



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Sep 27, 2018 – 03:53 PM EDT

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/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

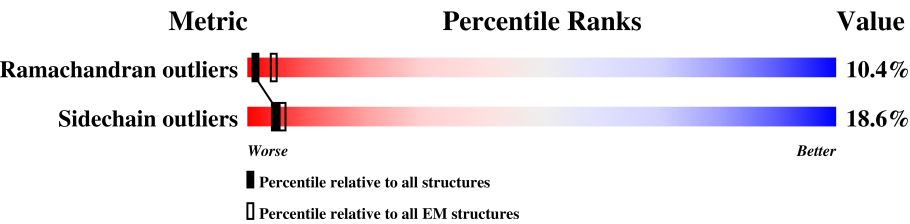
MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031172

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	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div><div>42%</div><div>17%</div><div>23%</div><div>18%</div></div>
1	16	183	<div><div>42%</div><div>17%</div><div>23%</div><div>18%</div></div>
1	1A	183	<div><div>42%</div><div>17%</div><div>23%</div><div>18%</div></div>
1	1E	183	<div><div>42%</div><div>17%</div><div>23%</div><div>18%</div></div>
1	1I	183	<div><div>42%</div><div>17%</div><div>23%</div><div>18%</div></div>
1	1M	183	<div><div>42%</div><div>17%</div><div>23%</div><div>18%</div></div>
1	1Q	183	<div><div>42%</div><div>17%</div><div>23%</div><div>18%</div></div>
1	1U	183	<div><div>42%</div><div>17%</div><div>23%</div><div>18%</div></div>
1	1Y	183	<div><div>42%</div><div>17%</div><div>23%</div><div>18%</div></div>
1	22	183	<div><div>42%</div><div>17%</div><div>23%</div><div>18%</div></div>
1	26	183	<div><div>42%</div><div>17%</div><div>23%</div><div>18%</div></div>

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

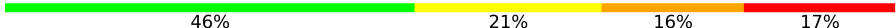
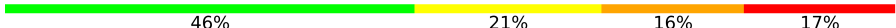
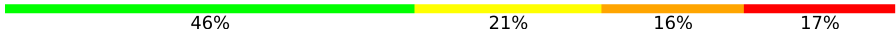

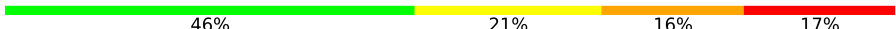
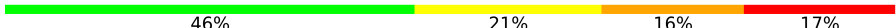
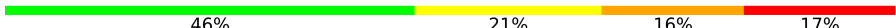
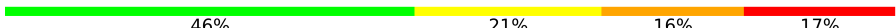
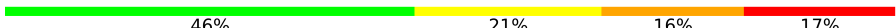





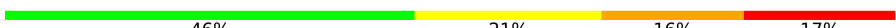
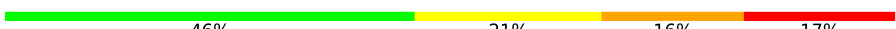


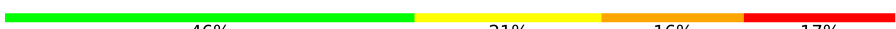
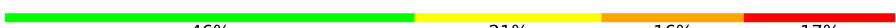
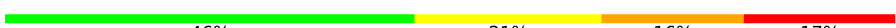
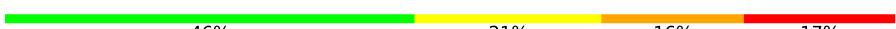
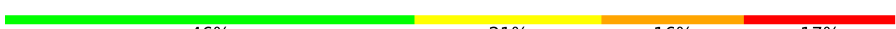
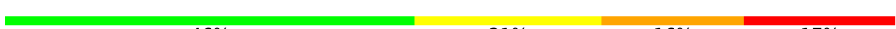
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Mol	Chain	Length	Quality of chain			
1	52	183	<div><div></div><div></div><div></div><div></div></div> <div>42%17%23%18%</div>			
1	56	183	<div><div></div><div></div><div></div><div></div></div> <div>42%17%23%18%</div>			
1	5A	183	<div><div></div><div></div><div></div><div></div></div> <div>42%17%23%18%</div>			
1	5E	183	<div><div></div><div></div><div></div><div></div></div> <div>42%17%23%18%</div>			
1	5I	183	<div><div></div><div></div><div></div><div></div></div> <div>42%17%23%18%</div>			
1	5M	183	<div><div></div><div></div><div></div><div></div></div> <div>42%17%23%18%</div>			
1	5Q	183	<div><div></div><div></div><div></div><div></div></div> <div>42%17%23%18%</div>			
1	5U	183	<div><div></div><div></div><div></div><div></div></div> <div>42%17%23%18%</div>			
1	5Y	183	<div><div></div><div></div><div></div><div></div></div> <div>42%17%23%18%</div>			
1	62	183	<div><div></div><div></div><div></div><div></div></div> <div>42%17%23%18%</div>			
1	66	183	<div><div></div><div></div><div></div><div></div></div> <div>42%17%23%18%</div>			
1	6A	183	<div><div></div><div></div><div></div><div></div></div> <div>42%17%23%18%</div>			
1	6E	183	<div><div></div><div></div><div></div><div></div></div> <div>42%17%23%18%</div>			
1	6I	183	<div><div></div><div></div><div></div><div></div></div> <div>42%17%23%18%</div>			
1	6M	183	<div><div></div><div></div><div></div><div></div></div> <div>42%17%23%18%</div>			
1	6Q	183	<div><div></div><div></div><div></div><div></div></div> <div>42%17%23%18%</div>			
1	6U	183	<div><div></div><div></div><div></div><div></div></div> <div>42%17%23%18%</div>			
1	6Y	183	<div><div></div><div></div><div></div><div></div></div> <div>42%17%23%18%</div>			
1	7A	183	<div><div></div><div></div><div></div><div></div></div> <div>42%17%23%18%</div>			
1	7E	183	<div><div></div><div></div><div></div><div></div></div> <div>42%17%23%18%</div>			
1	7I	183	<div><div></div><div></div><div></div><div></div></div> <div>42%17%23%18%</div>			
1	7M	183	<div><div></div><div></div><div></div><div></div></div> <div>42%17%23%18%</div>			
1	7Q	183	<div><div></div><div></div><div></div><div></div></div> <div>42%17%23%18%</div>			
1	7U	183	<div><div></div><div></div><div></div><div></div></div> <div>42%17%23%18%</div>			
2	13	229	<div><div></div><div></div><div></div><div></div></div> <div>46%21%16%17%</div>			

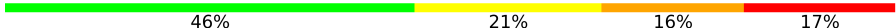
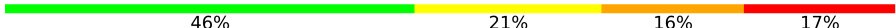
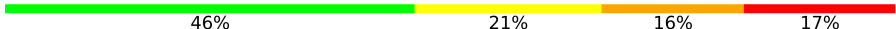

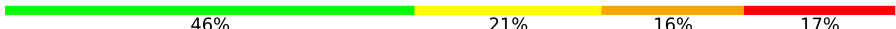
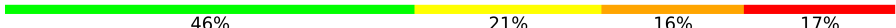
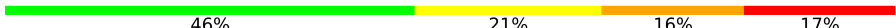
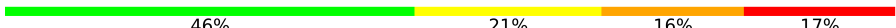
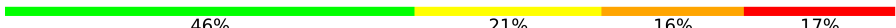






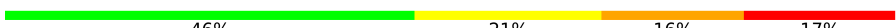
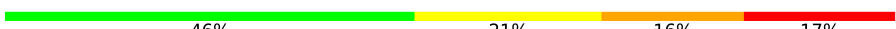


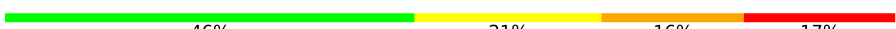
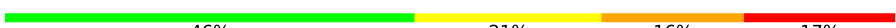
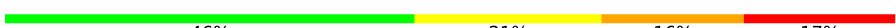
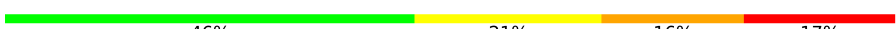
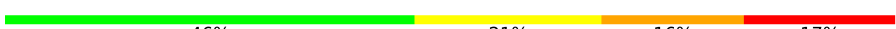
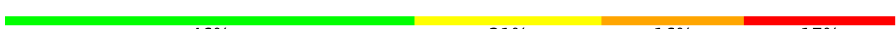
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Mol	Chain	Length	Quality of chain			
2	17	229		46%	21%	16% 17%
2	1B	229		46%	21%	16% 17%
2	1F	229		46%	21%	16% 17%
2	1J	229		46%	21%	16% 17%
2	1N	229		46%	21%	16% 17%
2	1R	229		46%	21%	16% 17%
2	1V	229		46%	21%	16% 17%
2	1Z	229		46%	21%	16% 17%
2	23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

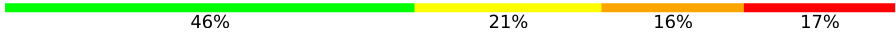
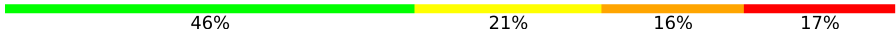
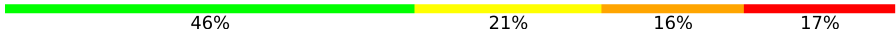

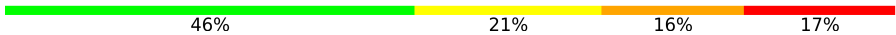

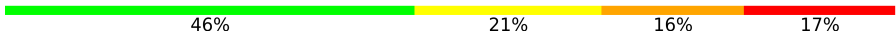
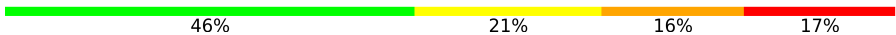
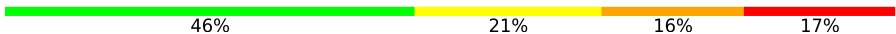
















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Mol	Chain	Length	Quality of chain			
2	3Z	229		46%	21%	16% 17%
2	43	229		46%	21%	16% 17%
2	47	229		46%	21%	16% 17%
2	4B	229		46%	21%	16% 17%
2	4F	229		46%	21%	16% 17%
2	4J	229		46%	21%	16% 17%
2	4N	229		46%	21%	16% 17%
2	4R	229		46%	21%	16% 17%
2	4V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














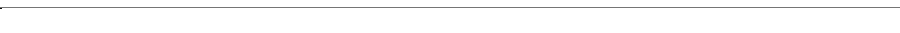


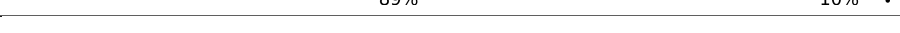
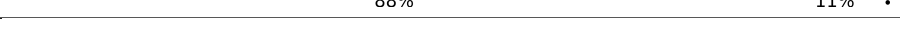







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Mol	Chain	Length	Quality of chain
2	6R	229	
2	6V	229	
2	6Z	229	
2	7B	229	
2	7F	229	
2	7J	229	
2	7N	229	
2	7R	229	
2	7V	229	
3	10	109	
3	14	109	
3	18	109	
3	1C	109	
3	1G	109	
3	1K	109	
3	1O	109	
3	1S	109	
3	1W	109	
3	20	109	
3	24	109	
3	28	109	
3	2C	109	
3	2G	109	
3	2K	109	
3	2O	109	














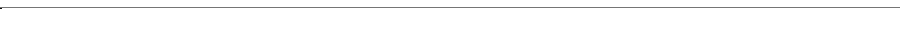


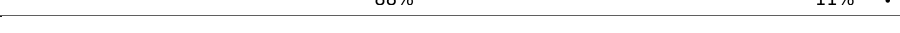
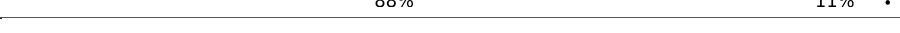







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Mol	Chain	Length	Quality of chain
3	2S	109	 88% 11% .
3	2W	109	 88% 11% .
3	30	109	 88% 11% .
3	34	109	 89% 10% .
3	38	109	 88% 11% .
3	3C	109	 89% 10% .
3	3G	109	 88% 11% .
3	3K	109	 89% 10% .
3	3O	109	 88% 11% .
3	3S	109	 88% 11% .
3	3W	109	 88% 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% .
3	5G	109	 88% 11% .


























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Mol	Chain	Length	Quality of chain
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% .
4	1L	122	 80% 16% .


























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Mol	Chain	Length	Quality of chain	
4	1P	122		80% 16% .
4	1T	122		80% 16% .
4	1X	122		80% 16% .
4	2I	122		80% 16% .
4	25	122		80% 16% .
4	29	122		80% 16% .
4	2D	122		80% 16% .
4	2H	122		80% 16% .
4	2L	122		80% 16% .
4	2P	122		80% 16% .
4	2T	122		80% 16% .
4	2X	122		80% 16% .
4	3I	122		80% 16% .
4	35	122		80% 16% .
4	39	122		80% 16% .
4	3D	122		80% 16% .
4	3H	122		80% 16% .
4	3L	122		80% 16% .
4	3P	122		80% 16% .
4	3T	122		80% 16% .
4	3X	122		80% 16% .
4	4I	122		80% 16% .
4	45	122		80% 16% .
4	49	122		80% 16% .
4	4D	122		80% 16% .





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Mol	Chain	Length	Quality of chain
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% .
4	7H	122	 80% 16% .

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Mol	Chain	Length	Quality of chain
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
1	1A	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	1E	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	1I	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	1M	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	1Q	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	1U	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	1Y	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	12	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	16	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	2A	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	2E	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	2I	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	2M	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	2Q	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	2U	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	2Y	183	Total 1449	C 926	N 244	O 272	S 7	0	0
1	22	183	Total 1449	C 926	N 244	O 272	S 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	52	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	62	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
1	7U	183	Total	C	N	O	S	0	0
			1449	926	244	272	7		

- Molecule 2 is a protein called Protein VP0.

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

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

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

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

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

- Molecule 4 is a protein called HUMAN MONOCLONAL ANTIBODY.

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

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Mol	Chain	Residues	Atoms						AltConf	Trace
4	1H	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	1L	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	1P	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	1T	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	1X	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	11	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	15	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	19	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	2D	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	2H	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	2L	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	2P	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	2T	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	2X	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	21	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	25	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	29	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	3D	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	3H	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	3L	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	3P	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
4	3T	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	3X	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	3I	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	35	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	39	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	4D	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	4H	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	4L	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	4P	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	4T	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	4X	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	4I	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	45	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	49	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	5D	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	5H	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	5L	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	5P	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	5T	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	5X	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	5I	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0

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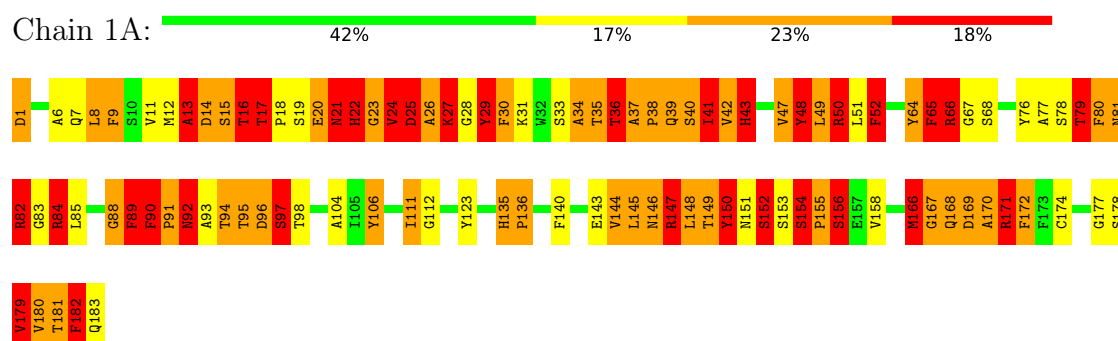
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Mol	Chain	Residues	Atoms						AltConf	Trace
4	55	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	59	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	6D	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	6H	122	Total 1126	C 573	H 208	N 155	O 186	S 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	6I	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

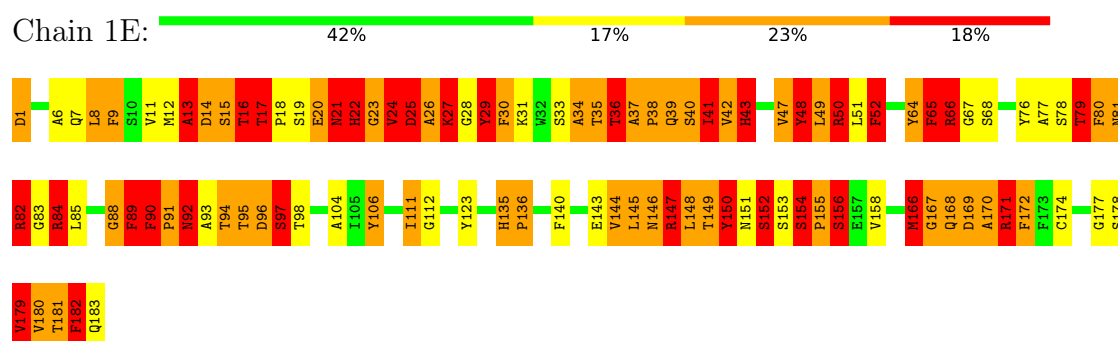
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

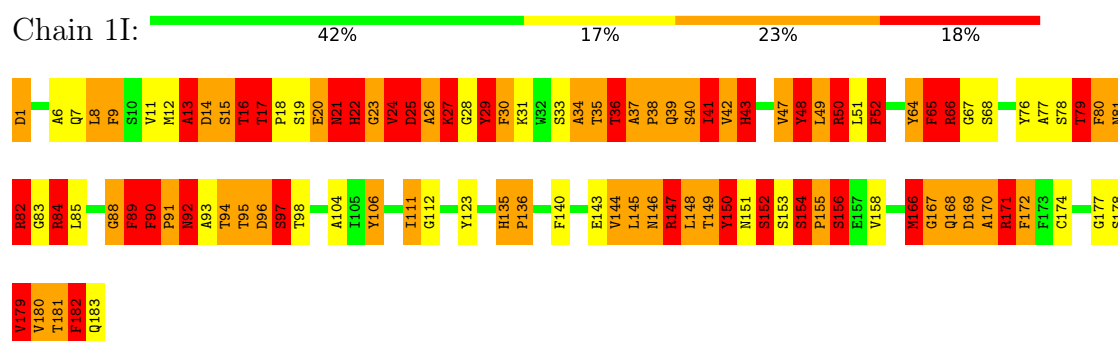
• Molecule 1: Protein VP3



• Molecule 1: Protein VP3

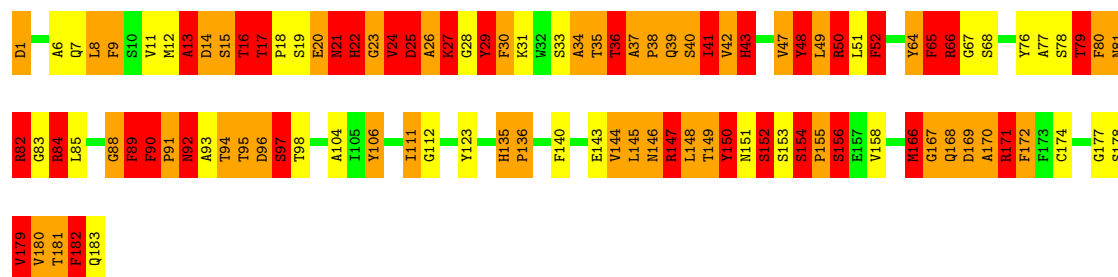


• Molecule 1: Protein VP3



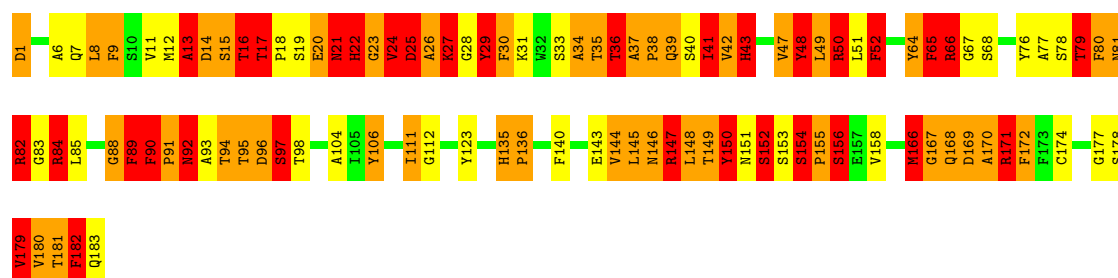
• Molecule 1: Protein VP3

Chain 1M: 



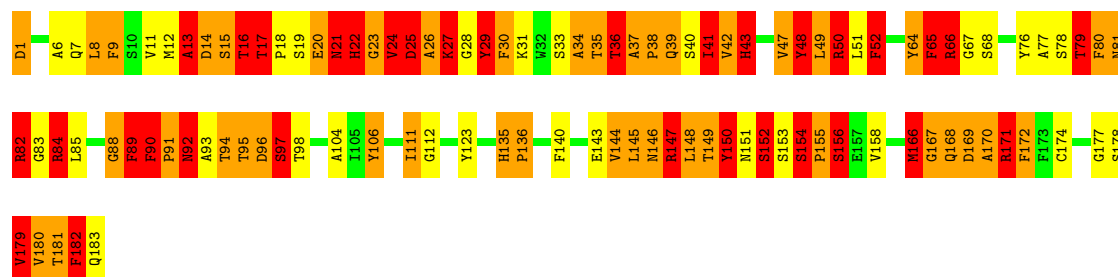
- Molecule 1: Protein VP3

Chain 1Q: 



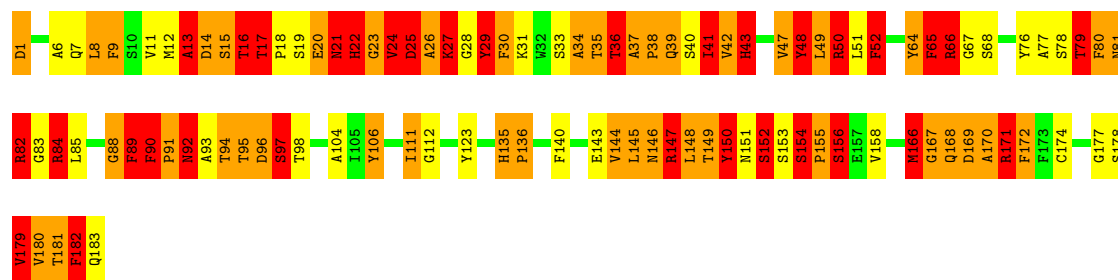
- Molecule 1: Protein VP3

Chain 1U: 

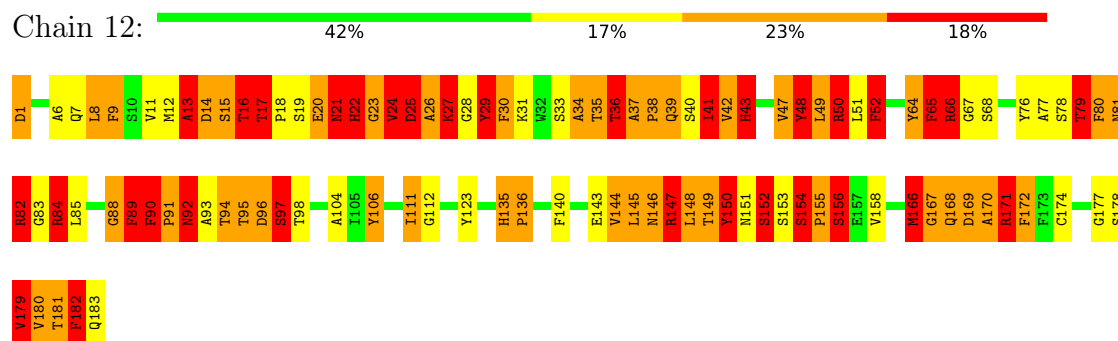


- Molecule 1: Protein VP3

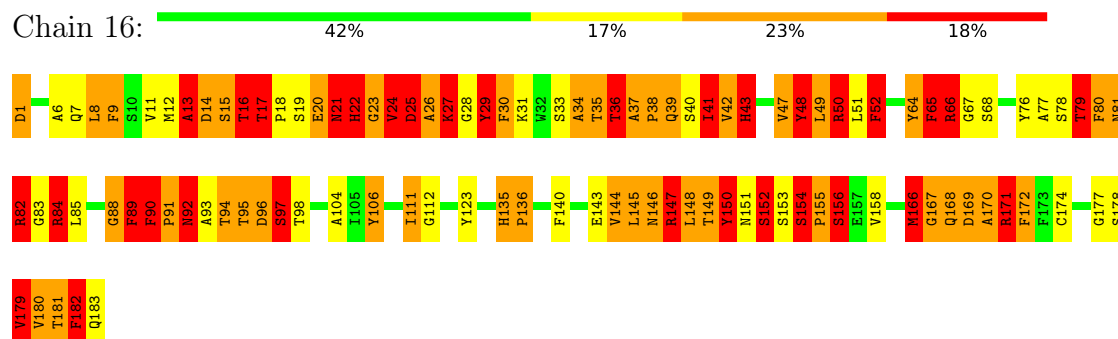
Chain 1Y: 



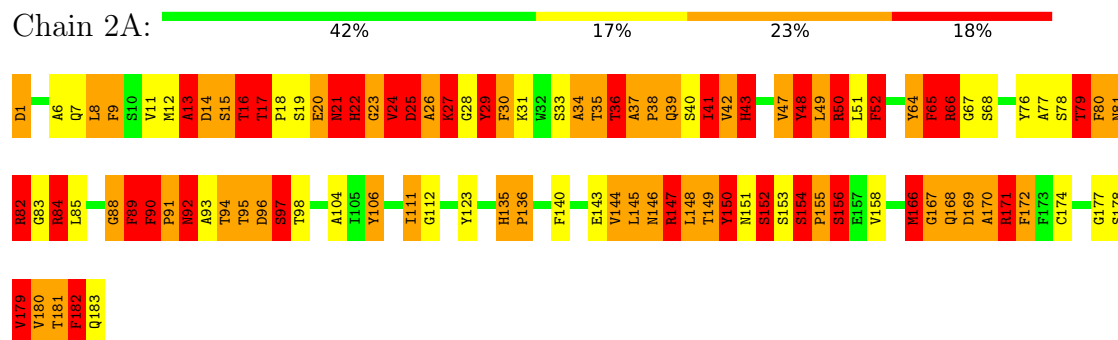
- Molecule 1: Protein VP3



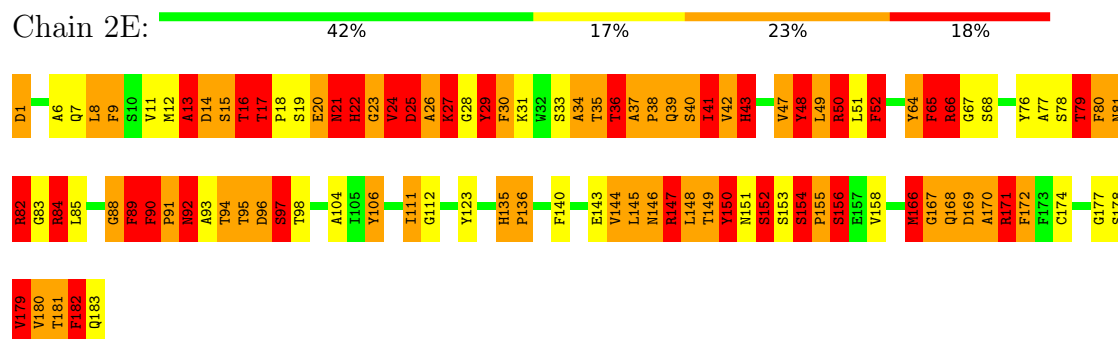
- Molecule 1: Protein VP3



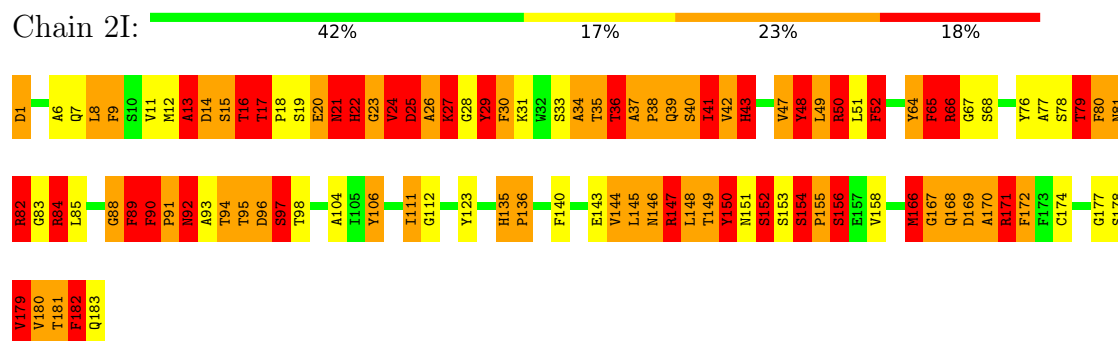
- Molecule 1: Protein VP3



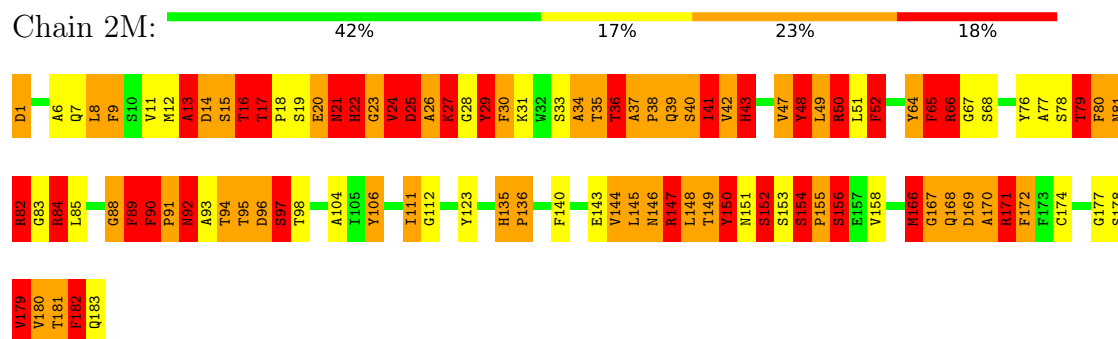
- Molecule 1: Protein VP3



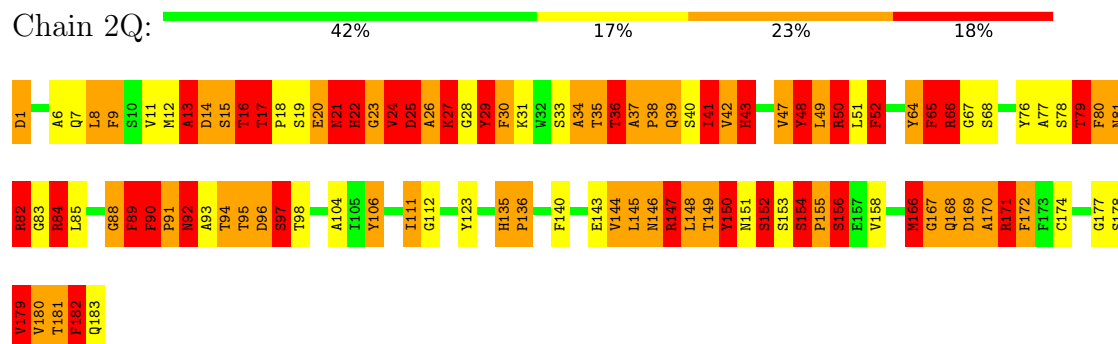
- Molecule 1: Protein VP3



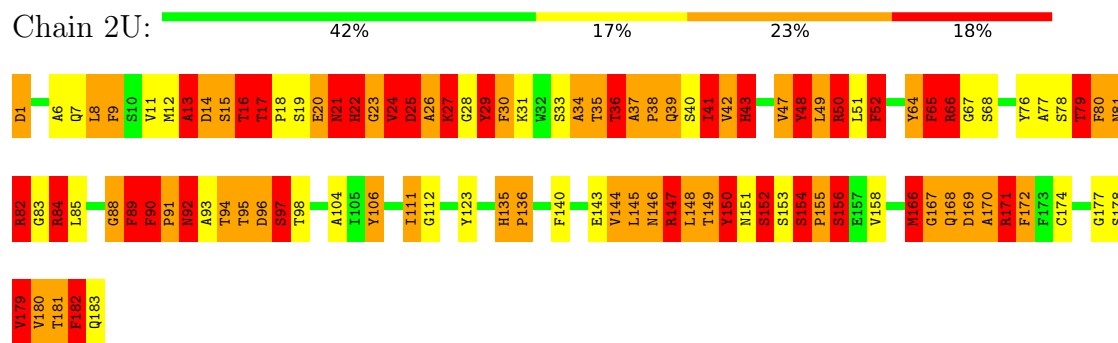
- Molecule 1: Protein VP3



- Molecule 1: Protein VP3

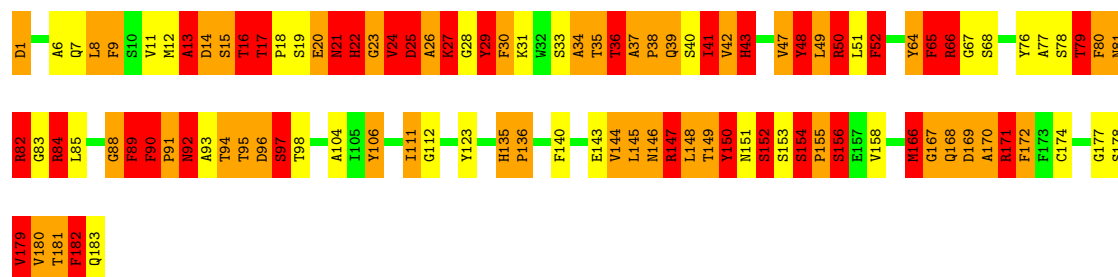


- Molecule 1: Protein VP3



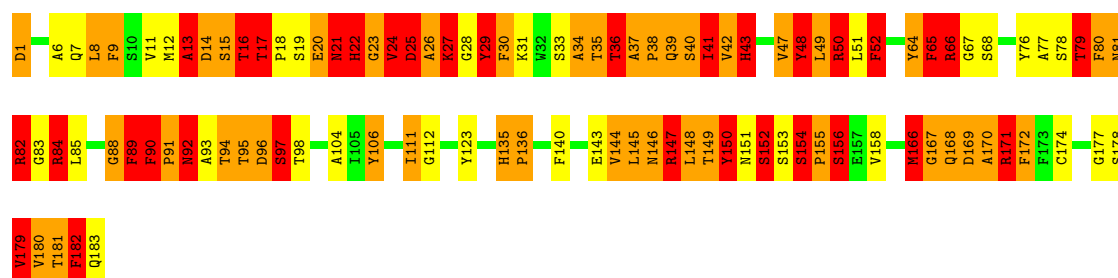
- Molecule 1: Protein VP3

Chain 2Y: 



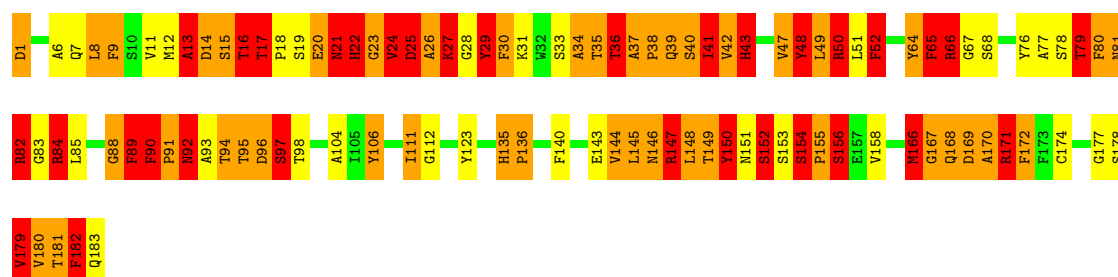
• Molecule 1: Protein VP3

Chain 22: 



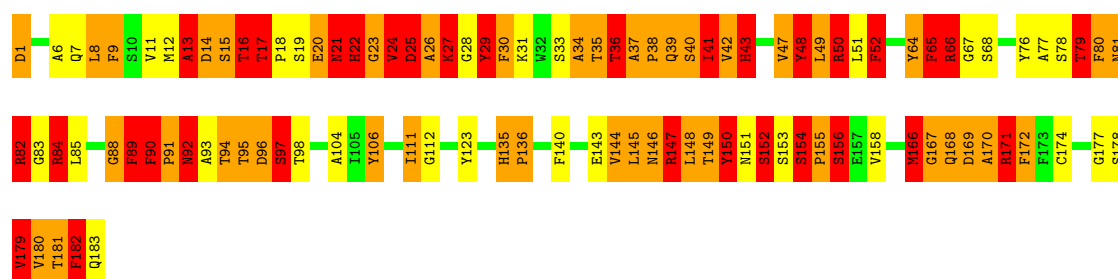
• Molecule 1: Protein VP3

Chain 26: 



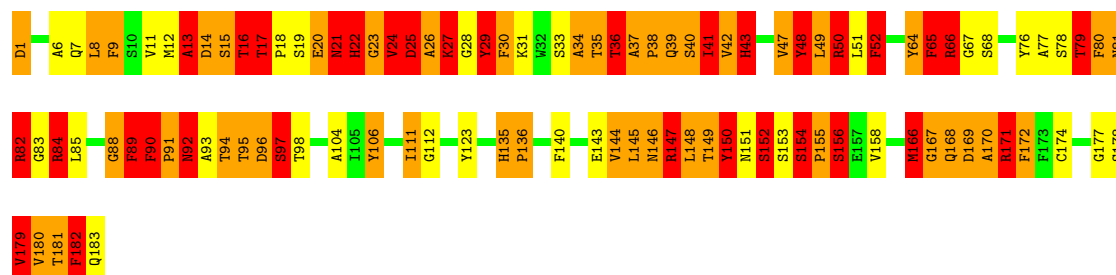
• Molecule 1: Protein VP3

Chain 3A: 



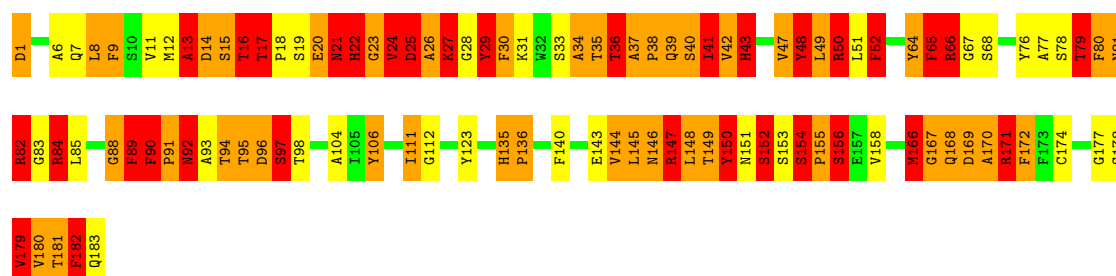
• Molecule 1: Protein VP3

Chain 3E: 



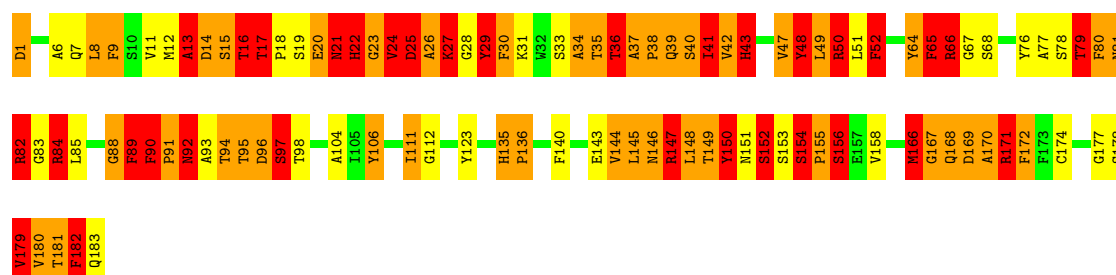
• Molecule 1: Protein VP3

Chain 3I: 



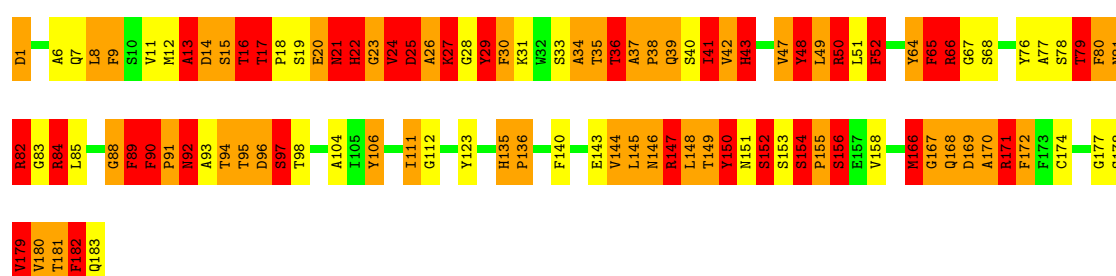
• Molecule 1: Protein VP3

Chain 3M: 



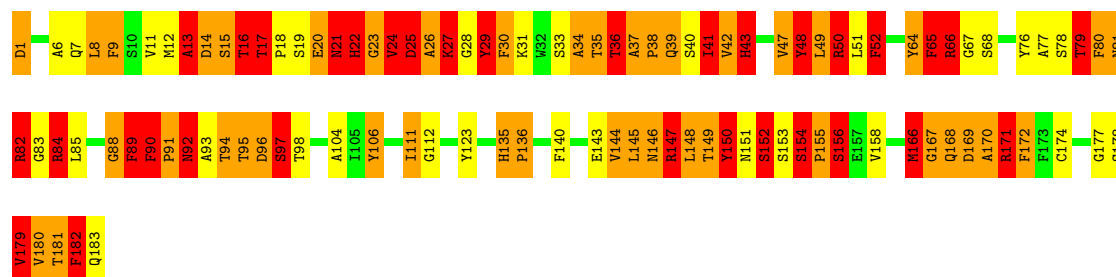
• Molecule 1: Protein VP3

Chain 3Q: 



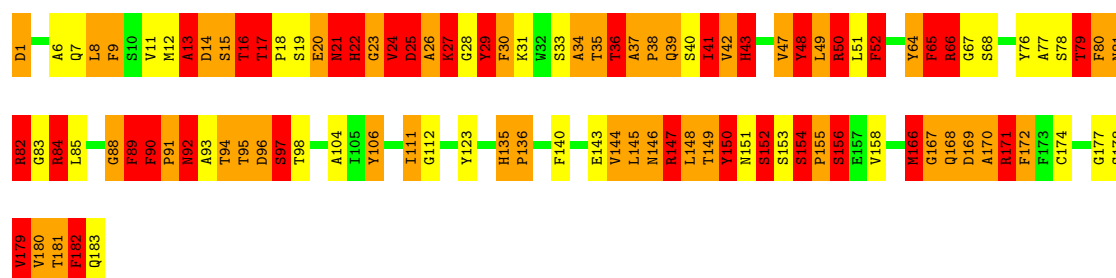
• Molecule 1: Protein VP3

Chain 3U: 



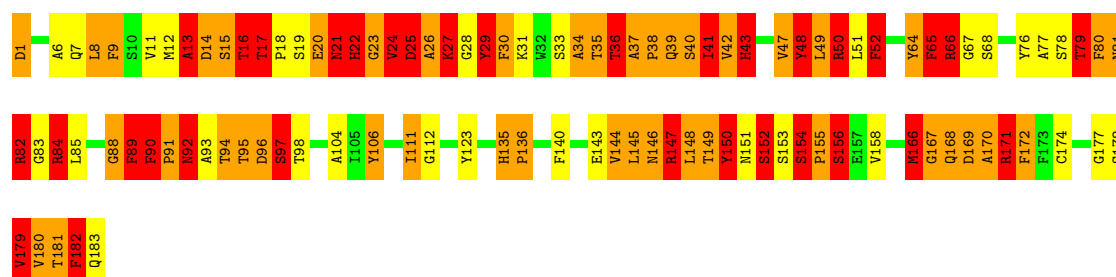
• Molecule 1: Protein VP3

Chain 3Y: 



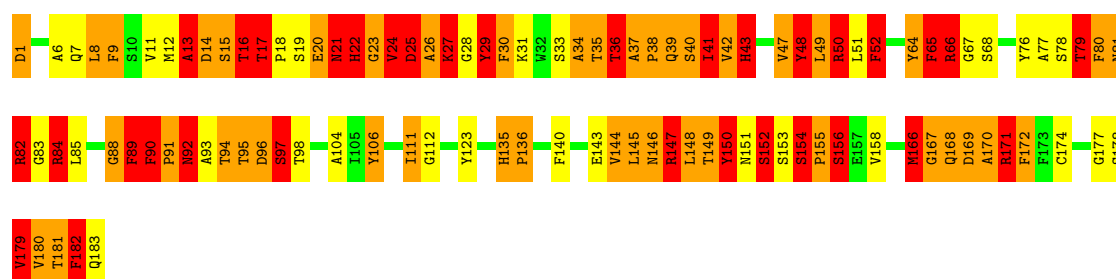
• Molecule 1: Protein VP3

Chain 32: 



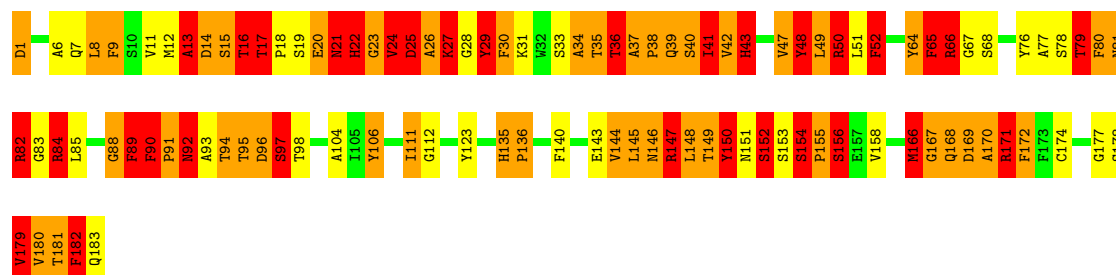
• Molecule 1: Protein VP3

Chain 36: 



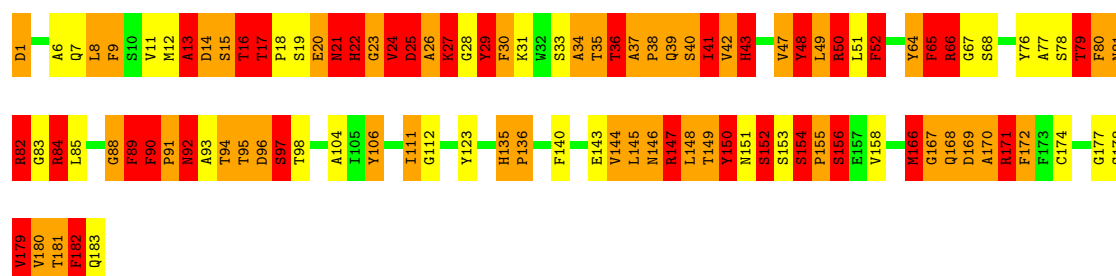
• Molecule 1: Protein VP3

Chain 4A: 



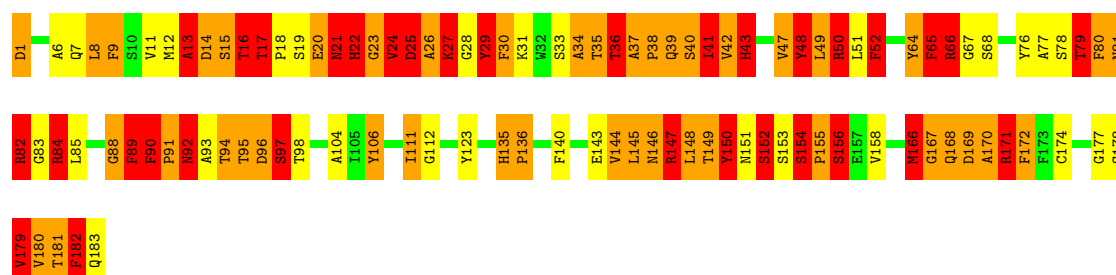
• Molecule 1: Protein VP3

Chain 4E: 



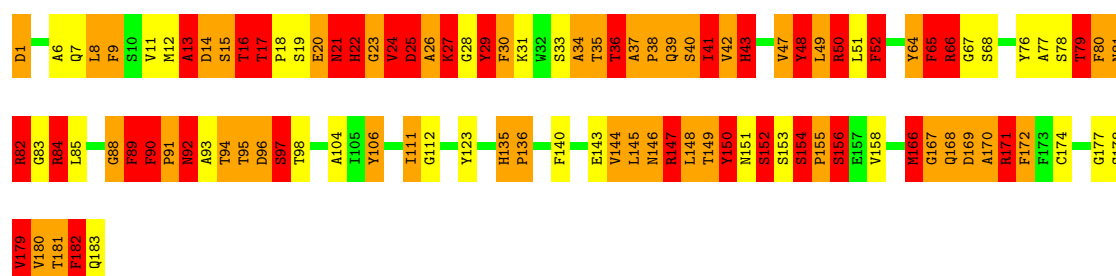
• Molecule 1: Protein VP3

Chain 4I: 



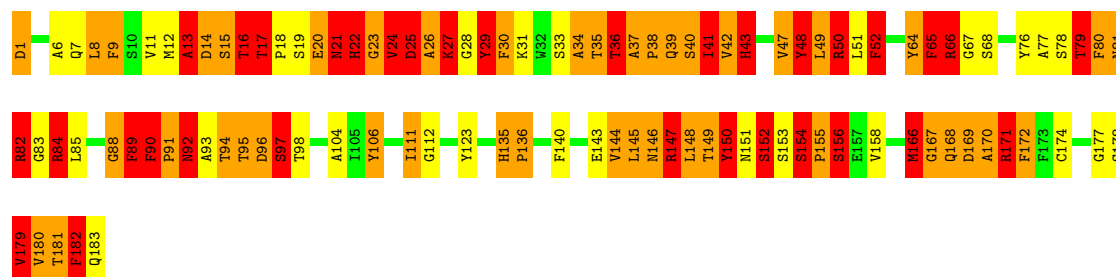
• Molecule 1: Protein VP3

Chain 4M: 



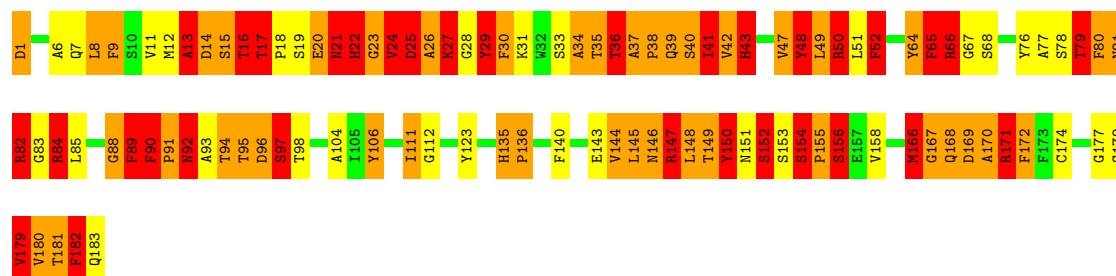
• Molecule 1: Protein VP3

Chain 4Q: 



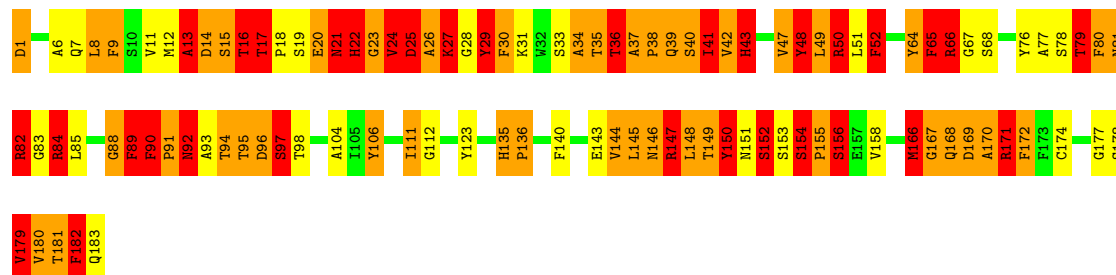
• Molecule 1: Protein VP3

Chain 4U: 



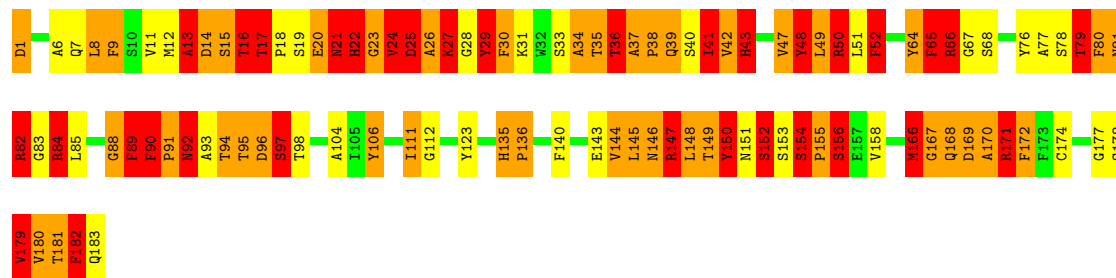
• Molecule 1: Protein VP3

Chain 4Y: 

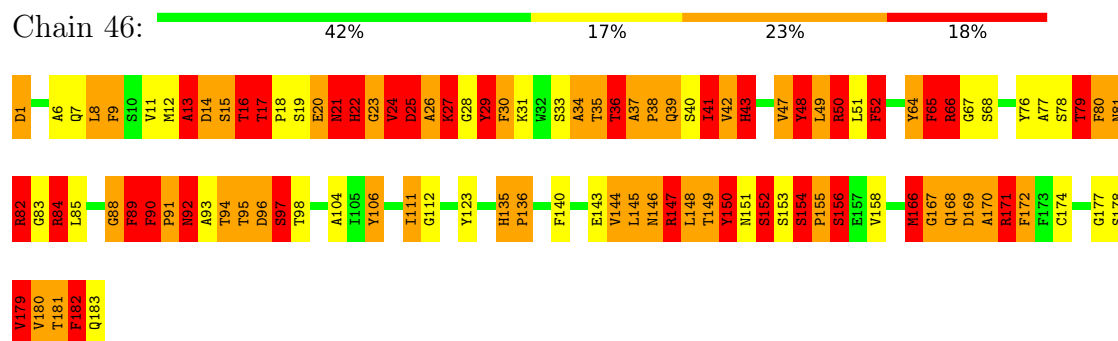


• Molecule 1: Protein VP3

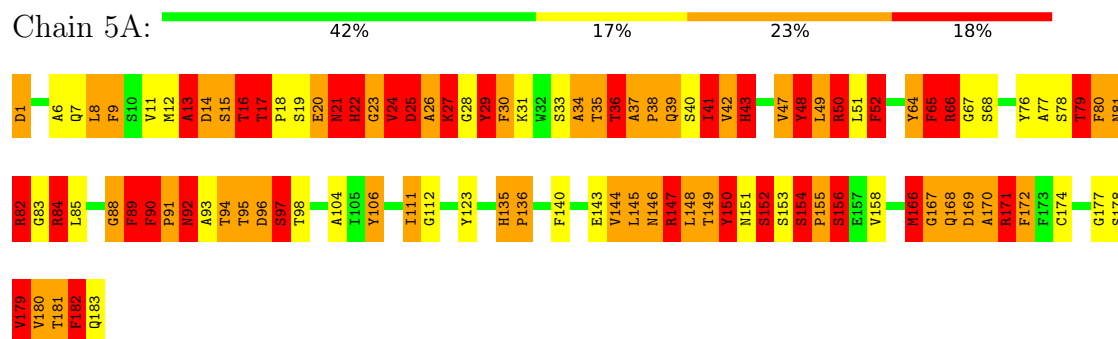
Chain 4Z: 



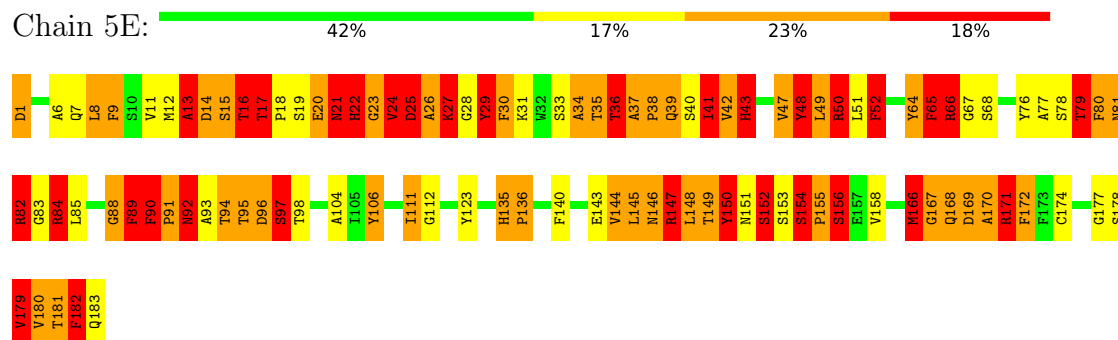
• Molecule 1: Protein VP3



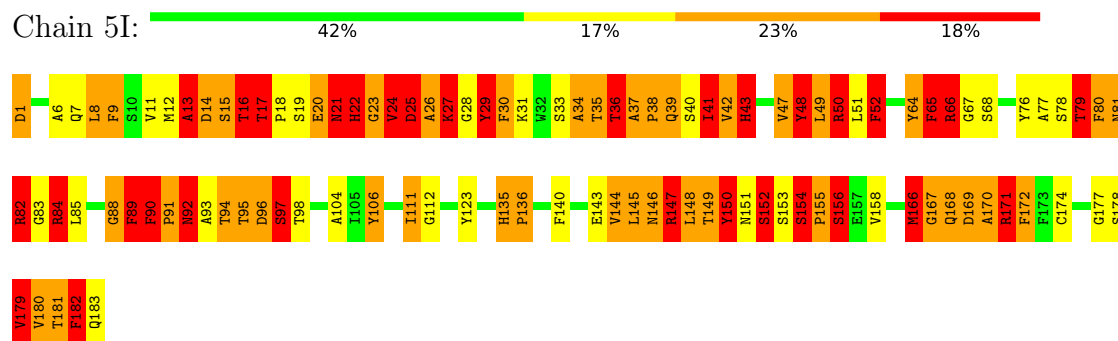
- Molecule 1: Protein VP3



- Molecule 1: Protein VP3

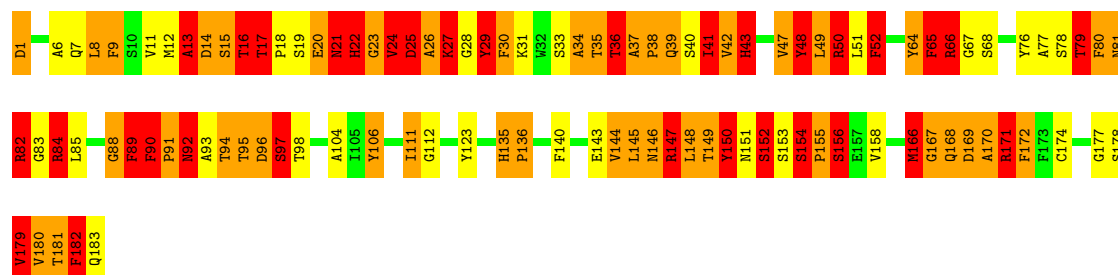


- Molecule 1: Protein VP3



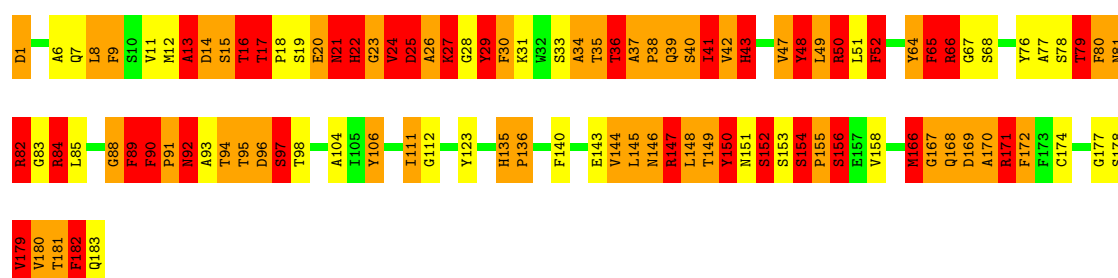
- Molecule 1: Protein VP3

Chain 5M: 



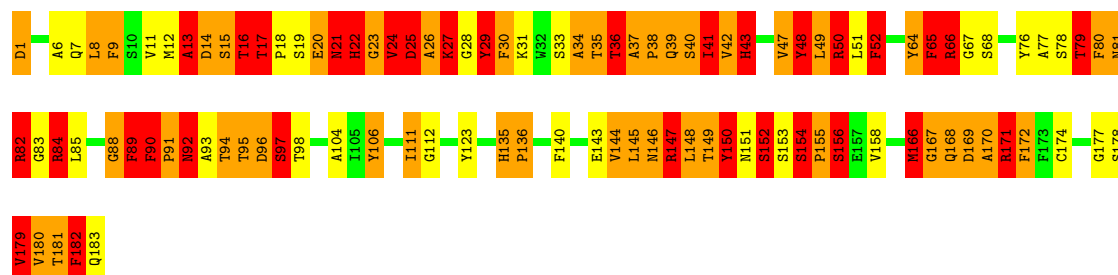
- Molecule 1: Protein VP3

Chain 5Q: 



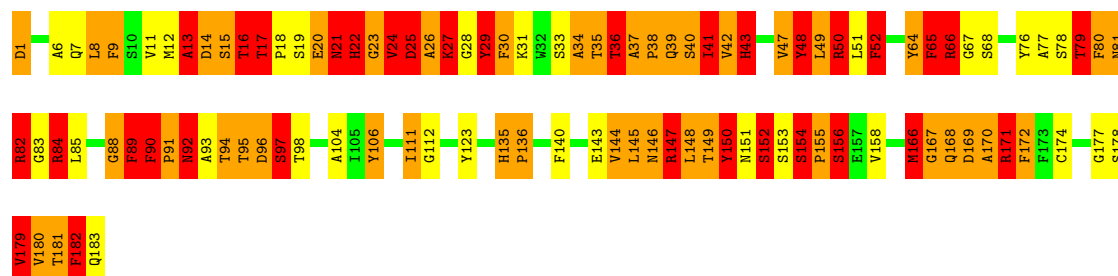
- Molecule 1: Protein VP3

Chain 5U: 

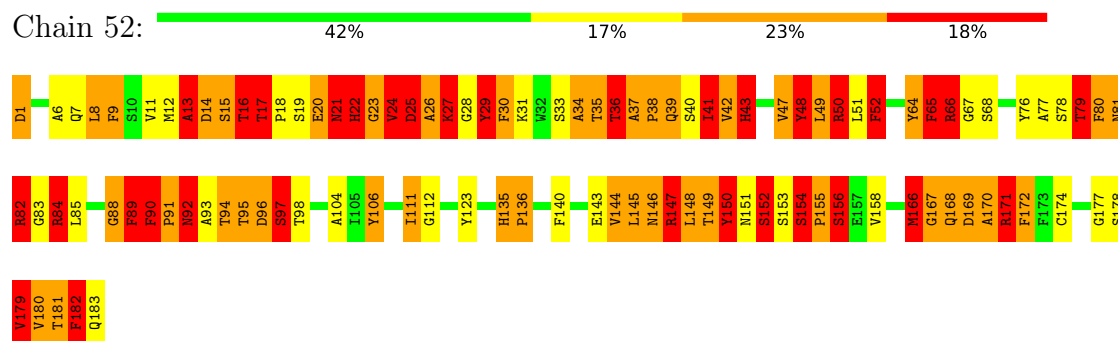


- Molecule 1: Protein VP3

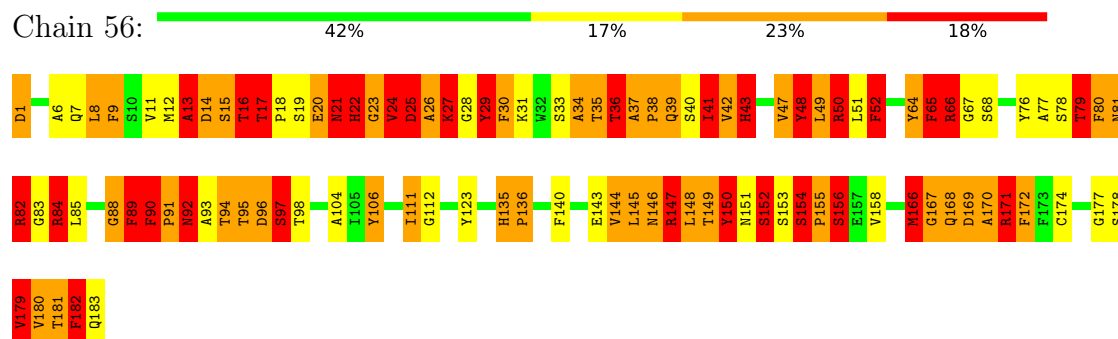
Chain 5Y: 



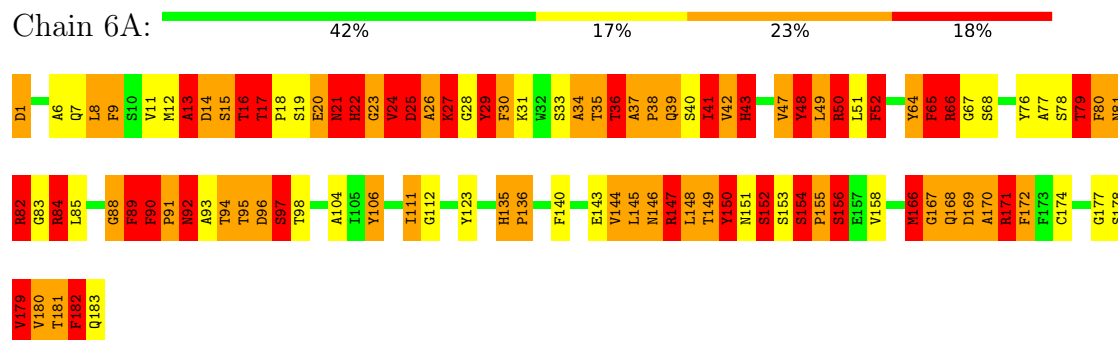
- Molecule 1: Protein VP3



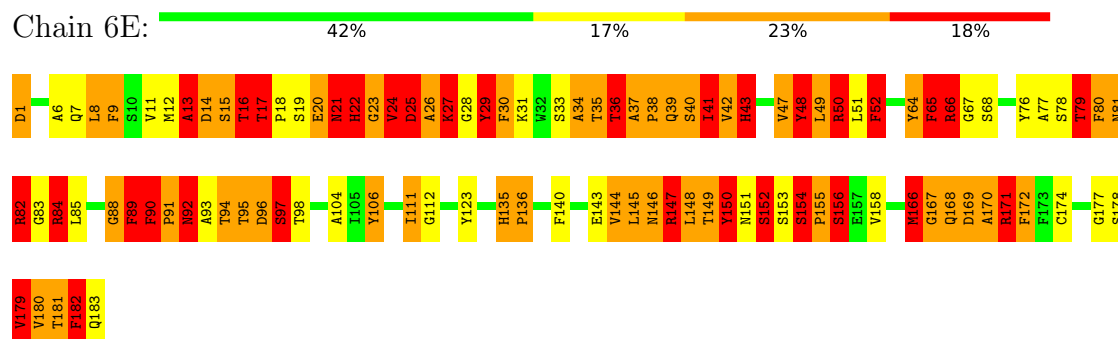
- Molecule 1: Protein VP3



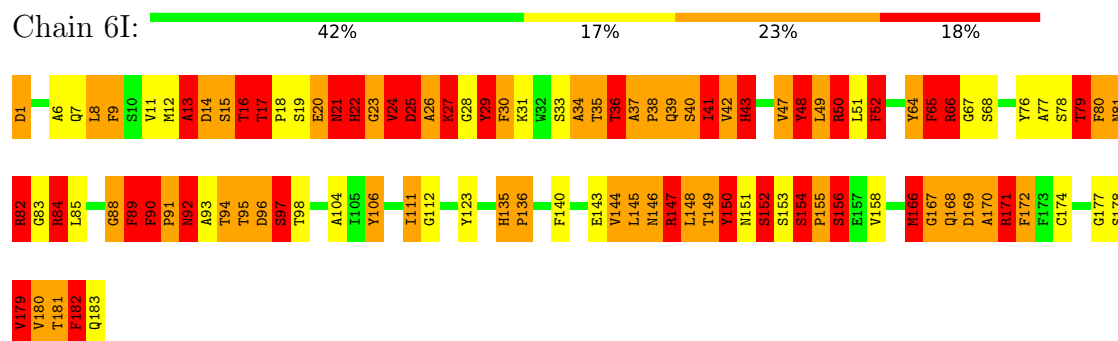
- Molecule 1: Protein VP3



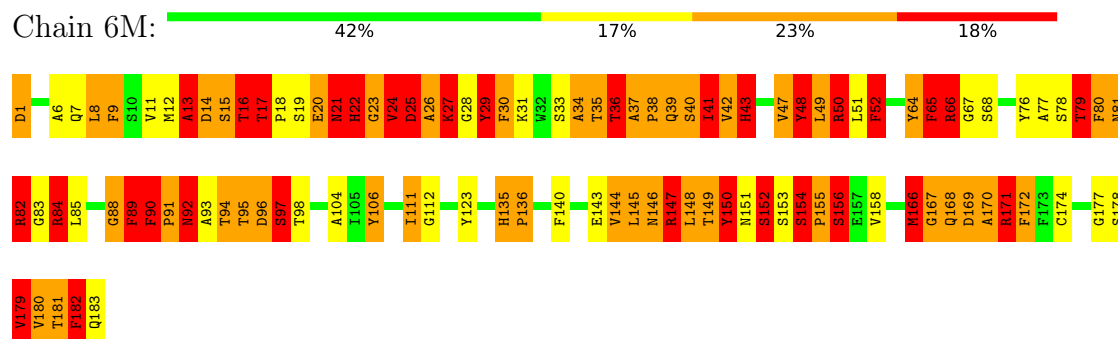
- Molecule 1: Protein VP3



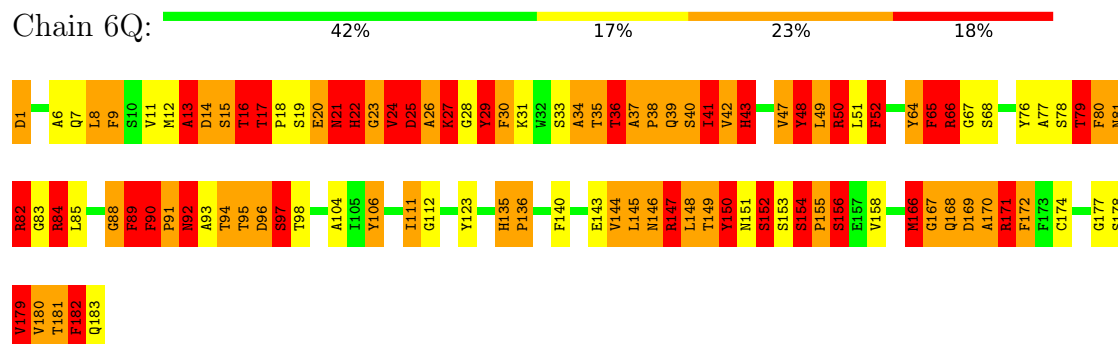
- Molecule 1: Protein VP3



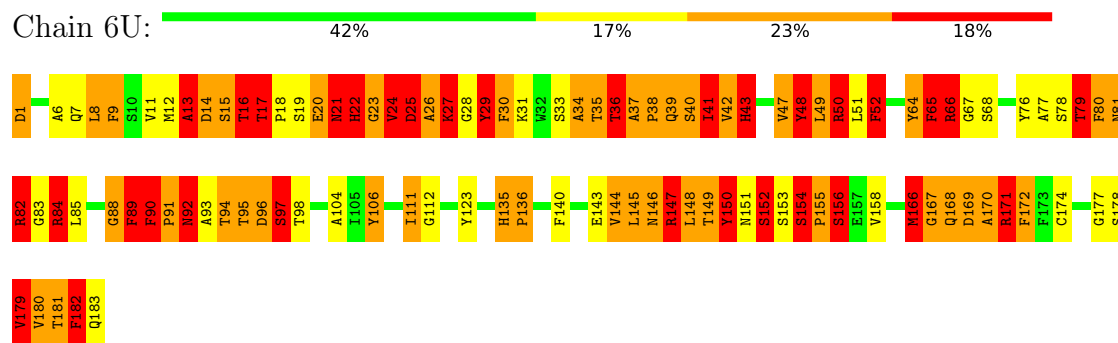
- Molecule 1: Protein VP3



- Molecule 1: Protein VP3

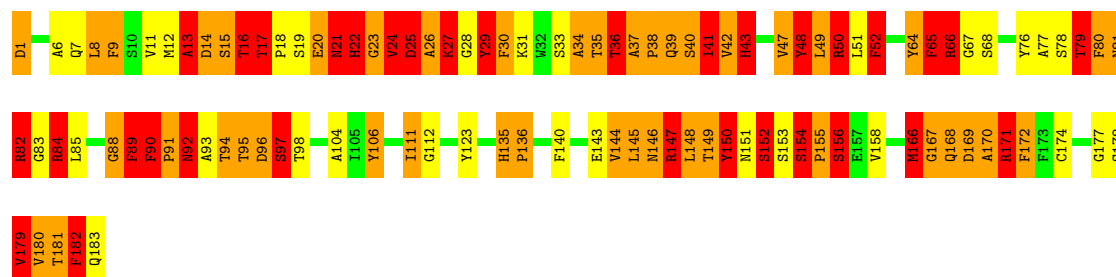


- Molecule 1: Protein VP3



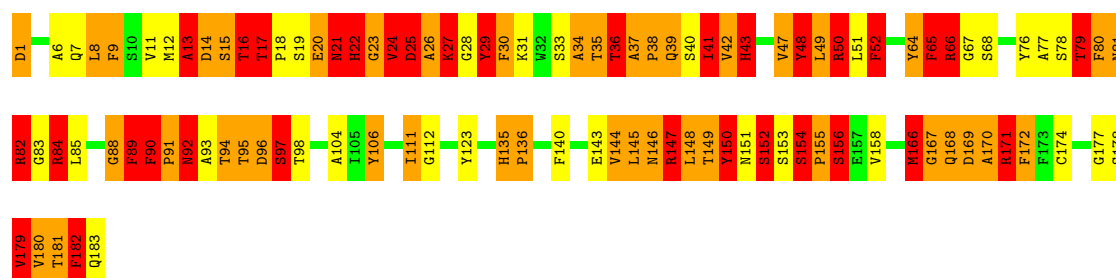
- Molecule 1: Protein VP3

Chain 6Y: 



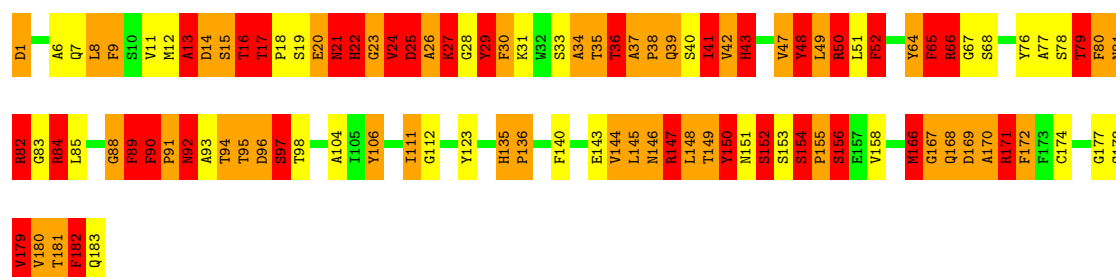
• Molecule 1: Protein VP3

Chain 62: 



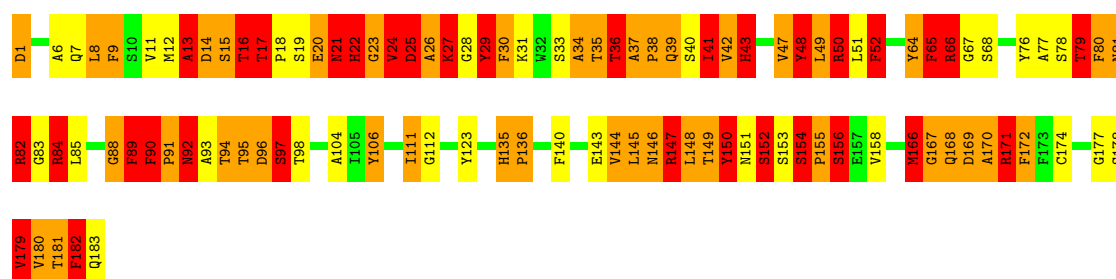
• Molecule 1: Protein VP3

Chain 66: 

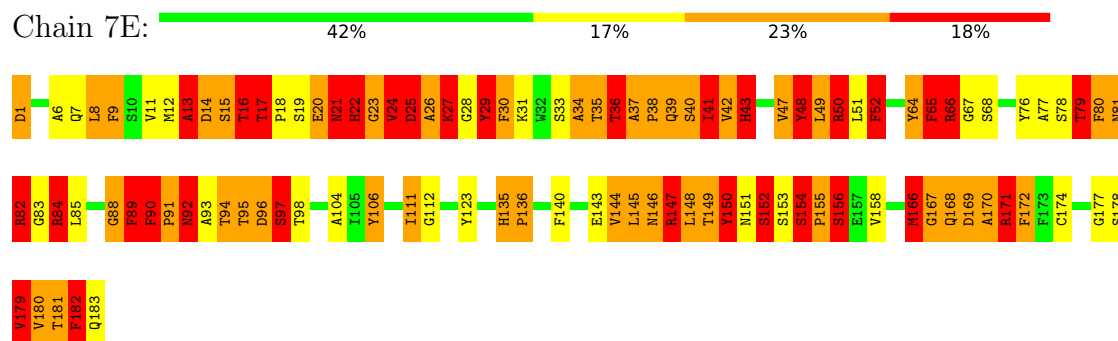


• Molecule 1: Protein VP3

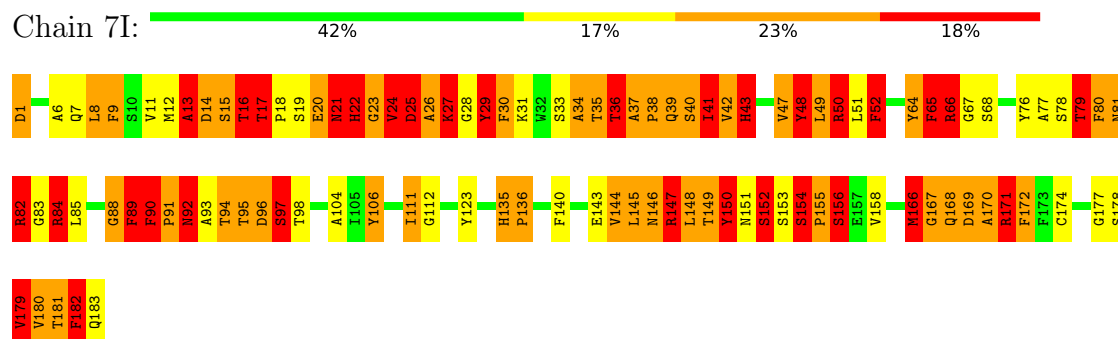
Chain 7A: 



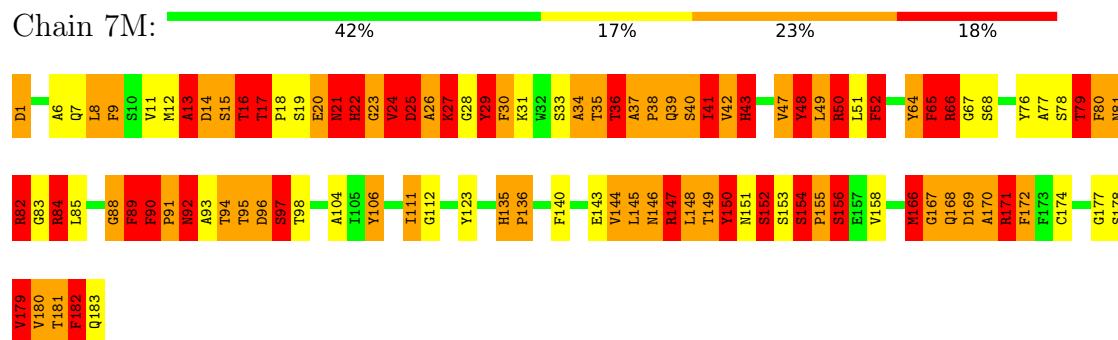
• Molecule 1: Protein VP3



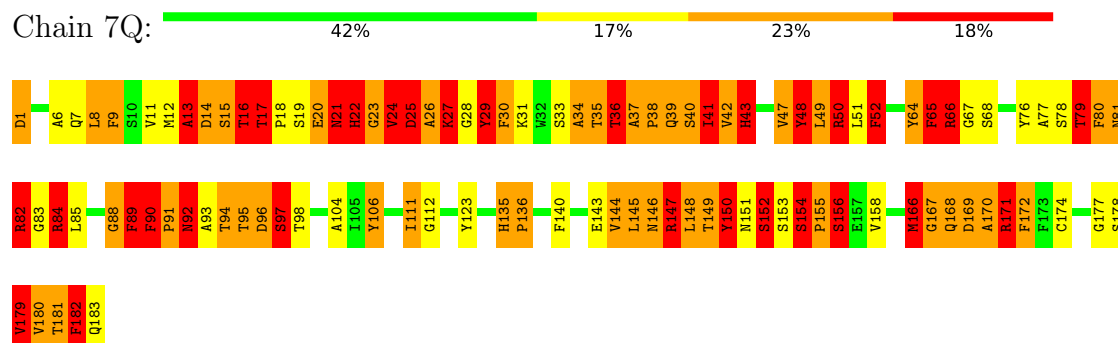
- Molecule 1: Protein VP3



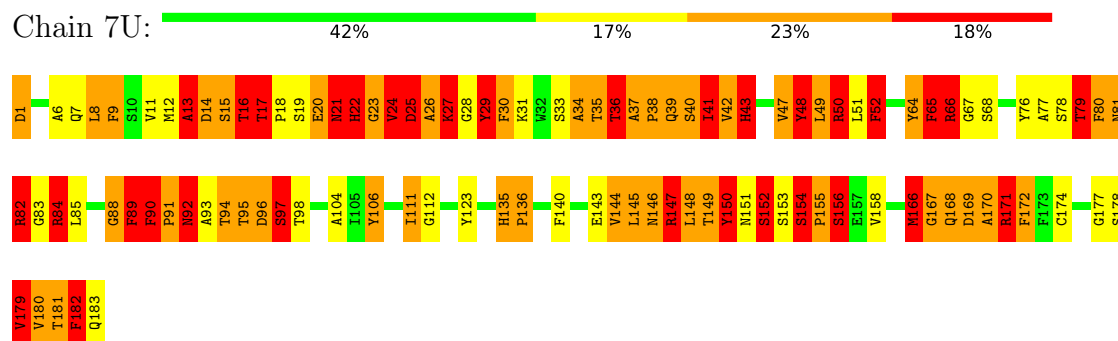
- Molecule 1: Protein VP3



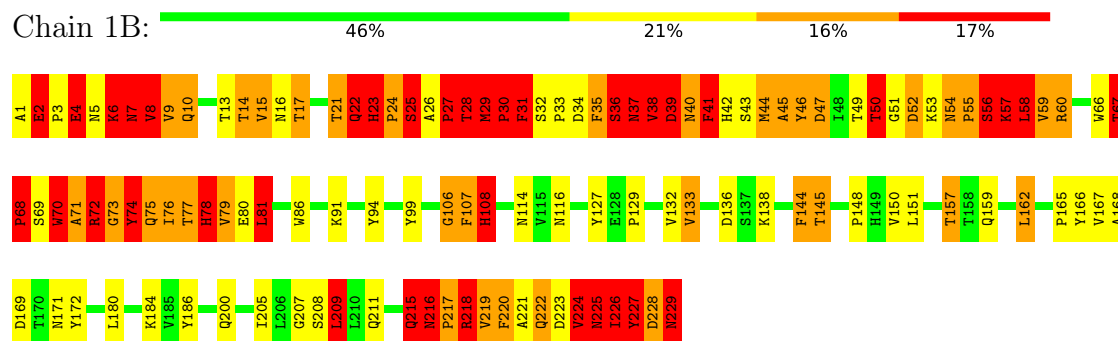
- Molecule 1: Protein VP3



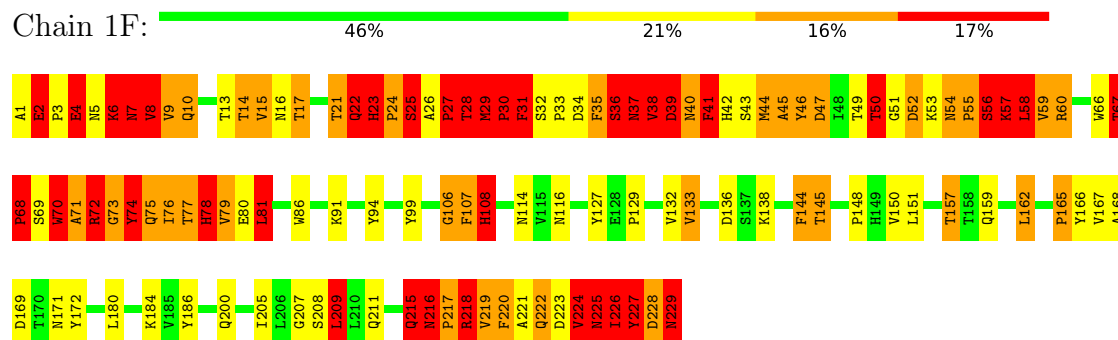
- Molecule 1: Protein VP3



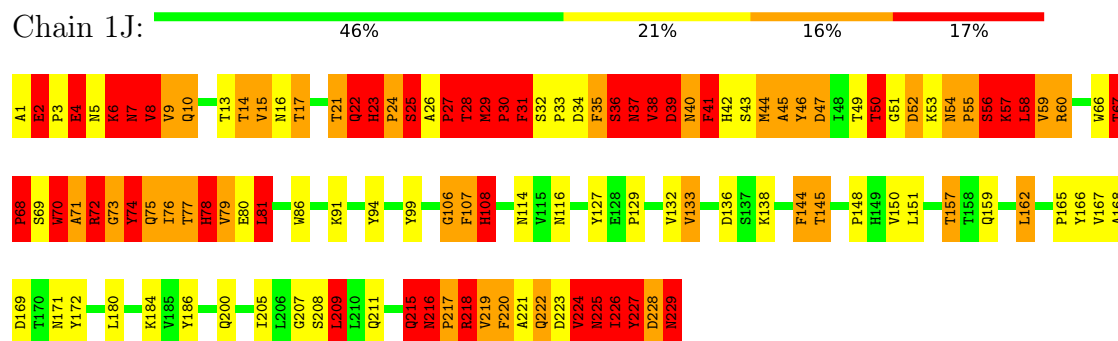
• Molecule 2: Protein VP0



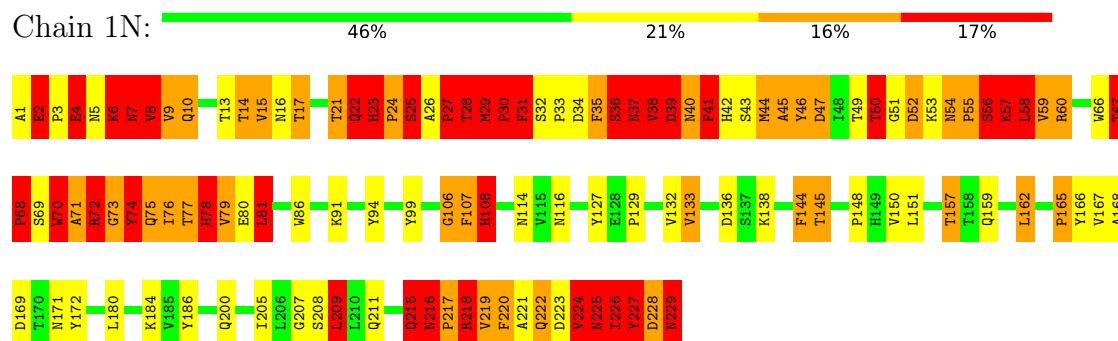
• Molecule 2: Protein VP0



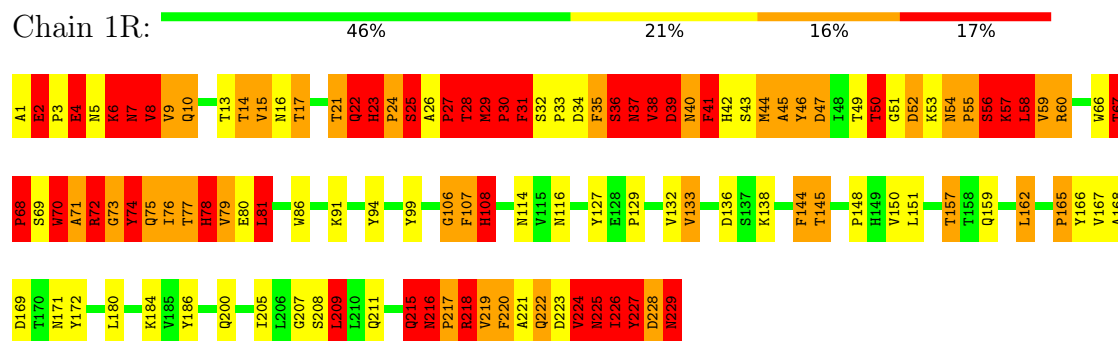
• Molecule 2: Protein VP0



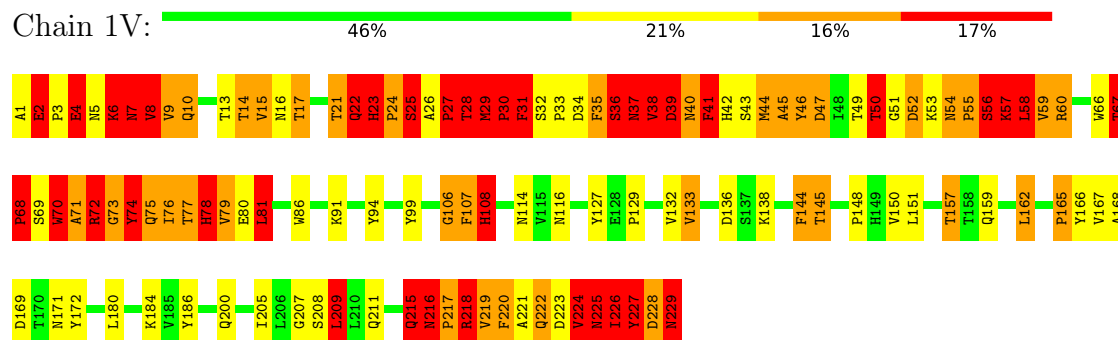
• Molecule 2: Protein VP0



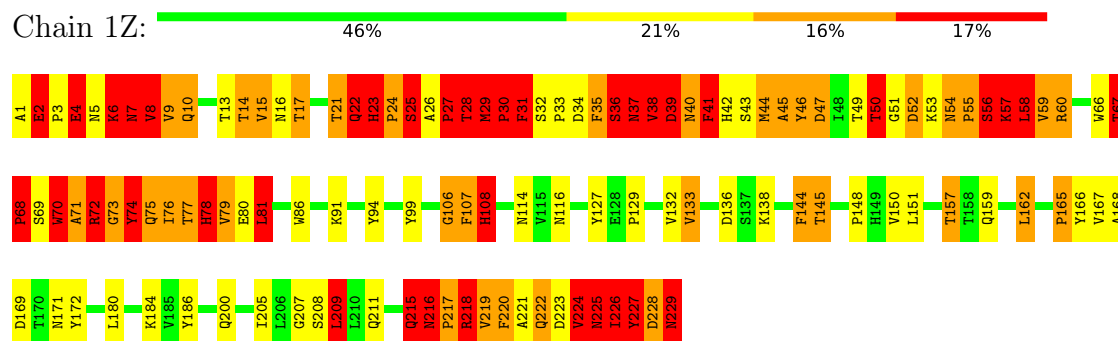
• Molecule 2: Protein VP0



• Molecule 2: Protein VP0

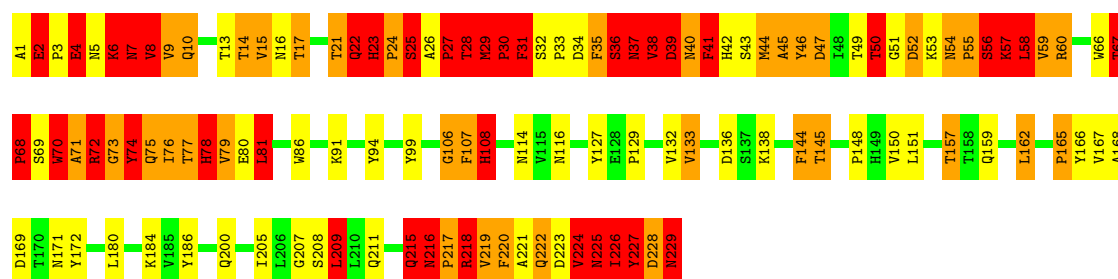


• Molecule 2: Protein VP0



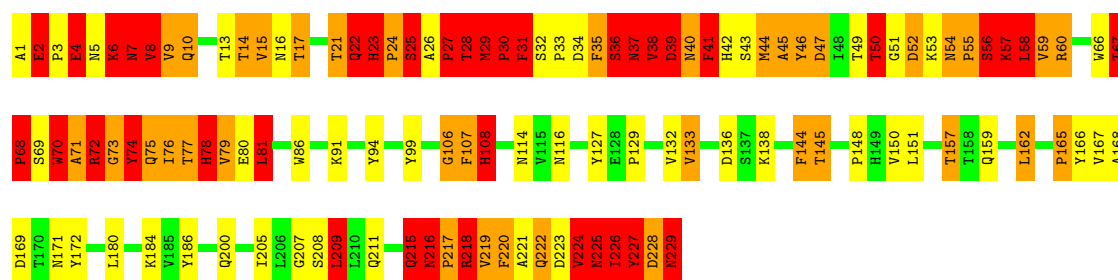
• Molecule 2: Protein VP0

Chain 13: 



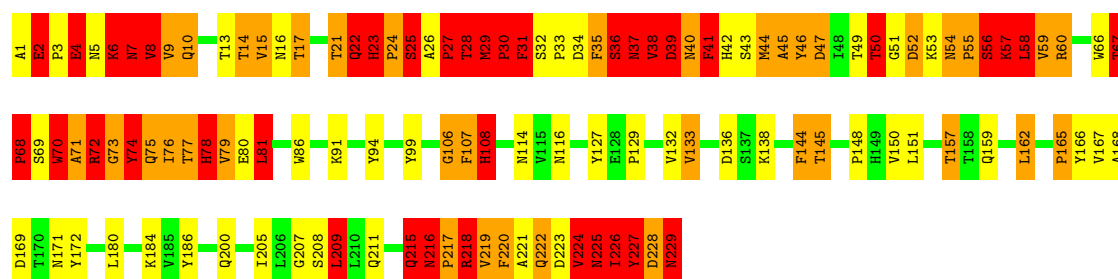
• Molecule 2: Protein VP0

Chain 17: 



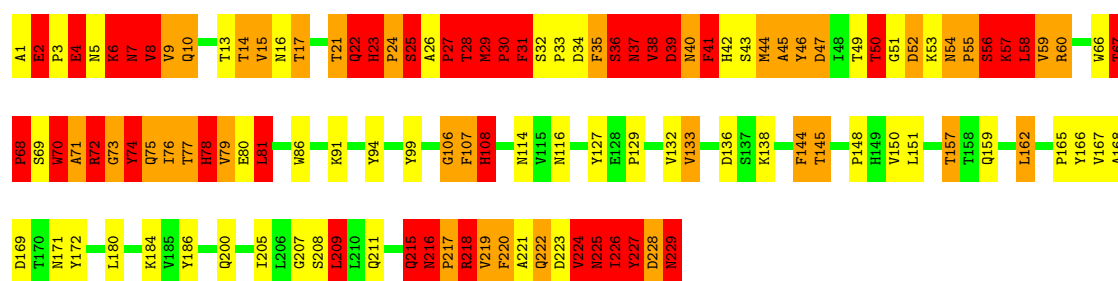
• Molecule 2: Protein VP0

Chain 2B: 

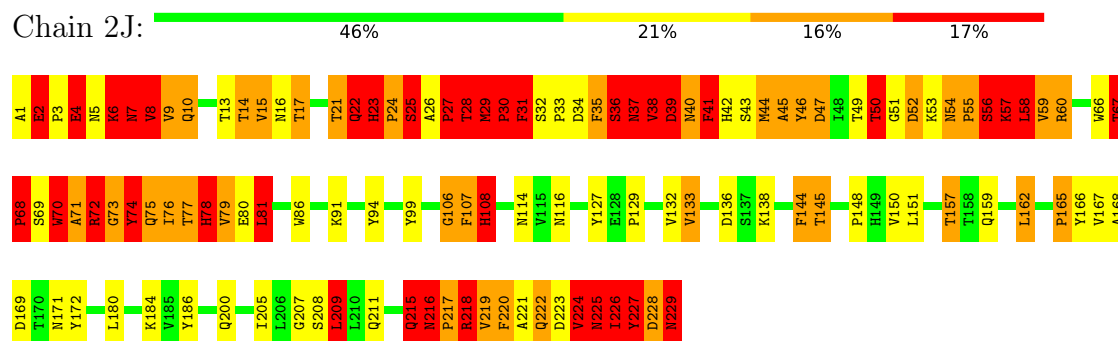


• Molecule 2: Protein VP0

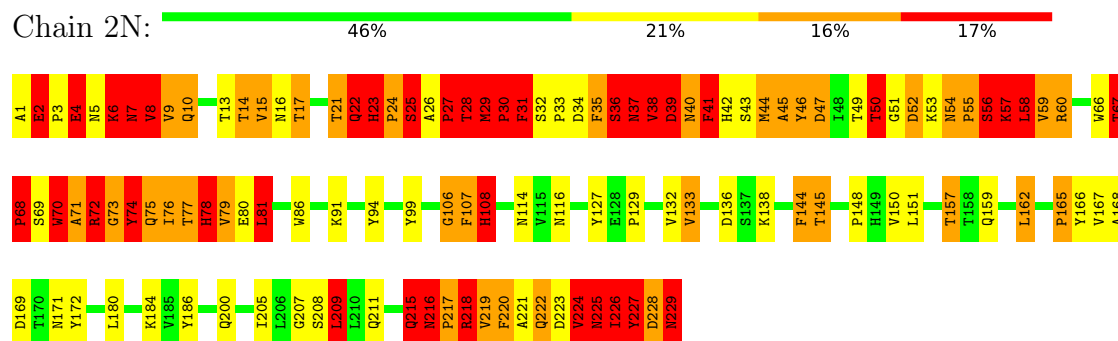
Chain 2F: 



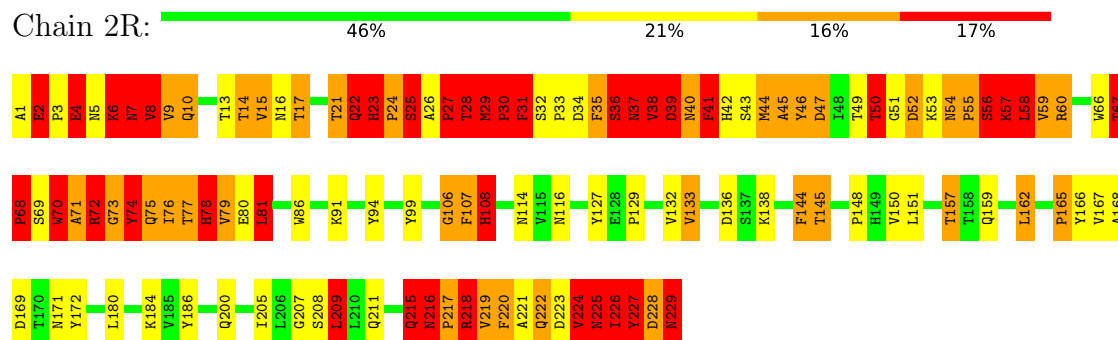
• Molecule 2: Protein VP0



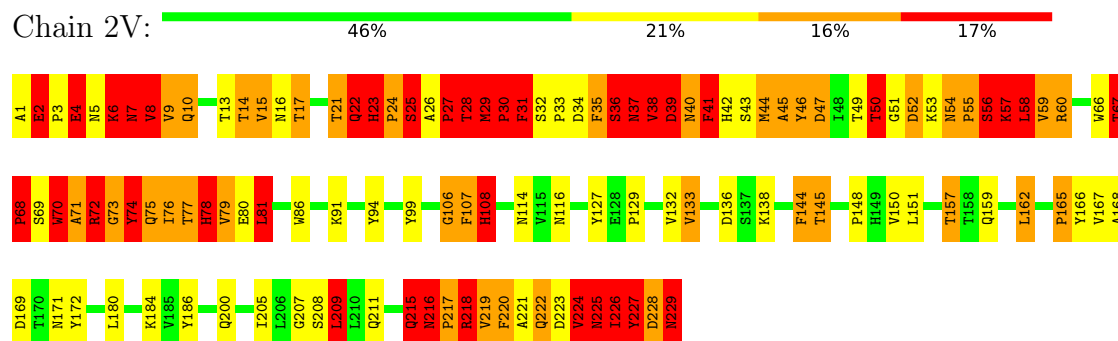
• Molecule 2: Protein VP0



• Molecule 2: Protein VP0

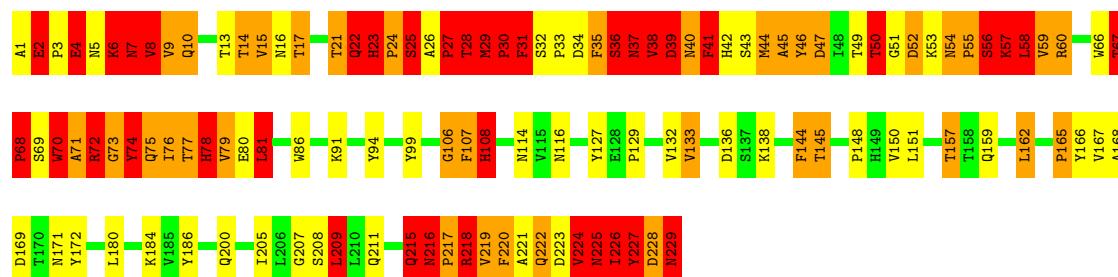


• Molecule 2: Protein VP0



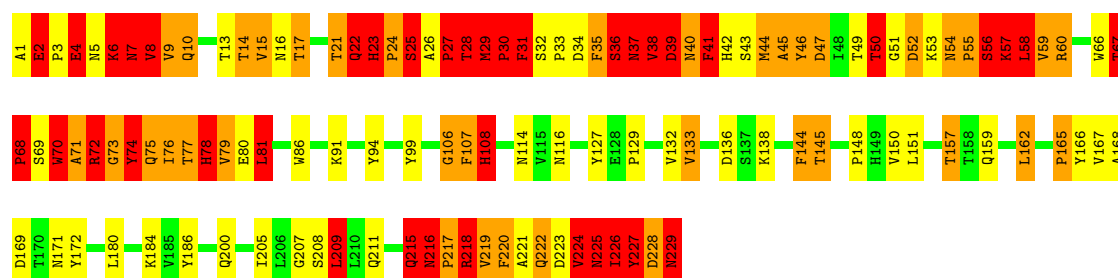
• Molecule 2: Protein VP0

Chain 2Z: 



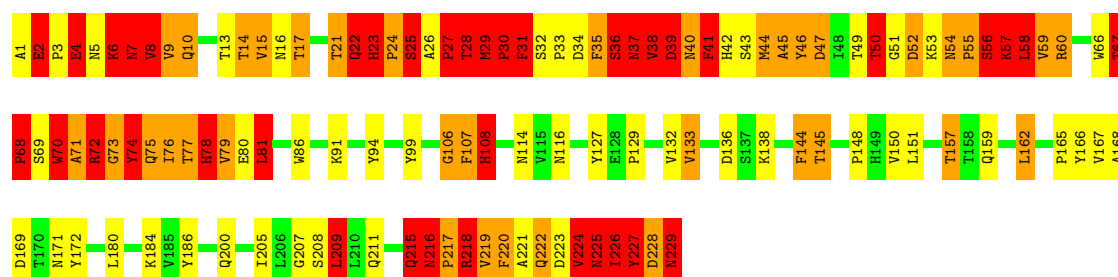
• Molecule 2: Protein VP0

Chain 23: 



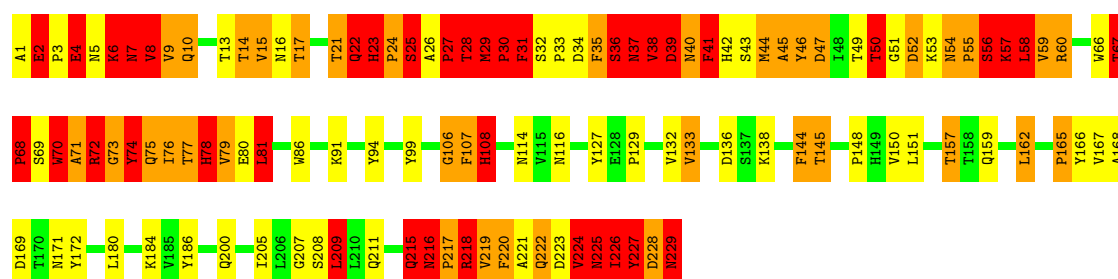
• Molecule 2: Protein VP0

Chain 27: 

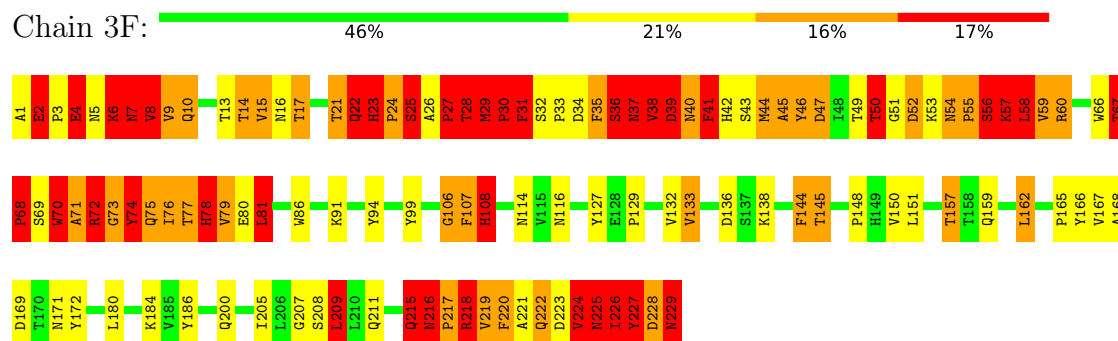


• Molecule 2: Protein VP0

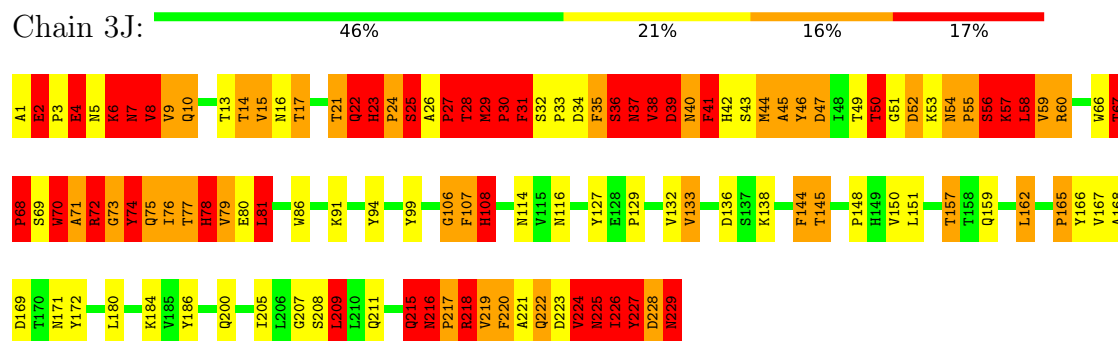
Chain 3B: 



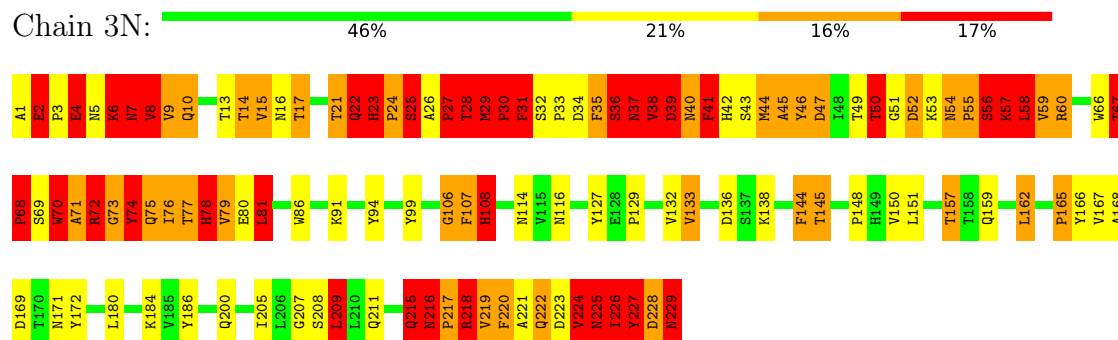
• Molecule 2: Protein VP0



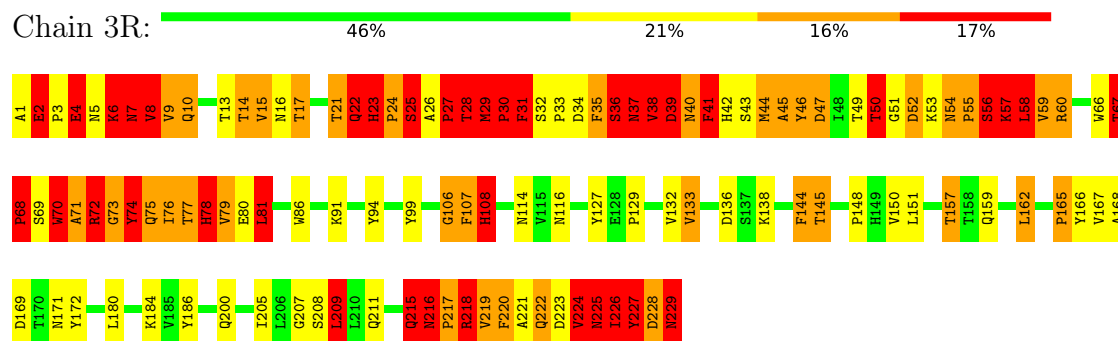
- Molecule 2: Protein VP0



- Molecule 2: Protein VP0

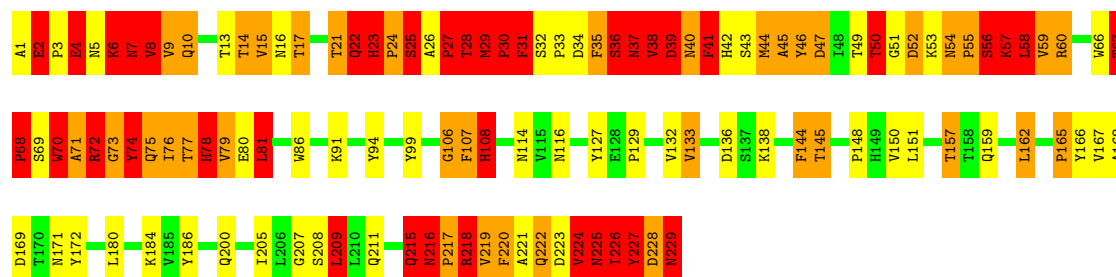


- Molecule 2: Protein VP0



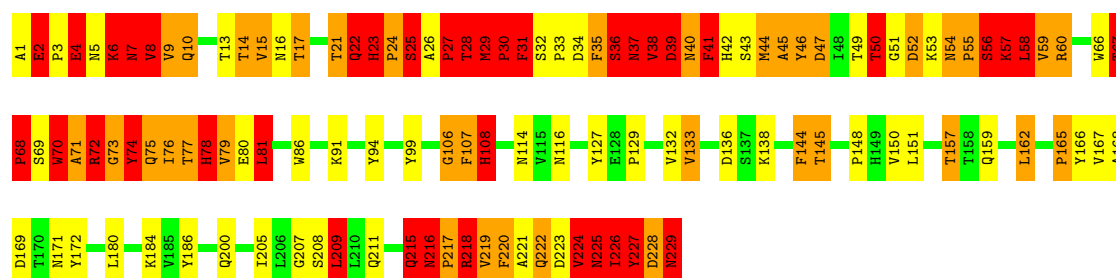
- Molecule 2: Protein VP0

Chain 3V: 



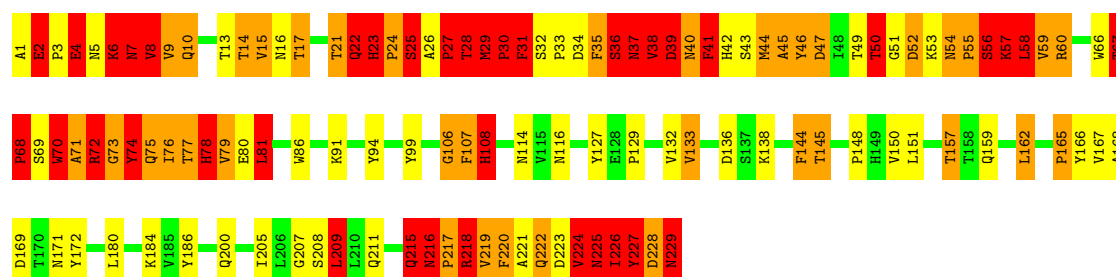
• Molecule 2: Protein VP0

Chain 3Z: 



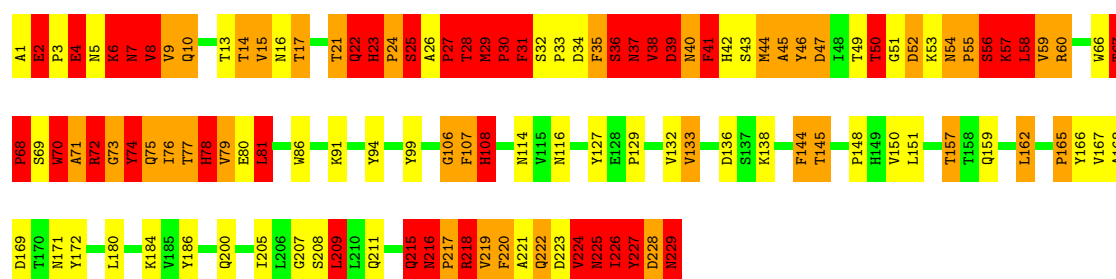
• Molecule 2: Protein VP0

Chain 33: 

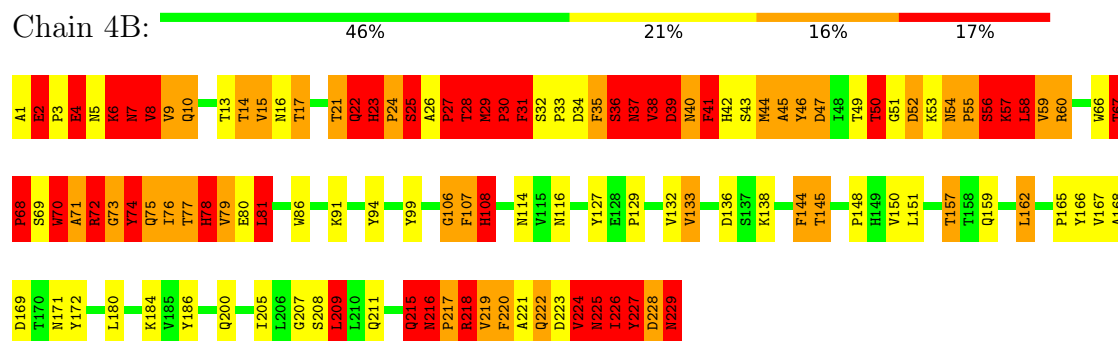


• Molecule 2: Protein VP0

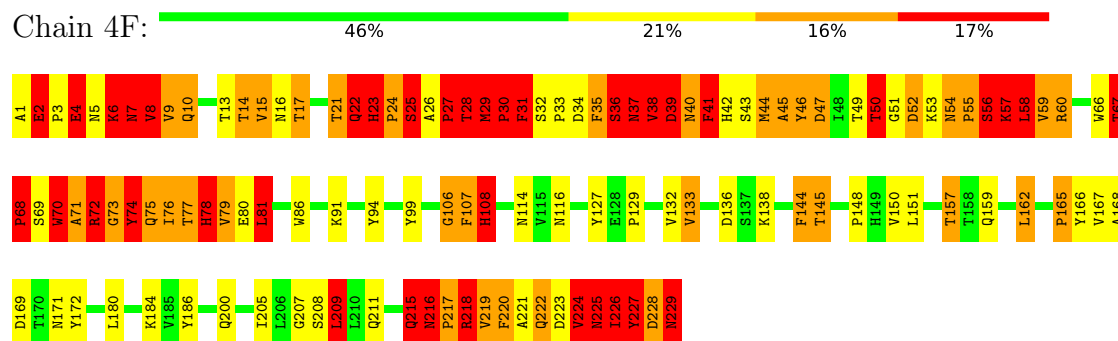
Chain 37: 



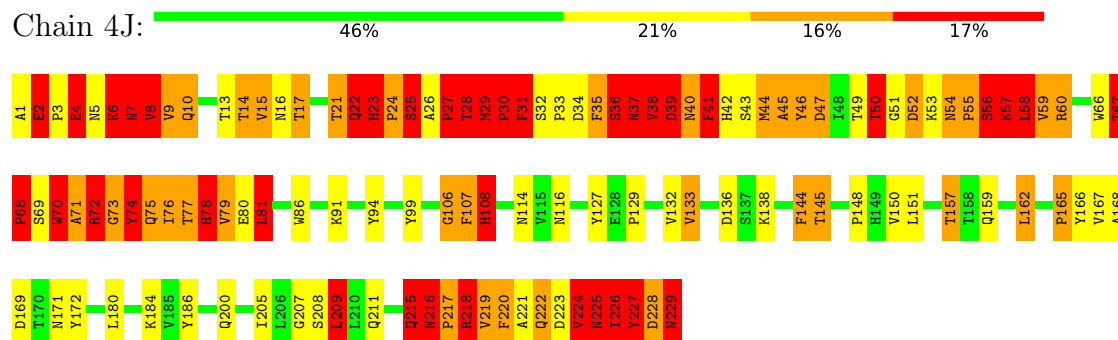
• Molecule 2: Protein VP0



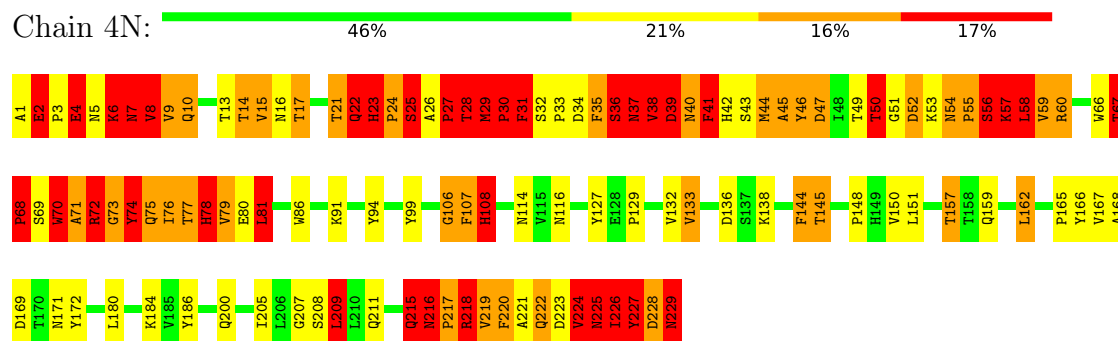
- Molecule 2: Protein VP0



- Molecule 2: Protein VP0

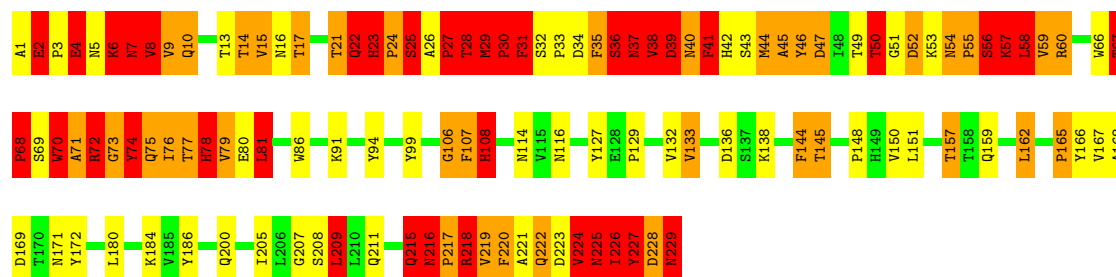


- Molecule 2: Protein VP0



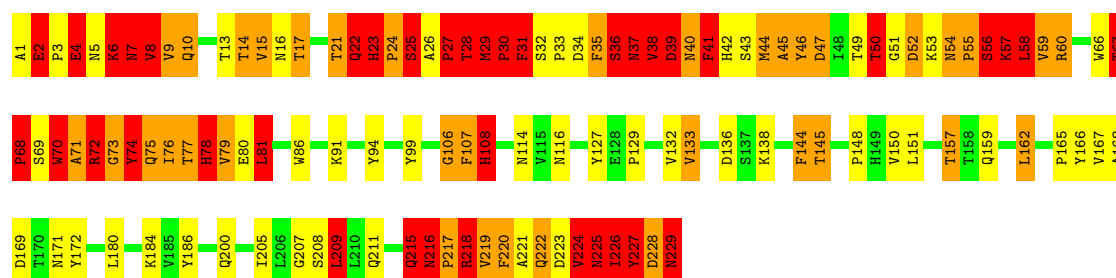
- Molecule 2: Protein VP0

Chain 4R: 



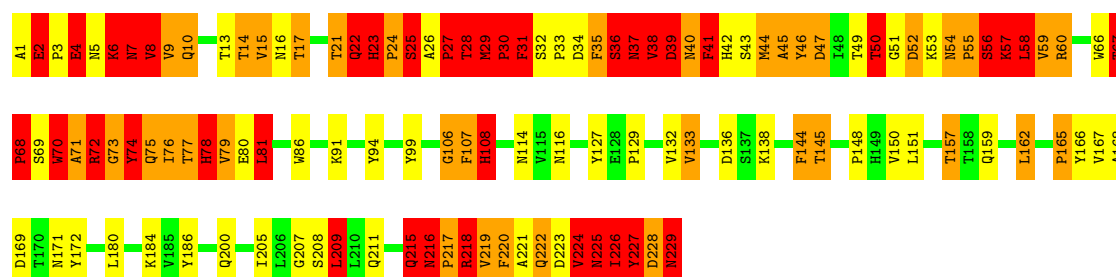
• Molecule 2: Protein VP0

Chain 4V: 



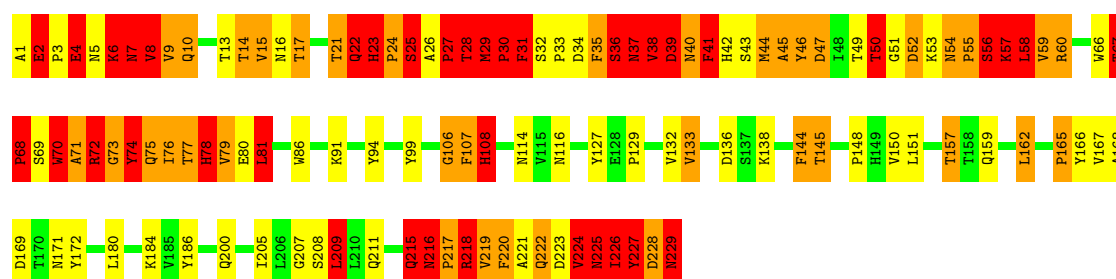
• Molecule 2: Protein VP0

Chain 4Z: 



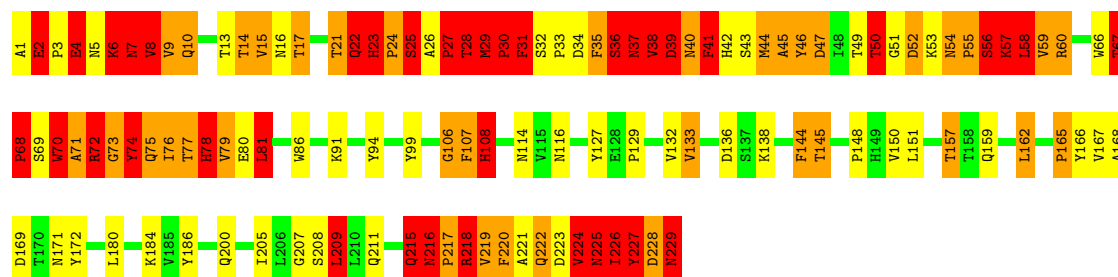
• Molecule 2: Protein VP0

Chain 43: 



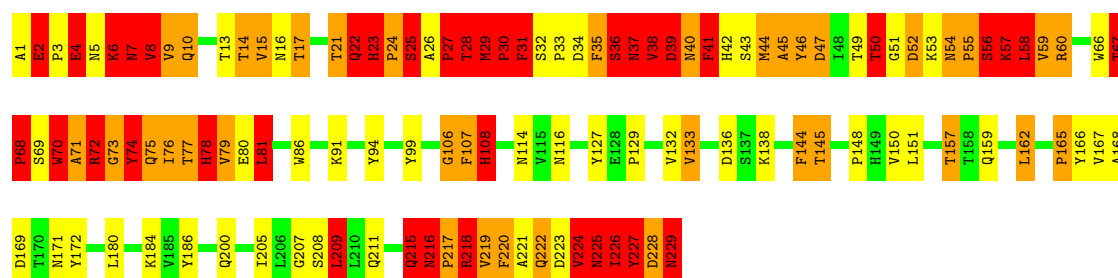
• Molecule 2: Protein VP0

Chain 47: 



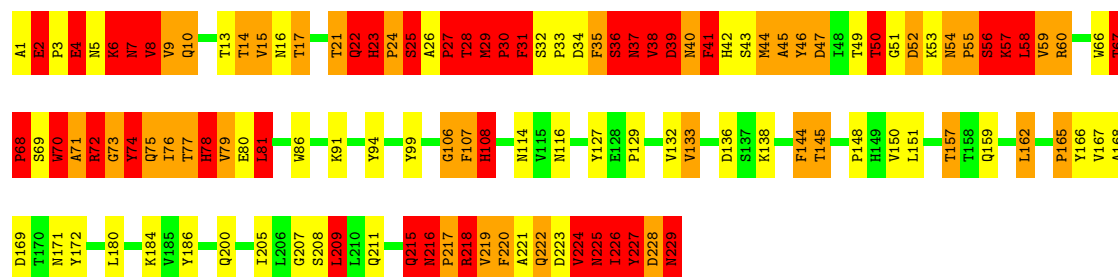
• Molecule 2: Protein VP0

Chain 5B: 



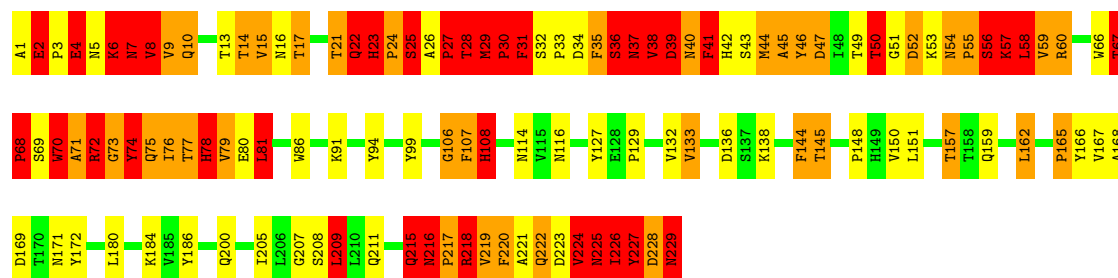
• Molecule 2: Protein VP0

Chain 5F: 

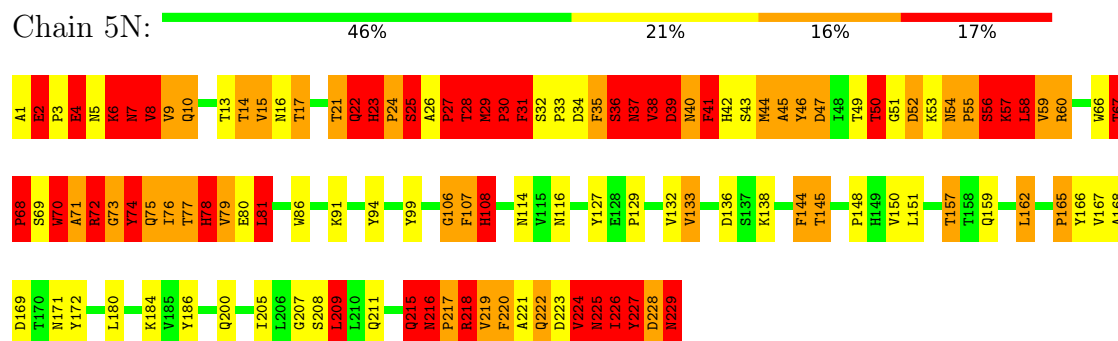


• Molecule 2: Protein VP0

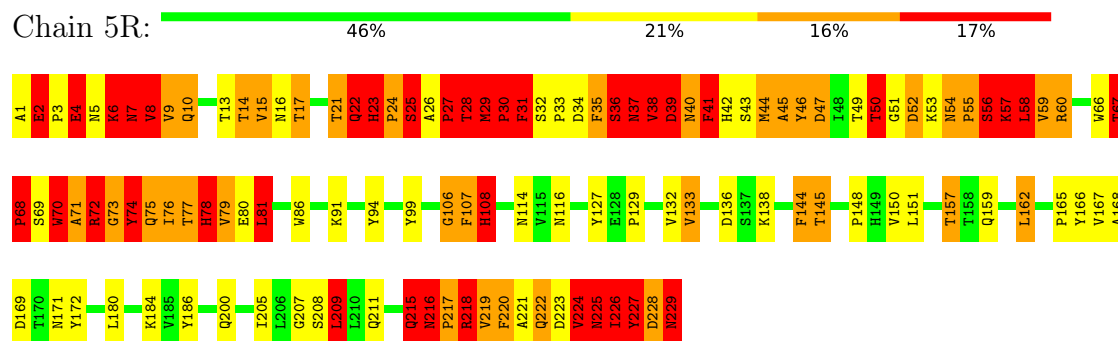
Chain 5J: 



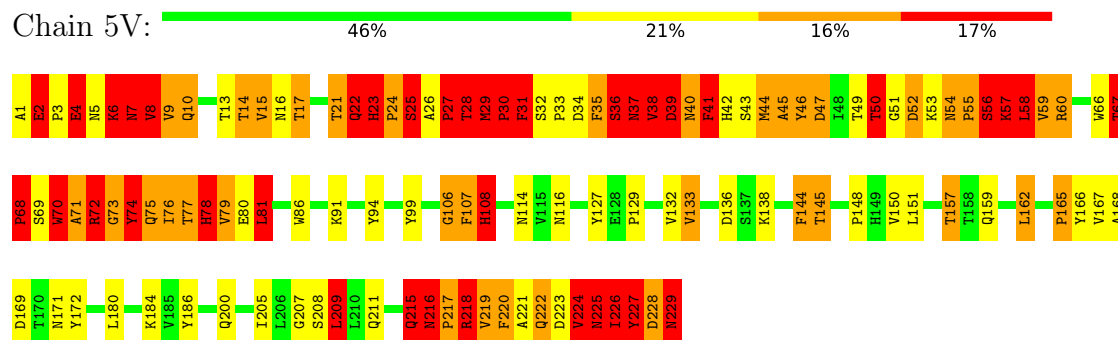
• Molecule 2: Protein VP0



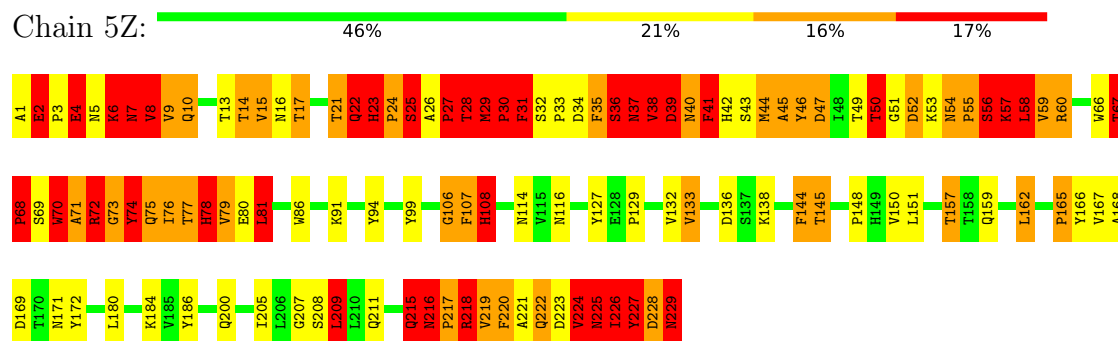
• Molecule 2: Protein VP0



• Molecule 2: Protein VP0

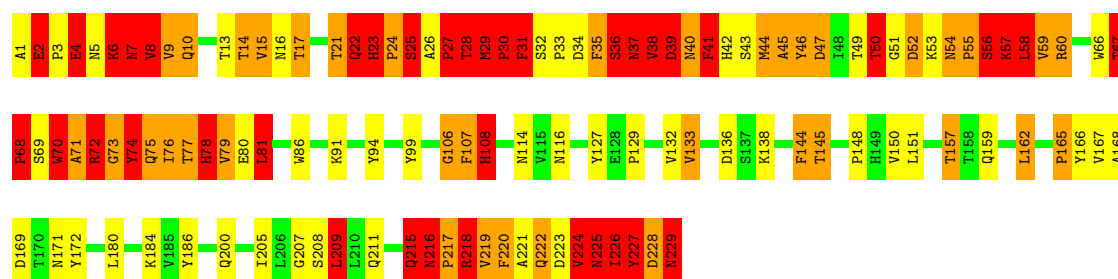


• Molecule 2: Protein VP0



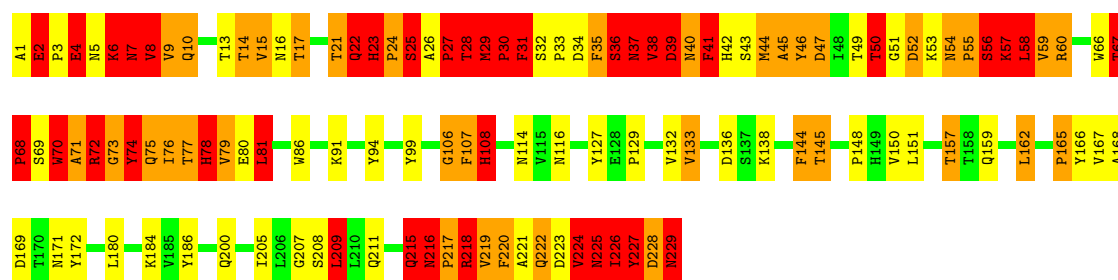
• Molecule 2: Protein VP0

Chain 53: 



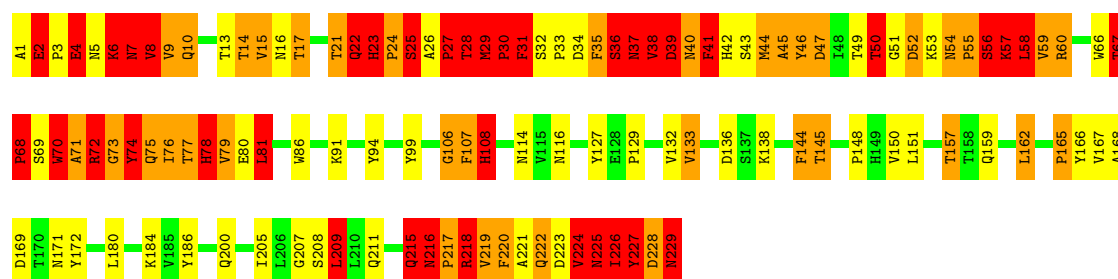
• Molecule 2: Protein VP0

Chain 57: 



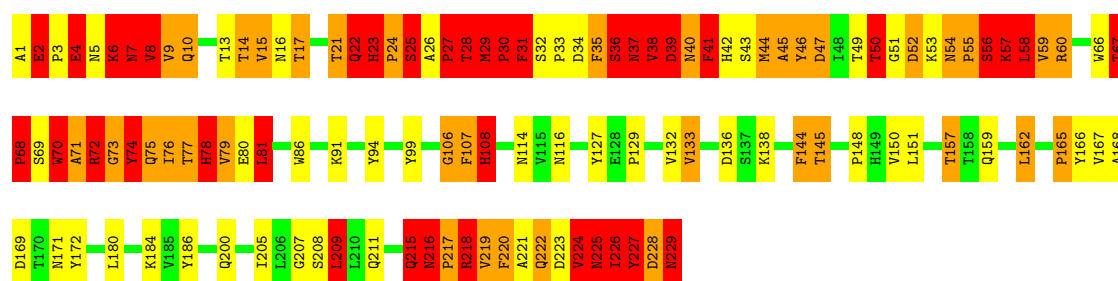
• Molecule 2: Protein VP0

Chain 6B: 

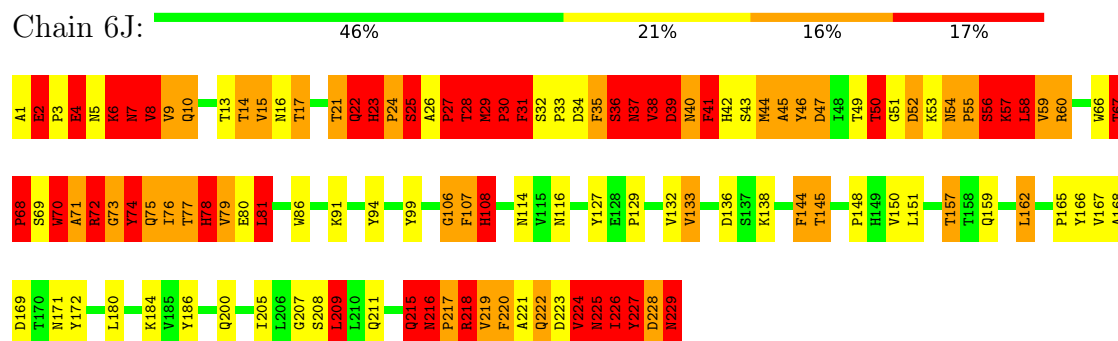


• Molecule 2: Protein VP0

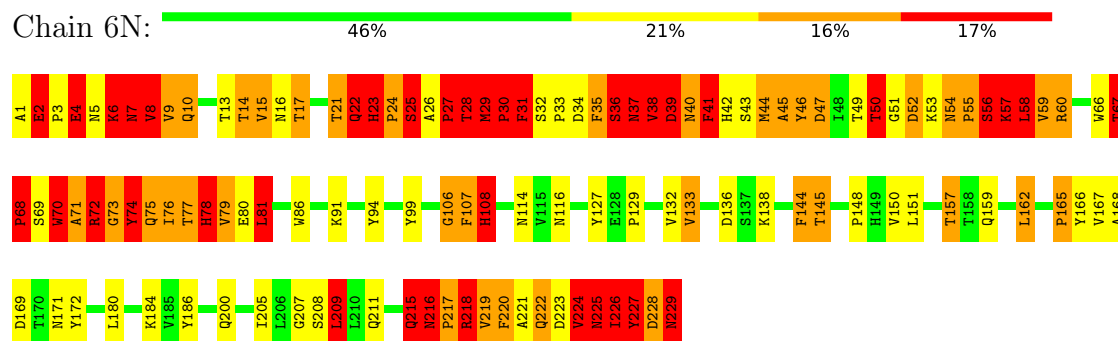
Chain 6F: 



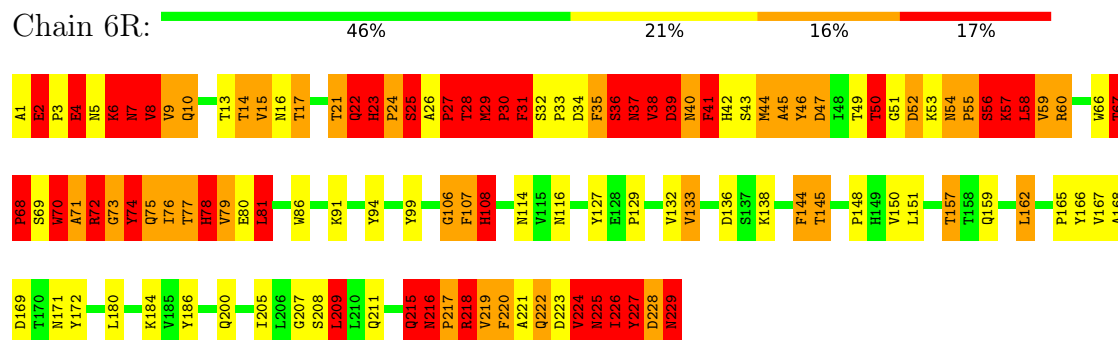
• Molecule 2: Protein VP0



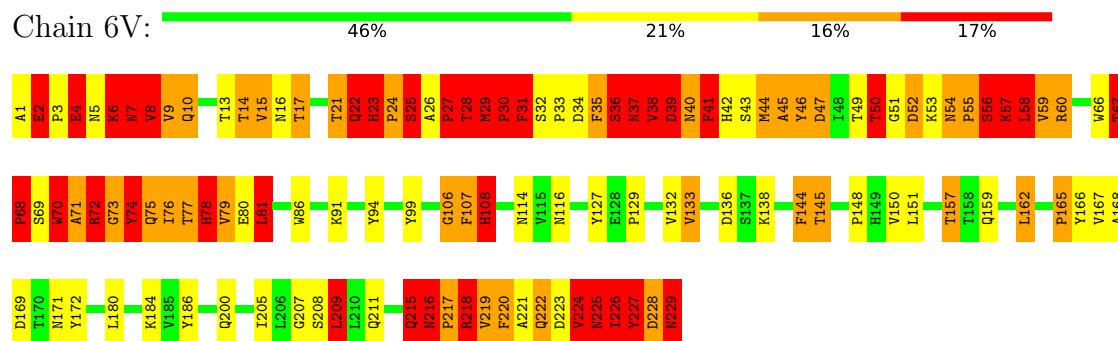
• Molecule 2: Protein VP0



• Molecule 2: Protein VP0

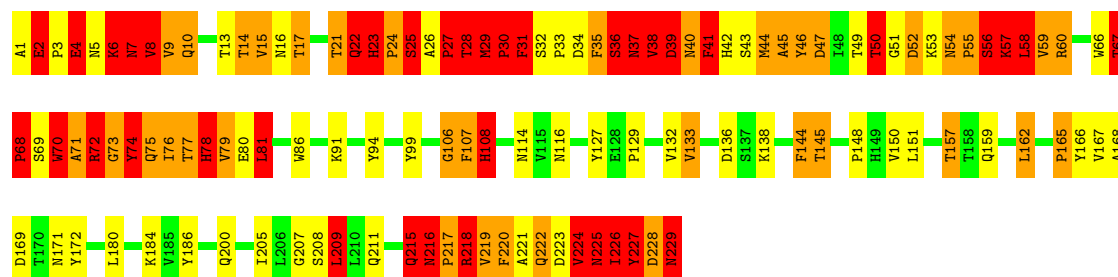


• Molecule 2: Protein VP0



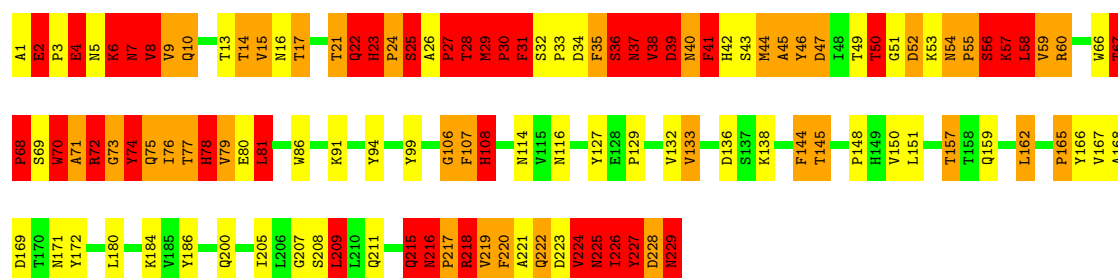
• Molecule 2: Protein VP0

Chain 6Z: 



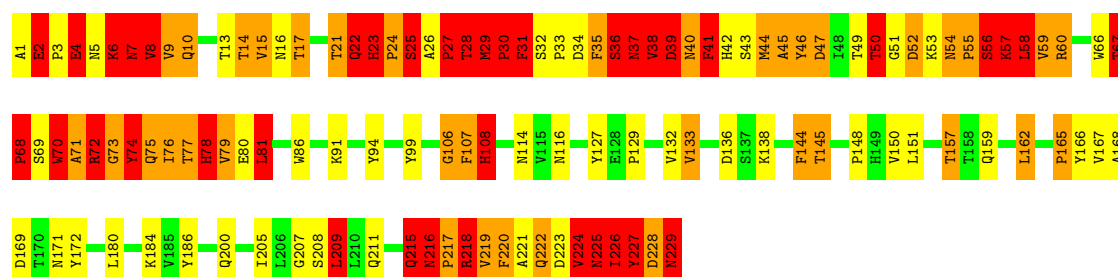
• Molecule 2: Protein VP0

Chain 63: 



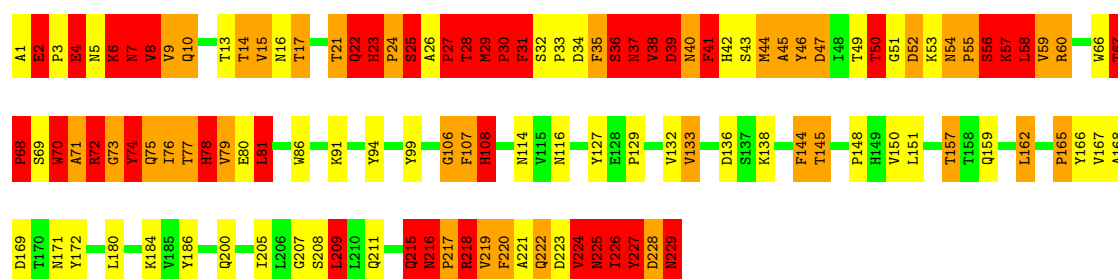
• Molecule 2: Protein VP0

Chain 67: 

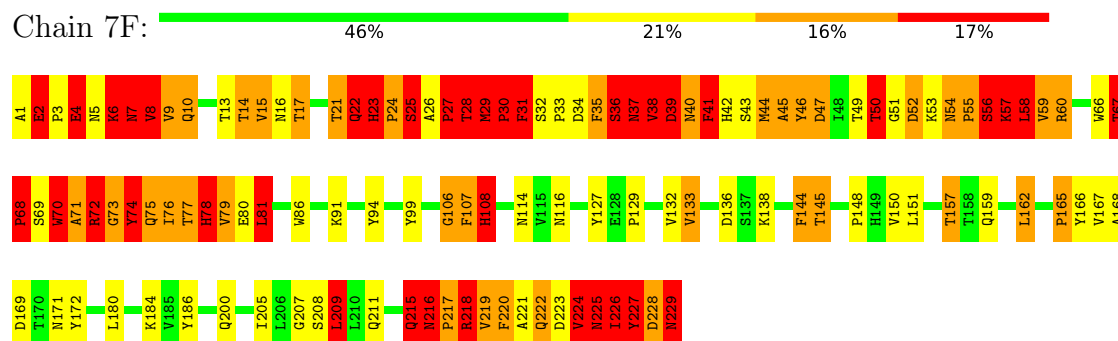


• Molecule 2: Protein VP0

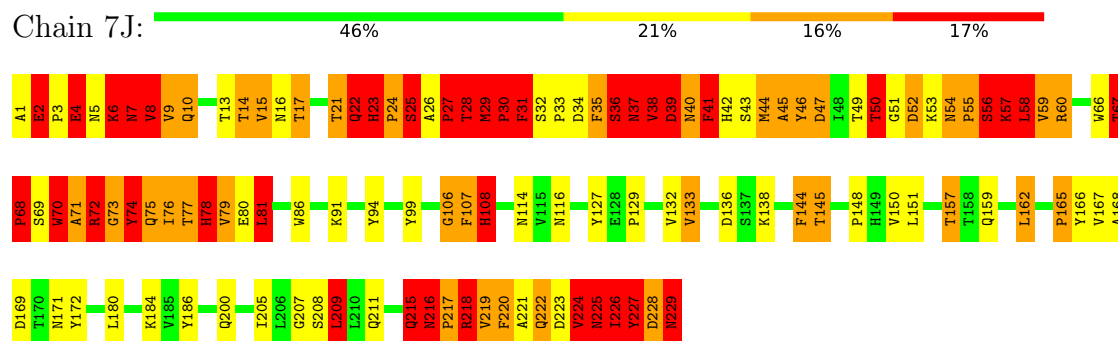
Chain 7B: 



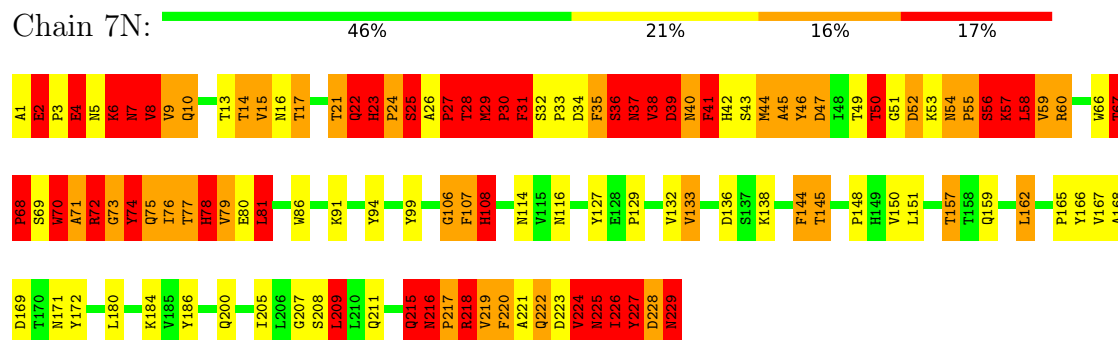
• Molecule 2: Protein VP0



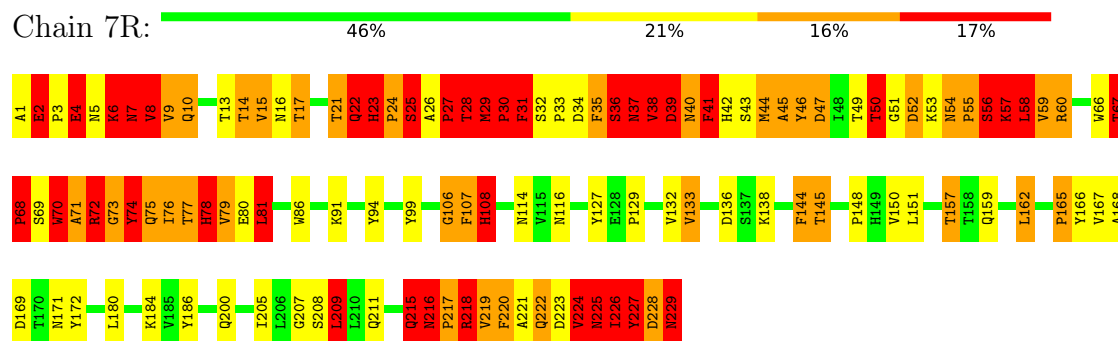
- Molecule 2: Protein VP0



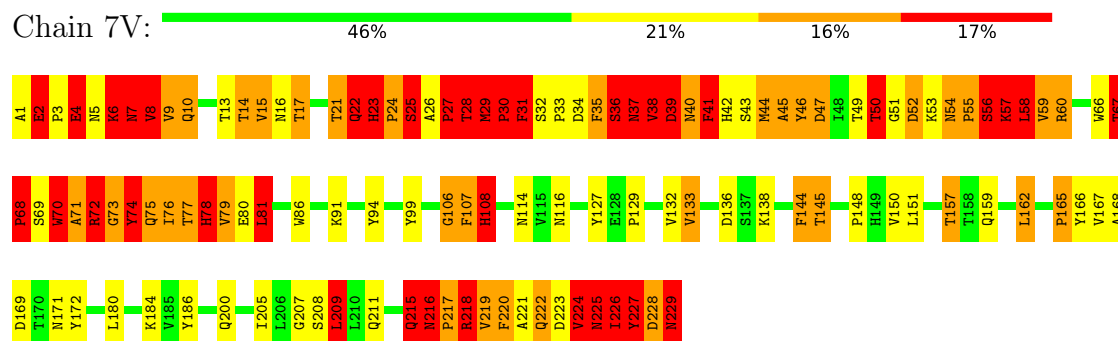
- Molecule 2: Protein VP0



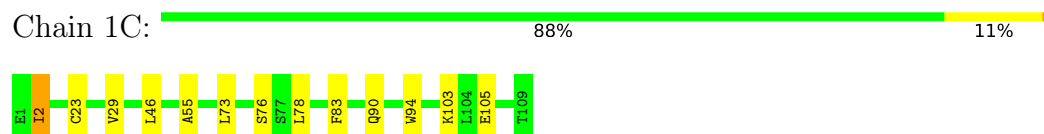
- Molecule 2: Protein VP0



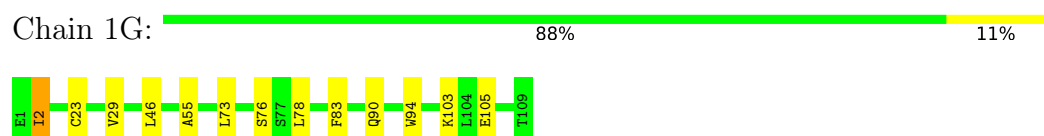
- Molecule 2: Protein VP0



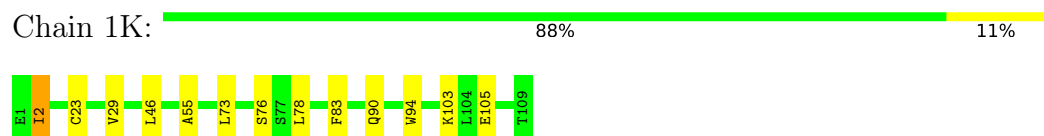
- Molecule 3: HUMAN MONOCLONAL ANTIBODY



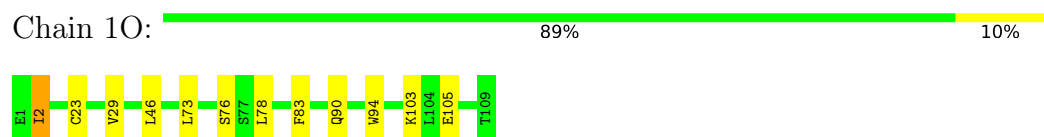
- Molecule 3: HUMAN MONOCLONAL ANTIBODY



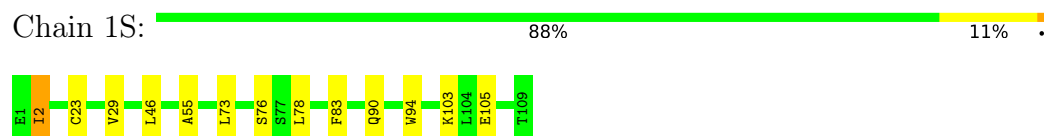
- Molecule 3: HUMAN MONOCLONAL ANTIBODY



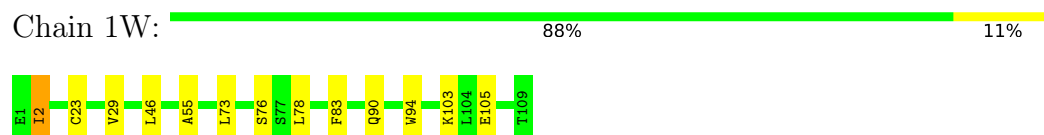
- Molecule 3: HUMAN MONOCLONAL ANTIBODY




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● Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 10:  88% 11%


● 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% .



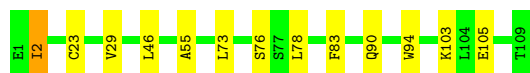
- Molecule 3: HUMAN MONOCLONAL ANTIBODY

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% .




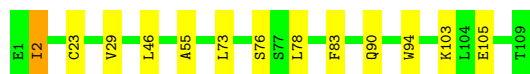
- Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 3O:  88% 11% .



• Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 3S:  88% 11% .




• Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 3W:  88% 11% .



• Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 30:  88% 11% .




• Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 34:  89% 10% .




• Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 38:  88% 11% .



• Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 4C:  88% 11% .



• Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 4G:  89% 10% .



- 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%




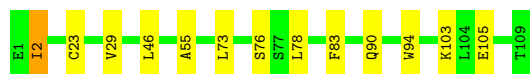
- Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 5C:  88% 11% .




- Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 5G:  88% 11% .




- Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 5K:  88% 11% .




- Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 5O:  88% 11% .



- Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 5S:  88% 11% .




- Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 5W:  89% 10% .




- Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 5O:  88% 11% .



- Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 54:  88% 11% .



- Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 58: 88% 11% .



- Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 6C: 88% 11% .



- Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 6G: 88% 11% .



- Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 6K: 88% 11% .



- Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 6O: 89% 10% .



- Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 6S: 88% 11% .




- Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 6W: 89% 10% .




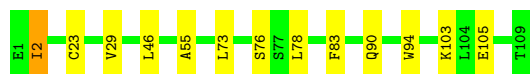
- Molecule 3: HUMAN MONOCLONAL ANTIBODY

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

Chain 7O:  88% 11% .



• Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 7S:  89% 10% .



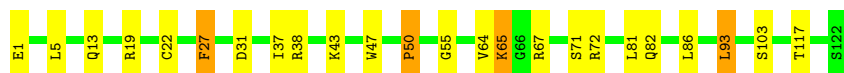
• Molecule 3: HUMAN MONOCLONAL ANTIBODY

Chain 7W: 88% 11%



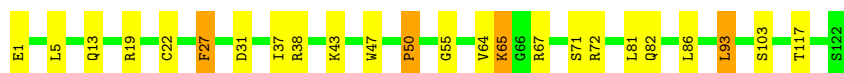
• Molecule 4: HUMAN MONOCLONAL ANTIBODY

Chain 1D: 80% 16%



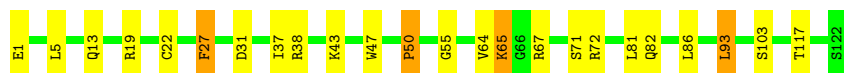
• Molecule 4: HUMAN MONOCLONAL ANTIBODY

Chain 1H: 80% 16%



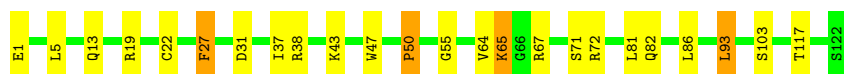
• Molecule 4: HUMAN MONOCLONAL ANTIBODY

Chain 1L: 80% 16%



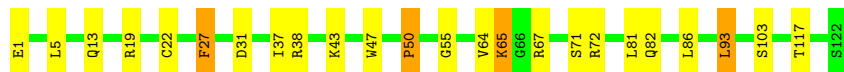
• Molecule 4: HUMAN MONOCLONAL ANTIBODY

Chain 1P: 80% 16%



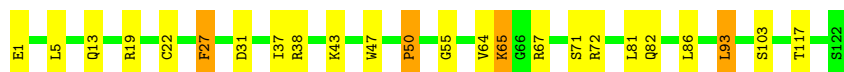
• Molecule 4: HUMAN MONOCLONAL ANTIBODY

Chain 1T: 80% 16%




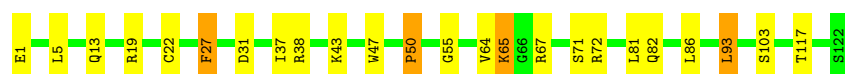
• Molecule 4: HUMAN MONOCLONAL ANTIBODY

Chain 1X: 80% 16%




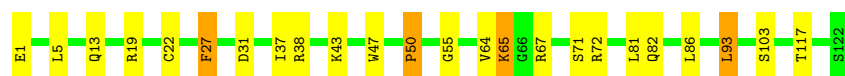
• Molecule 4: HUMAN MONOCLONAL ANTIBODY

Chain 11:  80% 16% .




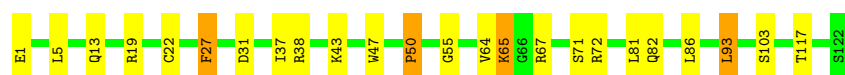
• Molecule 4: HUMAN MONOCLONAL ANTIBODY

Chain 15:  80% 16% .




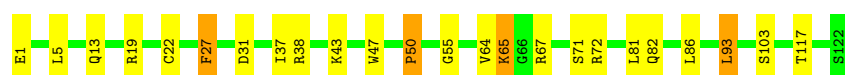
• Molecule 4: HUMAN MONOCLONAL ANTIBODY

Chain 19:  80% 16% .




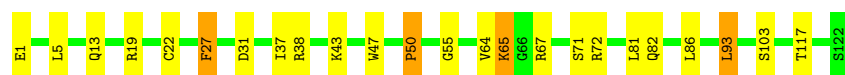
• Molecule 4: HUMAN MONOCLONAL ANTIBODY

Chain 2D:  80% 16% .




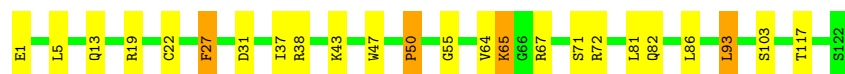
• Molecule 4: HUMAN MONOCLONAL ANTIBODY

Chain 2H:  80% 16% .




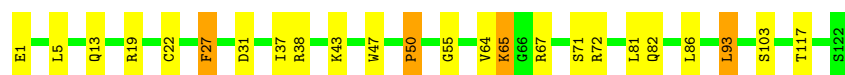
• Molecule 4: HUMAN MONOCLONAL ANTIBODY

Chain 2L:  80% 16% .




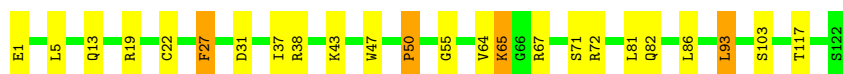
• Molecule 4: HUMAN MONOCLONAL ANTIBODY

Chain 2P:  80% 16% .

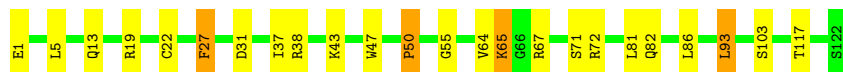
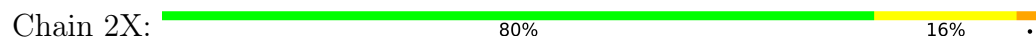


• Molecule 4: HUMAN MONOCLONAL ANTIBODY

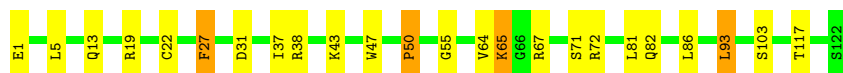
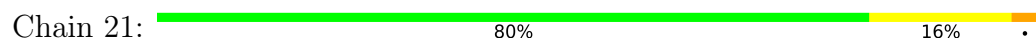
Chain 2T:  80% 16% .



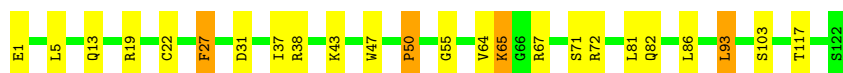
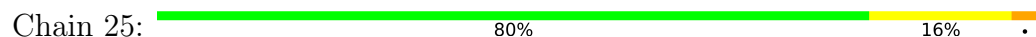
• Molecule 4: HUMAN MONOCLONAL ANTIBODY



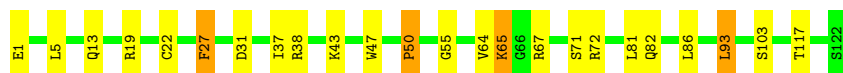
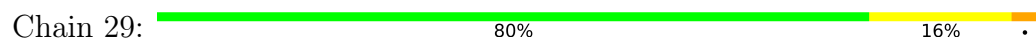
• Molecule 4: HUMAN MONOCLONAL ANTIBODY



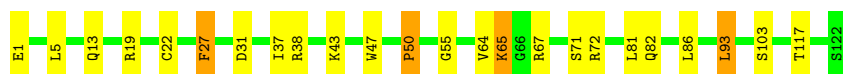
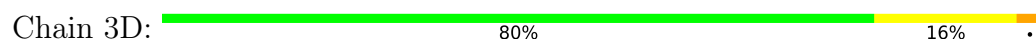
• Molecule 4: HUMAN MONOCLONAL ANTIBODY



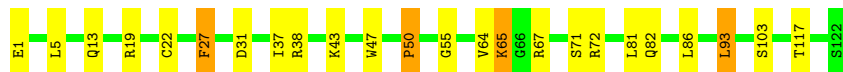
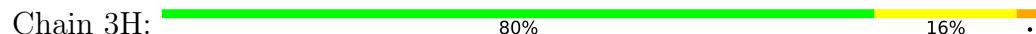
• Molecule 4: HUMAN MONOCLONAL ANTIBODY



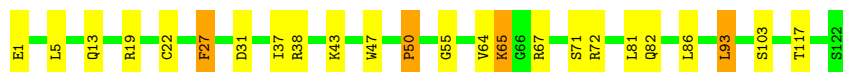
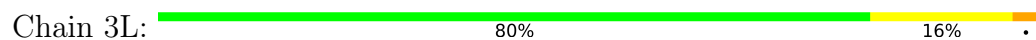
• Molecule 4: HUMAN MONOCLONAL ANTIBODY




• Molecule 4: HUMAN MONOCLONAL ANTIBODY

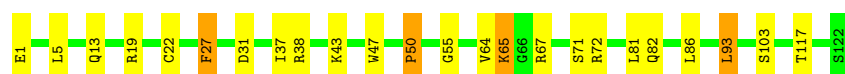


• Molecule 4: HUMAN MONOCLONAL ANTIBODY




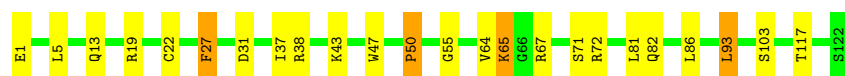
• Molecule 4: HUMAN MONOCLONAL ANTIBODY

Chain 3P:  80% 16% .




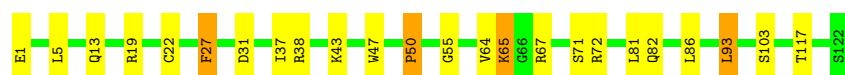
• Molecule 4: HUMAN MONOCLONAL ANTIBODY

Chain 3T:  80% 16% .




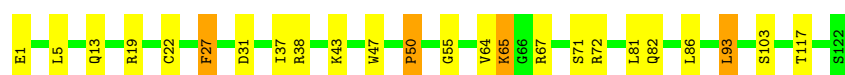
• Molecule 4: HUMAN MONOCLONAL ANTIBODY

Chain 3X:  80% 16% .



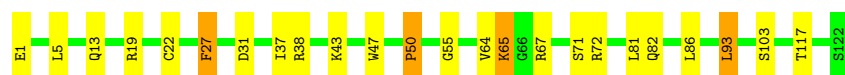
• Molecule 4: HUMAN MONOCLONAL ANTIBODY

Chain 3I:  80% 16% .




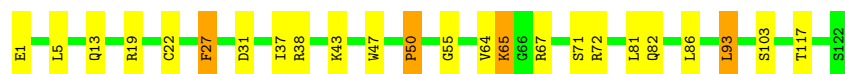
• Molecule 4: HUMAN MONOCLONAL ANTIBODY

Chain 35:  80% 16% .



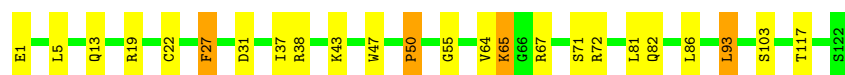
• Molecule 4: HUMAN MONOCLONAL ANTIBODY

Chain 39:  80% 16% .




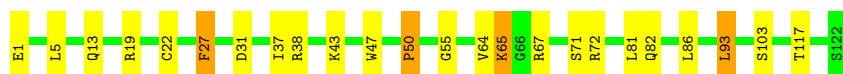
• Molecule 4: HUMAN MONOCLONAL ANTIBODY

Chain 4D:  80% 16% .

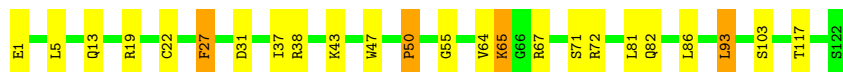
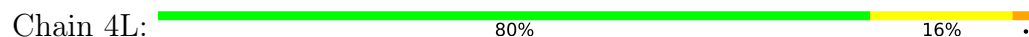


• Molecule 4: HUMAN MONOCLONAL ANTIBODY

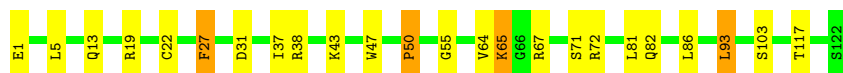
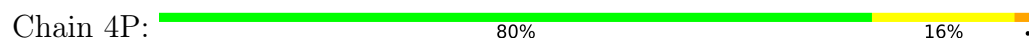
Chain 4H:  80% 16% .



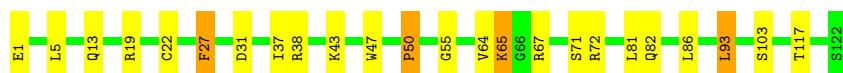
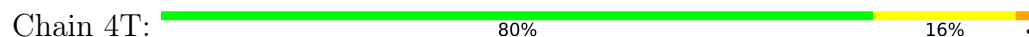
• Molecule 4: HUMAN MONOCLONAL ANTIBODY



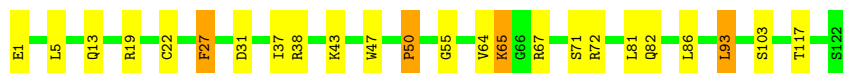
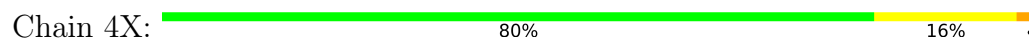
• Molecule 4: HUMAN MONOCLONAL ANTIBODY



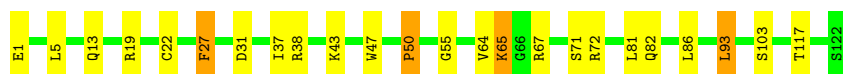
• Molecule 4: HUMAN MONOCLONAL ANTIBODY



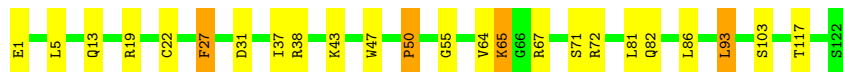
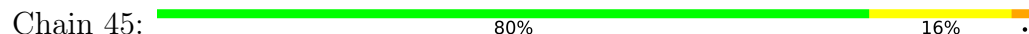
• Molecule 4: HUMAN MONOCLONAL ANTIBODY



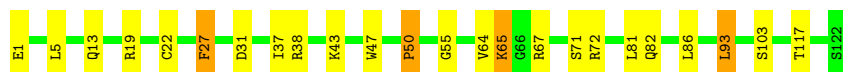
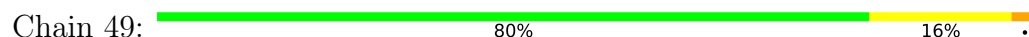
• Molecule 4: HUMAN MONOCLONAL ANTIBODY




• Molecule 4: HUMAN MONOCLONAL ANTIBODY

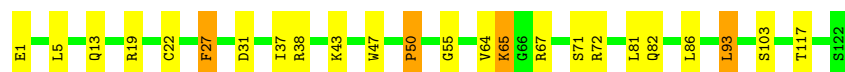


• Molecule 4: HUMAN MONOCLONAL ANTIBODY




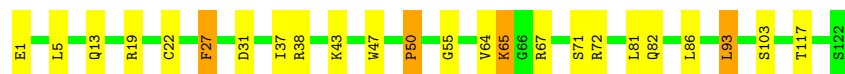
• Molecule 4: HUMAN MONOCLONAL ANTIBODY

Chain 5D:  80% 16% .




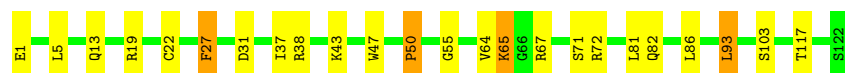
• Molecule 4: HUMAN MONOCLONAL ANTIBODY

Chain 5H:  80% 16% .




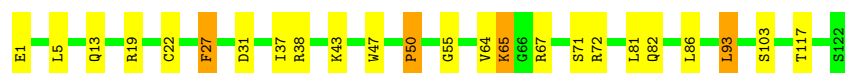
• Molecule 4: HUMAN MONOCLONAL ANTIBODY

Chain 5L:  80% 16% .




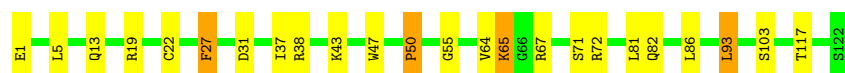
• Molecule 4: HUMAN MONOCLONAL ANTIBODY

Chain 5P:  80% 16% .




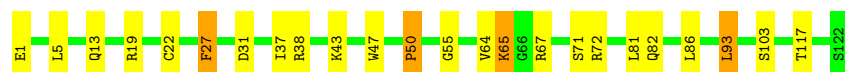
• Molecule 4: HUMAN MONOCLONAL ANTIBODY

Chain 5T:  80% 16% .




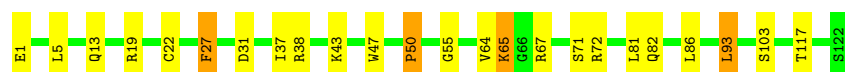
• Molecule 4: HUMAN MONOCLONAL ANTIBODY

Chain 5X:  80% 16% .




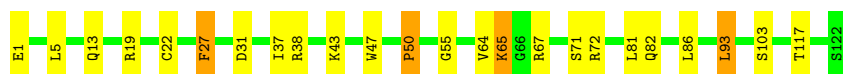
• Molecule 4: HUMAN MONOCLONAL ANTIBODY

Chain 5I:  80% 16% .

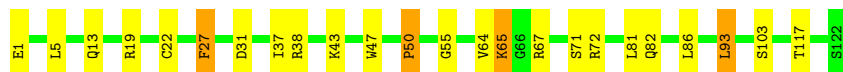
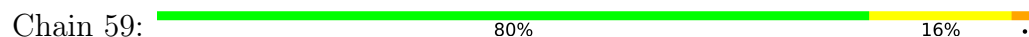


• Molecule 4: HUMAN MONOCLONAL ANTIBODY

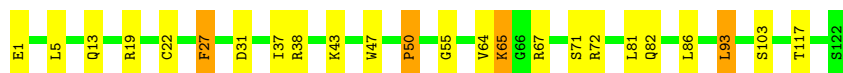
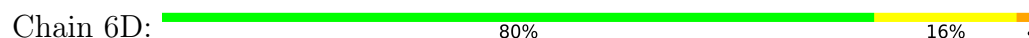
Chain 55:  80% 16% .



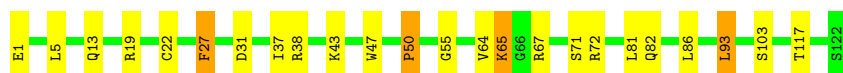
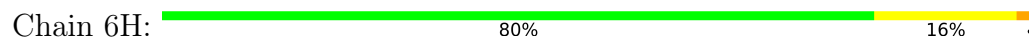
• Molecule 4: HUMAN MONOCLONAL ANTIBODY



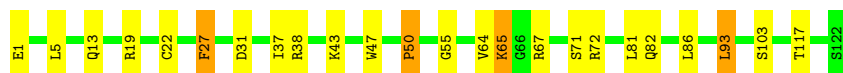
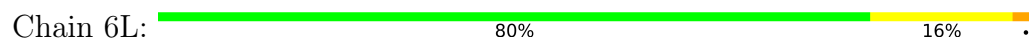
• Molecule 4: HUMAN MONOCLONAL ANTIBODY



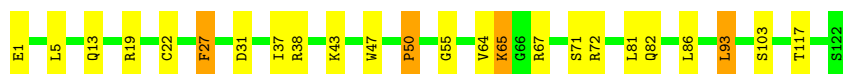
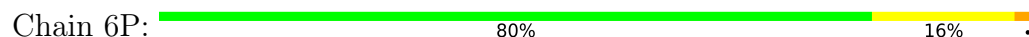
• Molecule 4: HUMAN MONOCLONAL ANTIBODY



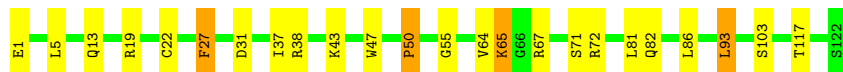
• Molecule 4: HUMAN MONOCLONAL ANTIBODY



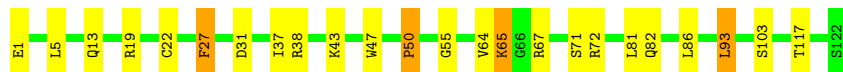
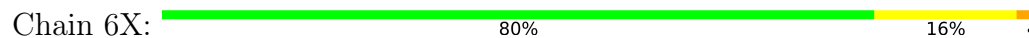
• Molecule 4: HUMAN MONOCLONAL ANTIBODY




• Molecule 4: HUMAN MONOCLONAL ANTIBODY

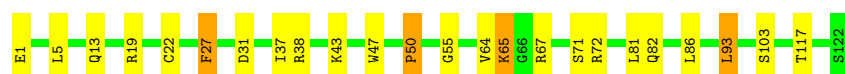


• Molecule 4: HUMAN MONOCLONAL ANTIBODY




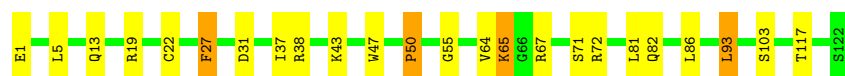
• Molecule 4: HUMAN MONOCLONAL ANTIBODY

Chain 61:  80% 16% .




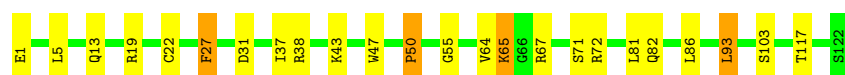
• Molecule 4: HUMAN MONOCLONAL ANTIBODY

Chain 65:  80% 16% .




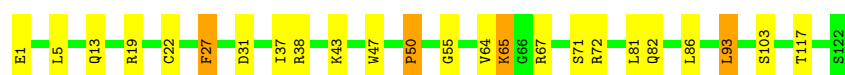
• Molecule 4: HUMAN MONOCLONAL ANTIBODY

Chain 69:  80% 16% .




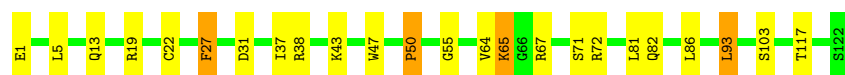
• Molecule 4: HUMAN MONOCLONAL ANTIBODY

Chain 7D:  80% 16% .




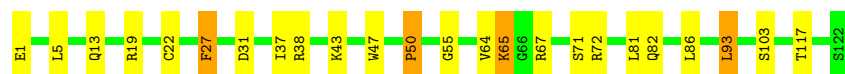
• Molecule 4: HUMAN MONOCLONAL ANTIBODY

Chain 7H:  80% 16% .




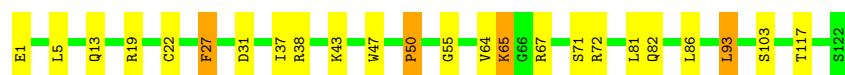
• Molecule 4: HUMAN MONOCLONAL ANTIBODY

Chain 7L:  80% 16% .




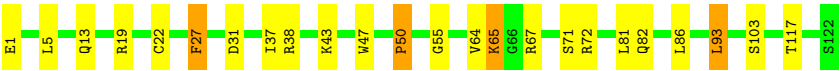
• Molecule 4: HUMAN MONOCLONAL ANTIBODY

Chain 7P:  80% 16% .

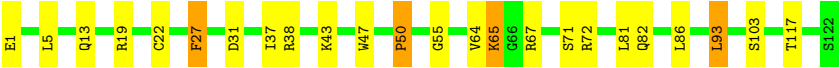
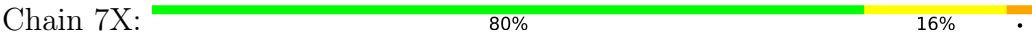


• Molecule 4: HUMAN MONOCLONAL ANTIBODY

Chain 7T:  80% 16% .



● Molecule 4: HUMAN MONOCLONAL ANTIBODY



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	270	Depositor
Resolution determination method	Not provided	Depositor
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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
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 >2	RMSZ	# Z >2
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 >2	RMSZ	# Z >2
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 >2	RMSZ	# Z >2
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 >2	RMSZ	# Z >2
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 >2	RMSZ	# Z >2
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

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%)	<div>07</div>
1	16	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	<div>07</div>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1A	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	1E	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	1I	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	1M	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	1Q	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	1U	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	1Y	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	22	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	26	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	2A	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	2E	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	2I	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	2M	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	2Q	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	2U	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	2Y	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	32	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	36	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	3A	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	3E	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	3I	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	3M	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	3Q	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	3U	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	3Y	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	42	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	46	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	4A	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	4E	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	4I	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	4M	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	4Q	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	4U	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	4Y	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	52	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	56	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	5A	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	5E	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	5I	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	5M	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	5Q	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	5U	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	5Y	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	62	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	66	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	6A	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	6E	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	6I	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	6M	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	6Q	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	6U	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	6Y	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	7A	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	7E	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	7I	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	7M	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	7Q	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
1	7U	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	7
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%)	21	65
3	14	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	18	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	1C	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	1G	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	1K	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1O	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	1S	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	1W	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	20	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	24	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	28	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	2C	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	2G	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	2K	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	2O	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	2S	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	2W	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	30	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	34	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	38	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	3C	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	3G	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	3K	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	3O	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	3S	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	3W	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	40	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	44	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	48	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	4C	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	4G	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	4K	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	4O	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	4S	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	4W	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	50	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	54	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	58	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	5C	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	5G	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	5K	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	5O	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	5S	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	5W	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	60	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	64	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	68	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	6C	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	6G	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	6K	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	6O	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	6S	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	6W	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	7C	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	7G	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	7K	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	7O	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	7S	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
3	7W	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	21	65
4	11	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	15	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	19	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	1D	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	1H	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	1L	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	1P	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	1T	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles		
4	1X	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42	
4	2I	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42	
4	25	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42	
4	29	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42	
4	2D	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42	
4	2H	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42	
4	2L	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42	
4	2P	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42	
4	2T	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42	
4	2X	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42	
4	3I	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42	
4	35	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42	
4	39	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42	
4	3D	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42	
4	3H	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42	
4	3L	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42	
4	3P	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42	
4	3T	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42	
4	3X	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42	
4	4I	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42	
4	45	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42	
4	49	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42	
4	4D	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42	
4	4H	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42	
4	4L	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42	
4	4P	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42	
4	4T	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42	
4	4X	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42	
4	5I	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42	
4	55	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42	
4	59	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42	

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	5D	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	5H	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	5L	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	5P	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	5T	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	5X	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	6I	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	6J	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	6K	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	6L	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	6M	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	6N	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	6O	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	6P	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	6Q	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	6R	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	6S	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	6T	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	6U	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	6V	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	6W	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	6X	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	6Y	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	6Z	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	7A	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	7B	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	7C	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	7D	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	7E	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	7F	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	7G	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	7H	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	7I	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	7J	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	7K	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	7L	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	7M	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	7N	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	7O	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	7P	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	7Q	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	7R	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	7S	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	7T	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	7U	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	7V	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	7W	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	7X	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	7Y	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
4	7Z	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	7	42
All	All	39780/38580 (103%)	32292 (81%)	3540 (9%)	3948 (10%)	1	12

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 ⓘ

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	10
1	16	163/163 (100%)	131 (80%)	32 (20%)	1	10
1	1A	163/163 (100%)	130 (80%)	33 (20%)	1	9
1	1E	163/163 (100%)	130 (80%)	33 (20%)	1	9
1	1I	163/163 (100%)	130 (80%)	33 (20%)	1	9
1	1M	163/163 (100%)	130 (80%)	33 (20%)	1	9
1	1Q	163/163 (100%)	131 (80%)	32 (20%)	1	10
1	1U	163/163 (100%)	131 (80%)	32 (20%)	1	10
1	1Y	163/163 (100%)	131 (80%)	32 (20%)	1	10
1	22	163/163 (100%)	130 (80%)	33 (20%)	1	9
1	26	163/163 (100%)	130 (80%)	33 (20%)	1	9
1	2A	163/163 (100%)	131 (80%)	32 (20%)	1	10
1	2E	163/163 (100%)	130 (80%)	33 (20%)	1	9
1	2I	163/163 (100%)	130 (80%)	33 (20%)	1	9
1	2M	163/163 (100%)	130 (80%)	33 (20%)	1	9
1	2Q	163/163 (100%)	131 (80%)	32 (20%)	1	10
1	2U	163/163 (100%)	131 (80%)	32 (20%)	1	10
1	2Y	163/163 (100%)	131 (80%)	32 (20%)	1	10
1	32	163/163 (100%)	130 (80%)	33 (20%)	1	9
1	36	163/163 (100%)	130 (80%)	33 (20%)	1	9
1	3A	163/163 (100%)	130 (80%)	33 (20%)	1	9
1	3E	163/163 (100%)	130 (80%)	33 (20%)	1	9
1	3I	163/163 (100%)	130 (80%)	33 (20%)	1	9
1	3M	163/163 (100%)	130 (80%)	33 (20%)	1	9
1	3Q	163/163 (100%)	131 (80%)	32 (20%)	1	10
1	3U	163/163 (100%)	131 (80%)	32 (20%)	1	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	3Y	163/163 (100%)	131 (80%)	32 (20%)	1	10
1	42	163/163 (100%)	131 (80%)	32 (20%)	1	10
1	46	163/163 (100%)	131 (80%)	32 (20%)	1	10
1	4A	163/163 (100%)	130 (80%)	33 (20%)	1	9
1	4E	163/163 (100%)	130 (80%)	33 (20%)	1	9
1	4I	163/163 (100%)	130 (80%)	33 (20%)	1	9
1	4M	163/163 (100%)	130 (80%)	33 (20%)	1	9
1	4Q	163/163 (100%)	130 (80%)	33 (20%)	1	9
1	4U	163/163 (100%)	130 (80%)	33 (20%)	1	9
1	4Y	163/163 (100%)	130 (80%)	33 (20%)	1	9
1	52	163/163 (100%)	131 (80%)	32 (20%)	1	10
1	56	163/163 (100%)	131 (80%)	32 (20%)	1	10
1	5A	163/163 (100%)	131 (80%)	32 (20%)	1	10
1	5E	163/163 (100%)	131 (80%)	32 (20%)	1	10
1	5I	163/163 (100%)	131 (80%)	32 (20%)	1	10
1	5M	163/163 (100%)	131 (80%)	32 (20%)	1	10
1	5Q	163/163 (100%)	130 (80%)	33 (20%)	1	9
1	5U	163/163 (100%)	130 (80%)	33 (20%)	1	9
1	5Y	163/163 (100%)	130 (80%)	33 (20%)	1	9
1	62	163/163 (100%)	131 (80%)	32 (20%)	1	10
1	66	163/163 (100%)	131 (80%)	32 (20%)	1	10
1	6A	163/163 (100%)	131 (80%)	32 (20%)	1	10
1	6E	163/163 (100%)	130 (80%)	33 (20%)	1	9
1	6I	163/163 (100%)	130 (80%)	33 (20%)	1	9
1	6M	163/163 (100%)	130 (80%)	33 (20%)	1	9
1	6Q	163/163 (100%)	130 (80%)	33 (20%)	1	9
1	6U	163/163 (100%)	130 (80%)	33 (20%)	1	9
1	6Y	163/163 (100%)	130 (80%)	33 (20%)	1	9
1	7A	163/163 (100%)	131 (80%)	32 (20%)	1	10
1	7E	163/163 (100%)	130 (80%)	33 (20%)	1	9
1	7I	163/163 (100%)	130 (80%)	33 (20%)	1	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	7M	163/163 (100%)	130 (80%)	33 (20%)	1	9
1	7Q	163/163 (100%)	130 (80%)	33 (20%)	1	9
1	7U	163/163 (100%)	130 (80%)	33 (20%)	1	9
2	13	203/203 (100%)	156 (77%)	47 (23%)	1	5
2	17	203/203 (100%)	156 (77%)	47 (23%)	1	5
2	1B	203/203 (100%)	156 (77%)	47 (23%)	1	5
2	1F	203/203 (100%)	156 (77%)	47 (23%)	1	5
2	1J	203/203 (100%)	156 (77%)	47 (23%)	1	5
2	1N	203/203 (100%)	156 (77%)	47 (23%)	1	5
2	1R	203/203 (100%)	156 (77%)	47 (23%)	1	5
2	1V	203/203 (100%)	156 (77%)	47 (23%)	1	5
2	1Z	203/203 (100%)	156 (77%)	47 (23%)	1	5
2	23	203/203 (100%)	156 (77%)	47 (23%)	1	5
2	27	203/203 (100%)	156 (77%)	47 (23%)	1	5
2	2B	203/203 (100%)	156 (77%)	47 (23%)	1	5
2	2F	203/203 (100%)	156 (77%)	47 (23%)	1	5
2	2J	203/203 (100%)	156 (77%)	47 (23%)	1	5
2	2N	203/203 (100%)	156 (77%)	47 (23%)	1	5
2	2R	203/203 (100%)	156 (77%)	47 (23%)	1	5
2	2V	203/203 (100%)	156 (77%)	47 (23%)	1	5
2	2Z	203/203 (100%)	156 (77%)	47 (23%)	1	5
2	33	203/203 (100%)	156 (77%)	47 (23%)	1	5
2	37	203/203 (100%)	156 (77%)	47 (23%)	1	5
2	3B	203/203 (100%)	156 (77%)	47 (23%)	1	5
2	3F	203/203 (100%)	156 (77%)	47 (23%)	1	5
2	3J	203/203 (100%)	156 (77%)	47 (23%)	1	5
2	3N	203/203 (100%)	156 (77%)	47 (23%)	1	5
2	3R	203/203 (100%)	156 (77%)	47 (23%)	1	5
2	3V	203/203 (100%)	156 (77%)	47 (23%)	1	5
2	3Z	203/203 (100%)	156 (77%)	47 (23%)	1	5
2	43	203/203 (100%)	156 (77%)	47 (23%)	1	5

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	7V	203/203 (100%)	156 (77%)	47 (23%)	1	5
3	10	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	14	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	18	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	1C	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	1G	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	1K	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	1O	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	1S	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	1W	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	20	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	24	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	28	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	2C	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	2G	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	2K	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	2O	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	2S	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	2W	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	30	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	34	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	38	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	3C	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	3G	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	3K	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	3O	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	3S	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	3W	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	40	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	44	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	48	110/93 (118%)	102 (93%)	8 (7%)	15	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	4C	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	4G	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	4K	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	4O	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	4S	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	4W	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	50	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	54	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	58	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	5C	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	5G	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	5K	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	5O	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	5S	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	5W	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	60	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	64	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	68	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	6C	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	6G	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	6K	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	6O	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	6S	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	6W	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	7C	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	7G	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	7K	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	7O	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	7S	110/93 (118%)	102 (93%)	8 (7%)	15	46
3	7W	110/93 (118%)	102 (93%)	8 (7%)	15	46
4	11	112/97 (116%)	93 (83%)	19 (17%)	2	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	15	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	19	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	1D	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	1H	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	1L	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	1P	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	1T	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	1X	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	21	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	25	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	29	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	2D	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	2H	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	2L	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	2P	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	2T	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	2X	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	31	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	35	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	39	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	3D	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	3H	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	3L	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	3P	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	3T	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	3X	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	41	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	45	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	49	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	4D	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	4H	112/97 (116%)	93 (83%)	19 (17%)	2	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	4L	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	4P	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	4T	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	4X	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	5I	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	55	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	59	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	5D	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	5H	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	5L	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	5P	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	5T	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	5X	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	6I	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	65	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	69	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	6D	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	6H	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	6L	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	6P	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	6T	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	6X	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	7D	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	7H	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	7L	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	7P	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	7T	112/97 (116%)	93 (83%)	19 (17%)	2	14
4	7X	112/97 (116%)	93 (83%)	19 (17%)	2	14
All	All	35280/33360 (106%)	28884 (82%)	6396 (18%)	5	12

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

Mol	Chain	Res	Type
1	4A	82	ARG
2	4Z	74	TYR
2	7F	39	ASP
4	4D	81	LEU
2	4N	39	ASP

Some 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 carbohydrates 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	6F	28
2	5Z	28
2	37	28
2	1F	28
2	4J	28

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Mol	Chain	Number of breaks
2	2N	28
2	7J	28
2	3N	28
2	4R	28
2	6Z	28
2	23	28
2	7V	28
2	1J	27
2	6N	27
2	1B	27
2	2F	27
2	7B	27
2	3R	27
2	7R	27
2	3B	27
2	2R	27
2	4N	27
2	5J	27
2	1N	27
2	13	27
2	2B	27
2	3V	27
2	57	27
2	4Z	27
2	7N	27
2	6R	27
2	47	27
2	1R	27
2	3F	27
2	5V	27
2	63	27
2	17	27
2	3Z	27
2	5F	27
2	53	27
2	6V	27
2	1V	27
2	3J	27
2	4V	27
2	6B	27
2	5R	27
2	43	27

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Mol	Chain	Number of breaks
2	27	27
2	67	27
2	2Z	27
2	4F	27
2	5B	27
2	6J	27
2	2J	27
2	7F	27
2	1Z	27
2	33	27
2	2V	27
2	4B	27
2	5N	27
1	1Y	26
1	6Q	26
1	5M	26
1	46	26
1	4M	26
1	1I	26
1	7E	26
1	3M	26
1	62	26
1	6E	26
1	5Y	26
1	3E	26
1	7U	26
1	4Y	26
1	32	26
1	6U	26
1	5I	26
1	2M	26
1	42	26
1	4I	26
1	1M	26
1	7A	26
1	3Q	26
1	26	26
1	66	26
1	2Y	26
1	7Q	26
1	1Q	26
1	3A	26

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Mol	Chain	Number of breaks
1	36	26
1	6I	26
1	5U	26
1	2I	26
1	4U	26
1	1A	26
1	12	26
1	6Y	26
1	3U	26
1	5E	26
1	22	26
1	56	26
1	2U	26
1	4E	26
1	7M	26
1	1U	26
1	6M	26
1	5Q	26
1	2E	26
1	4Q	26
1	1E	26
1	16	26
1	3Y	26
1	5A	26
1	52	26
1	2Q	26
1	4A	26
1	7I	26
1	3I	26
1	6A	26
1	2A	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