



## wwPDB EM Validation Summary Report ⓘ

Dec 10, 2022 – 05:37 pm GMT

PDB ID : 4UDF  
EMDB ID : EMD-2761  
Title : STRUCTURAL BASIS OF HUMAN PARECHOVIRUS NEUTRALIZATION  
BY HUMAN MONOCLONAL ANTIBODIES  
Authors : Shakeel, S.; Westerhuis, B.M.; Ora, A.; Koen, G.; Bakker, A.Q.; Claassen, Y.;  
Beaumont, T.; Wolthers, K.C.; Butcher, S.J.  
Deposited on : 2014-12-10  
Resolution : 20.00 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

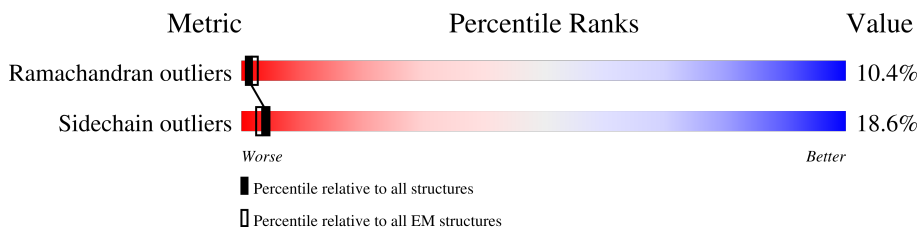
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 20.00 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	12	183	
1	16	183	
1	1A	183	
1	1E	183	
1	1I	183	
1	1M	183	
1	1Q	183	
1	1U	183	
1	1Y	183	
1	22	183	

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Mol	Chain	Length	Quality of chain			
1	26	183	42%	17%	23%	18%
1	2A	183	42%	17%	23%	18%
1	2E	183	42%	17%	23%	18%
1	2I	183	42%	17%	23%	18%
1	2M	183	42%	17%	23%	18%
1	2Q	183	42%	17%	23%	18%
1	2U	183	42%	17%	23%	18%
1	2Y	183	42%	17%	23%	18%
1	32	183	42%	17%	23%	18%
1	36	183	42%	17%	23%	18%
1	3A	183	42%	17%	23%	18%
1	3E	183	42%	17%	23%	18%
1	3I	183	42%	17%	23%	18%
1	3M	183	42%	17%	23%	18%
1	3Q	183	42%	17%	23%	18%
1	3U	183	42%	17%	23%	18%
1	3Y	183	42%	17%	23%	18%
1	42	183	42%	17%	23%	18%
1	46	183	42%	17%	23%	18%
1	4A	183	42%	17%	23%	18%
1	4E	183	42%	17%	23%	18%
1	4I	183	42%	17%	23%	18%
1	4M	183	42%	17%	23%	18%
1	4Q	183	42%	17%	23%	18%
1	4U	183	42%	17%	23%	18%

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Mol	Chain	Length	Quality of chain			
1	4Y	183	42%	17%	23%	18%
1	52	183	42%	17%	23%	18%
1	56	183	42%	17%	23%	18%
1	5A	183	42%	17%	23%	18%
1	5E	183	42%	17%	23%	18%
1	5I	183	42%	17%	23%	18%
1	5M	183	42%	17%	23%	18%
1	5Q	183	42%	17%	23%	18%
1	5U	183	42%	17%	23%	18%
1	5Y	183	42%	17%	23%	18%
1	62	183	42%	17%	23%	18%
1	66	183	42%	17%	23%	18%
1	6A	183	42%	17%	23%	18%
1	6E	183	42%	17%	23%	18%
1	6I	183	42%	17%	23%	18%
1	6M	183	42%	17%	23%	18%
1	6Q	183	42%	17%	23%	18%
1	6U	183	42%	17%	23%	18%
1	6Y	183	42%	17%	23%	18%
1	7A	183	42%	17%	23%	18%
1	7E	183	42%	17%	23%	18%
1	7I	183	42%	17%	23%	18%
1	7M	183	42%	17%	23%	18%
1	7Q	183	42%	17%	23%	18%
1	7U	183	42%	17%	23%	18%

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Mol	Chain	Length	Quality of chain			
2	13	229	46%	21%	16%	17%
2	17	229	46%	21%	16%	17%
2	1B	229	46%	21%	16%	17%
2	1F	229	46%	21%	16%	17%
2	1J	229	46%	21%	16%	17%
2	1N	229	46%	21%	16%	17%
2	1R	229	46%	21%	16%	17%
2	1V	229	46%	21%	16%	17%
2	1Z	229	46%	21%	16%	17%
2	23	229	46%	21%	16%	17%
2	27	229	46%	21%	16%	17%
2	2B	229	46%	21%	16%	17%
2	2F	229	46%	21%	16%	17%
2	2J	229	46%	21%	16%	17%
2	2N	229	46%	21%	16%	17%
2	2R	229	46%	21%	16%	17%
2	2V	229	46%	21%	16%	17%
2	2Z	229	46%	21%	16%	17%
2	33	229	46%	21%	16%	17%
2	37	229	46%	21%	16%	17%
2	3B	229	46%	21%	16%	17%
2	3F	229	46%	21%	16%	17%
2	3J	229	46%	21%	16%	17%
2	3N	229	46%	21%	16%	17%
2	3R	229	46%	21%	16%	17%




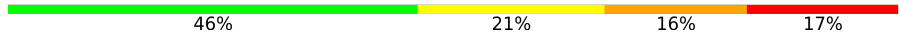
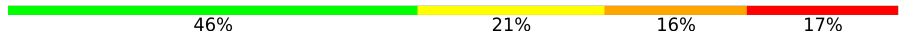
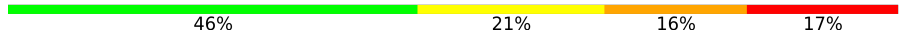
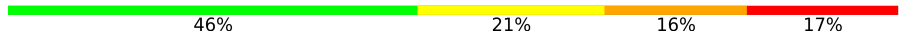
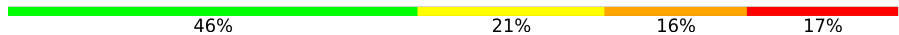
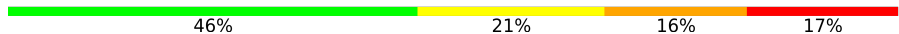
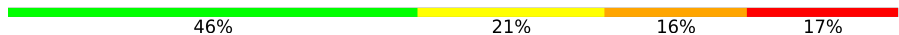















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Mol	Chain	Length	Quality of chain			
2	3V	229	46%	21%	16%	17%
2	3Z	229	46%	21%	16%	17%
2	43	229	46%	21%	16%	17%
2	47	229	46%	21%	16%	17%
2	4B	229	46%	21%	16%	17%
2	4F	229	46%	21%	16%	17%
2	4J	229	46%	21%	16%	17%
2	4N	229	46%	21%	16%	17%
2	4R	229	46%	21%	16%	17%
2	4V	229	46%	21%	16%	17%
2	4Z	229	46%	21%	16%	17%
2	53	229	46%	21%	16%	17%
2	57	229	46%	21%	16%	17%
2	5B	229	46%	21%	16%	17%
2	5F	229	46%	21%	16%	17%
2	5J	229	46%	21%	16%	17%
2	5N	229	46%	21%	16%	17%
2	5R	229	46%	21%	16%	17%
2	5V	229	46%	21%	16%	17%
2	5Z	229	46%	21%	16%	17%
2	63	229	46%	21%	16%	17%
2	67	229	46%	21%	16%	17%
2	6B	229	46%	21%	16%	17%
2	6F	229	46%	21%	16%	17%
2	6J	229	46%	21%	16%	17%


























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Mol	Chain	Length	Quality of chain
2	6N	229	 46% 21% 16% 17%
2	6R	229	 46% 21% 16% 17%
2	6V	229	 46% 21% 16% 17%
2	6Z	229	 46% 21% 16% 17%
2	7B	229	 46% 21% 16% 17%
2	7F	229	 46% 21% 16% 17%
2	7J	229	 46% 21% 16% 17%
2	7N	229	 46% 21% 16% 17%
2	7R	229	 46% 21% 16% 17%
2	7V	229	 46% 21% 16% 17%
3	10	109	 88% 11% .
3	14	109	 88% 11% .
3	18	109	 88% 11% .
3	1C	109	 88% 11% .
3	1G	109	 88% 11% .
3	1K	109	 88% 11% .
3	1O	109	 89% 10% .
3	1S	109	 88% 11% .
3	1W	109	 88% 11% .
3	20	109	 88% 11% .
3	24	109	 88% 11% .
3	28	109	 88% 11% .
3	2C	109	 88% 11% .
3	2G	109	 88% 11% .
3	2K	109	 89% 10% .

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Mol	Chain	Length	Quality of chain
3	2O	109	 88% 11%
3	2S	109	 88% 11%
3	2W	109	 88% 11%
3	30	109	 88% 11%
3	34	109	 89% 10%
3	38	109	 88% 11%
3	3C	109	 89% 10%
3	3G	109	 88% 11%
3	3K	109	 89% 10%
3	3O	109	 88% 11%
3	3S	109	 88% 11%
3	3W	109	 88% 11%
3	40	109	 89% 10%
3	44	109	 88% 11%
3	48	109	 88% 11%
3	4C	109	 88% 11%
3	4G	109	 89% 10%
3	4K	109	 88% 11%
3	4O	109	 88% 11%
3	4S	109	 88% 11%
3	4W	109	 88% 11%
3	50	109	 88% 11%
3	54	109	 88% 11%
3	58	109	 88% 11%
3	5C	109	 88% 11%

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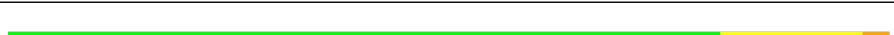

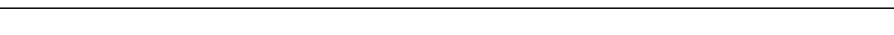
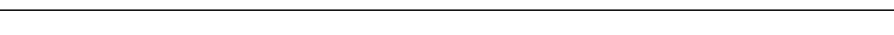
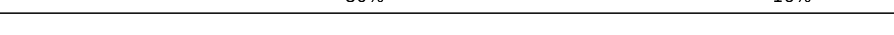

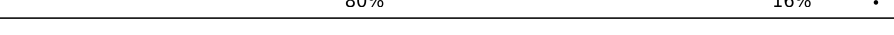









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Mol	Chain	Length	Quality of chain
3	5G	109	 88% 11%
3	5K	109	 88% 11%
3	5O	109	 88% 11%
3	5S	109	 88% 11%
3	5W	109	 89% 10%
3	60	109	 88% 11%
3	64	109	 88% 11%
3	68	109	 88% 11%
3	6C	109	 88% 11%
3	6G	109	 88% 11%
3	6K	109	 88% 11%
3	6O	109	 89% 10%
3	6S	109	 88% 11%
3	6W	109	 89% 10%
3	7C	109	 88% 11%
3	7G	109	 89% 10%
3	7K	109	 88% 11%
3	7O	109	 88% 11%
3	7S	109	 89% 10%
3	7W	109	 88% 11%
4	11	122	 80% 16%
4	15	122	 80% 16%
4	19	122	 80% 16%
4	1D	122	 80% 16%
4	1H	122	 80% 16%












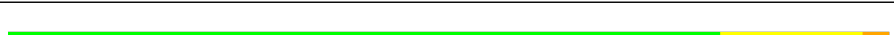

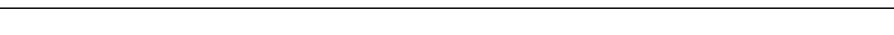
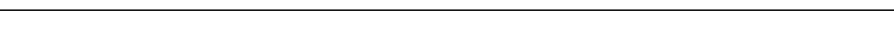
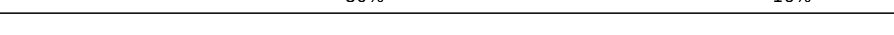

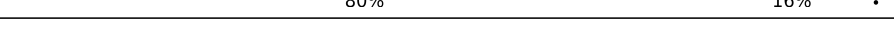







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Mol	Chain	Length	Quality of chain
4	1L	122	
4	1P	122	
4	1T	122	
4	1X	122	
4	2I	122	
4	25	122	
4	29	122	
4	2D	122	
4	2H	122	
4	2L	122	
4	2P	122	
4	2T	122	
4	2X	122	
4	3I	122	
4	35	122	
4	39	122	
4	3D	122	
4	3H	122	
4	3L	122	
4	3P	122	
4	3T	122	
4	3X	122	
4	4I	122	
4	45	122	
4	49	122	

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Mol	Chain	Length	Quality of chain
4	4D	122	 80% 16%
4	4H	122	 80% 16%
4	4L	122	 80% 16%
4	4P	122	 80% 16%
4	4T	122	 80% 16%
4	4X	122	 80% 16%
4	51	122	 80% 16%
4	55	122	 80% 16%
4	59	122	 80% 16%
4	5D	122	 80% 16%
4	5H	122	 80% 16%
4	5L	122	 80% 16%
4	5P	122	 80% 16%
4	5T	122	 80% 16%
4	5X	122	 80% 16%
4	61	122	 80% 16%
4	65	122	 80% 16%
4	69	122	 80% 16%
4	6D	122	 80% 16%
4	6H	122	 80% 16%
4	6L	122	 80% 16%
4	6P	122	 80% 16%
4	6T	122	 80% 16%
4	6X	122	 80% 16%
4	7D	122	 80% 16%

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Mol	Chain	Length	Quality of chain
4	7H	122	 80% 16% .
4	7L	122	 80% 16% .
4	7P	122	 80% 16% .
4	7T	122	 80% 16% .
4	7X	122	 80% 16% .

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 326520 atoms, of which 24420 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 Protein VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1A	183	1449	926	244	272	7	0	0
1	1E	183	1449	926	244	272	7	0	0
1	1I	183	1449	926	244	272	7	0	0
1	1M	183	1449	926	244	272	7	0	0
1	1Q	183	1449	926	244	272	7	0	0
1	1U	183	1449	926	244	272	7	0	0
1	1Y	183	1449	926	244	272	7	0	0
1	12	183	1449	926	244	272	7	0	0
1	16	183	1449	926	244	272	7	0	0
1	2A	183	1449	926	244	272	7	0	0
1	2E	183	1449	926	244	272	7	0	0
1	2I	183	1449	926	244	272	7	0	0
1	2M	183	1449	926	244	272	7	0	0
1	2Q	183	1449	926	244	272	7	0	0
1	2U	183	1449	926	244	272	7	0	0
1	2Y	183	1449	926	244	272	7	0	0
1	22	183	1449	926	244	272	7	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	26	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	3A	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	3E	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	3I	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	3M	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	3Q	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	3U	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	3Y	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	32	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	36	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	4A	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	4E	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	4I	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	4M	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	4Q	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	4U	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	4Y	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	42	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	46	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	5A	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	5E	183	Total 1449	C 926	N 244	O 272	S 7	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	5I	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	5M	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	5Q	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	5U	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	5Y	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	5Z	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	56	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	6A	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	6E	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	6I	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	6M	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	6Q	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	6U	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	6Y	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	6Z	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	66	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	7A	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	7E	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	7I	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	7M	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	7Q	183	Total 1449	C 926	N 244	O 272	S 7	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	7U	183	1449	926	244	272	7	0	0

- Molecule 2 is a protein called Protein VP0.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1B	229	1810	1151	301	353	5	0	0
2	1F	229	1810	1151	301	353	5	0	0
2	1J	229	1810	1151	301	353	5	0	0
2	1N	229	1810	1151	301	353	5	0	0
2	1R	229	1810	1151	301	353	5	0	0
2	1V	229	1810	1151	301	353	5	0	0
2	1Z	229	1810	1151	301	353	5	0	0
2	13	229	1810	1151	301	353	5	0	0
2	17	229	1810	1151	301	353	5	0	0
2	2B	229	1810	1151	301	353	5	0	0
2	2F	229	1810	1151	301	353	5	0	0
2	2J	229	1810	1151	301	353	5	0	0
2	2N	229	1810	1151	301	353	5	0	0
2	2R	229	1810	1151	301	353	5	0	0
2	2V	229	1810	1151	301	353	5	0	0
2	2Z	229	1810	1151	301	353	5	0	0
2	23	229	1810	1151	301	353	5	0	0
2	27	229	1810	1151	301	353	5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	3B	229	Total 1810	C 1151	N 301	O 353	S 5	0	0
2	3F	229	Total 1810	C 1151	N 301	O 353	S 5	0	0
2	3J	229	Total 1810	C 1151	N 301	O 353	S 5	0	0
2	3N	229	Total 1810	C 1151	N 301	O 353	S 5	0	0
2	3R	229	Total 1810	C 1151	N 301	O 353	S 5	0	0
2	3V	229	Total 1810	C 1151	N 301	O 353	S 5	0	0
2	3Z	229	Total 1810	C 1151	N 301	O 353	S 5	0	0
2	33	229	Total 1810	C 1151	N 301	O 353	S 5	0	0
2	37	229	Total 1810	C 1151	N 301	O 353	S 5	0	0
2	4B	229	Total 1810	C 1151	N 301	O 353	S 5	0	0
2	4F	229	Total 1810	C 1151	N 301	O 353	S 5	0	0
2	4J	229	Total 1810	C 1151	N 301	O 353	S 5	0	0
2	4N	229	Total 1810	C 1151	N 301	O 353	S 5	0	0
2	4R	229	Total 1810	C 1151	N 301	O 353	S 5	0	0
2	4V	229	Total 1810	C 1151	N 301	O 353	S 5	0	0
2	4Z	229	Total 1810	C 1151	N 301	O 353	S 5	0	0
2	43	229	Total 1810	C 1151	N 301	O 353	S 5	0	0
2	47	229	Total 1810	C 1151	N 301	O 353	S 5	0	0
2	5B	229	Total 1810	C 1151	N 301	O 353	S 5	0	0
2	5F	229	Total 1810	C 1151	N 301	O 353	S 5	0	0
2	5J	229	Total 1810	C 1151	N 301	O 353	S 5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	5N	229	Total	C	N	O	S	0	0
			1810	1151	301	353	5		
2	5R	229	Total	C	N	O	S	0	0
			1810	1151	301	353	5		
2	5V	229	Total	C	N	O	S	0	0
			1810	1151	301	353	5		
2	5Z	229	Total	C	N	O	S	0	0
			1810	1151	301	353	5		
2	53	229	Total	C	N	O	S	0	0
			1810	1151	301	353	5		
2	57	229	Total	C	N	O	S	0	0
			1810	1151	301	353	5		
2	6B	229	Total	C	N	O	S	0	0
			1810	1151	301	353	5		
2	6F	229	Total	C	N	O	S	0	0
			1810	1151	301	353	5		
2	6J	229	Total	C	N	O	S	0	0
			1810	1151	301	353	5		
2	6N	229	Total	C	N	O	S	0	0
			1810	1151	301	353	5		
2	6R	229	Total	C	N	O	S	0	0
			1810	1151	301	353	5		
2	6V	229	Total	C	N	O	S	0	0
			1810	1151	301	353	5		
2	6Z	229	Total	C	N	O	S	0	0
			1810	1151	301	353	5		
2	63	229	Total	C	N	O	S	0	0
			1810	1151	301	353	5		
2	67	229	Total	C	N	O	S	0	0
			1810	1151	301	353	5		
2	7B	229	Total	C	N	O	S	0	0
			1810	1151	301	353	5		
2	7F	229	Total	C	N	O	S	0	0
			1810	1151	301	353	5		
2	7J	229	Total	C	N	O	S	0	0
			1810	1151	301	353	5		
2	7N	229	Total	C	N	O	S	0	0
			1810	1151	301	353	5		
2	7R	229	Total	C	N	O	S	0	0
			1810	1151	301	353	5		
2	7V	229	Total	C	N	O	S	0	0
			1810	1151	301	353	5		

- Molecule 3 is a protein called HUMAN MONOCLONAL ANTIBODY.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
3	1C	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	1G	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	1K	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	1O	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	1S	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	1W	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	10	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	14	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	18	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	2C	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	2G	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	2K	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	2O	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	2S	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	2W	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	20	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	24	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	28	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	3C	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	3G	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	3K	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0

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Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	3O	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	3S	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	3W	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	30	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	34	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	38	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	4C	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	4G	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	4K	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	4O	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	4S	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	4W	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	40	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	44	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	48	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	5C	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	5G	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	5K	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	5O	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	5S	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	5W	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0

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Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
3	50	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	54	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	58	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	6C	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	6G	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	6K	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	6O	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	6S	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	6W	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	60	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	64	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	68	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	7C	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	7G	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	7K	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	7O	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	7S	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0
3	7W	109	Total 1057	C 541	H 199	N 144	O 170	S 3	17	0

- Molecule 4 is a protein called HUMAN MONOCLONAL ANTIBODY.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
4	1D	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0

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Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
4	1H	122	1126	573	208	155	186	4	15	0
4	1L	122	1126	573	208	155	186	4	15	0
4	1P	122	1126	573	208	155	186	4	15	0
4	1T	122	1126	573	208	155	186	4	15	0
4	1X	122	1126	573	208	155	186	4	15	0
4	11	122	1126	573	208	155	186	4	15	0
4	15	122	1126	573	208	155	186	4	15	0
4	19	122	1126	573	208	155	186	4	15	0
4	2D	122	1126	573	208	155	186	4	15	0
4	2H	122	1126	573	208	155	186	4	15	0
4	2L	122	1126	573	208	155	186	4	15	0
4	2P	122	1126	573	208	155	186	4	15	0
4	2T	122	1126	573	208	155	186	4	15	0
4	2X	122	1126	573	208	155	186	4	15	0
4	21	122	1126	573	208	155	186	4	15	0
4	25	122	1126	573	208	155	186	4	15	0
4	29	122	1126	573	208	155	186	4	15	0
4	3D	122	1126	573	208	155	186	4	15	0
4	3H	122	1126	573	208	155	186	4	15	0
4	3L	122	1126	573	208	155	186	4	15	0
4	3P	122	1126	573	208	155	186	4	15	0

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Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
4	3T	122	1126	573	208	155	186	4	15	0
4	3X	122	1126	573	208	155	186	4	15	0
4	3I	122	1126	573	208	155	186	4	15	0
4	35	122	1126	573	208	155	186	4	15	0
4	39	122	1126	573	208	155	186	4	15	0
4	4D	122	1126	573	208	155	186	4	15	0
4	4H	122	1126	573	208	155	186	4	15	0
4	4L	122	1126	573	208	155	186	4	15	0
4	4P	122	1126	573	208	155	186	4	15	0
4	4T	122	1126	573	208	155	186	4	15	0
4	4X	122	1126	573	208	155	186	4	15	0
4	4I	122	1126	573	208	155	186	4	15	0
4	45	122	1126	573	208	155	186	4	15	0
4	49	122	1126	573	208	155	186	4	15	0
4	5D	122	1126	573	208	155	186	4	15	0
4	5H	122	1126	573	208	155	186	4	15	0
4	5L	122	1126	573	208	155	186	4	15	0
4	5P	122	1126	573	208	155	186	4	15	0
4	5T	122	1126	573	208	155	186	4	15	0
4	5X	122	1126	573	208	155	186	4	15	0
4	5I	122	1126	573	208	155	186	4	15	0

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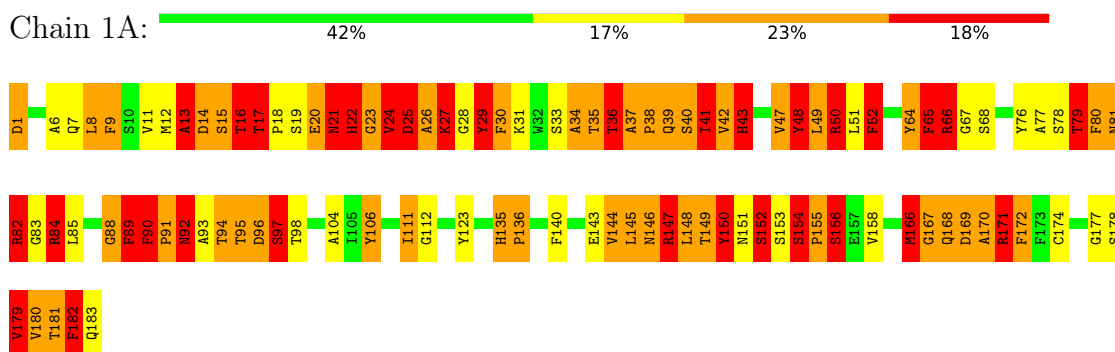
Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
4	55	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	59	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	6D	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	6H	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	6L	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	6P	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	6T	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	6X	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	61	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	65	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	69	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	7D	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	7H	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	7L	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	7P	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	7T	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	7X	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0



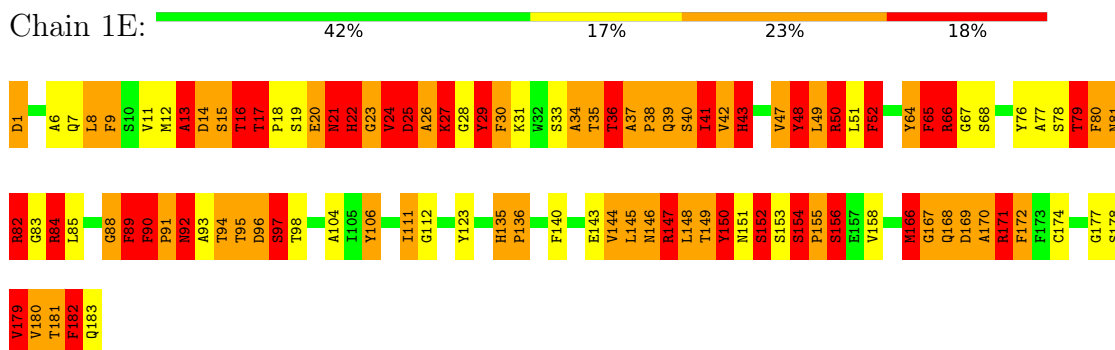
### 3 Residue-property plots [i](#)

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

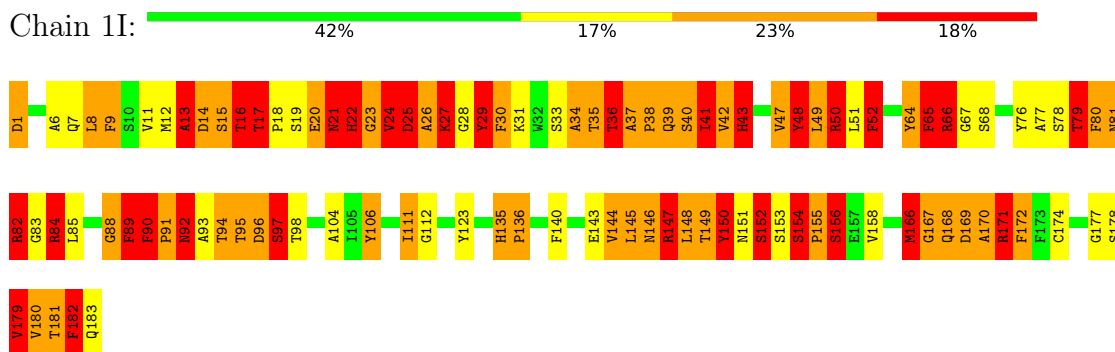
- Molecule 1: Protein VP3



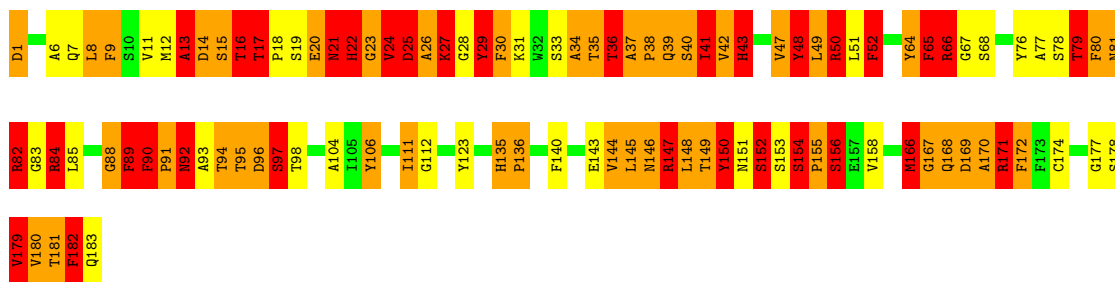
- Molecule 1: Protein VP3



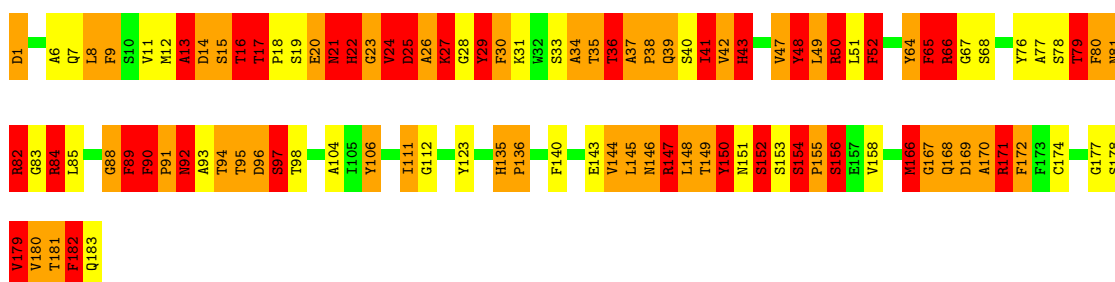
- Molecule 1: Protein VP3



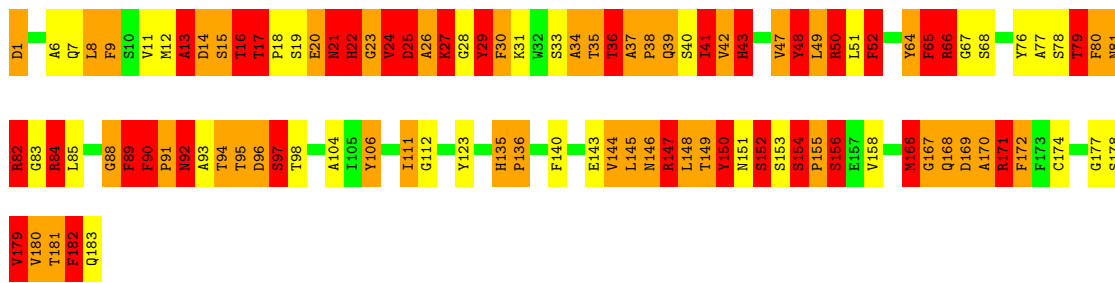
- Molecule 1: Protein VP3



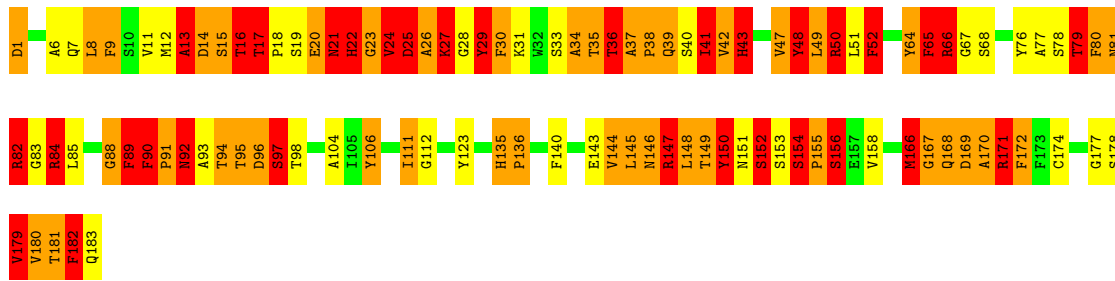
• Molecule 1: Protein VP3



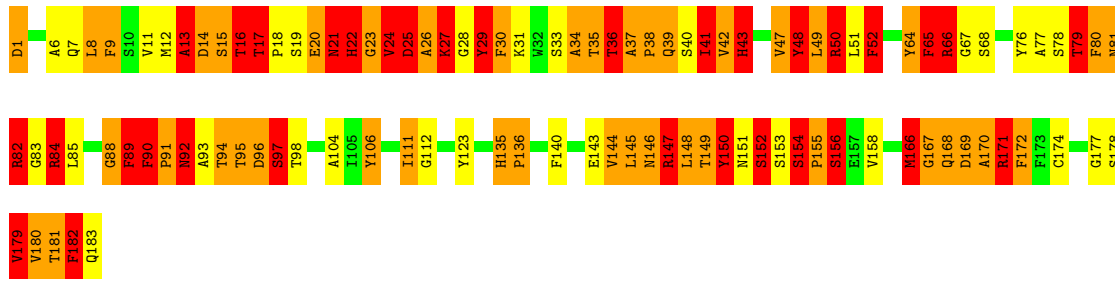
• Molecule 1: Protein VP3



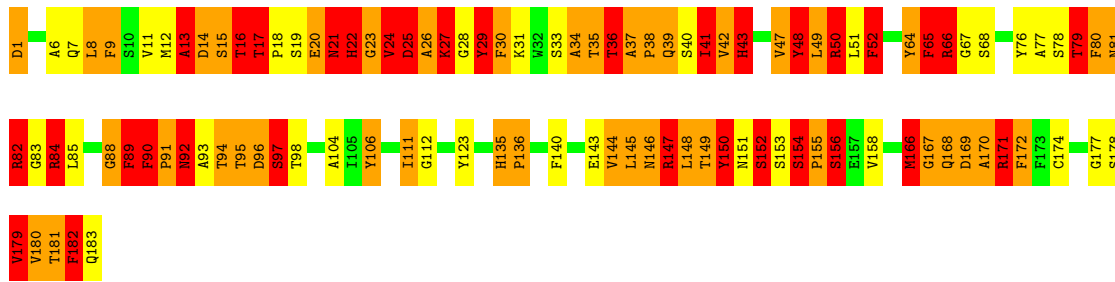
• Molecule 1: Protein VP3



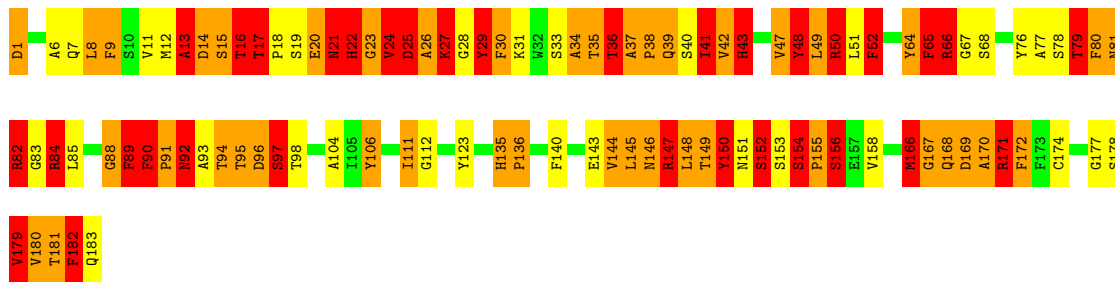
• Molecule 1: Protein VP3



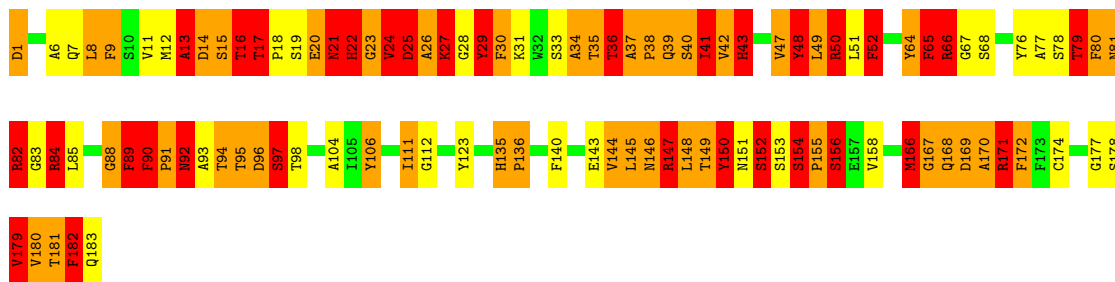
• Molecule 1: Protein VP3



• Molecule 1: Protein VP3

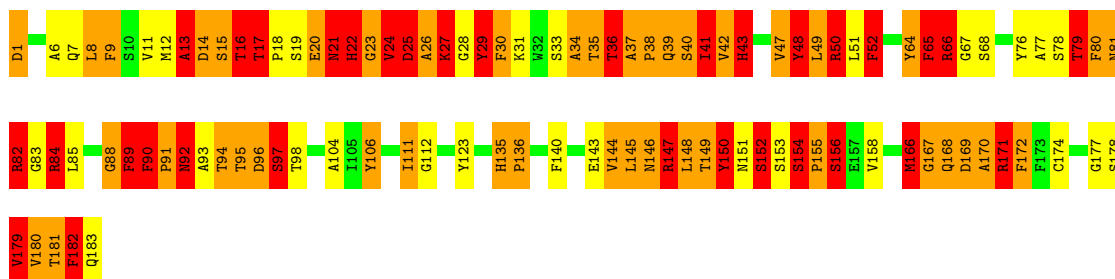


• Molecule 1: Protein VP3



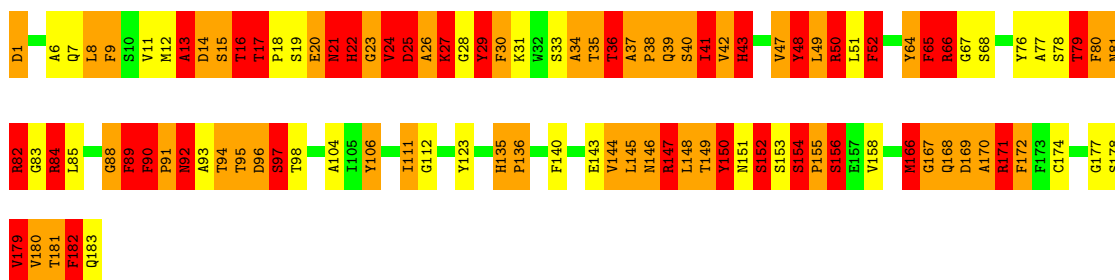
• Molecule 1: Protein VP3

Chain 2I:  42% 17% 23% 18%



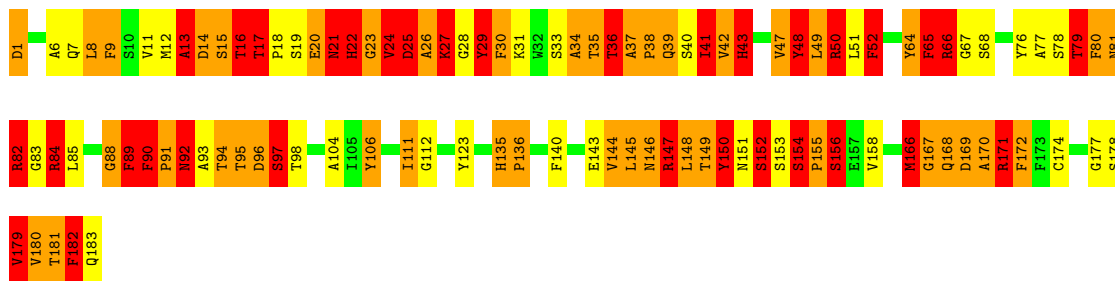
• Molecule 1: Protein VP3

Chain 2M:  42% 17% 23% 18%



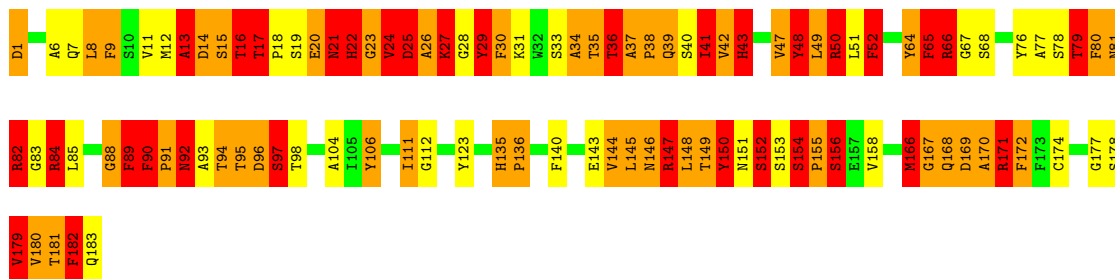
• Molecule 1: Protein VP3

Chain 2Q:  42% 17% 23% 18%

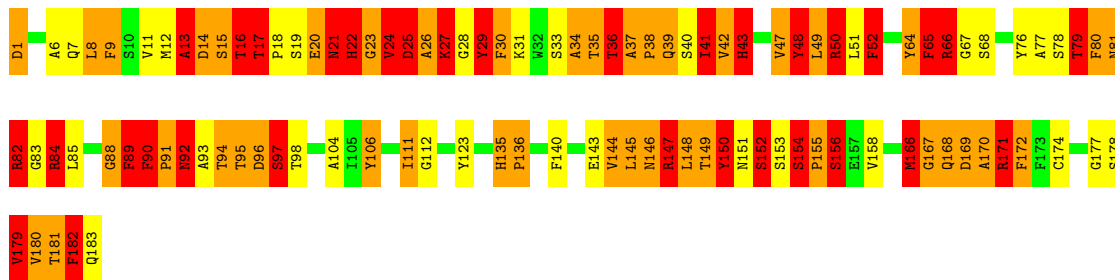


• Molecule 1: Protein VP3

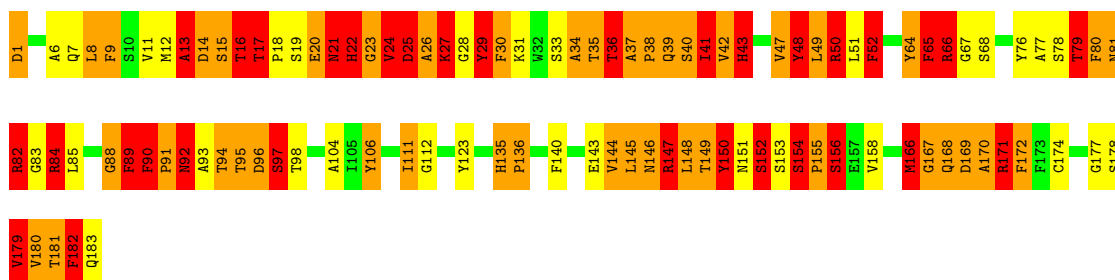
Chain 2U:  42% 17% 23% 18%



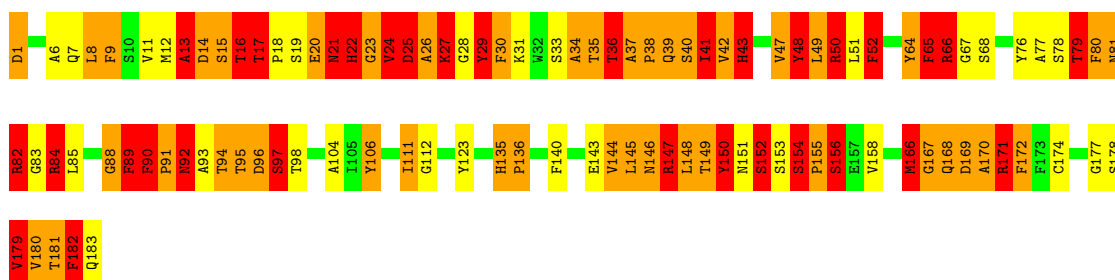
• Molecule 1: Protein VP3



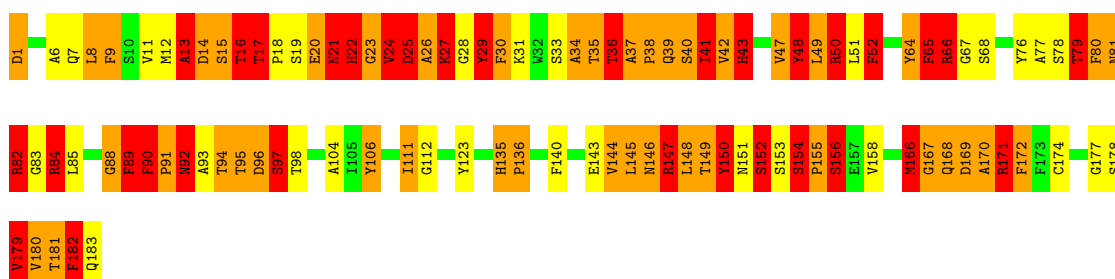
• Molecule 1: Protein VP3



• Molecule 1: Protein VP3



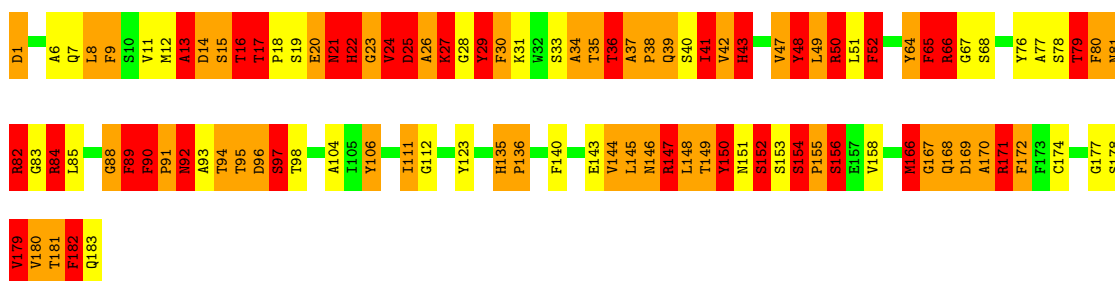
• Molecule 1: Protein VP3



• Molecule 1: Protein VP3

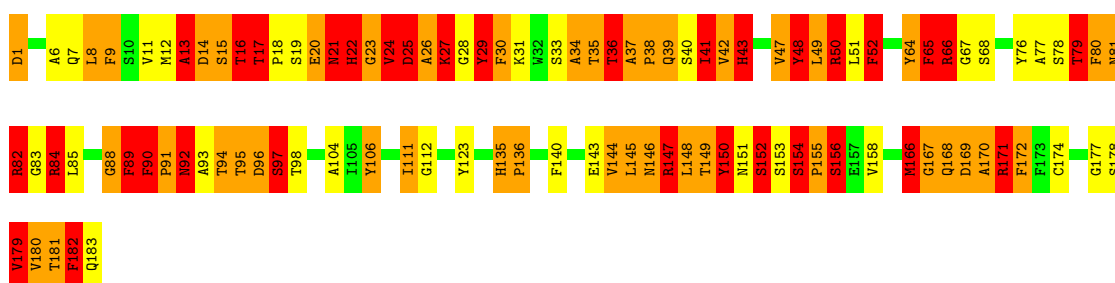


Chain 3U: 



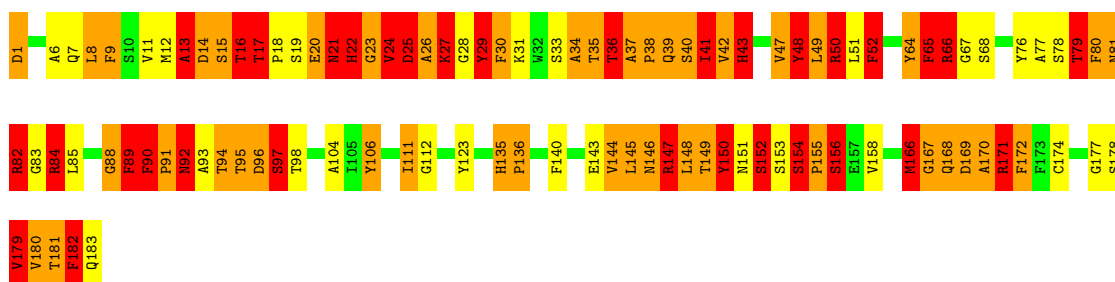
• Molecule 1: Protein VP3

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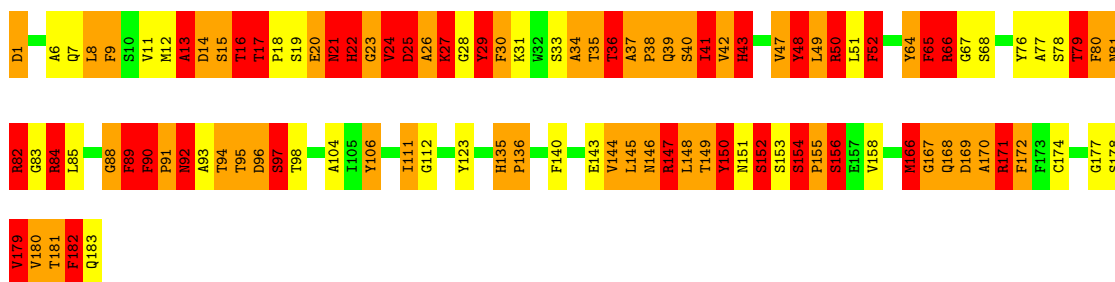
• Molecule 1: Protein VP3

Chain 32: 

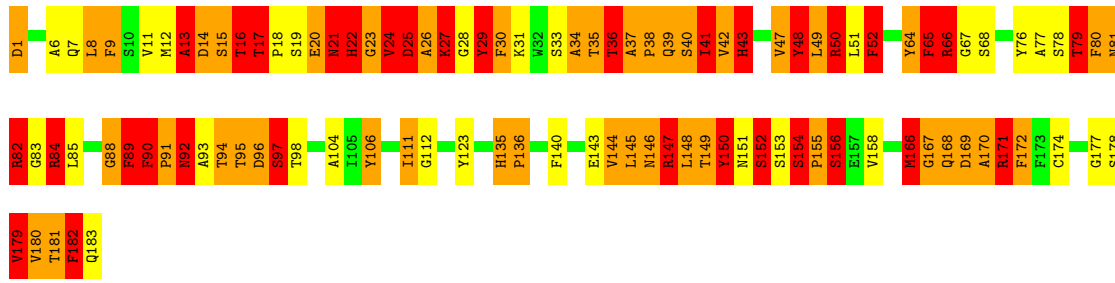


• Molecule 1: Protein VP3

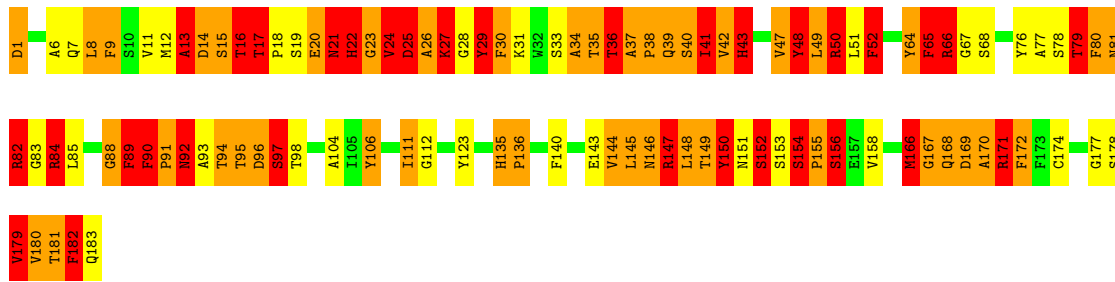
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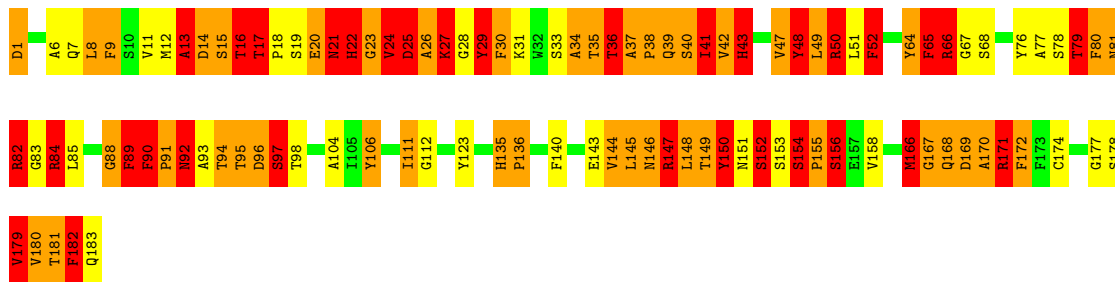
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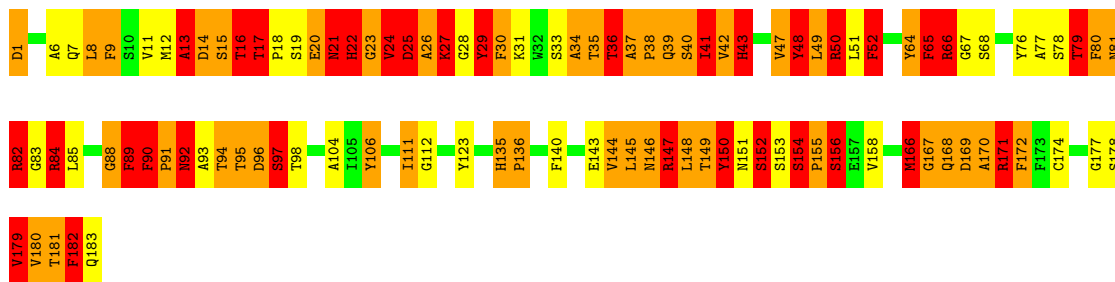
• Molecule 1: Protein VP3



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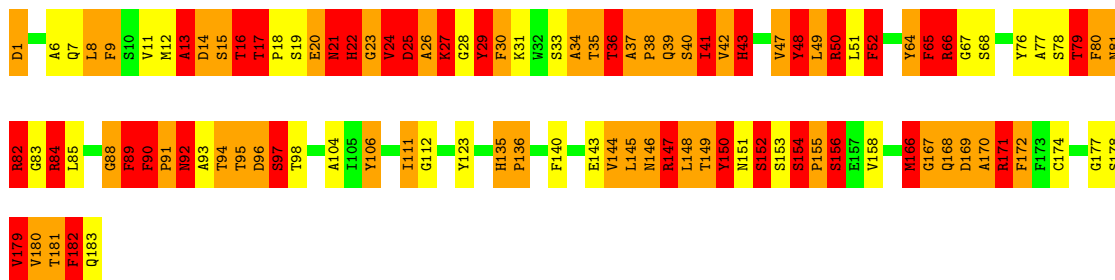


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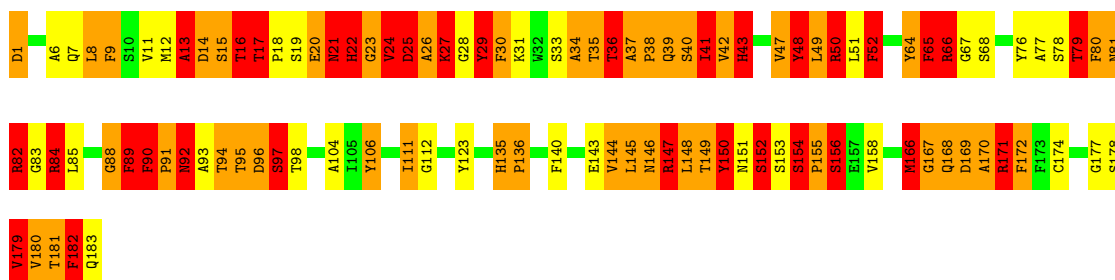


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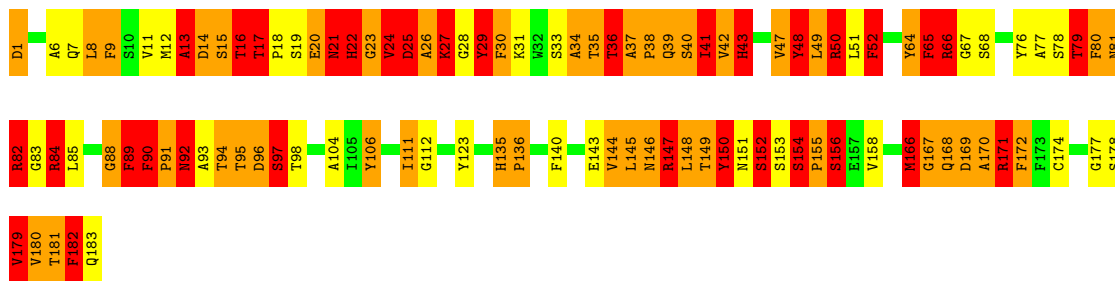




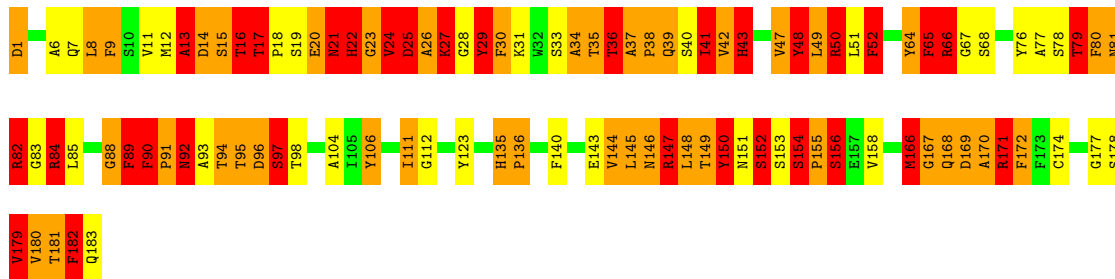
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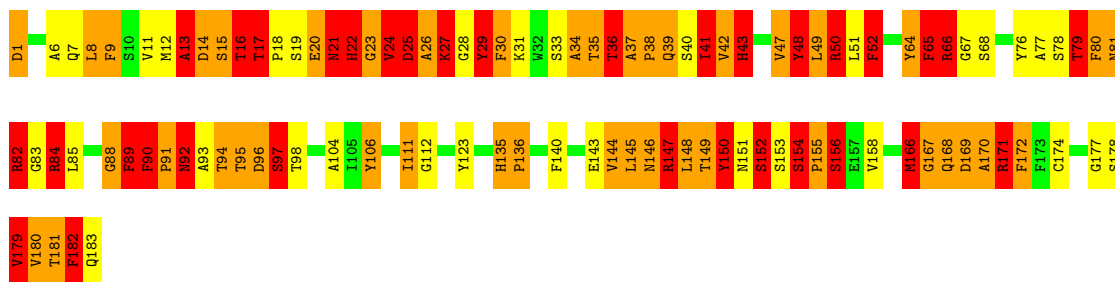
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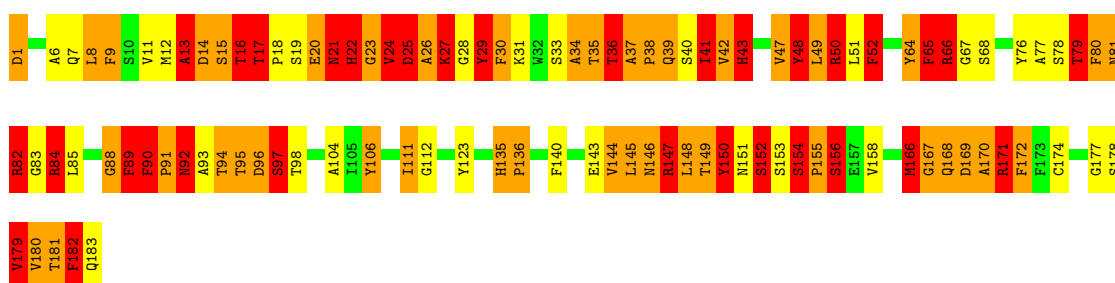
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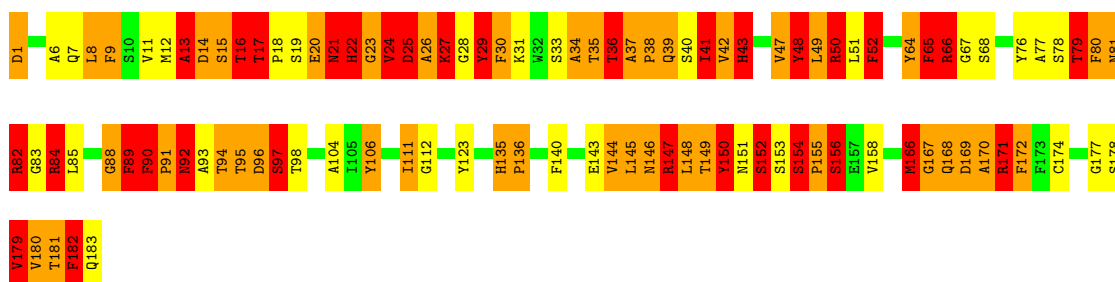
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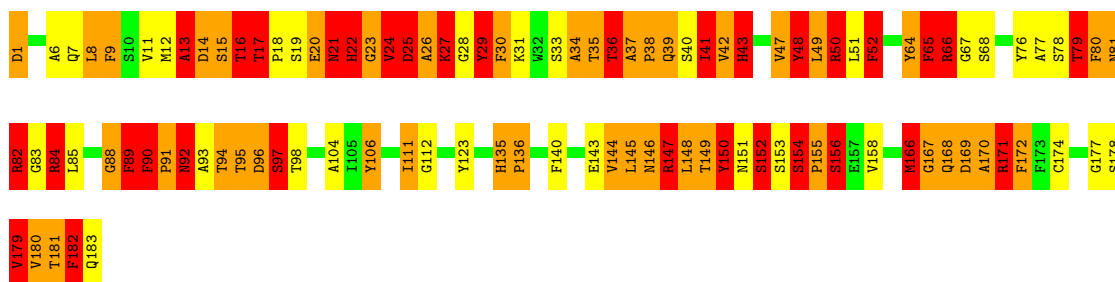
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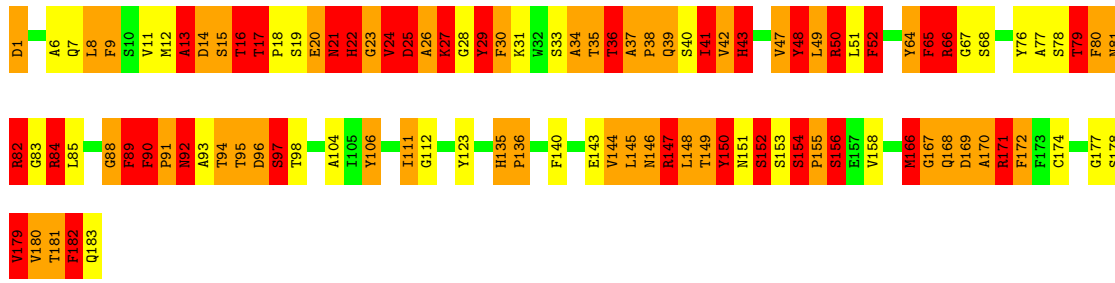


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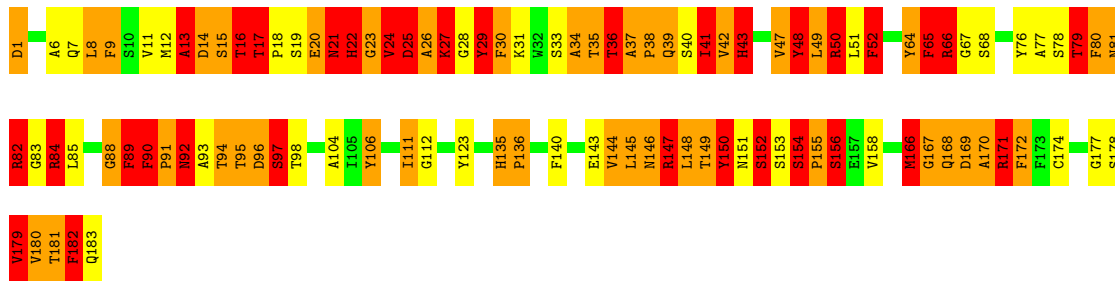


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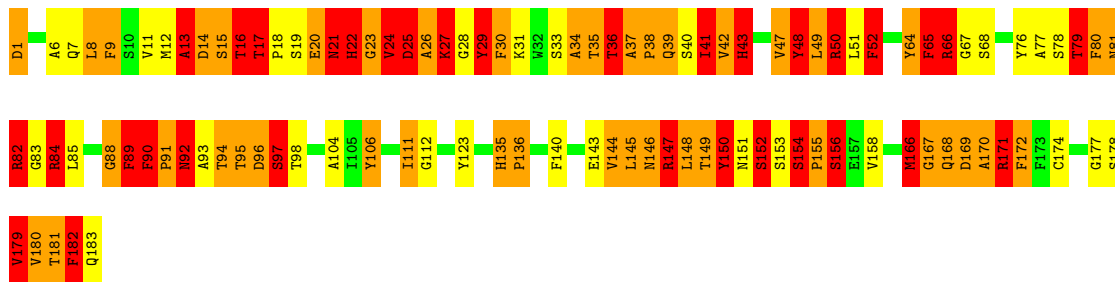




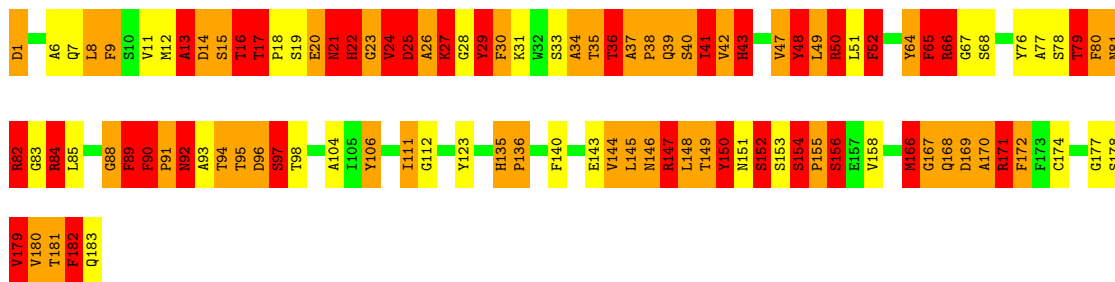
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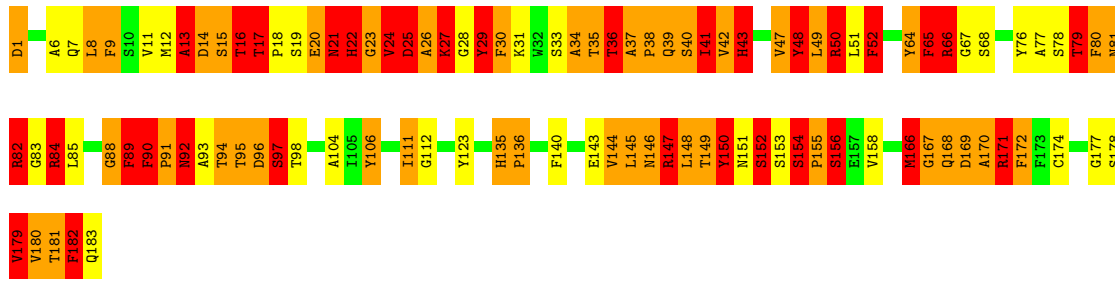
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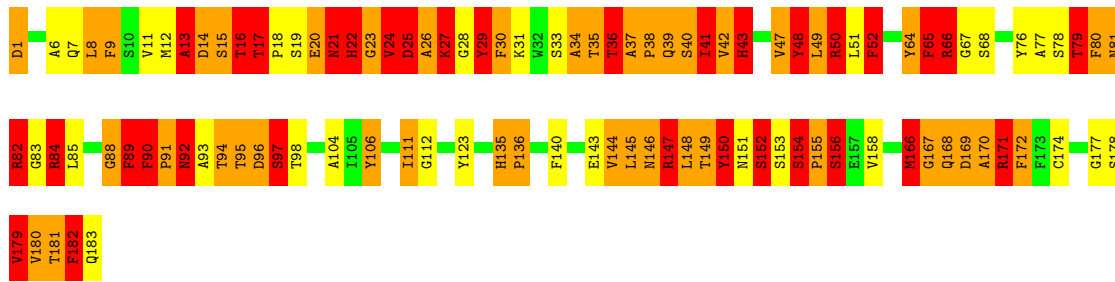
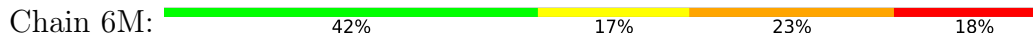
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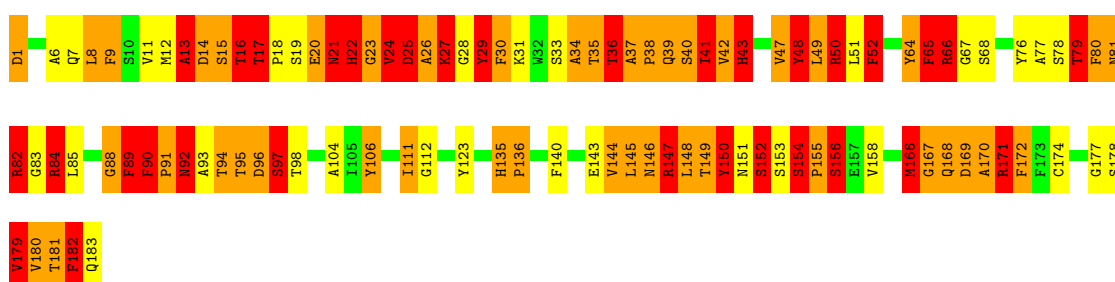
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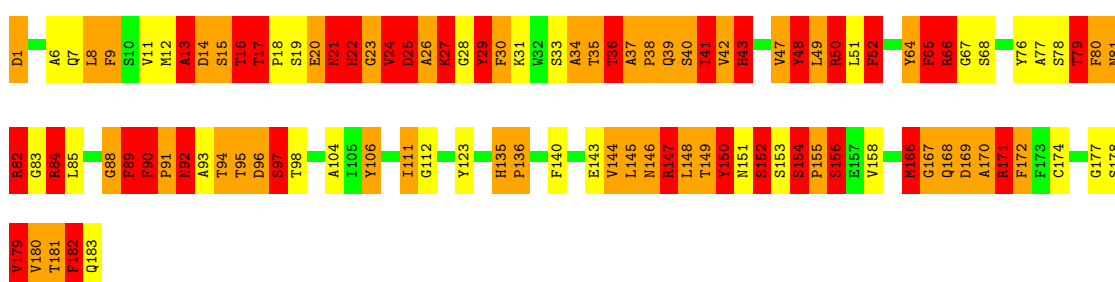
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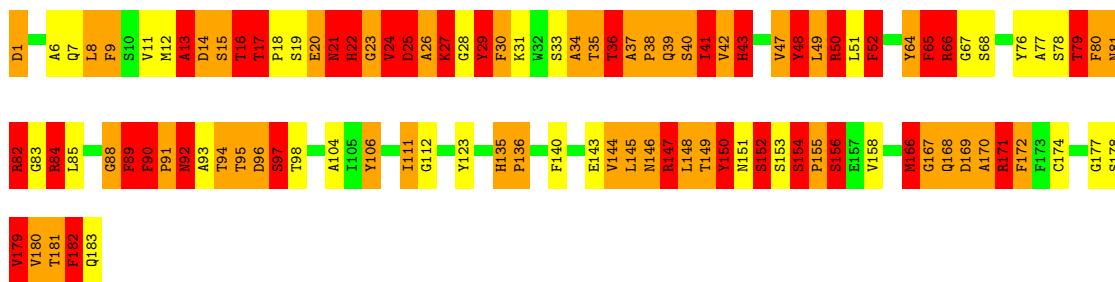
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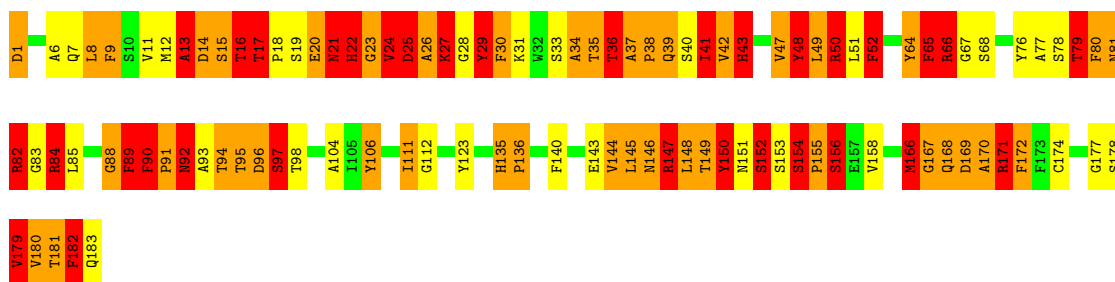
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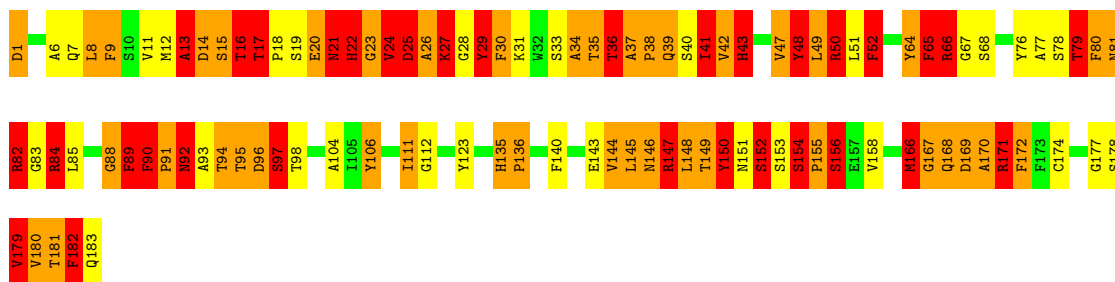
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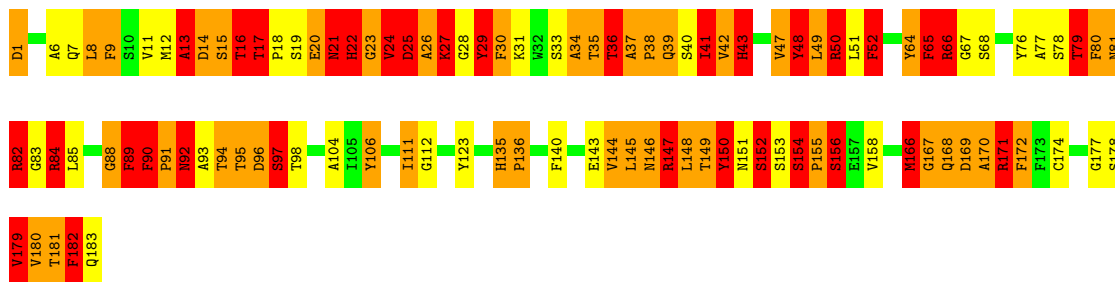
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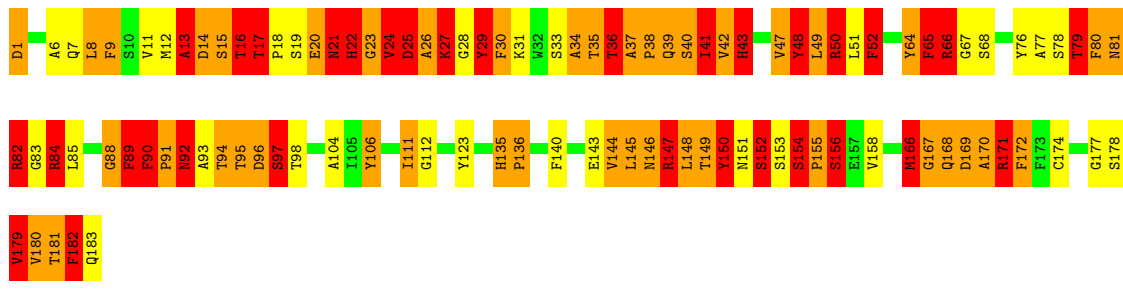
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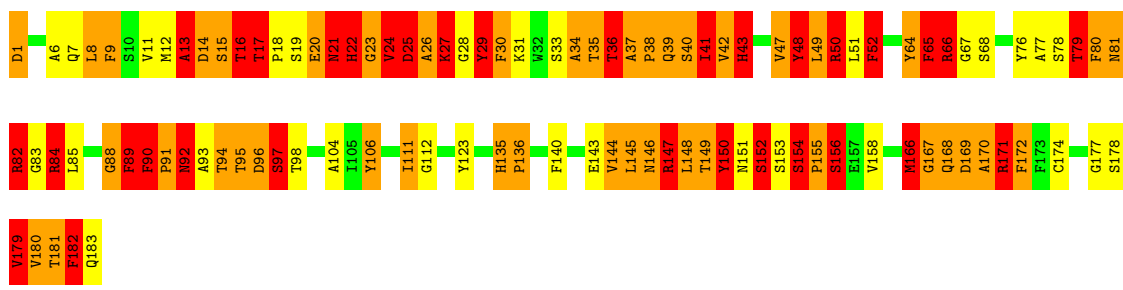
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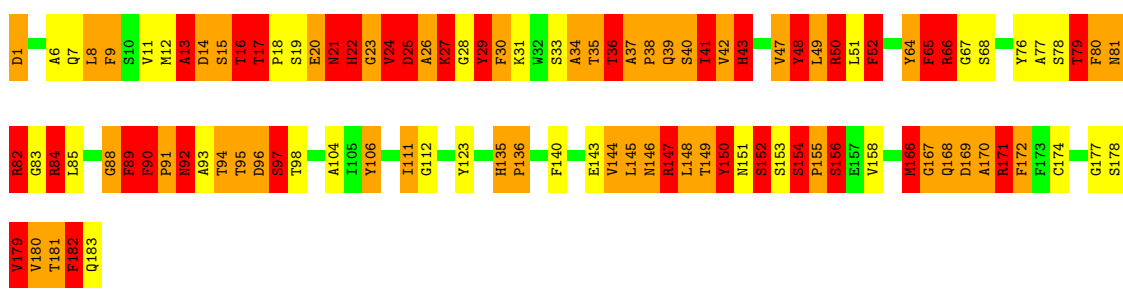
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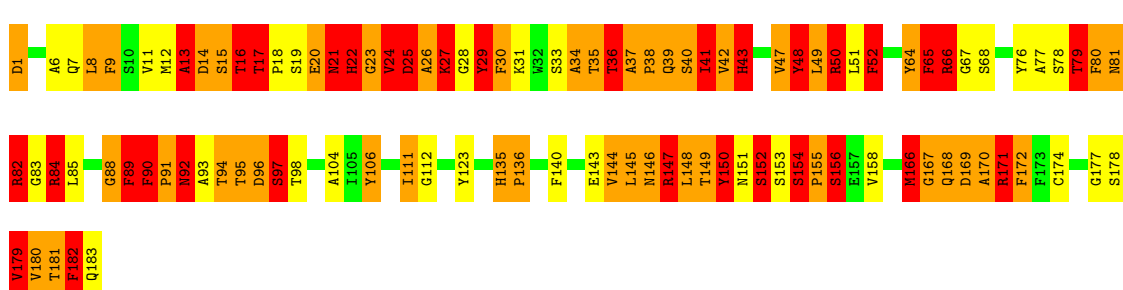
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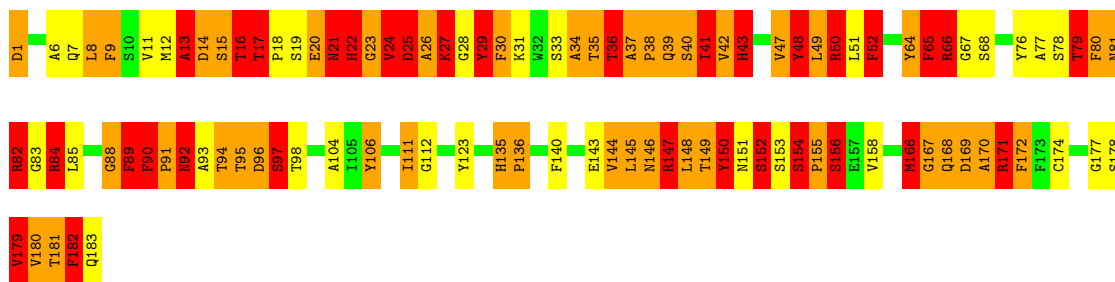
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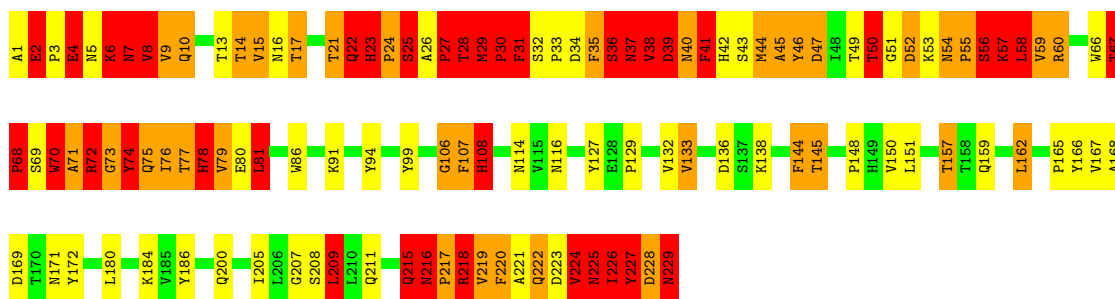
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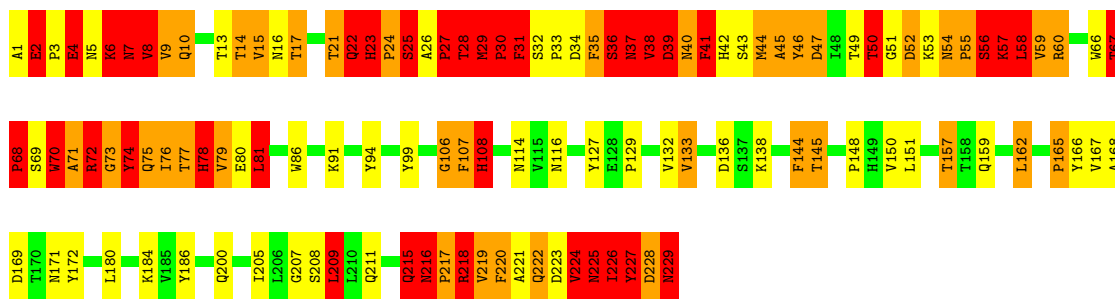
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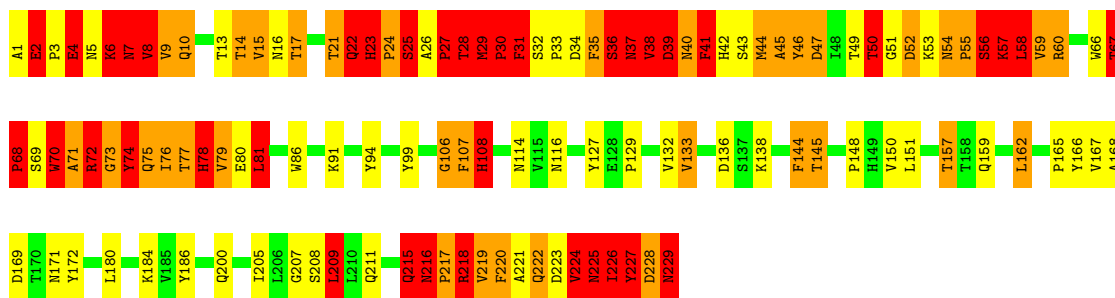
• Molecule 2: Protein VP0



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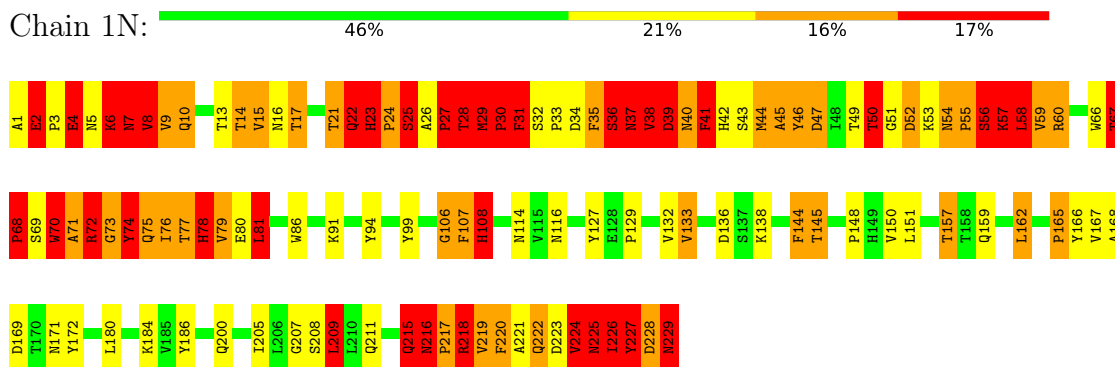


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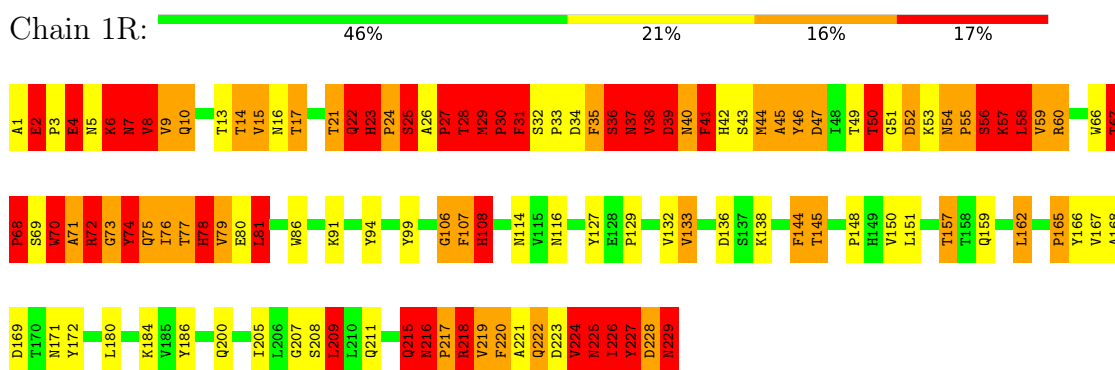




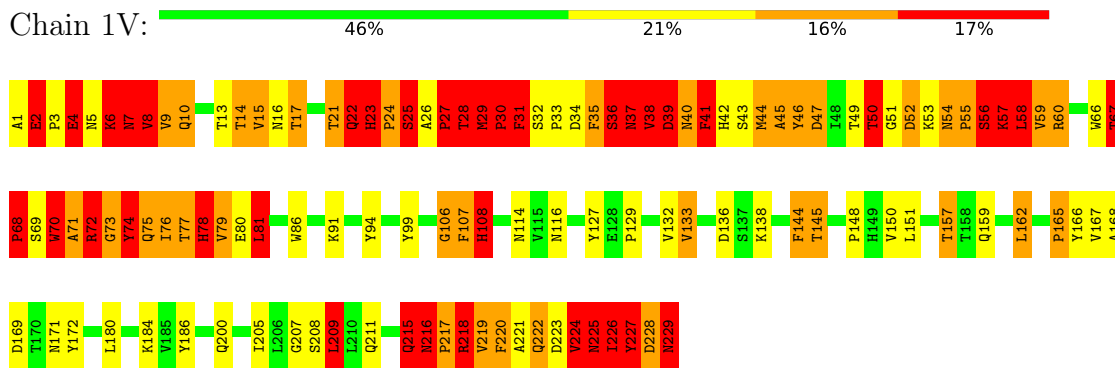
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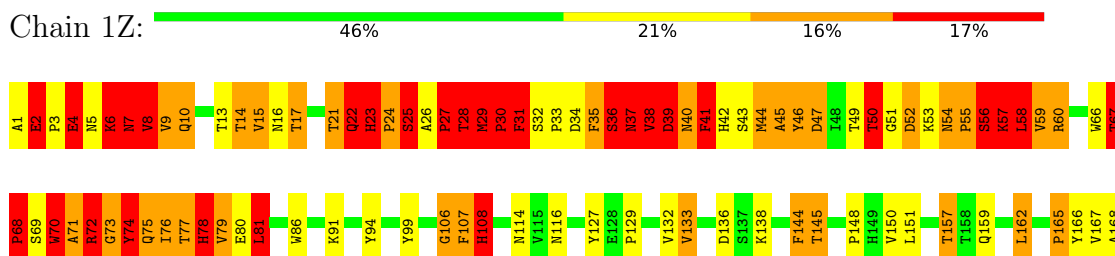
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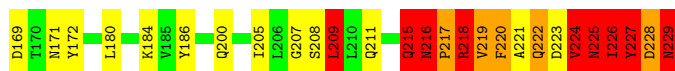


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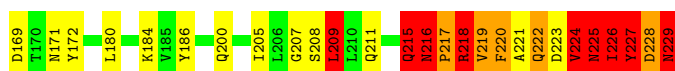
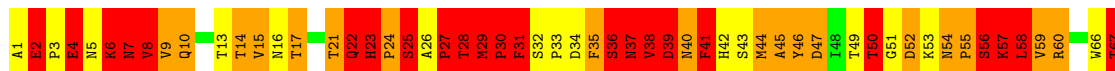


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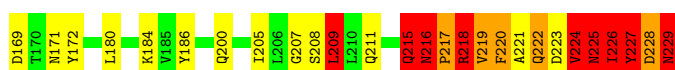
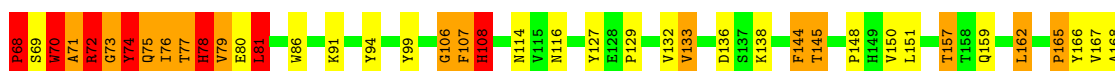
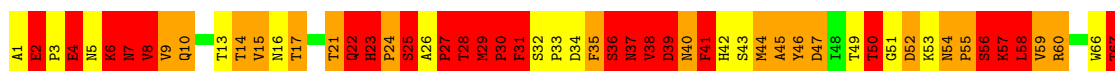




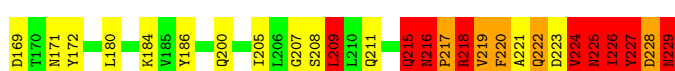
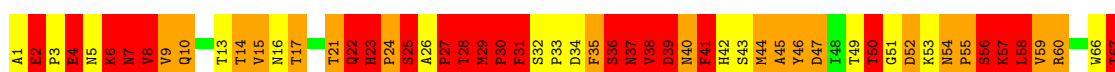
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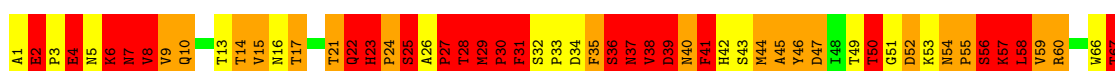
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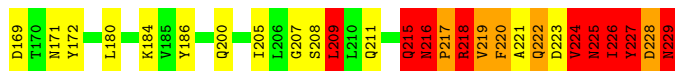


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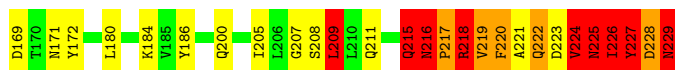
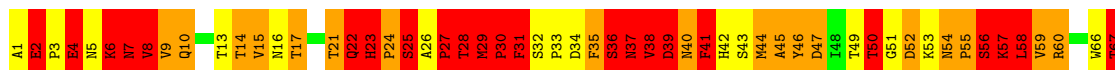


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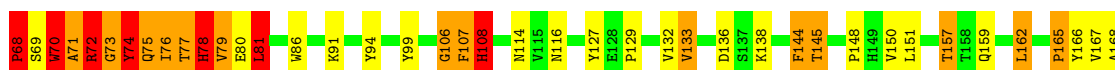
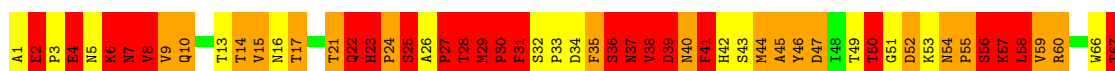




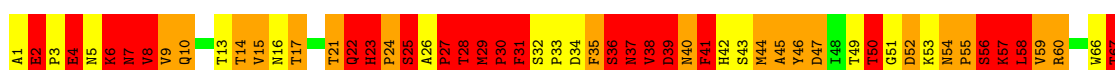
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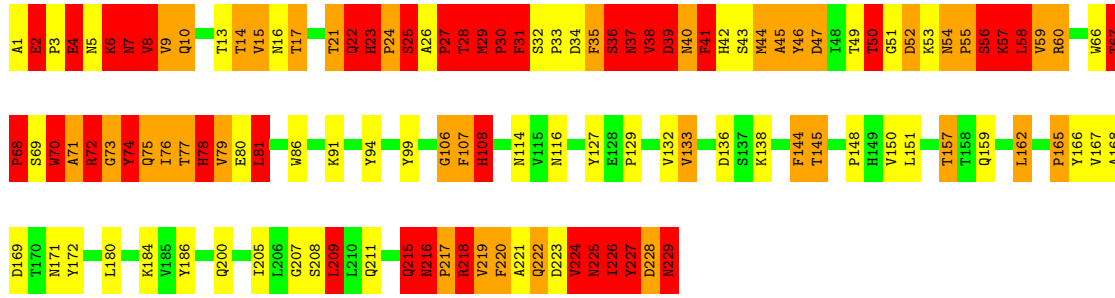


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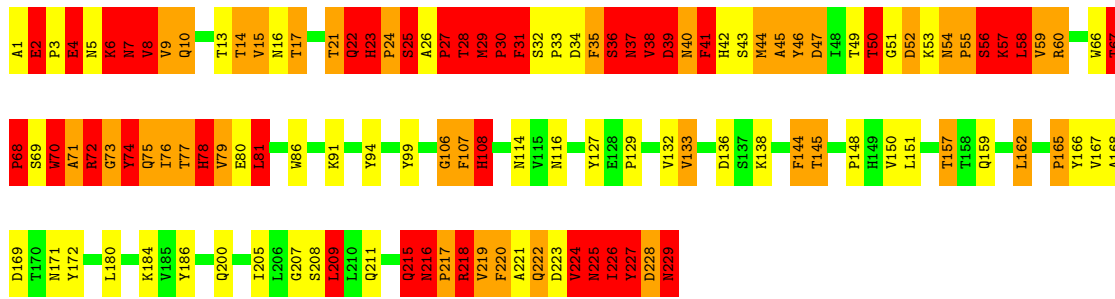


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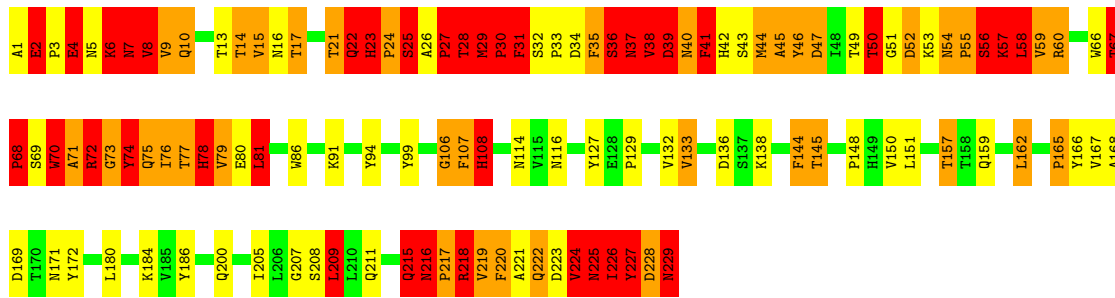




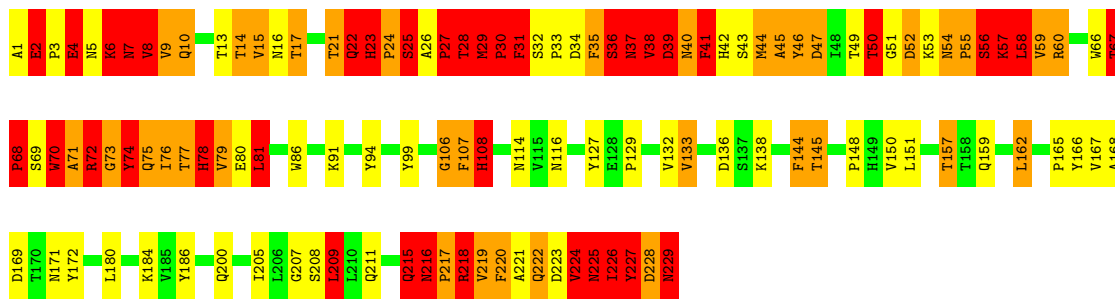
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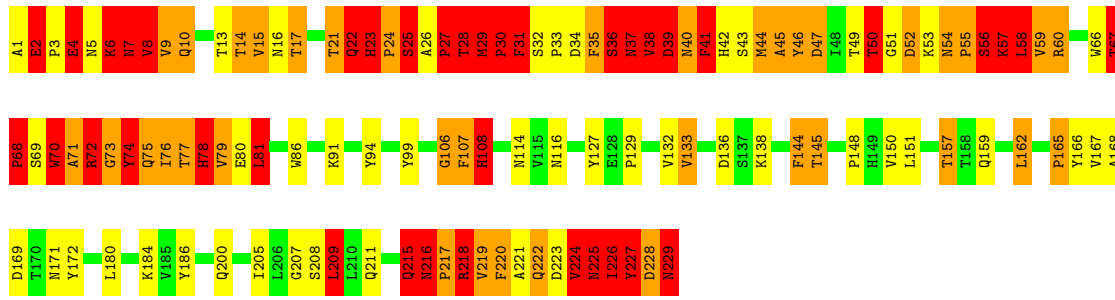
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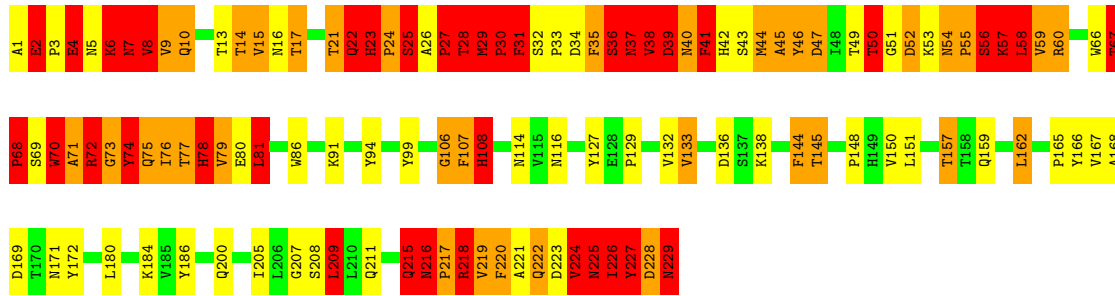
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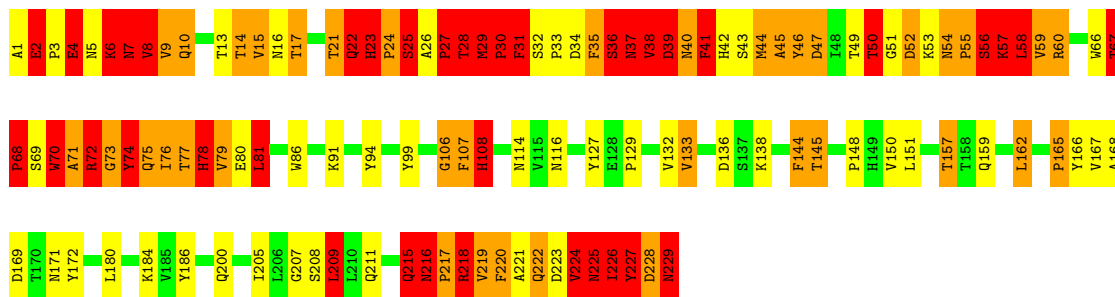
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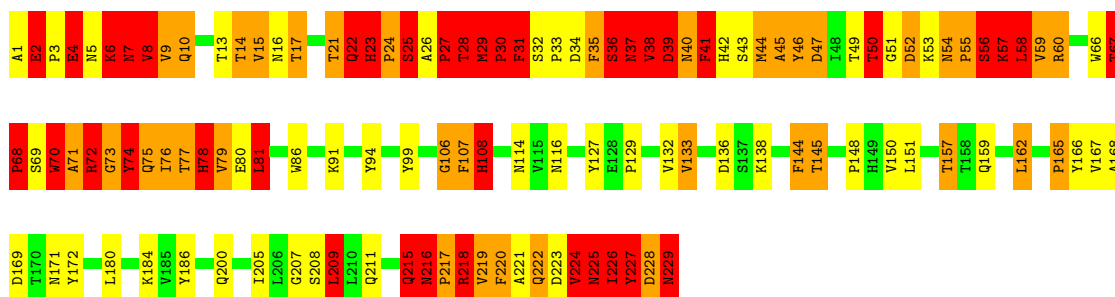
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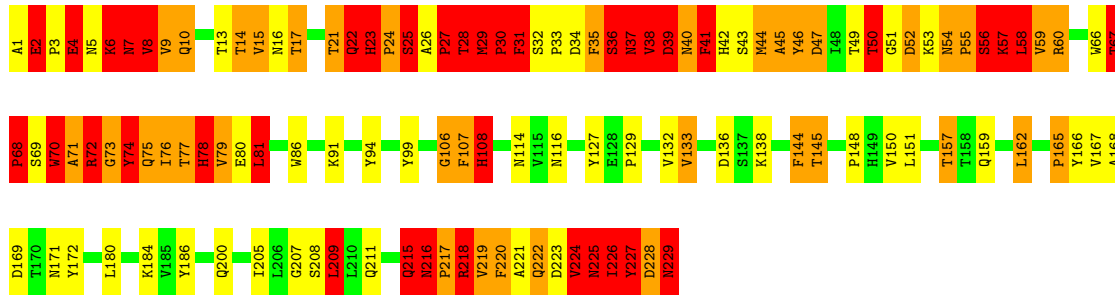
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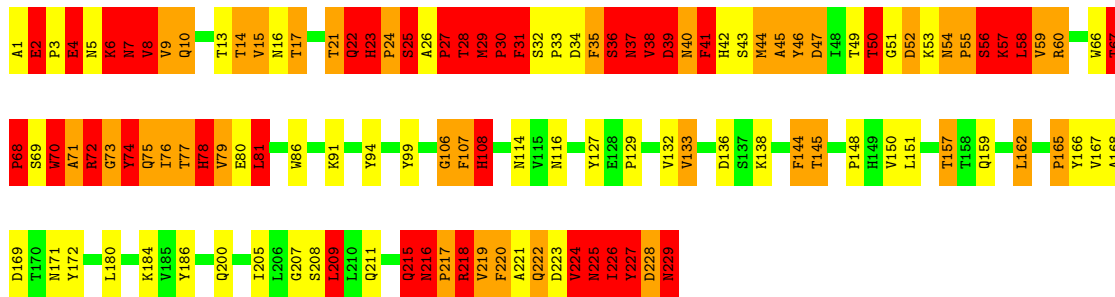
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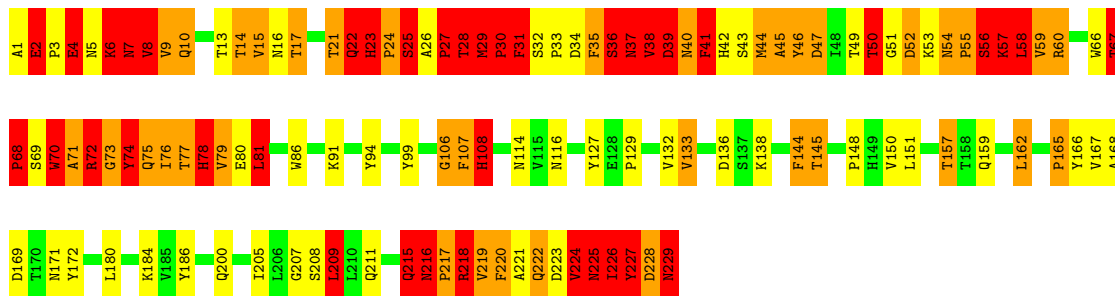
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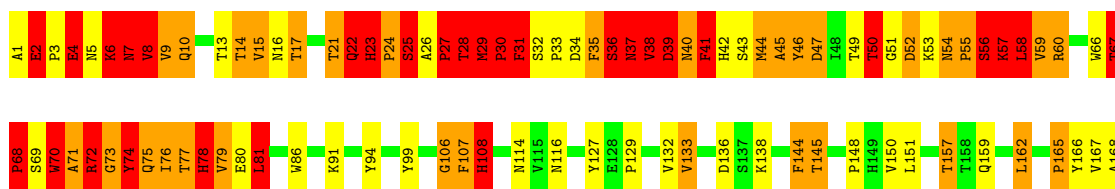
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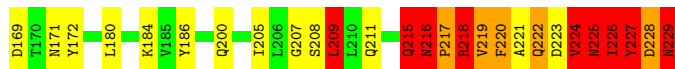


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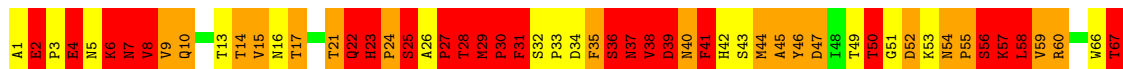


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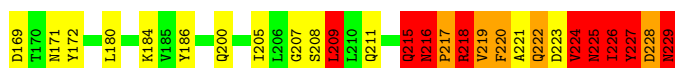
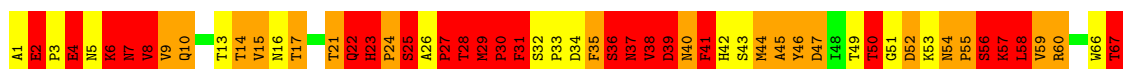




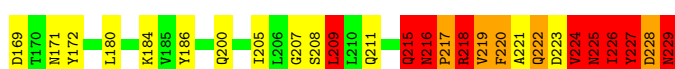
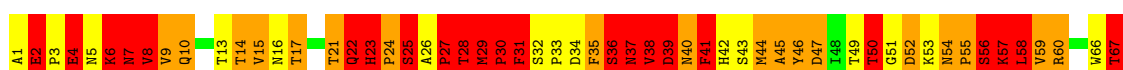
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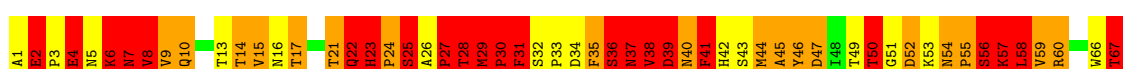
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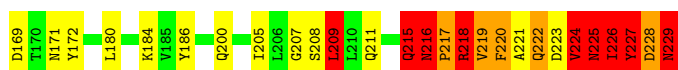
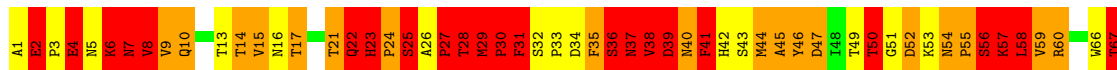


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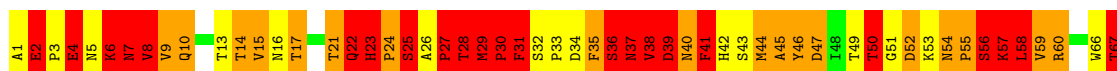




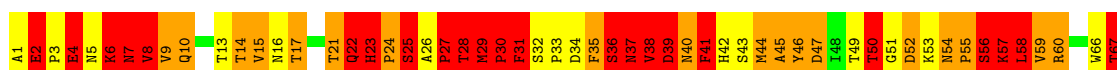
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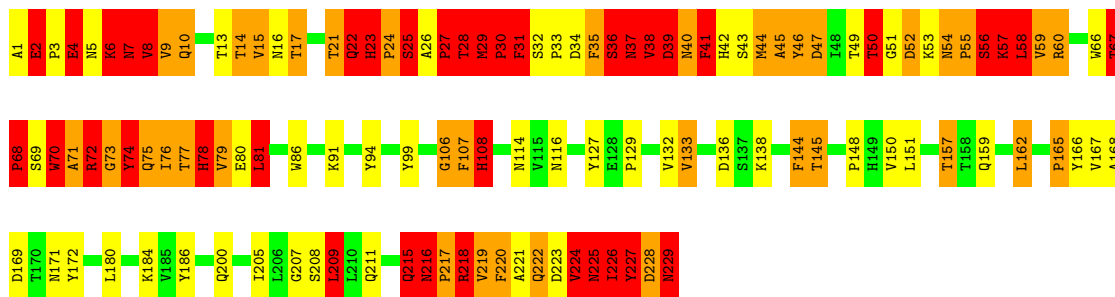
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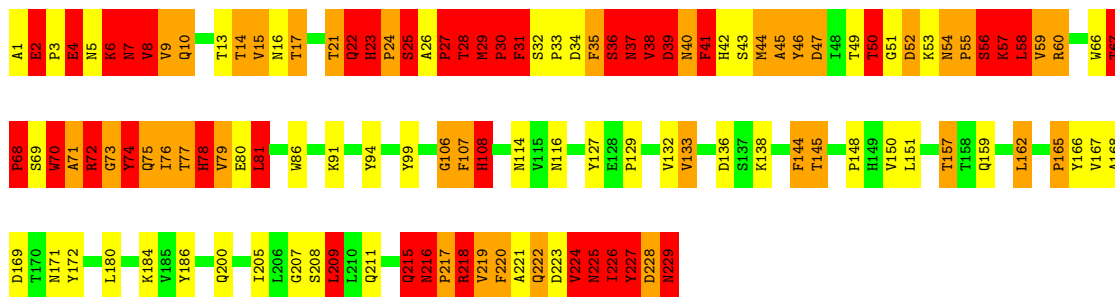
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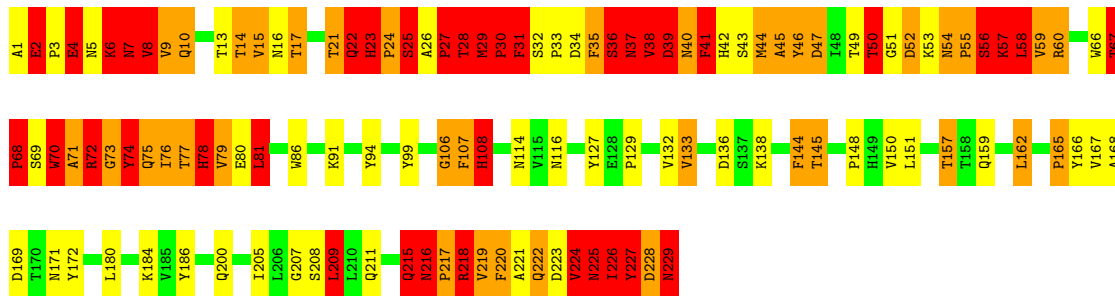




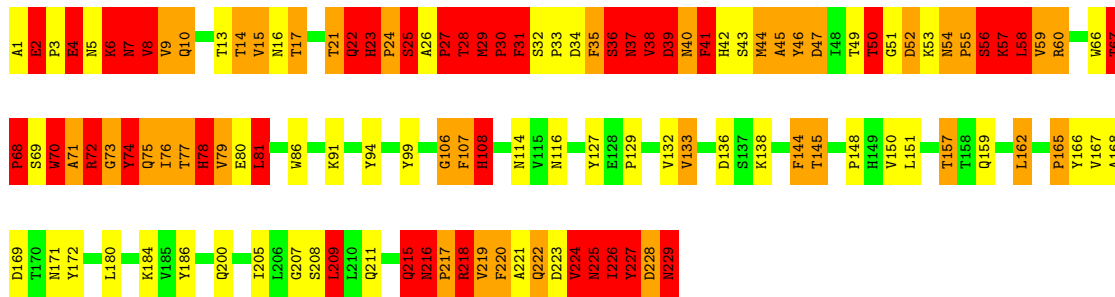
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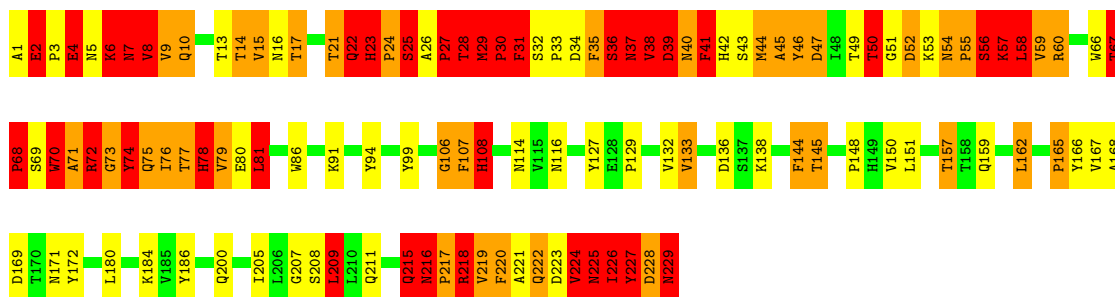
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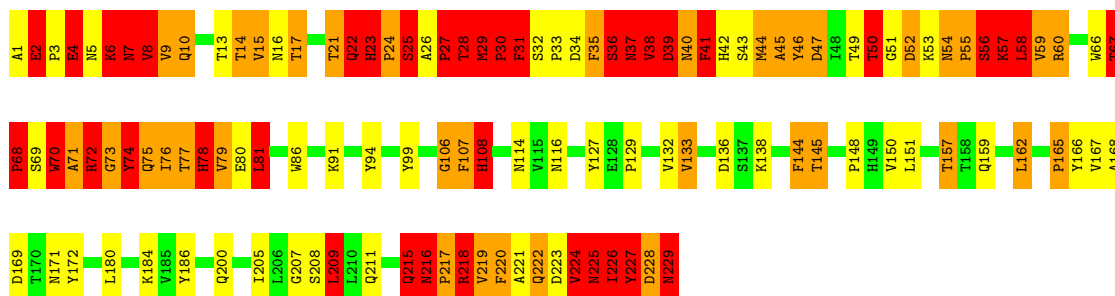
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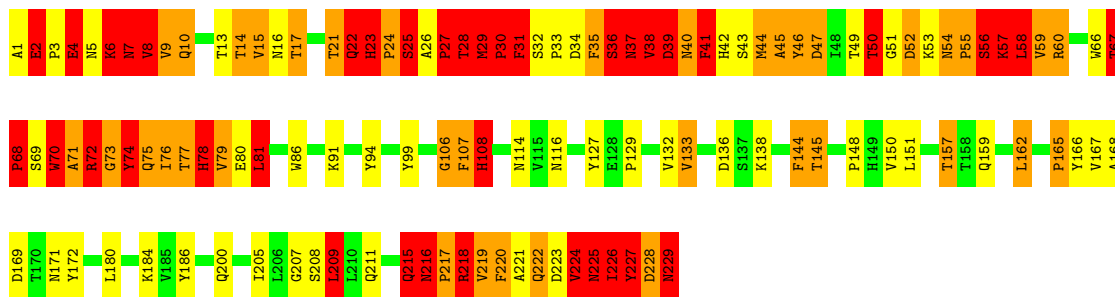
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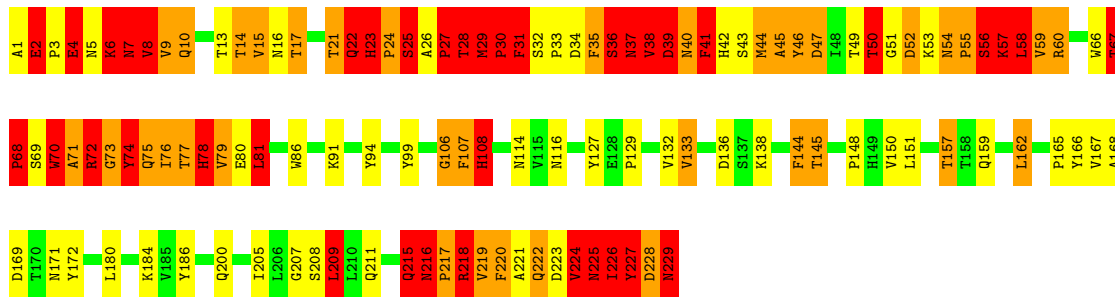
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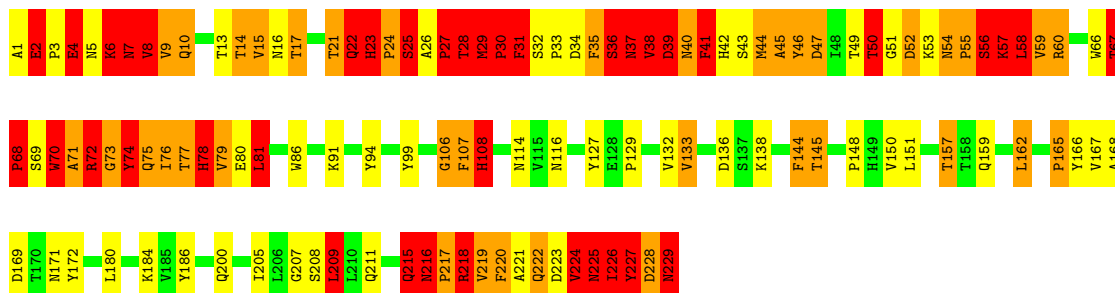
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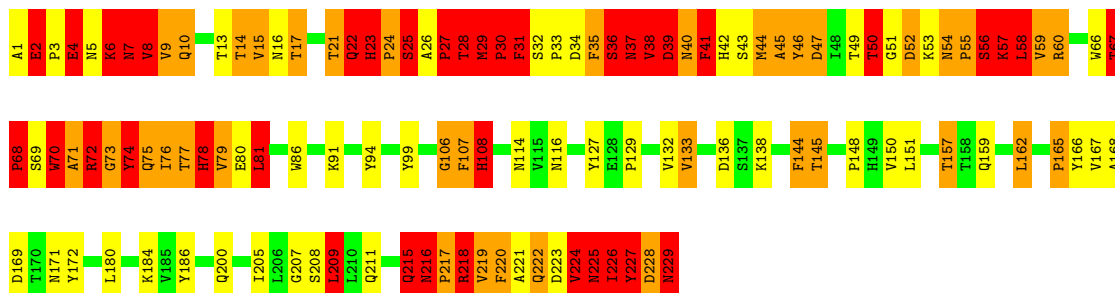
• Molecule 2: Protein VP0



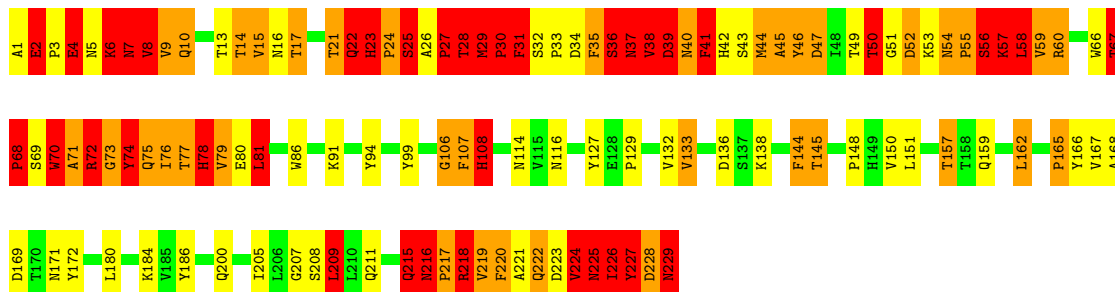
• Molecule 2: Protein VP0



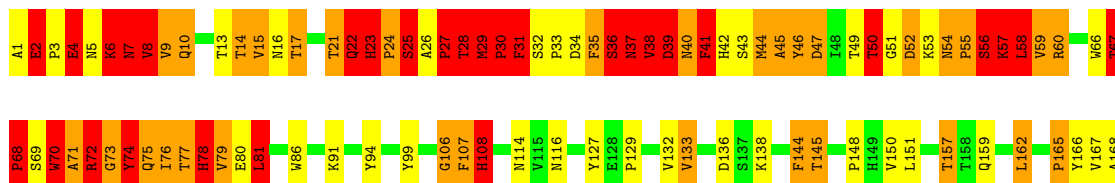
• Molecule 2: Protein VP0



• Molecule 2: Protein VP0

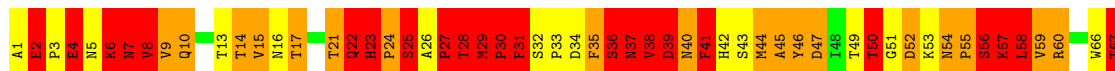


• Molecule 2: Protein VP0

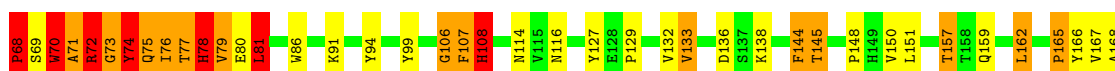
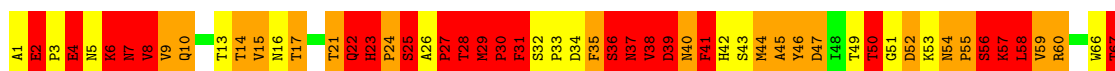




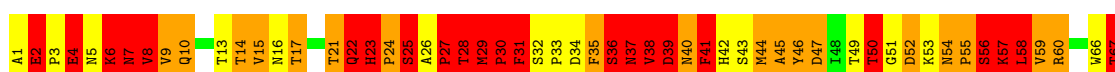
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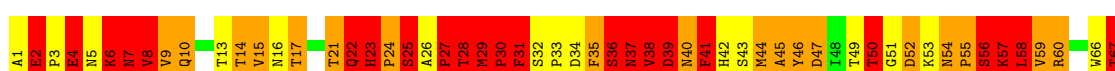
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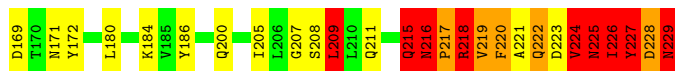


• Molecule 2: Protein VP0

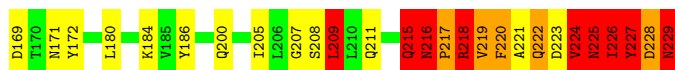
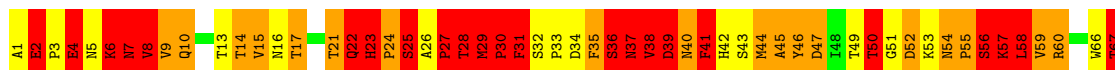


• Molecule 2: Protein VP0

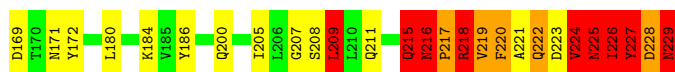
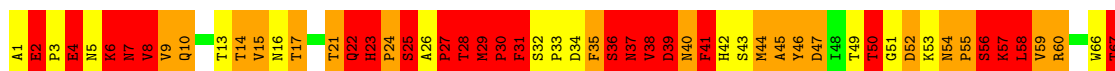




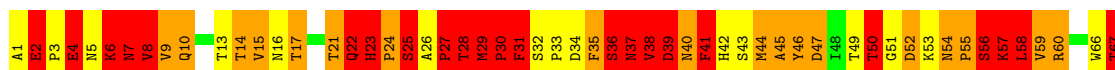
• Molecule 2: Protein VP0



• Molecule 2: Protein VP0

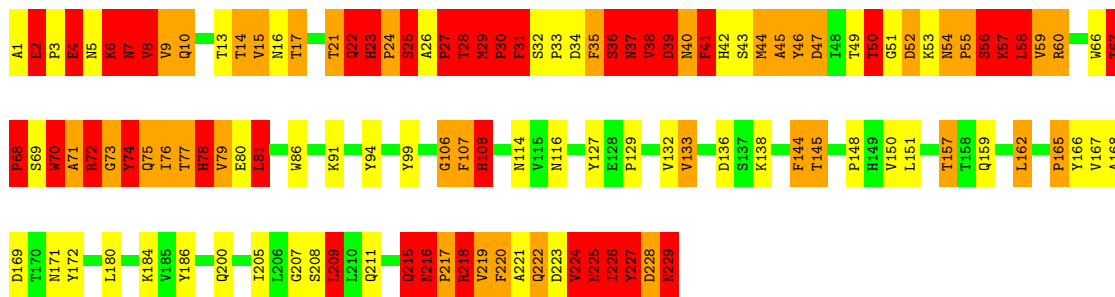


• Molecule 2: Protein VP0

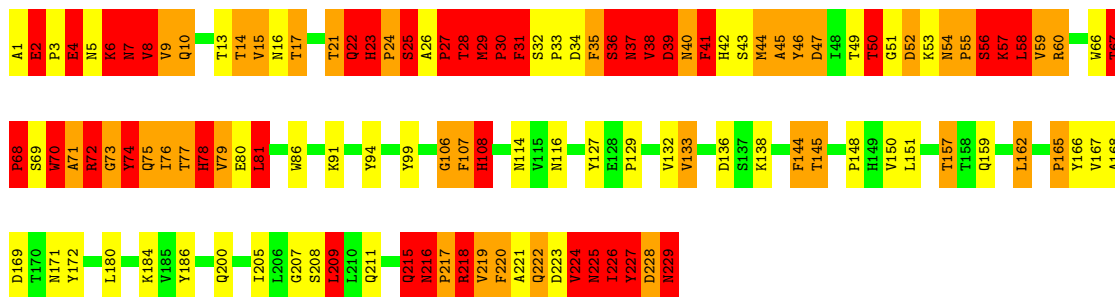


• Molecule 2: Protein VP0

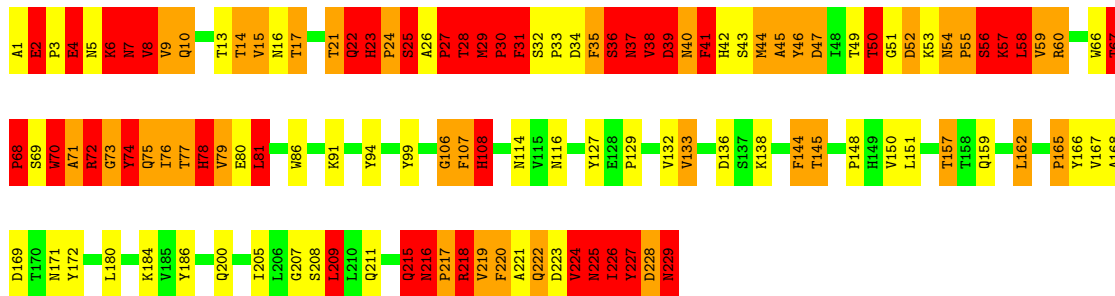




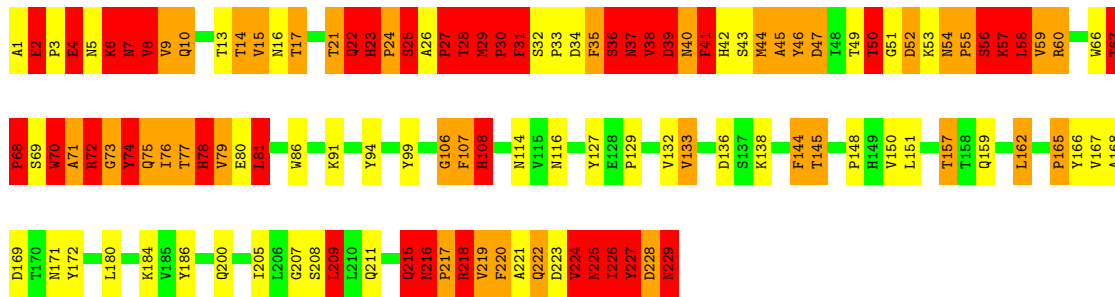
• Molecule 2: Protein VP0



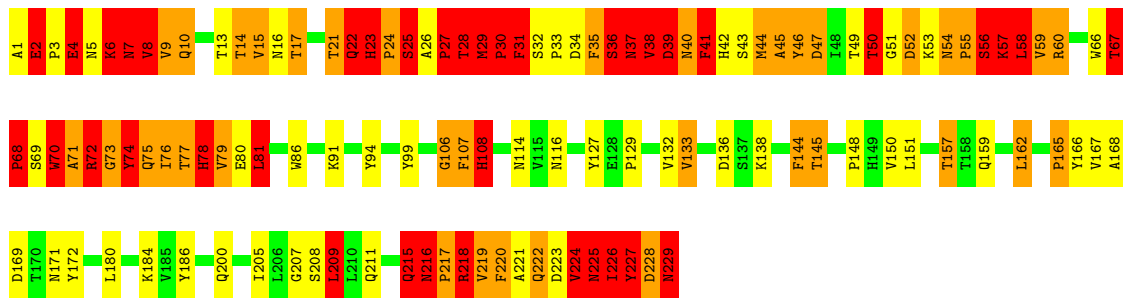
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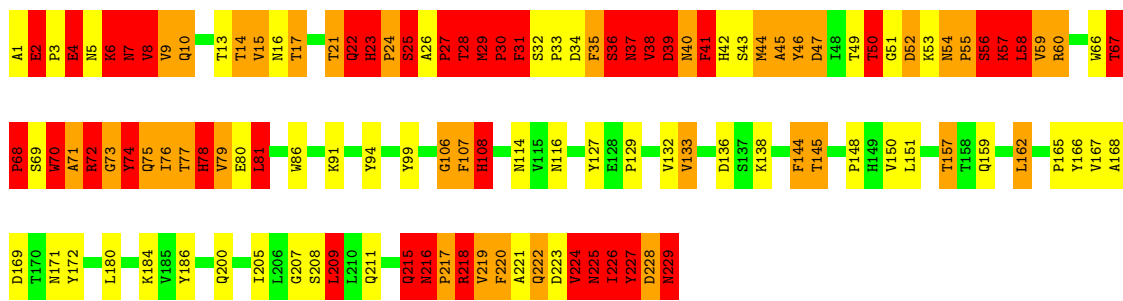
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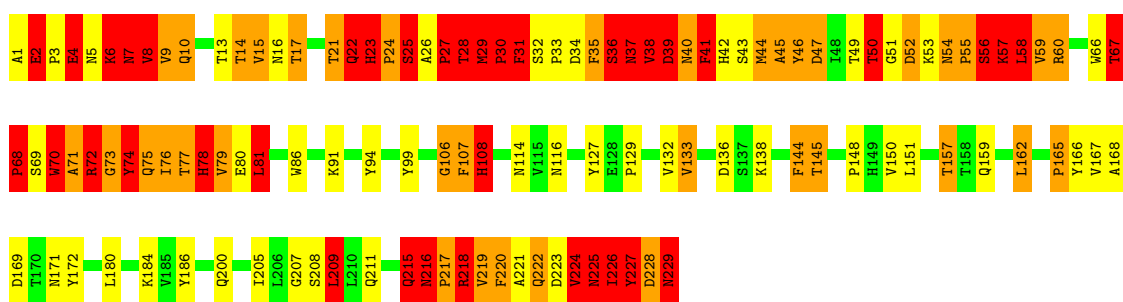
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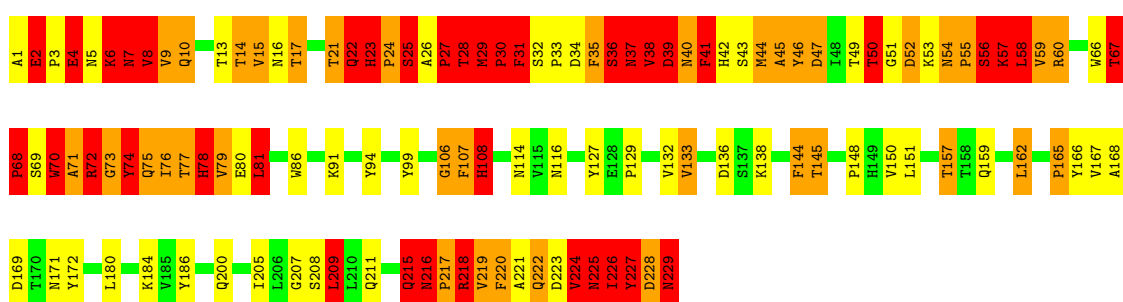
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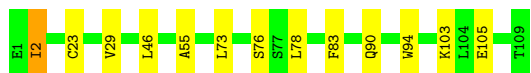
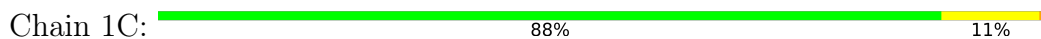
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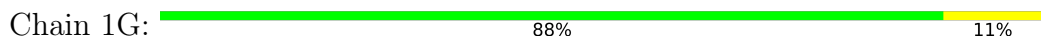
• Molecule 2: Protein VP0



• Molecule 3: HUMAN MONOCLONAL ANTIBODY



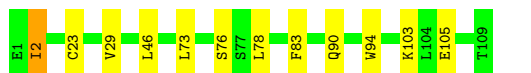
• Molecule 3: HUMAN MONOCLONAL ANTIBODY



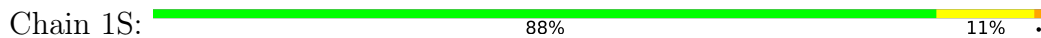
• Molecule 3: HUMAN MONOCLONAL ANTIBODY



• Molecule 3: HUMAN MONOCLONAL ANTIBODY



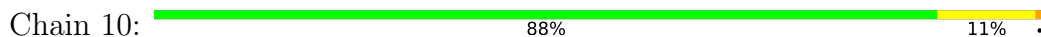
• Molecule 3: HUMAN MONOCLONAL ANTIBODY



• Molecule 3: HUMAN MONOCLONAL ANTIBODY




• Molecule 3: HUMAN MONOCLONAL ANTIBODY




• Molecule 3: HUMAN MONOCLONAL ANTIBODY



Chain 14:  88% 11%




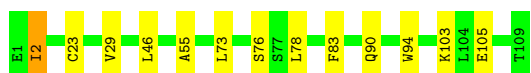
● Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 18:  88% 11%




● Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 2C:  88% 11%



● Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 2G:  88% 11%




● Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 2K:  89% 10%




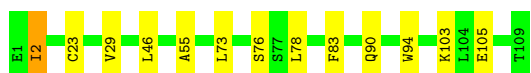
● Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 2O:  88% 11%



● Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 2S:  88% 11%



● Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 2W:  88% 11%



- Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 20: 88% 11%



- Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 24: 88% 11%



- Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 28: 88% 11%



- Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 3C: 89% 10%



- Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 3G: 88% 11%



- Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 3K: 89% 10%

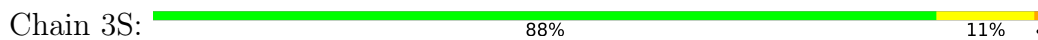


- Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 3O: 88% 11%



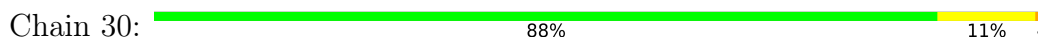
• Molecule 3: HUMAN MONOCLONAL ANTIBODY



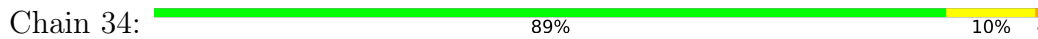
• Molecule 3: HUMAN MONOCLONAL ANTIBODY



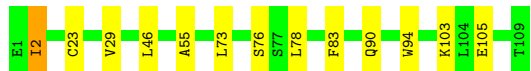
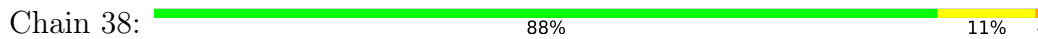
• Molecule 3: HUMAN MONOCLONAL ANTIBODY



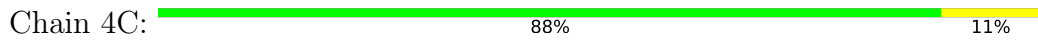
• Molecule 3: HUMAN MONOCLONAL ANTIBODY



• Molecule 3: HUMAN MONOCLONAL ANTIBODY



• Molecule 3: HUMAN MONOCLONAL ANTIBODY



• Molecule 3: HUMAN MONOCLONAL ANTIBODY





- Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 4K: 88% 11%



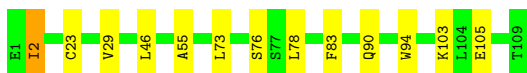
- Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 4O: 88% 11%



- Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 4S: 88% 11%



- Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 4W: 88% 11%



- Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 40: 89% 10%



- Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 44: 88% 11%

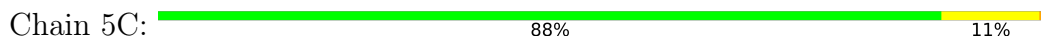


- Molecule 3: HUMAN MONOCLONAL ANTIBODY

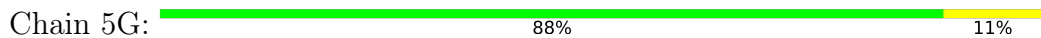
Chain 48: 88% 11%



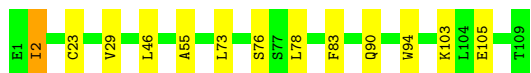
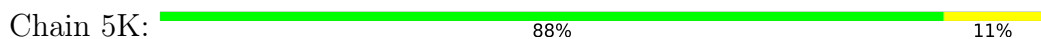
• Molecule 3: HUMAN MONOCLONAL ANTIBODY



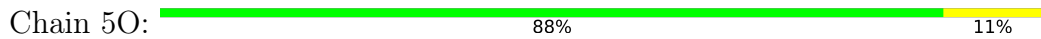
• Molecule 3: HUMAN MONOCLONAL ANTIBODY



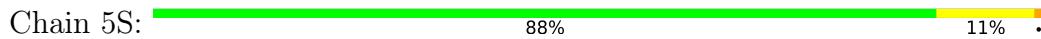
• Molecule 3: HUMAN MONOCLONAL ANTIBODY



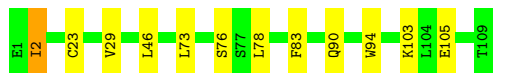
• Molecule 3: HUMAN MONOCLONAL ANTIBODY



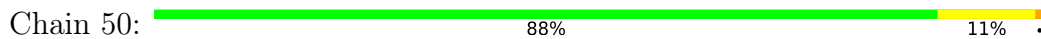
• Molecule 3: HUMAN MONOCLONAL ANTIBODY



• Molecule 3: HUMAN MONOCLONAL ANTIBODY

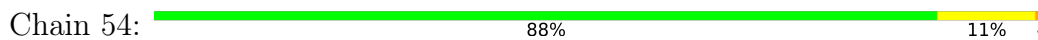


• Molecule 3: HUMAN MONOCLONAL ANTIBODY

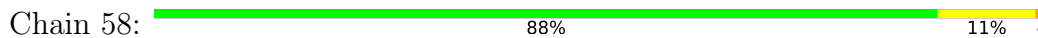




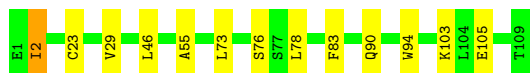
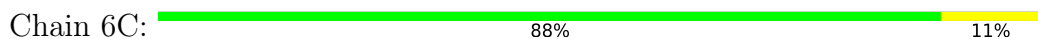
• Molecule 3: HUMAN MONOCLONAL ANTIBODY



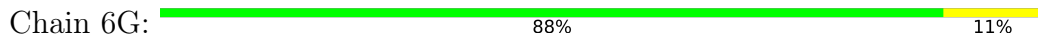
• Molecule 3: HUMAN MONOCLONAL ANTIBODY



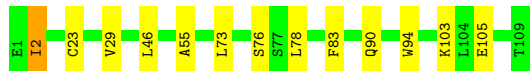
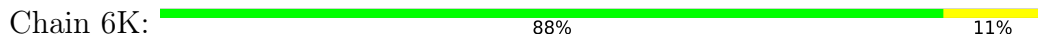
• Molecule 3: HUMAN MONOCLONAL ANTIBODY



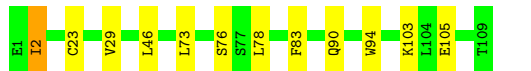
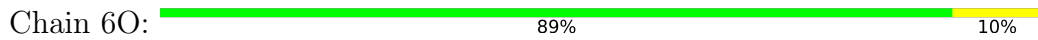
• Molecule 3: HUMAN MONOCLONAL ANTIBODY



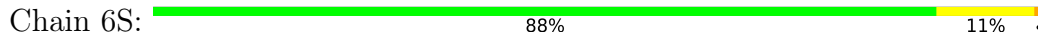
• Molecule 3: HUMAN MONOCLONAL ANTIBODY



• Molecule 3: HUMAN MONOCLONAL ANTIBODY



• Molecule 3: HUMAN MONOCLONAL ANTIBODY





- Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 6W:  89%  10%



- Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 60:  88%  11%



- Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 64:  88%  11%



- Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 68:  88%  11%



- Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 7C:  88%  11%



- Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 7G:  89%  10%

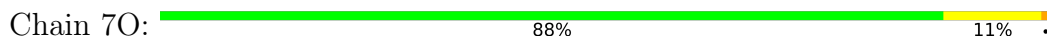


- Molecule 3: HUMAN MONOCLONAL ANTIBODY

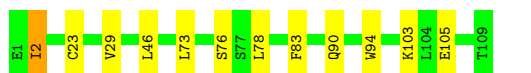
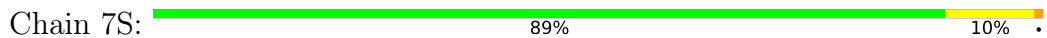
Chain 7K:  88%  11%



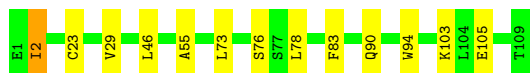
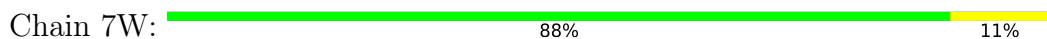
• Molecule 3: HUMAN MONOCLONAL ANTIBODY



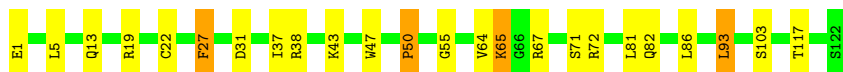
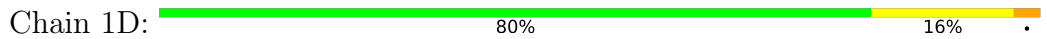
• Molecule 3: HUMAN MONOCLONAL ANTIBODY



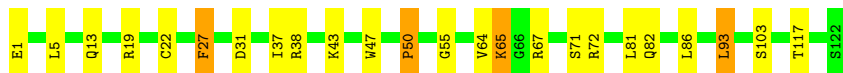
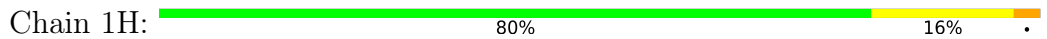
• Molecule 3: HUMAN MONOCLONAL ANTIBODY



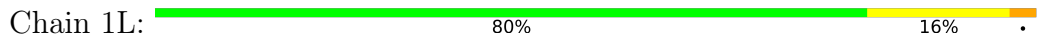
• Molecule 4: HUMAN MONOCLONAL ANTIBODY



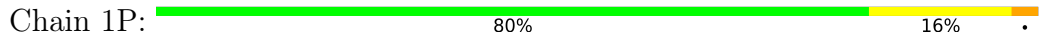
• Molecule 4: HUMAN MONOCLONAL ANTIBODY



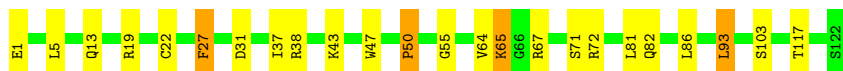
• Molecule 4: HUMAN MONOCLONAL ANTIBODY



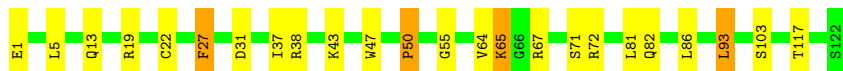
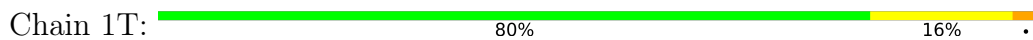
• Molecule 4: HUMAN MONOCLONAL ANTIBODY



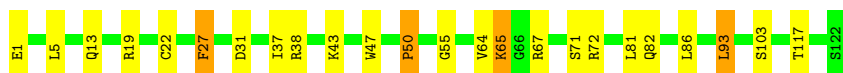
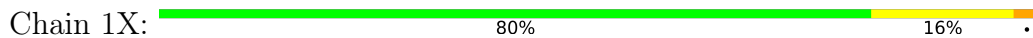




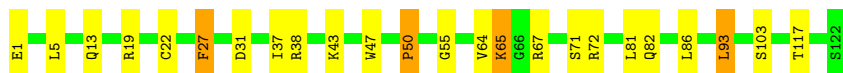
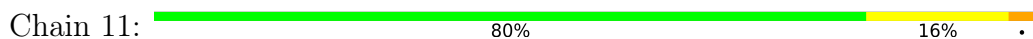
• Molecule 4: HUMAN MONOCLONAL ANTIBODY



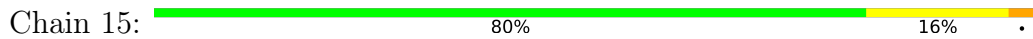
• Molecule 4: HUMAN MONOCLONAL ANTIBODY



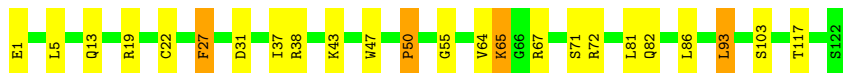
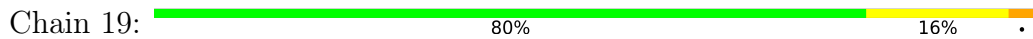
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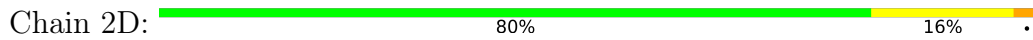
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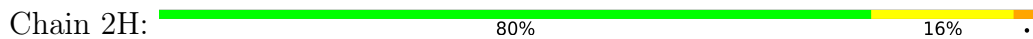
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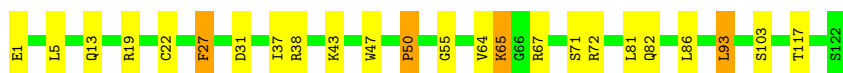


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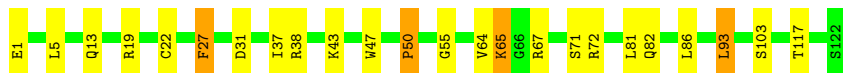
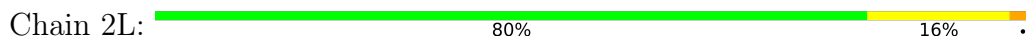


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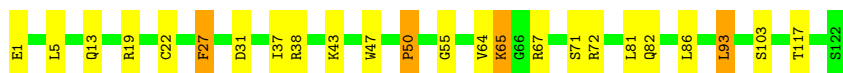
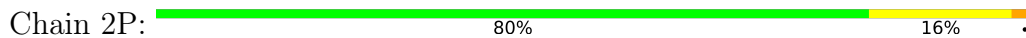




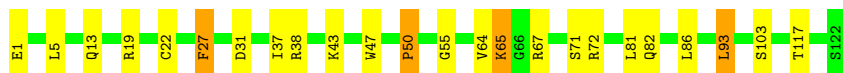
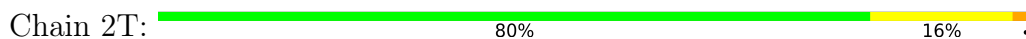
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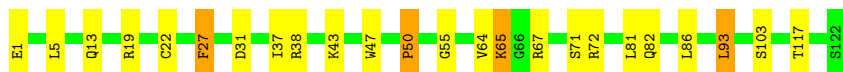
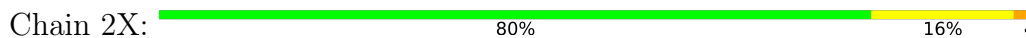
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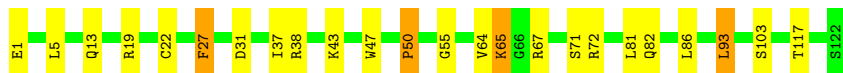
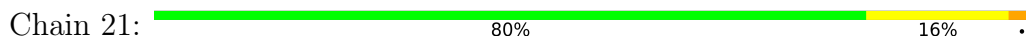
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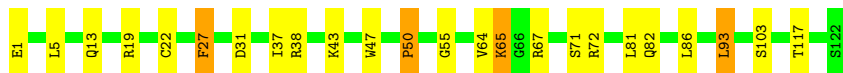
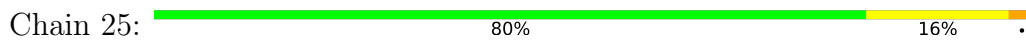
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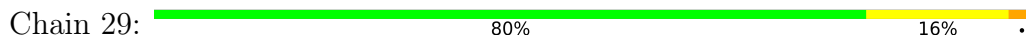
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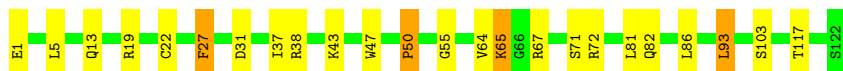


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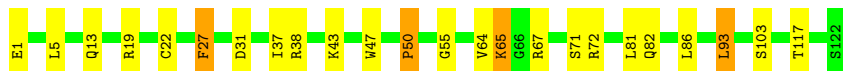
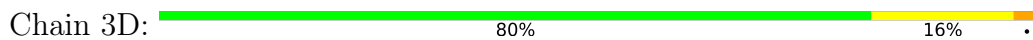


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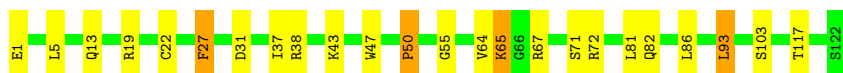
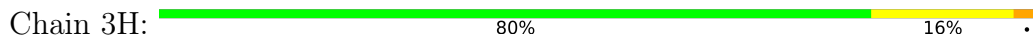




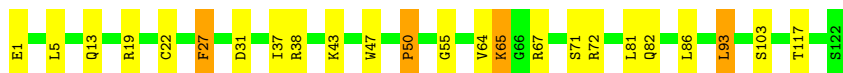
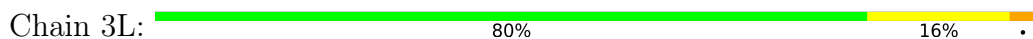
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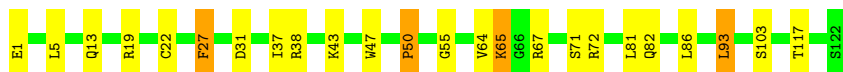
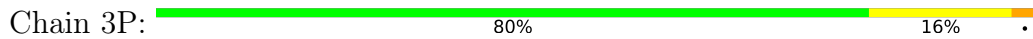
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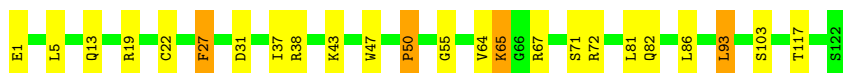
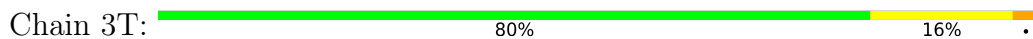
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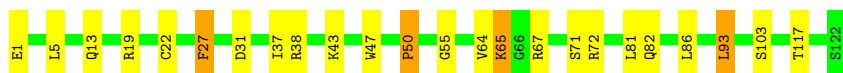
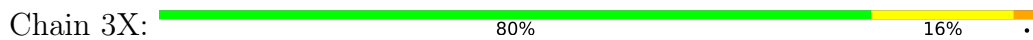
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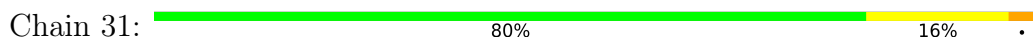
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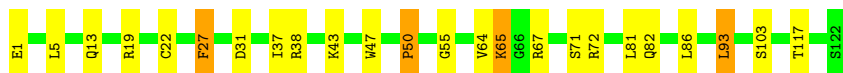


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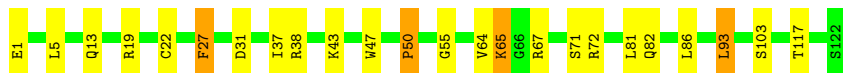
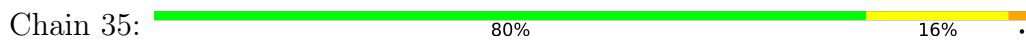


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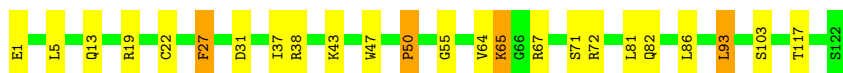
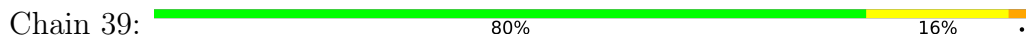




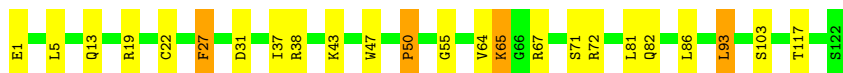
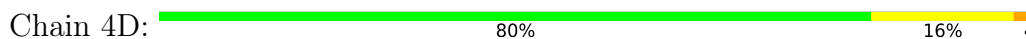
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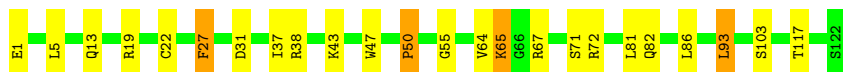
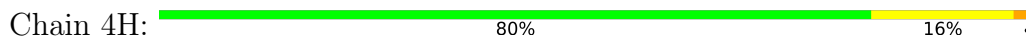
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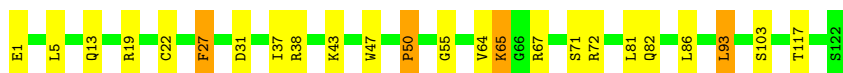
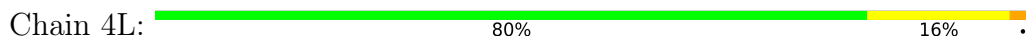
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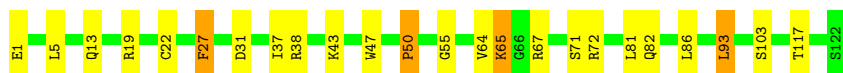
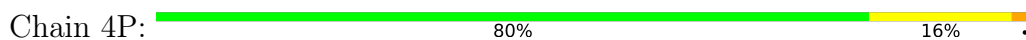
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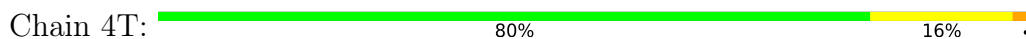
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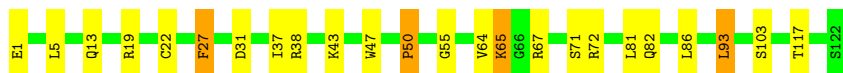


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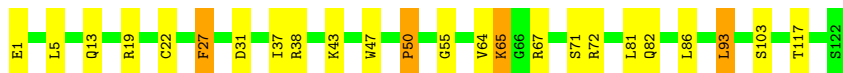
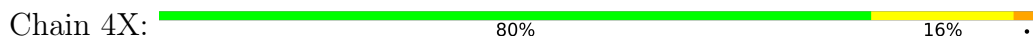


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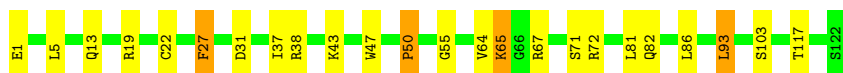
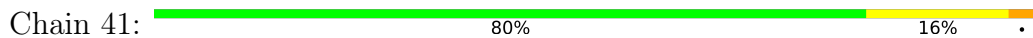




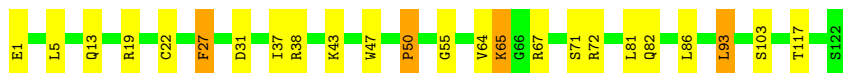
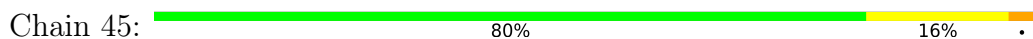
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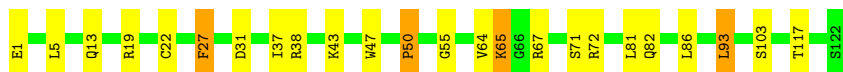
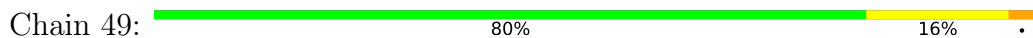
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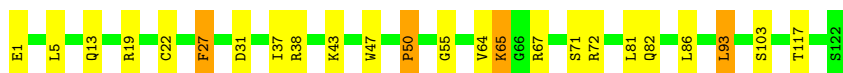
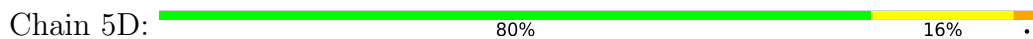
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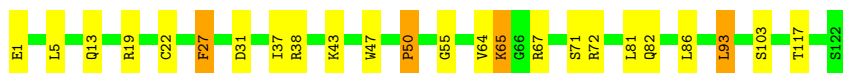
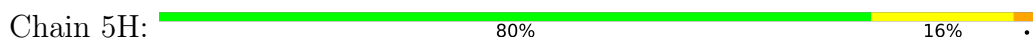
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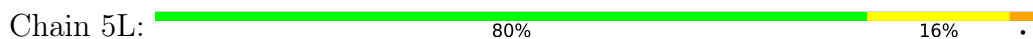
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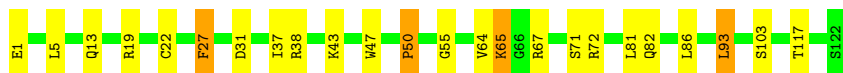


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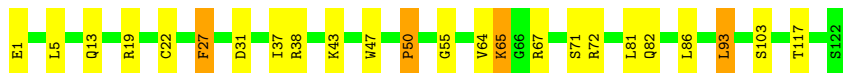
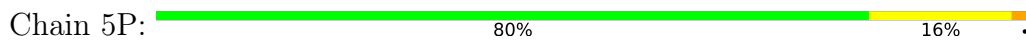


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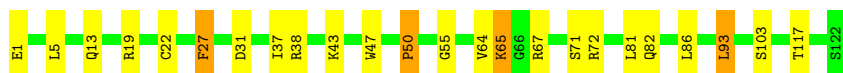
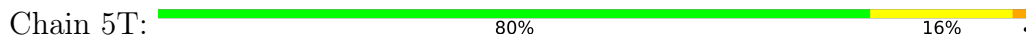




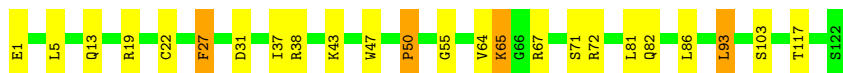
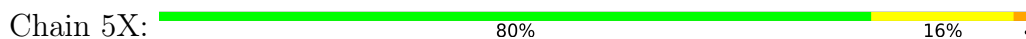
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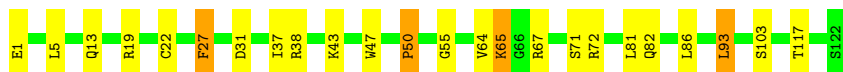
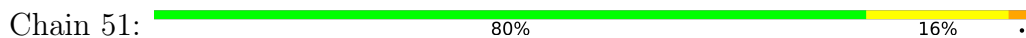
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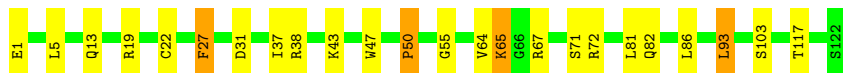
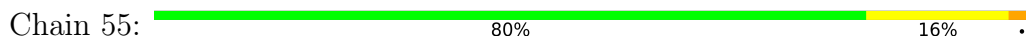
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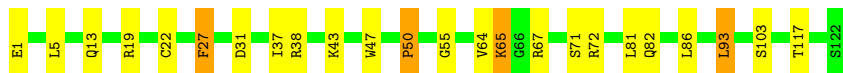
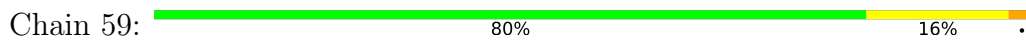
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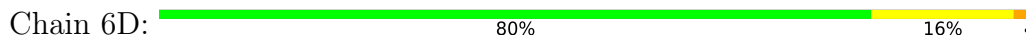
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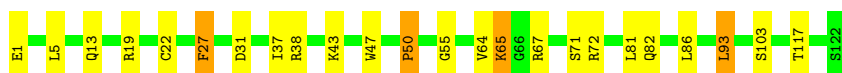


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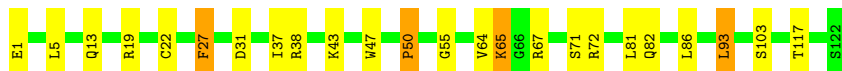
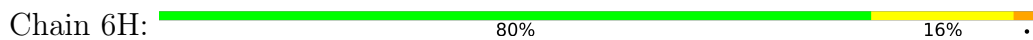


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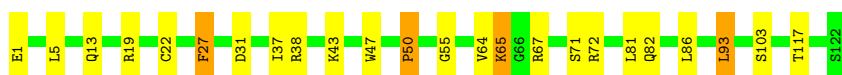
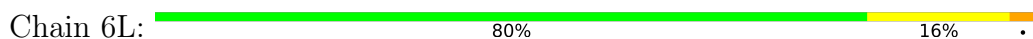




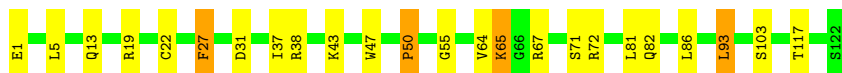
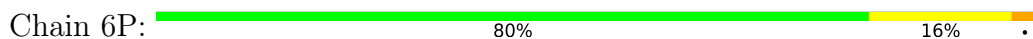
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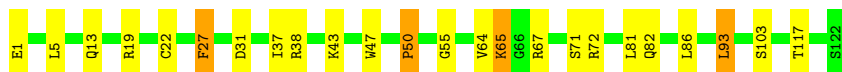
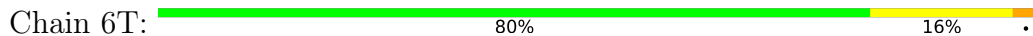
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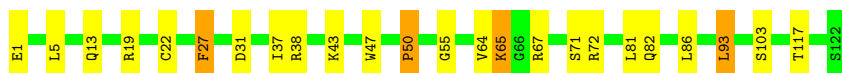
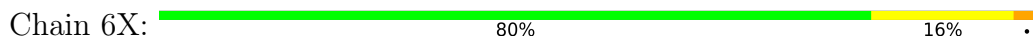
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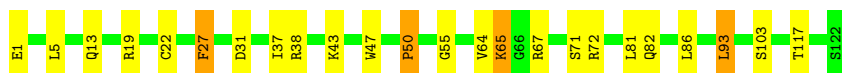
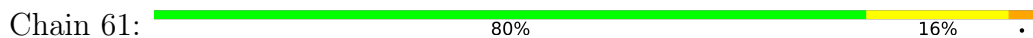
- Molecule 4: HUMAN MONOCLONAL ANTIBODY



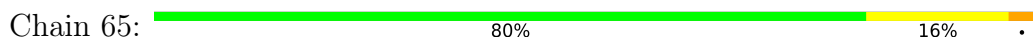
- Molecule 4: HUMAN MONOCLONAL ANTIBODY

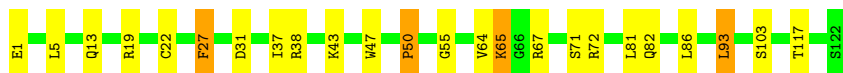


- Molecule 4: HUMAN MONOCLONAL ANTIBODY

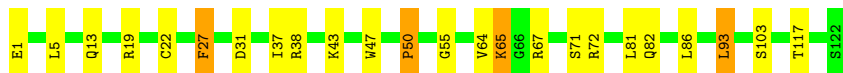
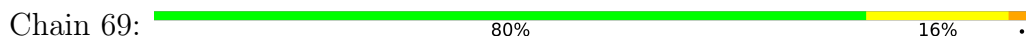


- Molecule 4: HUMAN MONOCLONAL ANTIBODY

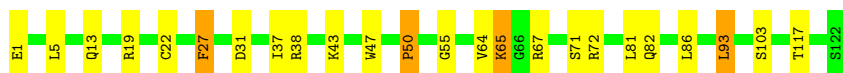
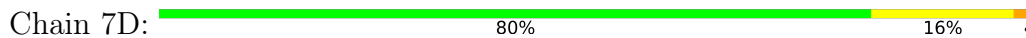




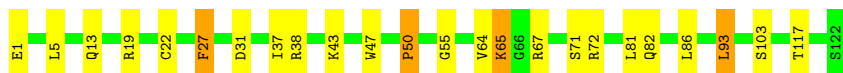
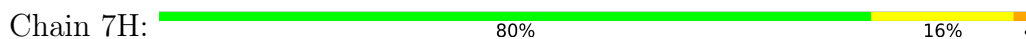
● Molecule 4: HUMAN MONOCLONAL ANTIBODY



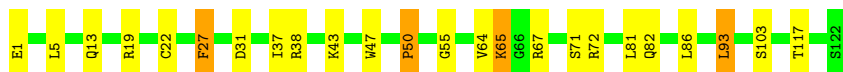
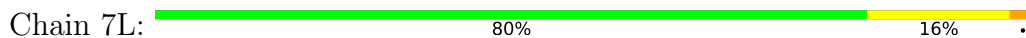
● Molecule 4: HUMAN MONOCLONAL ANTIBODY



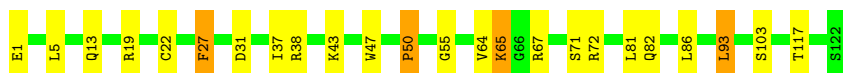
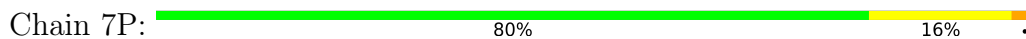
● Molecule 4: HUMAN MONOCLONAL ANTIBODY



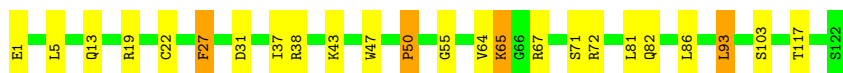
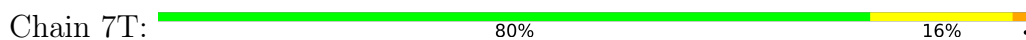
● Molecule 4: HUMAN MONOCLONAL ANTIBODY



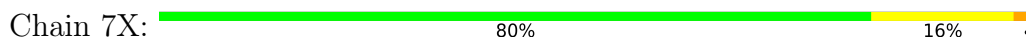
● Molecule 4: HUMAN MONOCLONAL ANTIBODY



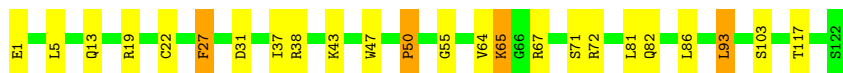
● Molecule 4: HUMAN MONOCLONAL ANTIBODY



● Molecule 4: HUMAN MONOCLONAL ANTIBODY







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	270	Depositor
Resolution determination method	Not provided	
CTF correction method	WHOLE MICROGRAPH	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	20	Depositor
Minimum defocus (nm)	1650	Depositor
Maximum defocus (nm)	4060	Depositor
Magnification	69000	Depositor
Image detector	GENERIC GATAN	Depositor
Maximum map value	32443.000	Depositor
Minimum map value	-4448.000	Depositor
Average map value	3666.095	Depositor
Map value standard deviation	7633.060	Depositor
Recommended contour level	7999.0	Depositor
Map size ( $\text{\AA}$ )	436.17, 436.17, 436.17	wwPDB
Map dimensions	201, 201, 201	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	2.17, 2.17, 2.17	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	12	8.47	446/1486 (30.0%)	9.04	510/2019 (25.3%)
1	16	8.47	446/1486 (30.0%)	9.04	510/2019 (25.3%)
1	1A	8.47	446/1486 (30.0%)	9.04	511/2019 (25.3%)
1	1E	8.47	446/1486 (30.0%)	9.04	510/2019 (25.3%)
1	1I	8.47	446/1486 (30.0%)	9.04	511/2019 (25.3%)
1	1M	8.47	446/1486 (30.0%)	9.04	511/2019 (25.3%)
1	1Q	8.47	446/1486 (30.0%)	9.04	510/2019 (25.3%)
1	1U	8.47	446/1486 (30.0%)	9.04	510/2019 (25.3%)
1	1Y	8.47	446/1486 (30.0%)	9.04	510/2019 (25.3%)
1	22	8.47	446/1486 (30.0%)	9.04	510/2019 (25.3%)
1	26	8.47	446/1486 (30.0%)	9.04	511/2019 (25.3%)
1	2A	8.47	446/1486 (30.0%)	9.04	510/2019 (25.3%)
1	2E	8.47	446/1486 (30.0%)	9.04	511/2019 (25.3%)
1	2I	8.47	446/1486 (30.0%)	9.04	511/2019 (25.3%)
1	2M	8.47	446/1486 (30.0%)	9.04	510/2019 (25.3%)
1	2Q	8.47	446/1486 (30.0%)	9.04	510/2019 (25.3%)
1	2U	8.47	446/1486 (30.0%)	9.04	510/2019 (25.3%)
1	2Y	8.47	446/1486 (30.0%)	9.04	510/2019 (25.3%)
1	32	8.47	446/1486 (30.0%)	9.04	511/2019 (25.3%)
1	36	8.47	446/1486 (30.0%)	9.04	510/2019 (25.3%)
1	3A	8.47	446/1486 (30.0%)	9.04	511/2019 (25.3%)
1	3E	8.47	446/1486 (30.0%)	9.04	511/2019 (25.3%)
1	3I	8.47	446/1486 (30.0%)	9.04	511/2019 (25.3%)
1	3M	8.47	446/1486 (30.0%)	9.04	510/2019 (25.3%)
1	3Q	8.47	446/1486 (30.0%)	9.04	510/2019 (25.3%)
1	3U	8.47	446/1486 (30.0%)	9.04	510/2019 (25.3%)
1	3Y	8.47	446/1486 (30.0%)	9.04	510/2019 (25.3%)
1	42	8.47	446/1486 (30.0%)	9.04	510/2019 (25.3%)
1	46	8.47	446/1486 (30.0%)	9.04	510/2019 (25.3%)
1	4A	8.47	446/1486 (30.0%)	9.04	511/2019 (25.3%)
1	4E	8.47	446/1486 (30.0%)	9.04	511/2019 (25.3%)
1	4I	8.47	446/1486 (30.0%)	9.04	510/2019 (25.3%)
1	4M	8.47	446/1486 (30.0%)	9.04	511/2019 (25.3%)
1	4Q	8.47	446/1486 (30.0%)	9.04	510/2019 (25.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	4U	8.47	446/1486 (30.0%)	9.04	511/2019 (25.3%)
1	4Y	8.47	446/1486 (30.0%)	9.04	511/2019 (25.3%)
1	52	8.47	446/1486 (30.0%)	9.04	510/2019 (25.3%)
1	56	8.47	446/1486 (30.0%)	9.04	510/2019 (25.3%)
1	5A	8.47	446/1486 (30.0%)	9.04	510/2019 (25.3%)
1	5E	8.47	446/1486 (30.0%)	9.04	510/2019 (25.3%)
1	5I	8.47	446/1486 (30.0%)	9.04	510/2019 (25.3%)
1	5M	8.47	446/1486 (30.0%)	9.04	510/2019 (25.3%)
1	5Q	8.47	446/1486 (30.0%)	9.04	511/2019 (25.3%)
1	5U	8.47	446/1486 (30.0%)	9.04	511/2019 (25.3%)
1	5Y	8.47	446/1486 (30.0%)	9.04	510/2019 (25.3%)
1	62	8.47	446/1486 (30.0%)	9.04	510/2019 (25.3%)
1	66	8.47	446/1486 (30.0%)	9.04	510/2019 (25.3%)
1	6A	8.47	446/1486 (30.0%)	9.04	510/2019 (25.3%)
1	6E	8.47	446/1486 (30.0%)	9.04	510/2019 (25.3%)
1	6I	8.47	446/1486 (30.0%)	9.04	511/2019 (25.3%)
1	6M	8.47	446/1486 (30.0%)	9.04	511/2019 (25.3%)
1	6Q	8.47	446/1486 (30.0%)	9.04	511/2019 (25.3%)
1	6U	8.47	446/1486 (30.0%)	9.04	511/2019 (25.3%)
1	6Y	8.47	446/1486 (30.0%)	9.04	510/2019 (25.3%)
1	7A	8.47	446/1486 (30.0%)	9.04	510/2019 (25.3%)
1	7E	8.47	446/1486 (30.0%)	9.04	511/2019 (25.3%)
1	7I	8.47	446/1486 (30.0%)	9.04	510/2019 (25.3%)
1	7M	8.47	446/1486 (30.0%)	9.04	511/2019 (25.3%)
1	7Q	8.47	446/1486 (30.0%)	9.04	511/2019 (25.3%)
1	7U	8.47	446/1486 (30.0%)	9.04	510/2019 (25.3%)
2	13	8.09	424/1857 (22.8%)	7.00	538/2542 (21.2%)
2	17	8.09	424/1857 (22.8%)	7.00	538/2542 (21.2%)
2	1B	8.09	424/1857 (22.8%)	7.00	538/2542 (21.2%)
2	1F	8.09	424/1857 (22.8%)	7.00	538/2542 (21.2%)
2	1J	8.09	424/1857 (22.8%)	7.00	538/2542 (21.2%)
2	1N	8.09	422/1857 (22.7%)	7.00	539/2542 (21.2%)
2	1R	8.09	424/1857 (22.8%)	7.00	539/2542 (21.2%)
2	1V	8.09	424/1857 (22.8%)	7.00	539/2542 (21.2%)
2	1Z	8.09	424/1857 (22.8%)	7.00	539/2542 (21.2%)
2	23	8.09	424/1857 (22.8%)	7.00	538/2542 (21.2%)
2	27	8.09	424/1857 (22.8%)	7.00	538/2542 (21.2%)
2	2B	8.09	424/1857 (22.8%)	7.00	538/2542 (21.2%)
2	2F	8.09	424/1857 (22.8%)	7.00	538/2542 (21.2%)
2	2J	8.09	422/1857 (22.7%)	7.00	539/2542 (21.2%)
2	2N	8.09	424/1857 (22.8%)	7.00	538/2542 (21.2%)
2	2R	8.09	424/1857 (22.8%)	7.00	539/2542 (21.2%)
2	2V	8.09	424/1857 (22.8%)	7.00	539/2542 (21.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
2	2Z	8.09	424/1857 (22.8%)	7.00	539/2542 (21.2%)
2	33	8.09	422/1857 (22.7%)	7.00	539/2542 (21.2%)
2	37	8.09	424/1857 (22.8%)	7.00	538/2542 (21.2%)
2	3B	8.09	422/1857 (22.7%)	7.00	539/2542 (21.2%)
2	3F	8.09	424/1857 (22.8%)	7.00	538/2542 (21.2%)
2	3J	8.09	422/1857 (22.7%)	7.00	539/2542 (21.2%)
2	3N	8.09	424/1857 (22.8%)	7.00	538/2542 (21.2%)
2	3R	8.09	424/1857 (22.8%)	7.00	538/2542 (21.2%)
2	3V	8.09	424/1857 (22.8%)	7.00	538/2542 (21.2%)
2	3Z	8.09	424/1857 (22.8%)	7.00	538/2542 (21.2%)
2	43	8.09	424/1857 (22.8%)	7.00	539/2542 (21.2%)
2	47	8.09	424/1857 (22.8%)	7.00	539/2542 (21.2%)
2	4B	8.09	424/1857 (22.8%)	7.00	538/2542 (21.2%)
2	4F	8.09	422/1857 (22.7%)	7.00	539/2542 (21.2%)
2	4J	8.09	424/1857 (22.8%)	7.00	538/2542 (21.2%)
2	4N	8.09	424/1857 (22.8%)	7.00	538/2542 (21.2%)
2	4R	8.09	424/1857 (22.8%)	7.00	538/2542 (21.2%)
2	4V	8.09	424/1857 (22.8%)	7.00	538/2542 (21.2%)
2	4Z	8.09	422/1857 (22.7%)	7.00	539/2542 (21.2%)
2	53	8.09	424/1857 (22.8%)	7.00	539/2542 (21.2%)
2	57	8.09	424/1857 (22.8%)	7.00	539/2542 (21.2%)
2	5B	8.09	424/1857 (22.8%)	7.00	539/2542 (21.2%)
2	5F	8.09	424/1857 (22.8%)	7.00	538/2542 (21.2%)
2	5J	8.09	424/1857 (22.8%)	7.00	538/2542 (21.2%)
2	5N	8.09	424/1857 (22.8%)	7.00	538/2542 (21.2%)
2	5R	8.09	424/1857 (22.8%)	7.00	538/2542 (21.2%)
2	5V	8.09	422/1857 (22.7%)	7.00	539/2542 (21.2%)
2	5Z	8.09	424/1857 (22.8%)	7.00	538/2542 (21.2%)
2	63	8.09	424/1857 (22.8%)	7.00	538/2542 (21.2%)
2	67	8.09	424/1857 (22.8%)	7.00	538/2542 (21.2%)
2	6B	8.09	424/1857 (22.8%)	7.00	539/2542 (21.2%)
2	6F	8.09	424/1857 (22.8%)	7.00	538/2542 (21.2%)
2	6J	8.09	424/1857 (22.8%)	7.00	538/2542 (21.2%)
2	6N	8.09	422/1857 (22.7%)	7.00	539/2542 (21.2%)
2	6R	8.09	424/1857 (22.8%)	7.00	538/2542 (21.2%)
2	6V	8.09	422/1857 (22.7%)	7.00	539/2542 (21.2%)
2	6Z	8.09	424/1857 (22.8%)	7.00	538/2542 (21.2%)
2	7B	8.09	424/1857 (22.8%)	7.00	538/2542 (21.2%)
2	7F	8.09	422/1857 (22.7%)	7.00	539/2542 (21.2%)
2	7J	8.09	424/1857 (22.8%)	7.00	538/2542 (21.2%)
2	7N	8.09	424/1857 (22.8%)	7.00	538/2542 (21.2%)
2	7R	8.09	422/1857 (22.7%)	7.00	539/2542 (21.2%)
2	7V	8.09	424/1857 (22.8%)	7.00	538/2542 (21.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
3	10	1.10	0/1043	1.19	6/1411 (0.4%)
3	14	1.10	1/1043 (0.1%)	1.19	6/1411 (0.4%)
3	18	1.10	1/1043 (0.1%)	1.19	6/1411 (0.4%)
3	1C	1.11	1/1043 (0.1%)	1.19	6/1411 (0.4%)
3	1G	1.10	1/1043 (0.1%)	1.19	6/1411 (0.4%)
3	1K	1.11	1/1043 (0.1%)	1.19	6/1411 (0.4%)
3	1O	1.10	1/1043 (0.1%)	1.19	5/1411 (0.4%)
3	1S	1.10	0/1043	1.19	6/1411 (0.4%)
3	1W	1.10	0/1043	1.19	6/1411 (0.4%)
3	20	1.10	0/1043	1.19	6/1411 (0.4%)
3	24	1.10	1/1043 (0.1%)	1.19	6/1411 (0.4%)
3	28	1.11	1/1043 (0.1%)	1.19	6/1411 (0.4%)
3	2C	1.10	1/1043 (0.1%)	1.19	6/1411 (0.4%)
3	2G	1.11	1/1043 (0.1%)	1.19	6/1411 (0.4%)
3	2K	1.10	1/1043 (0.1%)	1.19	5/1411 (0.4%)
3	2O	1.10	1/1043 (0.1%)	1.19	6/1411 (0.4%)
3	2S	1.10	0/1043	1.19	6/1411 (0.4%)
3	2W	1.10	0/1043	1.19	6/1411 (0.4%)
3	30	1.10	1/1043 (0.1%)	1.19	6/1411 (0.4%)
3	34	1.10	1/1043 (0.1%)	1.19	5/1411 (0.4%)
3	38	1.10	1/1043 (0.1%)	1.19	6/1411 (0.4%)
3	3C	1.10	1/1043 (0.1%)	1.19	5/1411 (0.4%)
3	3G	1.11	1/1043 (0.1%)	1.19	6/1411 (0.4%)
3	3K	1.10	1/1043 (0.1%)	1.19	5/1411 (0.4%)
3	3O	1.10	1/1043 (0.1%)	1.19	6/1411 (0.4%)
3	3S	1.10	1/1043 (0.1%)	1.19	6/1411 (0.4%)
3	3W	1.10	1/1043 (0.1%)	1.19	6/1411 (0.4%)
3	40	1.10	1/1043 (0.1%)	1.19	5/1411 (0.4%)
3	44	1.10	0/1043	1.19	6/1411 (0.4%)
3	48	1.10	0/1043	1.19	6/1411 (0.4%)
3	4C	1.11	1/1043 (0.1%)	1.19	6/1411 (0.4%)
3	4G	1.10	1/1043 (0.1%)	1.19	5/1411 (0.4%)
3	4K	1.10	1/1043 (0.1%)	1.19	6/1411 (0.4%)
3	4O	1.11	1/1043 (0.1%)	1.19	6/1411 (0.4%)
3	4S	1.10	1/1043 (0.1%)	1.19	6/1411 (0.4%)
3	4W	1.11	1/1043 (0.1%)	1.19	6/1411 (0.4%)
3	50	1.10	1/1043 (0.1%)	1.19	6/1411 (0.4%)
3	54	1.10	0/1043	1.19	6/1411 (0.4%)
3	58	1.10	0/1043	1.19	6/1411 (0.4%)
3	5C	1.10	0/1043	1.19	6/1411 (0.4%)
3	5G	1.10	1/1043 (0.1%)	1.19	6/1411 (0.4%)
3	5K	1.10	1/1043 (0.1%)	1.19	6/1411 (0.4%)
3	5O	1.10	1/1043 (0.1%)	1.19	6/1411 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
3	5S	1.11	1/1043 (0.1%)	1.19	6/1411 (0.4%)
3	5W	1.10	1/1043 (0.1%)	1.19	5/1411 (0.4%)
3	60	1.10	1/1043 (0.1%)	1.19	6/1411 (0.4%)
3	64	1.10	1/1043 (0.1%)	1.19	6/1411 (0.4%)
3	68	1.10	1/1043 (0.1%)	1.19	6/1411 (0.4%)
3	6C	1.10	0/1043	1.19	6/1411 (0.4%)
3	6G	1.10	1/1043 (0.1%)	1.19	6/1411 (0.4%)
3	6K	1.11	1/1043 (0.1%)	1.19	6/1411 (0.4%)
3	6O	1.10	1/1043 (0.1%)	1.19	5/1411 (0.4%)
3	6S	1.11	1/1043 (0.1%)	1.19	6/1411 (0.4%)
3	6W	1.10	1/1043 (0.1%)	1.19	5/1411 (0.4%)
3	7C	1.10	1/1043 (0.1%)	1.19	6/1411 (0.4%)
3	7G	1.10	1/1043 (0.1%)	1.19	5/1411 (0.4%)
3	7K	1.10	1/1043 (0.1%)	1.19	6/1411 (0.4%)
3	7O	1.11	1/1043 (0.1%)	1.19	6/1411 (0.4%)
3	7S	1.10	1/1043 (0.1%)	1.19	5/1411 (0.4%)
3	7W	1.10	1/1043 (0.1%)	1.19	6/1411 (0.4%)
4	11	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	15	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	19	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	1D	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	1H	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	1L	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	1P	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	1T	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	1X	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	21	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	25	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	29	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	2D	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	2H	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	2L	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	2P	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	2T	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	2X	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	31	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	35	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	39	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	3D	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	3H	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	3L	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	3P	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	3T	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
4	3X	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	4I	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	45	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	49	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	4D	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	4H	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	4L	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	4P	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	4T	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	4X	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	5I	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	55	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	59	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	5D	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	5H	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	5L	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	5P	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	5T	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	5X	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	6I	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	65	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	69	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	6D	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	6H	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	6L	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	6P	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	6T	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	6X	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	7D	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	7H	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	7L	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	7P	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	7T	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
4	7X	1.17	1/1081 (0.1%)	1.37	10/1461 (0.7%)
All	All	6.50	52284/328020 (15.9%)	6.29	63876/445980 (14.3%)

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	12	5	81

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	16	5	81
1	1A	5	81
1	1E	5	81
1	1I	5	81
1	1M	5	81
1	1Q	5	81
1	1U	5	81
1	1Y	5	81
1	22	5	81
1	26	5	81
1	2A	5	81
1	2E	5	81
1	2I	5	81
1	2M	5	81
1	2Q	5	81
1	2U	5	81
1	2Y	5	81
1	32	5	81
1	36	5	81
1	3A	5	81
1	3E	5	81
1	3I	5	81
1	3M	5	81
1	3Q	5	81
1	3U	5	81
1	3Y	5	81
1	42	5	81
1	46	5	81
1	4A	5	81
1	4E	5	81
1	4I	5	81
1	4M	5	81
1	4Q	5	81
1	4U	5	81
1	4Y	5	81
1	52	5	81
1	56	5	81
1	5A	5	81
1	5E	5	81
1	5I	5	81
1	5M	5	81
1	5Q	5	81

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	5U	5	81
1	5Y	5	81
1	62	5	81
1	66	5	81
1	6A	5	81
1	6E	5	81
1	6I	5	81
1	6M	5	81
1	6Q	5	81
1	6U	5	81
1	6Y	5	81
1	7A	5	81
1	7E	5	81
1	7I	5	81
1	7M	5	81
1	7Q	5	81
1	7U	5	81
2	13	4	72
2	17	4	72
2	1B	4	72
2	1F	4	72
2	1J	4	72
2	1N	4	72
2	1R	4	72
2	1V	4	72
2	1Z	4	72
2	23	4	72
2	27	4	72
2	2B	4	72
2	2F	4	72
2	2J	4	72
2	2N	4	72
2	2R	4	72
2	2V	4	72
2	2Z	4	72
2	33	4	72
2	37	4	72
2	3B	4	72
2	3F	4	72
2	3J	4	72
2	3N	4	72
2	3R	4	72

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	3V	4	72
2	3Z	4	72
2	43	4	72
2	47	4	72
2	4B	4	72
2	4F	4	72
2	4J	4	72
2	4N	4	72
2	4R	4	72
2	4V	4	72
2	4Z	4	72
2	53	4	72
2	57	4	72
2	5B	4	72
2	5F	4	72
2	5J	4	72
2	5N	4	72
2	5R	4	72
2	5V	4	72
2	5Z	4	72
2	63	4	72
2	67	4	72
2	6B	4	72
2	6F	4	72
2	6J	4	72
2	6N	4	72
2	6R	4	72
2	6V	4	72
2	6Z	4	72
2	7B	4	72
2	7F	4	72
2	7J	4	72
2	7N	4	72
2	7R	4	72
2	7V	4	72
3	10	1	0
3	14	1	0
3	18	1	0
3	1C	1	0
3	1G	1	0
3	1K	1	0
3	1O	1	0

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	1S	1	0
3	1W	1	0
3	20	1	0
3	24	1	0
3	28	1	0
3	2C	1	0
3	2G	1	0
3	2K	1	0
3	2O	1	0
3	2S	1	0
3	2W	1	0
3	30	1	0
3	34	1	0
3	38	1	0
3	3C	1	0
3	3G	1	0
3	3K	1	0
3	3O	1	0
3	3S	1	0
3	3W	1	0
3	40	1	0
3	44	1	0
3	48	1	0
3	4C	1	0
3	4G	1	0
3	4K	1	0
3	4O	1	0
3	4S	1	0
3	4W	1	0
3	50	1	0
3	54	1	0
3	58	1	0
3	5C	1	0
3	5G	1	0
3	5K	1	0
3	5O	1	0
3	5S	1	0
3	5W	1	0
3	60	1	0
3	64	1	0
3	68	1	0
3	6C	1	0

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	6G	1	0
3	6K	1	0
3	6O	1	0
3	6S	1	0
3	6W	1	0
3	7C	1	0
3	7G	1	0
3	7K	1	0
3	7O	1	0
3	7S	1	0
3	7W	1	0
4	11	1	1
4	15	1	1
4	19	1	1
4	1D	1	1
4	1H	1	1
4	1L	1	1
4	1P	1	1
4	1T	1	1
4	1X	1	1
4	21	1	1
4	25	1	1
4	29	1	1
4	2D	1	1
4	2H	1	1
4	2L	1	1
4	2P	1	1
4	2T	1	1
4	2X	1	1
4	31	1	1
4	35	1	1
4	39	1	1
4	3D	1	1
4	3H	1	1
4	3L	1	1
4	3P	1	1
4	3T	1	1
4	3X	1	1
4	41	1	1
4	45	1	1
4	49	1	1
4	4D	1	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	4H	1	1
4	4L	1	1
4	4P	1	1
4	4T	1	1
4	4X	1	1
4	51	1	1
4	55	1	1
4	59	1	1
4	5D	1	1
4	5H	1	1
4	5L	1	1
4	5P	1	1
4	5T	1	1
4	5X	1	1
4	61	1	1
4	65	1	1
4	69	1	1
4	6D	1	1
4	6H	1	1
4	6L	1	1
4	6P	1	1
4	6T	1	1
4	6X	1	1
4	7D	1	1
4	7H	1	1
4	7L	1	1
4	7P	1	1
4	7T	1	1
4	7X	1	1
All	All	660	9240

The worst 5 of 52284 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1R	74	TYR	CE2-CZ	59.78	2.16	1.38
2	1V	74	TYR	CE2-CZ	59.78	2.16	1.38
2	1Z	74	TYR	CE2-CZ	59.78	2.16	1.38
2	2R	74	TYR	CE2-CZ	59.78	2.16	1.38
2	2V	74	TYR	CE2-CZ	59.78	2.16	1.38

The worst 5 of 63876 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	12	150	TYR	CB-CG-CD2	-97.89	62.26	121.00
1	16	150	TYR	CB-CG-CD2	-97.89	62.26	121.00
1	2A	150	TYR	CB-CG-CD2	-97.89	62.26	121.00
1	3Q	150	TYR	CB-CG-CD2	-97.89	62.26	121.00
1	3U	150	TYR	CB-CG-CD2	-97.89	62.26	121.00

5 of 660 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	1A	13	ALA	CA
1	1A	17	THR	CA
1	1A	41	ILE	CA
1	1A	66	ARG	CA
1	1A	97	SER	CA

5 of 9240 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1A	1	ASP	Mainchain
1	1A	13	ALA	Mainchain
1	1A	14	ASP	Mainchain
1	1A	8	LEU	Peptide
1	1A	9	PHE	Sidechain

## 5.2 Too-close contacts [i](#)

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	12	1449	0	1386	0	0
1	16	1449	0	1386	0	0
1	1A	1449	0	1386	0	0
1	1E	1449	0	1386	0	0
1	1I	1449	0	1386	0	0
1	1M	1449	0	1386	0	0
1	1Q	1449	0	1386	0	0
1	1U	1449	0	1386	0	0
1	1Y	1449	0	1386	0	0
1	22	1449	0	1386	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	26	1449	0	1386	0	0
1	2A	1449	0	1386	0	0
1	2E	1449	0	1386	0	0
1	2I	1449	0	1386	0	0
1	2M	1449	0	1386	0	0
1	2Q	1449	0	1386	0	0
1	2U	1449	0	1386	0	0
1	2Y	1449	0	1386	0	0
1	32	1449	0	1386	0	0
1	36	1449	0	1386	0	0
1	3A	1449	0	1386	0	0
1	3E	1449	0	1386	0	0
1	3I	1449	0	1386	0	0
1	3M	1449	0	1386	0	0
1	3Q	1449	0	1386	0	0
1	3U	1449	0	1386	0	0
1	3Y	1449	0	1386	0	0
1	42	1449	0	1386	0	0
1	46	1449	0	1386	0	0
1	4A	1449	0	1386	0	0
1	4E	1449	0	1386	0	0
1	4I	1449	0	1386	0	0
1	4M	1449	0	1386	0	0
1	4Q	1449	0	1386	0	0
1	4U	1449	0	1386	0	0
1	4Y	1449	0	1386	0	0
1	52	1449	0	1386	0	0
1	56	1449	0	1386	0	0
1	5A	1449	0	1386	0	0
1	5E	1449	0	1386	0	0
1	5I	1449	0	1386	0	0
1	5M	1449	0	1386	0	0
1	5Q	1449	0	1386	0	0
1	5U	1449	0	1386	0	0
1	5Y	1449	0	1386	0	0
1	62	1449	0	1386	0	0
1	66	1449	0	1386	0	0
1	6A	1449	0	1386	0	0
1	6E	1449	0	1386	0	0
1	6I	1449	0	1386	0	0
1	6M	1449	0	1386	0	0
1	6Q	1449	0	1386	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	6U	1449	0	1386	0	0
1	6Y	1449	0	1386	0	0
1	7A	1449	0	1386	0	0
1	7E	1449	0	1386	0	0
1	7I	1449	0	1386	0	0
1	7M	1449	0	1386	0	0
1	7Q	1449	0	1386	0	0
1	7U	1449	0	1386	0	0
2	13	1810	0	1693	0	0
2	17	1810	0	1693	0	0
2	1B	1810	0	1693	0	0
2	1F	1810	0	1693	0	0
2	1J	1810	0	1693	0	0
2	1N	1810	0	1693	0	0
2	1R	1810	0	1693	0	0
2	1V	1810	0	1693	0	0
2	1Z	1810	0	1693	0	0
2	23	1810	0	1693	0	0
2	27	1810	0	1693	0	0
2	2B	1810	0	1693	0	0
2	2F	1810	0	1693	0	0
2	2J	1810	0	1693	0	0
2	2N	1810	0	1693	0	0
2	2R	1810	0	1693	0	0
2	2V	1810	0	1693	0	0
2	2Z	1810	0	1693	0	0
2	33	1810	0	1693	0	0
2	37	1810	0	1693	0	0
2	3B	1810	0	1693	0	0
2	3F	1810	0	1693	0	0
2	3J	1810	0	1693	0	0
2	3N	1810	0	1693	0	0
2	3R	1810	0	1693	0	0
2	3V	1810	0	1693	0	0
2	3Z	1810	0	1693	0	0
2	43	1810	0	1693	0	0
2	47	1810	0	1693	0	0
2	4B	1810	0	1693	0	0
2	4F	1810	0	1693	0	0
2	4J	1810	0	1693	0	0
2	4N	1810	0	1693	0	0
2	4R	1810	0	1693	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	4V	1810	0	1693	0	0
2	4Z	1810	0	1693	0	0
2	53	1810	0	1693	0	0
2	57	1810	0	1693	0	0
2	5B	1810	0	1693	0	0
2	5F	1810	0	1693	0	0
2	5J	1810	0	1693	0	0
2	5N	1810	0	1693	0	0
2	5R	1810	0	1693	0	0
2	5V	1810	0	1693	0	0
2	5Z	1810	0	1693	0	0
2	63	1810	0	1693	0	0
2	67	1810	0	1693	0	0
2	6B	1810	0	1693	0	0
2	6F	1810	0	1693	0	0
2	6J	1810	0	1693	0	0
2	6N	1810	0	1693	0	0
2	6R	1810	0	1693	0	0
2	6V	1810	0	1693	0	0
2	6Z	1810	0	1693	0	0
2	7B	1810	0	1693	0	0
2	7F	1810	0	1693	0	0
2	7J	1810	0	1693	0	0
2	7N	1810	0	1693	0	0
2	7R	1810	0	1693	0	0
2	7V	1810	0	1693	0	0
3	10	858	199	660	0	0
3	14	858	199	660	0	0
3	18	858	199	660	0	0
3	1C	858	199	660	0	0
3	1G	858	199	660	0	0
3	1K	858	199	660	0	0
3	1O	858	199	660	0	0
3	1S	858	199	660	0	0
3	1W	858	199	660	0	0
3	20	858	199	660	0	0
3	24	858	199	660	0	0
3	28	858	199	660	0	0
3	2C	858	199	660	0	0
3	2G	858	199	660	0	0
3	2K	858	199	660	0	0
3	2O	858	199	660	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	2S	858	199	660	0	0
3	2W	858	199	660	0	0
3	30	858	199	660	0	0
3	34	858	199	660	0	0
3	38	858	199	660	0	0
3	3C	858	199	660	0	0
3	3G	858	199	660	0	0
3	3K	858	199	660	0	0
3	3O	858	199	660	0	0
3	3S	858	199	660	0	0
3	3W	858	199	660	0	0
3	40	858	199	660	0	0
3	44	858	199	660	0	0
3	48	858	199	660	0	0
3	4C	858	199	660	0	0
3	4G	858	199	660	0	0
3	4K	858	199	660	0	0
3	4O	858	199	660	0	0
3	4S	858	199	660	0	0
3	4W	858	199	660	0	0
3	50	858	199	660	0	0
3	54	858	199	660	0	0
3	58	858	199	660	0	0
3	5C	858	199	660	0	0
3	5G	858	199	660	0	0
3	5K	858	199	660	0	0
3	5O	858	199	660	0	0
3	5S	858	199	660	0	0
3	5W	858	199	660	0	0
3	60	858	199	660	0	0
3	64	858	199	660	0	0
3	68	858	199	660	0	0
3	6C	858	199	660	0	0
3	6G	858	199	660	0	0
3	6K	858	199	660	0	0
3	6O	858	199	660	0	0
3	6S	858	199	660	0	0
3	6W	858	199	660	0	0
3	7C	858	199	660	0	0
3	7G	858	199	660	0	0
3	7K	858	199	660	0	0
3	7O	858	199	660	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	7S	858	199	660	0	0
3	7W	858	199	660	0	0
4	11	918	208	720	0	0
4	15	918	208	720	0	0
4	19	918	208	720	0	0
4	1D	918	208	720	0	0
4	1H	918	208	720	0	0
4	1L	918	208	720	0	0
4	1P	918	208	720	0	0
4	1T	918	208	720	0	0
4	1X	918	208	720	0	0
4	21	918	208	720	0	0
4	25	918	208	720	0	0
4	29	918	208	720	0	0
4	2D	918	208	720	0	0
4	2H	918	208	720	0	0
4	2L	918	208	720	0	0
4	2P	918	208	720	0	0
4	2T	918	208	720	0	0
4	2X	918	208	720	0	0
4	31	918	208	720	0	0
4	35	918	208	720	0	0
4	39	918	208	720	0	0
4	3D	918	208	720	0	0
4	3H	918	208	720	0	0
4	3L	918	208	720	0	0
4	3P	918	208	720	0	0
4	3T	918	208	720	0	0
4	3X	918	208	720	0	0
4	41	918	208	720	0	0
4	45	918	208	720	0	0
4	49	918	208	720	0	0
4	4D	918	208	720	0	0
4	4H	918	208	720	0	0
4	4L	918	208	720	0	0
4	4P	918	208	720	0	0
4	4T	918	208	720	0	0
4	4X	918	208	720	0	0
4	51	918	208	720	0	0
4	55	918	208	720	0	0
4	59	918	208	720	0	0
4	5D	918	208	720	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	5H	918	208	720	0	0
4	5L	918	208	720	0	0
4	5P	918	208	720	0	0
4	5T	918	208	720	0	0
4	5X	918	208	720	0	0
4	6I	918	208	720	0	0
4	65	918	208	720	0	0
4	69	918	208	720	0	0
4	6D	918	208	720	0	0
4	6H	918	208	720	0	0
4	6L	918	208	720	0	0
4	6P	918	208	720	0	0
4	6T	918	208	720	0	0
4	6X	918	208	720	0	0
4	7D	918	208	720	0	0
4	7H	918	208	720	0	0
4	7L	918	208	720	0	0
4	7P	918	208	720	0	0
4	7T	918	208	720	0	0
4	7X	918	208	720	0	0
All	All	302100	24420	267540	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	12	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	<b>0</b> <b>6</b>
1	16	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	<b>0</b> <b>6</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1A	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	1E	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	1I	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	1M	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	1Q	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	1U	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	1Y	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	22	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	26	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	2A	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	2E	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	2I	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	2M	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	2Q	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	2U	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	2Y	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	32	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	36	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	3A	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	3E	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	3I	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	3M	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	3Q	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	3U	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	3Y	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	42	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	46	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	4A	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	4E	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	4I	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	4M	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	4Q	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	4U	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	4Y	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	52	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	56	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	5A	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	5E	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	5I	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	5M	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	5Q	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	5U	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	5Y	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	62	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	66	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	6A	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	6E	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	6I	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	6M	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	6Q	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	6U	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	6Y	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	7A	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	7E	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	7I	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	7M	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	7Q	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
1	7U	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	6
2	13	223/229 (97%)	157 (70%)	27 (12%)	39 (18%)	0	3
2	17	223/229 (97%)	157 (70%)	27 (12%)	39 (18%)	0	3
2	1B	223/229 (97%)	157 (70%)	26 (12%)	40 (18%)	0	3
2	1F	223/229 (97%)	156 (70%)	27 (12%)	40 (18%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	1J	223/229 (97%)	157 (70%)	26 (12%)	40 (18%)	0	3
2	1N	223/229 (97%)	156 (70%)	27 (12%)	40 (18%)	0	3
2	1R	223/229 (97%)	155 (70%)	28 (13%)	40 (18%)	0	3
2	1V	223/229 (97%)	155 (70%)	28 (13%)	40 (18%)	0	3
2	1Z	223/229 (97%)	155 (70%)	28 (13%)	40 (18%)	0	3
2	23	223/229 (97%)	156 (70%)	27 (12%)	40 (18%)	0	3
2	27	223/229 (97%)	157 (70%)	26 (12%)	40 (18%)	0	3
2	2B	223/229 (97%)	157 (70%)	27 (12%)	39 (18%)	0	3
2	2F	223/229 (97%)	157 (70%)	26 (12%)	40 (18%)	0	3
2	2J	223/229 (97%)	156 (70%)	27 (12%)	40 (18%)	0	3
2	2N	223/229 (97%)	156 (70%)	27 (12%)	40 (18%)	0	3
2	2R	223/229 (97%)	155 (70%)	28 (13%)	40 (18%)	0	3
2	2V	223/229 (97%)	155 (70%)	28 (13%)	40 (18%)	0	3
2	2Z	223/229 (97%)	155 (70%)	28 (13%)	40 (18%)	0	3
2	33	223/229 (97%)	156 (70%)	27 (12%)	40 (18%)	0	3
2	37	223/229 (97%)	156 (70%)	27 (12%)	40 (18%)	0	3
2	3B	223/229 (97%)	156 (70%)	27 (12%)	40 (18%)	0	3
2	3F	223/229 (97%)	157 (70%)	26 (12%)	40 (18%)	0	3
2	3J	223/229 (97%)	156 (70%)	27 (12%)	40 (18%)	0	3
2	3N	223/229 (97%)	156 (70%)	27 (12%)	40 (18%)	0	3
2	3R	223/229 (97%)	157 (70%)	27 (12%)	39 (18%)	0	3
2	3V	223/229 (97%)	157 (70%)	27 (12%)	39 (18%)	0	3
2	3Z	223/229 (97%)	157 (70%)	27 (12%)	39 (18%)	0	3
2	43	223/229 (97%)	155 (70%)	28 (13%)	40 (18%)	0	3
2	47	223/229 (97%)	155 (70%)	28 (13%)	40 (18%)	0	3
2	4B	223/229 (97%)	157 (70%)	26 (12%)	40 (18%)	0	3
2	4F	223/229 (97%)	156 (70%)	27 (12%)	40 (18%)	0	3
2	4J	223/229 (97%)	156 (70%)	27 (12%)	40 (18%)	0	3
2	4N	223/229 (97%)	157 (70%)	26 (12%)	40 (18%)	0	3
2	4R	223/229 (97%)	156 (70%)	27 (12%)	40 (18%)	0	3
2	4V	223/229 (97%)	157 (70%)	26 (12%)	40 (18%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	4Z	223/229 (97%)	156 (70%)	27 (12%)	40 (18%)	0	3
2	53	223/229 (97%)	155 (70%)	28 (13%)	40 (18%)	0	3
2	57	223/229 (97%)	155 (70%)	28 (13%)	40 (18%)	0	3
2	5B	223/229 (97%)	155 (70%)	28 (13%)	40 (18%)	0	3
2	5F	223/229 (97%)	157 (70%)	27 (12%)	39 (18%)	0	3
2	5J	223/229 (97%)	157 (70%)	27 (12%)	39 (18%)	0	3
2	5N	223/229 (97%)	157 (70%)	27 (12%)	39 (18%)	0	3
2	5R	223/229 (97%)	157 (70%)	26 (12%)	40 (18%)	0	3
2	5V	223/229 (97%)	156 (70%)	27 (12%)	40 (18%)	0	3
2	5Z	223/229 (97%)	156 (70%)	27 (12%)	40 (18%)	0	3
2	63	223/229 (97%)	157 (70%)	27 (12%)	39 (18%)	0	3
2	67	223/229 (97%)	157 (70%)	27 (12%)	39 (18%)	0	3
2	6B	223/229 (97%)	155 (70%)	28 (13%)	40 (18%)	0	3
2	6F	223/229 (97%)	156 (70%)	27 (12%)	40 (18%)	0	3
2	6J	223/229 (97%)	157 (70%)	26 (12%)	40 (18%)	0	3
2	6N	223/229 (97%)	156 (70%)	27 (12%)	40 (18%)	0	3
2	6R	223/229 (97%)	157 (70%)	26 (12%)	40 (18%)	0	3
2	6V	223/229 (97%)	156 (70%)	27 (12%)	40 (18%)	0	3
2	6Z	223/229 (97%)	156 (70%)	27 (12%)	40 (18%)	0	3
2	7B	223/229 (97%)	157 (70%)	27 (12%)	39 (18%)	0	3
2	7F	223/229 (97%)	156 (70%)	27 (12%)	40 (18%)	0	3
2	7J	223/229 (97%)	156 (70%)	27 (12%)	40 (18%)	0	3
2	7N	223/229 (97%)	157 (70%)	26 (12%)	40 (18%)	0	3
2	7R	223/229 (97%)	156 (70%)	27 (12%)	40 (18%)	0	3
2	7V	223/229 (97%)	156 (70%)	27 (12%)	40 (18%)	0	3
3	10	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	14	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	18	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	1C	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	1G	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	1K	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1O	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	1S	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	1W	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	20	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	24	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	28	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	2C	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	2G	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	2K	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	2O	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	2S	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	2W	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	30	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	34	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	38	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	3C	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	3G	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	3K	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	3O	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	3S	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	3W	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	40	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	44	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	48	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	4C	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	4G	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	4K	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	4O	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	4S	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	4W	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	50	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	54	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	58	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	5C	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	5G	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	5K	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	5O	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	5S	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	5W	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	60	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	64	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	68	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	6C	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	6G	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	6K	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	6O	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	6S	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	6W	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	7C	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	7G	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	7K	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	7O	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	7S	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
3	7W	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	19	60
4	11	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	15	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	19	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	1D	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	1H	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	1L	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	1P	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	1T	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	1X	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	2I	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	25	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	29	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	2D	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	2H	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	2L	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	2P	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	2T	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	2X	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	3I	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	35	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	39	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	3D	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	3H	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	3L	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	3P	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	3T	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	3X	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	4I	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	45	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	49	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	4D	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	4H	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	4L	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	4P	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	4T	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	4X	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	5I	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	55	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	59	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	5D	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	5H	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	5L	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	5P	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	5T	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	5X	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	6I	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	65	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	69	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	6D	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	6H	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	6L	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	6P	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	6T	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	6X	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	7D	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	7H	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	7L	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	7P	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	7T	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
4	7X	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	6	35
All	All	39780/38580 (103%)	32292 (81%)	3540 (9%)	3948 (10%)	1	9

5 of 3948 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1A	25	ASP
1	1A	50	ARG
1	1A	52	PHE
1	1A	98	THR
1	1A	104	ALA

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	12	163/163 (100%)	131 (80%)	32 (20%)	1	8
1	16	163/163 (100%)	131 (80%)	32 (20%)	1	8
1	1A	163/163 (100%)	130 (80%)	33 (20%)	1	7
1	1E	163/163 (100%)	130 (80%)	33 (20%)	1	7
1	1I	163/163 (100%)	130 (80%)	33 (20%)	1	7
1	1M	163/163 (100%)	130 (80%)	33 (20%)	1	7
1	1Q	163/163 (100%)	131 (80%)	32 (20%)	1	8
1	1U	163/163 (100%)	131 (80%)	32 (20%)	1	8
1	1Y	163/163 (100%)	131 (80%)	32 (20%)	1	8
1	22	163/163 (100%)	130 (80%)	33 (20%)	1	7
1	26	163/163 (100%)	130 (80%)	33 (20%)	1	7
1	2A	163/163 (100%)	131 (80%)	32 (20%)	1	8
1	2E	163/163 (100%)	130 (80%)	33 (20%)	1	7
1	2I	163/163 (100%)	130 (80%)	33 (20%)	1	7
1	2M	163/163 (100%)	130 (80%)	33 (20%)	1	7
1	2Q	163/163 (100%)	131 (80%)	32 (20%)	1	8
1	2U	163/163 (100%)	131 (80%)	32 (20%)	1	8
1	2Y	163/163 (100%)	131 (80%)	32 (20%)	1	8
1	32	163/163 (100%)	130 (80%)	33 (20%)	1	7
1	36	163/163 (100%)	130 (80%)	33 (20%)	1	7
1	3A	163/163 (100%)	130 (80%)	33 (20%)	1	7
1	3E	163/163 (100%)	130 (80%)	33 (20%)	1	7
1	3I	163/163 (100%)	130 (80%)	33 (20%)	1	7
1	3M	163/163 (100%)	130 (80%)	33 (20%)	1	7
1	3Q	163/163 (100%)	131 (80%)	32 (20%)	1	8
1	3U	163/163 (100%)	131 (80%)	32 (20%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	3Y	163/163 (100%)	131 (80%)	32 (20%)	1	8
1	42	163/163 (100%)	131 (80%)	32 (20%)	1	8
1	46	163/163 (100%)	131 (80%)	32 (20%)	1	8
1	4A	163/163 (100%)	130 (80%)	33 (20%)	1	7
1	4E	163/163 (100%)	130 (80%)	33 (20%)	1	7
1	4I	163/163 (100%)	130 (80%)	33 (20%)	1	7
1	4M	163/163 (100%)	130 (80%)	33 (20%)	1	7
1	4Q	163/163 (100%)	130 (80%)	33 (20%)	1	7
1	4U	163/163 (100%)	130 (80%)	33 (20%)	1	7
1	4Y	163/163 (100%)	130 (80%)	33 (20%)	1	7
1	52	163/163 (100%)	131 (80%)	32 (20%)	1	8
1	56	163/163 (100%)	131 (80%)	32 (20%)	1	8
1	5A	163/163 (100%)	131 (80%)	32 (20%)	1	8
1	5E	163/163 (100%)	131 (80%)	32 (20%)	1	8
1	5I	163/163 (100%)	131 (80%)	32 (20%)	1	8
1	5M	163/163 (100%)	131 (80%)	32 (20%)	1	8
1	5Q	163/163 (100%)	130 (80%)	33 (20%)	1	7
1	5U	163/163 (100%)	130 (80%)	33 (20%)	1	7
1	5Y	163/163 (100%)	130 (80%)	33 (20%)	1	7
1	62	163/163 (100%)	131 (80%)	32 (20%)	1	8
1	66	163/163 (100%)	131 (80%)	32 (20%)	1	8
1	6A	163/163 (100%)	131 (80%)	32 (20%)	1	8
1	6E	163/163 (100%)	130 (80%)	33 (20%)	1	7
1	6I	163/163 (100%)	130 (80%)	33 (20%)	1	7
1	6M	163/163 (100%)	130 (80%)	33 (20%)	1	7
1	6Q	163/163 (100%)	130 (80%)	33 (20%)	1	7
1	6U	163/163 (100%)	130 (80%)	33 (20%)	1	7
1	6Y	163/163 (100%)	130 (80%)	33 (20%)	1	7
1	7A	163/163 (100%)	131 (80%)	32 (20%)	1	8
1	7E	163/163 (100%)	130 (80%)	33 (20%)	1	7
1	7I	163/163 (100%)	130 (80%)	33 (20%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	7M	163/163 (100%)	130 (80%)	33 (20%)	1	7
1	7Q	163/163 (100%)	130 (80%)	33 (20%)	1	7
1	7U	163/163 (100%)	130 (80%)	33 (20%)	1	7
2	13	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	17	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	1B	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	1F	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	1J	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	1N	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	1R	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	1V	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	1Z	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	23	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	27	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	2B	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	2F	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	2J	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	2N	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	2R	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	2V	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	2Z	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	33	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	37	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	3B	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	3F	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	3J	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	3N	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	3R	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	3V	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	3Z	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	43	203/203 (100%)	156 (77%)	47 (23%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	47	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	4B	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	4F	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	4J	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	4N	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	4R	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	4V	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	4Z	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	53	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	57	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	5B	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	5F	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	5J	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	5N	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	5R	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	5V	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	5Z	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	63	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	67	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	6B	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	6F	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	6J	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	6N	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	6R	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	6V	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	6Z	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	7B	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	7F	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	7J	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	7N	203/203 (100%)	156 (77%)	47 (23%)	1	4
2	7R	203/203 (100%)	156 (77%)	47 (23%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	7V	203/203 (100%)	156 (77%)	47 (23%)	1	4
3	10	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	14	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	18	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	1C	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	1G	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	1K	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	1O	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	1S	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	1W	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	20	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	24	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	28	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	2C	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	2G	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	2K	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	2O	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	2S	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	2W	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	30	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	34	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	38	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	3C	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	3G	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	3K	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	3O	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	3S	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	3W	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	40	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	44	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	48	110/93 (118%)	102 (93%)	8 (7%)	14	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	4C	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	4G	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	4K	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	4O	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	4S	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	4W	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	50	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	54	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	58	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	5C	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	5G	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	5K	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	5O	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	5S	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	5W	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	60	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	64	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	68	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	6C	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	6G	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	6K	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	6O	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	6S	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	6W	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	7C	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	7G	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	7K	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	7O	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	7S	110/93 (118%)	102 (93%)	8 (7%)	14	39
3	7W	110/93 (118%)	102 (93%)	8 (7%)	14	39
4	11	112/97 (116%)	93 (83%)	19 (17%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	15	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	19	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	1D	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	1H	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	1L	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	1P	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	1T	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	1X	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	21	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	25	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	29	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	2D	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	2H	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	2L	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	2P	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	2T	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	2X	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	31	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	35	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	39	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	3D	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	3H	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	3L	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	3P	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	3T	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	3X	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	41	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	45	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	49	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	4D	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	4H	112/97 (116%)	93 (83%)	19 (17%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	4L	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	4P	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	4T	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	4X	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	51	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	55	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	59	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	5D	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	5H	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	5L	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	5P	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	5T	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	5X	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	61	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	65	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	69	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	6D	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	6H	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	6L	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	6P	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	6T	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	6X	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	7D	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	7H	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	7L	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	7P	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	7T	112/97 (116%)	93 (83%)	19 (17%)	2	12
4	7X	112/97 (116%)	93 (83%)	19 (17%)	2	12
All	All	35280/33360 (106%)	28884 (82%)	6396 (18%)	4	10

5 of 6396 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	44	2	ILE
1	52	21	ASN
3	48	73	LEU
2	43	219	VAL
1	5M	24	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	1F	28
2	2N	28
2	23	28
2	3N	28
2	37	28

*Continued on next page...*

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<b>Mol</b>	<b>Chain</b>	<b>Number of breaks</b>
2	4J	28
2	4R	28
2	5Z	28
2	6F	28
2	6Z	28
2	7J	28
2	7V	28
2	1B	27
2	1J	27
2	1N	27
2	1R	27
2	1V	27
2	1Z	27
2	13	27
2	17	27
2	2B	27
2	2F	27
2	2J	27
2	2R	27
2	2V	27
2	2Z	27
2	27	27
2	3B	27
2	3F	27
2	3J	27
2	3R	27
2	3V	27
2	3Z	27
2	33	27
2	4B	27
2	4F	27
2	4N	27
2	4V	27
2	4Z	27
2	43	27
2	47	27
2	5B	27
2	5F	27
2	5J	27
2	5N	27
2	5R	27
2	5V	27

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Number of breaks</b>
2	53	27
2	57	27
2	6B	27
2	6J	27
2	6N	27
2	6R	27
2	6V	27
2	63	27
2	67	27
2	7B	27
2	7F	27
2	7N	27
2	7R	27
1	1A	26
1	1E	26
1	1I	26
1	1M	26
1	1Q	26
1	1U	26
1	1Y	26
1	12	26
1	16	26
1	2A	26
1	2E	26
1	2I	26
1	2M	26
1	2Q	26
1	2U	26
1	2Y	26
1	22	26
1	26	26
1	3A	26
1	3E	26
1	3I	26
1	3M	26
1	3Q	26
1	3U	26
1	3Y	26
1	32	26
1	36	26
1	4A	26
1	4E	26

*Continued on next page...*



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Mol	Chain	Number of breaks
1	4I	26
1	4M	26
1	4Q	26
1	4U	26
1	4Y	26
1	4Z	26
1	46	26
1	5A	26
1	5E	26
1	5I	26
1	5M	26
1	5Q	26
1	5U	26
1	5Y	26
1	5Z	26
1	56	26
1	6A	26
1	6E	26
1	6I	26
1	6M	26
1	6Q	26
1	6U	26
1	6Y	26
1	6Z	26
1	66	26
1	7A	26
1	7E	26
1	7I	26
1	7M	26
1	7Q	26
1	7U	26

The worst 5 of 3192 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1B	91:LYS	C	92:PRO	N	5.21
1	1F	91:LYS	C	92:PRO	N	5.21
1	1J	91:LYS	C	92:PRO	N	5.21
1	1N	91:LYS	C	92:PRO	N	5.21
1	1R	91:LYS	C	92:PRO	N	5.21

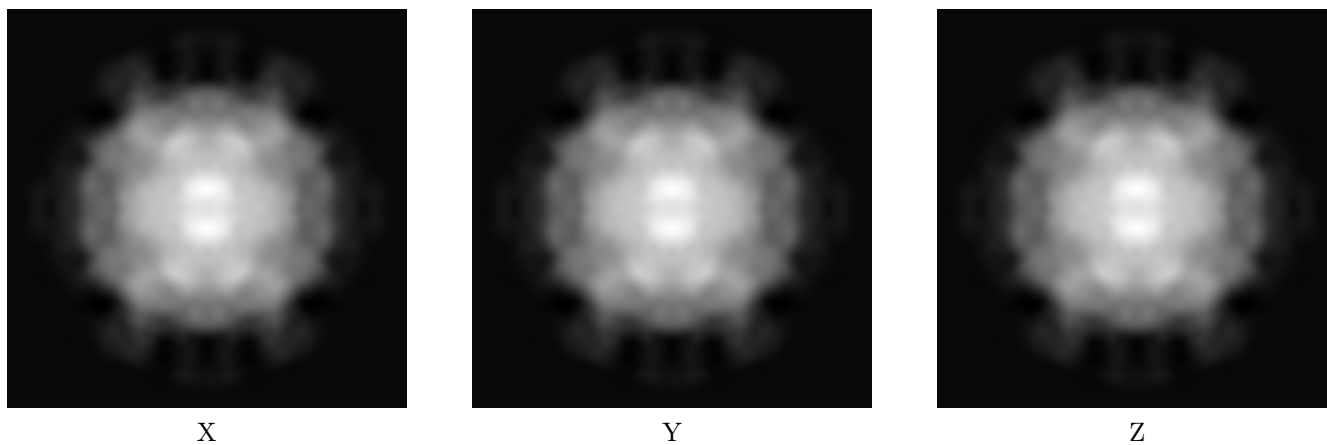
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2761. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

### 6.1 Orthogonal projections [i](#)

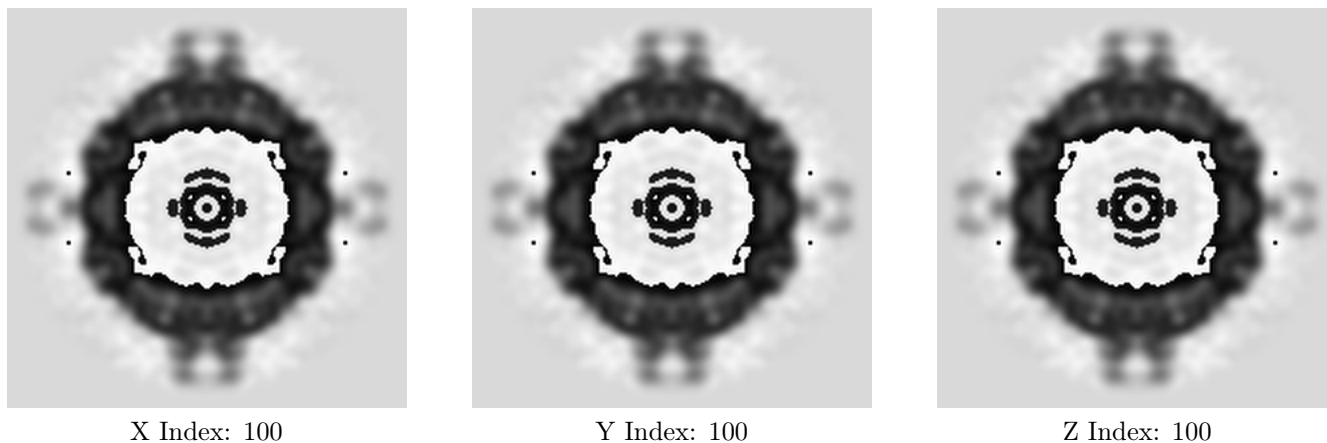
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

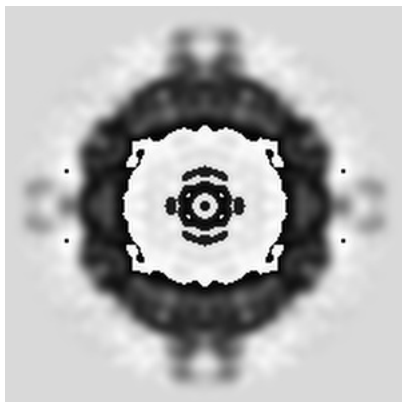
#### 6.2.1 Primary map



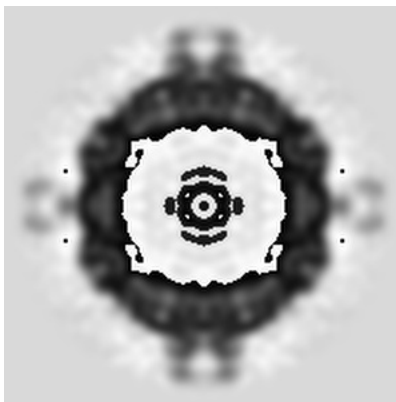
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

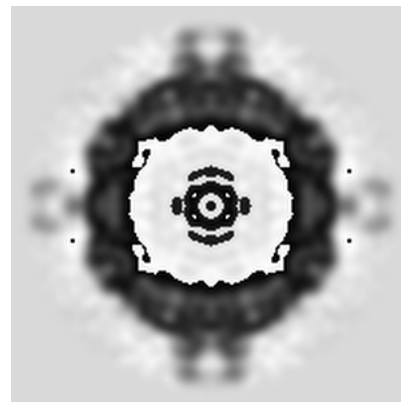
### 6.3.1 Primary map



X Index: 100



Y Index: 100

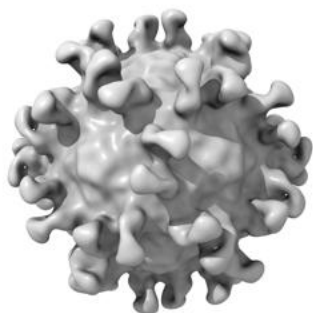


Z Index: 100

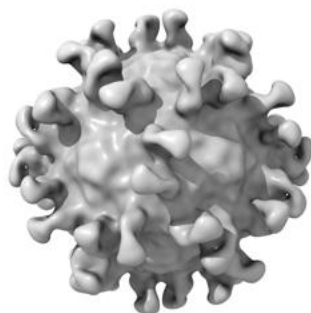
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

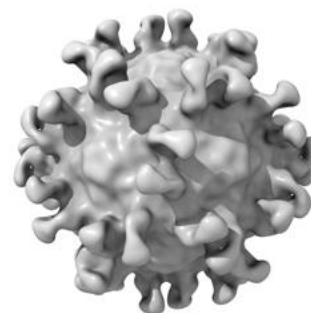
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 7999.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

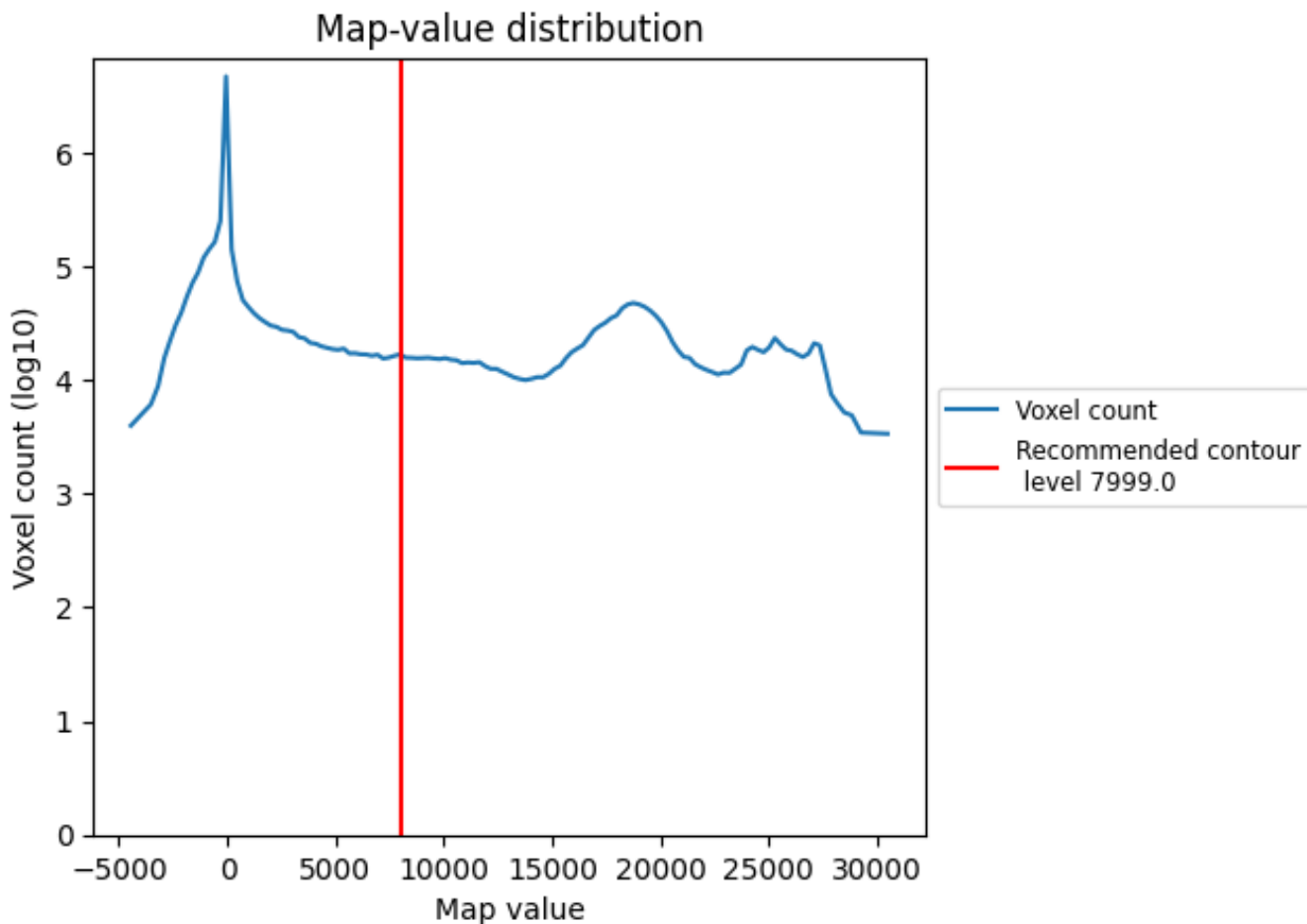
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

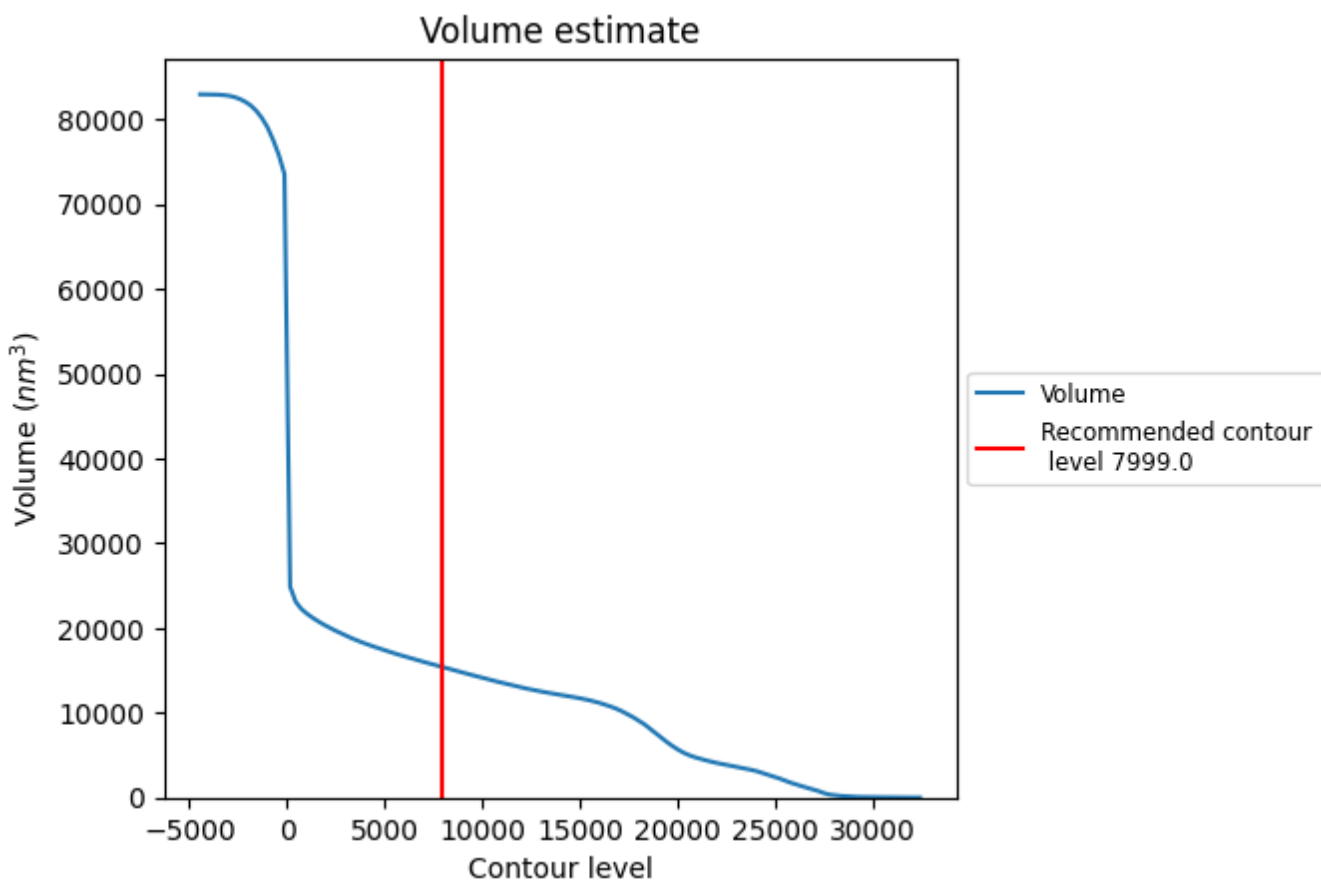
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

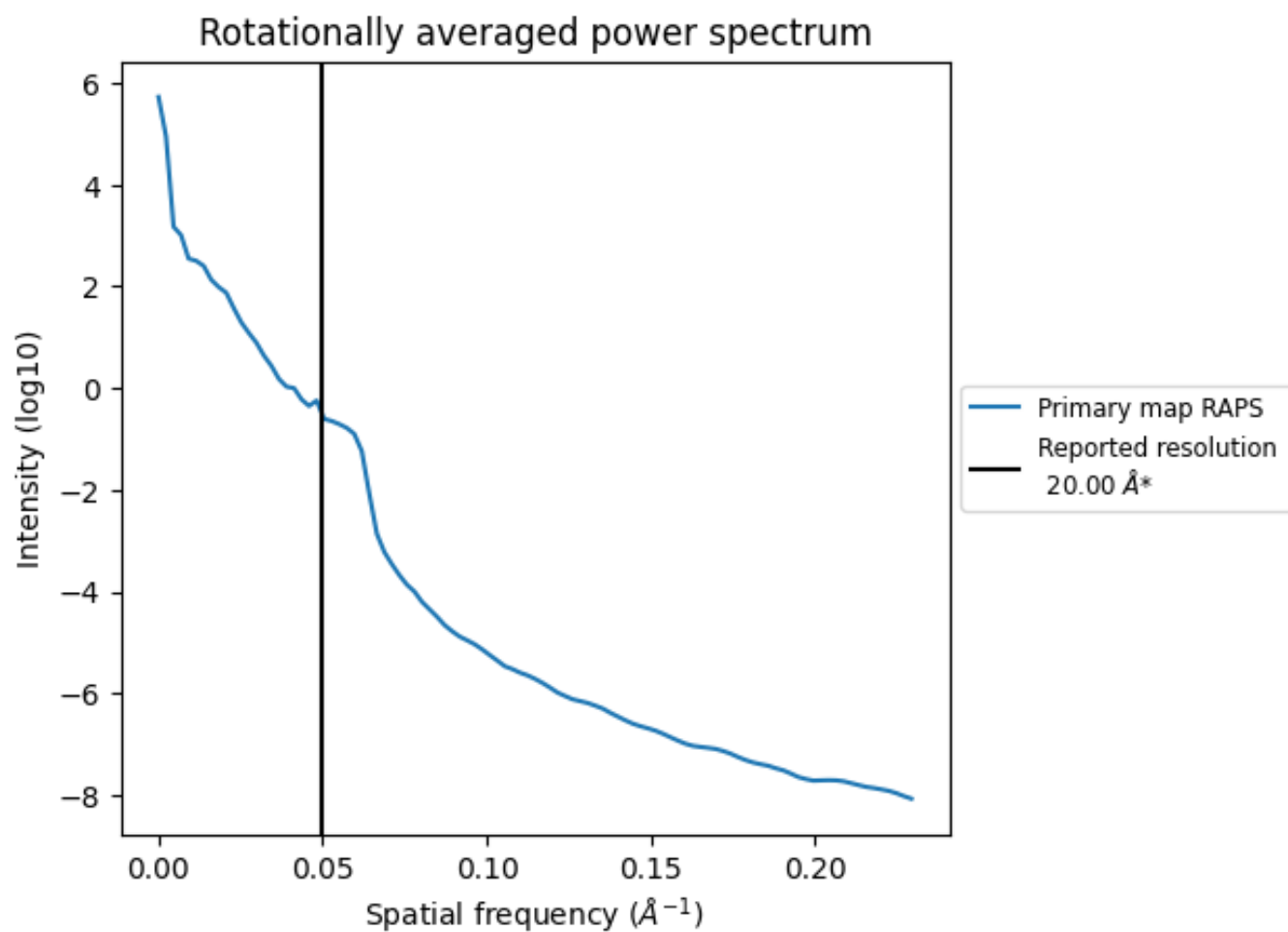
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 15383  $\text{nm}^3$ ; this corresponds to an approximate mass of 13896 kDa.

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

### 7.3 Rotationally averaged power spectrum [i](#)

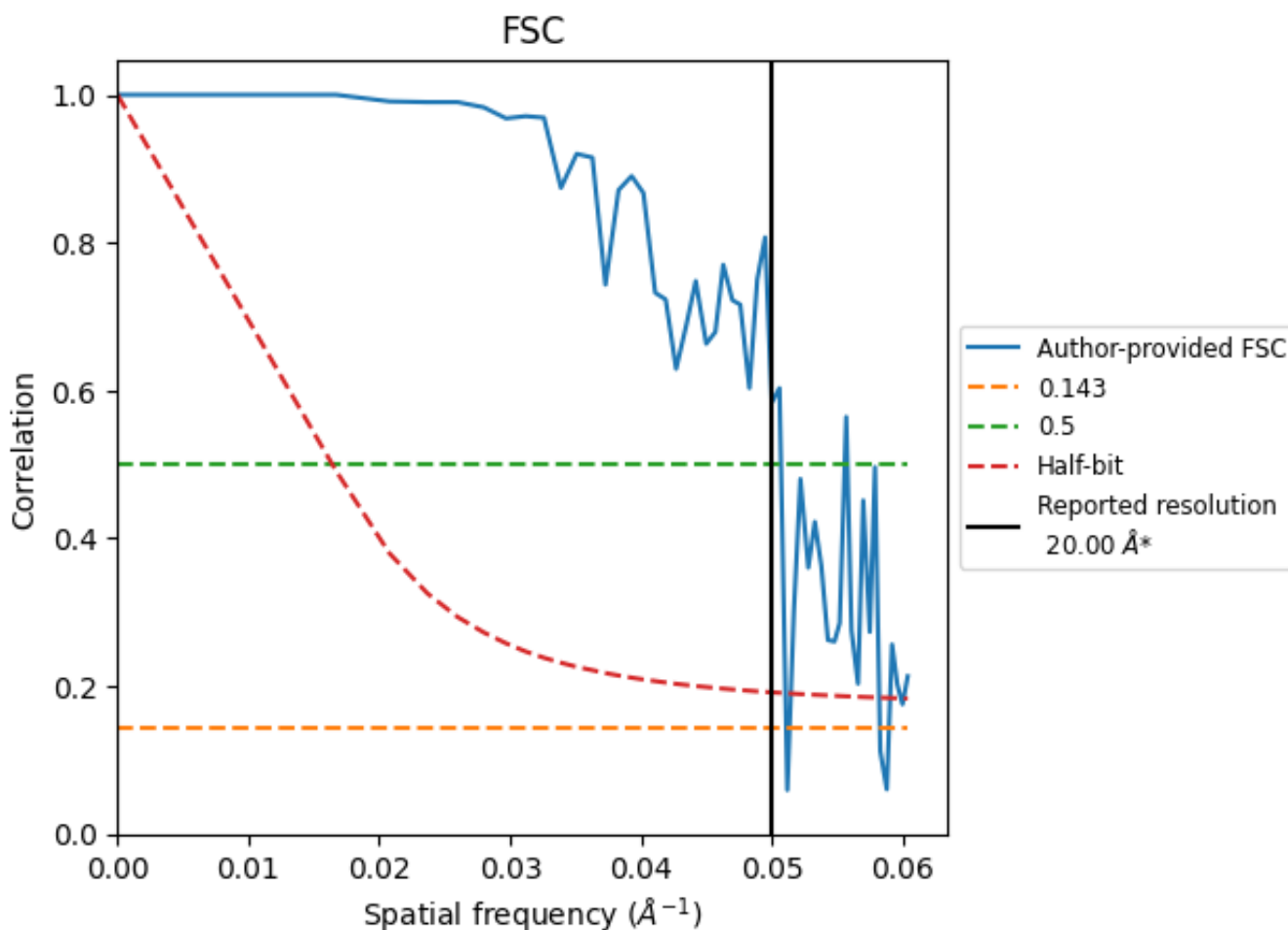


\*Reported resolution corresponds to spatial frequency of 0.050 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.050 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	19.57	19.72	19.61
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

## 9 Map-model fit

This section was not generated.