
1	5q	1800	0	1802	2	0
1	5r	1800	0	1802	3	0
1	5s	1800	0	1802	5	0
1	5t	1800	0	1802	3	0
1	5u	1800	0	1802	5	0
1	5v	1800	0	1802	0	0
1	5w	1800	0	1802	5	0
1	5x	1800	0	1802	5	0
1	5y	1800	0	1802	6	0
1	5z	1800	0	1802	5	0
1	6	1800	0	1802	6	0
1	60	1800	0	1802	2	0
1	61	1800	0	1802	2	0
1	62	1800	0	1802	2	0
1	63	1800	0	1802	5	0
1	64	1800	0	1802	5	0
1	65	1800	0	1802	3	0
1	66	1800	0	1802	6	0
1	67	1800	0	1802	5	0
1	68	1800	0	1802	3	0
1	69	1800	0	1802	4	0
1	6A	1800	0	1802	3	0
1	6B	1800	0	1802	4	0
1	6C	1800	0	1802	2	0
1	6D	1800	0	1802	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	6E	1800	0	1802	3	0
1	6F	1800	0	1802	2	0
1	6G	1800	0	1802	4	0
1	6H	1800	0	1802	6	0
1	6I	1800	0	1802	4	0
1	6J	1800	0	1802	3	0
1	6K	1800	0	1802	7	0
1	6L	1800	0	1802	5	0
1	6M	1800	0	1802	7	0
1	6N	1800	0	1802	5	0
1	6O	1800	0	1802	3	0
1	6P	1800	0	1802	2	0
1	6Q	1800	0	1802	3	0
1	6R	1800	0	1802	4	0
1	6S	1800	0	1802	2	0
1	6T	1800	0	1802	5	0
1	6U	1800	0	1802	2	0
1	6V	1800	0	1802	4	0
1	6W	1800	0	1802	4	0
1	6X	1800	0	1802	6	0
1	6Y	1800	0	1802	4	0
1	6Z	1800	0	1802	0	0
1	6a	1800	0	1802	1	0
1	6b	1800	0	1802	5	0
1	6c	1800	0	1802	6	0
1	6d	1800	0	1802	3	0
1	6e	1800	0	1802	6	0
1	6f	1800	0	1802	2	0
1	6g	1800	0	1802	3	0
1	6h	1800	0	1802	3	0
1	6i	1800	0	1802	6	0
1	6j	1800	0	1802	7	0
1	6k	1800	0	1802	5	0
1	6l	1800	0	1802	4	0
1	6m	1800	0	1802	5	0
1	6n	1800	0	1802	2	0
1	6o	1800	0	1802	0	0
1	6p	1800	0	1802	3	0
1	6q	1800	0	1802	3	0
1	6r	1800	0	1802	5	0
1	6s	1800	0	1802	6	0
1	6t	1800	0	1802	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	6u	1800	0	1802	7	0
1	6v	1800	0	1802	5	0
1	6w	1800	0	1802	5	0
1	6x	1800	0	1802	3	0
1	6y	1800	0	1802	4	0
1	6z	1800	0	1802	2	0
1	7	1800	0	1802	3	0
1	70	1800	0	1802	3	0
1	71	1800	0	1802	1	0
1	72	1800	0	1802	5	0
1	73	1800	0	1802	5	0
1	74	1800	0	1802	6	0
1	75	1800	0	1802	7	0
1	76	1800	0	1802	1	0
1	77	1800	0	1802	4	0
1	78	1800	0	1802	8	0
1	79	1800	0	1802	2	0
1	7A	1800	0	1802	0	0
1	7B	1800	0	1802	4	0
1	7C	1800	0	1802	1	0
1	7D	1800	0	1802	1	0
1	7E	1800	0	1802	6	0
1	7F	1800	0	1802	5	0
1	7G	1800	0	1802	3	0
1	7H	1800	0	1802	4	0
1	7I	1800	0	1802	3	0
1	7J	1800	0	1802	2	0
1	7K	1800	0	1802	4	0
1	7L	1800	0	1802	6	0
1	7M	1800	0	1802	5	0
1	7N	1800	0	1802	2	0
1	7O	1800	0	1802	2	0
1	7P	1800	0	1802	3	0
1	7Q	1800	0	1802	6	0
1	7R	1800	0	1802	3	0
1	7S	1800	0	1802	2	0
1	7T	1800	0	1802	8	0
1	7U	1800	0	1802	3	0
1	7V	1800	0	1802	3	0
1	7W	1800	0	1802	3	0
1	7X	1800	0	1802	2	0
1	7Y	1800	0	1802	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	7Z	1800	0	1802	1	0
1	7a	1800	0	1802	7	0
1	7b	1800	0	1802	2	0
1	7c	1800	0	1802	1	0
1	7d	1800	0	1802	3	0
1	7e	1800	0	1802	2	0
1	7f	1800	0	1802	5	0
1	7g	1800	0	1802	3	0
1	7h	1800	0	1802	5	0
1	7i	1800	0	1802	3	0
1	7j	1800	0	1802	4	0
1	7k	1800	0	1802	3	0
1	7l	1800	0	1802	4	0
1	7m	1800	0	1802	7	0
1	7n	1800	0	1802	2	0
1	7o	1800	0	1802	1	0
1	7p	1800	0	1802	5	0
1	7q	1800	0	1802	5	0
1	7r	1800	0	1802	4	0
1	7s	1800	0	1802	3	0
1	7t	1800	0	1802	1	0
1	7u	1800	0	1802	2	0
1	7v	1800	0	1802	5	0
1	7w	1800	0	1802	4	0
1	7x	1800	0	1802	3	0
1	7y	1800	0	1802	2	0
1	7z	1800	0	1802	1	0
1	8	1800	0	1802	3	0
1	80	1800	0	1802	1	0
1	81	1800	0	1802	5	0
1	82	1800	0	1802	4	0
1	83	1800	0	1802	1	0
1	84	1800	0	1802	3	0
1	85	1800	0	1802	6	0
1	86	1800	0	1802	7	0
1	87	1800	0	1802	2	0
1	88	1800	0	1802	4	0
1	89	1800	0	1802	7	0
1	8A	1800	0	1802	5	0
1	8B	1800	0	1802	4	0
1	8C	1800	0	1802	5	0
1	8D	1800	0	1802	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	8E	1800	0	1802	4	0
1	8F	1800	0	1802	1	0
1	8G	1800	0	1802	2	0
1	8H	1800	0	1802	4	0
1	8I	1800	0	1802	3	0
1	8J	1800	0	1802	6	0
1	8K	1800	0	1802	6	0
1	8L	1800	0	1802	5	0
1	8M	1800	0	1802	2	0
1	8N	1800	0	1802	8	0
1	8O	1800	0	1802	3	0
1	8P	1800	0	1802	2	0
1	8Q	1800	0	1802	2	0
1	8R	1800	0	1802	3	0
1	8S	1800	0	1802	6	0
1	8T	1800	0	1802	6	0
1	8U	1800	0	1802	4	0
1	8V	1800	0	1802	2	0
1	8W	1800	0	1802	4	0
1	8X	1800	0	1802	3	0
1	8Y	1800	0	1802	3	0
1	8Z	1800	0	1802	5	0
1	8a	1800	0	1802	3	0
1	8b	1800	0	1802	7	0
1	8c	1800	0	1802	4	0
1	8d	1800	0	1802	1	0
1	8e	1800	0	1802	5	0
1	8f	1800	0	1802	6	0
1	8g	1800	0	1802	5	0
1	8h	1800	0	1802	5	0
1	8i	1800	0	1802	7	0
1	8j	1800	0	1802	3	0
1	8k	1800	0	1802	3	0
1	8l	1800	0	1802	6	0
1	8m	1800	0	1802	4	0
1	8n	1800	0	1802	6	0
1	8o	1800	0	1802	2	0
1	8p	1800	0	1802	4	0
1	8q	1800	0	1802	4	0
1	8r	1800	0	1802	5	0
1	8s	1800	0	1802	1	0
1	8t	1800	0	1802	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	8u	1800	0	1802	5	0
1	8v	1800	0	1802	9	0
1	8w	1800	0	1802	8	0
1	8x	1800	0	1802	6	0
1	8y	1800	0	1802	4	0
1	8z	1800	0	1802	3	0
1	9	1800	0	1802	6	0
1	90	1800	0	1802	5	0
1	91	1800	0	1802	9	0
1	92	1800	0	1802	3	0
1	93	1800	0	1802	5	0
1	94	1800	0	1802	4	0
1	95	1800	0	1802	3	0
1	96	1800	0	1802	3	0
1	97	1800	0	1802	4	0
1	98	1800	0	1802	3	0
1	99	1800	0	1802	3	0
1	9A	1800	0	1802	2	0
1	9B	1800	0	1802	4	0
1	9C	1800	0	1802	0	0
1	9D	1800	0	1802	2	0
1	9E	1800	0	1802	2	0
1	9F	1800	0	1802	4	0
1	9G	1800	0	1802	0	0
1	9H	1800	0	1802	2	0
1	9I	1800	0	1802	2	0
1	9J	1800	0	1802	6	0
1	9K	1800	0	1802	2	0
1	9L	1800	0	1802	5	0
1	9M	1800	0	1802	4	0
1	9N	1800	0	1802	2	0
1	9O	1800	0	1802	4	0
1	9P	1800	0	1802	2	0
1	9Q	1800	0	1802	2	0
1	9R	1800	0	1802	4	0
1	9S	1800	0	1802	2	0
1	9T	1800	0	1802	6	0
1	9U	1800	0	1802	3	0
1	9V	1800	0	1802	5	0
1	9W	1800	0	1802	4	0
1	9X	1800	0	1802	2	0
1	9Y	1800	0	1802	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	9Z	1800	0	1802	5	0
1	9a	1800	0	1802	5	0
1	9b	1800	0	1802	3	0
1	9c	1800	0	1802	2	0
1	9d	1800	0	1802	5	0
1	9e	1800	0	1802	1	0
1	9f	1800	0	1802	2	0
1	9g	1800	0	1802	2	0
1	9h	1800	0	1802	5	0
1	9i	1800	0	1802	2	0
1	9j	1800	0	1802	3	0
1	9k	1800	0	1802	4	0
1	9l	1800	0	1802	3	0
1	9m	1800	0	1802	4	0
1	9n	1800	0	1802	3	0
1	9o	1800	0	1802	7	0
1	9p	1800	0	1802	3	0
1	9q	1800	0	1802	8	0
1	9r	1800	0	1802	7	0
1	9s	1800	0	1802	2	0
1	9t	1800	0	1802	5	0
1	9u	1800	0	1802	2	0
1	9v	1800	0	1802	3	0
1	9w	1800	0	1802	1	0
1	9x	1800	0	1802	5	0
1	9y	1800	0	1802	3	0
1	9z	1800	0	1802	4	0
1	A	1800	0	1802	3	0
1	B	1800	0	1802	3	0
1	C	1800	0	1802	6	0
1	D	1800	0	1802	1	0
1	E	1800	0	1802	3	0
1	F	1800	0	1802	5	0
1	G	1800	0	1802	7	0
1	H	1800	0	1802	2	0
1	I	1800	0	1802	2	0
1	J	1800	0	1802	5	0
1	K	1800	0	1802	3	0
1	L	1800	0	1802	3	0
1	M	1800	0	1802	6	0
1	N	1800	0	1802	8	0
1	O	1800	0	1802	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	1800	0	1802	4	0
1	Q	1800	0	1802	6	0
1	R	1800	0	1802	4	0
1	S	1800	0	1802	5	0
1	T	1800	0	1802	2	0
1	U	1800	0	1802	4	0
1	V	1800	0	1802	6	0
1	W	1800	0	1802	6	0
1	X	1800	0	1802	3	0
1	Y	1800	0	1802	5	0
1	Z	1800	0	1802	4	0
1	a	1800	0	1802	4	0
1	a0	1800	0	1802	6	0
1	a1	1800	0	1802	3	0
1	a2	1800	0	1802	7	0
1	a3	1800	0	1802	3	0
1	a4	1800	0	1802	3	0
1	a5	1800	0	1802	5	0
1	a6	1800	0	1802	6	0
1	a7	1800	0	1802	4	0
1	a8	1800	0	1802	5	0
1	a9	1800	0	1802	10	0
1	aA	1800	0	1802	4	0
1	aB	1800	0	1802	5	0
1	aC	1800	0	1802	1	0
1	aD	1800	0	1802	2	0
1	aE	1800	0	1802	6	0
1	aF	1800	0	1802	2	0
1	aG	1800	0	1802	2	0
1	aH	1800	0	1802	7	0
1	aI	1800	0	1802	2	0
1	aJ	1800	0	1802	3	0
1	aK	1800	0	1802	4	0
1	aL	1800	0	1802	4	0
1	aM	1800	0	1802	2	0
1	aN	1800	0	1802	10	0
1	aO	1800	0	1802	6	0
1	aP	1800	0	1802	5	0
1	aQ	1800	0	1802	5	0
1	aR	1800	0	1802	2	0
1	aS	1800	0	1802	3	0
1	aT	1800	0	1802	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	aU	1800	0	1802	7	0
1	aV	1800	0	1802	2	0
1	aW	1800	0	1802	3	0
1	aX	1800	0	1802	3	0
1	aY	1800	0	1802	6	0
1	aZ	1800	0	1802	2	0
1	aa	1800	0	1802	1	0
1	ab	1800	0	1802	1	0
1	ac	1800	0	1802	4	0
1	ad	1800	0	1802	2	0
1	ae	1800	0	1802	4	0
1	af	1800	0	1802	3	0
1	ag	1800	0	1802	3	0
1	ah	1800	0	1802	3	0
1	ai	1800	0	1802	5	0
1	aj	1800	0	1802	2	0
1	ak	1800	0	1802	2	0
1	al	1800	0	1802	6	0
1	am	1800	0	1802	0	0
1	an	1800	0	1802	5	0
1	ao	1800	0	1802	2	0
1	ap	1800	0	1802	5	0
1	aq	1800	0	1802	3	0
1	ar	1800	0	1802	5	0
1	as	1800	0	1802	5	0
1	at	1800	0	1802	6	0
1	au	1800	0	1802	5	0
1	av	1800	0	1802	6	0
1	aw	1800	0	1802	5	0
1	ax	1800	0	1802	5	0
1	ay	1800	0	1802	4	0
1	az	1800	0	1802	2	0
1	b	1800	0	1802	2	0
1	b0	1800	0	1802	9	0
1	b1	1800	0	1802	4	0
1	b2	1800	0	1802	10	0
1	b3	1800	0	1802	2	0
1	b4	1800	0	1802	1	0
1	b5	1800	0	1802	5	0
1	b6	1800	0	1802	2	0
1	b7	1800	0	1802	1	0
1	b8	1800	0	1802	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	b9	1800	0	1802	1	0
1	bA	1800	0	1802	4	0
1	bB	1800	0	1802	11	0
1	bC	1800	0	1802	8	0
1	bD	1800	0	1802	7	0
1	bE	1800	0	1802	3	0
1	bF	1800	0	1802	0	0
1	bG	1800	0	1802	1	0
1	bH	1800	0	1802	2	0
1	bI	1800	0	1802	6	0
1	bJ	1800	0	1802	4	0
1	bK	1800	0	1802	6	0
1	bL	1800	0	1802	8	0
1	bM	1800	0	1802	4	0
1	bN	1800	0	1802	4	0
1	bO	1800	0	1802	5	0
1	bP	1800	0	1802	1	0
1	bQ	1800	0	1802	3	0
1	bR	1800	0	1802	1	0
1	bS	1800	0	1802	4	0
1	bT	1800	0	1802	2	0
1	bU	1800	0	1802	2	0
1	bV	1800	0	1802	3	0
1	bW	1800	0	1802	1	0
1	bX	1800	0	1802	6	0
1	bY	1800	0	1802	2	0
1	bZ	1800	0	1802	1	0
1	ba	1800	0	1802	7	0
1	bb	1800	0	1802	3	0
1	bc	1800	0	1802	5	0
1	bd	1800	0	1802	4	0
1	be	1800	0	1802	2	0
1	bf	1800	0	1802	6	0
1	bg	1800	0	1802	8	0
1	bh	1800	0	1802	2	0
1	bi	1800	0	1802	2	0
1	bj	1800	0	1802	1	0
1	bk	1800	0	1802	4	0
1	bl	1800	0	1802	5	0
1	bm	1800	0	1802	9	0
1	bn	1800	0	1802	8	0
1	bo	1800	0	1802	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	bp	1800	0	1802	4	0
1	bq	1800	0	1802	4	0
1	br	1800	0	1802	3	0
1	bs	1800	0	1802	4	0
1	bt	1800	0	1802	5	0
1	bu	1800	0	1802	5	0
1	bv	1800	0	1802	5	0
1	bw	1800	0	1802	8	0
1	bx	1800	0	1802	6	0
1	by	1800	0	1802	5	0
1	bz	1800	0	1802	6	0
1	c	1800	0	1802	3	0
1	c0	1800	0	1802	4	0
1	c1	1800	0	1802	5	0
1	c2	1800	0	1802	5	0
1	c3	1800	0	1802	3	0
1	c4	1800	0	1802	4	0
1	c5	1800	0	1802	3	0
1	c6	1800	0	1802	4	0
1	c7	1800	0	1802	4	0
1	c8	1800	0	1802	5	0
1	c9	1800	0	1802	3	0
1	cA	1800	0	1802	3	0
1	cB	1800	0	1802	8	0
1	cC	1800	0	1802	10	0
1	cD	1800	0	1802	4	0
1	cE	1800	0	1802	1	0
1	cF	1800	0	1802	5	0
1	cG	1800	0	1802	5	0
1	cH	1800	0	1802	4	0
1	cI	1800	0	1802	8	0
1	cJ	1800	0	1802	4	0
1	cK	1800	0	1802	7	0
1	cL	1800	0	1802	4	0
1	cM	1800	0	1802	5	0
1	cN	1800	0	1802	6	0
1	cO	1800	0	1802	1	0
1	cP	1800	0	1802	0	0
1	cQ	1800	0	1802	2	0
1	cR	1800	0	1802	3	0
1	cS	1800	0	1802	5	0
1	cT	1800	0	1802	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	cU	1800	0	1802	4	0
1	cV	1800	0	1802	2	0
1	cW	1800	0	1802	0	0
1	cX	1800	0	1802	7	0
1	cY	1800	0	1802	6	0
1	cZ	1800	0	1802	2	0
1	ca	1800	0	1802	8	0
1	cb	1800	0	1802	5	0
1	cc	1800	0	1802	3	0
1	cd	1800	0	1802	6	0
1	ce	1800	0	1802	2	0
1	cf	1800	0	1802	5	0
1	cg	1800	0	1802	2	0
1	ch	1800	0	1802	5	0
1	ci	1800	0	1802	4	0
1	cj	1800	0	1802	2	0
1	ck	1800	0	1802	2	0
1	cl	1800	0	1802	2	0
1	cm	1800	0	1802	0	0
1	cn	1800	0	1802	2	0
1	co	1800	0	1802	1	0
1	cp	1800	0	1802	4	0
1	cq	1800	0	1802	7	0
1	cr	1800	0	1802	5	0
1	cs	1800	0	1802	3	0
1	ct	1800	0	1802	5	0
1	cu	1800	0	1802	5	0
1	cv	1800	0	1802	3	0
1	cw	1800	0	1802	4	0
1	cx	1800	0	1802	5	0
1	cy	1800	0	1802	6	0
1	cz	1800	0	1802	4	0
1	d	1800	0	1802	3	0
1	d0	1800	0	1802	2	0
1	d1	1800	0	1802	5	0
1	d2	1800	0	1802	3	0
1	d3	1800	0	1802	3	0
1	d4	1800	0	1802	2	0
1	d5	1800	0	1802	3	0
1	d6	1800	0	1802	5	0
1	d7	1800	0	1802	3	0
1	d8	1800	0	1802	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	d9	1800	0	1802	3	0
1	dA	1800	0	1802	6	0
1	dB	1800	0	1802	6	0
1	dC	1800	0	1802	5	0
1	dD	1800	0	1802	1	0
1	dE	1800	0	1802	2	0
1	dF	1800	0	1802	3	0
1	dG	1800	0	1802	1	0
1	dH	1800	0	1802	2	0
1	dI	1800	0	1802	3	0
1	dJ	1800	0	1802	3	0
1	dK	1800	0	1802	2	0
1	dL	1800	0	1802	2	0
1	dM	1800	0	1802	3	0
1	dN	1800	0	1802	3	0
1	dO	1800	0	1802	4	0
1	dP	1800	0	1802	1	0
1	dQ	1800	0	1802	2	0
1	dR	1800	0	1802	2	0
1	dS	1800	0	1802	2	0
1	dT	1800	0	1802	4	0
1	dU	1800	0	1802	4	0
1	dV	1800	0	1802	4	0
1	dW	1800	0	1802	2	0
1	dX	1800	0	1802	4	0
1	dY	1800	0	1802	7	0
1	dZ	1800	0	1802	1	0
1	da	1800	0	1802	1	0
1	db	1800	0	1802	1	0
1	dc	1800	0	1802	5	0
1	dd	1800	0	1802	4	0
1	de	1800	0	1802	4	0
1	df	1800	0	1802	3	0
1	dg	1800	0	1802	2	0
1	dh	1800	0	1802	4	0
1	di	1800	0	1802	2	0
1	dj	1800	0	1802	8	0
1	dk	1800	0	1802	4	0
1	dl	1800	0	1802	4	0
1	dm	1800	0	1802	2	0
1	dn	1800	0	1802	2	0
1	do	1800	0	1802	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	dp	1800	0	1802	1	0
1	dq	1800	0	1802	1	0
1	dr	1800	0	1802	0	0
1	ds	1800	0	1802	0	0
1	dt	1800	0	1802	6	0
1	du	1800	0	1802	3	0
1	dv	1800	0	1802	3	0
1	dw	1800	0	1802	6	0
1	dx	1800	0	1802	5	0
1	dy	1800	0	1802	6	0
1	dz	1800	0	1802	6	0
1	e	1800	0	1802	4	0
1	e0	1800	0	1802	4	0
1	e1	1800	0	1802	2	0
1	e2	1800	0	1802	1	0
1	e3	1800	0	1802	5	0
1	e4	1800	0	1802	3	0
1	e5	1800	0	1802	2	0
1	e6	1800	0	1802	3	0
1	e7	1800	0	1802	2	0
1	e8	1800	0	1802	2	0
1	e9	1800	0	1802	3	0
1	eA	1800	0	1802	3	0
1	eB	1800	0	1802	7	0
1	eC	1800	0	1802	7	0
1	eD	1800	0	1802	1	0
1	eE	1800	0	1802	4	0
1	eF	1800	0	1802	4	0
1	eG	1800	0	1802	4	0
1	eH	1800	0	1802	2	0
1	eI	1800	0	1802	4	0
1	eJ	1800	0	1802	6	0
1	eK	1800	0	1802	9	0
1	eL	1800	0	1802	5	0
1	eM	1800	0	1802	5	0
1	eN	1800	0	1802	6	0
1	eO	1800	0	1802	5	0
1	eP	1800	0	1802	3	0
1	eQ	1800	0	1802	7	0
1	eR	1800	0	1802	2	0
1	eS	1800	0	1802	5	0
1	eT	1800	0	1802	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	eU	1800	0	1802	2	0
1	eV	1800	0	1802	7	0
1	eW	1800	0	1802	4	0
1	eX	1800	0	1802	1	0
1	eY	1800	0	1802	2	0
1	eZ	1800	0	1802	5	0
1	ea	1800	0	1802	5	0
1	eb	1800	0	1802	4	0
1	ec	1800	0	1802	3	0
1	ed	1800	0	1802	2	0
1	ee	1800	0	1802	2	0
1	ef	1800	0	1802	4	0
1	eg	1800	0	1802	1	0
1	eh	1800	0	1802	3	0
1	ei	1800	0	1802	2	0
1	ej	1800	0	1802	3	0
1	ek	1800	0	1802	4	0
1	el	1800	0	1802	5	0
1	em	1800	0	1802	5	0
1	en	1800	0	1802	6	0
1	eo	1800	0	1802	8	0
1	ep	1800	0	1802	6	0
1	eq	1800	0	1802	3	0
1	er	1800	0	1802	3	0
1	es	1800	0	1802	1	0
1	et	1800	0	1802	7	0
1	eu	1800	0	1802	6	0
1	ev	1800	0	1802	3	0
1	ew	1800	0	1802	8	0
1	ex	1800	0	1802	3	0
1	ey	1800	0	1802	3	0
1	ez	1800	0	1802	4	0
1	f	1800	0	1802	3	0
1	f0	1800	0	1802	2	0
1	f1	1800	0	1802	4	0
1	f2	1800	0	1802	4	0
1	f3	1800	0	1802	4	0
1	f4	1800	0	1802	1	0
1	f5	1800	0	1802	3	0
1	f6	1800	0	1802	3	0
1	f7	1800	0	1802	8	0
1	f8	1800	0	1802	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	f9	1800	0	1802	3	0
1	fA	1800	0	1802	6	0
1	fB	1800	0	1802	3	0
1	fC	1800	0	1802	4	0
1	fD	1800	0	1802	2	0
1	fE	1800	0	1802	5	0
1	fF	1800	0	1802	6	0
1	fG	1800	0	1802	1	0
1	fH	1800	0	1802	2	0
1	fI	1800	0	1802	3	0
1	fJ	1800	0	1802	3	0
1	fK	1800	0	1802	2	0
1	fL	1800	0	1802	8	0
1	fM	1800	0	1802	2	0
1	fN	1800	0	1802	3	0
1	fO	1800	0	1802	4	0
1	fP	1800	0	1802	3	0
1	fQ	1800	0	1802	2	0
1	fR	1800	0	1802	2	0
1	fS	1800	0	1802	5	0
1	fT	1800	0	1802	5	0
1	fU	1800	0	1802	7	0
1	fV	1800	0	1802	3	0
1	fW	1800	0	1802	5	0
1	fX	1800	0	1802	3	0
1	fY	1800	0	1802	2	0
1	fZ	1800	0	1802	3	0
1	fa	1800	0	1802	2	0
1	fb	1800	0	1802	4	0
1	fc	1800	0	1802	7	0
1	fd	1800	0	1802	4	0
1	fe	1800	0	1802	0	0
1	ff	1800	0	1802	0	0
1	fg	1800	0	1802	3	0
1	fh	1800	0	1802	2	0
1	fi	1800	0	1802	3	0
1	fj	1800	0	1802	6	0
1	fk	1800	0	1802	5	0
1	fl	1800	0	1802	4	0
1	fm	1800	0	1802	5	0
1	fn	1800	0	1802	1	0
1	fo	1800	0	1802	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	fp	1800	0	1802	2	0
1	fq	1800	0	1802	5	0
1	fr	1800	0	1802	3	0
1	fs	1800	0	1802	1	0
1	ft	1800	0	1802	5	0
1	fu	1800	0	1802	6	0
1	fv	1800	0	1802	2	0
1	fw	1800	0	1802	3	0
1	fx	1800	0	1802	8	0
1	fy	1800	0	1802	3	0
1	fz	1800	0	1802	3	0
1	g	1800	0	1802	3	0
1	g0	1800	0	1802	3	0
1	g1	1800	0	1802	7	0
1	g2	1800	0	1802	8	0
1	g3	1800	0	1802	6	0
1	g4	1800	0	1802	1	0
1	g5	1800	0	1802	4	0
1	g6	1800	0	1802	5	0
1	g7	1800	0	1802	3	0
1	g8	1800	0	1802	3	0
1	g9	1800	0	1802	0	0
1	gA	1800	0	1802	1	0
1	gB	1800	0	1802	2	0
1	gC	1800	0	1802	4	0
1	gD	1800	0	1802	2	0
1	gE	1800	0	1802	7	0
1	gF	1800	0	1802	2	0
1	gG	1800	0	1802	3	0
1	gH	1800	0	1802	3	0
1	gI	1800	0	1802	2	0
1	gJ	1800	0	1802	3	0
1	gK	1800	0	1802	5	0
1	gL	1800	0	1802	3	0
1	gM	1800	0	1802	3	0
1	gN	1800	0	1802	2	0
1	gO	1800	0	1802	2	0
1	gP	1800	0	1802	7	0
1	gQ	1800	0	1802	2	0
1	gR	1800	0	1802	4	0
1	gS	1800	0	1802	5	0
1	gT	1800	0	1802	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	gU	1800	0	1802	4	0
1	gV	1800	0	1802	4	0
1	gW	1800	0	1802	9	0
1	gX	1800	0	1802	6	0
1	gY	1800	0	1802	3	0
1	gZ	1800	0	1802	2	0
1	ga	1800	0	1802	8	0
1	gb	1800	0	1802	1	0
1	gc	1800	0	1802	3	0
1	gd	1800	0	1802	4	0
1	ge	1800	0	1802	4	0
1	gf	1800	0	1802	3	0
1	gg	1800	0	1802	4	0
1	gh	1800	0	1802	2	0
1	gi	1800	0	1802	2	0
1	gj	1800	0	1802	3	0
1	gk	1800	0	1802	2	0
1	gl	1800	0	1802	5	0
1	gm	1800	0	1802	4	0
1	gn	1800	0	1802	2	0
1	go	1800	0	1802	5	0
1	gp	1800	0	1802	6	0
1	gq	1800	0	1802	2	0
1	gr	1800	0	1802	0	0
1	gs	1800	0	1802	2	0
1	gt	1800	0	1802	3	0
1	gu	1800	0	1802	3	0
1	gv	1800	0	1802	3	0
1	gw	1800	0	1802	6	0
1	gx	1800	0	1802	10	0
1	gy	1800	0	1802	3	0
1	gz	1800	0	1802	3	0
1	h	1800	0	1802	5	0
1	h0	1800	0	1802	5	0
1	h1	1800	0	1802	9	0
1	h2	1800	0	1802	2	0
1	h3	1800	0	1802	9	0
1	h4	1800	0	1802	3	0
1	h5	1800	0	1802	6	0
1	h6	1800	0	1802	5	0
1	h7	1800	0	1802	1	0
1	h8	1800	0	1802	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	h9	1800	0	1802	5	0
1	hA	1800	0	1802	4	0
1	hB	1800	0	1802	4	0
1	hC	1800	0	1802	8	0
1	hD	1800	0	1802	5	0
1	hE	1800	0	1802	8	0
1	hF	1800	0	1802	3	0
1	hG	1800	0	1802	5	0
1	hH	1800	0	1802	3	0
1	hI	1800	0	1802	3	0
1	hJ	1800	0	1802	0	0
1	hK	1800	0	1802	6	0
1	hL	1800	0	1802	8	0
1	hM	1800	0	1802	9	0
1	hN	1800	0	1802	3	0
1	hO	1800	0	1802	9	0
1	hP	1800	0	1802	3	0
1	hQ	1800	0	1802	3	0
1	hR	1800	0	1802	7	0
1	hS	1800	0	1802	3	0
1	hT	1800	0	1802	7	0
1	hU	1800	0	1802	5	0
1	hV	1800	0	1802	2	0
1	hW	1800	0	1802	6	0
1	hX	1800	0	1802	9	0
1	hY	1800	0	1802	7	0
1	hZ	1800	0	1802	7	0
1	ha	1800	0	1802	6	0
1	hb	1800	0	1802	7	0
1	hc	1800	0	1802	5	0
1	hd	1800	0	1802	1	0
1	he	1800	0	1802	4	0
1	hf	1800	0	1802	6	0
1	hg	1800	0	1802	8	0
1	hh	1800	0	1802	4	0
1	hi	1800	0	1802	4	0
1	hj	1800	0	1802	9	0
1	hk	1800	0	1802	2	0
1	hl	1800	0	1802	2	0
1	hm	1800	0	1802	0	0
1	hn	1800	0	1802	0	0
1	ho	1800	0	1802	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	hp	1800	0	1802	3	0
1	hq	1800	0	1802	6	0
1	hr	1800	0	1802	4	0
1	hs	1800	0	1802	9	0
1	ht	1800	0	1802	5	0
1	hu	1800	0	1802	5	0
1	hv	1800	0	1802	3	0
1	hw	1800	0	1802	2	0
1	hx	1800	0	1802	8	0
1	hy	1800	0	1802	6	0
1	hz	1800	0	1802	4	0
1	i	1800	0	1802	4	0
1	i0	1800	0	1802	3	0
1	i1	1800	0	1802	3	0
1	i2	1800	0	1802	6	0
1	i3	1800	0	1802	6	0
1	i4	1800	0	1802	4	0
1	i5	1800	0	1802	3	0
1	i6	1800	0	1802	2	0
1	i7	1800	0	1802	1	0
1	i8	1800	0	1802	3	0
1	i9	1800	0	1802	4	0
1	iA	1800	0	1802	2	0
1	iB	1800	0	1802	3	0
1	iC	1800	0	1802	3	0
1	iD	1800	0	1802	6	0
1	iE	1800	0	1802	8	0
1	iF	1800	0	1802	7	0
1	iG	1800	0	1802	7	0
1	iH	1800	0	1802	2	0
1	iI	1800	0	1802	0	0
1	iJ	1800	0	1802	4	0
1	iK	1800	0	1802	2	0
1	iL	1800	0	1802	2	0
1	iM	1800	0	1802	4	0
1	iN	1800	0	1802	6	0
1	iO	1800	0	1802	5	0
1	iP	1800	0	1802	3	0
1	iQ	1800	0	1802	2	0
1	iR	1800	0	1802	5	0
1	iS	1800	0	1802	6	0
1	iT	1800	0	1802	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	iU	1800	0	1802	4	0
1	iV	1800	0	1802	6	0
1	iW	1800	0	1802	6	0
1	iX	1800	0	1802	6	0
1	iY	1800	0	1802	4	0
1	iZ	1800	0	1802	2	0
1	ia	1800	0	1802	5	0
1	ib	1800	0	1802	4	0
1	ic	1800	0	1802	4	0
1	id	1800	0	1802	7	0
1	ie	1800	0	1802	5	0
1	if	1800	0	1802	5	0
1	ig	1800	0	1802	3	0
1	ih	1800	0	1802	3	0
1	ii	1800	0	1802	11	0
1	ij	1800	0	1802	9	0
1	ik	1800	0	1802	5	0
1	il	1800	0	1802	6	0
1	im	1800	0	1802	7	0
1	in	1800	0	1802	6	0
1	io	1800	0	1802	6	0
1	ip	1800	0	1802	4	0
1	iq	1800	0	1802	5	0
1	ir	1800	0	1802	8	0
1	is	1800	0	1802	2	0
1	it	1800	0	1802	6	0
1	iu	1800	0	1802	4	0
1	iv	1800	0	1802	3	0
1	iw	1800	0	1802	1	0
1	ix	1800	0	1802	3	0
1	iy	1800	0	1802	4	0
1	iz	1800	0	1802	3	0
1	j	1800	0	1802	4	0
1	j0	1800	0	1802	4	0
1	j1	1800	0	1802	5	0
1	j2	1800	0	1802	2	0
1	j3	1800	0	1802	3	0
1	j4	1800	0	1802	5	0
1	j5	1800	0	1802	5	0
1	j6	1800	0	1802	4	0
1	j7	1800	0	1802	4	0
1	j8	1800	0	1802	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	j9	1800	0	1802	3	0
1	jA	1800	0	1802	2	0
1	jB	1800	0	1802	8	0
1	jC	1800	0	1802	4	0
1	jD	1800	0	1802	4	0
1	jE	1800	0	1802	9	0
1	jF	1800	0	1802	5	0
1	jG	1800	0	1802	6	0
1	jH	1800	0	1802	4	0
1	jI	1800	0	1802	4	0
1	jJ	1800	0	1802	4	0
1	jK	1800	0	1802	5	0
1	jL	1800	0	1802	4	0
1	jM	1800	0	1802	6	0
1	jN	1800	0	1802	4	0
1	jO	1800	0	1802	1	0
1	jP	1800	0	1802	1	0
1	jQ	1800	0	1802	4	0
1	jR	1800	0	1802	5	0
1	jS	1800	0	1802	4	0
1	jT	1800	0	1802	3	0
1	jU	1800	0	1802	1	0
1	jV	1800	0	1802	6	0
1	jW	1800	0	1802	4	0
1	jX	1800	0	1802	3	0
1	jY	1800	0	1802	8	0
1	jZ	1800	0	1802	6	0
1	ja	1800	0	1802	3	0
1	jb	1800	0	1802	6	0
1	jc	1800	0	1802	4	0
1	jd	1800	0	1802	3	0
1	je	1800	0	1802	2	0
1	jf	1800	0	1802	2	0
1	yg	1800	0	1802	4	0
1	jh	1800	0	1802	4	0
1	ji	1800	0	1802	4	0
1	jj	1800	0	1802	3	0
1	jk	1800	0	1802	4	0
1	jl	1800	0	1802	3	0
1	jm	1800	0	1802	5	0
1	jn	1800	0	1802	4	0
1	jo	1800	0	1802	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	jp	1800	0	1802	5	0
1	jq	1800	0	1802	3	0
1	jr	1800	0	1802	6	0
1	js	1800	0	1802	3	0
1	jt	1800	0	1802	3	0
1	ju	1800	0	1802	10	0
1	jv	1800	0	1802	4	0
1	jw	1800	0	1802	6	0
1	jx	1800	0	1802	3	0
1	jy	1800	0	1802	7	0
1	jz	1800	0	1802	5	0
1	k	1800	0	1802	1	0
1	k0	1800	0	1802	7	0
1	k1	1800	0	1802	6	0
1	k2	1800	0	1802	2	0
1	k3	1800	0	1802	3	0
1	k4	1800	0	1802	3	0
1	k5	1800	0	1802	4	0
1	k6	1800	0	1802	2	0
1	k7	1800	0	1802	6	0
1	k8	1800	0	1802	3	0
1	k9	1800	0	1802	8	0
1	kA	1800	0	1802	6	0
1	kB	1800	0	1802	3	0
1	kC	1800	0	1802	4	0
1	kD	1800	0	1802	2	0
1	kE	1800	0	1802	3	0
1	kF	1800	0	1802	2	0
1	kG	1800	0	1802	2	0
1	kH	1800	0	1802	2	0
1	kI	1800	0	1802	3	0
1	kJ	1800	0	1802	5	0
1	kK	1800	0	1802	3	0
1	kL	1800	0	1802	4	0
1	kM	1800	0	1802	3	0
1	kN	1800	0	1802	3	0
1	kO	1800	0	1802	7	0
1	kP	1800	0	1802	4	0
1	kQ	1800	0	1802	2	0
1	kR	1800	0	1802	4	0
1	kS	1800	0	1802	5	0
1	kT	1800	0	1802	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	kU	1800	0	1802	7	0
1	kV	1800	0	1802	5	0
1	kW	1800	0	1802	1	0
1	kX	1800	0	1802	4	0
1	kY	1800	0	1802	5	0
1	kZ	1800	0	1802	4	0
1	ka	1800	0	1802	4	0
1	kb	1800	0	1802	4	0
1	kc	1800	0	1802	4	0
1	kd	1800	0	1802	3	0
1	ke	1800	0	1802	4	0
1	kf	1800	0	1802	3	0
1	kg	1800	0	1802	6	0
1	kh	1800	0	1802	2	0
1	ki	1800	0	1802	3	0
1	kj	1800	0	1802	1	0
1	kk	1800	0	1802	6	0
1	kl	1800	0	1802	4	0
1	km	1800	0	1802	3	0
1	kn	1800	0	1802	4	0
1	ko	1800	0	1802	1	0
1	kp	1800	0	1802	6	0
1	kq	1800	0	1802	5	0
1	kr	1800	0	1802	4	0
1	ks	1800	0	1802	4	0
1	kt	1800	0	1802	1	0
1	ku	1800	0	1802	4	0
1	kv	1800	0	1802	3	0
1	kw	1800	0	1802	4	0
1	kx	1800	0	1802	2	0
1	ky	1800	0	1802	2	0
1	kz	1800	0	1802	5	0
1	l	1800	0	1802	3	0
1	l0	1800	0	1802	6	0
1	l1	1800	0	1802	7	0
1	l2	1800	0	1802	4	0
1	l3	1800	0	1802	8	0
1	l4	1800	0	1802	5	0
1	l5	1800	0	1802	3	0
1	l6	1800	0	1802	7	0
1	l7	1800	0	1802	4	0
1	l8	1800	0	1802	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	l9	1800	0	1802	2	0
1	lA	1800	0	1802	6	0
1	lB	1800	0	1802	0	0
1	lC	1800	0	1802	6	0
1	lD	1800	0	1802	7	0
1	lE	1800	0	1802	5	0
1	lF	1800	0	1802	9	0
1	lG	1800	0	1802	3	0
1	lH	1800	0	1802	1	0
1	lI	1800	0	1802	5	0
1	lJ	1800	0	1802	2	0
1	lK	1800	0	1802	7	0
1	lL	1800	0	1802	4	0
1	lM	1800	0	1802	4	0
1	lN	1800	0	1802	8	0
1	lO	1800	0	1802	3	0
1	lP	1800	0	1802	4	0
1	lQ	1800	0	1802	2	0
1	lR	1800	0	1802	4	0
1	la	1800	0	1802	2	0
1	lb	1800	0	1802	1	0
1	lc	1800	0	1802	3	0
1	ld	1800	0	1802	1	0
1	le	1800	0	1802	6	0
1	lf	1800	0	1802	2	0
1	lg	1800	0	1802	3	0
1	lh	1800	0	1802	7	0
1	li	1800	0	1802	0	0
1	lj	1800	0	1802	3	0
1	lk	1800	0	1802	5	0
1	ll	1800	0	1802	3	0
1	lm	1800	0	1802	3	0
1	ln	1800	0	1802	7	0
1	lo	1800	0	1802	1	0
1	lp	1800	0	1802	1	0
1	lq	1800	0	1802	3	0
1	lr	1800	0	1802	4	0
1	ls	1800	0	1802	4	0
1	lt	1800	0	1802	5	0
1	lu	1800	0	1802	2	0
1	lv	1800	0	1802	9	0
1	lw	1800	0	1802	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	lx	1800	0	1802	4	0
1	ly	1800	0	1802	4	0
1	lz	1800	0	1802	2	0
1	m	1800	0	1802	6	0
1	n	1800	0	1802	3	0
1	o	1800	0	1802	2	0
1	p	1800	0	1802	3	0
1	q	1800	0	1802	3	0
1	r	1800	0	1802	3	0
1	s	1800	0	1802	6	0
1	t	1800	0	1802	4	0
1	u	1800	0	1802	4	0
1	v	1800	0	1802	0	0
1	w	1800	0	1802	3	0
1	x	1800	0	1802	8	0
1	y	1800	0	1802	5	0
1	z	1800	0	1802	4	0
All	All	2440800	0	2443512	4796	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

The worst 5 of 4796 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7y:209:ALA:HB3	1:7y:214:MET:HE2	1.57	0.85
1:78:83:LEU:HD23	1:78:84:HIS:CE1	2.14	0.81
1:3q:58:THR:HG21	1:3r:39:MET:HE2	1.62	0.81
1:d8:226:HIS:CG	1:d8:227:LYS:H	1.99	0.79
1:fT:13:GLN:HE22	1:fU:3:VAL:HG12	1.47	0.78

There are no symmetry-related clashes.

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.