



wwPDB EM Validation Summary Report i

Nov 14, 2022 – 04:52 PM EST

PDB ID : 7K8Y
EMDB ID : EMD-22735
Title : Structure of the SARS-CoV-2 S 2P trimer in complex with the human neutralizing antibody Fab fragment, C121 (State 2)
Authors : Abernathy, M.E.; Barnes, C.O.; Bjorkman, P.J.
Deposited on : 2020-09-27
Resolution : 4.40 Å(reported)
Based on initial models : 6VXX, 6W41

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 i 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](#) i) were used in the production of this report:

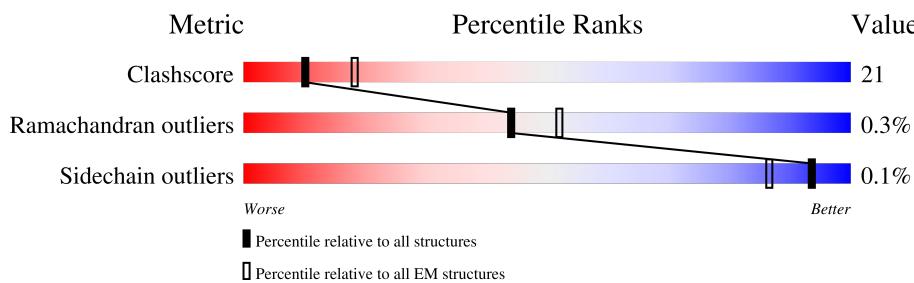
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

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

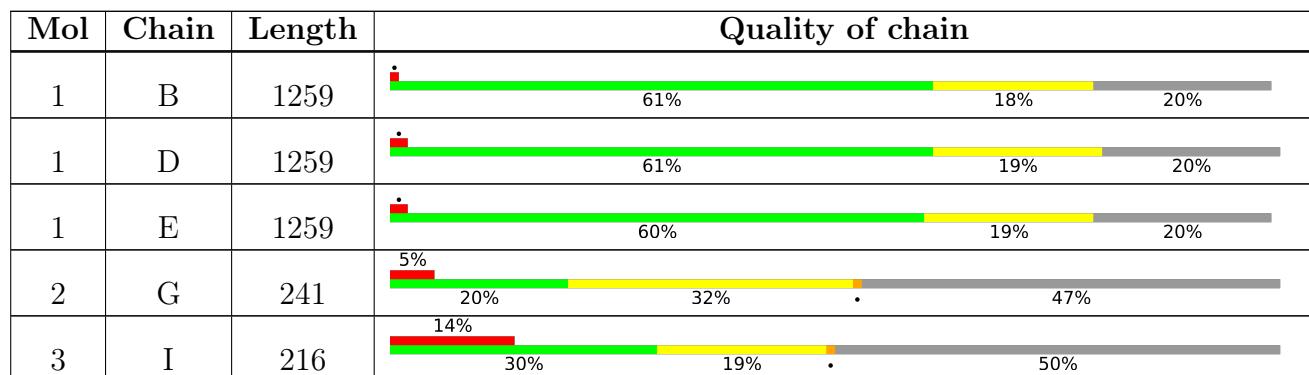
The reported resolution of this entry is 4.40 Å.

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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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.



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 25560 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
			7823	4996	1300	1492	35		
1	D	1002	Total	C	N	O	S	0	0
			7823	4996	1300	1492	35		
1	E	1002	Total	C	N	O	S	0	0
			7823	4996	1300	1492	35		

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
D	986	PRO	LYS	conflict	UNP P0DTC2
D	987	PRO	VAL	conflict	UNP P0DTC2
D	1214	SER	-	expression tag	UNP P0DTC2
D	1215	GLY	-	expression tag	UNP P0DTC2
D	1216	ARG	-	expression tag	UNP P0DTC2
D	1217	LEU	-	expression tag	UNP P0DTC2
D	1218	VAL	-	expression tag	UNP P0DTC2
D	1219	PRO	-	expression tag	UNP P0DTC2
D	1220	ARG	-	expression tag	UNP P0DTC2
D	1221	GLY	-	expression tag	UNP P0DTC2
D	1222	SER	-	expression tag	UNP P0DTC2
D	1223	PRO	-	expression tag	UNP P0DTC2
D	1224	GLY	-	expression tag	UNP P0DTC2
D	1225	SER	-	expression tag	UNP P0DTC2
D	1226	GLY	-	expression tag	UNP P0DTC2
D	1227	TYR	-	expression tag	UNP P0DTC2
D	1228	ILE	-	expression tag	UNP P0DTC2
D	1229	PRO	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1230	GLU	-	expression tag	UNP P0DTC2
D	1231	ALA	-	expression tag	UNP P0DTC2
D	1232	PRO	-	expression tag	UNP P0DTC2
D	1233	ARG	-	expression tag	UNP P0DTC2
D	1234	ASP	-	expression tag	UNP P0DTC2
D	1235	GLY	-	expression tag	UNP P0DTC2
D	1236	GLN	-	expression tag	UNP P0DTC2
D	1237	ALA	-	expression tag	UNP P0DTC2
D	1238	TYR	-	expression tag	UNP P0DTC2
D	1239	VAL	-	expression tag	UNP P0DTC2
D	1240	ARG	-	expression tag	UNP P0DTC2
D	1241	LYS	-	expression tag	UNP P0DTC2
D	1242	ASP	-	expression tag	UNP P0DTC2
D	1243	GLY	-	expression tag	UNP P0DTC2
D	1244	GLU	-	expression tag	UNP P0DTC2
D	1245	TRP	-	expression tag	UNP P0DTC2
D	1246	VAL	-	expression tag	UNP P0DTC2
D	1247	LEU	-	expression tag	UNP P0DTC2
D	1248	LEU	-	expression tag	UNP P0DTC2
D	1249	SER	-	expression tag	UNP P0DTC2
D	1250	THR	-	expression tag	UNP P0DTC2
D	1251	PHE	-	expression tag	UNP P0DTC2
D	1252	LEU	-	expression tag	UNP P0DTC2
D	1253	GLY	-	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	HIS	-	expression tag	UNP P0DTC2
D	1259	HIS	-	expression tag	UNP P0DTC2
E	986	PRO	LYS	conflict	UNP P0DTC2
E	987	PRO	VAL	conflict	UNP P0DTC2
E	1214	SER	-	expression tag	UNP P0DTC2
E	1215	GLY	-	expression tag	UNP P0DTC2
E	1216	ARG	-	expression tag	UNP P0DTC2
E	1217	LEU	-	expression tag	UNP P0DTC2
E	1218	VAL	-	expression tag	UNP P0DTC2
E	1219	PRO	-	expression tag	UNP P0DTC2
E	1220	ARG	-	expression tag	UNP P0DTC2
E	1221	GLY	-	expression tag	UNP P0DTC2
E	1222	SER	-	expression tag	UNP P0DTC2
E	1223	PRO	-	expression tag	UNP P0DTC2

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

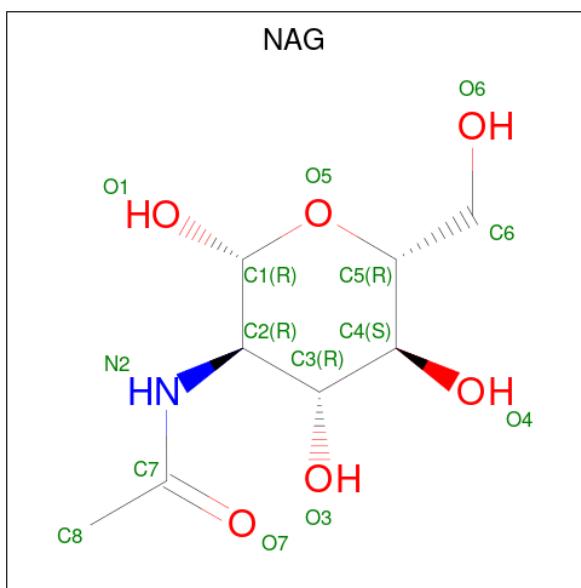
- Molecule 2 is a protein called C121 Fab Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	128	Total 991	C 631	N 166	O 187	S 7	0	0

- Molecule 3 is a protein called C121 Fab Light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	I	108	778	481	130	163	4	0	0

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



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O		
4	B	1	98	56	7	35	0	
4	B	1	98	56	7	35	0	
4	B	1	98	56	7	35	0	
4	B	1	98	56	7	35	0	
4	B	1	98	56	7	35	0	
4	B	1	98	56	7	35	0	
4	B	1	98	56	7	35	0	
4	D	1	112	64	8	40	0	
4	D	1	112	64	8	40	0	

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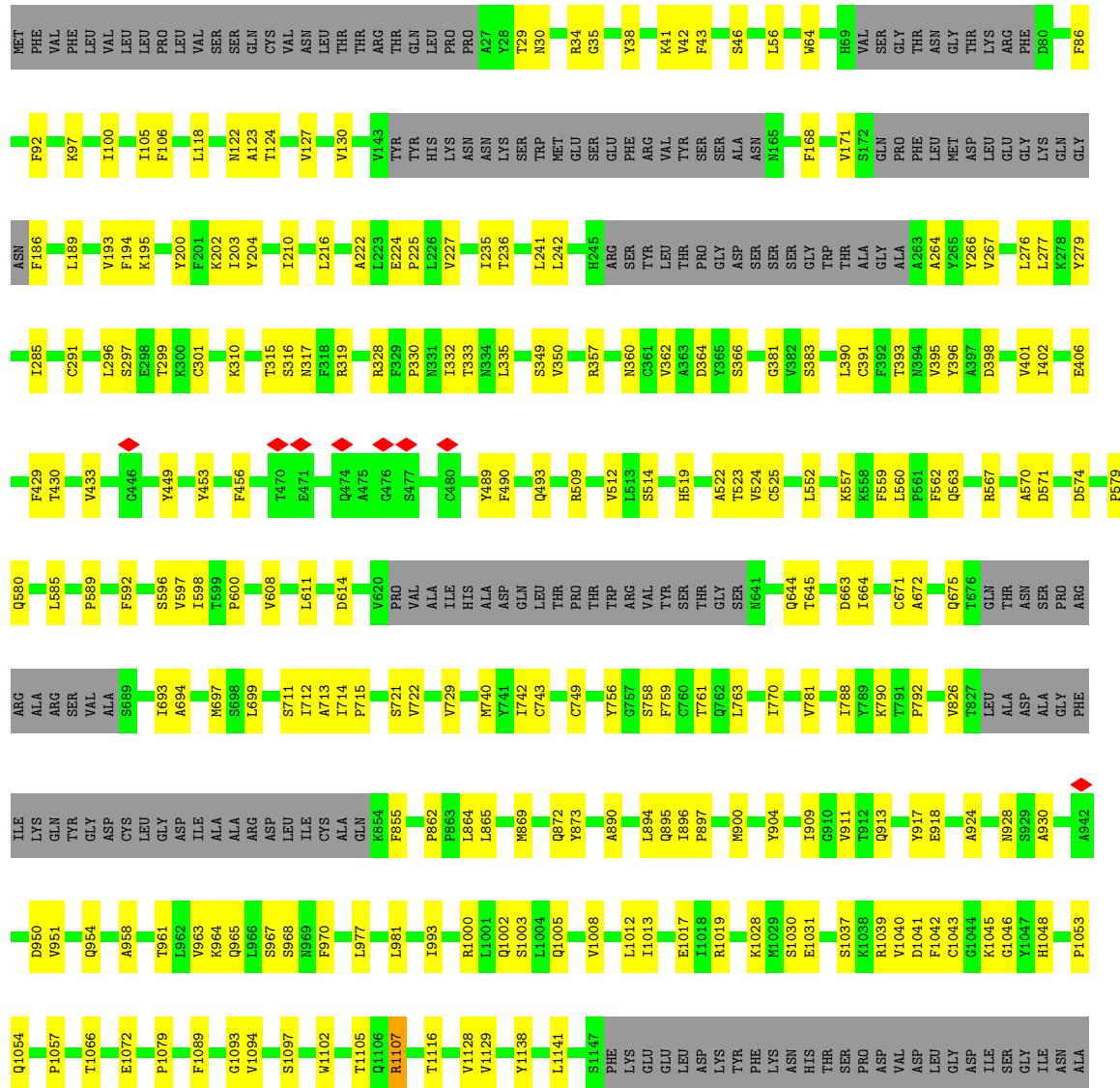
Mol	Chain	Residues	Atoms				AltConf
4	D	1	Total	C	N	O	0
			112	64	8	40	
4	D	1	Total	C	N	O	0
			112	64	8	40	
4	D	1	Total	C	N	O	0
			112	64	8	40	
4	D	1	Total	C	N	O	0
			112	64	8	40	
4	D	1	Total	C	N	O	0
			112	64	8	40	
4	D	1	Total	C	N	O	0
			112	64	8	40	
4	E	1	Total	C	N	O	0
			112	64	8	40	
4	E	1	Total	C	N	O	0
			112	64	8	40	
4	E	1	Total	C	N	O	0
			112	64	8	40	
4	E	1	Total	C	N	O	0
			112	64	8	40	
4	E	1	Total	C	N	O	0
			112	64	8	40	
4	E	1	Total	C	N	O	0
			112	64	8	40	
4	E	1	Total	C	N	O	0
			112	64	8	40	

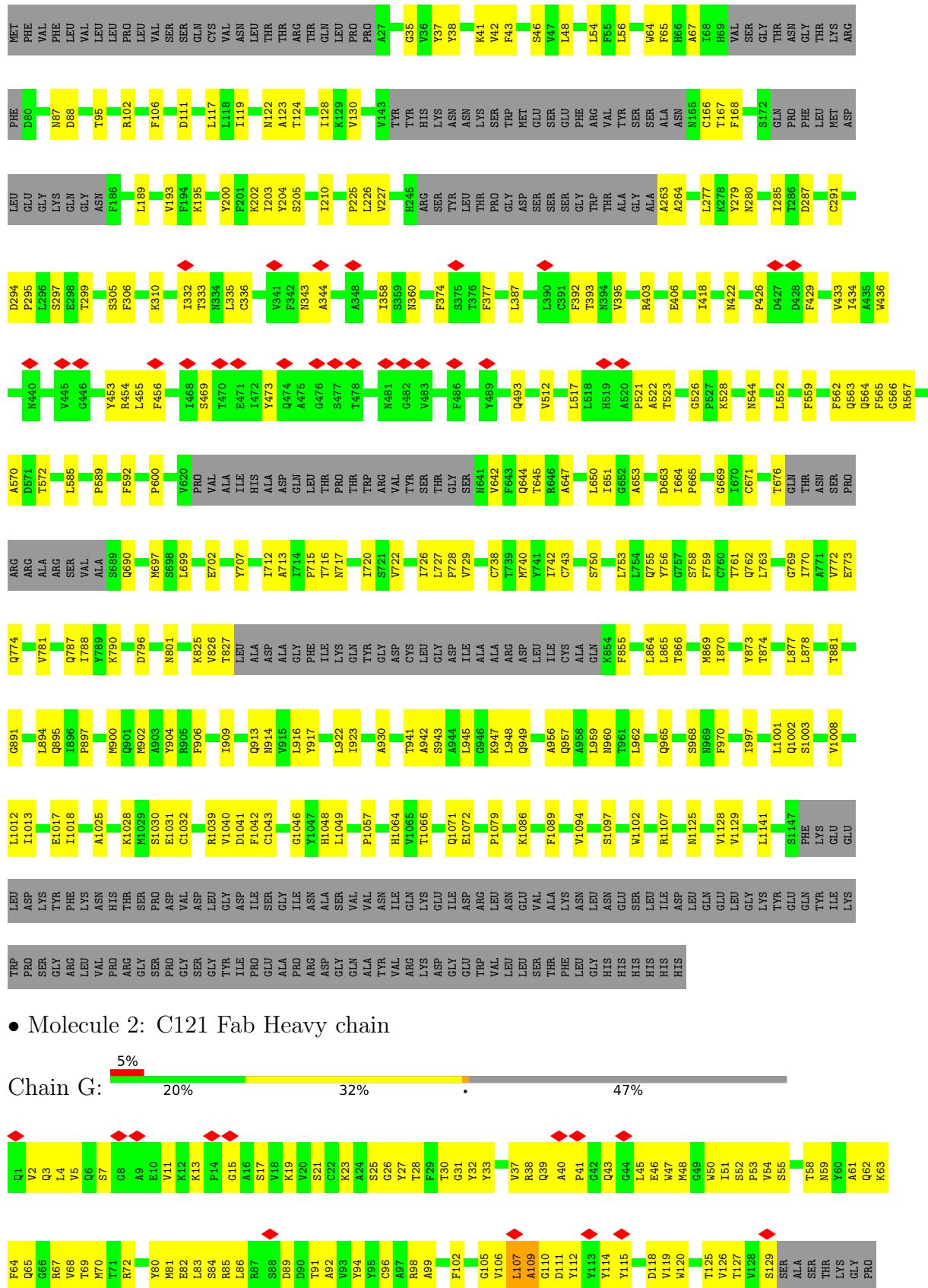
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

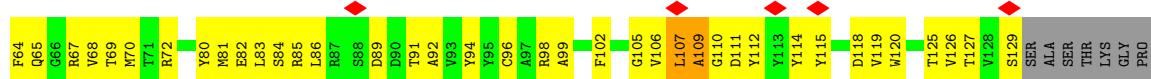
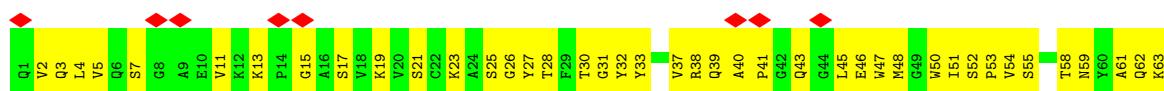
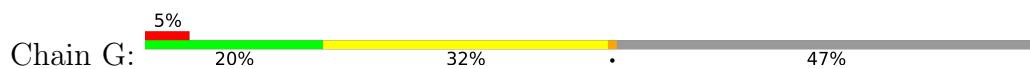
- Molecule 1: Spike glycoprotein

Chain B: 
 61% 18% 20%



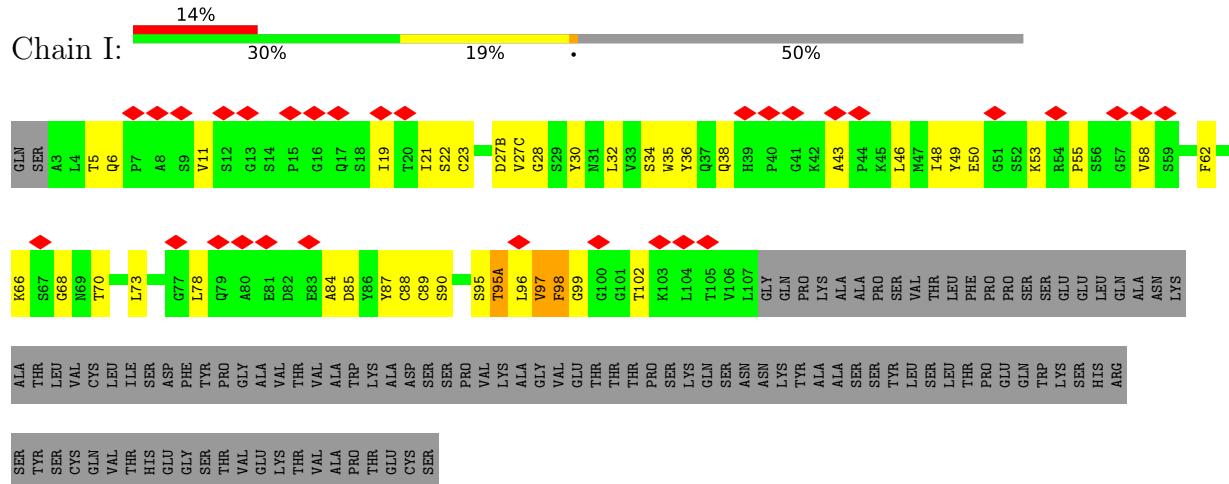


- Molecule 2: C121 Fab Heavy chain



SER	GLN	VAL	VAL	PHE	LEU	PRO	ALA	ALA	ALA
SER	SER	VAL	VAL	THR	VAL	PRO	SER	SER	SER
A3	A3	L4	T5	Q6	P7	A8	A8	S9	Lys
G68	GLN	VAL	VAL	VAL	VAL	VAL	VAL	LEU	LEU
LEU	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
CYS	CYS	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
GLN	GLN	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU
THR	ILE	I73	ASP						
HIS	SER	SER	ASP						
GLU	GLU	GLU	PHE						
GLY	GLY	GLY	TYR						
LYS	VAL	VAL	PRO						
VAL	VAL	VAL	TRP						
D82	THR	VAL	LYS						
VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
V11	Q79	S12	Q17	S18	D27B	V27C	V27C	D27B	V27C
W12	A84	W12	A85	W16	S95	W97	W98	S95	W97
S22	D85	S22	D85	S96	T95A	F98	F98	S22	T95A
C23	VAL	C23	VAL						
I21	ASP	I21	ASP	VAL	L96	W97	F98	ASP	L96
S20	ASP	S20	ASP	ASP	VAL	VAL	VAL	ASP	S20
I32	ASP	I32	ASP	ASP	ASP	ASP	ASP	ASP	I32
V33	ASP	V33	ASP	ASP	ASP	ASP	ASP	ASP	V33
L34	SER	L34	SER	SER	ASP	SER	SER	ASP	L34
W35	SER	W35	SER	SER	ASP	SER	SER	ASP	W35
Y36	LYS	Y36	LYS	LYS	ASP	Y36	Y36	ASP	Y36
Y30	GLU	Y30	GLU	GLU	VAL	Y30	Y30	VAL	Y30
M31	THR	M31	THR	THR	VAL	M31	M31	VAL	M31
L32	G100	L32	G100	G100	VAL	L32	L32	VAL	L32
L33	G101	L33	G101	G101	VAL	L33	L33	VAL	L33
V34	THR	V34	THR	THR	VAL	V34	V34	VAL	V34
W35	T102	W35	T102	T102	VAL	W35	W35	VAL	W35
Y36	K103	Y36	K103	K103	VAL	Y36	Y36	VAL	Y36
Y37	L104	Y37	L104	L104	VAL	Y37	Y37	VAL	Y37
K42	T105	K42	T105	T105	VAL	K42	K42	VAL	K42
A43	V106	A43	V106	V106	VAL	A43	A43	VAL	A43
P44	A44	P44	A44	A44	VAL	P44	P44	VAL	P44
K45	ASN	K45	ASN	ASN	VAL	K45	K45	VAL	K45
P46	GLY	P46	GLY	GLY	VAL	P46	P46	VAL	P46
G41	GLN	G41	GLN	GLN	VAL	G41	G41	VAL	G41
Q47	TYR	Q47	TYR	TYR	VAL	Q47	Q47	VAL	Q47
K53	ALA	K53	ALA	ALA	VAL	K53	K53	VAL	K53
R54	LYS	R54	LYS	LYS	VAL	R54	R54	VAL	R54
E50	PHE	E50	PHE	PHE	VAL	E50	E50	VAL	E50
P55	SER	P55	SER	SER	VAL	P55	P55	VAL	P55
S56	GLU	S56	GLU	GLU	VAL	S56	S56	VAL	S56
G57	LEU	G57	LEU	LEU	VAL	G57	G57	VAL	G57
V58	ALA	V58	ALA	ALA	VAL	V58	V58	VAL	V58
S59	ASN	S59	ASN	ASN	VAL	S59	S59	VAL	S59
LYS	LEU	LYS	LEU	LEU	VAL	LYS	LYS	VAL	LYS

- Molecule 3: C121 Fab Light chain



4 Experimental information i

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	14999	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	0.282	Depositor
Minimum map value	-0.090	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.0555	Depositor
Map size (Å)	377.872, 377.872, 377.872	wwPDB
Map dimensions	452, 452, 452	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	B	0.24	0/7999	0.42	0/10885
1	D	0.25	0/7999	0.42	0/10885
1	E	0.25	0/7999	0.42	0/10885
2	G	0.37	0/1018	0.53	0/1384
3	I	0.38	0/793	0.53	1/1075 (0.1%)
All	All	0.26	0/25808	0.43	1/35114 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	I	98	PHE	N-CA-C	5.52	125.89	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	527	PRO	Peptide

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	B	7823	0	7634	542	0
1	D	7823	0	7630	497	0
1	E	7823	0	7632	508	0
2	G	991	0	953	112	0
3	I	778	0	749	70	0
4	B	98	0	90	0	0
4	D	112	0	104	3	0
4	E	112	0	104	3	0
All	All	25560	0	24896	1084	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 21.

The worst 5 of 1084 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:D:589:PRO:HG2	1:E:855:PHE:CD1	1.30	1.63
3:I:87:TYR:CD1	3:I:98:PHE:CE1	1.80	1.63
1:B:1002:GLN:HE22	1:D:1001:LEU:CD1	1.15	1.53
1:B:559:PHE:CE1	1:D:43:PHE:CG	1.97	1.53
1:B:559:PHE:HE1	1:D:43:PHE:CD2	1.23	1.52

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	B	986/1259 (78%)	965 (98%)	20 (2%)	1 (0%)	51 85
1	D	986/1259 (78%)	956 (97%)	27 (3%)	3 (0%)	41 76
1	E	986/1259 (78%)	969 (98%)	16 (2%)	1 (0%)	51 85
2	G	126/241 (52%)	106 (84%)	19 (15%)	1 (1%)	19 60
3	I	106/216 (49%)	97 (92%)	7 (7%)	2 (2%)	8 41
All	All	3190/4234 (75%)	3093 (97%)	89 (3%)	8 (0%)	44 76

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	I	95(A)	THR
1	B	123	ALA
1	D	123	ALA
2	G	109	ALA
1	D	528	LYS

5.3.2 Protein sidechains [\(i\)](#)

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	B	876/1096 (80%)	875 (100%)	1 (0%)	93 97
1	D	876/1096 (80%)	875 (100%)	1 (0%)	93 97
1	E	876/1096 (80%)	876 (100%)	0	100 100
2	G	103/202 (51%)	101 (98%)	2 (2%)	57 75
3	I	87/180 (48%)	87 (100%)	0	100 100
All	All	2818/3670 (77%)	2814 (100%)	4 (0%)	93 97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1107	ARG
1	D	391	CYS
2	G	72	ARG

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Mol	Chain	Res	Type
2	G	107	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	542	ASN
1	E	913	GLN
1	E	751	ASN
1	E	953	ASN
1	B	1002	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

23 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	D	1305	1	14,14,15	0.47	0	17,19,21	1.26	1 (5%)
4	NAG	D	1303	1	14,14,15	0.22	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	E	1306	1	14,14,15	0.29	0	17,19,21	0.54	0
4	NAG	B	1303	1	14,14,15	0.22	0	17,19,21	0.42	0
4	NAG	B	1301	1	14,14,15	0.25	0	17,19,21	0.53	0
4	NAG	E	1303	1	14,14,15	0.25	0	17,19,21	0.43	0
4	NAG	D	1308	1	14,14,15	0.22	0	17,19,21	0.43	0
4	NAG	E	1304	1	14,14,15	0.26	0	17,19,21	0.52	0
4	NAG	D	1302	1	14,14,15	0.25	0	17,19,21	0.37	0
4	NAG	B	1306	1	14,14,15	0.24	0	17,19,21	0.44	0
4	NAG	E	1301	1	14,14,15	0.21	0	17,19,21	0.46	0
4	NAG	E	1305	-	14,14,15	0.23	0	17,19,21	0.42	0
4	NAG	E	1307	1	14,14,15	0.86	1 (7%)	17,19,21	1.00	1 (5%)
4	NAG	B	1304	1	14,14,15	0.26	0	17,19,21	0.53	0
4	NAG	D	1306	1	14,14,15	0.25	0	17,19,21	0.52	0
4	NAG	B	1302	1	14,14,15	0.21	0	17,19,21	0.41	0
4	NAG	E	1302	1	14,14,15	0.24	0	17,19,21	0.43	0
4	NAG	D	1307	1	14,14,15	0.24	0	17,19,21	0.41	0
4	NAG	B	1305	1	14,14,15	0.21	0	17,19,21	0.41	0
4	NAG	D	1301	1	14,14,15	0.49	0	17,19,21	0.60	0
4	NAG	D	1304	1	14,14,15	0.23	0	17,19,21	0.40	0
4	NAG	E	1308	1	14,14,15	0.23	0	17,19,21	0.45	0
4	NAG	B	1307	1	14,14,15	0.21	0	17,19,21	0.42	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	1305	1	-	4/6/23/26	0/1/1/1
4	NAG	D	1303	1	-	0/6/23/26	0/1/1/1
4	NAG	E	1306	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	1/6/23/26	0/1/1/1
4	NAG	E	1303	1	-	0/6/23/26	0/1/1/1
4	NAG	D	1308	1	-	1/6/23/26	0/1/1/1
4	NAG	E	1304	1	-	3/6/23/26	0/1/1/1
4	NAG	D	1302	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1306	1	-	1/6/23/26	0/1/1/1
4	NAG	E	1301	1	-	0/6/23/26	0/1/1/1
4	NAG	E	1305	-	-	1/6/23/26	0/1/1/1
4	NAG	E	1307	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	D	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
4	NAG	E	1302	1	-	4/6/23/26	0/1/1/1
4	NAG	D	1307	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	D	1301	1	-	3/6/23/26	0/1/1/1
4	NAG	D	1304	1	-	0/6/23/26	0/1/1/1
4	NAG	E	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1307	1	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1307	NAG	O5-C1	2.84	1.48	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1305	NAG	C2-N2-C7	4.31	129.03	122.90
4	E	1307	NAG	C1-O5-C5	3.87	117.43	112.19

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1302	NAG	O5-C5-C6-O6
4	D	1302	NAG	C4-C5-C6-O6
4	B	1303	NAG	O5-C5-C6-O6
4	E	1306	NAG	C4-C5-C6-O6
4	E	1306	NAG	O5-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1305	NAG	1	0
4	E	1306	NAG	1	0
4	E	1307	NAG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1306	NAG	1	0
4	D	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.

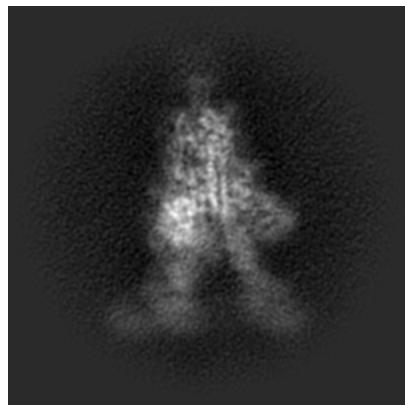
6 Map visualisation i

This section contains visualisations of the EMDB entry EMD-22735. These allow visual inspection of the internal detail of the map and identification of artifacts.

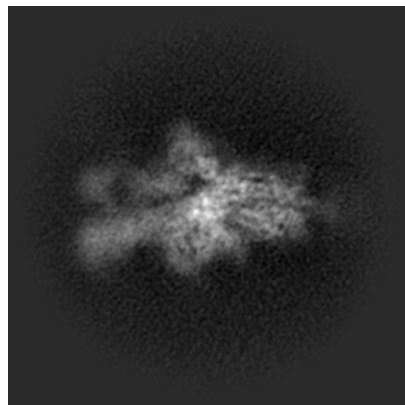
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections i

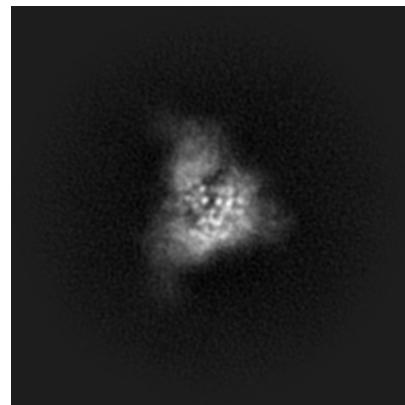
6.1.1 Primary map



X



Y

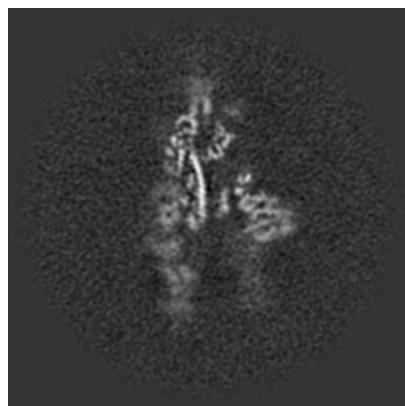


Z

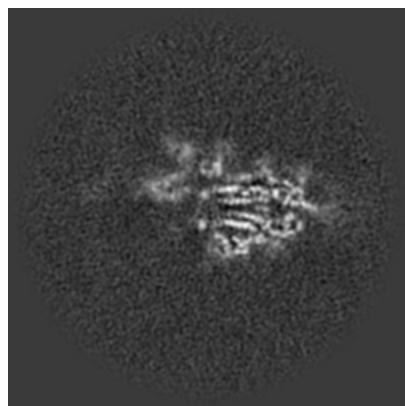
The images above show the map projected in three orthogonal directions.

6.2 Central slices i

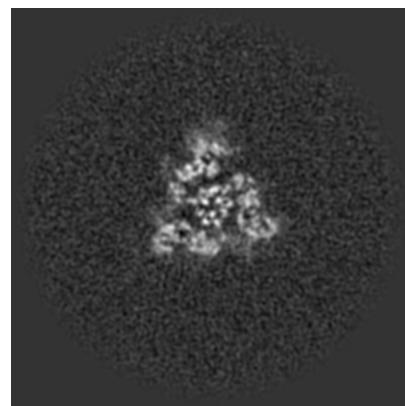
6.2.1 Primary map



X Index: 226



Y Index: 226

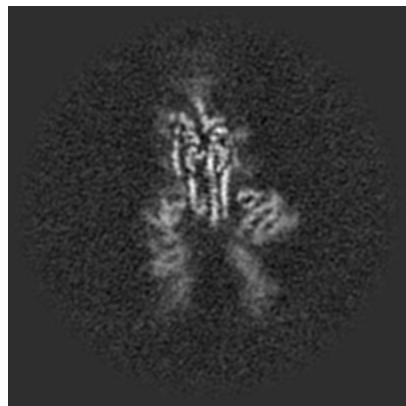


Z Index: 226

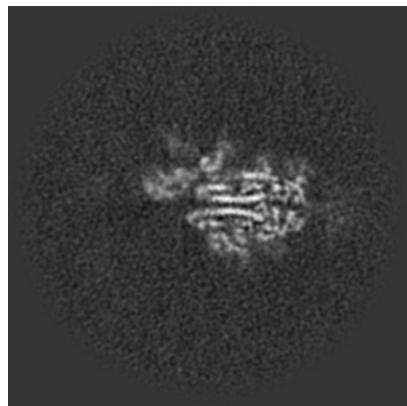
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [\(i\)](#)

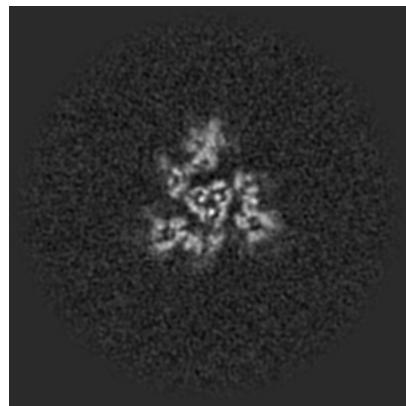
6.3.1 Primary map



X Index: 216



Y Index: 230



Z Index: 221

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

6.4 Orthogonal surface views [\(i\)](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0555. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

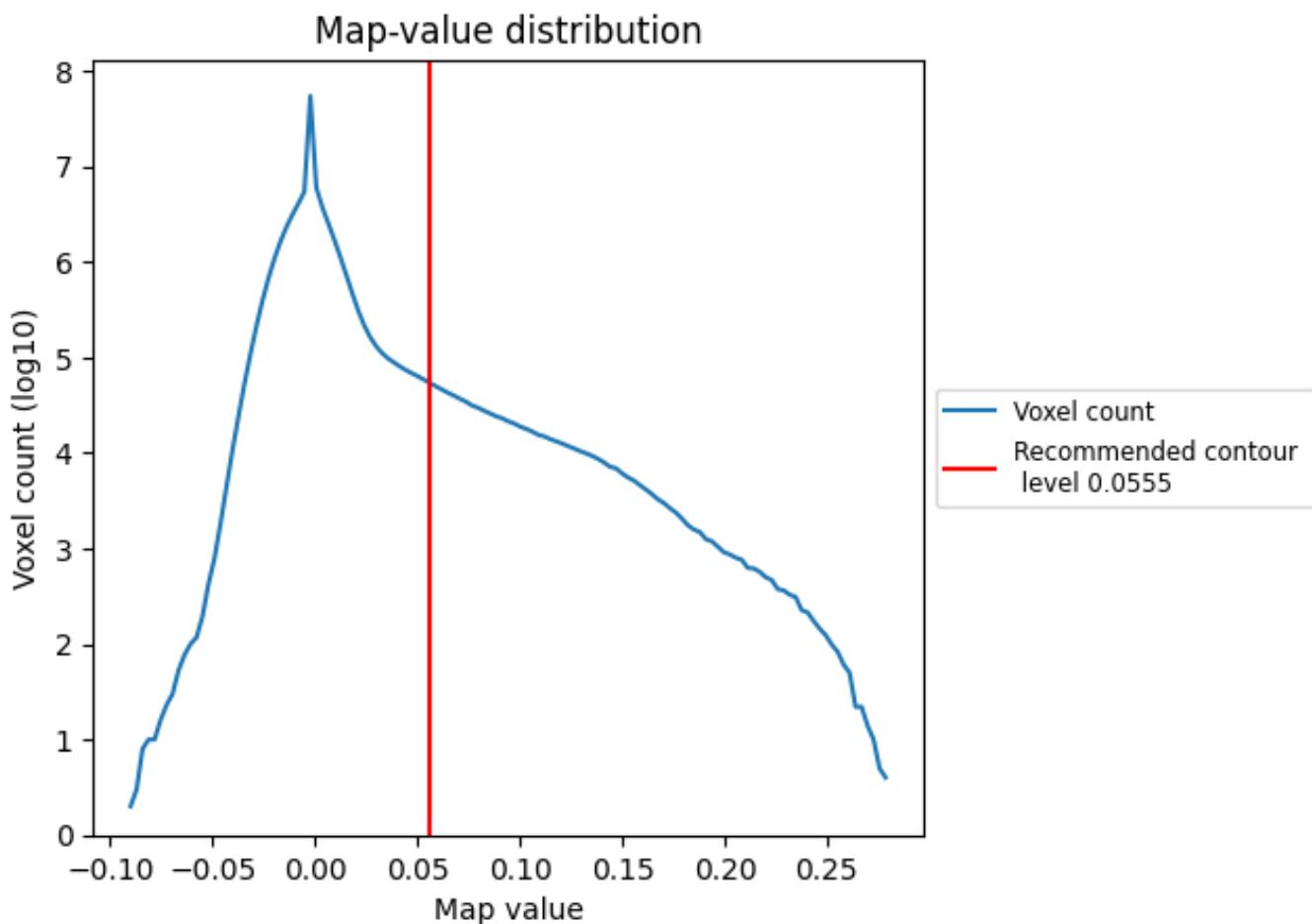
6.5 Mask visualisation

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

7 Map analysis (i)

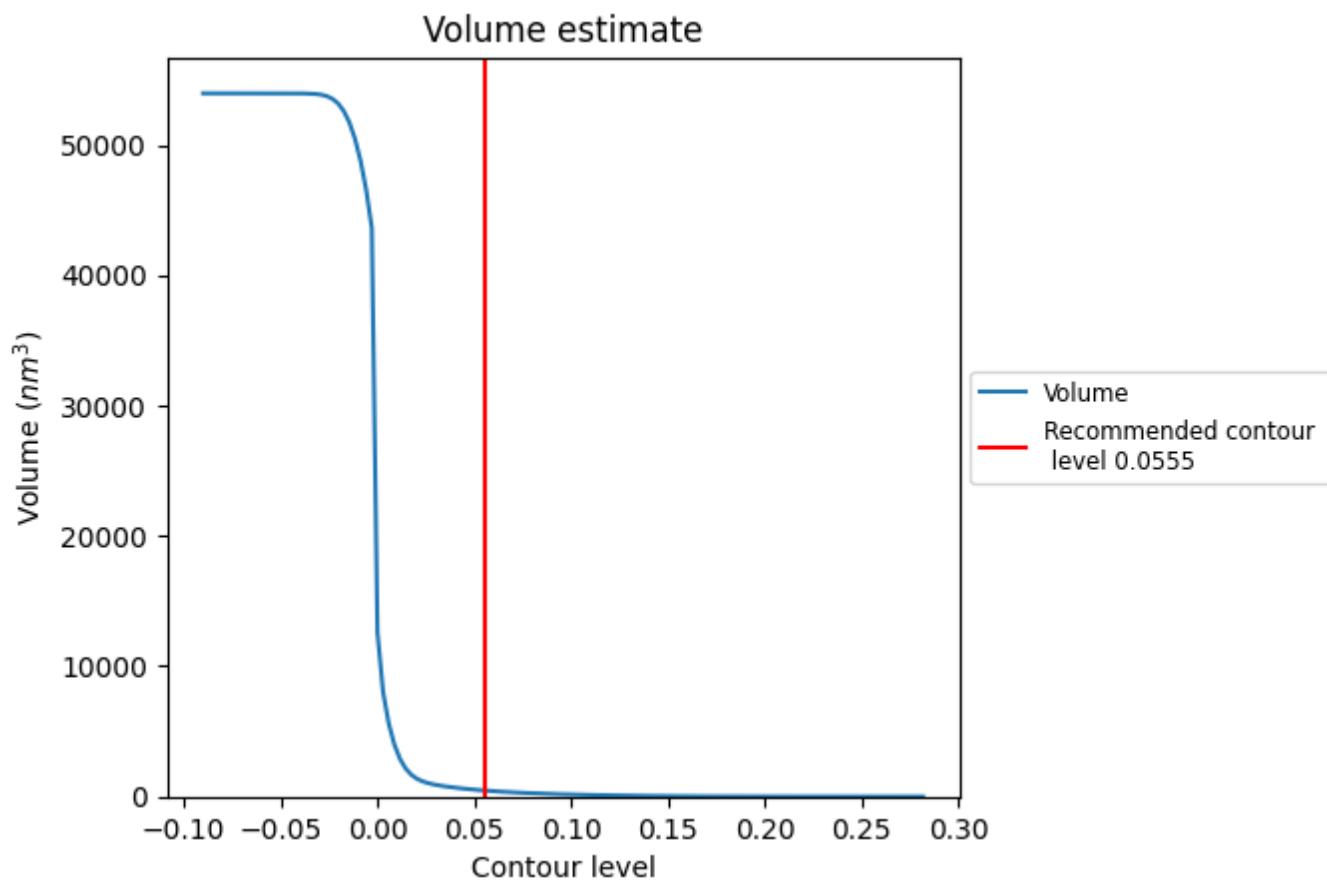
This section contains the results of statistical analysis of the map.

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.

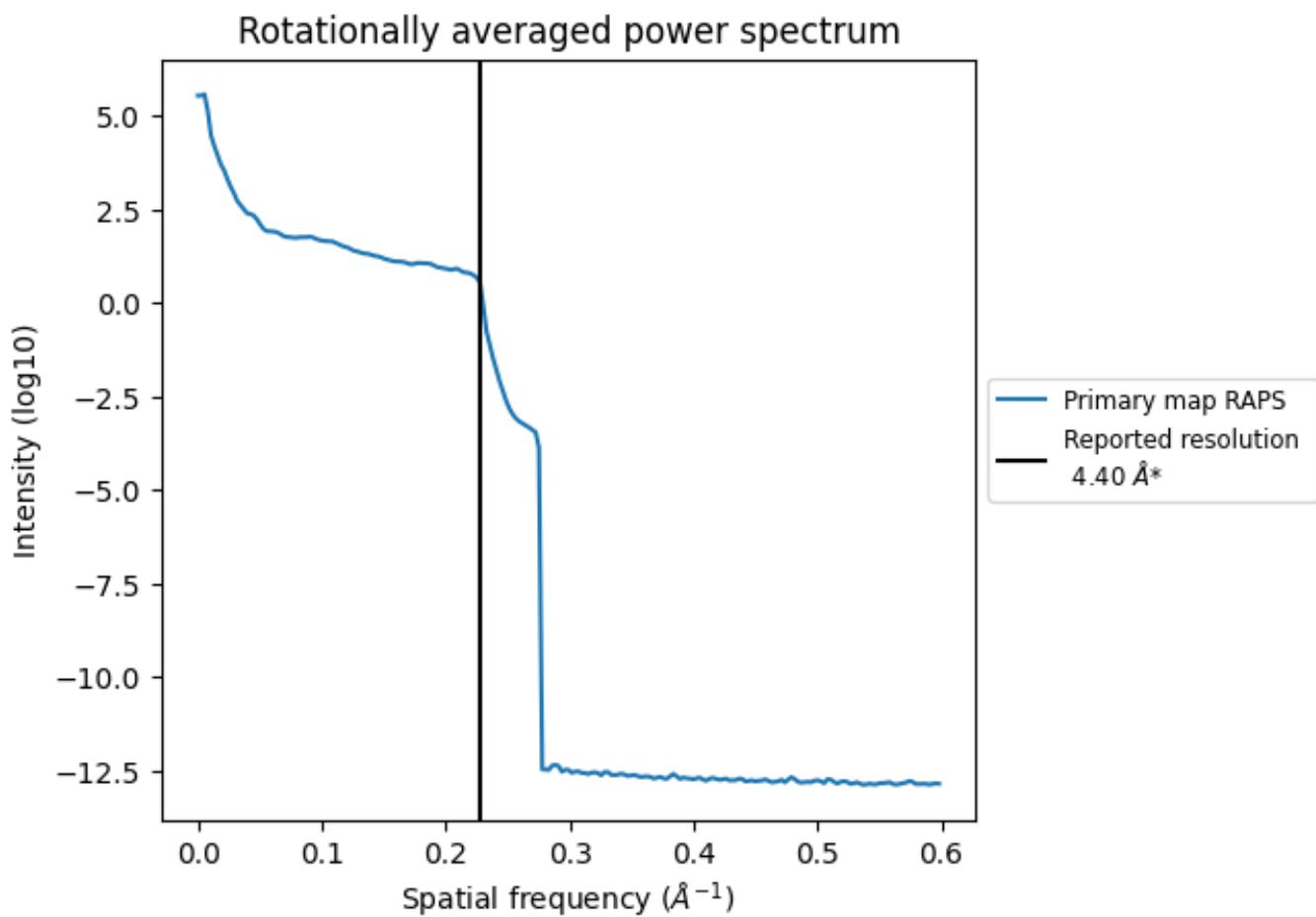
7.2 Volume estimate (i)



The volume at the recommended contour level is 461 nm^3 ; this corresponds to an approximate mass of 417 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 [\(i\)](#)

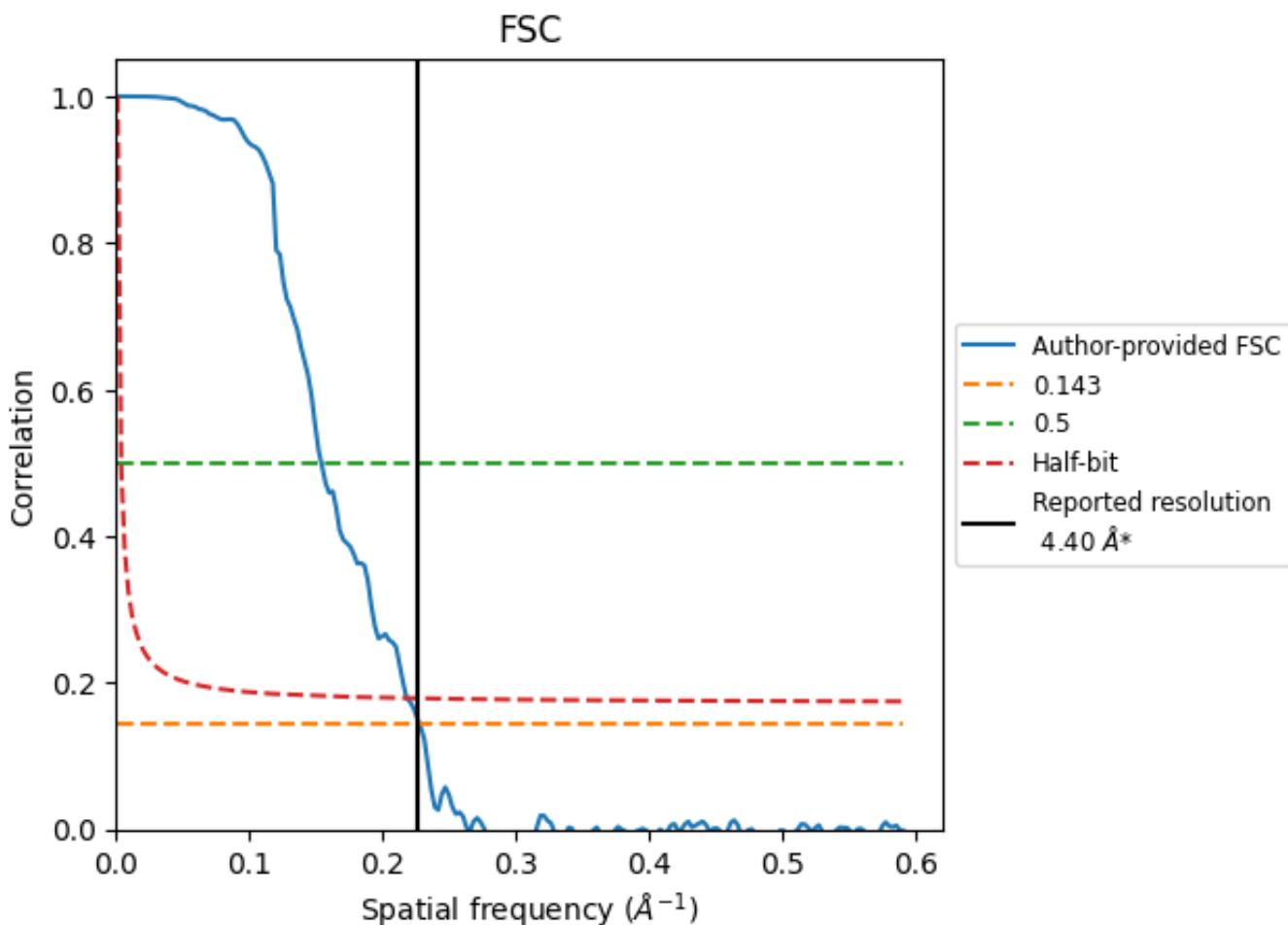


*Reported resolution corresponds to spatial frequency of 0.227 \AA^{-1}

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 0.227 \AA^{-1}

8.2 Resolution estimates [\(i\)](#)

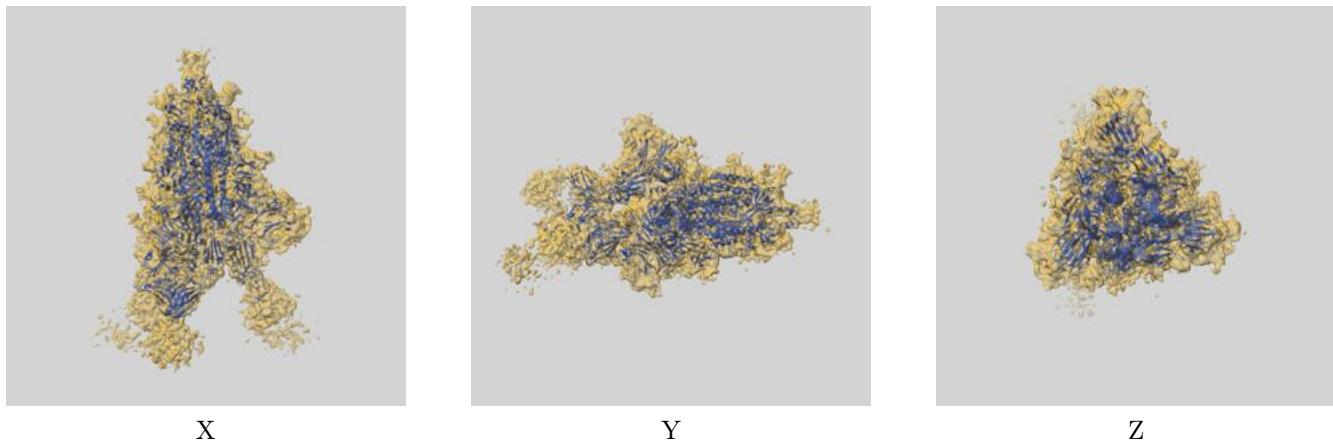
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.38	6.49	4.58
Unmasked-calculated*	-	-	-

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

9 Map-model fit (i)

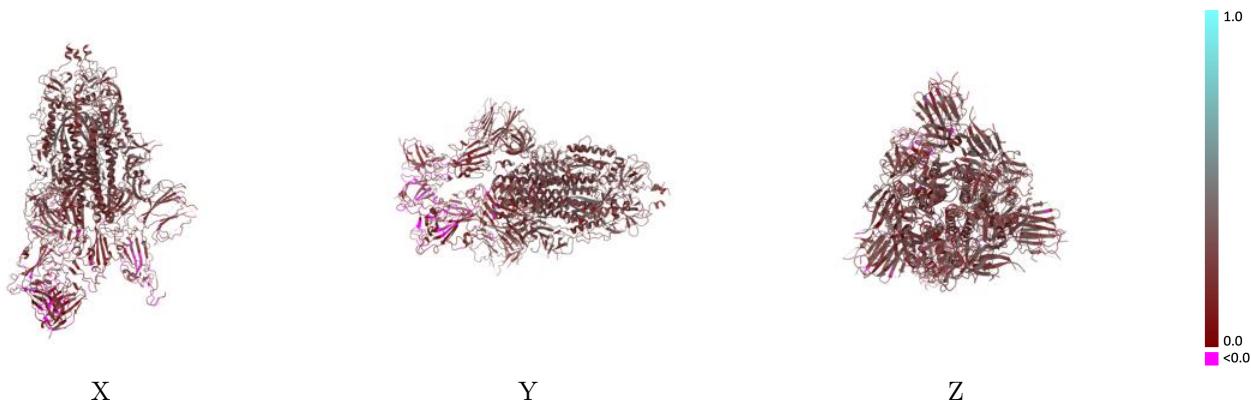
This section contains information regarding the fit between EMDB map EMD-22735 and PDB model 7K8Y. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay (i)



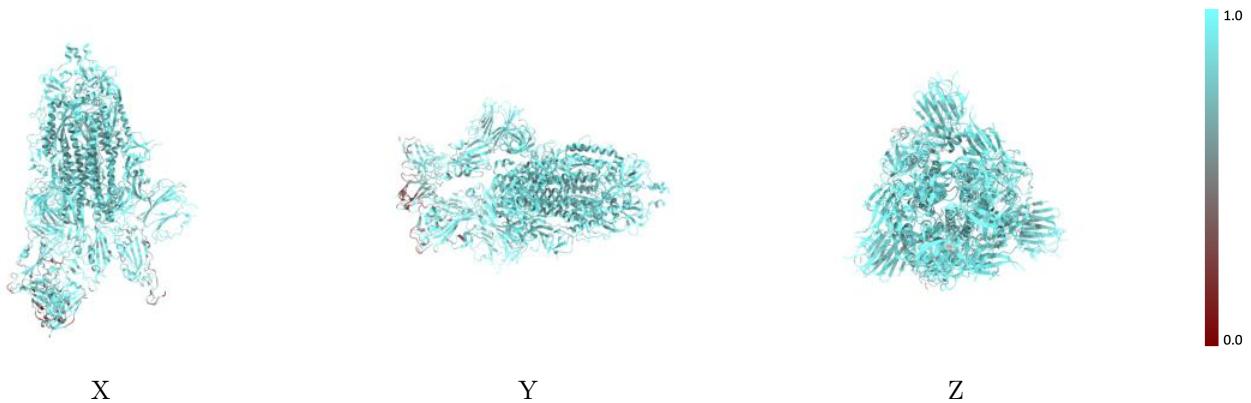
The images above show the 3D surface view of the map at the recommended contour level 0.0555 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



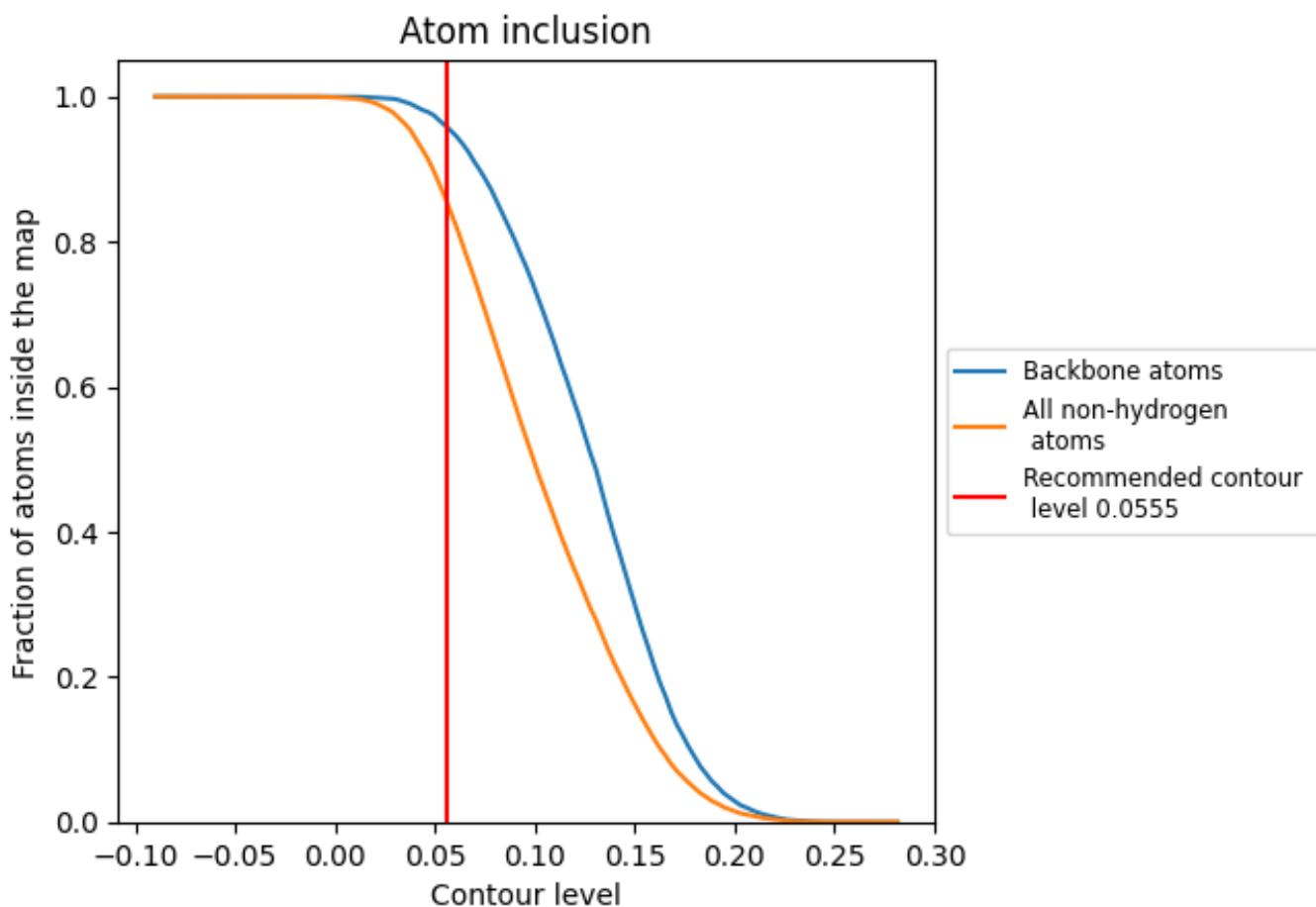
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0555).

9.4 Atom inclusion [\(i\)](#)



At the recommended contour level, 96% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [\(i\)](#)

The table lists the average atom inclusion at the recommended contour level (0.0555) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8584	0.2380
B	0.8828	0.2580
D	0.8635	0.2450
E	0.8668	0.2360
G	0.7801	0.1520
I	0.5724	0.1010

