



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 ⓘ 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.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

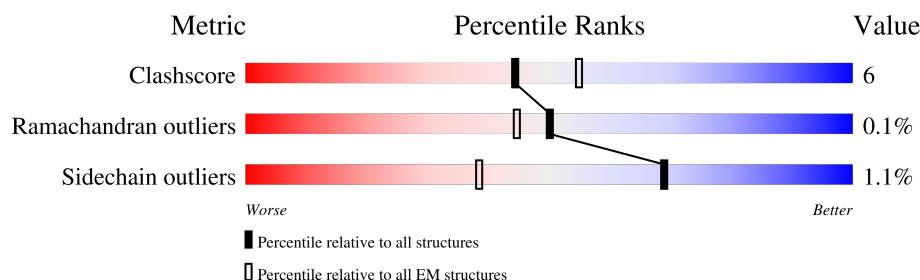
1 Overall quality at a glance

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.
















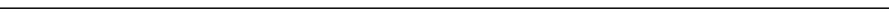











Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	
1	1-B	1230	
1	1-C	1230	
1	10-A	1230	
1	10-B	1230	
1	10-C	1230	
1	11-A	1230	
1	11-B	1230	














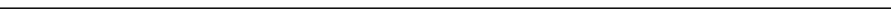











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Mol	Chain	Length	Quality of chain
1	11-C	1230	
1	12-A	1230	
1	12-B	1230	
1	12-C	1230	
1	13-A	1230	
1	13-B	1230	
1	13-C	1230	
1	14-A	1230	
1	14-B	1230	
1	14-C	1230	
1	15-A	1230	
1	15-B	1230	
1	15-C	1230	
1	16-A	1230	
1	16-B	1230	
1	16-C	1230	
1	17-A	1230	
1	17-B	1230	
1	17-C	1230	
1	18-A	1230	
1	18-B	1230	
1	18-C	1230	
1	19-A	1230	
1	19-B	1230	
1	19-C	1230	



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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	 70% 17% 12%
1	9-C	1230	 69% 18% 12%

2 Entry composition

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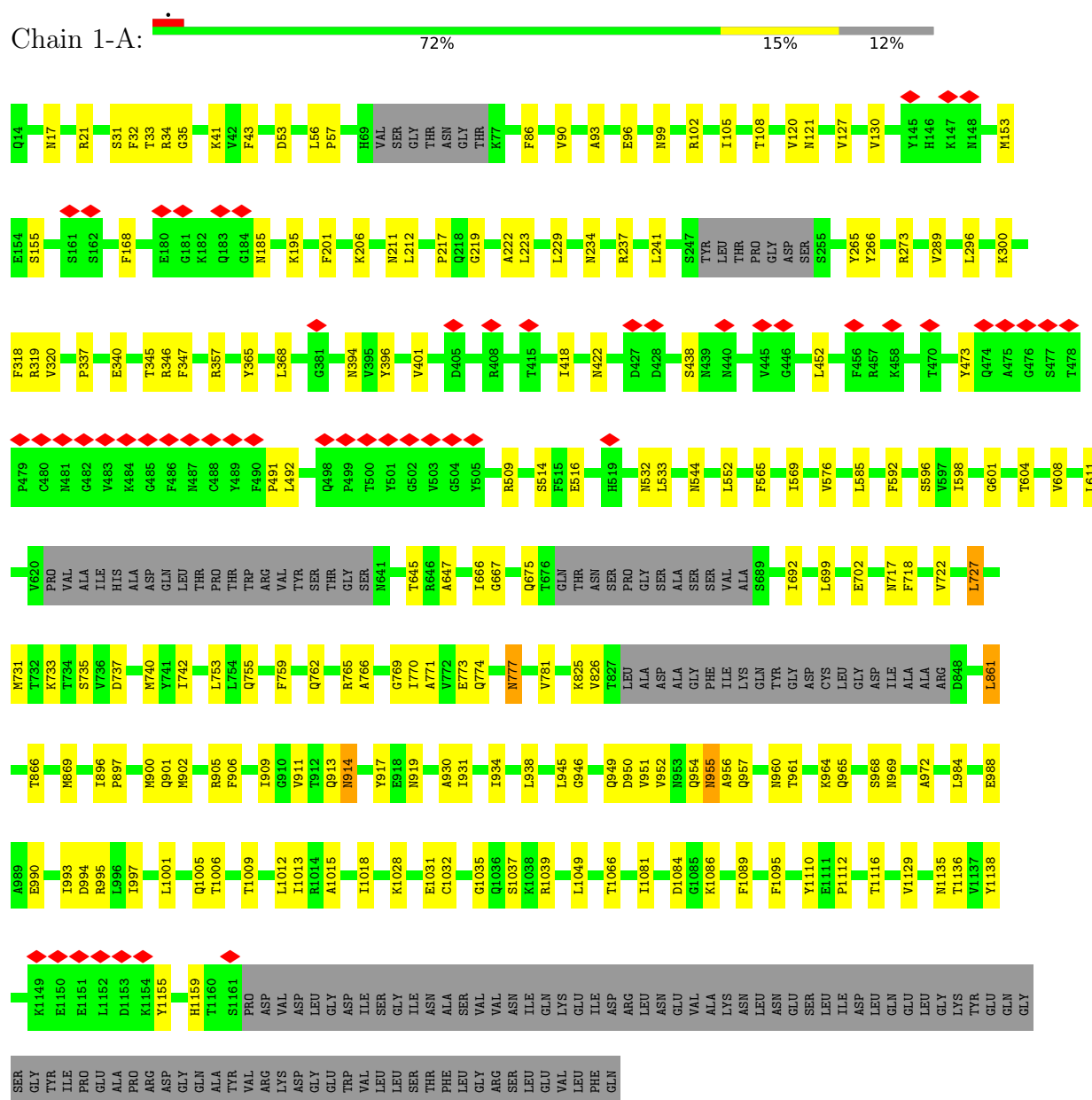
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1238	GLY	-	expression tag	UNP P10104
C	1239	ARG	-	expression tag	UNP P10104
C	1240	SER	-	expression tag	UNP P10104
C	1241	LEU	-	expression tag	UNP P10104
C	1242	GLU	-	expression tag	UNP P10104
C	1243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

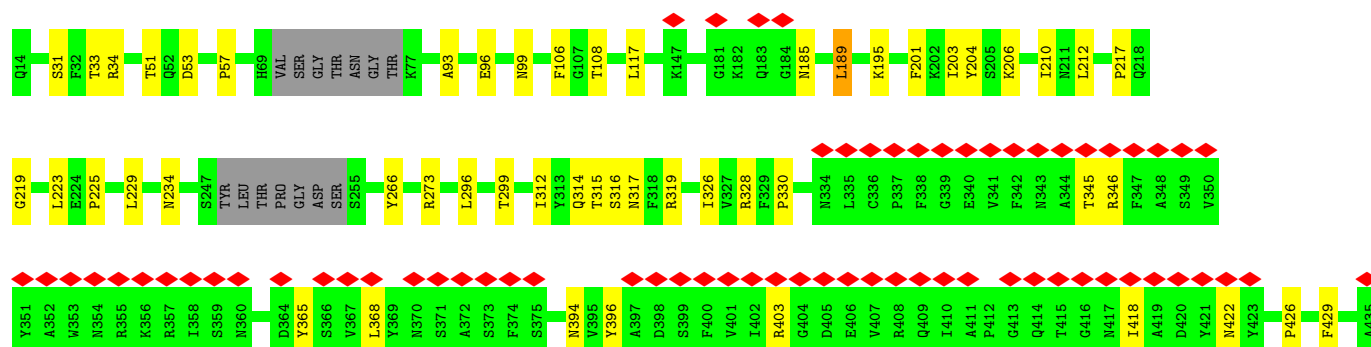
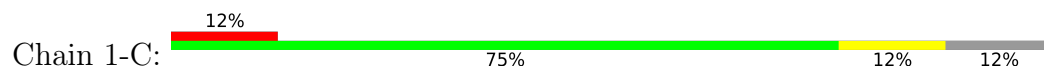
3 Residue-property plots

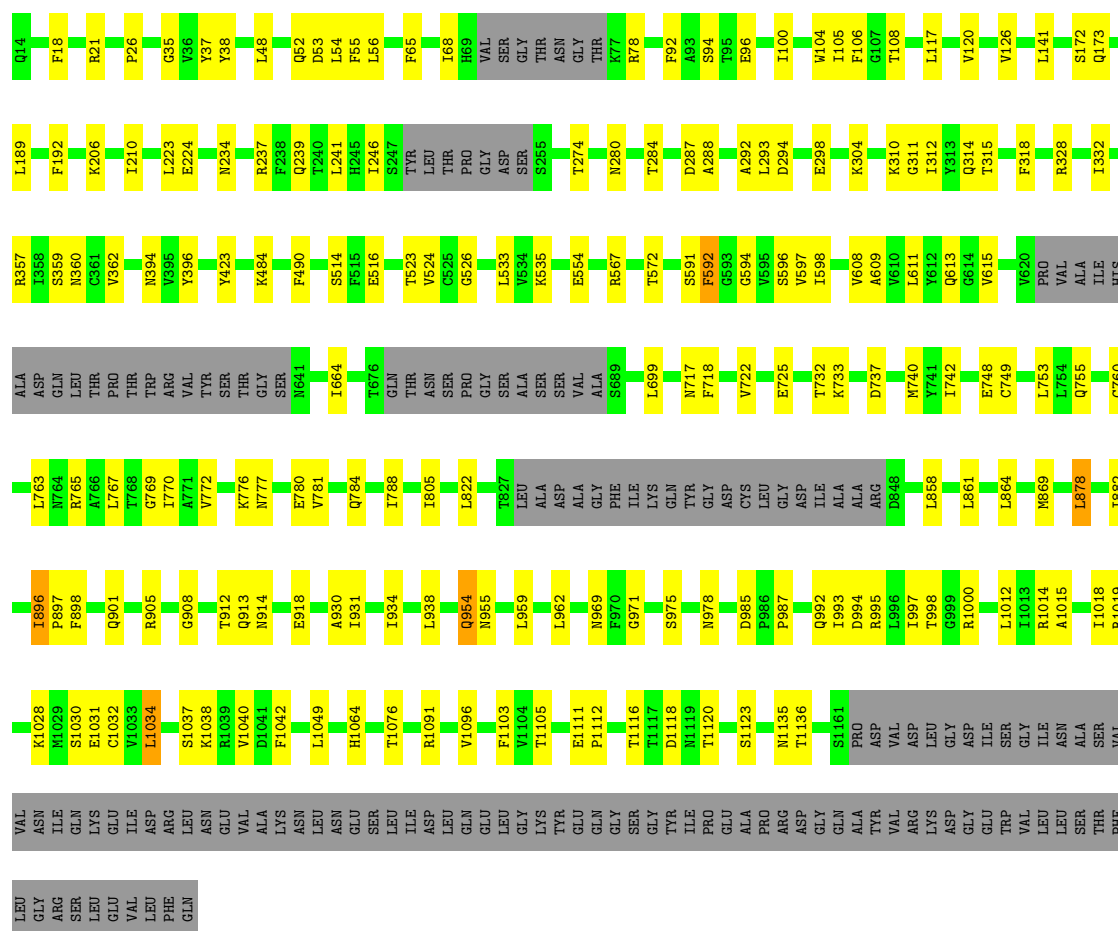
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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



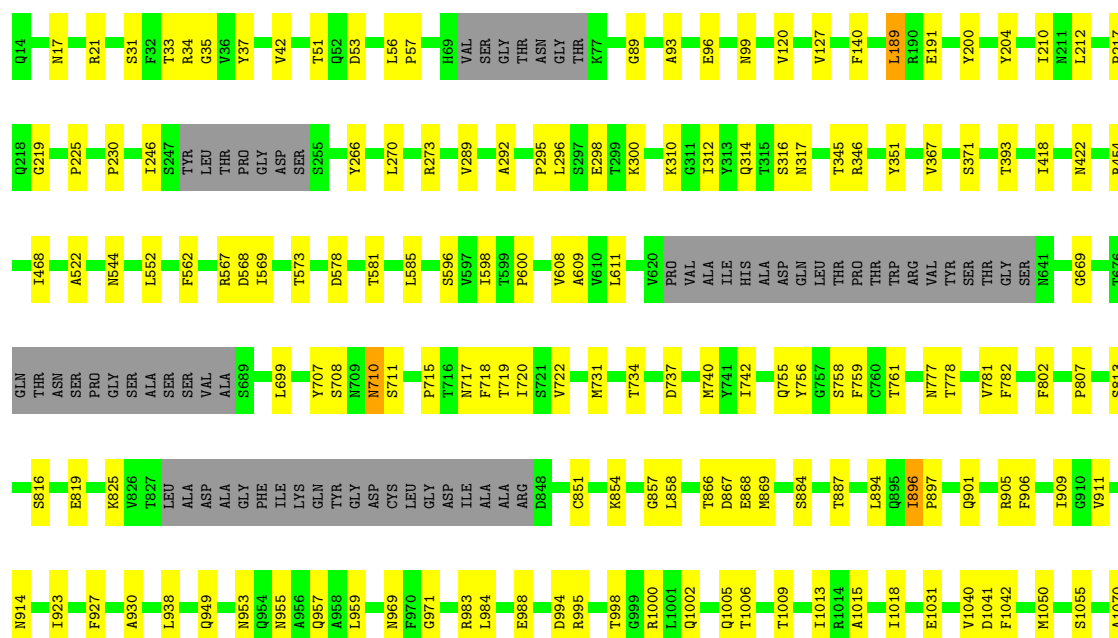
Chain 1-B: 74% 13% 12%



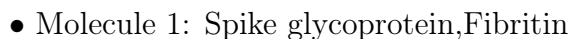


● Molecule 1: Spike glycoprotein, Fibrin

Chain 3-C: 74% 13% 12%



Response	Percentage
Used	75%
Not used	13%
Don't know	12%



Device Type	Percentage
Smartphone	76%
Tablet	12%
Feature Phone	12%

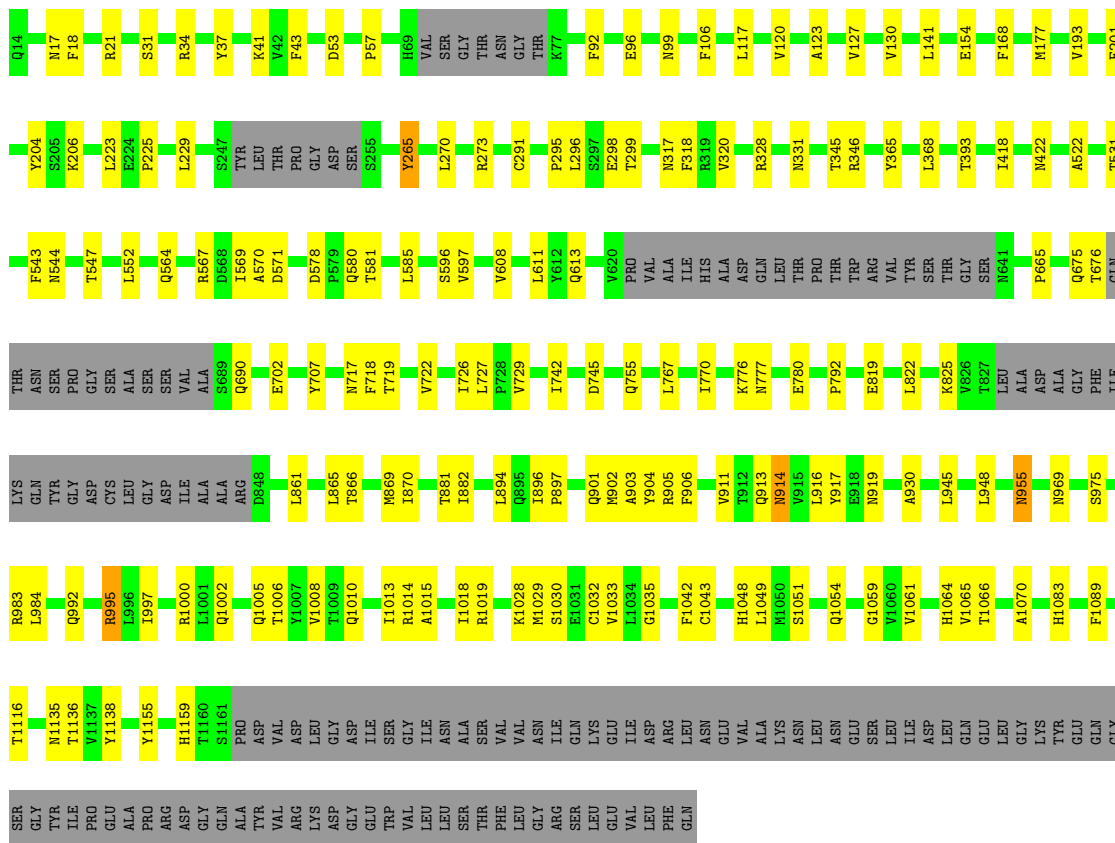
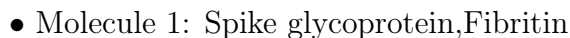


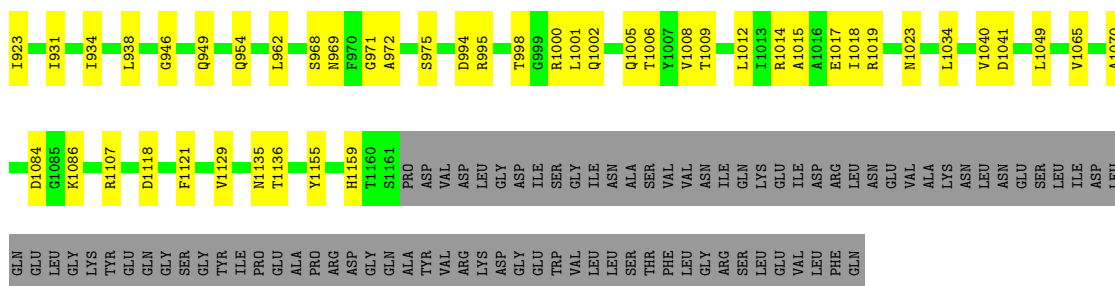
- Molecule 1: Spike glycoprotein, Fibrin

ARG	ASP	L981	ASP	ASP	SER	D578	L229	Q14
LYS	LEU	S982	CYS	VAL	VAL	D578	L229	Q14
ASP	GLY	R983	LEU	ALA	ALA	T581	P230	N17
GLY	ASP		GLY	S689	S689			
TRP	ILE	R1000	ASP	ILE	L699	L585	S247	R21
VAL	GLY	L1001	ILE				TYR	
LEU	GLY	Q1002	ALA				LEU	S31
LEU	ILE	S1003	ALA		Y707	S591	THR	F32
LEU	ASN	L1004	ARG	S708	S708	F592	PRO	T33
SER	ALA	Q1005	ARG	D848	N709		GLY	R34
THR	SER	T1006			N710	S596	ASP	
PHE	VAL	Y1007		L865	S711	V697	SER	Y37
LEU	VAL	V1008		T866		I598	S255	
GLY	ASN	T1009		D867	P715	P600		T51
ARG	ILE	Q1010		E868	P715	P600	Y266	D53
SER	GLN			M869	N717			
LEU	LYS	I1013		I870	F718	V608	P295	F65
GLY	GLY	R1014			T719	A609	L296	H66
VAL	ILE	A1015		T874	I720			
LEU	ASP				S721	V615	T299	
LEU	ARG	I1018		L878	V722			H69
PHE	LEU			A879		V620	K310	VAL
GLN	ASN	K1028			K733		G311	SER
	GLY			1882		VAL	I312	GLY
	VAL	E1031		T883	D737	ALA	T313	THR
ALA	ALA					ILE	Q314	ASN
LYS	LYS	V1040		W886	M740	HIS	T315	GLY
ASN	ASN				Y741	ALA	S316	THR
LEU	LEU	M1050		1896	I742	ASP	N317	K77
ASN	ASN			P897		GLN		
GLY	GLY	F1062		M902	S758	LEU	T345	F92
SER	SER	A1070			F759	THR	R346	A93
LEU	LEU					PRO	S94	
ILE	ILE			F906	Q762	THR	Y365	T95
ASP	ASP	A1080			L763	TRP		E96
LEU	LEU	I1081		V911		ARG	L368	
GLN	GLN	K1086			L767	VAL		N99
GLY	GLY			F927		TYR	N394	
LEU	LEU			A930	I770	SER	I418	F106
GLY	GLY	F1095		I931	A771	THR		
LYS	LYS				N777	GLY	M422	L117
TYR	TYR	I1115				SER		
GLY	GLY			I934		R641		V130
GLN	GLN	D1118			V781		P426	F168
GLY	GLY			G946		L650		
SER	SER	V1122			Q784		F429	
GLY	GLY			Q949	V785	A653		L189
TYR	TYR	V1129					L452	R190
ILE	ILE			N955	T827	I664		E191
PRO	PRO	N1135		A956	LEU		L492	
GLY	GLY	T1136		Q957	ALA	T676		Y200
ALA	ALA				ASP		E516	F201
PRO	PRO	Y1155			ALA	THR		
ARG	ARG			L962	GLY	ASN	N644	Y204
ASP	ASP	H1159		L966	PHE	SER		
GLY	GLY	T1160			ILE	PRO	L552	L216
GLN	GLN	S1161		S975	LYS	GLY	T553	
ALA	ALA			Y976	GLN	SER	E554	G219
ASP	ASP	PRO		L977	TYR	ALA		
VAL	VAL					SER	F552	F202

- Molecule 1: Spike glycoprotein, Fibrin

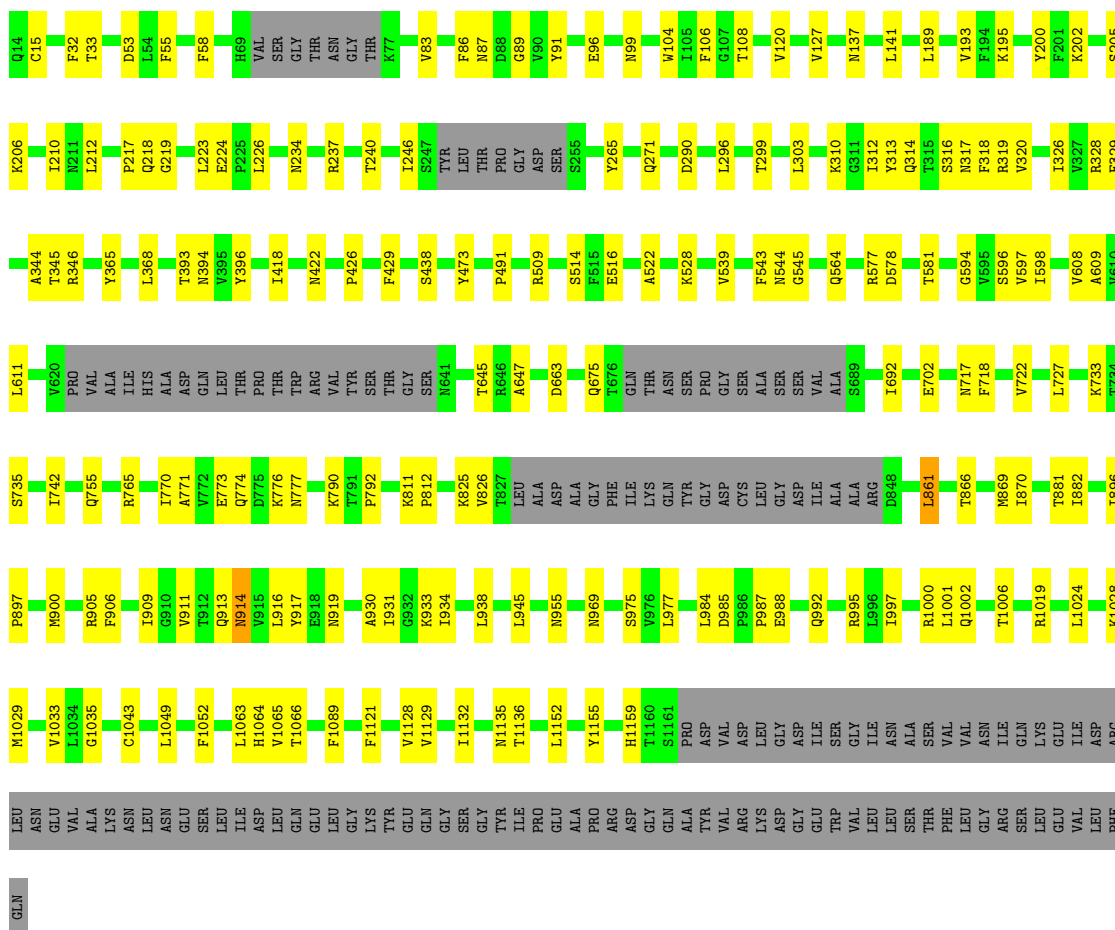
IIE	Q690	G566	I235	Q14
LYS	S691	G566	S247	N17
TYR	I692	D571	TYR	R21
GLY	L699	GLY	LEU	S31
ASP	E702	D578	THR	R34
CYS	E702	D578	PRO	L48
LEU	E702	T581	GLY	D53
GLY	N717	ASP	ASP	L54
GLY	F718	ASP	SER	P57
IIE	V722	F592	S255	
ALA	V722	F592		
ARG	I726	V608	T259	
D848	L727	A609	Y265	
	M731	V620	Y266	
L861	T732	PRO	R273	H99
T866	K733	VAL		VAL
D867		ALA	L276	SER
E668	Q755	IIE	GLY	THR
	F759	HIS	C291	ASN
L894	F759	ALA	A292	GLY
Q895	Q762	ASP	L296	THR
I896		GLN	S297	K77
P897	R765	LEU	E298	
	I770	THR		A93
R905	A771	PRO	F318	N99
F906		THR	P319	
I909	Q774	ARG	V320	R102
Q913	K776	VAL	I326	F106
N914	N777	SER	A344	V120
Y917	T778	THR	T345	V127
E918		GLY	R346	
N919	V781	SEA	F347	
A930	Q784	N641		M153
S939	P807	T645	Y365	N185
G946	S813	A647	L368	R190
K947	S816	G667	N394	I197
Q949	E819	Q675	I418	F201
D950	L822	T676	N422	K202
V951	K825	GLN	L452	I203
V952	N953	ASN	L492	Y204
Q954	N955	PRO	L492	H207
N955	T827	GLY	E516	L212
A956	LEU	ALA	V534	P225
Q957	ALA	SER	V539	L229
F960	ASP	SER	VAL	
T961	ALA	SER		
	GLY	ALA		
D969	D969	S690	N541	





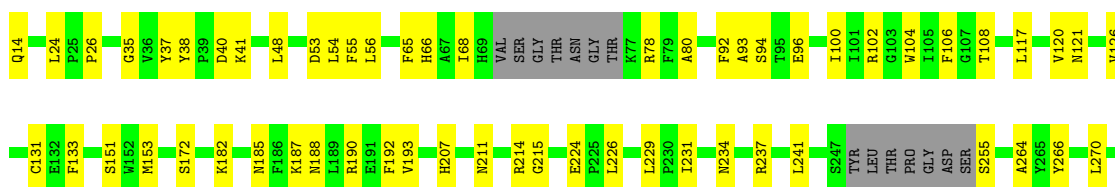
• Molecule 1: Spike glycoprotein,Fibritin

Chain 8-A: 73% 15% 12%



• Molecule 1: Spike glycoprotein,Fibritin

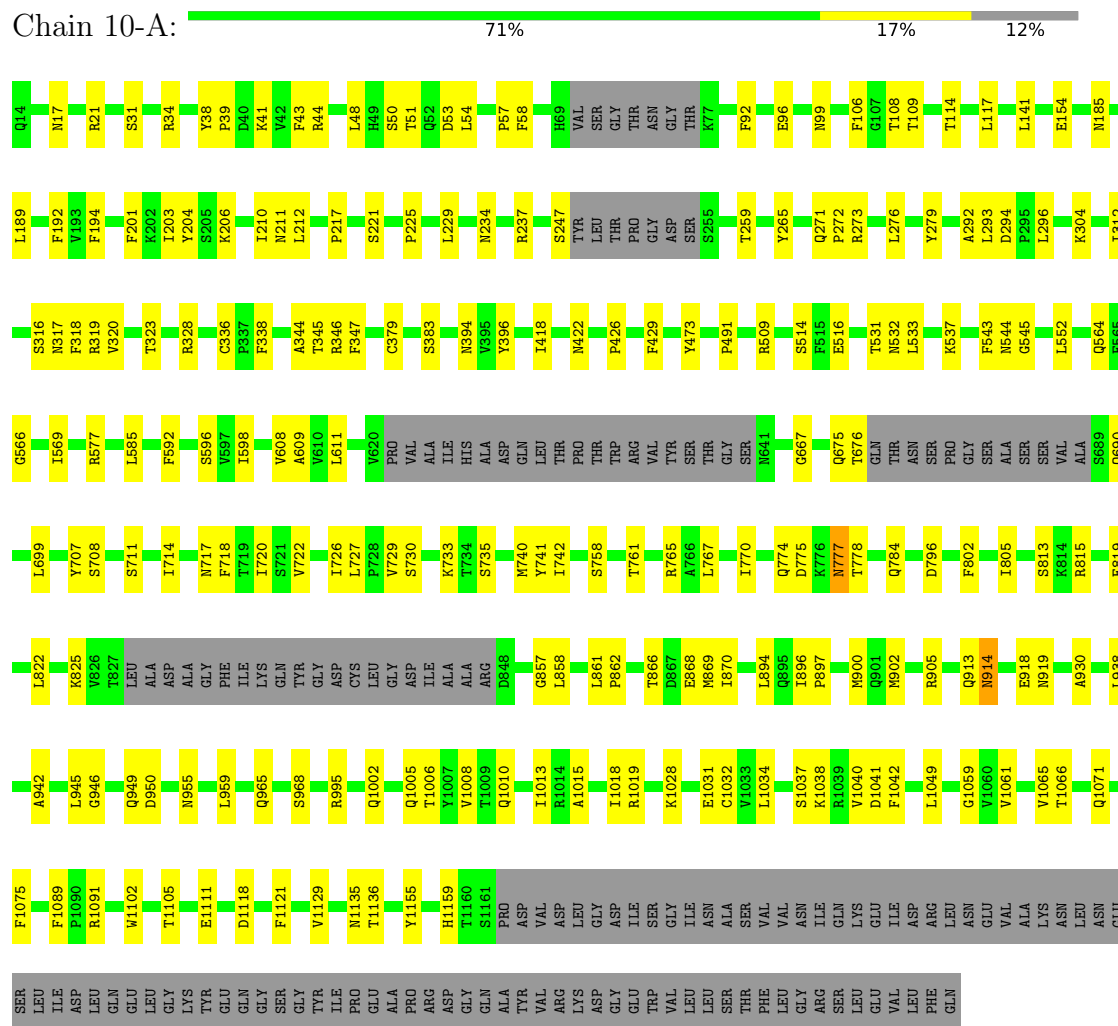
Chain 8-B: 69% 18% 12%



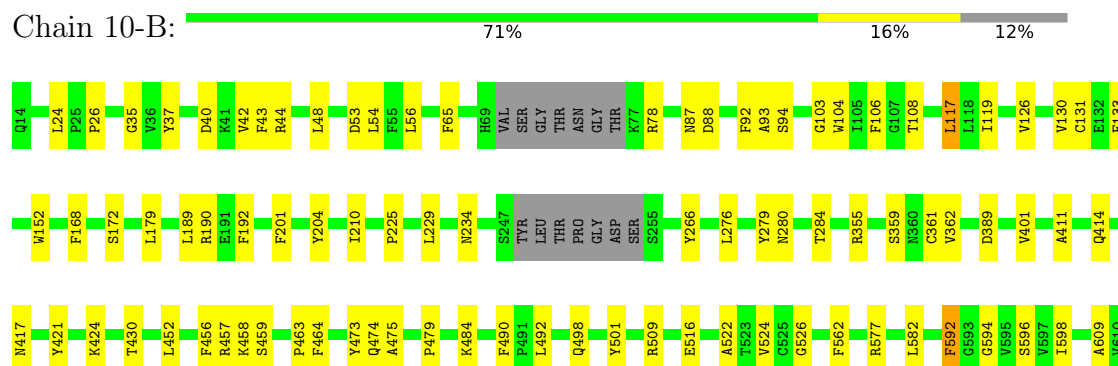


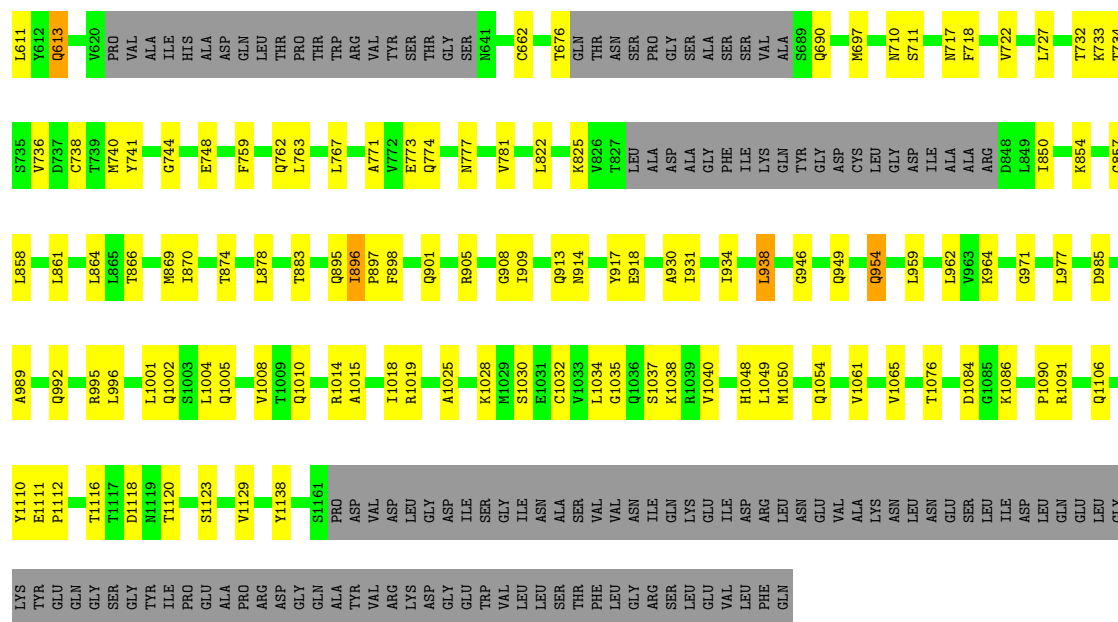
ALPHA	I993	ALA	7728	ILE	I326	M153	Q14
	I994	ALA	7729	HIS	I327	M154	Q15
	D994	ARG	7730	ALA	A344	D178	N17
	T998	D848	7731	ASN	T345	M185	F18
		T998	GLN	7732	GLN	R346	T19
		T998	LEU	7733	LEU	Y365	T20
	R1000	L858	7734	THR	Y366	L189	R21
	Q1002	L861	7742	PRO	THR	Y367	S31
	Q1005	T866	7746	THR	L368	F192	S31
	T1006	D867	7747	TRP	TRP	V193	S31
BETA	Q1005	T866	7750	ARG	T393	F201	R34
	R1014	E868	7756	VAL	N394	F201	Y37
	A1015	R869	7757	TYR	Y395	F202	Y38
	A1015	L870	7758	SER	Y396	I203	Y38
	I1018	T874	7759	THR	I418	Y204	F43
		T874	S758	GLY	I418	Y204	F43
		T874	F759	SER	I418	Y204	F43
	K1028	L878	7760	SER	N422	H207	L48
	M1029	L882	7761	ILE	N422	H207	L48
	V1040	I886	7765	ILE	N422	H207	L48
GAMMA	L1049	I886	7774	ILE	N422	H207	L48
	P1053	L894	7777	ILE	N422	H207	L48
	P1053	I896	7781	GLN	Y473	L229	VAL
	V1060	P897	7782	THR	Y473	L229	VAL
	V1065	A783	7783	ASN	P491	N234	GLY
	V1065	H902	7784	ASN	P491	I235	THR
	A1070	R905	7788	PRO	R509	T236	ASN
	F1089	F906	7789	GLY	R509	T236	ASN
	V1104	V911	7790	GLY	R509	T236	ASN
	I1115	L916	7791	SER	R509	T236	ASN
DELTA	S1123	I931	7792	ALA	V539	ASP	A93
	V1129	I934	7793	SER	N644	S255	E96
	M1135	L945	7796	VAL	L562	S256	E96
	T1136	G946	7797	ALA	L562	S256	E96
	K1149	Q949	7798	LEU	F562	Y266	N99
	L1152	Q957	7799	ASP	F562	Y266	N99
	Y1155	A958	7800	ASP	L655	L270	W104
	H1159	L959	7801	ASP	L655	L270	W104
	T1160	L977	7802	GLN	L655	L270	W104
	S1161	L983	7803	GLY	L655	L270	W104
Epsilon	ASP	L984	7804	ASP	S596	L276	G107
	VAL	L984	7805	PHE	V597	L296	T108
	ASP	L984	7806	ILE	L598	L296	T108
	ASP	L984	7807	LYS	L598	L296	T108
	ASP	L984	7808	GLN	L598	L296	T108
	ASP	L984	7809	TYR	L598	L296	T108
	ASP	L984	7810	GLY	L598	L296	T108
	ASP	L984	7811	ASP	L598	L296	T108
	ASP	L984	7812	ASP	L598	L296	T108
	ASP	L984	7813	ASP	L598	L296	T108

- Molecule 1: Spike glycoprotein, Fibrin



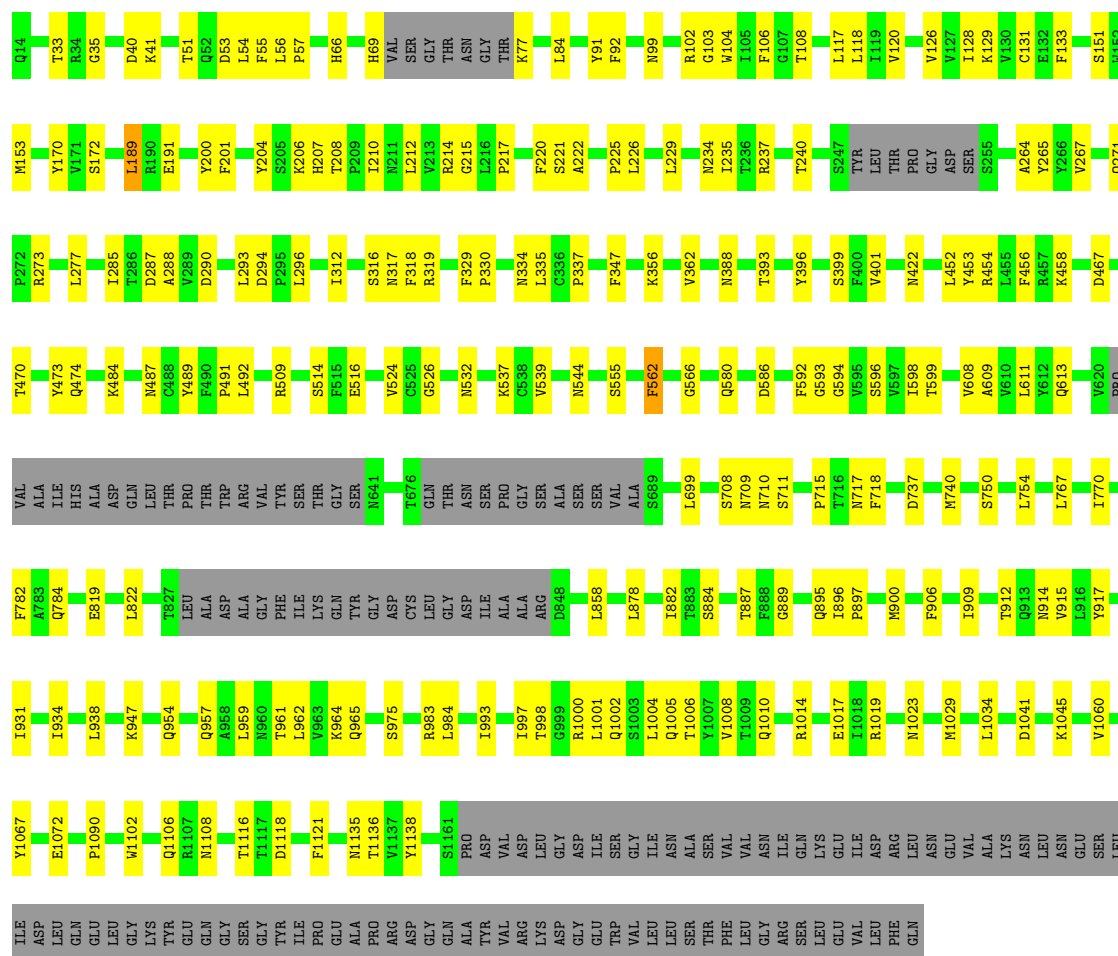
- Molecule 1: Spike glycoprotein, Fibrin



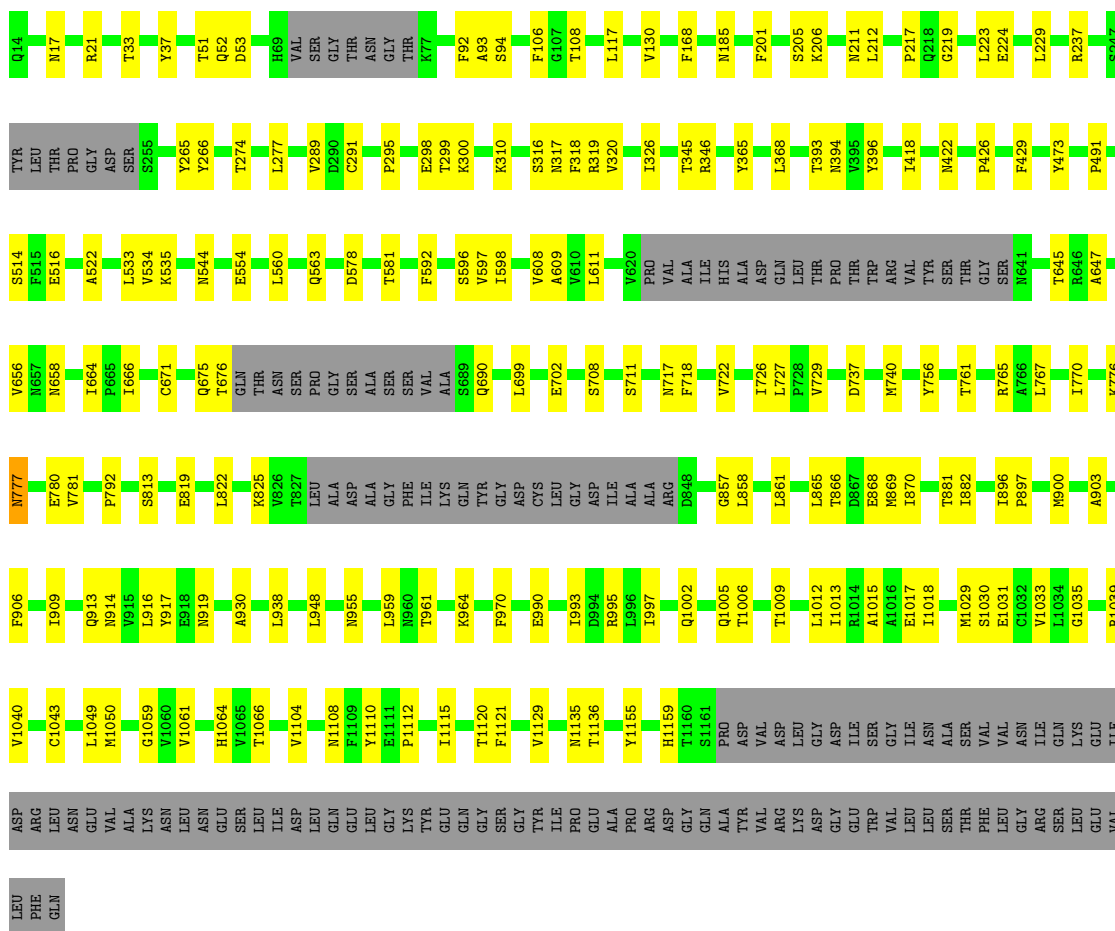


● Molecule 1: Spike glycoprotein,Fibrin

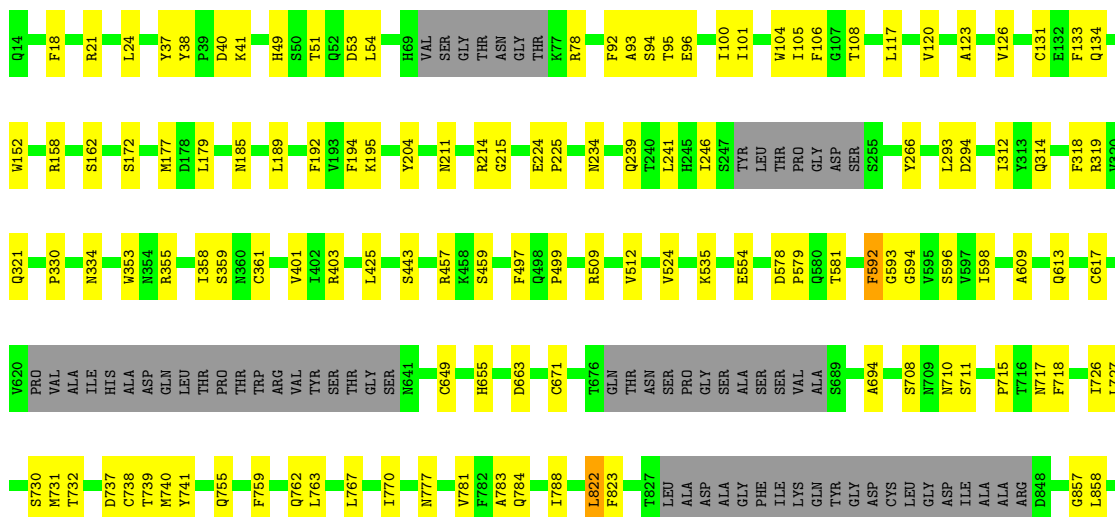
Chain 10-C: 71% 17% 12%

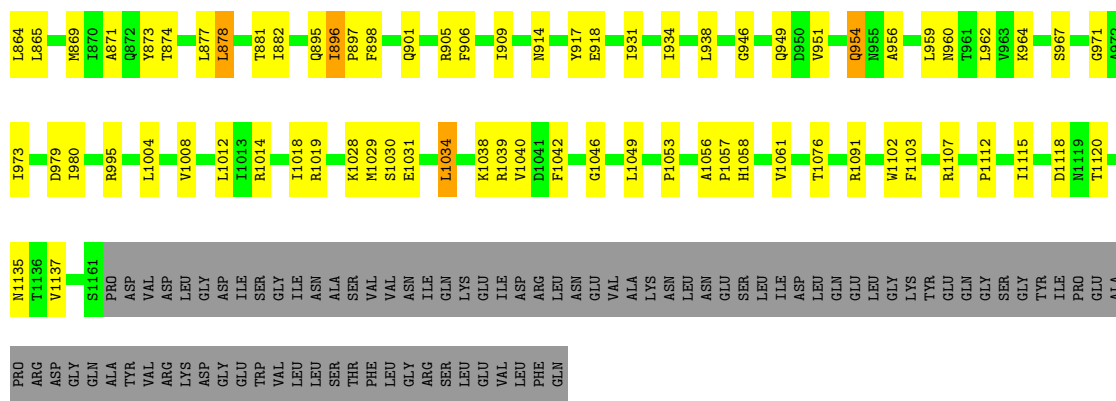


Chain 11-A: 73% 15% 12%



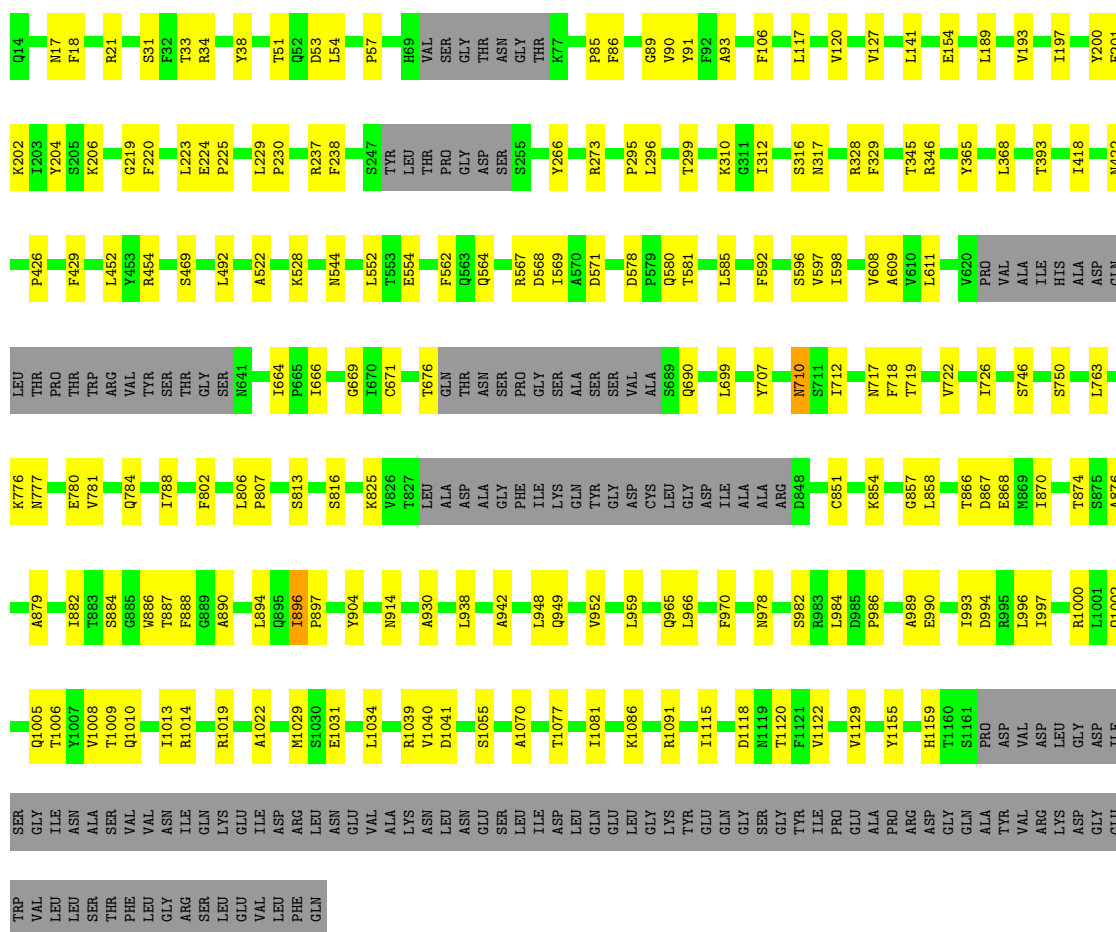
Chain 11-B:





● Molecule 1: Spike glycoprotein,Fibritin

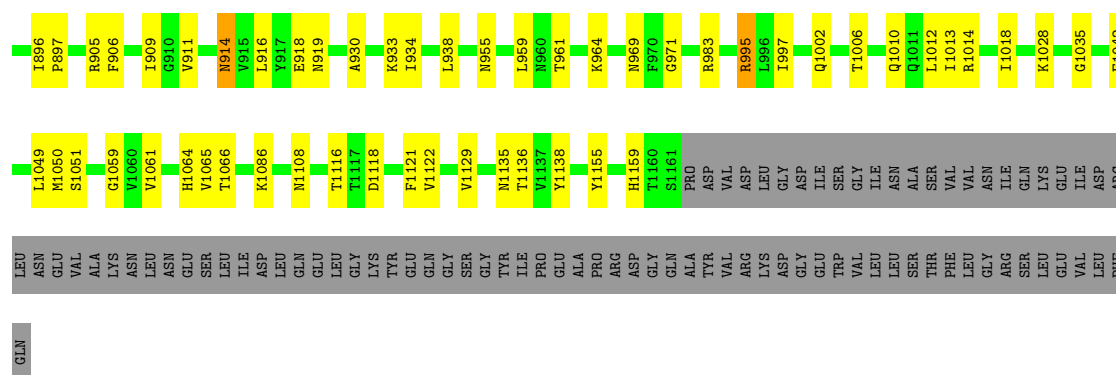
Chain 11-C: 72% 15% 12%



● Molecule 1: Spike glycoprotein,Fibritin

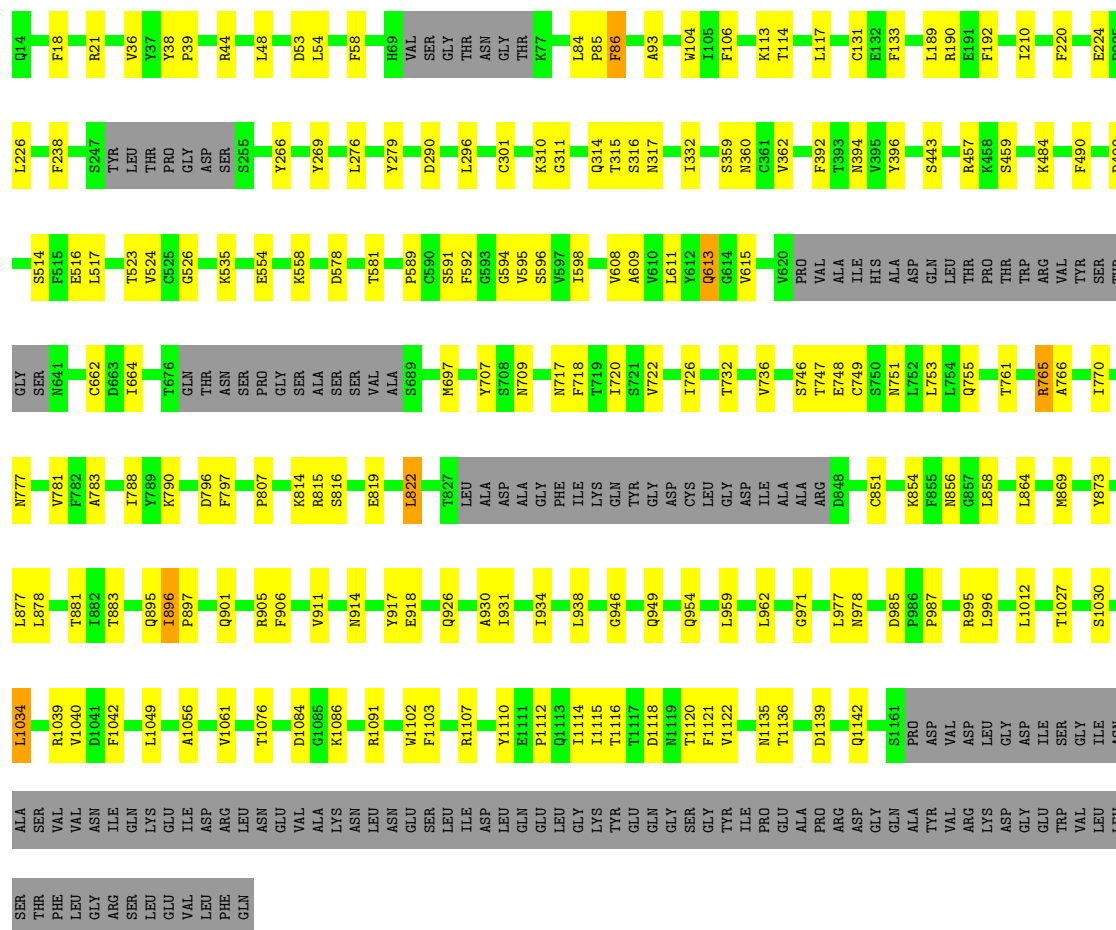
Chain 12-A: 73% 15% 12%





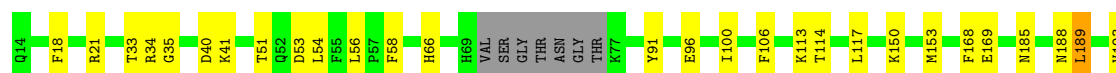
• Molecule 1: Spike glycoprotein,Fibritin

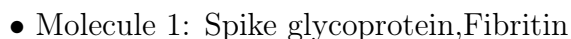
Chain 13-B: 73% 14% 12%



• Molecule 1: Spike glycoprotein,Fibritin

Chain 13-C: 72% 15% 12%



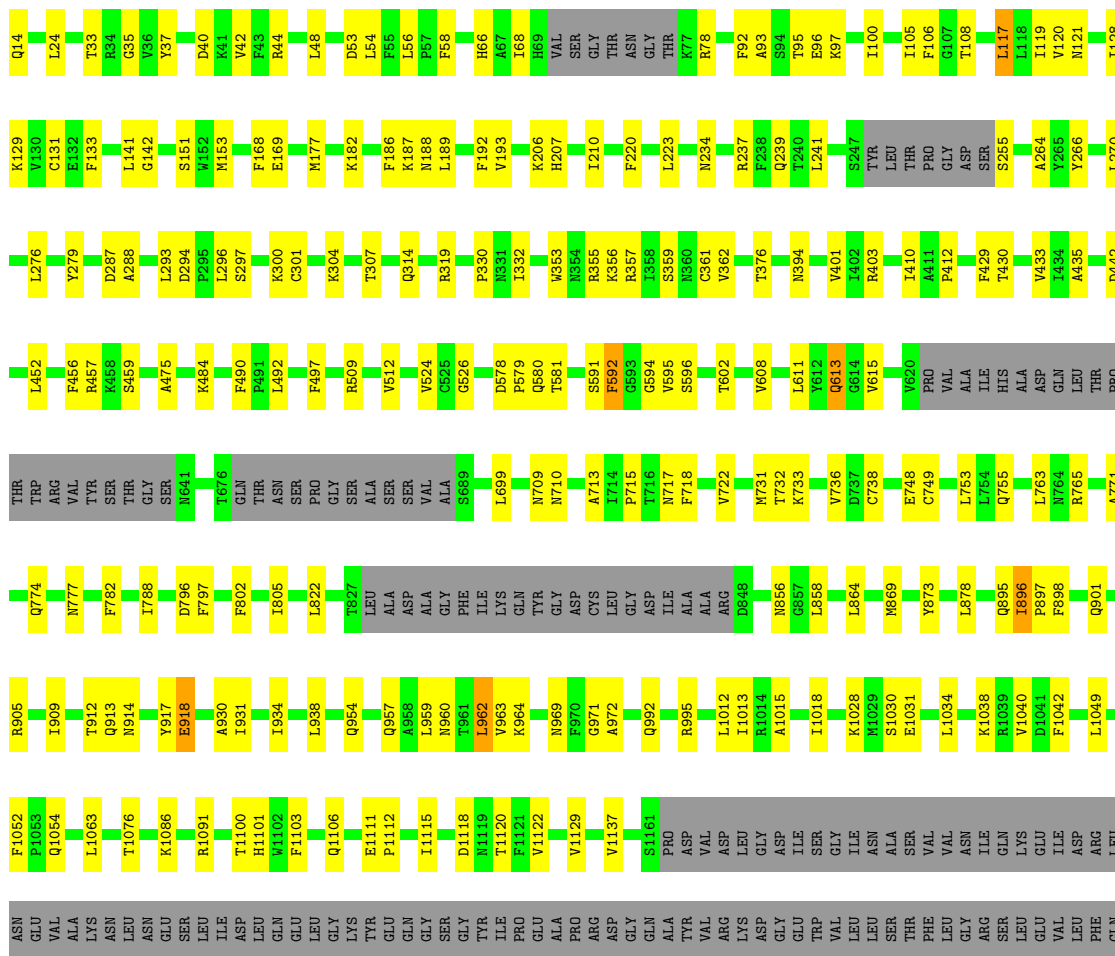


Q1011	L861	I712	V595	T323	F201	Q14
	P862		SS96	E324	K202	T33
		N717	V597		L203	
	T866	T718	I598	R328	Y204	Y37
		T719			S205	
	M869		A609	T345	K206	L48
	I870	V722	V610	R346	H207	
			L611		T208	
	T881	I726		F374	T209	Q52
	I882	L727	V620		L210	D53
M1029			PRO	D389	N211	L54
	I896	M731	VAL		L212	
	P897	T732	ALA	R394		P87
		K733	ILE	Y395	P217	
	F906		HIS	Y396	Q218	H69
		I742	ALA		G219	VAL
	V911		ASP	V401		SER
	T912	Q755	GLN		L223	GLY
	Q913	Y756	LEU	T418	E224	THR
	S1051		THR		P225	ASN
Q1054	V915	F759	PRO	N422	L226	GLY
	L916		THR			THR
		V772	TRP	P426	P230	K77
	N919	E773	ARG			
		Q774	VAL	F429	N234	V90
	A930	D775	TYR			Y91
	T1066	K776	SER	W436	F238	F92
	K933	N777	GLY	S443	L241	A93
	G946	Q784	THR			S94
	R947		SER	G476	S247	
F1089	Q949	E819	L650	N487	TYR	T100
		L822			LEU	G103
	N955		1666	P499	THR	W104
	A956		G667		PRO	I105
	Q957	T627	G667	R509	GLY	F106
		LEU			ASP	G107
	V963	ALA	C671	S514	SER	T108
	N969	GLY	Q675	F515		T109
	P970	PHE	T676	E516	S255	L110
	G971	ILE	THR		Y265	D111
Y1155		L977	LYS	F543	Y266	L117
	H1159		GLN	N544	R273	L118
	T1160	L977	SER	Q563	T774	I119
	S1161		TYR	Q564	A292	V120
	PRO	R983	ASP			
	VAL	L984	ASP			V127
	ASP		CYS	R567	L296	
	LEU	A989	LEU	D568		L141
	GLY	R995	SER	1569	T299	
	ASP		VAL	A570	K304	S151
S1161	ILE	R1000	ILE	D571		W152
	SER	Q1005	ALA		Q314	M153
	GLY		ALA	R577	F318	E154
	ILE		ARG	D578	R319	M185
	ASN	V1008	E702	T581		
	ALA	T1009			V320	L189
	SER	Q1010				
	ALA					
	SER					
	ALA					

[illegible]

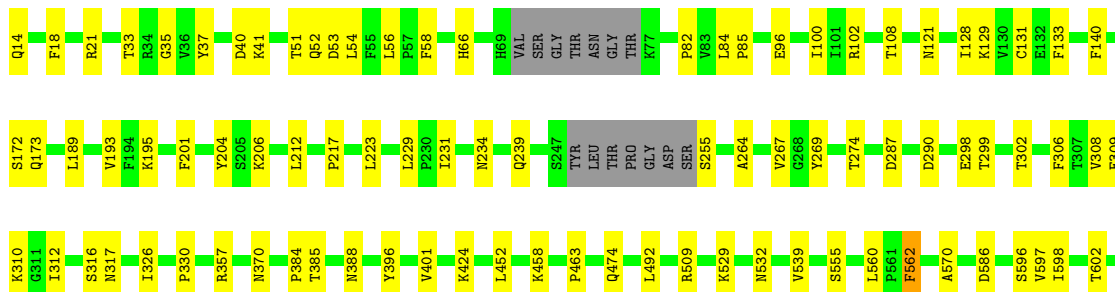
- Molecule 1: Spike glycoprotein, Fibrin

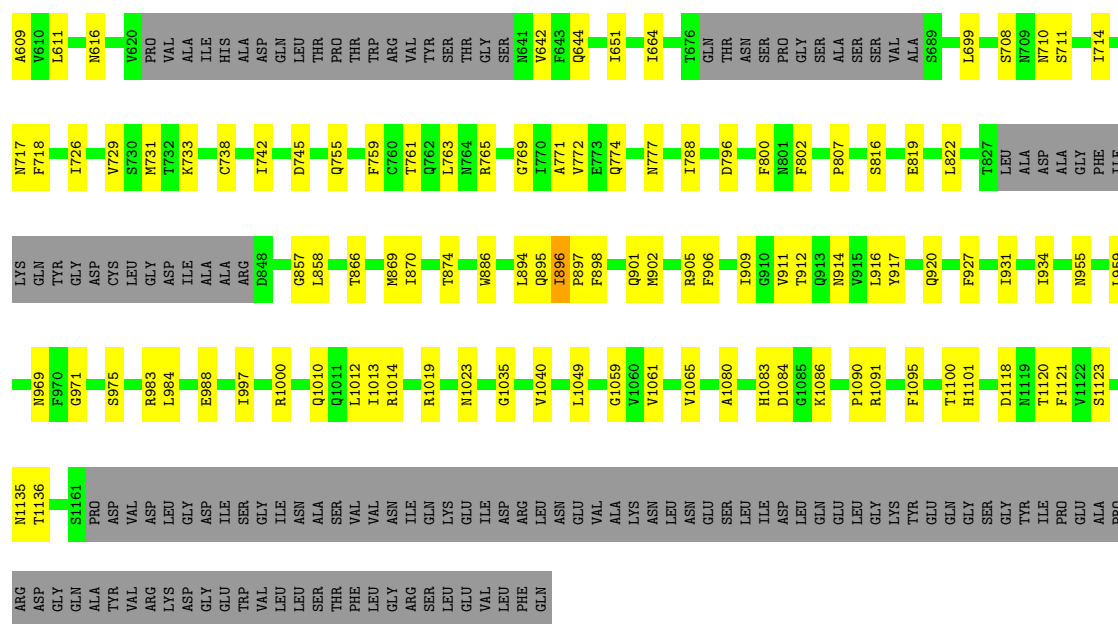
Chain 14-B:



- Molecule 1: Spike glycoprotein, Fibrin

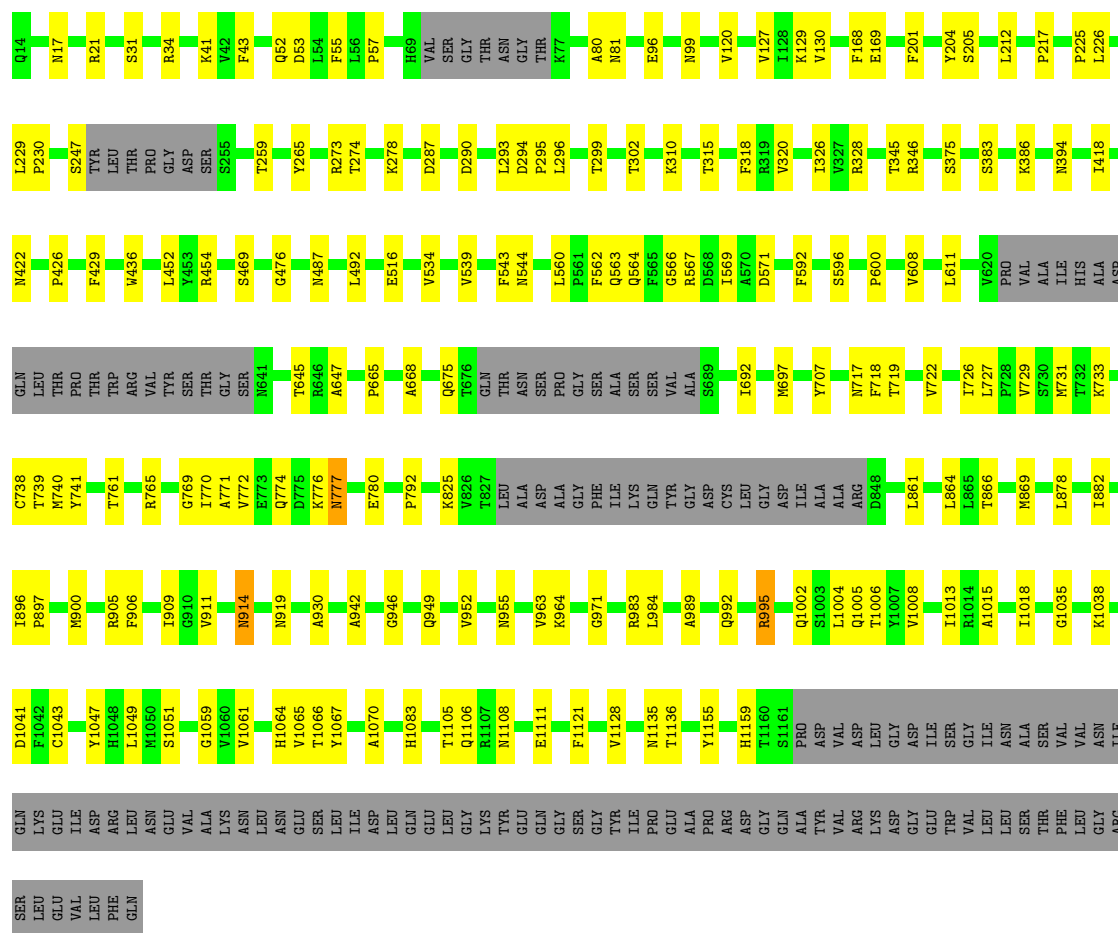
Chain 14-C: 72% 15% 12%



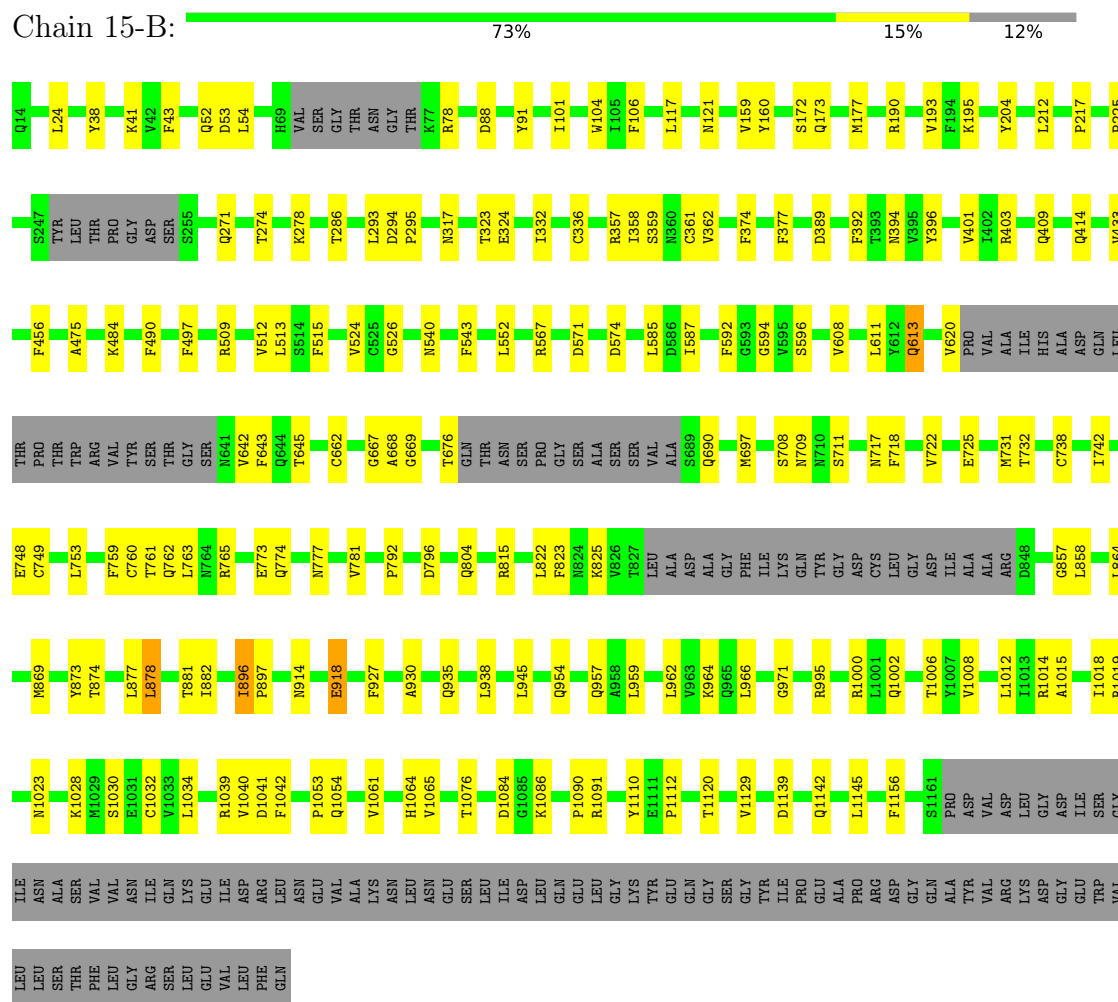


● Molecule 1: Spike glycoprotein,Fibrin

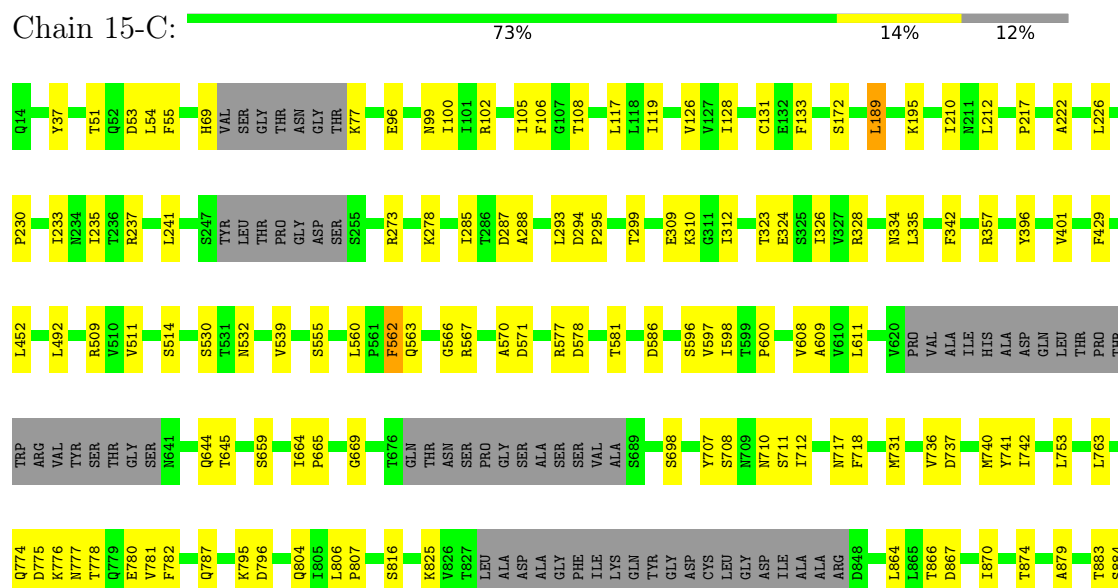
Chain 15-A: 73% 14% 12%

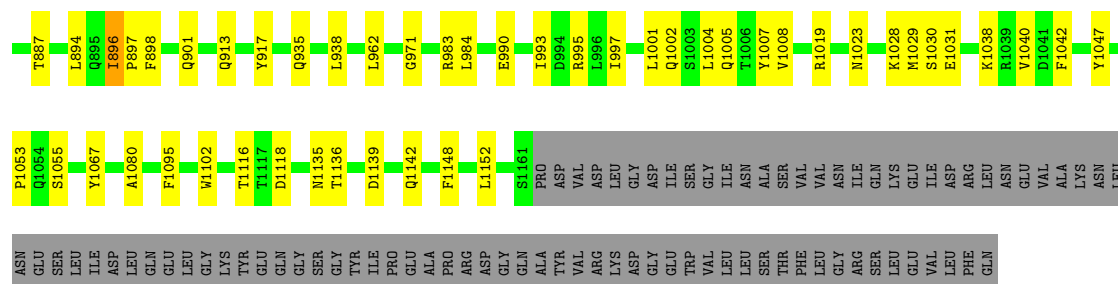


• Molecule 1: Spike glycoprotein,Fibritin



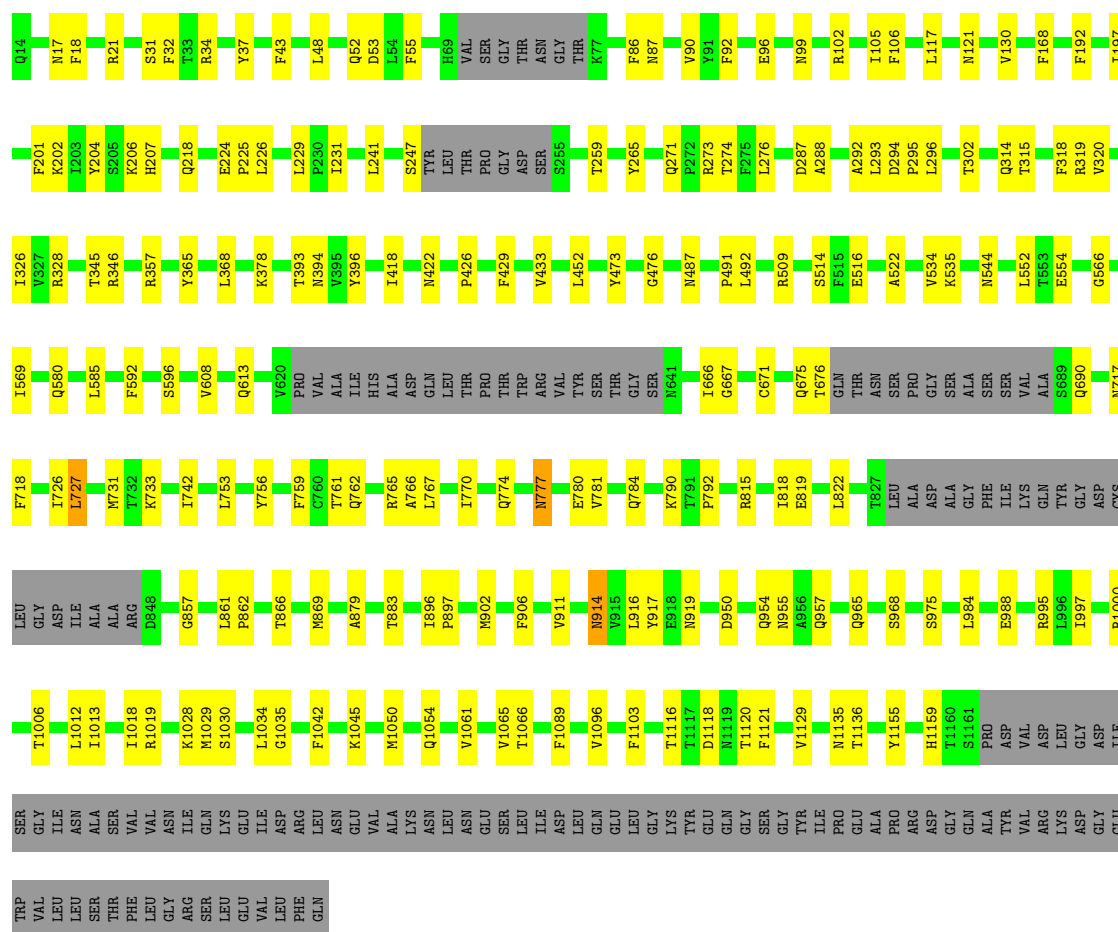
• Molecule 1: Spike glycoprotein,Fibritin





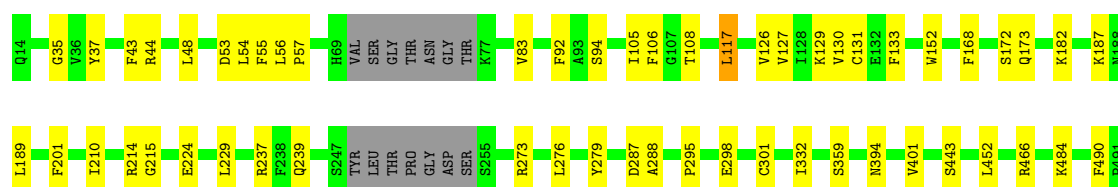
• Molecule 1: Spike glycoprotein,Fibrin

Chain 16-A: 72% 15% 12%

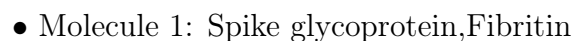


• Molecule 1: Spike glycoprotein,Fibrin

Chain 16-B: 74% 13% 12%

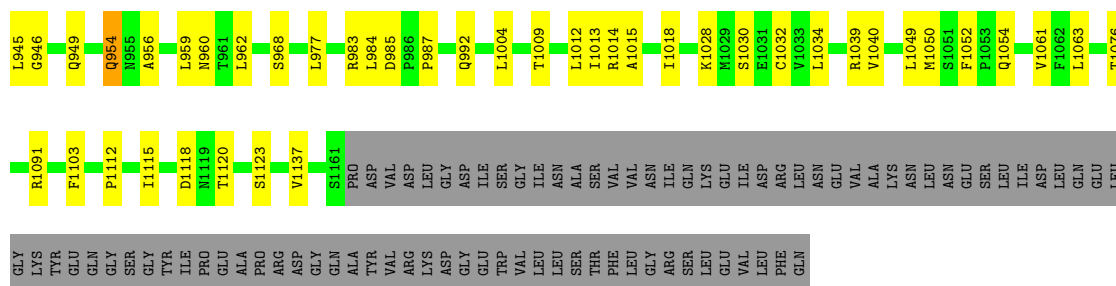


Digital Tool	Percentage
Video conferencing tool	73%
Digital whiteboard	14%
Digital sticky note	12%

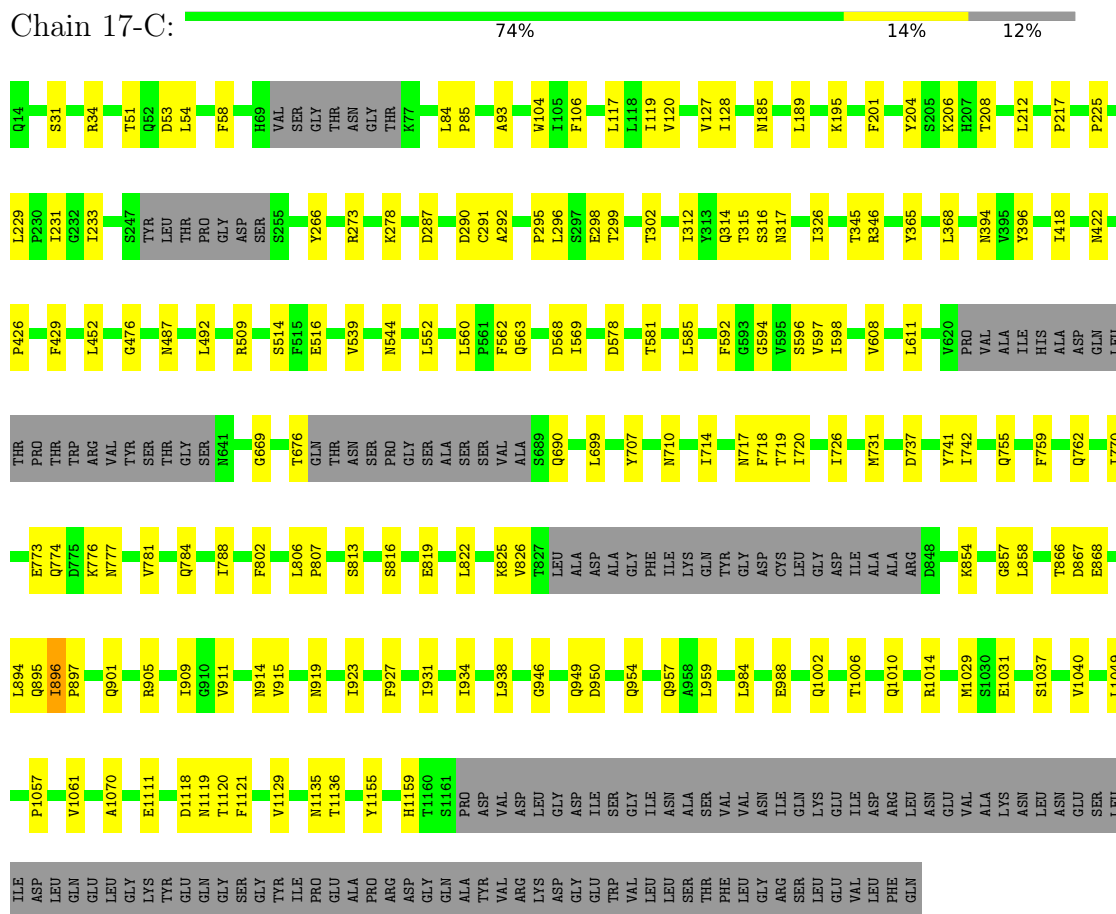


Response	Percentage
Best for the country	71%
Not the best for the country	17%
Don't know	12%

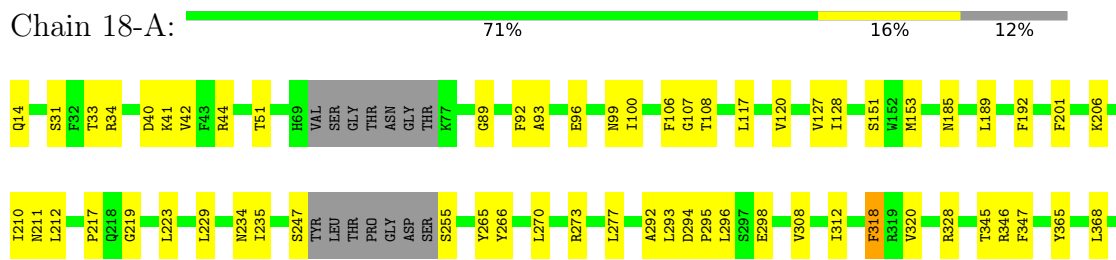


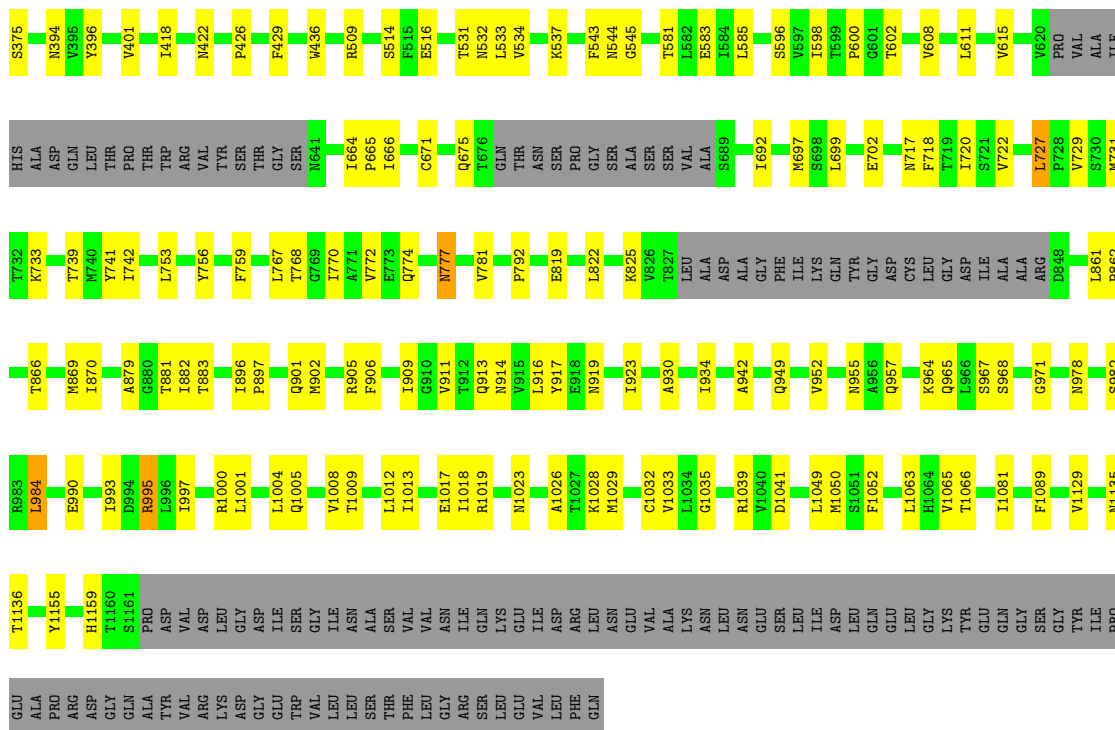


• Molecule 1: Spike glycoprotein,Fibrin

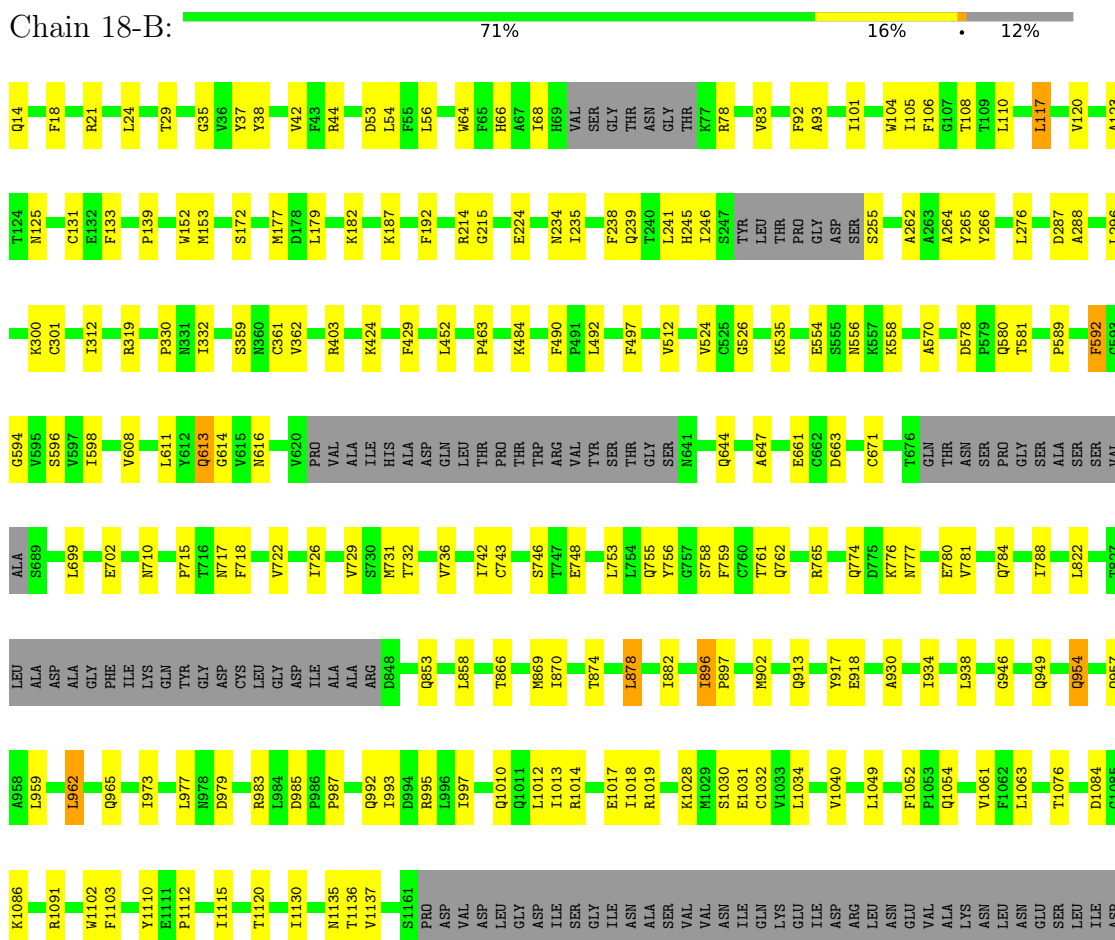


• Molecule 1: Spike glycoprotein,Fibrin

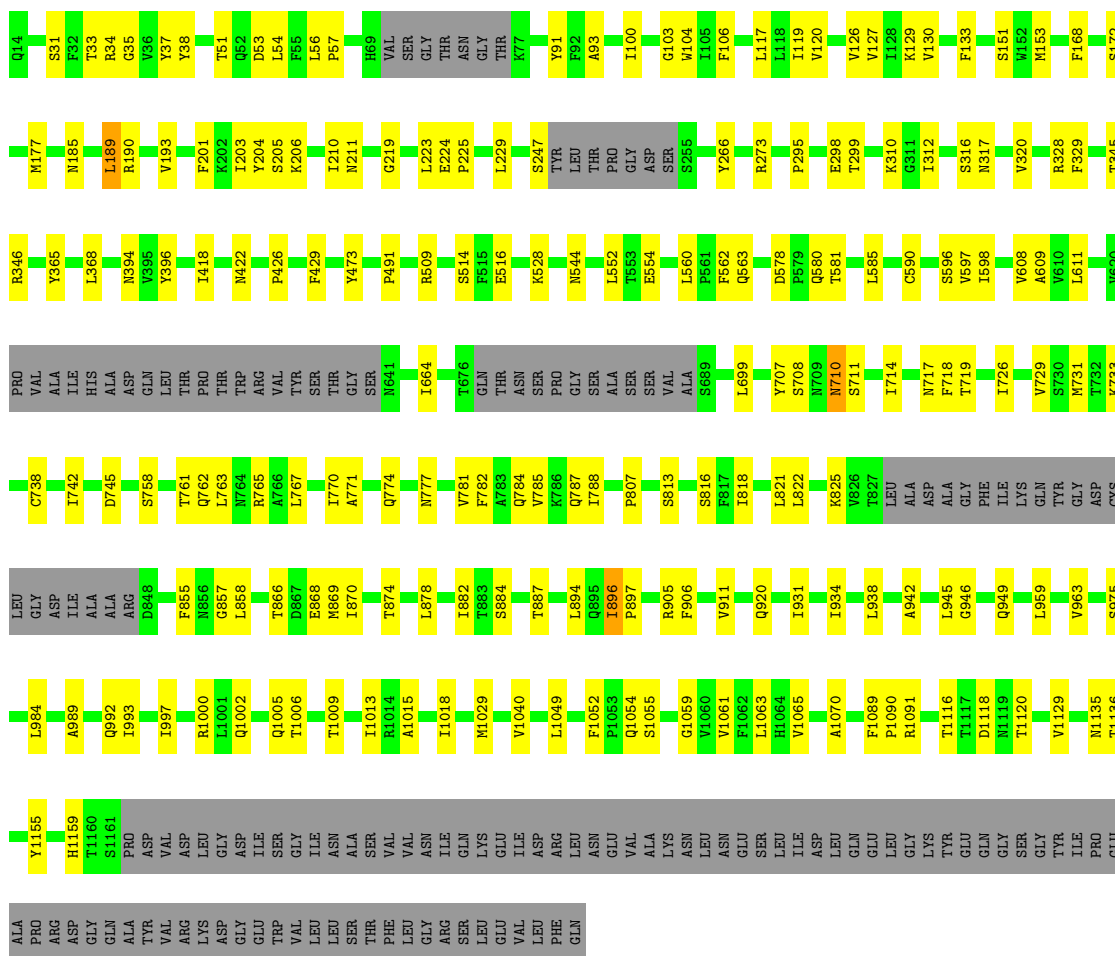




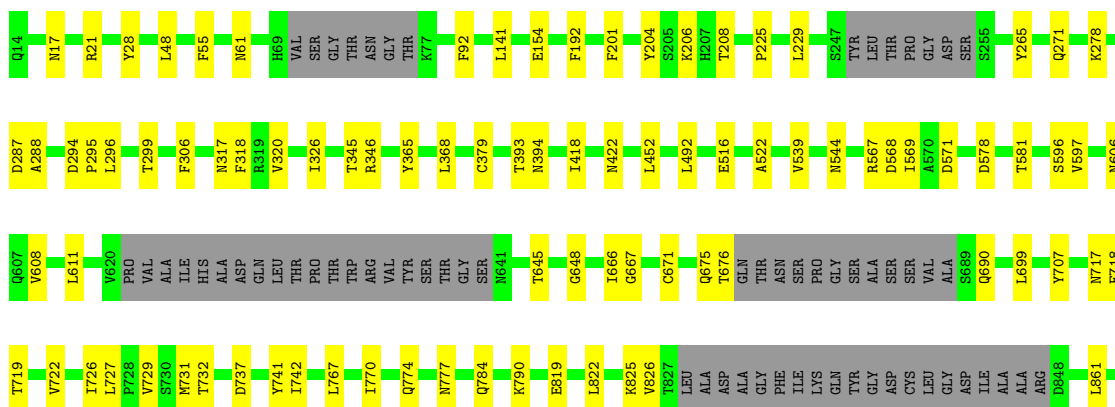
- Molecule 1: Spike glycoprotein, Fibrin

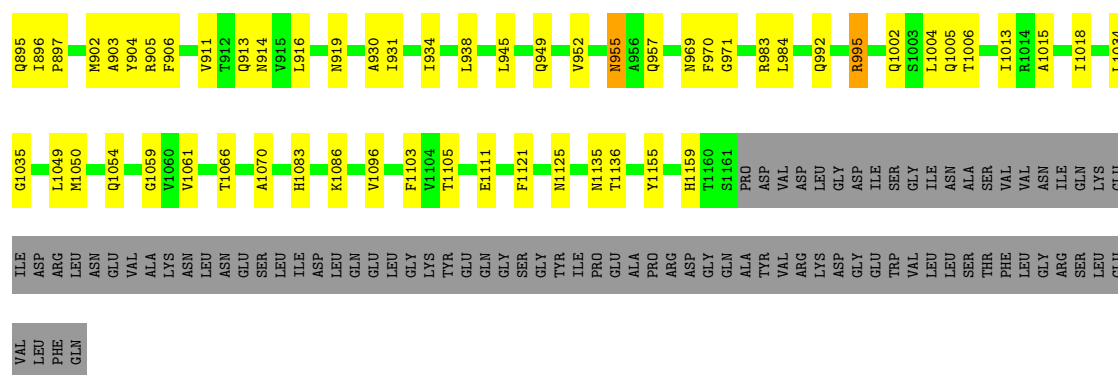


Chain 18-C: 72% 16% 12%




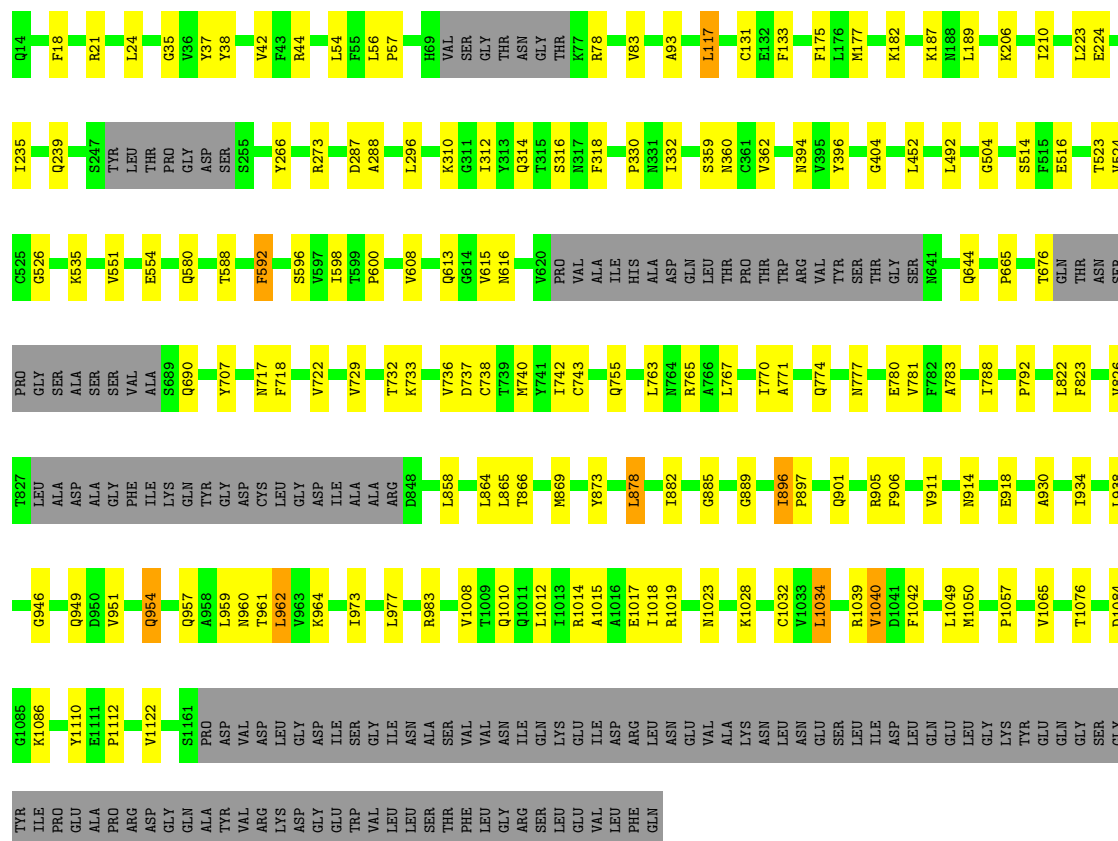
Chain 19-A: 76% 12% 12%






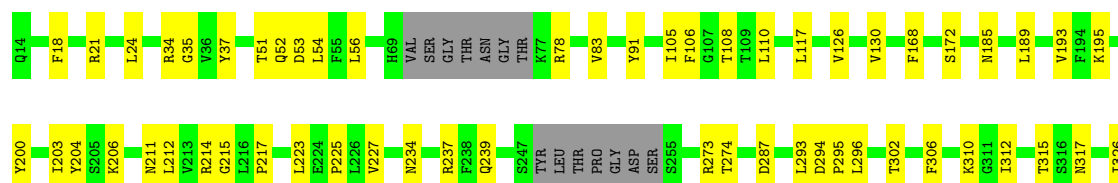
• Molecule 1: Spike glycoprotein,Fibrin

Chain 19-B:  75% 12% 12%




• Molecule 1: Spike glycoprotein,Fibrin

Chain 19-C:  74% 14% 12%



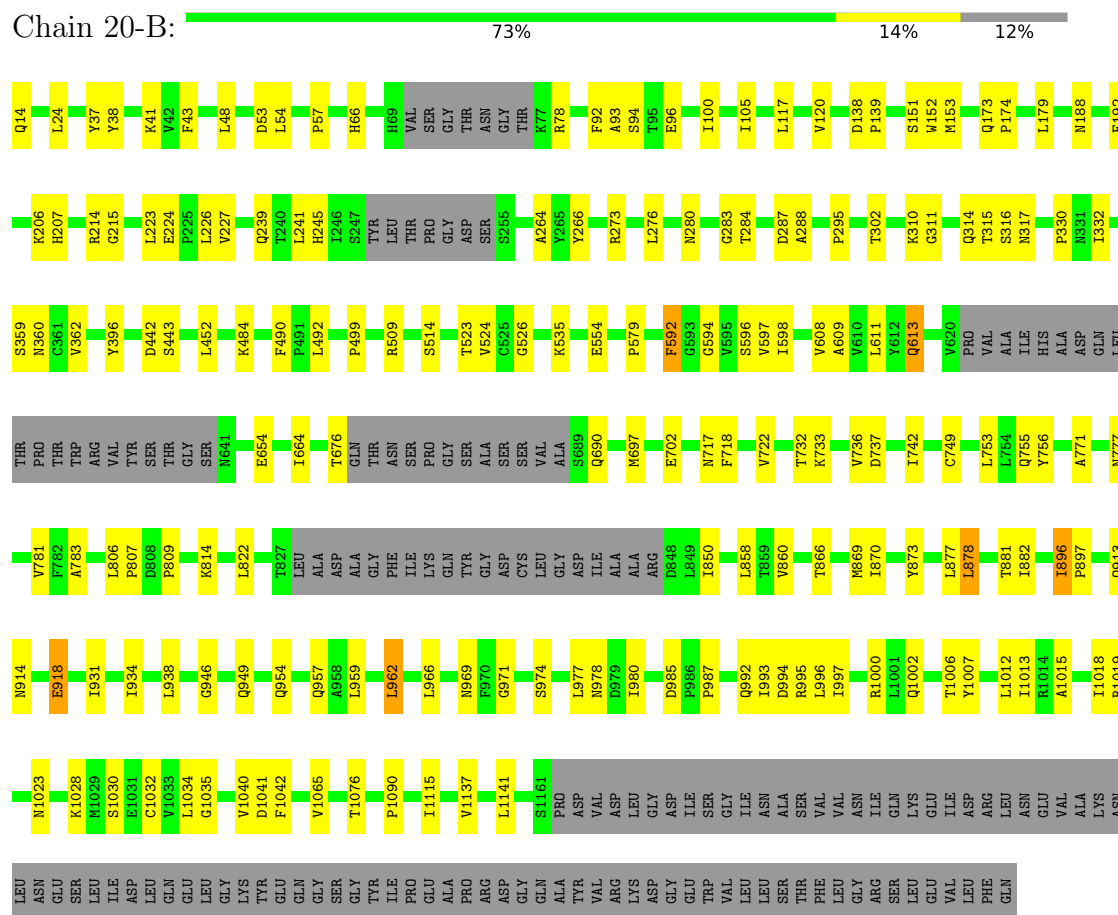
V327	V620	A766	P897	L1049	ASN
R328	PRO	L767	F898	M1050	LEU
N334	ASN	T768	Q901	S1051	ASN
L335	VAL	G769	M902	F1052	GLU
C336	ILE	I770	A903	P1053	SER
P337	HIS	A771	Y904	G1059	LEU
K356	ALA	E772	R905	V1060	ILE
V362	ASP	E773	Y906	V1061	ASP
K366	GLN	K774	I909	H1064	LEU
V362	LEU	K775	L916	A1080	GLN
V401	THR	N777	I931	F1095	LEU
V401	THR	T778	I934	R1107	GLY
K494	TRP	V781	Q954	I1114	LYS
N457	ARG	Q784	L959	D1118	THR
C488	VAL	P792	G971	N1135	GLY
Y489	TYR	I805	R995	T1136	ASN
F490	SER	P807	G999	D1139	GLY
R509	THR	S816	R1000	Q1142	THR
V524	SER	T827	L1001	S1161	ARG
N532	GLY	LEU	Q1002	PRO	ASP
L533	ALA	ALA	T1006	VAL	VAL
C538	ASP	ALA	Y1007	ASP	VAL
V539	GLN	ALA	V1008	LEU	ARG
F543	PRO	ALA	T1009	ASP	LYS
S555	GLY	PHE	Q1010	GLY	ASP
L560	SER	ILE	R1014	ILE	GLU
P561	VAL	GLY	A1015	SER	THR
F562	ALA	ASP	I1018	THR	THR
Q563	ALA	CYS	R1019	VAL	PHE
Q564	ALA	LEU	M1029	VAL	LEU
F565	LEU	GLY	S1030	VAL	GLY
V576	LEU	ASP	E1031	ILE	GLY
D586	ILE	ILE	C1032	ILE	ARG
I587	ALA	ALA	G1035	SER	SER
C590	ARG	ARG	K1038	GLU	LEU
F596	F718	D848	I1039	ASP	LEU
S597	E725	G857	V1040	LEU	ASN
I598	I726	L858	C1043	GLU	GLY
T599	V729	L864	G1044	VAL	ALA
P600	M740	L865	K1045	LYS	LYS
V608	L763	T866	H1048	GLU	
A609	N764	D867		VAL	
L611	R765	W886		ALA	
		I896		LYS	

• Molecule 1: Spike glycoprotein,Fibrin

Chain 20-A:  72% 15% 12%

Q14	Q218	R357	M731	I1013	ASP
T19	G219	N370	D737	L1024	ILE
S31	L223	N394	M740	A1025	SER
F32	E224	V395	F741	S1030	GLY
T33	P225	Y396	I742	L1034	THR
R34	L226	I418	Q755	G1035	SER
Q52	N234	N422	L767	V1040	VAL
D53	Q239	P426	L767	D1041	GLY
L54	T240	P426	I770	L1049	ARG
H69	S247	F429	Q774	Q901	GLN
VAL	TYR	S438	D775	M902	LYS
SER	LEU	Y473	K776	A903	GLU
THR	PRO	Q476	N777	Y904	VAL
GLY	GLY	N487	E780	G1059	ASP
THR	ASP	P491	V781	V1060	ARG
K77	SER	R509	E819	V1061	THR
N81	S256	S514	L822	T1066	GLN
W104	Y265	E516	K825	K1086	ASN
I105	T274	F515	V826	F1089	LEU
F106	K278	T108	T827	V1096	ASN
G107	D287	L117	LEU	F1103	SER
T108	A288	L118	ALA	V1104	ILE
L117	D294	L119	ASP	T1105	ASP
L118	P295	V120	ALA	E1111	LEU
V120	L296	V127	GLY	F1121	GLN
V127	S287	V130	LYS	N1125	LEU
V130	E298	Q134	GLN	V1128	LYS
Q134	T299	S161	THR	V1129	THR
S161	F306	F168	ASN	L1132	GLY
F168	T315	N185	ASN	N1135	GLY
N185	S316	L189	VAL	T1136	TYR
L189	N317	V320	ALA	L1141	ILE
Y204	F318	L326	ARG	Y1155	GLY
S205	R319	F329	D848	H1159	ARG
K206	V320	T345	L861	T1160	ASP
H207	S325	F329	L865	S1161	GLY
I210	I326	T345	T866	PRO	GLN
N211	F329	T345	M869	ASP	ALA
L212	T345	T345	I870	VAL	VAL
P217	T345	T345	T874	ASP	THR
				VAL	VAL
				ASP	VAL
				LEU	ARG
				GLY	LYS
				ASP	ASP

• Molecule 1: Spike glycoprotein,Fibrinin



K790	T791	P792	I805	I806	P807	S816	K825	V826	T827	LEU	ALA	ASP	ALA	GLY	PHE	ILE	LYS	GLN	TYR	GLY	ASP	CYS	LEU	GLY	ASP	ILE	ALA	ALA	D848	G857	T866	D867	E868	M869	I870	T874	S884	T887	F888	G889	I896	P897	F898	Q901	G908	Q913						
S929	A930	I931	K932	K933	I934	A942	Q954	Q957			N960	T961	L962	V963		L966		N969	L977		D994		I997		R1000	L1001	Q1002	S1003	L1004	Q1005	T1006	V1007	T1008	Q1009	Q1010	Q1011	L1012	I1013	R1014	L1024	K1028	M1029	S1030	F1031	C1032	V1033	L1034	K1038	R1039	V1040	D1041	F1042
M1050	S1051	F1052	P1053	H1064	V1065	H1083	M1102	D1118	F1121	V1129	N1135	T1136	D1153	F1156	S1161	PRO	ASP	VAL	ASP	ASP	LEU	GLY	ASP	ILE	TRP	GLY	VAL	ILE	ASN	ALA	SER	SER	VAL	VAL	ASN	ARG	LEU	ASN	ASN	GLY	VAL	ALA	LYS	ASN	ASN	ASN	ASN					
GLU	SER	LEU	ILE	LEU	GLN	GLU	GLY	LYS	TYR	GLU	GLN	GLY	SER	GLY	TYR	ILE	PRO	GLU	ALA	PRO	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

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 ($e^-/\text{\AA}^2$)	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	1.793	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 (\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	0.10	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(°)	Ideal(°)
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

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 ⓘ

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 ⓘ

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

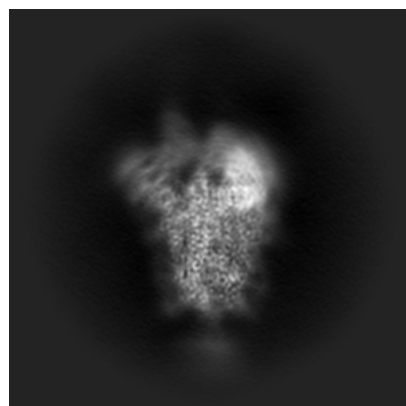
6 Map visualisation [i](#)

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.

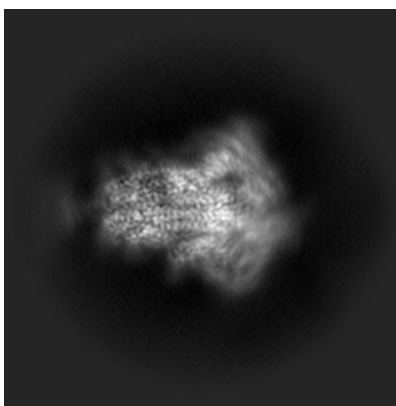
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

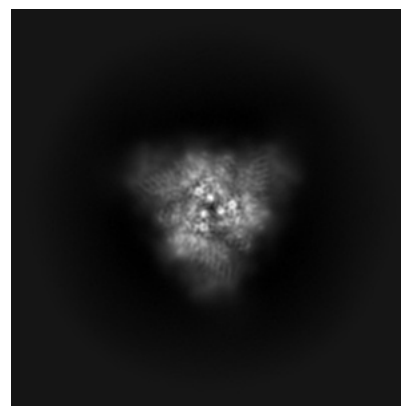
6.1.1 Primary map



X

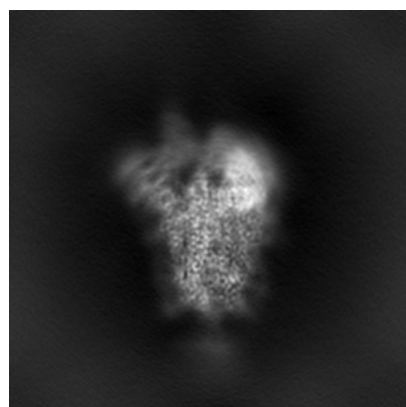


Y

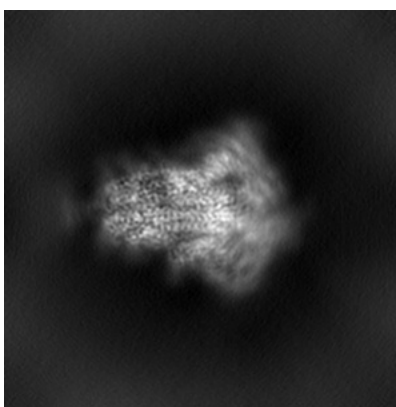


Z

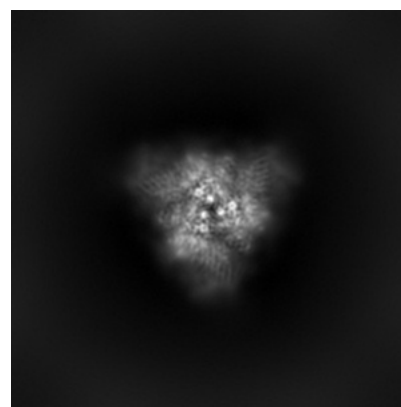
6.1.2 Raw map



X



Y

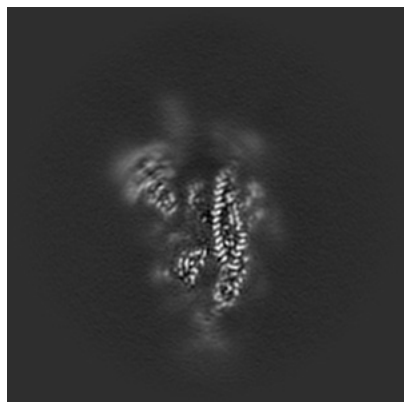


Z

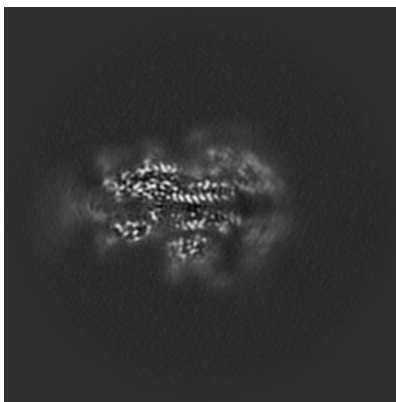
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

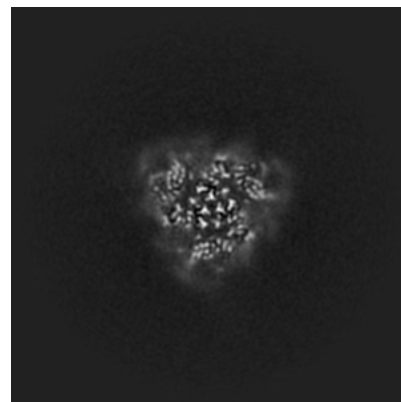
6.2.1 Primary map



X Index: 112

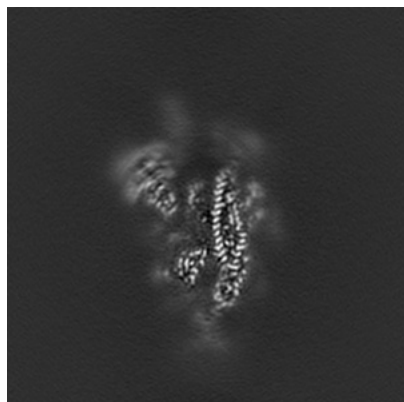


Y Index: 112

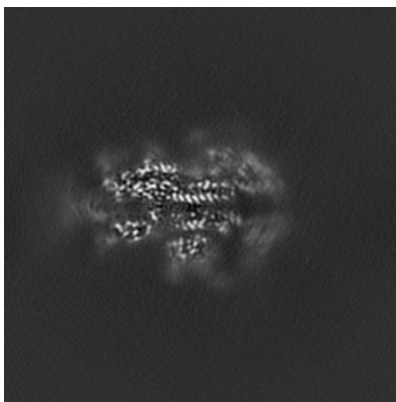


Z Index: 112

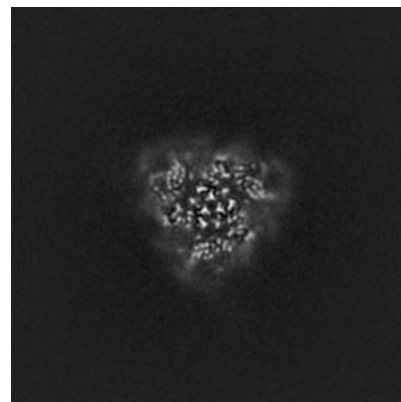
6.2.2 Raw map



X Index: 112



Y Index: 112

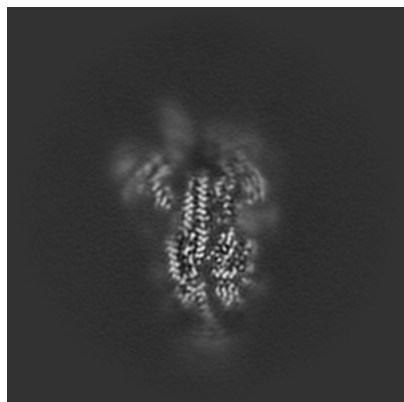


Z Index: 112

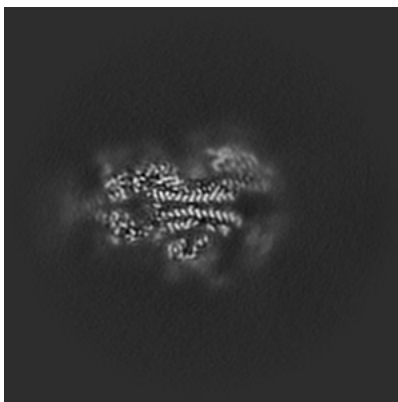
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

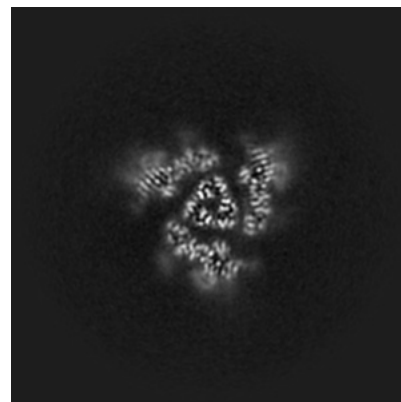
6.3.1 Primary map



X Index: 107

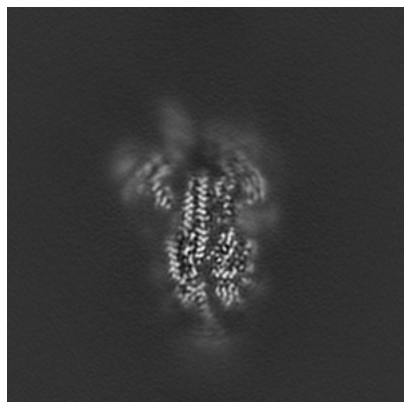


Y Index: 110

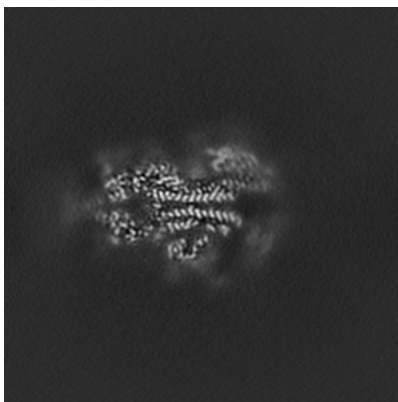


Z Index: 122

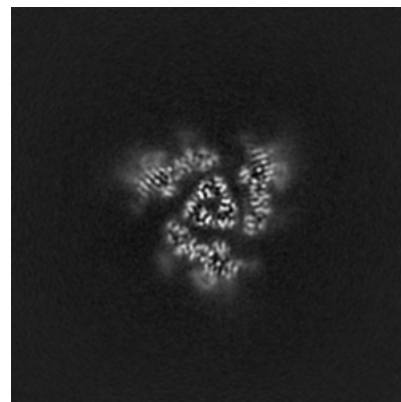
6.3.2 Raw map



X Index: 107



Y Index: 110

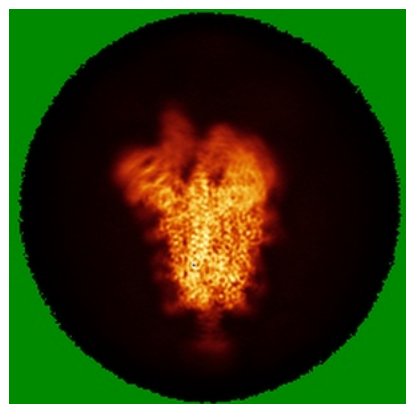


Z Index: 122

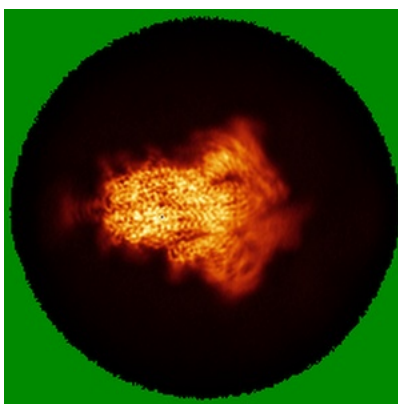
The images above show the largest variance slices of the map in three orthogonal directions.

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

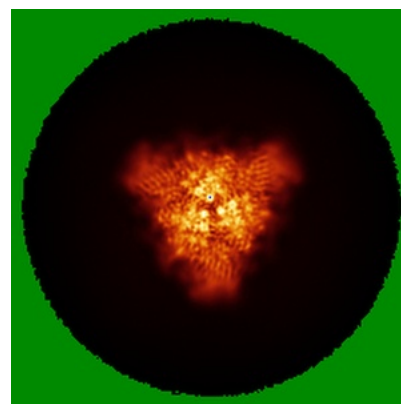
6.4.1 Primary map



X

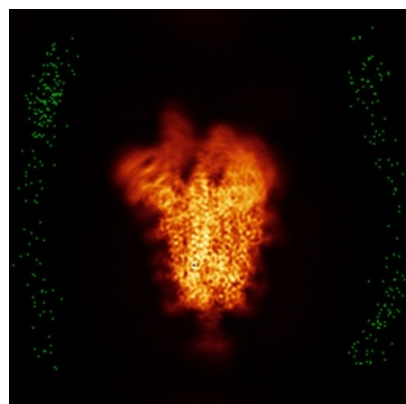


Y

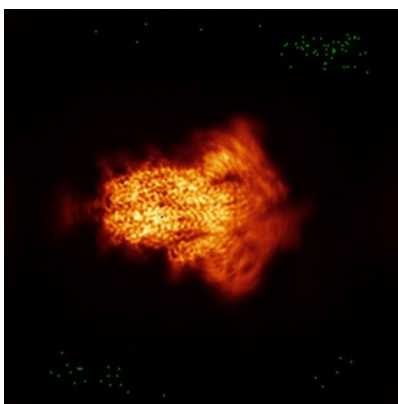


Z

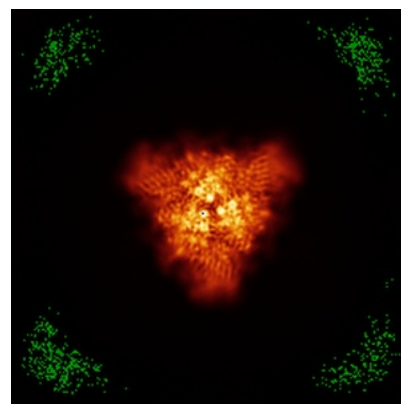
6.4.2 Raw map



X



Y



Z

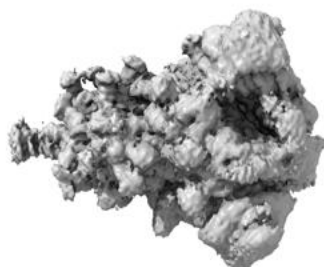
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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.

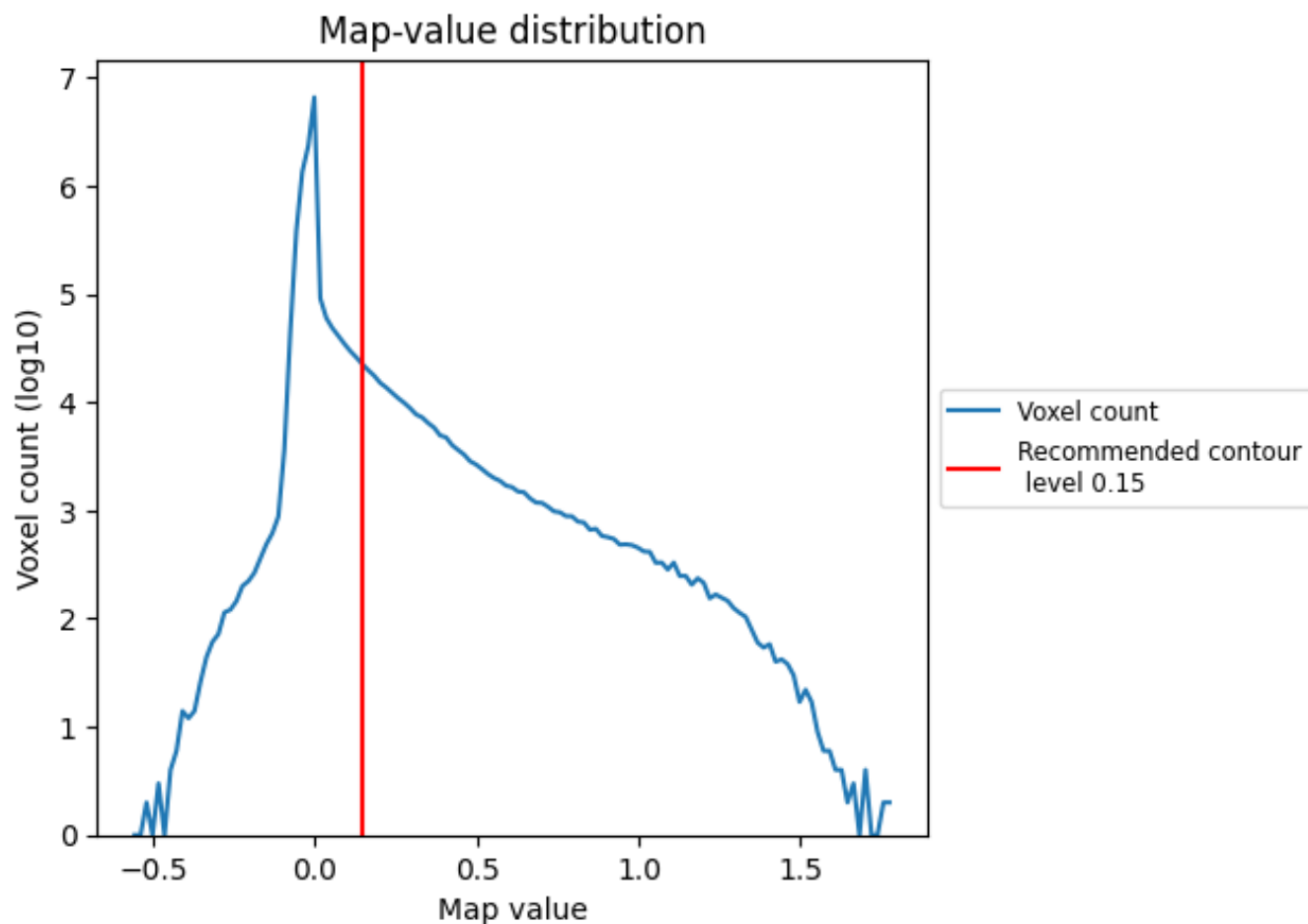
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

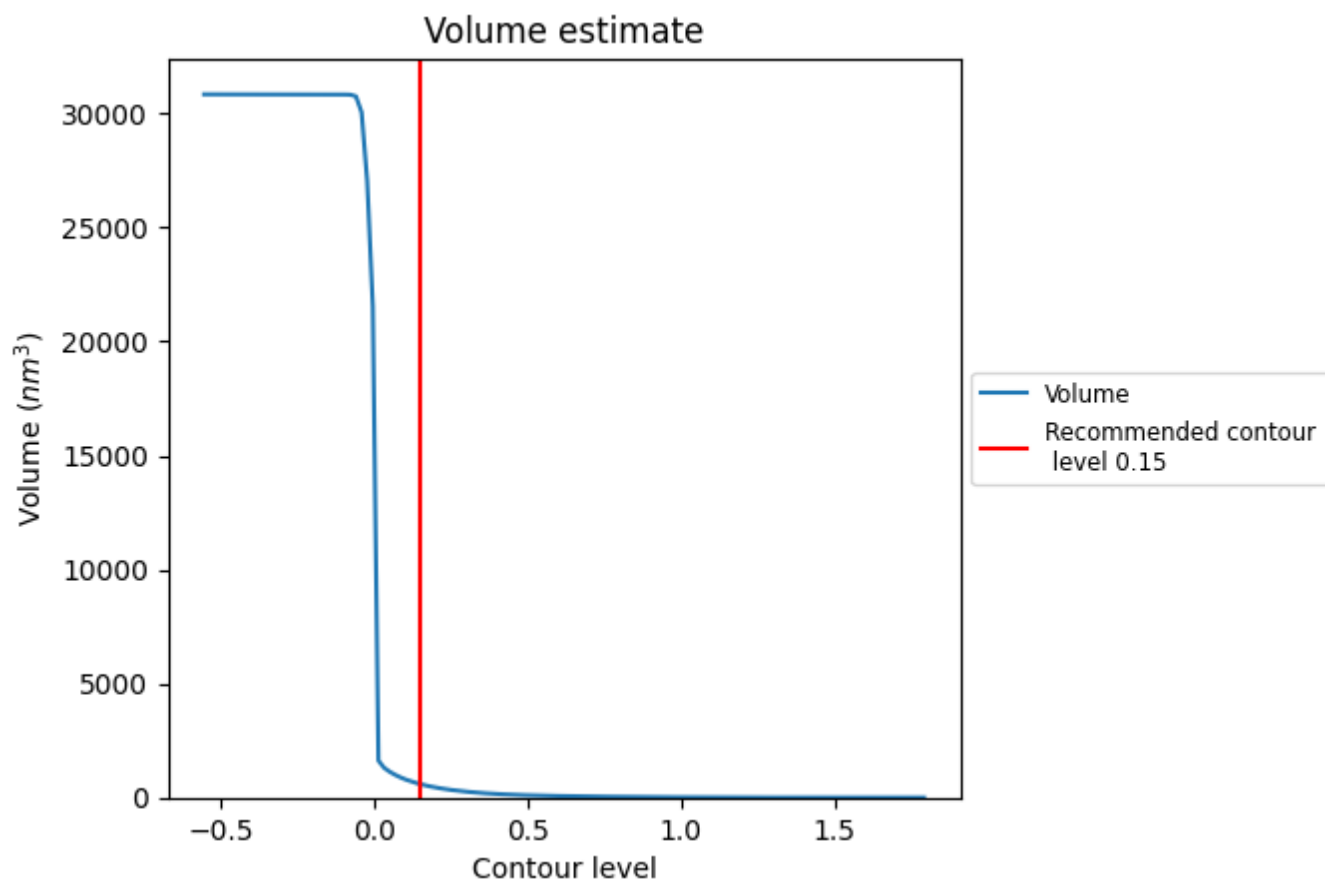
This section contains the results of statistical analysis of the map.

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.

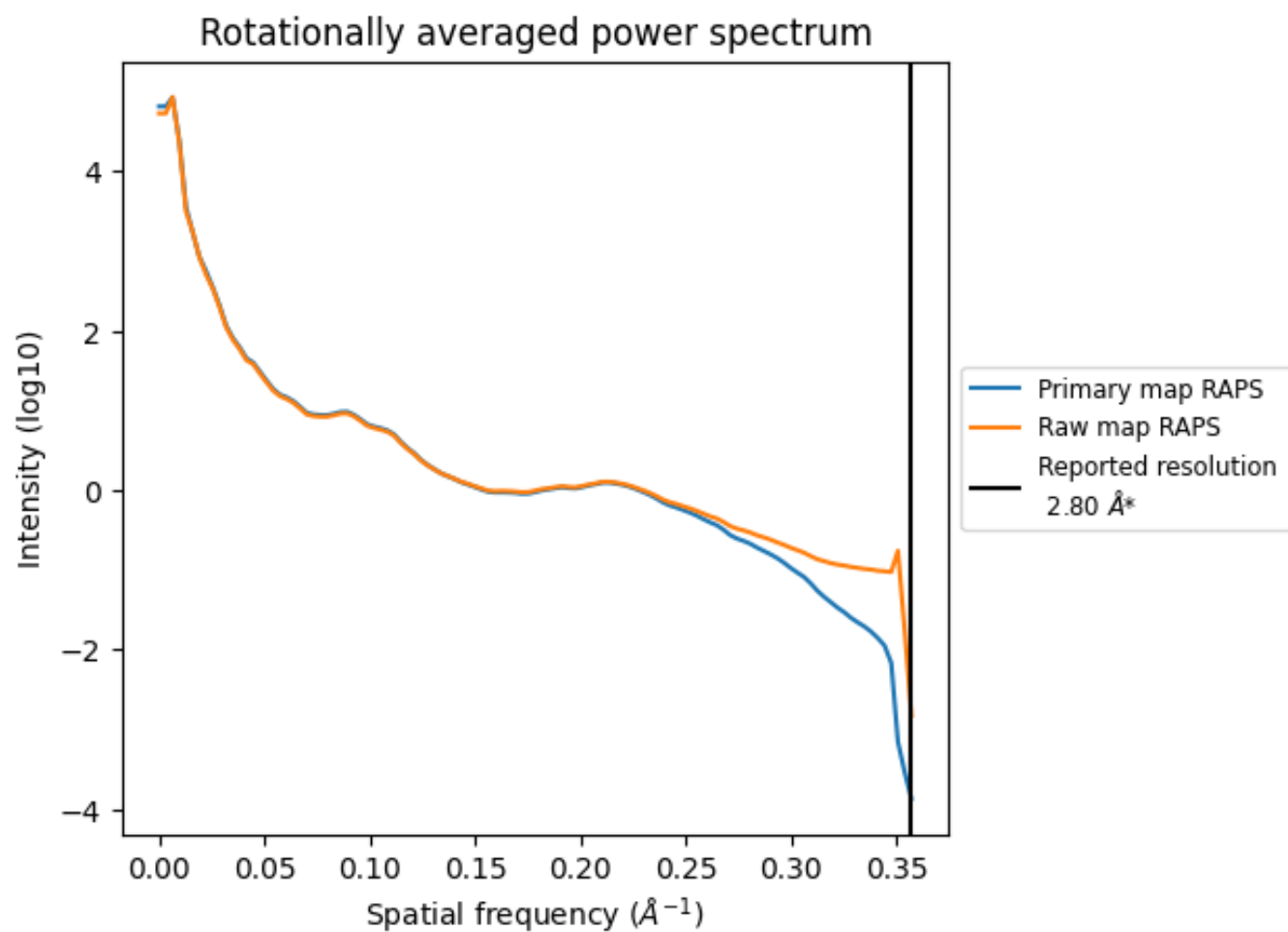
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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 ⓘ

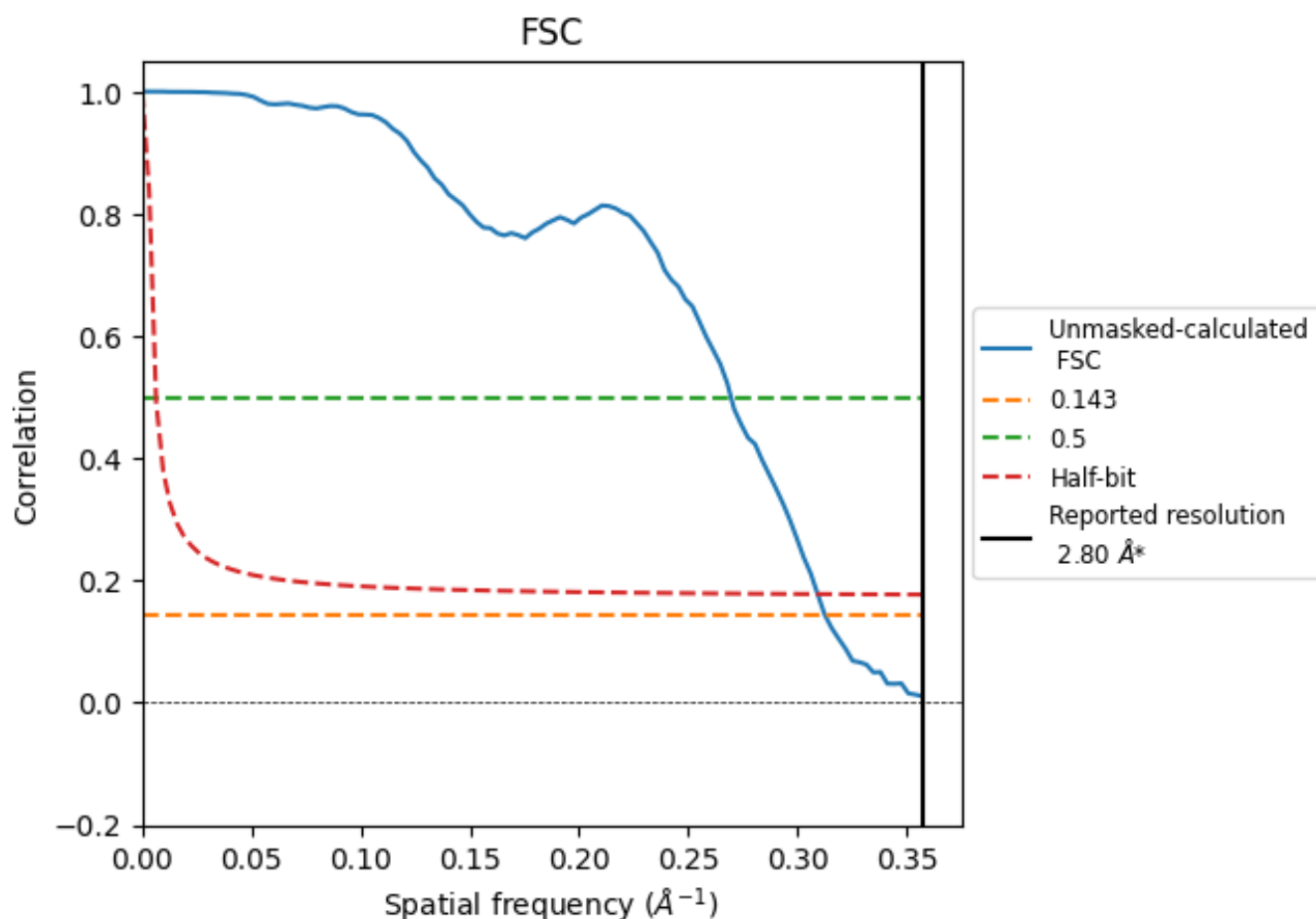


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

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](#)

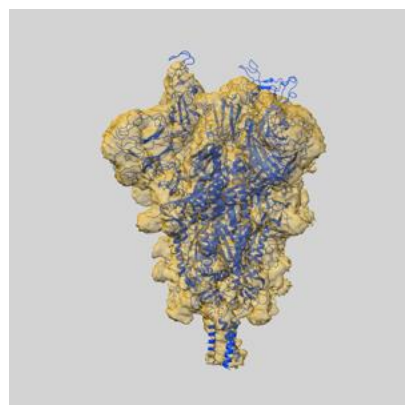
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.20	3.71	3.23

*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 %

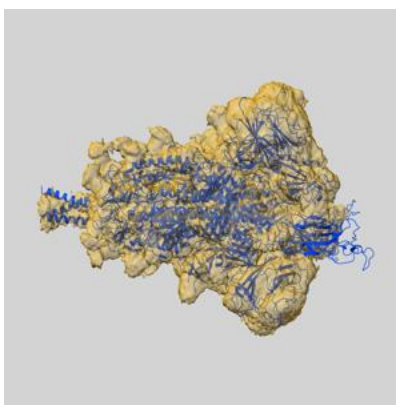
9 Map-model fit [i](#)

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](#).

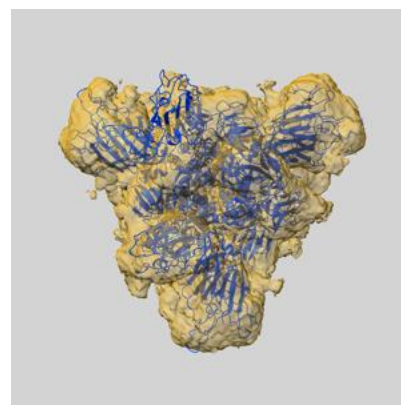
9.1 Map-model overlay [i](#)



X



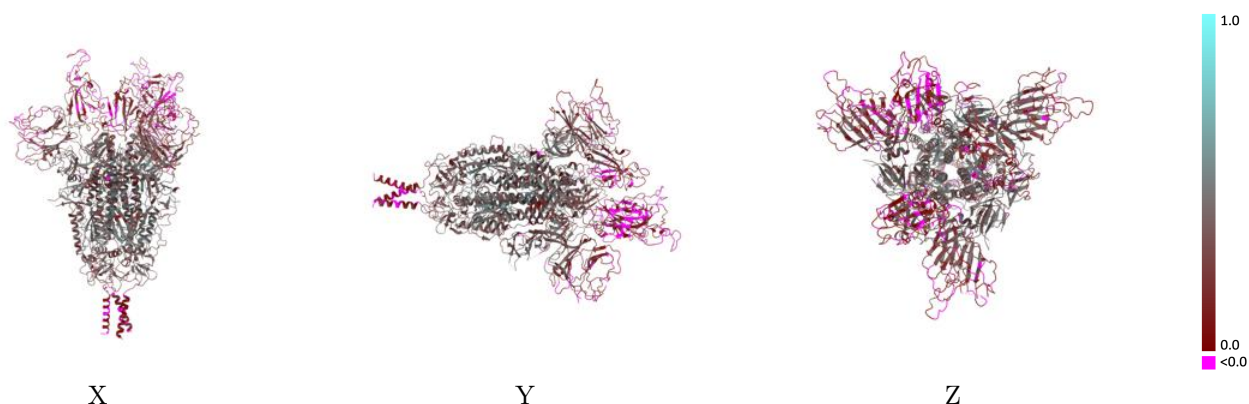
Y



Z

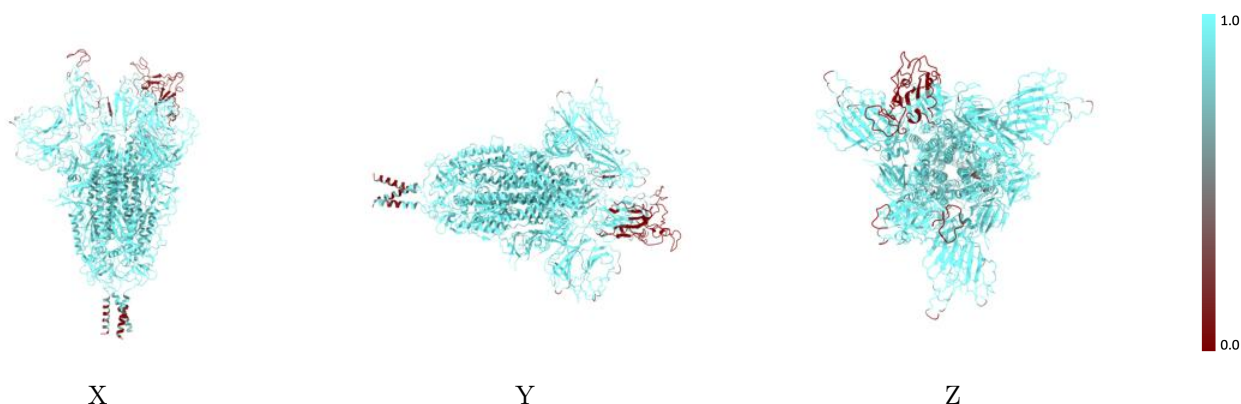
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



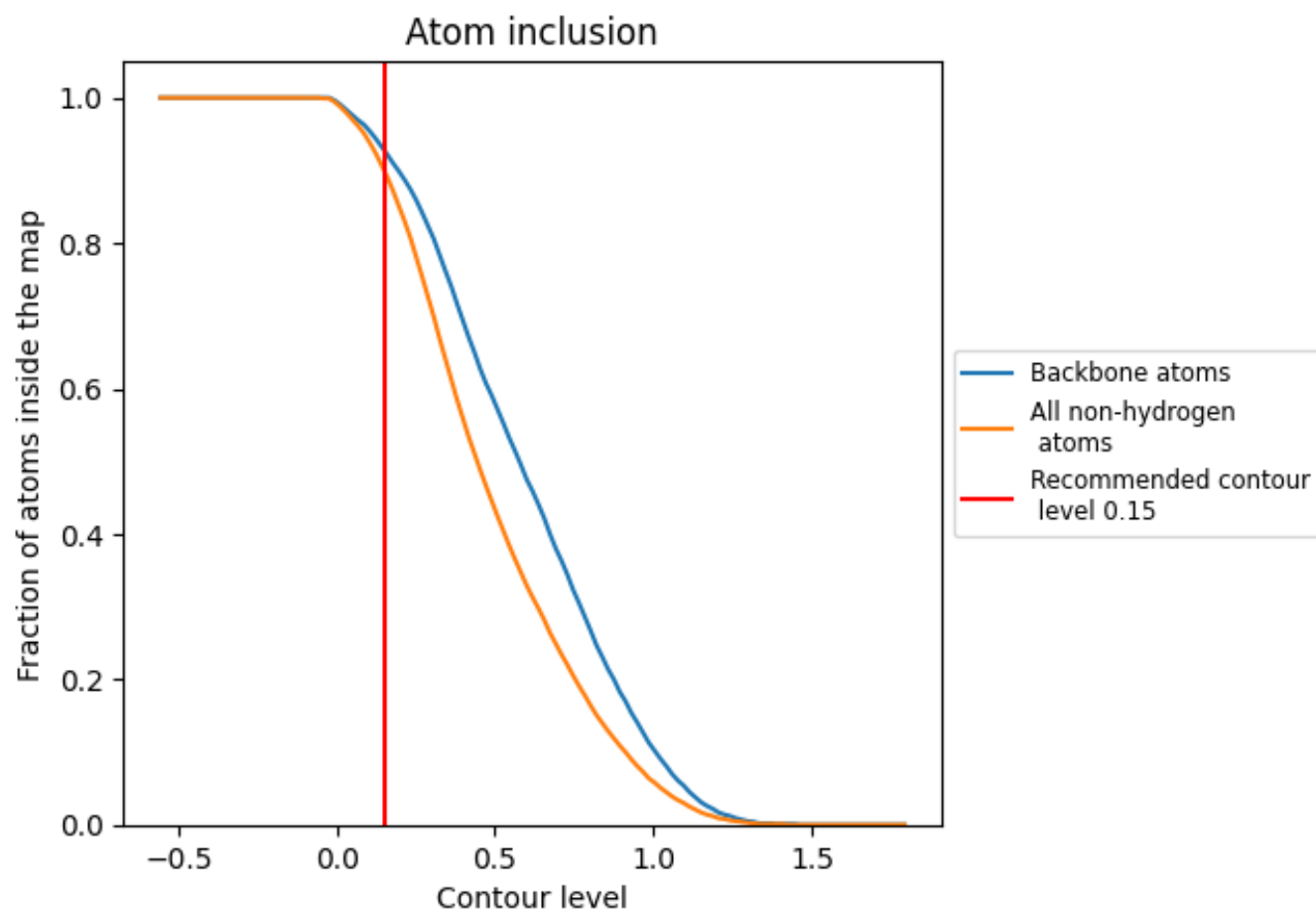
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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> 0.9000	<div></div> 0.2850
A	<div></div> 0.9220	<div></div> 0.2820
B	<div></div> 0.9440	<div></div> 0.2910
C	<div></div> 0.8350	<div></div> 0.2830

