



wwPDB EM Validation Summary Report ⓘ

Mar 4, 2026 – 11:36 PM UTC

PDB ID : 7K8U / pdb_00007k8u
EMDB ID : EMD-22731
Title : Structure of the SARS-CoV-2 S 6P trimer in complex with the human neutralizing antibody Fab fragment, C104
Authors : Barnes, C.O.; Malyutin, A.G.; Bjorkman, P.J.
Deposited on : 2020-09-27
Resolution : 3.80 Å(reported)
Based on initial model : 6VYB

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

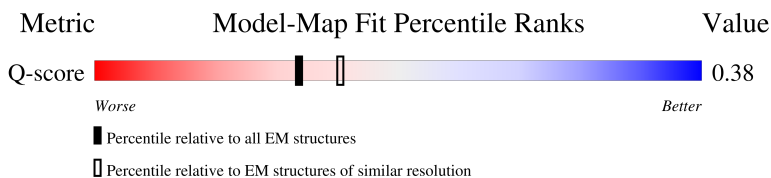
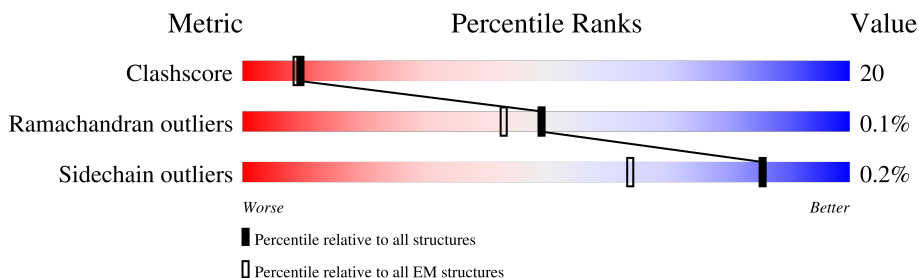
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	1259	
1	B	1259	
1	C	1259	
2	H	235	

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Mol	Chain	Length	Quality of chain
3	L	215	
4	D	2	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23915 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	A	991	Total	C	N	O	S	0	0
			7619	4877	1268	1440	34		
1	B	986	Total	C	N	O	S	0	0
			7586	4856	1260	1436	34		
1	C	991	Total	C	N	O	S	0	0
			7612	4877	1271	1430	34		

There are 147 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	607	GLU	GLN	conflict	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
A	1214	SER	-	expression tag	UNP P0DTC2
A	1215	GLY	-	expression tag	UNP P0DTC2
A	1216	ARG	-	expression tag	UNP P0DTC2
A	1217	LEU	-	expression tag	UNP P0DTC2
A	1218	VAL	-	expression tag	UNP P0DTC2
A	1219	PRO	-	expression tag	UNP P0DTC2
A	1220	ARG	-	expression tag	UNP P0DTC2
A	1221	GLY	-	expression tag	UNP P0DTC2
A	1222	SER	-	expression tag	UNP P0DTC2
A	1223	PRO	-	expression tag	UNP P0DTC2
A	1224	GLY	-	expression tag	UNP P0DTC2
A	1225	SER	-	expression tag	UNP P0DTC2
A	1226	GLY	-	expression tag	UNP P0DTC2
A	1227	TYR	-	expression tag	UNP P0DTC2
A	1228	ILE	-	expression tag	UNP P0DTC2
A	1229	PRO	-	expression tag	UNP P0DTC2
A	1230	GLU	-	expression tag	UNP P0DTC2
A	1231	ALA	-	expression tag	UNP P0DTC2
A	1232	PRO	-	expression tag	UNP P0DTC2
A	1233	ARG	-	expression tag	UNP P0DTC2
A	1234	ASP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1235	GLY	-	expression tag	UNP P0DTC2
A	1236	GLN	-	expression tag	UNP P0DTC2
A	1237	ALA	-	expression tag	UNP P0DTC2
A	1238	TYR	-	expression tag	UNP P0DTC2
A	1239	VAL	-	expression tag	UNP P0DTC2
A	1240	ARG	-	expression tag	UNP P0DTC2
A	1241	LYS	-	expression tag	UNP P0DTC2
A	1242	ASP	-	expression tag	UNP P0DTC2
A	1243	GLY	-	expression tag	UNP P0DTC2
A	1244	GLU	-	expression tag	UNP P0DTC2
A	1245	TRP	-	expression tag	UNP P0DTC2
A	1246	VAL	-	expression tag	UNP P0DTC2
A	1247	LEU	-	expression tag	UNP P0DTC2
A	1248	LEU	-	expression tag	UNP P0DTC2
A	1249	SER	-	expression tag	UNP P0DTC2
A	1250	THR	-	expression tag	UNP P0DTC2
A	1251	PHE	-	expression tag	UNP P0DTC2
A	1252	LEU	-	expression tag	UNP P0DTC2
A	1253	GLY	-	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	HIS	-	expression tag	UNP P0DTC2
A	1259	HIS	-	expression tag	UNP P0DTC2
B	607	GLU	GLN	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
B	1214	SER	-	expression tag	UNP P0DTC2
B	1215	GLY	-	expression tag	UNP P0DTC2
B	1216	ARG	-	expression tag	UNP P0DTC2
B	1217	LEU	-	expression tag	UNP P0DTC2
B	1218	VAL	-	expression tag	UNP P0DTC2
B	1219	PRO	-	expression tag	UNP P0DTC2
B	1220	ARG	-	expression tag	UNP P0DTC2
B	1221	GLY	-	expression tag	UNP P0DTC2
B	1222	SER	-	expression tag	UNP P0DTC2
B	1223	PRO	-	expression tag	UNP P0DTC2
B	1224	GLY	-	expression tag	UNP P0DTC2
B	1225	SER	-	expression tag	UNP P0DTC2
B	1226	GLY	-	expression tag	UNP P0DTC2
B	1227	TYR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1228	ILE	-	expression tag	UNP P0DTC2
B	1229	PRO	-	expression tag	UNP P0DTC2
B	1230	GLU	-	expression tag	UNP P0DTC2
B	1231	ALA	-	expression tag	UNP P0DTC2
B	1232	PRO	-	expression tag	UNP P0DTC2
B	1233	ARG	-	expression tag	UNP P0DTC2
B	1234	ASP	-	expression tag	UNP P0DTC2
B	1235	GLY	-	expression tag	UNP P0DTC2
B	1236	GLN	-	expression tag	UNP P0DTC2
B	1237	ALA	-	expression tag	UNP P0DTC2
B	1238	TYR	-	expression tag	UNP P0DTC2
B	1239	VAL	-	expression tag	UNP P0DTC2
B	1240	ARG	-	expression tag	UNP P0DTC2
B	1241	LYS	-	expression tag	UNP P0DTC2
B	1242	ASP	-	expression tag	UNP P0DTC2
B	1243	GLY	-	expression tag	UNP P0DTC2
B	1244	GLU	-	expression tag	UNP P0DTC2
B	1245	TRP	-	expression tag	UNP P0DTC2
B	1246	VAL	-	expression tag	UNP P0DTC2
B	1247	LEU	-	expression tag	UNP P0DTC2
B	1248	LEU	-	expression tag	UNP P0DTC2
B	1249	SER	-	expression tag	UNP P0DTC2
B	1250	THR	-	expression tag	UNP P0DTC2
B	1251	PHE	-	expression tag	UNP P0DTC2
B	1252	LEU	-	expression tag	UNP P0DTC2
B	1253	GLY	-	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	HIS	-	expression tag	UNP P0DTC2
B	1259	HIS	-	expression tag	UNP P0DTC2
C	607	GLU	GLN	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2
C	1214	SER	-	expression tag	UNP P0DTC2
C	1215	GLY	-	expression tag	UNP P0DTC2
C	1216	ARG	-	expression tag	UNP P0DTC2
C	1217	LEU	-	expression tag	UNP P0DTC2
C	1218	VAL	-	expression tag	UNP P0DTC2
C	1219	PRO	-	expression tag	UNP P0DTC2
C	1220	ARG	-	expression tag	UNP P0DTC2

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

- Molecule 2 is a protein called C104 Fab Heavy Chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	H	106	Total	C	N	O	0	0
			519	306	106	107		

- Molecule 3 is a protein called C104 Fab Light Chain.

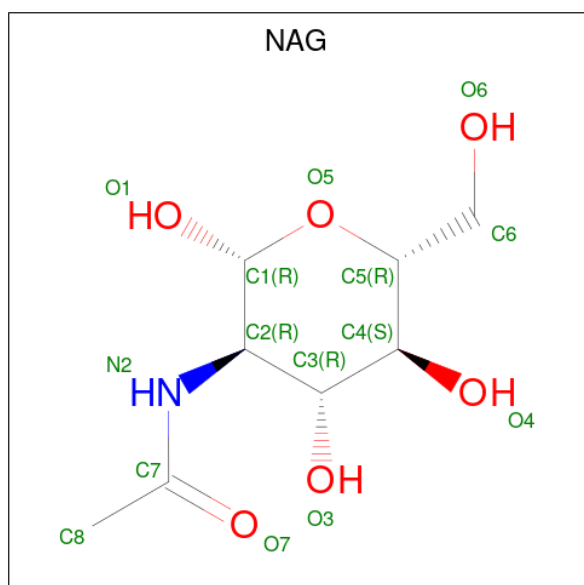
Mol	Chain	Residues	Atoms				AltConf	Trace
3	L	107	Total	C	N	O	0	0
			523	309	107	107		

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

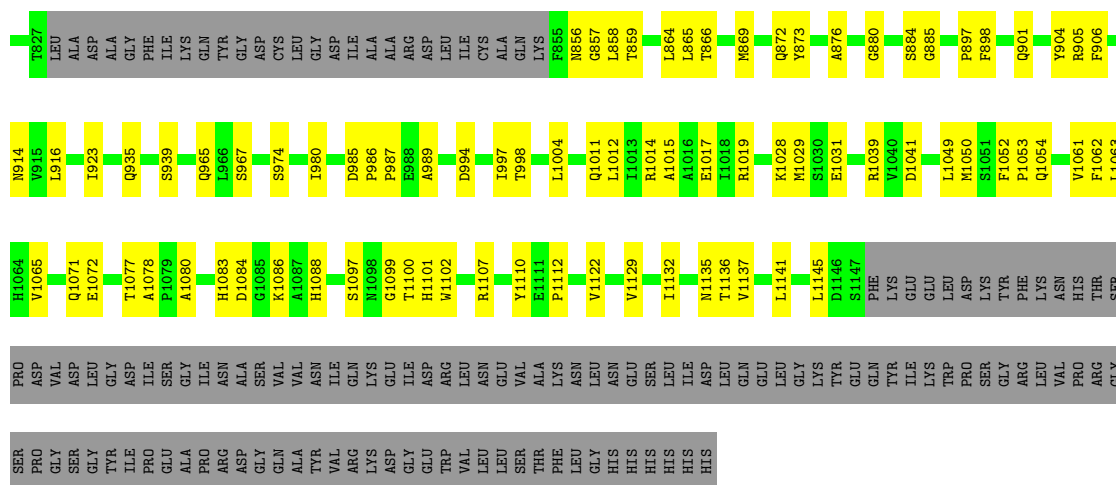


Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	

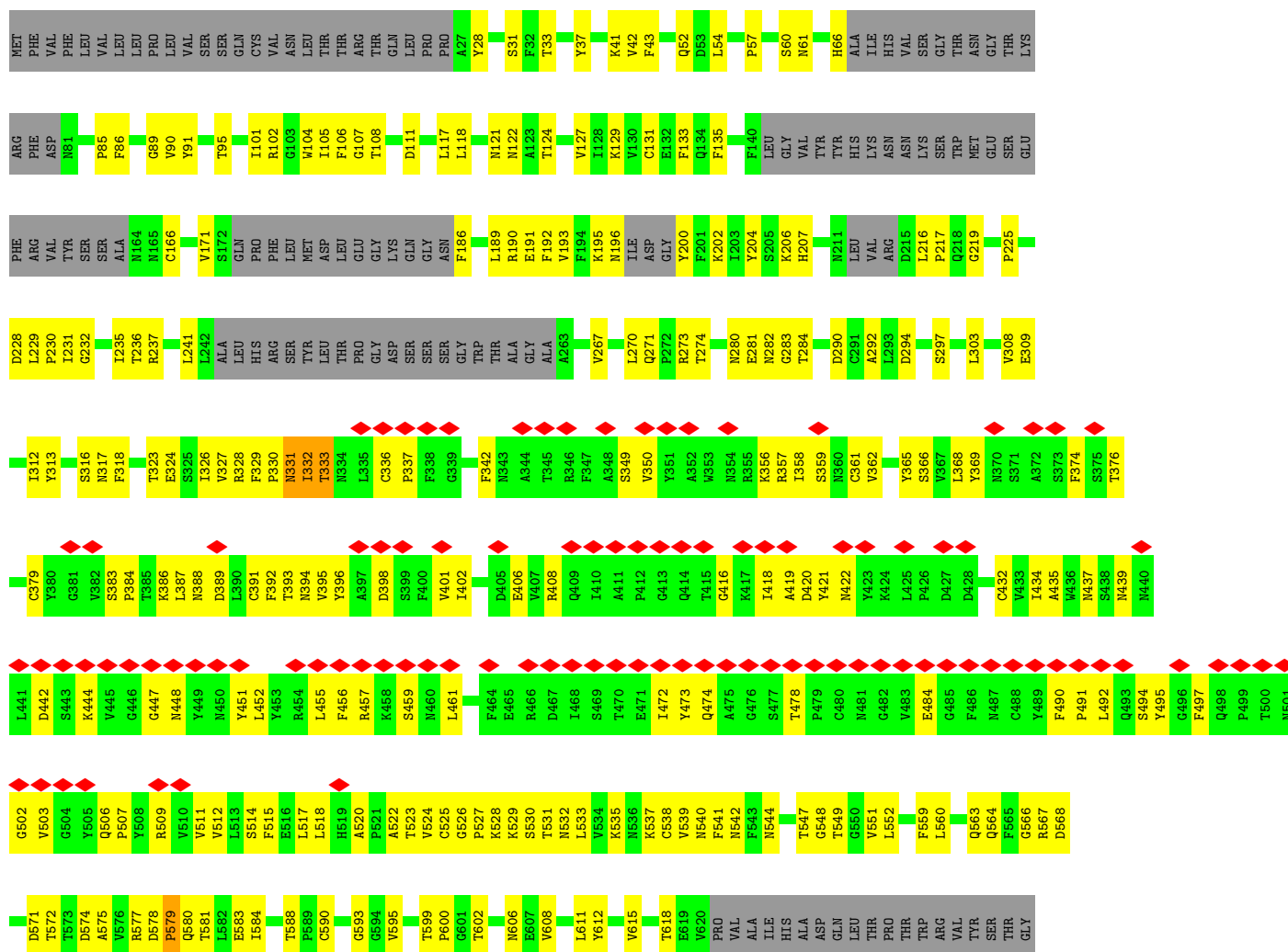
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	C	1	14	8	1	5	0



• Molecule 1: Spike glycoprotein

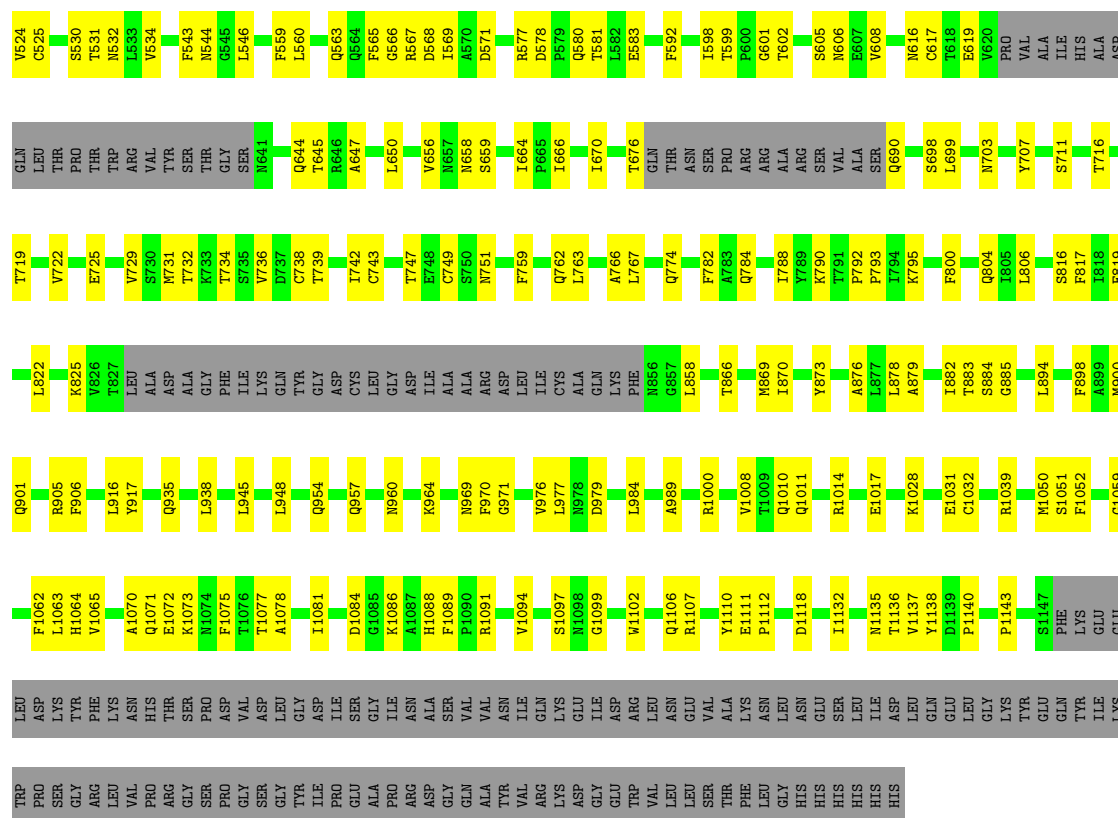


PRO	GLU	ALA	PRO	ARG	ASP	GLY	ILE	V1065	L959	LEU	E725	SER
							SER	N960	ALA	M641		
GLU	ALA	ASP	GLY	ILE	Q1071	ASP	GLY	A1070	T961	ASP	I726	THR
							ASN	Q1071	ALA	M642		
ASP	GLY	P1079	ALA	ASN	P1079	PHE	GLY	Q965	L966	GLY	V729	GLN
							ASN	L966	PHE	M644		
GLN	VAL	I1081	VAL	C1082	I1081	ILE	GLN	V976	GLN	LYS	M731	VAL
							VAL	I1081	LYS	G648		
VAL	ASN	H1083	ASN	H1083	VAL	ILE	ASN	N978	TYR	TRP	D737	ASP
							ASN	H1083	GLN	L650		
ARG	GLN	K1086	GLN	K1086	GLN	ASP	ASP	D979	GLY	ASP	T739	VAL
							ASP	L980	ASP	M740		
LYS	ASP	A1087	GLY	H1088	GLY	CYS	ASP	L981	CYS	ASP	C749	SER
							ASP	L981	CYS	M655		
GLY	ILE	G1093	ASP	G1093	ASP	GLY	GLY	D985	GLY	ASP	N657	THR
							ASP	D985	GLY	M658		
TRP	VAL	LEU	ARG	LEU	ASN	ILE	ILE	E988	ILE	ASP	L752	VAL
							LEU	E988	ILE	E661		
VAL	ASN	S1097	ASN	S1097	ASN	ALA	ALA	A989	ALA	ASP	G757	VAL
							ASN	A989	ALA	C662		
LEU	GLU	H1101	VAL	H1101	VAL	ARG	ARG	E990	ARG	ASP	L767	THR
							VAL	H1101	ARG	D663		
SER	THR	ALA	ALA	W1102	VAL	ASP	ASP	I993	ASP	LEU	I770	SER
							THR	I993	ASP	P665		
PHE	LEU	LYS	ASN	Q1106	ASN	ILE	ILE	I997	ILE	ASP	E773	VAL
							LEU	I997	ILE	C671		
GLY	HIS	ASN	LEU	E1111	ASN	CYS	CYS	R1000	CYS	ASP	Q774	THR
							LEU	R1000	CYS	A672		
HIS	HIS	HIS	HIS	N1125	SER	GLN	GLN	S1003	ALA	ASP	T778	THR
							SER	L1004	ALA	S673		
HIS	HIS	HIS	HIS	L1128	LEU	GLN	GLN	L1004	GLN	ASP	T778	THR
							LEU	L1004	GLN	T676		
HIS	HIS	HIS	HIS	V1129	ASP	ASN	ASN	Y1007	GLN	ASP	V781	THR
							ASN	Y1007	GLN	THR		
HIS	HIS	HIS	HIS	I1132	LEU	GLU	GLU	V1008	ASP	ASP	F782	THR
							LEU	V1008	ASP	ASN		
LEU	GLU	LEU	GLN	I1132	GLN	GLU	GLU	T1009	GLU	PRO	A783	THR
							GLU	T1009	PRO	ASN		
LEU	GLY	T1136	LEU	N1135	LEU	GLU	GLU	L1012	L877	ARG	V785	THR
							GLU	L877	ARG	ARG		
LYS	TYR	V1137	LYS	T1136	GLY	GLU	GLU	I1013	L878	ALA	Q787	THR
							GLU	I1013	ALA	ALA		
TYR	GLU	S1147	GLN	PHE	GLU	GLN	GLN	R1019	G880	ARG	I788	THR
							GLU	R1019	ARG	SER		
GLN	LYS	TYR	GLN	S1147	GLU	GLN	GLN	A1025	S884	VAL	K790	THR
							GLU	S884	VAL	ALA		
TYR	LYS	GLU	TYR	LYS	GLU	GLN	GLN	M1029	Q895	ASP	F797	THR
							GLU	Q895	ASP	S689		
LYS	TRP	LEU	TRP	LEU	GLU	GLY	GLY	S1030	Q895	ASP	G799	THR
							GLU	S1030	ASP	Q690		
PRO	SER	ASP	PRO	ASP	ASP	LYS	LYS	E1031	Q901	ASP	Q804	THR
							LYS	Q901	ASP	T696		
GLY	TYR	PHE	GLY	TYR	TYR	R905	TYR	V1033	A903	ASP	L806	THR
							TYR	A903	ASP	M697		
ARG	LEU	LYS	ARG	PHE	PHE	R906	PHE	R1039	R906	ASP	L699	THR
							LEU	R906	ASP	L699		
VAL	PRO	ASN	VAL	ASN	ASN	HIS	ASN	C1043	T912	ASP	E702	THR
							ASN	T912	ASP	S704		
ARG	GLY	THR	ARG	HIS	THR	HIS	HIS	Q913	Q913	ASP	S813	THR
							HIS	Q913	ASP	S704		
SER	PRO	GLY	SER	SER	GLY	SER	GLY	L1049	N914	ASP	S816	THR
							GLY	N914	ASP	Y707		
PRO	HIS	ASP	PRO	SER	GLY	SER	GLY	M1050	F817	ASP	I818	THR
							GLY	F817	ASP	S708		
GLY	VAL	ASP	PRO	ASP	GLY	VAL	VAL	S1051	L916	ASP	E819	THR
							VAL	L916	ASP	T716		
GLY	SER	ASP	SER	ASP	SER	VAL	VAL	G1059	Q935	ASP	D820	THR
							VAL	Q935	ASP	T716		
LEU	GLY	LEU	GLY	LEU	GLY	LEU	LEU	V1061	Q935	ASP	K325	THR
							LEU	V1061	ASP	T719		
ASP	GLY	SER	TYR	ILE	TYR	GLY	GLY	H1064	L938	ASP	V826	THR
							GLY	L938	ASP	V826		

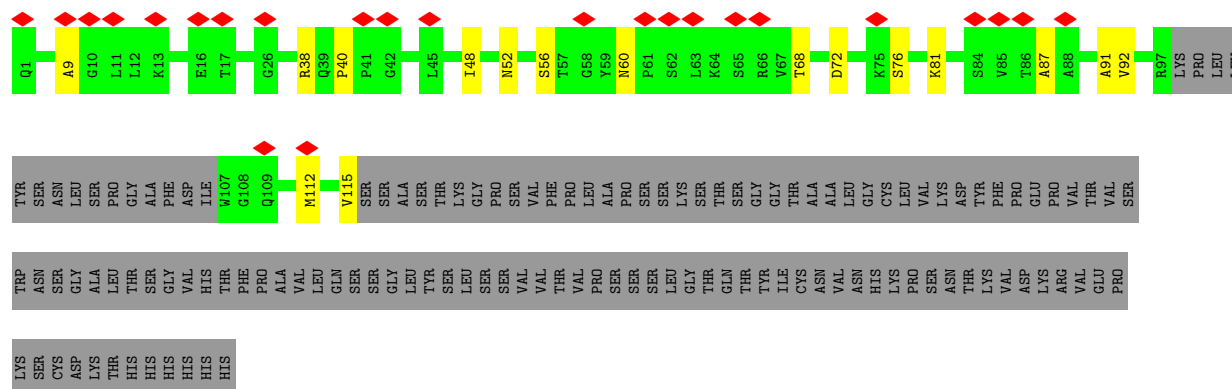
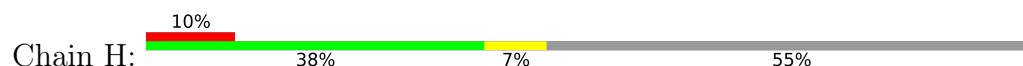
• Molecule 1: Spike glycoprotein

Chain C: 50% 29% 21%

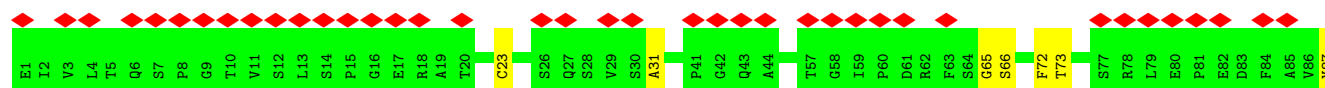
MET	PHE	VAL	PHE	LEU	VAL	LEU	LEU	PRO	LEU	VAL	SER	SER	GLN	CYS	VAL	ASN	LEU	THR	THR	ARG	THR	GLN	PRO	PRO	A27	Y28	T29	N30	S31	F32	T33	R34	Y37	Y38	P39	D40	K41	V42	F43	R44	L48	Q52	D53	L54	F55	L56	P57	F58	F59	W64	F65	H66	ALA	ILE	
HIS	VAL	SER	GLY	THR	ASN	GLY	THR	LYS	ARG	PHE	ASP	N81	L84	P85	F86	V90	A93	I101	R102	G103	W104	I105	F106	G107	S112	S116	L117	L118	I119	V120	N121	N122	T124	N125	V126	V127	I128	K129	F135	C136	P139	V143	TYR	THR	HIS	LYS	ASN	ASN	TYR						
LYS	SER	TRP	MET	GLU	SER	GLU	PHE	ARG	VAL	TYR	SER	SER	ASN	ASN	H165	C166	T167	GLN	PRO	PHE	MET	ASP	LEU	GLU	GLY	LYS	GLN	GLY	ASN	F186	K187	M188	L189	R190	F191	F192	V193	F194	K195	Y200	F201	I203	Y204	I210	N211	L212	V213	R214	P217	Q218					
G219	F220	S221	A222	L223	D228	T231	G232	I233	N234	I235	F238	L241	L242	ALA	LEU	HIS	ARG	SER	TYR	LEU	THR	PRO	GLY	ASP	SER	SER	GLY	LYS	THR	ALA	F186	K187	M188	L189	R190	F191	F192	V193	F194	K195	Y200	F201	I203	Y204	I210	N211	L212	V213	R214	P217	Q218				
C291	F306	T307	V308	E309	K310	Q311	S316	N317	F318	R319	I326	V327	R328	F329	P330	N331	I332	T333	C336	P337	G339	E340	G413	V414	F342	N343	A344	T345	R346	V350	Y351	A352	R357	I358	S359	N360	C361	T374	F275	Y279	N280	G283	T284	L285	T286	D287	A288	V289	D290						
S383	P384	T385	K386	D389	L390	C391	F392	N394	V395	V396	A397	D398	V401	L402	R403	E406	V407	R408	Q409	I410	A411	P412	G413	Q414	T415	G416	K417	I418	Y421	N422	Y423	K424	L425	P426	D427	G431	C432	V433	T434	A435	N436	N437	S438	N439	V445	G446	N450	R454	L455	F456					
R457	K458	S459	N460	L461	K462	R466	D467	L468	S469	T470	E471	L472	Y473	Q474	A475	G476	S477	T478	P479	C480	N481	G482	V483	E484	G485	F486	N487	C488	Y489	L492	F497	Q498	P499	T500	R501	G502	V503	G504	Y505	Q506	P507	Y508	R509	V510	V511	V512	L513	S514	F515	E516	L517	L518	H519	A520	T523

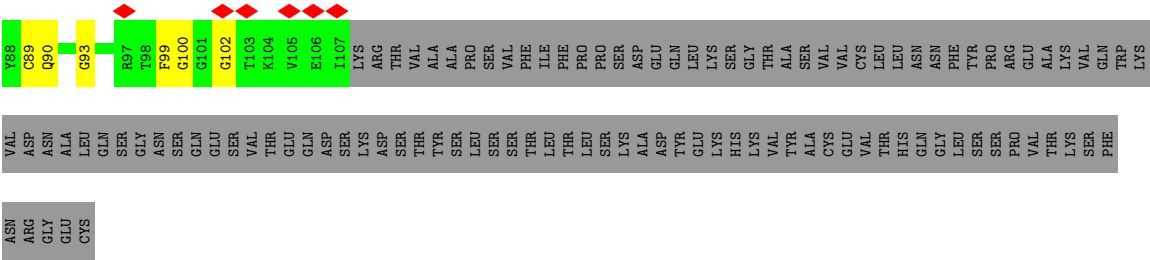


• Molecule 2: C104 Fab Heavy Chain

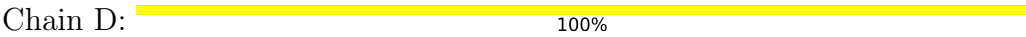


• Molecule 3: C104 Fab Light Chain





● Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	40469	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.416	Depositor
Minimum map value	-0.152	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	361.152, 361.152, 361.152	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.836, 0.836, 0.836	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	0.47	0/7789	0.51	0/10611
1	B	0.47	0/7756	0.53	3/10565 (0.0%)
1	C	0.45	0/7785	0.51	0/10611
2	H	0.16	0/517	0.32	0/713
3	L	0.15	0/522	0.37	0/722
All	All	0.45	0/24369	0.51	3/33222 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	333	THR	CA-C-N	-5.29	114.29	122.59
1	B	333	THR	C-N-CA	-5.29	114.29	122.59
1	B	618	THR	N-CA-C	-5.16	106.67	113.17

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	7619	0	7369	340	0
1	B	7586	0	7317	333	0
1	C	7612	0	7358	297	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	519	0	242	8	0
3	L	523	0	245	11	0
4	D	28	0	25	3	0
5	A	14	0	13	2	0
5	C	14	0	13	1	0
All	All	23915	0	22582	930	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 20.

The worst 5 of 930 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:ILE:HD13	1:B:332:ILE:H	1.17	1.06
1:A:336:CYS:HB2	1:A:337:PRO:HD2	1.07	1.04
1:B:332:ILE:HG22	1:B:527:PRO:HB3	1.37	1.04
1:A:336:CYS:HB2	1:A:337:PRO:CD	1.87	1.03
1:B:329:PHE:CD2	1:B:528:LYS:CB	2.42	1.02

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	971/1259 (77%)	881 (91%)	89 (9%)	1 (0%)	48	79
1	B	964/1259 (77%)	879 (91%)	84 (9%)	1 (0%)	48	79
1	C	975/1259 (77%)	897 (92%)	78 (8%)	0	100	100
2	H	102/235 (43%)	101 (99%)	1 (1%)	0	100	100
3	L	105/215 (49%)	100 (95%)	5 (5%)	0	100	100
All	All	3117/4227 (74%)	2858 (92%)	257 (8%)	2 (0%)	49	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	337	PRO
1	B	579	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	833/1096 (76%)	832 (100%)	1 (0%)	88	89
1	B	830/1096 (76%)	827 (100%)	3 (0%)	84	83
1	C	828/1096 (76%)	827 (100%)	1 (0%)	88	89
2	H	1/201 (0%)	1 (100%)	0	100	100
All	All	2492/3489 (71%)	2487 (100%)	5 (0%)	85	87

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	331	ASN
1	B	331	ASN
1	B	332	ILE
1	B	615	VAL
1	C	333	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	690	GLN
1	B	949	GLN
1	C	901	GLN
1	B	901	GLN
1	B	965	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

2 monosaccharides 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	D	1	4,1	14,14,15	0.27	0	17,19,21	0.56	0
4	NAG	D	2	4	14,14,15	0.27	0	17,19,21	0.69	0

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	D	1	4,1	-	5/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1	NAG	C1-C2-N2-C7
4	D	1	NAG	C8-C7-N2-C2

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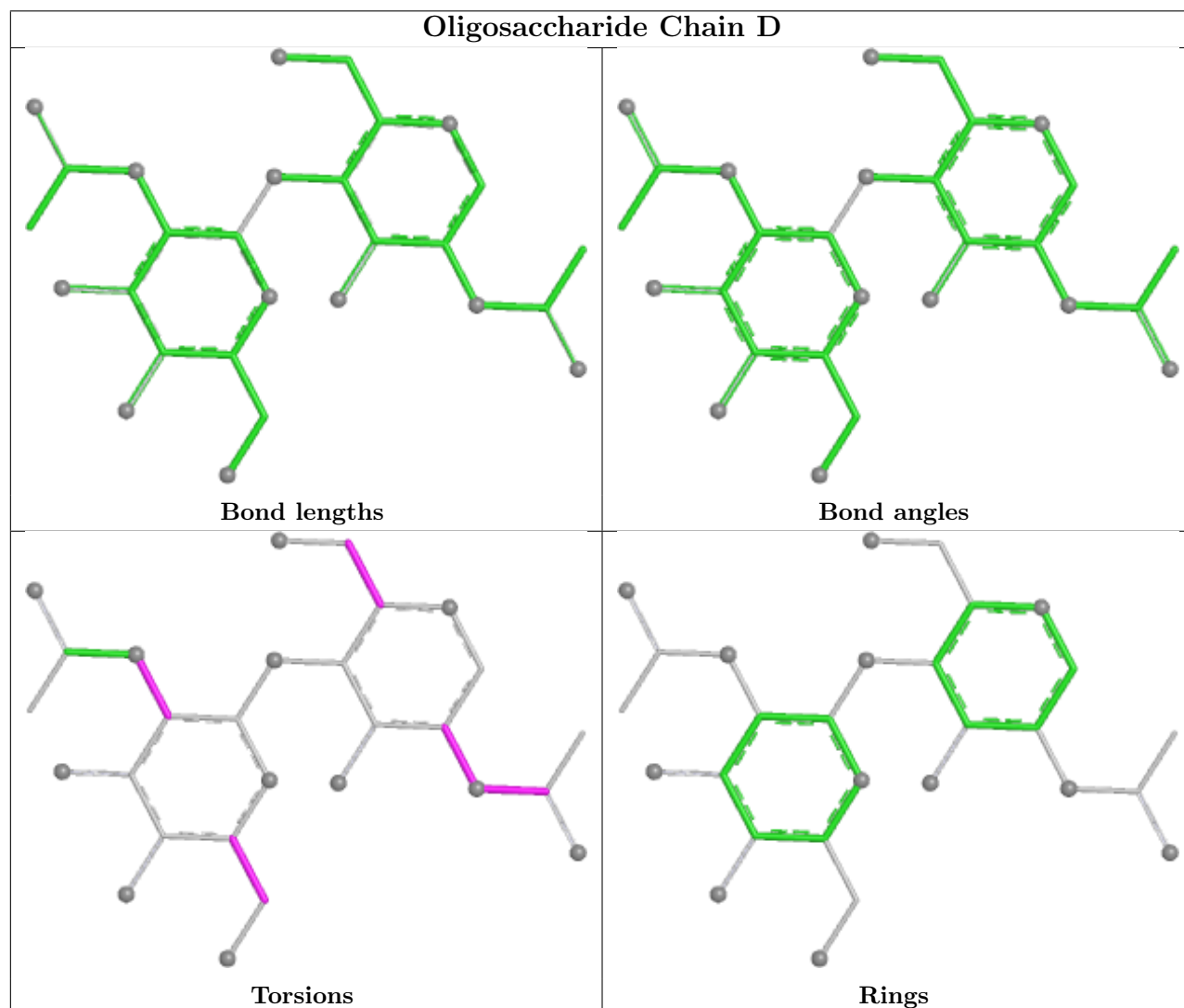
Mol	Chain	Res	Type	Atoms
4	D	1	NAG	O7-C7-N2-C2
4	D	1	NAG	O5-C5-C6-O6
4	D	2	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	2	NAG	2	0
4	D	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry

2 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
5	NAG	A	1301	1	14,14,15	0.28	0	17,19,21	0.60	0
5	NAG	C	1301	1	14,14,15	0.32	0	17,19,21	1.33	4 (23%)

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
5	NAG	A	1301	1	-	3/6/23/26	0/1/1/1
5	NAG	C	1301	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1301	NAG	O5-C1-C2	-2.67	107.15	111.29
5	C	1301	NAG	C2-N2-C7	-2.50	119.54	122.90
5	C	1301	NAG	C4-C3-C2	-2.24	107.73	111.02
5	C	1301	NAG	C3-C4-C5	-2.09	106.44	110.23

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1301	NAG	C3-C2-N2-C7
5	A	1301	NAG	C8-C7-N2-C2
5	A	1301	NAG	O7-C7-N2-C2
5	C	1301	NAG	C4-C5-C6-O6
5	C	1301	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1301	NAG	2	0
5	C	1301	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.

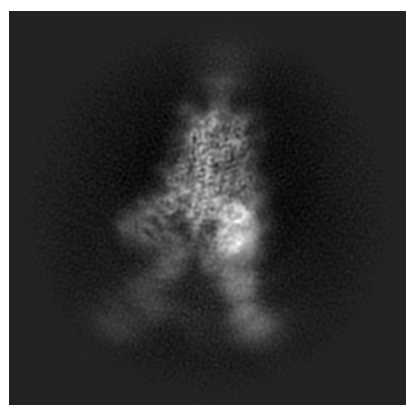
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22731. These allow visual inspection of the internal detail of the map and identification of artifacts.

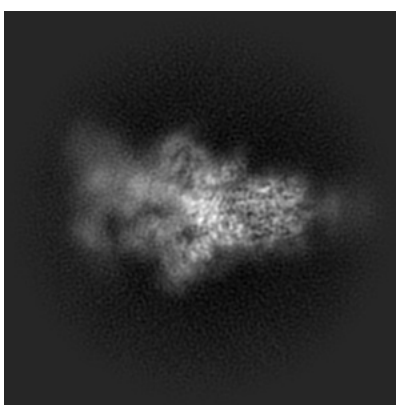
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

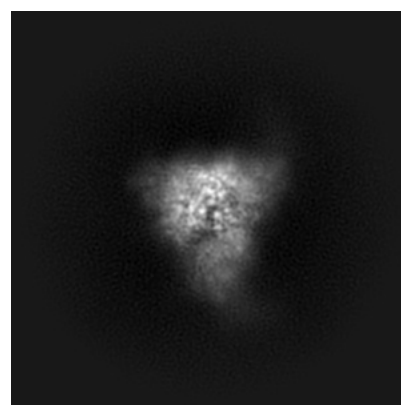
6.1.1 Primary map



X



Y

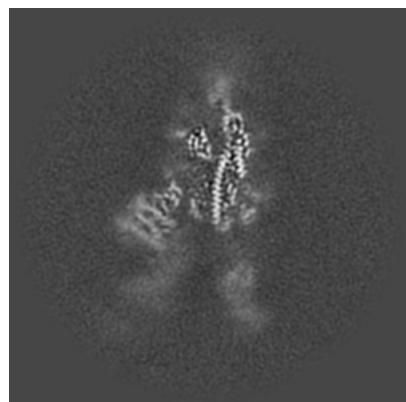


Z

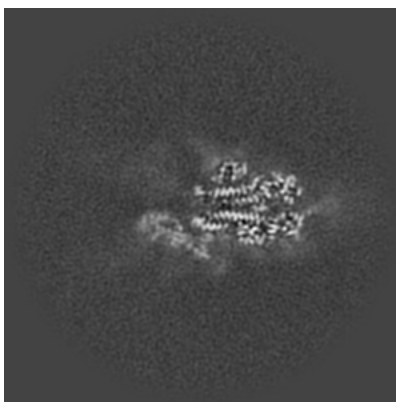
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

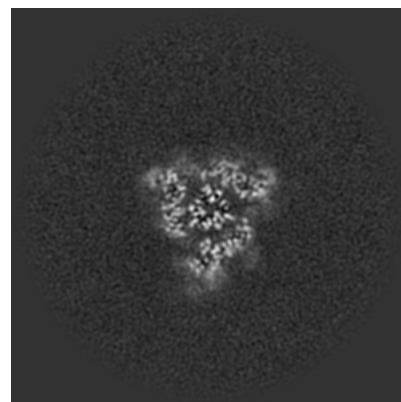
6.2.1 Primary map



X Index: 216



Y Index: 216

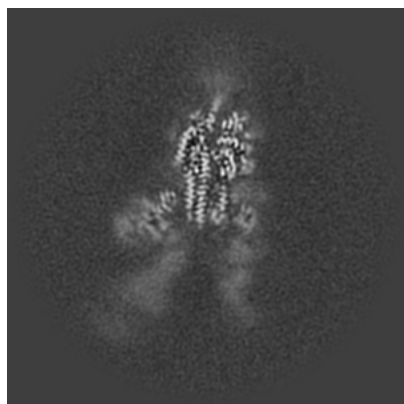


Z Index: 216

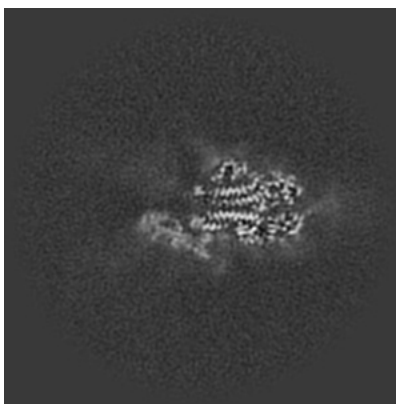
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

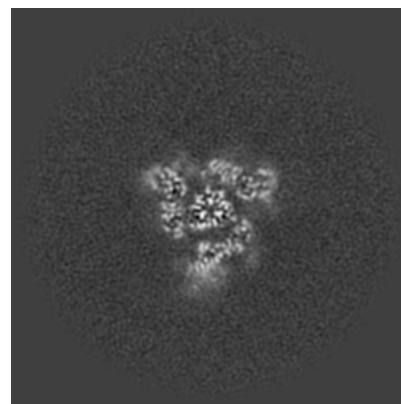
6.3.1 Primary map



X Index: 224



Y Index: 215

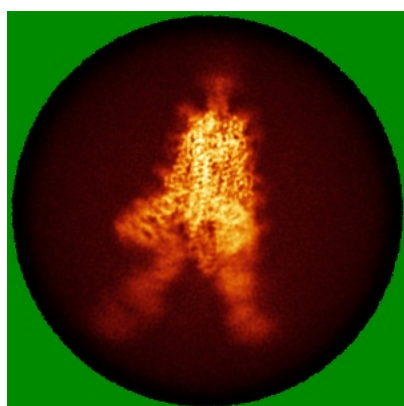


Z Index: 213

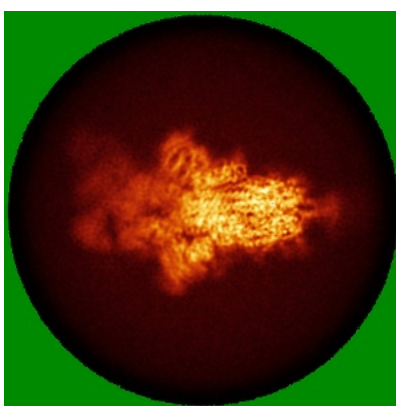
The images above show the largest variance slices of the map in three orthogonal directions.

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

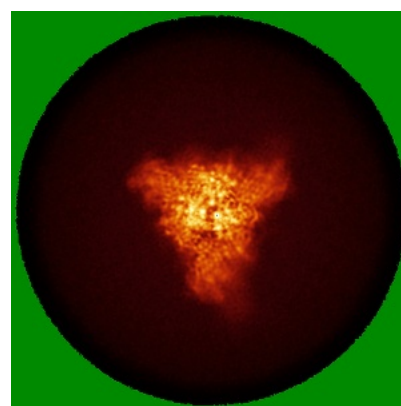
6.4.1 Primary map



X



Y

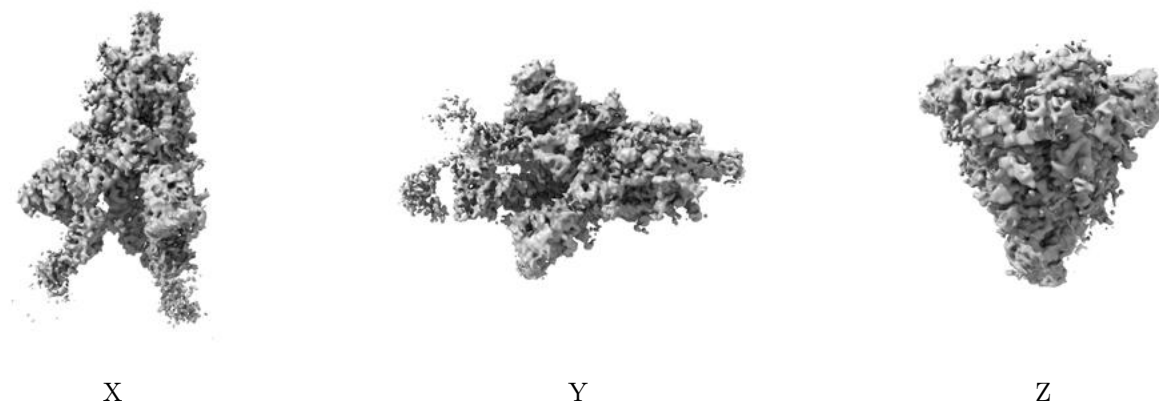


Z

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 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

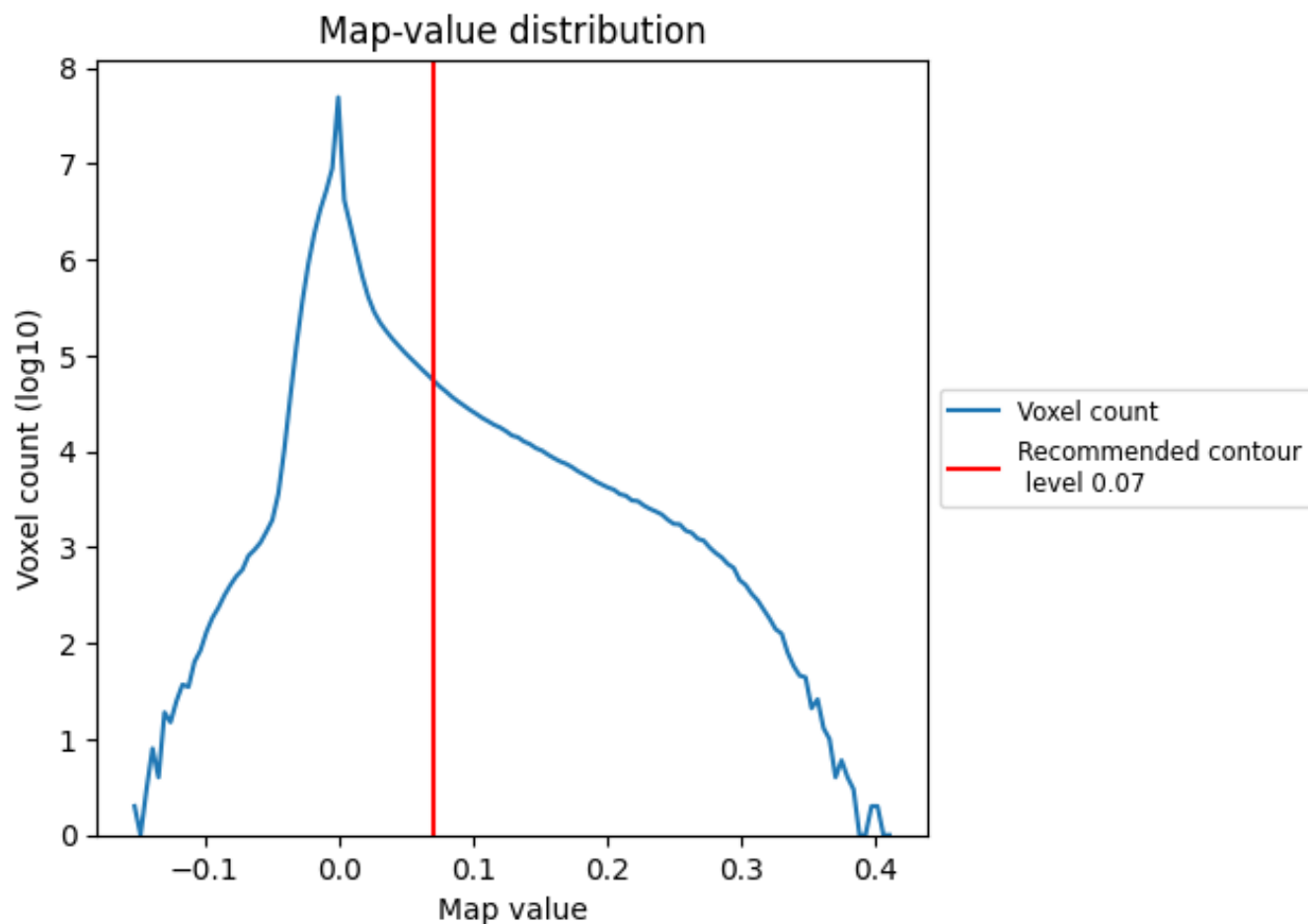
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

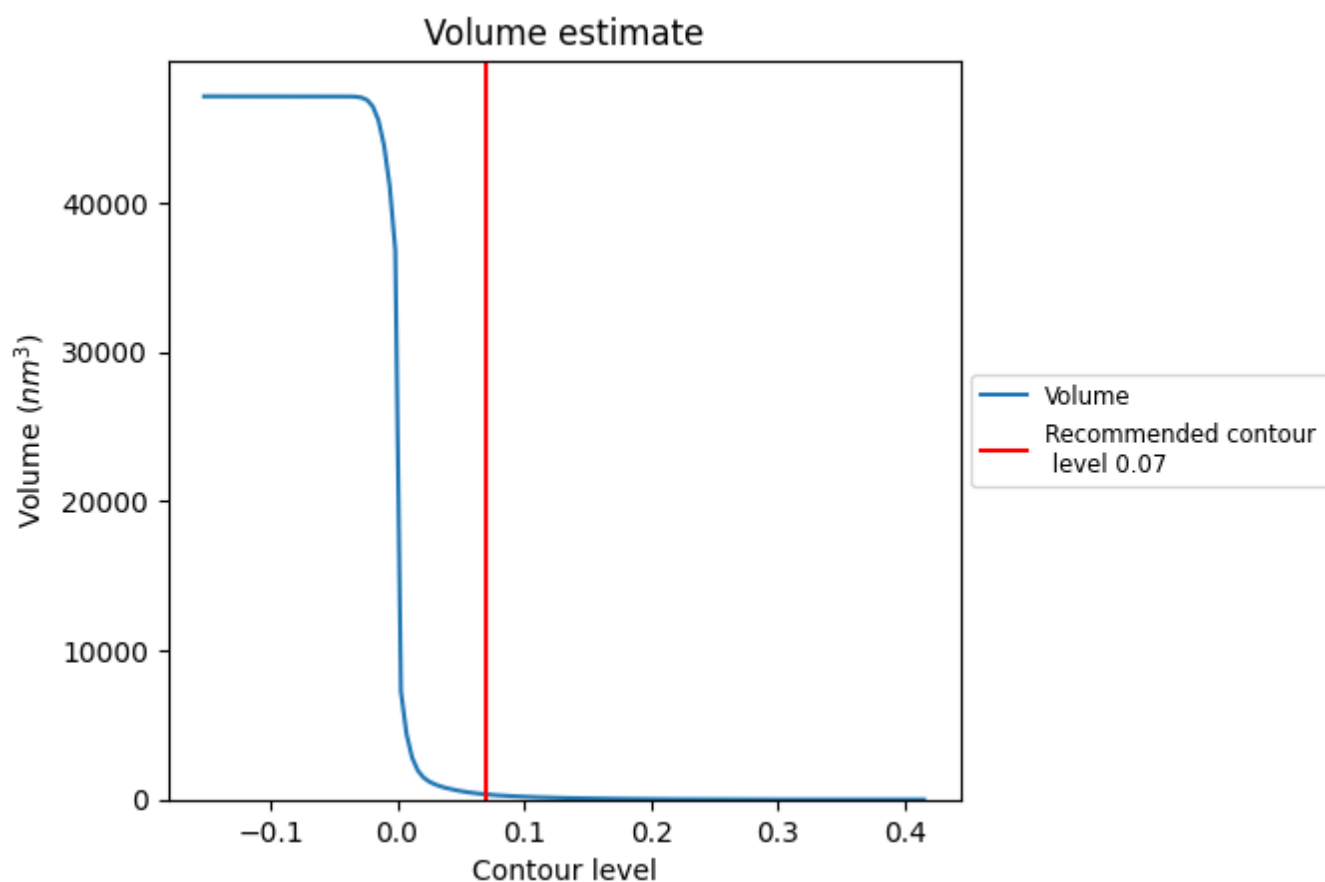
This section contains the results of statistical analysis of the map.

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.

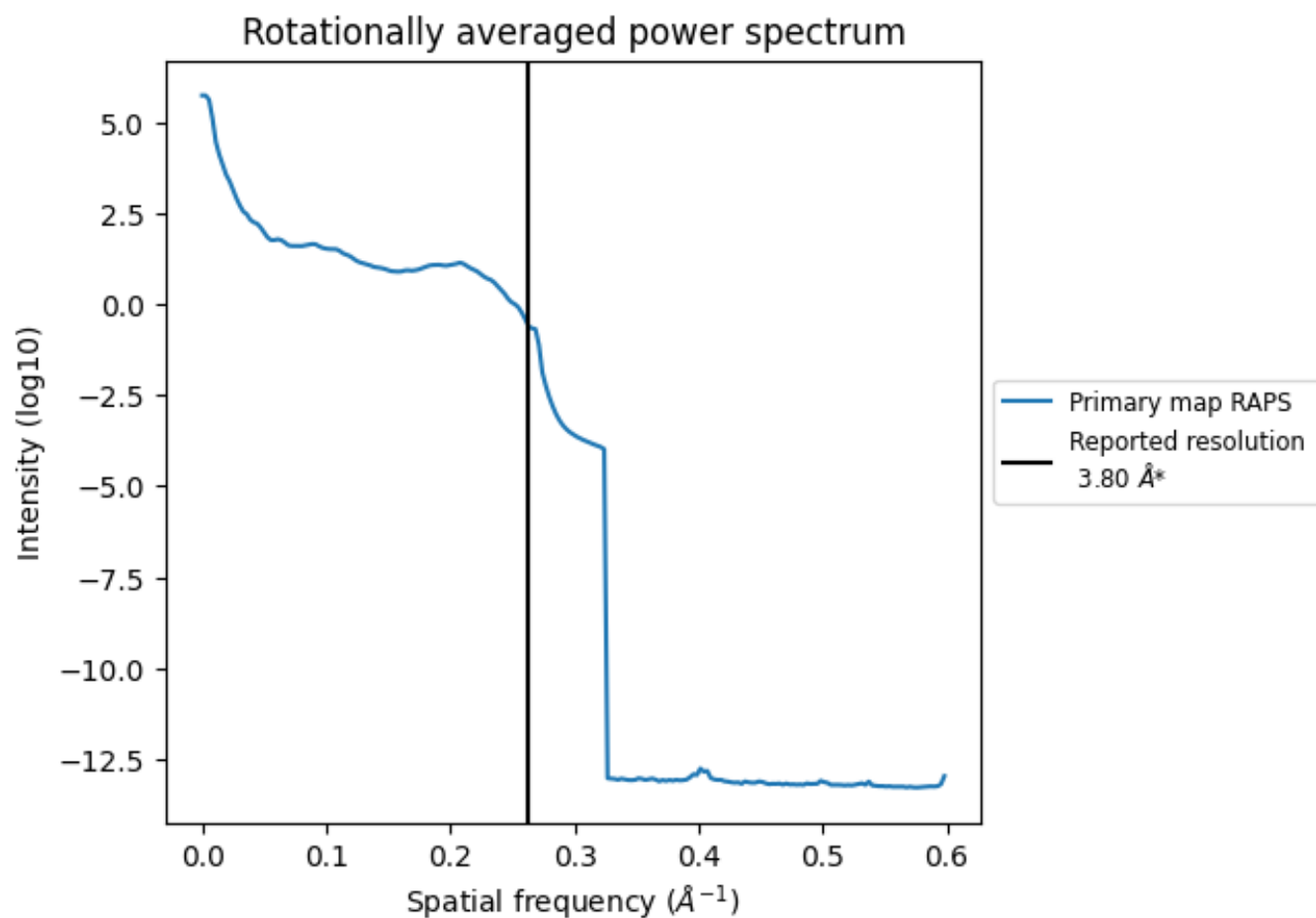
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 349 nm³; this corresponds to an approximate mass of 315 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 ⓘ

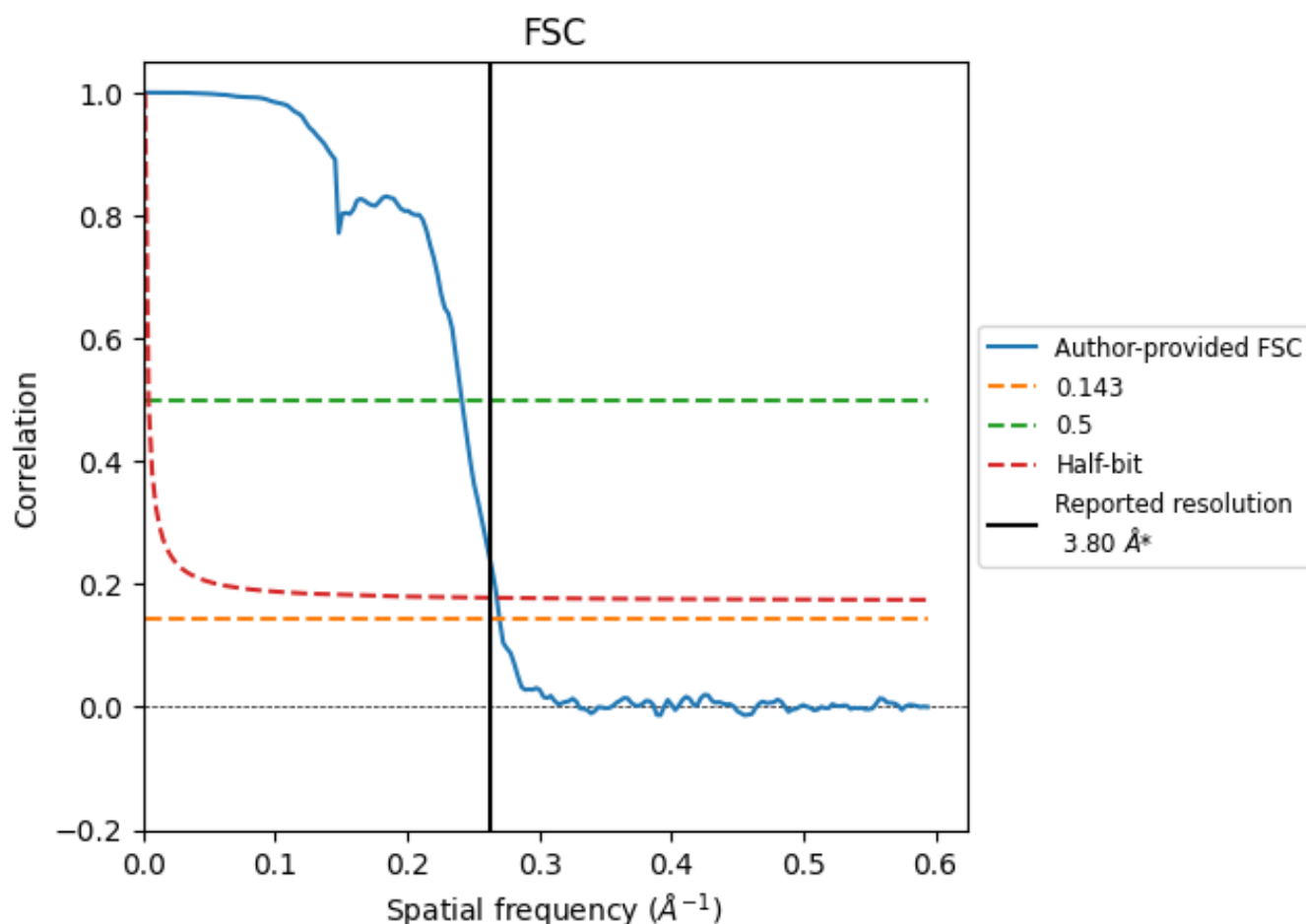


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.71	4.15	3.73
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

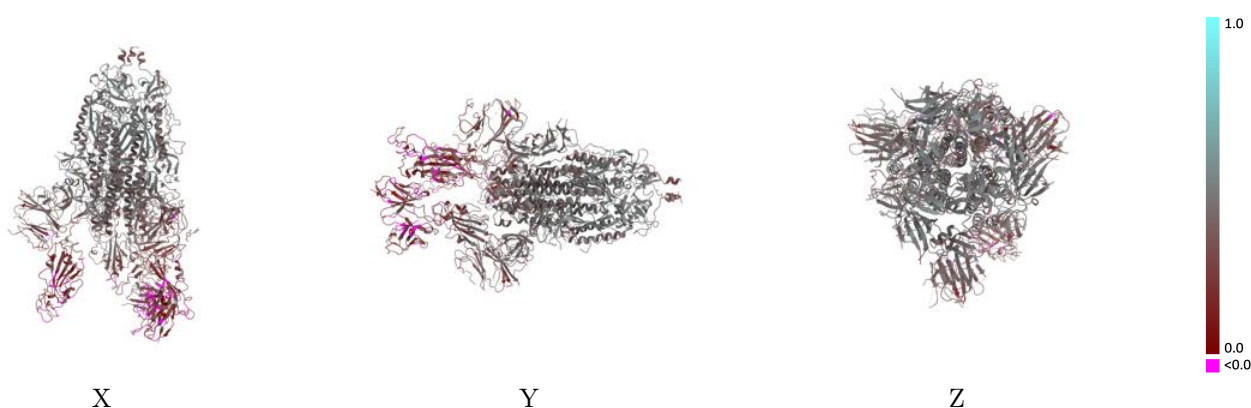
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-22731 and PDB model 7K8U. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)

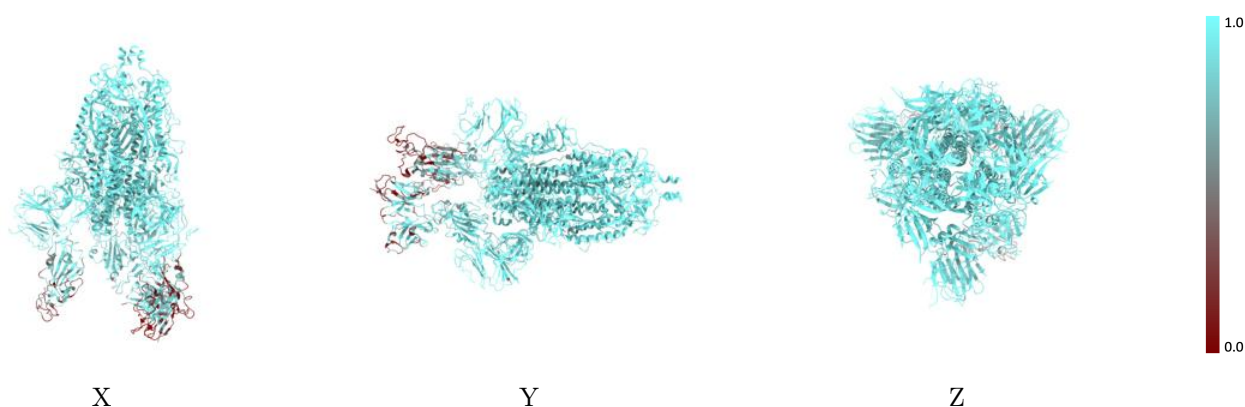
This section was not generated.

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



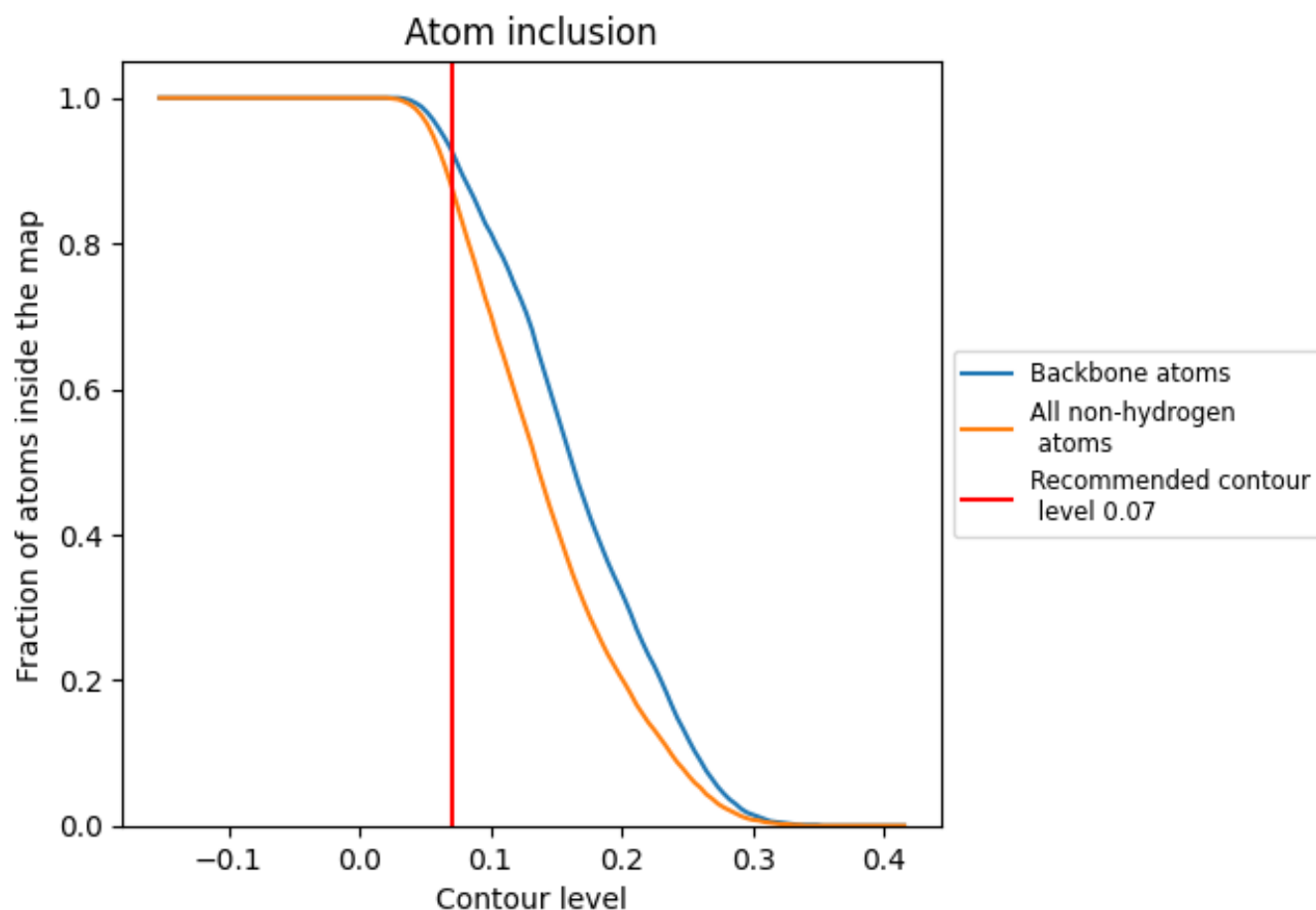
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.07).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8800	0.3800
A	0.9380	0.4080
B	0.8470	0.3790
C	0.8850	0.3760
D	0.8930	0.4150
H	0.7550	0.2100
L	0.5850	0.1860

1.0

0.0

<0.0