



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 12:19 AM UTC

PDB ID : 4UDF / pdb_00004udf
EMDB ID : EMD-2761
Title : STRUCTURAL BASIS OF HUMAN PARECHOVIRUS NEUTRALIZATION
BY HUMAN MONOCLONAL ANTIBODIES
Authors : Shakeel, S.; Westerhuis, B.M.; Ora, A.; Koen, G.; Bakker, A.Q.; Claassen, Y.;
Beaumont, T.; Wolthers, K.C.; Butcher, S.J.
Deposited on : 2014-12-10
Resolution : 20.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

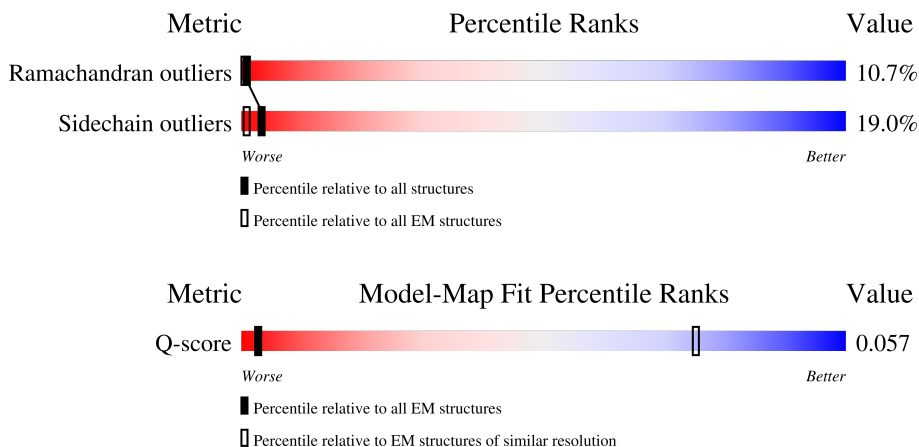
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 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.



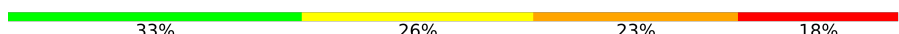
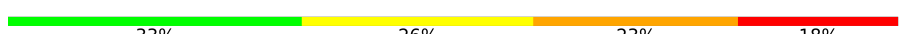
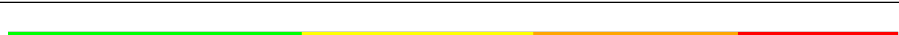
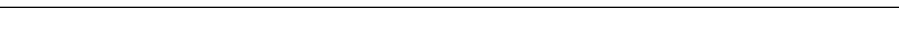
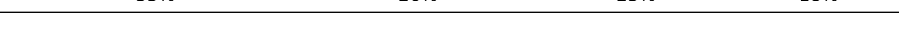
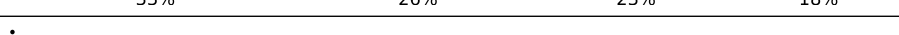
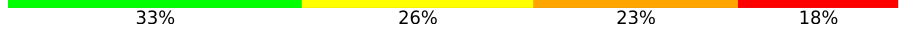
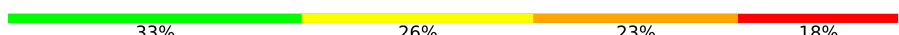
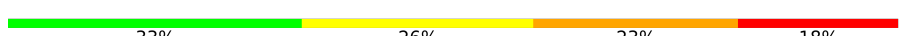
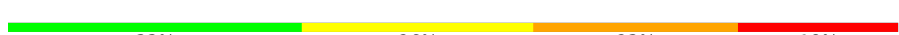
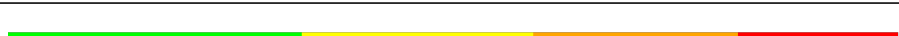

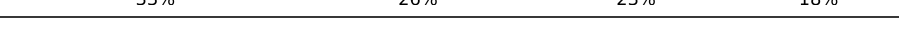
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	28 (19.40 - 20.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	12	183	33% 26% 23% 18%
1	16	183	33% 26% 23% 18%
1	1A	183	33% 26% 23% 18%
1	1E	183	33% 26% 23% 18%
1	1I	183	33% 26% 23% 18%

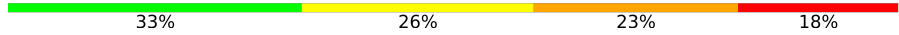
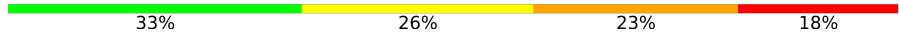
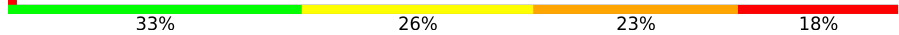

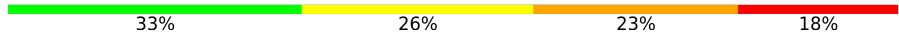

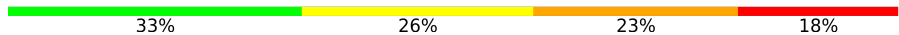
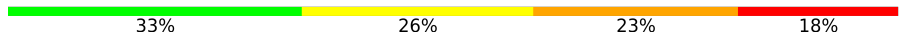
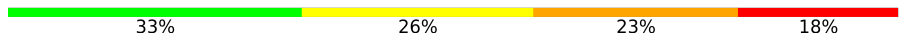
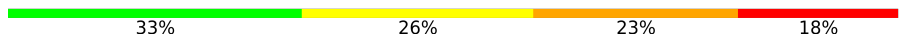
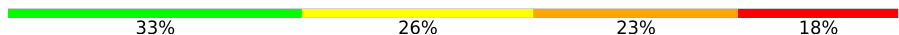
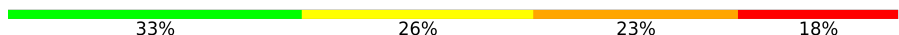
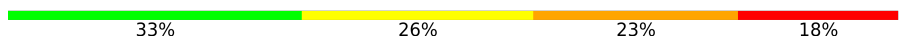
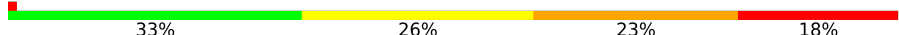
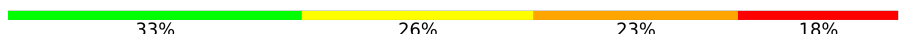
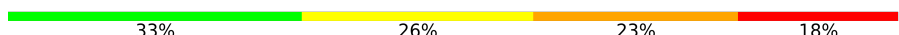
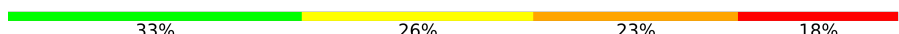
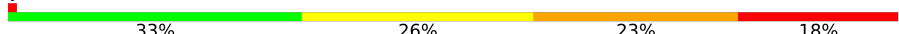
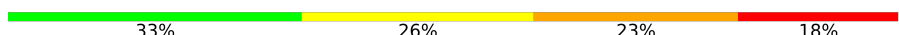
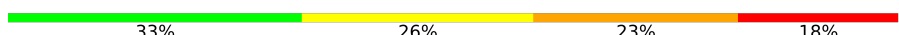
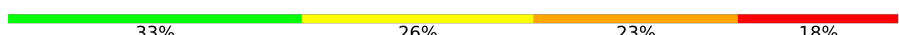
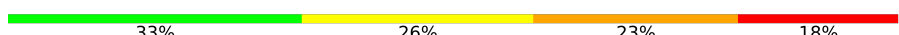
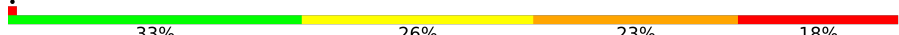
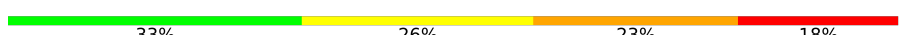
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Mol	Chain	Length	Quality of chain
1	1M	183	
1	1Q	183	
1	1U	183	
1	1Y	183	
1	22	183	
1	26	183	
1	2A	183	
1	2E	183	
1	2I	183	
1	2M	183	
1	2Q	183	
1	2U	183	
1	2Y	183	
1	32	183	
1	36	183	
1	3A	183	
1	3E	183	
1	3I	183	
1	3M	183	
1	3Q	183	
1	3U	183	
1	3Y	183	
1	42	183	
1	46	183	
1	4A	183	

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

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Mol	Chain	Length	Quality of chain
1	7E	183	33% 26% 23% 18%
1	7I	183	33% 26% 23% 18%
1	7M	183	33% 26% 23% 18%
1	7Q	183	33% 26% 23% 18%
1	7U	183	33% 26% 23% 18%
2	13	229	36% 30% 17% 17%
2	17	229	36% 30% 17% 17%
2	1B	229	36% 30% 17% 17%
2	1F	229	36% 30% 17% 17%
2	1J	229	36% 30% 17% 17%
2	1N	229	35% 31% 17% 17%
2	1R	229	35% 31% 17% 17%
2	1V	229	35% 31% 17% 17%
2	1Z	229	35% 31% 17% 17%
2	23	229	36% 30% 17% 17%
2	27	229	36% 30% 17% 17%
2	2B	229	36% 30% 17% 17%
2	2F	229	36% 30% 17% 17%
2	2J	229	35% 31% 17% 17%
2	2N	229	36% 30% 17% 17%
2	2R	229	35% 31% 17% 17%
2	2V	229	35% 31% 17% 17%
2	2Z	229	35% 31% 17% 17%
2	33	229	35% 31% 17% 17%
2	37	229	36% 30% 17% 17%

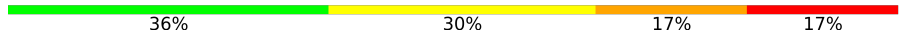
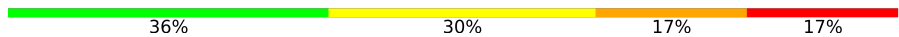
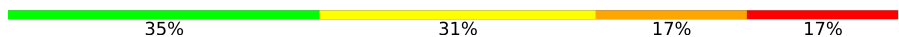
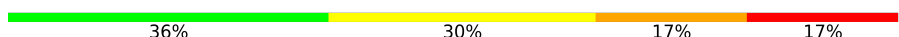
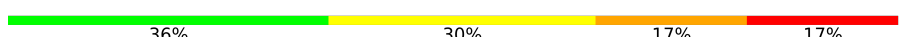
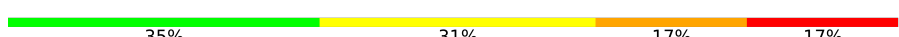
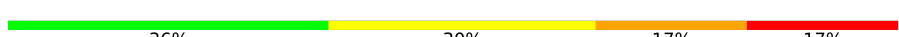

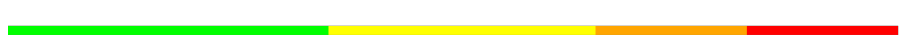

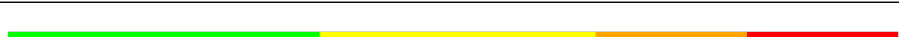
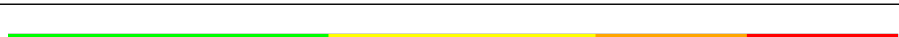

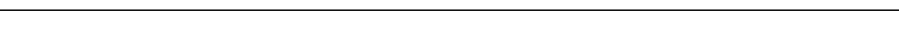
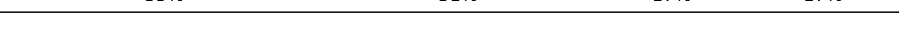
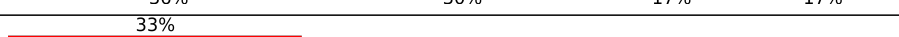



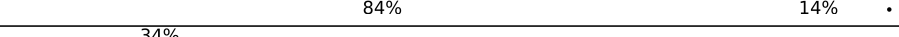





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Mol	Chain	Length	Quality of chain			
2	3B	229	35%	31%	17%	17%
2	3F	229	36%	30%	17%	17%
2	3J	229	35%	31%	17%	17%
2	3N	229	36%	30%	17%	17%
2	3R	229	36%	30%	17%	17%
2	3V	229	36%	30%	17%	17%
2	3Z	229	36%	30%	17%	17%
2	43	229	35%	31%	17%	17%
2	47	229	35%	31%	17%	17%
2	4B	229	36%	30%	17%	17%
2	4F	229	35%	31%	17%	17%
2	4J	229	36%	30%	17%	17%
2	4N	229	36%	30%	17%	17%
2	4R	229	36%	30%	17%	17%
2	4V	229	36%	30%	17%	17%
2	4Z	229	35%	31%	17%	17%
2	53	229	35%	31%	17%	17%
2	57	229	35%	31%	17%	17%
2	5B	229	35%	31%	17%	17%
2	5F	229	36%	30%	17%	17%
2	5J	229	36%	30%	17%	17%
2	5N	229	36%	30%	17%	17%
2	5R	229	36%	30%	17%	17%
2	5V	229	35%	31%	17%	17%
2	5Z	229	36%	30%	17%	17%

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Mol	Chain	Length	Quality of chain
2	63	229	
2	67	229	
2	6B	229	
2	6F	229	
2	6J	229	
2	6N	229	
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	

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Mol	Chain	Length	Quality of chain
3	24	109	34% 84% 14%
3	28	109	34% 84% 14%
3	2C	109	28% 84% 14%
3	2G	109	34% 84% 14%
3	2K	109	28% 84% 14%
3	2O	109	34% 84% 14%
3	2S	109	33% 84% 14%
3	2W	109	33% 84% 14%
3	30	109	28% 84% 14%
3	34	109	28% 84% 14%
3	38	109	34% 84% 14%
3	3C	109	28% 84% 14%
3	3G	109	34% 84% 14%
3	3K	109	28% 84% 14%
3	3O	109	34% 84% 14%
3	3S	109	28% 84% 14%
3	3W	109	28% 84% 14%
3	40	109	28% 84% 14%
3	44	109	33% 84% 14%
3	48	109	33% 84% 14%
3	4C	109	34% 84% 14%
3	4G	109	28% 84% 14%
3	4K	109	34% 84% 14%
3	4O	109	34% 84% 14%
3	4S	109	34% 84% 14%

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Mol	Chain	Length	Quality of chain
3	4W	109	34% 84% 14%
3	50	109	34% 84% 14%
3	54	109	33% 84% 14%
3	58	109	33% 84% 14%
3	5C	109	33% 84% 14%
3	5G	109	28% 84% 14%
3	5K	109	28% 84% 14%
3	5O	109	28% 84% 14%
3	5S	109	34% 84% 14%
3	5W	109	28% 84% 14%
3	60	109	34% 84% 14%
3	64	109	28% 84% 14%
3	68	109	28% 84% 14%
3	6C	109	33% 84% 14%
3	6G	109	34% 84% 14%
3	6K	109	34% 84% 14%
3	6O	109	28% 84% 14%
3	6S	109	34% 84% 14%
3	6W	109	28% 84% 14%
3	7C	109	28% 84% 14%
3	7G	109	28% 84% 14%
3	7K	109	34% 84% 14%
3	7O	109	34% 84% 14%
3	7S	109	28% 84% 14%
3	7W	109	34% 84% 14%

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Mol	Chain	Length	Quality of chain
4	11	122	22% 77% 19% .
4	15	122	19% 77% 19% .
4	19	122	19% 77% 19% .
4	1D	122	23% 77% 19% .
4	1H	122	21% 77% 19% .
4	1L	122	23% 77% 19% .
4	1P	122	20% 77% 19% .
4	1T	122	22% 77% 19% .
4	1X	122	22% 77% 19% .
4	21	122	22% 77% 19% .
4	25	122	21% 77% 19% .
4	29	122	23% 77% 19% .
4	2D	122	19% 77% 19% .
4	2H	122	23% 77% 19% .
4	2L	122	20% 77% 19% .
4	2P	122	21% 77% 19% .
4	2T	122	22% 77% 19% .
4	2X	122	22% 77% 19% .
4	31	122	19% 77% 19% .
4	35	122	20% 77% 19% .
4	39	122	21% 77% 19% .
4	3D	122	20% 77% 19% .
4	3H	122	23% 77% 19% .
4	3L	122	20% 77% 19% .
4	3P	122	21% 77% 19% .

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Mol	Chain	Length	Quality of chain	
4	3T	122	19%	77%
4	3X	122	19%	77%
4	4I	122	20%	77%
4	45	122	22%	77%
4	49	122	22%	77%
4	4D	122	23%	77%
4	4H	122	20%	77%
4	4L	122	21%	77%
4	4P	122	23%	77%
4	4T	122	21%	77%
4	4X	122	23%	77%
4	5I	122	21%	77%
4	55	122	22%	77%
4	59	122	22%	77%
4	5D	122	22%	77%
4	5H	122	19%	77%
4	5L	122	19%	77%
4	5P	122	19%	77%
4	5T	122	23%	77%
4	5X	122	20%	77%
4	6I	122	21%	77%
4	65	122	19%	77%
4	69	122	19%	77%
4	6D	122	22%	77%
4	6H	122	21%	77%

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Mol	Chain	Length	Quality of chain
4	6L	122	<p>23% 77% 19% .</p>
4	6P	122	<p>20% 77% 19% .</p>
4	6T	122	<p>23% 77% 19% .</p>
4	6X	122	<p>20% 77% 19% .</p>
4	7D	122	<p>19% 77% 19% .</p>
4	7H	122	<p>20% 77% 19% .</p>
4	7L	122	<p>21% 77% 19% .</p>
4	7P	122	<p>23% 77% 19% .</p>
4	7T	122	<p>20% 77% 19% .</p>
4	7X	122	<p>21% 77% 19% .</p>

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 Capsid protein VP3.

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

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

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

- Molecule 2 is a protein called Capsid protein VP0.

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

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	3B	229	Total 1810	C 1151	N 301	O 353	S 5	1	0
2	3F	229	Total 1810	C 1151	N 301	O 353	S 5	1	0
2	3J	229	Total 1810	C 1151	N 301	O 353	S 5	1	0
2	3N	229	Total 1810	C 1151	N 301	O 353	S 5	1	0
2	3R	229	Total 1810	C 1151	N 301	O 353	S 5	1	0
2	3V	229	Total 1810	C 1151	N 301	O 353	S 5	1	0
2	3Z	229	Total 1810	C 1151	N 301	O 353	S 5	1	0
2	33	229	Total 1810	C 1151	N 301	O 353	S 5	1	0
2	37	229	Total 1810	C 1151	N 301	O 353	S 5	1	0
2	4B	229	Total 1810	C 1151	N 301	O 353	S 5	1	0
2	4F	229	Total 1810	C 1151	N 301	O 353	S 5	1	0
2	4J	229	Total 1810	C 1151	N 301	O 353	S 5	1	0
2	4N	229	Total 1810	C 1151	N 301	O 353	S 5	1	0
2	4R	229	Total 1810	C 1151	N 301	O 353	S 5	1	0
2	4V	229	Total 1810	C 1151	N 301	O 353	S 5	1	0
2	4Z	229	Total 1810	C 1151	N 301	O 353	S 5	1	0
2	43	229	Total 1810	C 1151	N 301	O 353	S 5	1	0
2	47	229	Total 1810	C 1151	N 301	O 353	S 5	1	0
2	5B	229	Total 1810	C 1151	N 301	O 353	S 5	1	0
2	5F	229	Total 1810	C 1151	N 301	O 353	S 5	1	0
2	5J	229	Total 1810	C 1151	N 301	O 353	S 5	1	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	5N	229	Total 1810	C 1151	N 301	O 353	S 5	1	0
2	5R	229	Total 1810	C 1151	N 301	O 353	S 5	1	0
2	5V	229	Total 1810	C 1151	N 301	O 353	S 5	1	0
2	5Z	229	Total 1810	C 1151	N 301	O 353	S 5	1	0
2	53	229	Total 1810	C 1151	N 301	O 353	S 5	1	0
2	57	229	Total 1810	C 1151	N 301	O 353	S 5	1	0
2	6B	229	Total 1810	C 1151	N 301	O 353	S 5	1	0
2	6F	229	Total 1810	C 1151	N 301	O 353	S 5	1	0
2	6J	229	Total 1810	C 1151	N 301	O 353	S 5	1	0
2	6N	229	Total 1810	C 1151	N 301	O 353	S 5	1	0
2	6R	229	Total 1810	C 1151	N 301	O 353	S 5	1	0
2	6V	229	Total 1810	C 1151	N 301	O 353	S 5	1	0
2	6Z	229	Total 1810	C 1151	N 301	O 353	S 5	1	0
2	63	229	Total 1810	C 1151	N 301	O 353	S 5	1	0
2	67	229	Total 1810	C 1151	N 301	O 353	S 5	1	0
2	7B	229	Total 1810	C 1151	N 301	O 353	S 5	1	0
2	7F	229	Total 1810	C 1151	N 301	O 353	S 5	1	0
2	7J	229	Total 1810	C 1151	N 301	O 353	S 5	1	0
2	7N	229	Total 1810	C 1151	N 301	O 353	S 5	1	0
2	7R	229	Total 1810	C 1151	N 301	O 353	S 5	1	0
2	7V	229	Total 1810	C 1151	N 301	O 353	S 5	1	0

- Molecule 3 is a protein called HUMAN MONOCLONAL ANTIBODY.

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

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

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

- Molecule 4 is a protein called HUMAN MONOCLONAL ANTIBODY.

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

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

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Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
4	3T	122	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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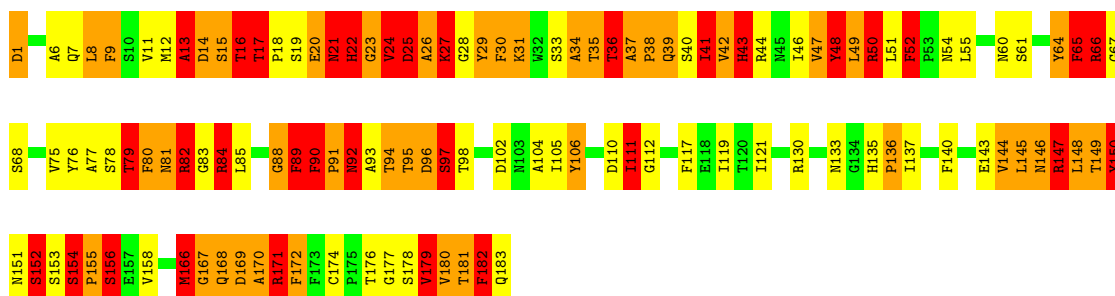
Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
4	55	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	59	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	6D	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	6H	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	6L	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	6P	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	6T	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	6X	122	Total 1126	C 573	H 208	N 155	O 186	S 4	15	0
4	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
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3 Residue-property plots [i](#)

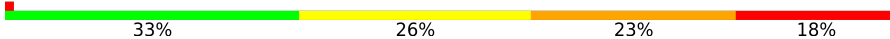
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

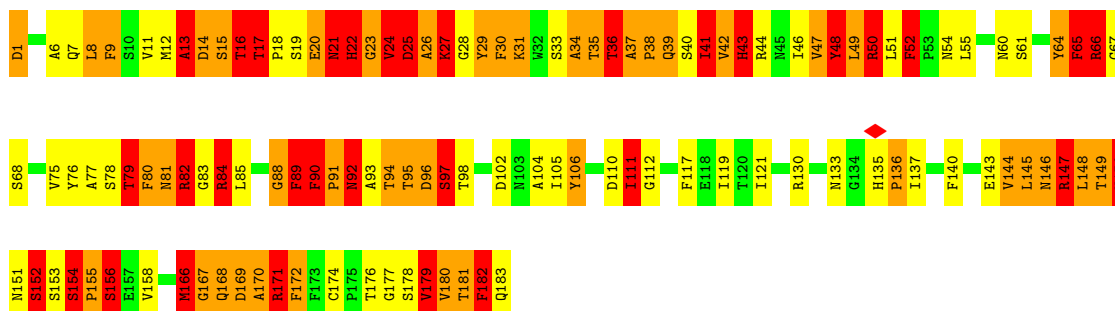
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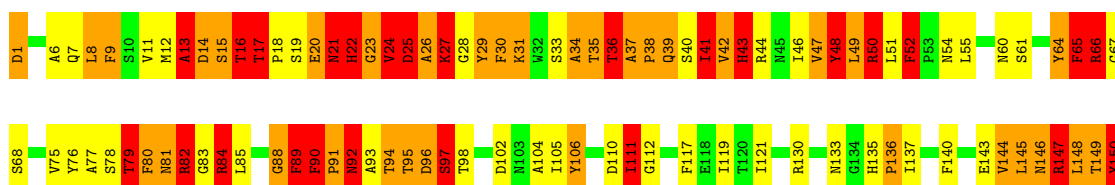
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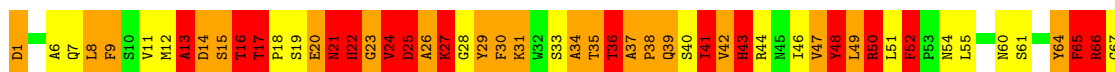
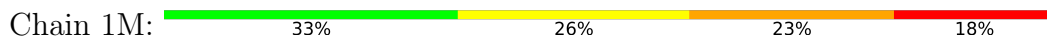
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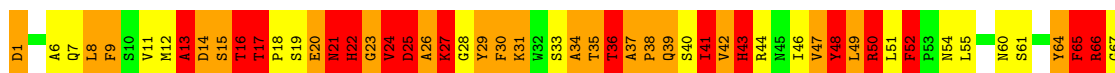
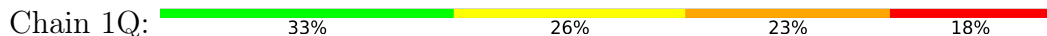




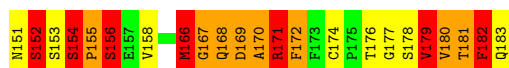
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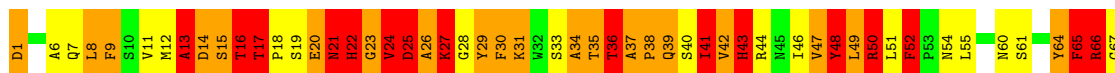
• Molecule 1: Capsid protein VP3



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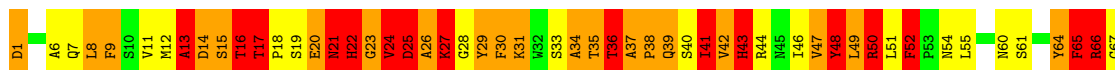
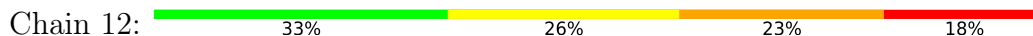


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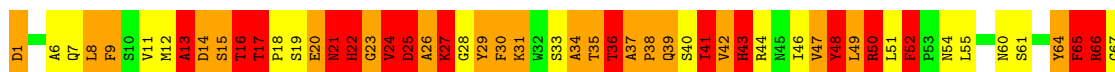




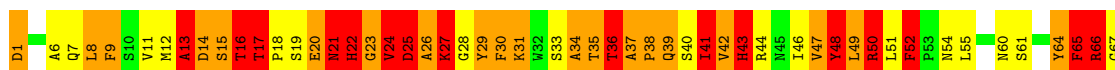
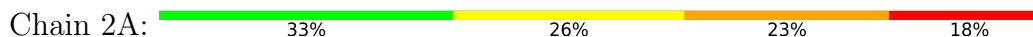
• Molecule 1: Capsid protein VP3



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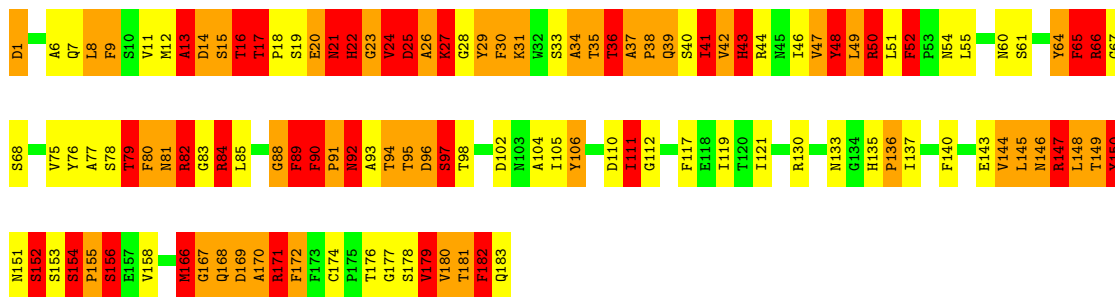


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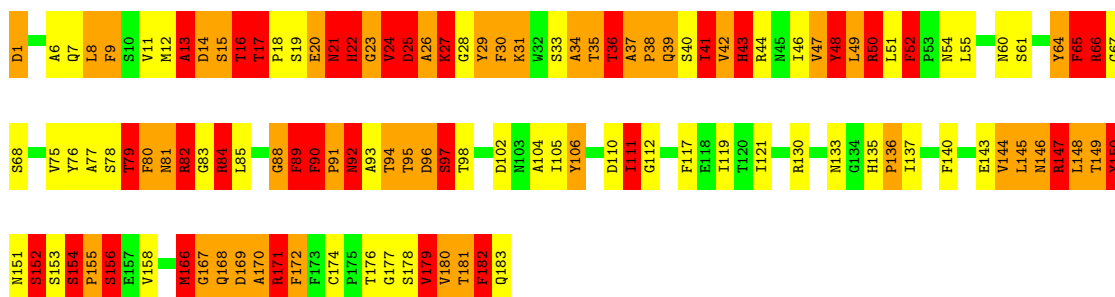


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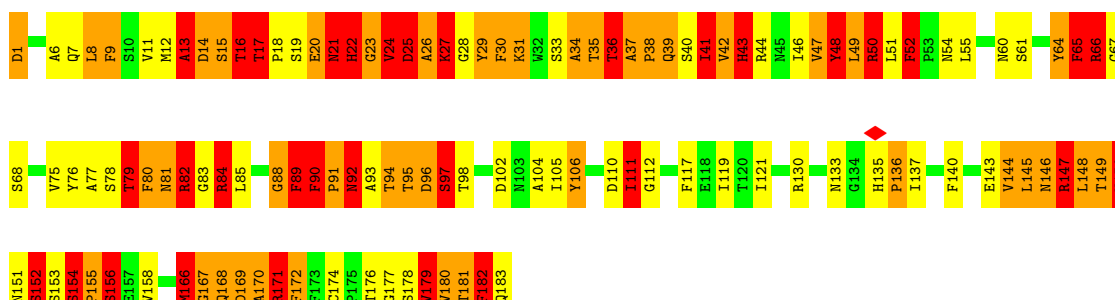




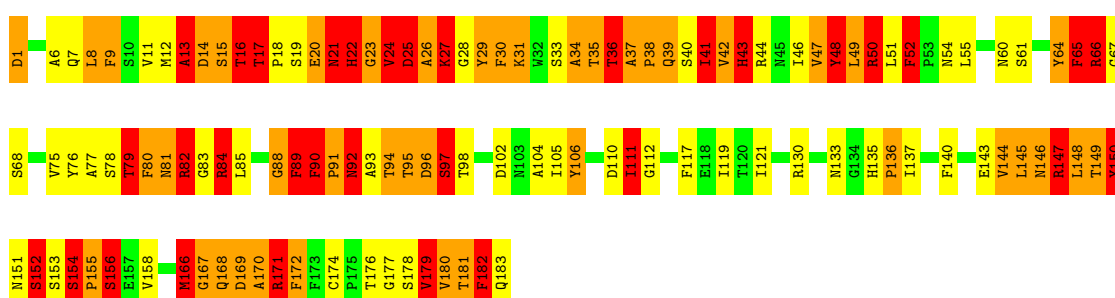
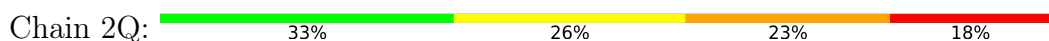
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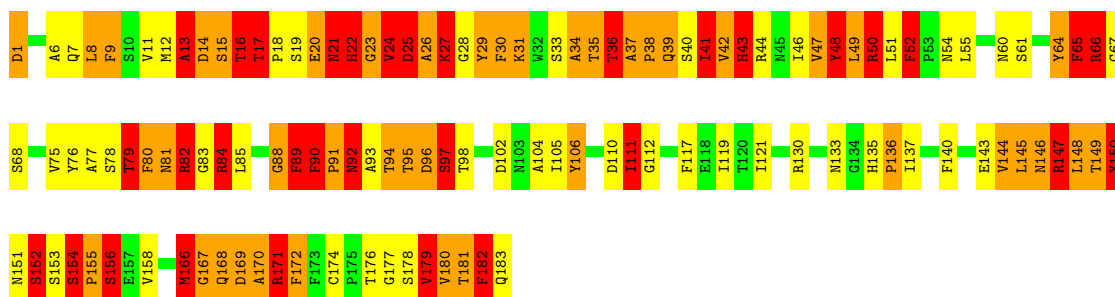
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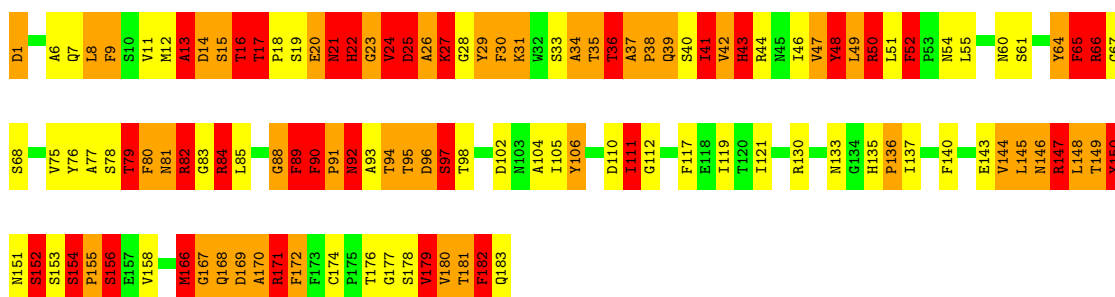
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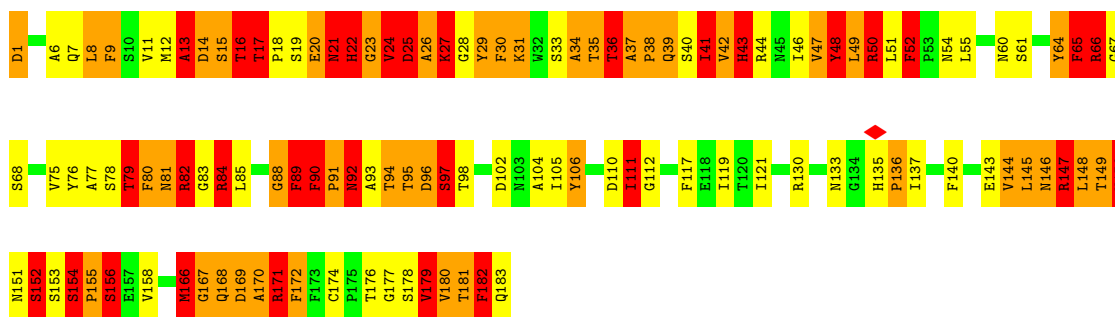
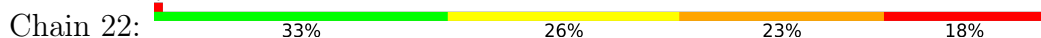
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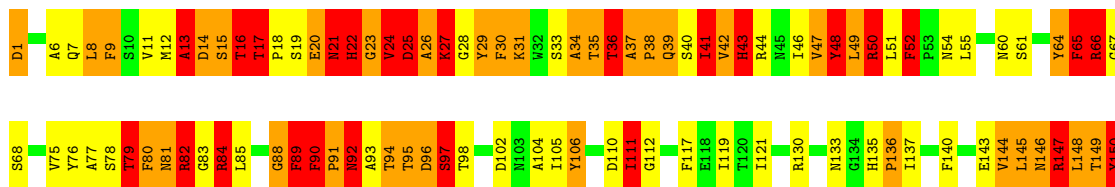
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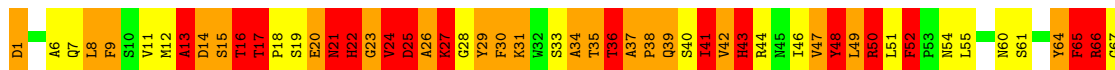
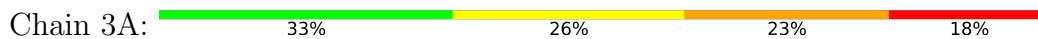


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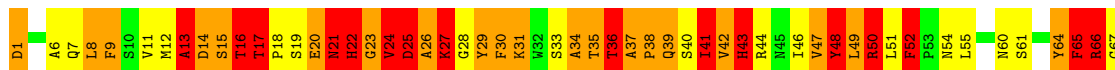
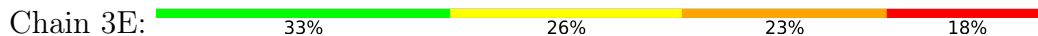




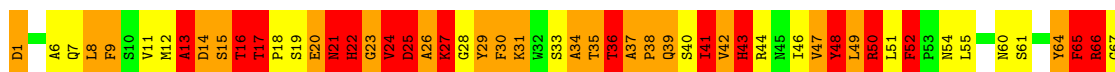
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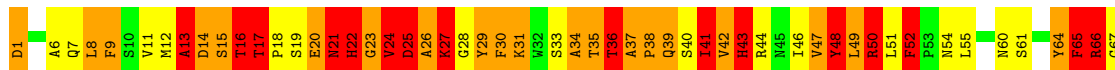
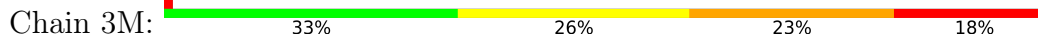
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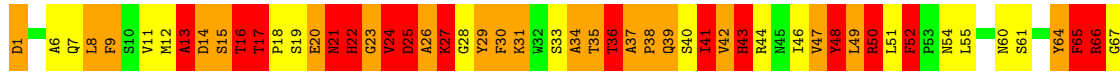


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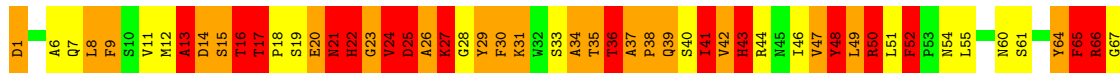




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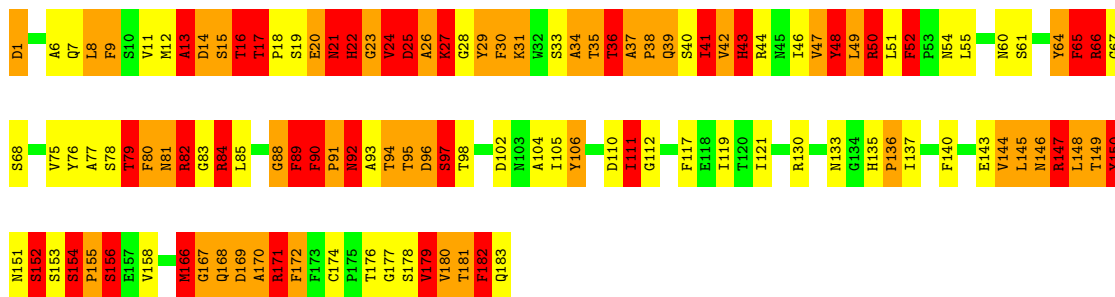


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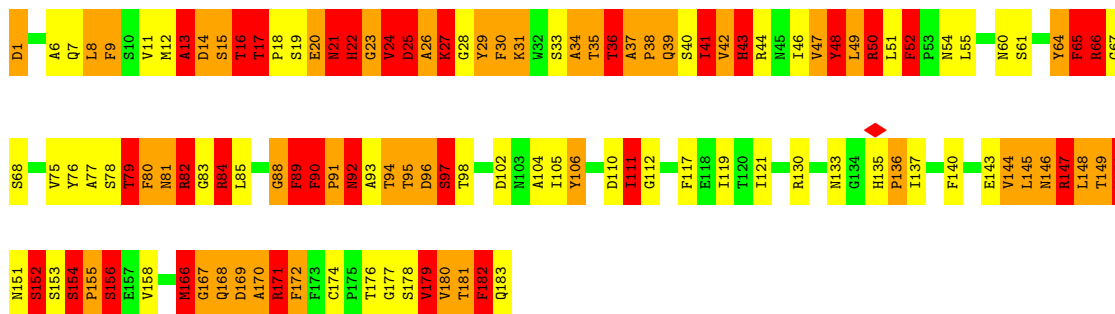


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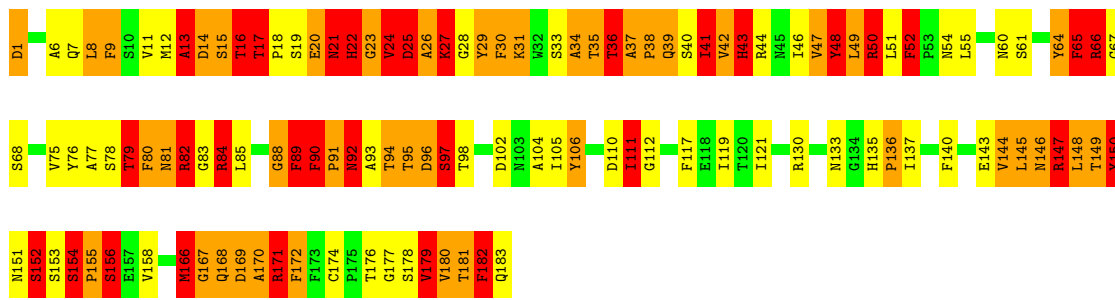




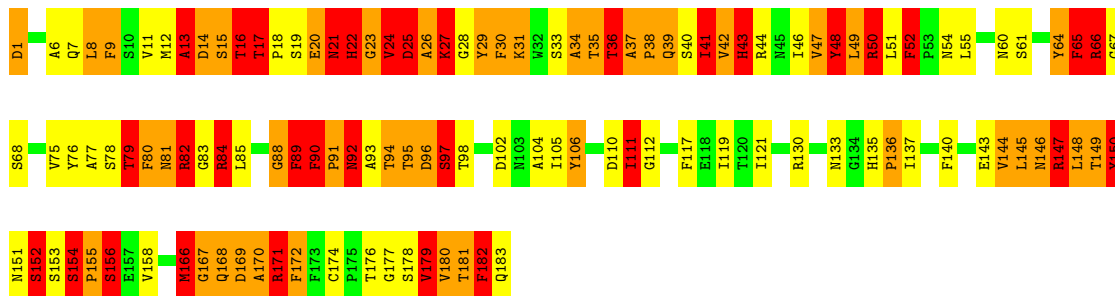
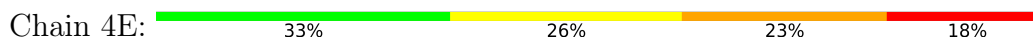
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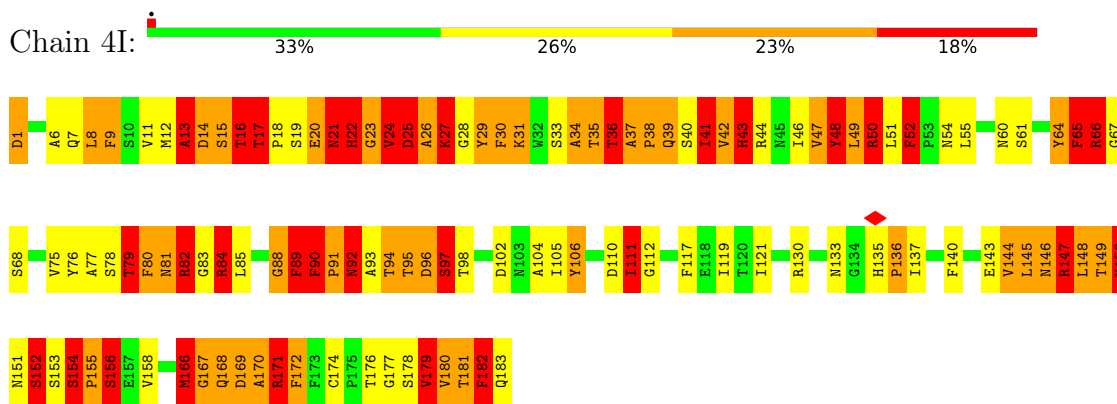
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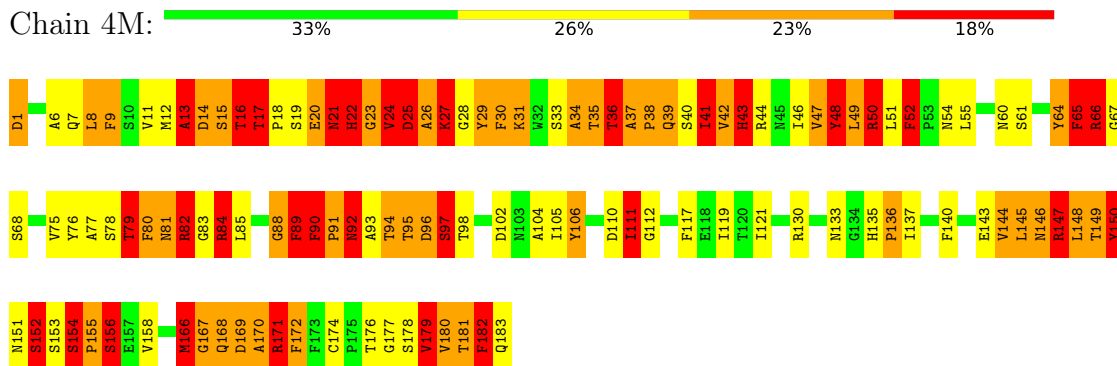
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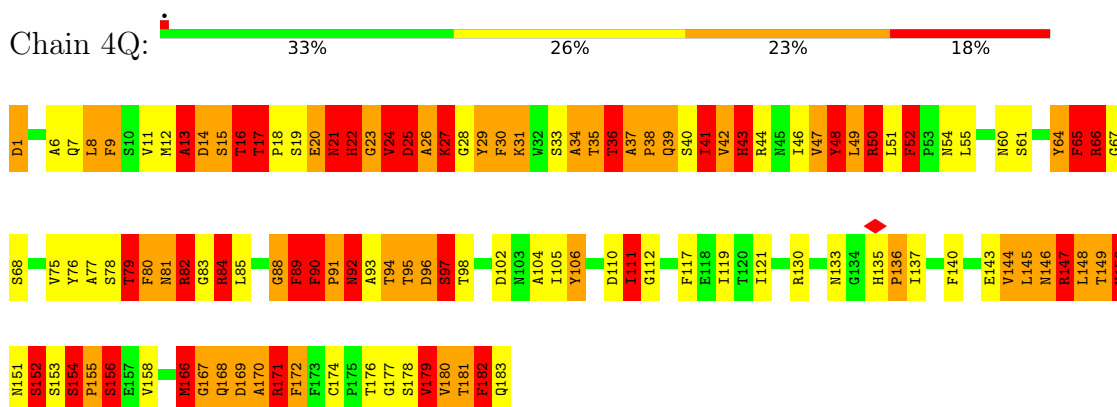
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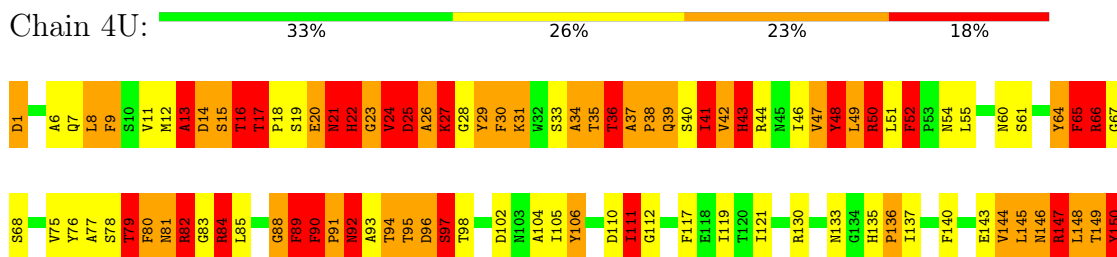
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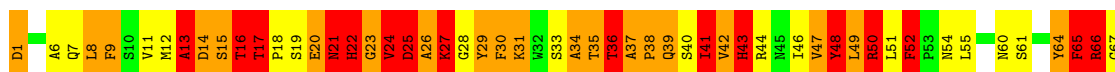


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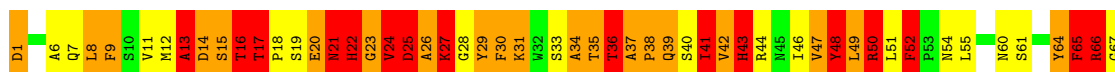
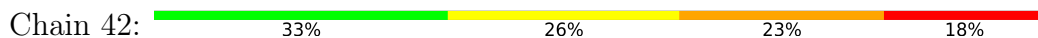




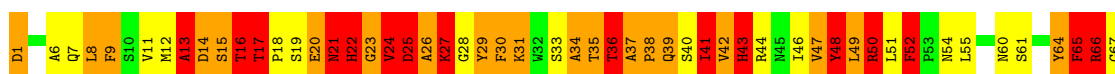
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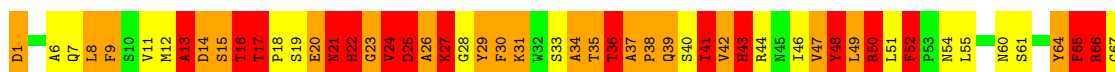
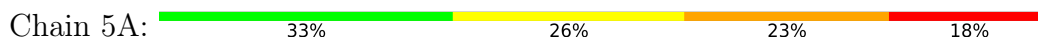
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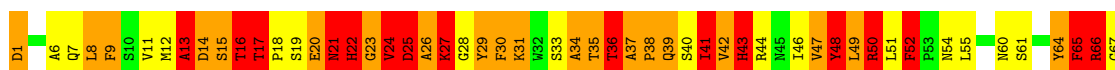
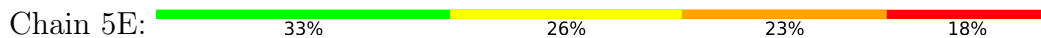


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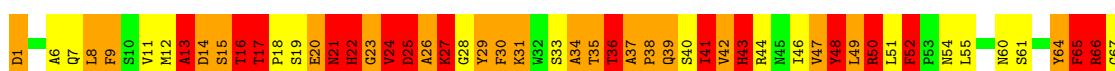
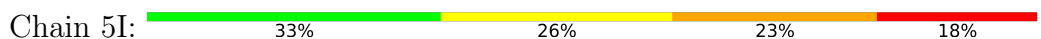




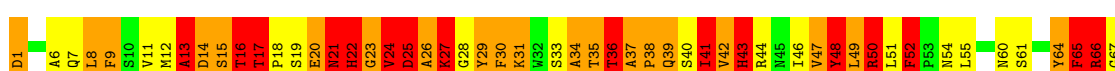
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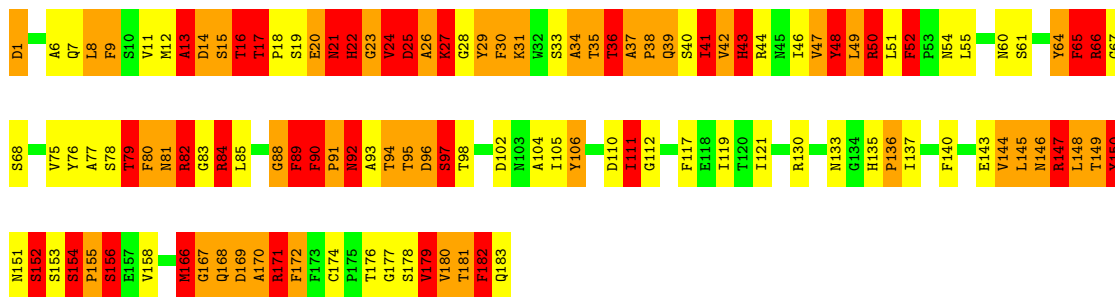


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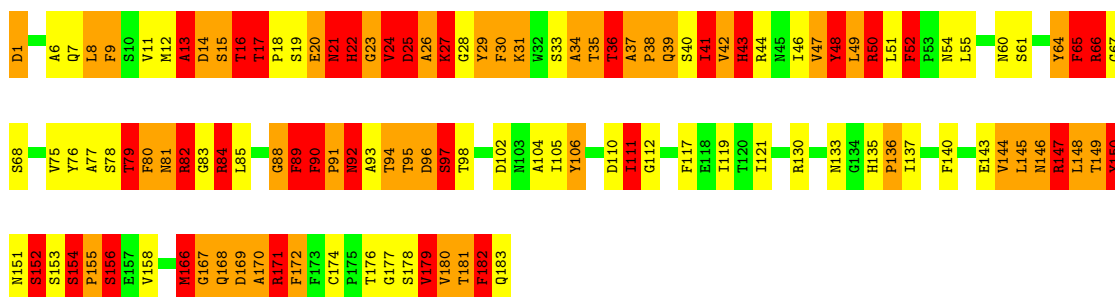


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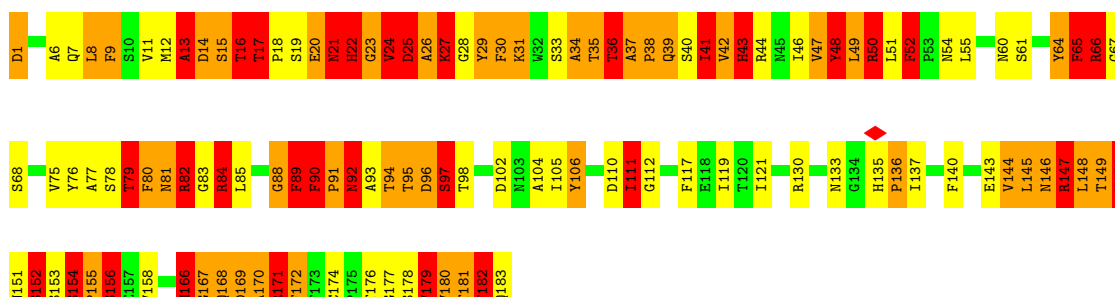




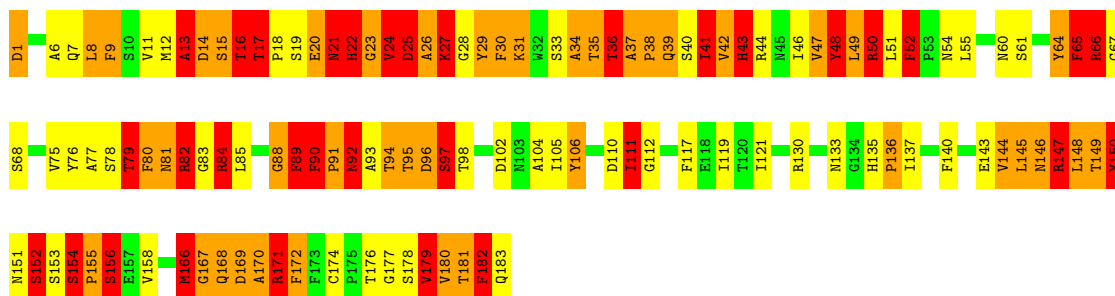
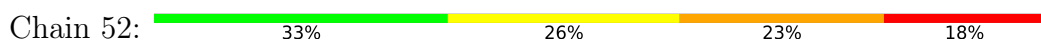
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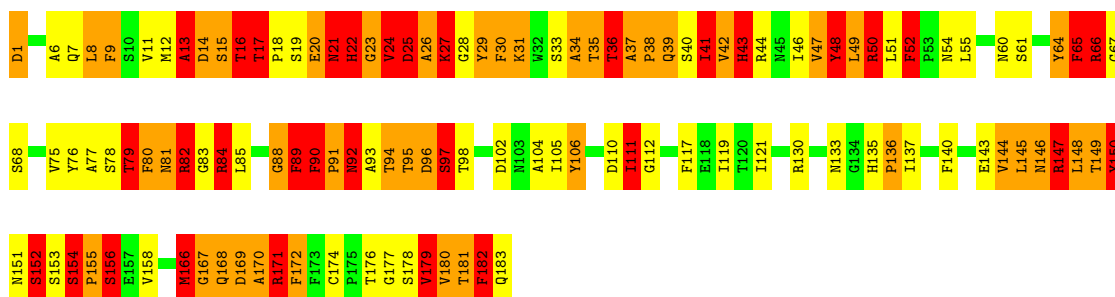
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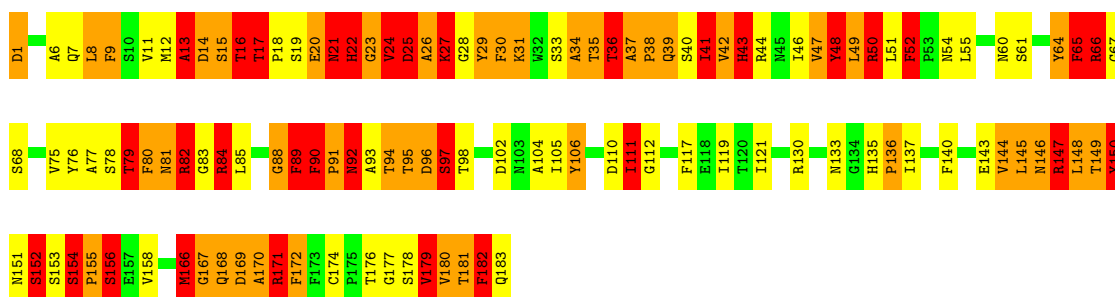
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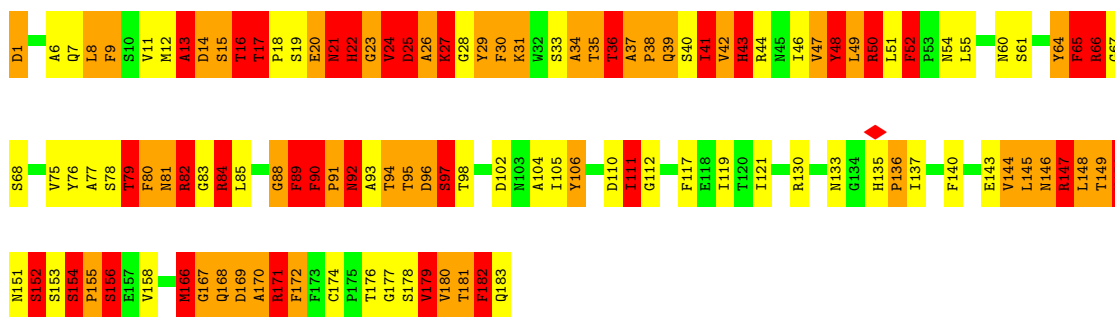
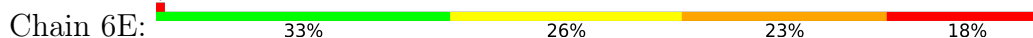
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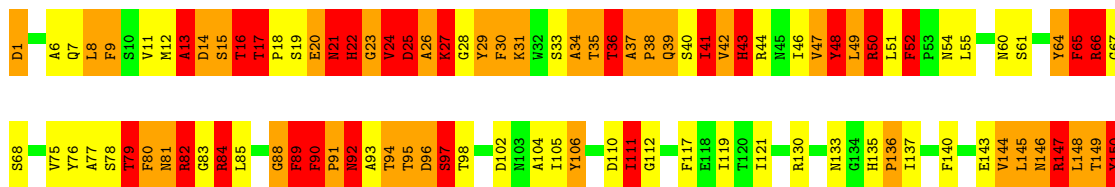
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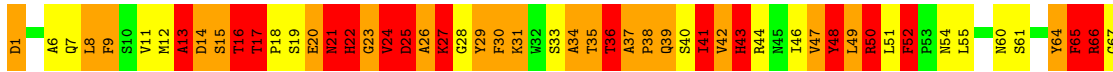


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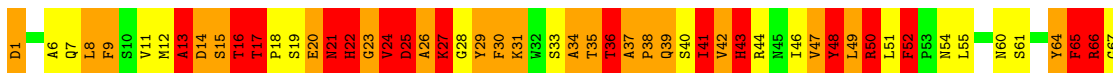
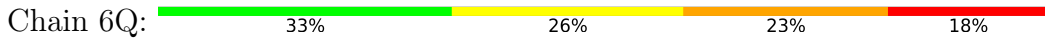




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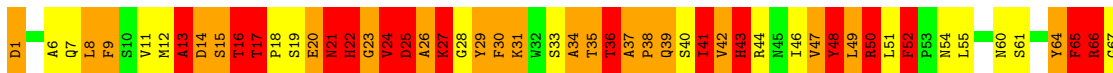
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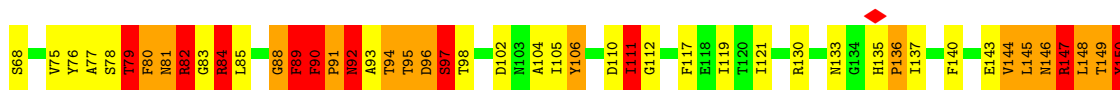


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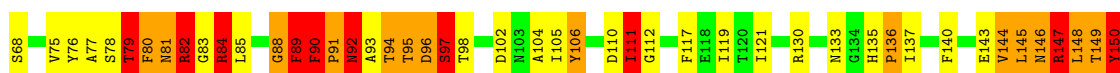


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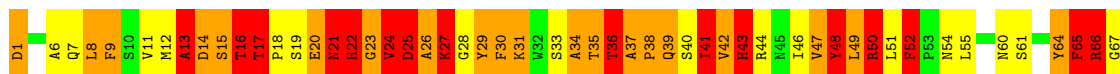
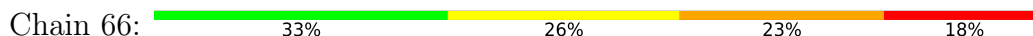




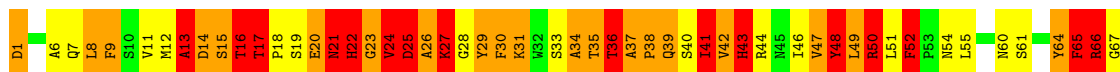
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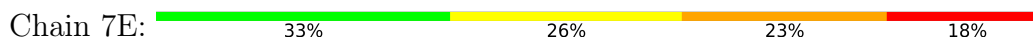
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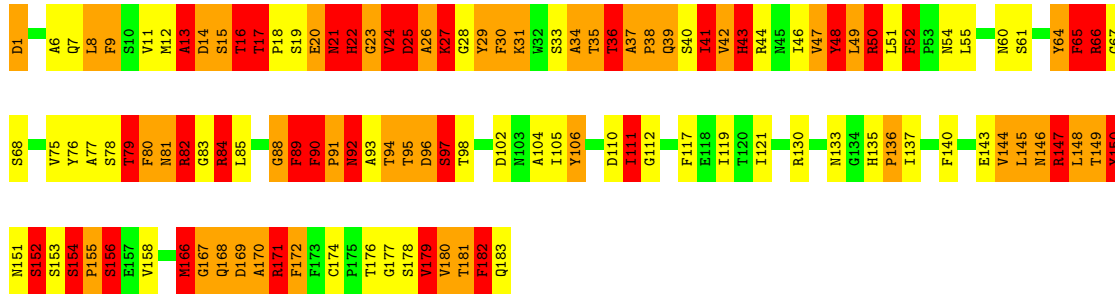


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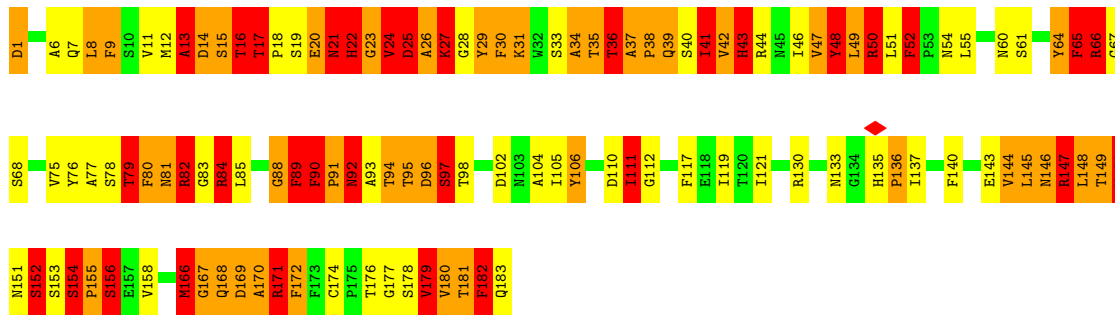
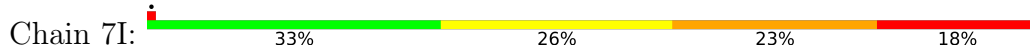


• Molecule 1: Capsid protein VP3

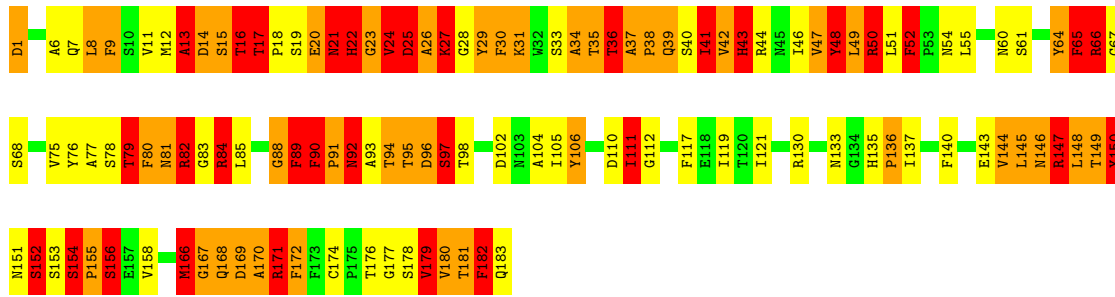
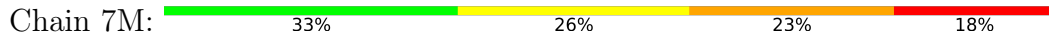




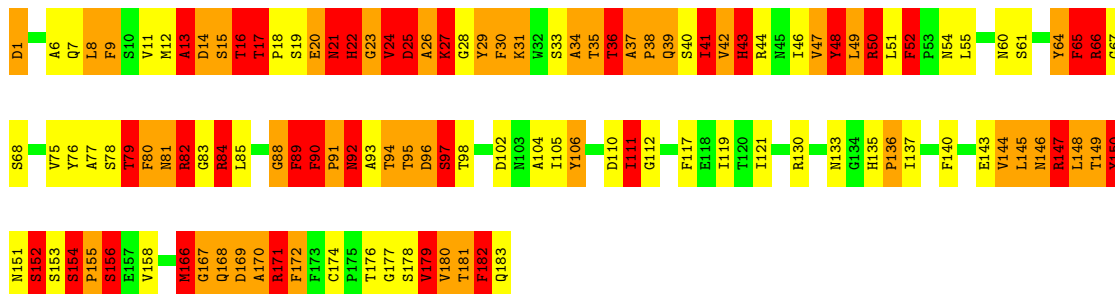
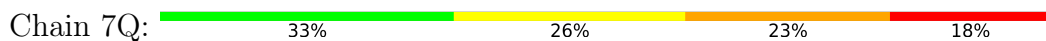
• Molecule 1: Capsid protein VP3



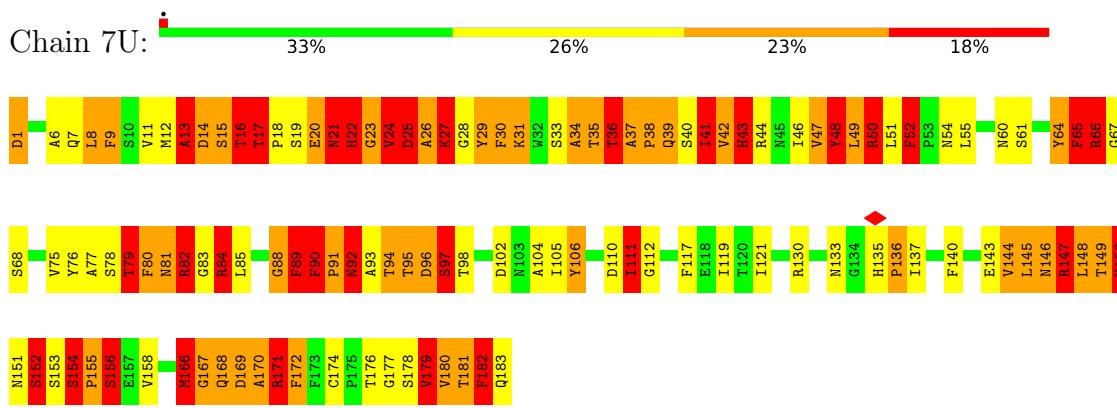
• Molecule 1: Capsid protein VP3



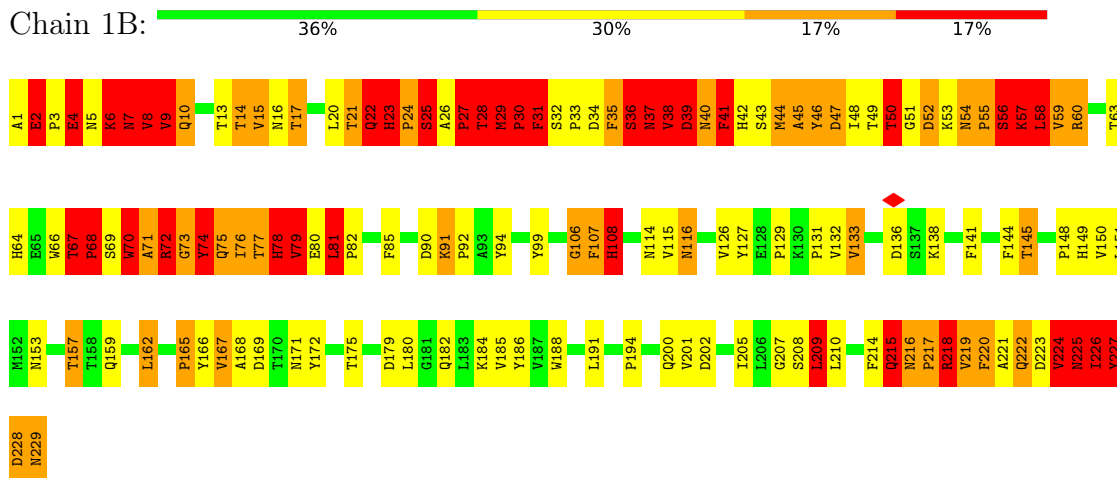
• Molecule 1: Capsid protein VP3



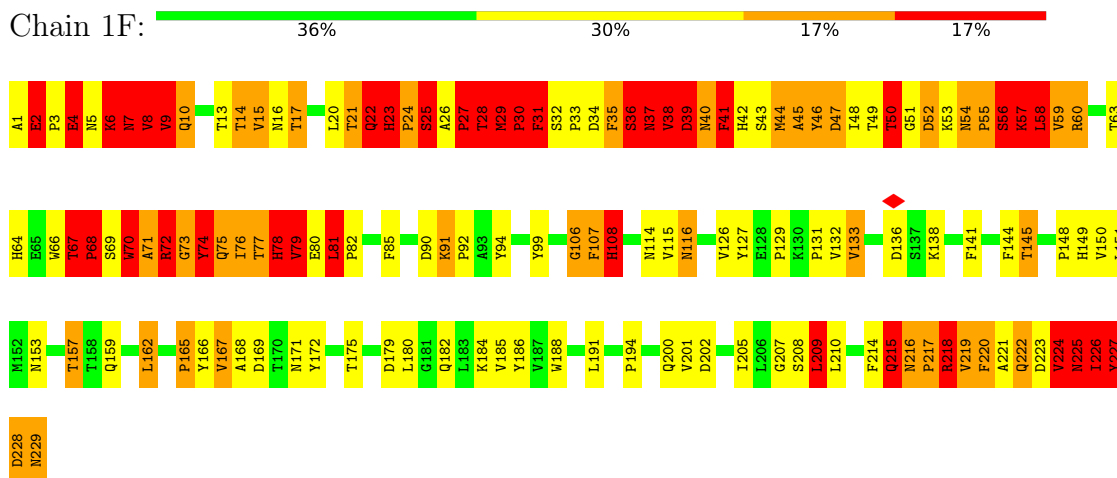
• Molecule 1: Capsid protein VP3



• Molecule 2: Capsid protein VP0

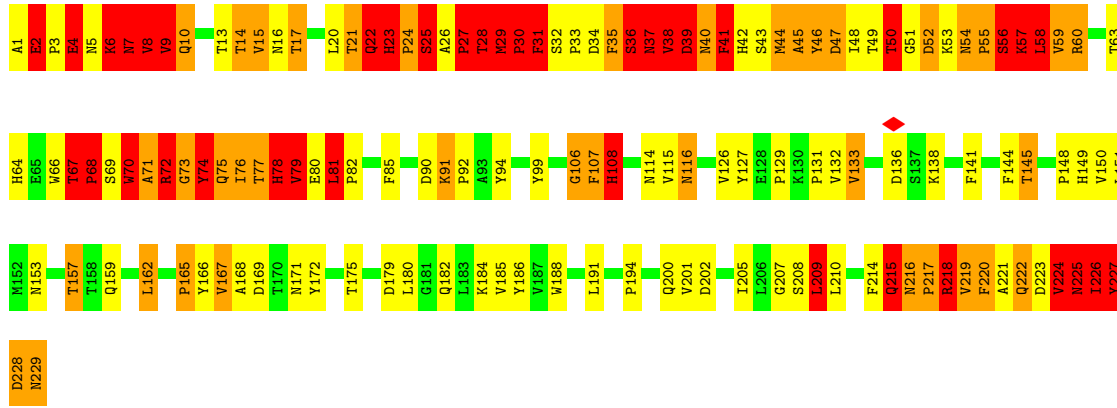


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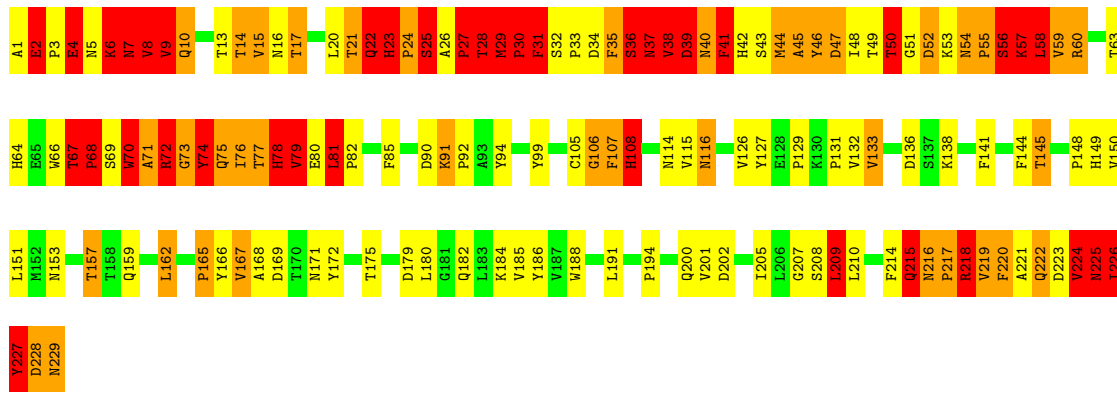
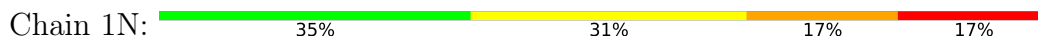


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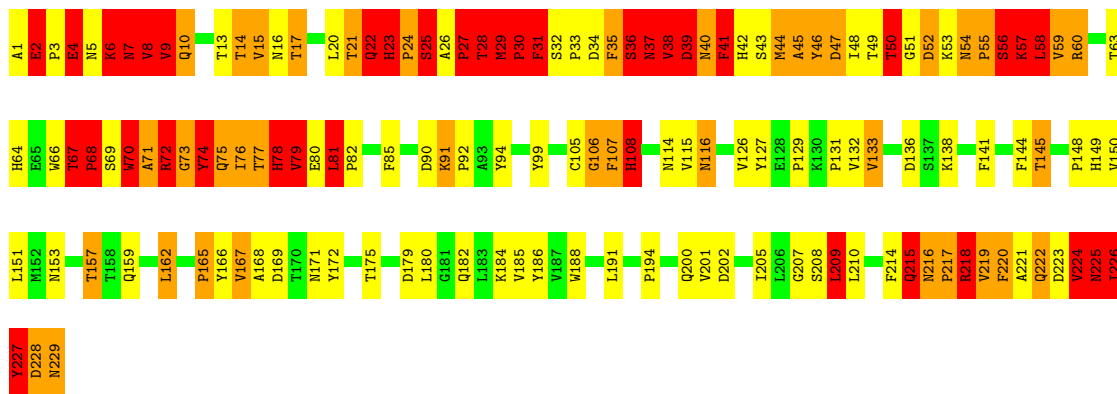
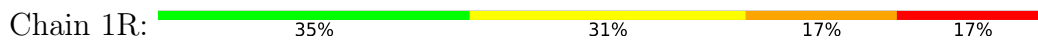




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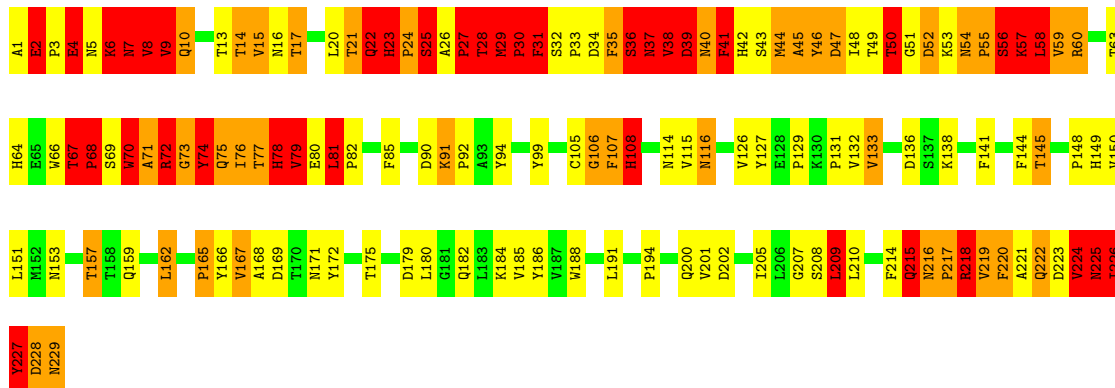


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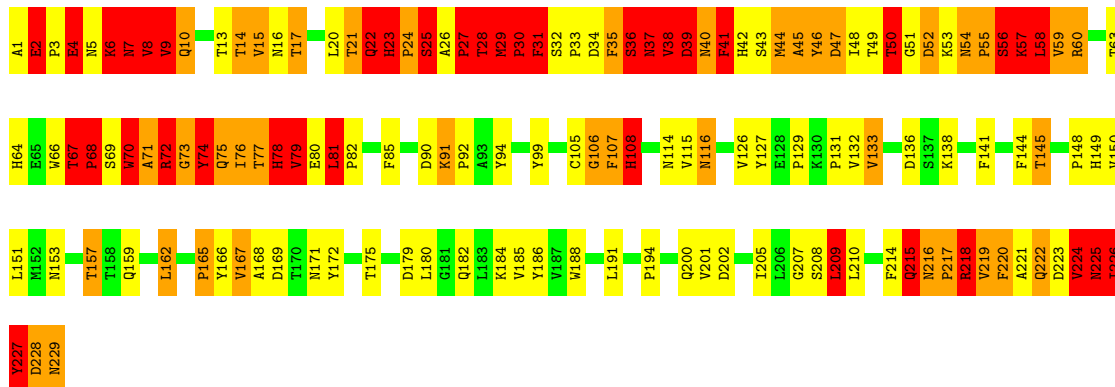


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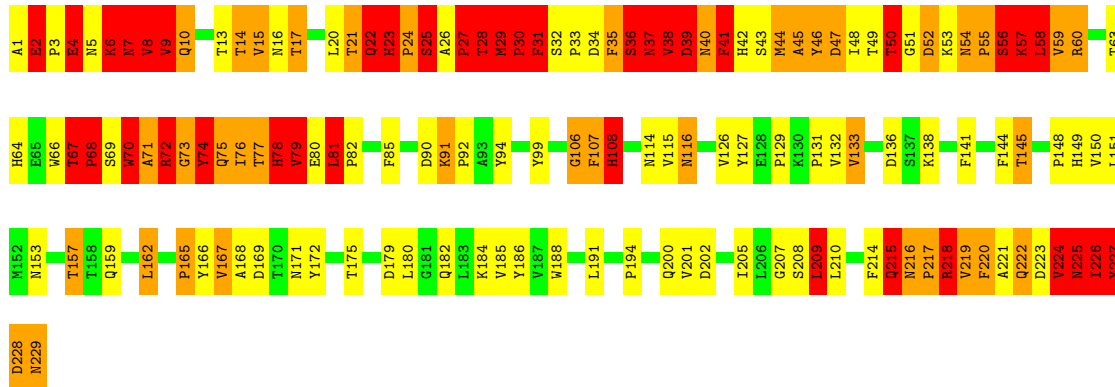




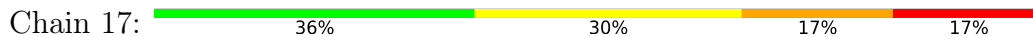
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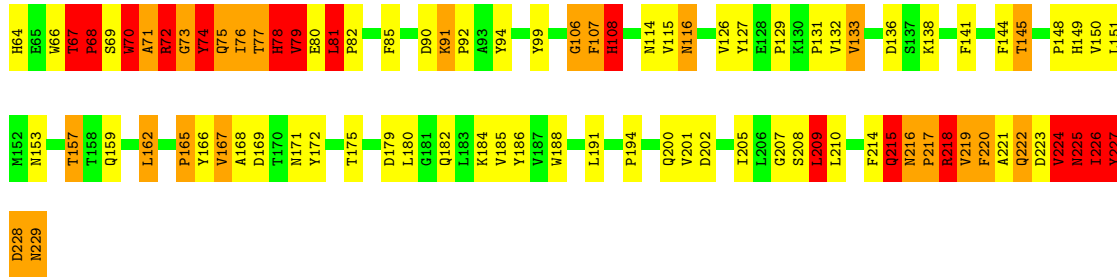


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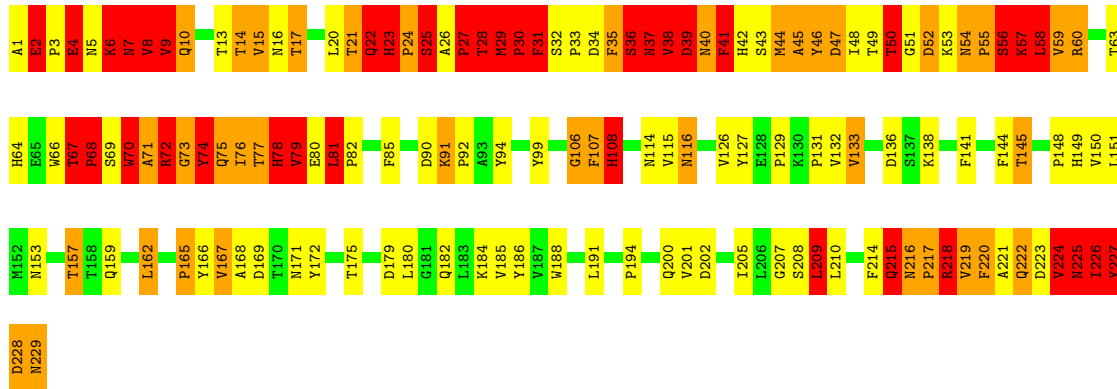
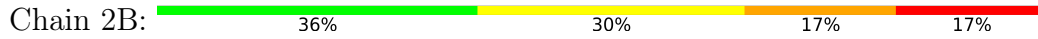


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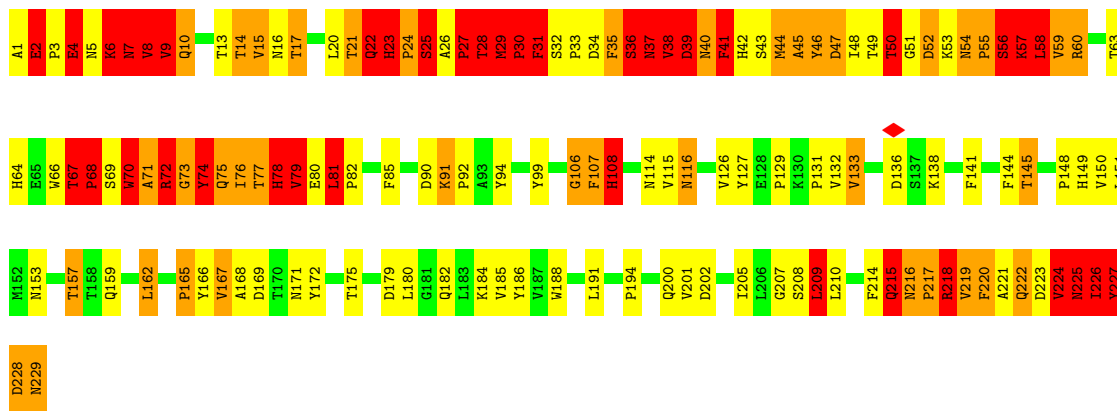
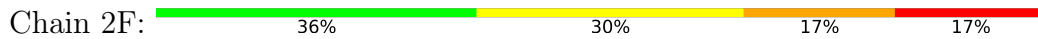




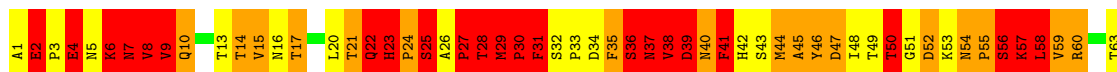
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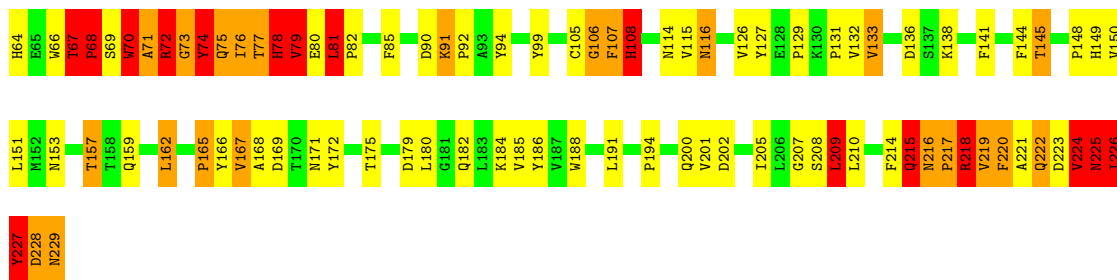


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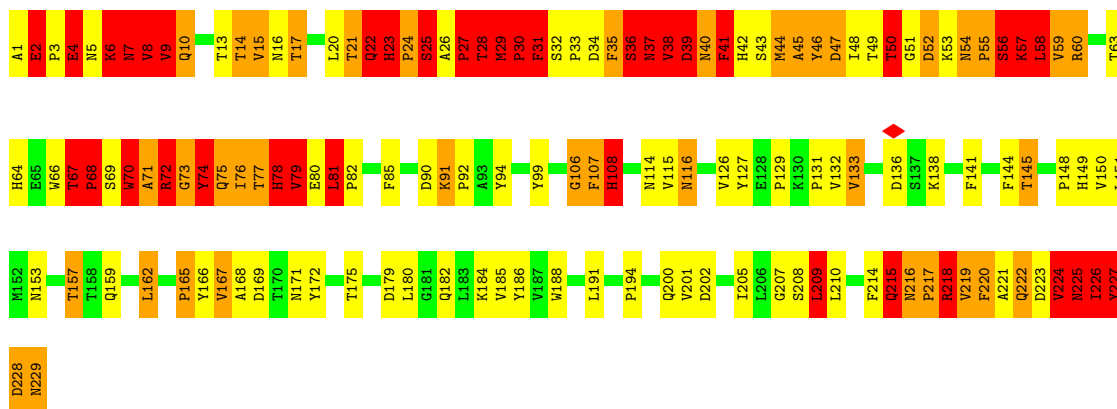
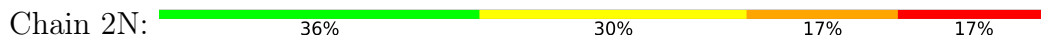


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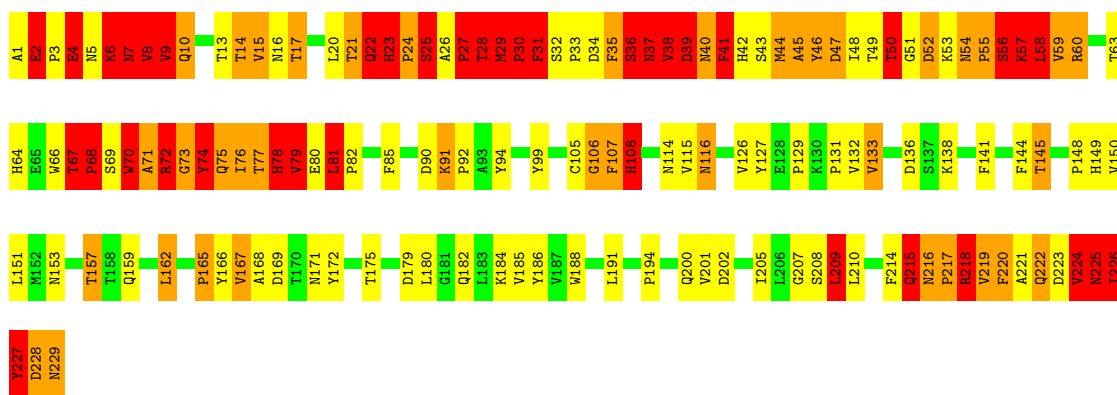




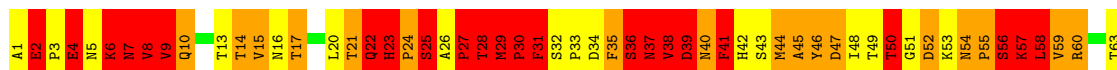
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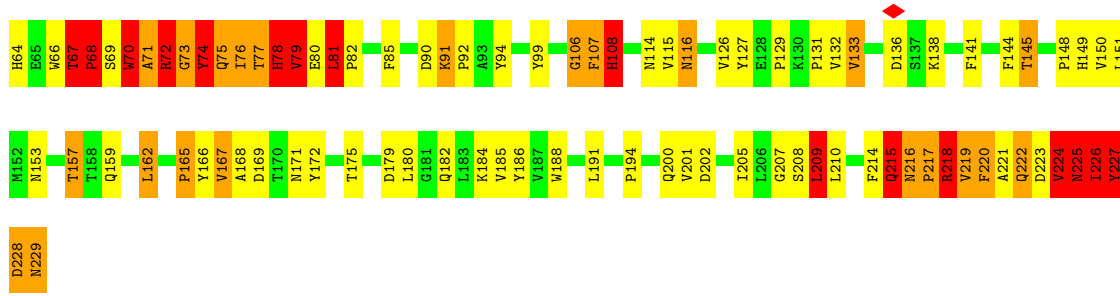


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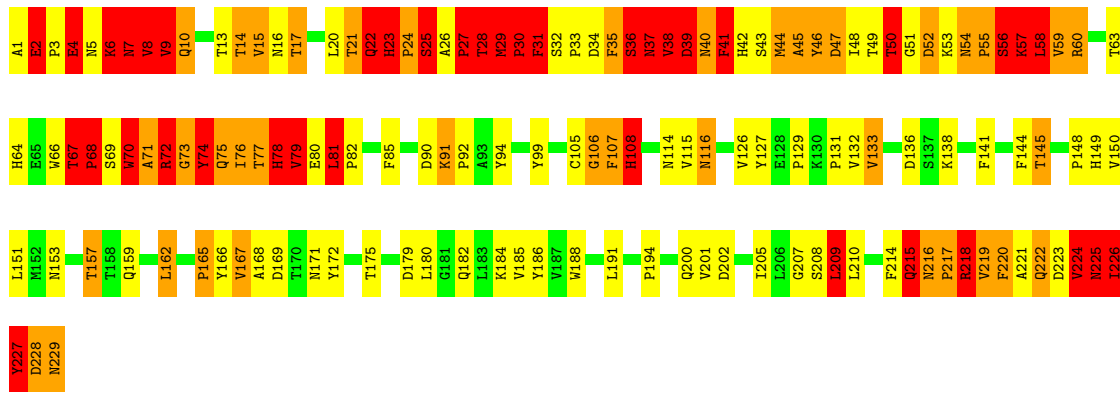


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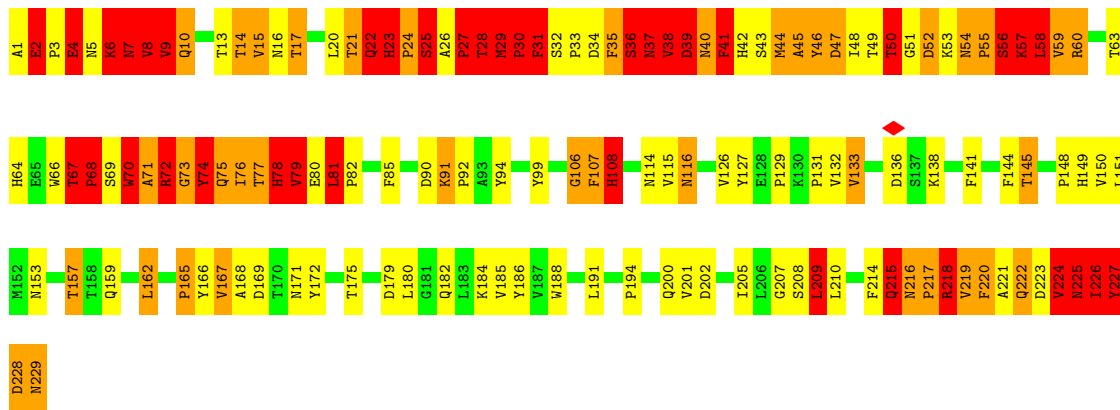




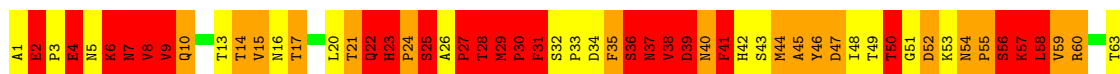
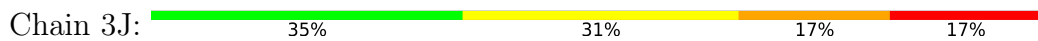
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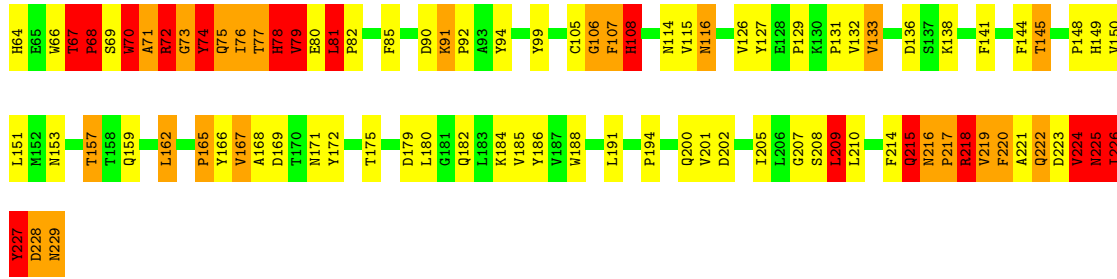


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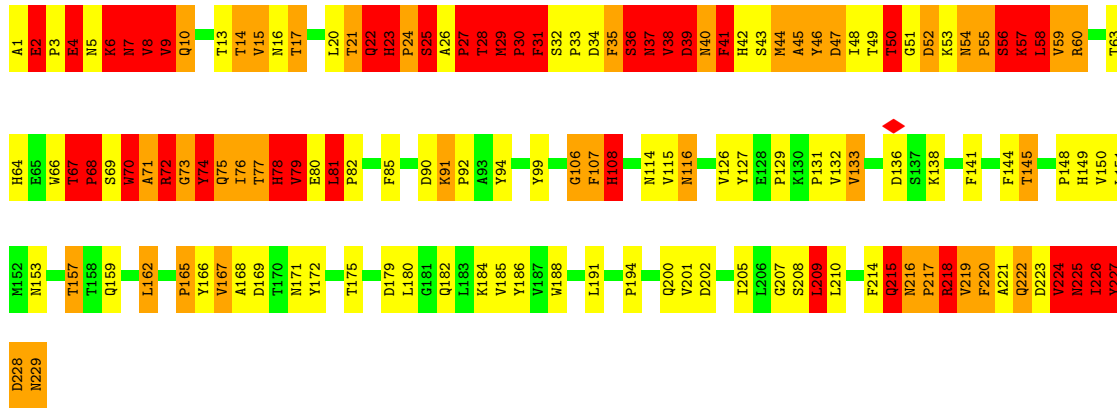
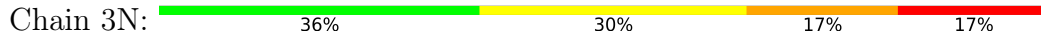


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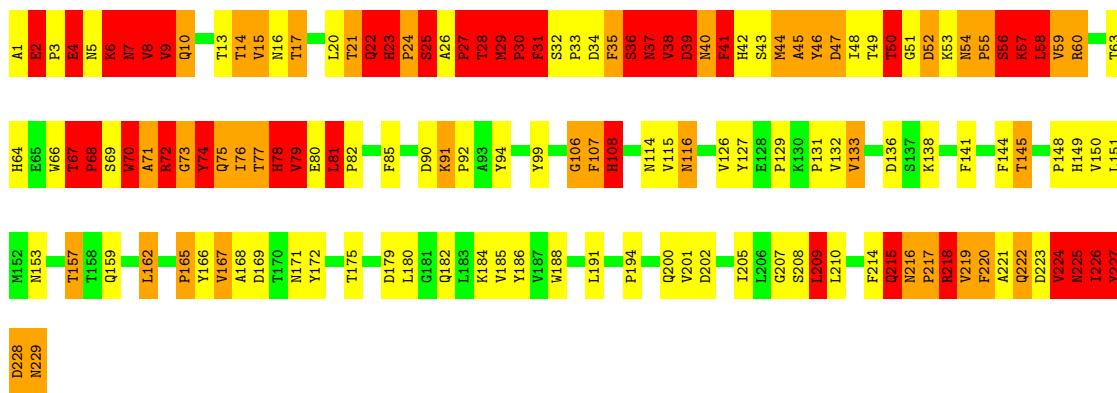




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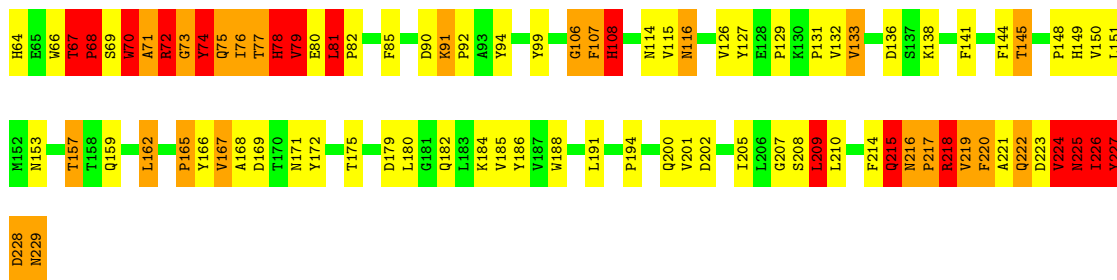


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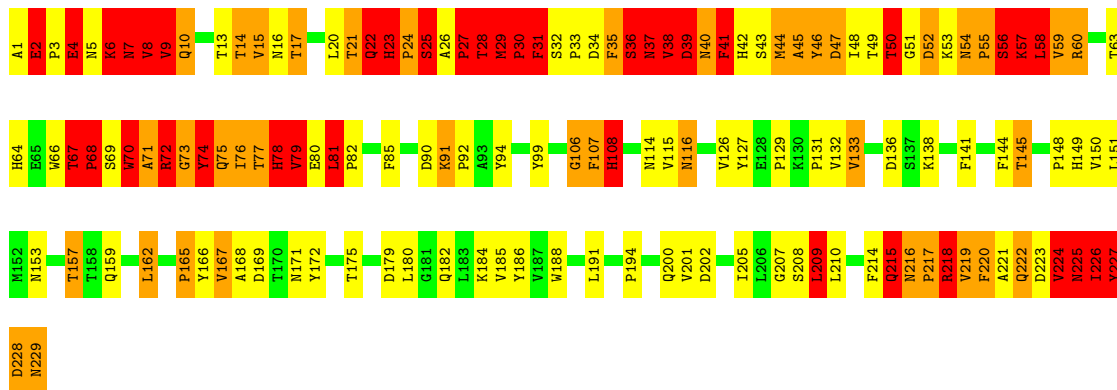
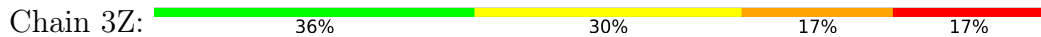


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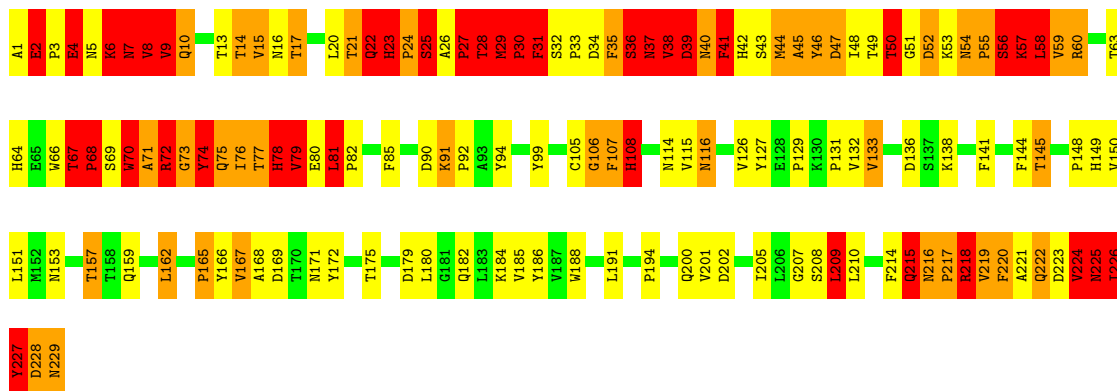
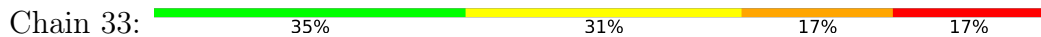




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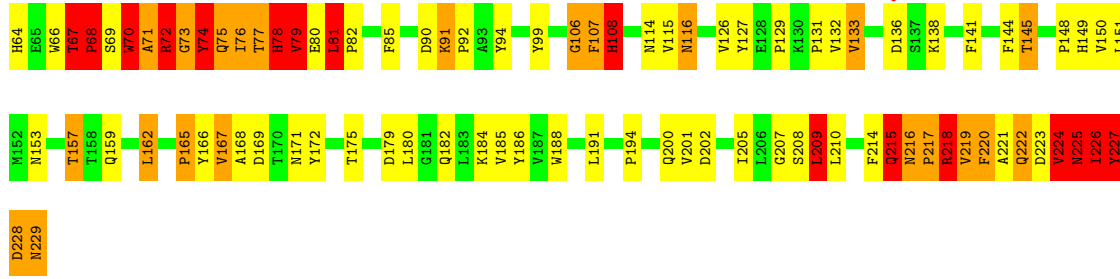


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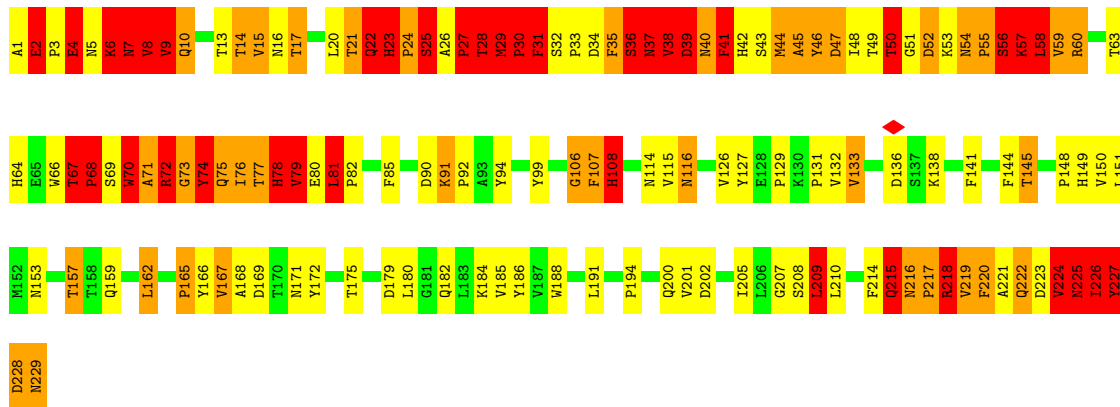


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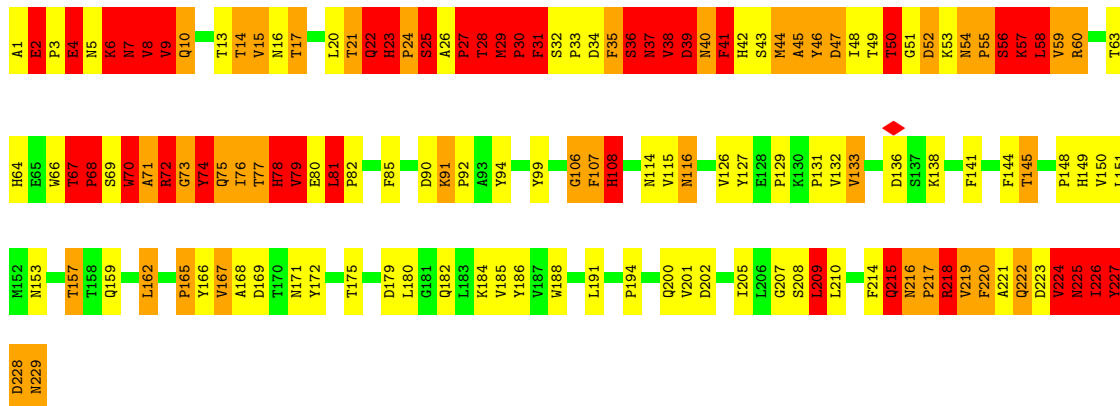




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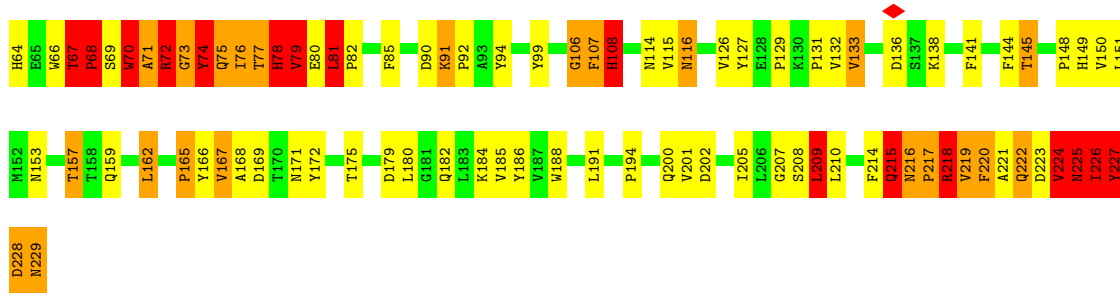


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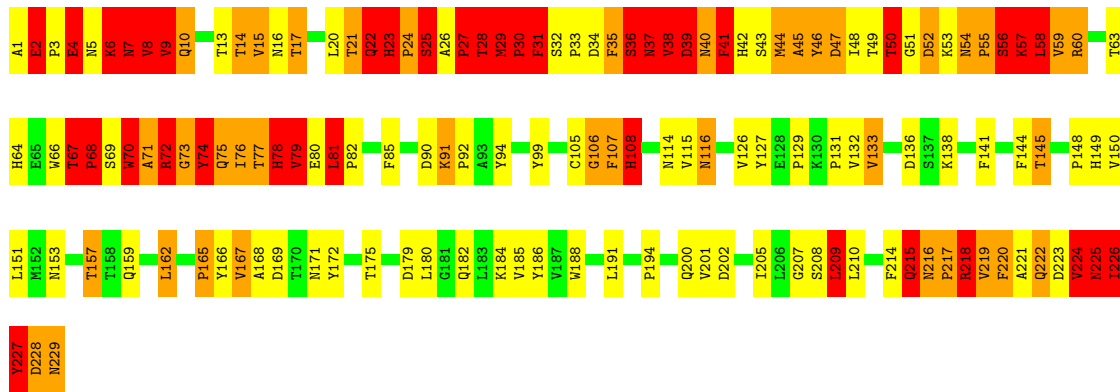


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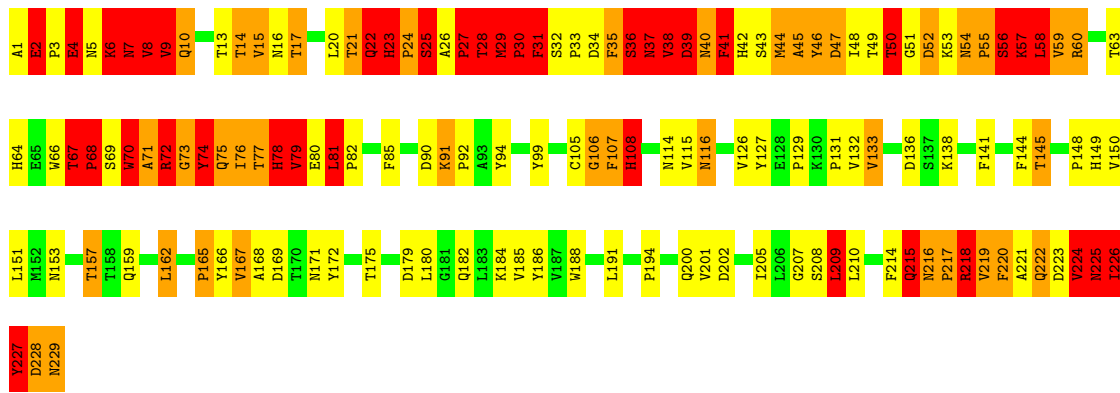




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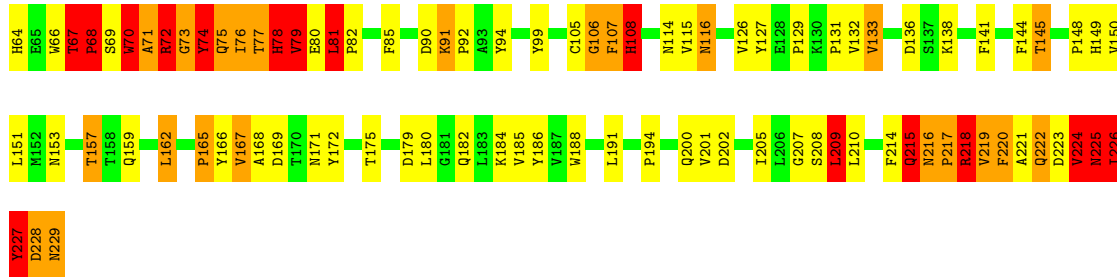


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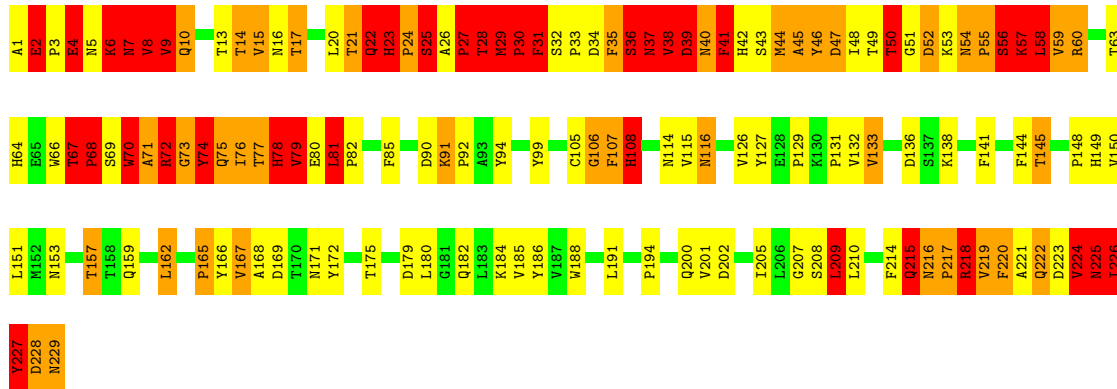
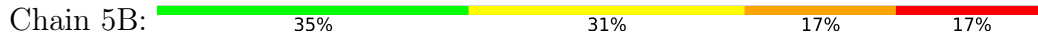


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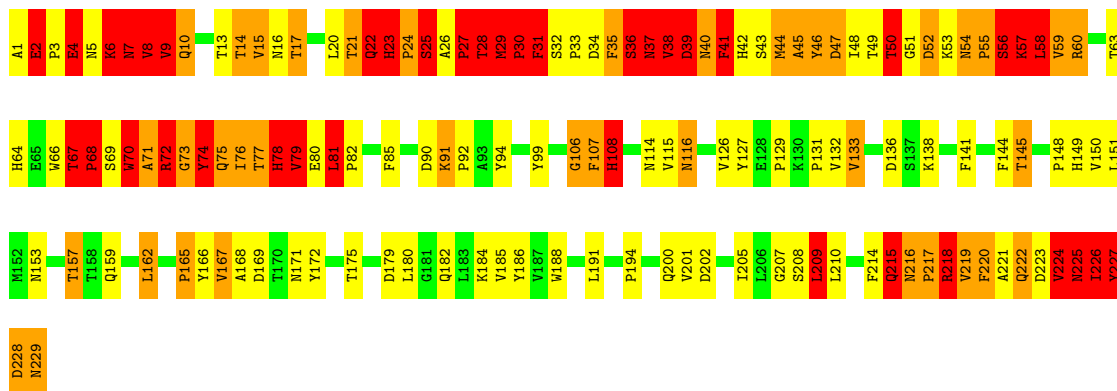
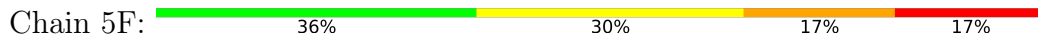




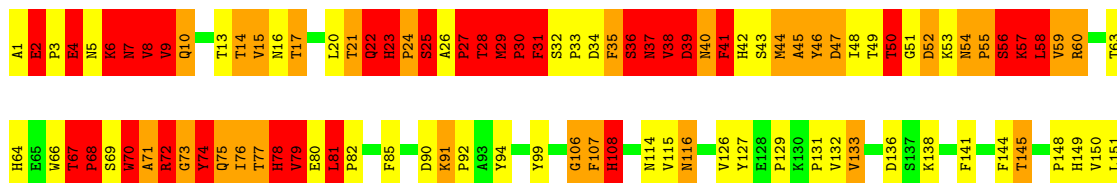
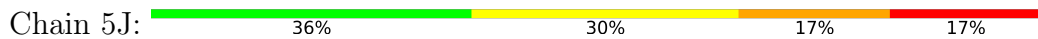
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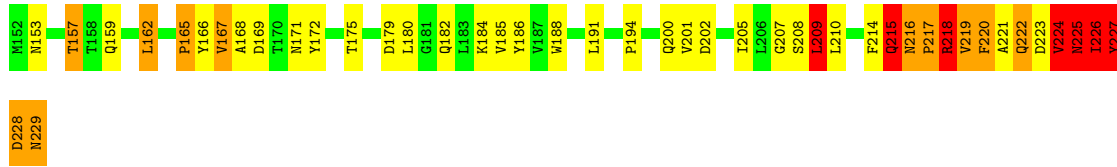


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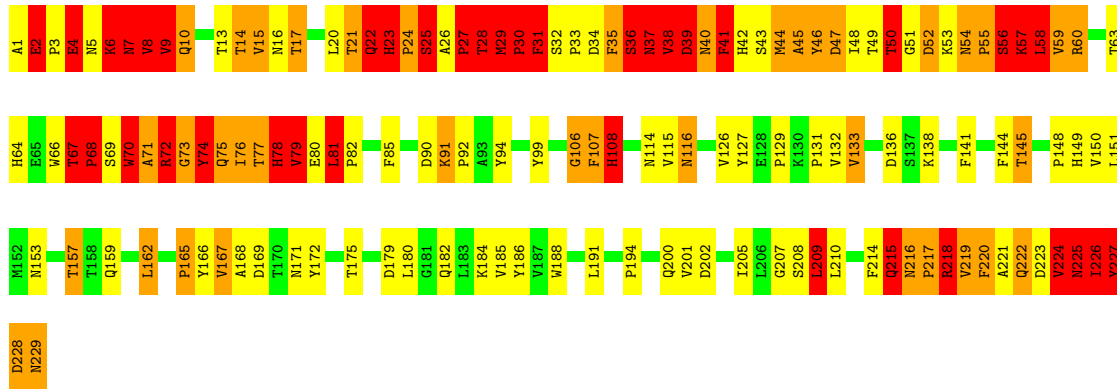
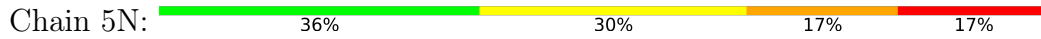


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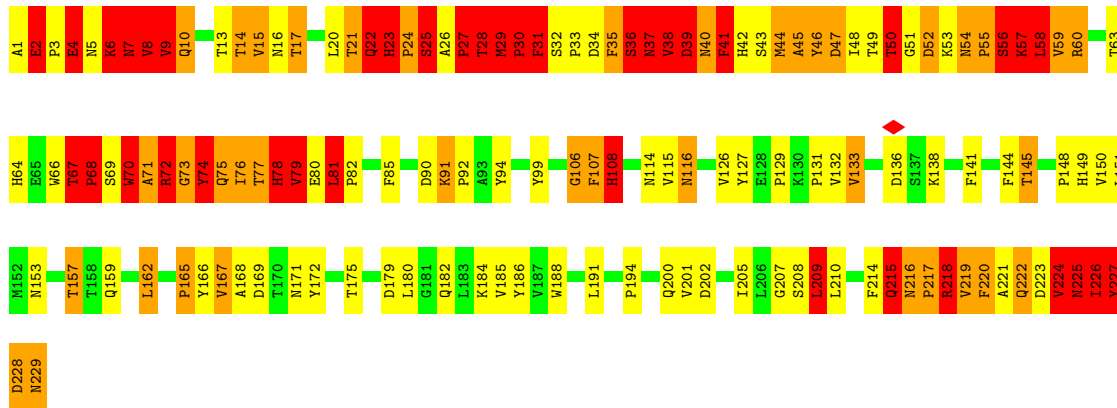




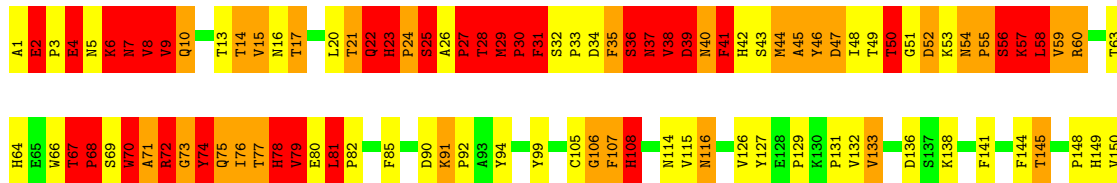
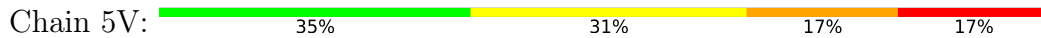
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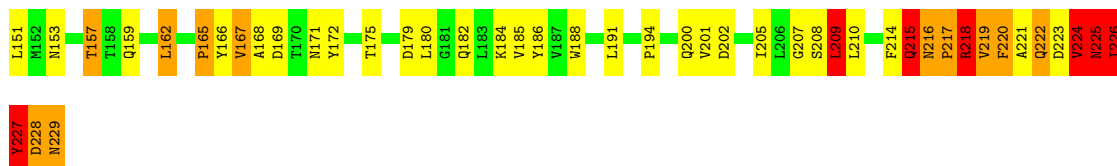


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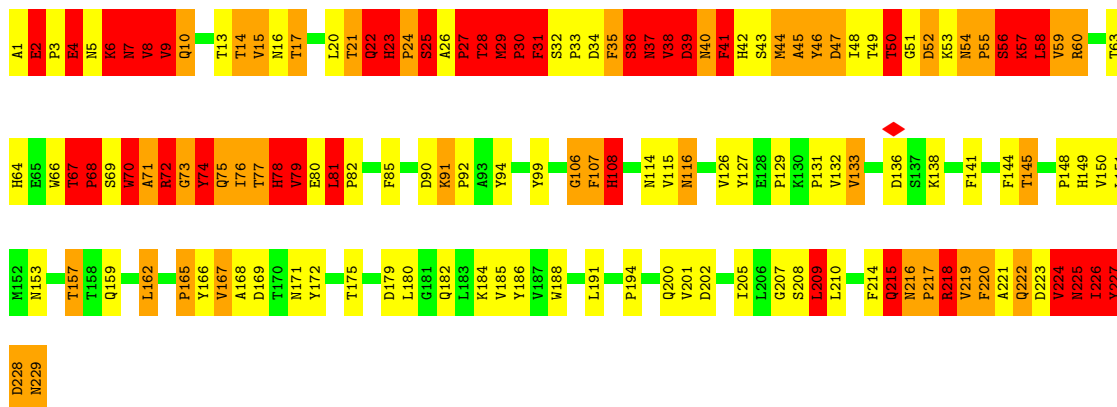


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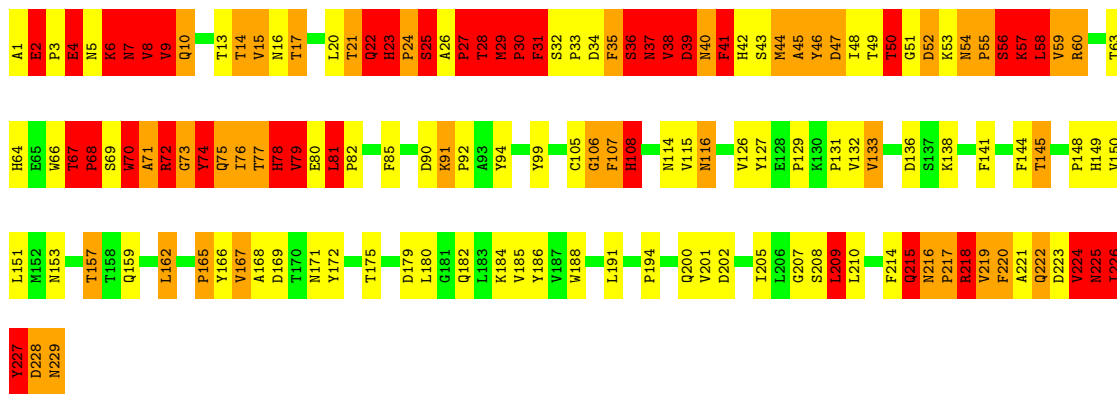




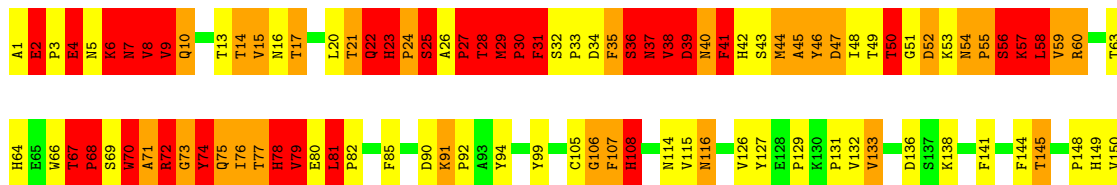
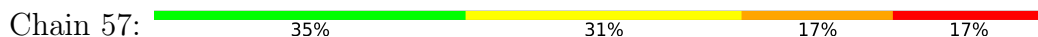
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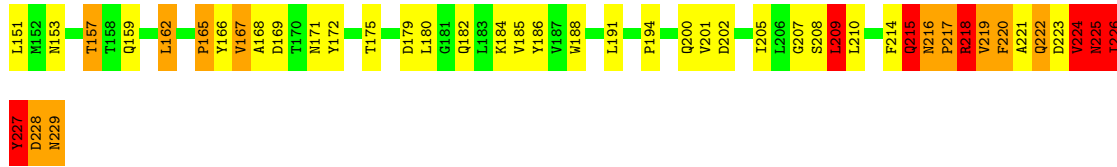


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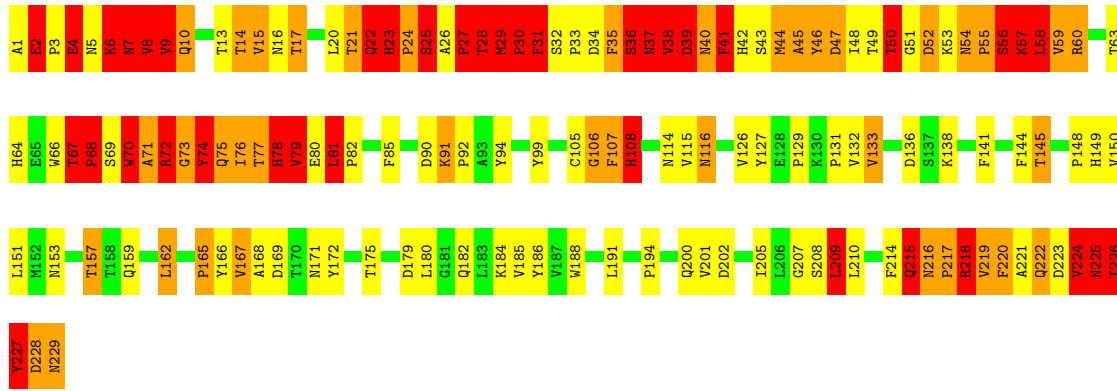
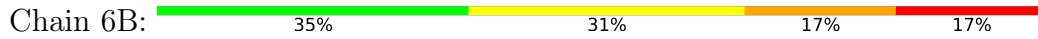


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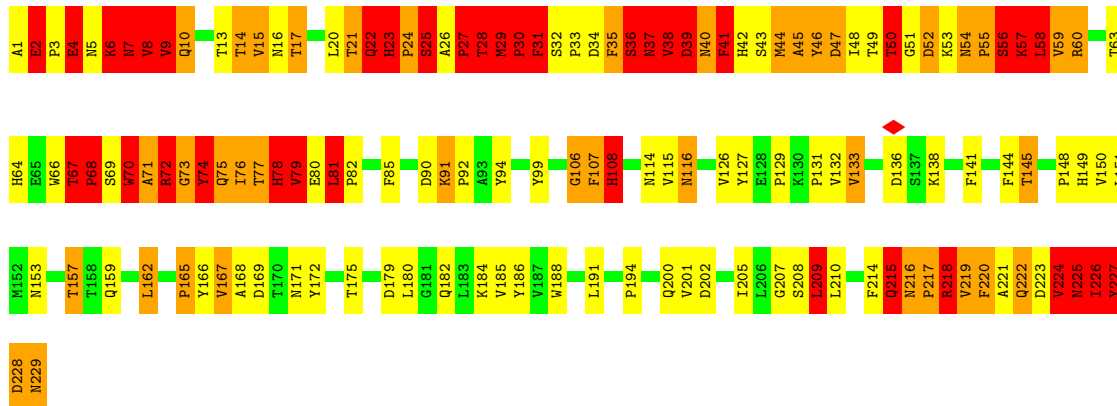




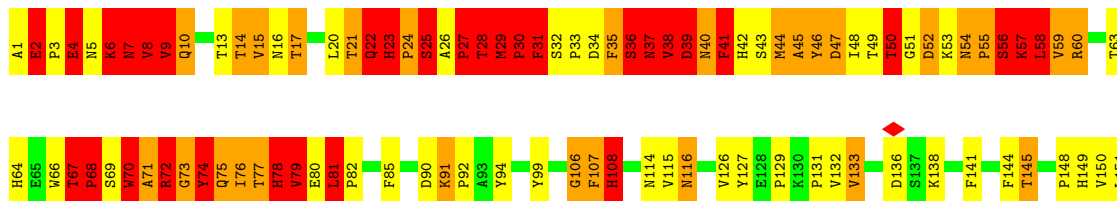
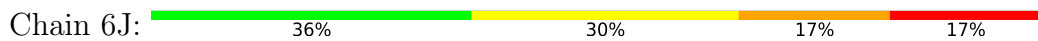
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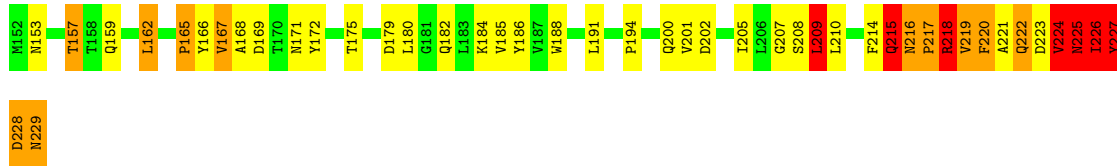


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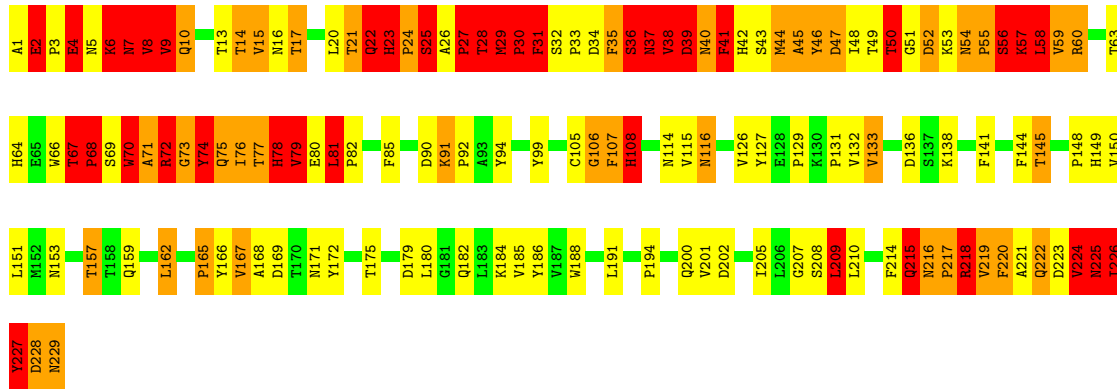
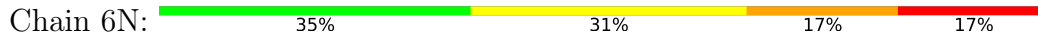


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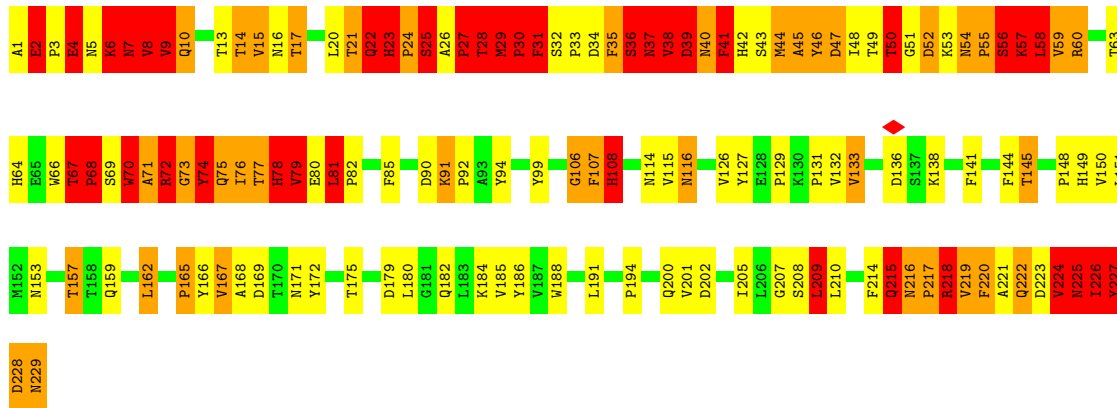




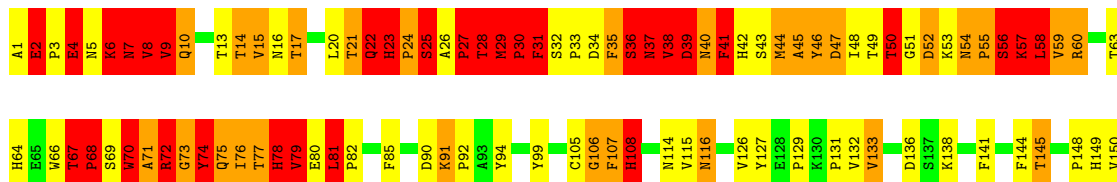
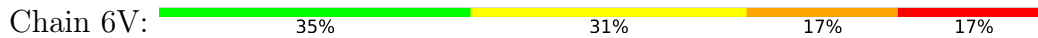
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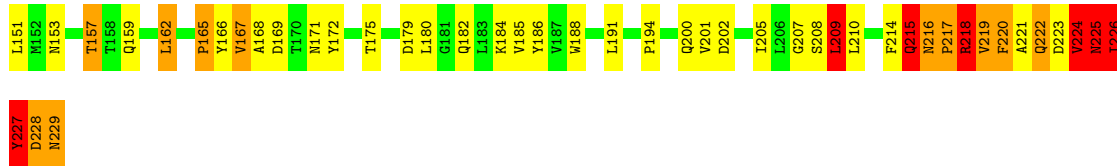


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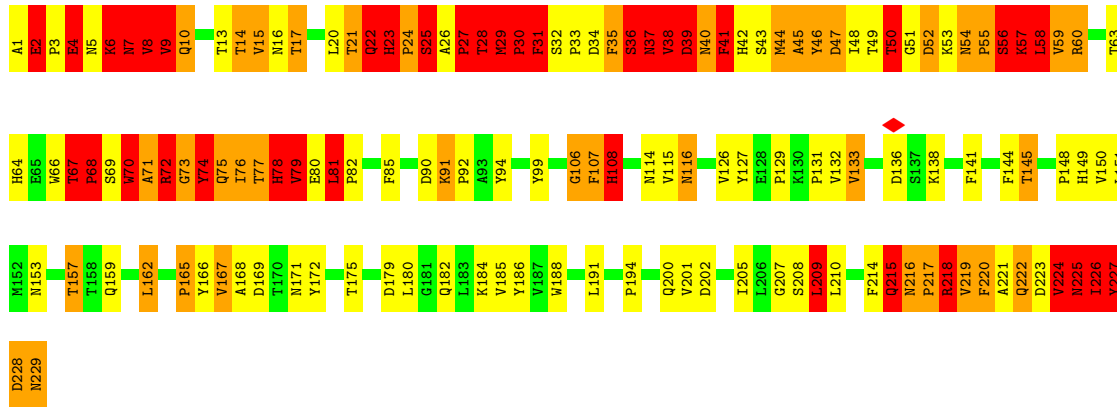
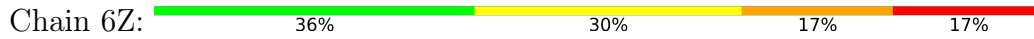


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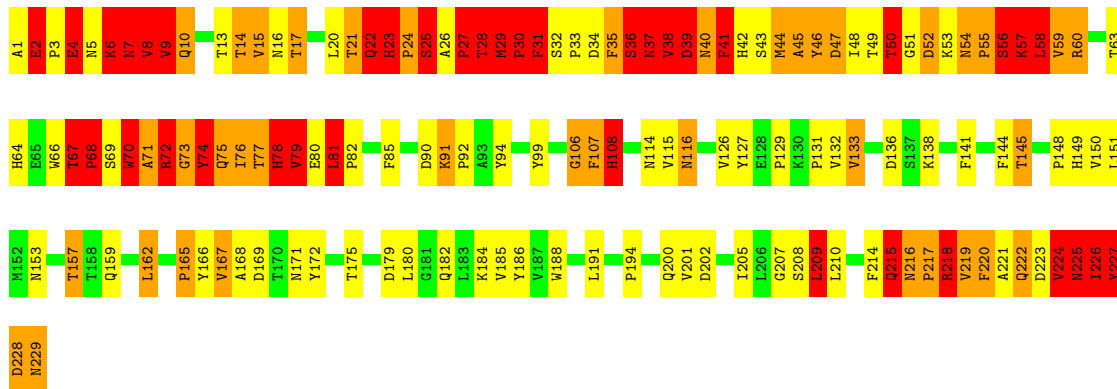
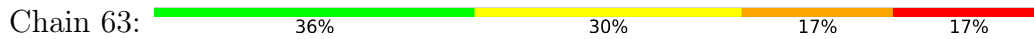




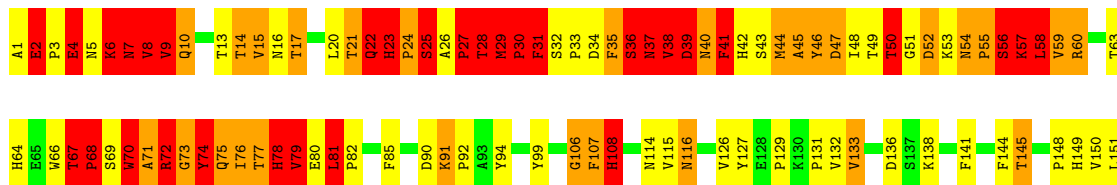
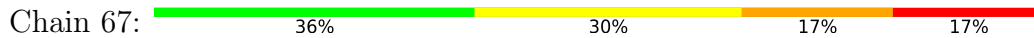
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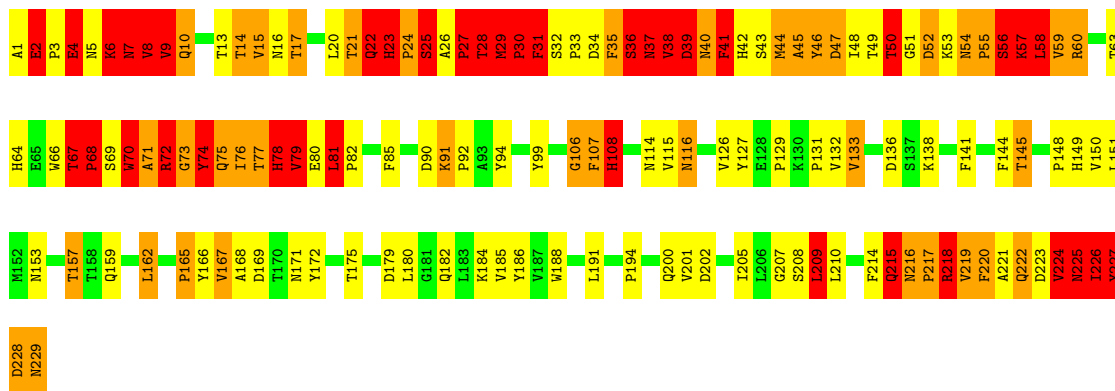


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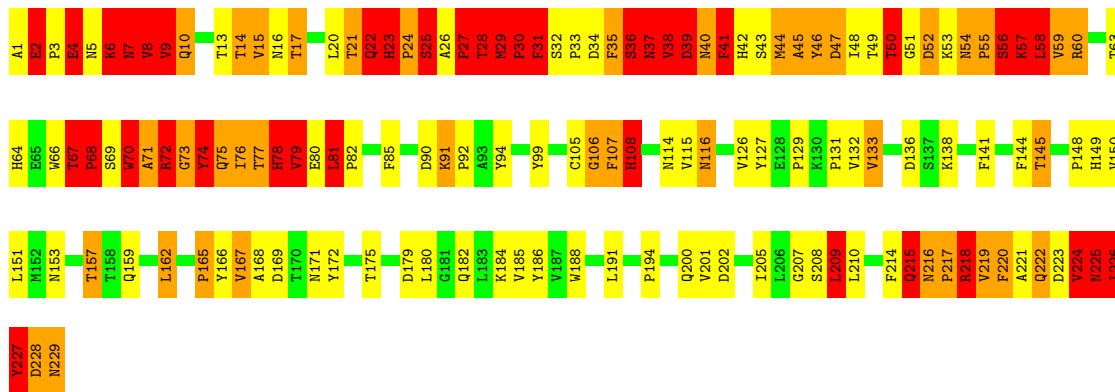




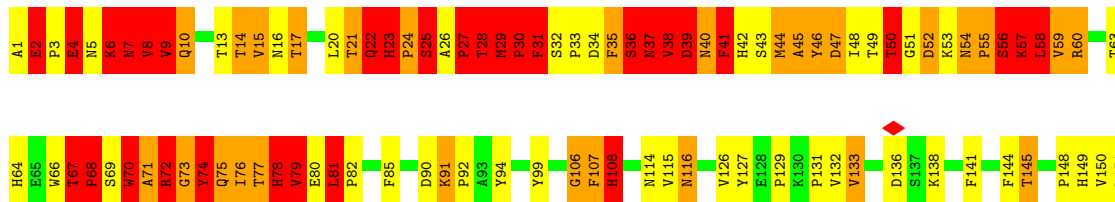
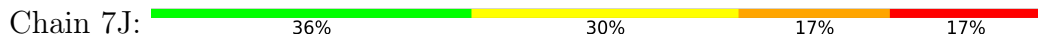
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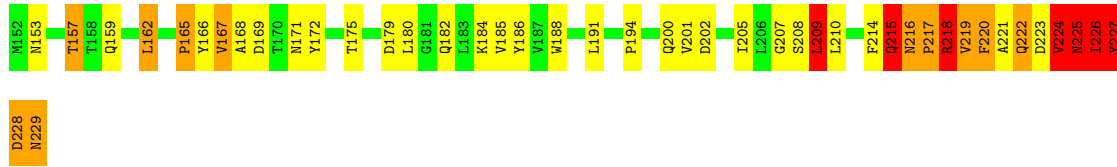


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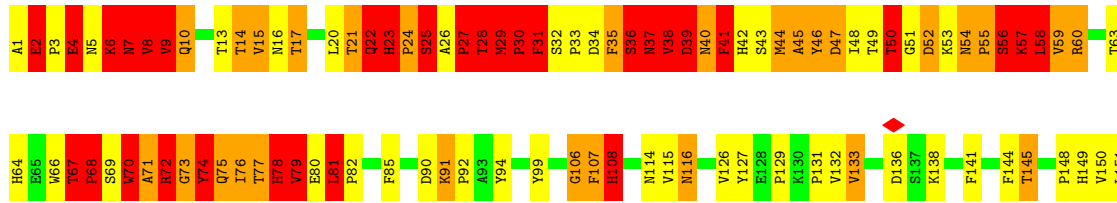
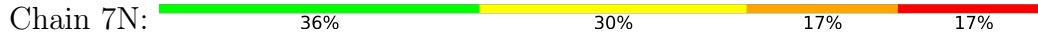


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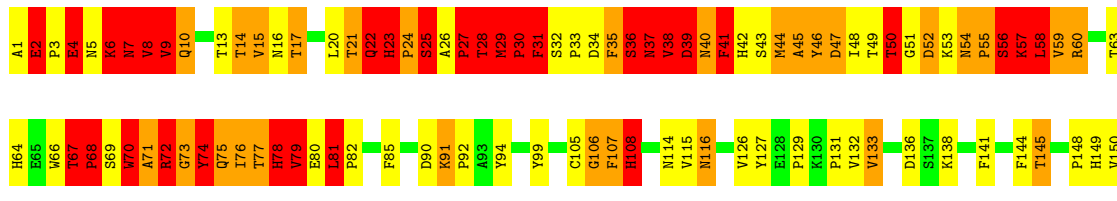
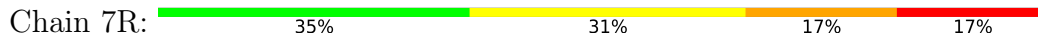




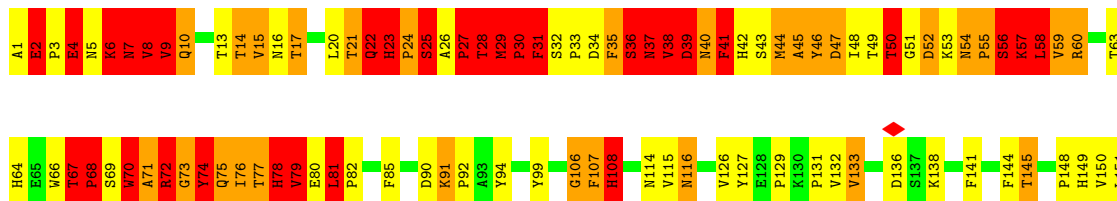
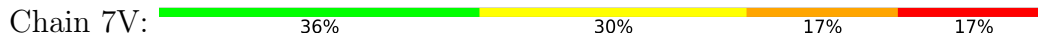
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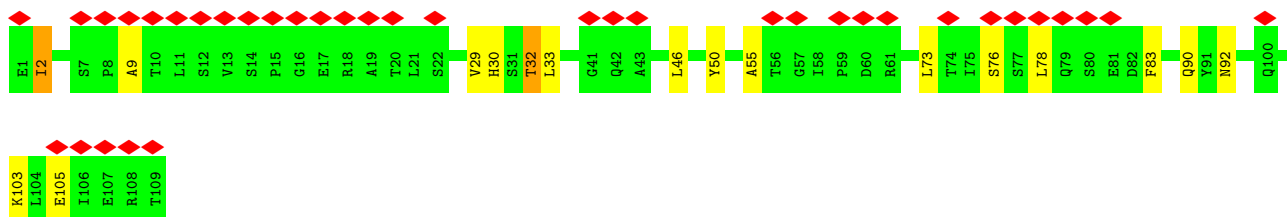
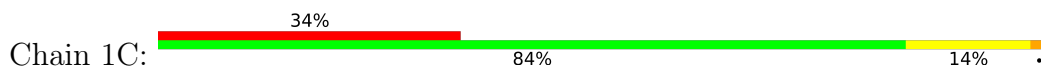


• Molecule 2: Capsid protein VP0

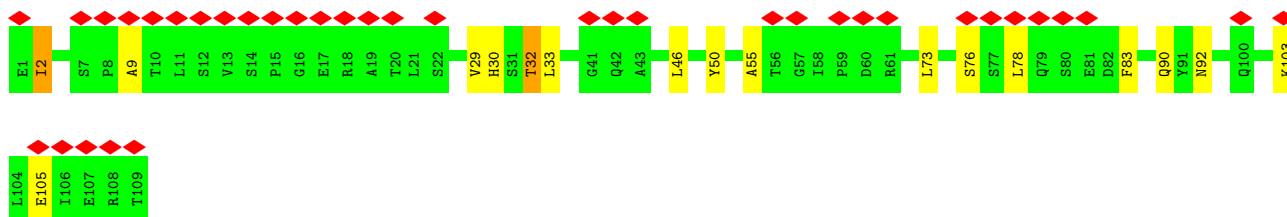
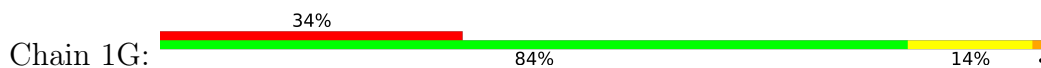




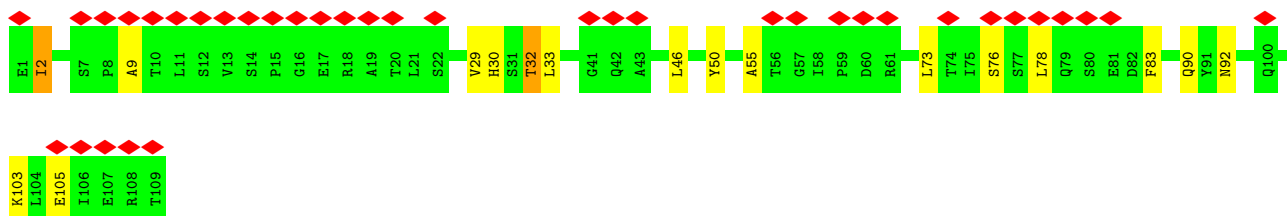
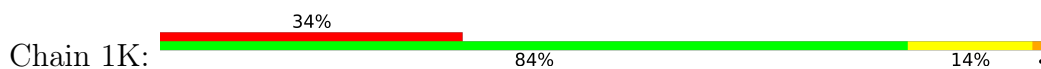
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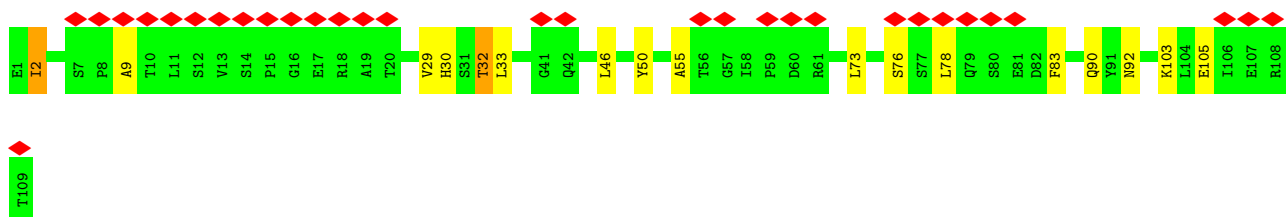
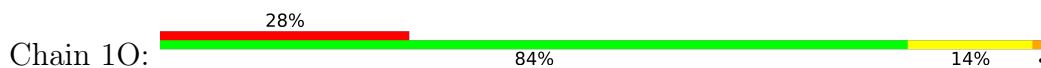
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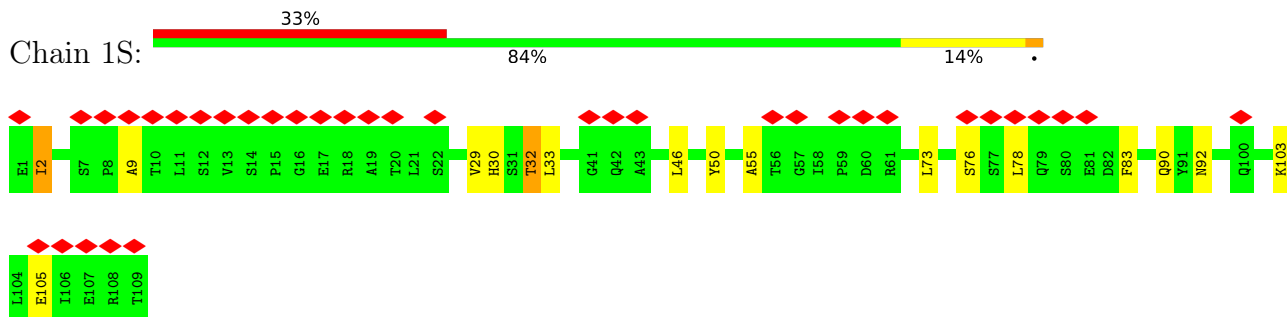
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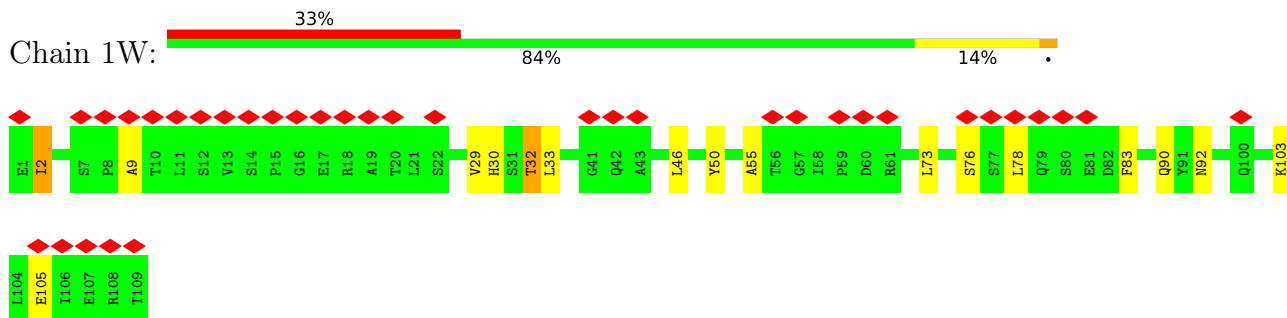
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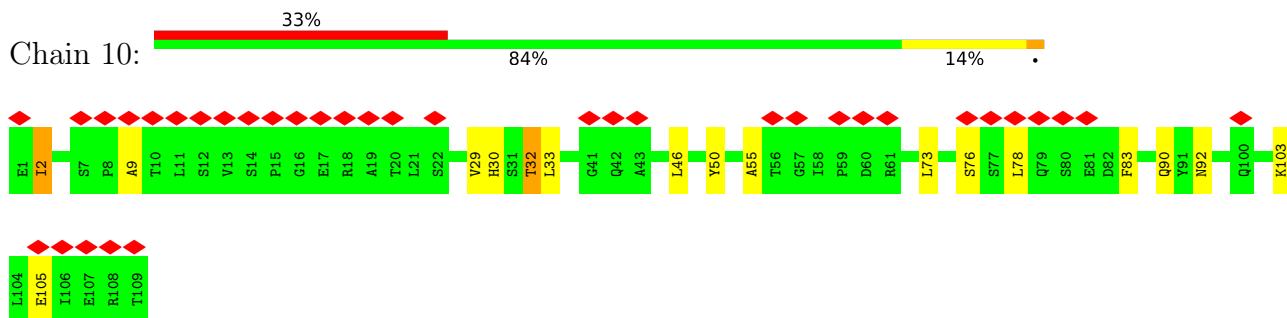
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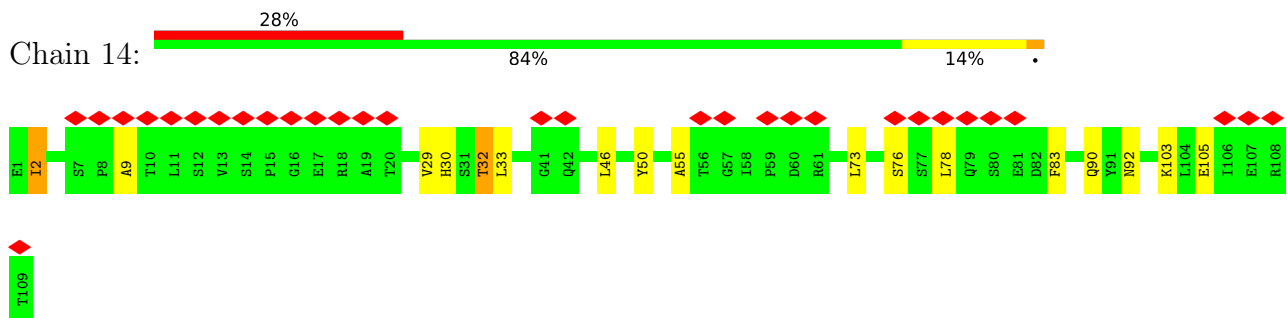
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• Molecule 3: HUMAN MONOCLONAL ANTIBODY

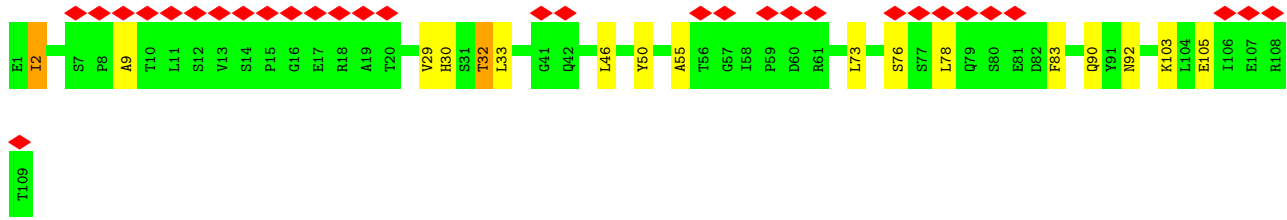


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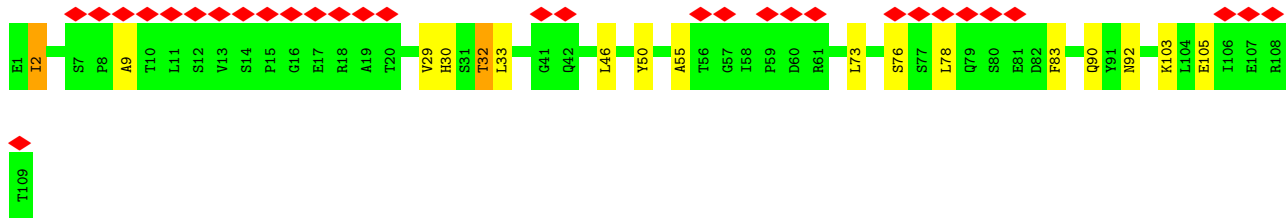
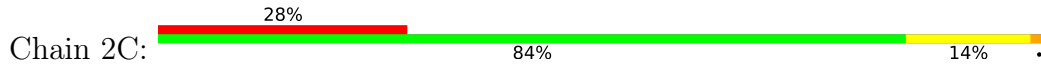


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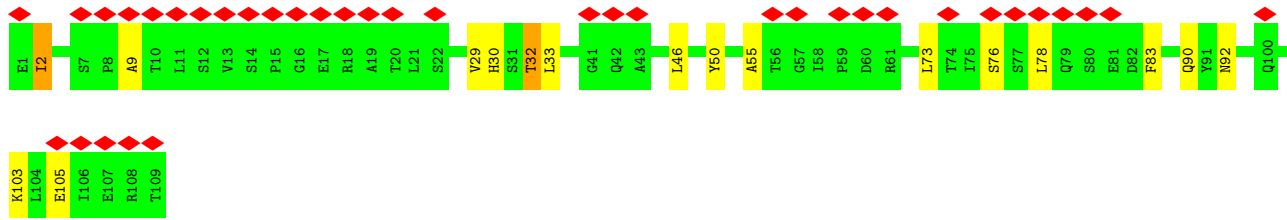
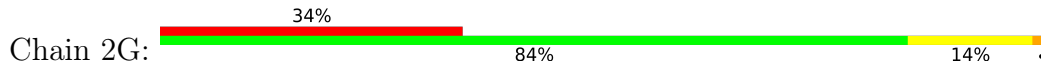




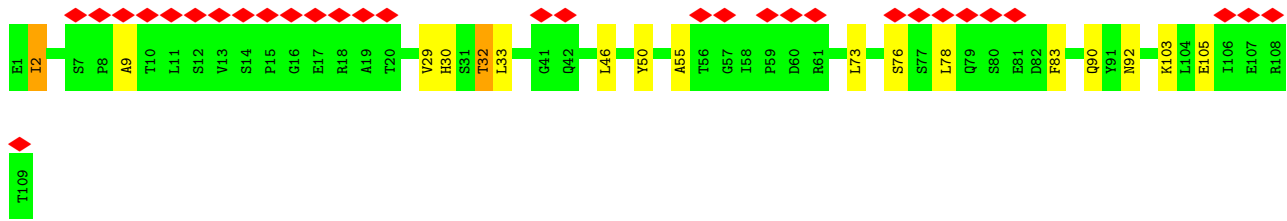
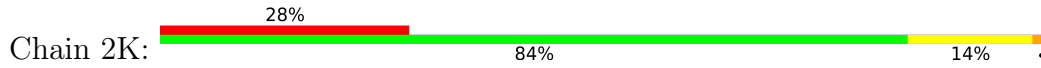
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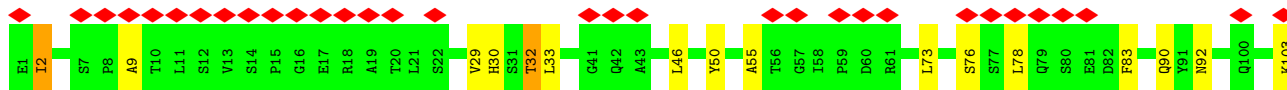
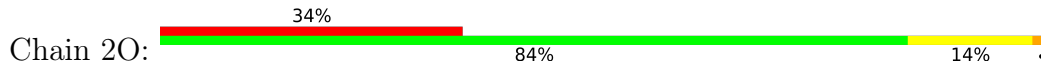
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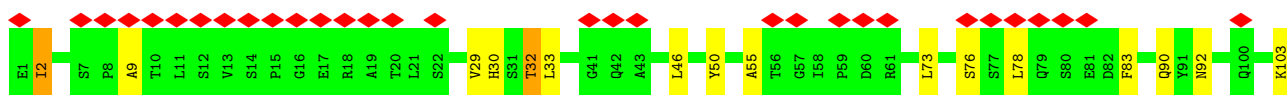
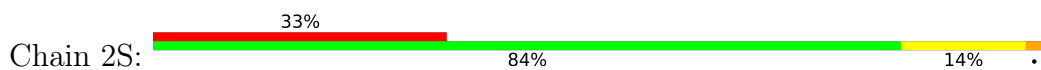


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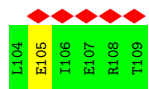
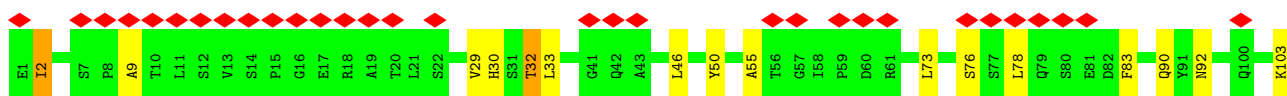
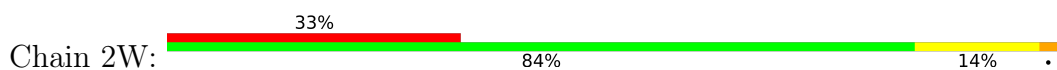




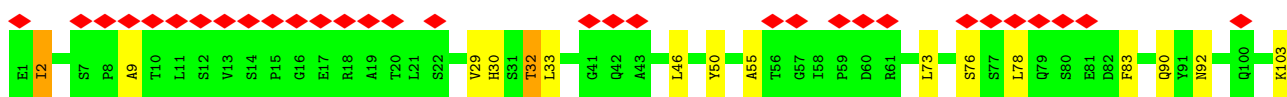
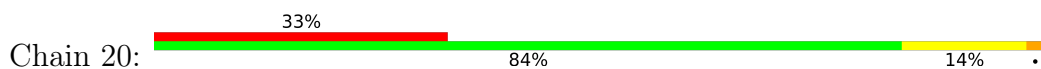
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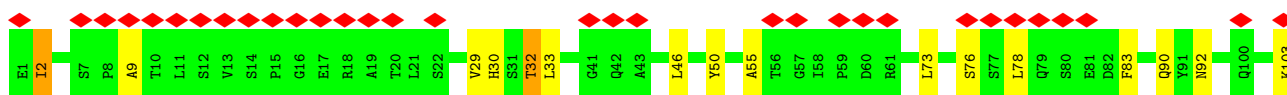
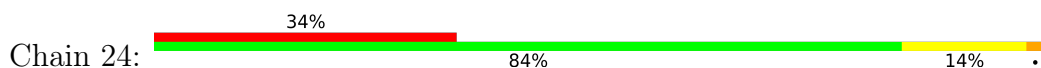
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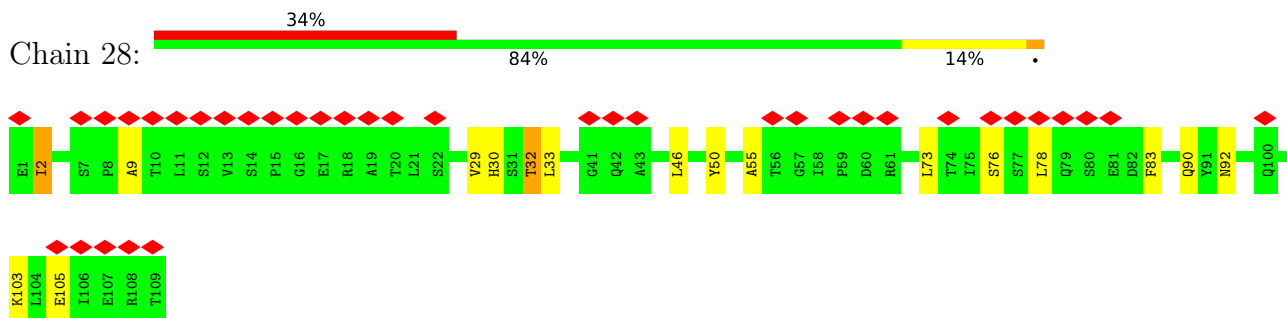
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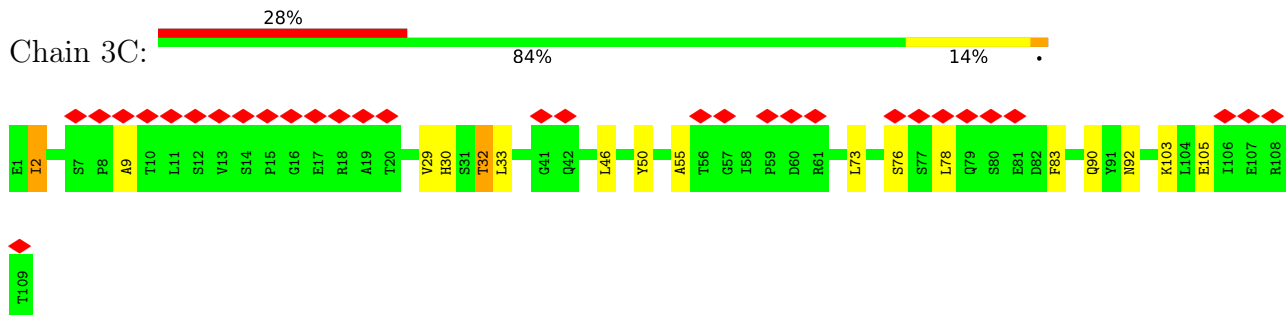
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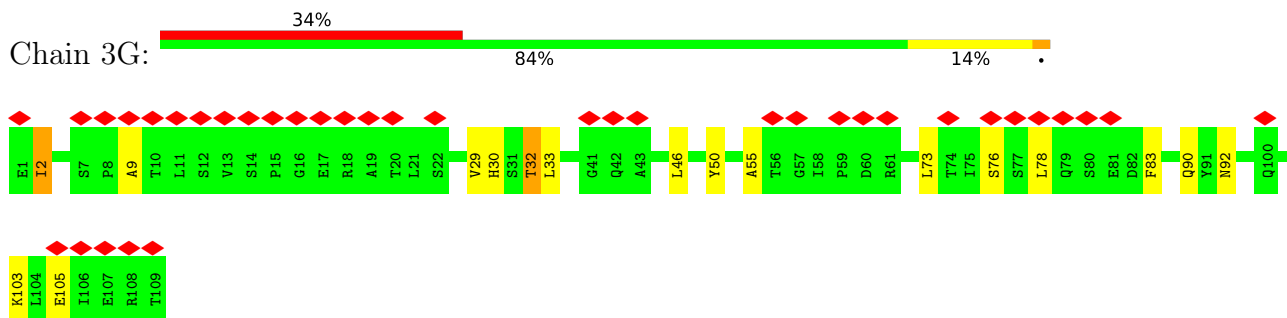
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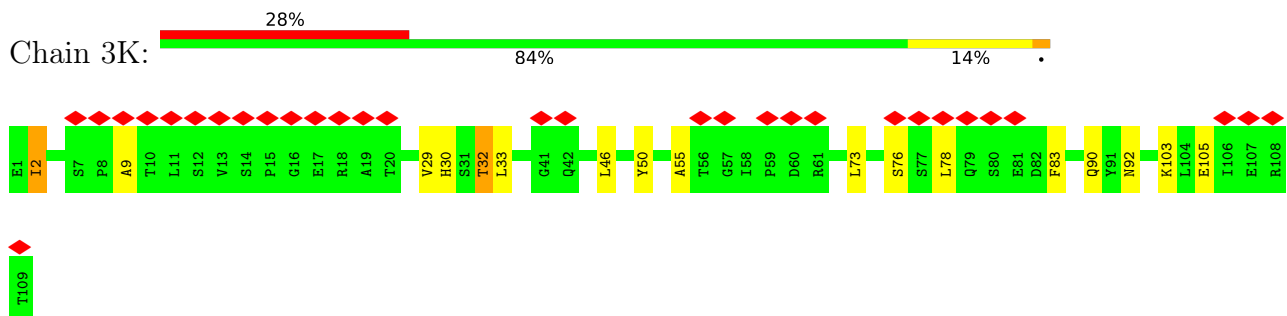
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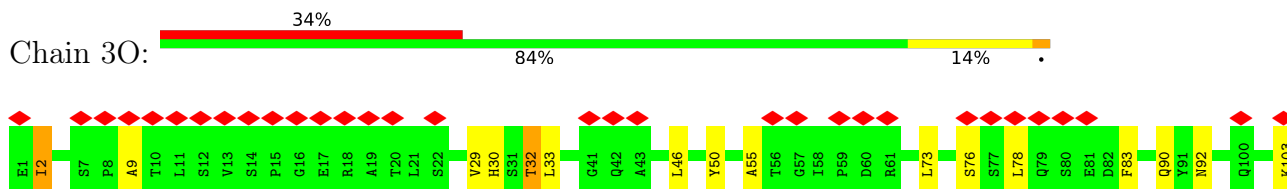
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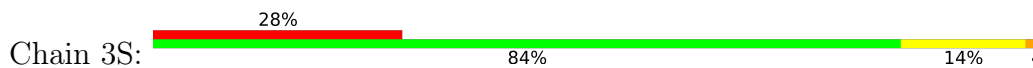


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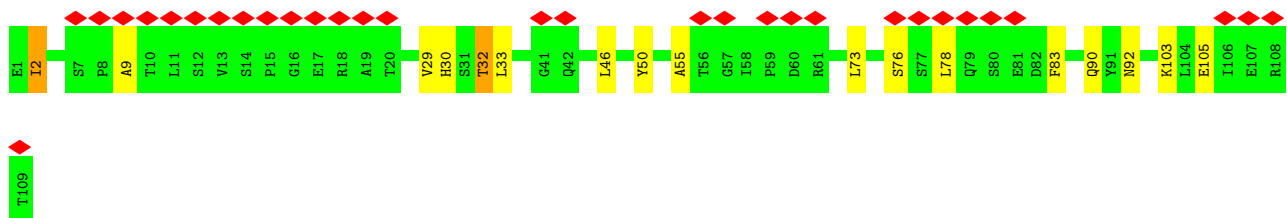




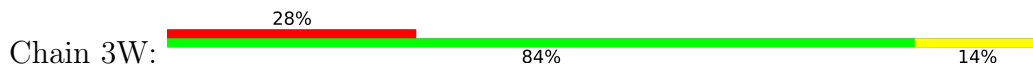
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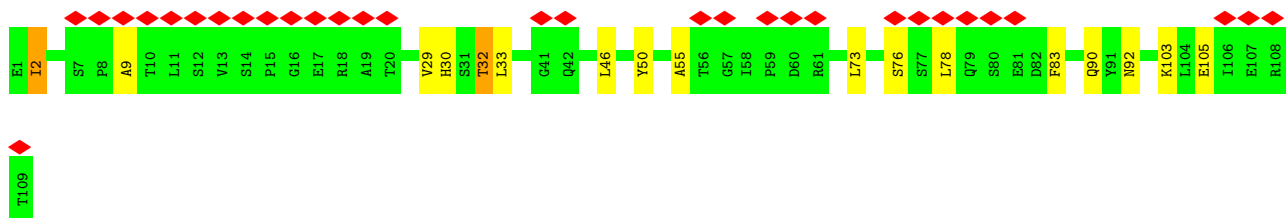
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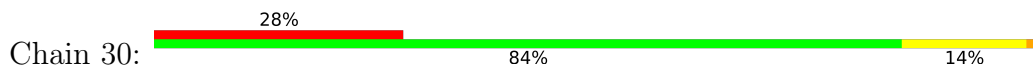
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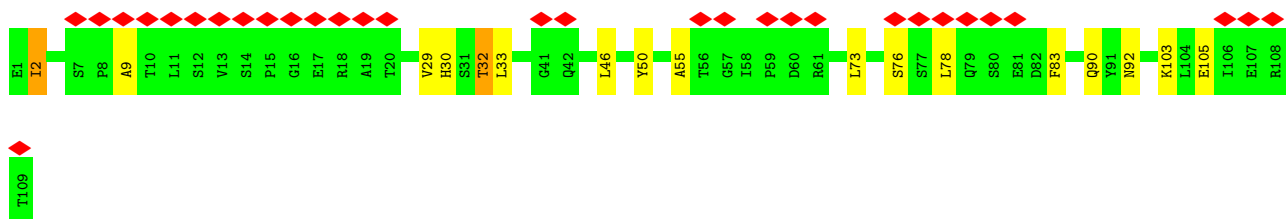
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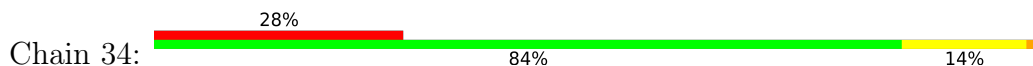
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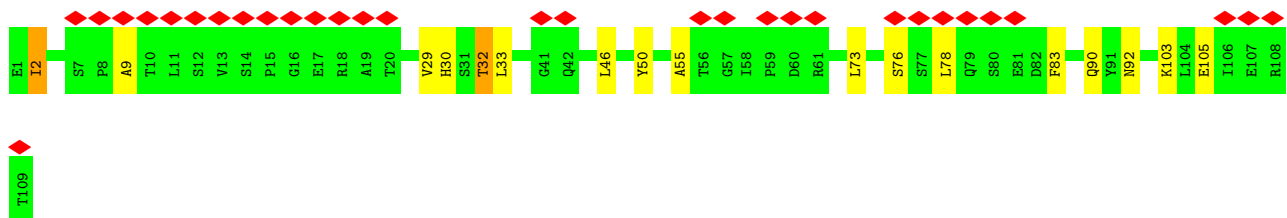
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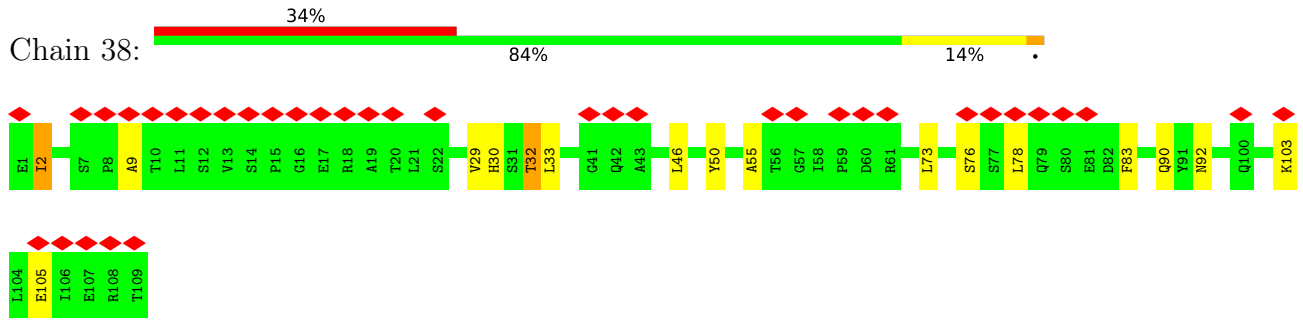
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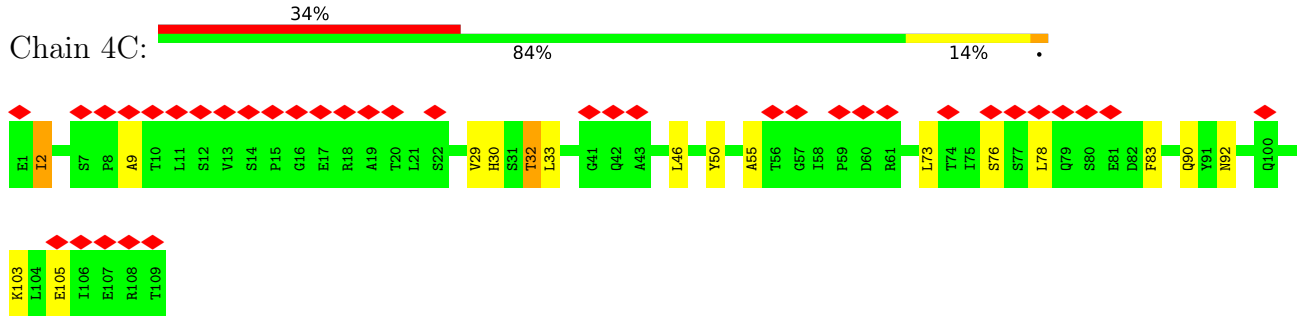
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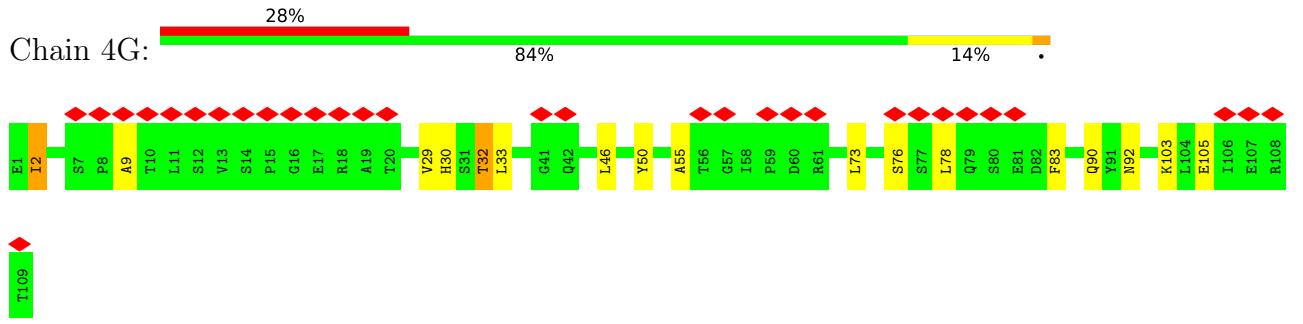
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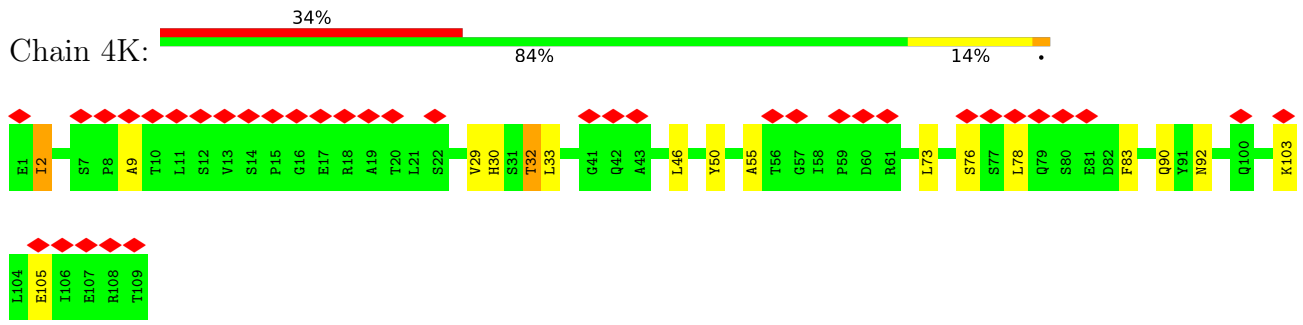
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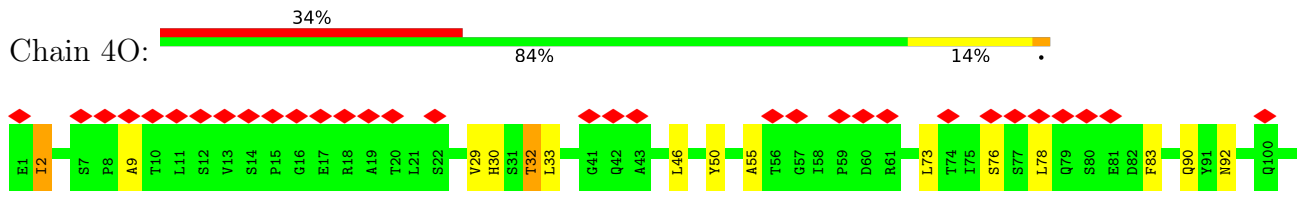
• Molecule 3: HUMAN MONOCLONAL ANTIBODY



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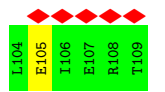
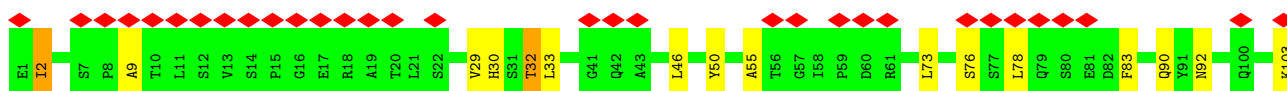
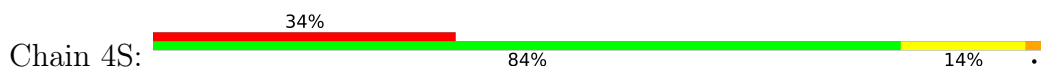


• Molecule 3: HUMAN MONOCLONAL ANTIBODY

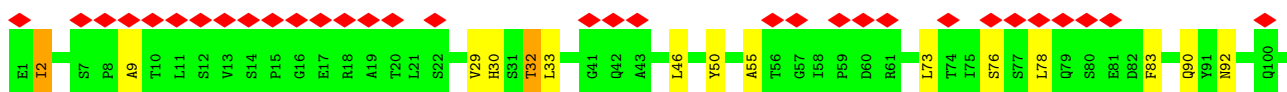
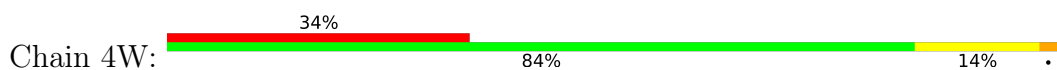




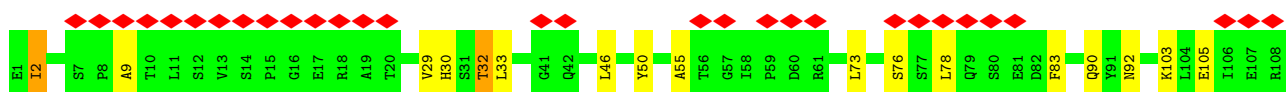
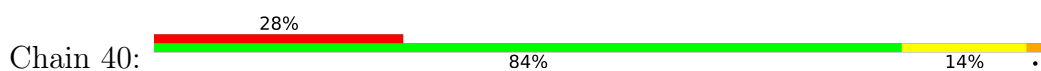
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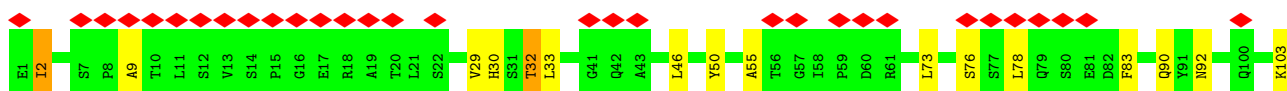
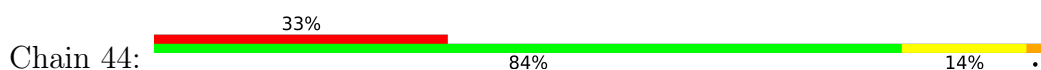
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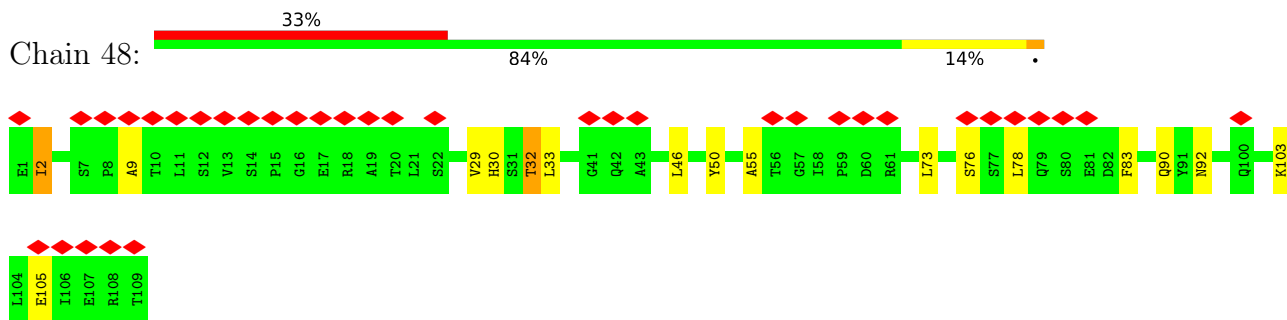
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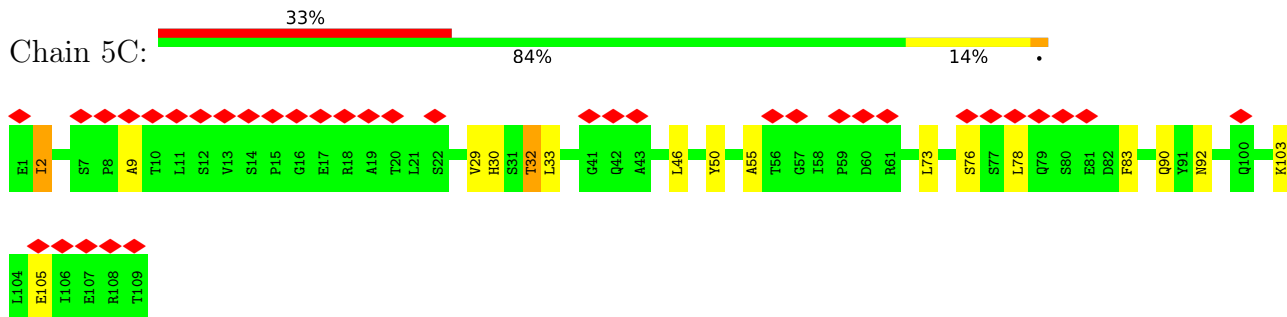
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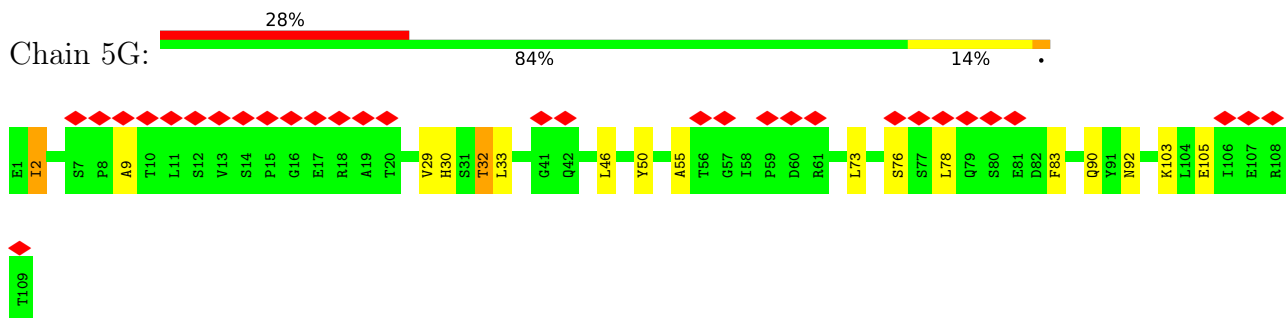
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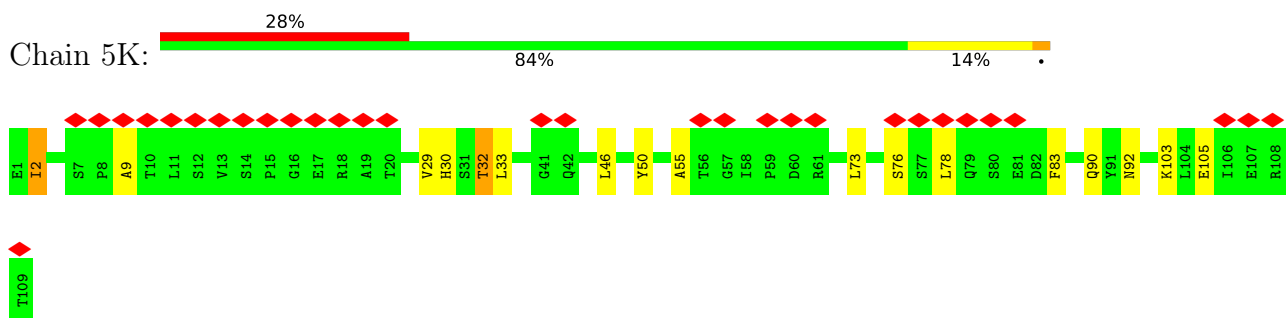
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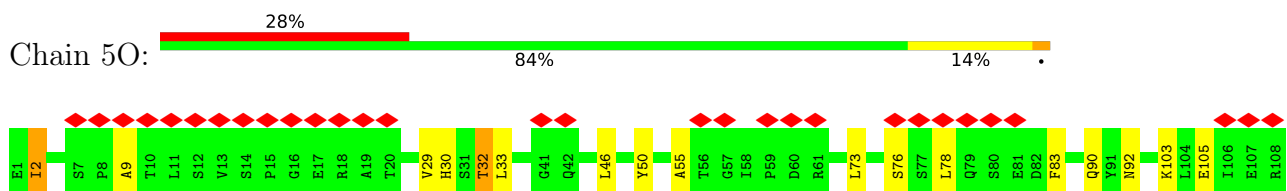
• Molecule 3: HUMAN MONOCLONAL ANTIBODY



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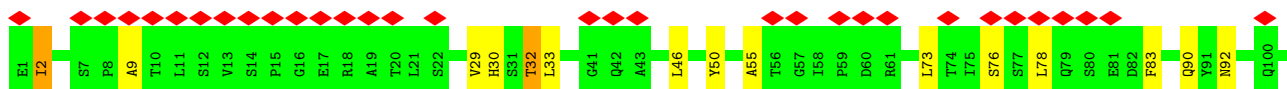
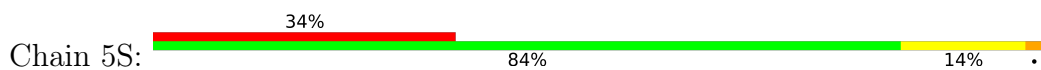


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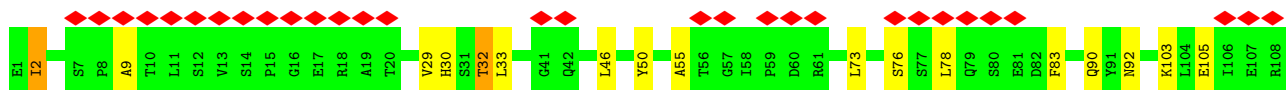
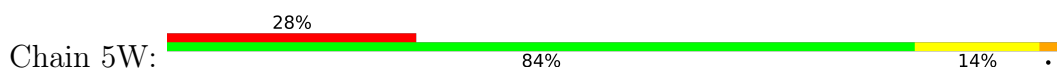
T109

• Molecule 3: HUMAN MONOCLONAL ANTIBODY



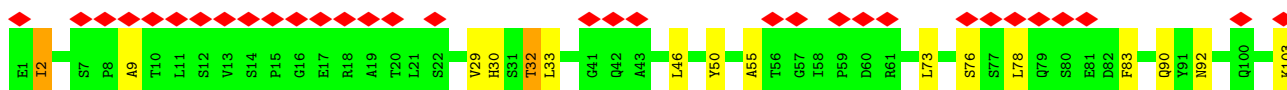
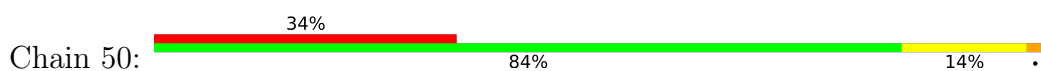
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• Molecule 3: HUMAN MONOCLONAL ANTIBODY



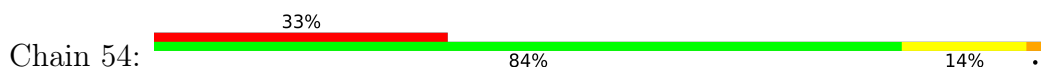
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• Molecule 3: HUMAN MONOCLONAL ANTIBODY



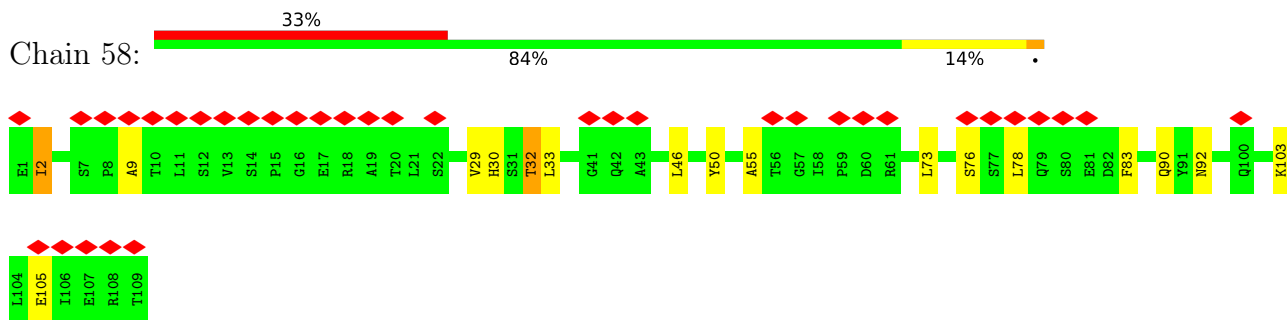
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• Molecule 3: HUMAN MONOCLONAL ANTIBODY

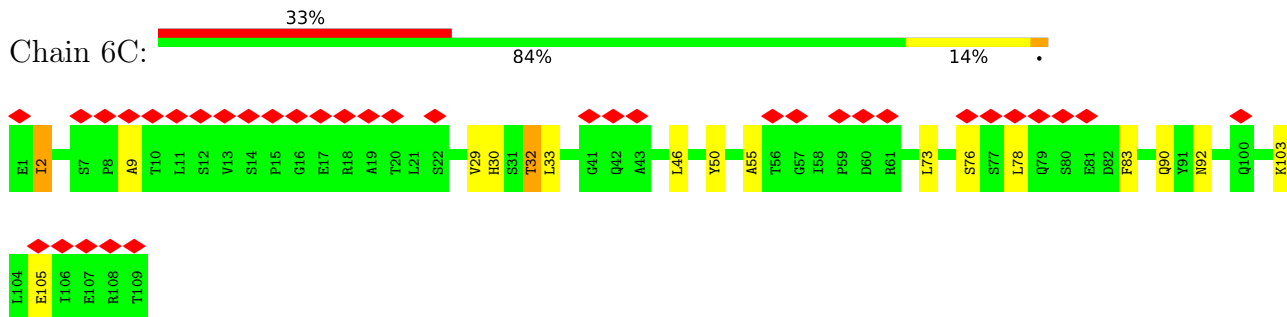


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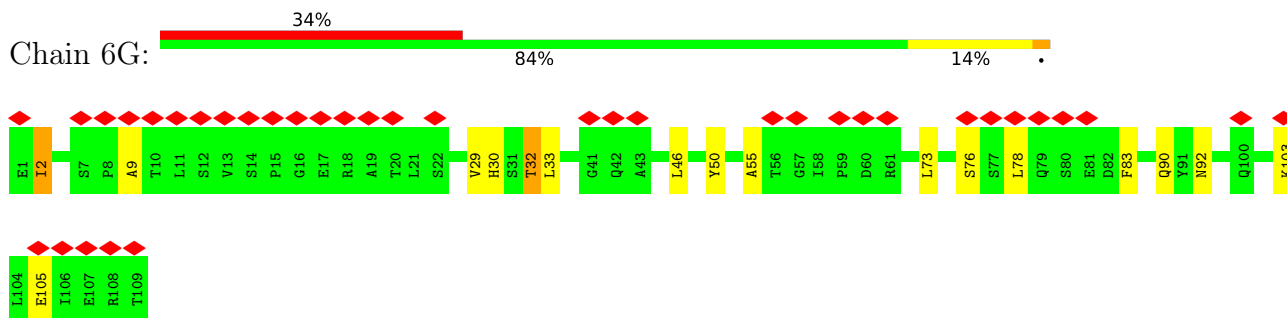
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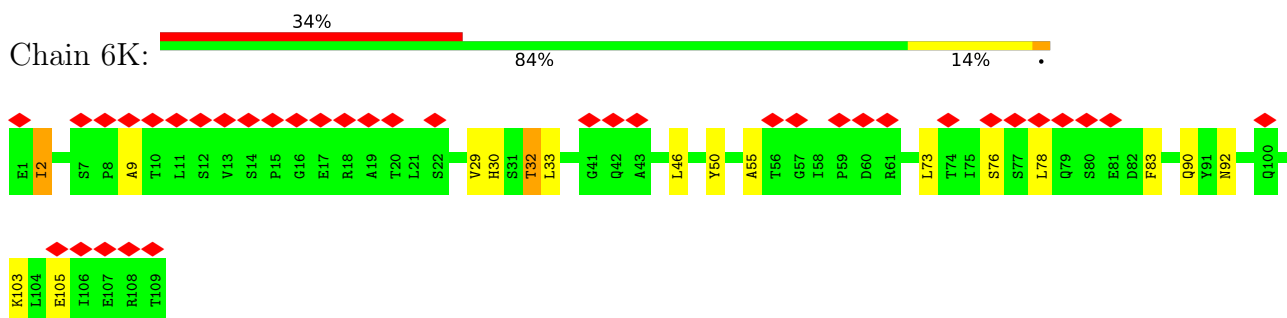
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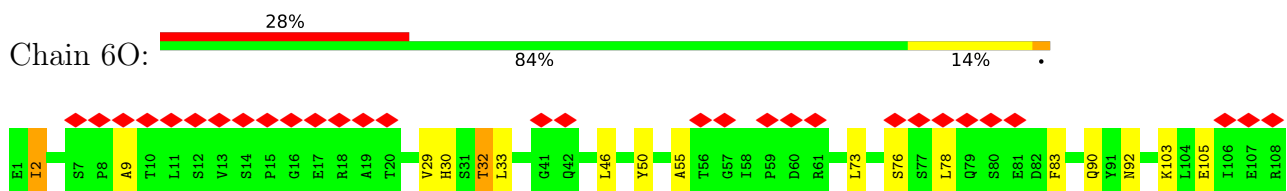
• Molecule 3: HUMAN MONOCLONAL ANTIBODY



• Molecule 3: HUMAN MONOCLONAL ANTIBODY

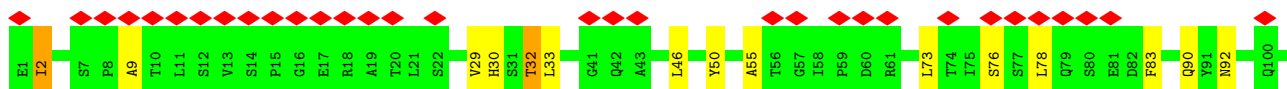
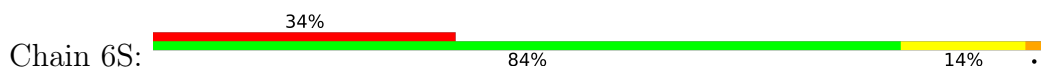


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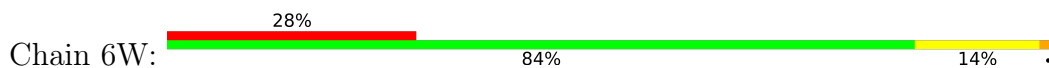
T109

• Molecule 3: HUMAN MONOCLONAL ANTIBODY



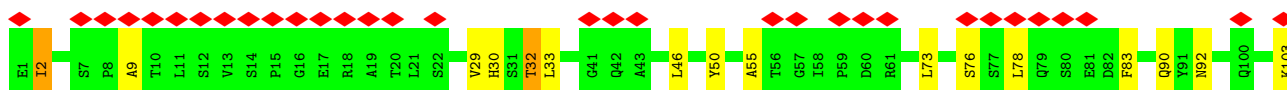
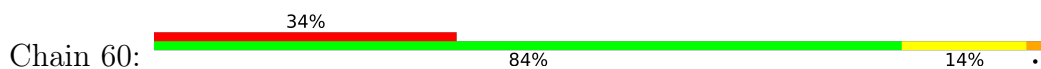
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• Molecule 3: HUMAN MONOCLONAL ANTIBODY



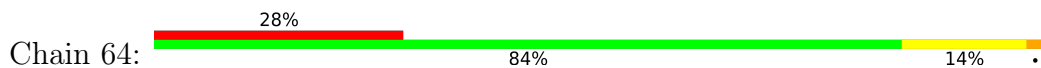
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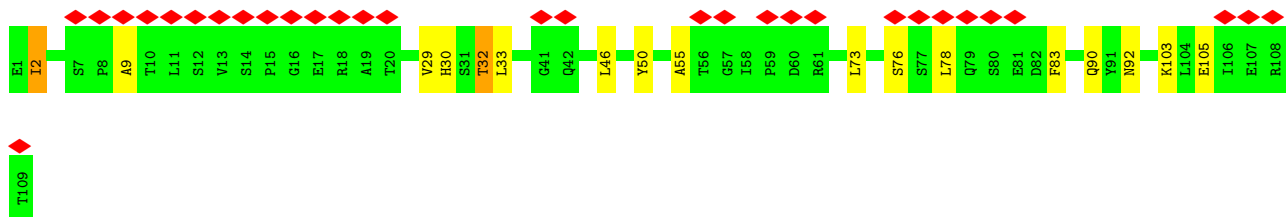
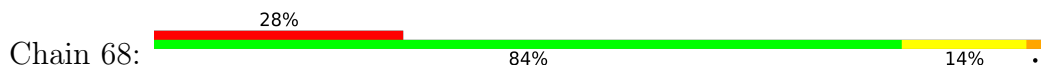
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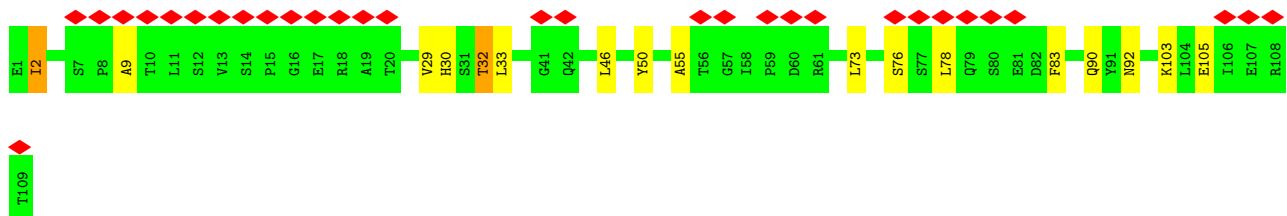
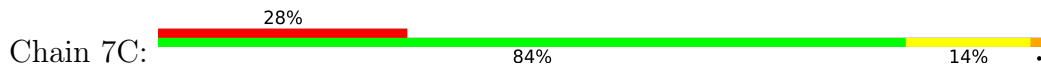


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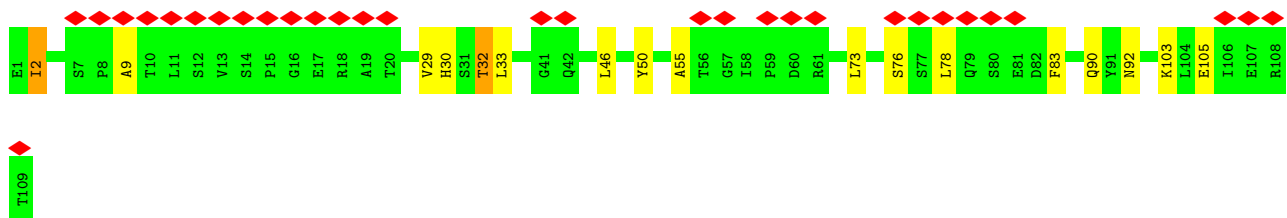
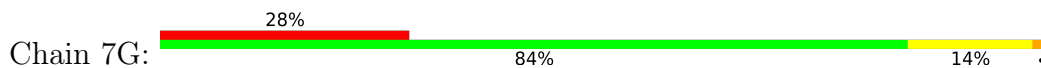
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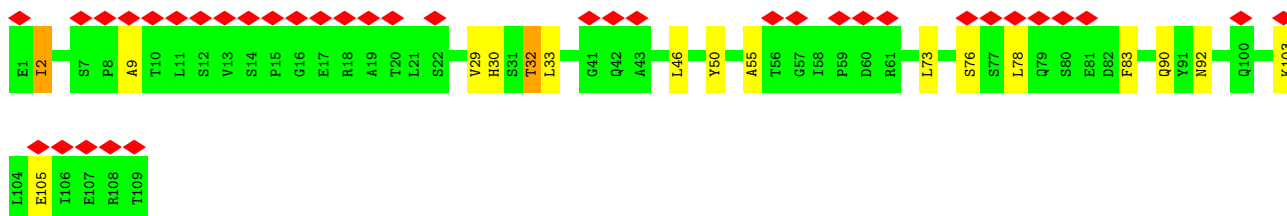
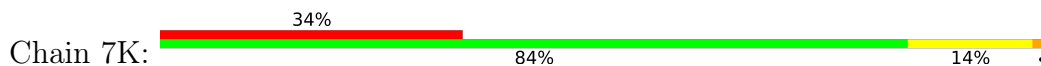
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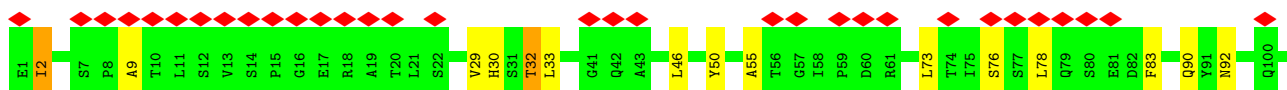
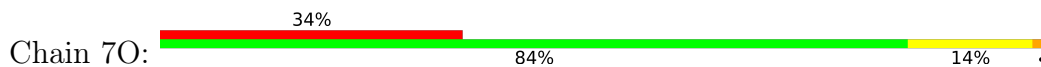
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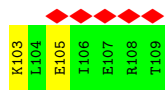


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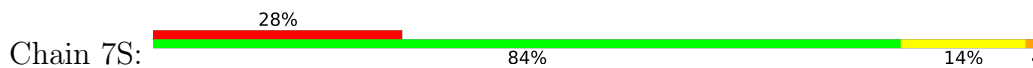


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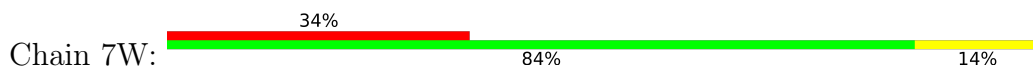
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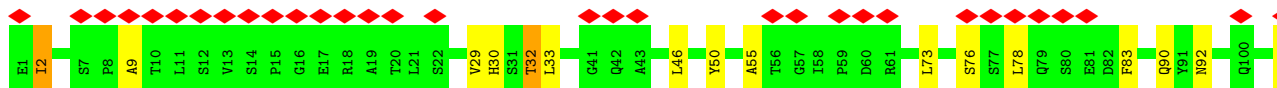
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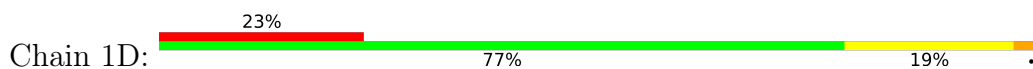
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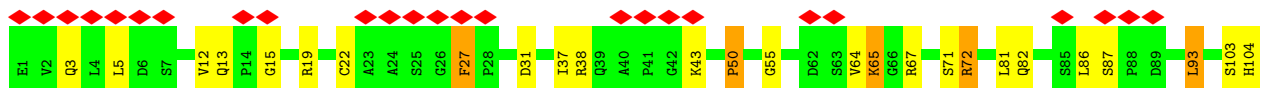
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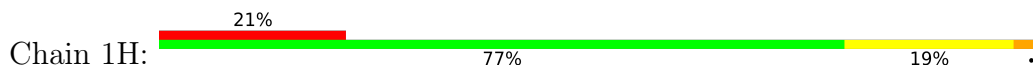
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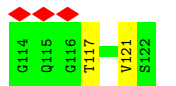
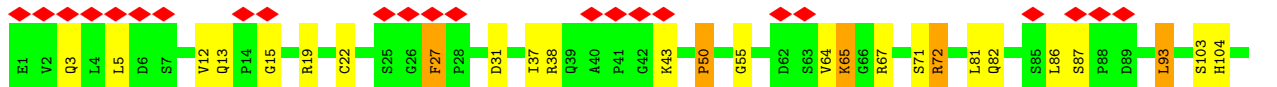
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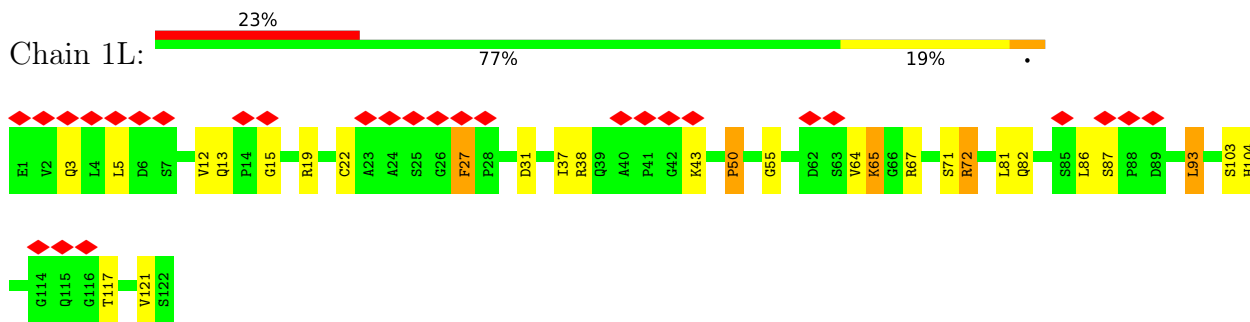
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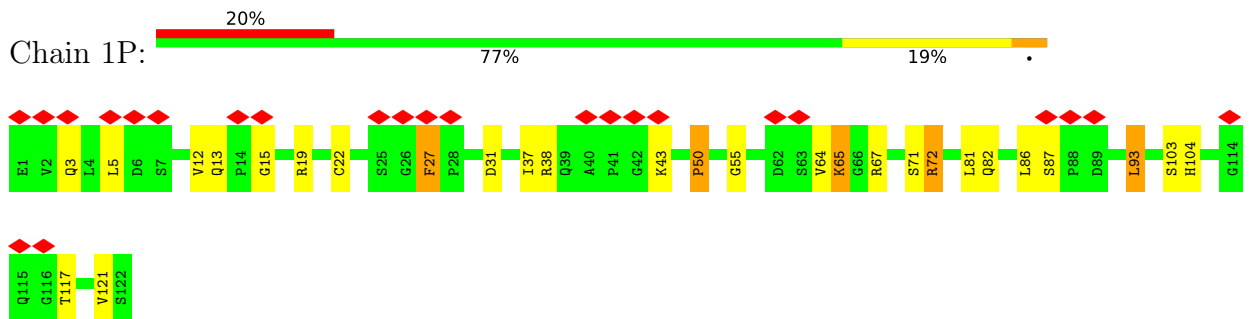
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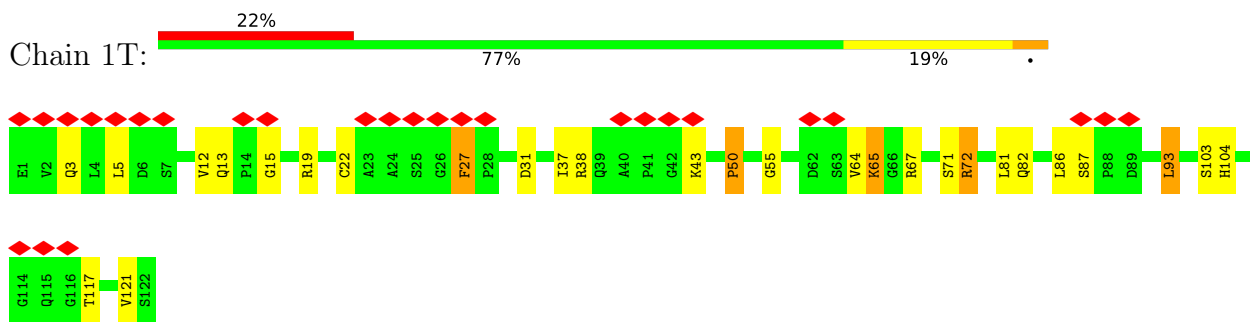
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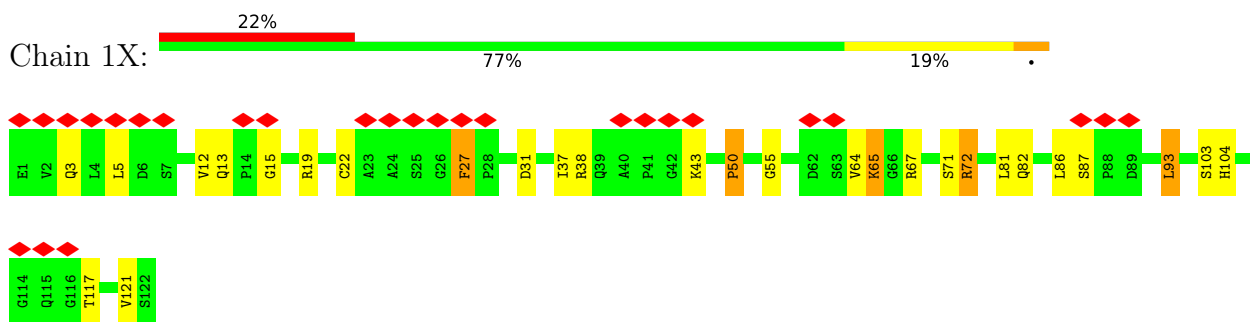
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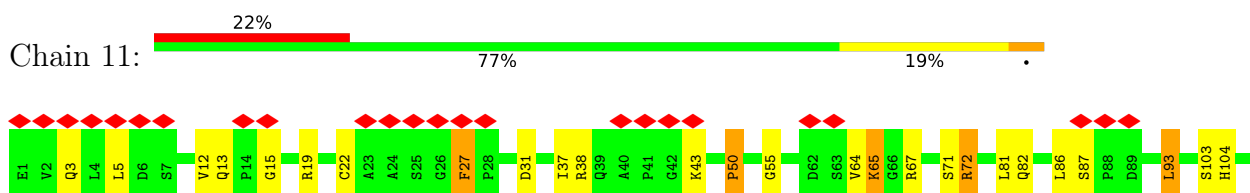
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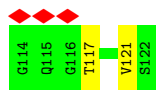


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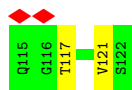
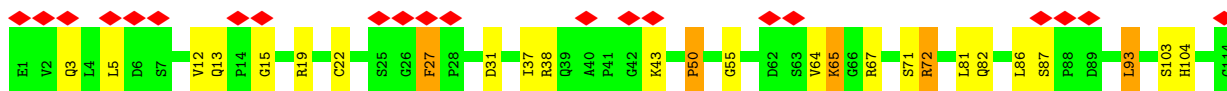
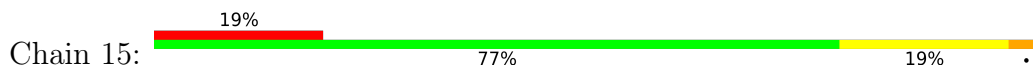


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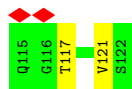
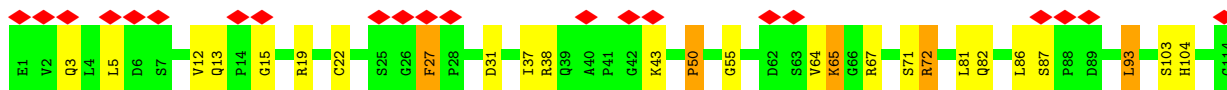
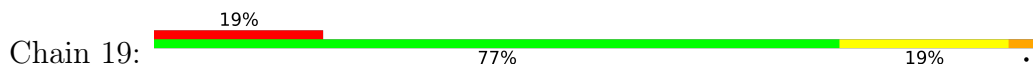




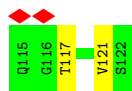
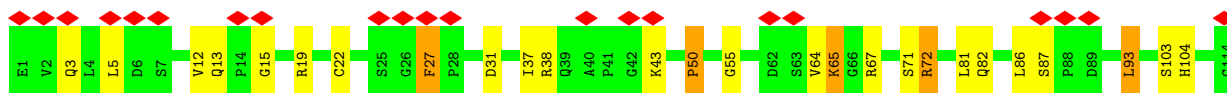
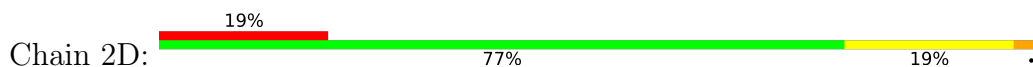
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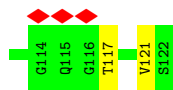
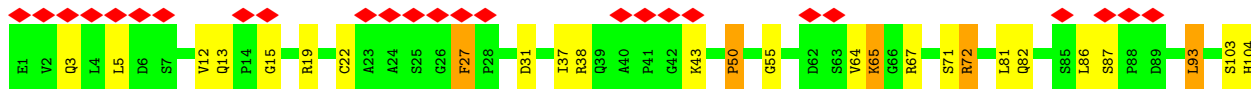
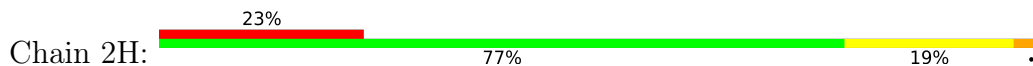
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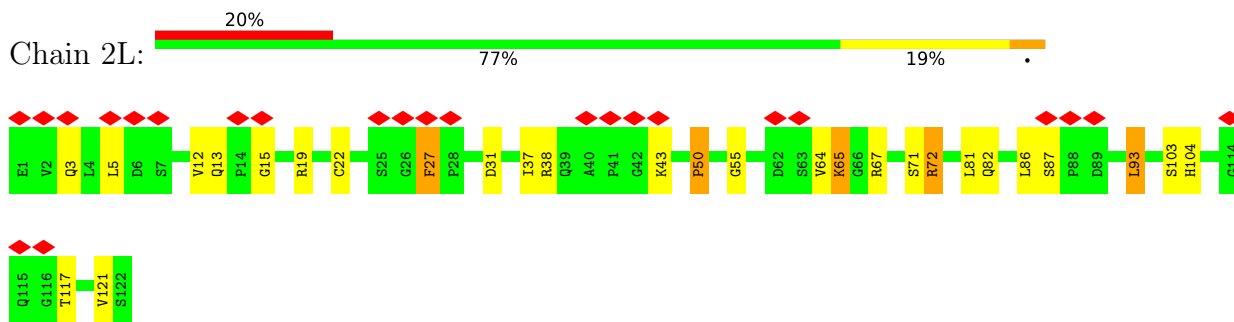
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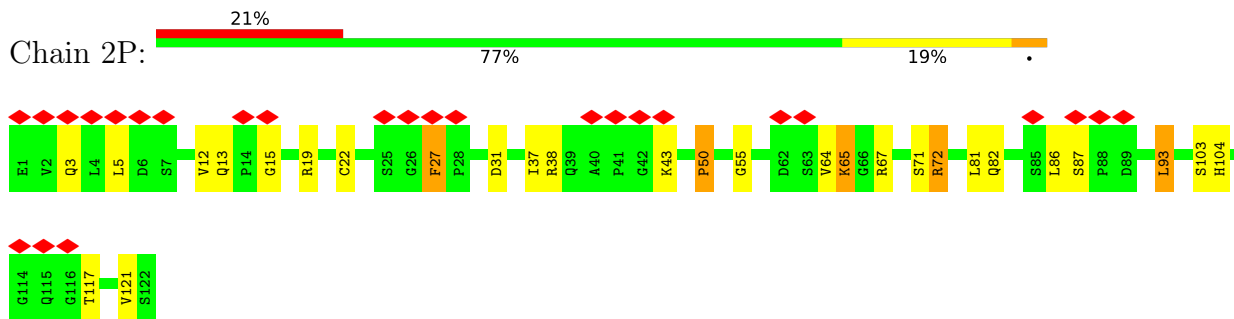
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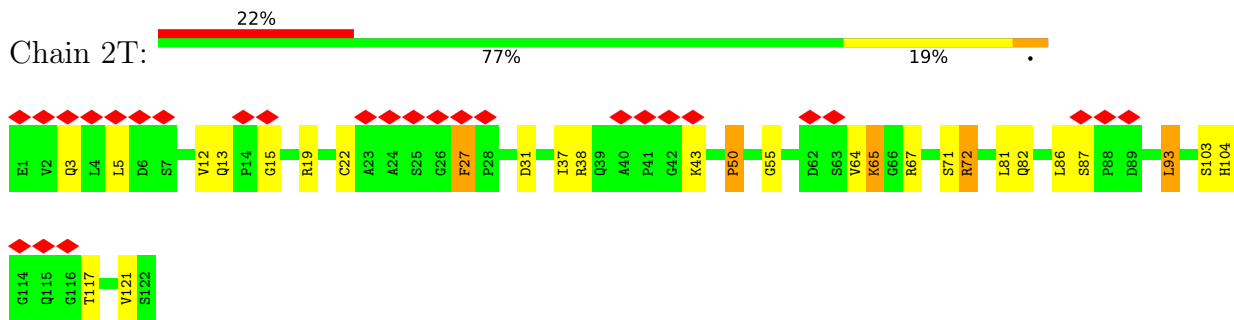
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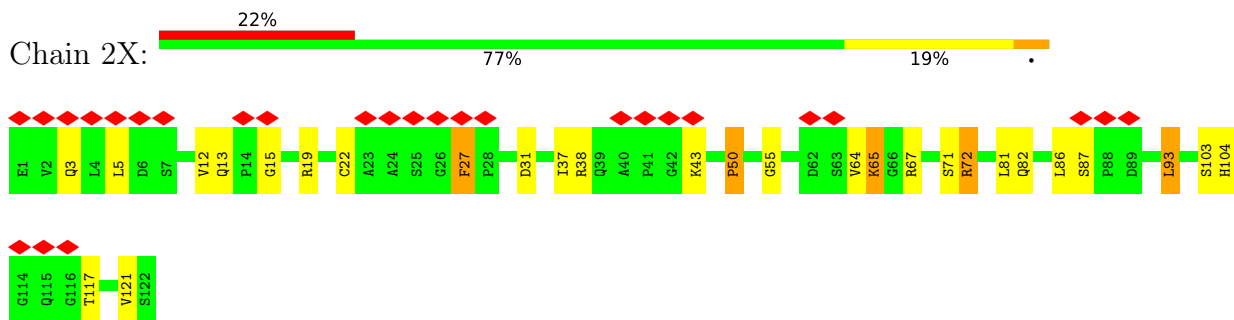
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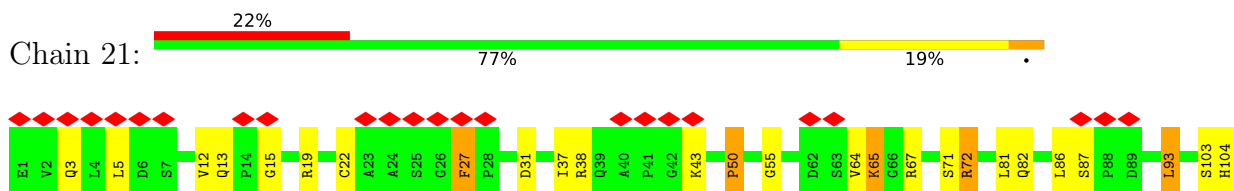
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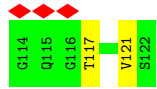


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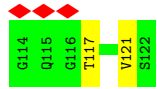
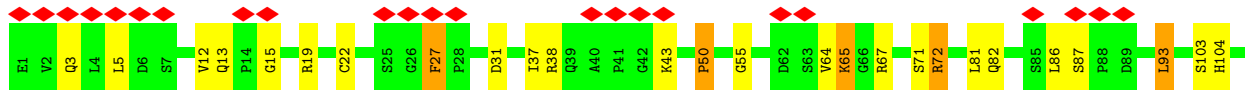
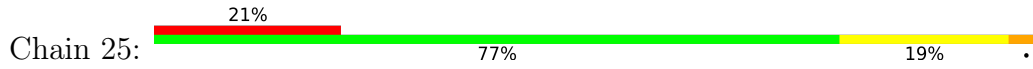


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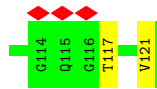
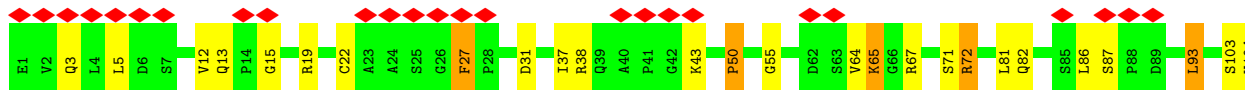
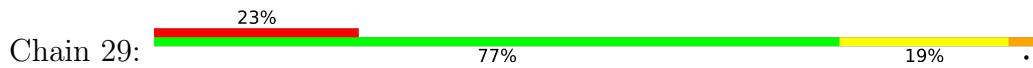




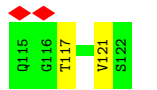
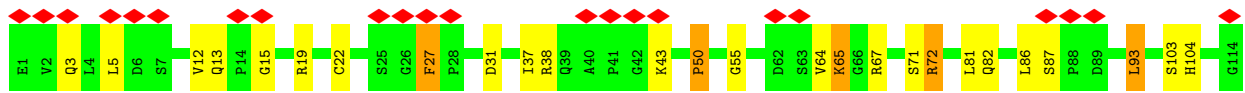
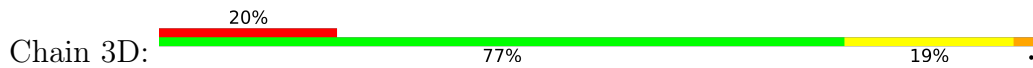
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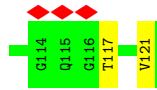
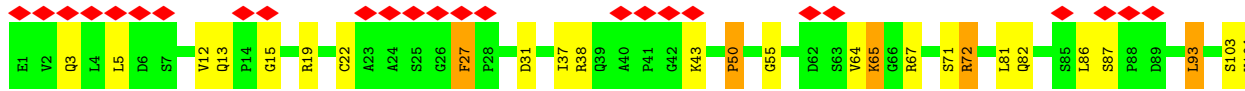
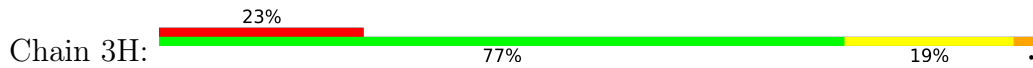
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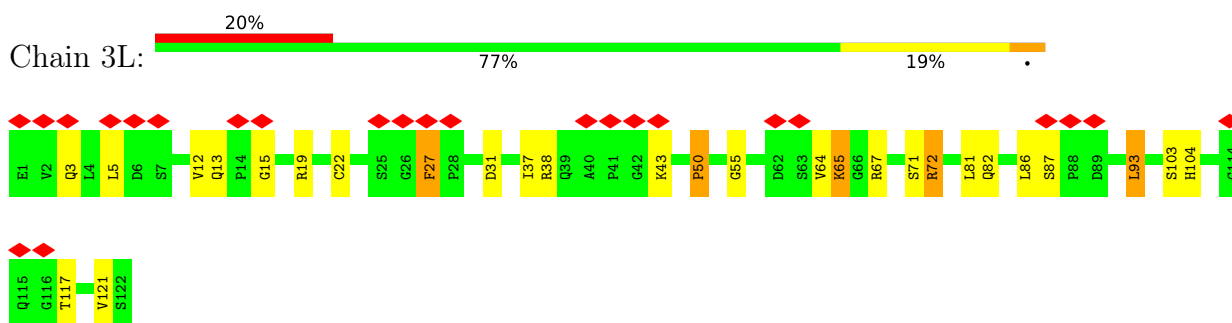
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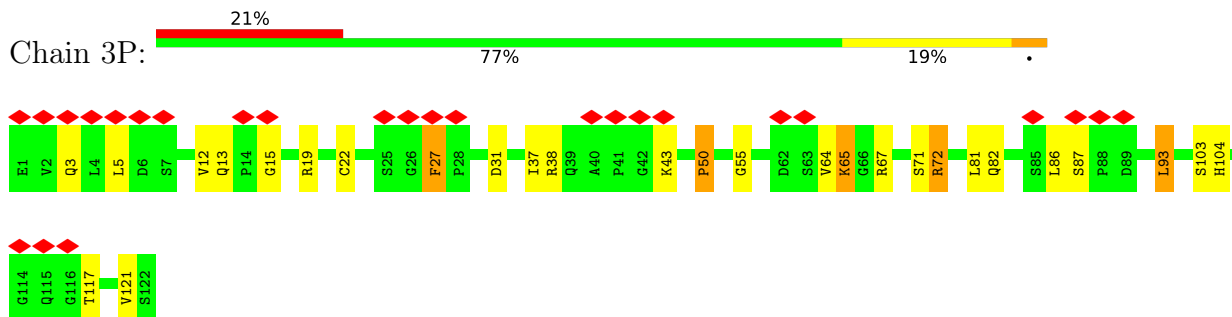
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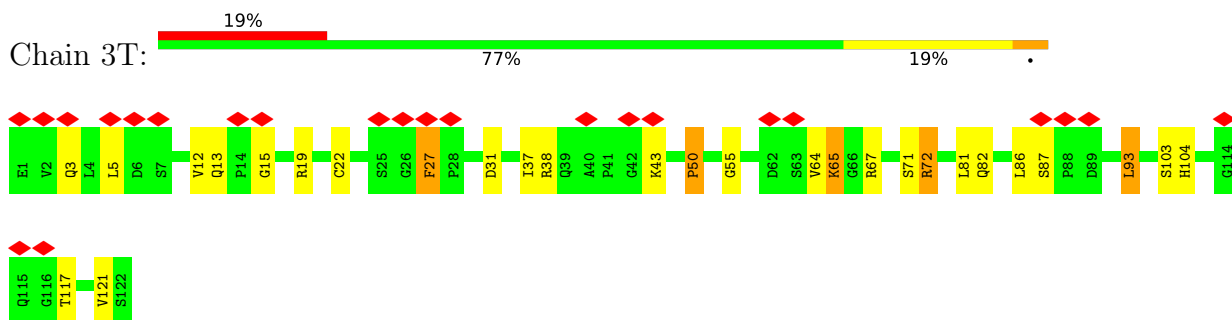
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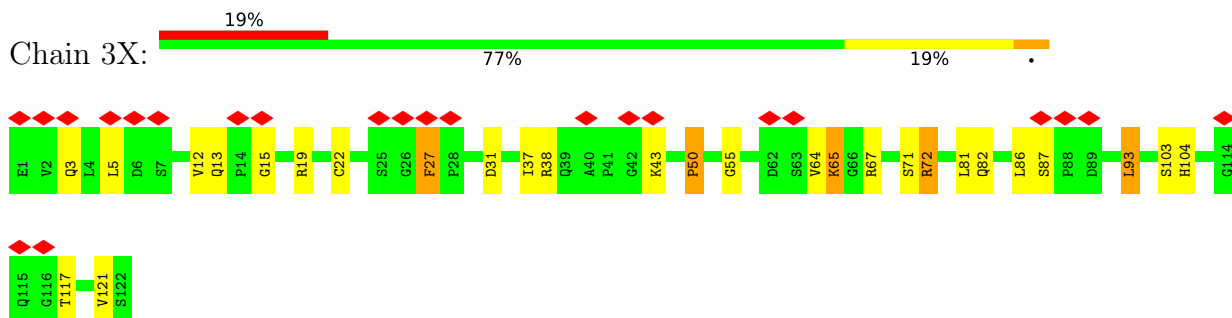
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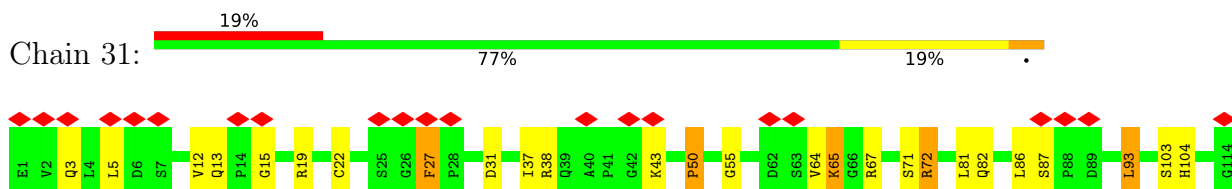
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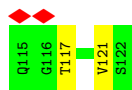


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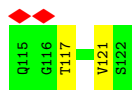
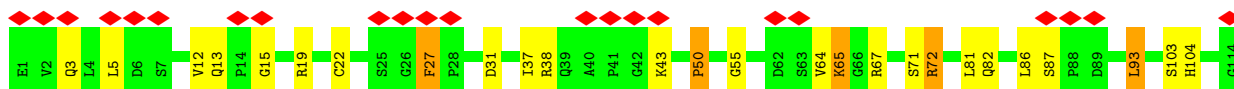
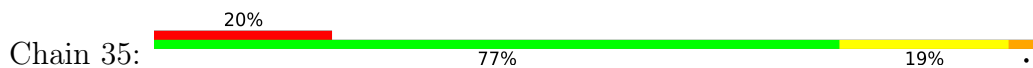


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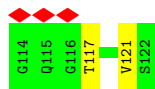
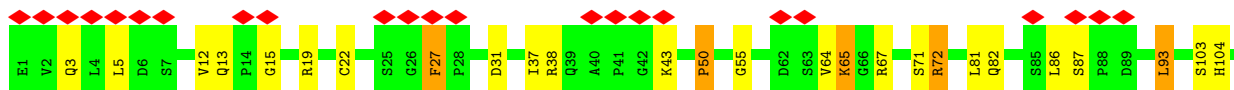
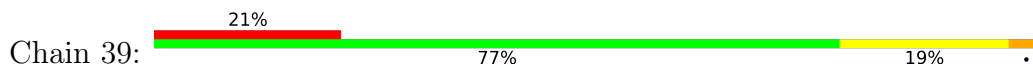




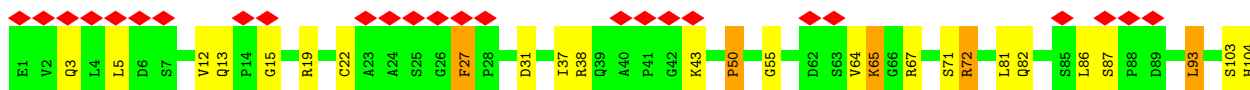
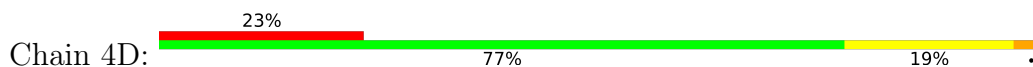
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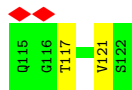
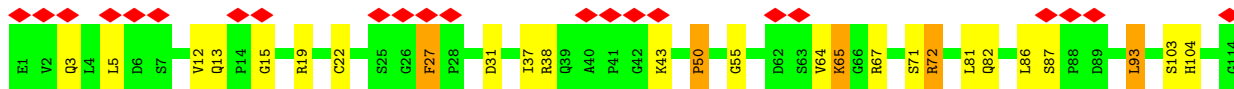
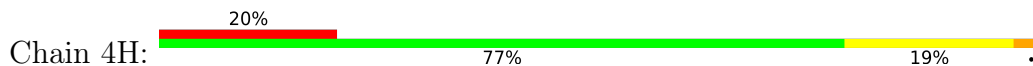
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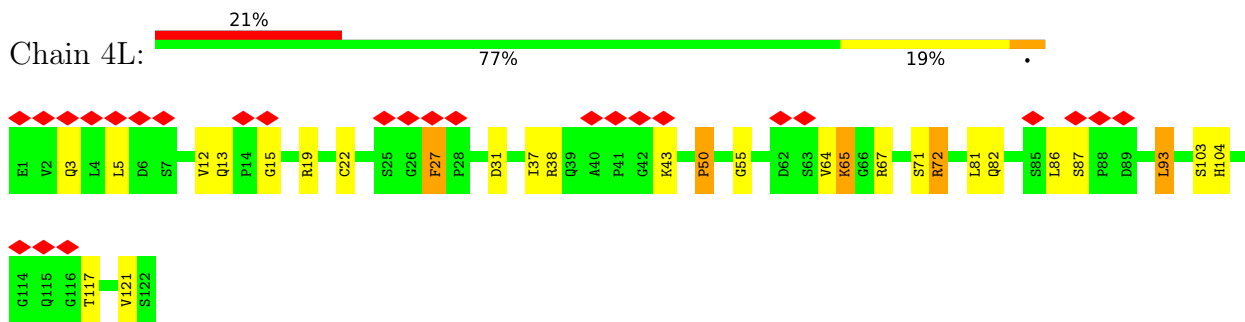
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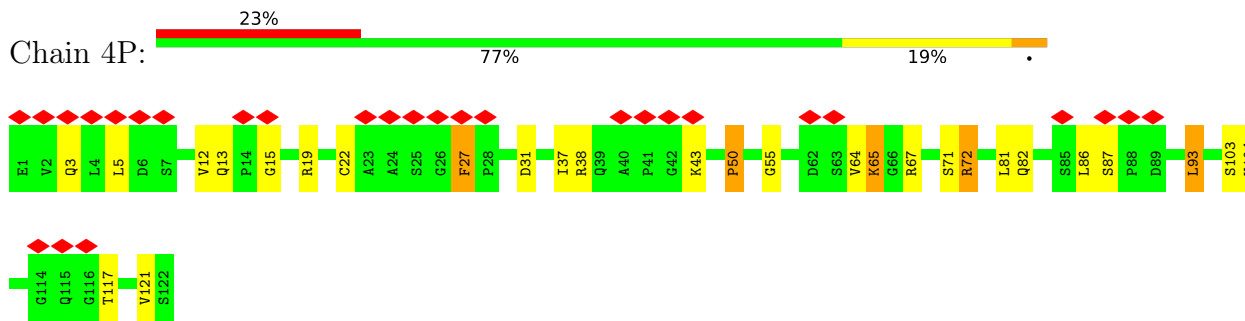
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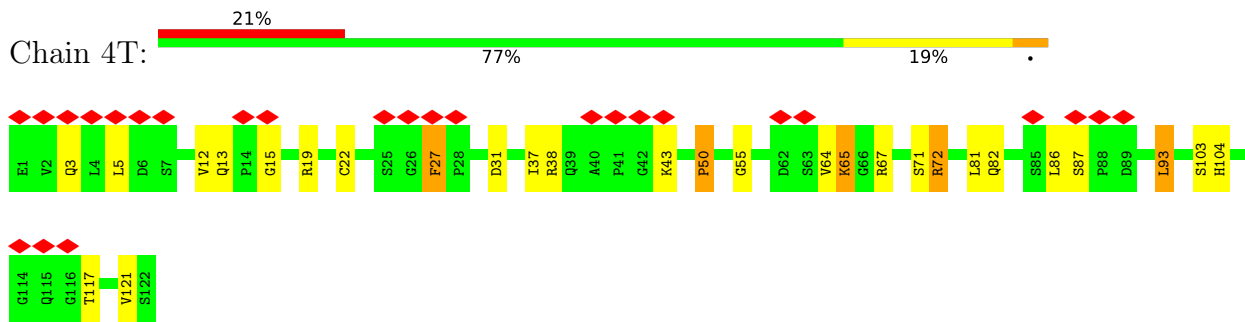
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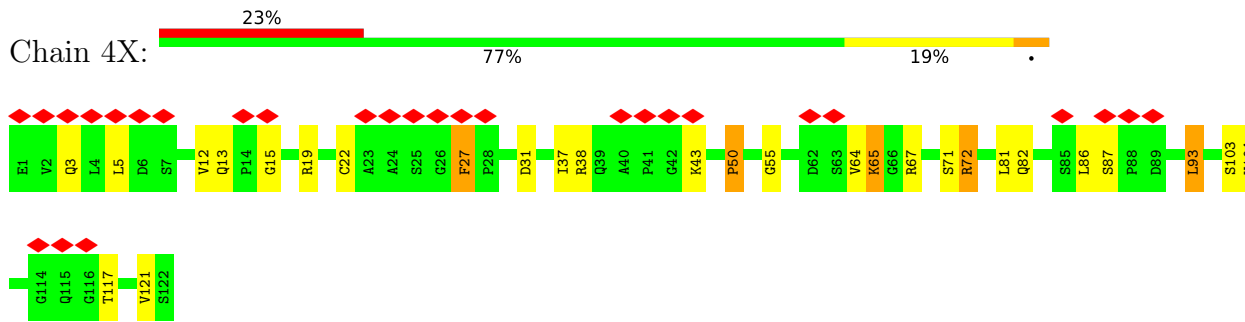
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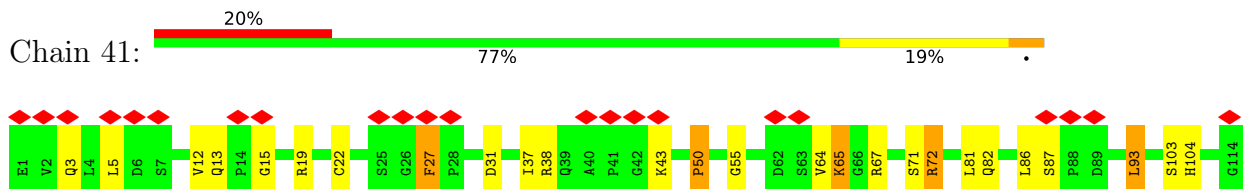
• Molecule 4: HUMAN MONOCLONAL ANTIBODY



• Molecule 4: HUMAN MONOCLONAL ANTIBODY

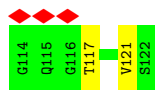
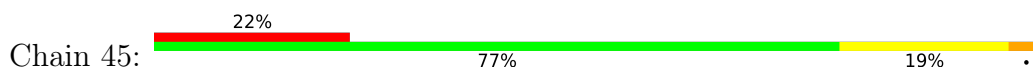


• Molecule 4: HUMAN MONOCLONAL ANTIBODY

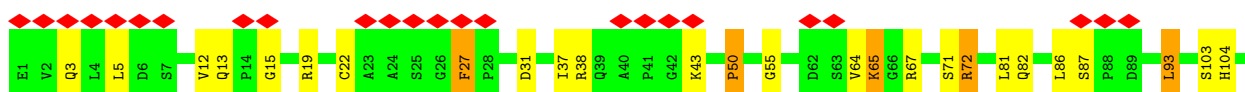
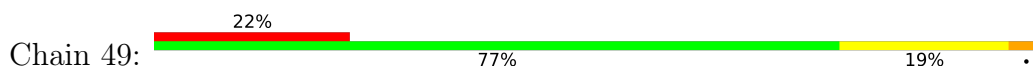




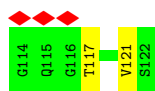
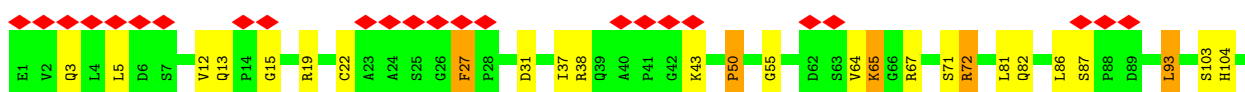
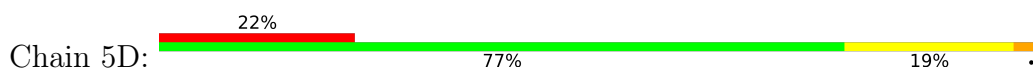
• Molecule 4: HUMAN MONOCLONAL ANTIBODY



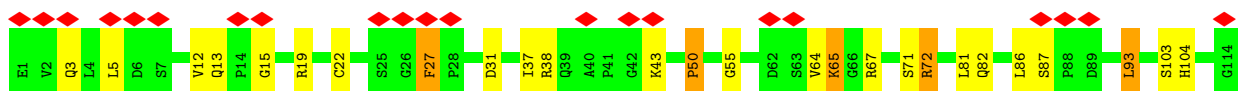
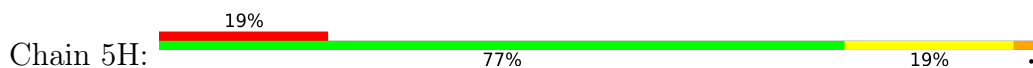
• Molecule 4: HUMAN MONOCLONAL ANTIBODY



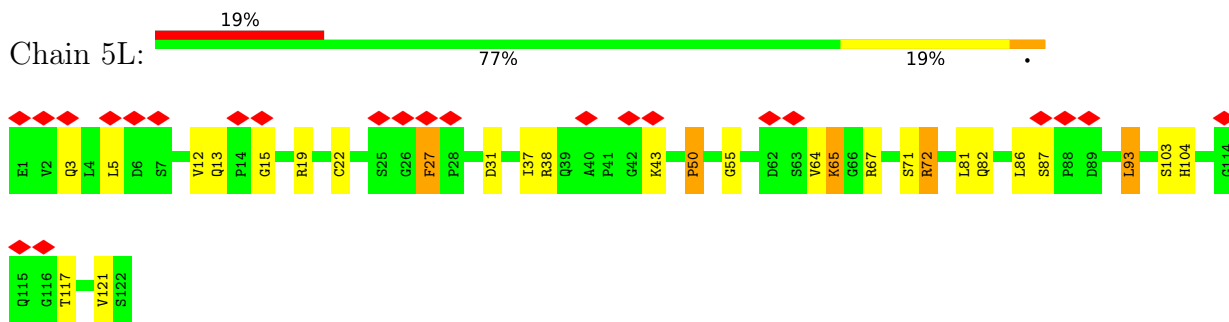
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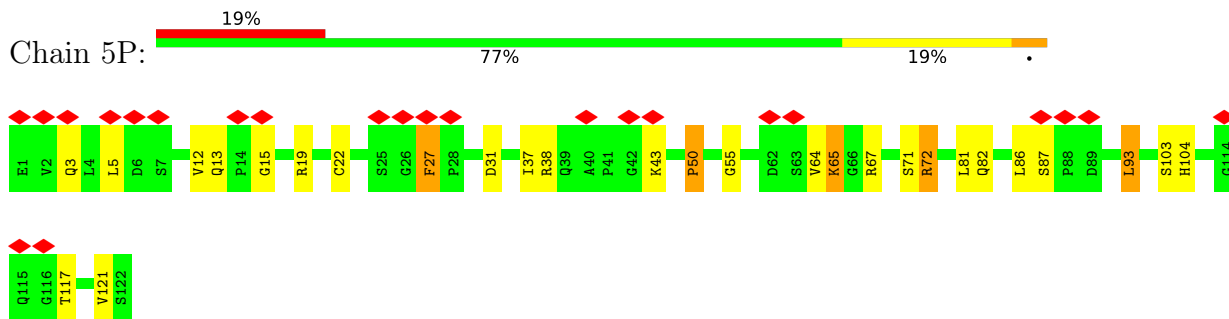
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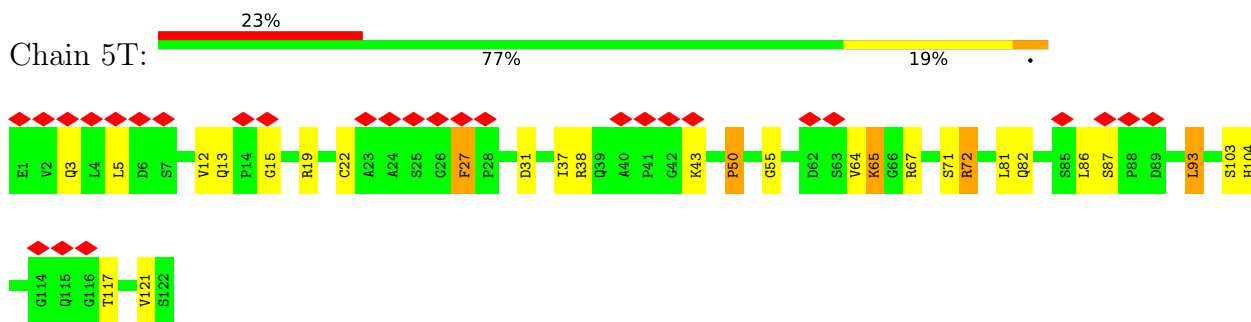
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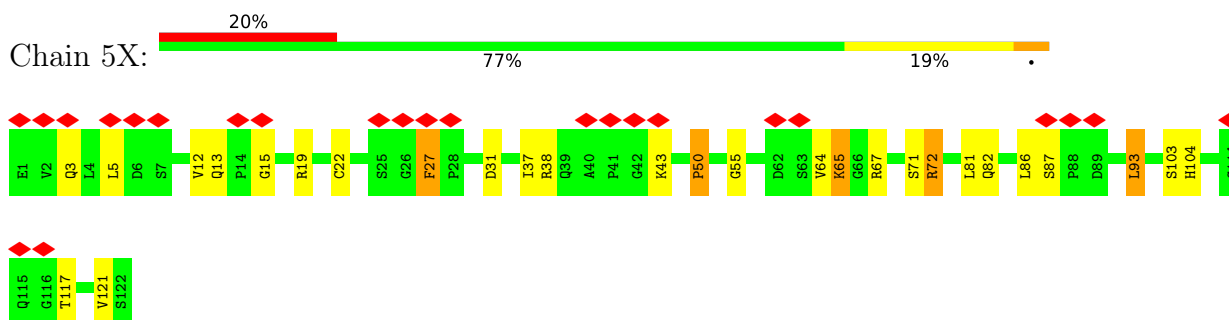
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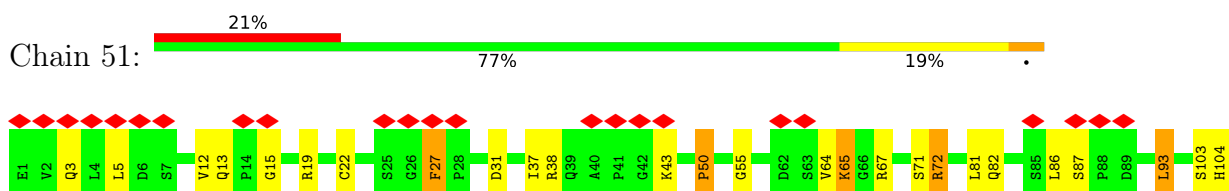
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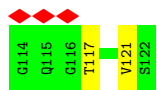


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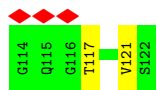
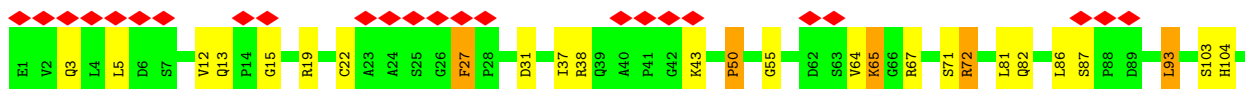
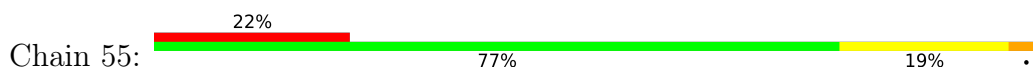


• Molecule 4: HUMAN MONOCLONAL ANTIBODY

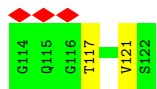
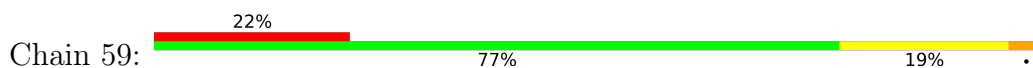




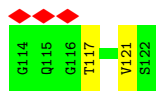
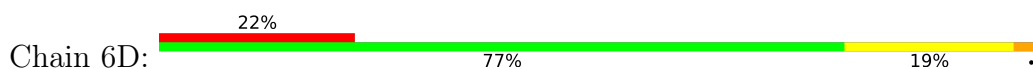
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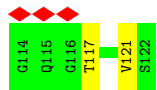
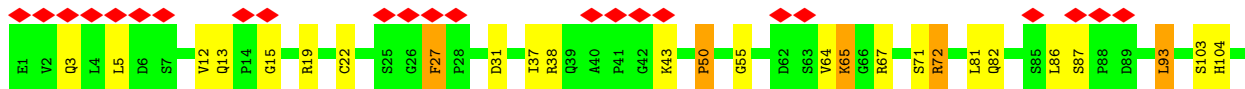
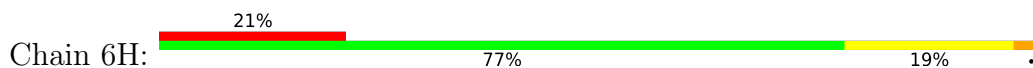
• Molecule 4: HUMAN MONOCLONAL ANTIBODY



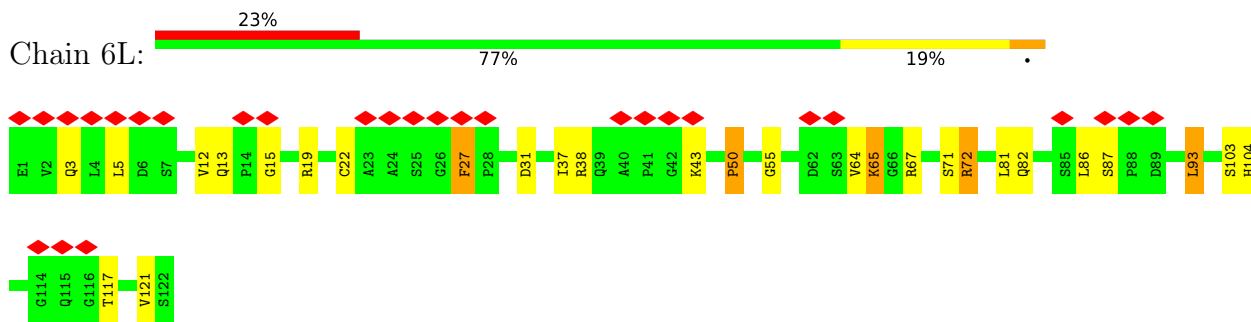
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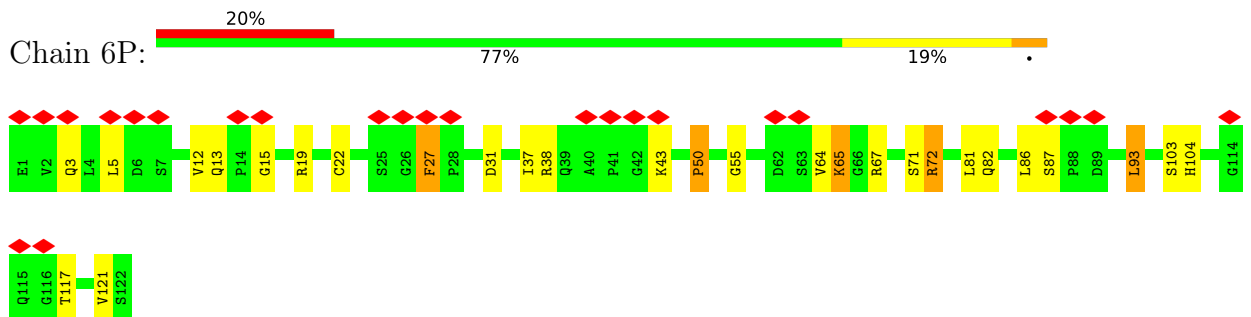
• Molecule 4: HUMAN MONOCLONAL ANTIBODY



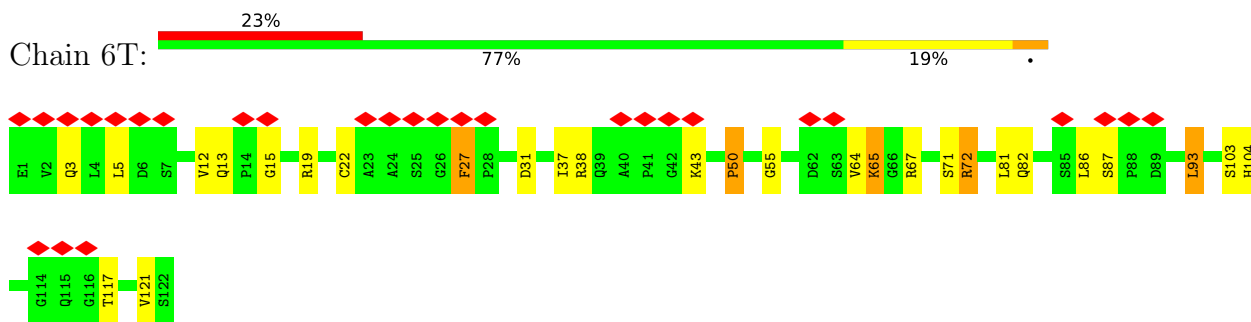
• Molecule 4: HUMAN MONOCLONAL ANTIBODY



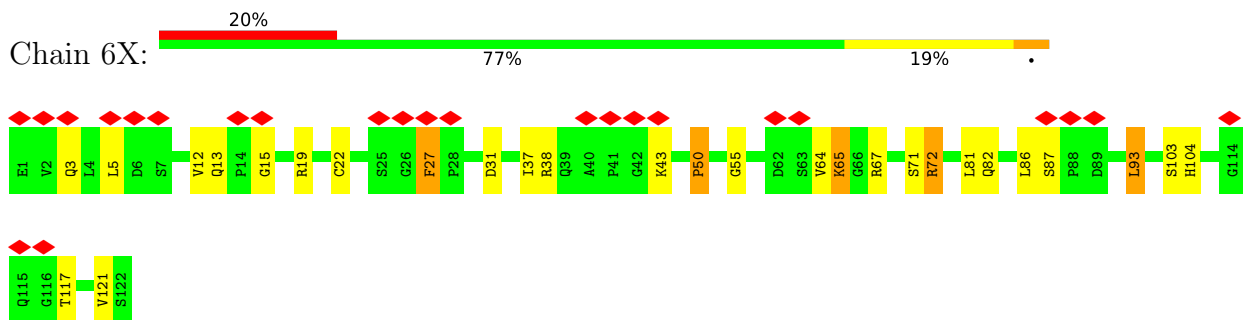
• Molecule 4: HUMAN MONOCLONAL ANTIBODY



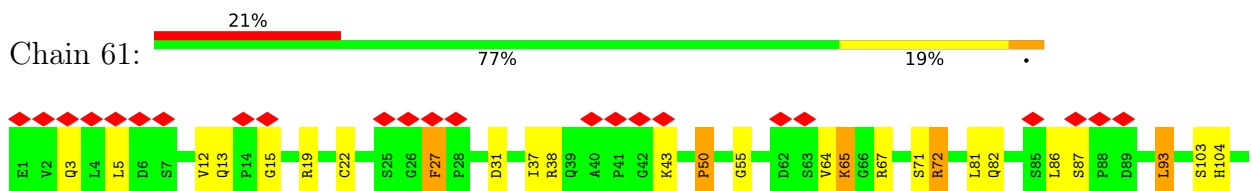
• Molecule 4: HUMAN MONOCLONAL ANTIBODY



• Molecule 4: HUMAN MONOCLONAL ANTIBODY

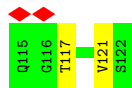
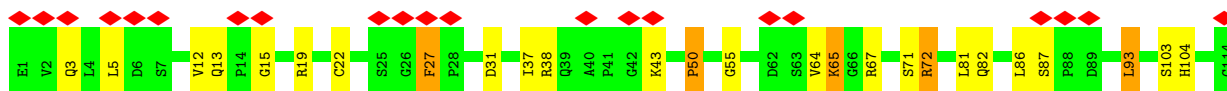
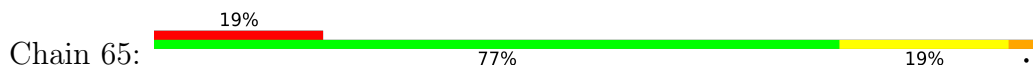


• Molecule 4: HUMAN MONOCLONAL ANTIBODY

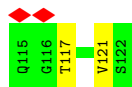
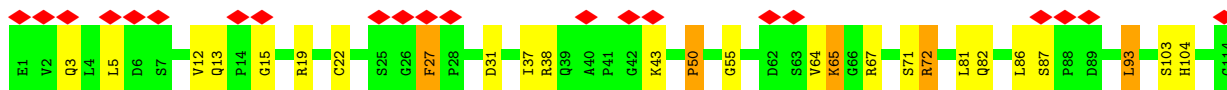
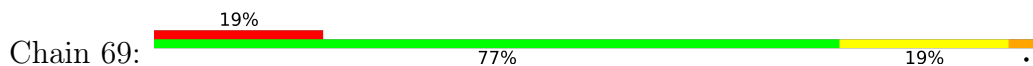




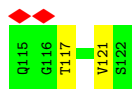
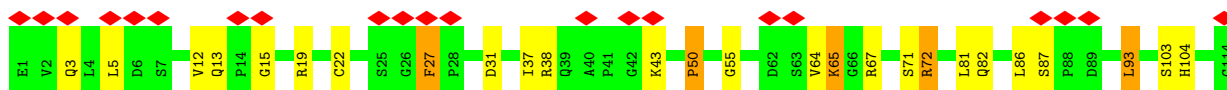
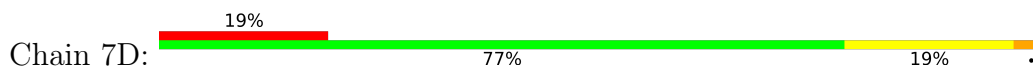
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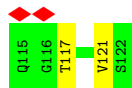
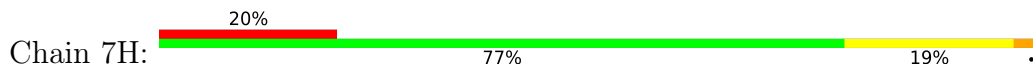
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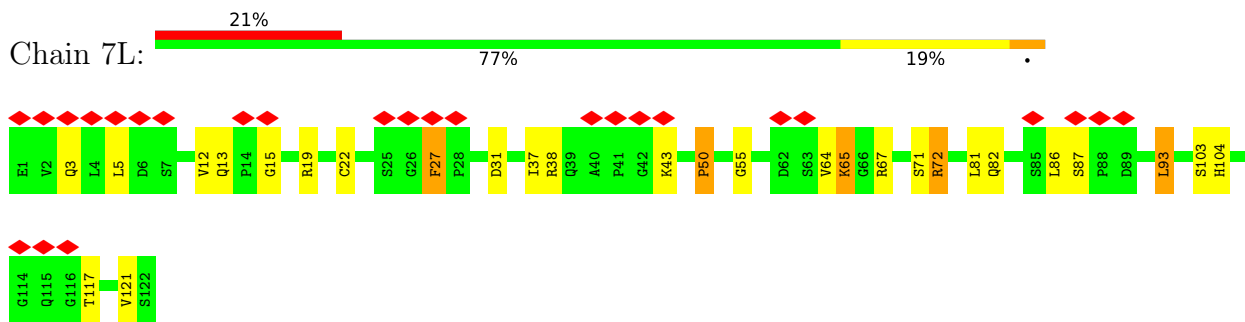
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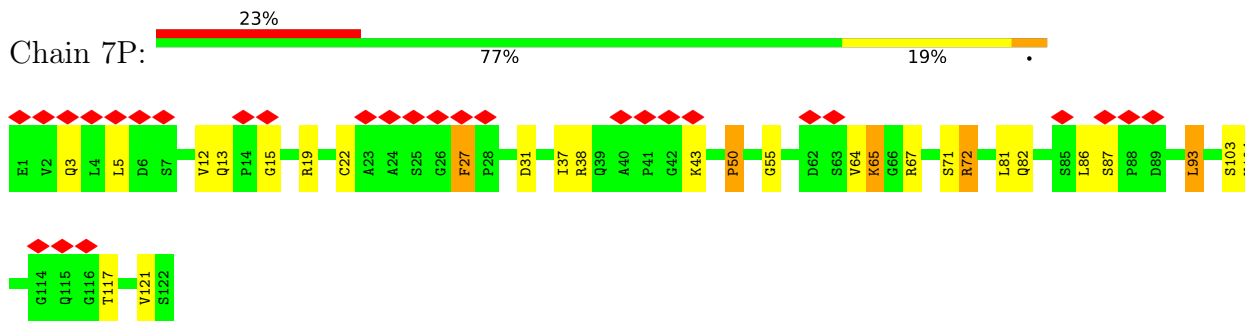
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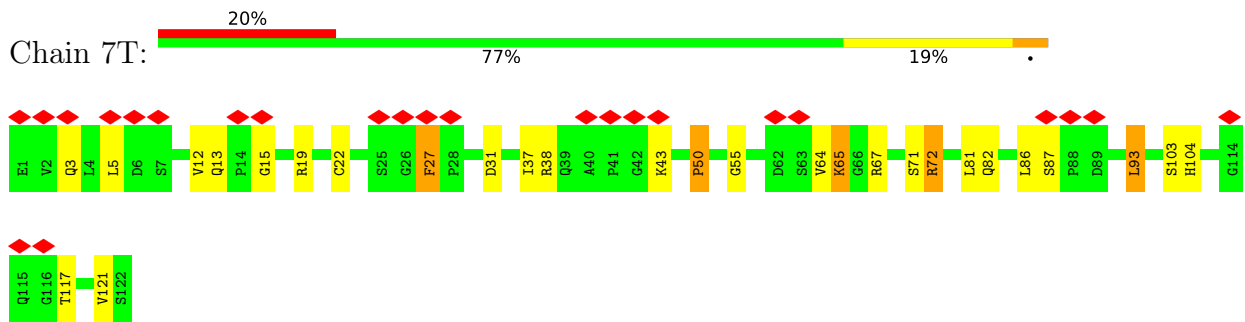
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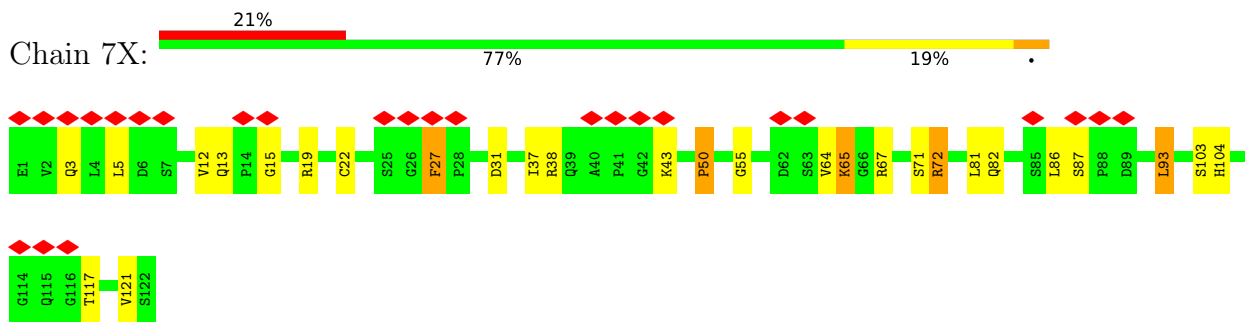
• Molecule 4: HUMAN MONOCLONAL ANTIBODY



• Molecule 4: HUMAN MONOCLONAL ANTIBODY



• Molecule 4: HUMAN MONOCLONAL ANTIBODY



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	270	Depositor
Resolution determination method	Not provided	
CTF correction method	WHOLE MICROGRAPH	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	1650	Depositor
Maximum defocus (nm)	4060	Depositor
Magnification	69000	Depositor
Image detector	GENERIC GATAN	Depositor
Maximum map value	32443.000	Depositor
Minimum map value	-4448.000	Depositor
Average map value	3666.095	Depositor
Map value standard deviation	7633.060	Depositor
Recommended contour level	7999	Depositor
Map size (\AA)	436.17, 436.17, 436.17	wwPDB
Map dimensions	201, 201, 201	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	2.17, 2.17, 2.17	Depositor

5 Model quality i

5.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	12	10.40	482/1486 (32.4%)	8.02	615/2019 (30.5%)
1	16	10.40	482/1486 (32.4%)	8.02	615/2019 (30.5%)
1	1A	10.41	482/1486 (32.4%)	8.02	614/2019 (30.4%)
1	1E	10.41	483/1486 (32.5%)	8.02	615/2019 (30.5%)
1	1I	10.41	482/1486 (32.4%)	8.02	614/2019 (30.4%)
1	1M	10.41	482/1486 (32.4%)	8.02	614/2019 (30.4%)
1	1Q	10.40	483/1486 (32.5%)	8.02	614/2019 (30.4%)
1	1U	10.40	483/1486 (32.5%)	8.02	614/2019 (30.4%)
1	1Y	10.40	483/1486 (32.5%)	8.02	614/2019 (30.4%)
1	22	10.41	483/1486 (32.5%)	8.02	615/2019 (30.5%)
1	26	10.41	482/1486 (32.4%)	8.02	614/2019 (30.4%)
1	2A	10.40	482/1486 (32.4%)	8.02	615/2019 (30.5%)
1	2E	10.41	482/1486 (32.4%)	8.02	614/2019 (30.4%)
1	2I	10.41	482/1486 (32.4%)	8.02	614/2019 (30.4%)
1	2M	10.41	483/1486 (32.5%)	8.02	615/2019 (30.5%)
1	2Q	10.40	483/1486 (32.5%)	8.02	614/2019 (30.4%)
1	2U	10.40	483/1486 (32.5%)	8.02	614/2019 (30.4%)
1	2Y	10.40	483/1486 (32.5%)	8.02	614/2019 (30.4%)
1	32	10.41	482/1486 (32.4%)	8.02	614/2019 (30.4%)
1	36	10.41	483/1486 (32.5%)	8.02	615/2019 (30.5%)
1	3A	10.41	482/1486 (32.4%)	8.02	614/2019 (30.4%)
1	3E	10.41	482/1486 (32.4%)	8.02	614/2019 (30.4%)
1	3I	10.41	482/1486 (32.4%)	8.02	614/2019 (30.4%)
1	3M	10.41	483/1486 (32.5%)	8.02	615/2019 (30.5%)
1	3Q	10.40	482/1486 (32.4%)	8.02	615/2019 (30.5%)
1	3U	10.40	482/1486 (32.4%)	8.02	615/2019 (30.5%)
1	3Y	10.40	482/1486 (32.4%)	8.02	615/2019 (30.5%)
1	42	10.40	483/1486 (32.5%)	8.02	614/2019 (30.4%)
1	46	10.40	483/1486 (32.5%)	8.02	614/2019 (30.4%)
1	4A	10.41	482/1486 (32.4%)	8.02	614/2019 (30.4%)
1	4E	10.41	482/1486 (32.4%)	8.02	614/2019 (30.4%)
1	4I	10.41	483/1486 (32.5%)	8.02	615/2019 (30.5%)
1	4M	10.41	482/1486 (32.4%)	8.02	614/2019 (30.4%)
1	4Q	10.41	483/1486 (32.5%)	8.02	615/2019 (30.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	4U	10.41	482/1486 (32.4%)	8.02	614/2019 (30.4%)
1	4Y	10.41	482/1486 (32.4%)	8.02	614/2019 (30.4%)
1	52	10.40	483/1486 (32.5%)	8.02	614/2019 (30.4%)
1	56	10.40	483/1486 (32.5%)	8.02	614/2019 (30.4%)
1	5A	10.40	483/1486 (32.5%)	8.02	614/2019 (30.4%)
1	5E	10.40	482/1486 (32.4%)	8.02	615/2019 (30.5%)
1	5I	10.40	482/1486 (32.4%)	8.02	615/2019 (30.5%)
1	5M	10.40	482/1486 (32.4%)	8.02	615/2019 (30.5%)
1	5Q	10.41	482/1486 (32.4%)	8.02	614/2019 (30.4%)
1	5U	10.41	482/1486 (32.4%)	8.02	614/2019 (30.4%)
1	5Y	10.41	483/1486 (32.5%)	8.02	615/2019 (30.5%)
1	62	10.40	482/1486 (32.4%)	8.02	615/2019 (30.5%)
1	66	10.40	482/1486 (32.4%)	8.02	615/2019 (30.5%)
1	6A	10.40	483/1486 (32.5%)	8.02	614/2019 (30.4%)
1	6E	10.41	483/1486 (32.5%)	8.02	615/2019 (30.5%)
1	6I	10.41	482/1486 (32.4%)	8.02	614/2019 (30.4%)
1	6M	10.41	482/1486 (32.4%)	8.02	614/2019 (30.4%)
1	6Q	10.41	482/1486 (32.4%)	8.02	614/2019 (30.4%)
1	6U	10.41	482/1486 (32.4%)	8.02	614/2019 (30.4%)
1	6Y	10.41	483/1486 (32.5%)	8.02	615/2019 (30.5%)
1	7A	10.40	482/1486 (32.4%)	8.02	615/2019 (30.5%)
1	7E	10.41	482/1486 (32.4%)	8.02	614/2019 (30.4%)
1	7I	10.41	483/1486 (32.5%)	8.02	615/2019 (30.5%)
1	7M	10.41	482/1486 (32.4%)	8.02	614/2019 (30.4%)
1	7Q	10.41	482/1486 (32.4%)	8.02	614/2019 (30.4%)
1	7U	10.41	483/1486 (32.5%)	8.02	615/2019 (30.5%)
2	13	9.87	497/1865 (26.6%)	7.04	646/2550 (25.3%)
2	17	9.87	497/1865 (26.6%)	7.04	646/2550 (25.3%)
2	1B	9.87	497/1865 (26.6%)	7.04	647/2550 (25.4%)
2	1F	9.87	497/1865 (26.6%)	7.04	647/2550 (25.4%)
2	1J	9.87	497/1865 (26.6%)	7.04	647/2550 (25.4%)
2	1N	9.87	497/1865 (26.6%)	7.04	648/2550 (25.4%)
2	1R	9.87	496/1865 (26.6%)	7.04	647/2550 (25.4%)
2	1V	9.87	496/1865 (26.6%)	7.04	647/2550 (25.4%)
2	1Z	9.87	496/1865 (26.6%)	7.04	647/2550 (25.4%)
2	23	9.87	497/1865 (26.6%)	7.04	647/2550 (25.4%)
2	27	9.87	497/1865 (26.6%)	7.04	647/2550 (25.4%)
2	2B	9.87	497/1865 (26.6%)	7.04	646/2550 (25.3%)
2	2F	9.87	497/1865 (26.6%)	7.04	647/2550 (25.4%)
2	2J	9.87	497/1865 (26.6%)	7.04	648/2550 (25.4%)
2	2N	9.87	497/1865 (26.6%)	7.04	647/2550 (25.4%)
2	2R	9.87	496/1865 (26.6%)	7.04	647/2550 (25.4%)
2	2V	9.87	496/1865 (26.6%)	7.04	647/2550 (25.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	2Z	9.87	496/1865 (26.6%)	7.04	647/2550 (25.4%)
2	33	9.87	497/1865 (26.6%)	7.04	648/2550 (25.4%)
2	37	9.87	497/1865 (26.6%)	7.04	647/2550 (25.4%)
2	3B	9.87	497/1865 (26.6%)	7.04	648/2550 (25.4%)
2	3F	9.87	497/1865 (26.6%)	7.04	647/2550 (25.4%)
2	3J	9.87	497/1865 (26.6%)	7.04	648/2550 (25.4%)
2	3N	9.87	497/1865 (26.6%)	7.04	647/2550 (25.4%)
2	3R	9.87	497/1865 (26.6%)	7.04	646/2550 (25.3%)
2	3V	9.87	497/1865 (26.6%)	7.04	646/2550 (25.3%)
2	3Z	9.87	497/1865 (26.6%)	7.04	646/2550 (25.3%)
2	43	9.87	496/1865 (26.6%)	7.04	647/2550 (25.4%)
2	47	9.87	496/1865 (26.6%)	7.04	647/2550 (25.4%)
2	4B	9.87	497/1865 (26.6%)	7.04	647/2550 (25.4%)
2	4F	9.87	497/1865 (26.6%)	7.04	648/2550 (25.4%)
2	4J	9.87	497/1865 (26.6%)	7.04	647/2550 (25.4%)
2	4N	9.87	497/1865 (26.6%)	7.04	647/2550 (25.4%)
2	4R	9.87	497/1865 (26.6%)	7.04	647/2550 (25.4%)
2	4V	9.87	497/1865 (26.6%)	7.04	647/2550 (25.4%)
2	4Z	9.87	497/1865 (26.6%)	7.04	648/2550 (25.4%)
2	53	9.87	496/1865 (26.6%)	7.04	647/2550 (25.4%)
2	57	9.87	496/1865 (26.6%)	7.04	647/2550 (25.4%)
2	5B	9.87	496/1865 (26.6%)	7.04	647/2550 (25.4%)
2	5F	9.87	497/1865 (26.6%)	7.04	646/2550 (25.3%)
2	5J	9.87	497/1865 (26.6%)	7.04	646/2550 (25.3%)
2	5N	9.87	497/1865 (26.6%)	7.04	646/2550 (25.3%)
2	5R	9.87	497/1865 (26.6%)	7.04	647/2550 (25.4%)
2	5V	9.87	497/1865 (26.6%)	7.04	648/2550 (25.4%)
2	5Z	9.87	497/1865 (26.6%)	7.04	647/2550 (25.4%)
2	63	9.87	497/1865 (26.6%)	7.04	646/2550 (25.3%)
2	67	9.87	497/1865 (26.6%)	7.04	646/2550 (25.3%)
2	6B	9.87	496/1865 (26.6%)	7.04	647/2550 (25.4%)
2	6F	9.87	497/1865 (26.6%)	7.04	647/2550 (25.4%)
2	6J	9.87	497/1865 (26.6%)	7.04	647/2550 (25.4%)
2	6N	9.87	497/1865 (26.6%)	7.04	648/2550 (25.4%)
2	6R	9.87	497/1865 (26.6%)	7.04	647/2550 (25.4%)
2	6V	9.87	497/1865 (26.6%)	7.04	648/2550 (25.4%)
2	6Z	9.87	497/1865 (26.6%)	7.04	647/2550 (25.4%)
2	7B	9.87	497/1865 (26.6%)	7.04	646/2550 (25.3%)
2	7F	9.87	497/1865 (26.6%)	7.04	648/2550 (25.4%)
2	7J	9.87	497/1865 (26.6%)	7.04	647/2550 (25.4%)
2	7N	9.87	497/1865 (26.6%)	7.04	647/2550 (25.4%)
2	7R	9.87	497/1865 (26.6%)	7.04	648/2550 (25.4%)
2	7V	9.87	497/1865 (26.6%)	7.04	647/2550 (25.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	10	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	14	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	18	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	1C	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	1G	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	1K	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	1O	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	1S	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	1W	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	20	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	24	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	28	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	2C	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	2G	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	2K	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	2O	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	2S	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	2W	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	30	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	34	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	38	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	3C	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	3G	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	3K	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	3O	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	3S	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	3W	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	40	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	44	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	48	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	4C	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	4G	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	4K	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	4O	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	4S	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	4W	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	50	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	54	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	58	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	5C	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	5G	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	5K	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	5O	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	5S	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	5W	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	60	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	64	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	68	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	6C	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	6G	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	6K	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	6O	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	6S	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	6W	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	7C	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	7G	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	7K	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	7O	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	7S	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
3	7W	1.00	1/1043 (0.1%)	1.60	18/1411 (1.3%)
4	11	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	15	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	19	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	1D	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	1H	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	1L	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	1P	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	1T	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	1X	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	21	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	25	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	29	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	2D	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	2H	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	2L	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	2P	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	2T	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	2X	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	31	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	35	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	39	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	3D	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	3H	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	3L	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	3P	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	3T	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	3X	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	4I	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	45	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	49	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	4D	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	4H	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	4L	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	4P	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	4T	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	4X	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	51	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	55	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	59	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	5D	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	5H	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	5L	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	5P	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	5T	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	5X	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	61	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	65	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	69	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	6D	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	6H	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	6L	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	6P	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	6T	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	6X	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	7D	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	7H	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	7L	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	7P	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	7T	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
4	7X	1.10	1/1081 (0.1%)	1.69	21/1461 (1.4%)
All	All	7.94	58872/328500 (17.9%)	5.96	78024/446460 (17.5%)

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	5	70
2	17	5	70
2	1B	5	70
2	1F	5	70
2	1J	5	70
2	1N	5	70
2	1R	5	70
2	1V	5	70
2	1Z	5	70
2	23	5	70
2	27	5	70
2	2B	5	70
2	2F	5	70
2	2J	5	70
2	2N	5	70
2	2R	5	70
2	2V	5	70
2	2Z	5	70
2	33	5	70
2	37	5	70
2	3B	5	70
2	3F	5	70
2	3J	5	70
2	3N	5	70
2	3R	5	70

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	3V	5	70
2	3Z	5	70
2	43	5	70
2	47	5	70
2	4B	5	70
2	4F	5	70
2	4J	5	70
2	4N	5	70
2	4R	5	70
2	4V	5	70
2	4Z	5	70
2	53	5	70
2	57	5	70
2	5B	5	70
2	5F	5	70
2	5J	5	70
2	5N	5	70
2	5R	5	70
2	5V	5	70
2	5Z	5	70
2	63	5	70
2	67	5	70
2	6B	5	70
2	6F	5	70
2	6J	5	70
2	6N	5	70
2	6R	5	70
2	6V	5	70
2	6Z	5	70
2	7B	5	70
2	7F	5	70
2	7J	5	70
2	7N	5	70
2	7R	5	70
2	7V	5	70
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	720	9120

The worst 5 of 58872 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1F	108	HIS	ND1-CE1	73.61	2.06	1.32
2	2N	108	HIS	ND1-CE1	73.61	2.06	1.32
2	23	108	HIS	ND1-CE1	73.61	2.06	1.32
2	3N	108	HIS	ND1-CE1	73.61	2.06	1.32
2	37	108	HIS	ND1-CE1	73.61	2.06	1.32

The worst 5 of 78024 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1M	151	ASN	N-CA-CB	52.12	162.68	109.51
1	2I	151	ASN	N-CA-CB	52.12	162.68	109.51
1	3A	151	ASN	N-CA-CB	52.12	162.68	109.51
1	3I	151	ASN	N-CA-CB	52.12	162.68	109.51
1	32	151	ASN	N-CA-CB	52.12	162.68	109.51

5 of 720 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 9120 planarity outliers are listed below:

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

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	12	1449	0	1392	0	0
1	16	1449	0	1392	0	0
1	1A	1449	0	1392	0	0
1	1E	1449	0	1392	0	0
1	1I	1449	0	1392	0	0
1	1M	1449	0	1392	0	0
1	1Q	1449	0	1392	0	0
1	1U	1449	0	1392	0	0
1	1Y	1449	0	1392	0	0
1	22	1449	0	1392	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	26	1449	0	1392	0	0
1	2A	1449	0	1392	0	0
1	2E	1449	0	1392	0	0
1	2I	1449	0	1392	0	0
1	2M	1449	0	1392	0	0
1	2Q	1449	0	1392	0	0
1	2U	1449	0	1392	0	0
1	2Y	1449	0	1392	0	0
1	32	1449	0	1392	0	0
1	36	1449	0	1392	0	0
1	3A	1449	0	1392	0	0
1	3E	1449	0	1392	0	0
1	3I	1449	0	1392	0	0
1	3M	1449	0	1392	0	0
1	3Q	1449	0	1392	0	0
1	3U	1449	0	1392	0	0
1	3Y	1449	0	1392	0	0
1	42	1449	0	1392	0	0
1	46	1449	0	1392	0	0
1	4A	1449	0	1392	0	0
1	4E	1449	0	1392	0	0
1	4I	1449	0	1392	0	0
1	4M	1449	0	1392	0	0
1	4Q	1449	0	1392	0	0
1	4U	1449	0	1392	0	0
1	4Y	1449	0	1392	0	0
1	52	1449	0	1392	0	0
1	56	1449	0	1392	0	0
1	5A	1449	0	1392	0	0
1	5E	1449	0	1392	0	0
1	5I	1449	0	1392	0	0
1	5M	1449	0	1392	0	0
1	5Q	1449	0	1392	0	0
1	5U	1449	0	1392	0	0
1	5Y	1449	0	1392	0	0
1	62	1449	0	1392	0	0
1	66	1449	0	1392	0	0
1	6A	1449	0	1392	0	0
1	6E	1449	0	1392	0	0
1	6I	1449	0	1392	0	0
1	6M	1449	0	1392	0	0
1	6Q	1449	0	1392	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	6U	1449	0	1392	0	0
1	6Y	1449	0	1392	0	0
1	7A	1449	0	1392	0	0
1	7E	1449	0	1392	0	0
1	7I	1449	0	1392	0	0
1	7M	1449	0	1392	0	0
1	7Q	1449	0	1392	0	0
1	7U	1449	0	1392	0	0
2	13	1810	0	1683	0	0
2	17	1810	0	1683	0	0
2	1B	1810	0	1683	0	0
2	1F	1810	0	1683	0	0
2	1J	1810	0	1683	0	0
2	1N	1810	0	1683	0	0
2	1R	1810	0	1683	0	0
2	1V	1810	0	1683	0	0
2	1Z	1810	0	1683	0	0
2	23	1810	0	1683	0	0
2	27	1810	0	1683	0	0
2	2B	1810	0	1683	0	0
2	2F	1810	0	1683	0	0
2	2J	1810	0	1683	0	0
2	2N	1810	0	1683	0	0
2	2R	1810	0	1683	0	0
2	2V	1810	0	1683	0	0
2	2Z	1810	0	1683	0	0
2	33	1810	0	1683	0	0
2	37	1810	0	1683	0	0
2	3B	1810	0	1683	0	0
2	3F	1810	0	1683	0	0
2	3J	1810	0	1683	0	0
2	3N	1810	0	1683	0	0
2	3R	1810	0	1683	0	0
2	3V	1810	0	1683	0	0
2	3Z	1810	0	1683	0	0
2	43	1810	0	1683	0	0
2	47	1810	0	1683	0	0
2	4B	1810	0	1683	0	0
2	4F	1810	0	1683	0	0
2	4J	1810	0	1683	0	0
2	4N	1810	0	1683	0	0
2	4R	1810	0	1683	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	4V	1810	0	1683	0	0
2	4Z	1810	0	1683	0	0
2	53	1810	0	1683	0	0
2	57	1810	0	1683	0	0
2	5B	1810	0	1683	0	0
2	5F	1810	0	1683	0	0
2	5J	1810	0	1683	0	0
2	5N	1810	0	1683	0	0
2	5R	1810	0	1683	0	0
2	5V	1810	0	1683	0	0
2	5Z	1810	0	1683	0	0
2	63	1810	0	1683	0	0
2	67	1810	0	1683	0	0
2	6B	1810	0	1683	0	0
2	6F	1810	0	1683	0	0
2	6J	1810	0	1683	0	0
2	6N	1810	0	1683	0	0
2	6R	1810	0	1683	0	0
2	6V	1810	0	1683	0	0
2	6Z	1810	0	1683	0	0
2	7B	1810	0	1683	0	0
2	7F	1810	0	1683	0	0
2	7J	1810	0	1683	0	0
2	7N	1810	0	1683	0	0
2	7R	1810	0	1683	0	0
2	7V	1810	0	1683	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	267300	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%)	0 4
1	16	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0 4

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	4Q	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	4
1	4U	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	4
1	4Y	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	4
1	52	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	4
1	56	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	4
1	5A	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	4
1	5E	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	4
1	5I	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	4
1	5M	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	4
1	5Q	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	4
1	5U	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	4
1	5Y	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	4
1	62	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	4
1	66	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	4
1	6A	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	4
1	6E	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	4
1	6I	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	4
1	6M	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	4
1	6Q	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	4
1	6U	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	4
1	6Y	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	4
1	7A	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	4
1	7E	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	4
1	7I	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	4
1	7M	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	4
1	7Q	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	4
1	7U	181/183 (99%)	142 (78%)	17 (9%)	22 (12%)	0	4
2	13	226/229 (99%)	157 (70%)	27 (12%)	42 (19%)	0	2
2	17	226/229 (99%)	157 (70%)	27 (12%)	42 (19%)	0	2
2	1B	226/229 (99%)	157 (70%)	26 (12%)	43 (19%)	0	2
2	1F	226/229 (99%)	156 (69%)	27 (12%)	43 (19%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	1J	226/229 (99%)	157 (70%)	26 (12%)	43 (19%)	0	2
2	1N	226/229 (99%)	156 (69%)	27 (12%)	43 (19%)	0	2
2	1R	226/229 (99%)	155 (69%)	28 (12%)	43 (19%)	0	2
2	1V	226/229 (99%)	155 (69%)	28 (12%)	43 (19%)	0	2
2	1Z	226/229 (99%)	155 (69%)	28 (12%)	43 (19%)	0	2
2	23	226/229 (99%)	156 (69%)	27 (12%)	43 (19%)	0	2
2	27	226/229 (99%)	157 (70%)	26 (12%)	43 (19%)	0	2
2	2B	226/229 (99%)	157 (70%)	27 (12%)	42 (19%)	0	2
2	2F	226/229 (99%)	157 (70%)	26 (12%)	43 (19%)	0	2
2	2J	226/229 (99%)	156 (69%)	27 (12%)	43 (19%)	0	2
2	2N	226/229 (99%)	156 (69%)	27 (12%)	43 (19%)	0	2
2	2R	226/229 (99%)	155 (69%)	28 (12%)	43 (19%)	0	2
2	2V	226/229 (99%)	155 (69%)	28 (12%)	43 (19%)	0	2
2	2Z	226/229 (99%)	155 (69%)	28 (12%)	43 (19%)	0	2
2	33	226/229 (99%)	156 (69%)	27 (12%)	43 (19%)	0	2
2	37	226/229 (99%)	156 (69%)	27 (12%)	43 (19%)	0	2
2	3B	226/229 (99%)	156 (69%)	27 (12%)	43 (19%)	0	2
2	3F	226/229 (99%)	157 (70%)	26 (12%)	43 (19%)	0	2
2	3J	226/229 (99%)	156 (69%)	27 (12%)	43 (19%)	0	2
2	3N	226/229 (99%)	156 (69%)	27 (12%)	43 (19%)	0	2
2	3R	226/229 (99%)	157 (70%)	27 (12%)	42 (19%)	0	2
2	3V	226/229 (99%)	157 (70%)	27 (12%)	42 (19%)	0	2
2	3Z	226/229 (99%)	157 (70%)	27 (12%)	42 (19%)	0	2
2	43	226/229 (99%)	155 (69%)	28 (12%)	43 (19%)	0	2
2	47	226/229 (99%)	155 (69%)	28 (12%)	43 (19%)	0	2
2	4B	226/229 (99%)	157 (70%)	26 (12%)	43 (19%)	0	2
2	4F	226/229 (99%)	156 (69%)	27 (12%)	43 (19%)	0	2
2	4J	226/229 (99%)	156 (69%)	27 (12%)	43 (19%)	0	2
2	4N	226/229 (99%)	157 (70%)	26 (12%)	43 (19%)	0	2
2	4R	226/229 (99%)	156 (69%)	27 (12%)	43 (19%)	0	2
2	4V	226/229 (99%)	157 (70%)	26 (12%)	43 (19%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	4Z	226/229 (99%)	156 (69%)	27 (12%)	43 (19%)	0	2
2	53	226/229 (99%)	155 (69%)	28 (12%)	43 (19%)	0	2
2	57	226/229 (99%)	155 (69%)	28 (12%)	43 (19%)	0	2
2	5B	226/229 (99%)	155 (69%)	28 (12%)	43 (19%)	0	2
2	5F	226/229 (99%)	157 (70%)	27 (12%)	42 (19%)	0	2
2	5J	226/229 (99%)	157 (70%)	27 (12%)	42 (19%)	0	2
2	5N	226/229 (99%)	157 (70%)	27 (12%)	42 (19%)	0	2
2	5R	226/229 (99%)	157 (70%)	26 (12%)	43 (19%)	0	2
2	5V	226/229 (99%)	156 (69%)	27 (12%)	43 (19%)	0	2
2	5Z	226/229 (99%)	156 (69%)	27 (12%)	43 (19%)	0	2
2	63	226/229 (99%)	157 (70%)	27 (12%)	42 (19%)	0	2
2	67	226/229 (99%)	157 (70%)	27 (12%)	42 (19%)	0	2
2	6B	226/229 (99%)	155 (69%)	28 (12%)	43 (19%)	0	2
2	6F	226/229 (99%)	156 (69%)	27 (12%)	43 (19%)	0	2
2	6J	226/229 (99%)	157 (70%)	26 (12%)	43 (19%)	0	2
2	6N	226/229 (99%)	156 (69%)	27 (12%)	43 (19%)	0	2
2	6R	226/229 (99%)	157 (70%)	26 (12%)	43 (19%)	0	2
2	6V	226/229 (99%)	156 (69%)	27 (12%)	43 (19%)	0	2
2	6Z	226/229 (99%)	156 (69%)	27 (12%)	43 (19%)	0	2
2	7B	226/229 (99%)	157 (70%)	27 (12%)	42 (19%)	0	2
2	7F	226/229 (99%)	156 (69%)	27 (12%)	43 (19%)	0	2
2	7J	226/229 (99%)	156 (69%)	27 (12%)	43 (19%)	0	2
2	7N	226/229 (99%)	157 (70%)	26 (12%)	43 (19%)	0	2
2	7R	226/229 (99%)	156 (69%)	27 (12%)	43 (19%)	0	2
2	7V	226/229 (99%)	156 (69%)	27 (12%)	43 (19%)	0	2
3	10	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	14	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	18	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	1C	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	1G	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	1K	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1O	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	1S	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	1W	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	20	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	24	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	28	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	2C	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	2G	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	2K	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	2O	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	2S	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	2W	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	30	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	34	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	38	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	3C	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	3G	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	3K	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	3O	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	3S	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	3W	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	40	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	44	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	48	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	4C	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	4G	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	4K	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	4O	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	4S	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	4W	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	50	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	54	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	58	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	5C	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	5G	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	5K	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	5O	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	5S	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	5W	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	60	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	64	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	68	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	6C	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	6G	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	6K	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	6O	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	6S	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	6W	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	7C	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	7G	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	7K	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	7O	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	7S	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
3	7W	124/109 (114%)	116 (94%)	7 (6%)	1 (1%)	16	54
4	11	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	5	29
4	15	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	5	29
4	19	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	5	29
4	1D	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	5	29
4	1H	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	5	29
4	1L	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	5	29
4	1P	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	5	29
4	1T	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	5	29

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	5D	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	5	29
4	5H	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	5	29
4	5L	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	5	29
4	5P	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	5	29
4	5T	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	5	29
4	5X	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	5	29
4	6I	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	5	29
4	65	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	5	29
4	69	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	5	29
4	6D	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	5	29
4	6H	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	5	29
4	6L	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	5	29
4	6P	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	5	29
4	6T	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	5	29
4	6X	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	5	29
4	7D	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	5	29
4	7H	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	5	29
4	7L	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	5	29
4	7P	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	5	29
4	7T	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	5	29
4	7X	135/122 (111%)	124 (92%)	8 (6%)	3 (2%)	5	29
All	All	39960/38580 (104%)	32292 (81%)	3540 (9%)	4128 (10%)	1	6

5 of 4128 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains [i](#)

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

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

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	7M	163/163 (100%)	131 (80%)	32 (20%)	1	7
1	7Q	163/163 (100%)	130 (80%)	33 (20%)	1	7
1	7U	163/163 (100%)	131 (80%)	32 (20%)	1	7
2	13	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	17	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	1B	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	1F	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	1J	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	1N	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	1R	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	1V	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	1Z	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	23	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	27	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	2B	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	2F	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	2J	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	2N	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	2R	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	2V	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	2Z	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	33	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	37	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	3B	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	3F	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	3J	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	3N	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	3R	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	3V	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	3Z	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	43	204/203 (100%)	157 (77%)	47 (23%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	47	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	4B	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	4F	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	4J	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	4N	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	4R	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	4V	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	4Z	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	53	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	57	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	5B	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	5F	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	5J	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	5N	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	5R	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	5V	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	5Z	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	63	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	67	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	6B	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	6F	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	6J	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	6N	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	6R	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	6V	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	6Z	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	7B	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	7F	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	7J	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	7N	204/203 (100%)	157 (77%)	47 (23%)	1	6
2	7R	204/203 (100%)	157 (77%)	47 (23%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	7V	204/203 (100%)	157 (77%)	47 (23%)	1	6
3	10	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	14	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	18	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	1C	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	1G	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	1K	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	1O	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	1S	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	1W	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	20	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	24	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	28	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	2C	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	2G	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	2K	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	2O	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	2S	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	2W	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	30	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	34	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	38	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	3C	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	3G	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	3K	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	3O	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	3S	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	3W	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	40	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	44	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	48	110/93 (118%)	101 (92%)	9 (8%)	10	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	4C	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	4G	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	4K	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	4O	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	4S	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	4W	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	50	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	54	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	58	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	5C	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	5G	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	5K	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	5O	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	5S	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	5W	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	60	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	64	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	68	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	6C	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	6G	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	6K	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	6O	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	6S	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	6W	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	7C	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	7G	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	7K	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	7O	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	7S	110/93 (118%)	101 (92%)	9 (8%)	10	31
3	7W	110/93 (118%)	101 (92%)	9 (8%)	10	31
4	11	112/97 (116%)	92 (82%)	20 (18%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	15	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	19	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	1D	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	1H	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	1L	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	1P	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	1T	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	1X	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	21	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	25	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	29	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	2D	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	2H	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	2L	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	2P	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	2T	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	2X	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	31	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	35	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	39	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	3D	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	3H	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	3L	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	3P	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	3T	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	3X	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	41	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	45	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	49	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	4D	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	4H	112/97 (116%)	92 (82%)	20 (18%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	4L	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	4P	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	4T	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	4X	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	51	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	55	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	59	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	5D	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	5H	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	5L	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	5P	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	5T	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	5X	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	61	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	65	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	69	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	6D	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	6H	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	6L	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	6P	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	6T	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	6X	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	7D	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	7H	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	7L	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	7P	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	7T	112/97 (116%)	92 (82%)	20 (18%)	2	9
4	7X	112/97 (116%)	92 (82%)	20 (18%)	2	9
All	All	35340/33360 (106%)	28836 (82%)	6504 (18%)	3	8

5 of 6504 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	42	97	SER
2	5Z	2	GLU
1	7U	22	HIS
1	46	111	ILE
1	42	84	ARG

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

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

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

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

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

The worst 5 of 3192 chain breaks are listed below:

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

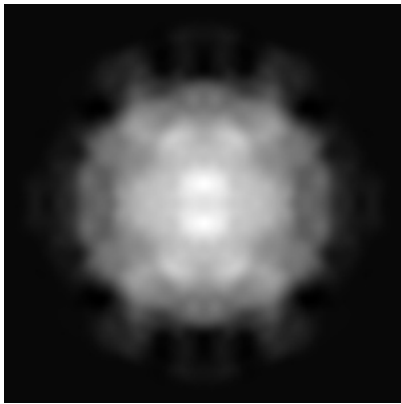
6 Map visualisation [i](#)

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

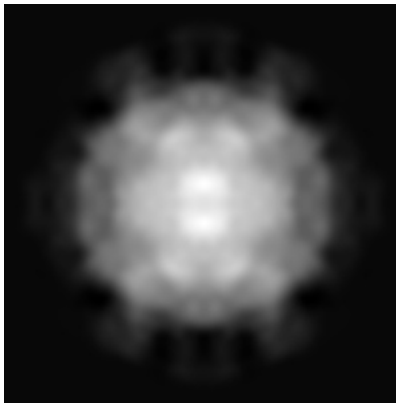
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

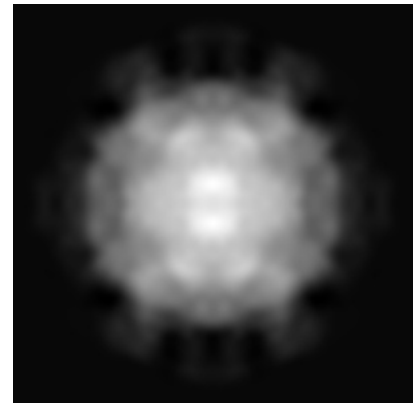
6.1.1 Primary map



X



Y

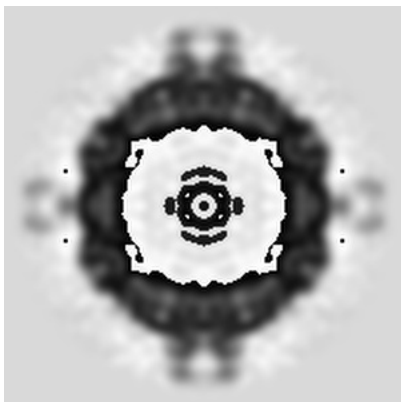


Z

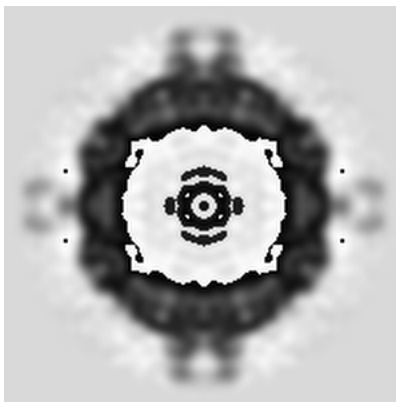
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

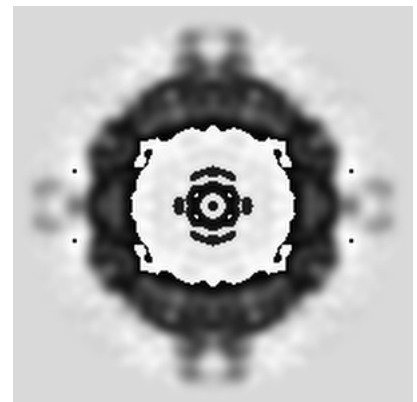
6.2.1 Primary map



X Index: 100



Y Index: 100

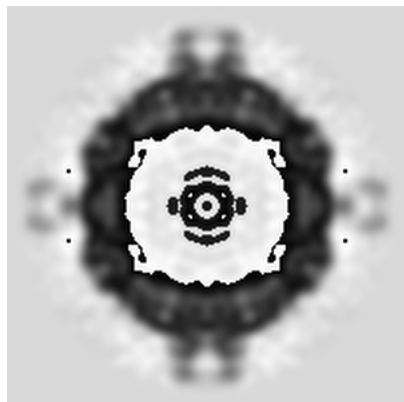


Z Index: 100

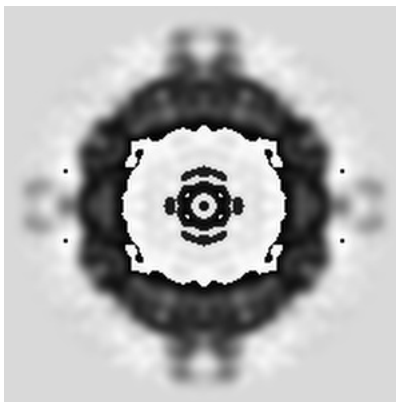
The images above show central slices of the map in three orthogonal directions.

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

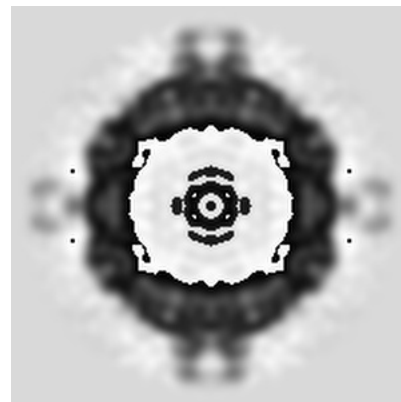
6.3.1 Primary map



X Index: 100



Y Index: 100

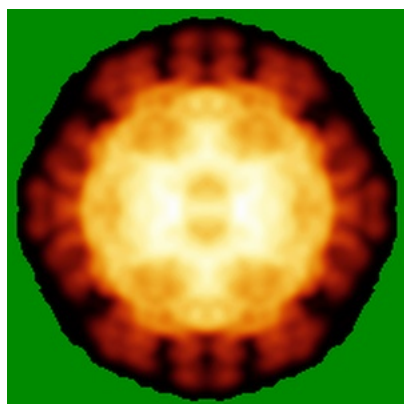


Z Index: 100

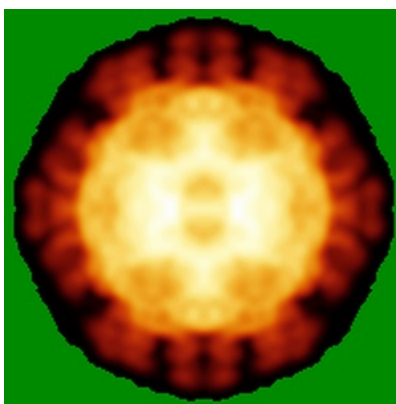
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [\(i\)](#)

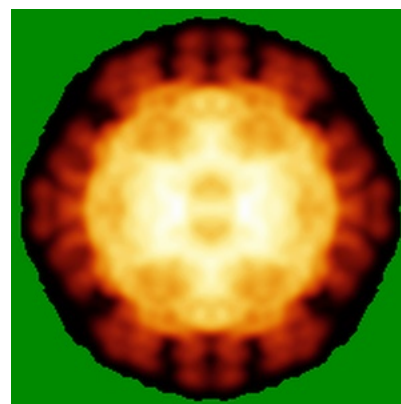
6.4.1 Primary map



X



Y

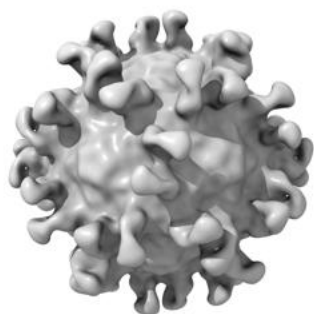


Z

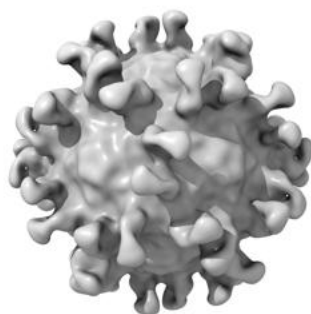
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

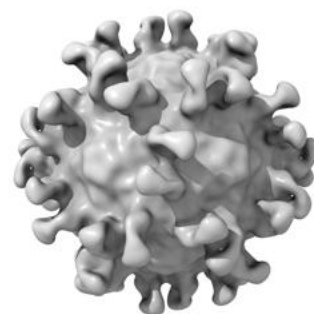
6.5.1 Primary map



X



Y



Z

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

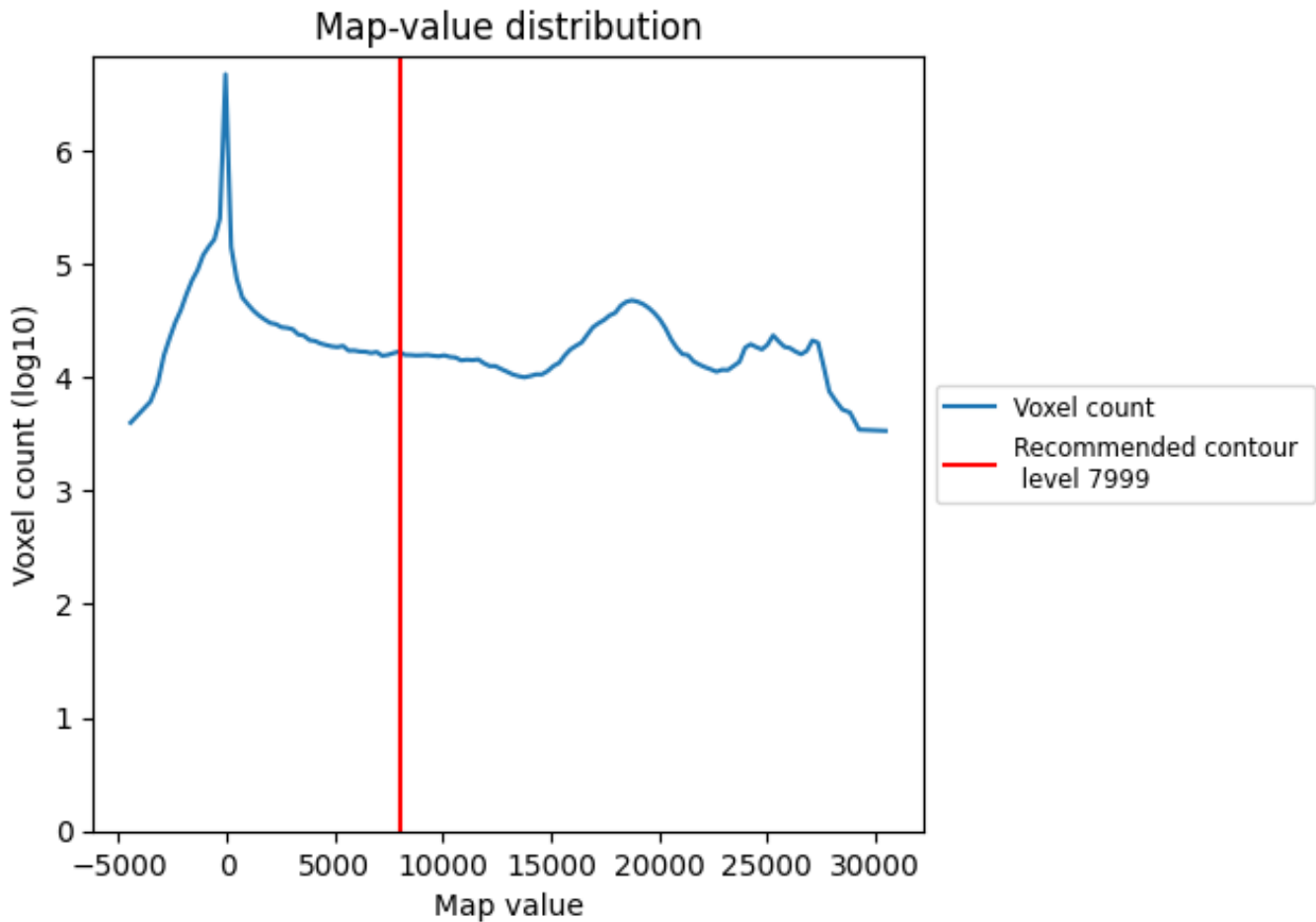
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

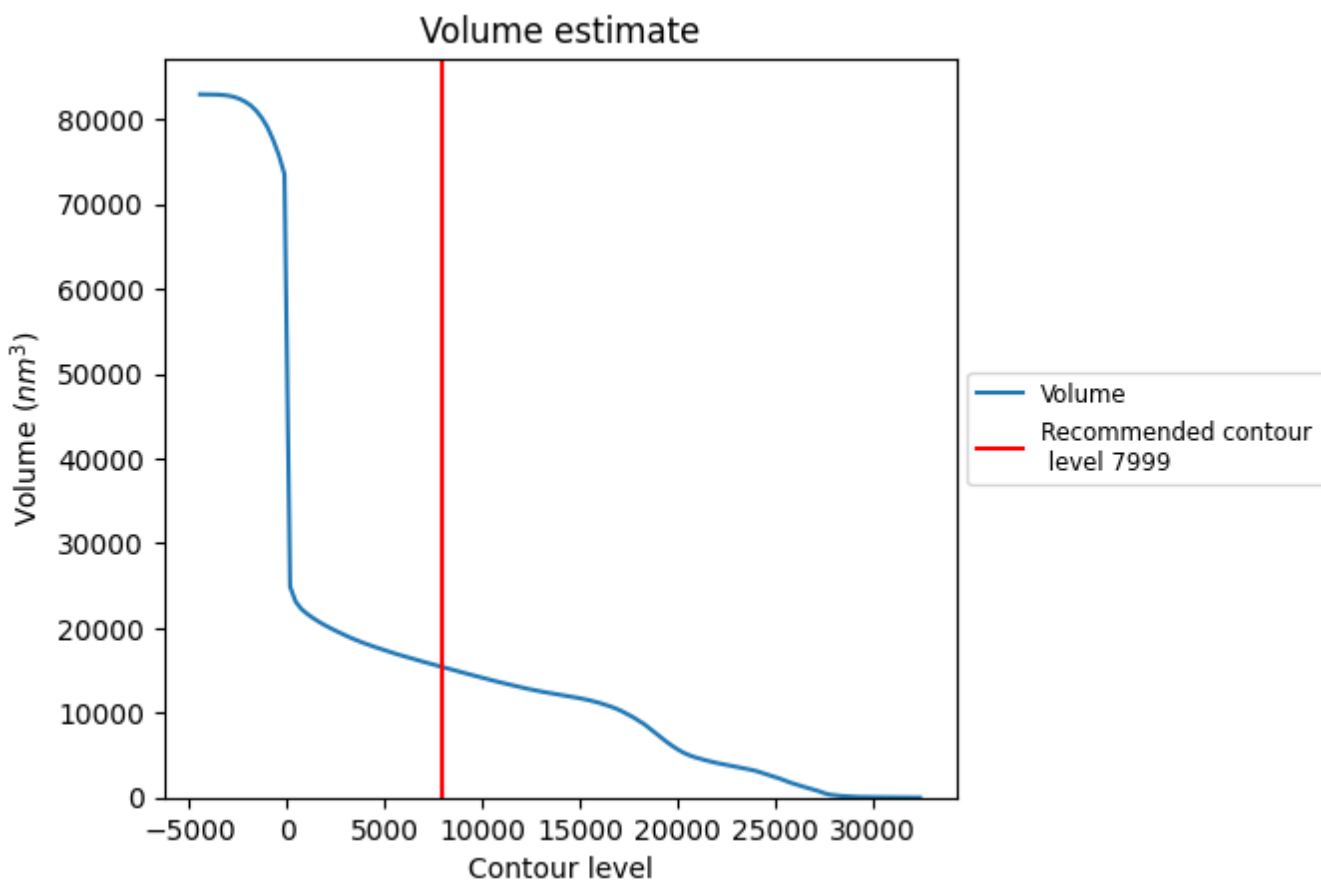
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

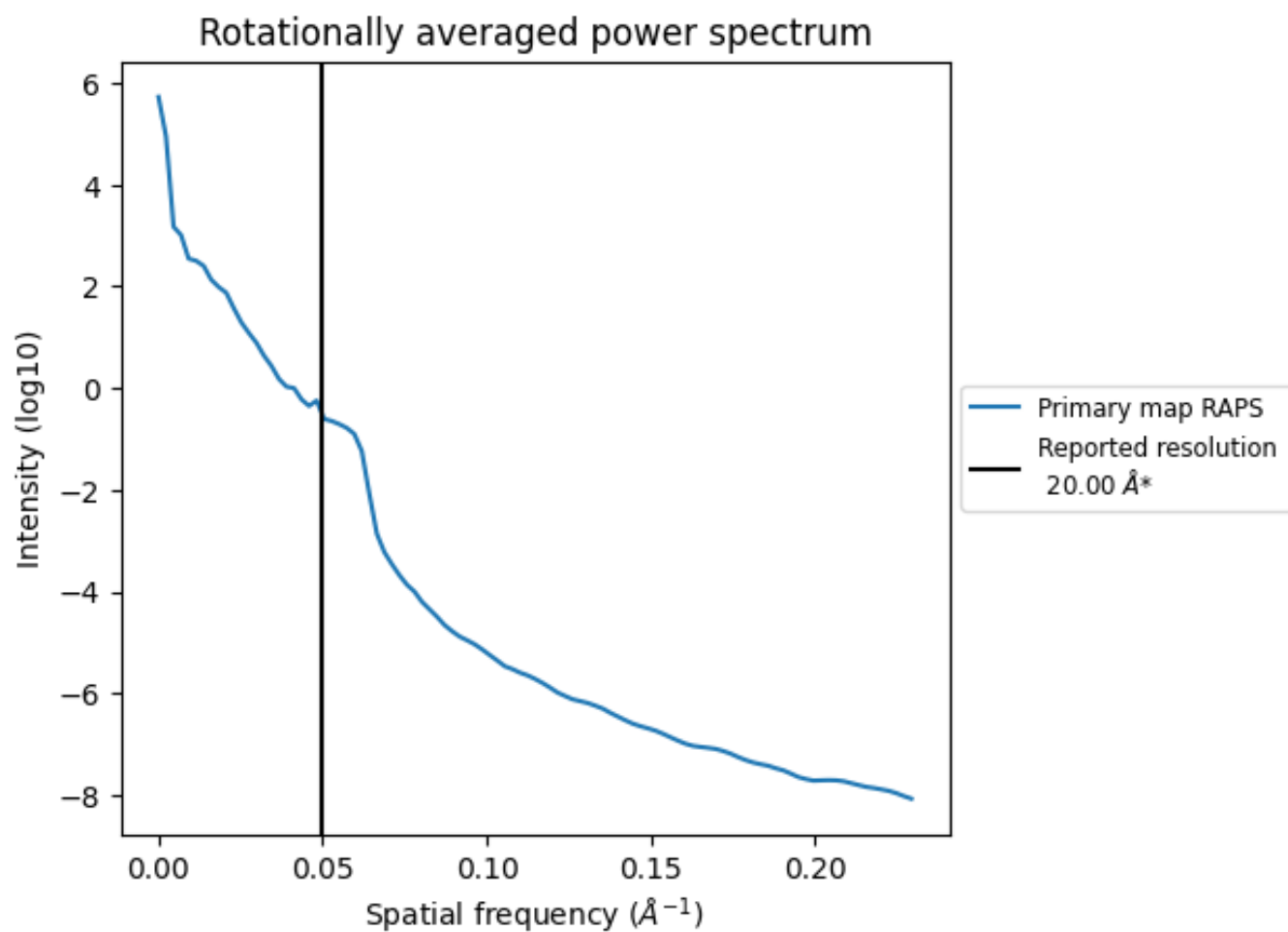
7.2 Volume estimate [\(i\)](#)



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

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

7.3 Rotationally averaged power spectrum [i](#)

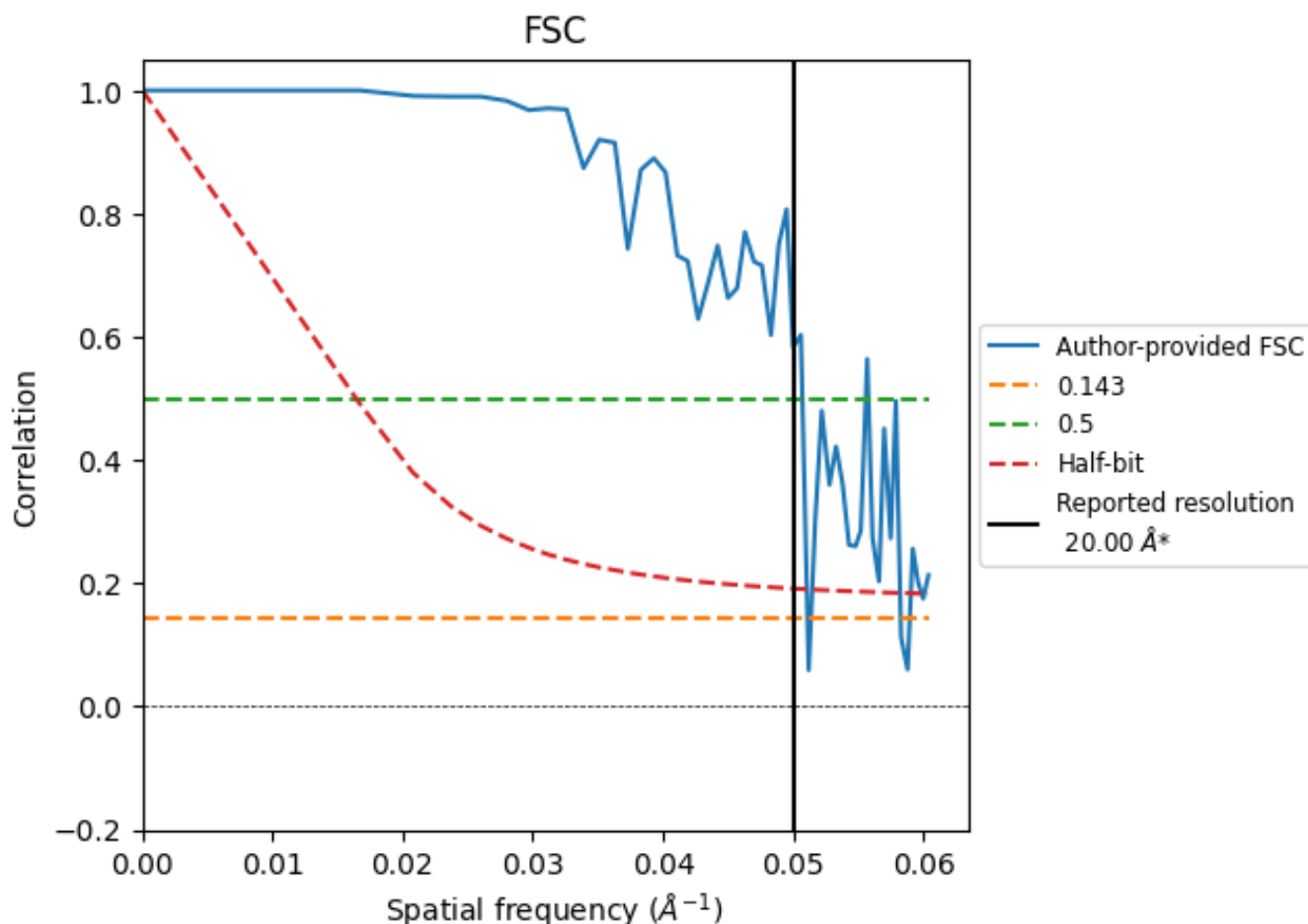


*Reported resolution corresponds to spatial frequency of 0.050 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.050 Å⁻¹

8.2 Resolution estimates [i](#)

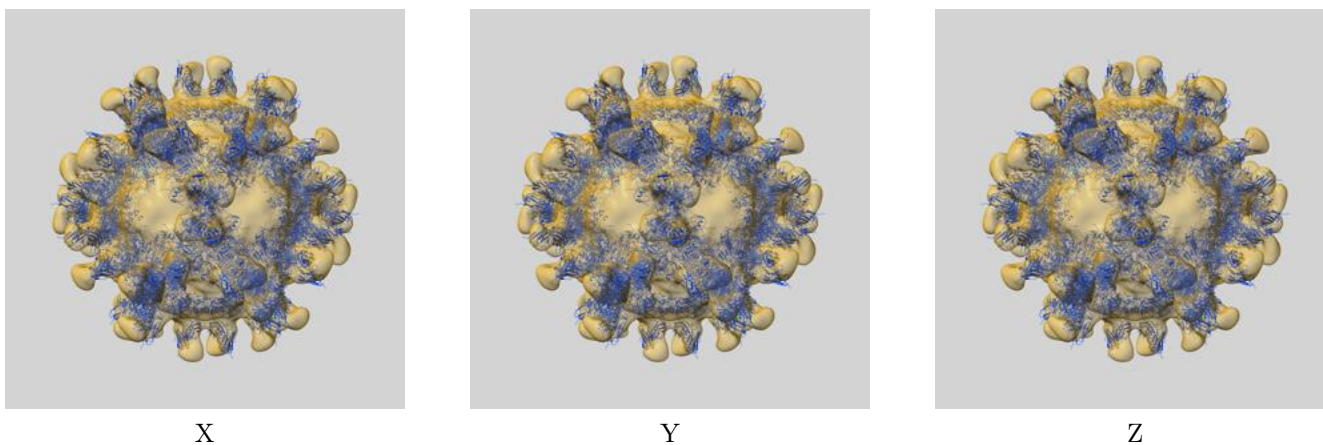
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	19.57	19.72	19.61
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

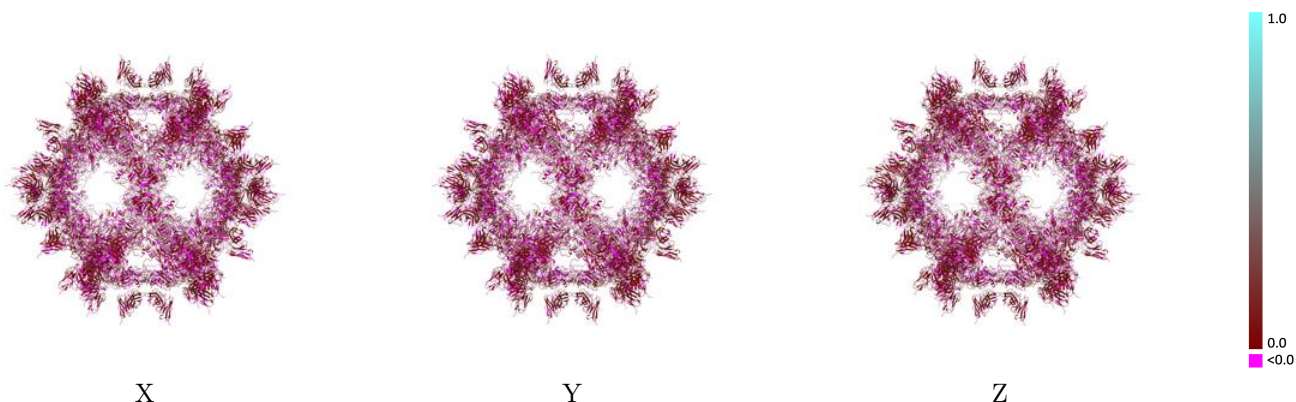
This section contains information regarding the fit between EMDB map EMD-2761 and PDB model 4UDF. Per-residue inclusion information can be found in section 3 on page 25.

9.1 Map-model overlay [i](#)



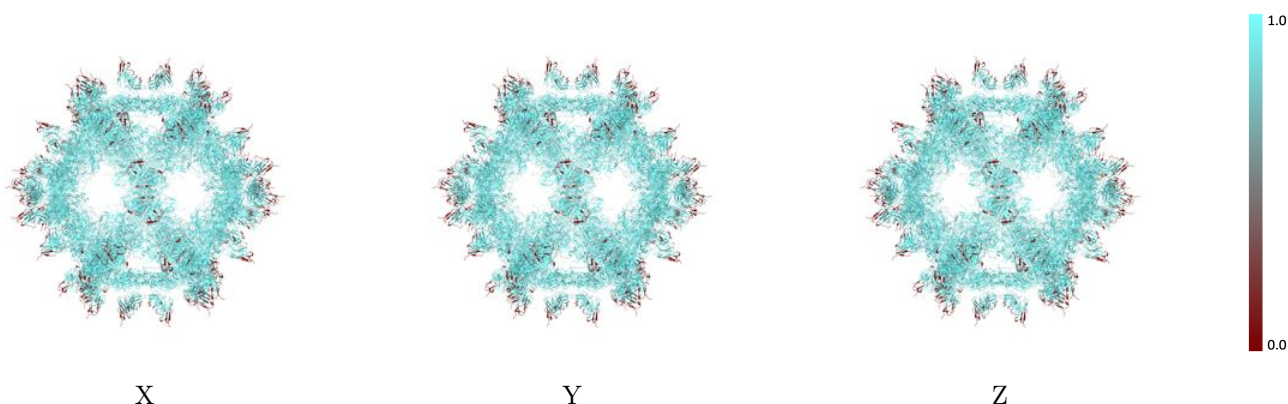
The images above show the 3D surface view of the map at the recommended contour level 7999.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



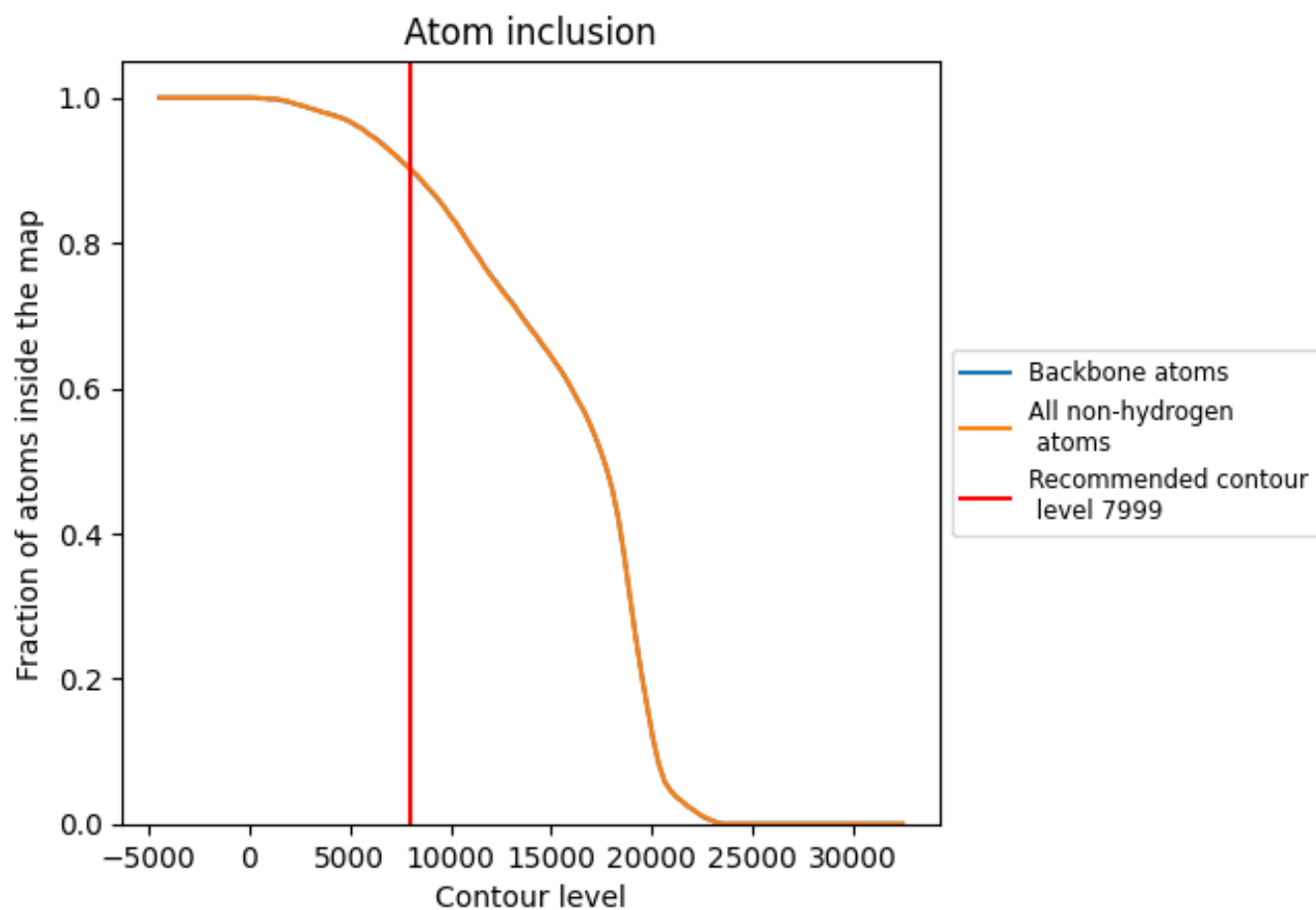
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (7999).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary





















































































The table lists the average atom inclusion at the recommended contour level (7999) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9020	 0.0570
10	 0.6390	 0.0440
11	 0.8000	 0.0460
12	 0.9940	 0.0680
13	 0.9970	 0.0550
14	 0.6900	 0.0530
15	 0.8160	 0.0400
16	 0.9940	 0.0760
17	 0.9970	 0.0550
18	 0.6900	 0.0660
19	 0.8160	 0.0590
1A	 0.9940	 0.0640
1B	 0.9960	 0.0460
1C	 0.6300	 0.0570
1D	 0.7840	 0.0460
1E	 0.9920	 0.0660
1F	 0.9970	 0.0480
1G	 0.6360	 0.0470
1H	 0.7890	 0.0450
1I	 0.9940	 0.0710
1J	 0.9960	 0.0520
1K	 0.6300	 0.0570
1L	 0.7840	 0.0520
1M	 0.9940	 0.0700
1N	 0.9970	 0.0550
1O	 0.6910	 0.0610
1P	 0.8100	 0.0570
1Q	 0.9940	 0.0750
1R	 0.9970	 0.0580
1S	 0.6390	 0.0580
1T	 0.8000	 0.0580
1U	 0.9940	 0.0690
1V	 0.9970	 0.0500
1W	 0.6390	 0.0520
1X	 0.8000	 0.0510



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Chain	Atom inclusion	Q-score
1Y	 0.9940	 0.0670
1Z	 0.9970	 0.0500
20	 0.6390	 0.0500
21	 0.8000	 0.0450
22	 0.9920	 0.0700
23	 0.9970	 0.0520
24	 0.6360	 0.0470
25	 0.7890	 0.0540
26	 0.9940	 0.0660
27	 0.9960	 0.0480
28	 0.6300	 0.0410
29	 0.7840	 0.0460
2A	 0.9940	 0.0710
2B	 0.9970	 0.0500
2C	 0.6900	 0.0580
2D	 0.8160	 0.0470
2E	 0.9940	 0.0750
2F	 0.9960	 0.0550
2G	 0.6300	 0.0620
2H	 0.7840	 0.0530
2I	 0.9940	 0.0640
2J	 0.9970	 0.0480
2K	 0.6910	 0.0490
2L	 0.8100	 0.0450
2M	 0.9920	 0.0690
2N	 0.9970	 0.0530
2O	 0.6360	 0.0530
2P	 0.7890	 0.0560
2Q	 0.9940	 0.0690
2R	 0.9970	 0.0550
2S	 0.6390	 0.0570
2T	 0.8000	 0.0520
2U	 0.9940	 0.0770
2V	 0.9970	 0.0560
2W	 0.6390	 0.0620
2X	 0.8000	 0.0590
2Y	 0.9940	 0.0680
2Z	 0.9970	 0.0490
30	 0.6900	 0.0520
31	 0.8160	 0.0560
32	 0.9940	 0.0620
33	 0.9970	 0.0470





















































































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Chain	Atom inclusion	Q-score
34	0.6910	0.0440
35	0.8100	0.0500
36	0.9920	0.0690
37	0.9970	0.0560
38	0.6360	0.0500
39	0.7890	0.0580
3A	0.9940	0.0730
3B	0.9970	0.0560
3C	0.6910	0.0550
3D	0.8100	0.0600
3E	0.9940	0.0680
3F	0.9960	0.0470
3G	0.6300	0.0500
3H	0.7840	0.0560
3I	0.9940	0.0730
3J	0.9970	0.0560
3K	0.6910	0.0490
3L	0.8100	0.0610
3M	0.9920	0.0690
3N	0.9970	0.0510
3O	0.6360	0.0390
3P	0.7890	0.0490
3Q	0.9940	0.0720
3R	0.9970	0.0490
3S	0.6900	0.0450
3T	0.8160	0.0550
3U	0.9940	0.0690
3V	0.9970	0.0510
3W	0.6900	0.0480
3X	0.8160	0.0560
3Y	0.9940	0.0780
3Z	0.9970	0.0570
40	0.6910	0.0560
41	0.8100	0.0470
42	0.9940	0.0720
43	0.9970	0.0540
44	0.6390	0.0590
45	0.8000	0.0430
46	0.9940	0.0670
47	0.9970	0.0510
48	0.6390	0.0620
49	0.8000	0.0460

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Chain	Atom inclusion	Q-score
4A	 0.9940	 0.0730
4B	 0.9960	 0.0490
4C	 0.6300	 0.0540
4D	 0.7840	 0.0610
4E	 0.9940	 0.0680
4F	 0.9970	 0.0520
4G	 0.6910	 0.0480
4H	 0.8100	 0.0590
4I	 0.9920	 0.0720
4J	 0.9970	 0.0510
4K	 0.6360	 0.0500
4L	 0.7890	 0.0550
4M	 0.9940	 0.0650
4N	 0.9960	 0.0430
4O	 0.6300	 0.0450
4P	 0.7840	 0.0520
4Q	 0.9920	 0.0740
4R	 0.9970	 0.0590
4S	 0.6360	 0.0620
4T	 0.7890	 0.0520
4U	 0.9940	 0.0710
4V	 0.9960	 0.0470
4W	 0.6300	 0.0580
4X	 0.7840	 0.0450
4Y	 0.9940	 0.0650
4Z	 0.9970	 0.0530
50	 0.6360	 0.0640
51	 0.7890	 0.0590
52	 0.9940	 0.0740
53	 0.9970	 0.0530
54	 0.6390	 0.0570
55	 0.8000	 0.0620
56	 0.9940	 0.0680
57	 0.9970	 0.0500
58	 0.6390	 0.0440
59	 0.8000	 0.0490
5A	 0.9940	 0.0740
5B	 0.9970	 0.0550
5C	 0.6390	 0.0620
5D	 0.8000	 0.0510
5E	 0.9940	 0.0740
5F	 0.9970	 0.0590













































































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Chain	Atom inclusion	Q-score
5G	0.6900	0.0610
5H	0.8160	0.0600
5I	0.9940	0.0720
5J	0.9970	0.0500
5K	0.6900	0.0500
5L	0.8160	0.0490
5M	0.9940	0.0670
5N	0.9970	0.0460
5O	0.6900	0.0470
5P	0.8160	0.0480
5Q	0.9940	0.0630
5R	0.9960	0.0480
5S	0.6300	0.0480
5T	0.7840	0.0400
5U	0.9940	0.0720
5V	0.9970	0.0580
5W	0.6910	0.0570
5X	0.8100	0.0520
5Y	0.9920	0.0730
5Z	0.9970	0.0530
60	0.6360	0.0530
61	0.7890	0.0620
62	0.9940	0.0720
63	0.9970	0.0550
64	0.6900	0.0550
65	0.8160	0.0520
66	0.9940	0.0770
67	0.9970	0.0540
68	0.6900	0.0650
69	0.8160	0.0590
6A	0.9940	0.0730
6B	0.9970	0.0560
6C	0.6390	0.0500
6D	0.8000	0.0510
6E	0.9920	0.0630
6F	0.9970	0.0490
6G	0.6360	0.0450
6H	0.7890	0.0470
6I	0.9940	0.0750
6J	0.9960	0.0570
6K	0.6300	0.0550
6L	0.7840	0.0560

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Chain	Atom inclusion	Q-score
6M	 0.9940	 0.0700
6N	 0.9970	 0.0540
6O	 0.6910	 0.0530
6P	 0.8100	 0.0500
6Q	 0.9940	 0.0690
6R	 0.9960	 0.0460
6S	 0.6300	 0.0540
6T	 0.7840	 0.0510
6U	 0.9940	 0.0620
6V	 0.9970	 0.0500
6W	 0.6910	 0.0440
6X	 0.8100	 0.0470
6Y	 0.9920	 0.0750
6Z	 0.9970	 0.0590
7A	 0.9940	 0.0660
7B	 0.9970	 0.0490
7C	 0.6900	 0.0520
7D	 0.8160	 0.0430
7E	 0.9940	 0.0680
7F	 0.9970	 0.0520
7G	 0.6910	 0.0580
7H	 0.8100	 0.0480
7I	 0.9920	 0.0650
7J	 0.9970	 0.0500
7K	 0.6360	 0.0510
7L	 0.7890	 0.0440
7M	 0.9940	 0.0730
7N	 0.9960	 0.0510
7O	 0.6300	 0.0650
7P	 0.7840	 0.0540
7Q	 0.9940	 0.0670
7R	 0.9970	 0.0550
7S	 0.6910	 0.0630
7T	 0.8100	 0.0510
7U	 0.9920	 0.0700
7V	 0.9970	 0.0530
7W	 0.6360	 0.0600
7X	 0.7890	 0.0480