wwPDB EM Validation Summary Report

Apr 29, 2025 – 07:23 pm BST

PDB ID	:	9GDX / pdb_00009gdx
EMDB ID	:	EMD-51279
Title	:	SARS-CoV-2 Spike protein Beta Variant at 4C structural flexibility / heterogeneity analyses
Authors	:	Herreros, D.; Mata, C.P.; Noddings, C.; Irene, D.; Agard, D.A.; Tsai, M.-D.; Sorzano, C.O.S.; Carazo, J.M.
Deposited on	:	2024-08-06
Resolution	:	2.80 Å(reported)
Based on initial model	:	7VX1

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 (i) 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 (i)) were used in the production of this report:

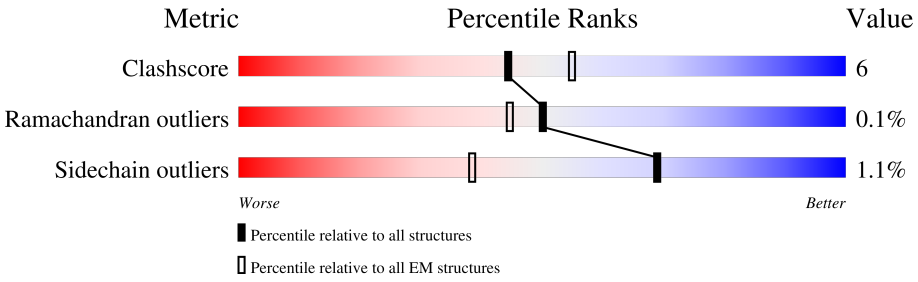
EMDB validation analysis	:	0.0.1.dev118
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 <=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	1-A	1230	72% 15% 12%
1	1-B	1230	74% 13% 12%
1	1-C	1230	12% 75% 12% 12%
1	10-A	1230	71% 17% 12%
1	10-B	1230	71% 16% 12%
1	10-C	1230	71% 17% 12%
1	11-A	1230	73% 15% 12%
1	11-B	1230	72% 16% 12%

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Mol	Chain	Length	Quality of chain
1	11-C	1230	72% 15% 12%
1	12-A	1230	73% 15% 12%
1	12-B	1230	76% 11% 12%
1	12-C	1230	73% 14% 12%
1	13-A	1230	73% 14% 12%
1	13-B	1230	73% 14% 12%
1	13-C	1230	72% 15% 12%
1	14-A	1230	72% 15% 12%
1	14-B	1230	70% 17% 12%
1	14-C	1230	72% 15% 12%
1	15-A	1230	73% 14% 12%
1	15-B	1230	73% 15% 12%
1	15-C	1230	73% 14% 12%
1	16-A	1230	72% 15% 12%
1	16-B	1230	74% 13% 12%
1	16-C	1230	75% 13% 12%
1	17-A	1230	73% 14% 12%
1	17-B	1230	71% 17% 12%
1	17-C	1230	74% 14% 12%
1	18-A	1230	71% 16% 12%
1	18-B	1230	71% 16% 12%
1	18-C	1230	72% 16% 12%
1	19-A	1230	76% 12% 12%
1	19-B	1230	75% 12% 12%
1	19-C	1230	74% 14% 12%

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Mol	Chain	Length	Quality of chain
1	2-A	1230	71% 16% 12%
1	2-B	1230	73% 15% 12%
1	2-C	1230	73% 14% 12%
1	20-A	1230	72% 15% 12%
1	20-B	1230	73% 14% 12%
1	20-C	1230	71% 17% 12%
1	3-A	1230	72% 15% 12%
1	3-B	1230	73% 15% 12%
1	3-C	1230	74% 13% 12%
1	4-A	1230	71% 17% 12%
1	4-B	1230	73% 14% 12%
1	4-C	1230	73% 15% 12%
1	5-A	1230	75% 13% 12%
1	5-B	1230	76% 12% 12%
1	5-C	1230	75% 12% 12%
1	6-A	1230	76% 12% 12%
1	6-B	1230	71% 16% 12%
1	6-C	1230	73% 14% 12%
1	7-A	1230	74% 13% 12%
1	7-B	1230	74% 14% 12%
1	7-C	1230	74% 14% 12%
1	8-A	1230	73% 15% 12%
1	8-B	1230	69% 18% 12%
1	8-C	1230	72% 15% 12%
1	9-A	1230	70% 17% 12%

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Mol	Chain	Length	Quality of chain
1	9-B	1230	
1	9-C	1230	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 507240 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike glycoprotein,Fibritin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1-A	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	2-A	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	3-A	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	4-A	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	5-A	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	6-A	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	7-A	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	8-A	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	9-A	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	10-A	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	11-A	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	12-A	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	13-A	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	14-A	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	15-A	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	16-A	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	17-A	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	18-A	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	19-A	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	20-A	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	1-B	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	2-B	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	3-B	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	4-B	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	5-B	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	6-B	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	7-B	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	8-B	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	9-B	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	10-B	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	11-B	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	12-B	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	13-B	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	14-B	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	15-B	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	16-B	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	17-B	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	18-B	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	19-B	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	20-B	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	1-C	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	2-C	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	3-C	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	4-C	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	5-C	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	6-C	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	7-C	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	8-C	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	9-C	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	10-C	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	11-C	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	12-C	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	13-C	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	14-C	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	15-C	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	16-C	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	17-C	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	18-C	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	19-C	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	20-C	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		

There are 87 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	PHE	LEU	variant	UNP P0DTC2
A	80	ALA	ASP	variant	UNP P0DTC2
A	215	GLY	ASP	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	246	ILE	ARG	conflict	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	484	LYS	GLU	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	701	VAL	ALA	variant	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1209	GLY	-	linker	UNP P0DTC2
A	1210	SER	-	linker	UNP P0DTC2
A	1232	LEU	PHE	engineered mutation	UNP P10104
A	1238	GLY	-	expression tag	UNP P10104
A	1239	ARG	-	expression tag	UNP P10104
A	1240	SER	-	expression tag	UNP P10104
A	1241	LEU	-	expression tag	UNP P10104
A	1242	GLU	-	expression tag	UNP P10104
A	1243	VAL	-	expression tag	UNP P10104
A	1244	LEU	-	expression tag	UNP P10104
A	1245	PHE	-	expression tag	UNP P10104
A	1246	GLN	-	expression tag	UNP P10104
B	18	PHE	LEU	variant	UNP P0DTC2
B	80	ALA	ASP	variant	UNP P0DTC2
B	215	GLY	ASP	variant	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	ALA	deletion	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	246	ILE	ARG	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	417	ASN	LYS	variant	UNP P0DTC2
B	484	LYS	GLU	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	701	VAL	ALA	variant	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1209	GLY	-	linker	UNP P0DTC2
B	1210	SER	-	linker	UNP P0DTC2
B	1232	LEU	PHE	engineered mutation	UNP P10104
B	1238	GLY	-	expression tag	UNP P10104
B	1239	ARG	-	expression tag	UNP P10104
B	1240	SER	-	expression tag	UNP P10104
B	1241	LEU	-	expression tag	UNP P10104
B	1242	GLU	-	expression tag	UNP P10104
B	1243	VAL	-	expression tag	UNP P10104
B	1244	LEU	-	expression tag	UNP P10104
B	1245	PHE	-	expression tag	UNP P10104
B	1246	GLN	-	expression tag	UNP P10104
C	18	PHE	LEU	variant	UNP P0DTC2
C	80	ALA	ASP	variant	UNP P0DTC2
C	215	GLY	ASP	variant	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	246	ILE	ARG	conflict	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	484	LYS	GLU	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	701	VAL	ALA	variant	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1209	GLY	-	linker	UNP P0DTC2
C	1210	SER	-	linker	UNP P0DTC2
C	1232	LEU	PHE	engineered mutation	UNP P10104

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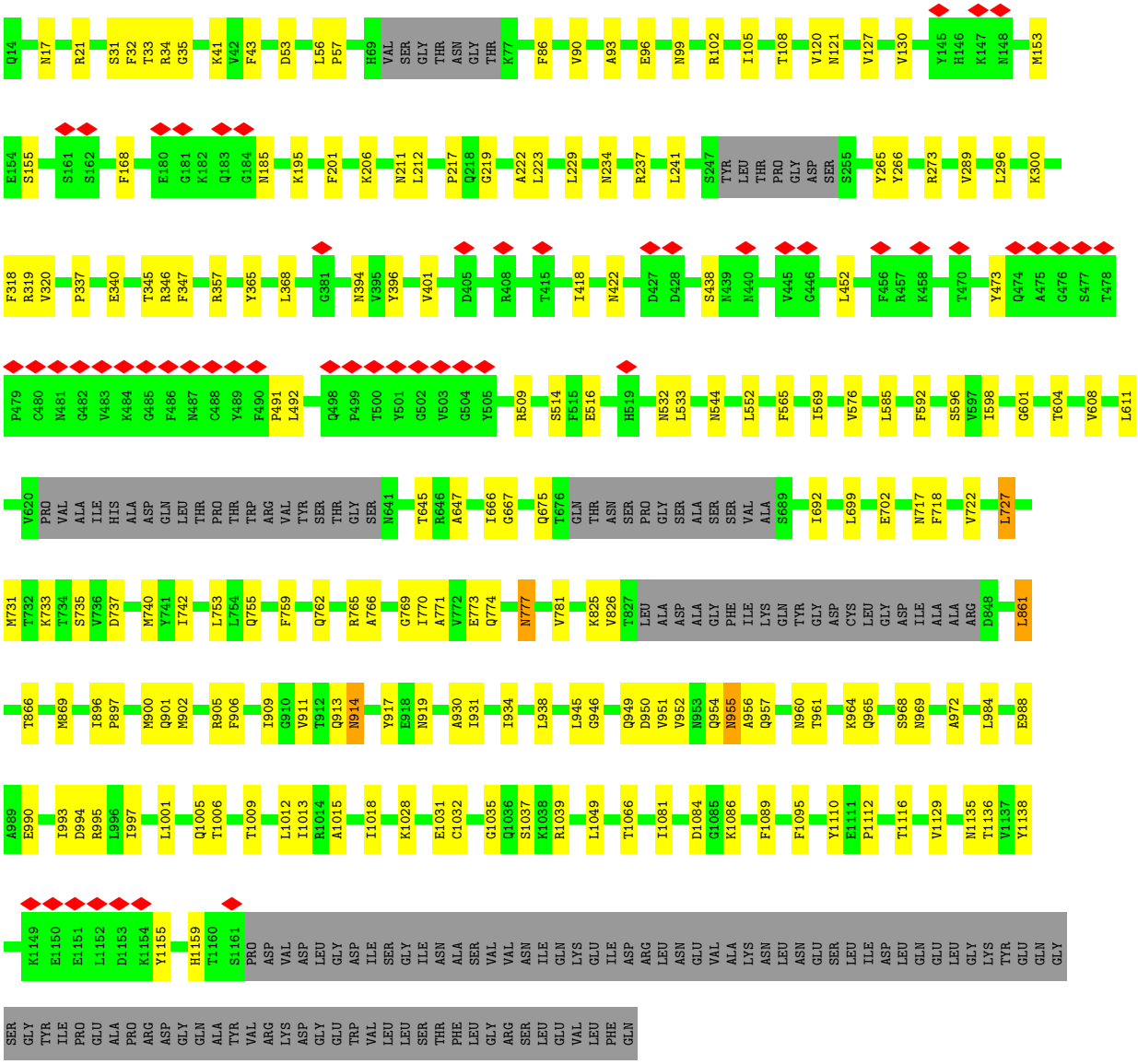
Chain	Residue	Modelled	Actual	Comment	Reference
C	1238	GLY	-	expression tag	UNP P10104
C	1239	ARG	-	expression tag	UNP P10104
C	1240	SER	-	expression tag	UNP P10104
C	1241	LEU	-	expression tag	UNP P10104
C	1242	GLU	-	expression tag	UNP P10104
C	1243	VAL	-	expression tag	UNP P10104
C	1244	LEU	-	expression tag	UNP P10104
C	1245	PHE	-	expression tag	UNP P10104
C	1246	GLN	-	expression tag	UNP P10104

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.

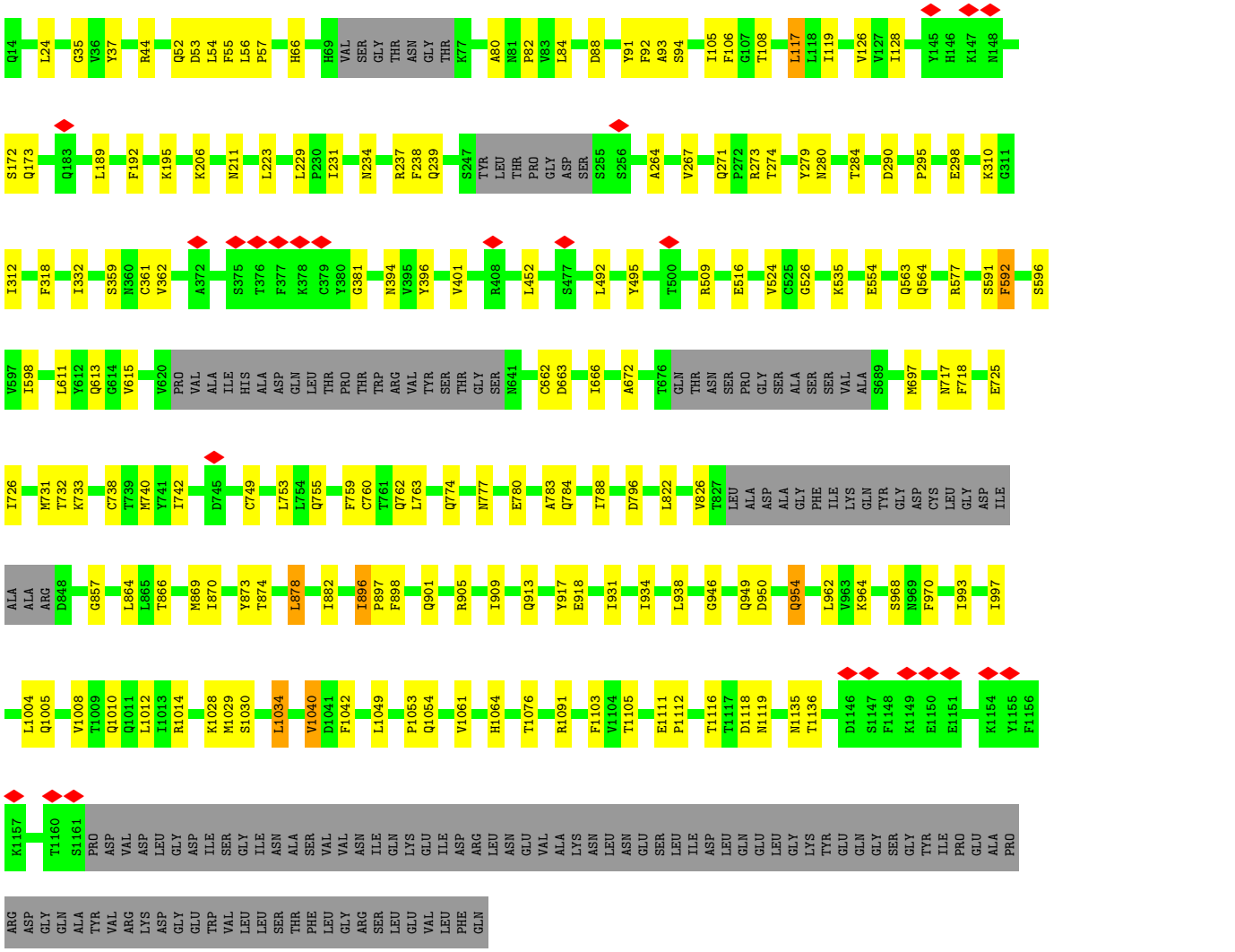
- Molecule 1: Spike glycoprotein,Fibritin

Chain 1-A:



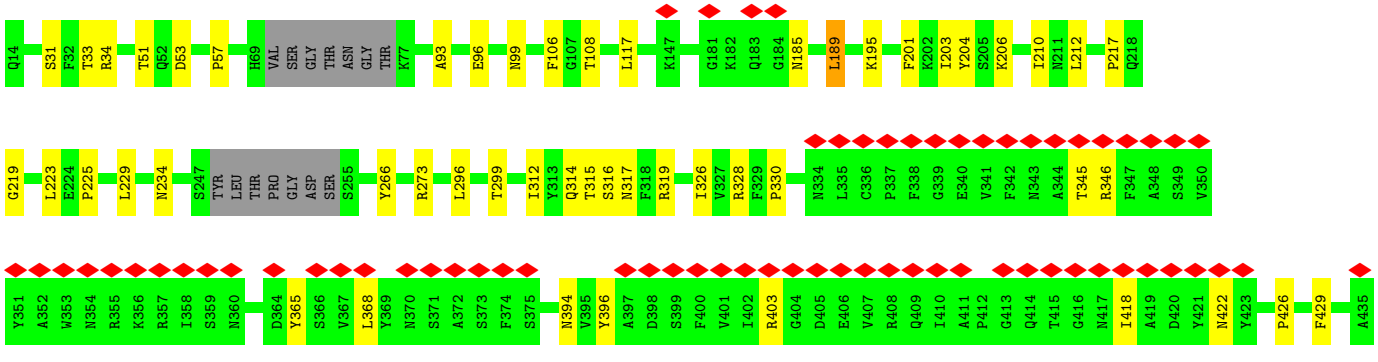
• Molecule 1: Spike glycoprotein,Fibritin

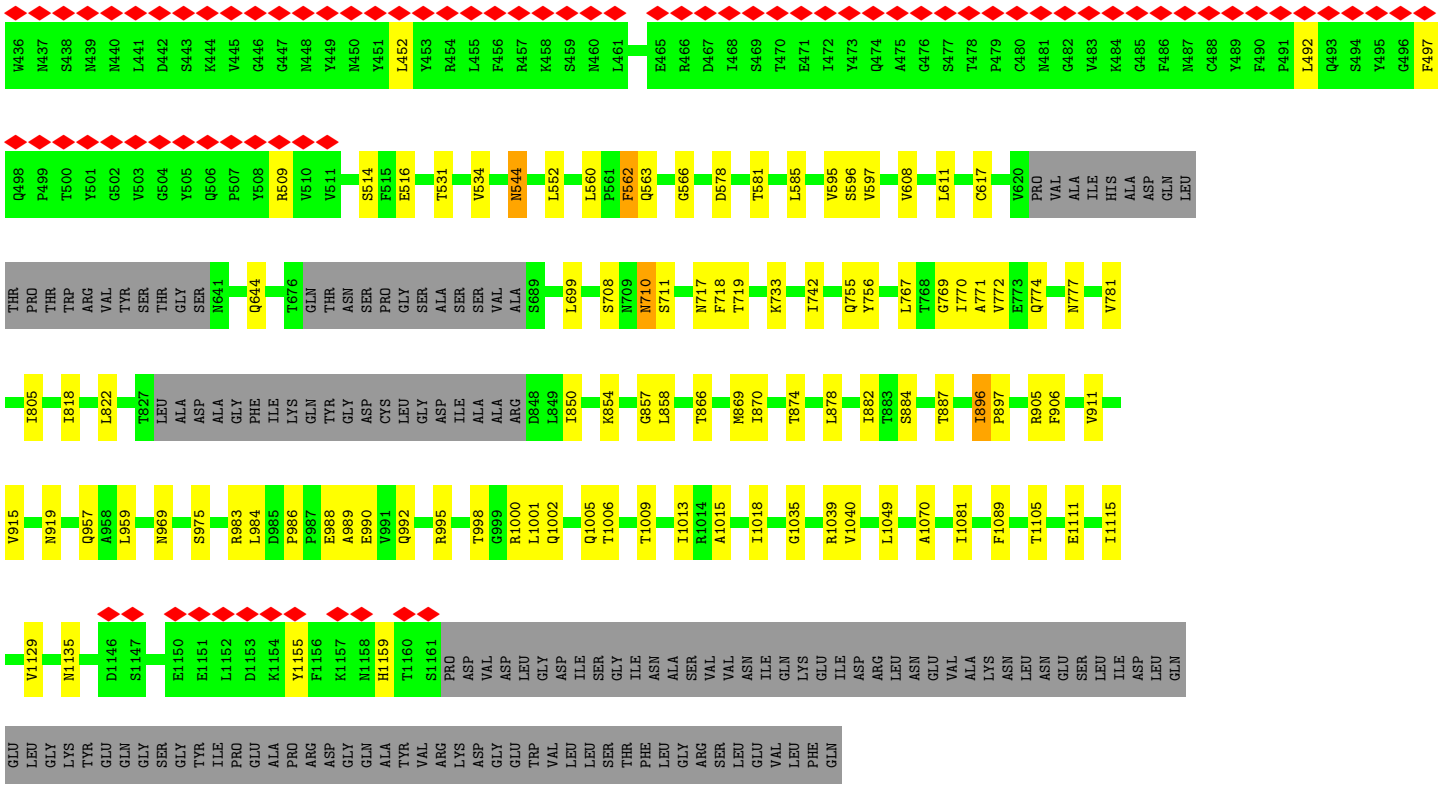
Chain 1-B:



• Molecule 1: Spike glycoprotein,Fibritin

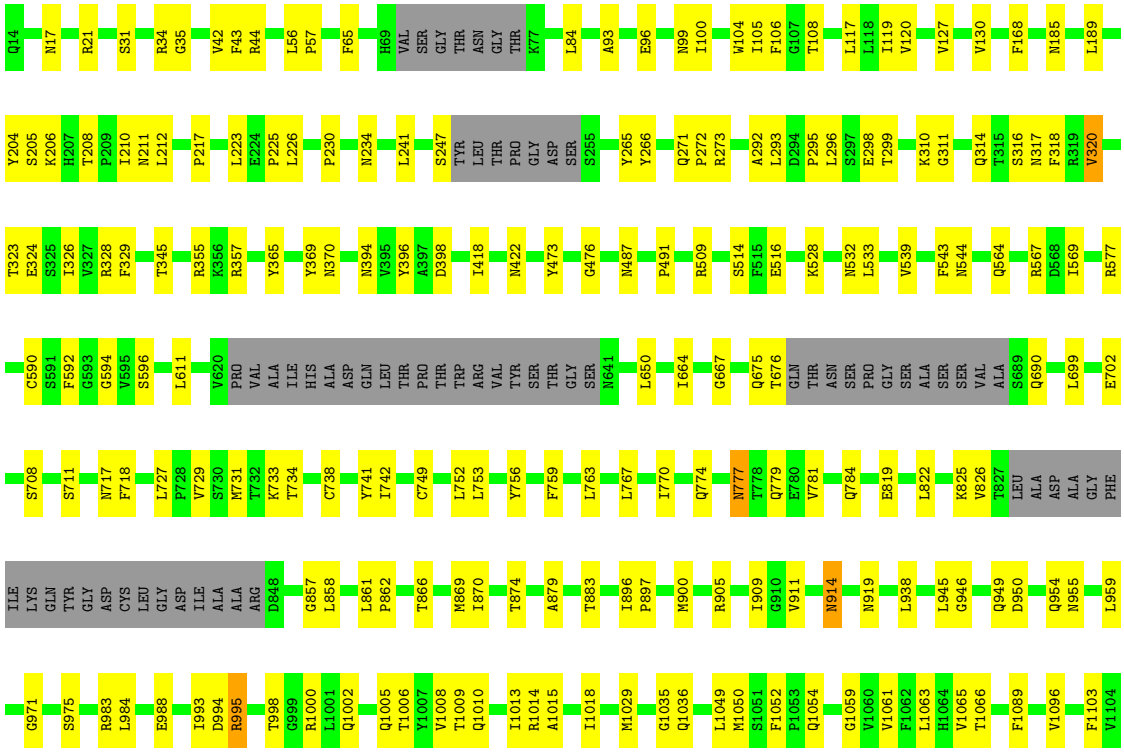
Chain 1-C:

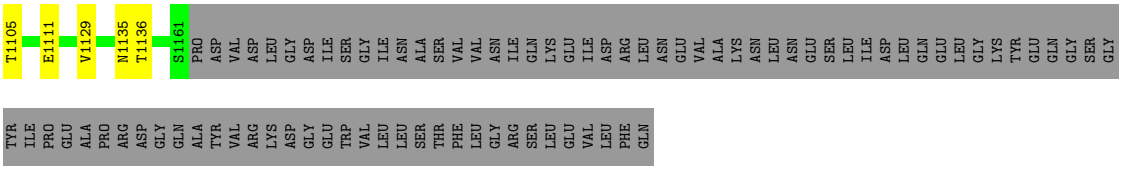




• Molecule 1: Spike glycoprotein,Fibritin

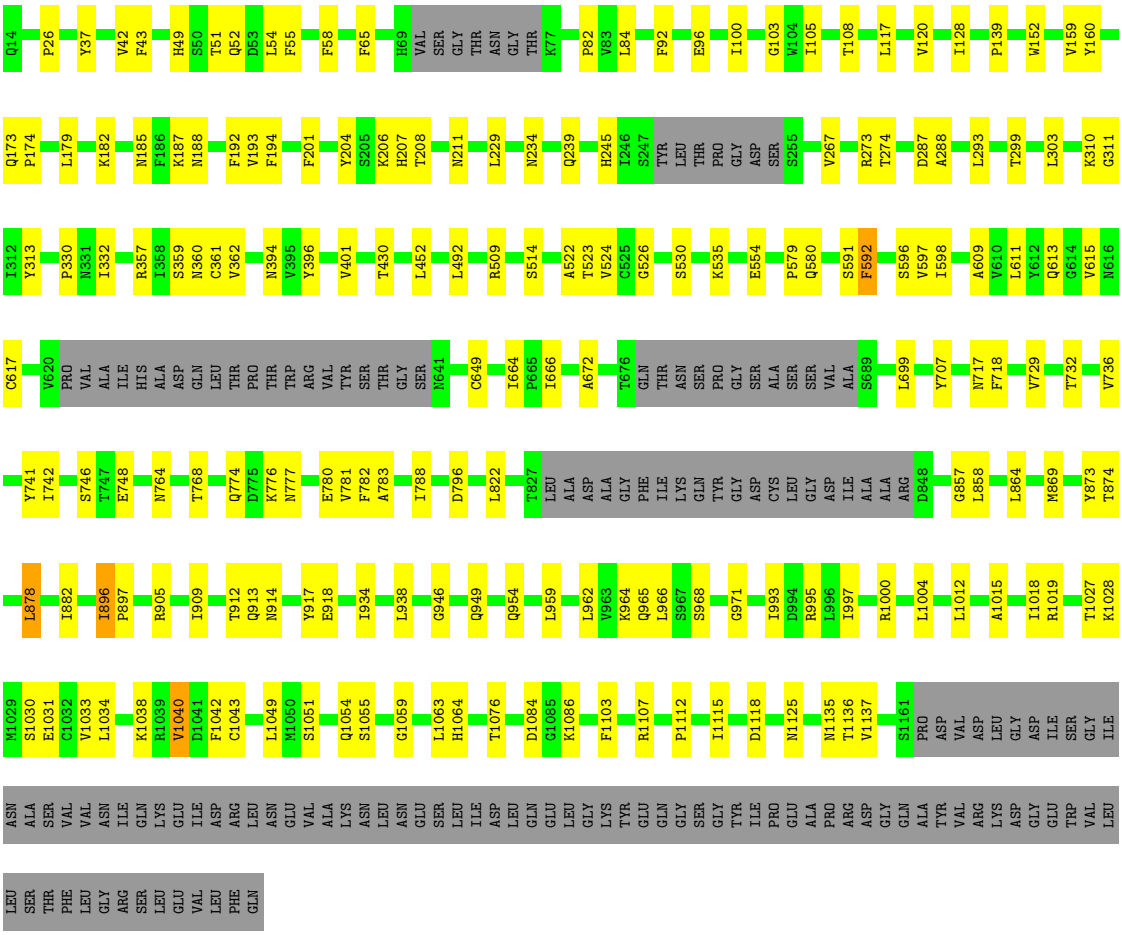
Chain 2-A: 71% 16% 12%





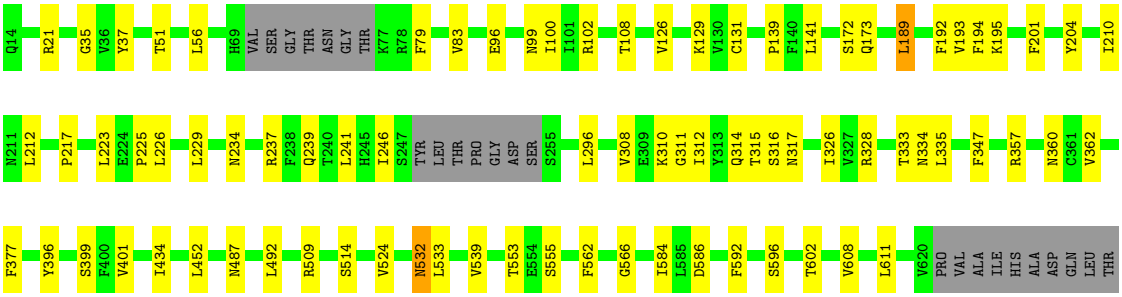
• Molecule 1: Spike glycoprotein,Fibritin

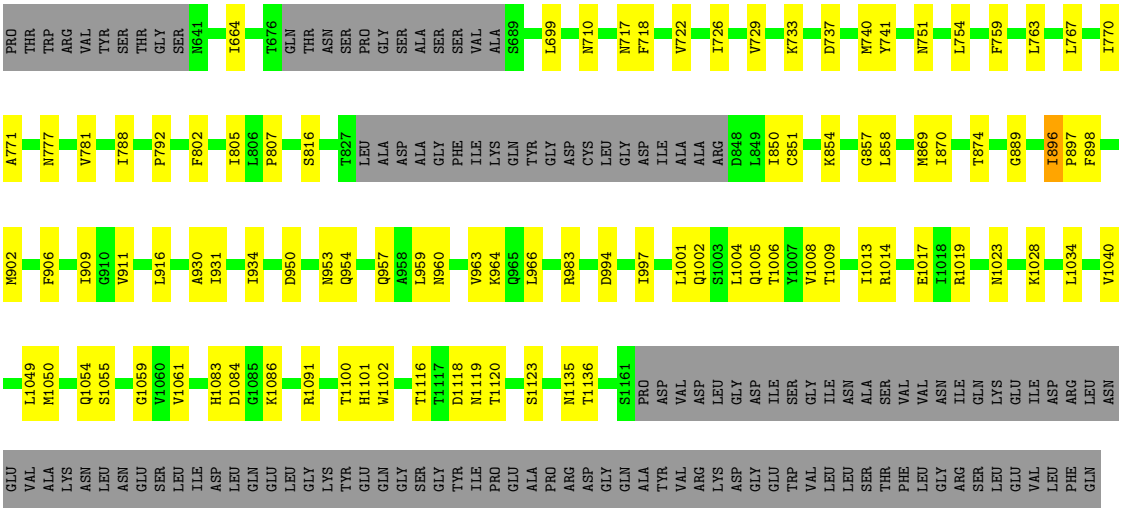
Chain 2-B:



• Molecule 1: Spike glycoprotein,Fibritin

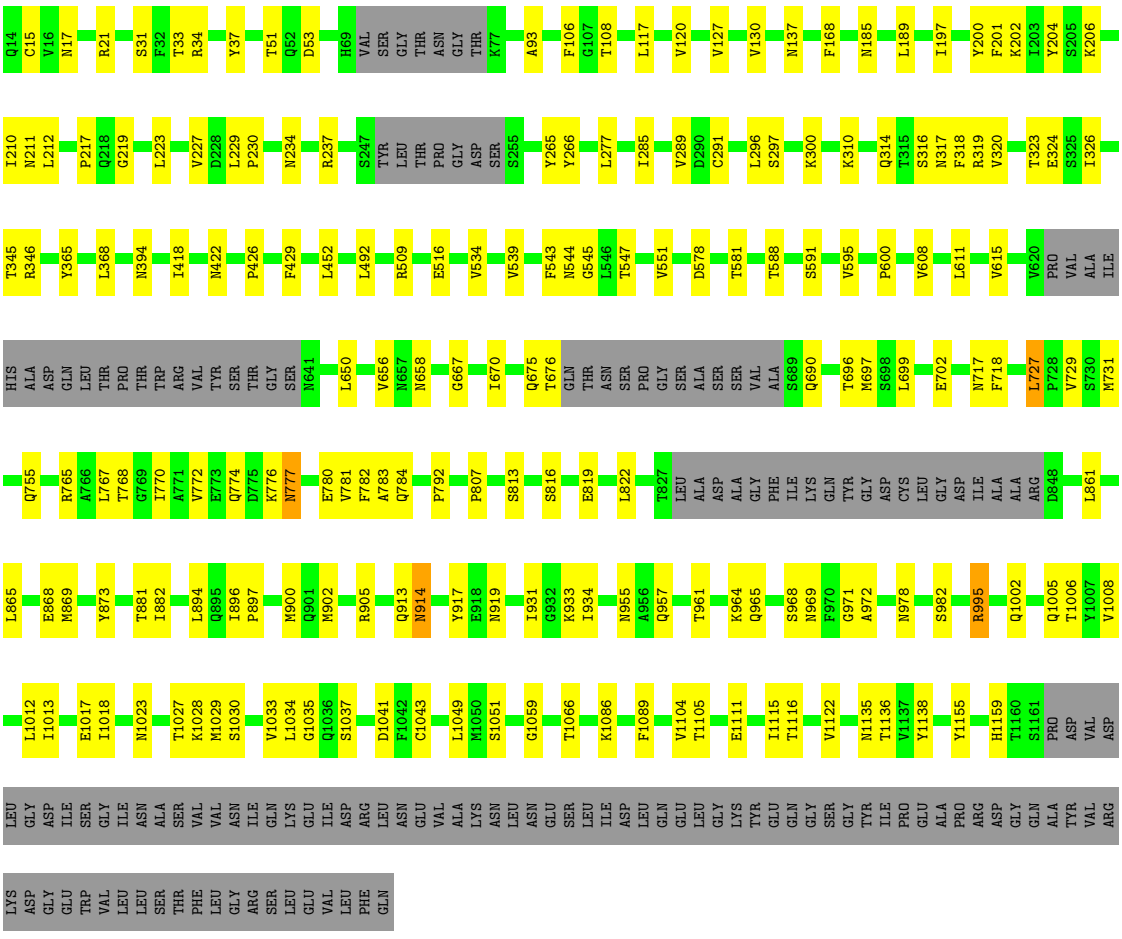
Chain 2-C:





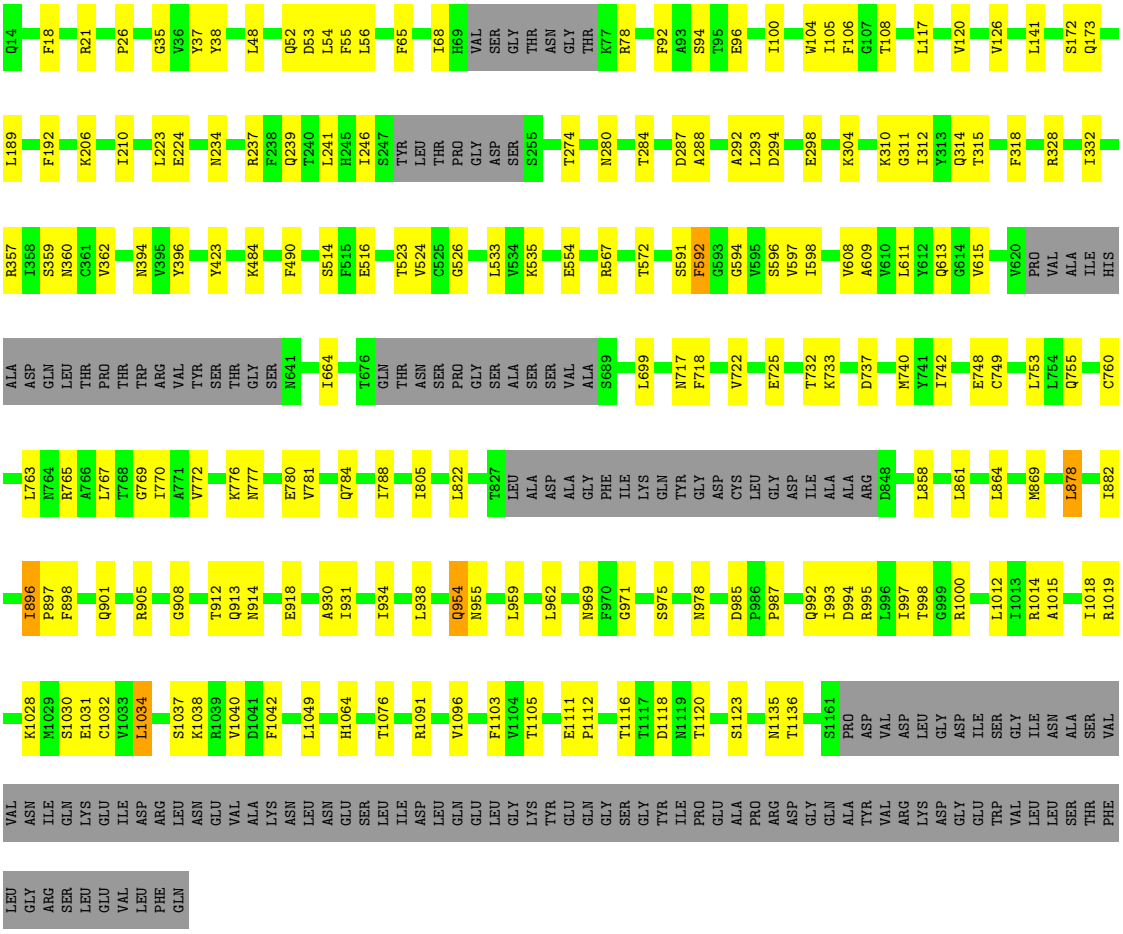
• Molecule 1: Spike glycoprotein,Fibritin

Chain 3-A:



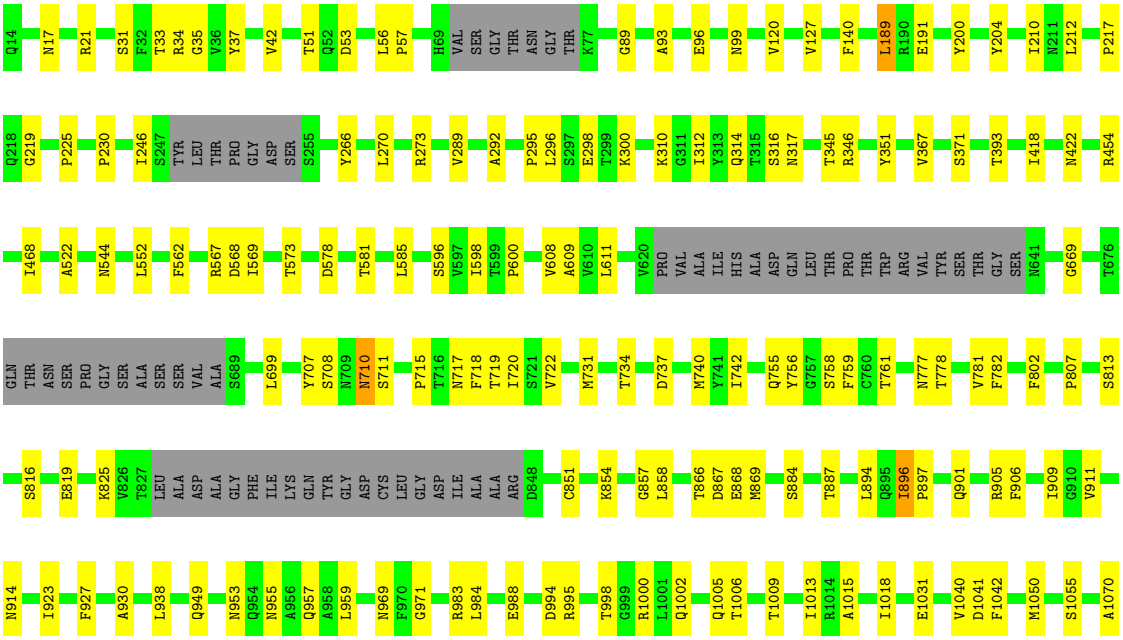
• Molecule 1: Spike glycoprotein,Fibritin

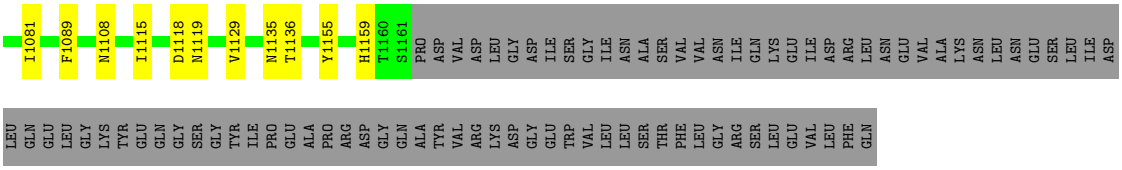
Chain 3-B:



• Molecule 1: Spike glycoprotein,Fibritin

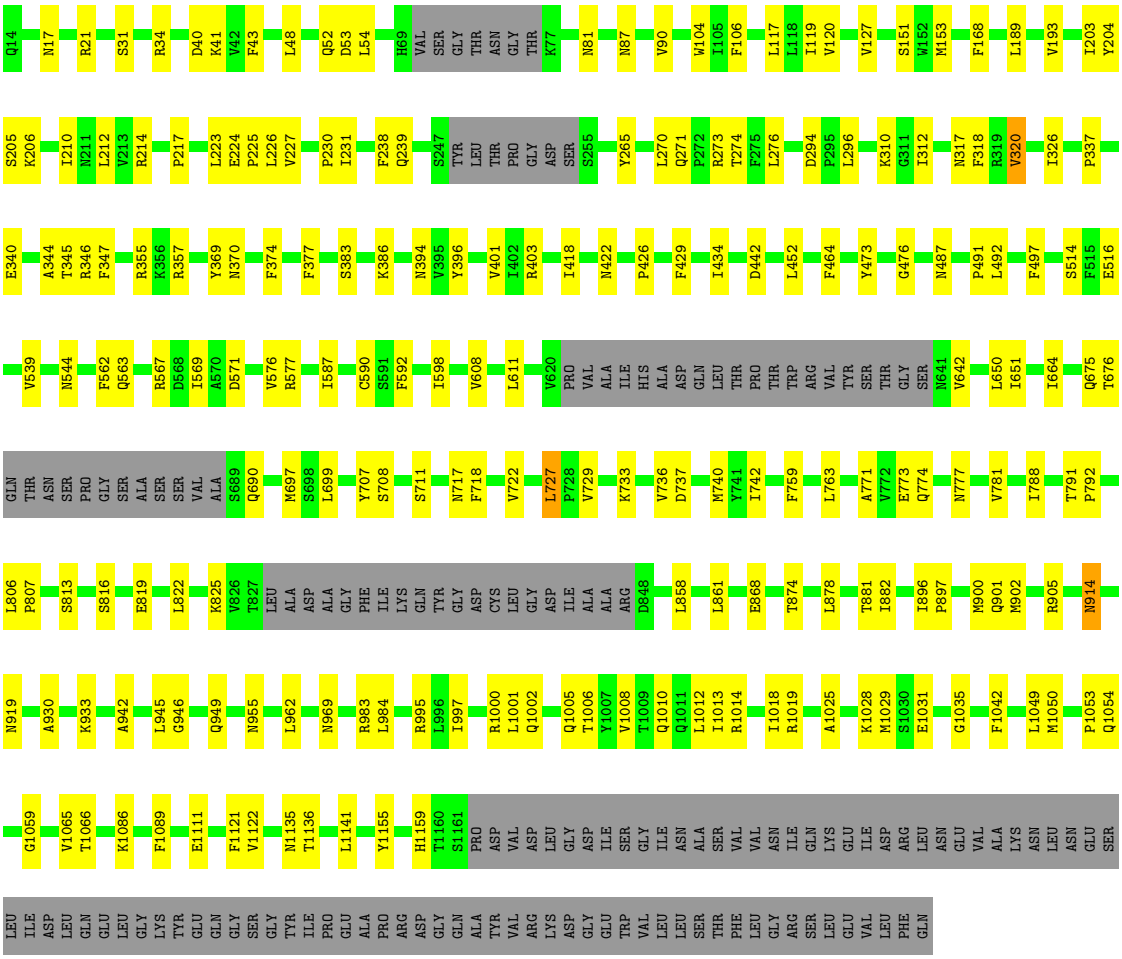
Chain 3-C:





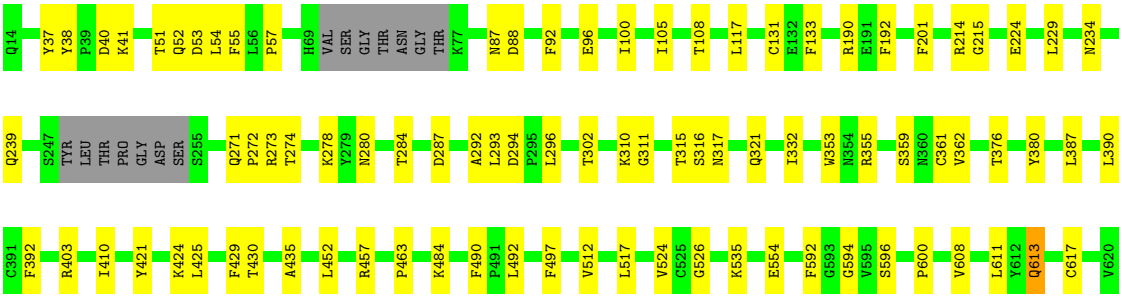
• Molecule 1: Spike glycoprotein,Fibritin

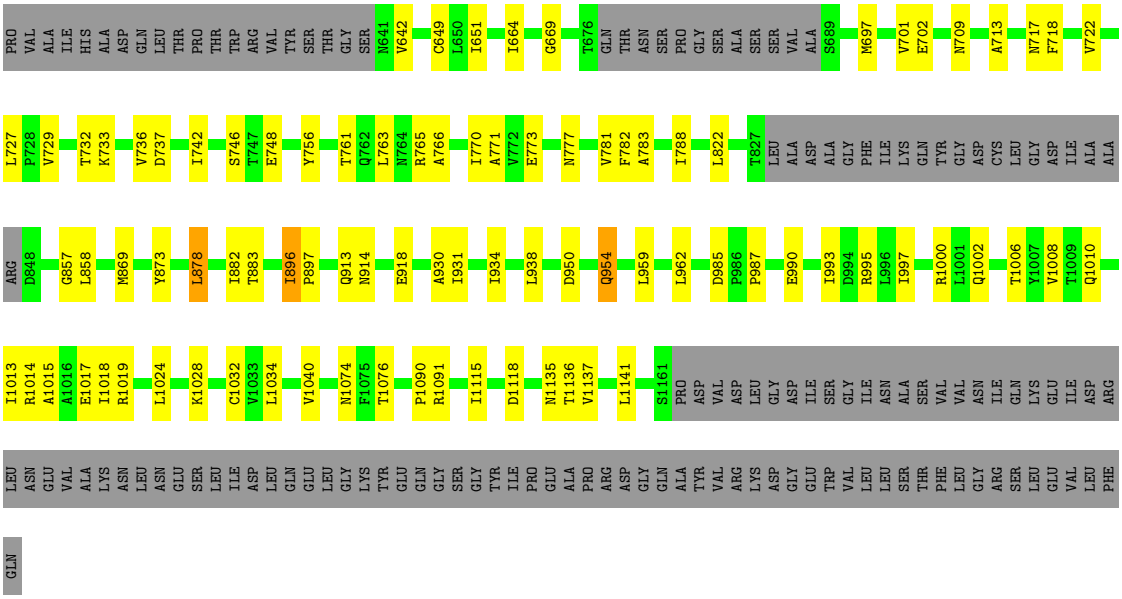
Chain 4-A:



• Molecule 1: Spike glycoprotein,Fibritin

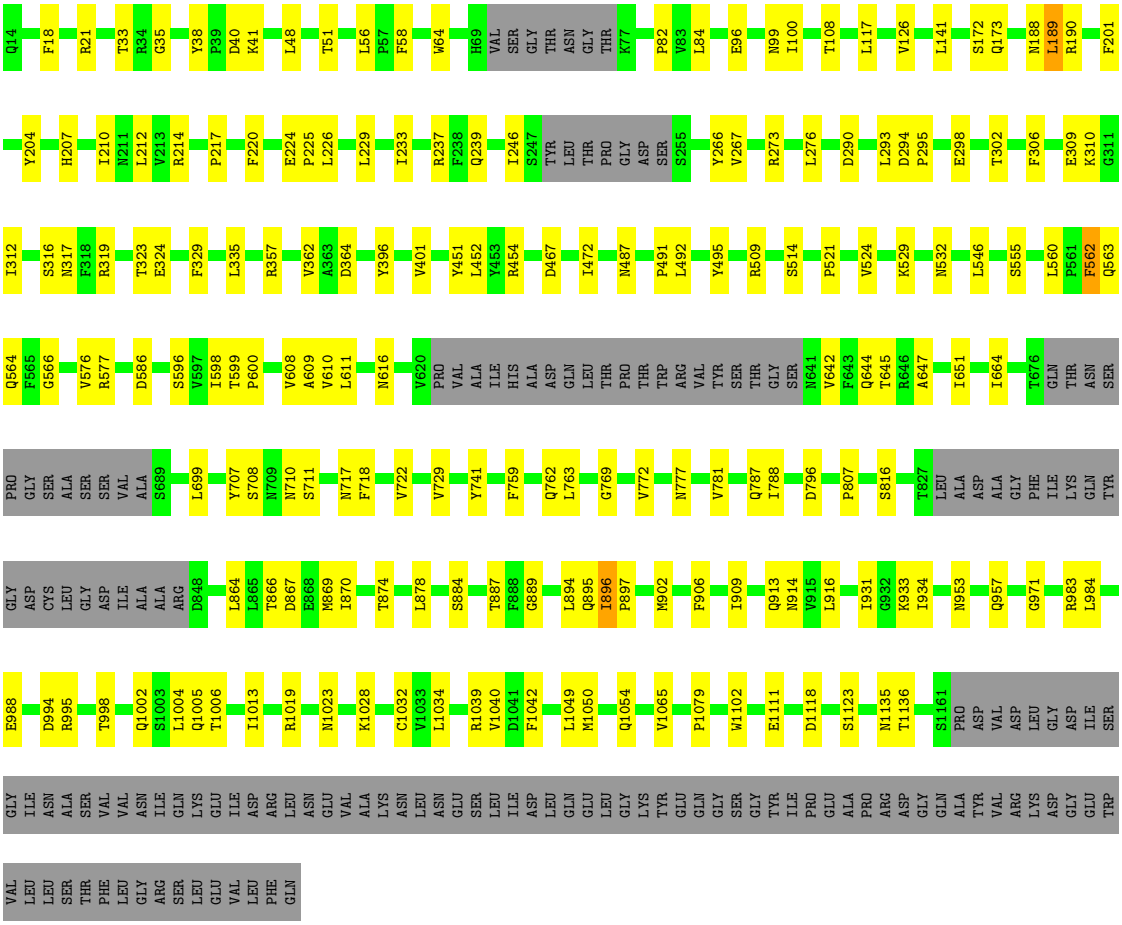
Chain 4-B:





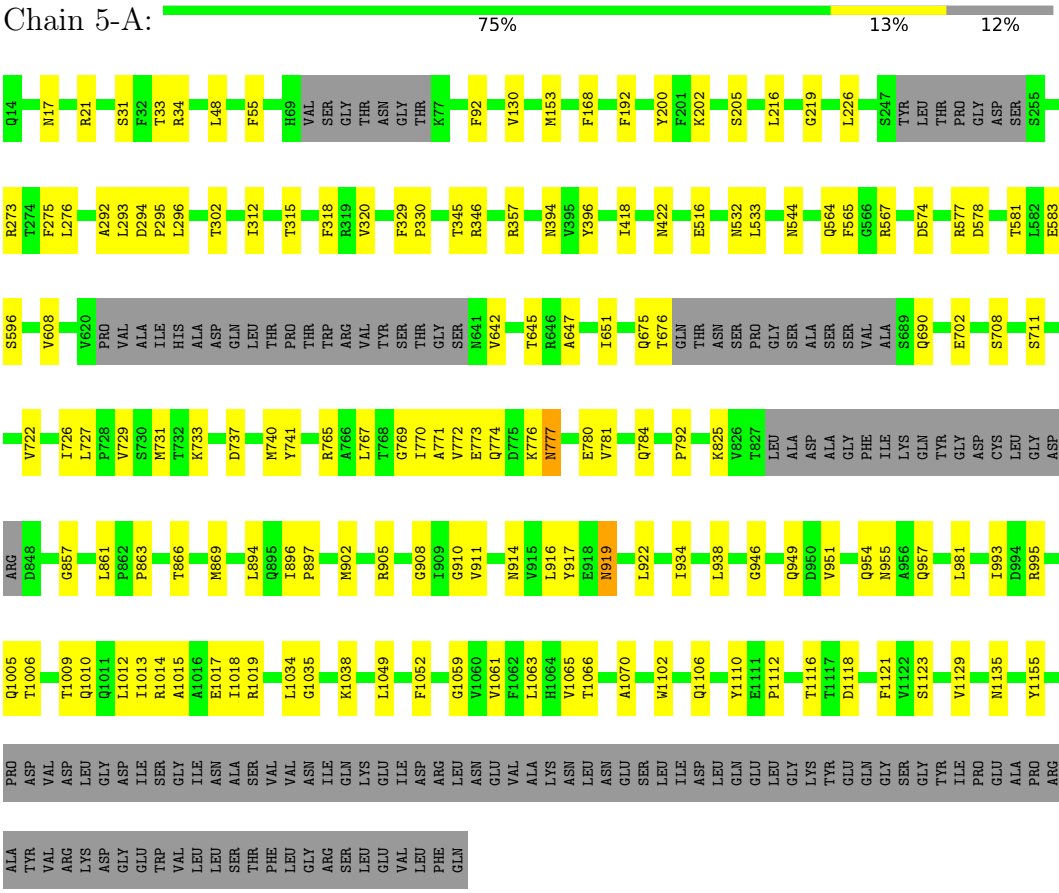
• Molecule 1: Spike glycoprotein,Fibritin

Chain 4-C:



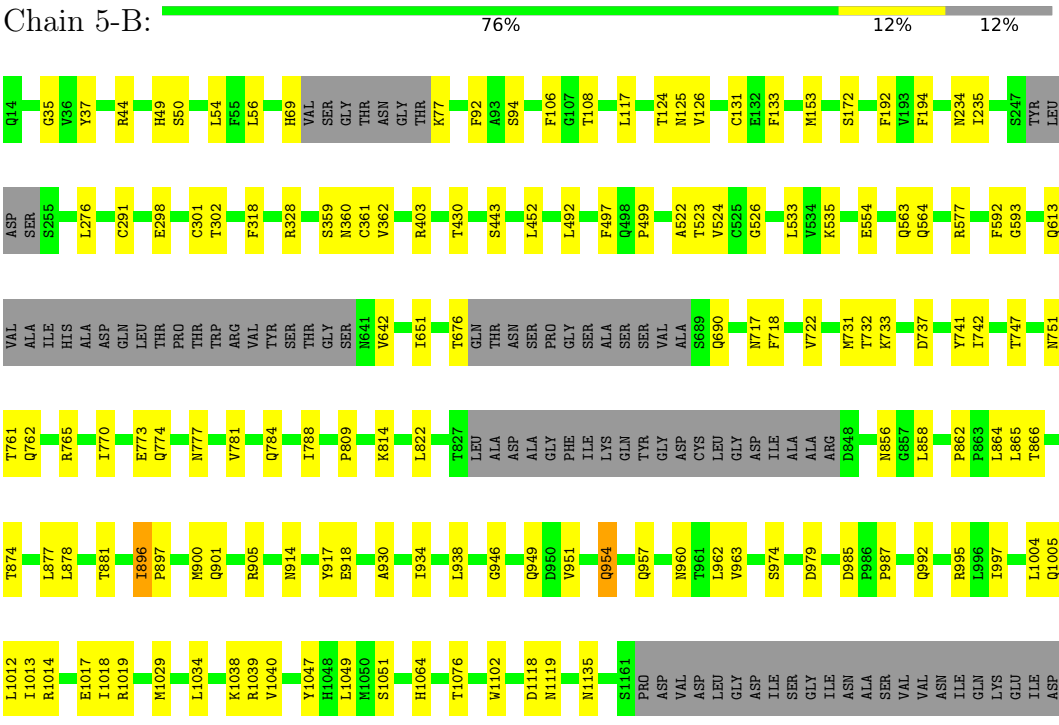
• Molecule 1: Spike glycoprotein,Fibritin

Chain 5-A:



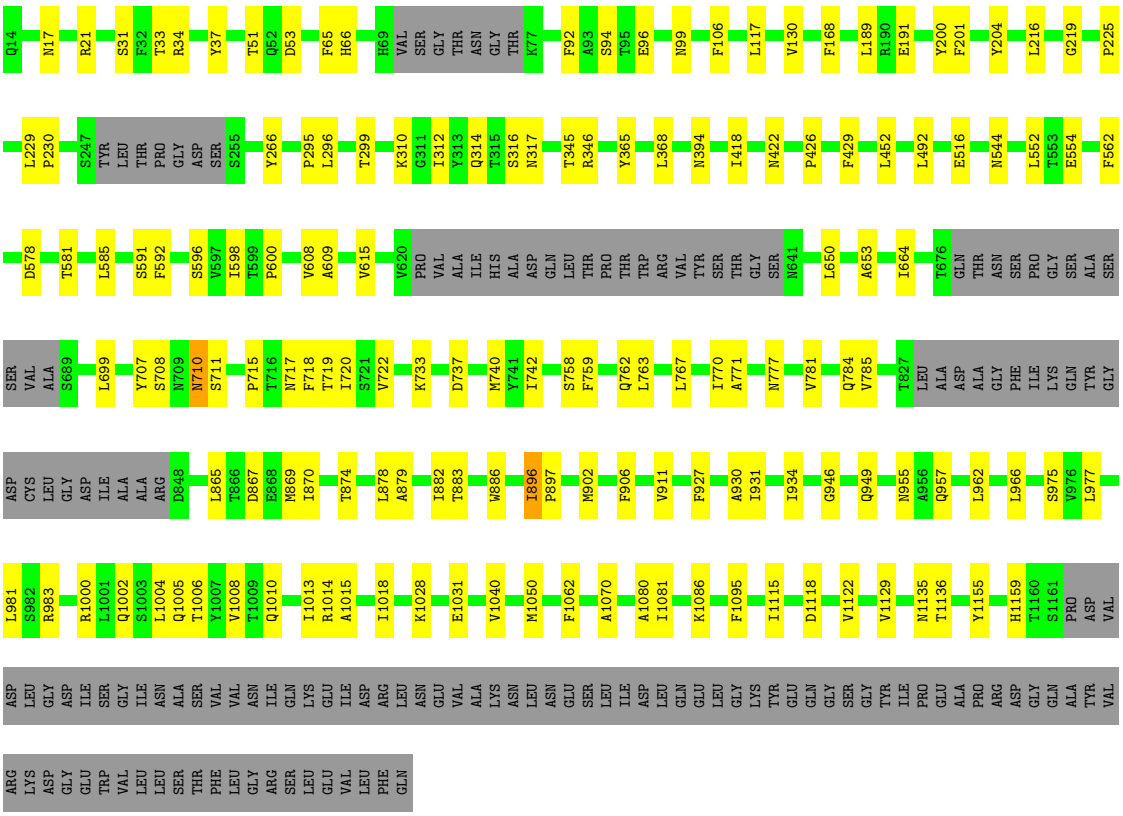
• Molecule 1: Spike glycoprotein,Fibritin

Chain 5-B:



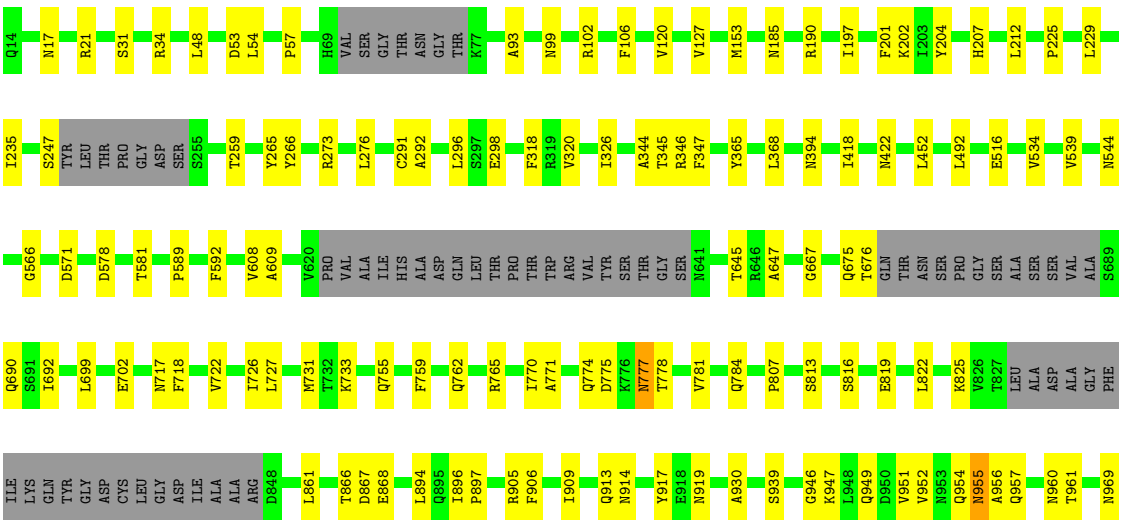
• Molecule 1: Spike glycoprotein,Fibritin

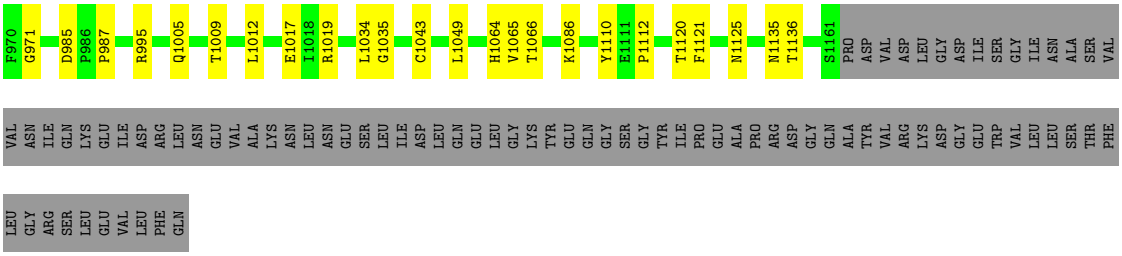
Chain 5-C:



• Molecule 1: Spike glycoprotein,Fibritin

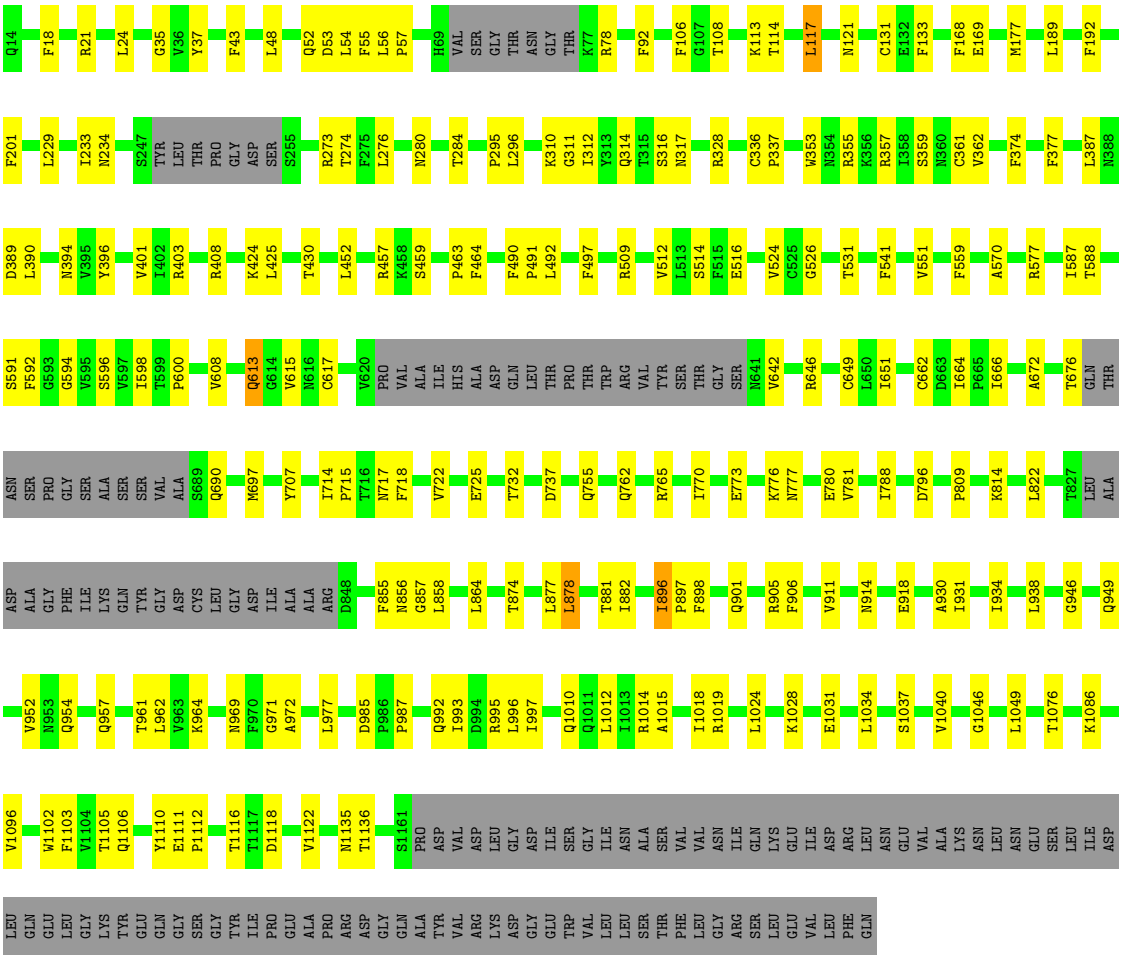
Chain 6-A:





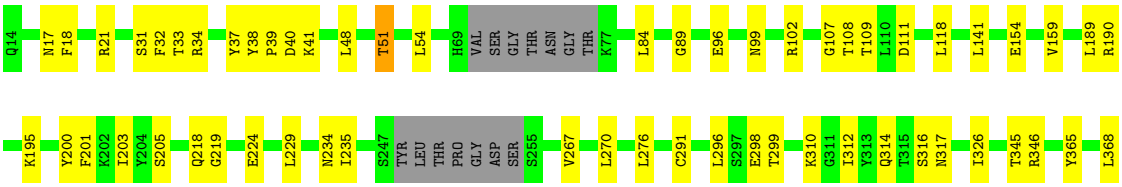
• Molecule 1: Spike glycoprotein,Fibritin

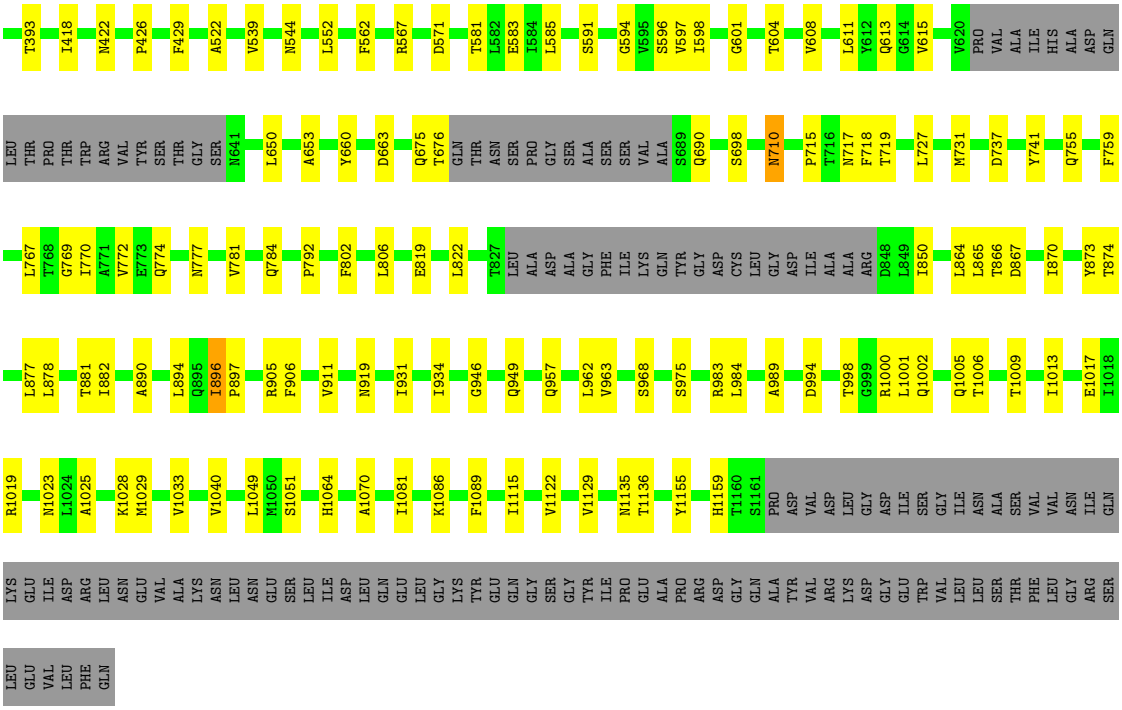
Chain 6-B:



• Molecule 1: Spike glycoprotein,Fibritin

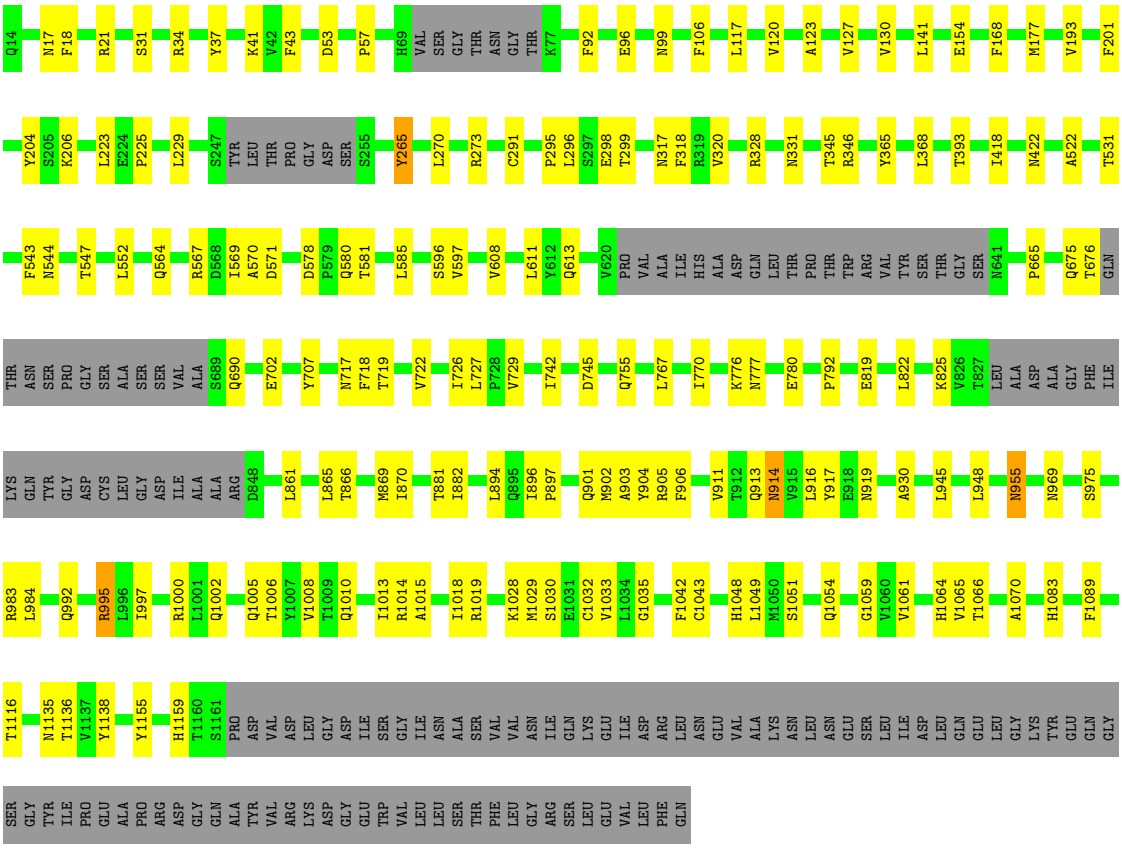
Chain 6-C:





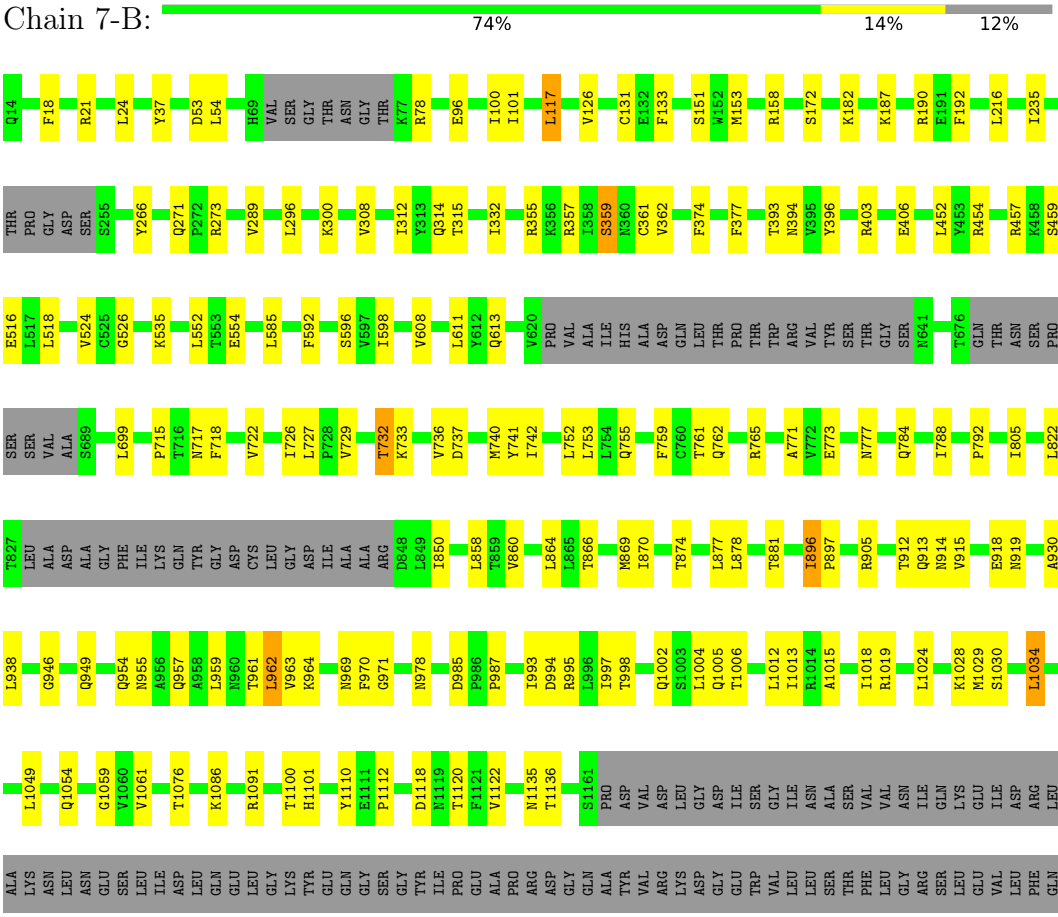
• Molecule 1: Spike glycoprotein,Fibritin

Chain 7-A:



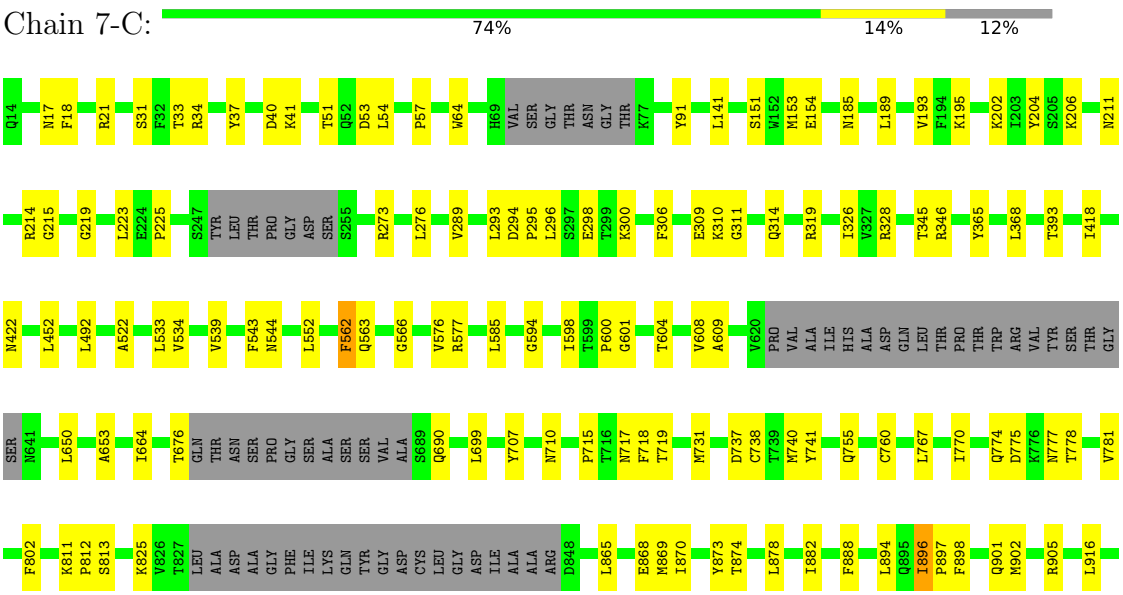
• Molecule 1: Spike glycoprotein,Fibritin

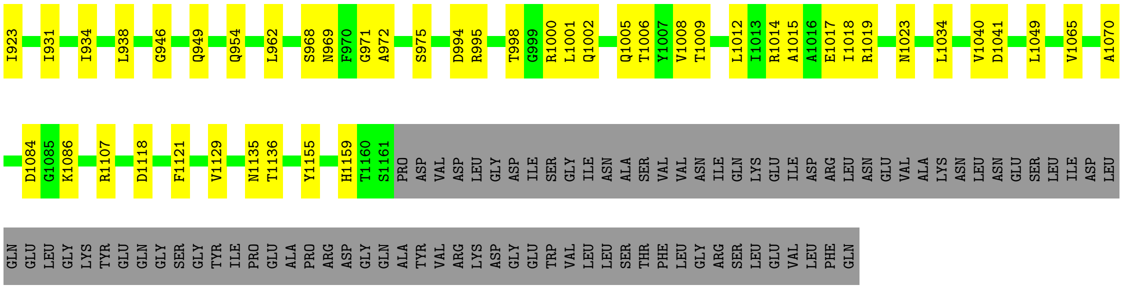
Chain 7-B:



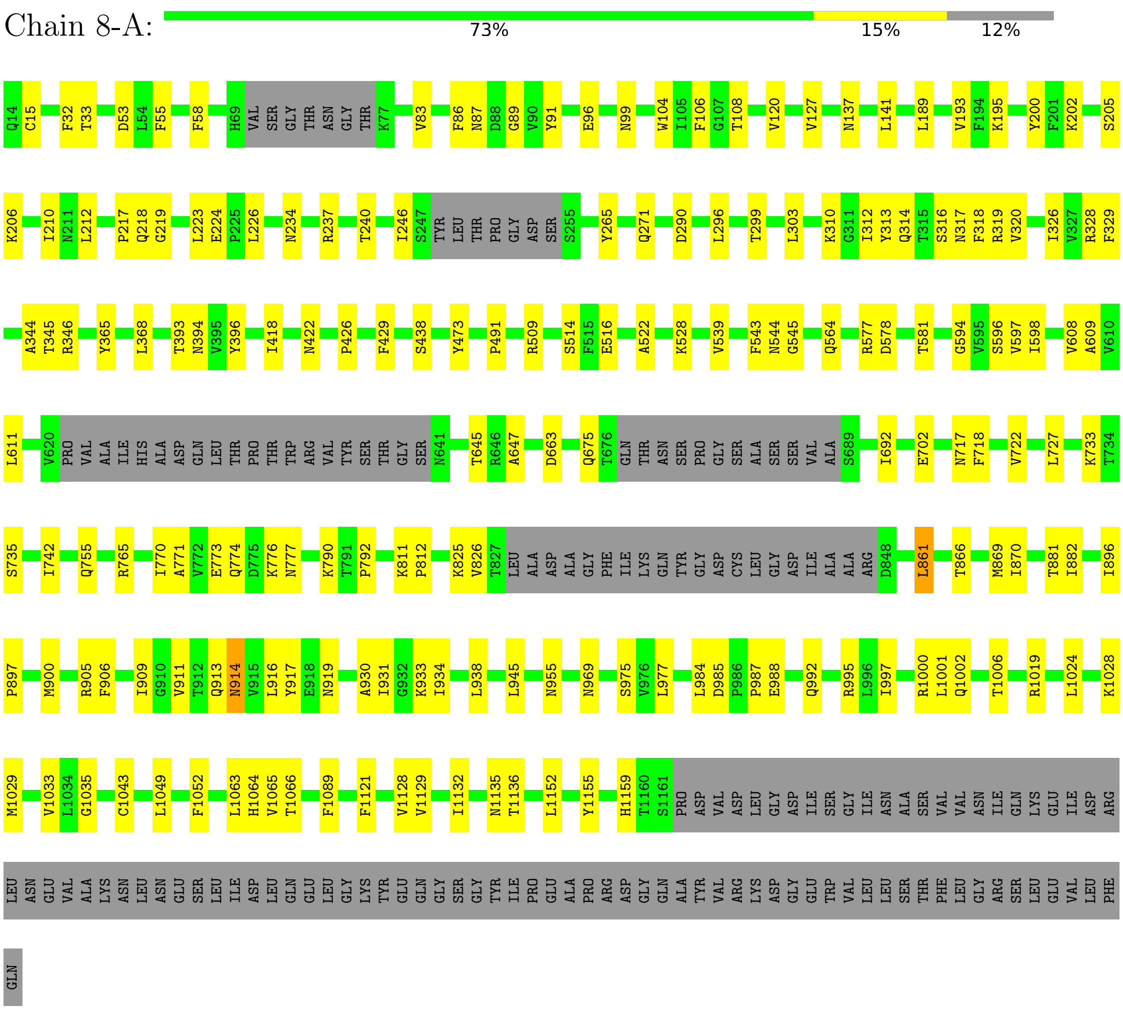
• Molecule 1: Spike glycoprotein,Fibritin

Chain 7-C:

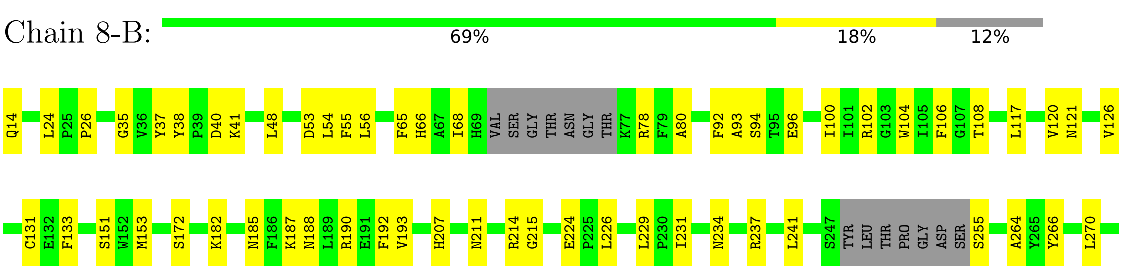


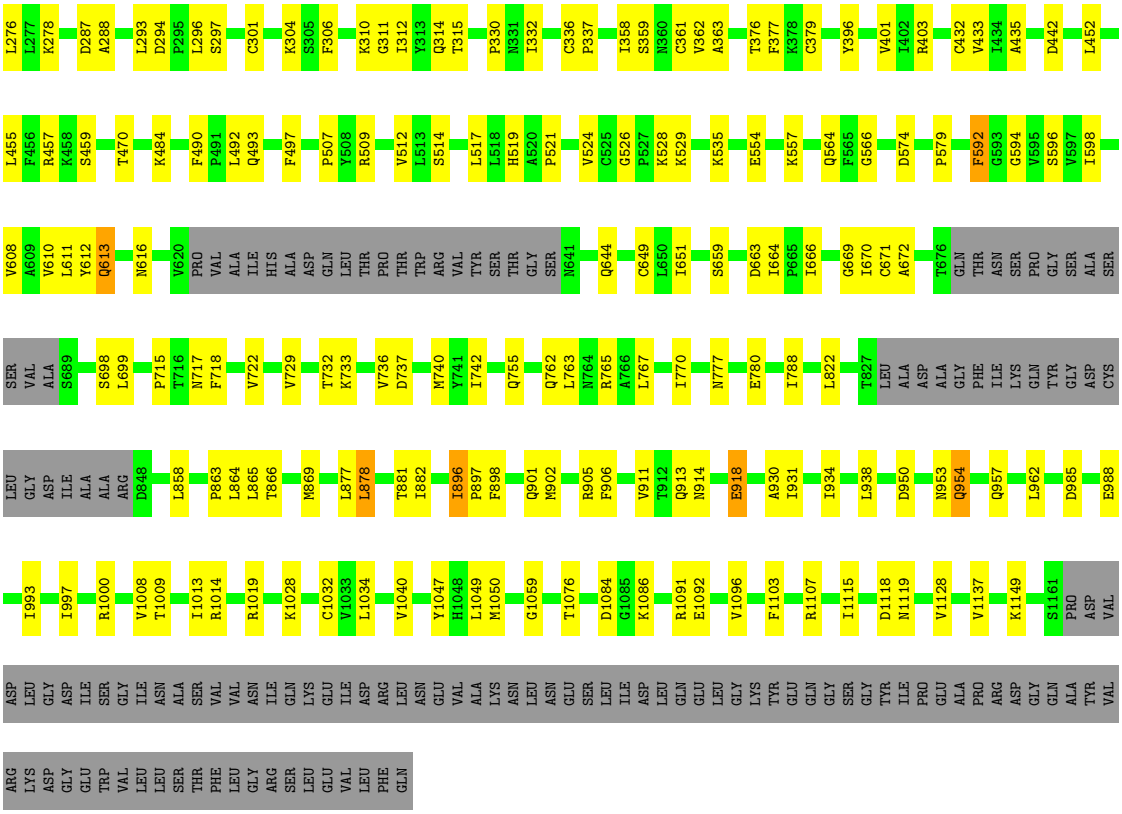


- Molecule 1: Spike glycoprotein,Fibritin



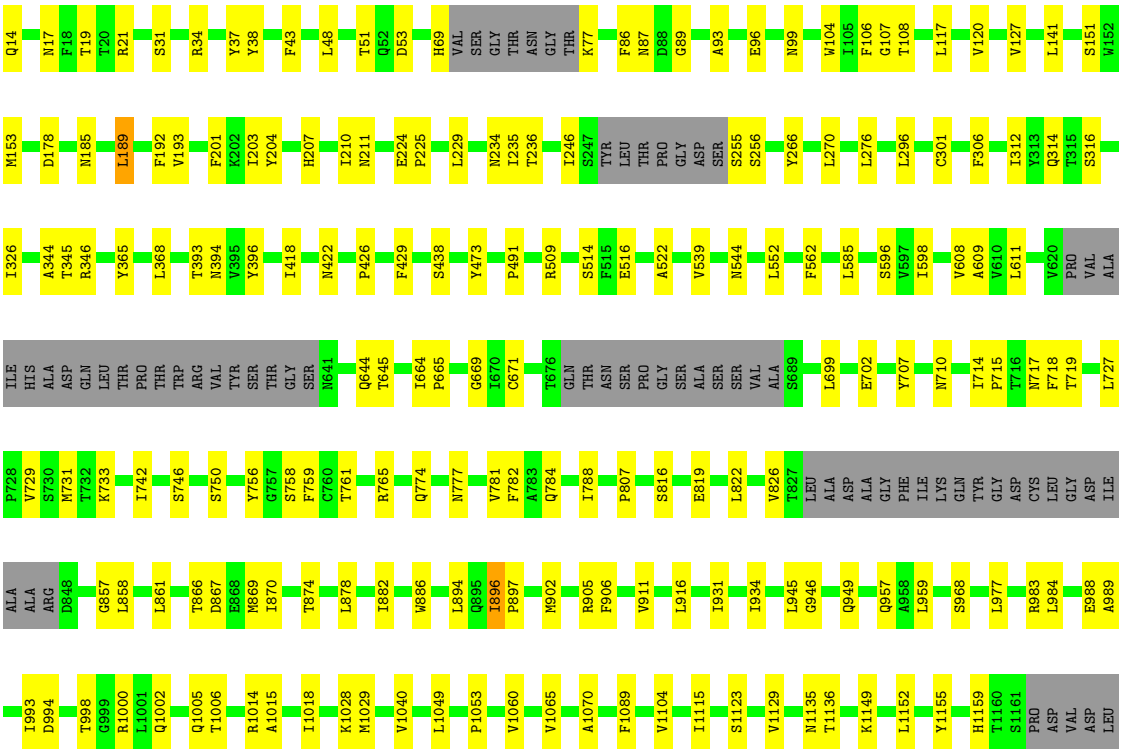
- Molecule 1: Spike glycoprotein,Fibritin

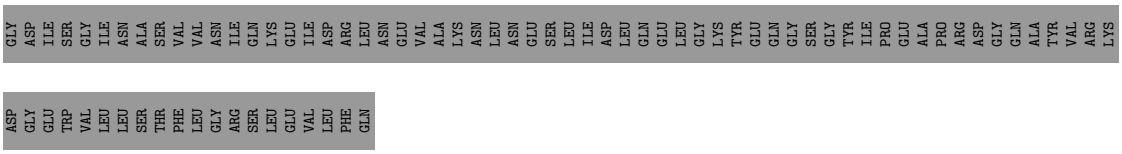




• Molecule 1: Spike glycoprotein,Fibritin

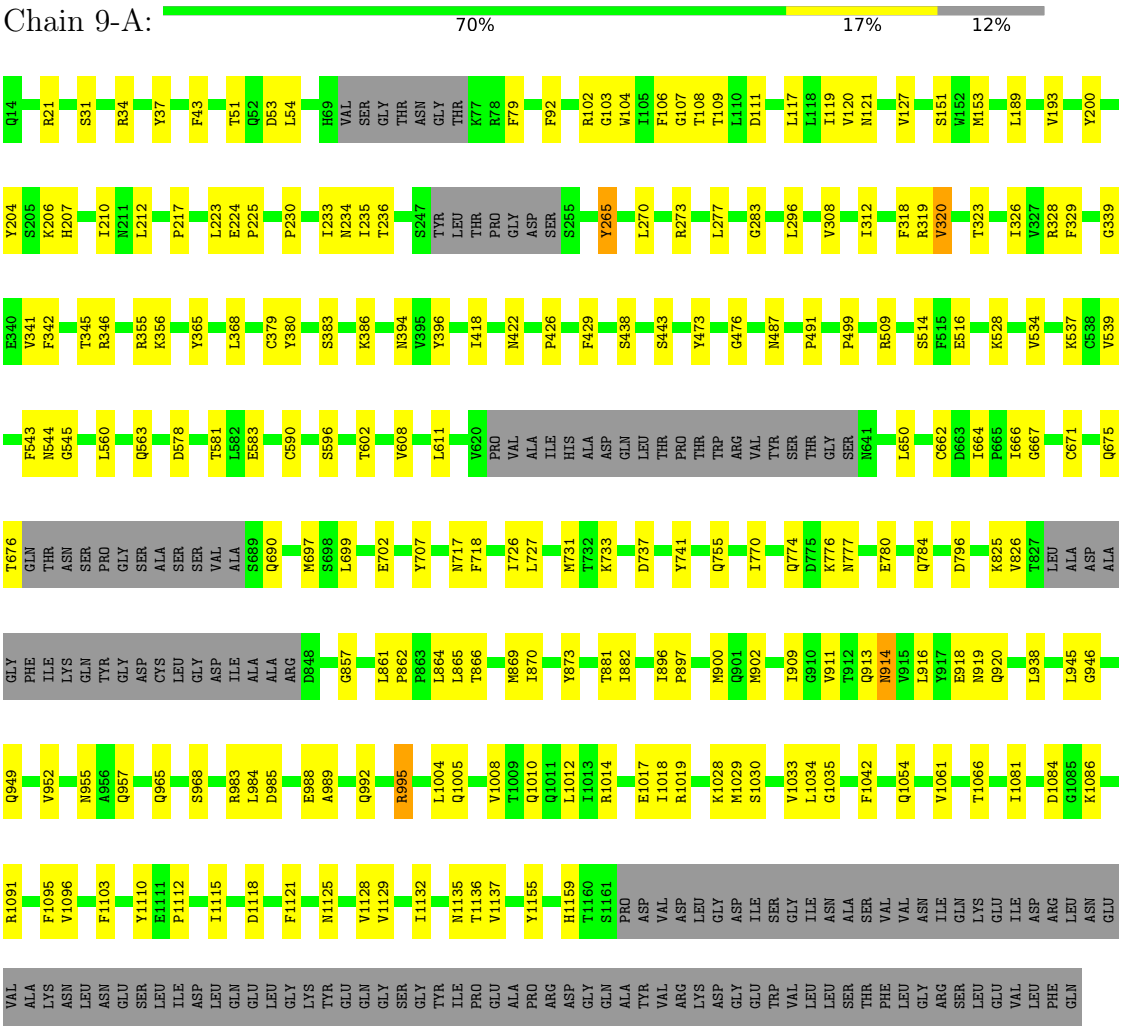
Chain 8-C:





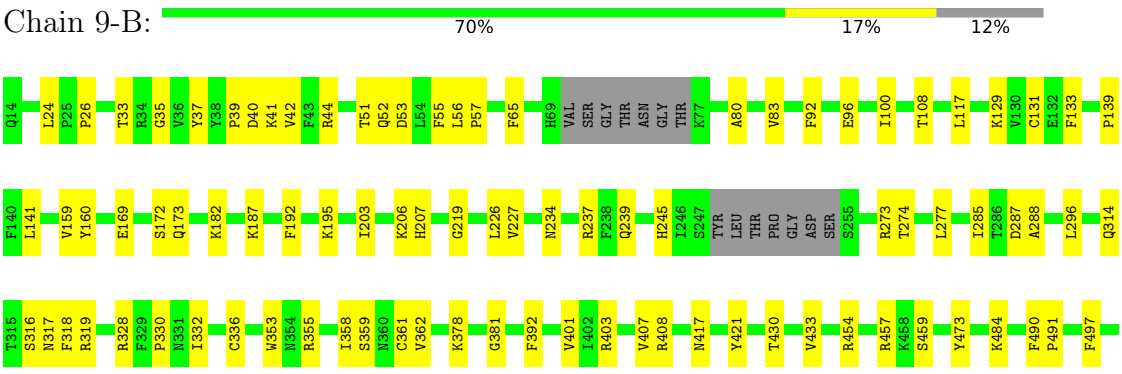
• Molecule 1: Spike glycoprotein,Fibritin

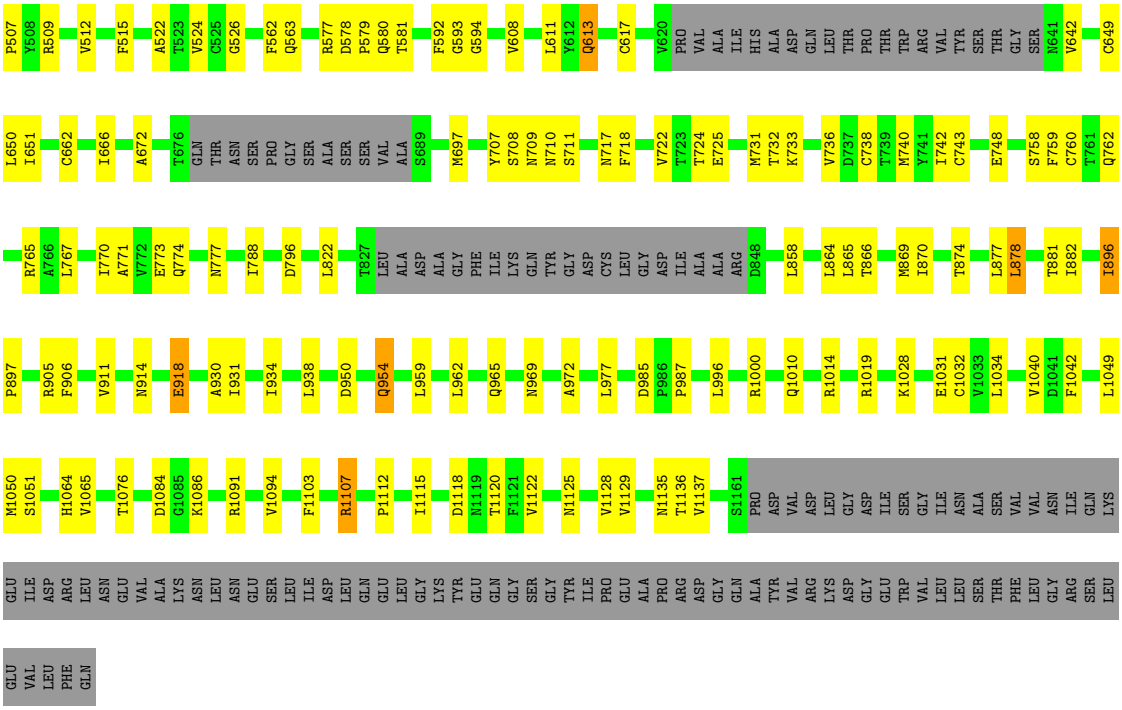
Chain 9-A:



• Molecule 1: Spike glycoprotein,Fibritin

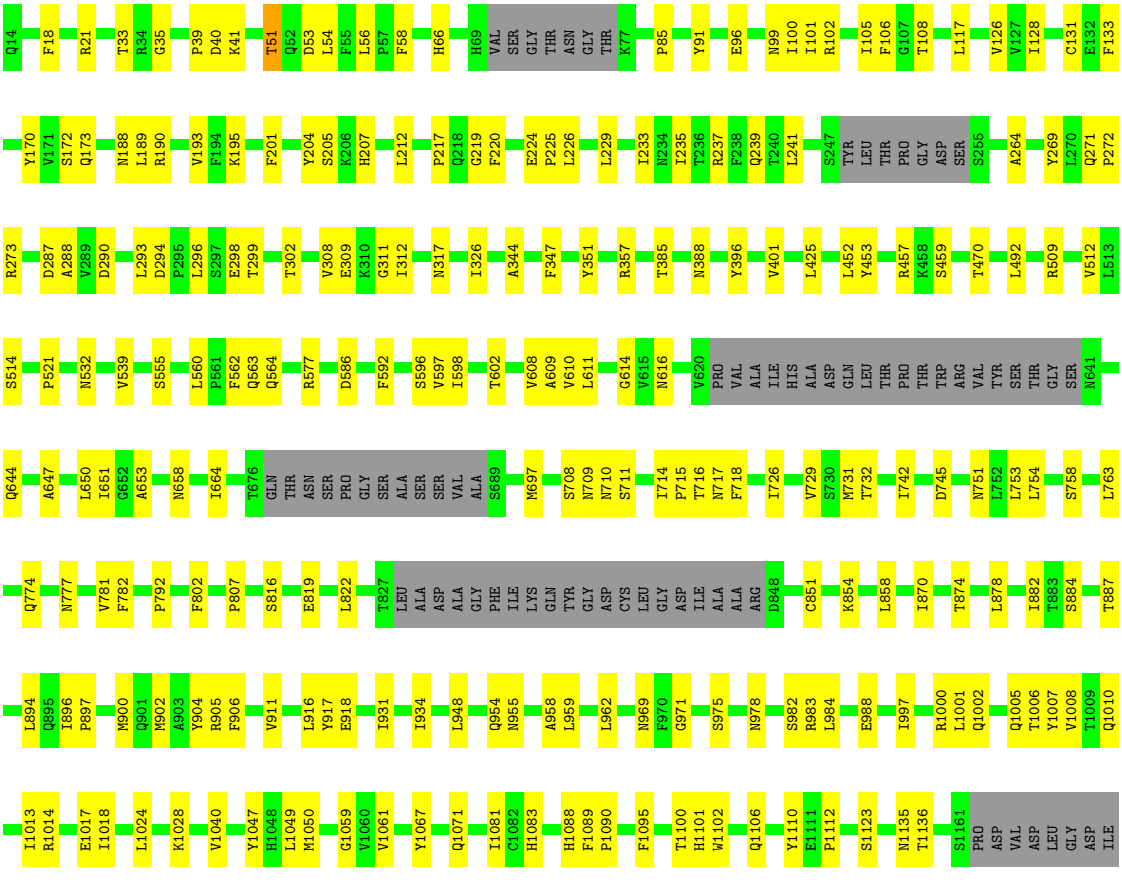
Chain 9-B:

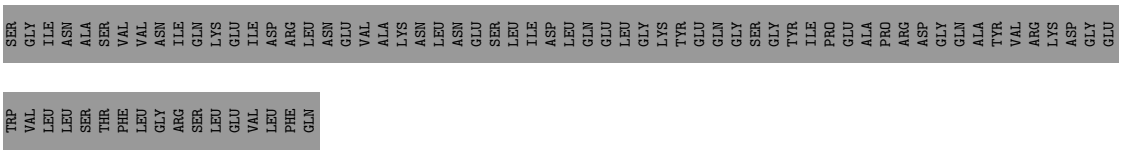




• Molecule 1: Spike glycoprotein,Fibritin

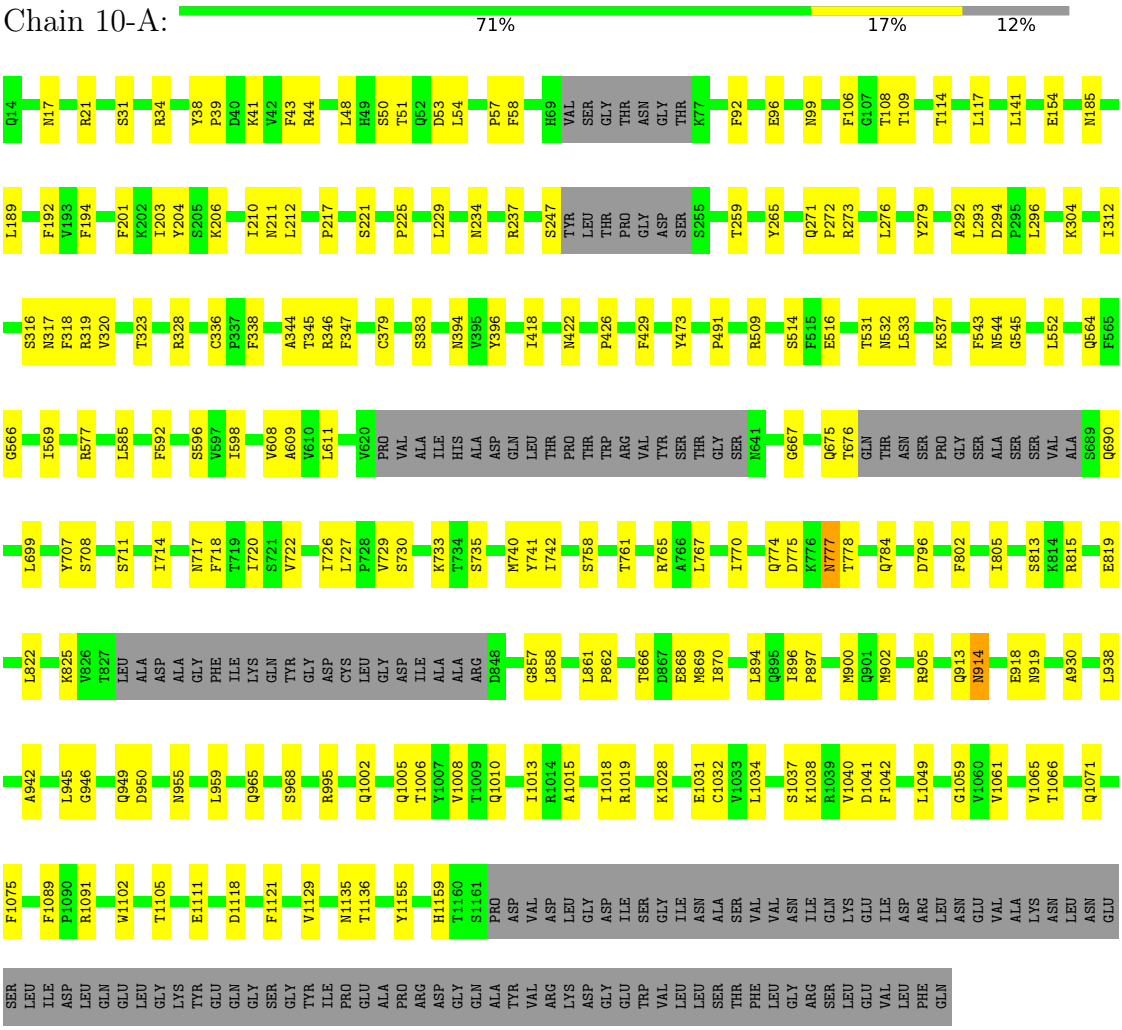
Chain 9-C:





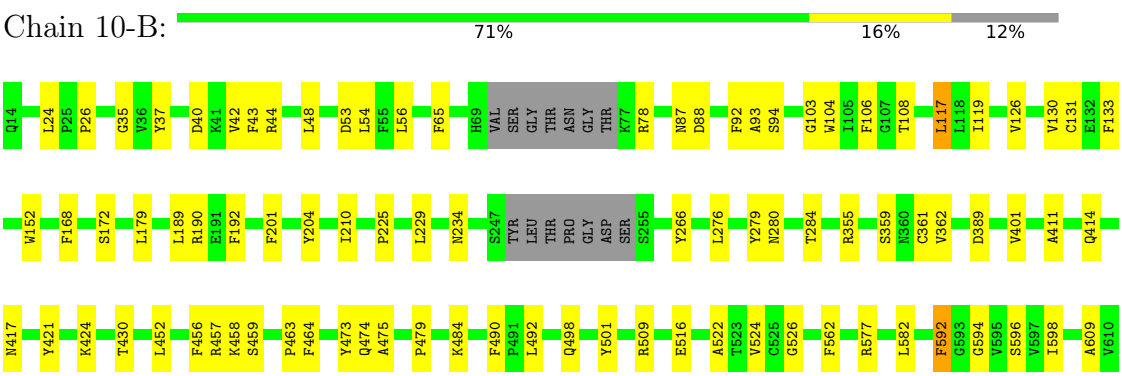
• Molecule 1: Spike glycoprotein,Fibritin

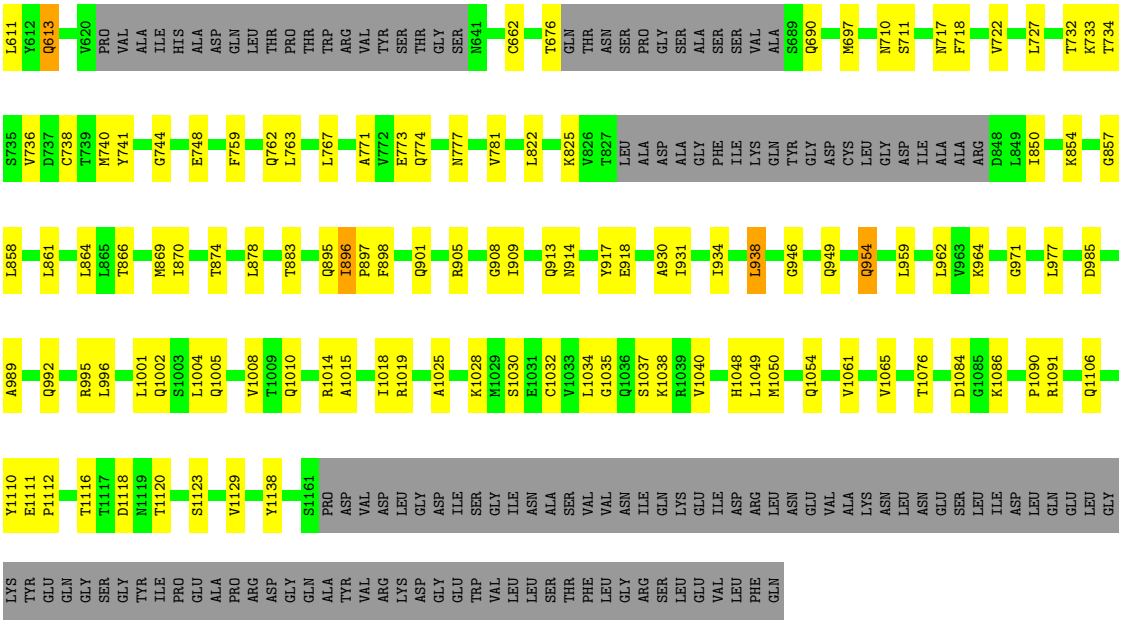
Chain 10-A:



• Molecule 1: Spike glycoprotein,Fibritin

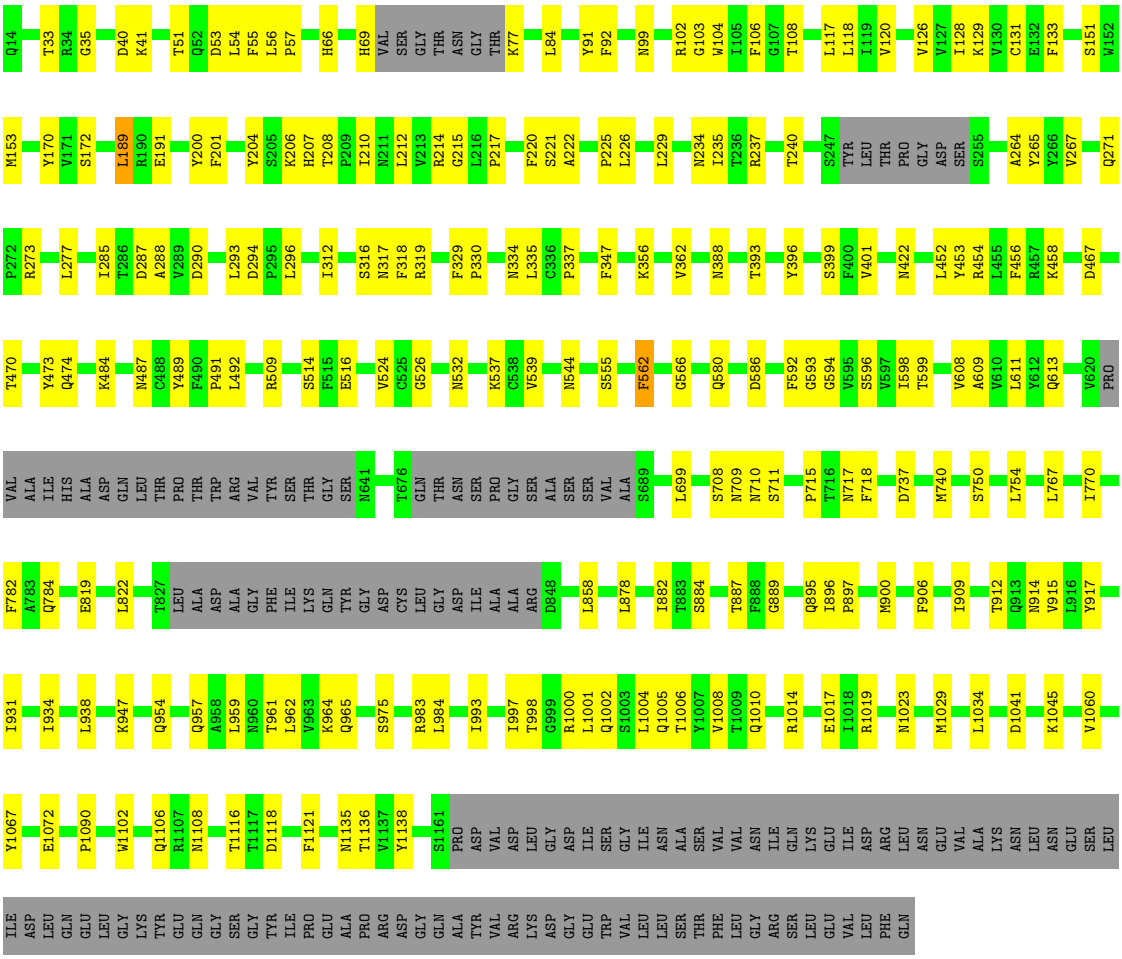
Chain 10-B:





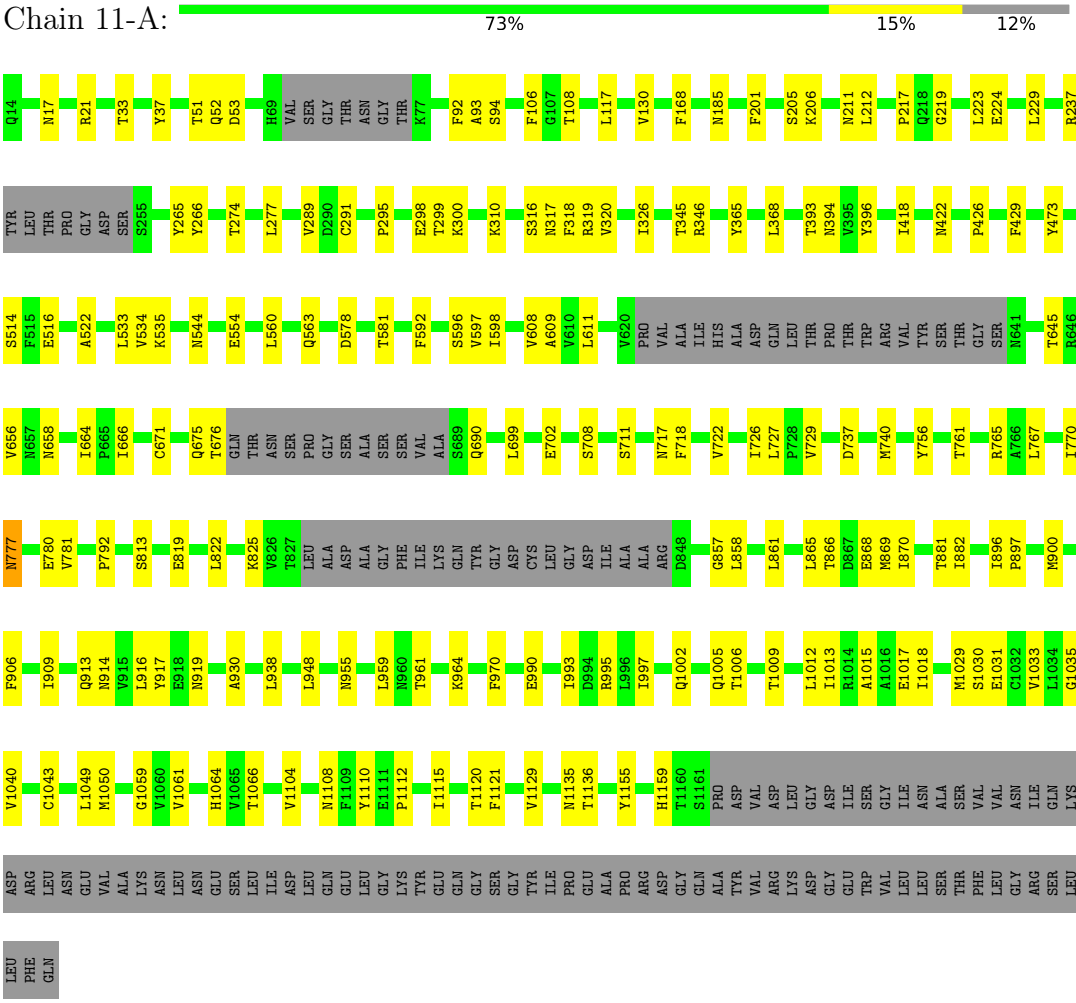
• Molecule 1: Spike glycoprotein,Fibritin

Chain 10-C:



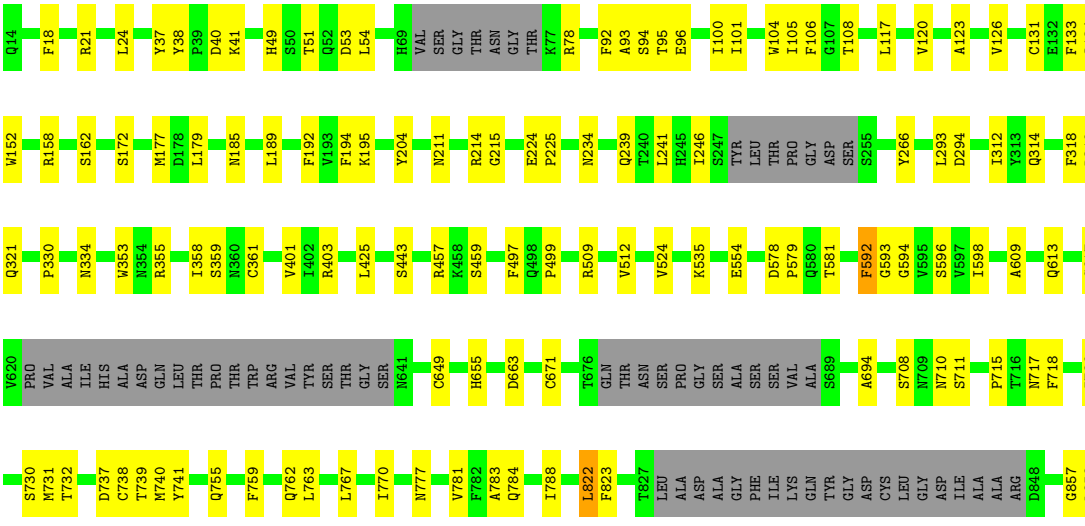
• Molecule 1: Spike glycoprotein,Fibritin

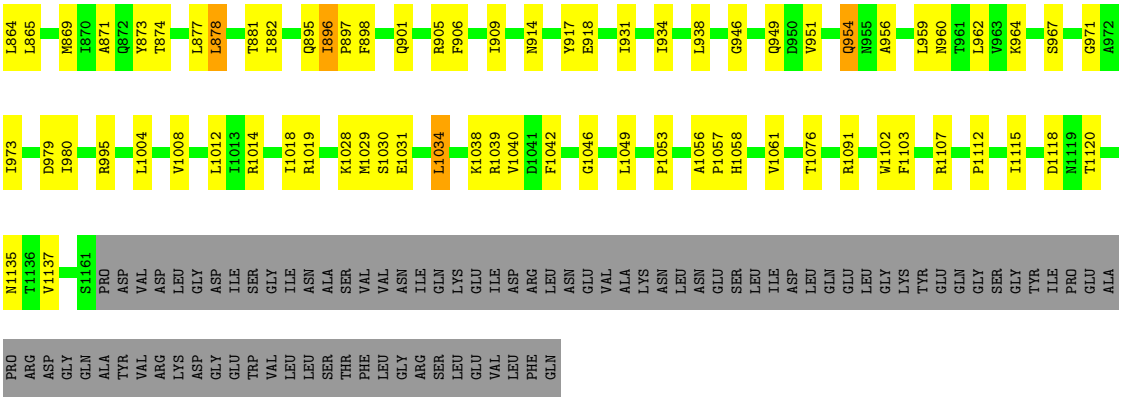
Chain 11-A:



• Molecule 1: Spike glycoprotein,Fibritin

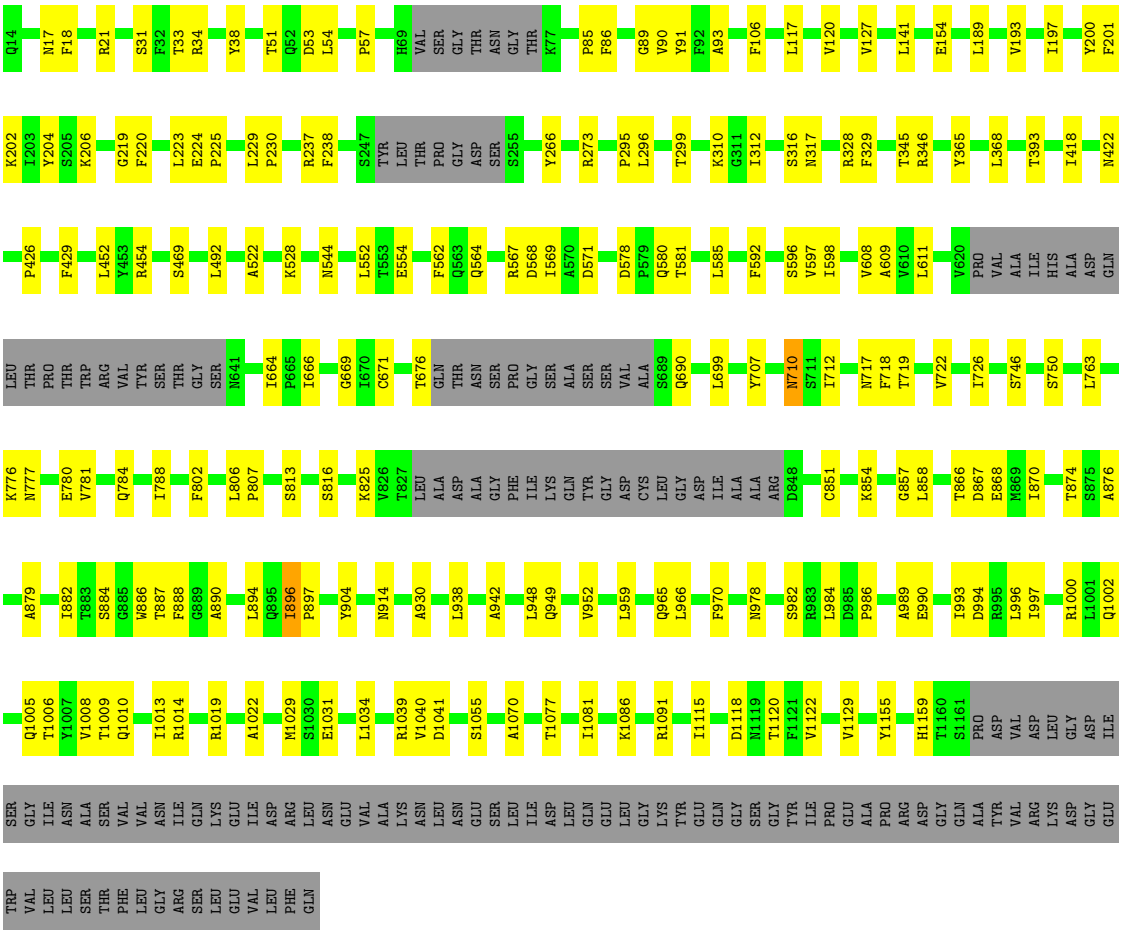
Chain 11-B:





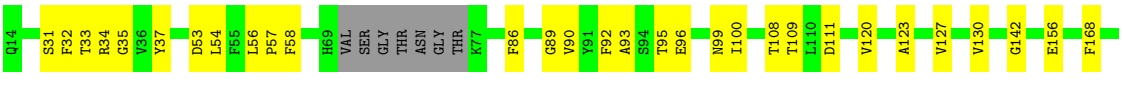
• Molecule 1: Spike glycoprotein,Fibritin

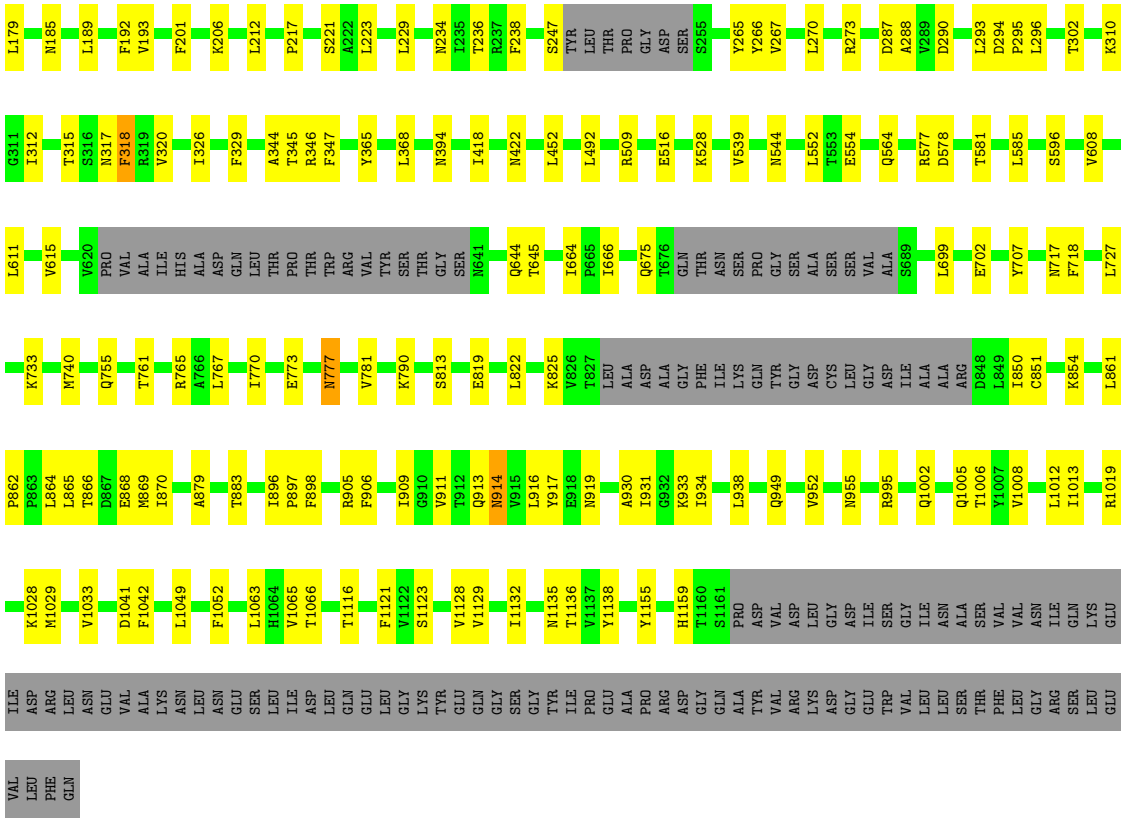
Chain 11-C:



• Molecule 1: Spike glycoprotein,Fibritin

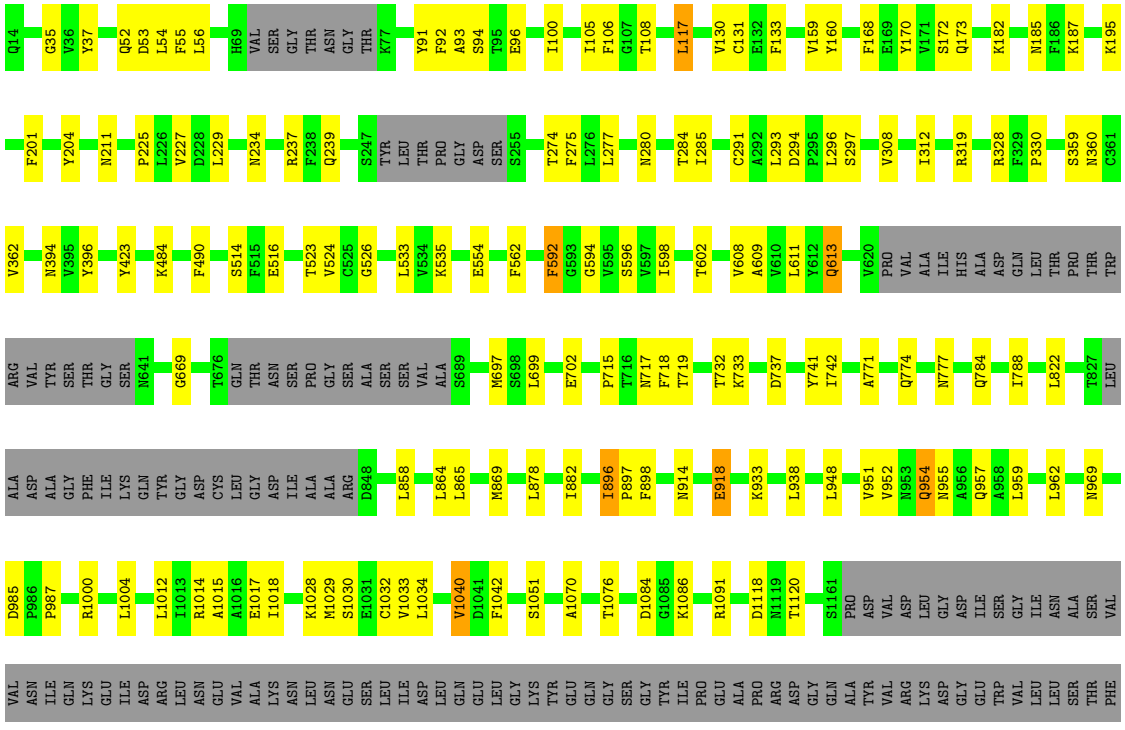
Chain 12-A:

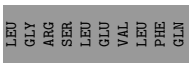




• Molecule 1: Spike glycoprotein,Fibritin

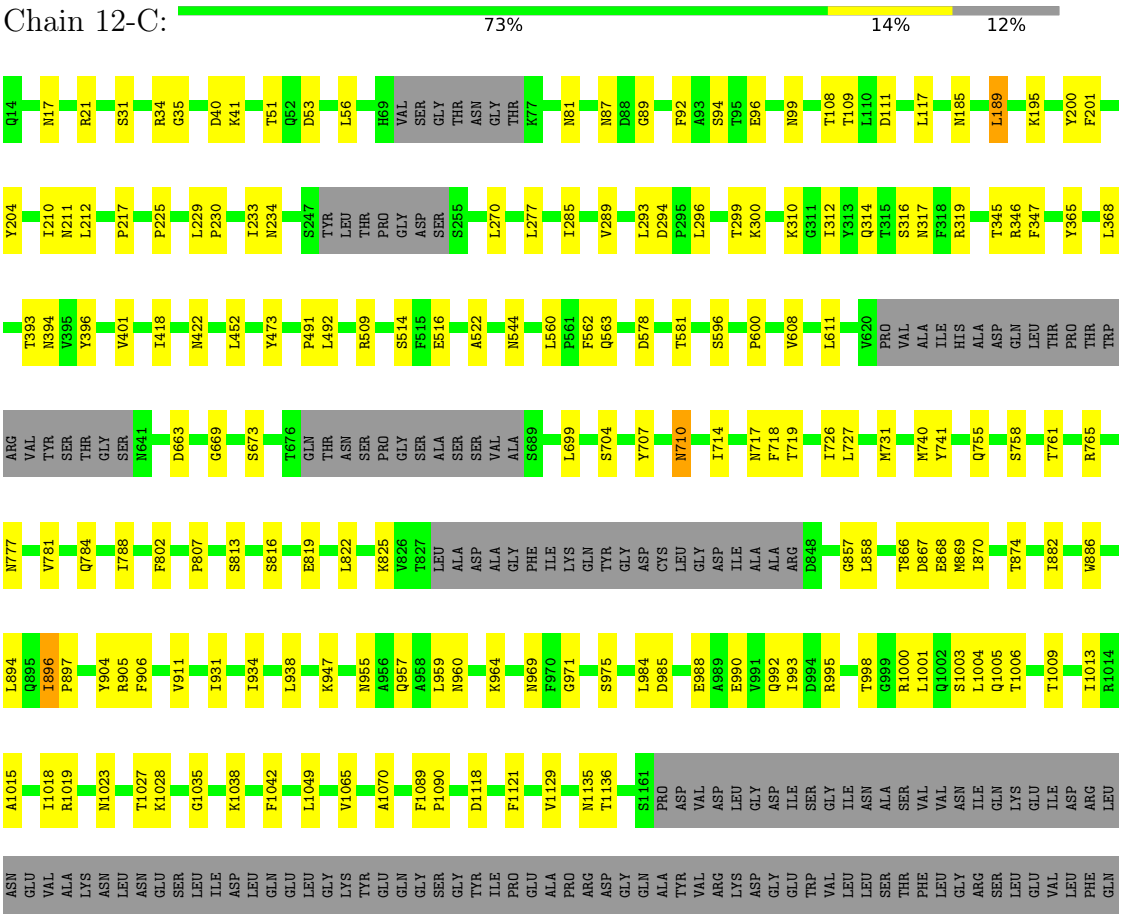
Chain 12-B:





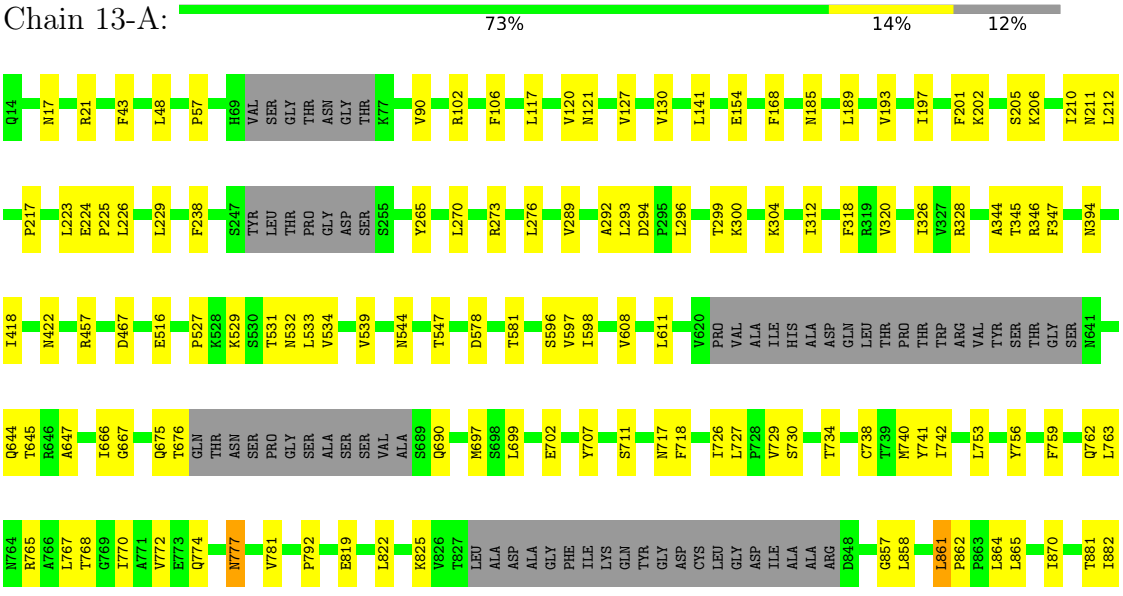
• Molecule 1: Spike glycoprotein,Fibritin

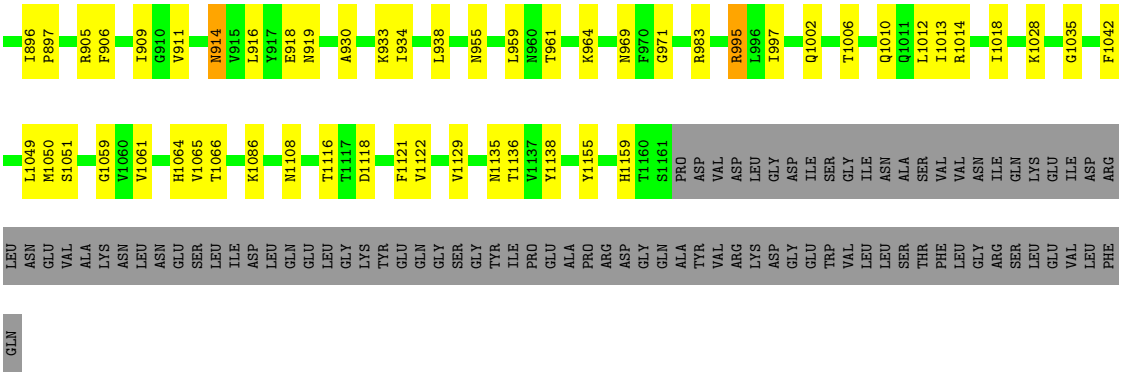
Chain 12-C:



• Molecule 1: Spike glycoprotein,Fibritin

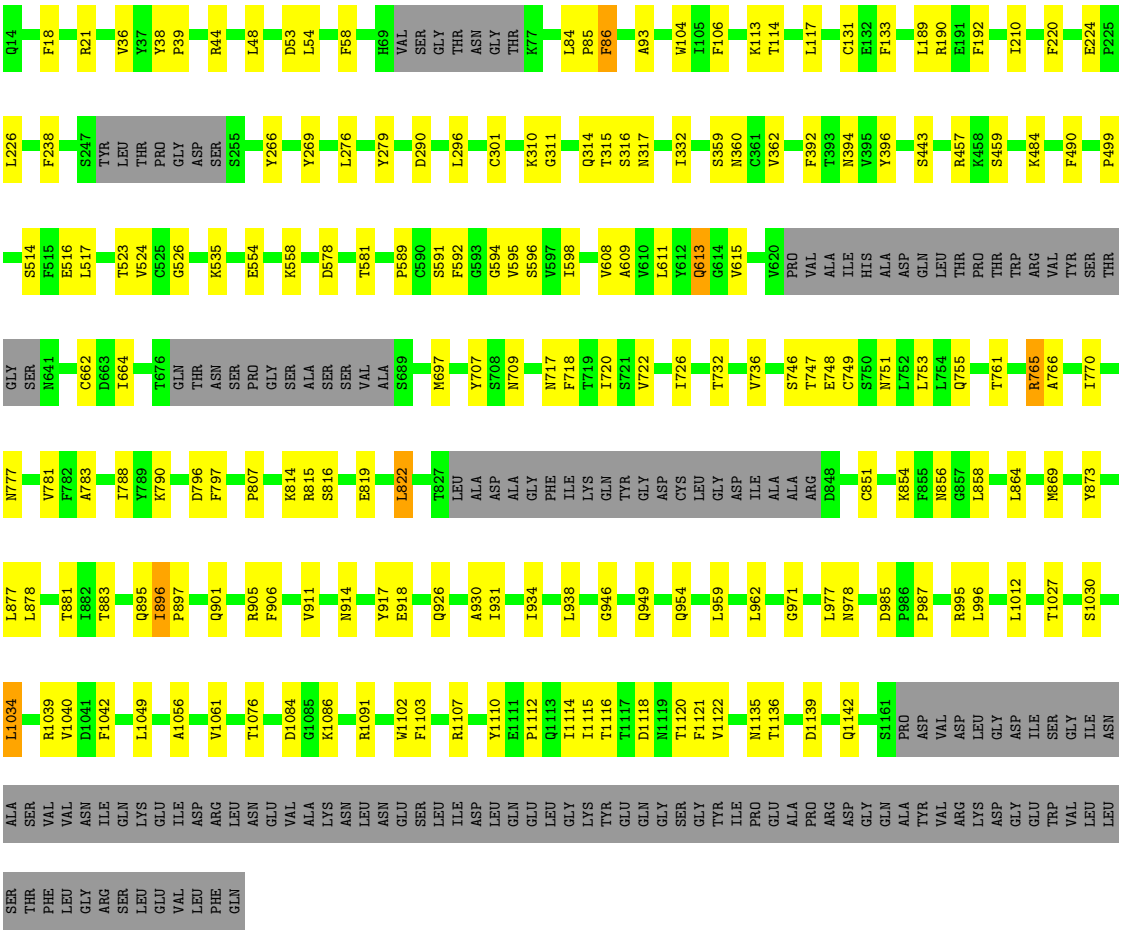
Chain 13-A:





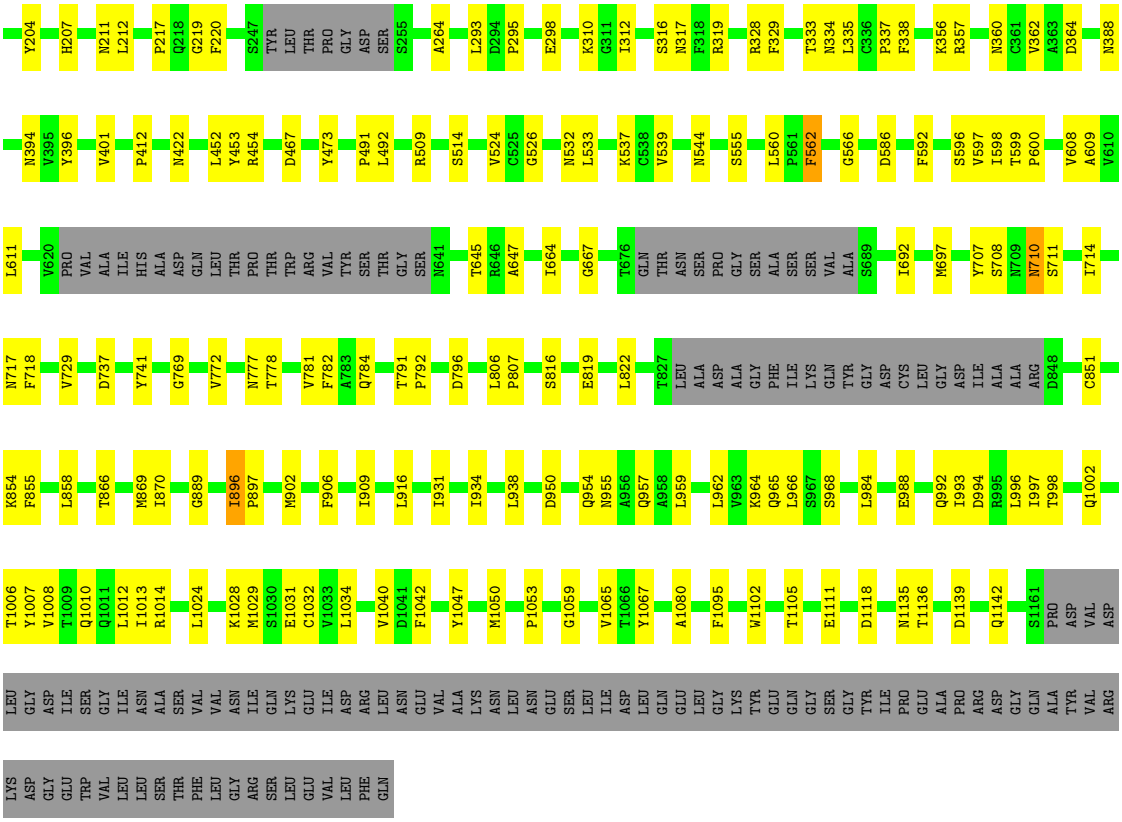
• Molecule 1: Spike glycoprotein,Fibritin

Chain 13-B:



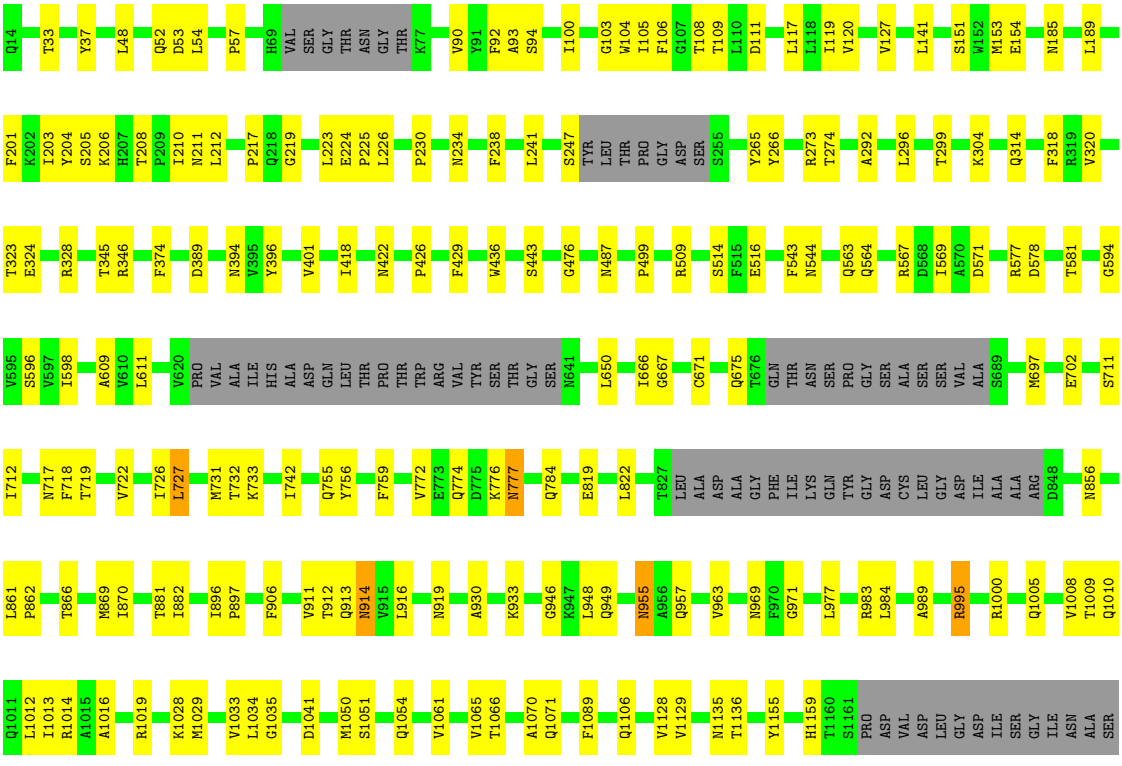
• Molecule 1: Spike glycoprotein,Fibritin

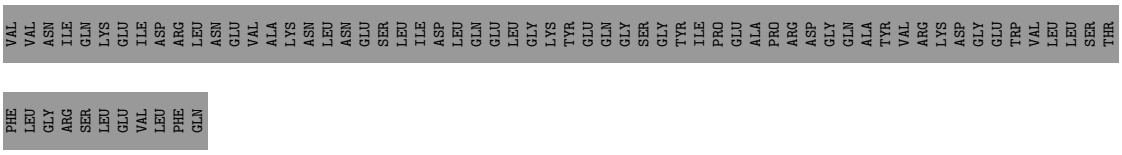
Chain 13-C:



• Molecule 1: Spike glycoprotein,Fibritin

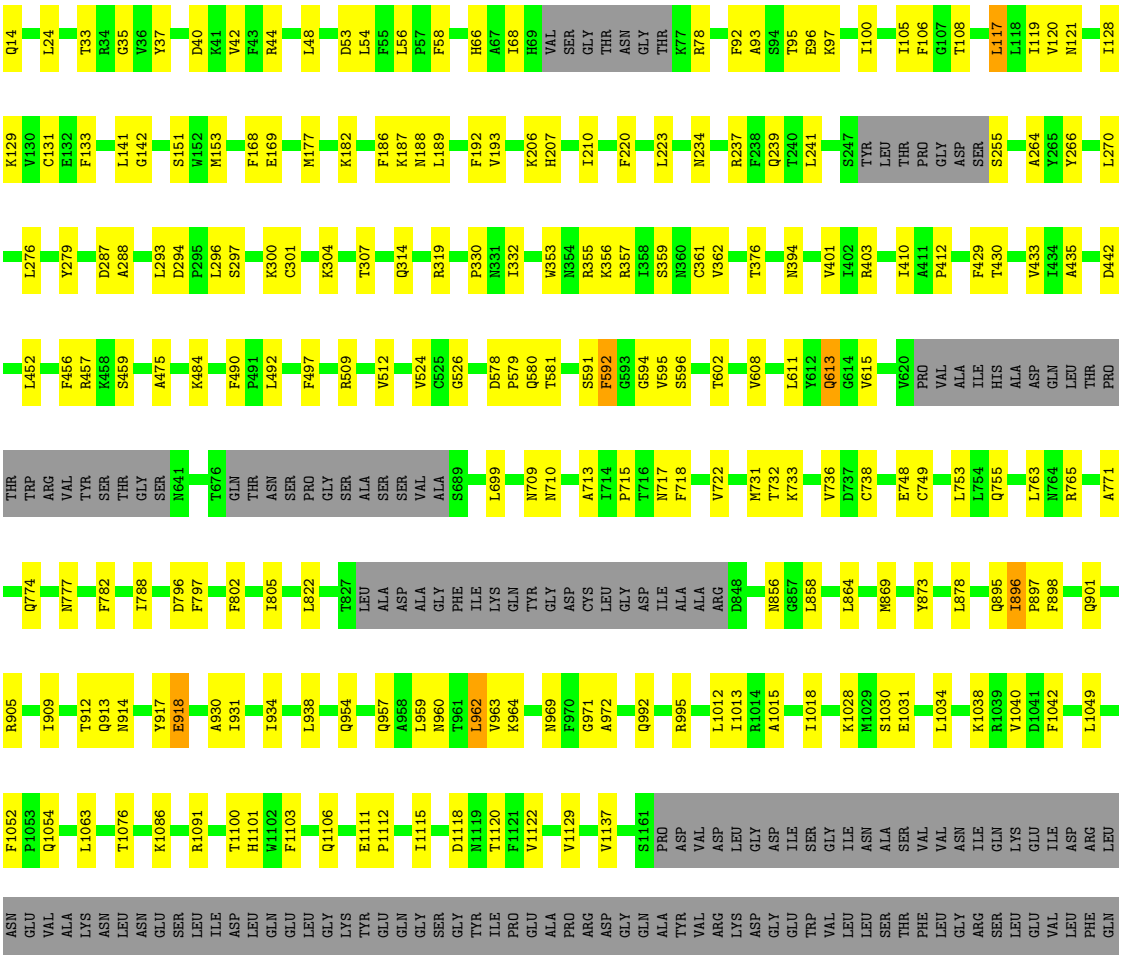
Chain 14-A:





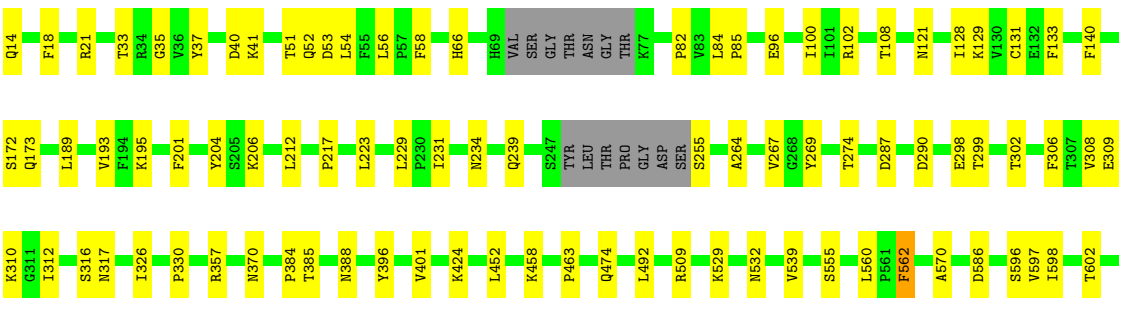
• Molecule 1: Spike glycoprotein,Fibritin

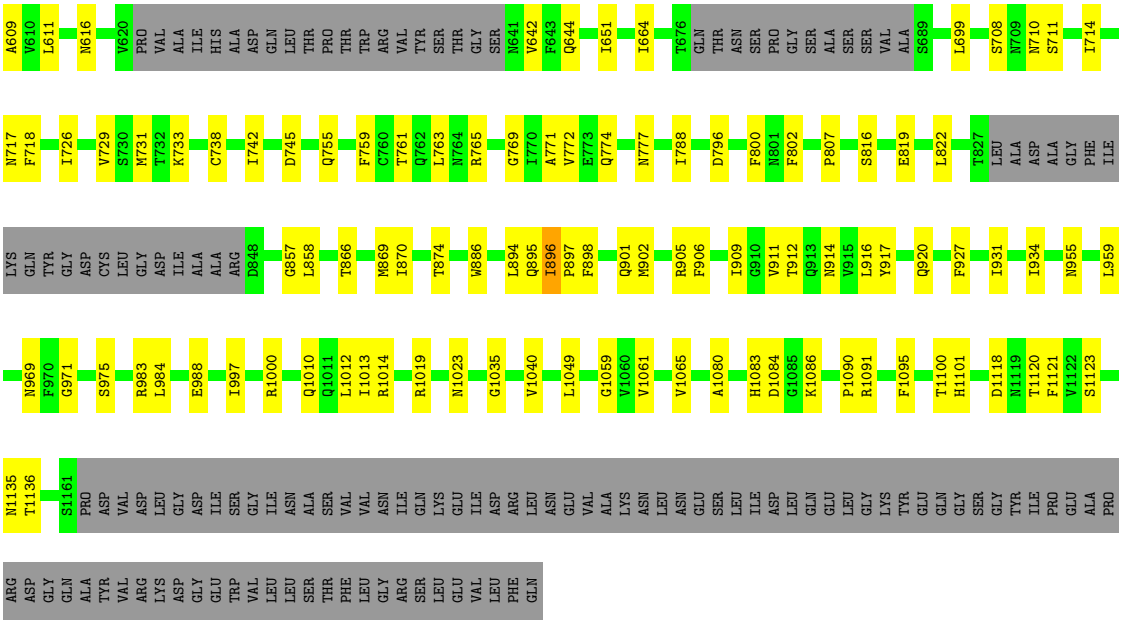
Chain 14-B:



• Molecule 1: Spike glycoprotein,Fibritin

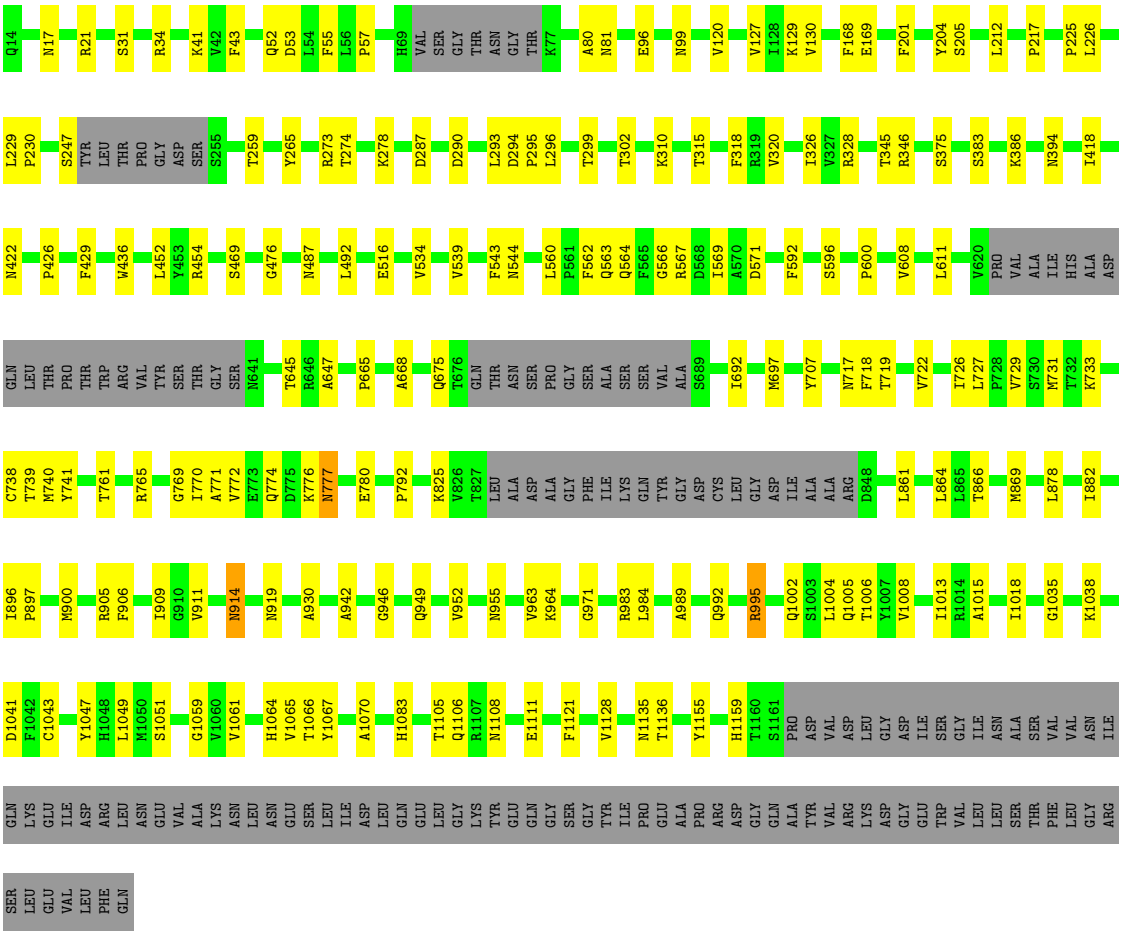
Chain 14-C:





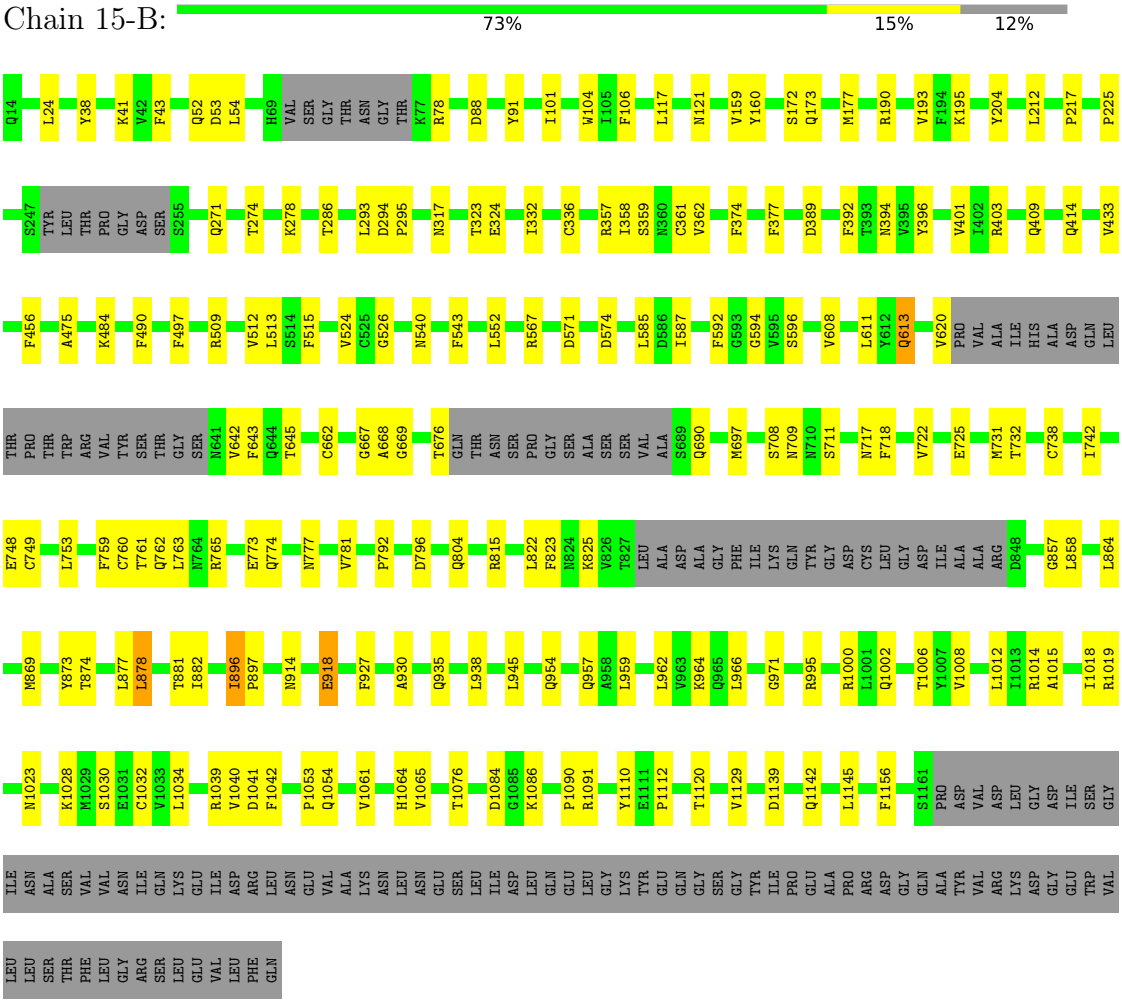
• Molecule 1: Spike glycoprotein,Fibritin

Chain 15-A:



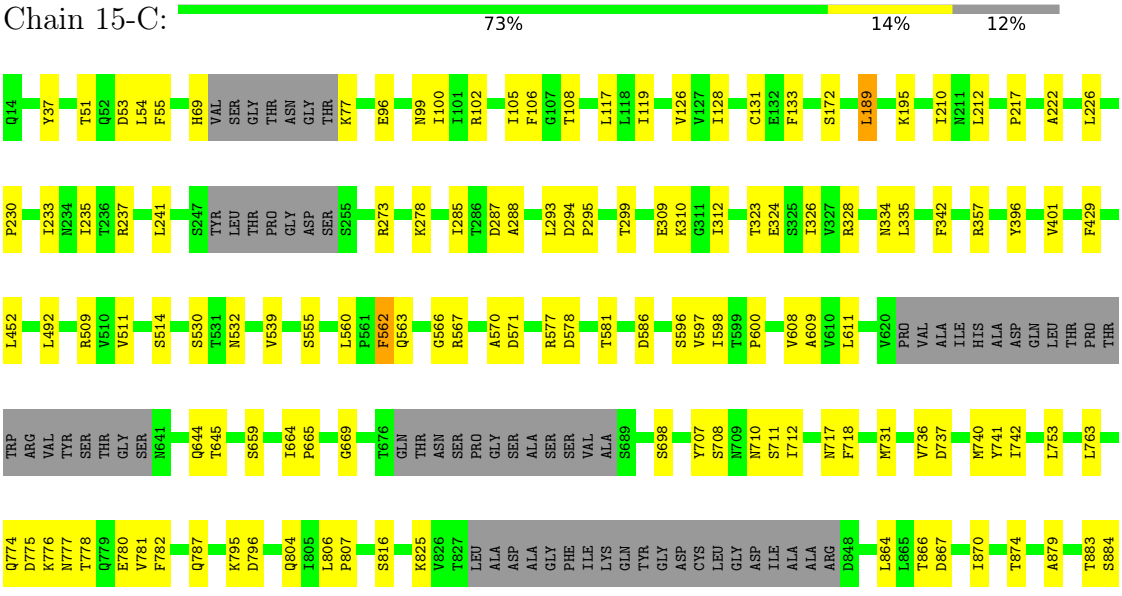
• Molecule 1: Spike glycoprotein,Fibritin

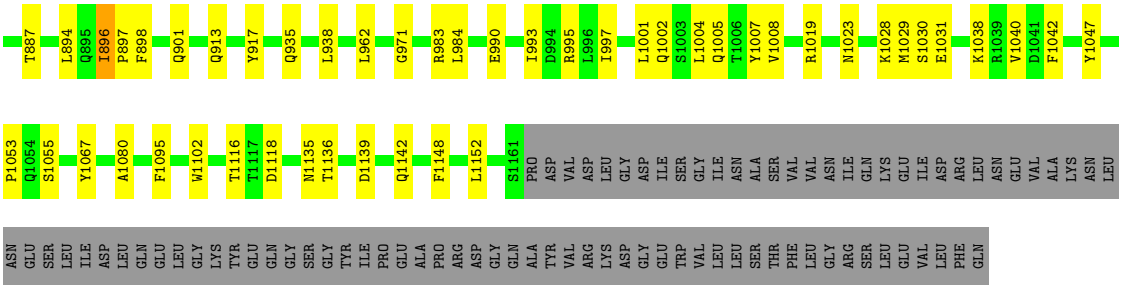
Chain 15-B:



• Molecule 1: Spike glycoprotein,Fibritin

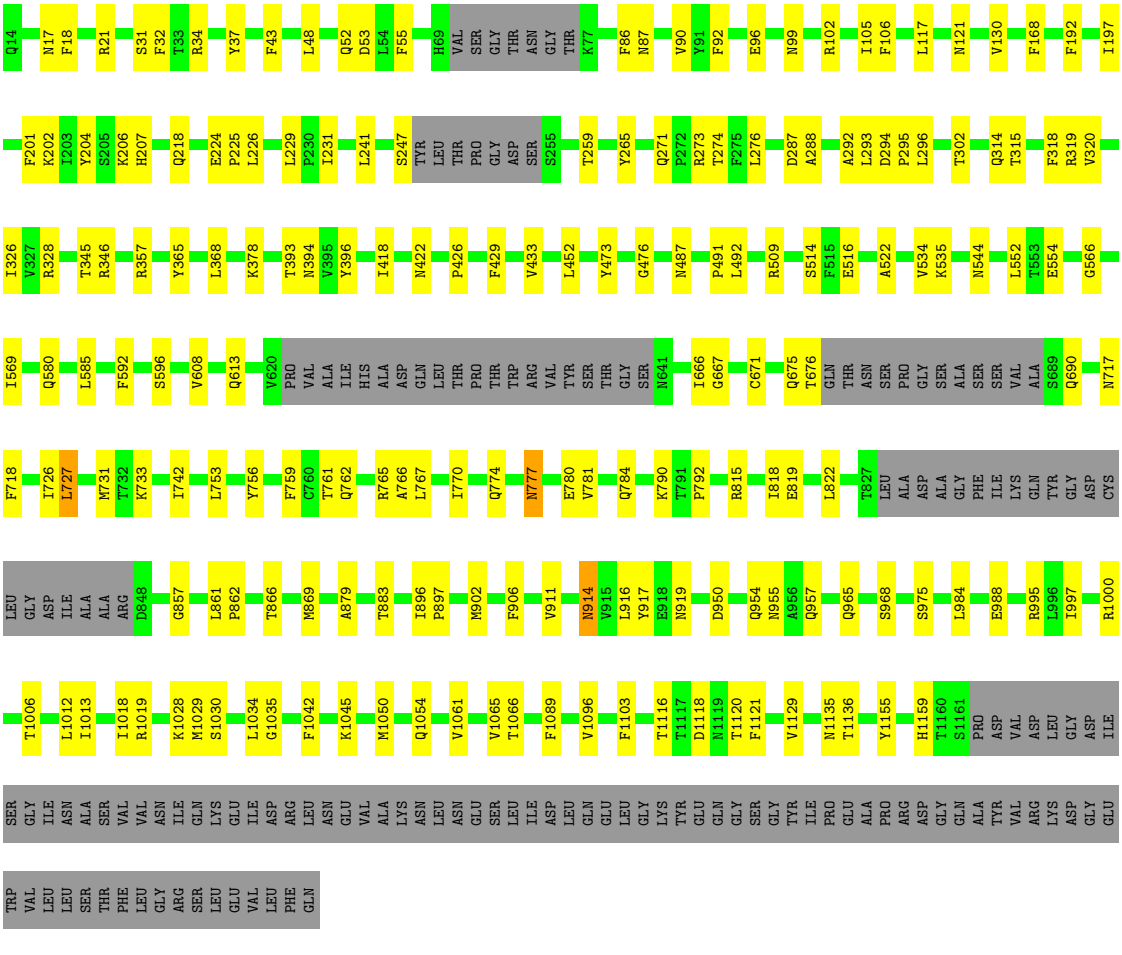
Chain 15-C:





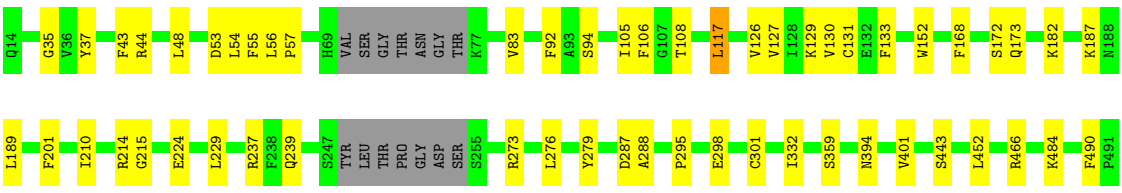
• Molecule 1: Spike glycoprotein,Fibritin

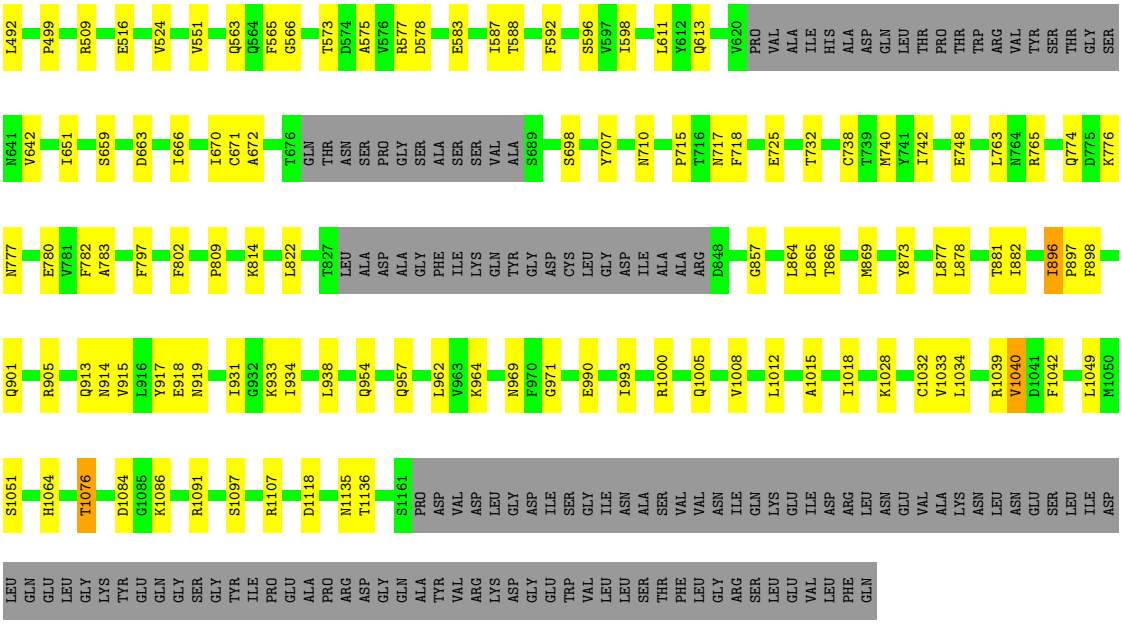
Chain 16-A:



• Molecule 1: Spike glycoprotein,Fibritin

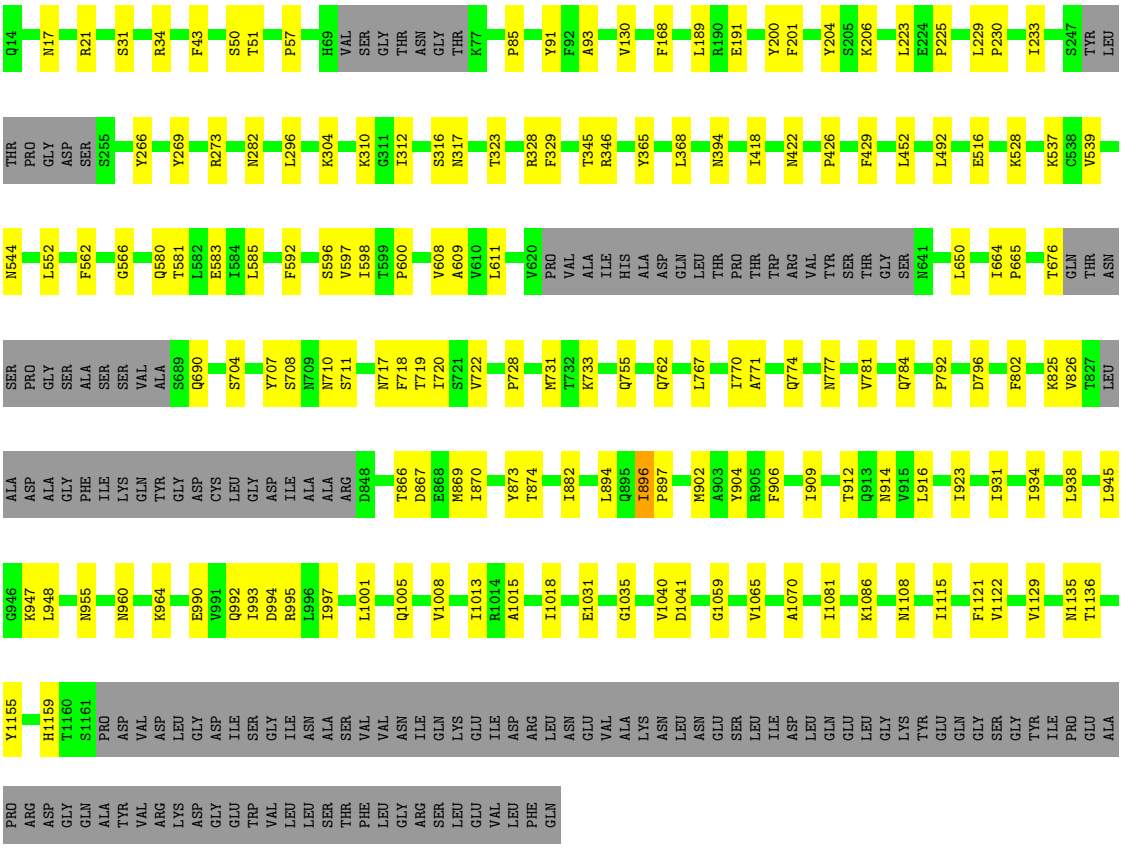
Chain 16-B:





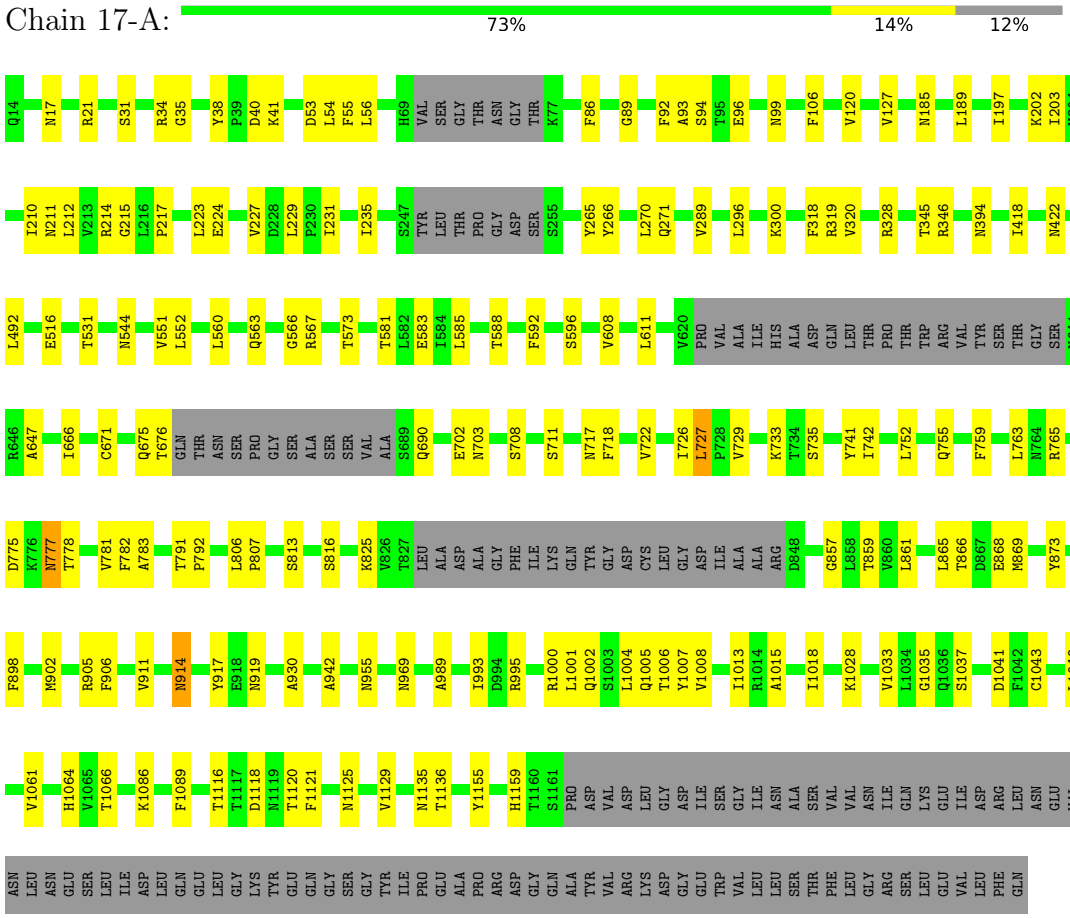
• Molecule 1: Spike glycoprotein,Fibritin

Chain 16-C:



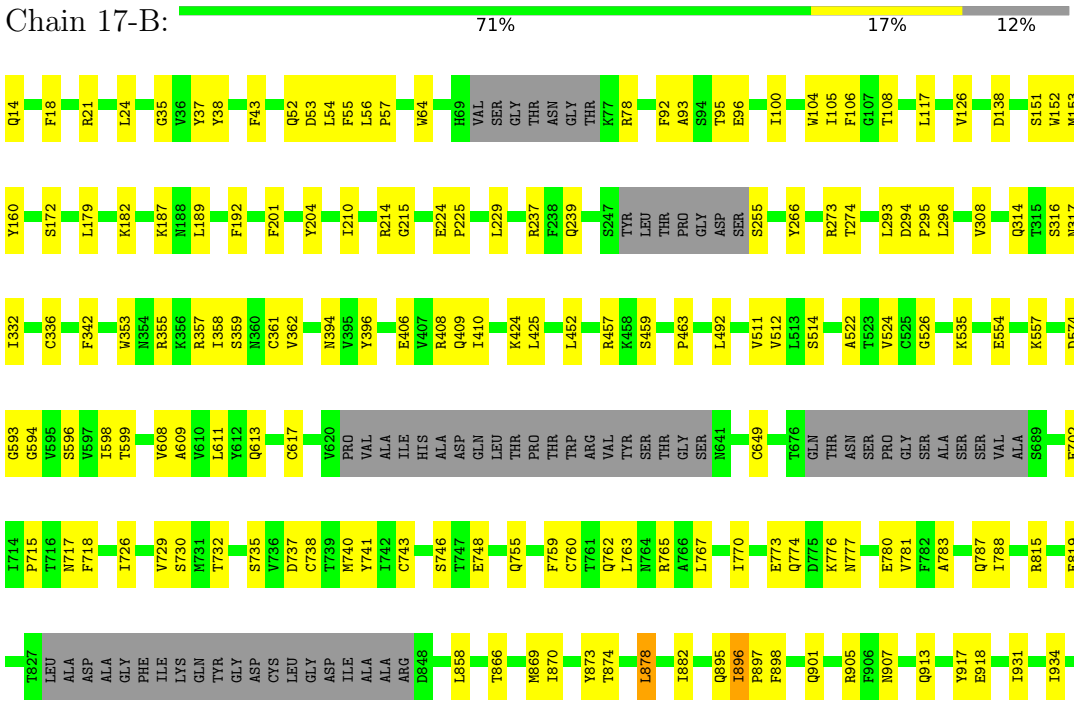
• Molecule 1: Spike glycoprotein,Fibritin

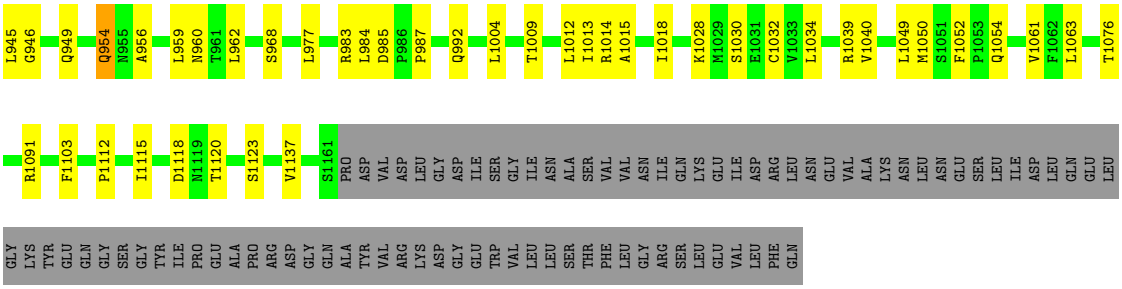
Chain 17-A:



• Molecule 1: Spike glycoprotein,Fibritin

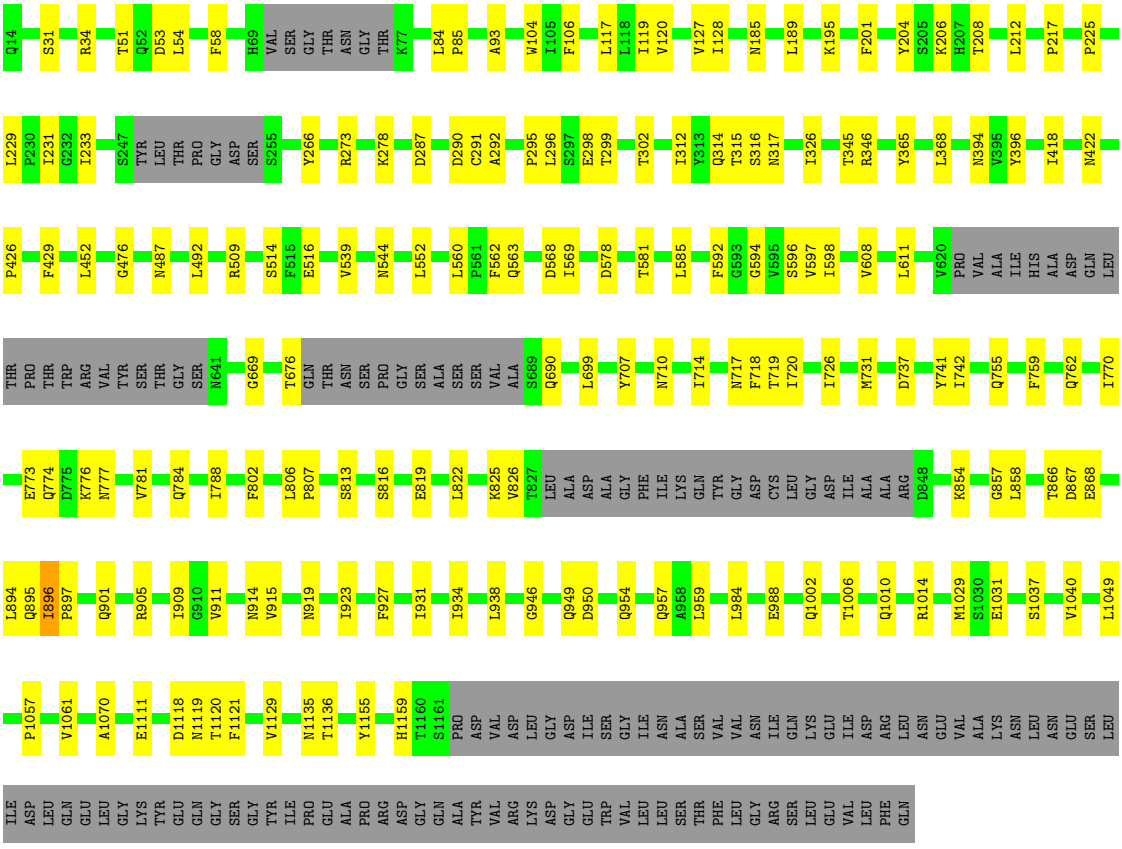
Chain 17-B:





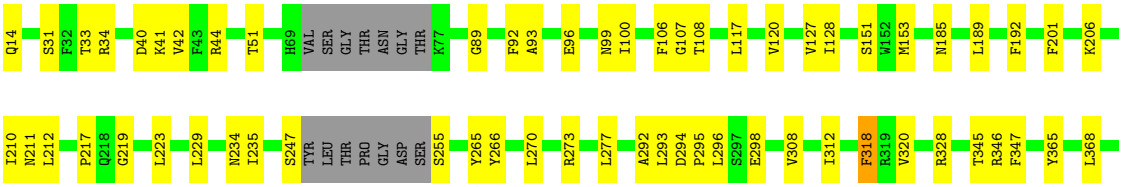
• Molecule 1: Spike glycoprotein,Fibritin

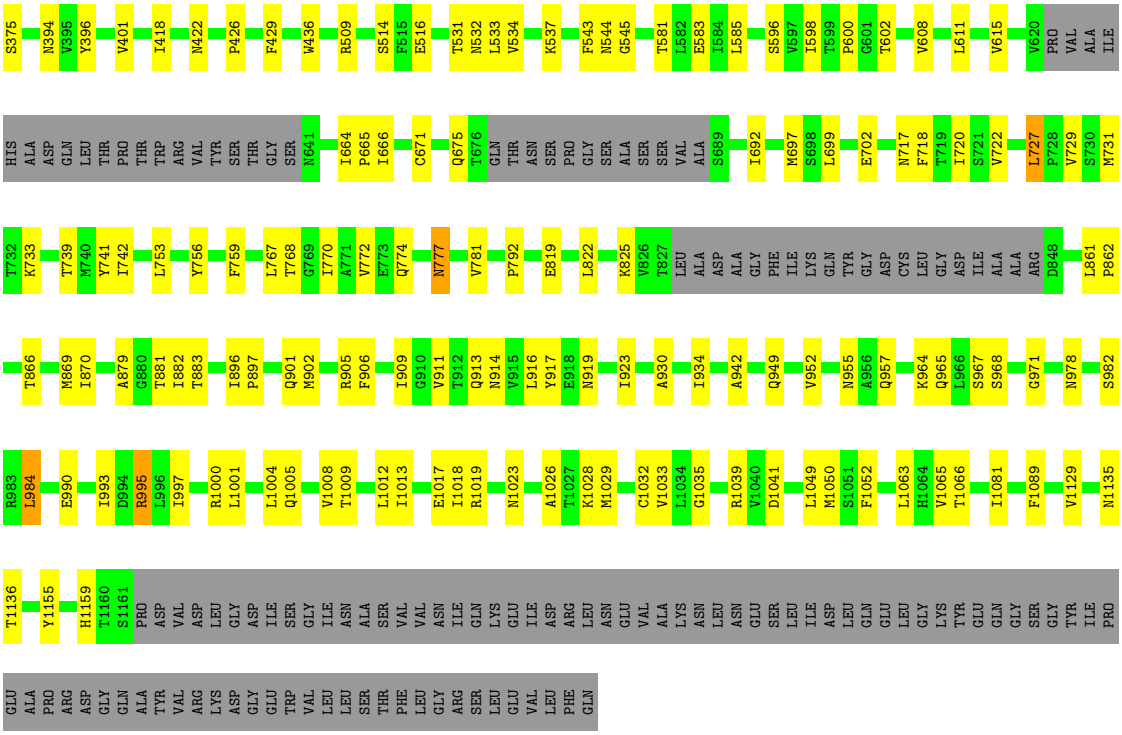
Chain 17-C:



• Molecule 1: Spike glycoprotein,Fibritin

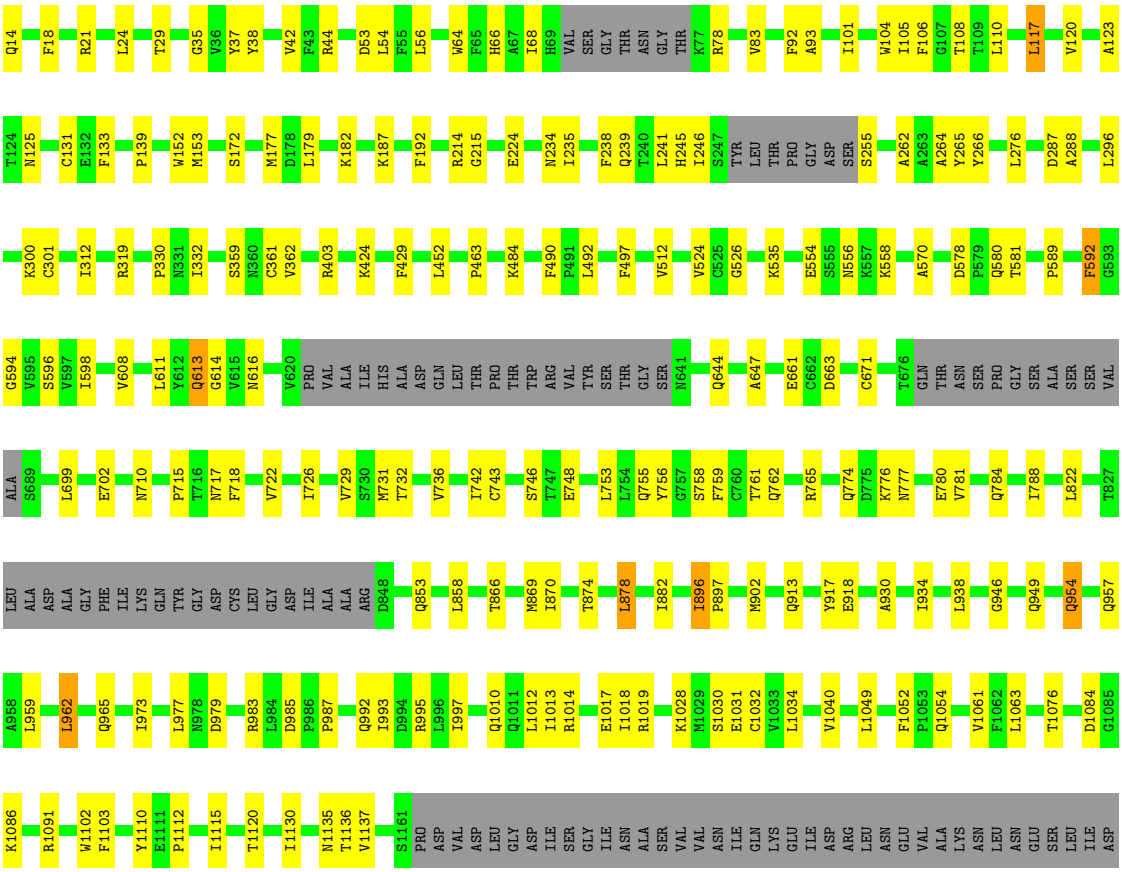
Chain 18-A:

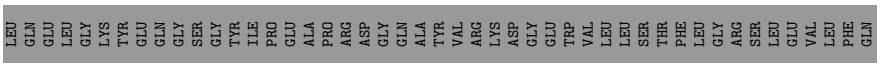




• Molecule 1: Spike glycoprotein,Fibritin

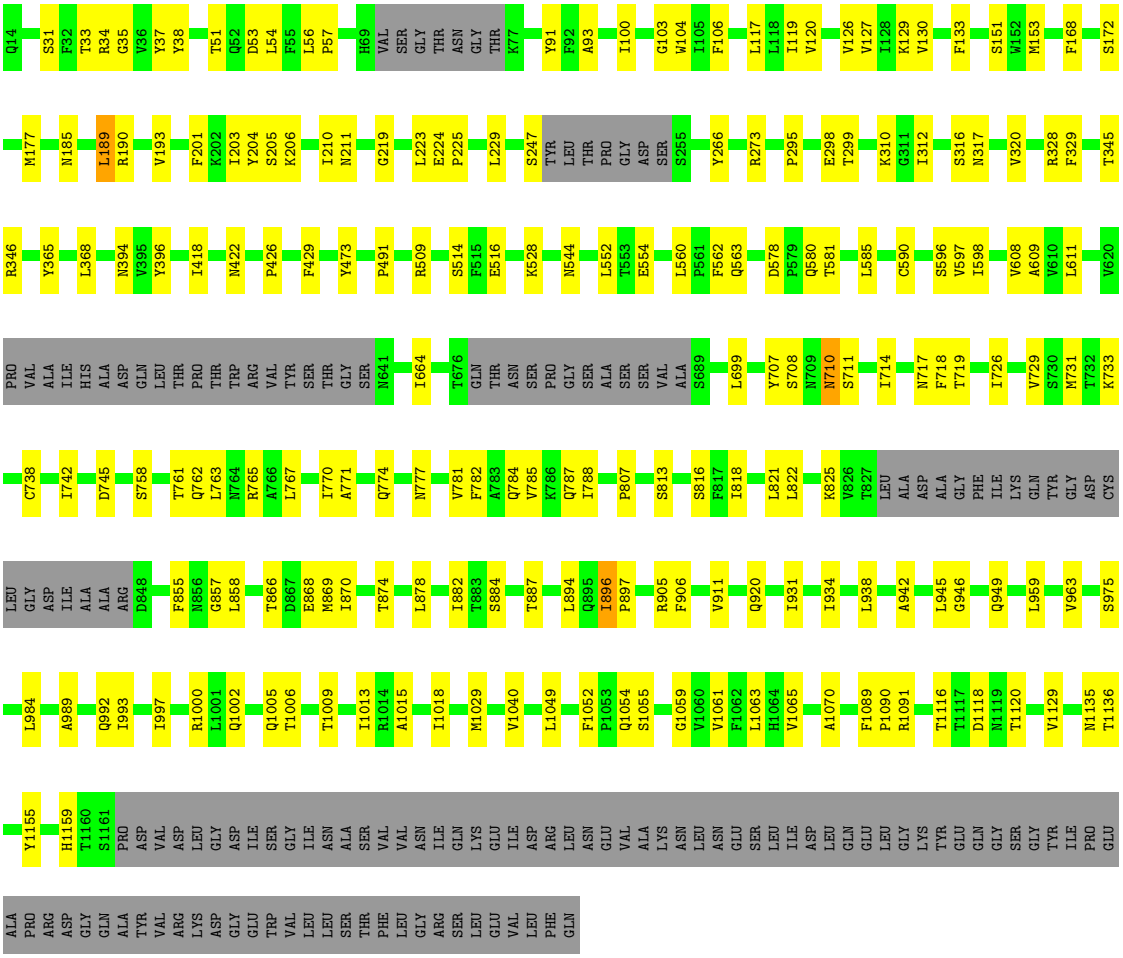
Chain 18-B:





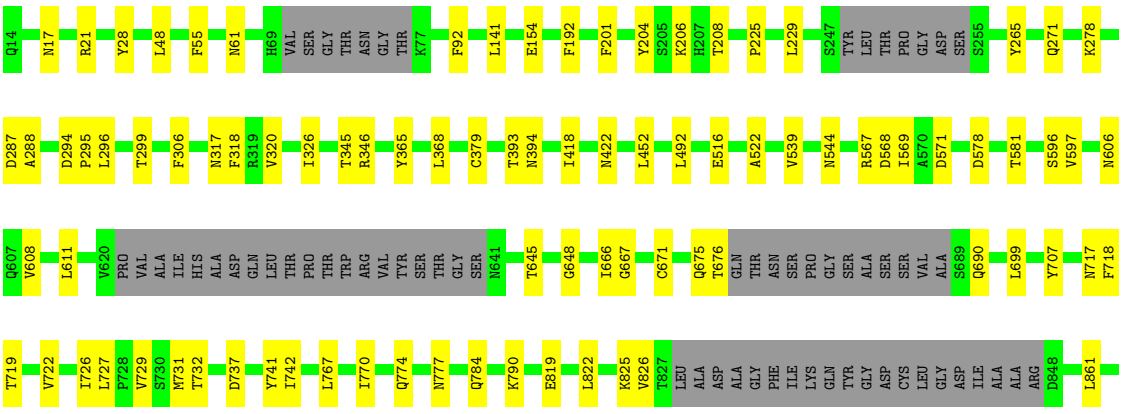
• Molecule 1: Spike glycoprotein,Fibritin

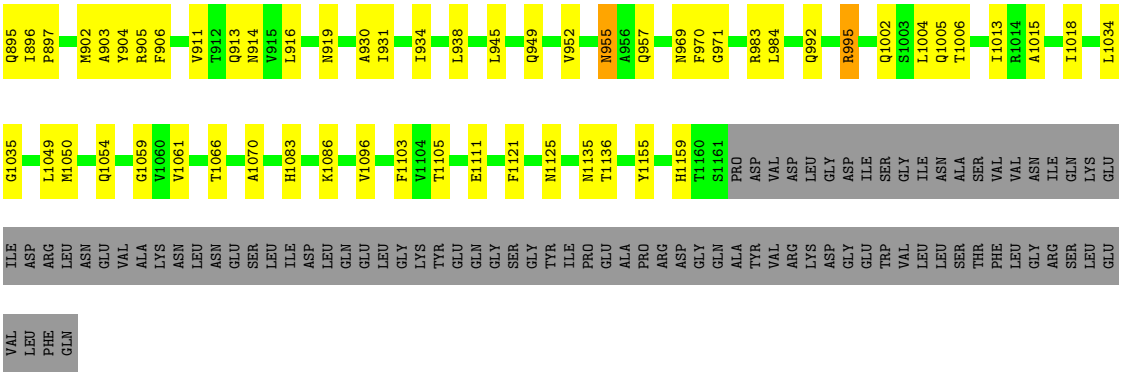
Chain 18-C:



• Molecule 1: Spike glycoprotein,Fibritin

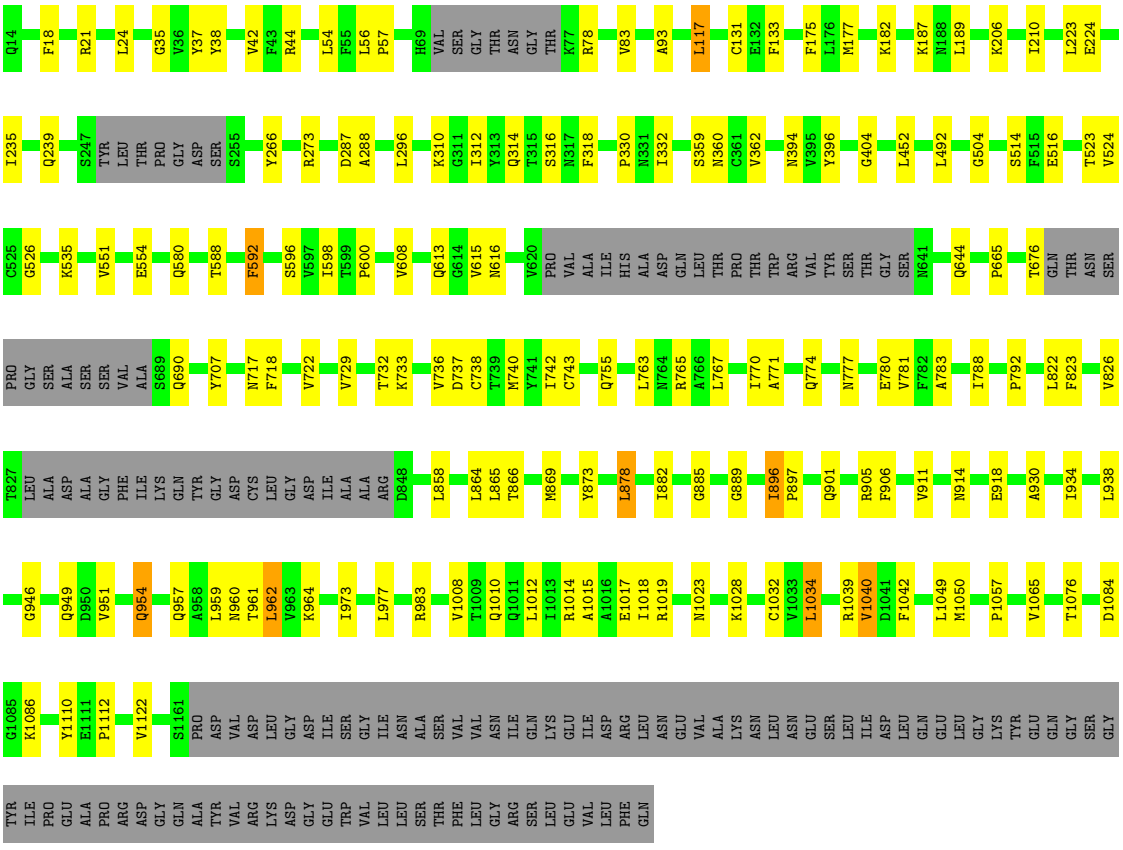
Chain 19-A:





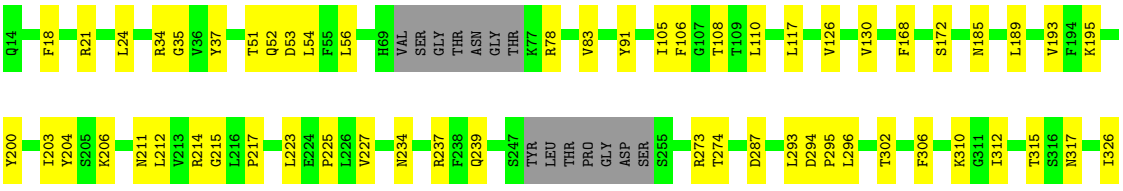
• Molecule 1: Spike glycoprotein,Fibritin

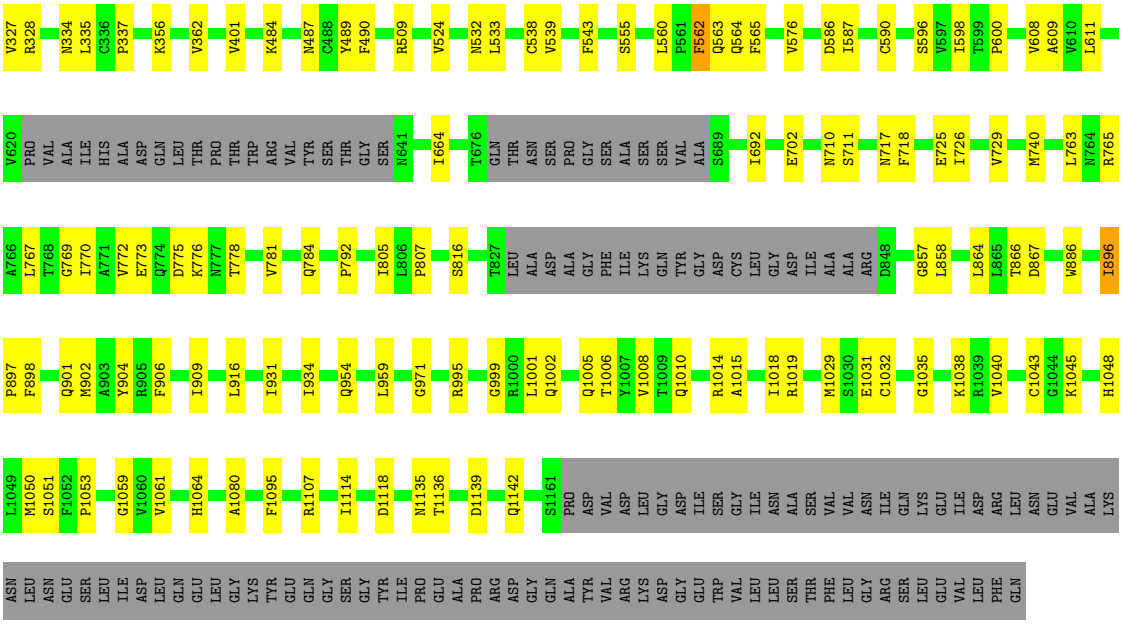
Chain 19-B:

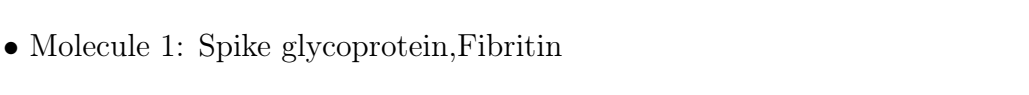


• Molecule 1: Spike glycoprotein,Fibritin

Chain 19-C:

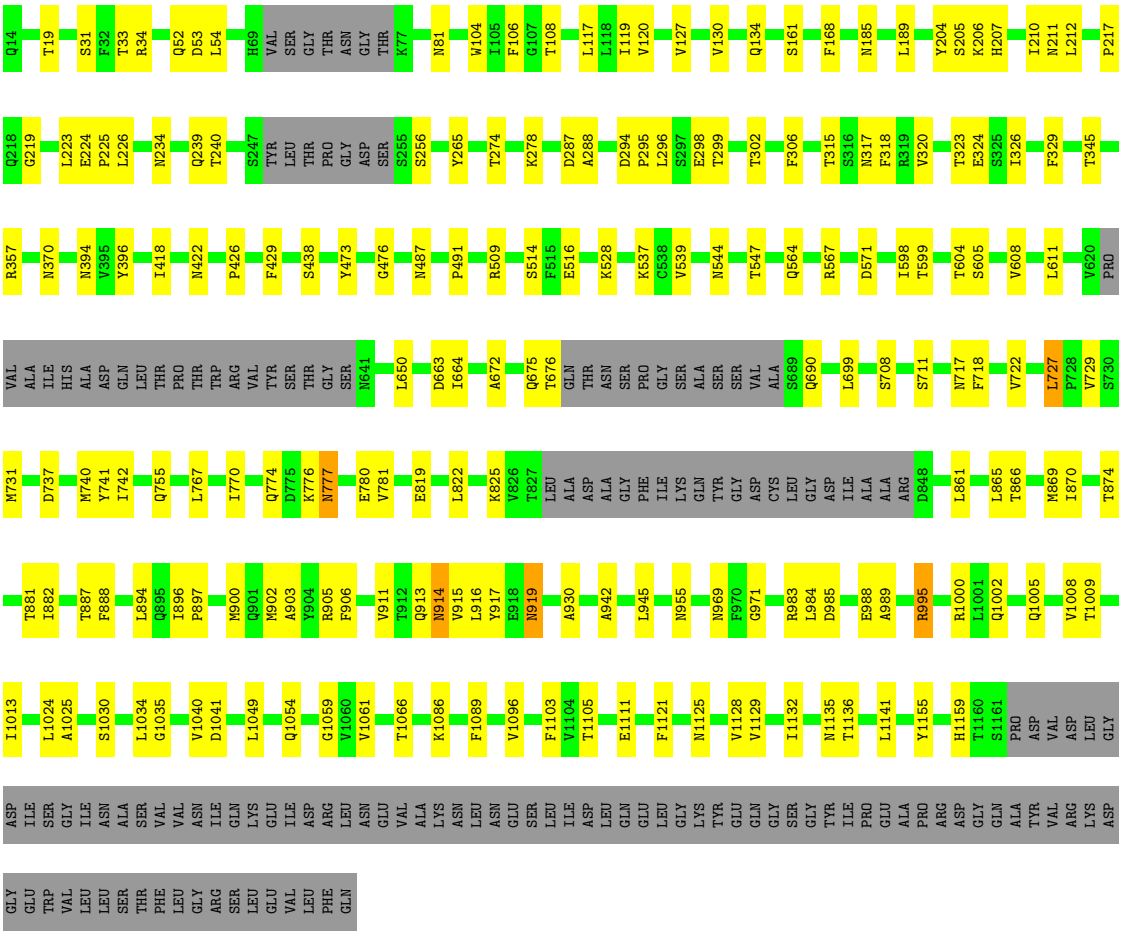






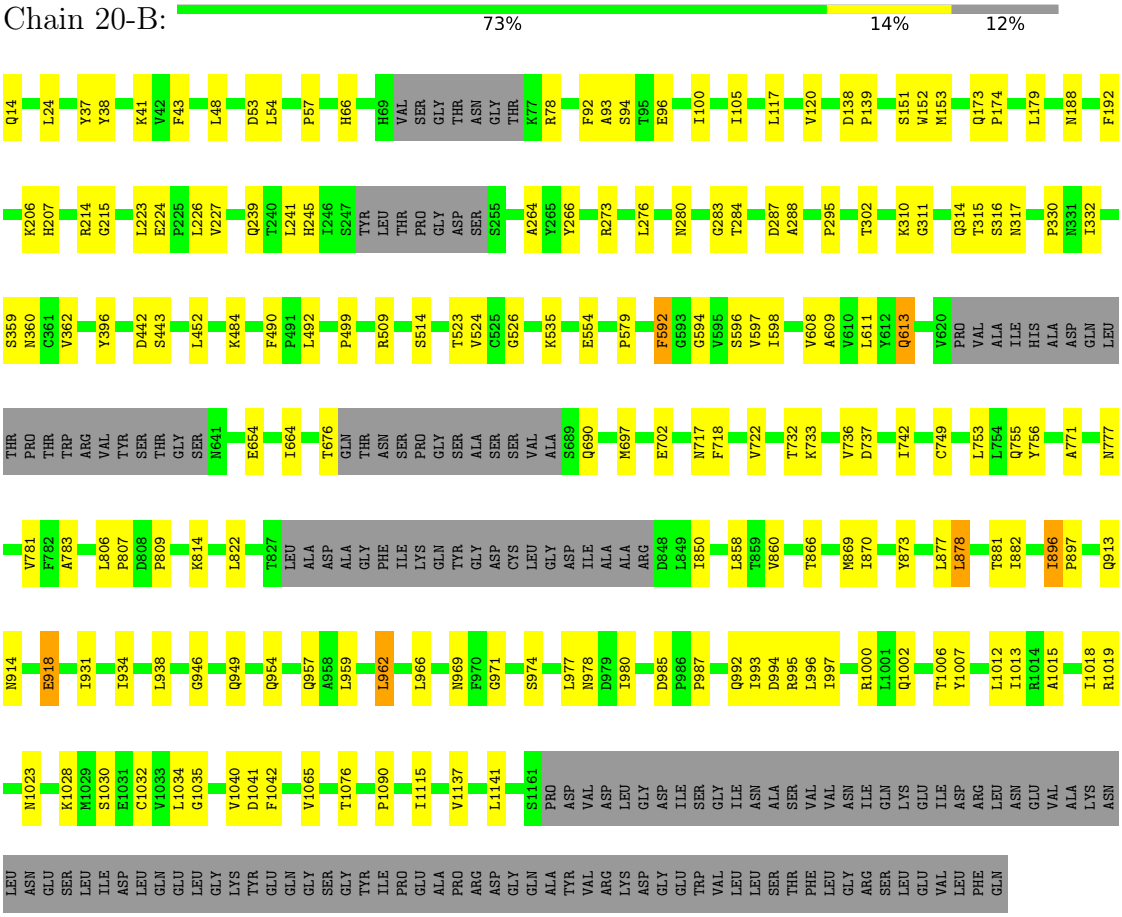
• Molecule 1: Spike glycoprotein,Fibritin

Chain 20-A:



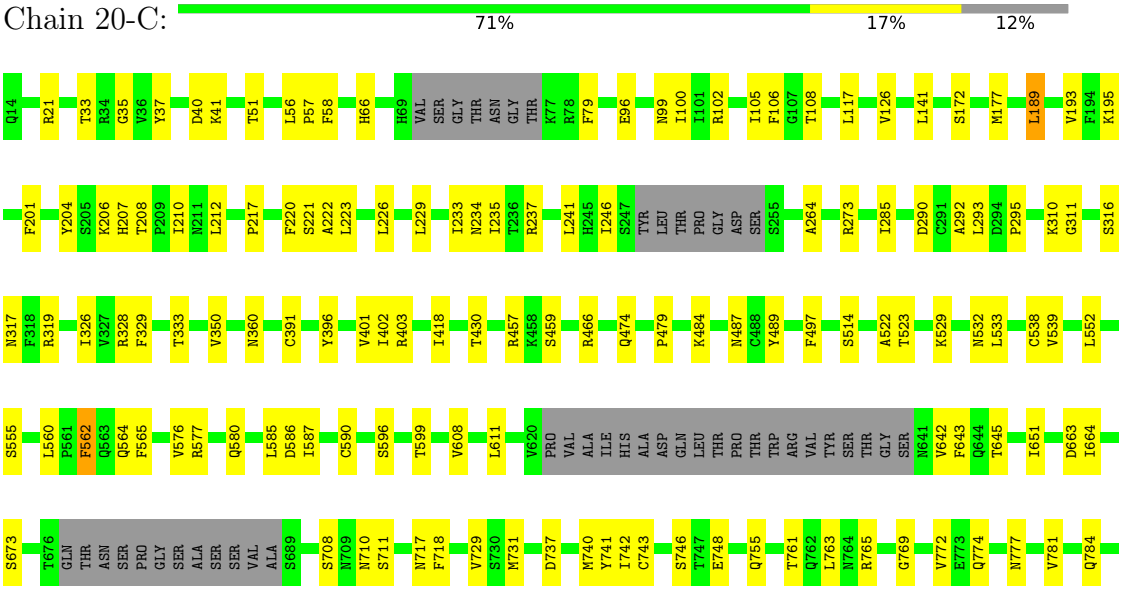
• Molecule 1: Spike glycoprotein,Fibritin

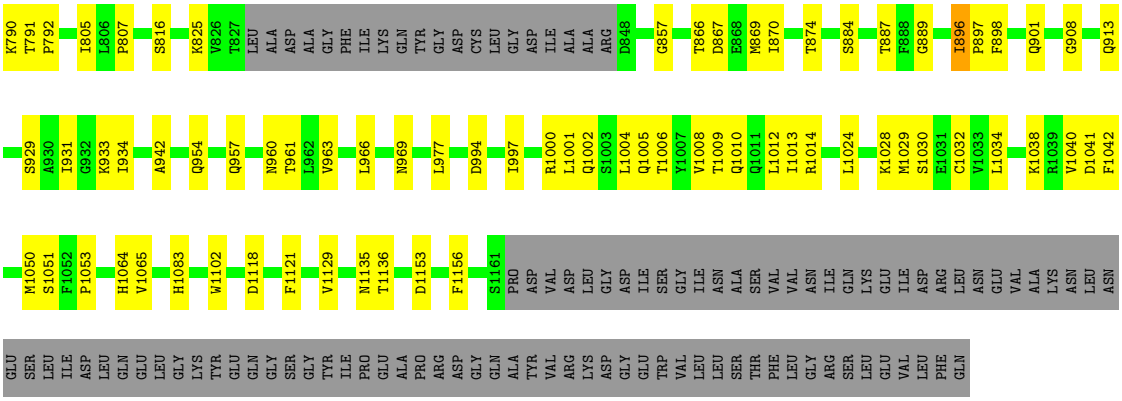
Chain 20-B:



• Molecule 1: Spike glycoprotein,Fibritin

Chain 20-C:




K790 T791 P792 I805 L806 P807 S816 K825 V826 T827 LEU ALA ASP ALA GLY PHE ILE LYS GLN TYR GLY ASP CYS LEU GLY ASP ILE ALA ALA ARG D848 G857 T866 D867 E868 M869 I870 T874 S884 T887 F888 G889 I896 P897 F898 Q901 G908 Q913
S929 A930 I931 G932 K933 I934 A942 Q954 Q957 N960 T961 L962 V963 L966 N969 L977 D994 I997 R1000 L1001 Q1002 S1003 L1004 Q1005 T1006 Y1007 V1008 T1009 Q1010 Q1011 L1012 I1013 R1014 L1024 K1028 M1029 S1030 E1031 C1032 V1033 L1034 K1038 R1039 V1040 D1041 F1042
M1050 S1051 F1052 P1053 H1064 V1065 H1083 W1102 D1118 F1121 V1129 N1135 T1136 D1153 F1156 S1161 PRO ASP VAL ASP LEU GLY ASP ILE SER GLY ILE ASN ALA SER VAL VAL ASN ILE GLN LYS GLU ILE ASP ARG LEU ASN GLU VAL ALA LYS ASN LEU ASN
GLU SER LEU ILE ASP LEU GLN GLU LEU GLY LYS TYR GLU GLN GLY SER GLY TYR ILE PRO GLU ALA PRO ARG ASP GLY GLN ALA TYR VAL ARG LYS ASP GLY GLU TRP VAL LEU LEU SER THR PHE LEU GLY ARG SER LEU GLU VAL LEU PHE GLN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	479908	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.793	Depositor
Minimum map value	-0.556	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.060	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	313.6, 313.6, 313.6	wwPDB
Map dimensions	224, 224, 224	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	1-A	0.10	0/8652	0.27	0/11768
1	1-B	0.10	0/8652	0.29	2/11768 (0.0%)
1	1-C	0.08	0/8652	0.23	0/11768
1	2-A	0.10	0/8652	0.27	0/11768
1	2-B	0.10	0/8652	0.29	2/11768 (0.0%)
1	2-C	0.08	0/8652	0.23	0/11768
1	3-A	0.10	0/8652	0.27	0/11768
1	3-B	0.10	0/8652	0.29	2/11768 (0.0%)
1	3-C	0.08	0/8652	0.23	0/11768
1	4-A	0.10	0/8652	0.27	0/11768
1	4-B	0.10	0/8652	0.29	2/11768 (0.0%)
1	4-C	0.08	0/8652	0.23	0/11768
1	5-A	0.10	0/8652	0.27	0/11768
1	5-B	0.10	0/8652	0.29	2/11768 (0.0%)
1	5-C	0.08	0/8652	0.23	0/11768
1	6-A	0.10	0/8652	0.27	0/11768
1	6-B	0.10	0/8652	0.29	2/11768 (0.0%)
1	6-C	0.08	0/8652	0.23	0/11768
1	7-A	0.10	0/8652	0.27	0/11768
1	7-B	0.10	0/8652	0.29	2/11768 (0.0%)
1	7-C	0.08	0/8652	0.23	0/11768
1	8-A	0.10	0/8652	0.27	0/11768
1	8-B	0.10	0/8652	0.29	2/11768 (0.0%)
1	8-C	0.08	0/8652	0.23	0/11768
1	9-A	0.10	0/8652	0.27	0/11768
1	9-B	0.10	0/8652	0.29	2/11768 (0.0%)
1	9-C	0.08	0/8652	0.23	0/11768
1	10-A	0.10	0/8652	0.27	0/11768
1	10-B	0.10	0/8652	0.29	2/11768 (0.0%)
1	10-C	0.08	0/8652	0.23	0/11768
1	11-A	0.10	0/8652	0.27	0/11768
1	11-B	0.10	0/8652	0.29	2/11768 (0.0%)
1	11-C	0.08	0/8652	0.23	0/11768
1	12-A	0.10	0/8652	0.27	0/11768

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	12-B	0.10	0/8652	0.29	2/11768 (0.0%)
1	12-C	0.08	0/8652	0.23	0/11768
1	13-A	0.10	0/8652	0.27	0/11768
1	13-B	0.10	0/8652	0.29	2/11768 (0.0%)
1	13-C	0.08	0/8652	0.23	0/11768
1	14-A	0.10	0/8652	0.27	0/11768
1	14-B	0.10	0/8652	0.29	2/11768 (0.0%)
1	14-C	0.08	0/8652	0.23	0/11768
1	15-A	0.10	0/8652	0.27	0/11768
1	15-B	0.10	0/8652	0.29	2/11768 (0.0%)
1	15-C	0.08	0/8652	0.23	0/11768
1	16-A	0.10	0/8652	0.27	0/11768
1	16-B	0.10	0/8652	0.29	2/11768 (0.0%)
1	16-C	0.08	0/8652	0.23	0/11768
1	17-A	0.10	0/8652	0.27	0/11768
1	17-B	0.10	0/8652	0.29	2/11768 (0.0%)
1	17-C	0.08	0/8652	0.23	0/11768
1	18-A	0.10	0/8652	0.27	0/11768
1	18-B	0.10	0/8652	0.29	2/11768 (0.0%)
1	18-C	0.08	0/8652	0.23	0/11768
1	19-A	0.10	0/8652	0.27	0/11768
1	19-B	0.10	0/8652	0.29	2/11768 (0.0%)
1	19-C	0.08	0/8652	0.23	0/11768
1	20-A	0.10	0/8652	0.27	0/11768
1	20-B	0.10	0/8652	0.29	2/11768 (0.0%)
1	20-C	0.08	0/8652	0.23	0/11768
All	All	0.09	0/519120	0.27	40/706080 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	9-B	0	1
1	13-B	0	3
1	16-B	0	1
1	17-C	0	1
1	18-A	0	1
All	All	0	7

There are no bond length outliers.

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1-B	359	SER	CA-C-N	5.08	131.24	121.54
1	1-B	359	SER	C-N-CA	5.08	131.24	121.54
1	2-B	359	SER	CA-C-N	5.08	131.24	121.54
1	2-B	359	SER	C-N-CA	5.08	131.24	121.54
1	3-B	359	SER	CA-C-N	5.08	131.24	121.54

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	13-B	1107	ARG	Sidechain
1	13-B	765	ARG	Sidechain
1	13-B	86	PHE	Sidechain
1	16-B	152	TRP	Mainchain
1	9-B	1107	ARG	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	1-A	8454	0	8246	123	0
1	1-B	8454	0	8246	111	0
1	1-C	8454	0	8246	96	0
1	2-A	8454	0	8246	122	0
1	2-B	8454	0	8246	111	0
1	2-C	8454	0	8248	111	0
1	3-A	8454	0	8246	115	0
1	3-B	8454	0	8246	118	0
1	3-C	8454	0	8246	103	0
1	4-A	8454	0	8246	122	0
1	4-B	8454	0	8246	104	0
1	4-C	8454	0	8248	123	0
1	5-A	8454	0	8246	93	0
1	5-B	8454	0	8246	90	0
1	5-C	8454	0	8246	89	0
1	6-A	8454	0	8246	85	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	6-B	8454	0	8246	126	0
1	6-C	8454	0	8246	111	0
1	7-A	8454	0	8246	100	0
1	7-B	8454	0	8246	102	0
1	7-C	8454	0	8246	109	0
1	8-A	8454	0	8246	107	0
1	8-B	8454	0	8246	135	0
1	8-C	8454	0	8246	112	0
1	9-A	8454	0	8246	135	0
1	9-B	8454	0	8246	136	0
1	9-C	8454	0	8248	148	0
1	10-A	8454	0	8246	132	0
1	10-B	8454	0	8246	126	0
1	10-C	8454	0	8248	135	0
1	11-A	8454	0	8246	106	0
1	11-B	8454	0	8246	121	0
1	11-C	8454	0	8246	116	0
1	12-A	8454	0	8246	108	0
1	12-B	8454	0	8246	96	0
1	12-C	8454	0	8246	109	0
1	13-A	8454	0	8246	114	0
1	13-B	8454	0	8246	109	0
1	13-C	8454	0	8248	124	0
1	14-A	8454	0	8246	118	0
1	14-B	8454	0	8246	141	0
1	14-C	8454	0	8248	118	0
1	15-A	8454	0	8246	111	0
1	15-B	8454	0	8246	113	0
1	15-C	8454	0	8248	114	0
1	16-A	8454	0	8246	117	0
1	16-B	8454	0	8246	103	0
1	16-C	8454	0	8246	98	0
1	17-A	8454	0	8246	103	0
1	17-B	8454	0	8246	129	0
1	17-C	8454	0	8246	101	0
1	18-A	8454	0	8246	122	0
1	18-B	8454	0	8246	135	0
1	18-C	8454	0	8246	128	0
1	19-A	8454	0	8246	86	0
1	19-B	8454	0	8246	97	0
1	19-C	8454	0	8248	113	0
1	20-A	8454	0	8246	116	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	20-B	8454	0	8246	111	0
1	20-C	8454	0	8248	136	0
All	All	507240	0	494778	6228	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 6228 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:GLN:N	1:B:255:SER:HG	1.69	0.90
1:B:14:GLN:N	1:B:255:SER:HG	1.73	0.87
1:B:14:GLN:N	1:B:255:SER:HG	1.75	0.84
1:C:214:ARG:HH11	1:C:215:GLY:H	1.25	0.83
1:C:312:ILE:HD11	1:C:596:SER:HB3	1.61	0.82

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	1-A	1067/1230 (87%)	1026 (96%)	40 (4%)	1 (0%)	48 77
1	1-B	1067/1230 (87%)	1019 (96%)	48 (4%)	0	100 100
1	1-C	1067/1230 (87%)	1027 (96%)	39 (4%)	1 (0%)	48 77
1	2-A	1067/1230 (87%)	1025 (96%)	41 (4%)	1 (0%)	48 77
1	2-B	1067/1230 (87%)	1019 (96%)	48 (4%)	0	100 100
1	2-C	1067/1230 (87%)	1018 (95%)	48 (4%)	1 (0%)	48 77
1	3-A	1067/1230 (87%)	1026 (96%)	40 (4%)	1 (0%)	48 77
1	3-B	1067/1230 (87%)	1019 (96%)	48 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	3-C	1067/1230 (87%)	1026 (96%)	40 (4%)	1 (0%)	48	77
1	4-A	1067/1230 (87%)	1026 (96%)	40 (4%)	1 (0%)	48	77
1	4-B	1067/1230 (87%)	1019 (96%)	48 (4%)	0	100	100
1	4-C	1067/1230 (87%)	1018 (95%)	48 (4%)	1 (0%)	48	77
1	5-A	1067/1230 (87%)	1028 (96%)	38 (4%)	1 (0%)	48	77
1	5-B	1067/1230 (87%)	1020 (96%)	47 (4%)	0	100	100
1	5-C	1067/1230 (87%)	1026 (96%)	40 (4%)	1 (0%)	48	77
1	6-A	1067/1230 (87%)	1025 (96%)	41 (4%)	1 (0%)	48	77
1	6-B	1067/1230 (87%)	1019 (96%)	48 (4%)	0	100	100
1	6-C	1067/1230 (87%)	1026 (96%)	40 (4%)	1 (0%)	48	77
1	7-A	1067/1230 (87%)	1027 (96%)	39 (4%)	1 (0%)	48	77
1	7-B	1067/1230 (87%)	1020 (96%)	47 (4%)	0	100	100
1	7-C	1067/1230 (87%)	1027 (96%)	39 (4%)	1 (0%)	48	77
1	8-A	1067/1230 (87%)	1025 (96%)	41 (4%)	1 (0%)	48	77
1	8-B	1067/1230 (87%)	1020 (96%)	47 (4%)	0	100	100
1	8-C	1067/1230 (87%)	1025 (96%)	41 (4%)	1 (0%)	48	77
1	9-A	1067/1230 (87%)	1027 (96%)	39 (4%)	1 (0%)	48	77
1	9-B	1067/1230 (87%)	1019 (96%)	48 (4%)	0	100	100
1	9-C	1067/1230 (87%)	1018 (95%)	48 (4%)	1 (0%)	48	77
1	10-A	1067/1230 (87%)	1026 (96%)	40 (4%)	1 (0%)	48	77
1	10-B	1067/1230 (87%)	1018 (95%)	49 (5%)	0	100	100
1	10-C	1067/1230 (87%)	1018 (95%)	48 (4%)	1 (0%)	48	77
1	11-A	1067/1230 (87%)	1027 (96%)	39 (4%)	1 (0%)	48	77
1	11-B	1067/1230 (87%)	1019 (96%)	48 (4%)	0	100	100
1	11-C	1067/1230 (87%)	1026 (96%)	40 (4%)	1 (0%)	48	77
1	12-A	1067/1230 (87%)	1025 (96%)	41 (4%)	1 (0%)	48	77
1	12-B	1067/1230 (87%)	1019 (96%)	48 (4%)	0	100	100
1	12-C	1067/1230 (87%)	1026 (96%)	40 (4%)	1 (0%)	48	77
1	13-A	1067/1230 (87%)	1026 (96%)	40 (4%)	1 (0%)	48	77
1	13-B	1067/1230 (87%)	1020 (96%)	47 (4%)	0	100	100
1	13-C	1067/1230 (87%)	1016 (95%)	49 (5%)	2 (0%)	44	73

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	14-A	1067/1230 (87%)	1028 (96%)	38 (4%)	1 (0%)	48	77
1	14-B	1067/1230 (87%)	1018 (95%)	49 (5%)	0	100	100
1	14-C	1067/1230 (87%)	1016 (95%)	50 (5%)	1 (0%)	48	77
1	15-A	1067/1230 (87%)	1027 (96%)	39 (4%)	1 (0%)	48	77
1	15-B	1067/1230 (87%)	1022 (96%)	45 (4%)	0	100	100
1	15-C	1067/1230 (87%)	1017 (95%)	49 (5%)	1 (0%)	48	77
1	16-A	1067/1230 (87%)	1026 (96%)	40 (4%)	1 (0%)	48	77
1	16-B	1067/1230 (87%)	1019 (96%)	48 (4%)	0	100	100
1	16-C	1067/1230 (87%)	1026 (96%)	40 (4%)	1 (0%)	48	77
1	17-A	1067/1230 (87%)	1027 (96%)	39 (4%)	1 (0%)	48	77
1	17-B	1067/1230 (87%)	1019 (96%)	48 (4%)	0	100	100
1	17-C	1067/1230 (87%)	1026 (96%)	40 (4%)	1 (0%)	48	77
1	18-A	1067/1230 (87%)	1024 (96%)	41 (4%)	2 (0%)	44	73
1	18-B	1067/1230 (87%)	1019 (96%)	48 (4%)	0	100	100
1	18-C	1067/1230 (87%)	1027 (96%)	39 (4%)	1 (0%)	48	77
1	19-A	1067/1230 (87%)	1027 (96%)	39 (4%)	1 (0%)	48	77
1	19-B	1067/1230 (87%)	1020 (96%)	47 (4%)	0	100	100
1	19-C	1067/1230 (87%)	1017 (95%)	49 (5%)	1 (0%)	48	77
1	20-A	1067/1230 (87%)	1027 (96%)	39 (4%)	1 (0%)	48	77
1	20-B	1067/1230 (87%)	1019 (96%)	48 (4%)	0	100	100
1	20-C	1067/1230 (87%)	1017 (95%)	49 (5%)	1 (0%)	48	77
All	All	64020/73800 (87%)	61354 (96%)	2624 (4%)	42 (0%)	50	77

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	18-A	984	LEU
1	1-A	544	ASN
1	1-C	544	ASN
1	2-A	544	ASN
1	3-A	544	ASN

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	1-A	944/1067 (88%)	932 (99%)	12 (1%)	65	88
1	1-B	944/1067 (88%)	930 (98%)	14 (2%)	60	86
1	1-C	944/1067 (88%)	939 (100%)	5 (0%)	86	95
1	2-A	944/1067 (88%)	932 (99%)	12 (1%)	65	88
1	2-B	944/1067 (88%)	930 (98%)	14 (2%)	60	86
1	2-C	944/1067 (88%)	939 (100%)	5 (0%)	86	95
1	3-A	944/1067 (88%)	932 (99%)	12 (1%)	65	88
1	3-B	944/1067 (88%)	930 (98%)	14 (2%)	60	86
1	3-C	944/1067 (88%)	939 (100%)	5 (0%)	86	95
1	4-A	944/1067 (88%)	932 (99%)	12 (1%)	65	88
1	4-B	944/1067 (88%)	930 (98%)	14 (2%)	60	86
1	4-C	944/1067 (88%)	939 (100%)	5 (0%)	86	95
1	5-A	944/1067 (88%)	932 (99%)	12 (1%)	65	88
1	5-B	944/1067 (88%)	930 (98%)	14 (2%)	60	86
1	5-C	944/1067 (88%)	939 (100%)	5 (0%)	86	95
1	6-A	944/1067 (88%)	932 (99%)	12 (1%)	65	88
1	6-B	944/1067 (88%)	930 (98%)	14 (2%)	60	86
1	6-C	944/1067 (88%)	939 (100%)	5 (0%)	86	95
1	7-A	944/1067 (88%)	932 (99%)	12 (1%)	65	88
1	7-B	944/1067 (88%)	930 (98%)	14 (2%)	60	86
1	7-C	944/1067 (88%)	939 (100%)	5 (0%)	86	95
1	8-A	944/1067 (88%)	932 (99%)	12 (1%)	65	88
1	8-B	944/1067 (88%)	930 (98%)	14 (2%)	60	86
1	8-C	944/1067 (88%)	939 (100%)	5 (0%)	86	95
1	9-A	944/1067 (88%)	932 (99%)	12 (1%)	65	88
1	9-B	944/1067 (88%)	930 (98%)	14 (2%)	60	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	9-C	944/1067 (88%)	939 (100%)	5 (0%)	86 95
1	10-A	944/1067 (88%)	932 (99%)	12 (1%)	65 88
1	10-B	944/1067 (88%)	930 (98%)	14 (2%)	60 86
1	10-C	944/1067 (88%)	939 (100%)	5 (0%)	86 95
1	11-A	944/1067 (88%)	932 (99%)	12 (1%)	65 88
1	11-B	944/1067 (88%)	930 (98%)	14 (2%)	60 86
1	11-C	944/1067 (88%)	939 (100%)	5 (0%)	86 95
1	12-A	944/1067 (88%)	932 (99%)	12 (1%)	65 88
1	12-B	944/1067 (88%)	930 (98%)	14 (2%)	60 86
1	12-C	944/1067 (88%)	939 (100%)	5 (0%)	86 95
1	13-A	944/1067 (88%)	932 (99%)	12 (1%)	65 88
1	13-B	944/1067 (88%)	930 (98%)	14 (2%)	60 86
1	13-C	944/1067 (88%)	939 (100%)	5 (0%)	86 95
1	14-A	944/1067 (88%)	932 (99%)	12 (1%)	65 88
1	14-B	944/1067 (88%)	930 (98%)	14 (2%)	60 86
1	14-C	944/1067 (88%)	939 (100%)	5 (0%)	86 95
1	15-A	944/1067 (88%)	932 (99%)	12 (1%)	65 88
1	15-B	944/1067 (88%)	930 (98%)	14 (2%)	60 86
1	15-C	944/1067 (88%)	939 (100%)	5 (0%)	86 95
1	16-A	944/1067 (88%)	932 (99%)	12 (1%)	65 88
1	16-B	944/1067 (88%)	930 (98%)	14 (2%)	60 86
1	16-C	944/1067 (88%)	939 (100%)	5 (0%)	86 95
1	17-A	944/1067 (88%)	932 (99%)	12 (1%)	65 88
1	17-B	944/1067 (88%)	930 (98%)	14 (2%)	60 86
1	17-C	944/1067 (88%)	939 (100%)	5 (0%)	86 95
1	18-A	944/1067 (88%)	932 (99%)	12 (1%)	65 88
1	18-B	944/1067 (88%)	930 (98%)	14 (2%)	60 86
1	18-C	944/1067 (88%)	939 (100%)	5 (0%)	86 95
1	19-A	944/1067 (88%)	932 (99%)	12 (1%)	65 88
1	19-B	944/1067 (88%)	930 (98%)	14 (2%)	60 86
1	19-C	944/1067 (88%)	939 (100%)	5 (0%)	86 95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	20-A	944/1067 (88%)	932 (99%)	12 (1%)	65 88
1	20-B	944/1067 (88%)	930 (98%)	14 (2%)	60 86
1	20-C	944/1067 (88%)	939 (100%)	5 (0%)	86 95
All	All	56640/64020 (88%)	56020 (99%)	620 (1%)	69 90

5 of 620 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	15-C	710	ASN
1	19-B	732	THR
1	16-A	1066	THR
1	15-C	562	PHE
1	17-B	1040	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 698 such sidechains are listed below:

Mol	Chain	Res	Type
1	14-C	949	GLN
1	17-B	1054	GLN
1	15-A	613	GLN
1	14-C	777	ASN
1	16-A	957	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

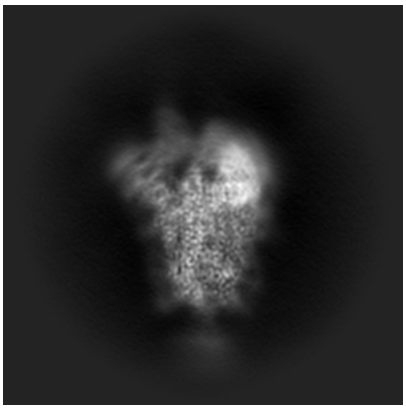
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-51279. These allow visual inspection of the internal detail of the map and identification of artifacts.

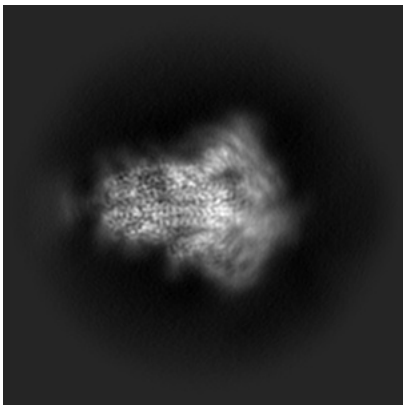
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

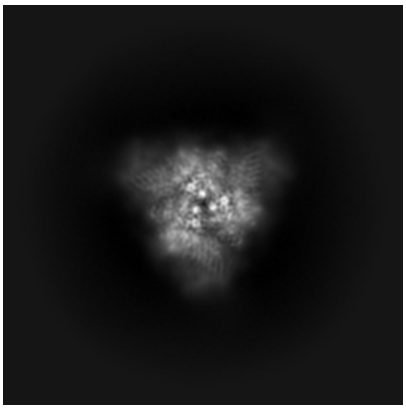
6.1.1 Primary map



X

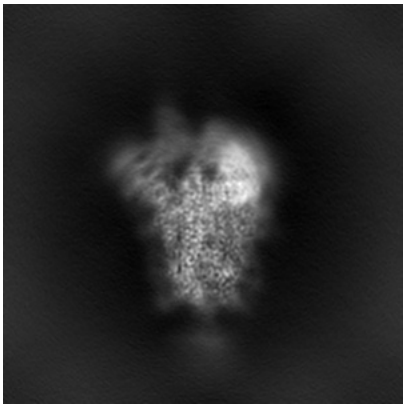


Y

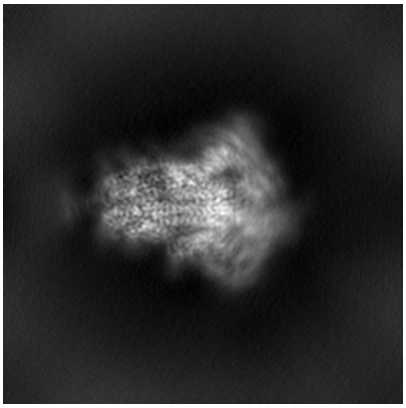


Z

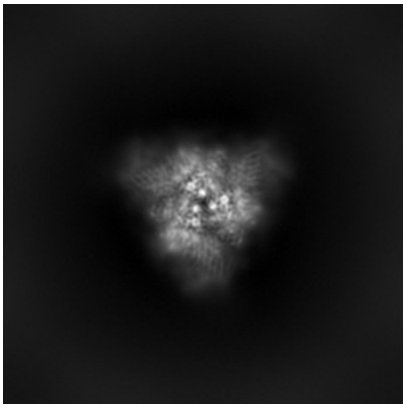
6.1.2 Raw map



X



Y

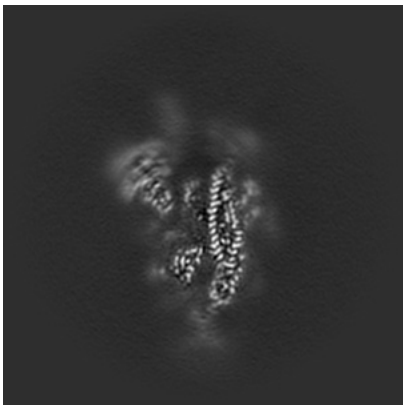


Z

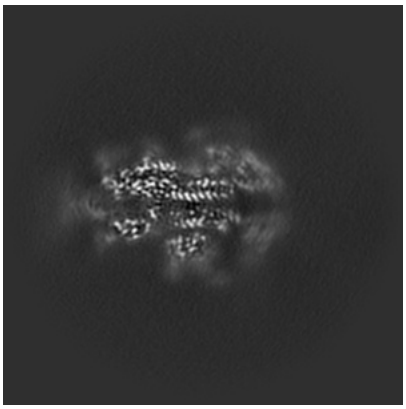
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

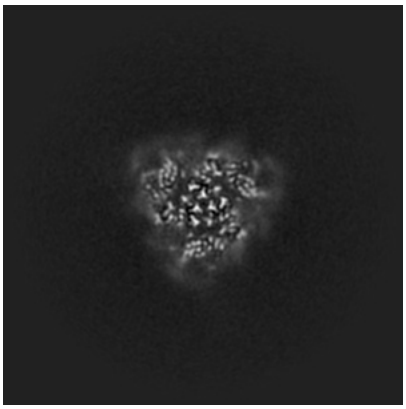
6.2.1 Primary map



X Index: 112

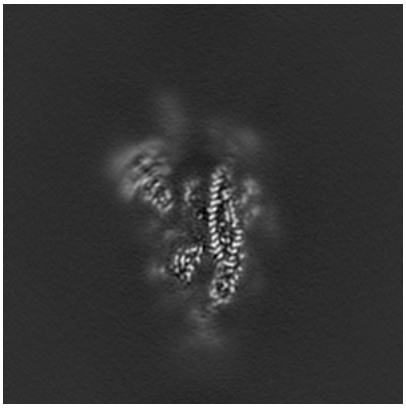


Y Index: 112

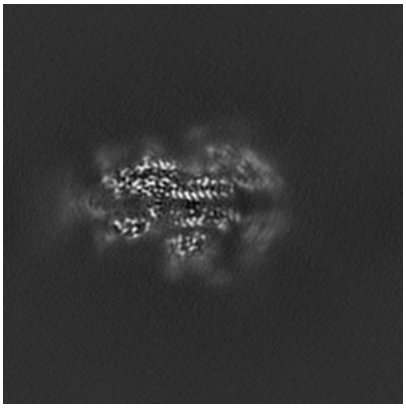


Z Index: 112

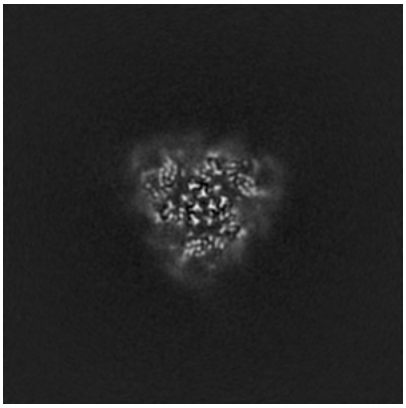
6.2.2 Raw map



X Index: 112



Y Index: 112

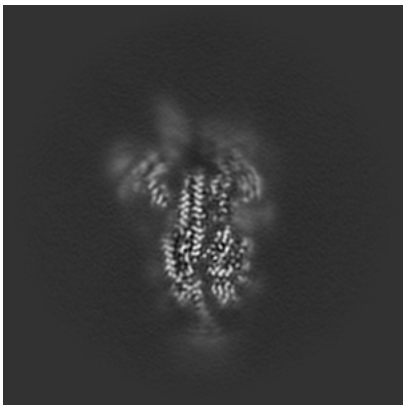


Z Index: 112

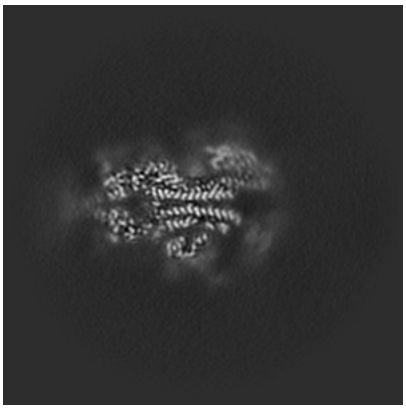
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

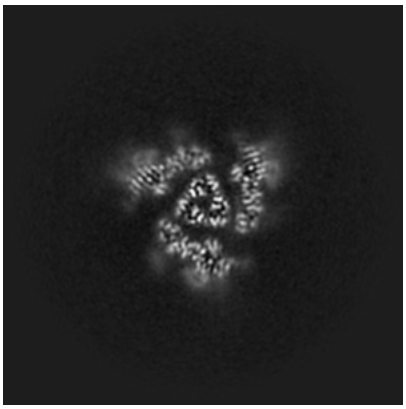
6.3.1 Primary map



X Index: 107

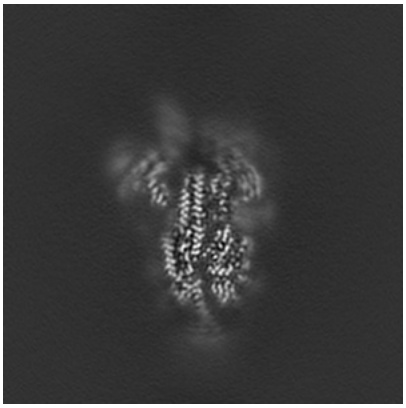


Y Index: 110

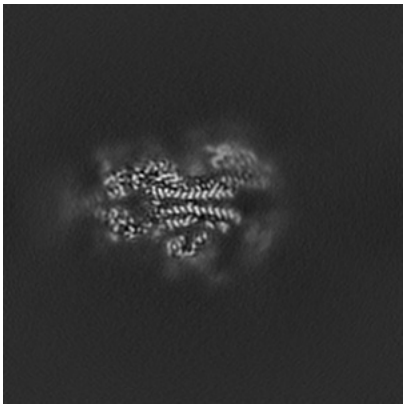


Z Index: 122

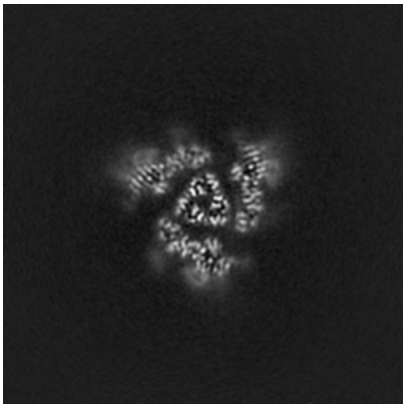
6.3.2 Raw map



X Index: 107



Y Index: 110

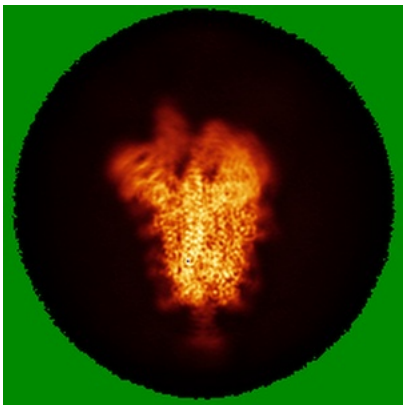


Z Index: 122

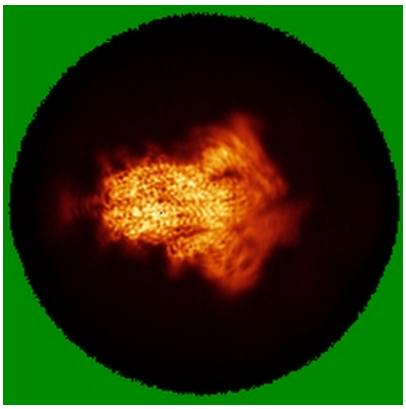
The images above show the largest variance slices of the map in three orthogonal directions.

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

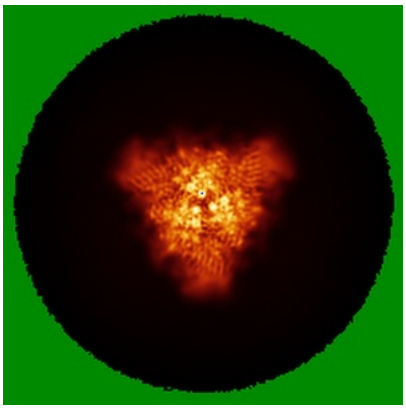
6.4.1 Primary map



X

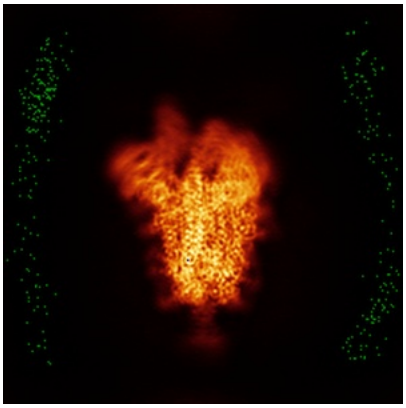


Y

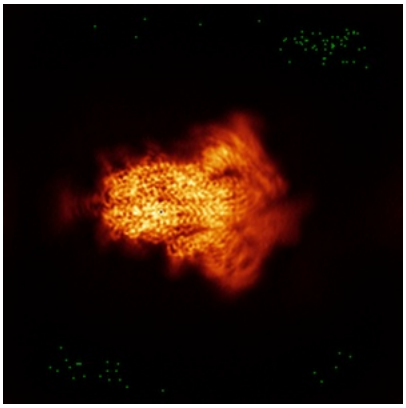


Z

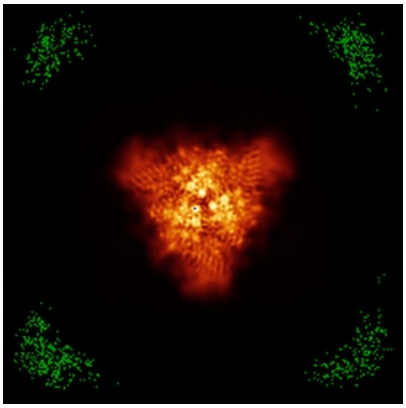
6.4.2 Raw map



X



Y

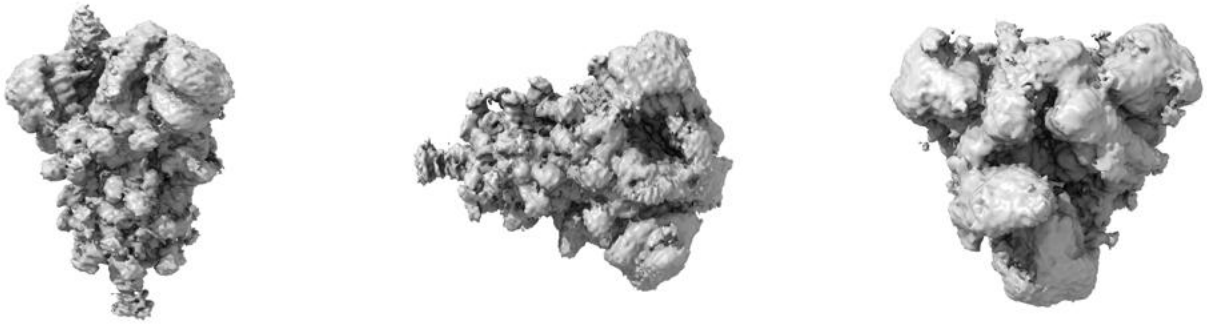


Z

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)

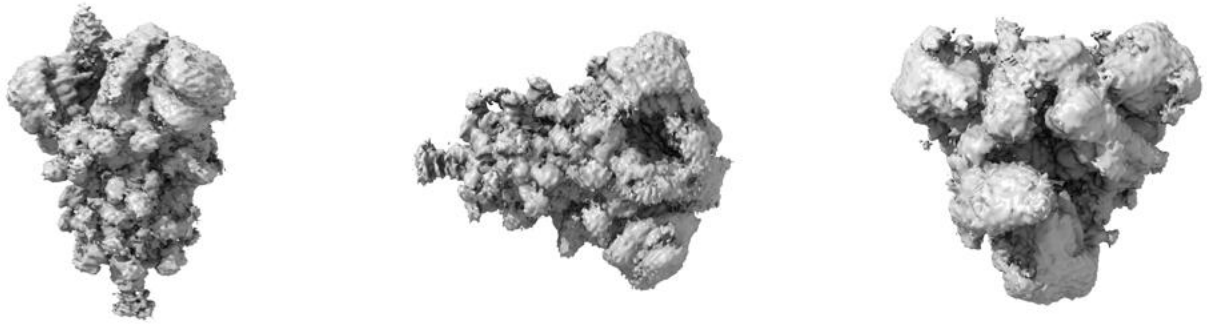
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

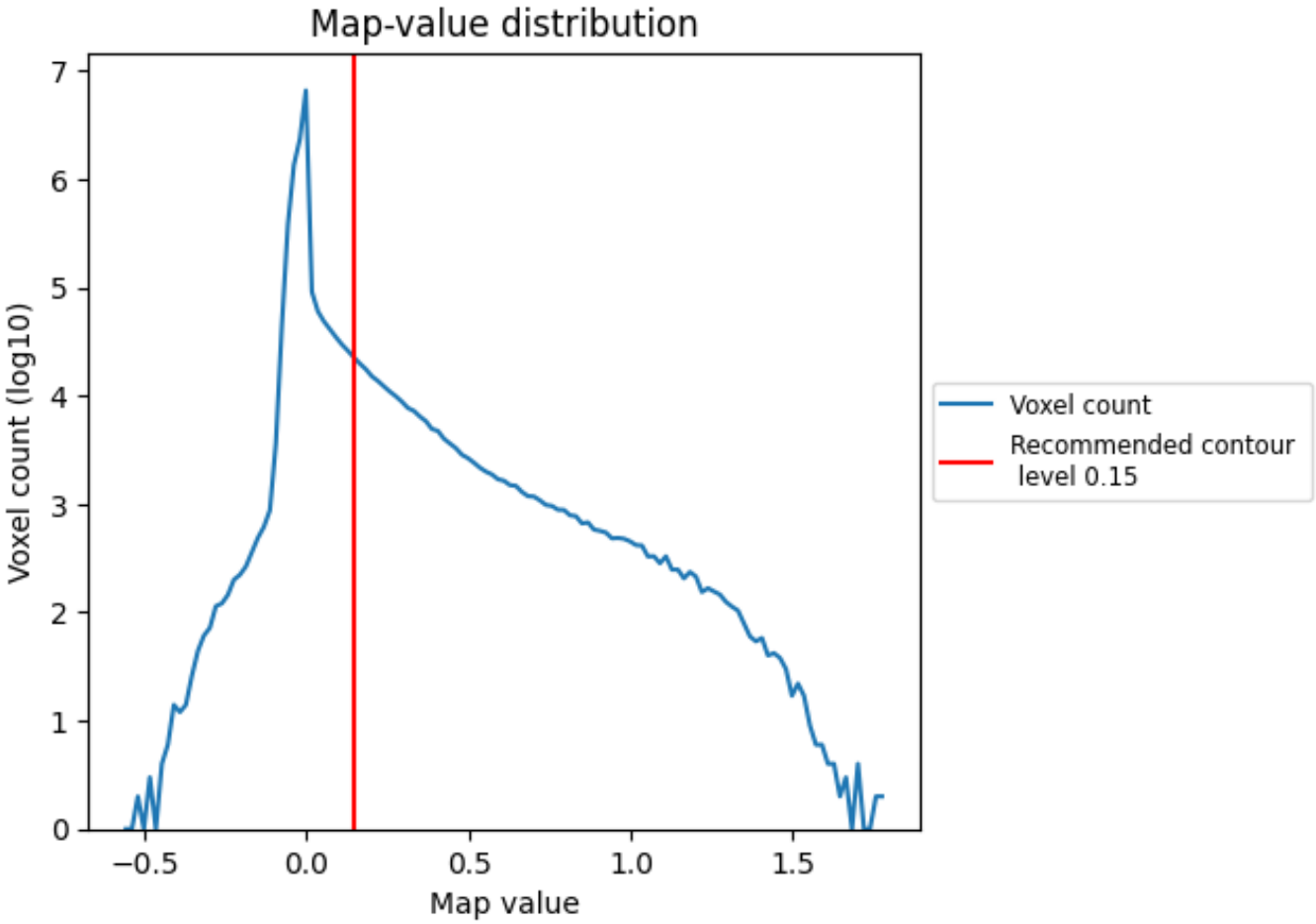
6.6 Mask visualisation (i)

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

7 Map analysis

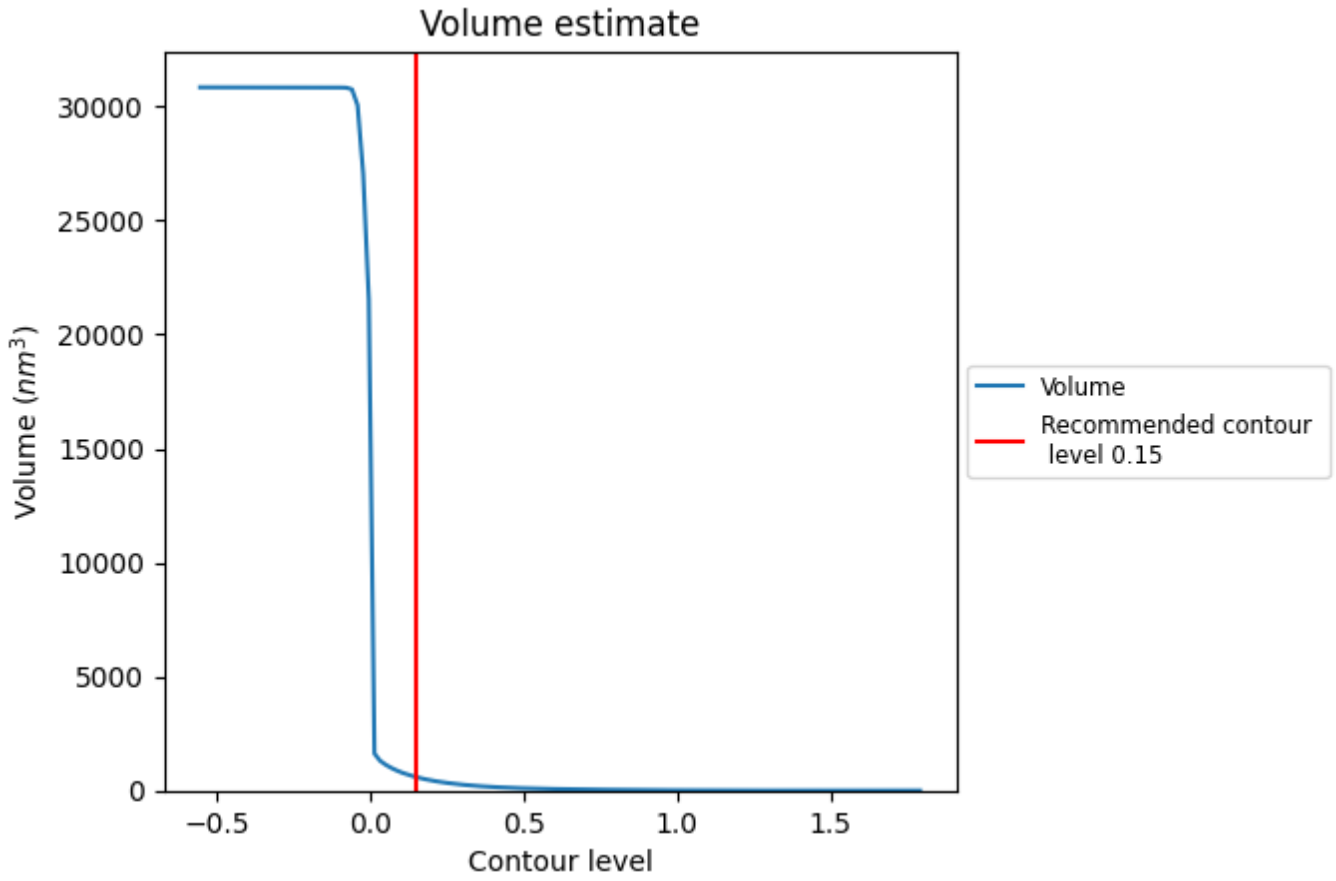
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

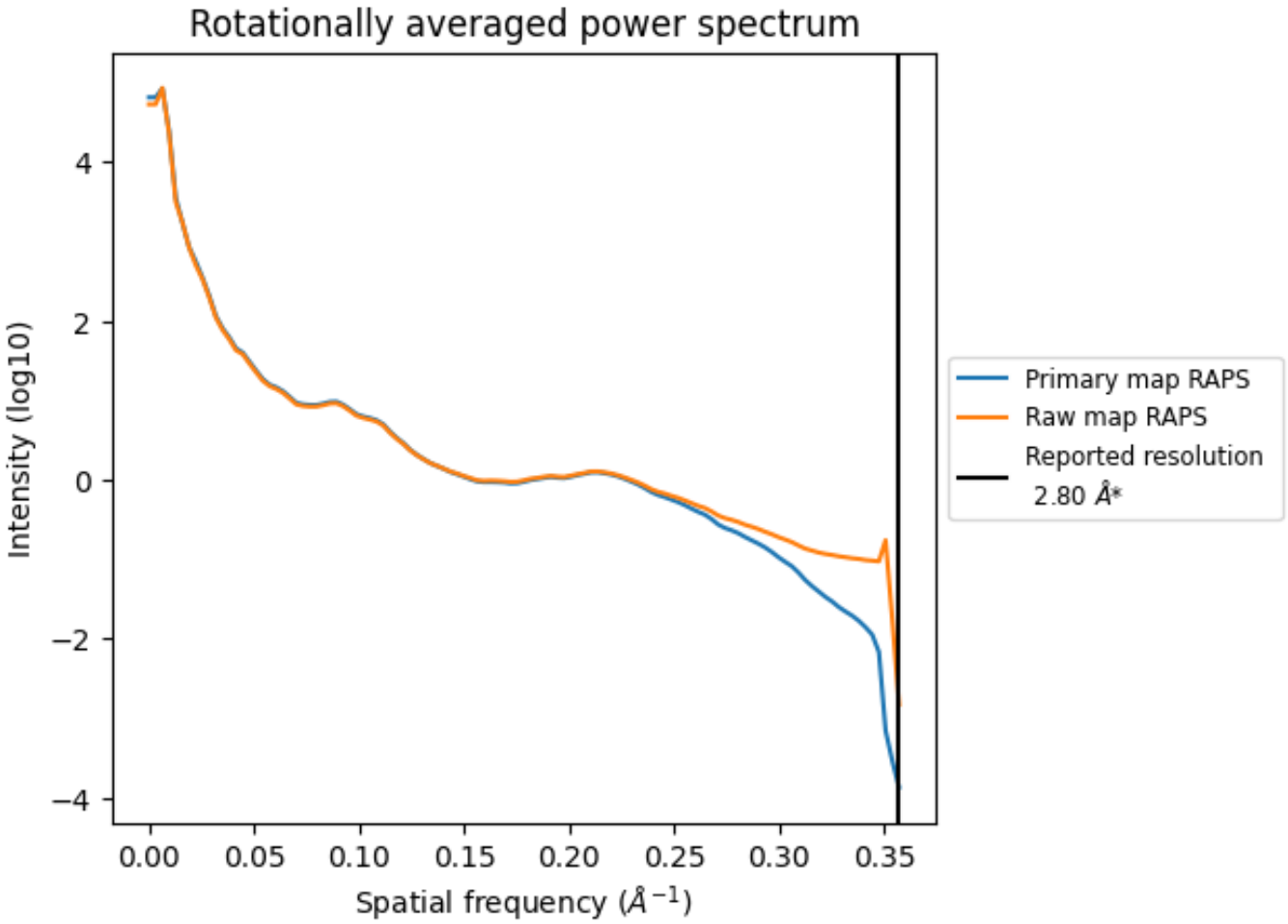
7.2 Volume estimate (i)



The volume at the recommended contour level is 588 nm^3; this corresponds to an approximate mass of 531 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)

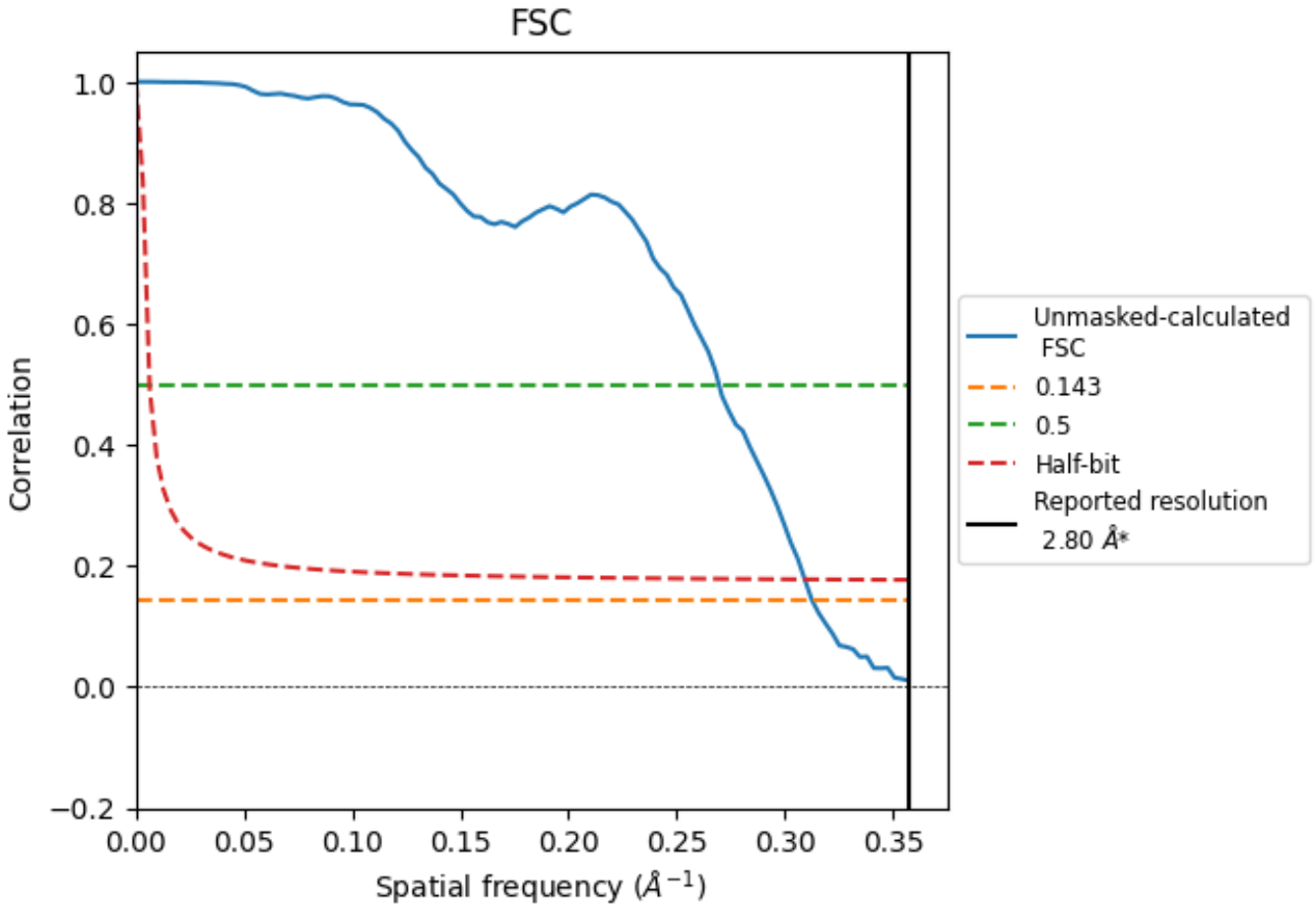


*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

8.2 Resolution estimates (i)

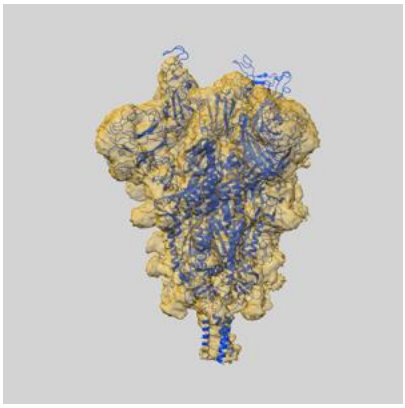
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.20	3.71	3.23

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.20 differs from the reported value 2.8 by more than 10 %

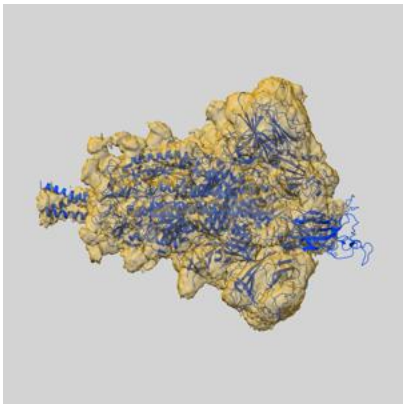
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-51279 and PDB model 9GDX. Per-residue inclusion information can be found in section 3 on page 12.

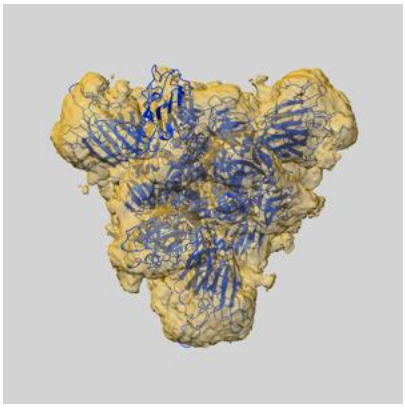
9.1 Map-model overlay



X



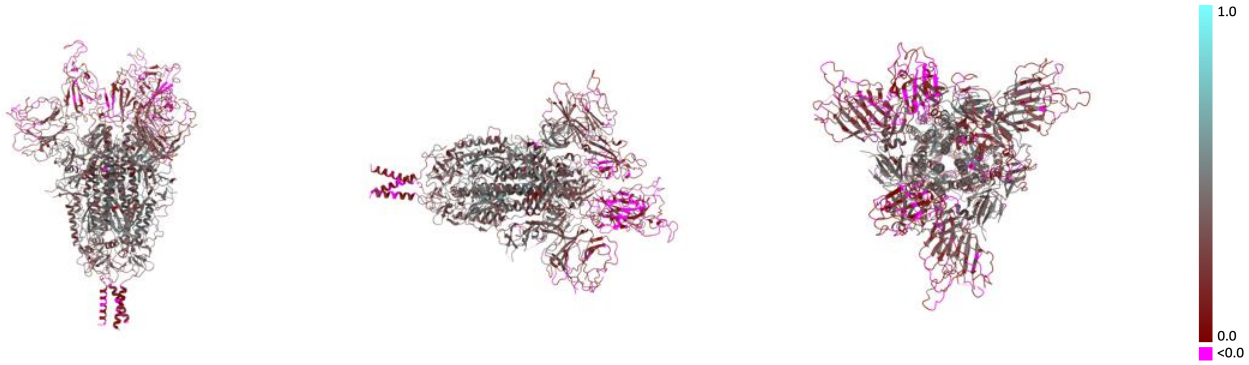
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15 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.

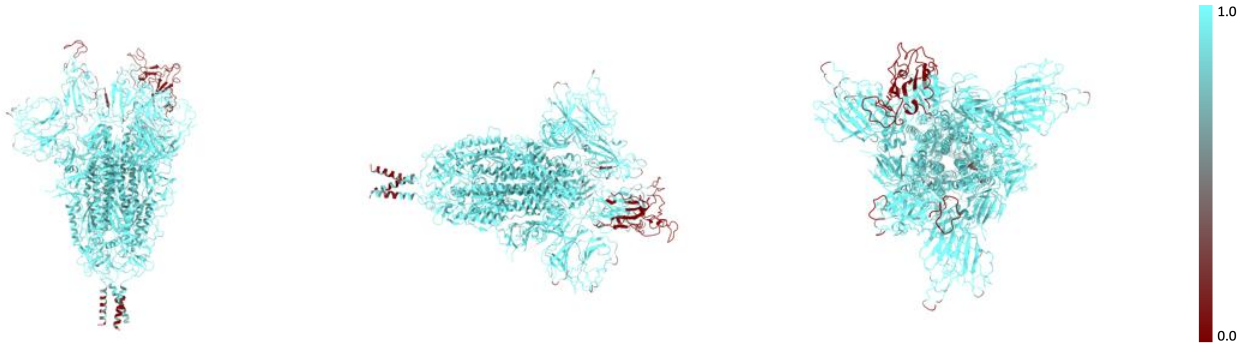
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

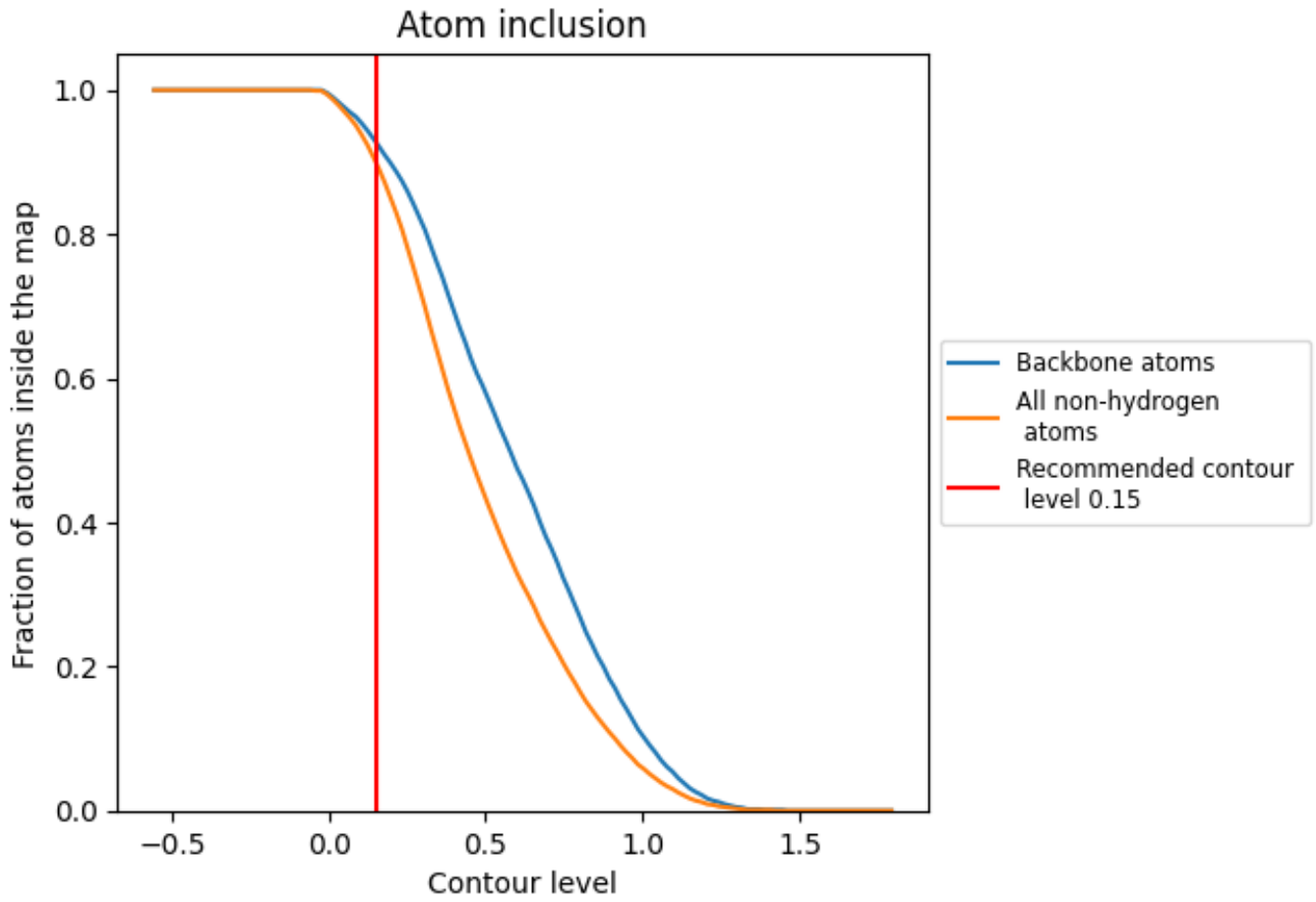
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.15).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9000	0.2850
A	0.9220	0.2820
B	0.9440	0.2910
C	0.8350	0.2830