



wwPDB EM Validation Summary Report ⓘ

Mar 24, 2026 – 01:53 PM UTC

PDB ID : 7E9O / pdb_00007e9o
EMDB ID : EMD-31034
Title : Cryo-EM structure of the SARS-CoV-2 S-6P in complex with 35B5 Fab(3 up RBDs, state2)
Authors : Wang, X.F.; Zhu, Y.Q.
Deposited on : 2021-03-04
Resolution : 3.41 Å(reported)

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

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

A user guide is available at
<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

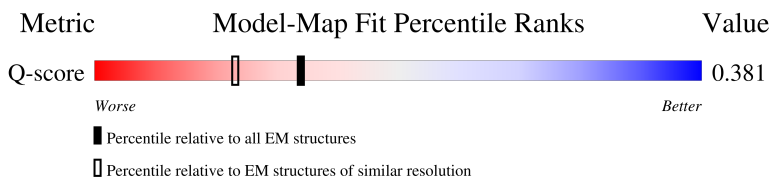
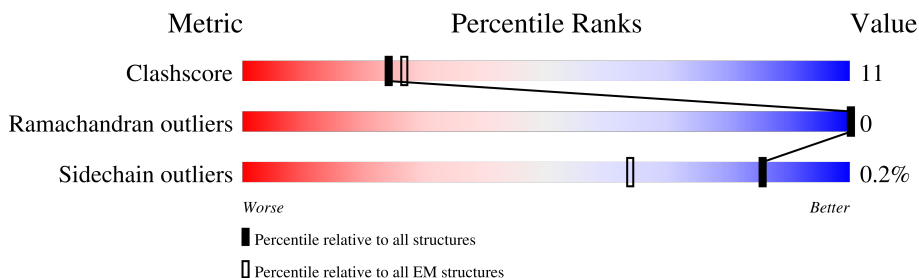
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.41 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13997 (2.91 - 3.91)

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	A	1288	
1	B	1288	
1	C	1288	
2	L	219	

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Mol	Chain	Length	Quality of chain
2	O	219	89% 69% 30%
2	X	219	74% 70% 29%
3	H	237	44% 67% 29% 5%
3	P	237	82% 65% 31% 5%
3	Y	237	65% 59% 36% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 33876 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	1002	Total	C	N	O	S	0	0
			7825	4998	1300	1492	35		
1	A	1002	Total	C	N	O	S	0	0
			7825	4998	1300	1492	35		
1	C	1002	Total	C	N	O	S	0	0
			7825	4998	1300	1492	35		

There are 267 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	TYR	-	expression tag	UNP P0DTC2
B	1213	ILE	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2
B	1215	GLU	-	expression tag	UNP P0DTC2
B	1216	ALA	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	ARG	-	expression tag	UNP P0DTC2
B	1219	ASP	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	ALA	-	expression tag	UNP P0DTC2
B	1223	TYR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1224	VAL	-	expression tag	UNP P0DTC2
B	1225	ARG	-	expression tag	UNP P0DTC2
B	1226	LYS	-	expression tag	UNP P0DTC2
B	1227	ASP	-	expression tag	UNP P0DTC2
B	1228	GLY	-	expression tag	UNP P0DTC2
B	1229	GLU	-	expression tag	UNP P0DTC2
B	1230	TRP	-	expression tag	UNP P0DTC2
B	1231	VAL	-	expression tag	UNP P0DTC2
B	1232	LEU	-	expression tag	UNP P0DTC2
B	1233	LEU	-	expression tag	UNP P0DTC2
B	1234	SER	-	expression tag	UNP P0DTC2
B	1235	THR	-	expression tag	UNP P0DTC2
B	1236	PHE	-	expression tag	UNP P0DTC2
B	1237	LEU	-	expression tag	UNP P0DTC2
B	1238	GLY	-	expression tag	UNP P0DTC2
B	1239	ARG	-	expression tag	UNP P0DTC2
B	1240	SER	-	expression tag	UNP P0DTC2
B	1241	LEU	-	expression tag	UNP P0DTC2
B	1242	GLU	-	expression tag	UNP P0DTC2
B	1243	VAL	-	expression tag	UNP P0DTC2
B	1244	LEU	-	expression tag	UNP P0DTC2
B	1245	PHE	-	expression tag	UNP P0DTC2
B	1246	GLN	-	expression tag	UNP P0DTC2
B	1247	GLY	-	expression tag	UNP P0DTC2
B	1248	PRO	-	expression tag	UNP P0DTC2
B	1249	GLY	-	expression tag	UNP P0DTC2
B	1250	HIS	-	expression tag	UNP P0DTC2
B	1251	HIS	-	expression tag	UNP P0DTC2
B	1252	HIS	-	expression tag	UNP P0DTC2
B	1253	HIS	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2
B	1258	SER	-	expression tag	UNP P0DTC2
B	1259	ALA	-	expression tag	UNP P0DTC2
B	1260	TRP	-	expression tag	UNP P0DTC2
B	1261	SER	-	expression tag	UNP P0DTC2
B	1262	HIS	-	expression tag	UNP P0DTC2
B	1263	PRO	-	expression tag	UNP P0DTC2
B	1264	GLN	-	expression tag	UNP P0DTC2
B	1265	PHE	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1266	GLU	-	expression tag	UNP P0DTC2
B	1267	LYS	-	expression tag	UNP P0DTC2
B	1268	GLY	-	expression tag	UNP P0DTC2
B	1269	GLY	-	expression tag	UNP P0DTC2
B	1270	GLY	-	expression tag	UNP P0DTC2
B	1271	SER	-	expression tag	UNP P0DTC2
B	1272	GLY	-	expression tag	UNP P0DTC2
B	1273	GLY	-	expression tag	UNP P0DTC2
B	1274	GLY	-	expression tag	UNP P0DTC2
B	1275	GLY	-	expression tag	UNP P0DTC2
B	1276	SER	-	expression tag	UNP P0DTC2
B	1277	GLY	-	expression tag	UNP P0DTC2
B	1278	GLY	-	expression tag	UNP P0DTC2
B	1279	SER	-	expression tag	UNP P0DTC2
B	1280	ALA	-	expression tag	UNP P0DTC2
B	1281	TRP	-	expression tag	UNP P0DTC2
B	1282	SER	-	expression tag	UNP P0DTC2
B	1283	HIS	-	expression tag	UNP P0DTC2
B	1284	PRO	-	expression tag	UNP P0DTC2
B	1285	GLN	-	expression tag	UNP P0DTC2
B	1286	PHE	-	expression tag	UNP P0DTC2
B	1287	GLU	-	expression tag	UNP P0DTC2
B	1288	LYS	-	expression tag	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	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2
A	1226	LYS	-	expression tag	UNP P0DTC2
A	1227	ASP	-	expression tag	UNP P0DTC2
A	1228	GLY	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	TRP	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2
A	1232	LEU	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2
A	1235	THR	-	expression tag	UNP P0DTC2
A	1236	PHE	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	GLY	-	expression tag	UNP P0DTC2
A	1239	ARG	-	expression tag	UNP P0DTC2
A	1240	SER	-	expression tag	UNP P0DTC2
A	1241	LEU	-	expression tag	UNP P0DTC2
A	1242	GLU	-	expression tag	UNP P0DTC2
A	1243	VAL	-	expression tag	UNP P0DTC2
A	1244	LEU	-	expression tag	UNP P0DTC2
A	1245	PHE	-	expression tag	UNP P0DTC2
A	1246	GLN	-	expression tag	UNP P0DTC2
A	1247	GLY	-	expression tag	UNP P0DTC2
A	1248	PRO	-	expression tag	UNP P0DTC2
A	1249	GLY	-	expression tag	UNP P0DTC2
A	1250	HIS	-	expression tag	UNP P0DTC2
A	1251	HIS	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	HIS	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	SER	-	expression tag	UNP P0DTC2
A	1259	ALA	-	expression tag	UNP P0DTC2
A	1260	TRP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1261	SER	-	expression tag	UNP P0DTC2
A	1262	HIS	-	expression tag	UNP P0DTC2
A	1263	PRO	-	expression tag	UNP P0DTC2
A	1264	GLN	-	expression tag	UNP P0DTC2
A	1265	PHE	-	expression tag	UNP P0DTC2
A	1266	GLU	-	expression tag	UNP P0DTC2
A	1267	LYS	-	expression tag	UNP P0DTC2
A	1268	GLY	-	expression tag	UNP P0DTC2
A	1269	GLY	-	expression tag	UNP P0DTC2
A	1270	GLY	-	expression tag	UNP P0DTC2
A	1271	SER	-	expression tag	UNP P0DTC2
A	1272	GLY	-	expression tag	UNP P0DTC2
A	1273	GLY	-	expression tag	UNP P0DTC2
A	1274	GLY	-	expression tag	UNP P0DTC2
A	1275	GLY	-	expression tag	UNP P0DTC2
A	1276	SER	-	expression tag	UNP P0DTC2
A	1277	GLY	-	expression tag	UNP P0DTC2
A	1278	GLY	-	expression tag	UNP P0DTC2
A	1279	SER	-	expression tag	UNP P0DTC2
A	1280	ALA	-	expression tag	UNP P0DTC2
A	1281	TRP	-	expression tag	UNP P0DTC2
A	1282	SER	-	expression tag	UNP P0DTC2
A	1283	HIS	-	expression tag	UNP P0DTC2
A	1284	PRO	-	expression tag	UNP P0DTC2
A	1285	GLN	-	expression tag	UNP P0DTC2
A	1286	PHE	-	expression tag	UNP P0DTC2
A	1287	GLU	-	expression tag	UNP P0DTC2
A	1288	LYS	-	expression tag	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	817	PRO	PHE	engineered mutation	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	899	PRO	ALA	engineered mutation	UNP P0DTC2
C	942	PRO	ALA	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

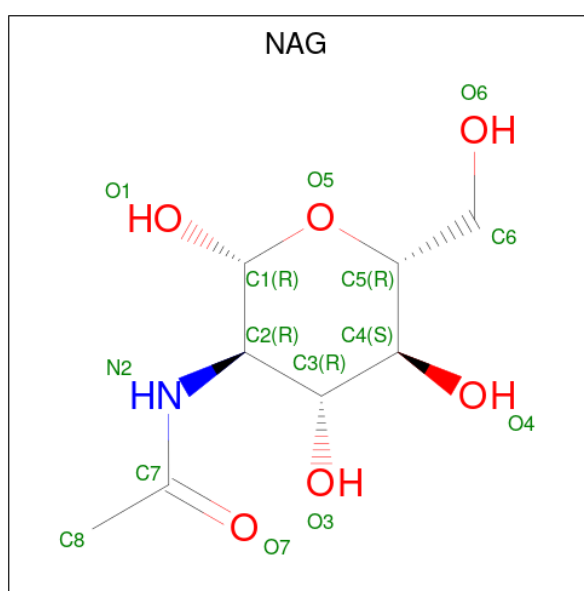
- Molecule 2 is a protein called Light chain of 35B5 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	218	Total	C	N	O	S	0	0
			1673	1050	280	337	6		
2	O	218	Total	C	N	O	S	0	0
			1673	1050	280	337	6		
2	X	218	Total	C	N	O	S	0	0
			1673	1050	280	337	6		

- Molecule 3 is a protein called Heavy chain of 35B5 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	226	Total	C	N	O	S	0	0
			1668	1048	285	327	8		
3	P	226	Total	C	N	O	S	0	0
			1668	1048	285	327	8		
3	Y	226	Total	C	N	O	S	0	0
			1668	1048	285	327	8		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	

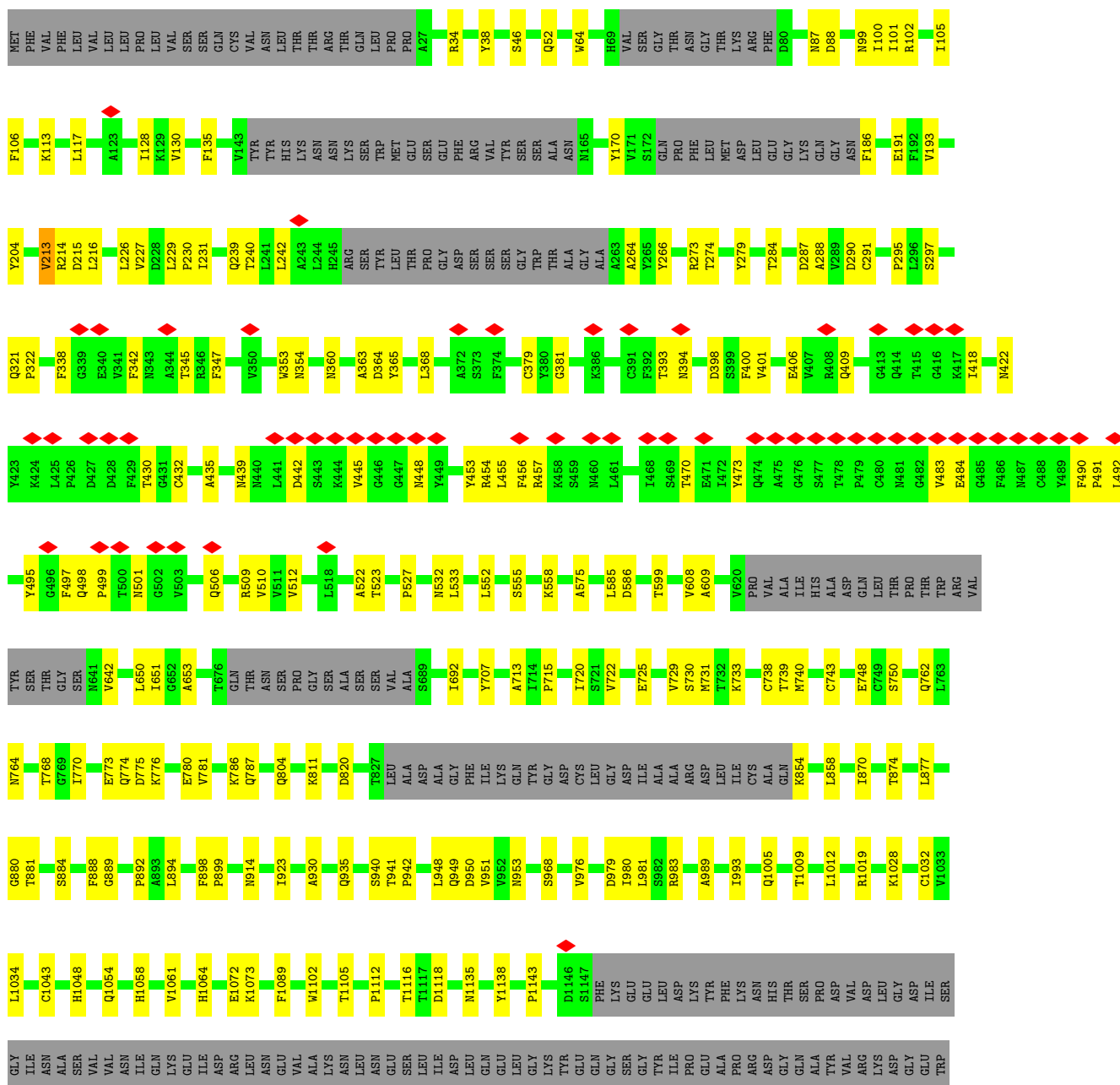
LYS	GLY	TRP	VAL	LEU	SER	THR	PHE	LEU	GLY	ARG	SER	GLN	GLY	PRO	GLY	HIS	HIS	HIS	ALA	TRP	SER	HIS	PRO	GLN	GLY	PHE	LYS	GLY	GLY	SER	GLY	GLY	GLY	GLY	SER	GLY	GLY	GLY	GLY	THR	PRO	GLN	PHE	GLU																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
	ASP	ILE	SER	ILE	ASN	VAL	VAL	ASN	GLN	LYS	GLU	ILE	ASP	ARG	LEU	ASN	GLU	VAL	ALA	LYS	LEU	GLN	ASN	GLY	GLN	GLY	GLY	TYR	GLN	SER	GLY	PRO	ALA	GLY	ARG	ASP	VAL	ASP	LEU	GLY																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
	V1060	V1061	E1072	G1093	V1094	F1096	V1097	N1098	G1099	W1102	F1103	V1104	T1105	Q1106	R1107	Y1110	E1111	P1112	N1119	C1126	V1129	I1132	N1135	T1136	L1141	L1145	D1146	S1147	PHE	LYS	GLU	GLU	LEU	ASP	LYS	PRO	GLY	PHE	LYS	ASN	HIS	THR	PRO	ASP	VAL	ASP	LYS	ASP	GLY																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														

● Molecule 1: Spike glycoprotein



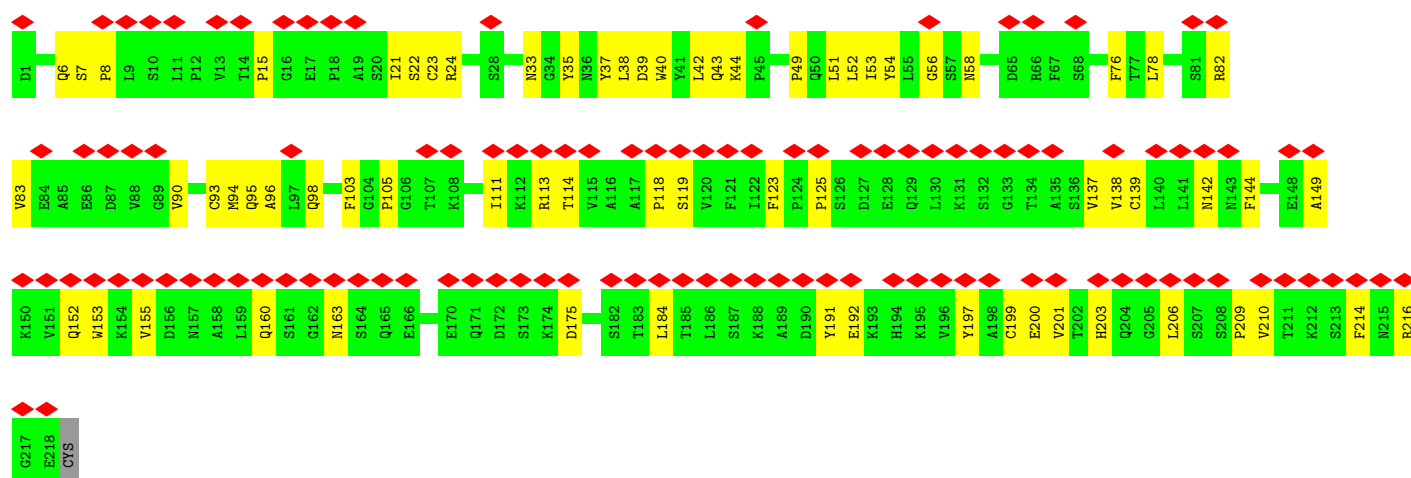
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G107	T108	D111	S112	Q115	S116	L117	L118	L119	V120	N121	N122	A123	T124	N125	V126	V127	I128	K129	V130	C131	E132	F133	Q134	V143	TYR	TYR	HIS	LYS	ASN	ASN	LYS	SER	TRP	MET	GLU	VAL	SER	GLU	GLY	PHE	ARG	VAL	THR	ASN	GLY	VAL	ASP	SER	SER	SER	ALA	ASN	N165	D172	GLN	PRO	PHE	LEU	MET	ASP	LEU	GLU	
GLY	LYS	GLN	GLY	F186	K187	N188	L189	G199	I203	I210	R214	D215	L216	F220	V227	I231	G232	T236	R237	F238	G239	T240	L241	A243	L244	H245	ARG	SER	TYR	LEU	THR	PRO	GLY	ASP	SER	SER	SER	SER	GLY	TRP	THR	ALA	ALA	A263	A264	Y265	Y266	L277															
K278	Y279	N282	I285	D290	C291	D294	S297	E298	L303	K304	S305	F306	T307	V308	K310	R328	F329	N334	L335	F342	R346	S349	V353	N354	R357	I358	S359	N360	A363	D364	Y365	S366	Y369	A372	K378	V382	S383	L384	F385	K386																							
L387	N388	D389	L390	C391	N394	V395	Y396	A397	D398	V401	D405	E406	Q409	T410	A411	Q414	T415	G416	D420	Y421	N422	L425	P426	D427	D428	F429	T430	C431	C432	V433	N437	S438	L441	V445	G446	G447	N448	Y449	L452	Y453	R454	L455	F456	R457	K458	S459	K462																
P463	F464	E465	R466	E471	I472	Y473	Q474	A475	G476	S477	T478	P479	C480	M481	G482	E483	E484	G485	N487	C488	Y489	P491	S494	T500	R509	V510	V511	V512	H519	T523	V524	C525	G526	N532	L533	V534	K535	C538	G550	V551	E554	K557	R558	F559	B577																		
D578	P579	Q580	T581	L582	F583	I584	T599	V608	V615	M616	C617	V620	PRO	VAL	ALA	ILE	ALA	ASP	GLN	LEU	THR	THR	TRP	ARG	VAL	TYR	SER	THR	GLY	SER	M641	E661	C662	D663	I664	P665	C671	T676	GLN	THR	ASN	PRO	GLY	ASP	ALA	SER	GLY	VAL	ALA														
S689	Q690	V695	V722	I726	V729	S735	C738	T739	C743	C749	L752	F759	Q762	I770	E773	E780	V781	Q784	V785	K786	K790	N801	F802	S803	Q804	I805	N811	P817	D820	T827	LEU	ALA	ASP	ALA	GLY	ASP	ALA	SER	GLY	PHE	ILE	LYS																					
GLN	TYR	GLY	ASP	CYS	GLY	ASP	ILE	ALA	ALA	ASP	ARG	LEU	ILE	CYS	GLN	K854	T859	E868	M869	S1030	E1031	A871	Q872	T874	F888	P892	I896	P897	F898	P899	I909	G910	V911	T912	G913	N914	A930	I934	Q935	D950	V951	T961	L962	V963	E1144	L1145	D1146																
P986	P987	E988	A989	Q992	I993	D994	R995	L996	I997	Y1007	V1008	T1009	I1012	I1013	R1019	K1028	M1029	S1030	E1031	C1032	C1043	H1048	V1061	H1064	E1072	K1073	N1074	T1077	A1078	G1082	K1086	V1122	C1126	V1129	I1132	P1140	L1141	E1144	L1145	D1146																							

- Molecule 1: Spike glycoprotein

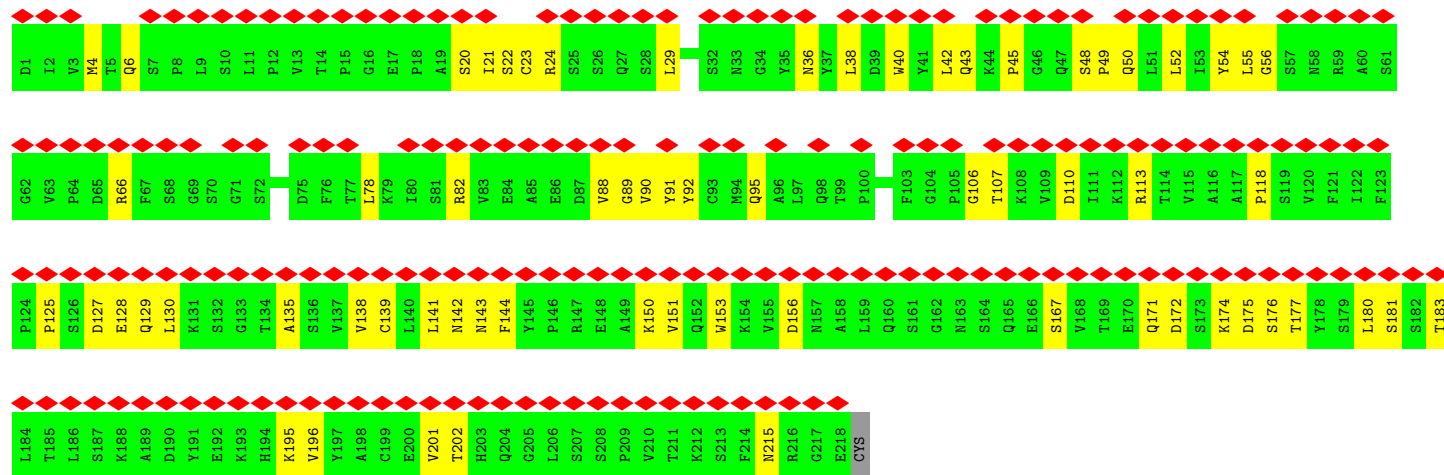
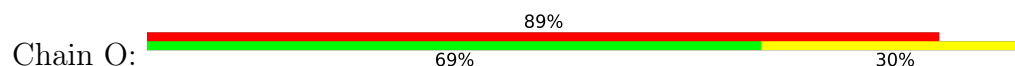


VAL LEU LEU SER THR PHE LEU LEU GLY ARG SER SER LEU VAL VAL LEU PHE GLN GLY PRO PRO HIS HIS HIS HIS HIS HIS ALA ALA TRP SER HIS HIS PRO GLN PHE PHE GLU LYS LYS

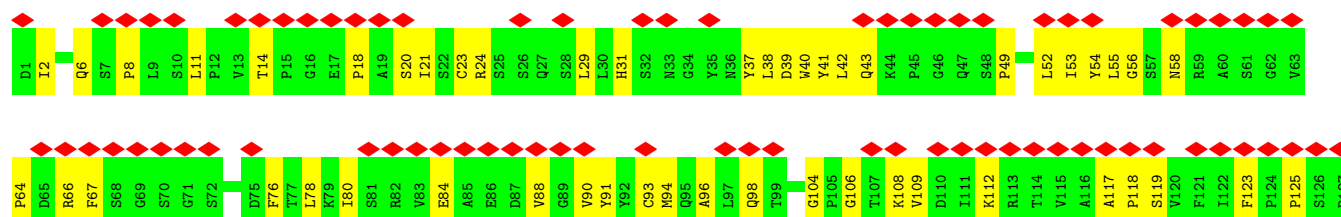
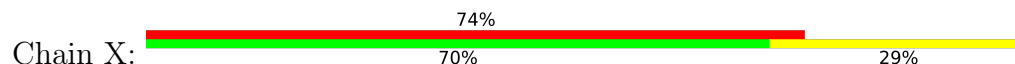
• Molecule 2: Light chain of 35B5 Fab

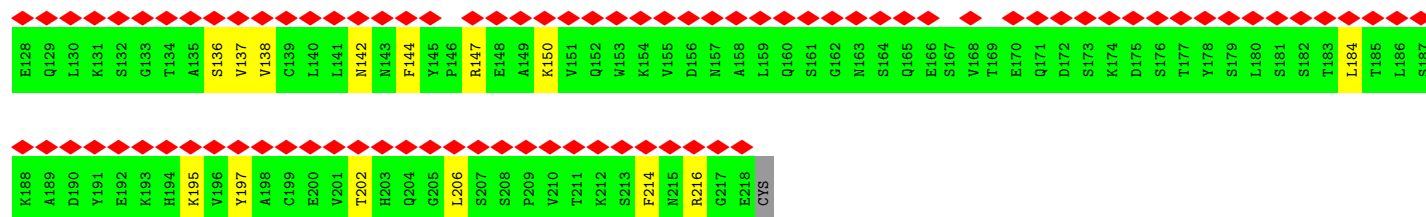


• Molecule 2: Light chain of 35B5 Fab

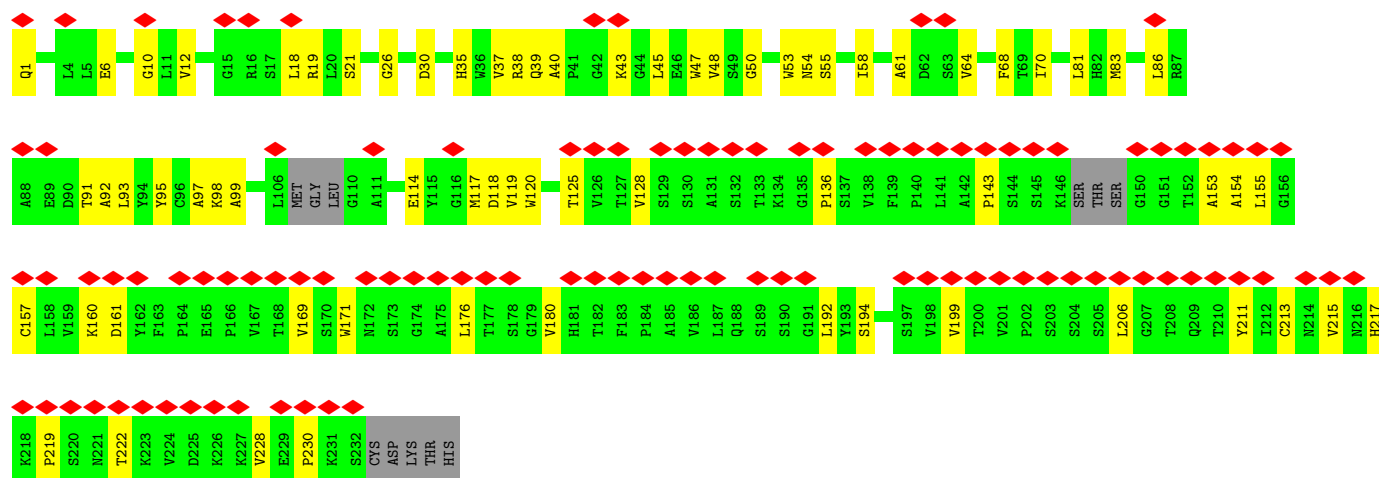
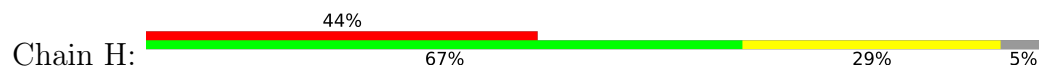


• Molecule 2: Light chain of 35B5 Fab

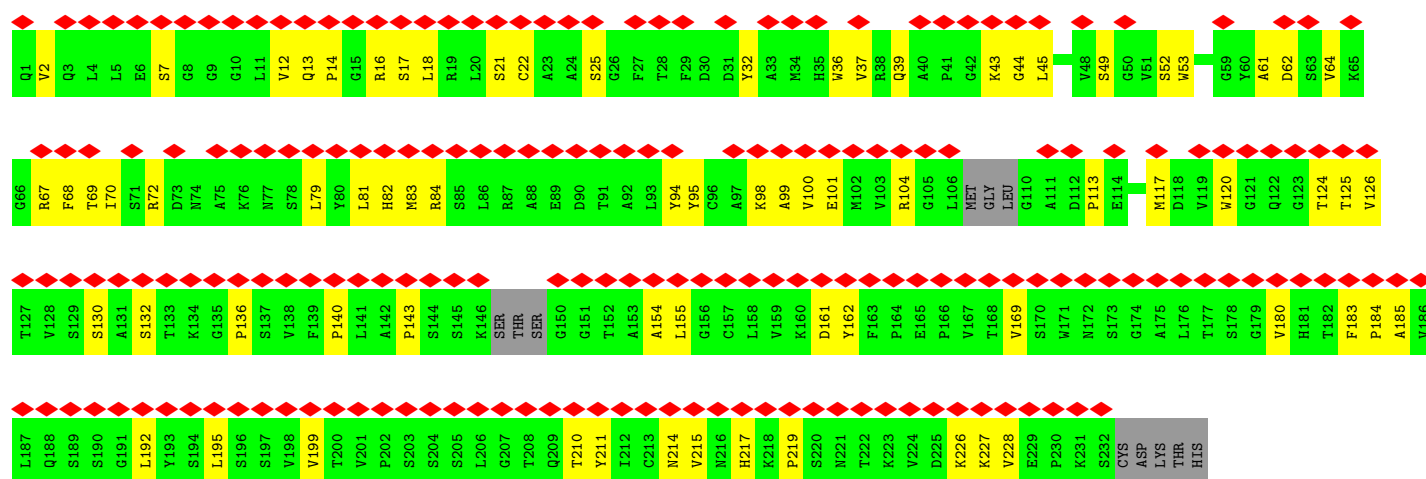
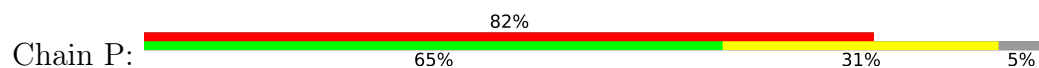




• Molecule 3: Heavy chain of 35B5 Fab

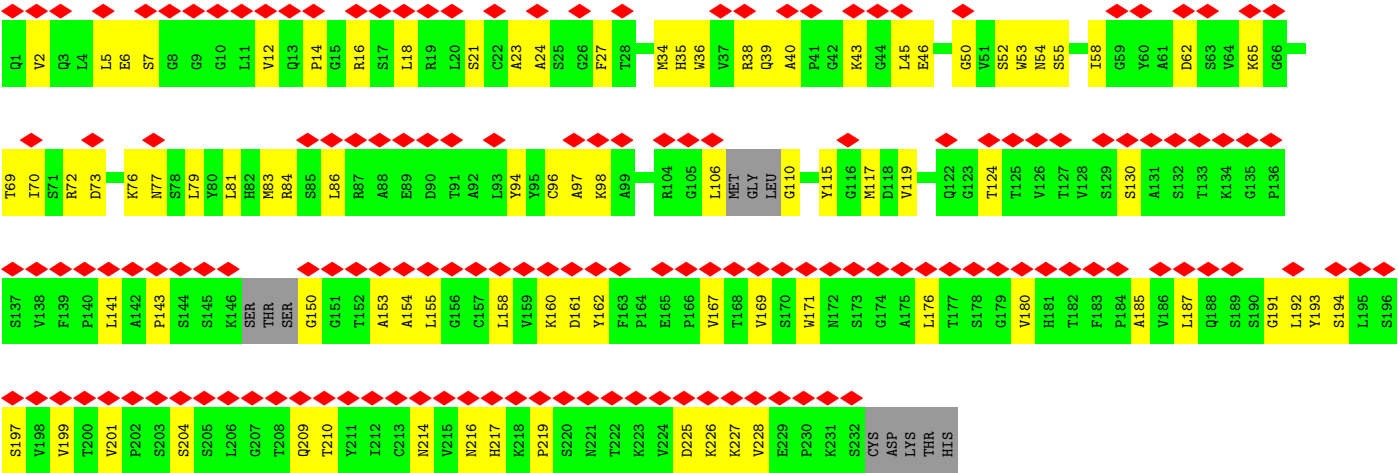


• Molecule 3: Heavy chain of 35B5 Fab



• Molecule 3: Heavy chain of 35B5 Fab





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	122887	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	44.154	Depositor
Minimum map value	-26.918	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4	Depositor
Map size (Å)	361.35, 361.35, 361.35	wwPDB
Map dimensions	330, 330, 330	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.095, 1.095, 1.095	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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	0.26	0/8004	0.49	4/10896 (0.0%)
1	B	0.28	0/8004	0.52	4/10896 (0.0%)
1	C	0.24	0/8004	0.48	3/10896 (0.0%)
2	L	0.14	0/1711	0.39	0/2326
2	O	0.15	0/1711	0.43	0/2326
2	X	0.22	0/1711	0.43	0/2326
3	H	0.19	0/1706	0.40	0/2323
3	P	0.21	0/1706	0.44	0/2323
3	Y	0.23	0/1706	0.44	0/2323
All	All	0.24	0/34263	0.48	11/46635 (0.0%)

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	909	ILE	N-CA-C	-8.99	102.35	111.88
1	C	942	PRO	N-CA-C	7.71	123.72	113.40
1	B	906	PHE	CB-CA-C	-6.59	100.49	110.90
1	A	888	PHE	CA-CB-CG	6.37	120.17	113.80
1	A	892	PRO	CB-CA-C	-6.15	103.53	111.46

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7825	0	7635	155	0
1	B	7825	0	7637	160	0
1	C	7825	0	7637	127	0
2	L	1673	0	1628	58	0
2	O	1673	0	1628	48	0
2	X	1673	0	1628	44	0
3	H	1668	0	1609	55	0
3	P	1668	0	1609	50	0
3	Y	1668	0	1609	58	0
4	A	126	0	117	2	0
4	B	126	0	117	3	0
4	C	126	0	117	0	0
All	All	33876	0	32971	722	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 11.

The worst 5 of 722 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:P:37:VAL:O	3:P:95:TYR:HB2	1.69	0.93
3:Y:83:MET:HB3	3:Y:86:LEU:HD21	1.57	0.87
1:B:105:ILE:HG13	1:B:241:LEU:HD11	1.58	0.85
3:P:2:VAL:HA	3:P:25:SER:O	1.78	0.84
2:L:94:MET:HE3	2:L:103:PHE:HE1	1.43	0.83

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	A	986/1288 (77%)	938 (95%)	48 (5%)	0	100	100
1	B	986/1288 (77%)	934 (95%)	52 (5%)	0	100	100
1	C	986/1288 (77%)	935 (95%)	51 (5%)	0	100	100
2	L	216/219 (99%)	207 (96%)	9 (4%)	0	100	100
2	O	216/219 (99%)	209 (97%)	7 (3%)	0	100	100
2	X	216/219 (99%)	206 (95%)	10 (5%)	0	100	100
3	H	220/237 (93%)	211 (96%)	9 (4%)	0	100	100
3	P	220/237 (93%)	207 (94%)	13 (6%)	0	100	100
3	Y	220/237 (93%)	211 (96%)	9 (4%)	0	100	100
All	All	4266/5232 (82%)	4058 (95%)	208 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	879/1116 (79%)	878 (100%)	1 (0%)	88	88
1	B	879/1116 (79%)	876 (100%)	3 (0%)	86	84
1	C	879/1116 (79%)	876 (100%)	3 (0%)	86	84
2	L	192/193 (100%)	192 (100%)	0	100	100
2	O	192/193 (100%)	192 (100%)	0	100	100
2	X	192/193 (100%)	192 (100%)	0	100	100
3	H	181/195 (93%)	181 (100%)	0	100	100
3	P	181/195 (93%)	180 (99%)	1 (1%)	78	80
3	Y	181/195 (93%)	180 (99%)	1 (1%)	78	80
All	All	3756/4512 (83%)	3747 (100%)	9 (0%)	85	85

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	P	132	SER
3	Y	201	VAL
1	A	382	VAL
1	C	213	VAL
1	C	214	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
3	H	3	GLN
3	P	172	ASN
3	H	209	GLN
3	P	3	GLN
3	Y	82	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

27 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	1301	1	14,14,15	1.90	4 (28%)	17,19,21	1.06	1 (5%)
4	NAG	C	1309	1	14,14,15	1.90	4 (28%)	17,19,21	1.30	3 (17%)
4	NAG	B	1308	1	14,14,15	0.53	0	17,19,21	0.78	1 (5%)
4	NAG	C	1304	1	14,14,15	2.00	4 (28%)	17,19,21	1.57	4 (23%)
4	NAG	A	1303	1	14,14,15	1.97	4 (28%)	17,19,21	1.38	3 (17%)
4	NAG	A	1301	1	14,14,15	1.94	4 (28%)	17,19,21	1.05	1 (5%)
4	NAG	B	1304	1	14,14,15	1.99	4 (28%)	17,19,21	0.95	0
4	NAG	B	1303	1	14,14,15	1.90	4 (28%)	17,19,21	1.21	2 (11%)
4	NAG	A	1304	1	14,14,15	1.94	4 (28%)	17,19,21	1.56	3 (17%)
4	NAG	B	1305	1	14,14,15	1.88	4 (28%)	17,19,21	1.13	2 (11%)
4	NAG	A	1309	1	14,14,15	1.89	4 (28%)	17,19,21	1.16	2 (11%)
4	NAG	C	1308	1	14,14,15	1.90	4 (28%)	17,19,21	1.08	2 (11%)
4	NAG	B	1307	1	14,14,15	1.91	4 (28%)	17,19,21	1.19	2 (11%)
4	NAG	B	1302	1	14,14,15	1.99	4 (28%)	17,19,21	1.42	3 (17%)
4	NAG	B	1306	1	14,14,15	1.91	4 (28%)	17,19,21	1.11	2 (11%)
4	NAG	C	1303	1	14,14,15	2.17	4 (28%)	17,19,21	2.24	5 (29%)
4	NAG	A	1308	1	14,14,15	1.92	4 (28%)	17,19,21	1.14	2 (11%)
4	NAG	B	1309	1	14,14,15	1.92	4 (28%)	17,19,21	1.12	2 (11%)
4	NAG	C	1307	1	14,14,15	1.91	3 (21%)	17,19,21	1.29	3 (17%)
4	NAG	A	1306	1	14,14,15	1.97	4 (28%)	17,19,21	0.99	0
4	NAG	C	1306	1	14,14,15	1.91	4 (28%)	17,19,21	1.04	2 (11%)
4	NAG	C	1305	1	14,14,15	1.87	4 (28%)	17,19,21	1.20	2 (11%)
4	NAG	C	1302	1	14,14,15	1.93	4 (28%)	17,19,21	1.07	2 (11%)
4	NAG	B	1301	1	14,14,15	1.93	4 (28%)	17,19,21	1.11	1 (5%)
4	NAG	A	1305	1	14,14,15	1.98	4 (28%)	17,19,21	1.21	2 (11%)
4	NAG	A	1307	1	14,14,15	1.86	4 (28%)	17,19,21	1.13	2 (11%)
4	NAG	A	1302	1	14,14,15	1.92	4 (28%)	17,19,21	1.10	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1309	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1304	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1307	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1303	1	-	5/6/23/26	0/1/1/1
4	NAG	A	1308	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1307	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1306	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1306	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1302	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	2/6/23/26	0/1/1/1

The worst 5 of 103 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1303	NAG	O5-C1	4.80	1.51	1.43
4	C	1304	NAG	O5-C1	4.70	1.51	1.43
4	B	1302	NAG	O5-C1	4.59	1.51	1.43
4	A	1305	NAG	O5-C1	4.48	1.51	1.43
4	B	1309	NAG	O5-C1	4.32	1.51	1.43

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1303	NAG	C8-C7-N2	5.49	125.23	116.12
4	C	1303	NAG	C2-N2-C7	4.30	128.67	122.90
4	C	1303	NAG	C1-O5-C5	3.58	116.98	112.19
4	C	1304	NAG	O5-C1-C2	3.38	116.52	111.29
4	C	1304	NAG	C1-O5-C5	3.38	116.71	112.19

There are no chirality outliers.

5 of 61 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1307	NAG	C4-C5-C6-O6
4	B	1305	NAG	C4-C5-C6-O6
4	A	1306	NAG	O5-C5-C6-O6
4	B	1307	NAG	O5-C5-C6-O6
4	B	1306	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1308	NAG	3	0
4	A	1301	NAG	1	0
4	A	1305	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

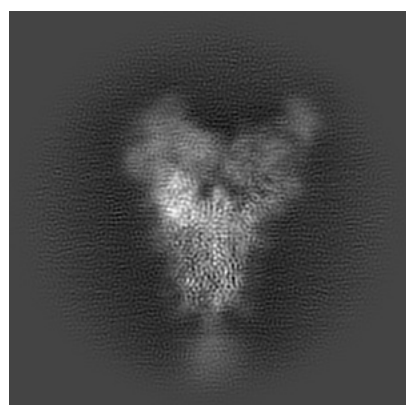
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31034. These allow visual inspection of the internal detail of the map and identification of artifacts.

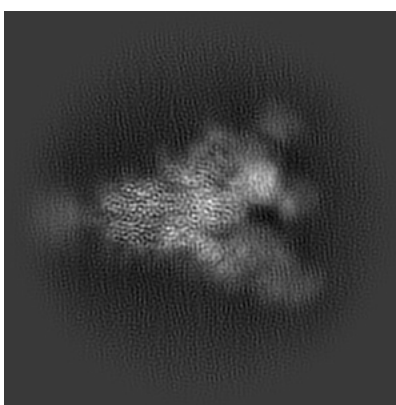
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

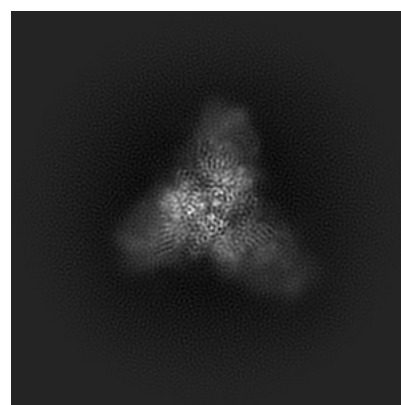
6.1.1 Primary map



X



Y

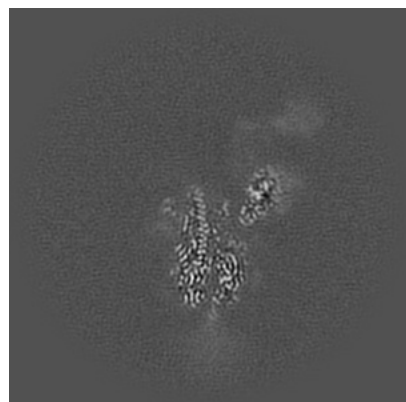


Z

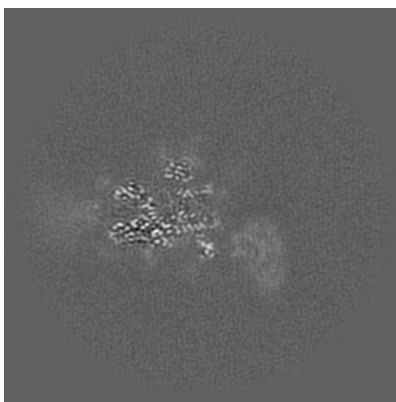
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

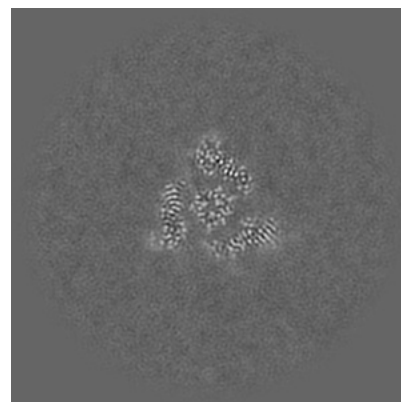
6.2.1 Primary map



X Index: 165



Y Index: 165

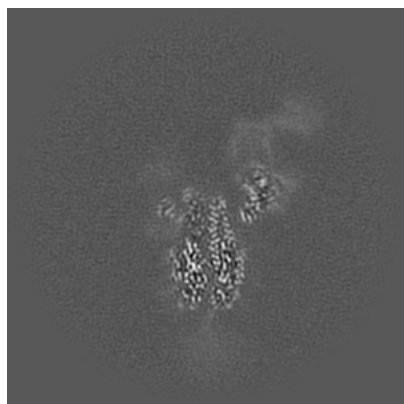


Z Index: 165

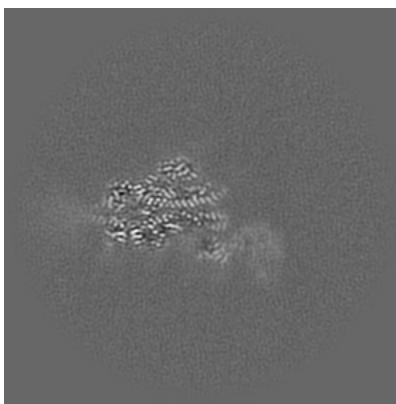
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

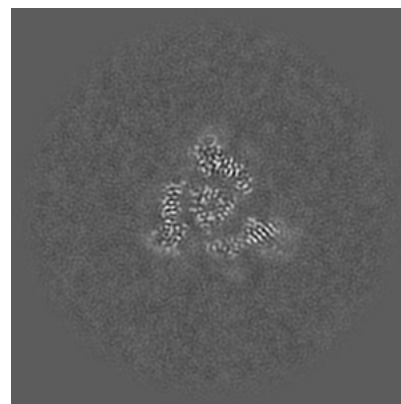
6.3.1 Primary map



X Index: 169



Y Index: 171

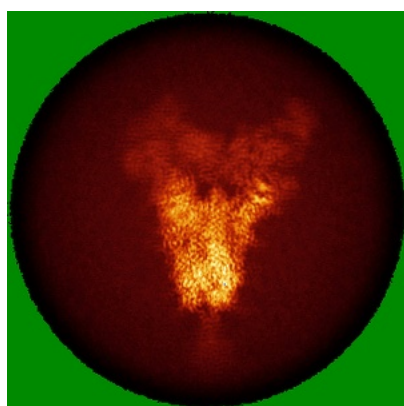


Z Index: 167

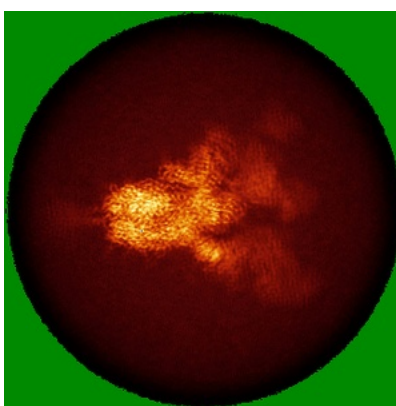
The images above show the largest variance slices of the map in three orthogonal directions.

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

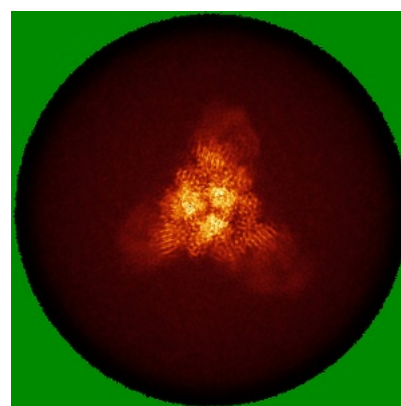
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

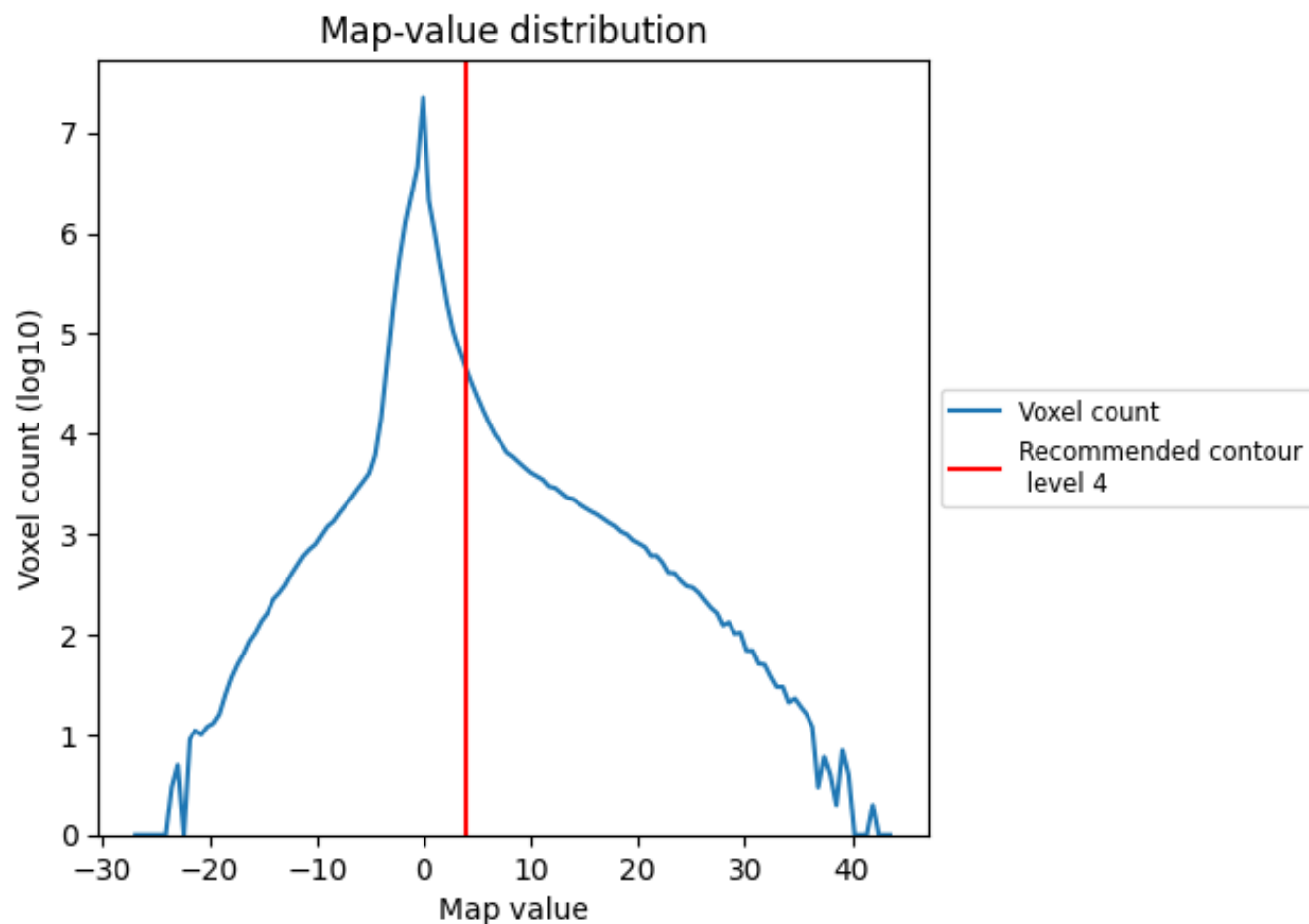
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

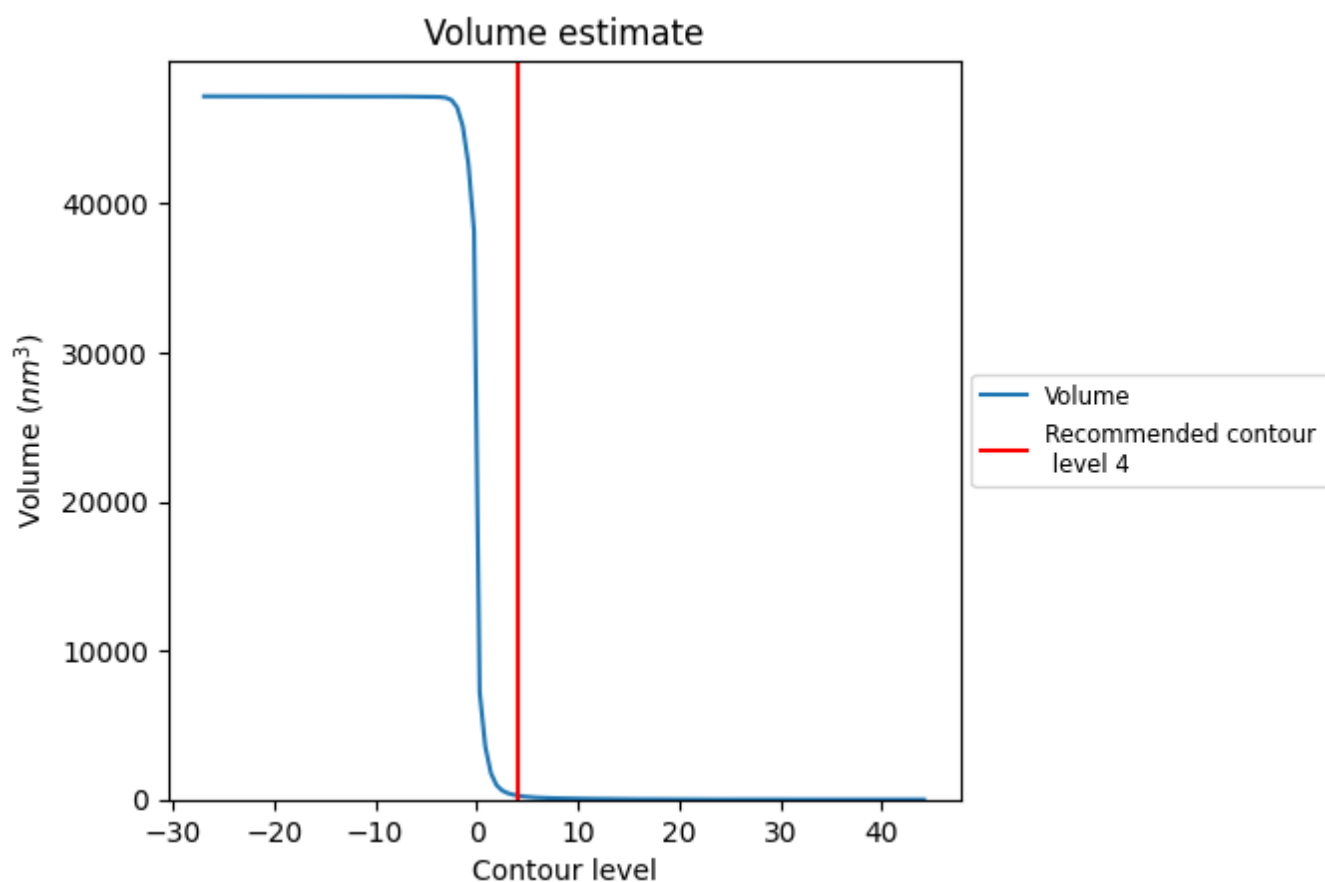
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

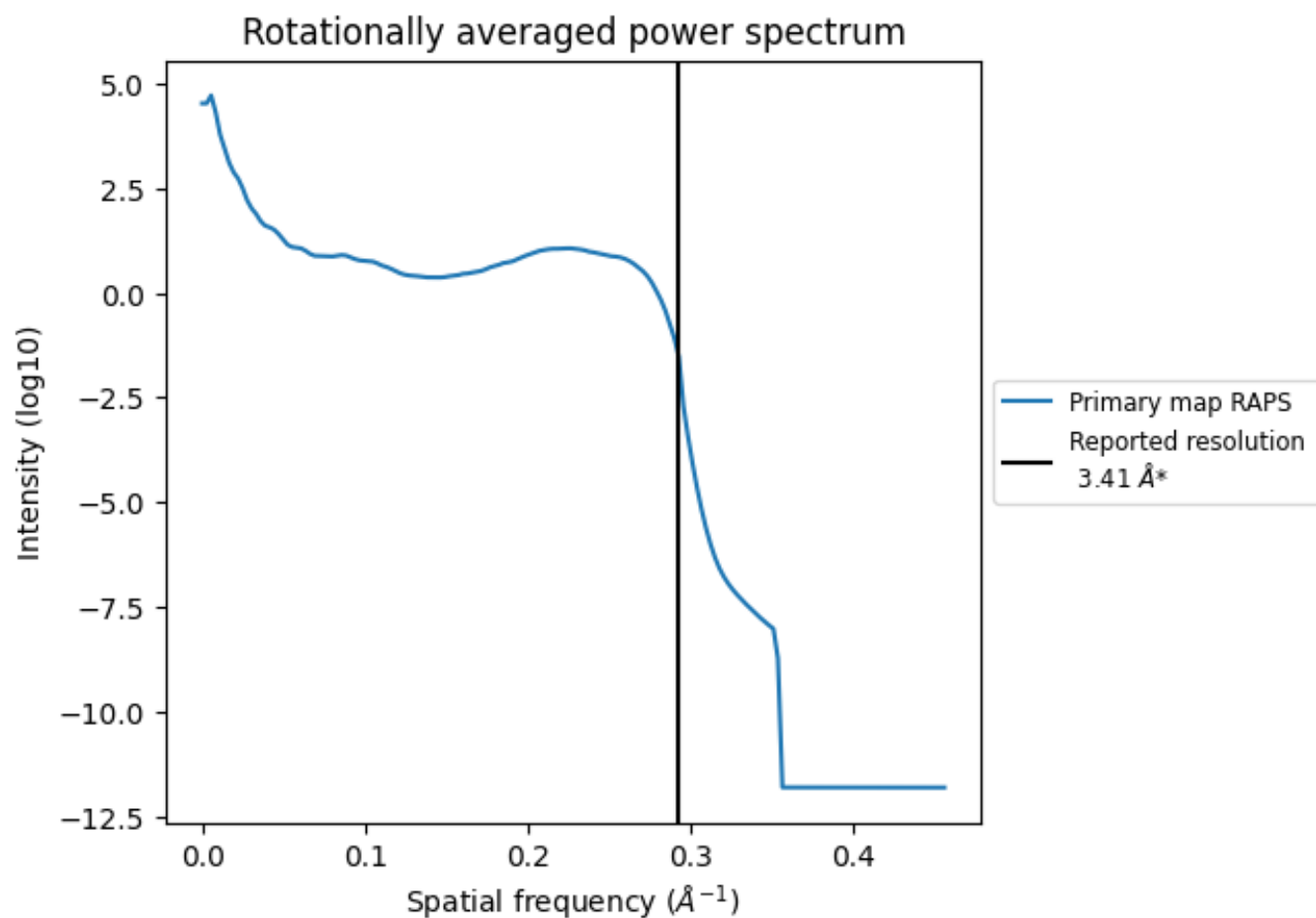
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 273 nm³; this corresponds to an approximate mass of 246 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 0.293 Å⁻¹

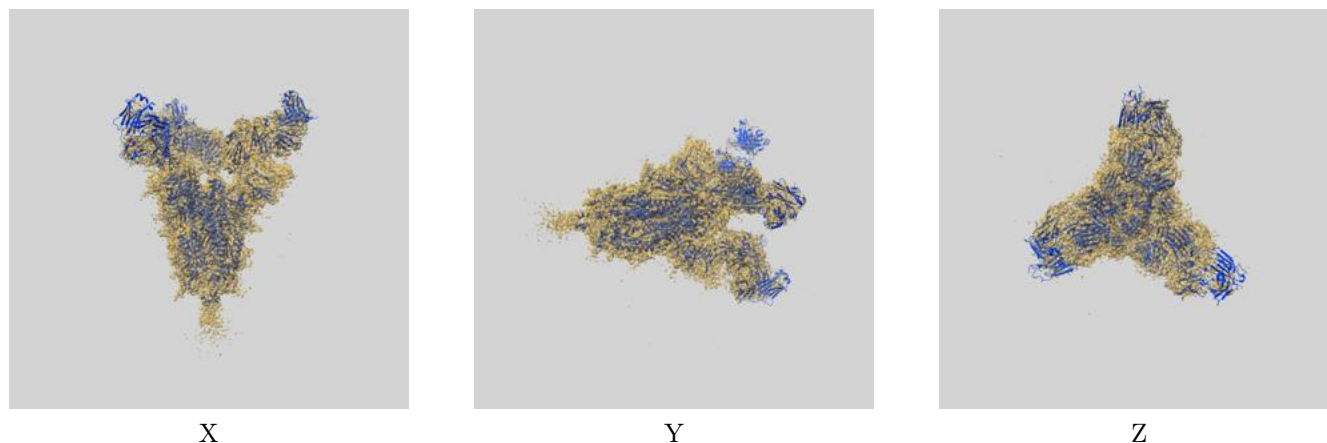
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

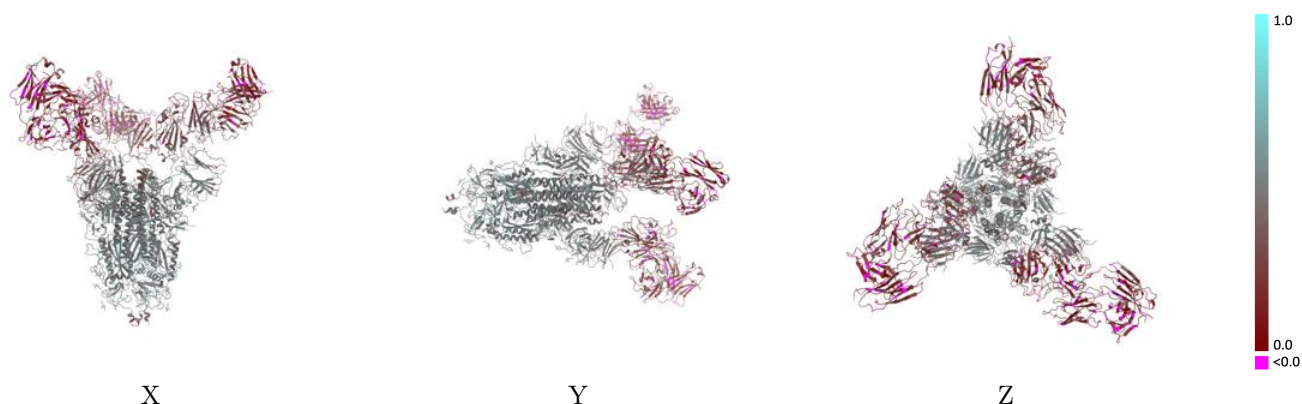
This section contains information regarding the fit between EMDB map EMD-31034 and PDB model 7E9O. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



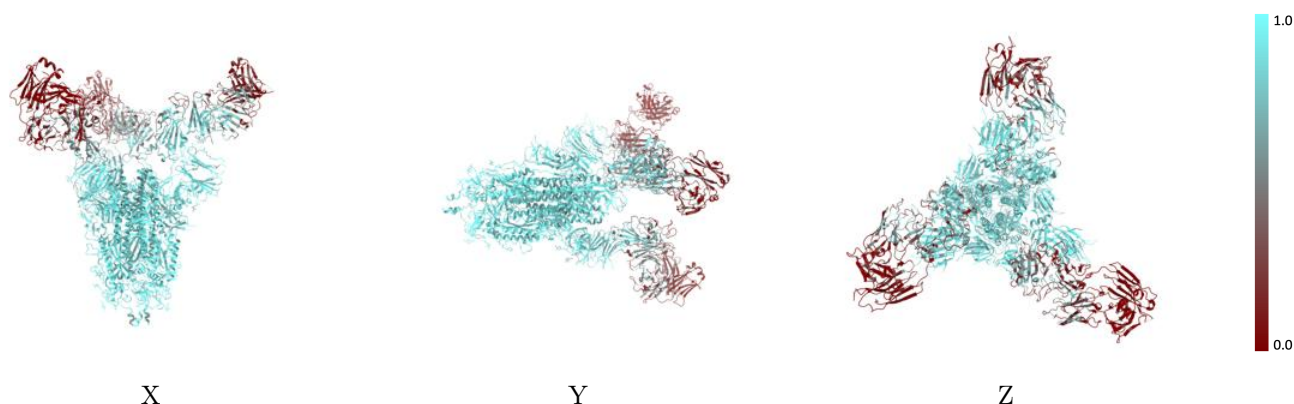
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



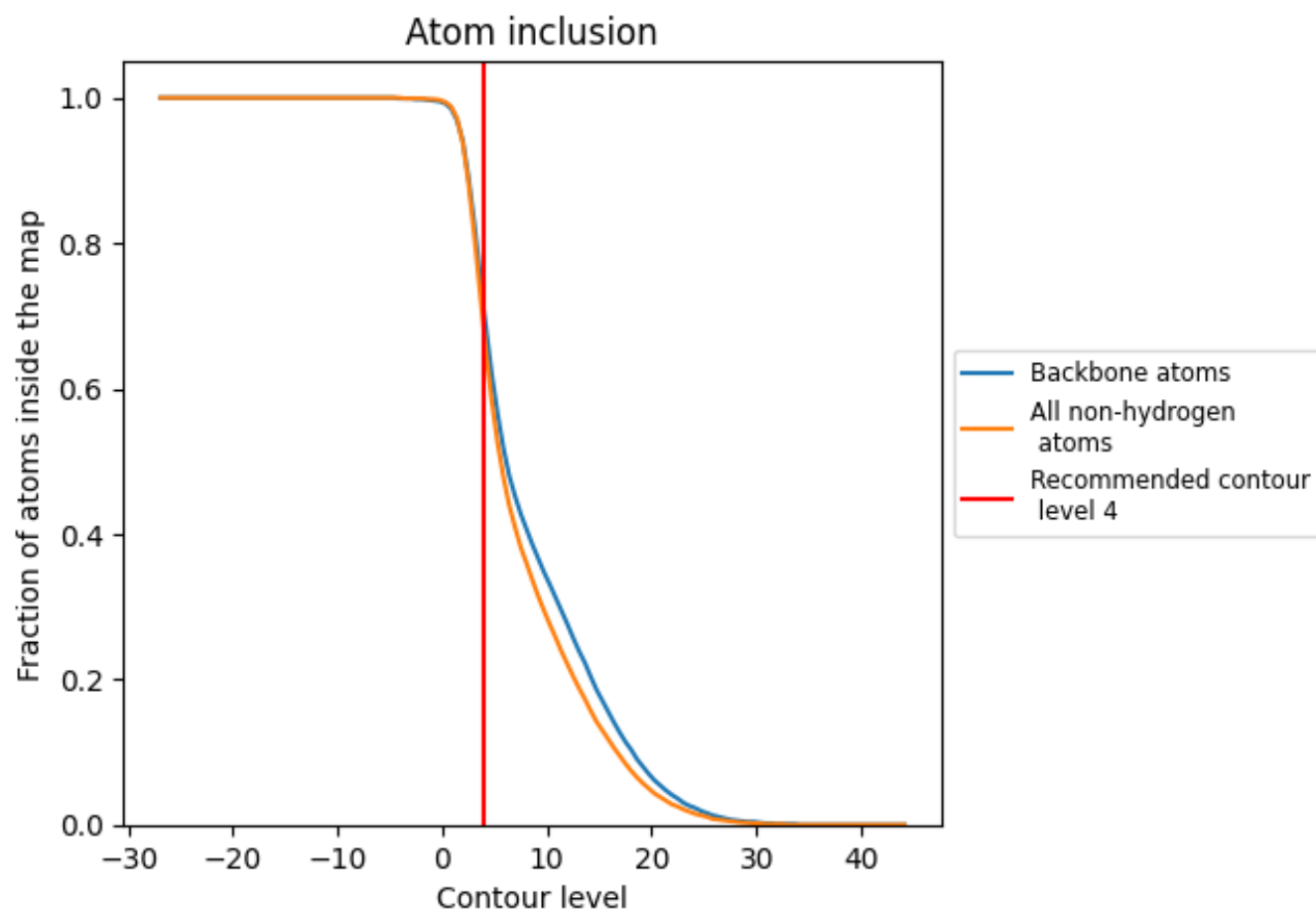
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 67% 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 (4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6730	0.3810
A	0.8570	0.4540
B	0.8060	0.4400
C	0.8360	0.4530
H	0.4680	0.2780
L	0.4030	0.2370
O	0.1510	0.1850
P	0.1650	0.1940
X	0.2480	0.2110
Y	0.3050	0.2190

1.0

0.0

<0.0