wwPDB EM Validation Summary Report ⓘ

Nov 9, 2024 – 11:04 pm GMT

PDB ID	:	8Q5Y
EMDB ID	:	EMD-18180
Title	:	cryoEM structure of SARS-CoV2 Spike trimer in complex with Fab23
Authors	:	Hallberg, M.; Das, H.
Deposited on	:	2023-08-10
Resolution	:	2.60 Å(reported)

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

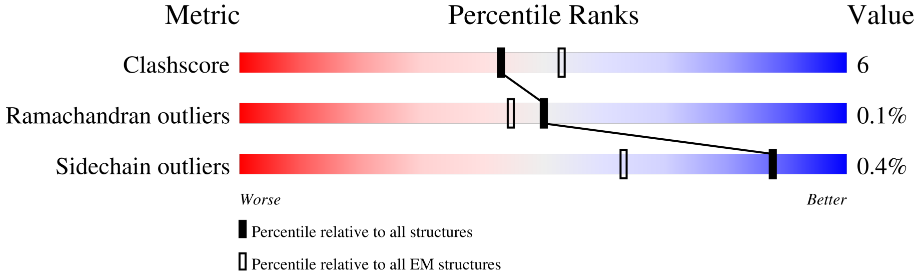
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance ⓘ

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

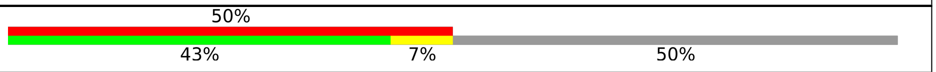
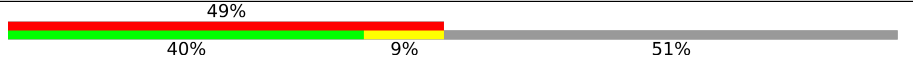
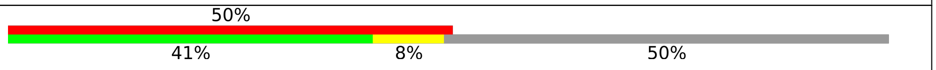
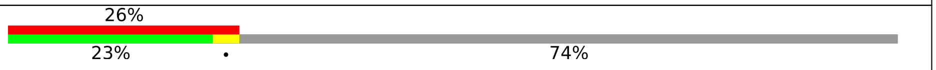
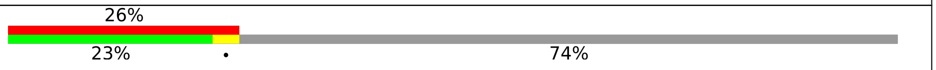
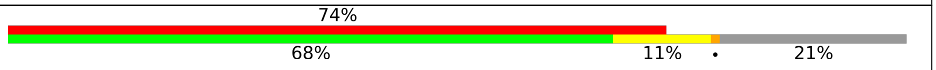
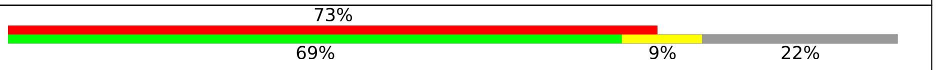
The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

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

Mol	Chain	Length	Quality of chain
1	A	214	
1	H	214	
1	L	214	
2	B	447	
2	G	447	
2	R	447	
3	C	1288	
3	D	1288	

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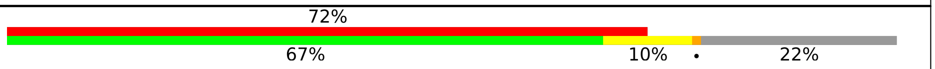
Mol	Chain	Length	Quality of chain
3	E	1288	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 28689 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 Monoclonal antibody Mab 23 (Light chain).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	L	106	798	505	133	157	3	0	0
1	H	104	778	491	131	153	3	0	0
1	A	106	798	505	133	157	3	0	0

- Molecule 2 is a protein called Monoclonal antibody Mab 23 (Heavy Chain).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	R	115	896	567	151	174	4	0	0
2	G	115	896	567	151	174	4	0	0
2	B	116	902	570	152	176	4	0	0

- Molecule 3 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	1002	7825	4998	1300	1492	35	0	0
3	E	1001	7818	4993	1299	1491	35	0	0
3	C	1022	7978	5095	1327	1521	35	0	0

There are 267 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	682	GLY	ARG	conflict	UNP P0DTC2
D	683	SER	ARG	conflict	UNP P0DTC2
D	685	SER	ARG	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	817	PRO	PHE	conflict	UNP P0DTC2
D	899	PRO	ALA	conflict	UNP P0DTC2
D	942	PRO	ALA	conflict	UNP P0DTC2
D	944	PRO	ALA	conflict	UNP P0DTC2
D	986	PRO	LYS	conflict	UNP P0DTC2
D	987	PRO	VAL	conflict	UNP P0DTC2
D	1209	GLY	-	expression tag	UNP P0DTC2
D	1210	SER	-	expression tag	UNP P0DTC2
D	1211	GLY	-	expression tag	UNP P0DTC2
D	1212	TYR	-	expression tag	UNP P0DTC2
D	1213	ILE	-	expression tag	UNP P0DTC2
D	1214	PRO	-	expression tag	UNP P0DTC2
D	1215	GLU	-	expression tag	UNP P0DTC2
D	1216	ALA	-	expression tag	UNP P0DTC2
D	1217	PRO	-	expression tag	UNP P0DTC2
D	1218	ARG	-	expression tag	UNP P0DTC2
D	1219	ASP	-	expression tag	UNP P0DTC2
D	1220	GLY	-	expression tag	UNP P0DTC2
D	1221	GLN	-	expression tag	UNP P0DTC2
D	1222	ALA	-	expression tag	UNP P0DTC2
D	1223	TYR	-	expression tag	UNP P0DTC2
D	1224	VAL	-	expression tag	UNP P0DTC2
D	1225	ARG	-	expression tag	UNP P0DTC2
D	1226	LYS	-	expression tag	UNP P0DTC2
D	1227	ASP	-	expression tag	UNP P0DTC2
D	1228	GLY	-	expression tag	UNP P0DTC2
D	1229	GLU	-	expression tag	UNP P0DTC2
D	1230	TRP	-	expression tag	UNP P0DTC2
D	1231	VAL	-	expression tag	UNP P0DTC2
D	1232	LEU	-	expression tag	UNP P0DTC2
D	1233	LEU	-	expression tag	UNP P0DTC2
D	1234	SER	-	expression tag	UNP P0DTC2
D	1235	THR	-	expression tag	UNP P0DTC2
D	1236	PHE	-	expression tag	UNP P0DTC2
D	1237	LEU	-	expression tag	UNP P0DTC2
D	1238	GLY	-	expression tag	UNP P0DTC2
D	1239	ARG	-	expression tag	UNP P0DTC2
D	1240	SER	-	expression tag	UNP P0DTC2
D	1241	LEU	-	expression tag	UNP P0DTC2
D	1242	GLU	-	expression tag	UNP P0DTC2
D	1243	VAL	-	expression tag	UNP P0DTC2
D	1244	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1245	PHE	-	expression tag	UNP P0DTC2
D	1246	GLN	-	expression tag	UNP P0DTC2
D	1247	GLY	-	expression tag	UNP P0DTC2
D	1248	PRO	-	expression tag	UNP P0DTC2
D	1249	GLY	-	expression tag	UNP P0DTC2
D	1250	HIS	-	expression tag	UNP P0DTC2
D	1251	HIS	-	expression tag	UNP P0DTC2
D	1252	HIS	-	expression tag	UNP P0DTC2
D	1253	HIS	-	expression tag	UNP P0DTC2
D	1254	HIS	-	expression tag	UNP P0DTC2
D	1255	HIS	-	expression tag	UNP P0DTC2
D	1256	HIS	-	expression tag	UNP P0DTC2
D	1257	HIS	-	expression tag	UNP P0DTC2
D	1258	SER	-	expression tag	UNP P0DTC2
D	1259	ALA	-	expression tag	UNP P0DTC2
D	1260	TRP	-	expression tag	UNP P0DTC2
D	1261	SER	-	expression tag	UNP P0DTC2
D	1262	HIS	-	expression tag	UNP P0DTC2
D	1263	PRO	-	expression tag	UNP P0DTC2
D	1264	GLN	-	expression tag	UNP P0DTC2
D	1265	PHE	-	expression tag	UNP P0DTC2
D	1266	GLU	-	expression tag	UNP P0DTC2
D	1267	LYS	-	expression tag	UNP P0DTC2
D	1268	GLY	-	expression tag	UNP P0DTC2
D	1269	GLY	-	expression tag	UNP P0DTC2
D	1270	GLY	-	expression tag	UNP P0DTC2
D	1271	SER	-	expression tag	UNP P0DTC2
D	1272	GLY	-	expression tag	UNP P0DTC2
D	1273	GLY	-	expression tag	UNP P0DTC2
D	1274	GLY	-	expression tag	UNP P0DTC2
D	1275	GLY	-	expression tag	UNP P0DTC2
D	1276	SER	-	expression tag	UNP P0DTC2
D	1277	GLY	-	expression tag	UNP P0DTC2
D	1278	GLY	-	expression tag	UNP P0DTC2
D	1279	SER	-	expression tag	UNP P0DTC2
D	1280	ALA	-	expression tag	UNP P0DTC2
D	1281	TRP	-	expression tag	UNP P0DTC2
D	1282	SER	-	expression tag	UNP P0DTC2
D	1283	HIS	-	expression tag	UNP P0DTC2
D	1284	PRO	-	expression tag	UNP P0DTC2
D	1285	GLN	-	expression tag	UNP P0DTC2
D	1286	PHE	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1287	GLU	-	expression tag	UNP P0DTC2
D	1288	LYS	-	expression tag	UNP P0DTC2
E	682	GLY	ARG	conflict	UNP P0DTC2
E	683	SER	ARG	conflict	UNP P0DTC2
E	685	SER	ARG	conflict	UNP P0DTC2
E	817	PRO	PHE	conflict	UNP P0DTC2
E	899	PRO	ALA	conflict	UNP P0DTC2
E	942	PRO	ALA	conflict	UNP P0DTC2
E	944	PRO	ALA	conflict	UNP P0DTC2
E	986	PRO	LYS	conflict	UNP P0DTC2
E	987	PRO	VAL	conflict	UNP P0DTC2
E	1209	GLY	-	expression tag	UNP P0DTC2
E	1210	SER	-	expression tag	UNP P0DTC2
E	1211	GLY	-	expression tag	UNP P0DTC2
E	1212	TYR	-	expression tag	UNP P0DTC2
E	1213	ILE	-	expression tag	UNP P0DTC2
E	1214	PRO	-	expression tag	UNP P0DTC2
E	1215	GLU	-	expression tag	UNP P0DTC2
E	1216	ALA	-	expression tag	UNP P0DTC2
E	1217	PRO	-	expression tag	UNP P0DTC2
E	1218	ARG	-	expression tag	UNP P0DTC2
E	1219	ASP	-	expression tag	UNP P0DTC2
E	1220	GLY	-	expression tag	UNP P0DTC2
E	1221	GLN	-	expression tag	UNP P0DTC2
E	1222	ALA	-	expression tag	UNP P0DTC2
E	1223	TYR	-	expression tag	UNP P0DTC2
E	1224	VAL	-	expression tag	UNP P0DTC2
E	1225	ARG	-	expression tag	UNP P0DTC2
E	1226	LYS	-	expression tag	UNP P0DTC2
E	1227	ASP	-	expression tag	UNP P0DTC2
E	1228	GLY	-	expression tag	UNP P0DTC2
E	1229	GLU	-	expression tag	UNP P0DTC2
E	1230	TRP	-	expression tag	UNP P0DTC2
E	1231	VAL	-	expression tag	UNP P0DTC2
E	1232	LEU	-	expression tag	UNP P0DTC2
E	1233	LEU	-	expression tag	UNP P0DTC2
E	1234	SER	-	expression tag	UNP P0DTC2
E	1235	THR	-	expression tag	UNP P0DTC2
E	1236	PHE	-	expression tag	UNP P0DTC2
E	1237	LEU	-	expression tag	UNP P0DTC2
E	1238	GLY	-	expression tag	UNP P0DTC2
E	1239	ARG	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1240	SER	-	expression tag	UNP P0DTC2
E	1241	LEU	-	expression tag	UNP P0DTC2
E	1242	GLU	-	expression tag	UNP P0DTC2
E	1243	VAL	-	expression tag	UNP P0DTC2
E	1244	LEU	-	expression tag	UNP P0DTC2
E	1245	PHE	-	expression tag	UNP P0DTC2
E	1246	GLN	-	expression tag	UNP P0DTC2
E	1247	GLY	-	expression tag	UNP P0DTC2
E	1248	PRO	-	expression tag	UNP P0DTC2
E	1249	GLY	-	expression tag	UNP P0DTC2
E	1250	HIS	-	expression tag	UNP P0DTC2
E	1251	HIS	-	expression tag	UNP P0DTC2
E	1252	HIS	-	expression tag	UNP P0DTC2
E	1253	HIS	-	expression tag	UNP P0DTC2
E	1254	HIS	-	expression tag	UNP P0DTC2
E	1255	HIS	-	expression tag	UNP P0DTC2
E	1256	HIS	-	expression tag	UNP P0DTC2
E	1257	HIS	-	expression tag	UNP P0DTC2
E	1258	SER	-	expression tag	UNP P0DTC2
E	1259	ALA	-	expression tag	UNP P0DTC2
E	1260	TRP	-	expression tag	UNP P0DTC2
E	1261	SER	-	expression tag	UNP P0DTC2
E	1262	HIS	-	expression tag	UNP P0DTC2
E	1263	PRO	-	expression tag	UNP P0DTC2
E	1264	GLN	-	expression tag	UNP P0DTC2
E	1265	PHE	-	expression tag	UNP P0DTC2
E	1266	GLU	-	expression tag	UNP P0DTC2
E	1267	LYS	-	expression tag	UNP P0DTC2
E	1268	GLY	-	expression tag	UNP P0DTC2
E	1269	GLY	-	expression tag	UNP P0DTC2
E	1270	GLY	-	expression tag	UNP P0DTC2
E	1271	SER	-	expression tag	UNP P0DTC2
E	1272	GLY	-	expression tag	UNP P0DTC2
E	1273	GLY	-	expression tag	UNP P0DTC2
E	1274	GLY	-	expression tag	UNP P0DTC2
E	1275	GLY	-	expression tag	UNP P0DTC2
E	1276	SER	-	expression tag	UNP P0DTC2
E	1277	GLY	-	expression tag	UNP P0DTC2
E	1278	GLY	-	expression tag	UNP P0DTC2
E	1279	SER	-	expression tag	UNP P0DTC2
E	1280	ALA	-	expression tag	UNP P0DTC2
E	1281	TRP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1282	SER	-	expression tag	UNP P0DTC2
E	1283	HIS	-	expression tag	UNP P0DTC2
E	1284	PRO	-	expression tag	UNP P0DTC2
E	1285	GLN	-	expression tag	UNP P0DTC2
E	1286	PHE	-	expression tag	UNP P0DTC2
E	1287	GLU	-	expression tag	UNP P0DTC2
E	1288	LYS	-	expression tag	UNP P0DTC2
C	682	GLY	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2
C	685	SER	ARG	conflict	UNP P0DTC2
C	817	PRO	PHE	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2
C	942	PRO	ALA	conflict	UNP P0DTC2
C	944	PRO	ALA	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	TYR	-	expression tag	UNP P0DTC2
C	1213	ILE	-	expression tag	UNP P0DTC2
C	1214	PRO	-	expression tag	UNP P0DTC2
C	1215	GLU	-	expression tag	UNP P0DTC2
C	1216	ALA	-	expression tag	UNP P0DTC2
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	ARG	-	expression tag	UNP P0DTC2
C	1219	ASP	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	GLN	-	expression tag	UNP P0DTC2
C	1222	ALA	-	expression tag	UNP P0DTC2
C	1223	TYR	-	expression tag	UNP P0DTC2
C	1224	VAL	-	expression tag	UNP P0DTC2
C	1225	ARG	-	expression tag	UNP P0DTC2
C	1226	LYS	-	expression tag	UNP P0DTC2
C	1227	ASP	-	expression tag	UNP P0DTC2
C	1228	GLY	-	expression tag	UNP P0DTC2
C	1229	GLU	-	expression tag	UNP P0DTC2
C	1230	TRP	-	expression tag	UNP P0DTC2
C	1231	VAL	-	expression tag	UNP P0DTC2
C	1232	LEU	-	expression tag	UNP P0DTC2
C	1233	LEU	-	expression tag	UNP P0DTC2
C	1234	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1235	THR	-	expression tag	UNP P0DTC2
C	1236	PHE	-	expression tag	UNP P0DTC2
C	1237	LEU	-	expression tag	UNP P0DTC2
C	1238	GLY	-	expression tag	UNP P0DTC2
C	1239	ARG	-	expression tag	UNP P0DTC2
C	1240	SER	-	expression tag	UNP P0DTC2
C	1241	LEU	-	expression tag	UNP P0DTC2
C	1242	GLU	-	expression tag	UNP P0DTC2
C	1243	VAL	-	expression tag	UNP P0DTC2
C	1244	LEU	-	expression tag	UNP P0DTC2
C	1245	PHE	-	expression tag	UNP P0DTC2
C	1246	GLN	-	expression tag	UNP P0DTC2
C	1247	GLY	-	expression tag	UNP P0DTC2
C	1248	PRO	-	expression tag	UNP P0DTC2
C	1249	GLY	-	expression tag	UNP P0DTC2
C	1250	HIS	-	expression tag	UNP P0DTC2
C	1251	HIS	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	HIS	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	SER	-	expression tag	UNP P0DTC2
C	1259	ALA	-	expression tag	UNP P0DTC2
C	1260	TRP	-	expression tag	UNP P0DTC2
C	1261	SER	-	expression tag	UNP P0DTC2
C	1262	HIS	-	expression tag	UNP P0DTC2
C	1263	PRO	-	expression tag	UNP P0DTC2
C	1264	GLN	-	expression tag	UNP P0DTC2
C	1265	PHE	-	expression tag	UNP P0DTC2
C	1266	GLU	-	expression tag	UNP P0DTC2
C	1267	LYS	-	expression tag	UNP P0DTC2
C	1268	GLY	-	expression tag	UNP P0DTC2
C	1269	GLY	-	expression tag	UNP P0DTC2
C	1270	GLY	-	expression tag	UNP P0DTC2
C	1271	SER	-	expression tag	UNP P0DTC2
C	1272	GLY	-	expression tag	UNP P0DTC2
C	1273	GLY	-	expression tag	UNP P0DTC2
C	1274	GLY	-	expression tag	UNP P0DTC2
C	1275	GLY	-	expression tag	UNP P0DTC2
C	1276	SER	-	expression tag	UNP P0DTC2

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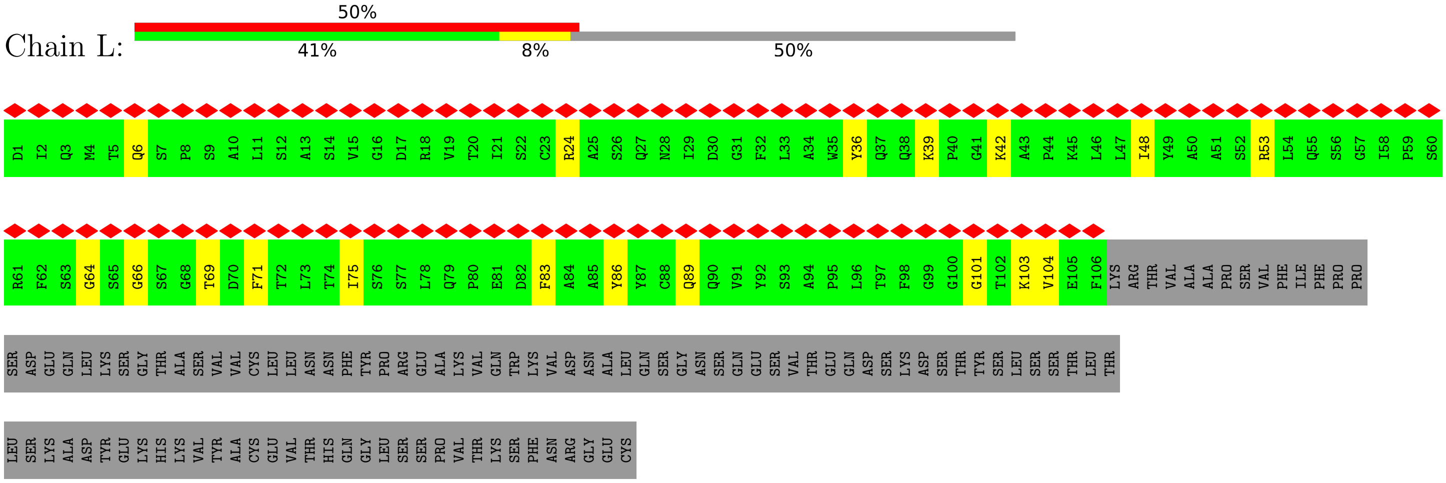
Chain	Residue	Modelled	Actual	Comment	Reference
C	1277	GLY	-	expression tag	UNP P0DTC2
C	1278	GLY	-	expression tag	UNP P0DTC2
C	1279	SER	-	expression tag	UNP P0DTC2
C	1280	ALA	-	expression tag	UNP P0DTC2
C	1281	TRP	-	expression tag	UNP P0DTC2
C	1282	SER	-	expression tag	UNP P0DTC2
C	1283	HIS	-	expression tag	UNP P0DTC2
C	1284	PRO	-	expression tag	UNP P0DTC2
C	1285	GLN	-	expression tag	UNP P0DTC2
C	1286	PHE	-	expression tag	UNP P0DTC2
C	1287	GLU	-	expression tag	UNP P0DTC2
C	1288	LYS	-	expression tag	UNP P0DTC2

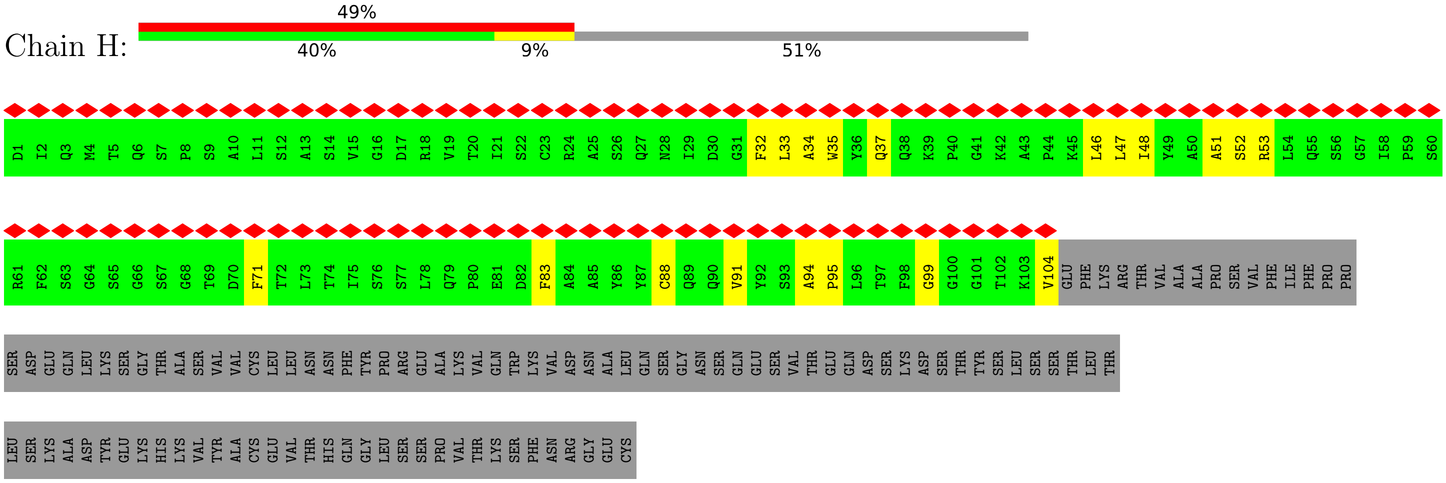
3 Residue-property plots ⓘ

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.

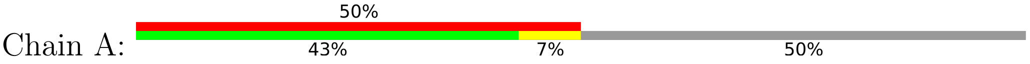
- Molecule 1: Monoclonal antibody Mab 23 (Light chain)

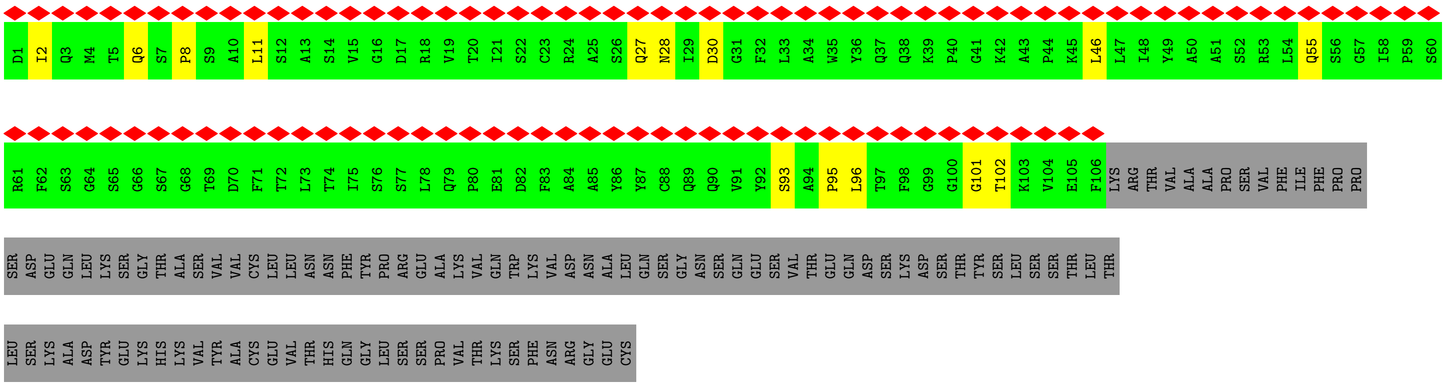


- Molecule 1: Monoclonal antibody Mab 23 (Light chain)



- Molecule 1: Monoclonal antibody Mab 23 (Light chain)

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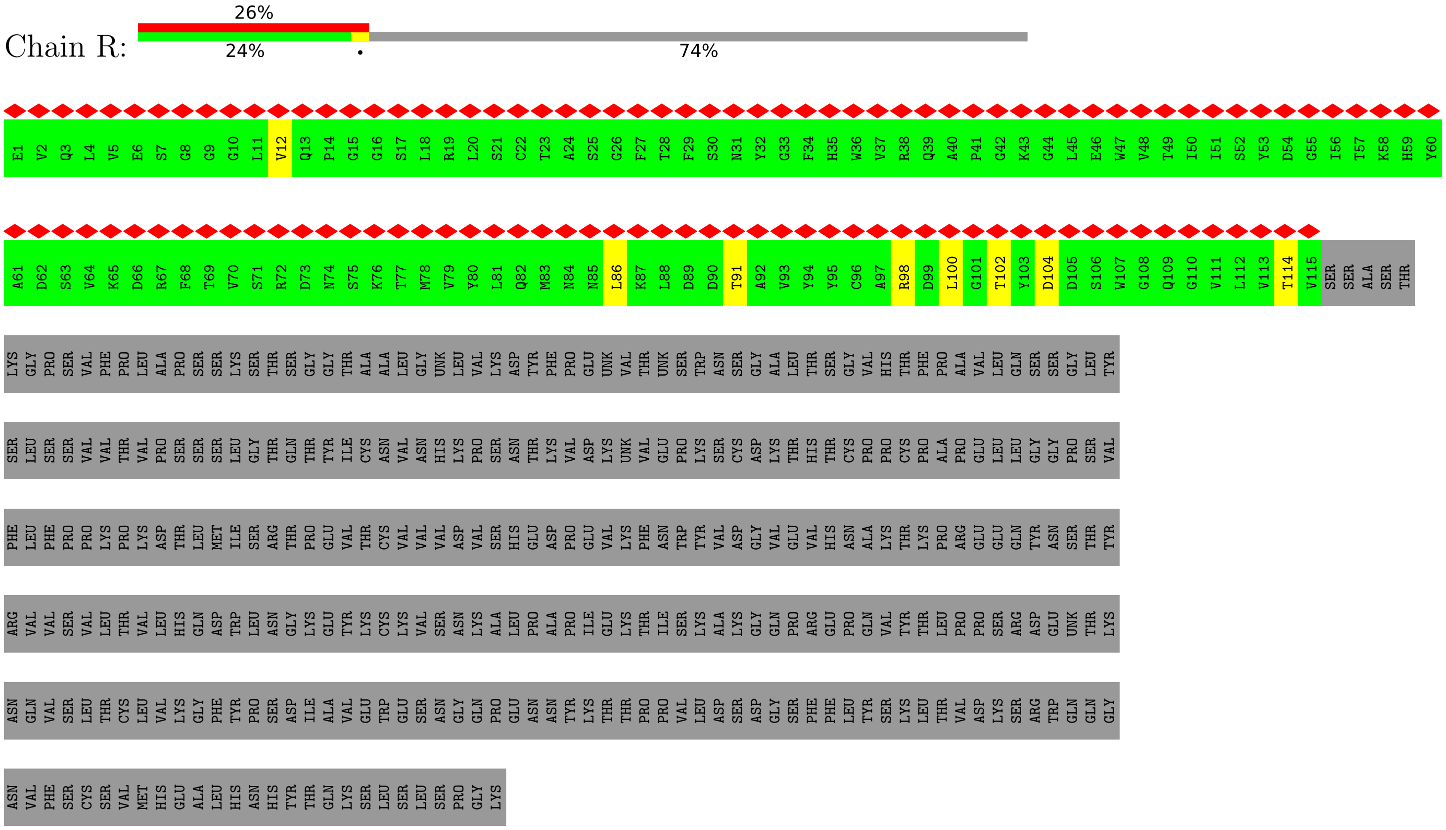
R61 F62 S63 G64 S65 G66 S67 G68 T69 D70 F71 T72 L73 T74 I75 S76 S77 L78 Q79 P80 E81 D82 F83 A84 A85 Y86 Y87 C88 Q89 Q90 V91 Y92 S93 A94 P95 L96 T97 F98 G99 G100 G101 T102 K103 V104 E105 F106 LYS ARG THR VAL ALA ALA PRO SER VAL PHE ILE PHE PRO PRO

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

LEU SER LYS ALA ASP TYR GLU LYS HIS LYS VAL TYR ALA CYS GLU VAL THR HIS GLN GLY LEU SER SER PRO VAL THR LYS SER PHE ASN ARG GLY GLU CYS

- Molecule 2: Monoclonal antibody Mab 23 (Heavy Chain)


Chain R:

26%

24%

•

74%

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A61 D62 S63 V64 K65 D66 R67 F68 T69 V70 S71 R72 D73 N74 S75 K76 T77 M78 V79 Y80 L81 Q82 M83 N84 N85 L86 K87 L88 D89 D90 T91 A92 V93 Y94 Y95 C96 A97 R98 D99 L100 G101 T102 Y103 D104 D105 S106 W107 G108 Q109 G110 V111 L112 V113 T114 V115 SER SER ALA SER THR

LYS GLY PRO SER VAL PHE PRO LEU ALA PRO SER SER LYS SER THR SER GLY GLY THR ALA ALA LEU GLY UNK LEU VAL LYS ASP TYR PHE PRO GLU UNK VAL THR UNK SER TRP ASN SER GLY ALA LEU THR SER GLY VAL HIS THR PHE PRO ALA VAL LEU GLN SER SER GLY LEU TYR

SER LEU SER SER VAL VAL THR VAL PRO SER SER SER LEU GLY THR GLN THR TYR ILE CYS ASN VAL ASN HIS LYS PRO SER ASN THR LYS VAL ASP LYS UNK VAL GLU PRO LYS SER CYS ASP LYS THR HIS THR CYS PRO PRO CYS PRO ALA PRO GLU LEU LEU GLY GLY PRO SER VAL

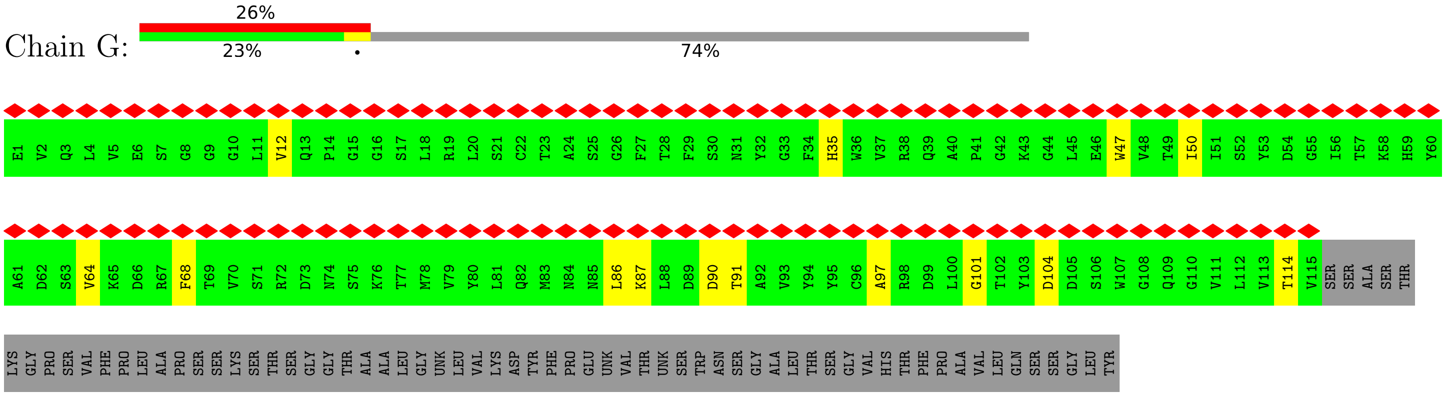
PHE LEU PHE PRO PRO LYS PRO LYS ASP THR LEU MET ILE SER ARG THR PRO GLU VAL THR CYS VAL VAL VAL ASP VAL SER HIS GLU ASP PRO GLU VAL LYS PHE ASN TRP TYR VAL ASP GLY VAL GLU VAL HIS ASN ALA LYS THR LYS PRO ARG GLU GLU GLN TYR ASN SER THR TYR

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

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

ASN VAL PHE SER CYS SER VAL MET HIS GLU ALA LEU HIS ASN HIS TYR THR GLN LYS SER LEU SER LEU SER PRO GLY LYS

- Molecule 2: Monoclonal antibody Mab 23 (Heavy Chain)


Chain G:

26%

23%

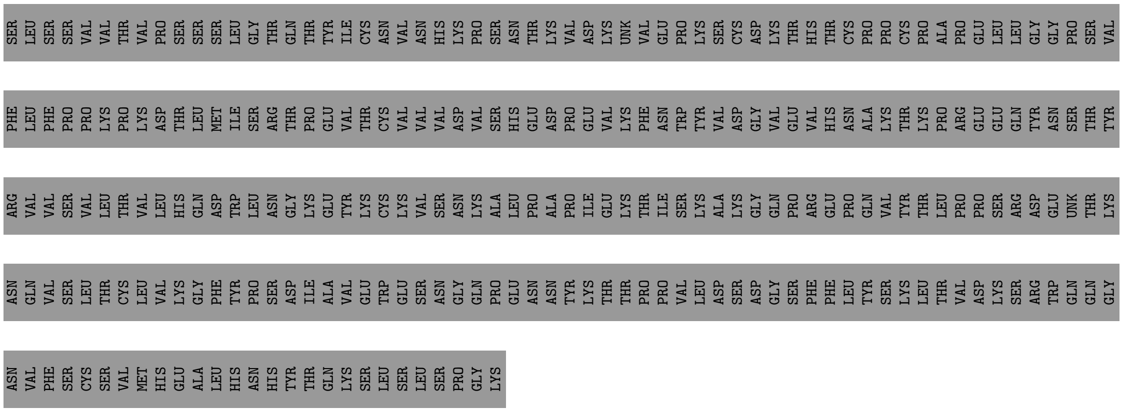
•

74%

E1 V2 Q3 L4 V5 E6 S7 G8 G9 G10 L11 V12 Q13 P14 G15 G16 S17 L18 R19 L20 S21 C22 T23 A24 S25 G26 F27 T28 F29 S30 N31 Y32 G33 F34 H35 W36 V37 R38 Q39 A40 P41 G42 K43 G44 L45 E46 W47 V48 T49 I50 I51 S52 Y53 D54 G55 I56 T57 K58 H59 Y60

A61 D62 S63 V64 K65 D66 R67 F68 T69 V70 S71 R72 D73 N74 S75 K76 T77 M78 V79 Y80 L81 Q82 M83 N84 N85 L86 K87 L88 D89 D90 T91 A92 V93 Y94 Y95 C96 A97 R98 D99 L100 G101 T102 Y103 D104 D105 S106 W107 G108 Q109 G110 V111 L112 V113 T114 V115 SER SER ALA SER THR

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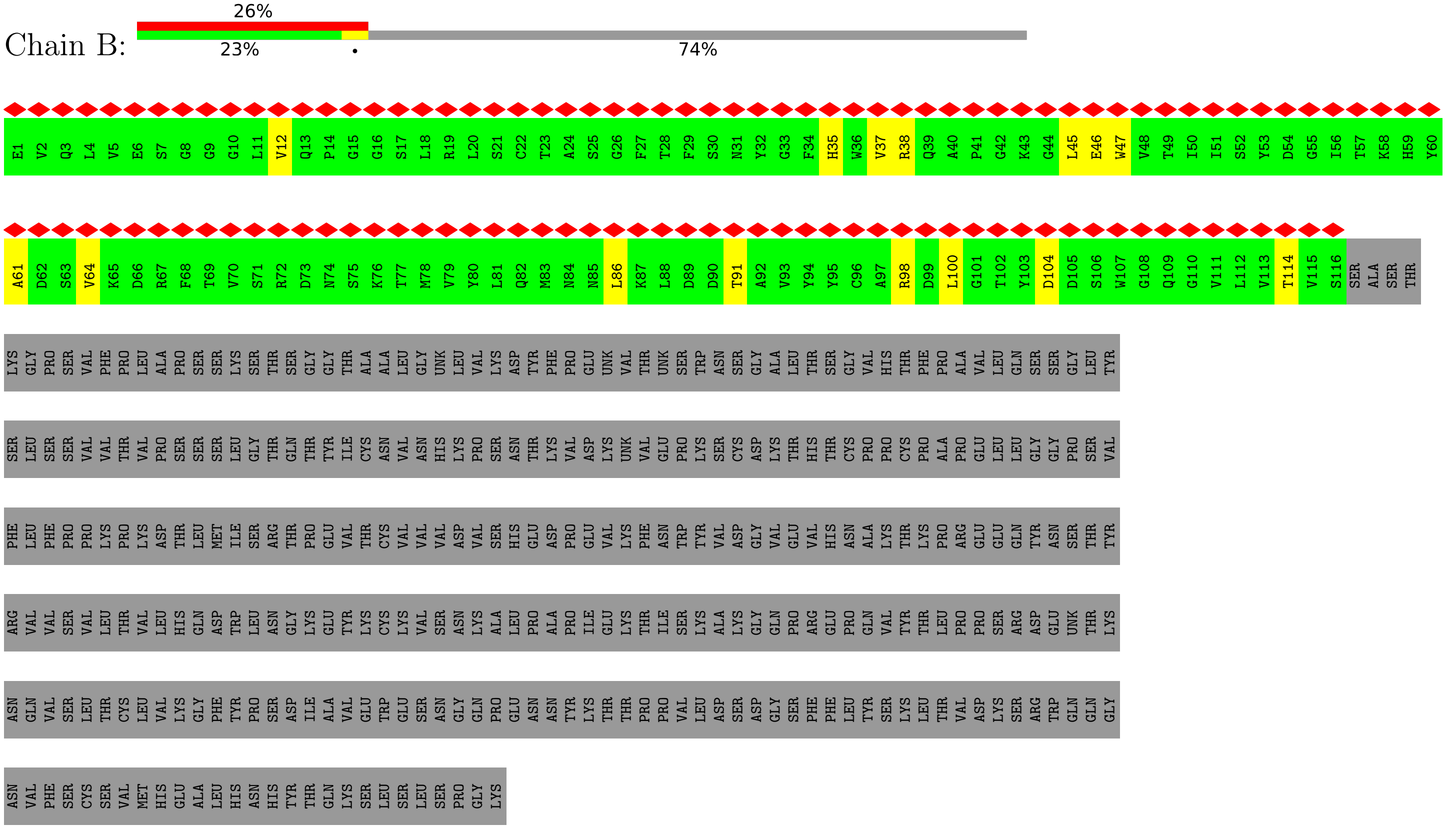
PHE LEU PHE PRO PRO LYS PRO LYS ASP THR LEU MET ILE SER ARG THR PRO GLU VAL THR CYS VAL VAL VAL ASP VAL SER HIS GLU ASP PRO GLU VAL LYS PHE ASN TRP TYR VAL ASP GLY VAL GLU VAL HIS ASN ALA LYS THR LYS PRO ARG GLU GLU GLN TYR ASN SER THR TYR

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

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

ASN VAL PHE SER CYS SER VAL MET HIS GLU ALA LEU HIS ASN HIS TYR THR GLN LYS SER LEU SER LEU SER PRO GLY LYS

- Molecule 2: Monoclonal antibody Mab 23 (Heavy Chain)



E1 V2 Q3 L4 V5 E6 S7 G8 G9 G10 L11 V12 Q13 P14 G15 G16 S17 L18 R19 L20 S21 C22 T23 A24 S25 G26 F27 T28 F29 S30 N31 Y32 G33 F34 H35 W36 V37 R38 Q39 A40 P41 G42 K43 G44 L45 E46 W47 V48 T49 I50 I51 S52 Y53 D54 G55 I56 T57 K58 H59 Y60

A61 D62 S63 V64 K65 D66 R67 F68 T69 V70 S71 R72 D73 N74 S75 K76 T77 M78 V79 Y80 L81 Q82 M83 N84 N85 L86 K87 L88 D89 D90 T91 A92 V93 Y94 Y95 C96 A97 R98 D99 L100 G101 T102 Y103 D104 D105 S106 W107 G108 Q109 G110 V111 L112 V113 T114 V115 S116 SER ALA SER THR

LYS GLY PRO SER VAL PHE PRO LEU ALA PRO SER SER LYS SER THR SER GLY GLY THR ALA ALA LEU GLY UNK LEU VAL LYS ASP TYR PHE PRO GLU UNK VAL THR UNK SER TRP ASN SER GLY ALA LEU THR SER GLY VAL HIS THR PHE PRO ALA VAL LEU GLN SER SER GLY LEU TYR

SER LEU SER SER VAL VAL THR VAL PRO SER SER SER LEU GLY THR GLN THR TYR ILE CYS ASN VAL ASN HIS LYS PRO SER ASN THR LYS VAL ASP LYS UNK VAL GLU PRO LYS SER CYS ASP LYS THR HIS THR CYS PRO PRO CYS PRO ALA PRO GLU LEU LEU GLY GLY PRO SER VAL

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

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

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

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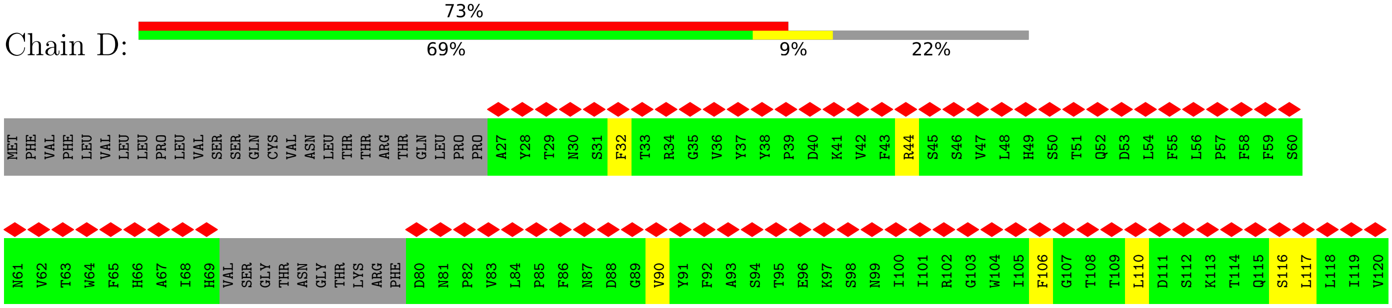
- Molecule 3: Spike glycoprotein



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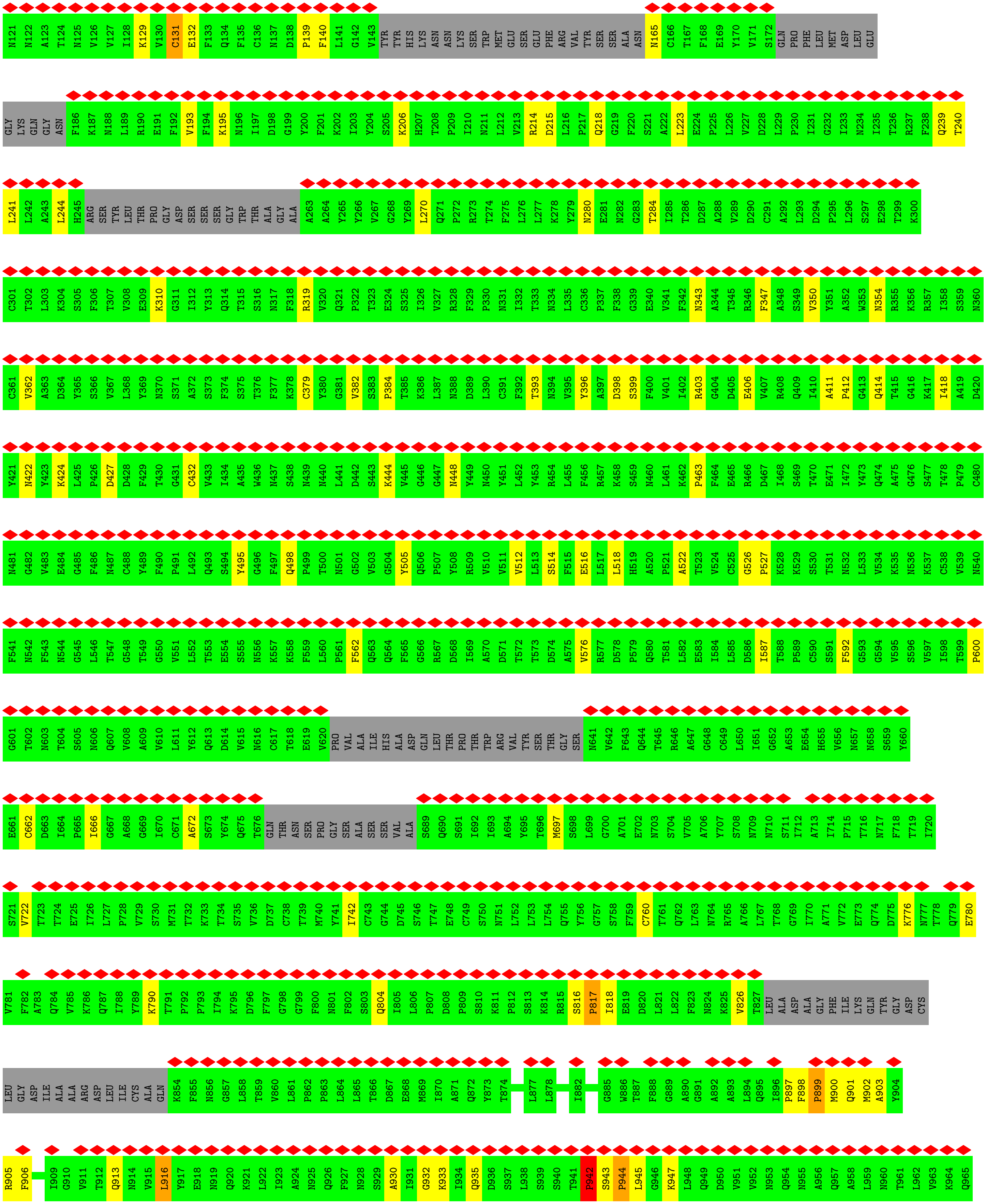
N61 V62 T63 W64 F65 H66 A67 I68 H69 VAL SER GLY THR ASN GLY THR LYS ARG PHE D80 N81 P82 V83 L84 P85 F86 N87 D88 G89 V90 Y91 F92 A93 S94 T95 E96 K97 S98 N99 I100 I101 R102 G103 W104 I105 F106 G107 T108 T109 L110 D111 S112 K113 T114 Q115 S116 L117 L118 I119 V120


N121 N122 A123 T124 N125 V126 V127 I128 K129 V130 C131 E132 F133 Q134 F135 C136 N137 D138 P139 F140 L141 G142 V143 TYR TYR HIS LYS ASN ASN LYS SER TRP MET GLU SER GLU PHE ARG VAL TYR SER SER ALA ASN N165 C166 T167 F168 E169 Y170 V171 S172 GLN PRO PHE LEU MET ASP LEU GLU
GLY LYS GLN GLY ASN F186 K187 N188 L189 R190 E191 F192 V193 F194 K195 N196 I197 D198 G199 Y200 F201 K202 I203 Y204 S205 K206 H207 T208 P209 I210 N211 L212 V213 R214 D215 L216 P217 Q218 G219 F220 S221 A222 L223 E224 P225 L226 V227 D228 L229 P230 I231 G232 I233 N234 I235 T236 R237 F238 Q239 T240
L241 L242 A243 L244 H245 ARG SER TYR LEU THR PRO GLY ASP SER SER SER GLY TRP THR ALA GLY ALA A263 A264 Y265 Y266 V267 G268 Y269 L270 Q271 P272 R273 T274 F275 L276 L277 K278 Y279 N280 E281 N282 G283 T284 I285 T286 D287 A288 V289 D290 C291 A292 L293 D294 P295 L296 S297 E298 T299 K300
C301 T302 L303 K304 S305 F306 T307 V308 E309 K310 G311 I312 Y313 Q314 T315 S316 N317 F318 R319 V320 Q321 P322 T323 E324 S325 I326 V327 R328 F329 P330 N331 I332 T333 N334 L335 C336 P337 F338 G339 E340 V341 F342 N343 A344 T345 R346 F347 A348 S349 V350 Y351 A352 W353 N354 R355 K356 R357 I358 S359 N360
C361 V362 A363 D364 Y365 S366 V367 L368 Y369 N370 S371 A372 S373 F374 S375 T376 F377 K378 C379 Y380 G381 V382 S383 P384 T385 K386 L387 N388 D389 L390 C391 F392 T393 N394 V395 Y396 A397 D398 S399 F400 V401 I402 R403 G404 D405 E406 V407 R408 Q409 I410 A411 P412 G413 Q414 T415 G416 K417 I418 A419 D420
Y421 N422 Y423 K424 L425 P426 D427 D428 F429 T430 G431 C432 V433 I434 A435 W436 N437 S438 N439 N440 L441 D442 S443 K444 V445 G446 G447 N448 Y449 N450 Y451 L452 Y453 R454 L455 F456 R457 K458 S459 N460 L461 K462 P463 F464 E465 R466 D467 I468 S469 T470 E471 I472 Y473 Q474 A475 G476 S477 T478 P479 C480
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F541 N542 F543 N544 G545 L546 T547 G548 T549 G550 V551 L552 T553 E554 S555 N556 K557 K558 F559 L560 P561 F562 Q563 Q564 F565 G566 R567 D568 I569 A570 D571 T572 T573 D574 A575 V576 R577 D578 P579 Q580 T581 L582 E583 I584 L585 D586 I587 T588 P589 C590 S591 F592 G593 G594 V595 S596 V597 I598 T599 P600
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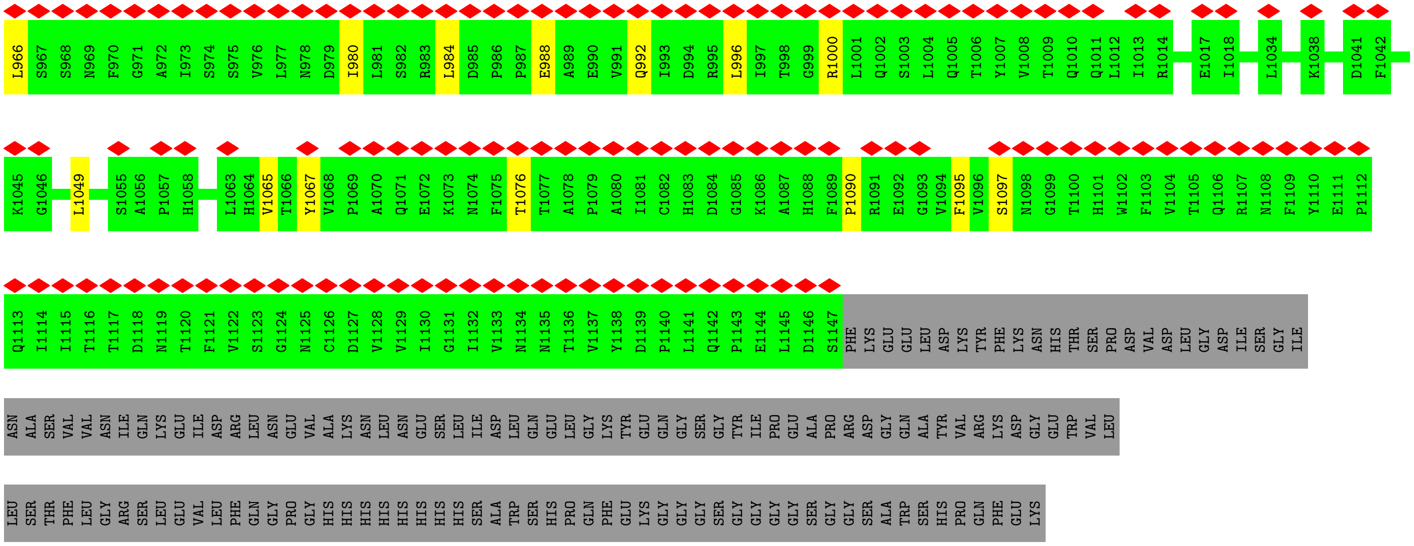
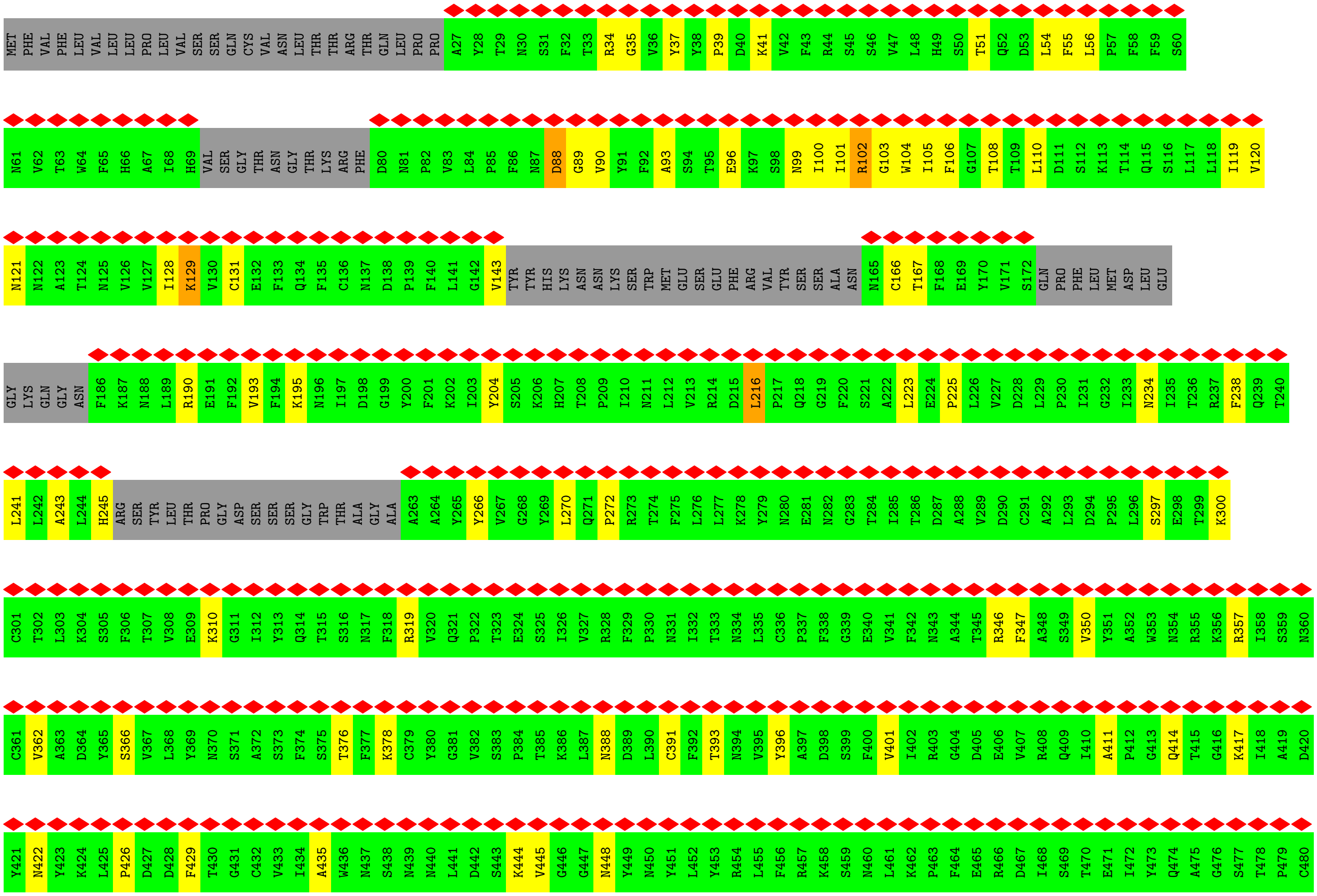
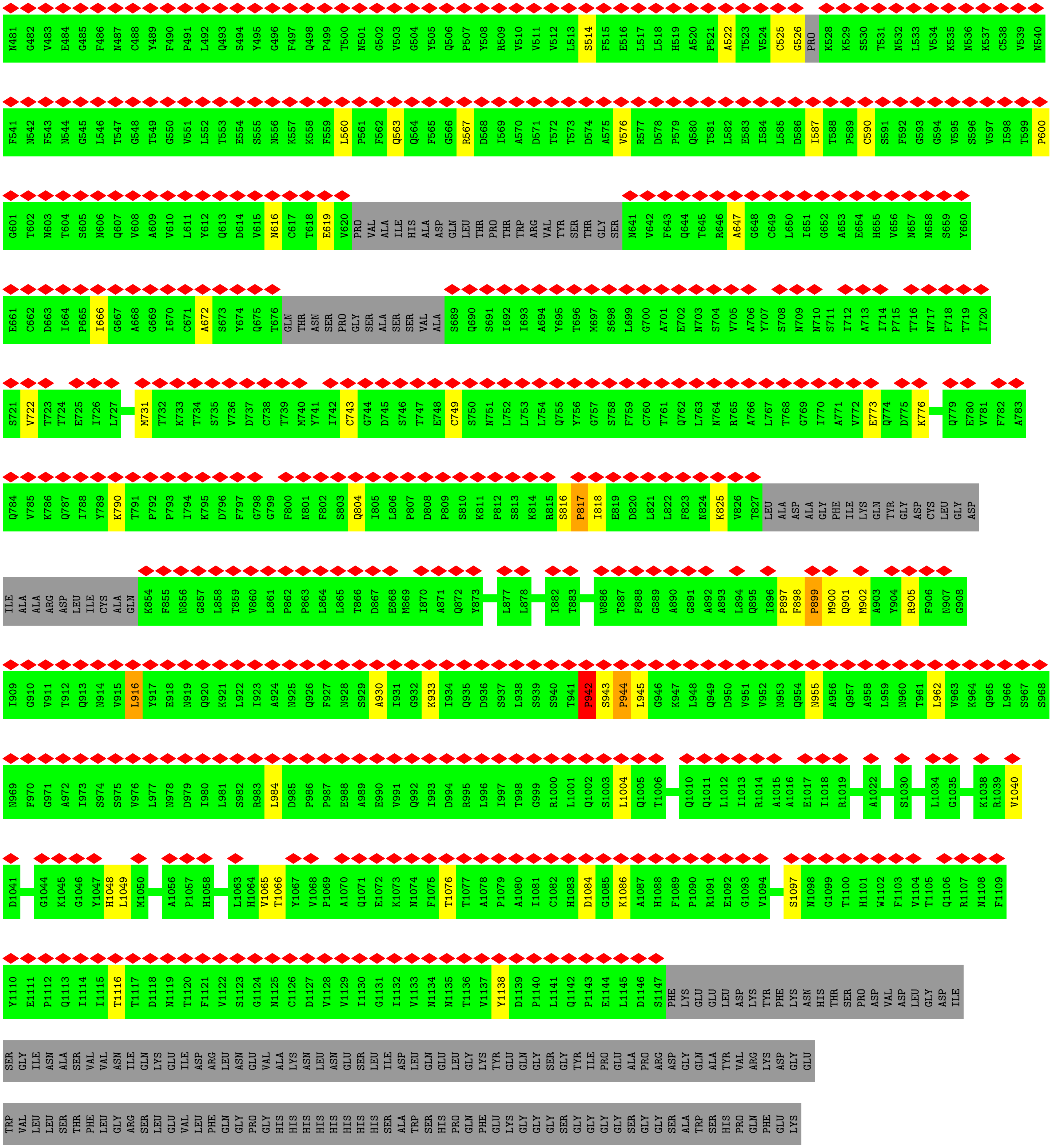
S721 V722 T723 T724 E725 I726 L727 P728 V729 S730 M731 T732 K733 T734 S735 V736 D737 C738 T739 M740 Y741 I742 C743 G744 D745 S746 T747 E748 C749 S750 N751 L752 L753 L754 Q755 Y756 G757 S758 F759 C760 T761 Q762 L763 N764 R765 A766 L767 T768 G769 I770 A771 V772 E773 Q774 D775 K776 N777 T778 Q779 E780
V781 F782 A783 Q784 V785 K786 Q787 I788 Y789 K790 T791 P792 P793 I794 K795 D796 F797 G798 G799 F800 N801 F802 S803 Q804 I805 L806 P807 D808 P809 S810 K811 P812 S813 K814 R815 S816 P817 I818 E819 D820 L821 L822 F823 N824 K825 V826 T827 LEU ALA ASP ALA GLY PHE ILE LYS GLN TYR GLY ASP CYS
LEU GLY ASP ILE ALA ALA ARG ASP LEU ILE CYS ALA GLN K854 F855 N856 G857 L858 T859 V860 L861 P862 P863 L864 L865 T866 D867 E868 M869 I870 A871 Q872 Y873 T874 L877 L878 I882 G885 W886 T887 F888 G889 A890 G891 A892 A893 L894 Q895 I896 P897 F898 P899 M900 Q901 M902 A903 Y904
R905 F906 I909 G910 V911 T912 Q913 N914 V915 L916 Y917 E918 N919 Q920 K921 L922 I923 A924 N925 Q926 F927 N928 S929 A930 I931 G932 K933 I934 Q935 D936 S937 L938 S939 S940 T941 P942 S943 P944 A945 G946 K947 L948 Q949 D950 V951 V952 N953 Q954 N955 A956 Q957 A958 L959 N960 T961 L962 V963 K964 Q965



- Molecule 3: Spike glycoprotein

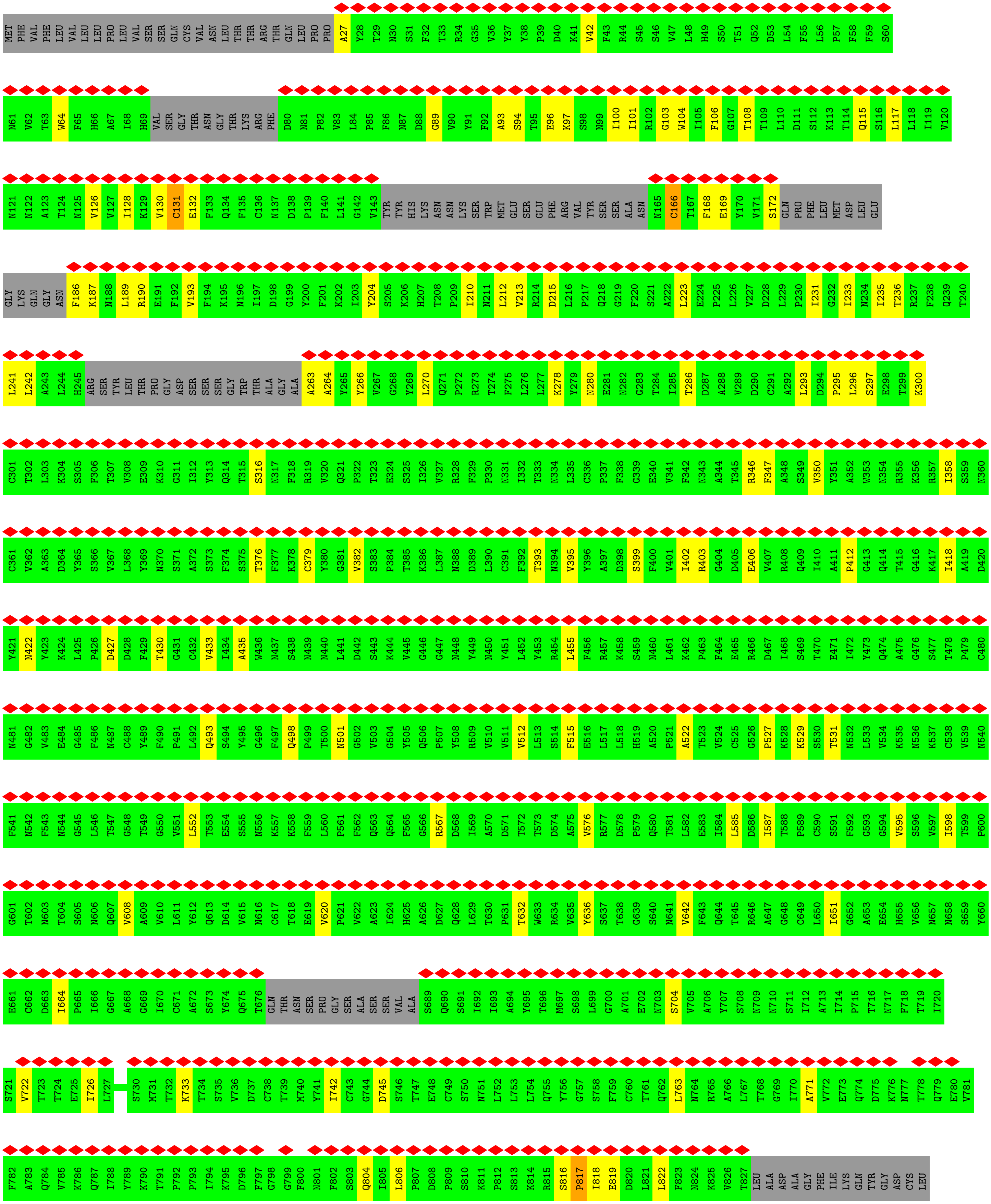
Chain E:





- Molecule 3: Spike glycoprotein

Chain C:


MET PHE VAL PHE LEU VAL LEU LEU PRO LEU VAL SER SER GLN CYS VAL ASN LEU THR THR ARG THR GLN LEU PRO PRO A27 Y28 T29 N30 S31 F32 T33 R34 G35 V36 Y37 Y38 P39 D40 K41 V42 F43 R44 S45 S46 V47 L48 H49 S50 T51 Q52 D53 L54 F55 L56 P57 F58 F59 S60
N61 V62 T63 W64 F65 H66 A67 I68 H69 VAL SER GLY THR ASN GLY THR LYS ARG PHE D80 N81 P82 V83 L84 P85 F86 N87 D88 G89 V90 Y91 F92 A93 S94 T95 E96 K97 S98 N99 I100 I101 R102 G103 W104 I105 F106 G107 T108 T109 L110 D111 S112 K113 T114 Q115 S116 L117 L118 I119 V120
N121 N122 A123 T124 N125 V126 V127 I128 K129 V130 C131 E132 F133 Q134 F135 C136 N137 D138 P139 F140 L141 G142 V143 TYR TYR HIS LYS ASN ASN LYS SER TRP MET GLU SER GLU PHE ARG VAL TYR SER SER ALA ASN N165 C166 T167 F168 E169 Y170 V171 S172 GLN PRO PHE LEU MET ASP LEU GLU
GLY LYS GLN GLY ASN F186 K187 N188 L189 R190 E191 F192 V193 F194 K195 N196 I197 D198 G199 Y200 F201 K202 I203 Y204 S205 K206 H207 T208 P209 I210 N211 L212 V213 R214 D215 L216 P217 Q218 G219 F220 S221 A222 L223 E224 P225 L226 V227 D228 L229 P230 I231 G232 I233 N234 I235 T236 R237 F238 Q239 T240
L241 L242 A243 L244 H245 ARG SER TYR LEU THR PRO GLY ASP SER SER SER GLY TRP THR ALA GLY ALA A263 A264 Y265 Y266 V267 G268 Y269 L270 Q271 P272 R273 T274 F275 L276 L277 K278 Y279 N280 E281 N282 G283 T284 I285 T286 D287 A288 V289 D290 C291 A292 L293 D294 P295 L296 S297 E298 T299 K300
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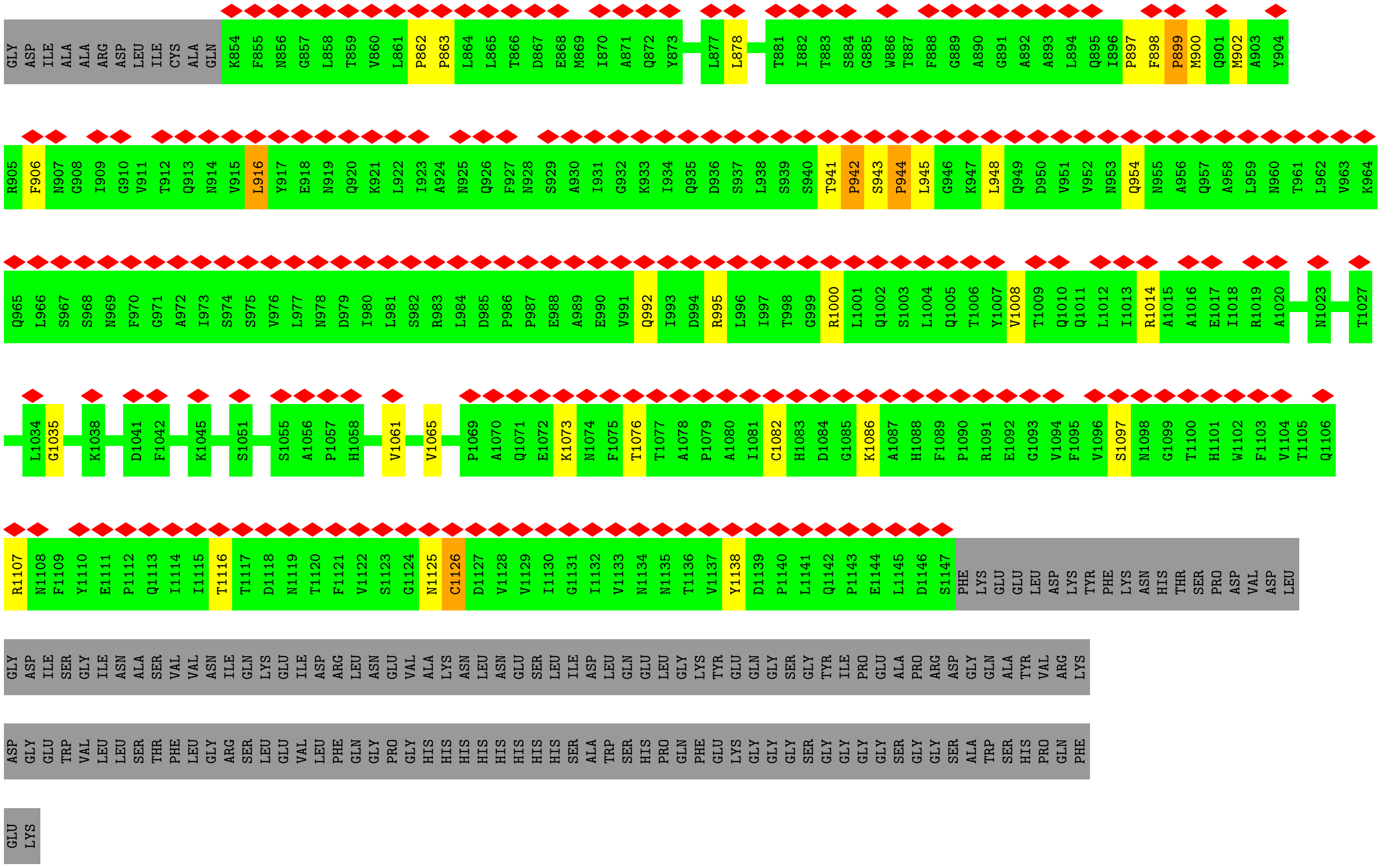
F541 N542 F543 N544 G545 L546 T547 G548 T549 G550 V551 L552 T553 E554 S555 N556 K557 K558 F559 L560 P561 F562 Q563 Q564 F565 G566 R567 D568 I569 A570 D571 T572 T573 D574 A575 V576 R577 D578 P579 Q580 T581 L582 E583 I584 L585 D586 I587 T588 P589 C590 S591 F592 G593 G594 V595 S596 V597 I598 T599 P600
G601 T602 N603 T604 S605 N606 Q607 V608 A609 V610 L611 Y612 Q613 D614 V615 N616 C617 T618 E619 V620 P621 V622 A623 I624 H625 A626 D627 Q628 L629 T630 P631 T632 W633 R634 V635 Y636 S637 T638 G639 S640 N641 V642 F643 Q644 T645 R646 A647 G648 C649 L650 I651 G652 A653 E654 H655 V656 N657 N658 S659 Y660
E661 C662 D663 I664 P665 I666 G667 A668 G669 I670 C671 A672 S673 Y674 Q675 T676 GLN THR ASN SER PRO GLY SER ALA SER SER VAL ALA S689 Q690 S691 I692 I693 A694 Y695 T696 M697 S698 L699 G700 A701 E702 N703 S704 V705 A706 Y707 S708 N709 N710 S711 I712 A713 I714 P715 T716 N717 F718 T719 I720
S721 V722 T723 T724 E725 I726 L727 S730 M731 T732 K733 T734 S735 V736 D737 C738 T739 M740 Y741 I742 C743 G744 D745 S746 T747 E748 C749 S750 N751 L752 L753 L754 Q755 Y756 G757 S758 F759 C760 T761 Q762 L763 N764 R765 A766 L767 T768 G769 I770 A771 V772 E773 Q774 D775 K776 N777 T778 Q779 E780 V781
F782 A783 Q784 V785 K786 Q787 I788 Y789 K790 T791 P792 P793 I794 K795 D796 F797 G798 G799 F800 N801 F802 S803 Q804 I805 L806 P807 D808 P809 S810 K811 P812 S813 K814 R815 S816 P817 I818 E819 D820 L821 L822 F823 N824 K825 V826 T827 LEU ALA ASP ALA GLY PHE ILE LYS GLN TYR GLY ASP CYS LEU


GLY ASP ILE ALA ALA ARG ASP LEU ILE CYS ALA GLN K854 F855 N856 G857 L858 T859 V860 L861 P862 P863 L864 L865 T866 D867 E868 M869 I870 A871 Q872 Y873 L877 L878 T881 I882 T883 S884 G885 W886 T887 F888 G889 A890 G891 A892 A893 L894 Q895 I896 P897 F898 P899 M900 Q901 M902 A903 Y904
R905 F906 N907 G908 I909 G910 V911 T912 Q913 N914 V915 L916 Y917 E918 N919 Q920 K921 L922 I923 A924 N925 Q926 F927 N928 S929 A930 I931 G932 K933 I934 Q935 D936 S937 L938 S939 S940 T941 P942 S943 P944 L945 G946 K947 L948 Q949 D950 V951 V952 N953 Q954 N955 A956 Q957 A958 L959 N960 T961 L962 V963 K964
Q965 L966 S967 S968 N969 F970 G971 A972 I973 S974 S975 V976 L977 N978 D979 I980 L981 S982 R983 L984 D985 P986 P987 E988 A989 E990 V991 Q992 I993 D994 R995 L996 I997 T998 G999 R1000 L1001 Q1002 S1003 L1004 Q1005 T1006 Y1007 V1008 T1009 Q1010 Q1011 L1012 I1013 R1014 A1015 A1016 E1017 I1018 R1019 A1020 N1023 T1027
L1034 G1035 K1038 D1041 F1042 K1045 S1051 S1055 A1056 P1057 H1058 V1061 V1065 P1069 A1070 Q1071 E1072 K1073 N1074 F1075 T1076 T1077 A1078 P1079 A1080 I1081 C1082 H1083 D1084 G1085 K1086 A1087 H1088 F1089 P1090 R1091 E1092 G1093 V1094 F1095 V1096 S1097 N1098 G1099 T1100 H1101 W1102 F1103 V1104 T1105 Q1106
R1107 N1108 F1109 Y1110 E1111 P1112 Q1113 I1114 I1115 T1116 T1117 D1118 N1119 T1120 F1121 V1122 S1123 G1124 N1125 C1126 D1127 V1128 V1129 I1130 G1131 I1132 V1133 N1134 N1135 T1136 V1137 Y1138 D1139 P1140 L1141 Q1142 P1143 E1144 L1145 D1146 S1147 PHE LYS GLU GLU LEU ASP LYS TYR PHE LYS ASN HIS THR SER PRO ASP VAL ASP LEU
GLY ASP ILE SER GLY ILE ASN ALA SER VAL VAL ASN ILE GLN LYS GLU ILE ASP ARG LEU ASN GLU VAL ALA LYS ASN LEU ASN GLU SER LEU ILE ASP LEU GLN GLU LEU GLY LYS TYR GLU GLN GLY SER GLY TYR ILE PRO GLU ALA PRO ARG ASP GLY GLN ALA TYR VAL ARG LYS
ASP GLY GLU TRP VAL LEU LEU SER THR PHE LEU GLY ARG SER LEU GLU VAL LEU PHE GLN GLY PRO GLY HIS HIS HIS HIS HIS HIS HIS HIS SER ALA TRP SER HIS PRO GLN PHE GLU LYS GLY GLY GLY SER GLY GLY GLY GLY SER GLY GLY SER ALA TRP SER HIS PRO GLN PHE
GLU LYS

4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	135612	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	48	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	165000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.808	Depositor
Minimum map value	-3.324	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	1.9	Depositor
Map size (Å)	517.12, 517.12, 517.12	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.01, 1.01, 1.01	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	A	0.31	0/816	0.67	0/1106
1	H	0.38	0/795	0.64	0/1078
1	L	0.35	0/816	0.68	0/1106
2	B	0.31	0/922	0.61	0/1251
2	G	0.31	0/916	0.63	0/1243
2	R	0.30	0/916	0.59	0/1243
3	C	0.35	0/8163	0.65	9/11118 (0.1%)
3	D	0.38	2/8004 (0.0%)	0.63	6/10896 (0.1%)
3	E	0.35	0/7995	0.63	7/10881 (0.1%)
All	All	0.36	2/29343 (0.0%)	0.64	22/39922 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	131	CYS	CB-SG	-5.41	1.73	1.81
3	D	760	CYS	CB-SG	-5.15	1.73	1.81

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	942	PRO	CA-N-CD	-9.04	98.85	111.50
3	E	944	PRO	CA-N-CD	-9.00	98.90	111.50
3	E	899	PRO	CA-N-CD	-8.98	98.93	111.50
3	E	88	ASP	CB-CG-OD1	8.83	126.24	118.30
3	C	944	PRO	CA-N-CD	-8.81	99.17	111.50

There are no chirality outliers.

There are no planarity outliers.

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	A	798	0	778	9	0
1	H	778	0	763	13	0
1	L	798	0	778	11	0
2	B	902	0	866	10	0
2	G	896	0	861	9	0
2	R	896	0	861	5	0
3	C	7978	0	7788	113	0
3	D	7825	0	7644	98	0
3	E	7818	0	7636	112	0
All	All	28689	0	27975	363	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 363 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)
3:E:804:GLN:O	3:E:817:PRO:CD	1.82	1.26
3:C:804:GLN:O	3:C:817:PRO:CD	1.92	1.16
3:C:899:PRO:HD2	3:C:900:MET:H	1.10	1.15
3:D:944:PRO:HD2	3:D:945:LEU:H	1.10	1.15
3:E:899:PRO:HD2	3:E:900:MET:H	1.11	1.15

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	A	104/214 (49%)	100 (96%)	4 (4%)	0	100	100
1	H	102/214 (48%)	93 (91%)	9 (9%)	0	100	100
1	L	104/214 (49%)	96 (92%)	8 (8%)	0	100	100
2	B	114/447 (26%)	114 (100%)	0	0	100	100
2	G	113/447 (25%)	110 (97%)	3 (3%)	0	100	100
2	R	113/447 (25%)	113 (100%)	0	0	100	100
3	C	1008/1288 (78%)	983 (98%)	25 (2%)	0	100	100
3	D	986/1288 (77%)	964 (98%)	21 (2%)	1 (0%)	48	71
3	E	983/1288 (76%)	962 (98%)	20 (2%)	1 (0%)	48	71
All	All	3627/5847 (62%)	3535 (98%)	90 (2%)	2 (0%)	50	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	942	PRO
3	E	942	PRO

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	A	86/183 (47%)	86 (100%)	0	100	100
1	H	84/183 (46%)	84 (100%)	0	100	100
1	L	86/183 (47%)	86 (100%)	0	100	100
2	B	98/393 (25%)	98 (100%)	0	100	100
2	G	97/393 (25%)	97 (100%)	0	100	100
2	R	97/393 (25%)	97 (100%)	0	100	100
3	C	895/1116 (80%)	892 (100%)	3 (0%)	91	97
3	D	879/1116 (79%)	876 (100%)	3 (0%)	91	97
3	E	878/1116 (79%)	872 (99%)	6 (1%)	81	93

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3200/5076 (63%)	3188 (100%)	12 (0%)	88 96

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	167	THR
3	E	916	LEU
3	C	1107	ARG
3	C	166	CYS
3	E	102	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	89	GLN
3	D	448	ASN
3	D	450	ASN
3	D	498	GLN
3	E	907	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 ⓘ

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.

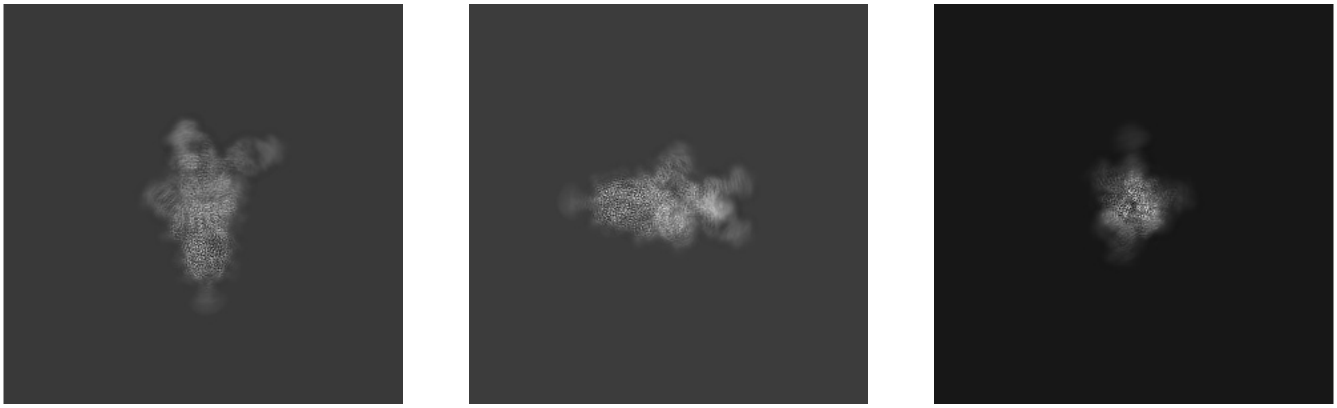
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-18180. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

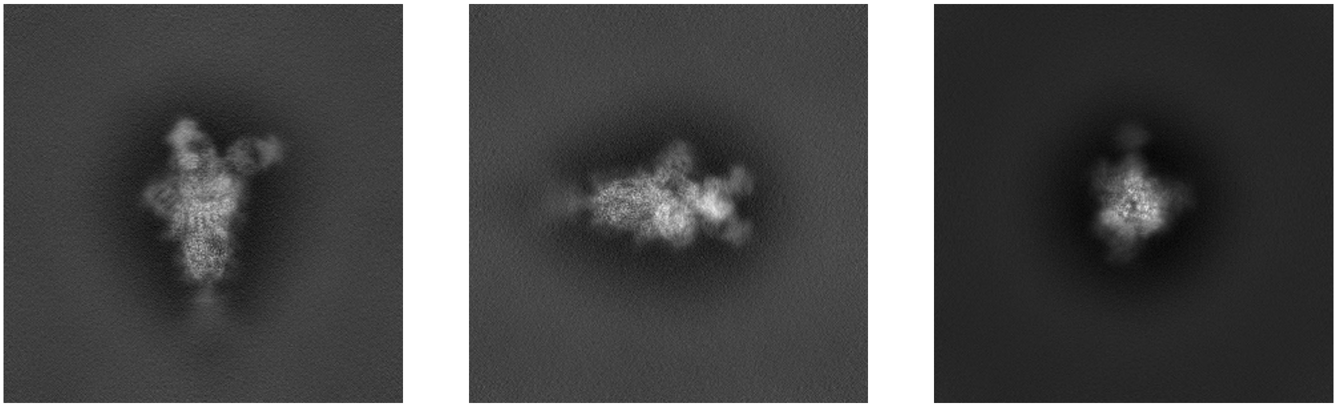
6.1 Orthogonal projections ⓘ

6.1.1 Primary map



X Y Z

6.1.2 Raw map

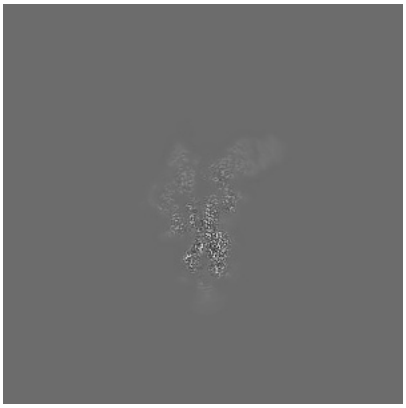


X Y Z

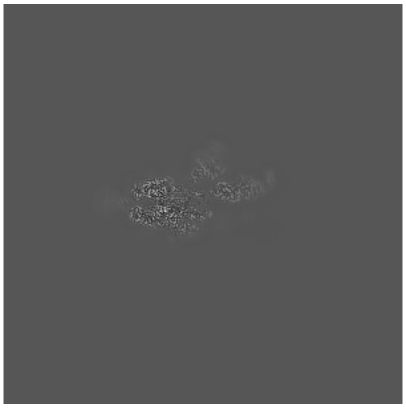
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

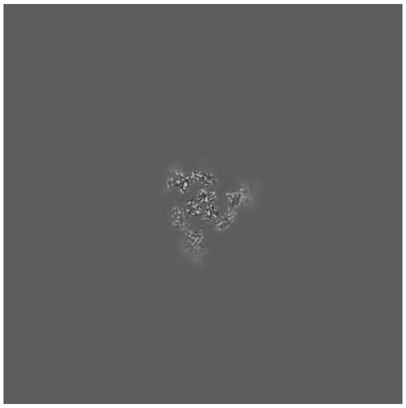
6.2.1 Primary map



X Index: 256

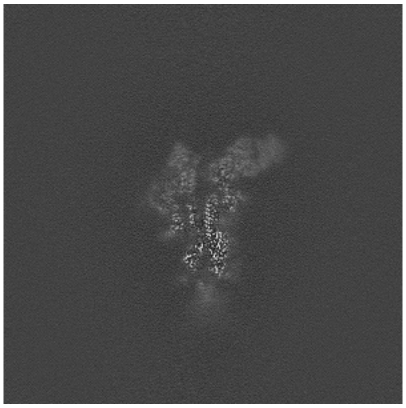


Y Index: 256

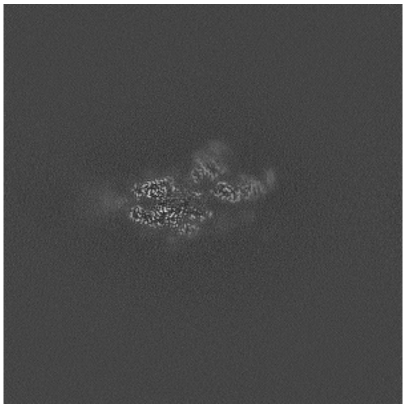


Z Index: 256

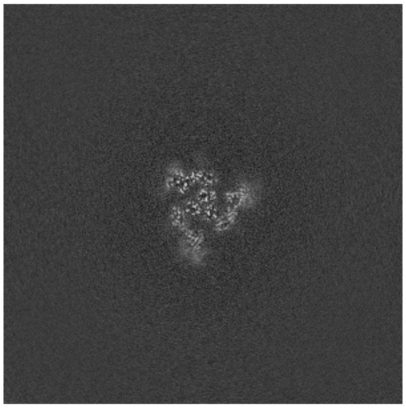
6.2.2 Raw map



X Index: 256



Y Index: 256

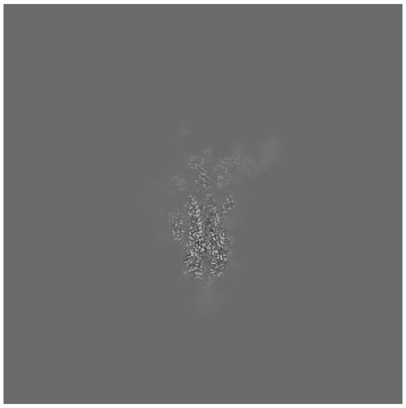


Z Index: 256

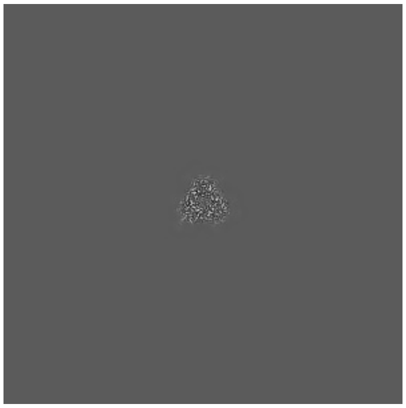
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ

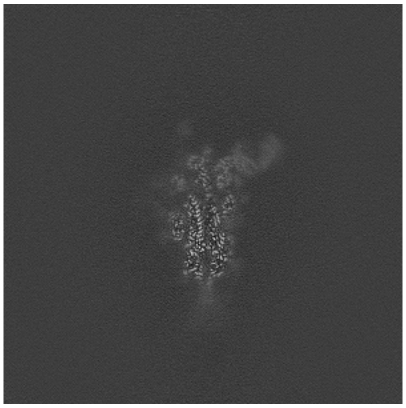
6.3.1 Primary map


X Index: 263

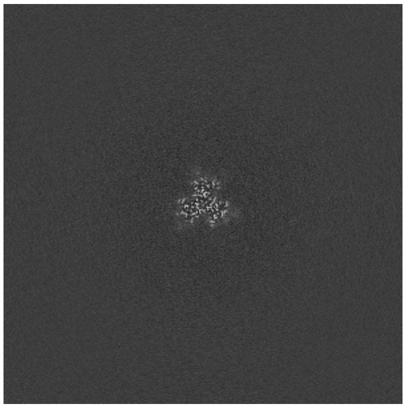

Y Index: 251


Z Index: 193

6.3.2 Raw map


X Index: 263

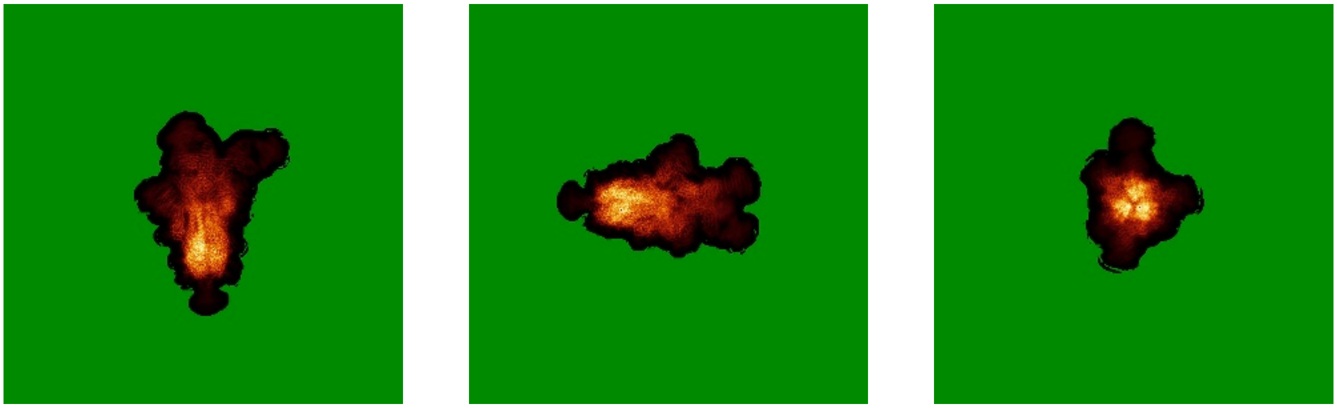

Y Index: 252


Z Index: 201

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

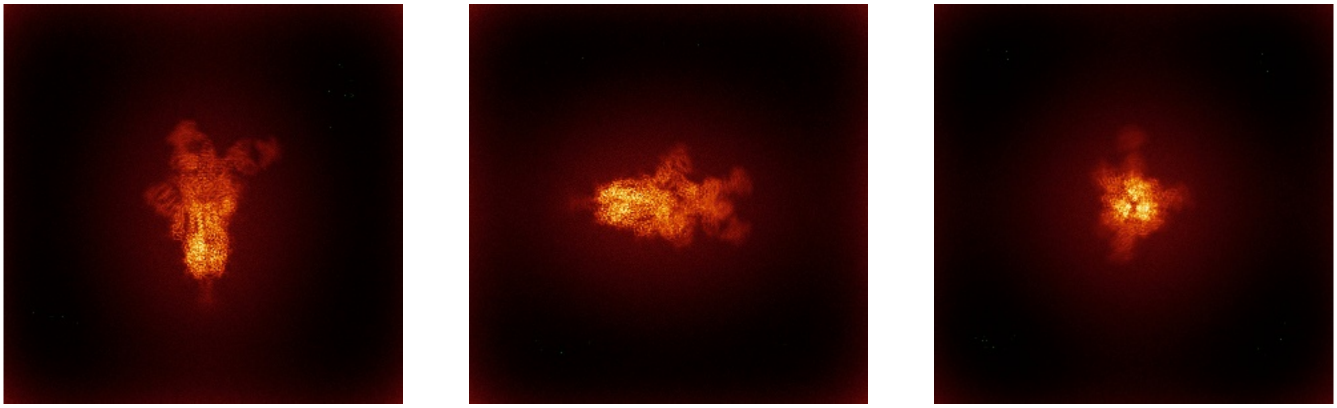
6.4 Orthogonal standard-deviation projections (False-color) ⓘ

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 ⓘ

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 1.9. 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.

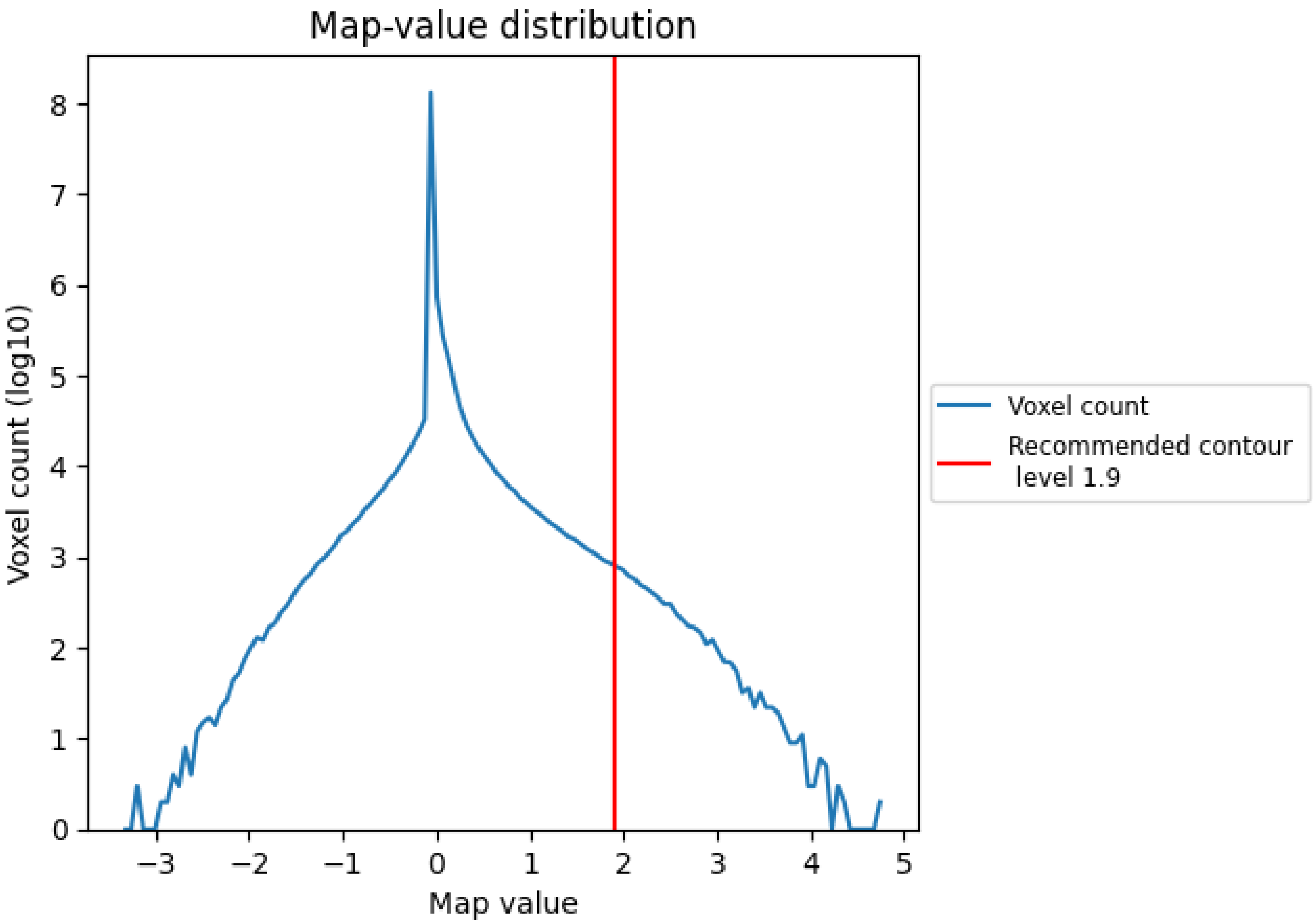
6.6 Mask visualisation ⓘ

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

7 Map analysis ⓘ

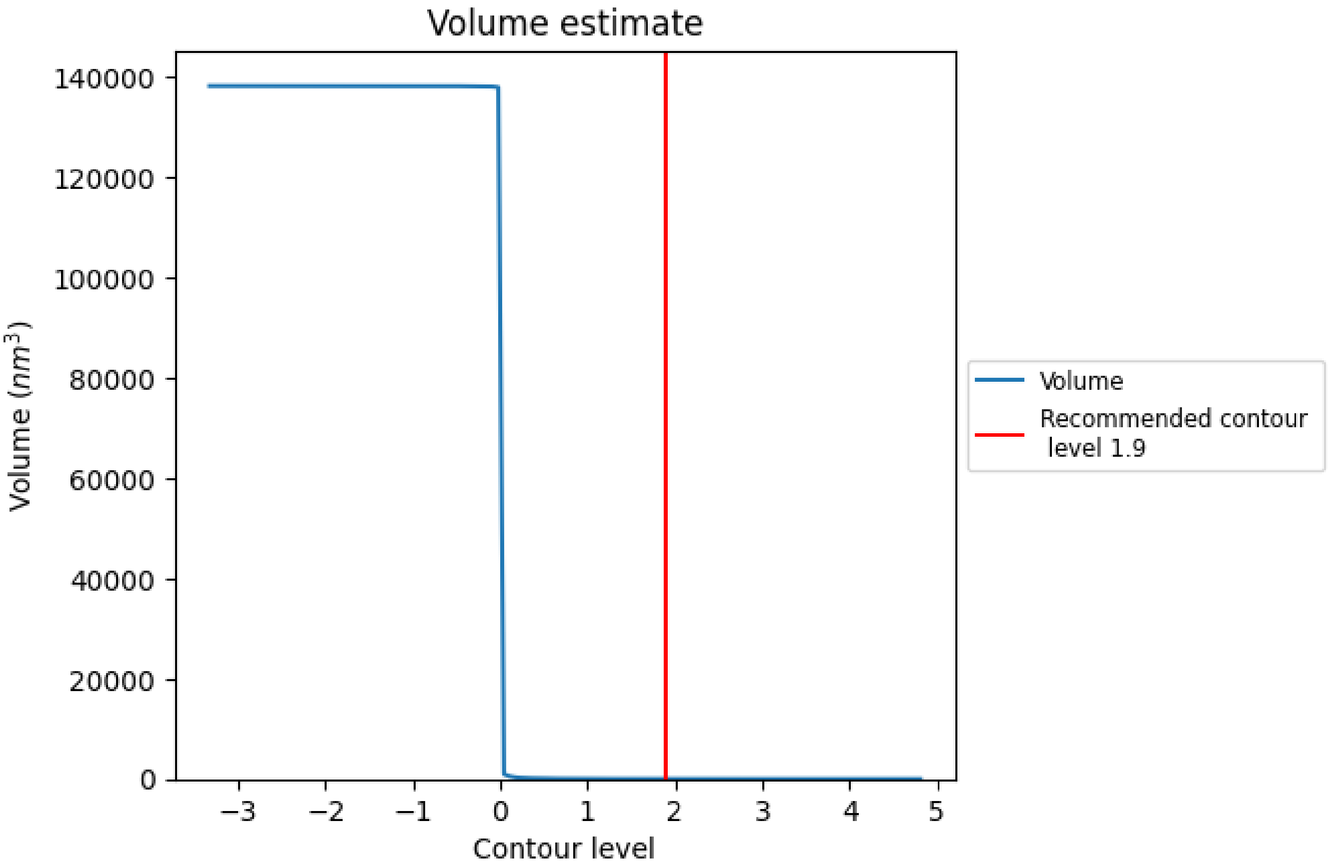
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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

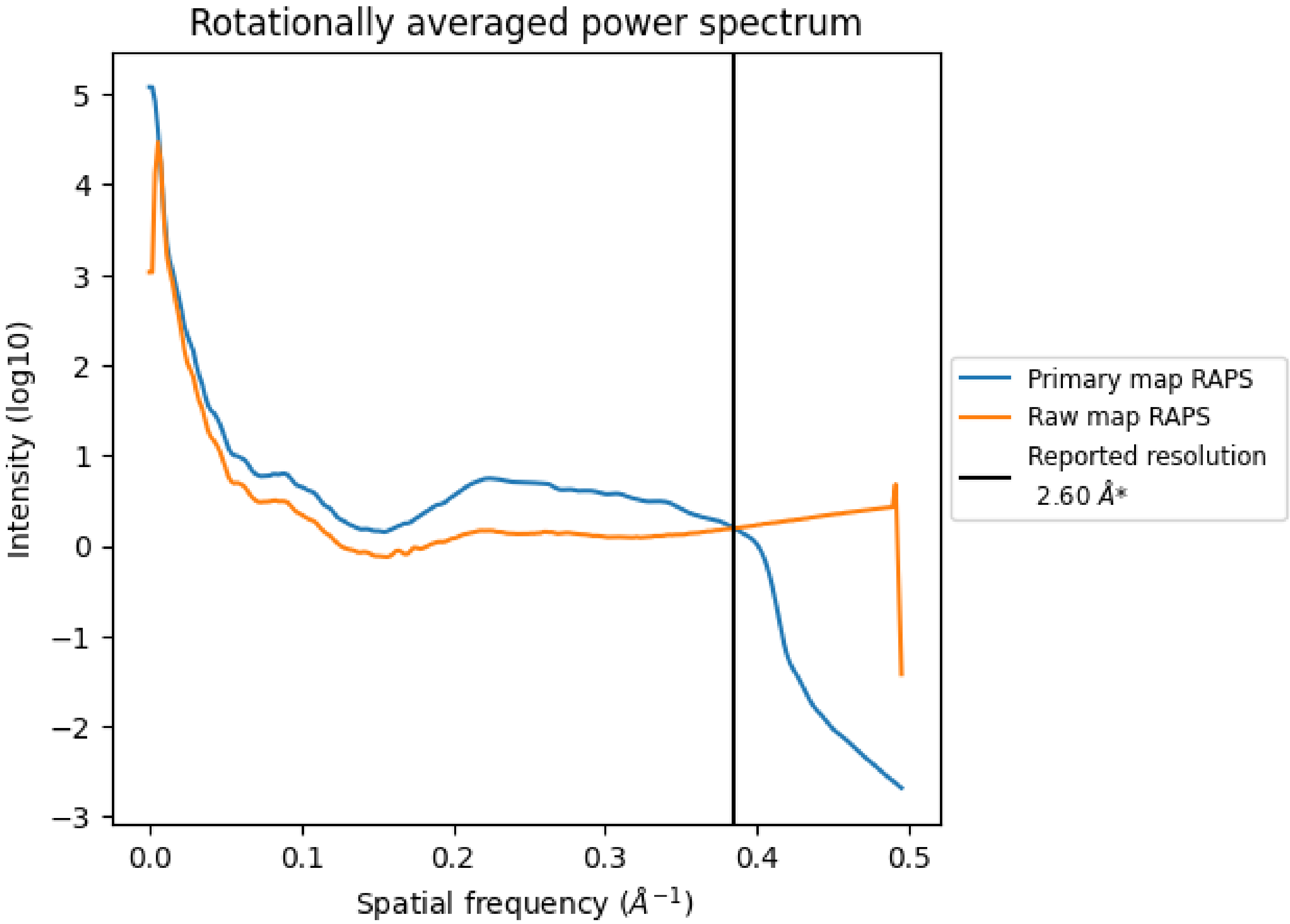
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 7 nm^3; this corresponds to an approximate mass of 7 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 ⓘ

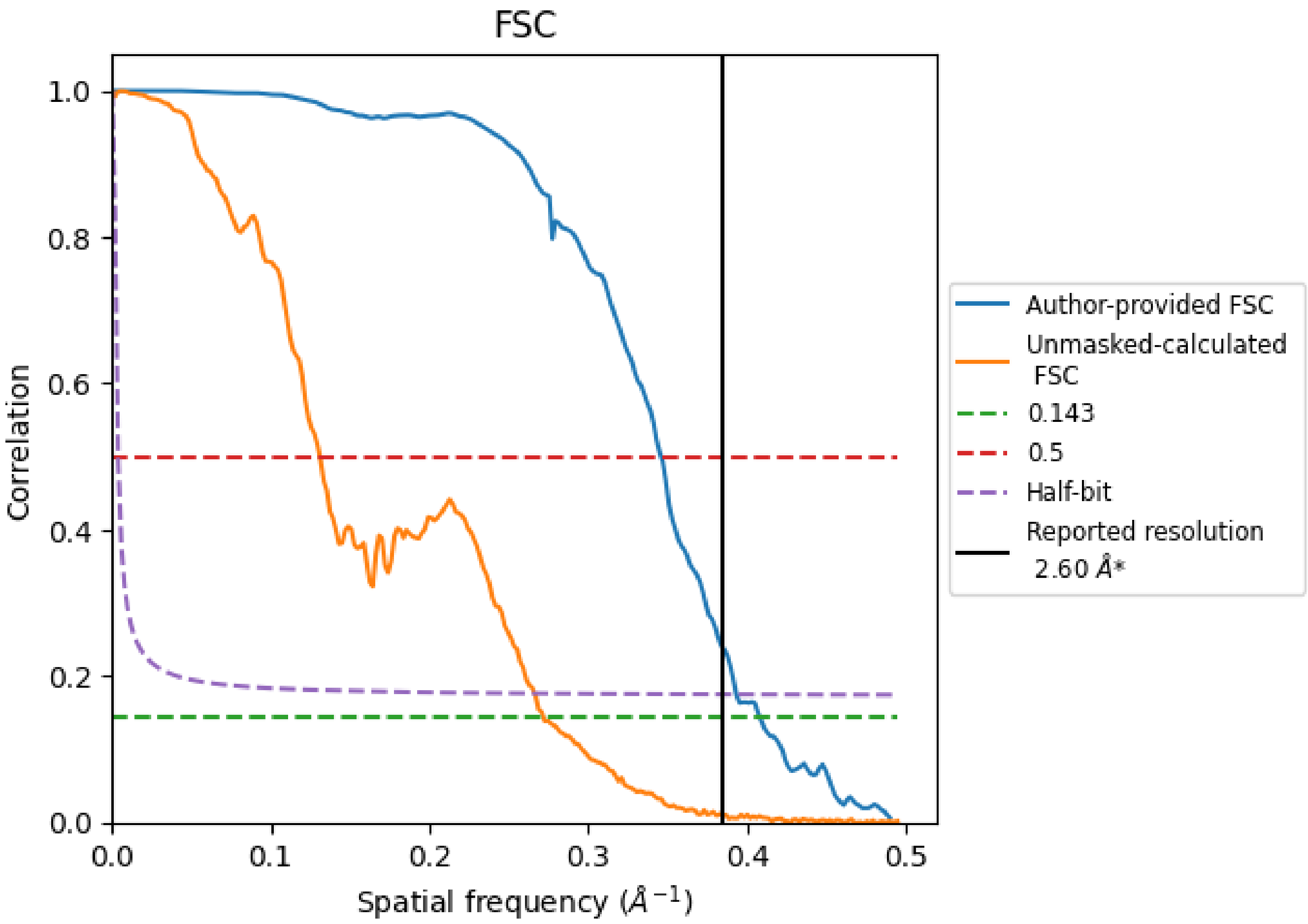


*Reported resolution corresponds to spatial frequency of 0.385 $Å^{-1}$

8 Fourier-Shell correlation ⓘ

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

8.1 FSC ⓘ



*Reported resolution corresponds to spatial frequency of 0.385 Å^{-1}

8.2 Resolution estimates ⓘ

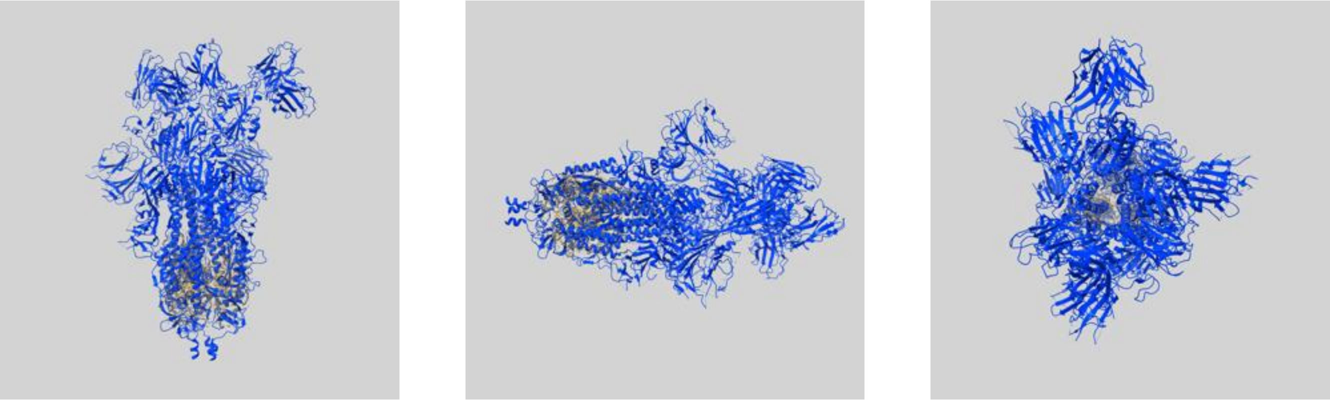
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.45	2.89	2.54
Unmasked-calculated*	3.68	7.64	3.76

*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 3.68 differs from the reported value 2.6 by more than 10 %

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-18180 and PDB model 8Q5Y. Per-residue inclusion information can be found in section 3 on page 12.

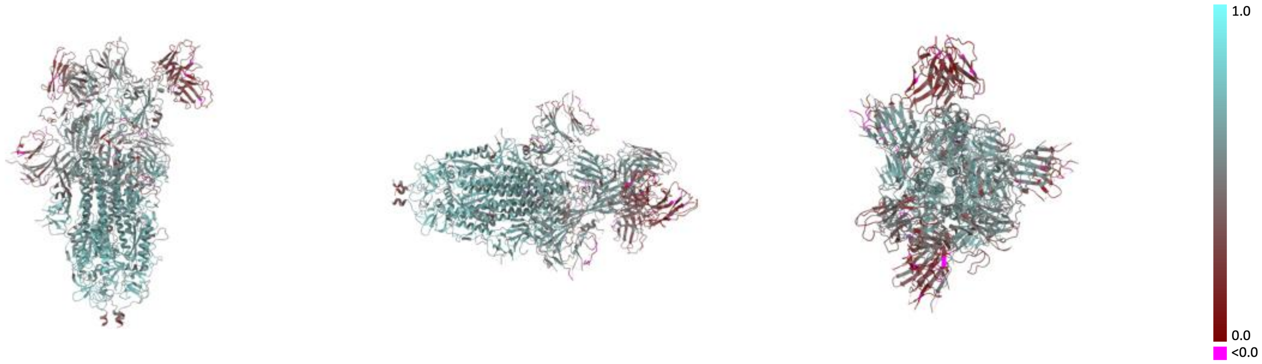
9.1 Map-model overlay ⓘ



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 1.9 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.

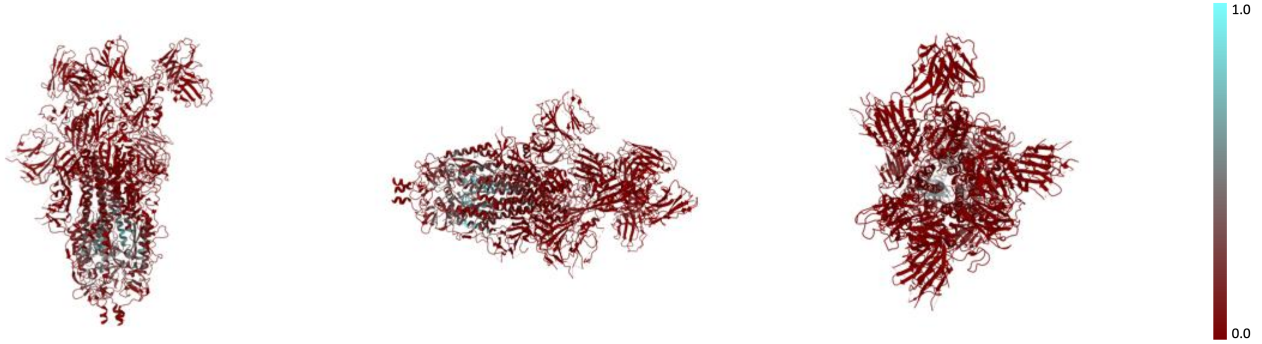
9.2 Q-score mapped to coordinate model ⓘ



X Y Z

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

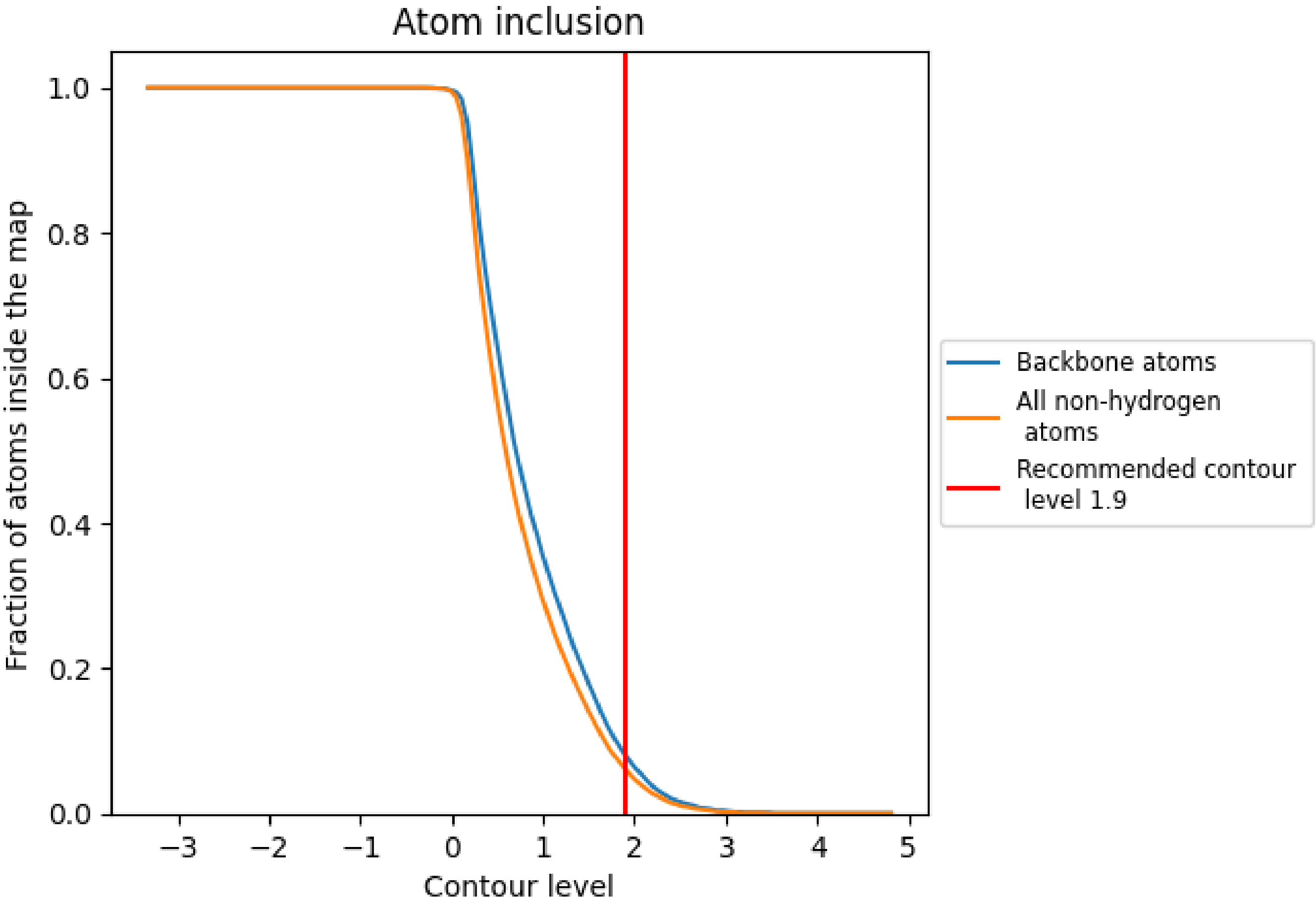
9.3 Atom inclusion mapped to coordinate model ⓘ



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.9).

9.4 Atom inclusion ⓘ



At the recommended contour level, 8% of all backbone atoms, 6% 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 (1.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.0610	0.5160
A	0.0000	0.2410
B	0.0000	0.2370
C	0.0730	0.5490
D	0.0700	0.5660
E	0.0790	0.5510
G	0.0000	0.4750
H	0.0000	0.4750
L	0.0000	0.3510
R	0.0000	0.2370