



wwPDB EM Validation Summary Report ⓘ

Apr 24, 2025 – 08:03 pm BST

PDB ID : 9GDY / pdb_00009gdy
EMDB ID : EMD-51280
Title : SARS-CoV-2 Spike protein Beta Variant at 37C 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 models : 7VX1, 7WEV

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.dev117
MolProbity : 4.02b-467
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) : 2.42

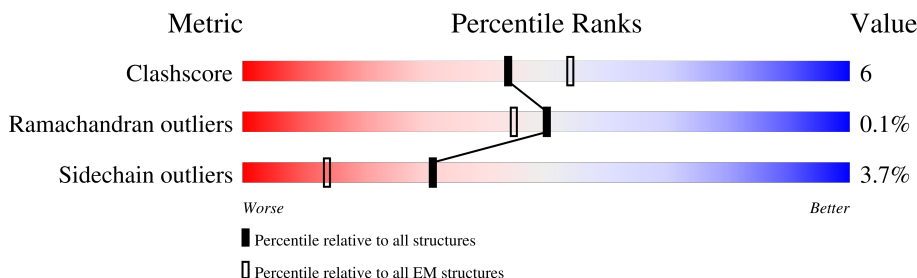
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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.














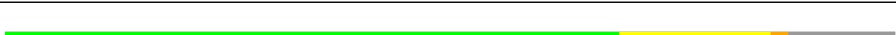

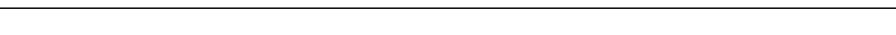
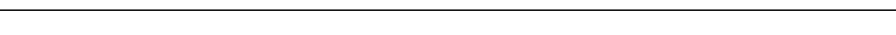
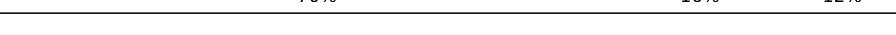

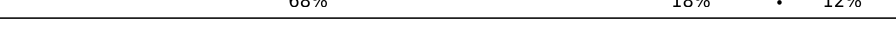







Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 $\leq 5\%$. 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	1-A	1230	<div> <div>12%</div> <div>69%</div> <div>17%</div> <div>•</div> <div>12%</div> </div>
1	1-B	1230	<div> <div>6%</div> <div>69%</div> <div>16%</div> <div>•</div> <div>12%</div> </div>
1	1-C	1230	<div> <div>7%</div> <div>70%</div> <div>16%</div> <div>•</div> <div>12%</div> </div>
1	10-A	1230	<div> <div>68%</div> <div>18%</div> <div>•</div> <div>12%</div> </div>
1	10-B	1230	<div> <div>72%</div> <div>14%</div> <div>•</div> <div>12%</div> </div>
1	10-C	1230	<div> <div>69%</div> <div>16%</div> <div>•</div> <div>12%</div> </div>
1	11-A	1230	<div> <div>71%</div> <div>15%</div> <div>•</div> <div>12%</div> </div>
1	11-B	1230	<div> <div>72%</div> <div>15%</div> <div>•</div> <div>12%</div> </div>


























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Mol	Chain	Length	Quality of chain
1	11-C	1230	 70%16%12%
1	12-A	1230	 70%16%12%
1	12-B	1230	 68%18%12%
1	12-C	1230	 69%17%12%
1	13-A	1230	 68%17%12%
1	13-B	1230	 70%16%12%
1	13-C	1230	 69%17%12%
1	14-A	1230	 69%17%12%
1	14-B	1230	 71%15%12%
1	14-C	1230	 68%18%12%
1	15-A	1230	 69%17%12%
1	15-B	1230	 69%17%12%
1	15-C	1230	 68%18%12%
1	16-A	1230	 68%17%12%
1	16-B	1230	 70%16%12%
1	16-C	1230	 70%16%12%
1	17-A	1230	 68%18%12%
1	17-B	1230	 70%16%12%
1	17-C	1230	 67%19%12%
1	18-A	1230	 71%16%12%
1	18-B	1230	 71%15%12%
1	18-C	1230	 70%17%12%
1	19-A	1230	 69%17%12%
1	19-B	1230	 70%17%12%
1	19-C	1230	 68%18%12%

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Mol	Chain	Length	Quality of chain
1	2-A	1230	
1	2-B	1230	
1	2-C	1230	
1	20-A	1230	
1	20-B	1230	
1	20-C	1230	
1	3-A	1230	
1	3-B	1230	
1	3-C	1230	
1	4-A	1230	
1	4-B	1230	
1	4-C	1230	
1	5-A	1230	
1	5-B	1230	
1	5-C	1230	
1	6-A	1230	
1	6-B	1230	
1	6-C	1230	
1	7-A	1230	
1	7-B	1230	
1	7-C	1230	
1	8-A	1230	
1	8-B	1230	
1	8-C	1230	
1	9-A	1230	

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Mol	Chain	Length	Quality of chain
1	9-B	1230	<div><div></div><div>68%</div><div>17%</div><div>•</div><div>12%</div></div>
1	9-C	1230	<div><div></div><div>69%</div><div>17%</div><div>•</div><div>12%</div></div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 509160 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	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	4-A	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	5-A	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	6-A	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	7-A	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	8-A	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	9-A	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	10-A	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	11-A	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	12-A	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	13-A	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	14-A	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	15-A	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	16-A	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	17-A	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	18-A	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	19-A	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	20-A	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
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	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	4-B	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	5-B	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	6-B	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	7-B	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	8-B	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	9-B	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	10-B	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	11-B	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	12-B	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	13-B	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	14-B	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	15-B	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	16-B	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	17-B	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	18-B	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	19-B	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	20-B	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
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	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	4-C	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	5-C	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	6-C	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	7-C	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	8-C	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	9-C	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	10-C	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	11-C	1079	Total	C	N	O	S	0	0
			8454	5399	1410	1606	39		
1	12-C	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	13-C	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	14-C	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	15-C	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	16-C	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	17-C	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	18-C	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		
1	19-C	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	20-C	1085	Total	C	N	O	S	0	0
			8494	5425	1416	1615	38		

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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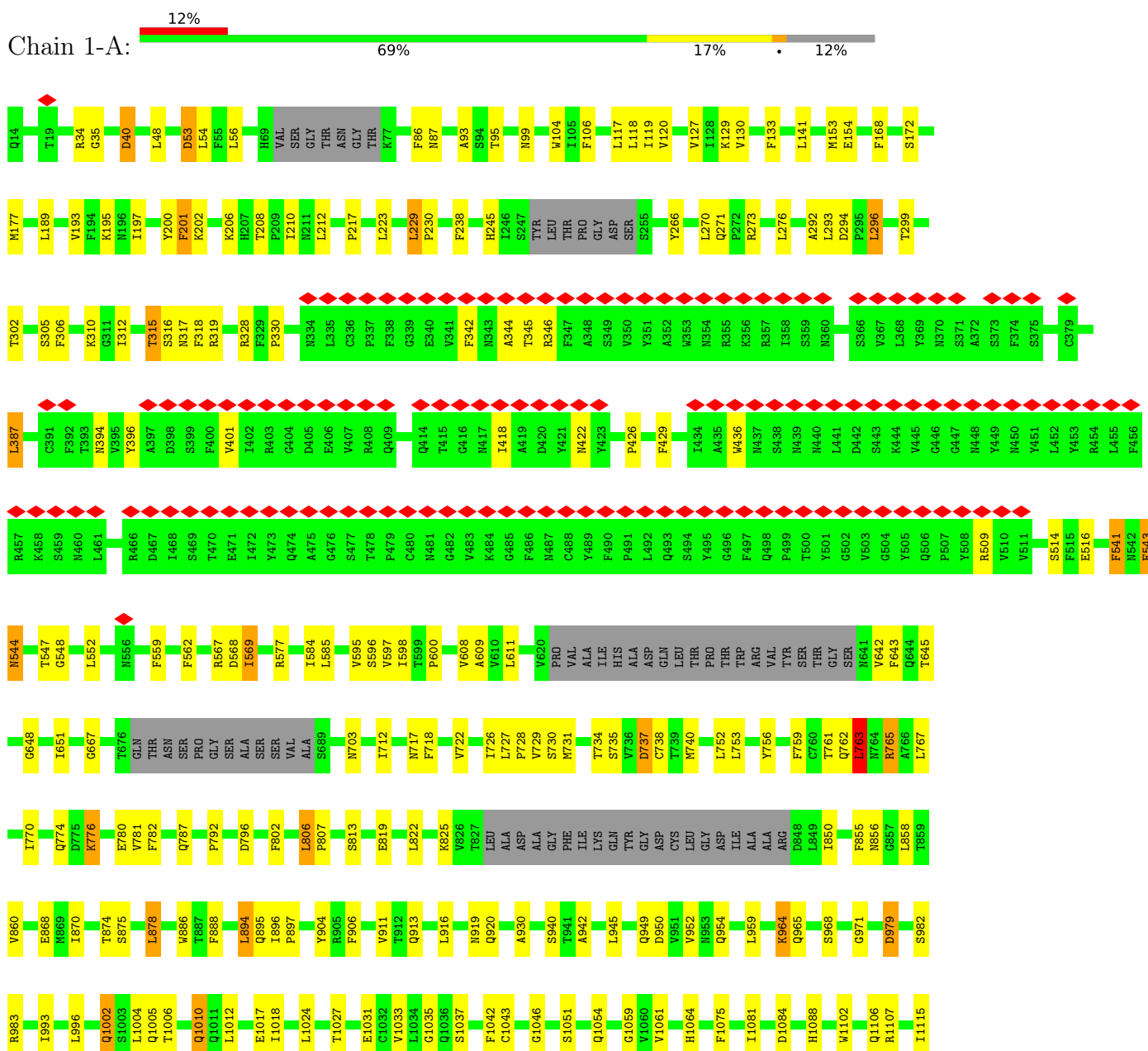
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1238	GLY	-	expression tag	UNP P10104
C	1239	ARG	-	expression tag	UNP P10104
C	1240	SER	-	expression tag	UNP P10104
C	1241	LEU	-	expression tag	UNP P10104
C	1242	GLU	-	expression tag	UNP P10104
C	1243	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

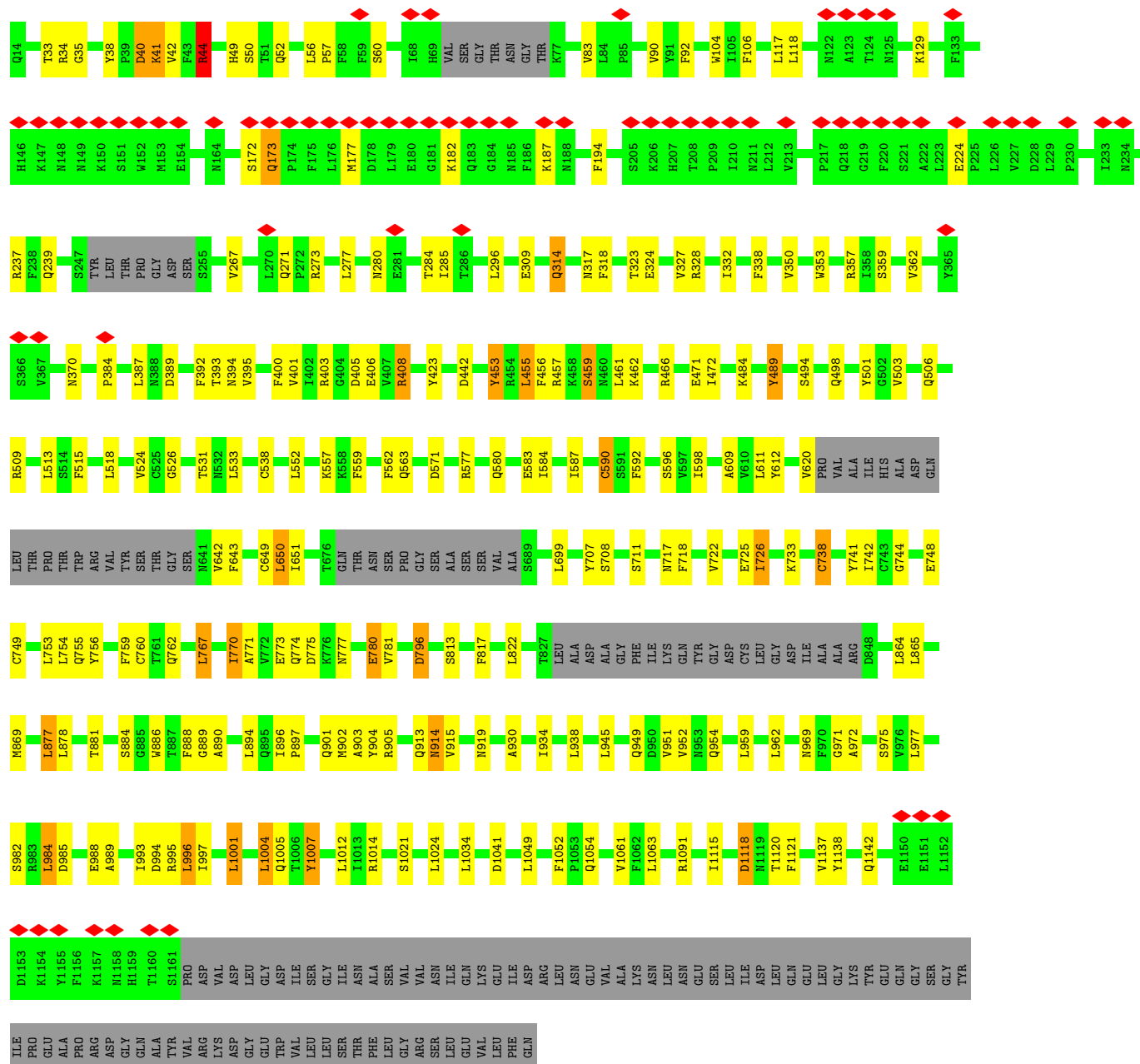
3 Residue-property plots

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

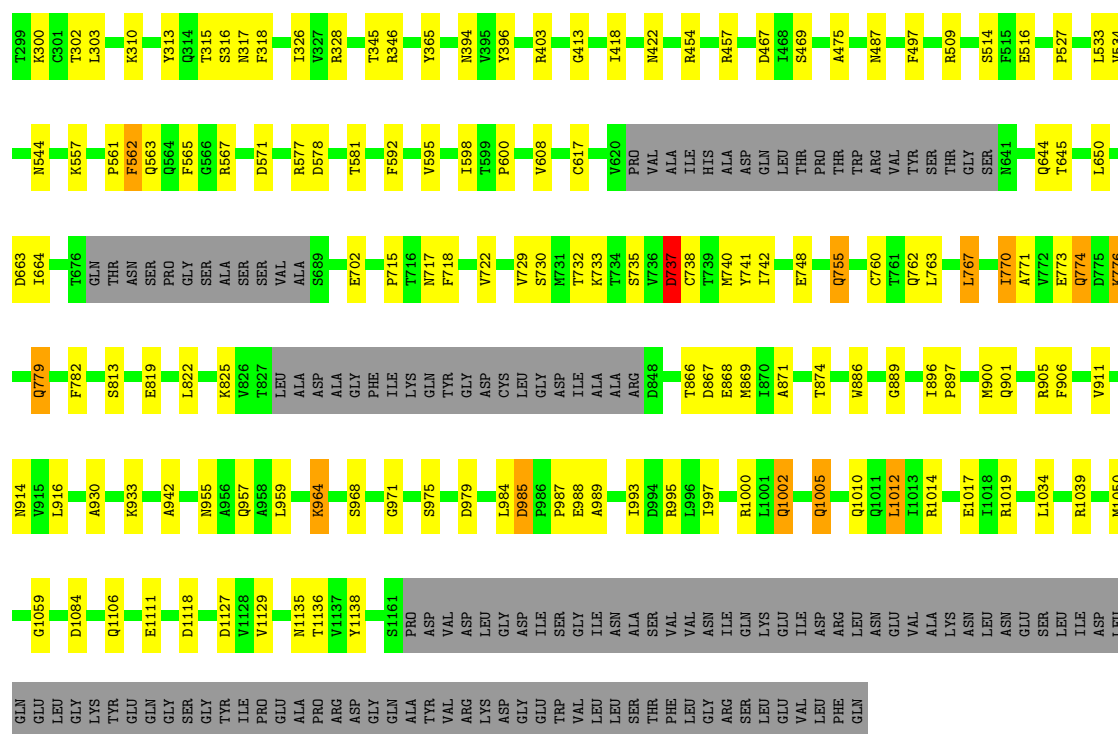


- Molecule 1: Spike glycoprotein, Fibrin



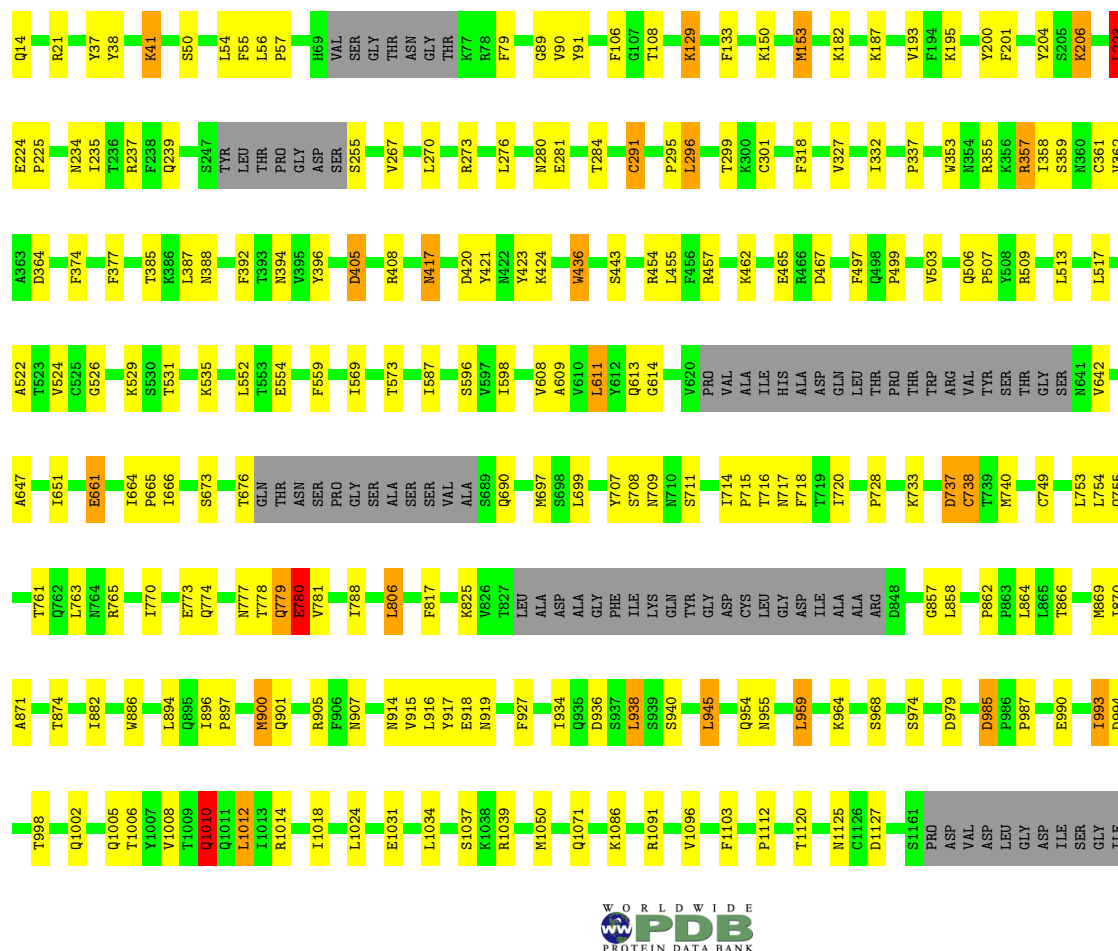
- Molecule 1: Spike glycoprotein, Fibrin





• Molecule 1: Spike glycoprotein,Fibritin

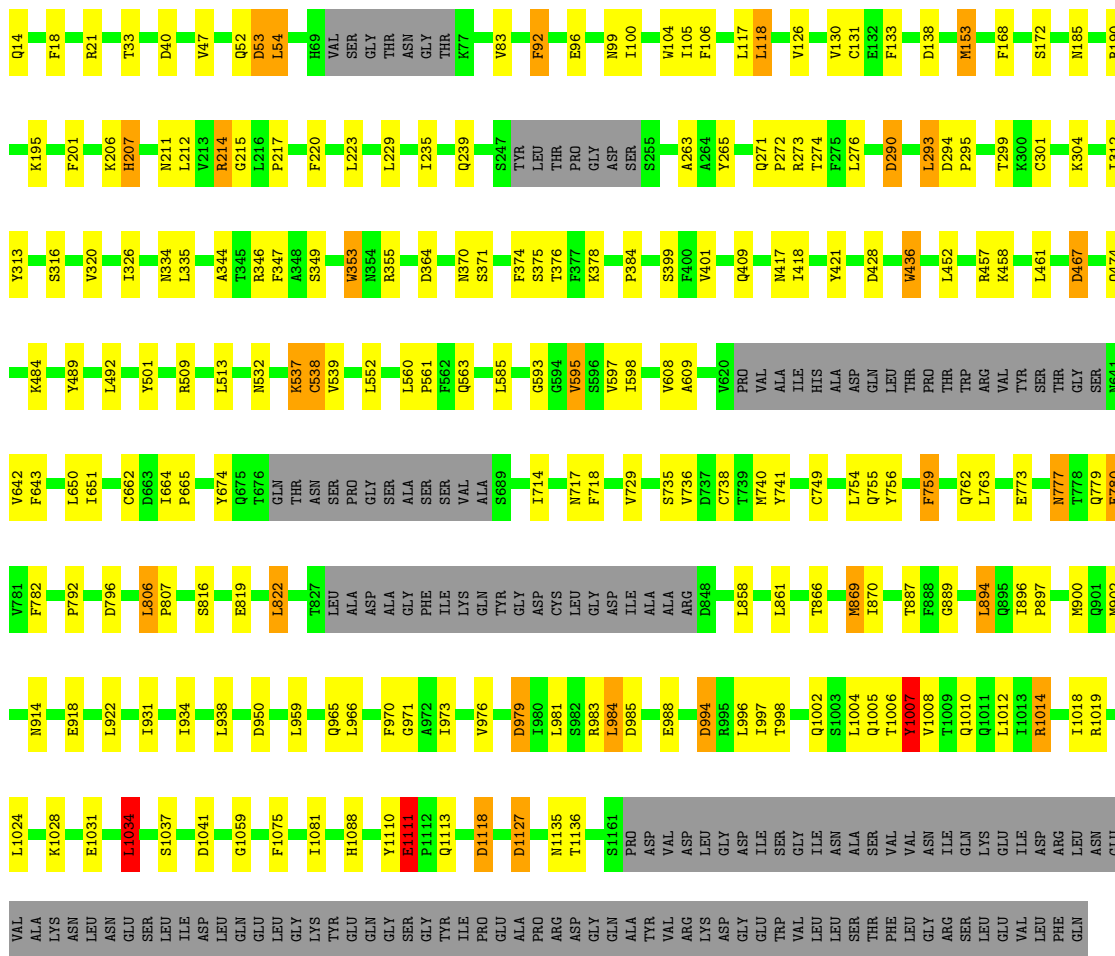
Chain 2-B: 70% 16% 12%



[illegible]

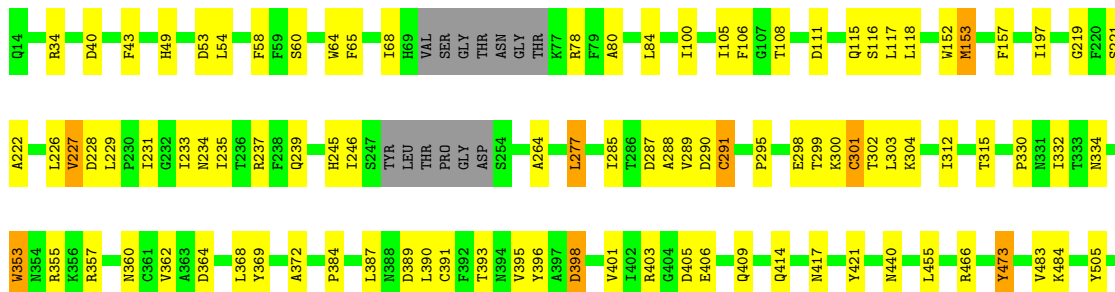
- Molecule 1: Spike glycoprotein, Fibrin

Chain 2-C: 70% 15% 2% 12%



- Molecule 1: Spike glycoprotein, Fibrin

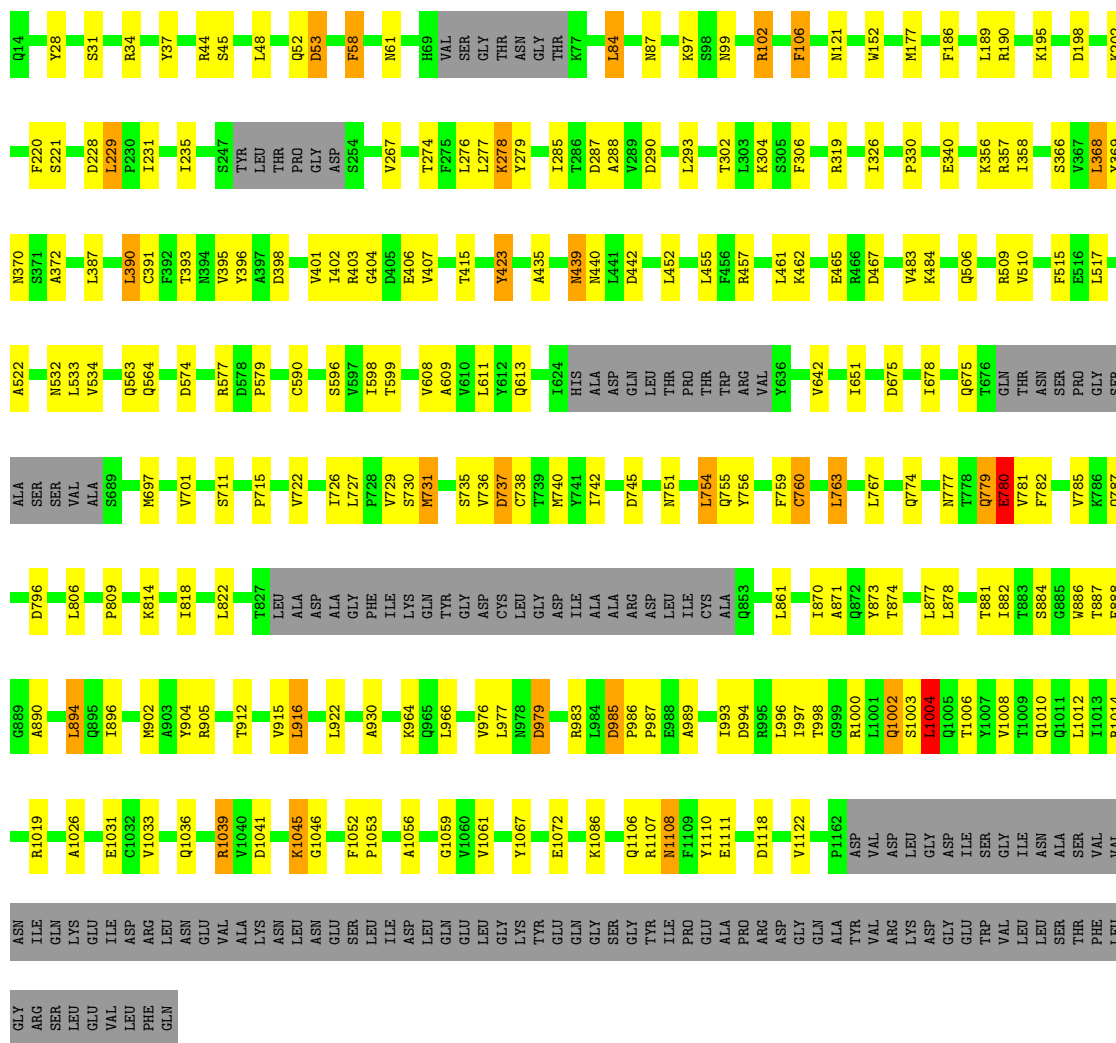
Chain 3-A: 69% 17% • 12%



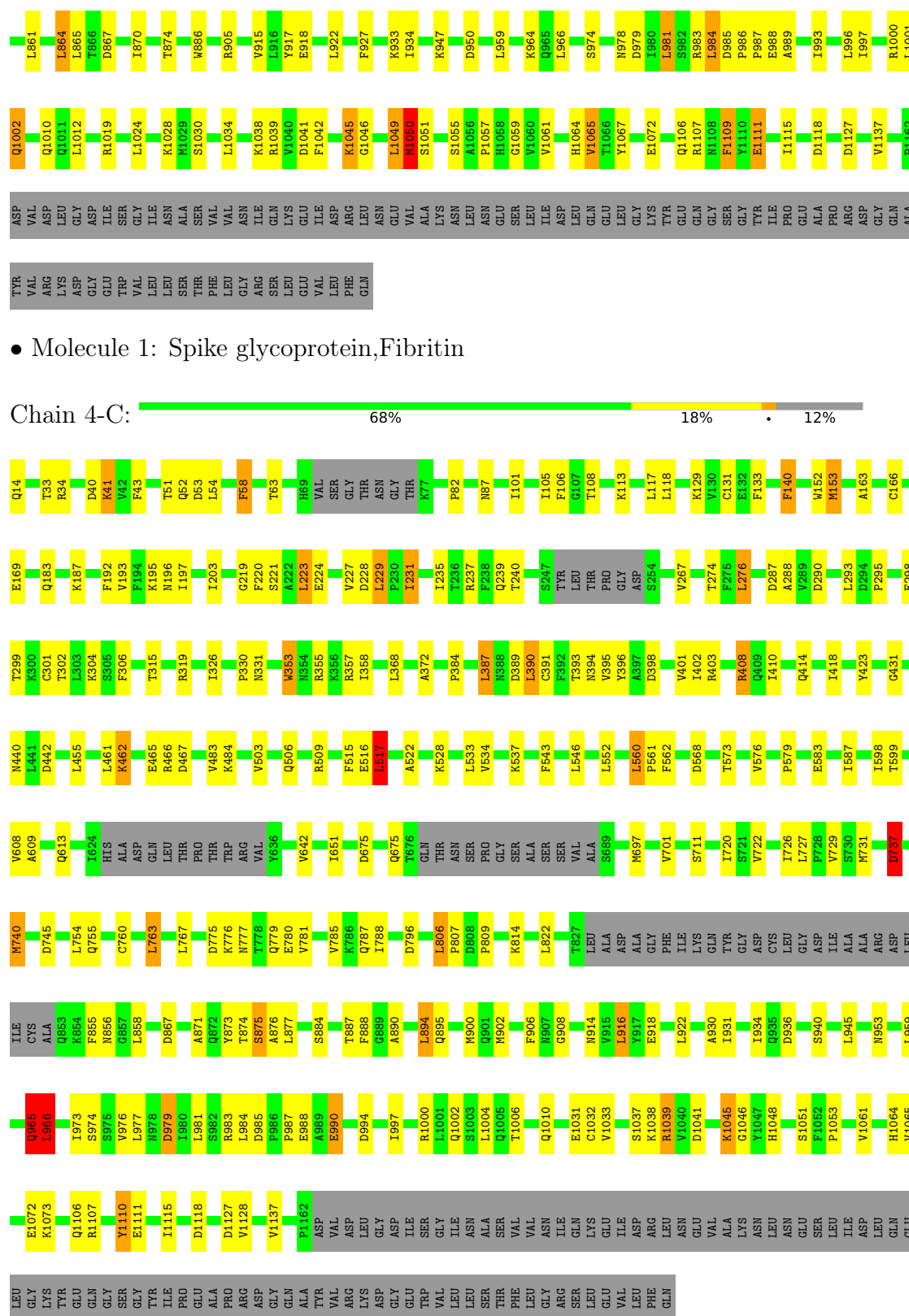
LEU ASN
GLU SER
LEU ILE
ASP LEU
GLN
LEU GLY
LYS TYR
GLU
GLN
GLY
SER
GLY
TYR
ILE
GLU
ALA
PRO
ARG
ASP
GLY
GLN
ALA
TYR
VAL
ARG
LYS
ASP
GLY
TRP
VAL
LEU
SER
THR
PHE
LEU
GLY
ARG
SER
LEU
VAL
PHE
GLN

• Molecule 1: Spike glycoprotein,Fibrin

Chain 3-C: 70% 16% 12%







• Molecule 1: Spike glycoprotein,Fibrin

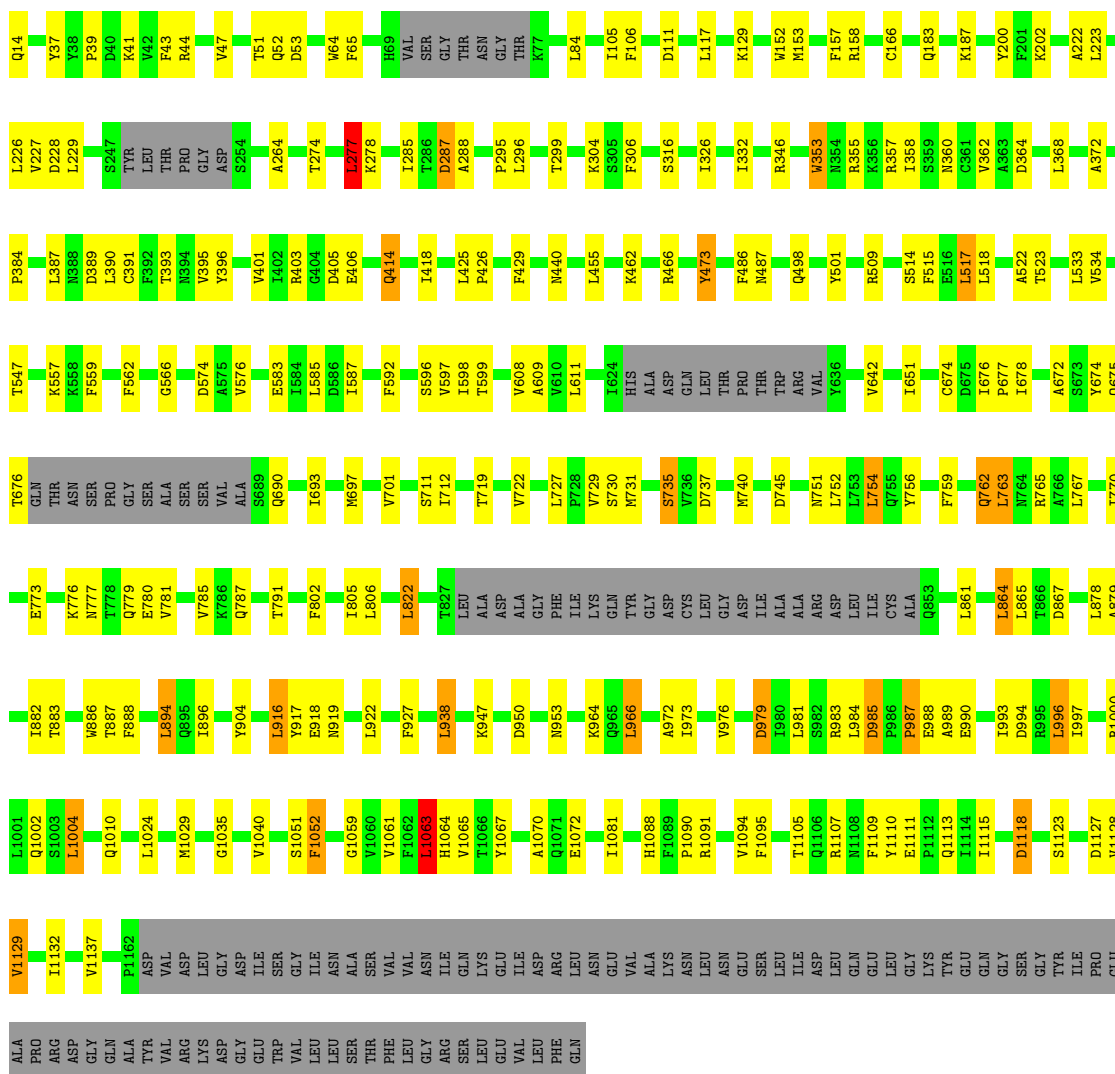
Chain 5-A:



LEU
PHE
GLN

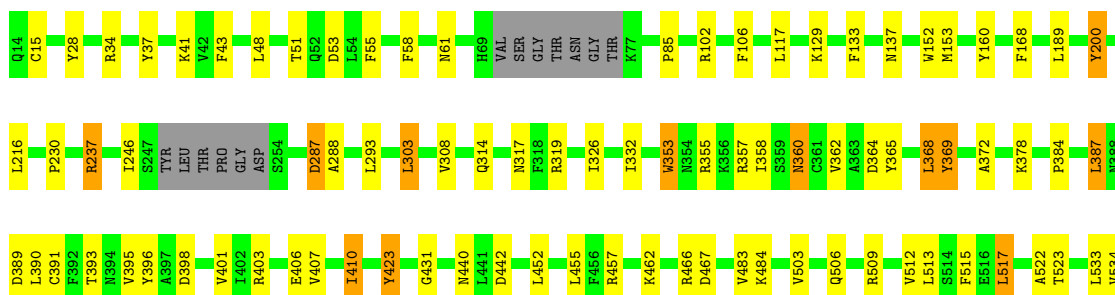
• Molecule 1: Spike glycoprotein,Fibrin

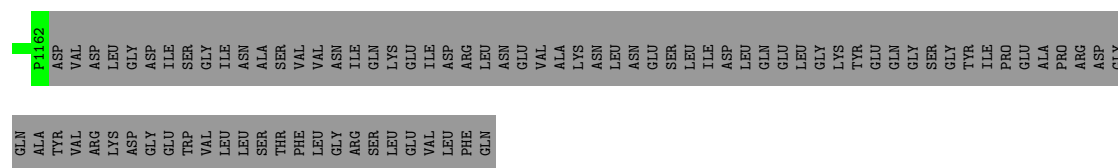
Chain 7-A: 69% 17% 12%



• Molecule 1: Spike glycoprotein,Fibrin

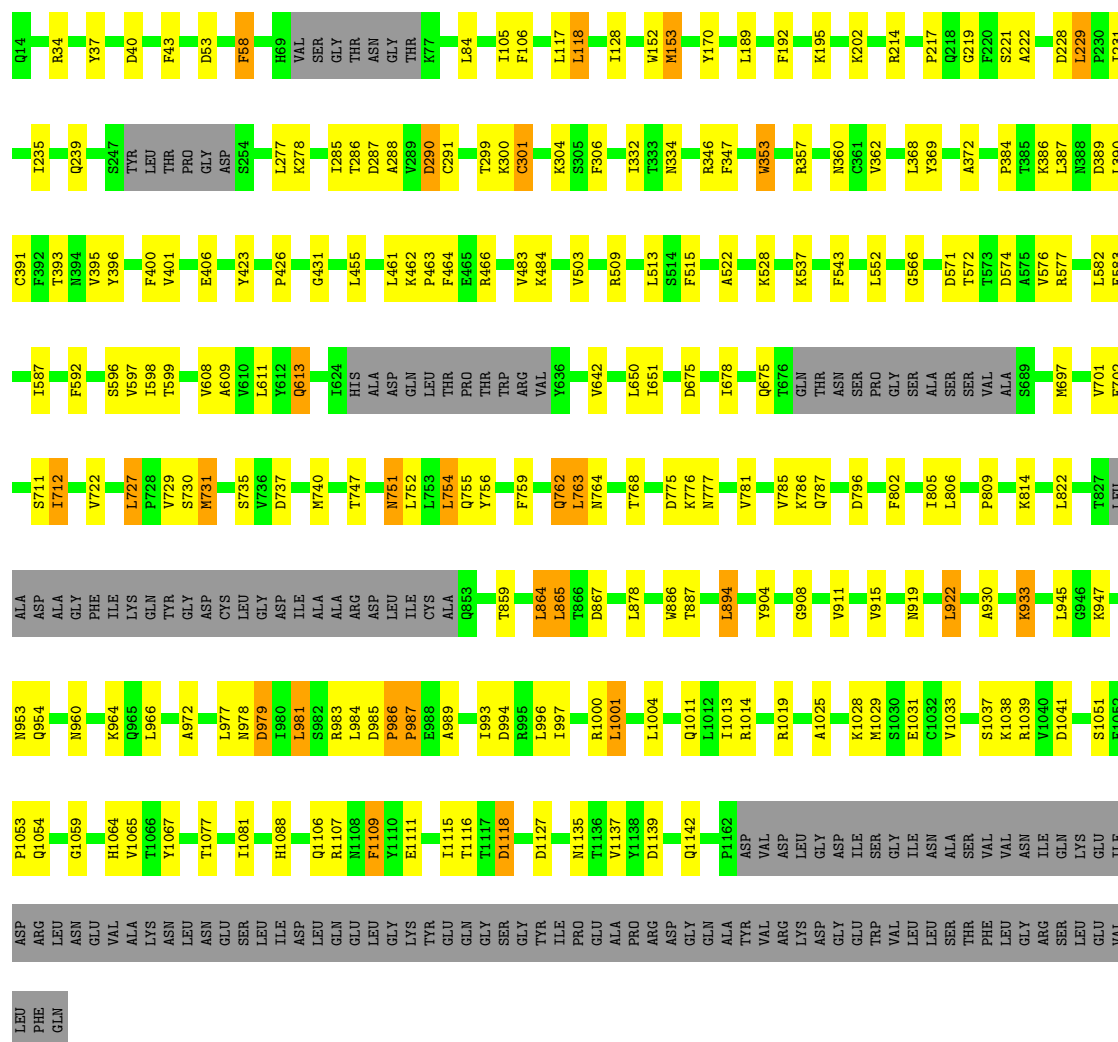
Chain 7-B: 70% 16% 12%





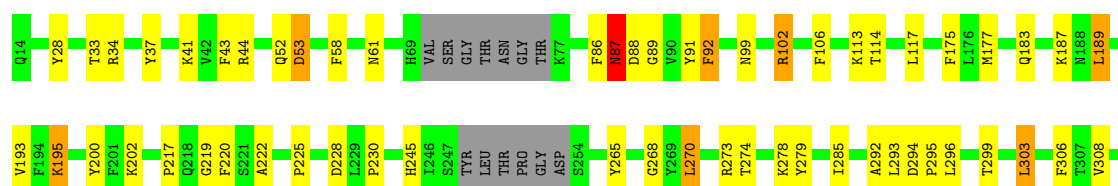
• Molecule 1: Spike glycoprotein,Fibritin

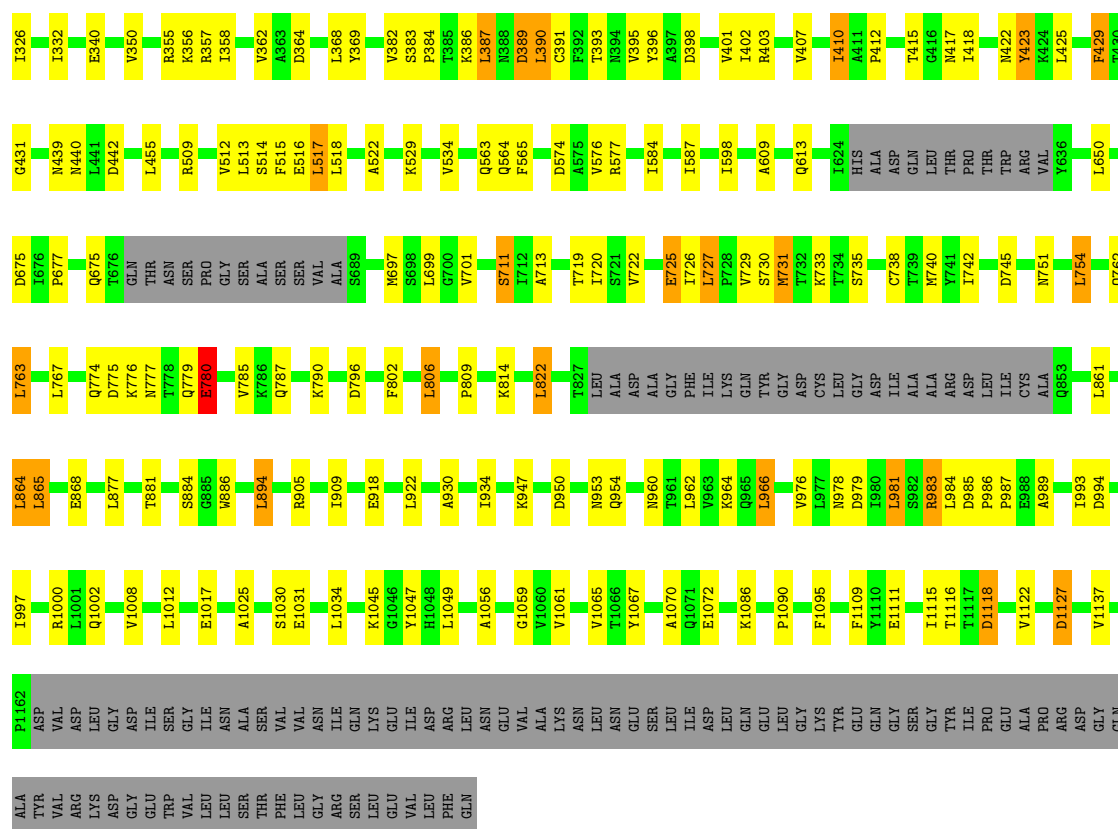
Chain 8-A: 70% 16% 12%



• Molecule 1: Spike glycoprotein,Fibritin

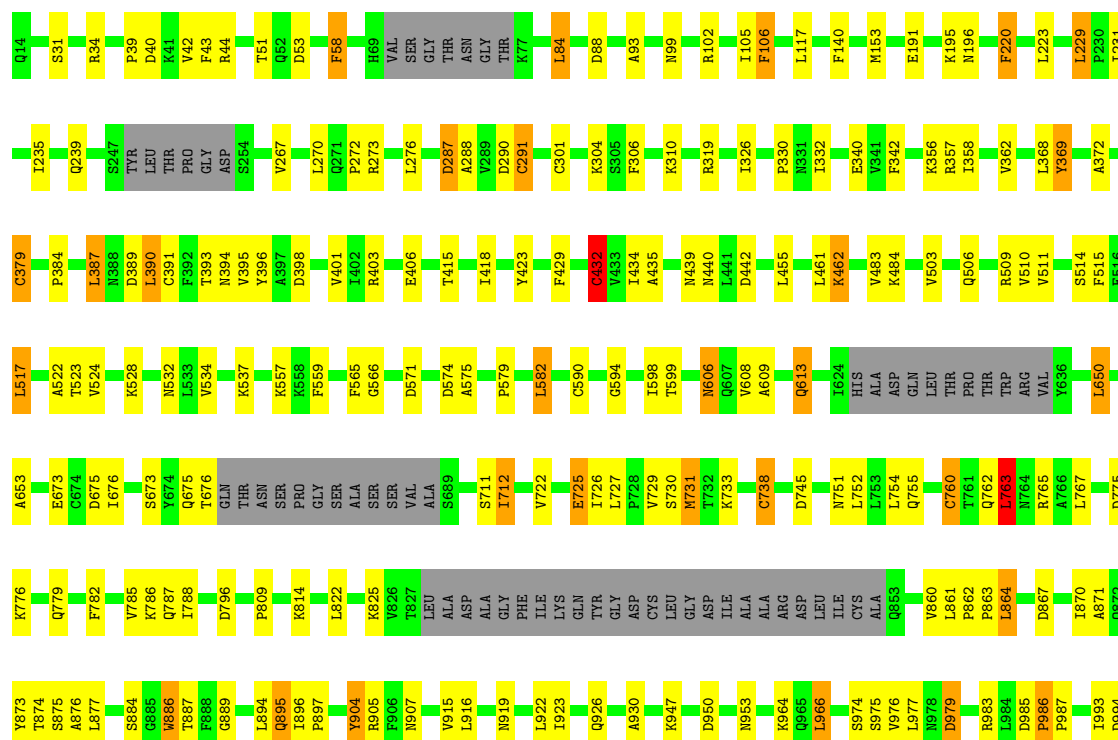
Chain 8-B: 69% 16% 12%

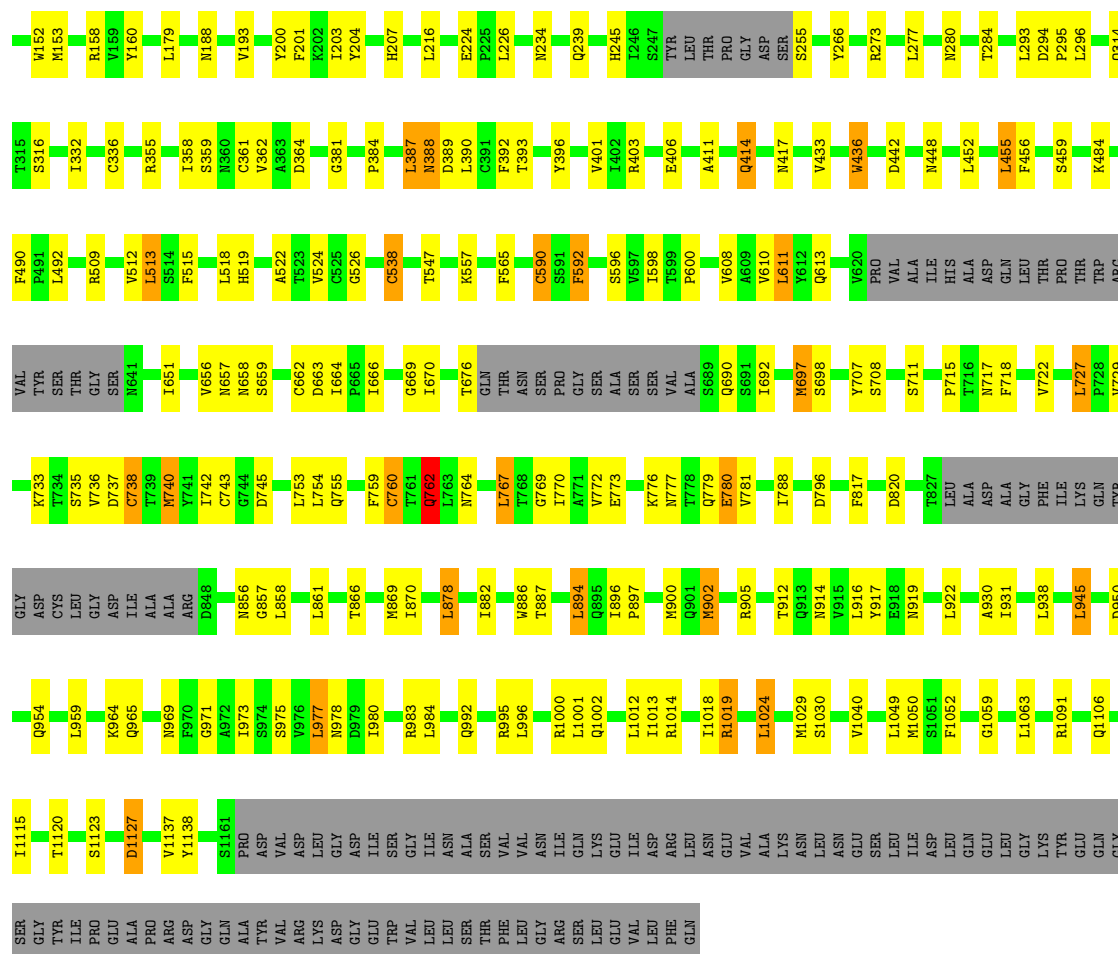




• Molecule 1: Spike glycoprotein,Fibritin

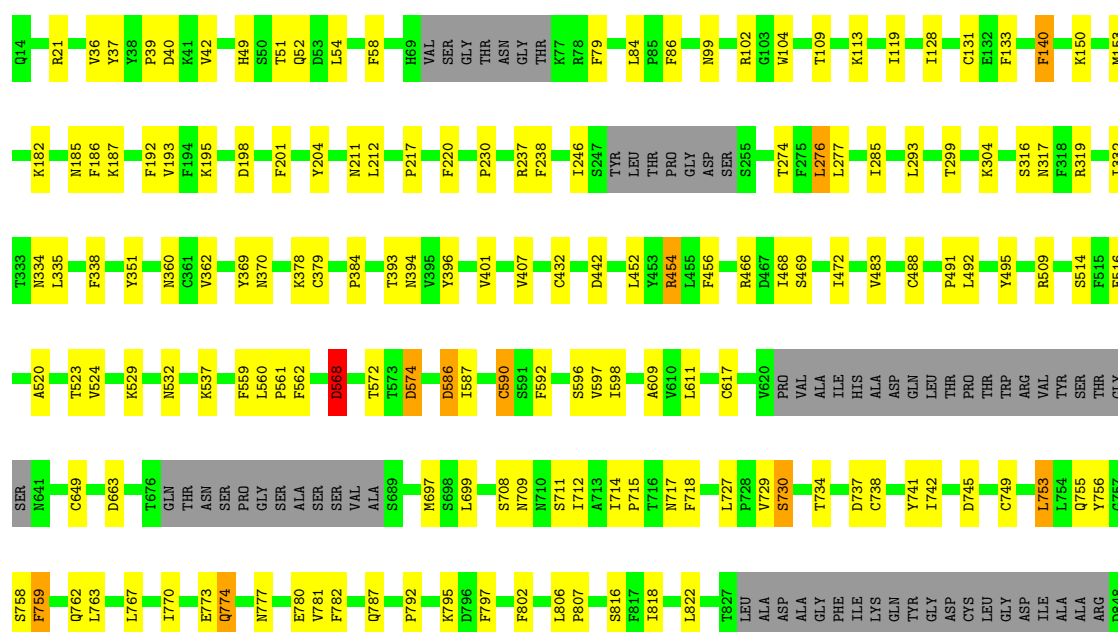
Chain 8-C: 69% 17% 12%





• Molecule 1: Spike glycoprotein,Fibritin

Chain 9-C: 69% 17% 12%



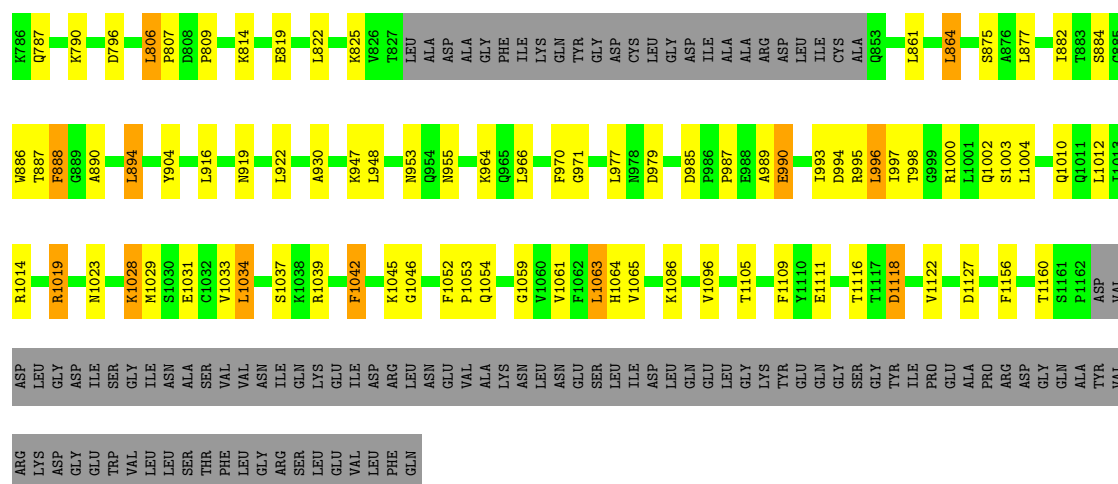


Device Type	Percentage
Smartphones	72%
Tablets	14%
Smart TVs	12%



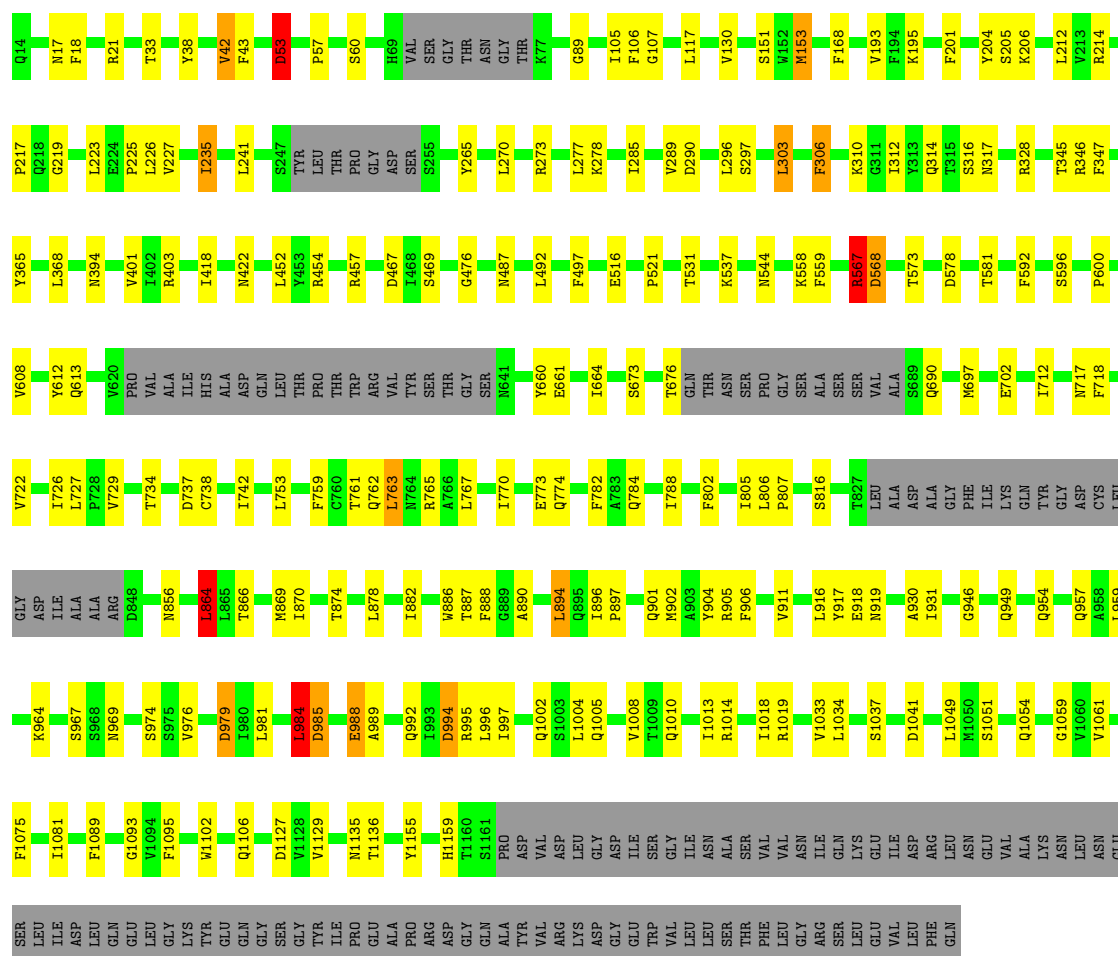
Category	Percentage
Very bad	69%
Bad	16%
Good	12%
Very good	1%





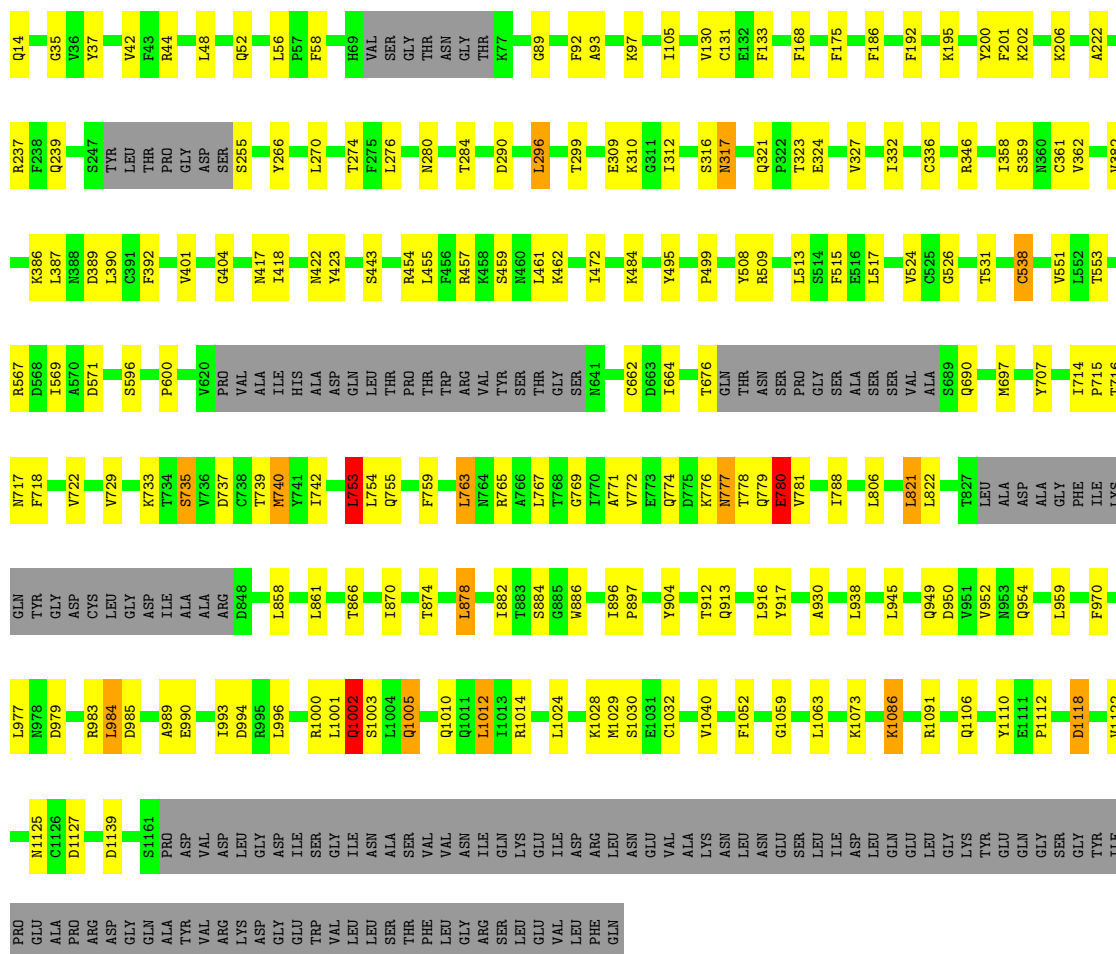
• Molecule 1: Spike glycoprotein,Fibrin

Chain 11-A: 71% 15% 12%



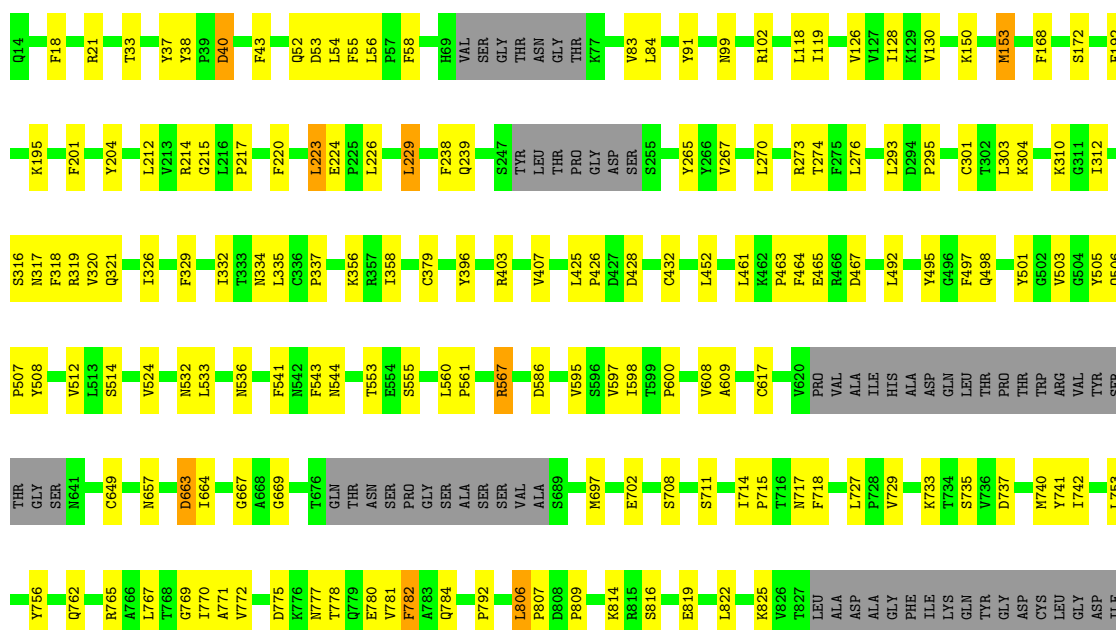
• Molecule 1: Spike glycoprotein,Fibrin

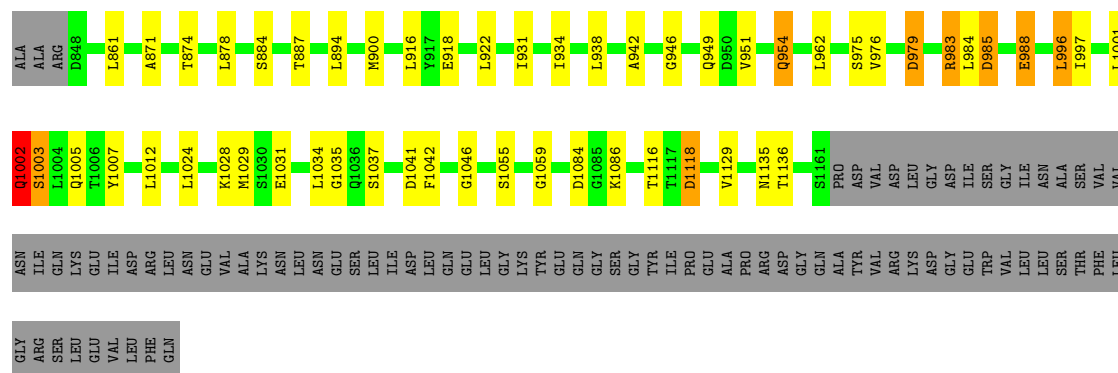
Chain 11-B: 72% 15% 12%



• Molecule 1: Spike glycoprotein,Fibritin

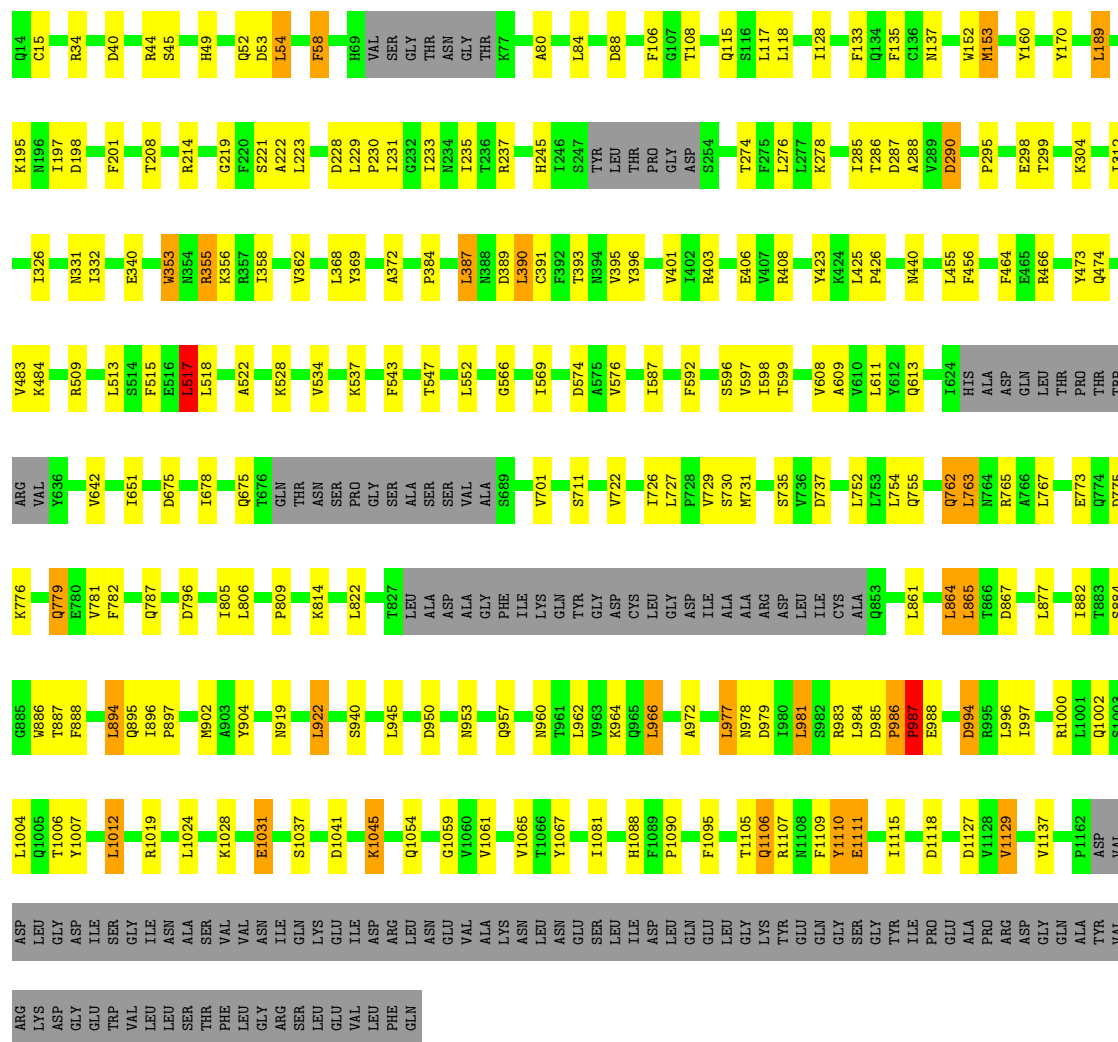
Chain 11-C: 70% 16% 12%





• Molecule 1: Spike glycoprotein,Fibritin


Chain 12-A: 70% 16% 12%

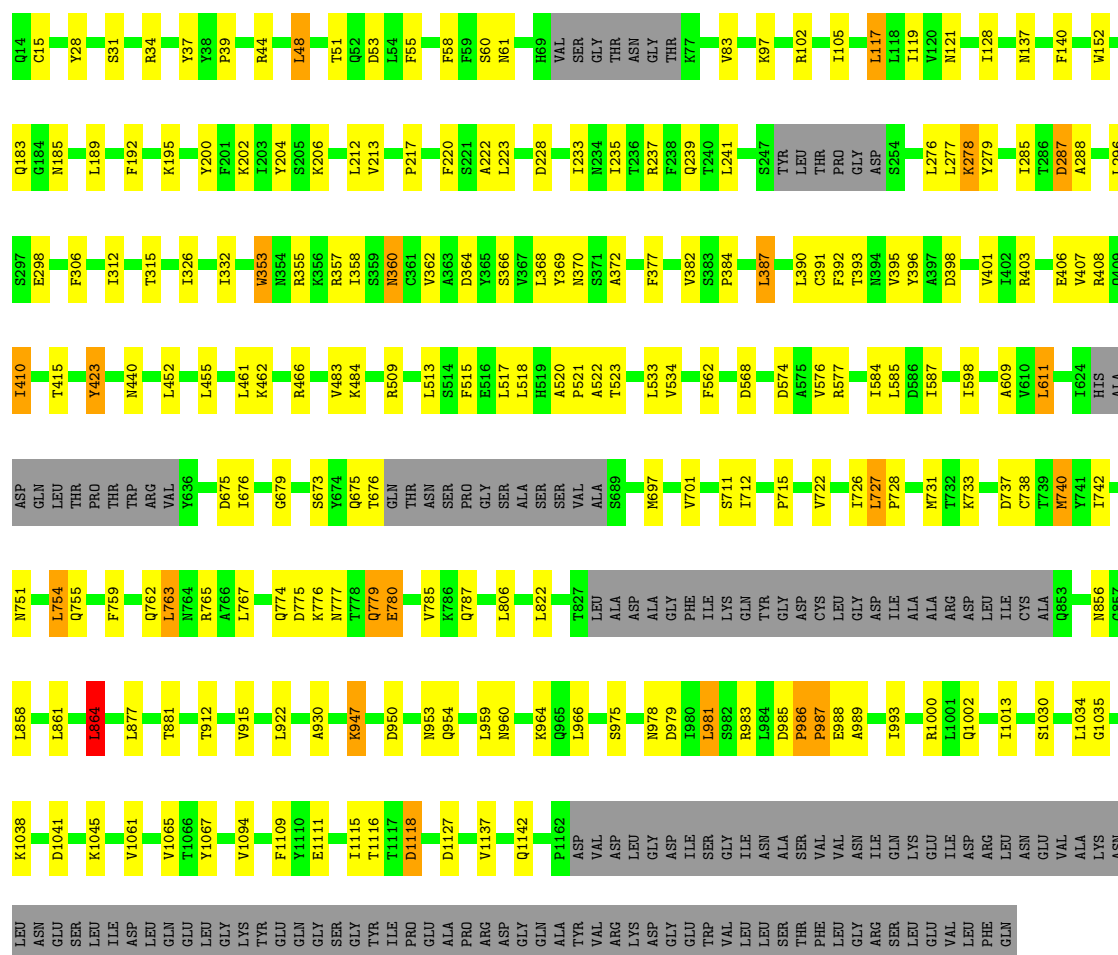


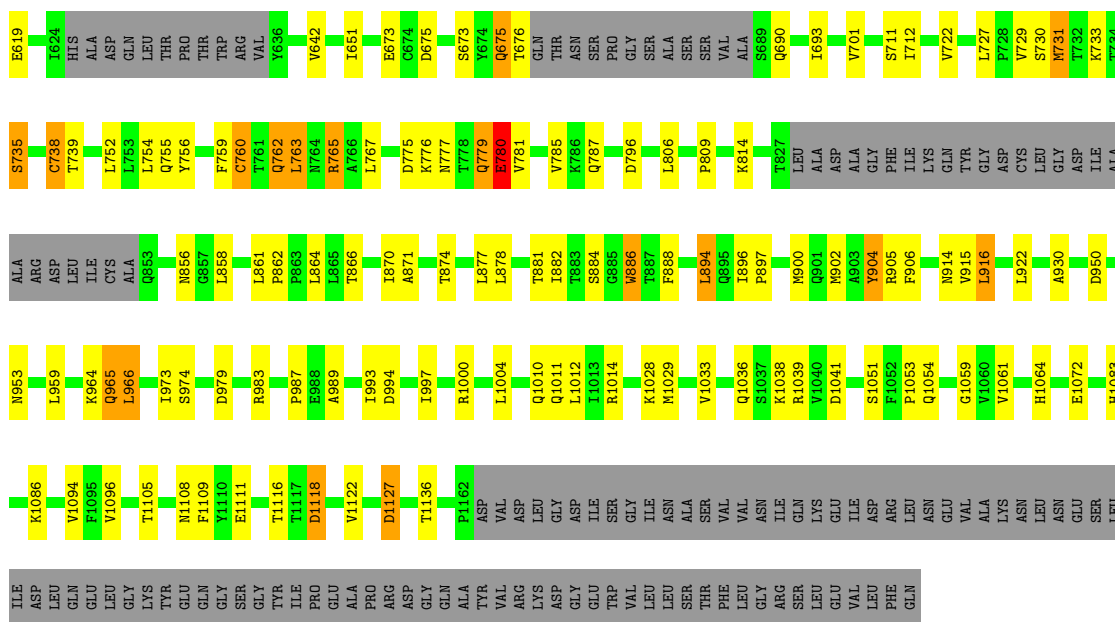


PRO
GLU
ALA
PRO
ARG
ASP
GLY
GLN
ALA
VAL
TYR
ARG
LYS
ASP
GLY
TRP
VAL
LEU
SER
THR
PHE
LEU
GLY
ARG
SER
LEU
VAL
PHE
GLN

• Molecule 1: Spike glycoprotein,Fibrin

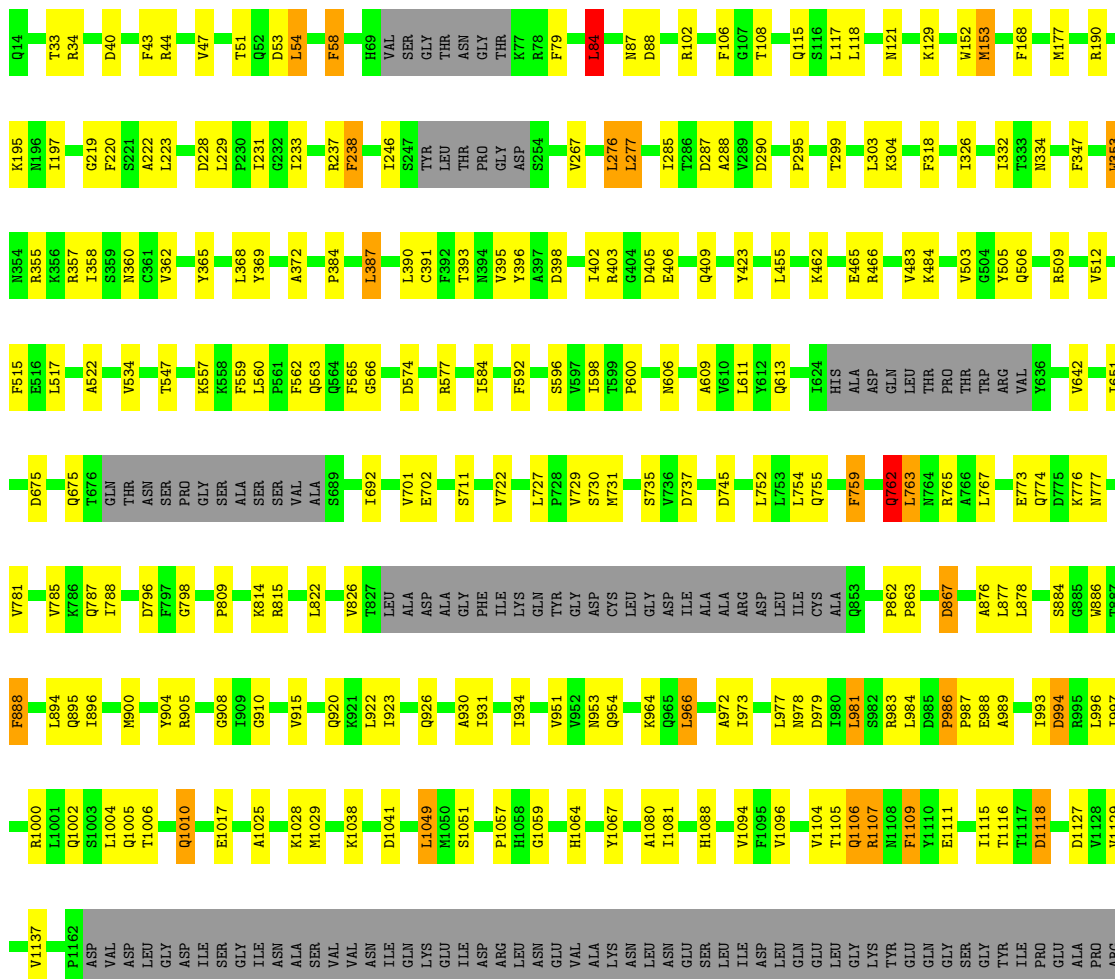
Chain 14-B:  71% 15% 12%





- Molecule 1: Spike glycoprotein, Fibrin

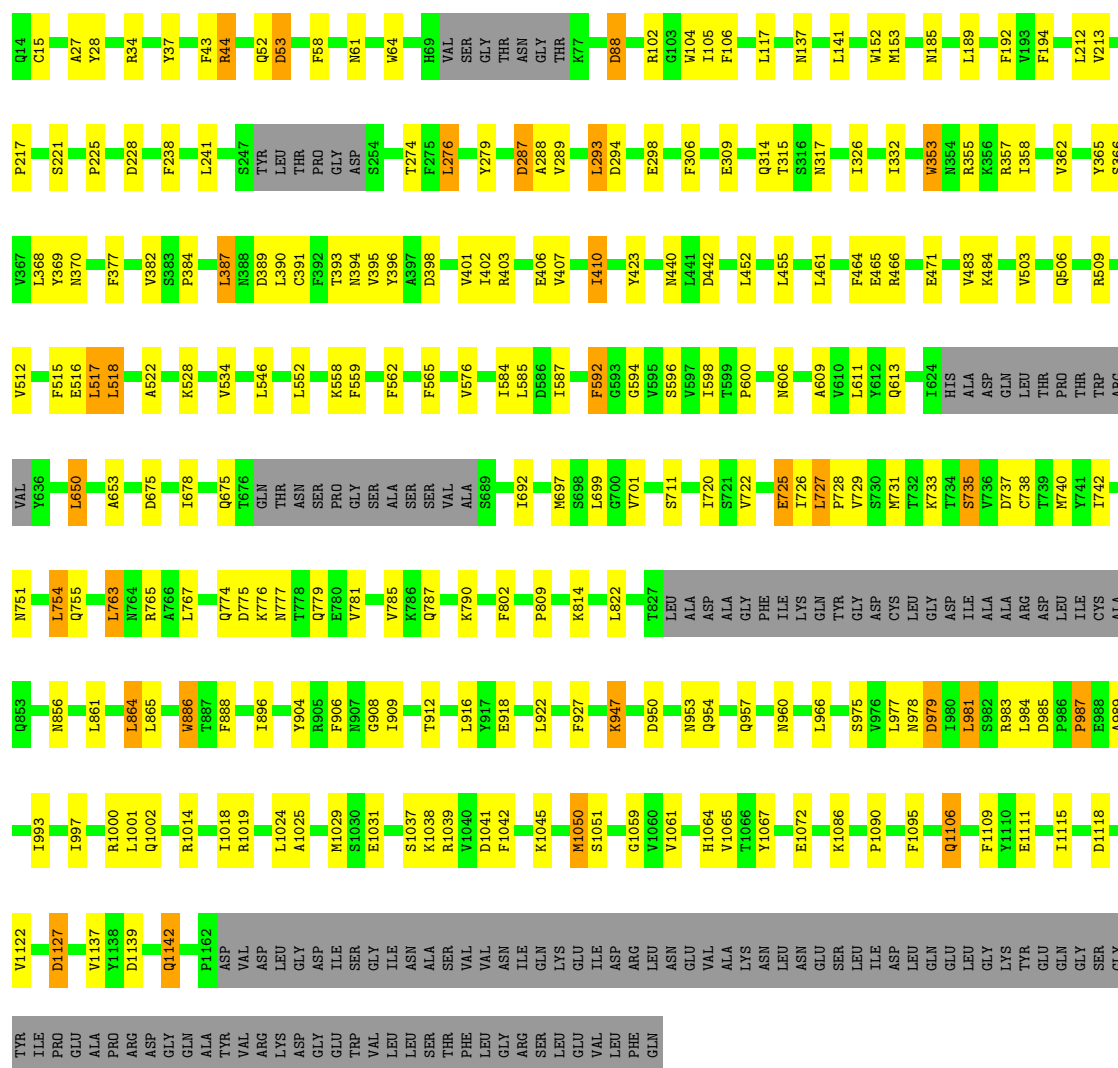
Chain 15-A:  69% 17% 1% 12%



ASP
GLY
GLN
ALA
TYR
VAL
ARG
LYS
ASP
GLY
GLU
TRP
VAL
LEU
LEU
SER
THR
PHE
LEU
GLY
ARG
SER
SER
GLU
VAL
LEU
PHE
GLN

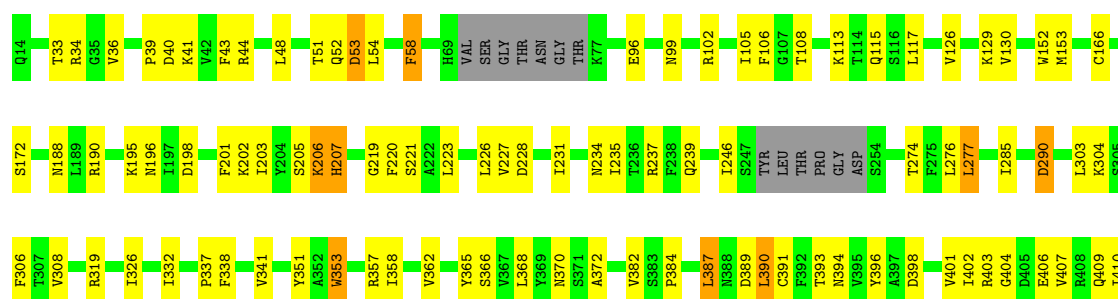
• Molecule 1: Spike glycoprotein,Fibritin

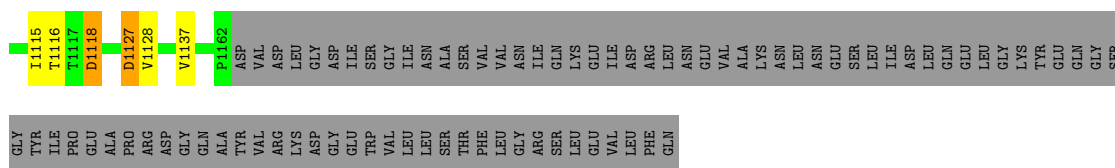
Chain 15-B: 69% 17% 12%



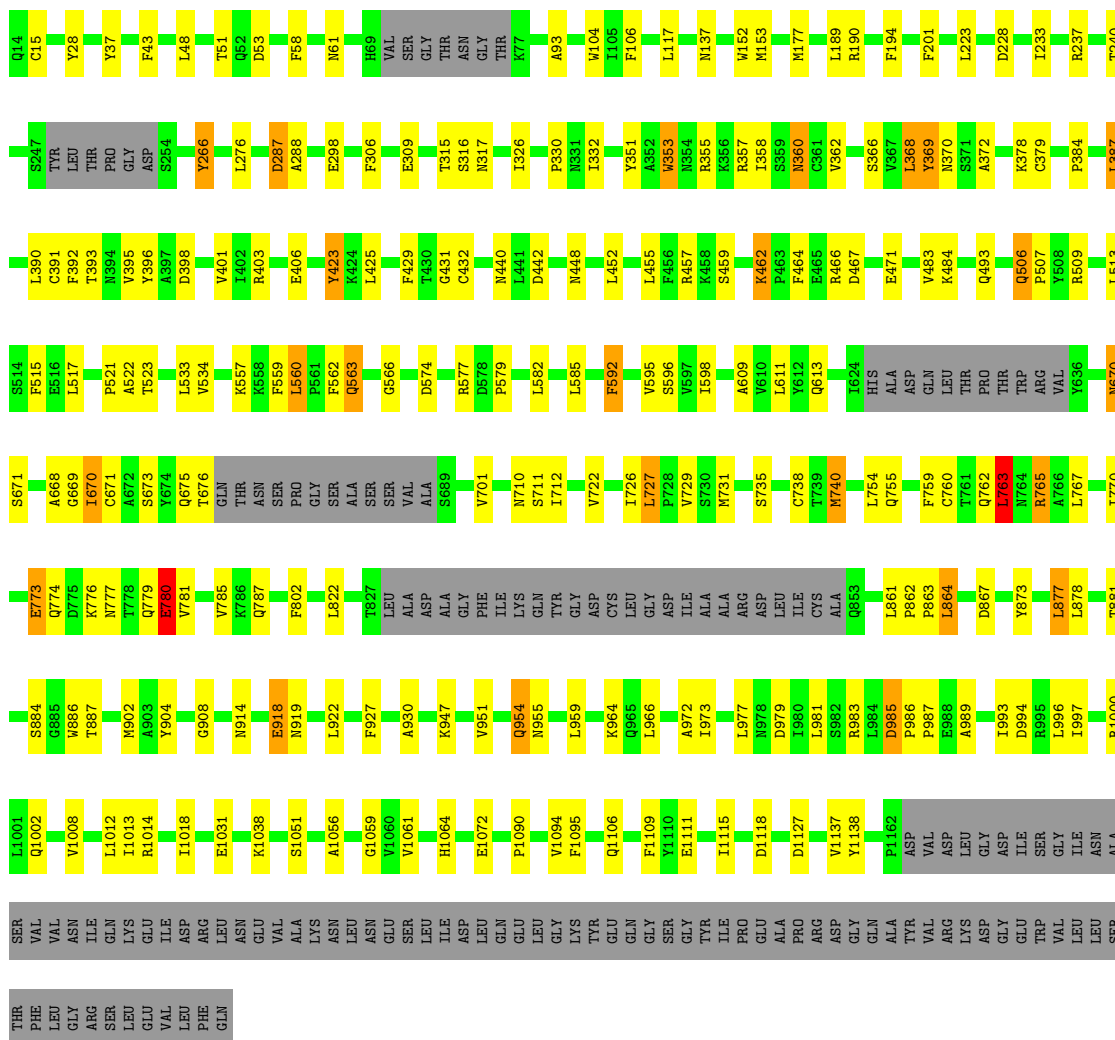
• Molecule 1: Spike glycoprotein,Fibritin

Chain 15-C: 68% 18% 12%

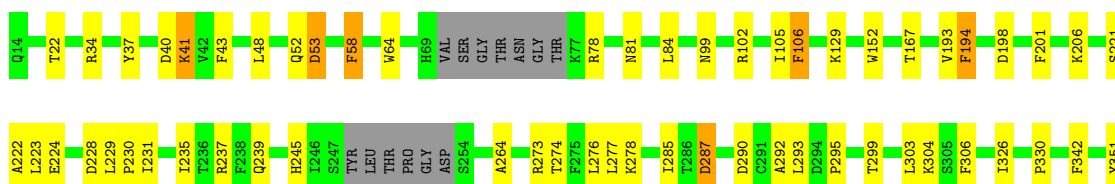


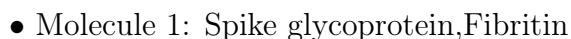


- Molecule 1: Spike glycoprotein, Fibrin

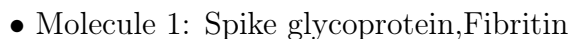
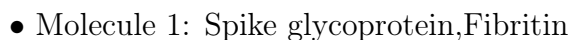


- Molecule 1: Spike glycoprotein, Fibrin



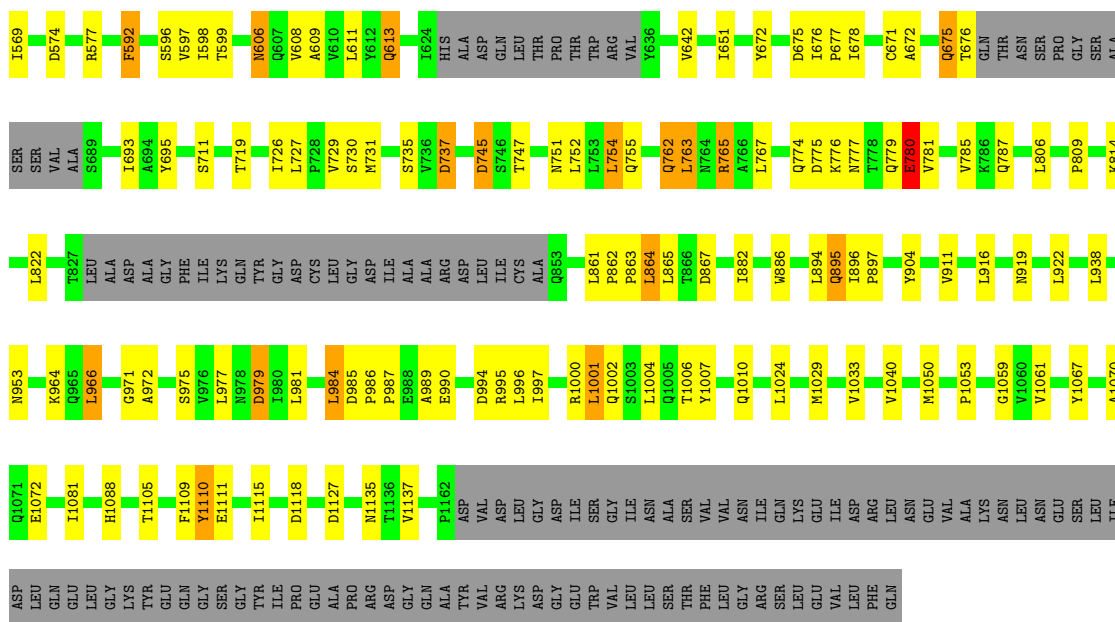


PRO	T761	L858	V510	R346	F201	Q14
	Q762	L864	F515	R353	K206	T22
	TRP	L763	F516	W353		
	ARG	N764	L517	N354	P217	R34
	VAL	R765	L665	R355	Q218	
	Y636	A766		K356	G219	D40
	L767	D867	P621	R357	F220	
			A522	S358	S221	V47
	E773	Y873	K629	S359	A222	
	L650	L877	V634	N360	L226	Q52
I651	L878	K335	C361	V227	D53	
D676			V362	D228		
I678	Q779	T547	L368	I231	P57	
	W780	L552	Y369	I231	F58	
V781	Q787	T676	A372	I233	I68	
GLN	T791	THR	P384	F238	H69	
ASN	D796	Q563	Q564	I246	VAL	
SER	L806	F665	S947	T246	GLY	
GLY	L809	G566	L390	TYR	THR	
SER	P809	D574	C391	LEU	GLY	
ALA	K814	A575	F392	THR	THR	
SER		V576	N394	GLY		
VAL	L822	P579	V395	ASP		
ALA			Y396	S954	P85	
S689	K825	L585	V401	R273	L84	
Q690	W826	D586	I402	T274	P86	
I693	T827	I587	R403	F275	N87	
LEU			L276	L277	E96	
ALA		F592	E406		K97	
ASP	L953	G593	V407	I285	I100	
GLY	Q954	G594	I410	I286	I101	
ALA	L959	V595		D287	R102	
PHE	K964	S596	Y423	A288	K113	
ILE	Q965	V597			T114	
LYS	L966	I598	D427	A292	Q115	
GLN		T599		P295	S116	
TYR	G971	N606	A435	L117	L118	
GLY	A972	Q607		E298		
ASP		W728	N440	T299	N121	
CYS	L977	S730	L441			
LEU	N978	M731	D442	F306	V126	
GLY	D979	I742	L455			
ASP	L980	I611		T315	W152	
ILE		Y612			M153	
ALA	L981	Q613		I326	S172	
ALA	R983	I624	L461	K462		
ARG	L984	H15	P463	F464		
ASP	D985	ALA		P330		
ILE	P986	ASP	E465	N331	L189	
CYS	P987	S758	GLN	I332		
W759	E988	LEU	R466	T333	G199	
F759					W506	
C682		THR	P500	N324		



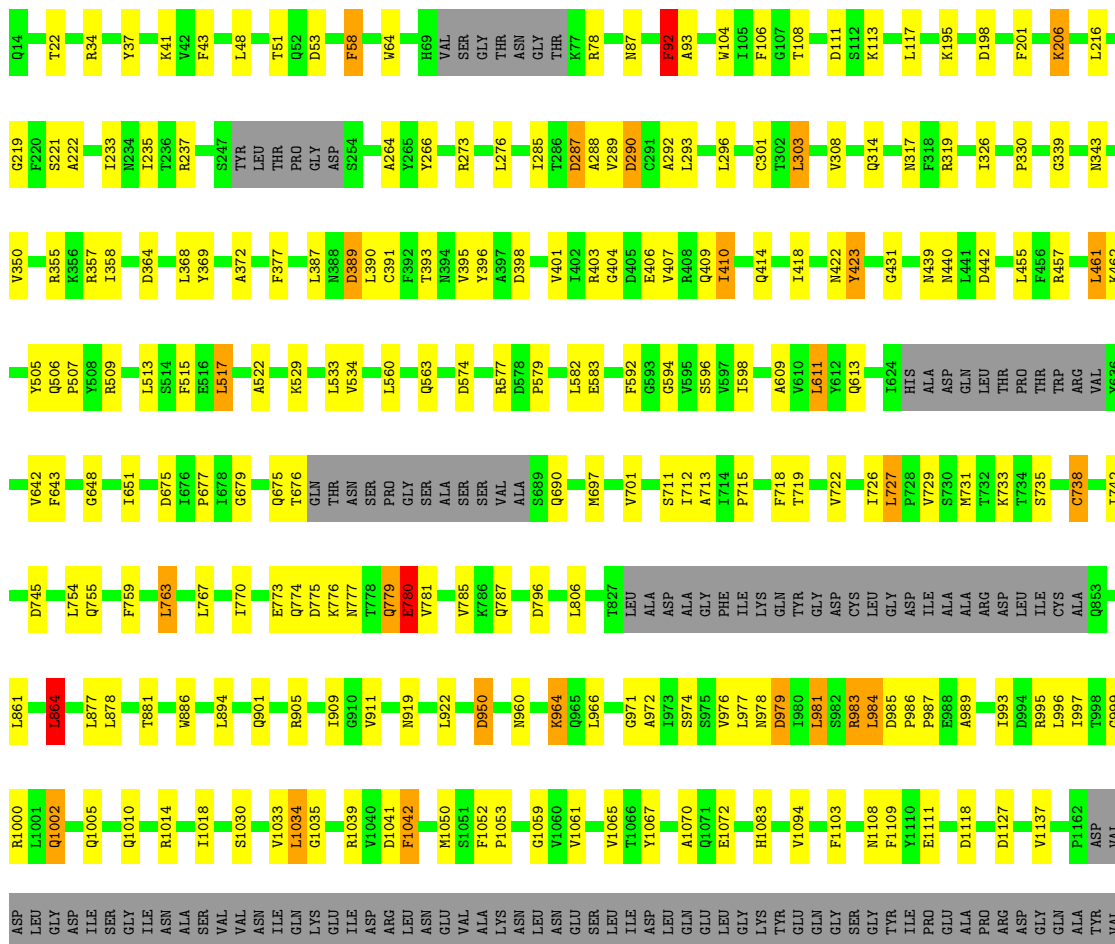


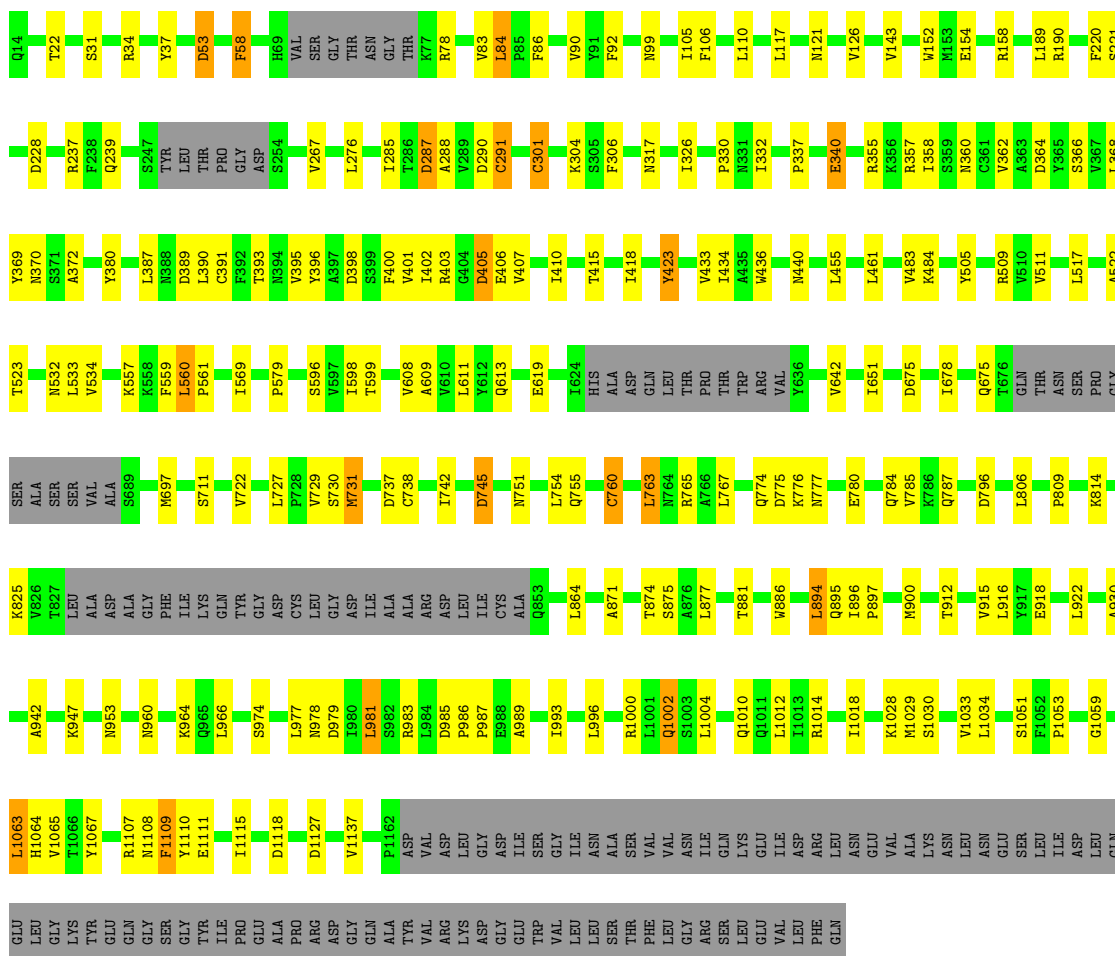




- Molecule 1: Spike glycoprotein, Fibrin

Chain 20-B:  70% 16% 2% 12%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	309062	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 ($e^-/\text{\AA}^2$)	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	1.384	Depositor
Minimum map value	-0.335	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.057	Depositor
Recommended contour level	0.15	Depositor
Map size (\AA)	313.6, 313.6, 313.6	wwPDB
Map dimensions	224, 224, 224	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	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	0.39	0/8652	0.86	28/11768 (0.2%)
1	1-B	0.43	2/8652 (0.0%)	0.93	48/11768 (0.4%)
1	1-C	0.43	2/8652 (0.0%)	0.90	36/11768 (0.3%)
1	2-A	0.38	1/8652 (0.0%)	0.87	38/11768 (0.3%)
1	2-B	0.41	1/8652 (0.0%)	0.92	41/11768 (0.3%)
1	2-C	0.42	3/8652 (0.0%)	0.94	43/11768 (0.4%)
1	3-A	0.41	0/8695	0.97	54/11829 (0.5%)
1	3-B	0.41	0/8695	0.93	46/11829 (0.4%)
1	3-C	0.42	0/8695	0.95	40/11829 (0.3%)
1	4-A	0.43	0/8695	0.99	50/11829 (0.4%)
1	4-B	0.45	0/8695	1.00	62/11829 (0.5%)
1	4-C	0.45	0/8695	1.05	64/11829 (0.5%)
1	5-A	0.45	1/8695 (0.0%)	1.03	63/11829 (0.5%)
1	5-B	0.44	0/8695	0.98	51/11829 (0.4%)
1	5-C	0.45	0/8695	0.99	47/11829 (0.4%)
1	6-A	0.43	0/8695	0.98	55/11829 (0.5%)
1	6-B	0.42	0/8695	0.94	37/11829 (0.3%)
1	6-C	0.43	1/8695 (0.0%)	0.99	49/11829 (0.4%)
1	7-A	0.46	0/8695	1.01	57/11829 (0.5%)
1	7-B	0.46	0/8695	0.95	45/11829 (0.4%)
1	7-C	0.46	2/8695 (0.0%)	0.99	48/11829 (0.4%)
1	8-A	0.43	0/8695	1.02	63/11829 (0.5%)
1	8-B	0.42	0/8695	0.97	47/11829 (0.4%)
1	8-C	0.46	2/8695 (0.0%)	1.01	56/11829 (0.5%)
1	9-A	0.38	0/8652	0.85	28/11768 (0.2%)
1	9-B	0.41	2/8652 (0.0%)	0.91	45/11768 (0.4%)
1	9-C	0.40	0/8652	0.90	34/11768 (0.3%)
1	10-A	0.41	0/8695	0.96	48/11829 (0.4%)
1	10-B	0.41	0/8695	0.93	45/11829 (0.4%)
1	10-C	0.43	1/8695 (0.0%)	1.00	56/11829 (0.5%)
1	11-A	0.37	0/8652	0.83	26/11768 (0.2%)
1	11-B	0.38	0/8652	0.90	41/11768 (0.3%)
1	11-C	0.40	1/8652 (0.0%)	0.89	34/11768 (0.3%)
1	12-A	0.44	0/8695	0.99	58/11829 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	12-B	0.44	0/8695	0.99	53/11829 (0.4%)
1	12-C	0.45	1/8695 (0.0%)	1.01	60/11829 (0.5%)
1	13-A	0.42	0/8695	0.98	60/11829 (0.5%)
1	13-B	0.43	0/8695	0.97	56/11829 (0.5%)
1	13-C	0.43	2/8695 (0.0%)	0.96	51/11829 (0.4%)
1	14-A	0.43	0/8695	0.99	58/11829 (0.5%)
1	14-B	0.41	0/8695	0.93	45/11829 (0.4%)
1	14-C	0.43	0/8695	0.99	49/11829 (0.4%)
1	15-A	0.42	0/8695	0.97	47/11829 (0.4%)
1	15-B	0.42	0/8695	0.95	51/11829 (0.4%)
1	15-C	0.43	0/8695	0.97	42/11829 (0.4%)
1	16-A	0.42	0/8695	1.02	65/11829 (0.5%)
1	16-B	0.43	0/8695	0.95	49/11829 (0.4%)
1	16-C	0.44	2/8695 (0.0%)	1.01	54/11829 (0.5%)
1	17-A	0.42	0/8695	0.99	57/11829 (0.5%)
1	17-B	0.41	0/8695	0.97	55/11829 (0.5%)
1	17-C	0.43	0/8695	1.01	54/11829 (0.5%)
1	18-A	0.42	0/8695	0.96	44/11829 (0.4%)
1	18-B	0.42	0/8695	0.95	43/11829 (0.4%)
1	18-C	0.41	0/8695	0.96	50/11829 (0.4%)
1	19-A	0.43	0/8695	1.00	50/11829 (0.4%)
1	19-B	0.42	1/8695 (0.0%)	0.99	53/11829 (0.4%)
1	19-C	0.43	1/8695 (0.0%)	1.01	63/11829 (0.5%)
1	20-A	0.42	0/8695	0.98	58/11829 (0.5%)
1	20-B	0.41	1/8695 (0.0%)	0.94	47/11829 (0.4%)
1	20-C	0.41	1/8695 (0.0%)	0.98	41/11829 (0.3%)
All	All	0.42	28/521184 (0.0%)	0.96	2938/709008 (0.4%)

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	1-B	0	1
1	1-C	0	2
1	2-C	0	1
1	8-B	0	1
1	10-B	0	1
1	11-C	0	1
1	17-C	0	1
1	20-B	0	1
All	All	0	9

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1-C	320	VAL	C-N	15.62	1.70	1.34
1	8-C	379	CYS	CB-SG	7.88	1.95	1.82
1	6-C	291	CYS	CB-SG	-7.63	1.69	1.82
1	19-C	291	CYS	CB-SG	-7.59	1.69	1.82
1	13-C	432	CYS	CB-SG	-7.09	1.70	1.82

The worst 5 of 2938 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	12-C	745	ASP	CB-CG-OD2	15.96	132.66	118.30
1	3-A	1034	LEU	CA-CB-CG	15.12	150.08	115.30
1	16-C	745	ASP	CB-CG-OD1	14.75	131.57	118.30
1	8-B	745	ASP	CB-CG-OD1	14.48	131.33	118.30
1	17-A	1034	LEU	CA-CB-CG	14.18	147.91	115.30

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-B	338	PHE	Sidechain
1	1-C	590	CYS	Peptide
1	1-C	592	PHE	Peptide
1	2-C	595	VAL	Peptide
1	8-B	87	ASN	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-A	8454	0	8245	121	0
1	1-B	8454	0	8246	111	0
1	1-C	8454	0	8248	120	0
1	2-A	8454	0	8246	100	0
1	2-B	8454	0	8246	114	0
1	2-C	8454	0	8248	109	0
1	3-A	8494	0	8289	110	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	3-B	8494	0	8289	98	0
1	3-C	8494	0	8289	116	0
1	4-A	8494	0	8289	142	0
1	4-B	8494	0	8289	140	0
1	4-C	8494	0	8289	125	0
1	5-A	8494	0	8289	135	0
1	5-B	8494	0	8289	112	0
1	5-C	8494	0	8289	124	0
1	6-A	8494	0	8289	115	0
1	6-B	8494	0	8289	102	0
1	6-C	8494	0	8289	114	0
1	7-A	8494	0	8289	119	0
1	7-B	8494	0	8289	110	0
1	7-C	8494	0	8289	112	0
1	8-A	8494	0	8289	99	0
1	8-B	8494	0	8289	123	0
1	8-C	8494	0	8289	121	0
1	9-A	8454	0	8245	116	0
1	9-B	8454	0	8246	130	0
1	9-C	8454	0	8248	126	0
1	10-A	8494	0	8289	113	0
1	10-B	8494	0	8289	90	0
1	10-C	8494	0	8289	105	0
1	11-A	8454	0	8246	103	0
1	11-B	8454	0	8246	97	0
1	11-C	8454	0	8248	111	0
1	12-A	8494	0	8289	117	0
1	12-B	8494	0	8289	116	0
1	12-C	8494	0	8289	112	0
1	13-A	8494	0	8289	123	0
1	13-B	8494	0	8289	109	0
1	13-C	8494	0	8289	118	0
1	14-A	8494	0	8289	112	0
1	14-B	8494	0	8289	93	0
1	14-C	8494	0	8289	122	0
1	15-A	8494	0	8289	112	0
1	15-B	8494	0	8289	110	0
1	15-C	8494	0	8289	123	0
1	16-A	8494	0	8289	120	0
1	16-B	8494	0	8289	99	0
1	16-C	8494	0	8289	110	0
1	17-A	8494	0	8289	128	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	17-B	8494	0	8289	115	0
1	17-C	8494	0	8289	130	0
1	18-A	8494	0	8289	103	0
1	18-B	8494	0	8289	100	0
1	18-C	8494	0	8289	115	0
1	19-A	8494	0	8289	120	0
1	19-B	8494	0	8289	105	0
1	19-C	8494	0	8289	126	0
1	20-A	8494	0	8289	89	0
1	20-B	8494	0	8289	110	0
1	20-C	8494	0	8289	94	0
All	All	509160	0	496830	6304	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 6304 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:C:320:VAL:C	1:C:321:GLN:N	1.70	1.45
1:A:14:GLN:HE21	1:A:14:GLN:N	1.41	1.18
1:C:853:GLN:N	1:C:853:GLN:HE21	1.62	0.97
1:B:1051:SER:HG	1:B:1064:HIS:HD1	1.23	0.86
1:C:353:TRP:HE1	1:C:466:ARG:HB2	1.41	0.84

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	1024 (96%)	42 (4%)	1 (0%)	48 77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-B	1067/1230 (87%)	1020 (96%)	47 (4%)	0	100	100
1	1-C	1067/1230 (87%)	1011 (95%)	54 (5%)	2 (0%)	44	73
1	2-A	1067/1230 (87%)	1025 (96%)	41 (4%)	1 (0%)	48	77
1	2-B	1067/1230 (87%)	1019 (96%)	47 (4%)	1 (0%)	48	77
1	2-C	1067/1230 (87%)	1013 (95%)	53 (5%)	1 (0%)	48	77
1	3-A	1073/1230 (87%)	1038 (97%)	34 (3%)	1 (0%)	48	77
1	3-B	1073/1230 (87%)	1033 (96%)	39 (4%)	1 (0%)	48	77
1	3-C	1073/1230 (87%)	1035 (96%)	37 (3%)	1 (0%)	48	77
1	4-A	1073/1230 (87%)	1038 (97%)	34 (3%)	1 (0%)	48	77
1	4-B	1073/1230 (87%)	1037 (97%)	35 (3%)	1 (0%)	48	77
1	4-C	1073/1230 (87%)	1038 (97%)	34 (3%)	1 (0%)	48	77
1	5-A	1073/1230 (87%)	1038 (97%)	34 (3%)	1 (0%)	48	77
1	5-B	1073/1230 (87%)	1033 (96%)	39 (4%)	1 (0%)	48	77
1	5-C	1073/1230 (87%)	1036 (97%)	36 (3%)	1 (0%)	48	77
1	6-A	1073/1230 (87%)	1036 (97%)	36 (3%)	1 (0%)	48	77
1	6-B	1073/1230 (87%)	1035 (96%)	37 (3%)	1 (0%)	48	77
1	6-C	1073/1230 (87%)	1039 (97%)	33 (3%)	1 (0%)	48	77
1	7-A	1073/1230 (87%)	1037 (97%)	35 (3%)	1 (0%)	48	77
1	7-B	1073/1230 (87%)	1036 (97%)	36 (3%)	1 (0%)	48	77
1	7-C	1073/1230 (87%)	1034 (96%)	38 (4%)	1 (0%)	48	77
1	8-A	1073/1230 (87%)	1037 (97%)	35 (3%)	1 (0%)	48	77
1	8-B	1073/1230 (87%)	1035 (96%)	37 (3%)	1 (0%)	48	77
1	8-C	1073/1230 (87%)	1037 (97%)	35 (3%)	1 (0%)	48	77
1	9-A	1067/1230 (87%)	1023 (96%)	43 (4%)	1 (0%)	48	77
1	9-B	1067/1230 (87%)	1022 (96%)	45 (4%)	0	100	100
1	9-C	1067/1230 (87%)	1016 (95%)	49 (5%)	2 (0%)	44	73
1	10-A	1073/1230 (87%)	1037 (97%)	35 (3%)	1 (0%)	48	77
1	10-B	1073/1230 (87%)	1037 (97%)	35 (3%)	1 (0%)	48	77
1	10-C	1073/1230 (87%)	1038 (97%)	34 (3%)	1 (0%)	48	77
1	11-A	1067/1230 (87%)	1026 (96%)	40 (4%)	1 (0%)	48	77
1	11-B	1067/1230 (87%)	1019 (96%)	48 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	11-C	1067/1230 (87%)	1013 (95%)	51 (5%)	3 (0%)	37	67
1	12-A	1073/1230 (87%)	1039 (97%)	33 (3%)	1 (0%)	48	77
1	12-B	1073/1230 (87%)	1037 (97%)	35 (3%)	1 (0%)	48	77
1	12-C	1073/1230 (87%)	1037 (97%)	35 (3%)	1 (0%)	48	77
1	13-A	1073/1230 (87%)	1040 (97%)	32 (3%)	1 (0%)	48	77
1	13-B	1073/1230 (87%)	1036 (97%)	36 (3%)	1 (0%)	48	77
1	13-C	1073/1230 (87%)	1036 (97%)	36 (3%)	1 (0%)	48	77
1	14-A	1073/1230 (87%)	1038 (97%)	34 (3%)	1 (0%)	48	77
1	14-B	1073/1230 (87%)	1036 (97%)	36 (3%)	1 (0%)	48	77
1	14-C	1073/1230 (87%)	1038 (97%)	34 (3%)	1 (0%)	48	77
1	15-A	1073/1230 (87%)	1037 (97%)	35 (3%)	1 (0%)	48	77
1	15-B	1073/1230 (87%)	1039 (97%)	33 (3%)	1 (0%)	48	77
1	15-C	1073/1230 (87%)	1036 (97%)	36 (3%)	1 (0%)	48	77
1	16-A	1073/1230 (87%)	1036 (97%)	36 (3%)	1 (0%)	48	77
1	16-B	1073/1230 (87%)	1037 (97%)	35 (3%)	1 (0%)	48	77
1	16-C	1073/1230 (87%)	1037 (97%)	35 (3%)	1 (0%)	48	77
1	17-A	1073/1230 (87%)	1038 (97%)	34 (3%)	1 (0%)	48	77
1	17-B	1073/1230 (87%)	1037 (97%)	35 (3%)	1 (0%)	48	77
1	17-C	1073/1230 (87%)	1032 (96%)	38 (4%)	3 (0%)	37	67
1	18-A	1073/1230 (87%)	1035 (96%)	37 (3%)	1 (0%)	48	77
1	18-B	1073/1230 (87%)	1037 (97%)	35 (3%)	1 (0%)	48	77
1	18-C	1073/1230 (87%)	1040 (97%)	32 (3%)	1 (0%)	48	77
1	19-A	1073/1230 (87%)	1040 (97%)	32 (3%)	1 (0%)	48	77
1	19-B	1073/1230 (87%)	1037 (97%)	35 (3%)	1 (0%)	48	77
1	19-C	1073/1230 (87%)	1038 (97%)	33 (3%)	2 (0%)	44	73
1	20-A	1073/1230 (87%)	1038 (97%)	34 (3%)	1 (0%)	48	77
1	20-B	1073/1230 (87%)	1035 (96%)	37 (3%)	1 (0%)	48	77
1	20-C	1073/1230 (87%)	1040 (97%)	32 (3%)	1 (0%)	48	77
All	All	64308/73800 (87%)	62001 (96%)	2243 (4%)	64 (0%)	50	77

5 of 64 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	11-C	319	ARG
1	1-C	590	CYS
1	17-C	445	VAL
1	19-C	385	THR
1	2-A	544	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1-A	944/1067 (88%)	907 (96%)	37 (4%)	27	61
1	1-B	944/1067 (88%)	907 (96%)	37 (4%)	27	61
1	1-C	944/1067 (88%)	917 (97%)	27 (3%)	37	71
1	2-A	944/1067 (88%)	916 (97%)	28 (3%)	36	70
1	2-B	944/1067 (88%)	910 (96%)	34 (4%)	30	64
1	2-C	944/1067 (88%)	911 (96%)	33 (4%)	31	65
1	3-A	949/1067 (89%)	910 (96%)	39 (4%)	26	59
1	3-B	949/1067 (89%)	910 (96%)	39 (4%)	26	59
1	3-C	949/1067 (89%)	917 (97%)	32 (3%)	32	66
1	4-A	949/1067 (89%)	914 (96%)	35 (4%)	29	63
1	4-B	949/1067 (89%)	904 (95%)	45 (5%)	22	54
1	4-C	949/1067 (89%)	913 (96%)	36 (4%)	28	62
1	5-A	949/1067 (89%)	915 (96%)	34 (4%)	30	64
1	5-B	949/1067 (89%)	912 (96%)	37 (4%)	27	61
1	5-C	949/1067 (89%)	916 (96%)	33 (4%)	31	65
1	6-A	949/1067 (89%)	912 (96%)	37 (4%)	27	61
1	6-B	949/1067 (89%)	913 (96%)	36 (4%)	28	62
1	6-C	949/1067 (89%)	915 (96%)	34 (4%)	30	64
1	7-A	949/1067 (89%)	919 (97%)	30 (3%)	34	68
1	7-B	949/1067 (89%)	911 (96%)	38 (4%)	27	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	7-C	949/1067 (89%)	918 (97%)	31 (3%)	33	67
1	8-A	949/1067 (89%)	915 (96%)	34 (4%)	30	64
1	8-B	949/1067 (89%)	917 (97%)	32 (3%)	32	66
1	8-C	949/1067 (89%)	915 (96%)	34 (4%)	30	64
1	9-A	944/1067 (88%)	924 (98%)	20 (2%)	48	80
1	9-B	944/1067 (88%)	908 (96%)	36 (4%)	28	62
1	9-C	944/1067 (88%)	916 (97%)	28 (3%)	36	70
1	10-A	949/1067 (89%)	912 (96%)	37 (4%)	27	61
1	10-B	949/1067 (89%)	922 (97%)	27 (3%)	38	72
1	10-C	949/1067 (89%)	906 (96%)	43 (4%)	23	55
1	11-A	944/1067 (88%)	909 (96%)	35 (4%)	29	63
1	11-B	944/1067 (88%)	914 (97%)	30 (3%)	34	68
1	11-C	944/1067 (88%)	921 (98%)	23 (2%)	44	77
1	12-A	949/1067 (89%)	916 (96%)	33 (4%)	31	65
1	12-B	949/1067 (89%)	909 (96%)	40 (4%)	25	58
1	12-C	949/1067 (89%)	910 (96%)	39 (4%)	26	59
1	13-A	949/1067 (89%)	914 (96%)	35 (4%)	29	63
1	13-B	949/1067 (89%)	907 (96%)	42 (4%)	24	56
1	13-C	949/1067 (89%)	918 (97%)	31 (3%)	33	67
1	14-A	949/1067 (89%)	918 (97%)	31 (3%)	33	67
1	14-B	949/1067 (89%)	914 (96%)	35 (4%)	29	63
1	14-C	949/1067 (89%)	912 (96%)	37 (4%)	27	61
1	15-A	949/1067 (89%)	911 (96%)	38 (4%)	27	60
1	15-B	949/1067 (89%)	905 (95%)	44 (5%)	23	55
1	15-C	949/1067 (89%)	916 (96%)	33 (4%)	31	65
1	16-A	949/1067 (89%)	911 (96%)	38 (4%)	27	60
1	16-B	949/1067 (89%)	903 (95%)	46 (5%)	21	53
1	16-C	949/1067 (89%)	910 (96%)	39 (4%)	26	59
1	17-A	949/1067 (89%)	916 (96%)	33 (4%)	31	65
1	17-B	949/1067 (89%)	917 (97%)	32 (3%)	32	66
1	17-C	949/1067 (89%)	906 (96%)	43 (4%)	23	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	18-A	949/1067 (89%)	919 (97%)	30 (3%)	34	68
1	18-B	949/1067 (89%)	904 (95%)	45 (5%)	22	54
1	18-C	949/1067 (89%)	909 (96%)	40 (4%)	25	58
1	19-A	949/1067 (89%)	916 (96%)	33 (4%)	31	65
1	19-B	949/1067 (89%)	914 (96%)	35 (4%)	29	63
1	19-C	949/1067 (89%)	915 (96%)	34 (4%)	30	64
1	20-A	949/1067 (89%)	911 (96%)	38 (4%)	27	60
1	20-B	949/1067 (89%)	913 (96%)	36 (4%)	28	62
1	20-C	949/1067 (89%)	910 (96%)	39 (4%)	26	59
All	All	56880/64020 (89%)	54770 (96%)	2110 (4%)	31	63

5 of 2110 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	18-B	1050	MET
1	19-A	517	LEU
1	18-B	1042	PHE
1	20-C	400	PHE
1	8-B	429	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 120 such sidechains are listed below:

Mol	Chain	Res	Type
1	9-C	969	ASN
1	19-A	115	GLN
1	12-A	957	GLN
1	18-C	762	GLN
1	20-C	777	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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
1	1-C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	320:VAL	C	321:GLN	N	1.70

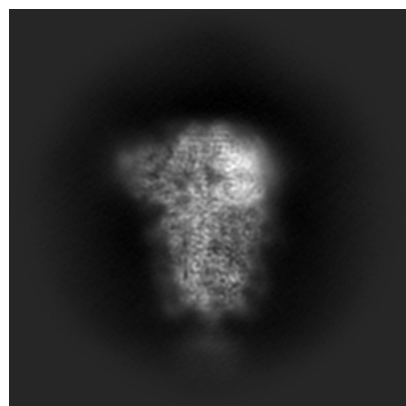
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51280. These allow visual inspection of the internal detail of the map and identification of artifacts.

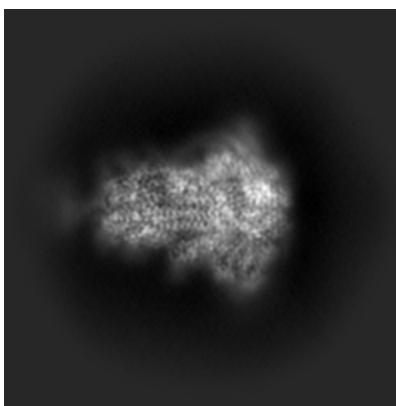
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

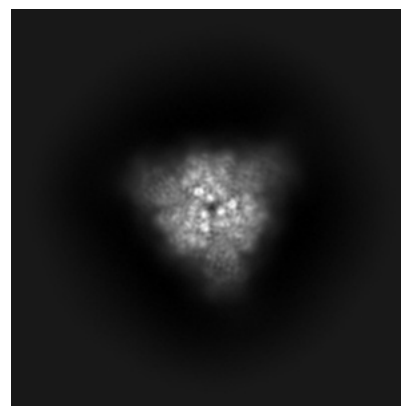
6.1.1 Primary map



X

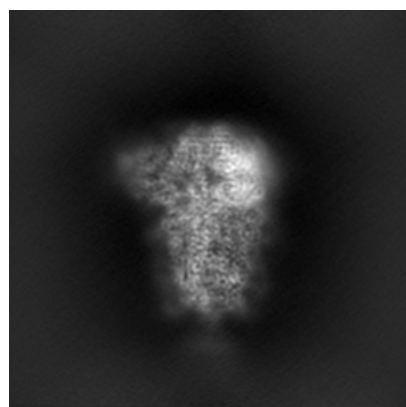


Y

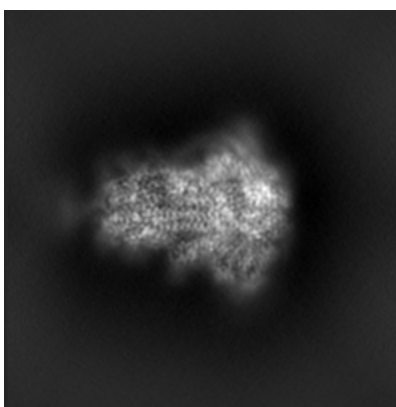


Z

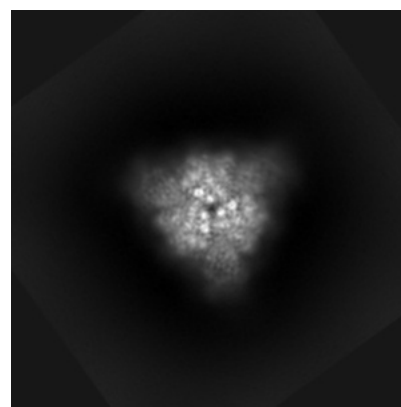
6.1.2 Raw map



X



Y

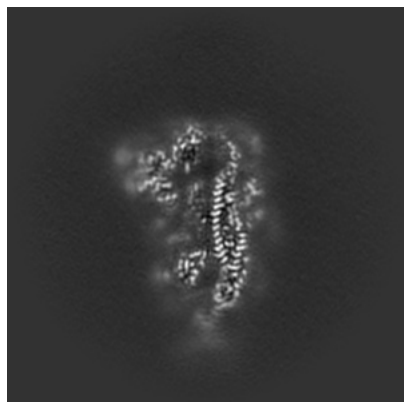


Z

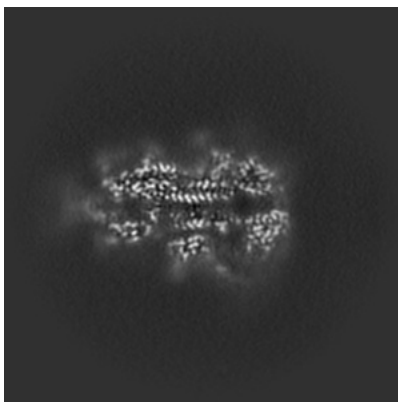
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

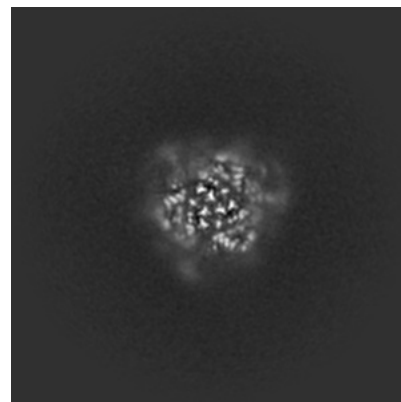
6.2.1 Primary map



X Index: 112

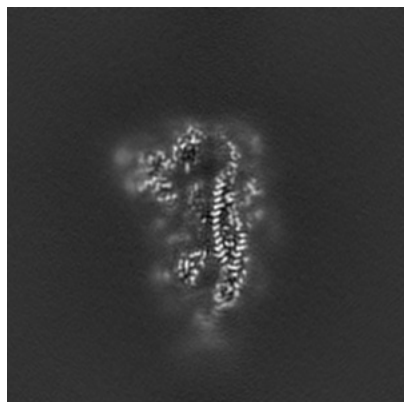


Y Index: 112

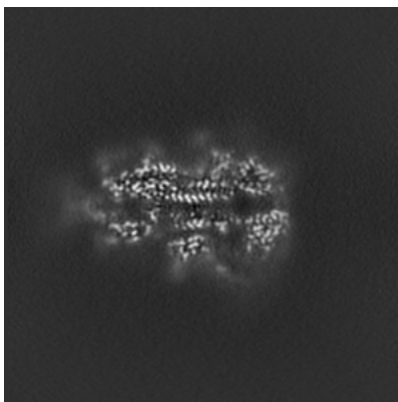


Z Index: 112

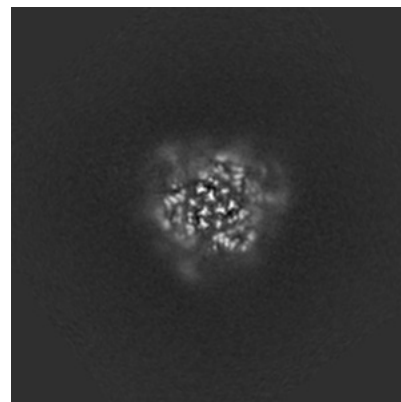
6.2.2 Raw map



X Index: 112



Y Index: 112

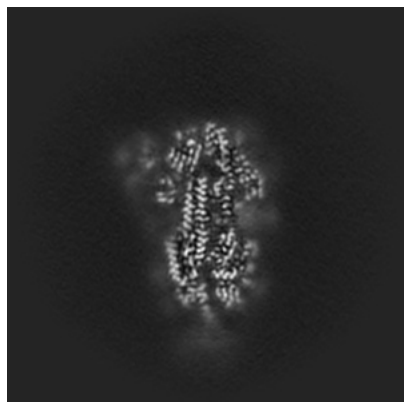


Z Index: 112

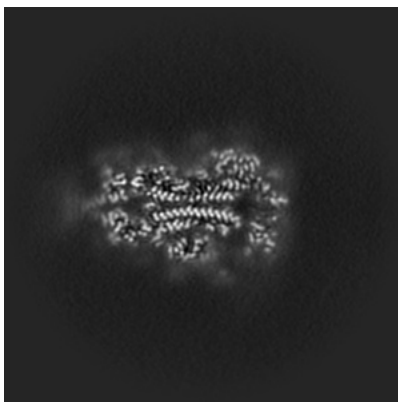
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

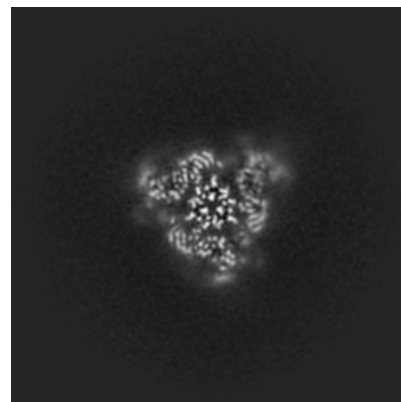
6.3.1 Primary map



X Index: 107

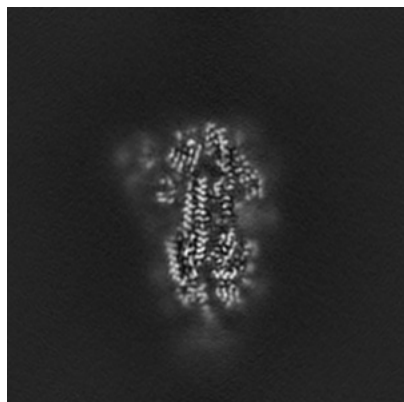


Y Index: 109

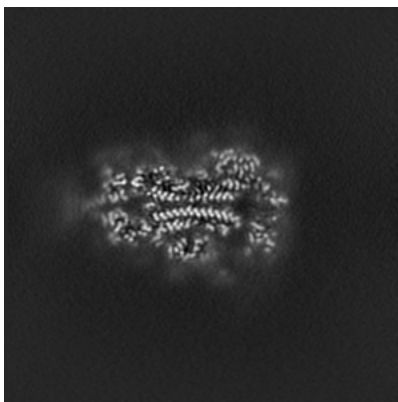


Z Index: 119

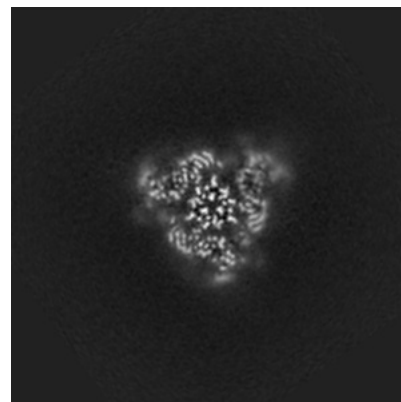
6.3.2 Raw map



X Index: 107



Y Index: 109

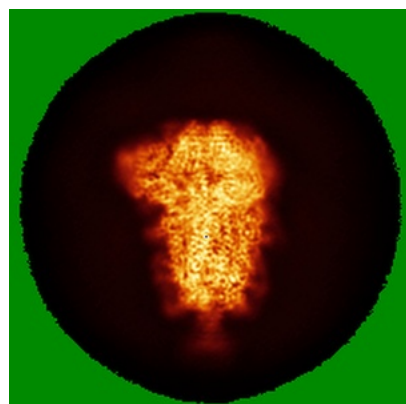


Z Index: 119

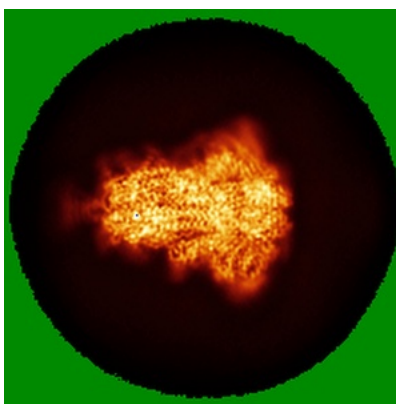
The images above show the largest variance slices of the map in three orthogonal directions.

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

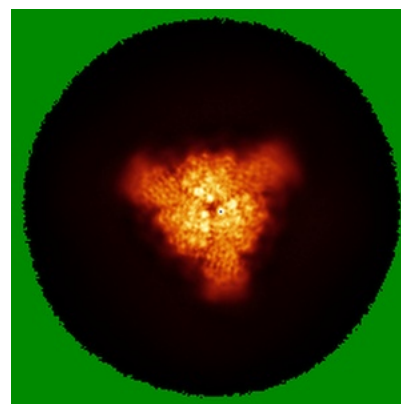
6.4.1 Primary map



X



Y

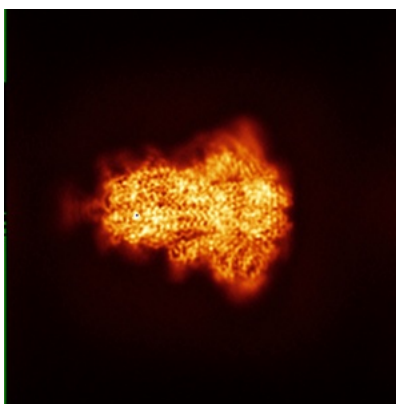


Z

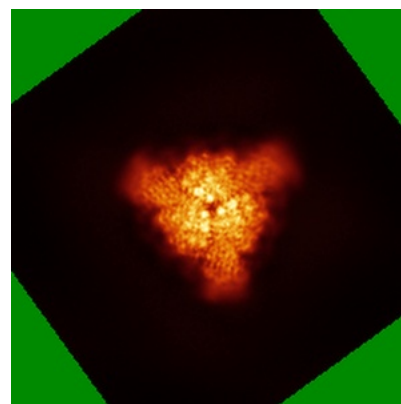
6.4.2 Raw map



X



Y

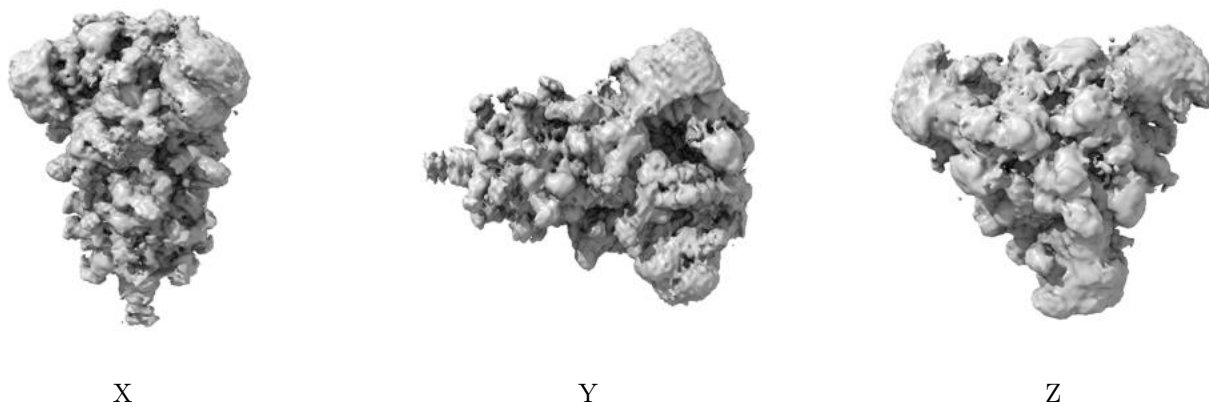


Z

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.

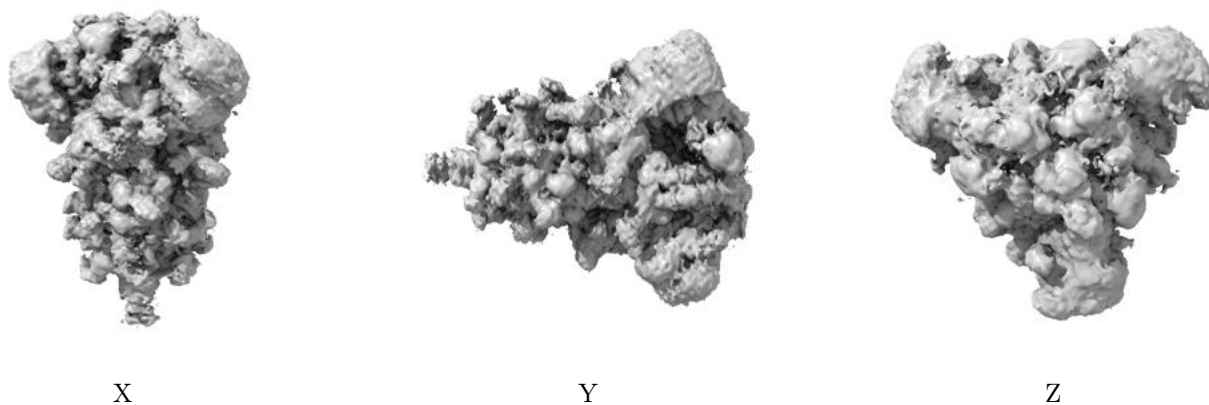
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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



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.

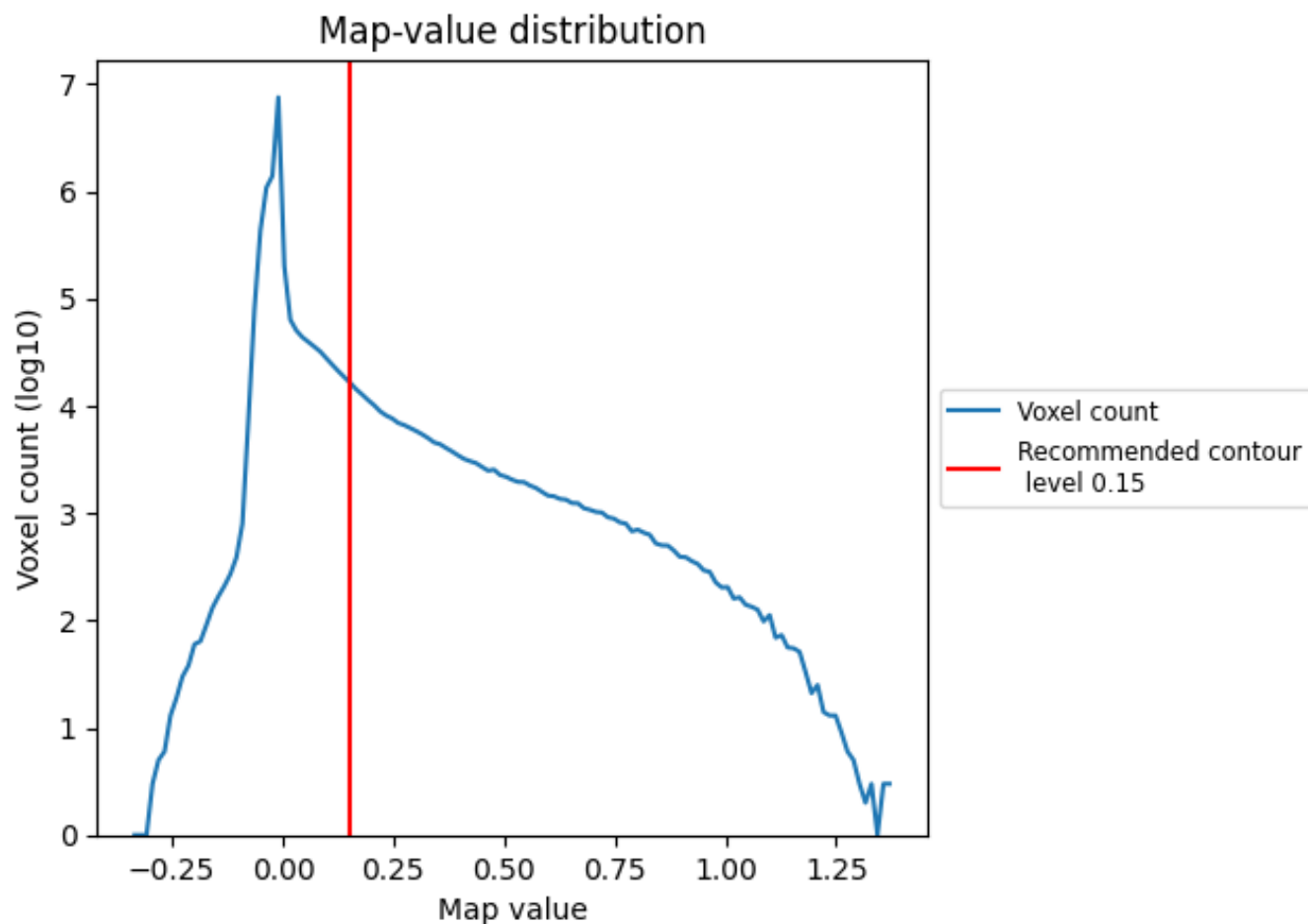
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

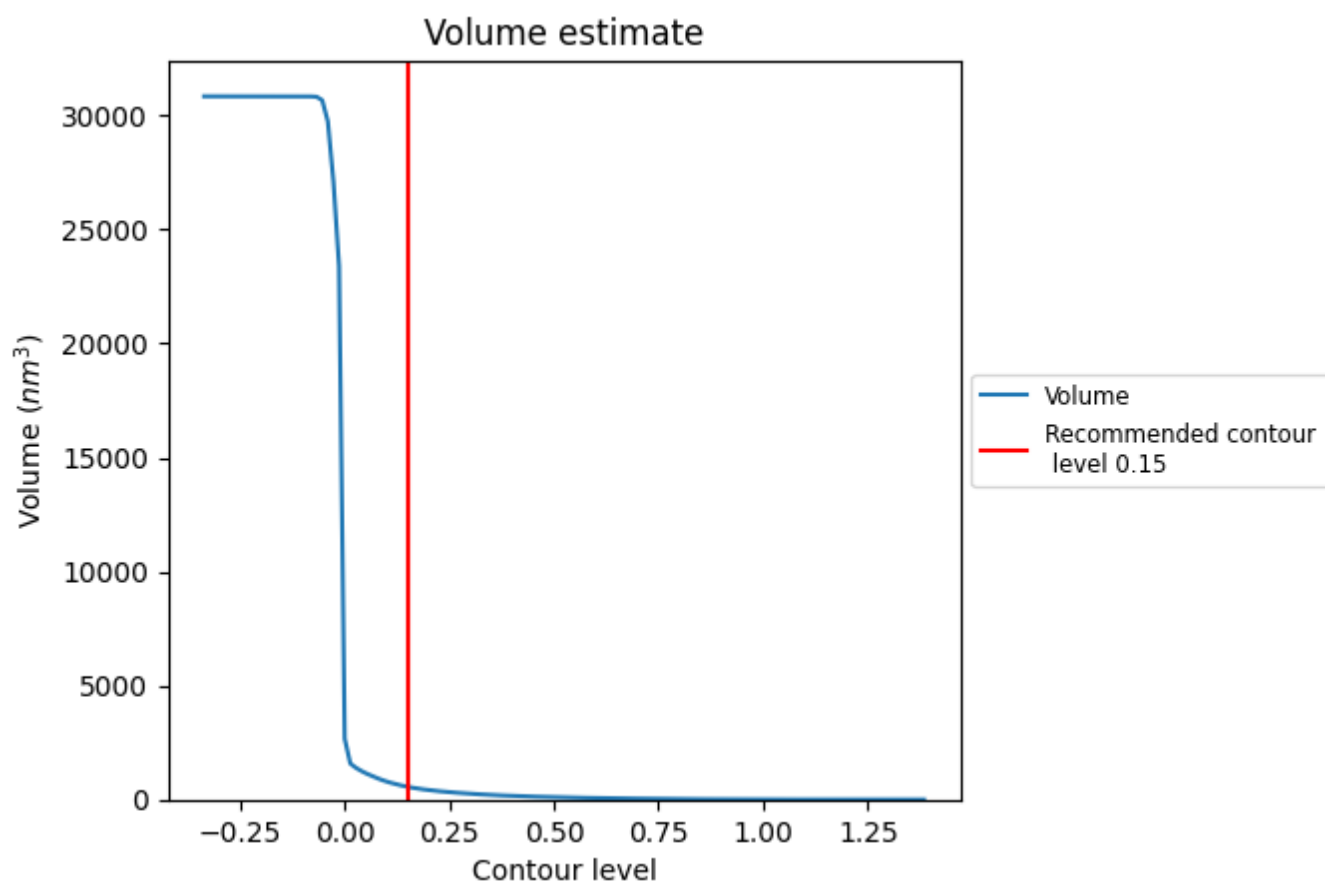
This section contains the results of statistical analysis of the map.

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.

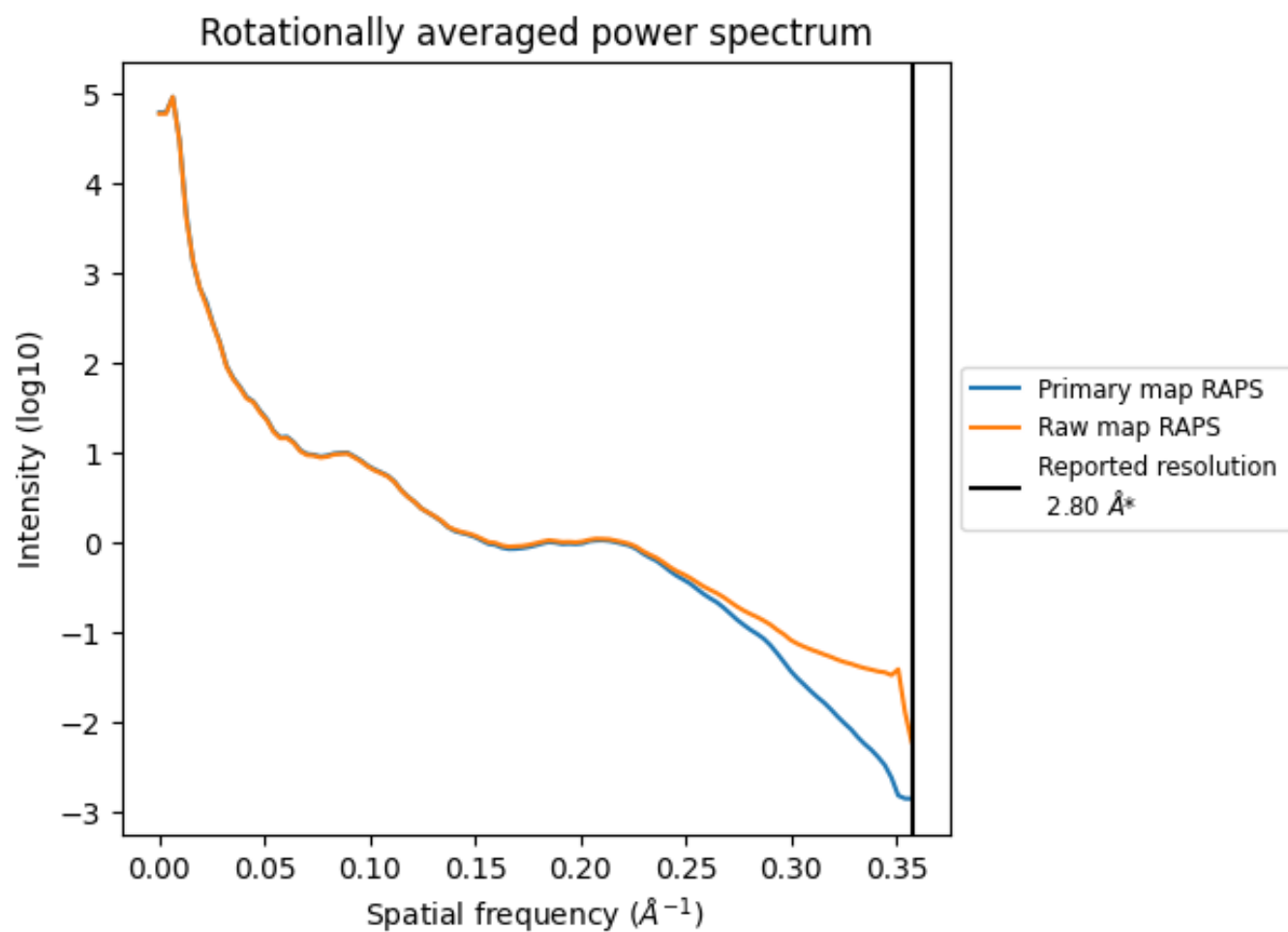
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 564 nm^3 ; this corresponds to an approximate mass of 510 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 ⓘ

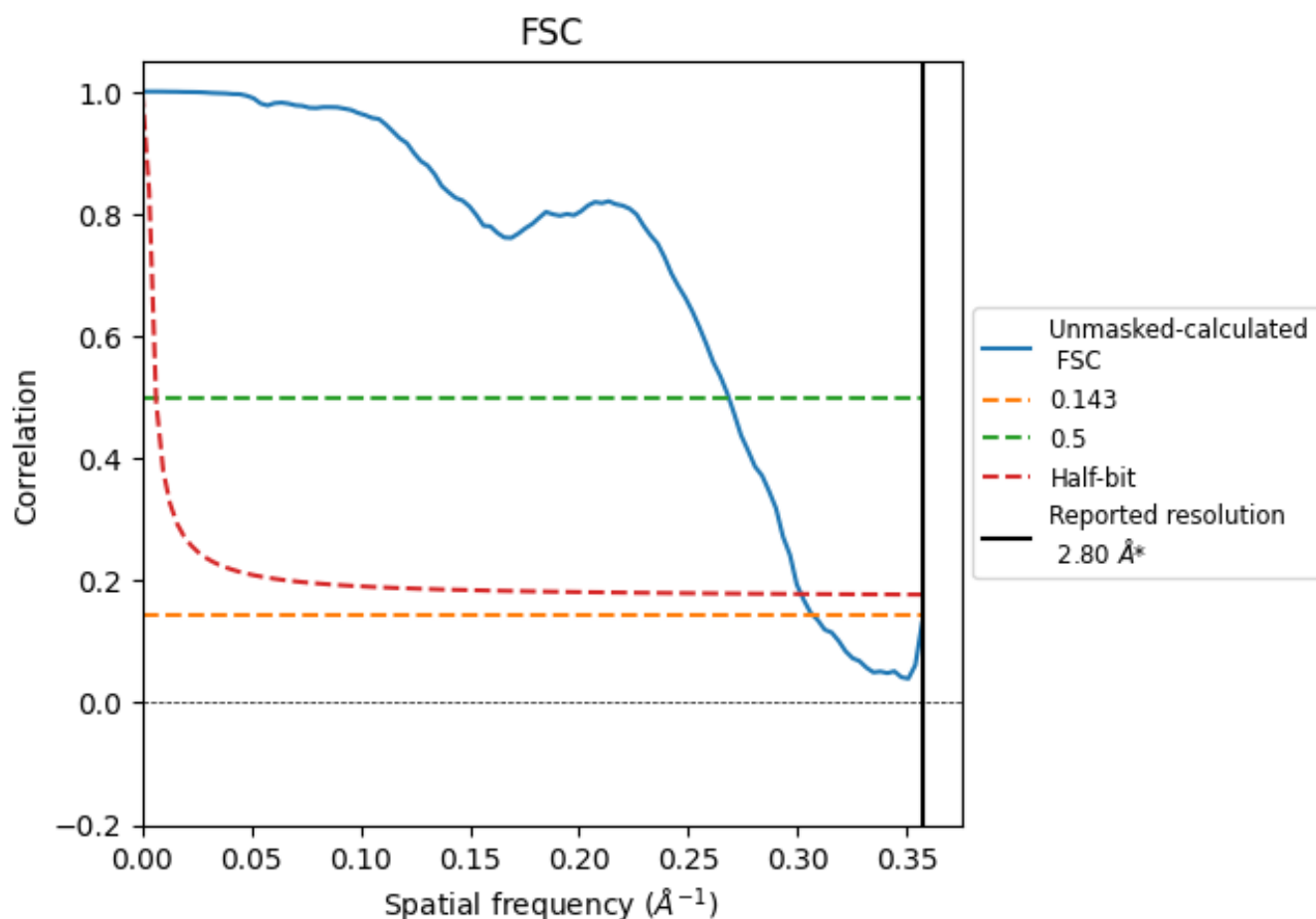


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

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 0.357 Å⁻¹

8.2 Resolution estimates [i](#)

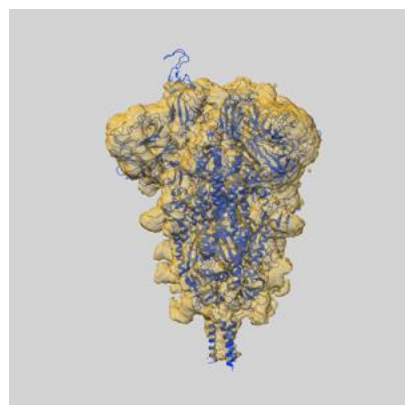
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.26	3.73	3.31

*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 3.26 differs from the reported value 2.8 by more than 10 %

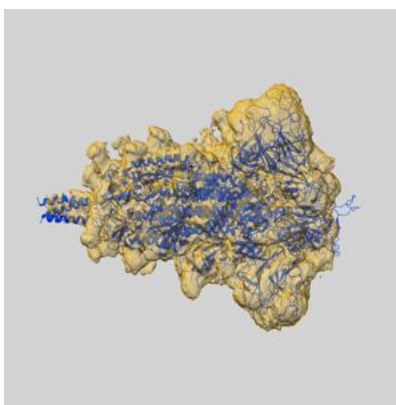
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51280 and PDB model 9GDY. Per-residue inclusion information can be found in section [3](#) on page [12](#).

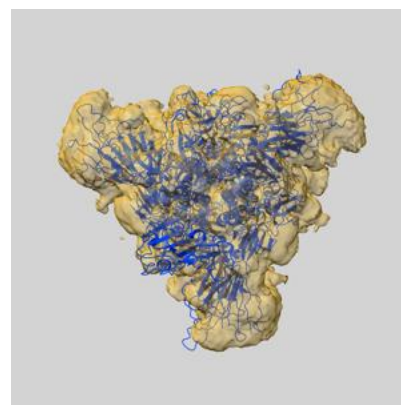
9.1 Map-model overlay [i](#)



X



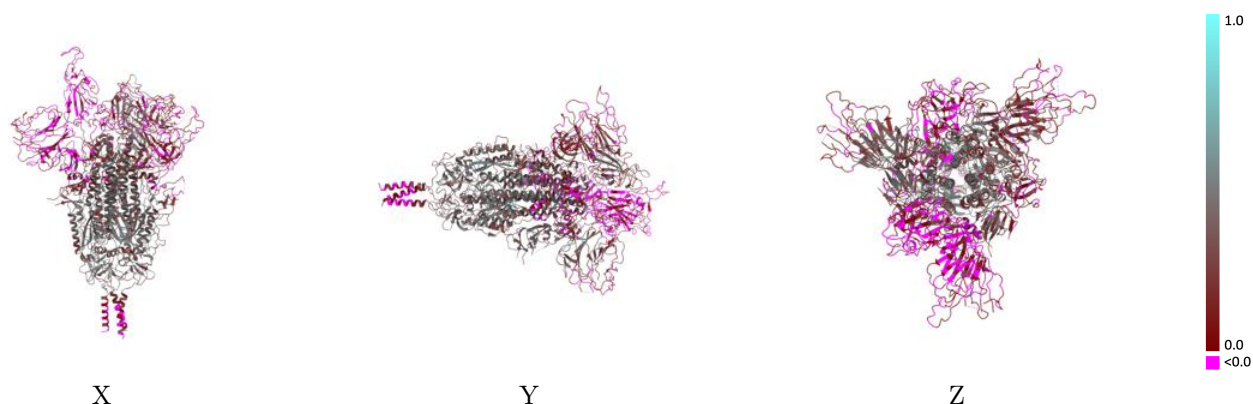
Y



Z

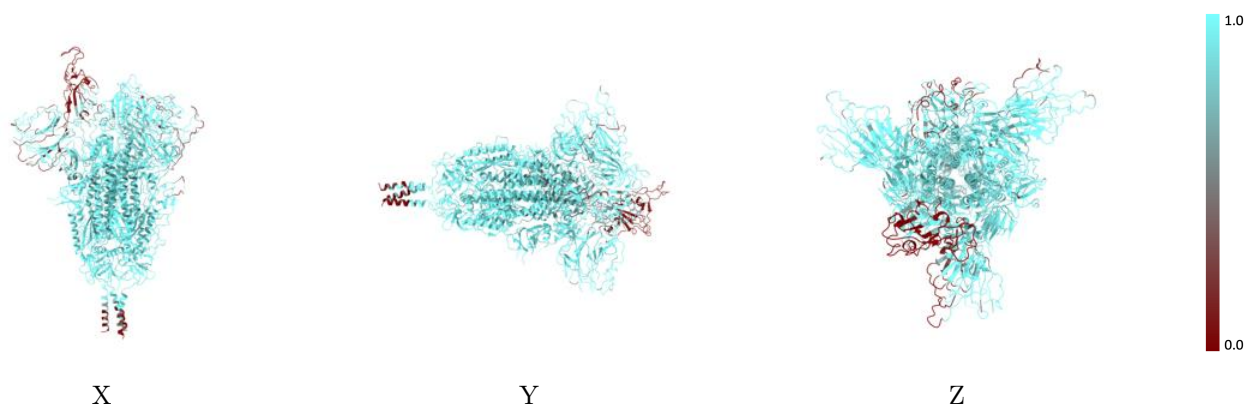
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



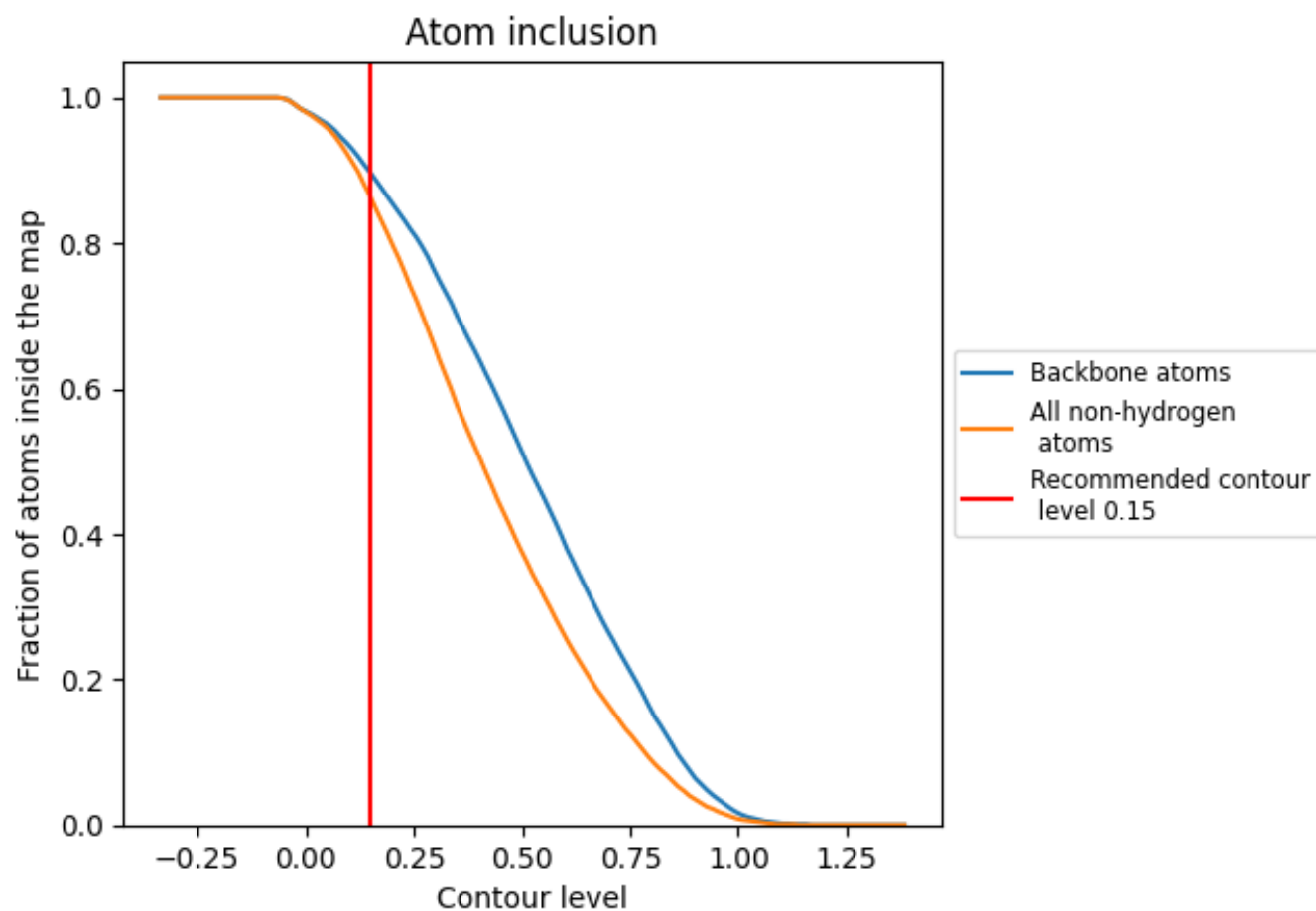
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion ⓘ



At the recommended contour level, 90% of all backbone atoms, 86% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8640	<div></div> 0.2390
A	<div></div> 0.8260	<div></div> 0.2590
B	<div></div> 0.8900	<div></div> 0.2410
C	<div></div> 0.8750	<div></div> 0.2170

