



wwPDB EM Validation Summary Report ⓘ

Nov 2, 2025 – 06:17 am GMT

PDB ID : 9R6Q / pdb_00009r6q
EMDB ID : EMD-53684
Title : Local refinement of the N-terminal domain (NTD) and receptor binding domain (RBD) from the Porcine hemagglutinating encephalomyelitis virus (PHEV) Spike in the closed conformation bound to 9-O-Ac-Sia
Authors : Fernandez, I.; Rey, F.A.
Deposited on : 2025-05-13
Resolution : 3.50 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.dev129
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

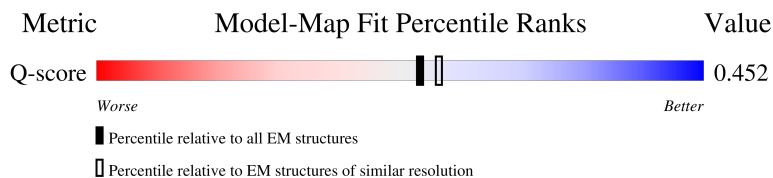
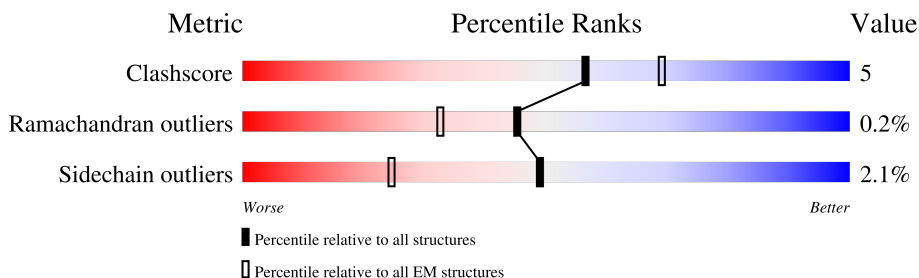
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	1333	
1	B	1333	
2	D	3	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4280 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	266	Total	C	N	O	S	0	0
			2136	1398	331	397	10		
1	B	269	Total	C	N	O	S	0	0
			2053	1275	359	394	25		

There are 146 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1275	GLY	-	expression tag	UNP Q2QKN3
A	1276	SER	-	expression tag	UNP Q2QKN3
A	1277	GLY	-	expression tag	UNP Q2QKN3
A	1278	TYR	-	expression tag	UNP Q2QKN3
A	1279	ILE	-	expression tag	UNP Q2QKN3
A	1280	PRO	-	expression tag	UNP Q2QKN3
A	1281	GLU	-	expression tag	UNP Q2QKN3
A	1282	ALA	-	expression tag	UNP Q2QKN3
A	1283	PRO	-	expression tag	UNP Q2QKN3
A	1284	ARG	-	expression tag	UNP Q2QKN3
A	1285	ASP	-	expression tag	UNP Q2QKN3
A	1286	GLY	-	expression tag	UNP Q2QKN3
A	1287	GLN	-	expression tag	UNP Q2QKN3
A	1288	ALA	-	expression tag	UNP Q2QKN3
A	1289	TYR	-	expression tag	UNP Q2QKN3
A	1290	VAL	-	expression tag	UNP Q2QKN3
A	1291	ARG	-	expression tag	UNP Q2QKN3
A	1292	LYS	-	expression tag	UNP Q2QKN3
A	1293	ASP	-	expression tag	UNP Q2QKN3
A	1294	GLY	-	expression tag	UNP Q2QKN3
A	1295	GLU	-	expression tag	UNP Q2QKN3
A	1296	TRP	-	expression tag	UNP Q2QKN3
A	1297	VAL	-	expression tag	UNP Q2QKN3
A	1298	LEU	-	expression tag	UNP Q2QKN3
A	1299	LEU	-	expression tag	UNP Q2QKN3
A	1300	SER	-	expression tag	UNP Q2QKN3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1301	THR	-	expression tag	UNP Q2QKN3
A	1302	PHE	-	expression tag	UNP Q2QKN3
A	1303	LEU	-	expression tag	UNP Q2QKN3
A	1304	GLY	-	expression tag	UNP Q2QKN3
A	1305	SER	-	expression tag	UNP Q2QKN3
A	1306	LEU	-	expression tag	UNP Q2QKN3
A	1307	VAL	-	expression tag	UNP Q2QKN3
A	1308	PRO	-	expression tag	UNP Q2QKN3
A	1309	ARG	-	expression tag	UNP Q2QKN3
A	1310	GLY	-	expression tag	UNP Q2QKN3
A	1311	SER	-	expression tag	UNP Q2QKN3
A	1312	HIS	-	expression tag	UNP Q2QKN3
A	1313	HIS	-	expression tag	UNP Q2QKN3
A	1314	HIS	-	expression tag	UNP Q2QKN3
A	1315	HIS	-	expression tag	UNP Q2QKN3
A	1316	HIS	-	expression tag	UNP Q2QKN3
A	1317	HIS	-	expression tag	UNP Q2QKN3
A	1318	HIS	-	expression tag	UNP Q2QKN3
A	1319	HIS	-	expression tag	UNP Q2QKN3
A	1320	SER	-	expression tag	UNP Q2QKN3
A	1321	ALA	-	expression tag	UNP Q2QKN3
A	1322	TRP	-	expression tag	UNP Q2QKN3
A	1323	SER	-	expression tag	UNP Q2QKN3
A	1324	HIS	-	expression tag	UNP Q2QKN3
A	1325	PRO	-	expression tag	UNP Q2QKN3
A	1326	GLN	-	expression tag	UNP Q2QKN3
A	1327	PHE	-	expression tag	UNP Q2QKN3
A	1328	GLU	-	expression tag	UNP Q2QKN3
A	1329	LYS	-	expression tag	UNP Q2QKN3
A	1330	GLY	-	expression tag	UNP Q2QKN3
A	1331	THR	-	expression tag	UNP Q2QKN3
A	1332	GLY	-	expression tag	UNP Q2QKN3
A	1333	GLY	-	expression tag	UNP Q2QKN3
A	1334	LEU	-	expression tag	UNP Q2QKN3
A	1335	ASN	-	expression tag	UNP Q2QKN3
A	1336	ASP	-	expression tag	UNP Q2QKN3
A	1337	ILE	-	expression tag	UNP Q2QKN3
A	1338	PHE	-	expression tag	UNP Q2QKN3
A	1339	GLU	-	expression tag	UNP Q2QKN3
A	1340	ALA	-	expression tag	UNP Q2QKN3
A	1341	GLN	-	expression tag	UNP Q2QKN3
A	1342	LYS	-	expression tag	UNP Q2QKN3

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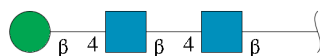
Chain	Residue	Modelled	Actual	Comment	Reference
A	1343	ILE	-	expression tag	UNP Q2QKN3
A	1344	GLU	-	expression tag	UNP Q2QKN3
A	1345	TRP	-	expression tag	UNP Q2QKN3
A	1346	HIS	-	expression tag	UNP Q2QKN3
A	1347	GLU	-	expression tag	UNP Q2QKN3
B	1275	GLY	-	expression tag	UNP Q2QKN3
B	1276	SER	-	expression tag	UNP Q2QKN3
B	1277	GLY	-	expression tag	UNP Q2QKN3
B	1278	TYR	-	expression tag	UNP Q2QKN3
B	1279	ILE	-	expression tag	UNP Q2QKN3
B	1280	PRO	-	expression tag	UNP Q2QKN3
B	1281	GLU	-	expression tag	UNP Q2QKN3
B	1282	ALA	-	expression tag	UNP Q2QKN3
B	1283	PRO	-	expression tag	UNP Q2QKN3
B	1284	ARG	-	expression tag	UNP Q2QKN3
B	1285	ASP	-	expression tag	UNP Q2QKN3
B	1286	GLY	-	expression tag	UNP Q2QKN3
B	1287	GLN	-	expression tag	UNP Q2QKN3
B	1288	ALA	-	expression tag	UNP Q2QKN3
B	1289	TYR	-	expression tag	UNP Q2QKN3
B	1290	VAL	-	expression tag	UNP Q2QKN3
B	1291	ARG	-	expression tag	UNP Q2QKN3
B	1292	LYS	-	expression tag	UNP Q2QKN3
B	1293	ASP	-	expression tag	UNP Q2QKN3
B	1294	GLY	-	expression tag	UNP Q2QKN3
B	1295	GLU	-	expression tag	UNP Q2QKN3
B	1296	TRP	-	expression tag	UNP Q2QKN3
B	1297	VAL	-	expression tag	UNP Q2QKN3
B	1298	LEU	-	expression tag	UNP Q2QKN3
B	1299	LEU	-	expression tag	UNP Q2QKN3
B	1300	SER	-	expression tag	UNP Q2QKN3
B	1301	THR	-	expression tag	UNP Q2QKN3
B	1302	PHE	-	expression tag	UNP Q2QKN3
B	1303	LEU	-	expression tag	UNP Q2QKN3
B	1304	GLY	-	expression tag	UNP Q2QKN3
B	1305	SER	-	expression tag	UNP Q2QKN3
B	1306	LEU	-	expression tag	UNP Q2QKN3
B	1307	VAL	-	expression tag	UNP Q2QKN3
B	1308	PRO	-	expression tag	UNP Q2QKN3
B	1309	ARG	-	expression tag	UNP Q2QKN3
B	1310	GLY	-	expression tag	UNP Q2QKN3
B	1311	SER	-	expression tag	UNP Q2QKN3

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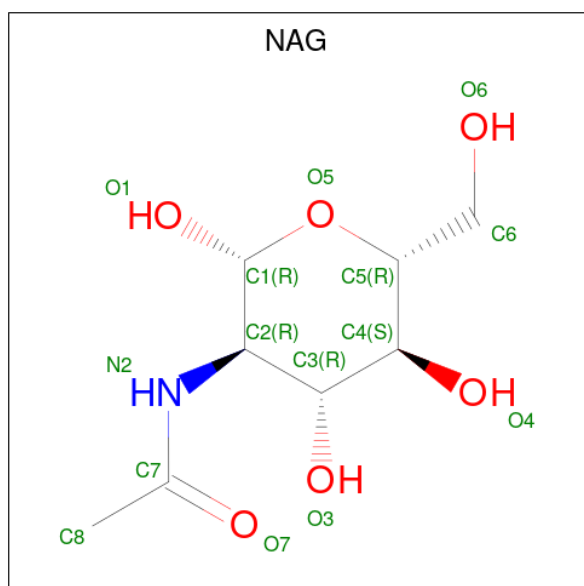
Chain	Residue	Modelled	Actual	Comment	Reference
B	1312	HIS	-	expression tag	UNP Q2QKN3
B	1313	HIS	-	expression tag	UNP Q2QKN3
B	1314	HIS	-	expression tag	UNP Q2QKN3
B	1315	HIS	-	expression tag	UNP Q2QKN3
B	1316	HIS	-	expression tag	UNP Q2QKN3
B	1317	HIS	-	expression tag	UNP Q2QKN3
B	1318	HIS	-	expression tag	UNP Q2QKN3
B	1319	HIS	-	expression tag	UNP Q2QKN3
B	1320	SER	-	expression tag	UNP Q2QKN3
B	1321	ALA	-	expression tag	UNP Q2QKN3
B	1322	TRP	-	expression tag	UNP Q2QKN3
B	1323	SER	-	expression tag	UNP Q2QKN3
B	1324	HIS	-	expression tag	UNP Q2QKN3
B	1325	PRO	-	expression tag	UNP Q2QKN3
B	1326	GLN	-	expression tag	UNP Q2QKN3
B	1327	PHE	-	expression tag	UNP Q2QKN3
B	1328	GLU	-	expression tag	UNP Q2QKN3
B	1329	LYS	-	expression tag	UNP Q2QKN3
B	1330	GLY	-	expression tag	UNP Q2QKN3
B	1331	THR	-	expression tag	UNP Q2QKN3
B	1332	GLY	-	expression tag	UNP Q2QKN3
B	1333	GLY	-	expression tag	UNP Q2QKN3
B	1334	LEU	-	expression tag	UNP Q2QKN3
B	1335	ASN	-	expression tag	UNP Q2QKN3
B	1336	ASP	-	expression tag	UNP Q2QKN3
B	1337	ILE	-	expression tag	UNP Q2QKN3
B	1338	PHE	-	expression tag	UNP Q2QKN3
B	1339	GLU	-	expression tag	UNP Q2QKN3
B	1340	ALA	-	expression tag	UNP Q2QKN3
B	1341	GLN	-	expression tag	UNP Q2QKN3
B	1342	LYS	-	expression tag	UNP Q2QKN3
B	1343	ILE	-	expression tag	UNP Q2QKN3
B	1344	GLU	-	expression tag	UNP Q2QKN3
B	1345	TRP	-	expression tag	UNP Q2QKN3
B	1346	HIS	-	expression tag	UNP Q2QKN3
B	1347	GLU	-	expression tag	UNP Q2QKN3

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



Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	3	Total	C	N	O	0	0
			39	22	2	15		

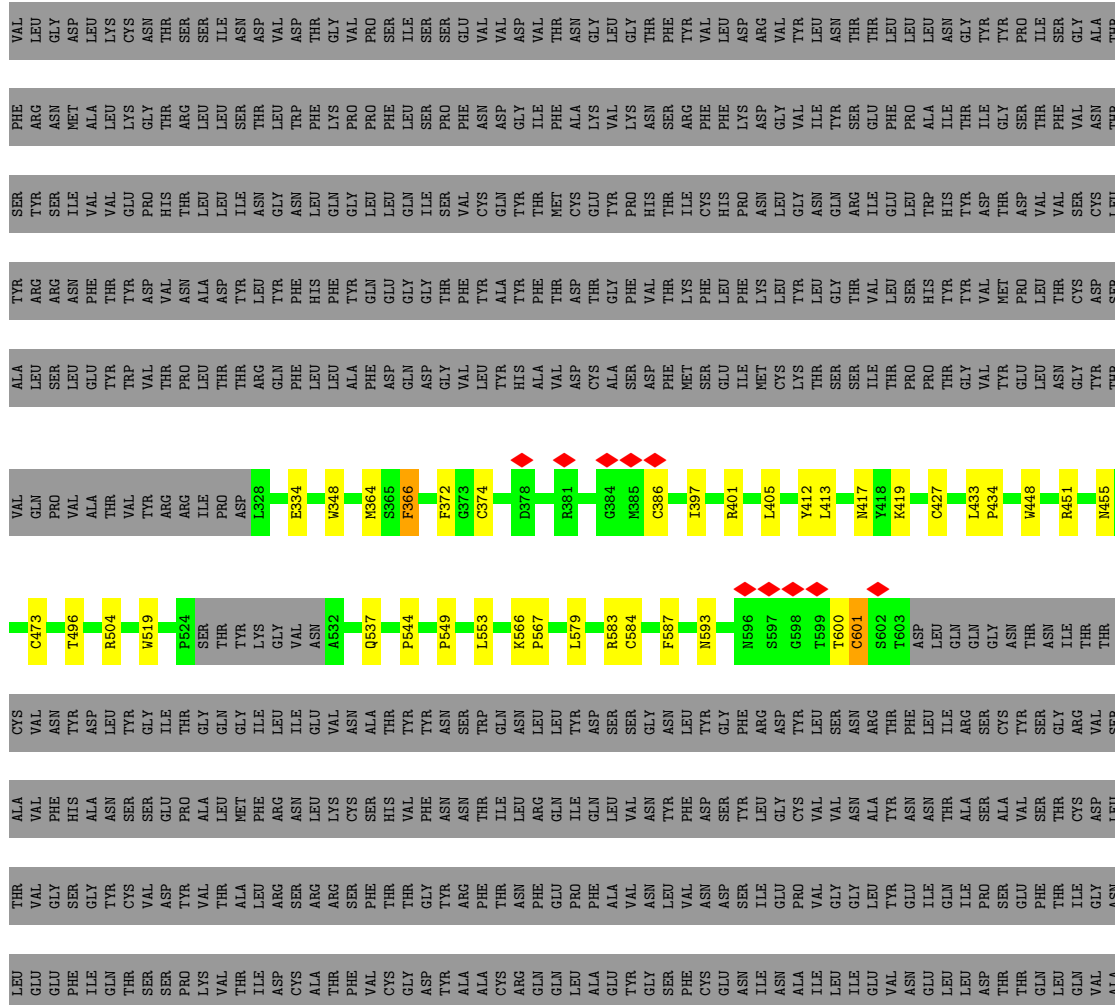
- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 4 is 9-O-acetyl-5-acetamido-3,5-dideoxy-D-glycero-alpha-D-galacto-non-2-ulopyranosonic acid (CCD ID: 5N6) (formula: $C_{13}H_{21}NO_{10}$) (labeled as "Ligand of Interest" by depositor).





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

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

Chain D: 33% 67%

NAG1	NAG2	BMA3
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	203953	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	240000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.552	Depositor
Minimum map value	-0.208	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0576	Depositor
Map size (Å)	292.31998, 292.31998, 292.31998	wwPDB
Map dimensions	252, 252, 252	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.16, 1.16, 1.16	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: BMA, 5N6, 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	0.20	0/2199	0.27	0/3004
1	B	0.17	0/2104	0.27	0/2861
All	All	0.18	0/4303	0.27	0/5865

There are no bond length outliers.

There are no bond angle outliers.

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	2136	0	2051	19	0
1	B	2053	0	1921	21	0
2	D	39	0	34	0	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
4	A	24	0	0	0	0
All	All	4280	0	4032	39	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 5.

The worst 5 of 39 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:A:211:HIS:HB2	1:A:222:TYR:HB2	1.69	0.75
1:B:504:ARG:HG3	1:B:519:TRP:HE1	1.65	0.60
1:A:75:PHE:HB3	1:A:261:TRP:HB3	1.85	0.59
1:B:537:GLN:HE22	1:B:553:LEU:HB3	1.71	0.56
1:A:132:VAL:HG23	1:A:134:THR:H	1.73	0.54

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	262/1333 (20%)	248 (95%)	13 (5%)	1 (0%)	30	64
1	B	265/1333 (20%)	260 (98%)	5 (2%)	0	100	100
All	All	527/2666 (20%)	508 (96%)	18 (3%)	1 (0%)	45	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	THR

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	A	239/1160 (21%)	233 (98%)	6 (2%)	42	67
1	B	233/1160 (20%)	229 (98%)	4 (2%)	56	75
All	All	472/2320 (20%)	462 (98%)	10 (2%)	49	71

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	496	THR
1	B	600	THR
1	B	601	CYS
1	A	160	CYS
1	A	165	CYS

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

Mol	Chain	Res	Type
1	A	161	GLN
1	B	347	ASN
1	B	376	ASN
1	B	442	HIS
1	B	593	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

3 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	$\# Z > 2$
2	NAG	D	1	2,1	14,14,15	0.74	0	17,19,21	0.89	0
2	NAG	D	2	2	14,14,15	0.73	0	17,19,21	0.90	1 (5%)
2	BMA	D	3	2	11,11,12	0.87	0	15,15,17	2.09	4 (26%)

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
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	BMA	C1-O5-C5	5.87	120.14	112.19
2	D	3	BMA	C3-C4-C5	2.80	115.22	110.24
2	D	2	NAG	O5-C1-C2	-2.45	107.43	111.29
2	D	3	BMA	C2-C3-C4	2.21	114.71	110.89
2	D	3	BMA	O4-C4-C3	-2.18	105.31	110.35

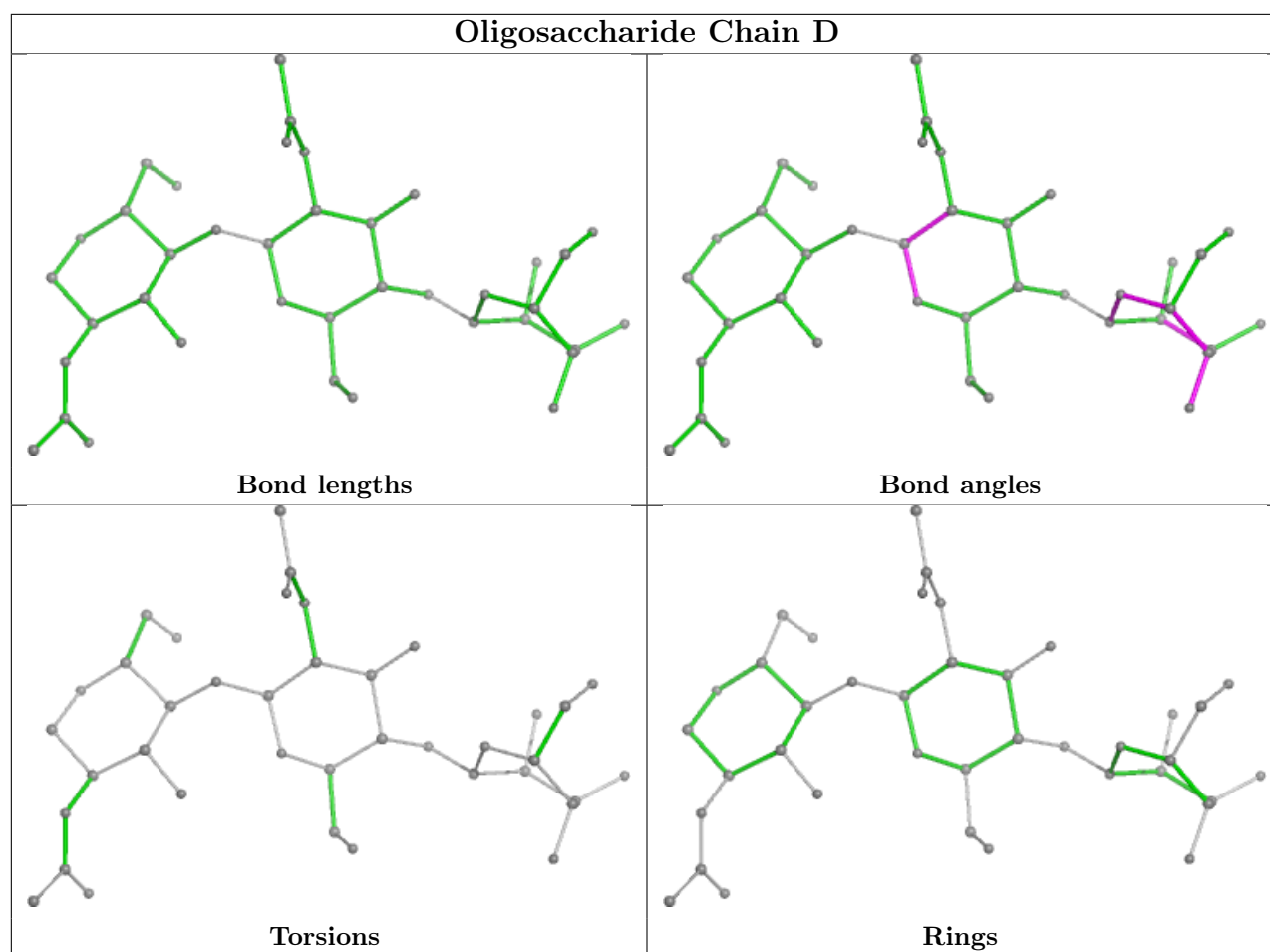
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

3 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	$\# Z > 2$
3	NAG	A	1401	1	14,14,15	0.75	0	17,19,21	0.85	0
3	NAG	B	1401	1	14,14,15	0.75	0	17,19,21	0.77	0
4	5N6	A	1402	-	24,24,24	1.37	2 (8%)	29,35,35	2.49	13 (44%)

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
3	NAG	A	1401	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1401	1	-	0/6/23/26	0/1/1/1
4	5N6	A	1402	-	-	5/23/41/41	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1402	5N6	O6-C6	-2.37	1.40	1.44
4	A	1402	5N6	O8-C8	-2.26	1.38	1.43

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1402	5N6	O1A-C1-C2	-5.00	116.01	123.59
4	A	1402	5N6	O10-C10-C11	-4.94	112.88	122.06
4	A	1402	5N6	C9-C8-C7	-4.40	103.70	112.20
4	A	1402	5N6	C9-O9-CAG	-3.87	107.37	117.10
4	A	1402	5N6	C5-N5-C10	3.17	130.89	123.18

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

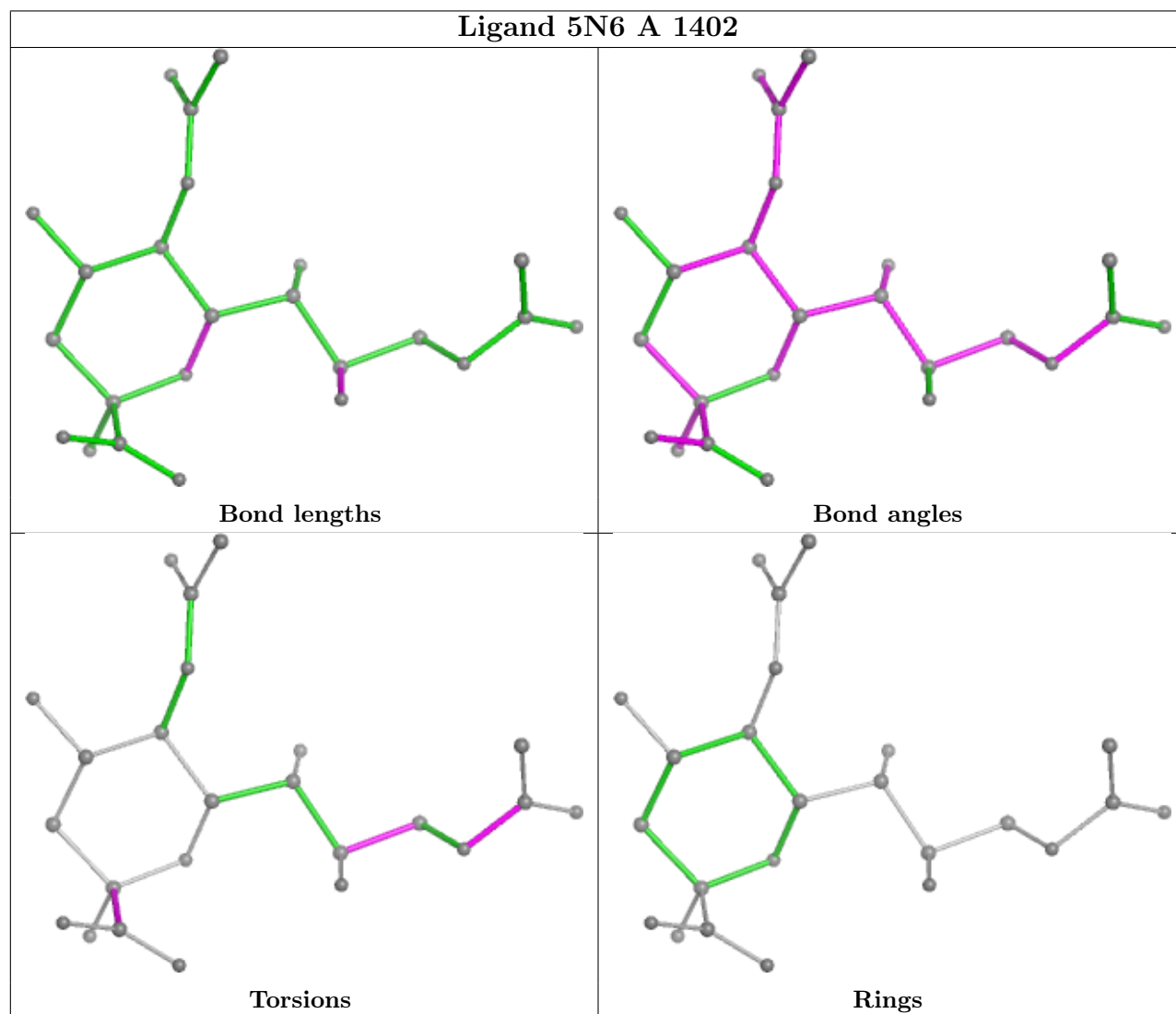
Mol	Chain	Res	Type	Atoms
4	A	1402	5N6	C7-C8-C9-O9
4	A	1402	5N6	O8-C8-C9-O9
4	A	1402	5N6	CAF-CAG-O9-C9
4	A	1402	5N6	OBJ-CAG-O9-C9
3	A	1401	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

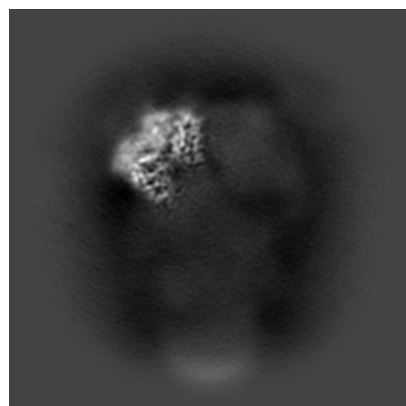
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53684. These allow visual inspection of the internal detail of the map and identification of artifacts.

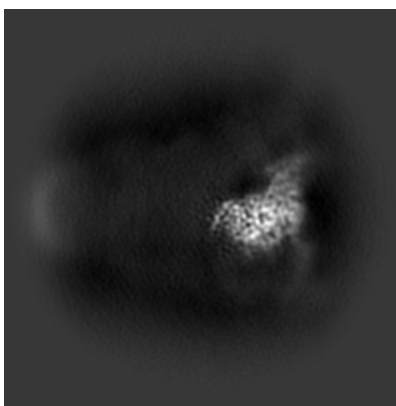
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

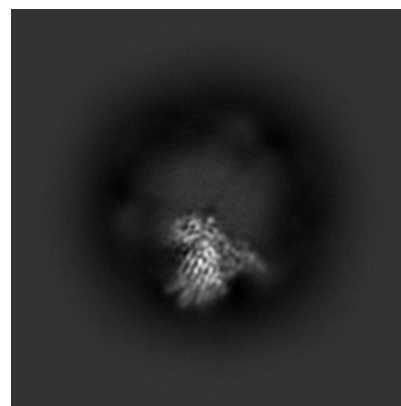
6.1.1 Primary map



X

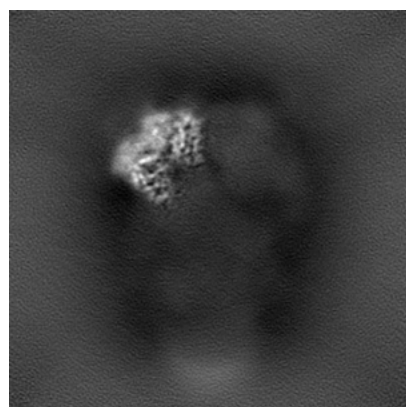


Y

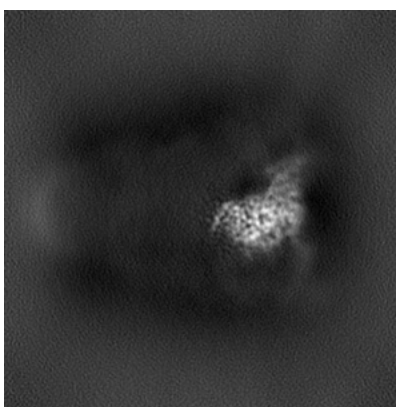


Z

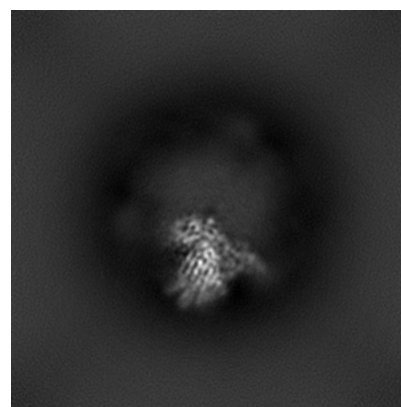
6.1.2 Raw map



X



Y

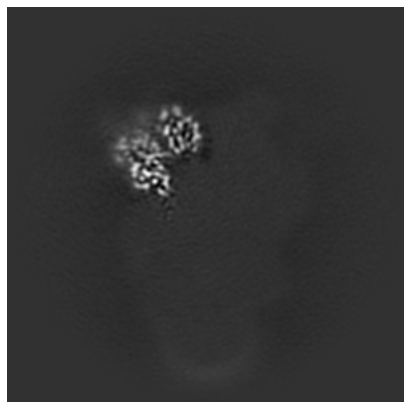


Z

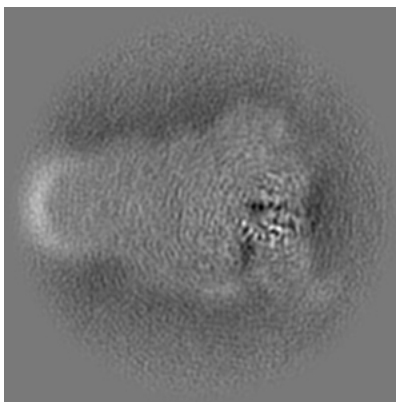
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

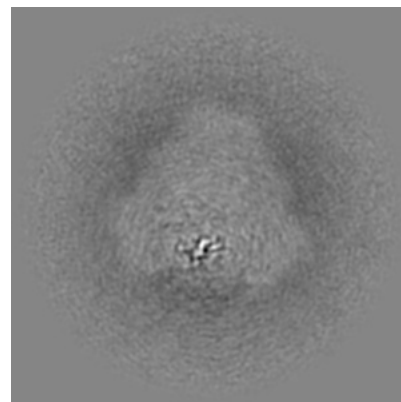
6.2.1 Primary map



X Index: 126

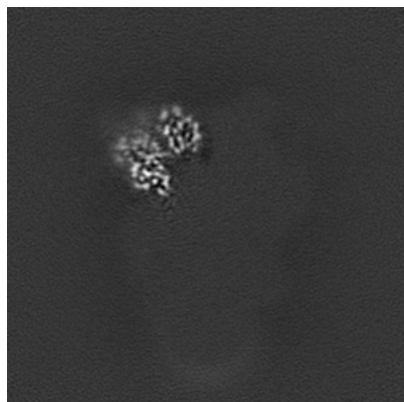


Y Index: 126

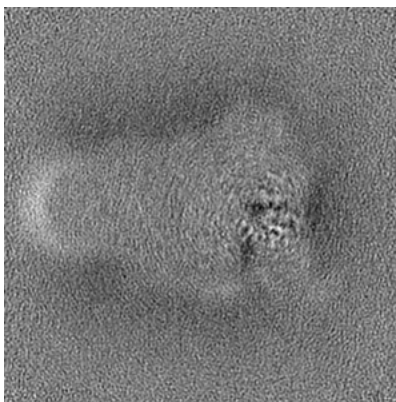


Z Index: 126

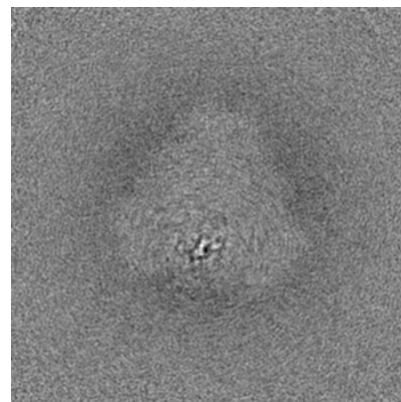
6.2.2 Raw map



X Index: 126



Y Index: 126

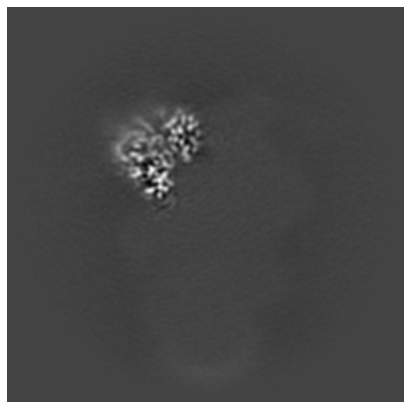


Z Index: 126

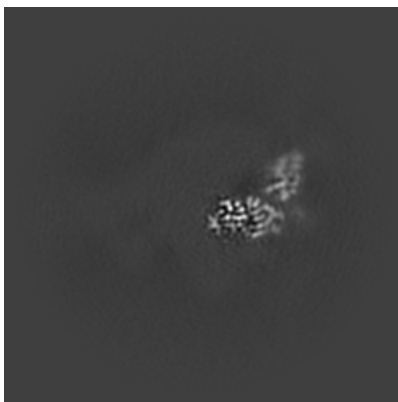
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

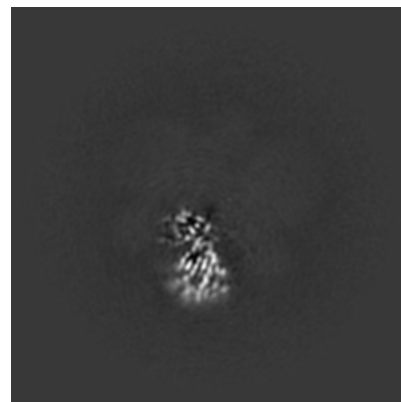
6.3.1 Primary map



X Index: 123

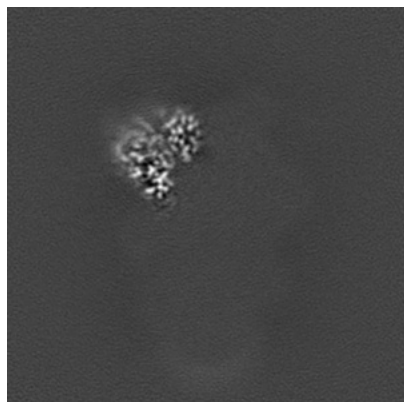


Y Index: 92

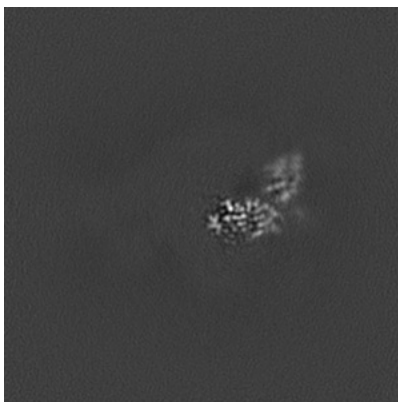


Z Index: 158

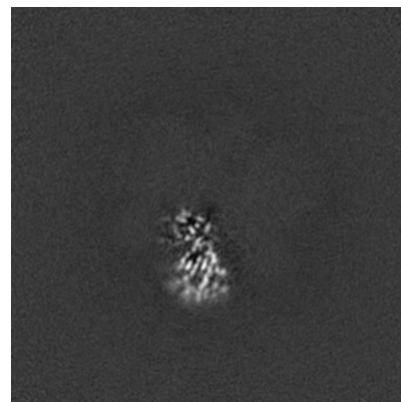
6.3.2 Raw map



X Index: 123



Y Index: 93

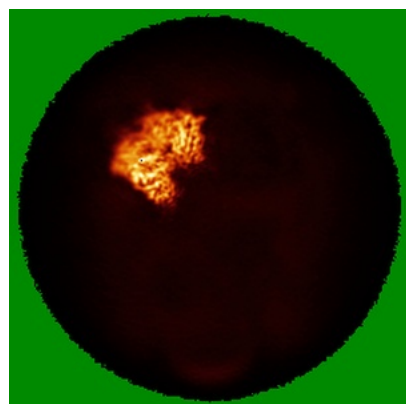


Z Index: 158

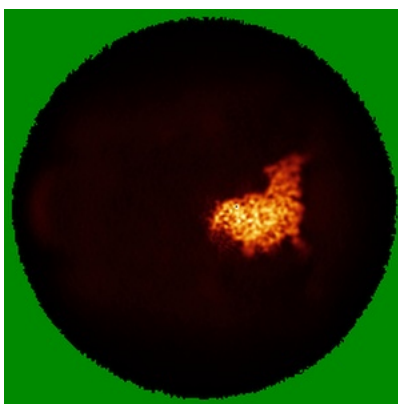
The images above show the largest variance slices of the map in three orthogonal directions.

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

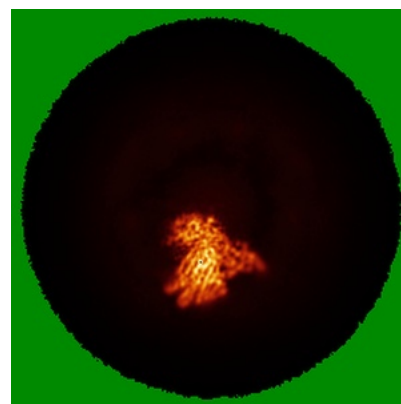
6.4.1 Primary map



X

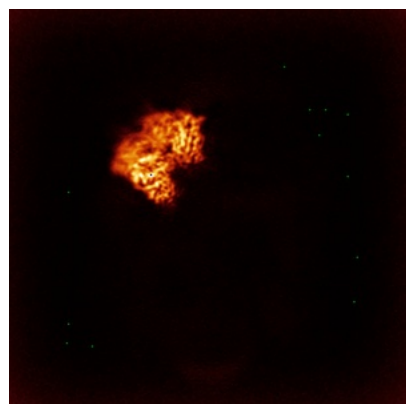


Y

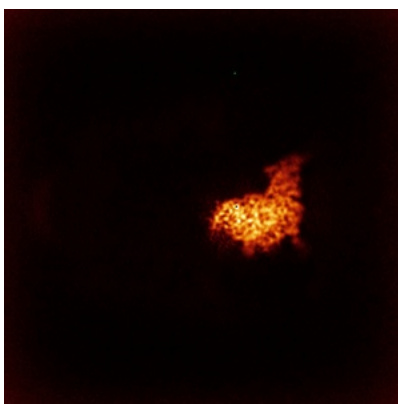


Z

6.4.2 Raw map



X



Y

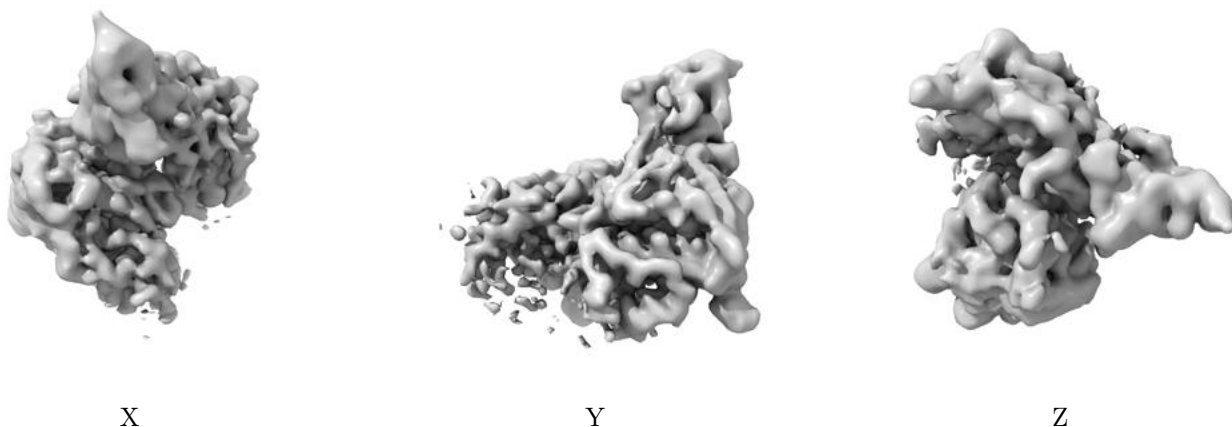


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0576. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

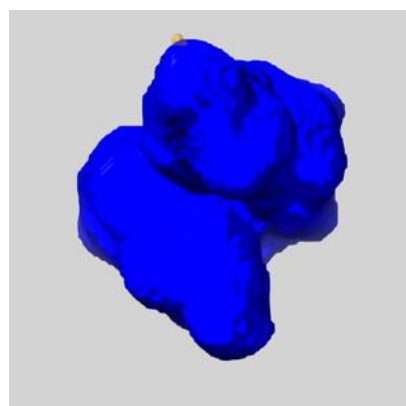
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

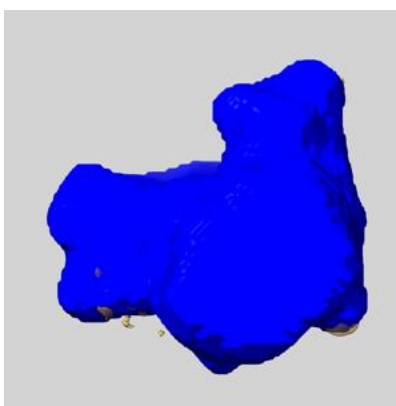
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

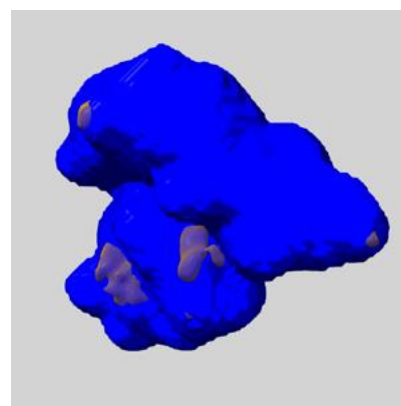
6.6.1 emd_53684_msk_1.map [i](#)



X



Y

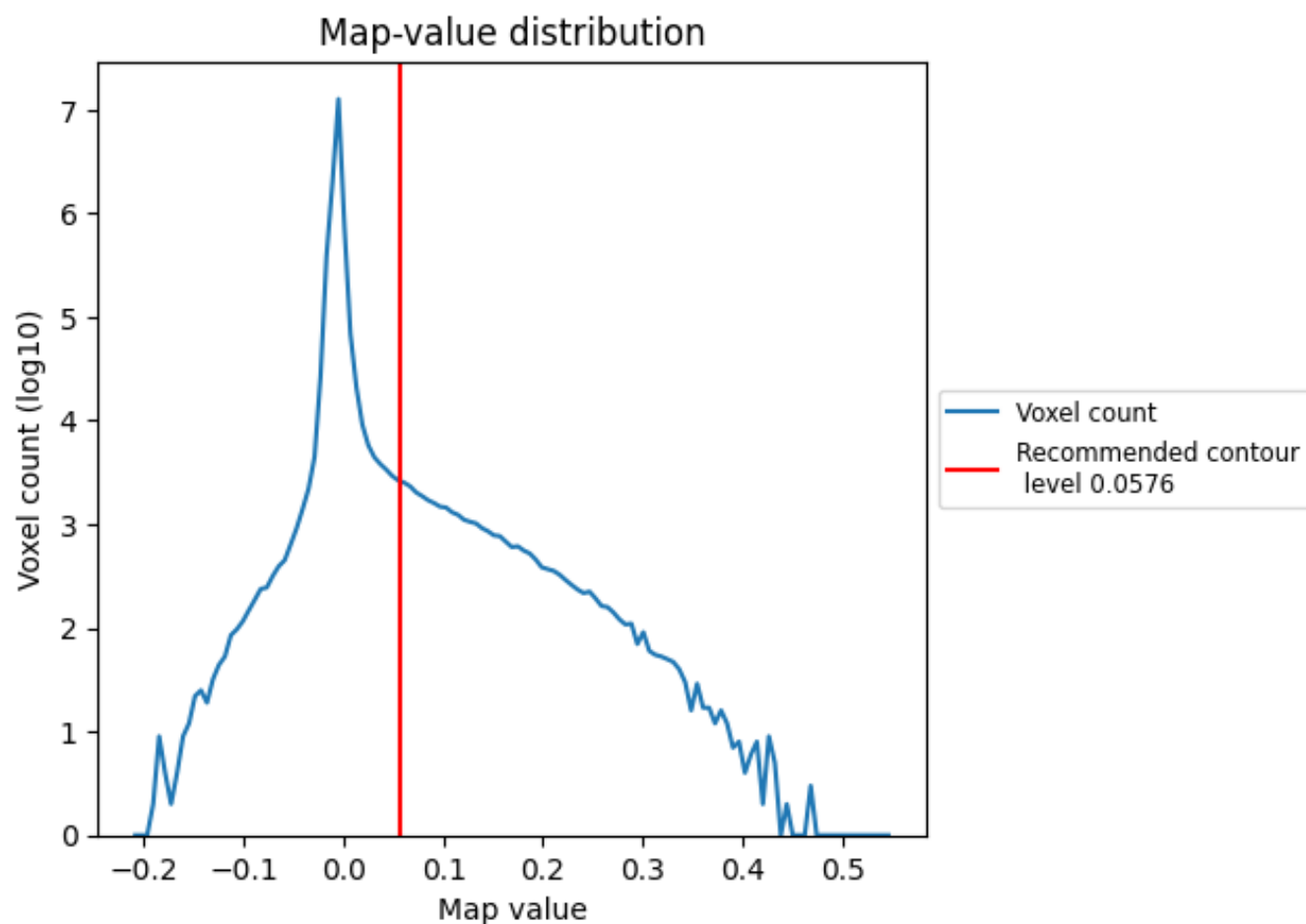


Z

7 Map analysis [i](#)

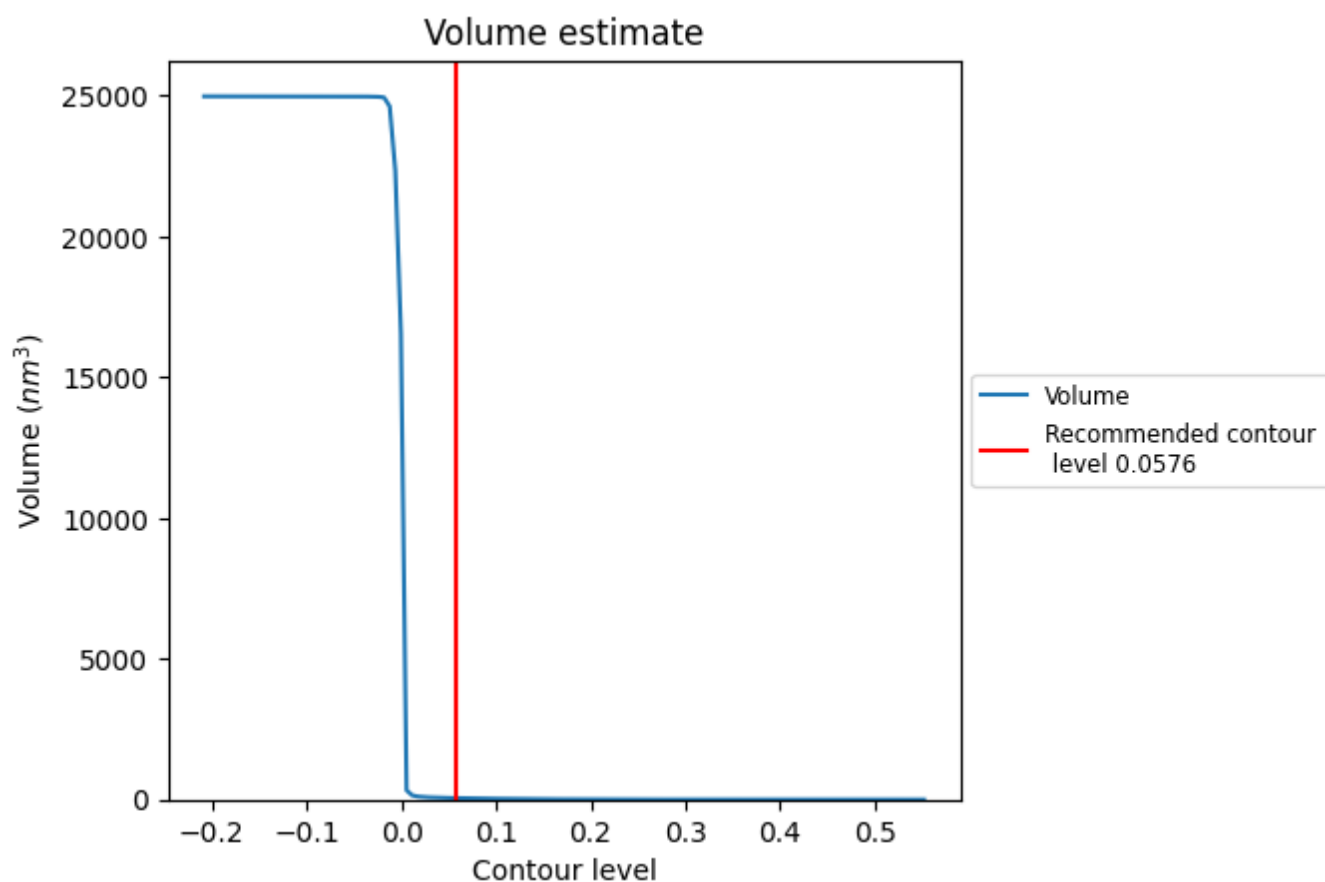
This section contains the results of statistical analysis of the map.

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.

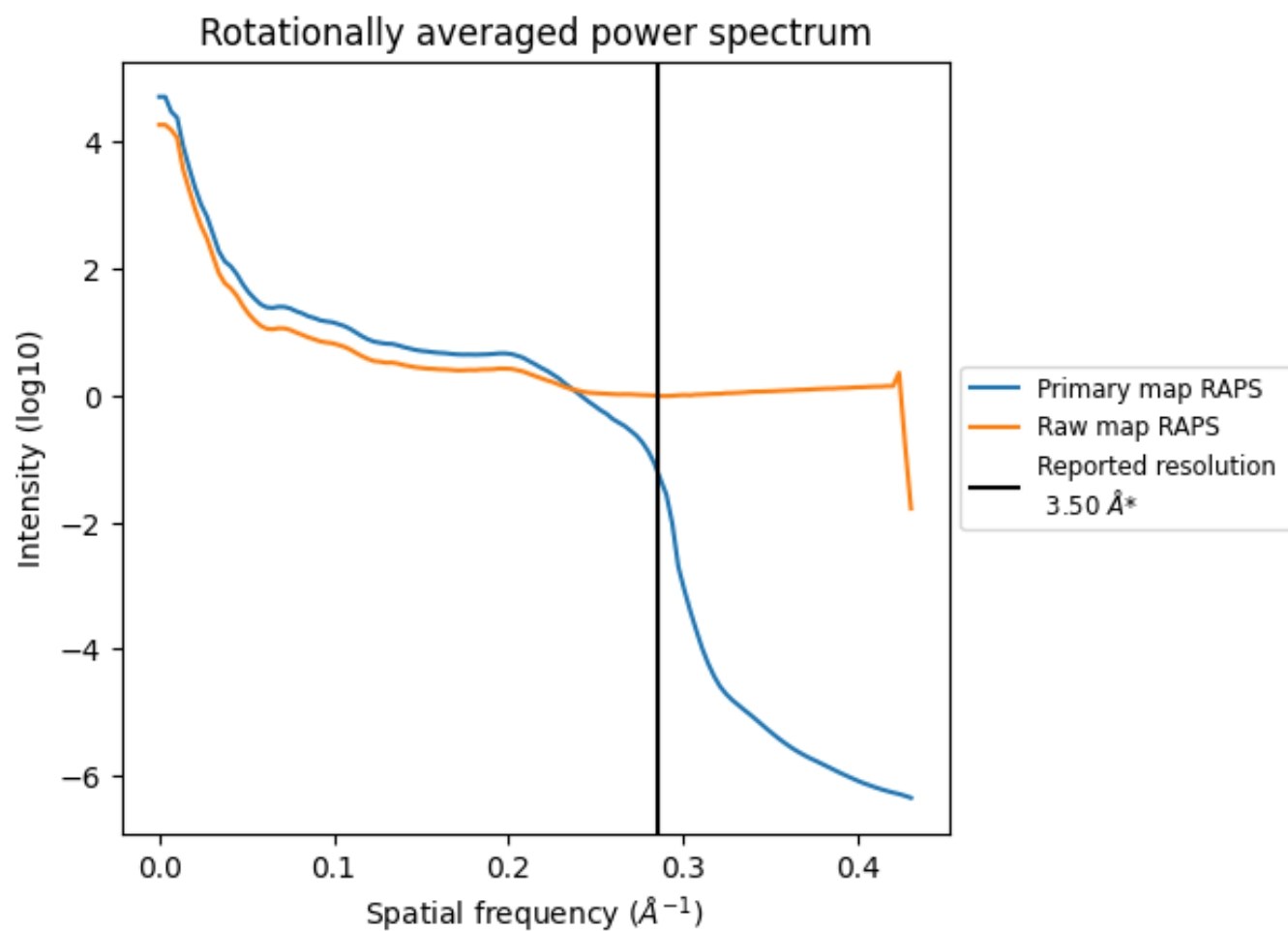
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 52 nm³; this corresponds to an approximate mass of 47 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 ⓘ

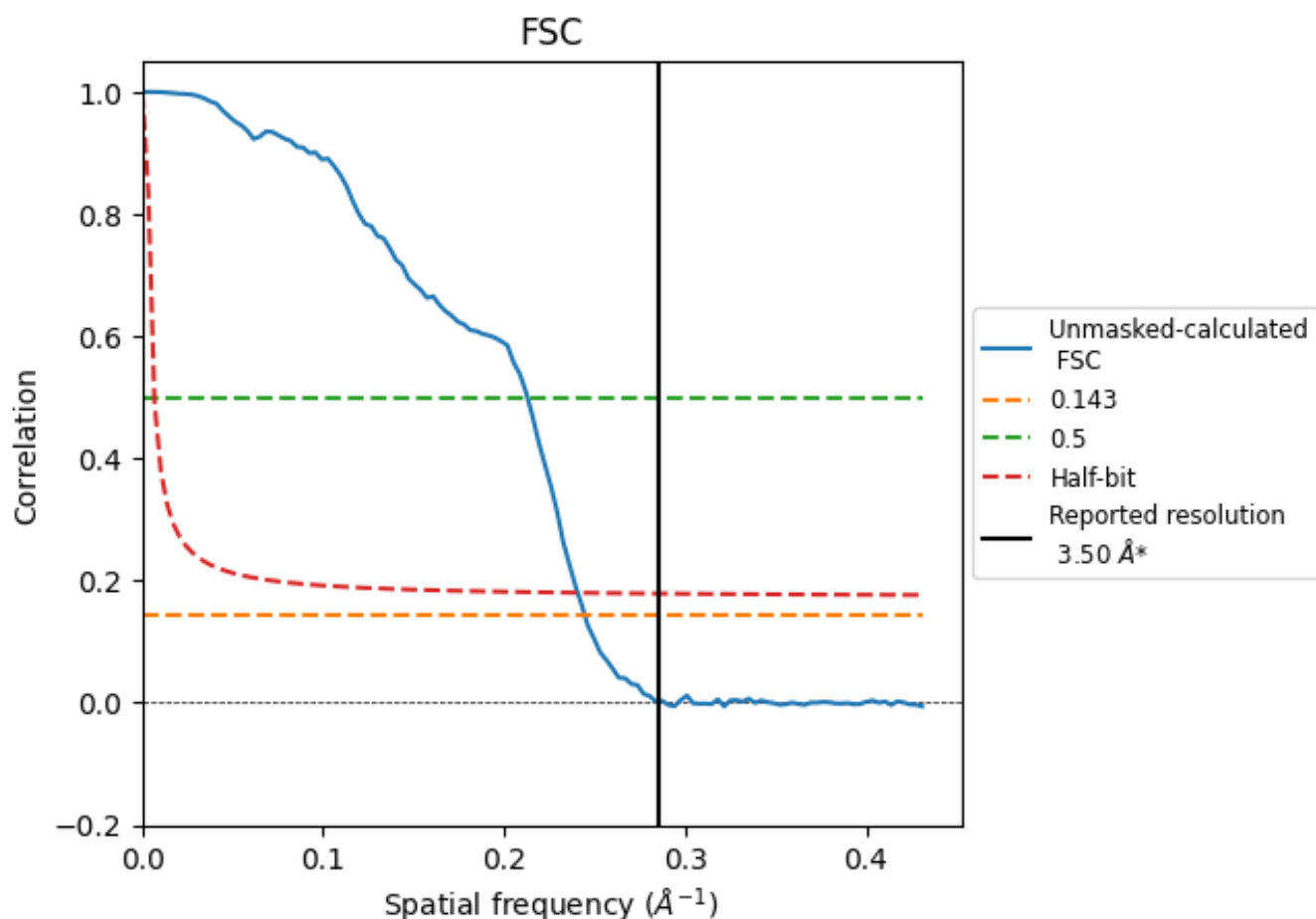


*Reported resolution corresponds to spatial frequency of 0.286 \AA^{-1}

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 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

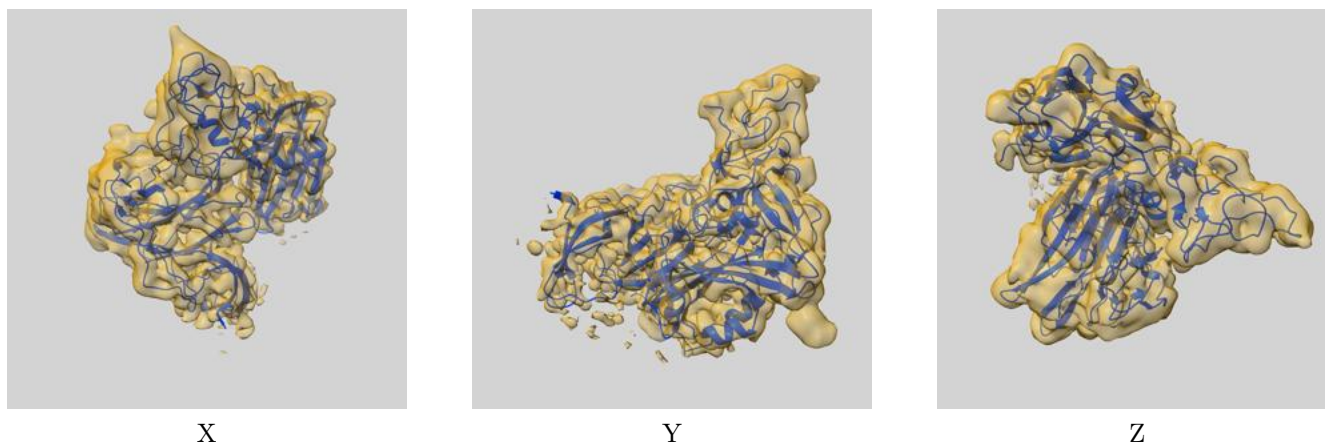
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.09	4.70	4.16

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.09 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

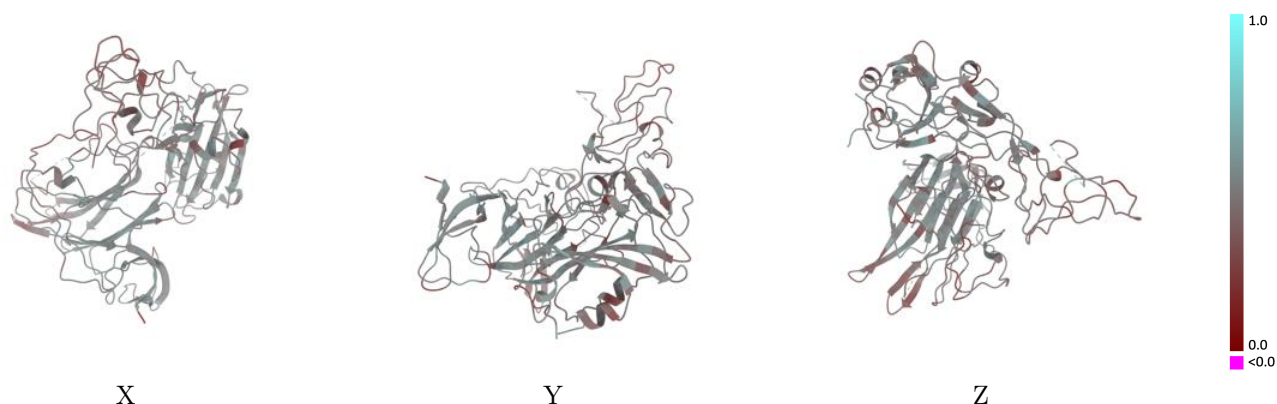
This section contains information regarding the fit between EMDB map EMD-53684 and PDB model 9R6Q. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

9.1 Map-model overlay [i](#)



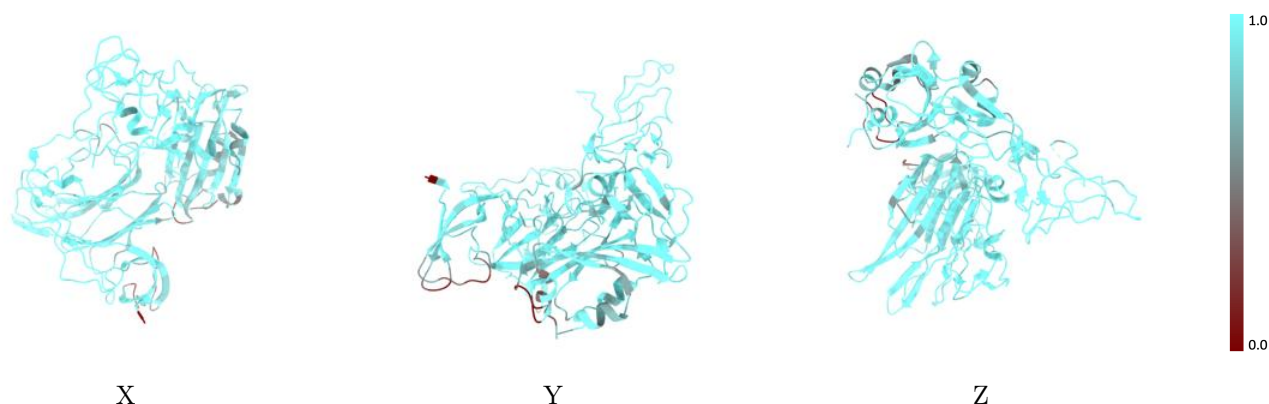
The images above show the 3D surface view of the map at the recommended contour level 0.0576 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



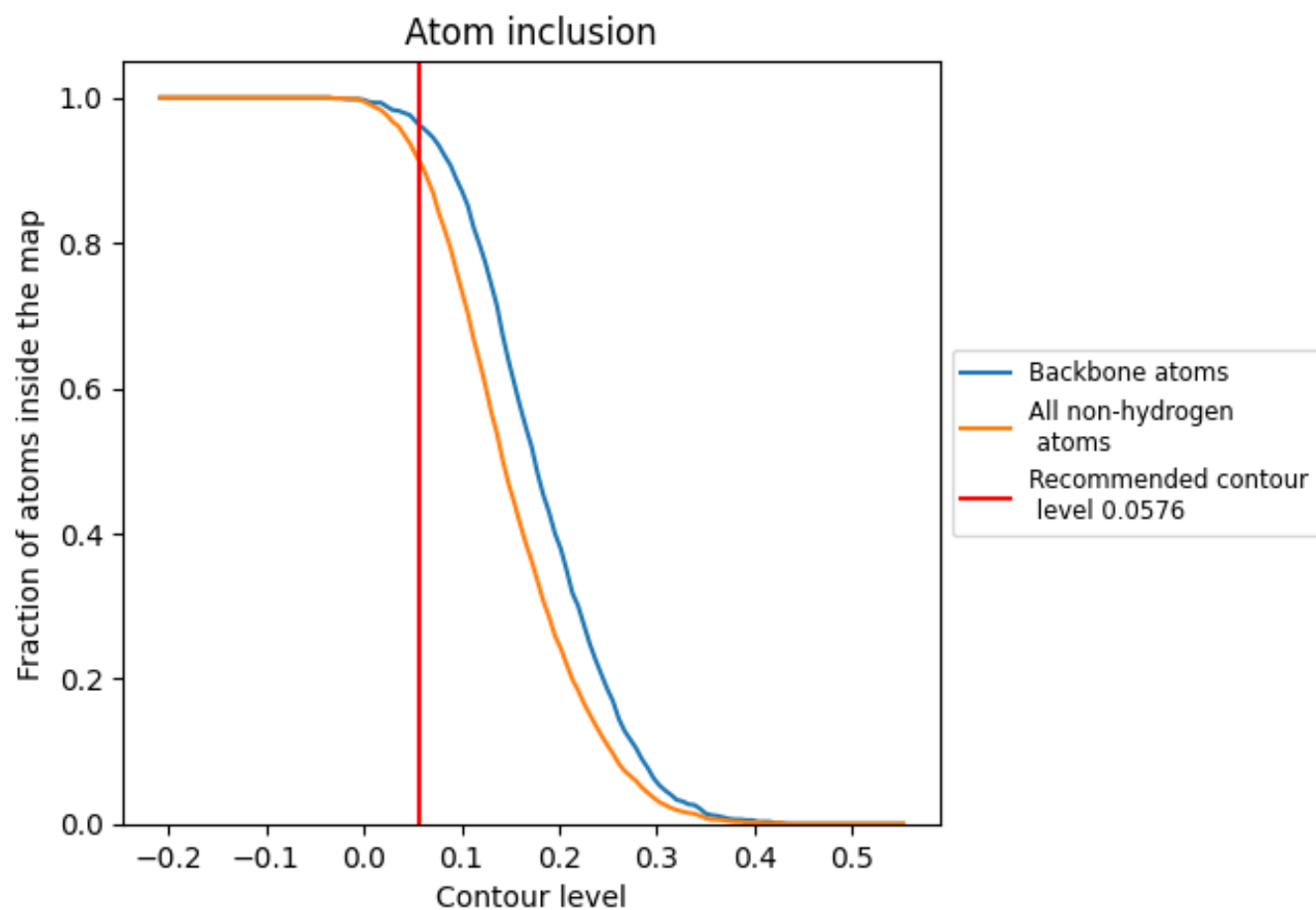
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0576).

9.4 Atom inclusion ⓘ



At the recommended contour level, 96% of all backbone atoms, 91% 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 (0.0576) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9100	<div></div> 0.4520
A	<div></div> 0.9250	<div></div> 0.4580
B	<div></div> 0.8950	<div></div> 0.4460
D	<div></div> 0.9490	<div></div> 0.4660

