



Full wwPDB EM Validation Report ⓘ

May 14, 2025 – 08:39 AM EDT

PDB ID : 8USZ / pdb_00008usz
EMDB ID : EMD-42524
Title : Cryo-EM Structure of Full-Length Spike Protein of Omicron XBB.1.5
Authors : Huynh, K.W.; Chang, J.S.; Fennell, K.F.; Che, Y.; Wu, H.
Deposited on : 2023-10-30
Resolution : 2.98 Å(reported)

This is a Full wwPDB EM Validation 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.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

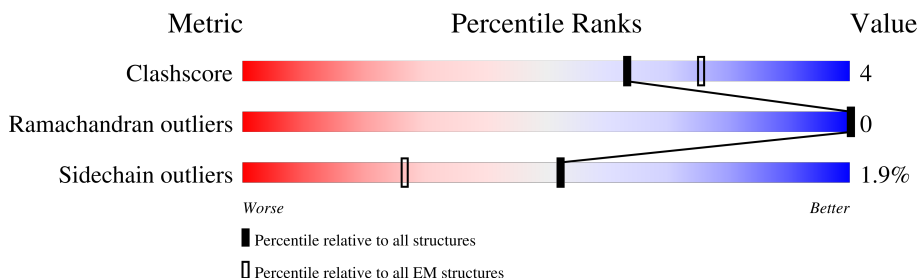
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.98 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1290	
1	B	1290	
1	C	1290	
2	D	2	
2	E	2	
2	F	2	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21179 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	958	Total	C	N	O	S	0	0
			6989	4434	1187	1337	31		
1	B	914	Total	C	N	O	S	1	0
			6981	4469	1160	1319	33		
1	C	886	Total	C	N	O	S	1	0
			6859	4402	1139	1287	31		

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ILE	THR	conflict	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	27	SER	ALA	conflict	UNP P0DTC2
A	83	ALA	VAL	conflict	UNP P0DTC2
A	143	ASP	GLY	conflict	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	146	GLN	HIS	conflict	UNP P0DTC2
A	183	GLU	GLN	conflict	UNP P0DTC2
A	213	GLU	VAL	conflict	UNP P0DTC2
A	252	VAL	GLY	conflict	UNP P0DTC2
A	339	HIS	GLY	conflict	UNP P0DTC2
A	346	THR	ARG	conflict	UNP P0DTC2
A	368	ILE	LEU	conflict	UNP P0DTC2
A	371	PHE	SER	conflict	UNP P0DTC2
A	373	PRO	SER	conflict	UNP P0DTC2
A	375	PHE	SER	conflict	UNP P0DTC2
A	376	ALA	THR	conflict	UNP P0DTC2
A	405	ASN	ASP	conflict	UNP P0DTC2
A	408	SER	ARG	conflict	UNP P0DTC2
A	417	ASN	LYS	conflict	UNP P0DTC2
A	440	LYS	ASN	conflict	UNP P0DTC2
A	445	PRO	VAL	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	446	SER	GLY	conflict	UNP P0DTC2
A	460	LYS	ASN	conflict	UNP P0DTC2
A	477	ASN	SER	conflict	UNP P0DTC2
A	478	LYS	THR	conflict	UNP P0DTC2
A	484	ALA	GLU	conflict	UNP P0DTC2
A	486	PRO	PHE	conflict	UNP P0DTC2
A	490	SER	PHE	conflict	UNP P0DTC2
A	498	ARG	GLN	conflict	UNP P0DTC2
A	501	TYR	ASN	conflict	UNP P0DTC2
A	505	HIS	TYR	conflict	UNP P0DTC2
A	614	GLY	ASP	conflict	UNP P0DTC2
A	655	TYR	HIS	conflict	UNP P0DTC2
A	679	LYS	ASN	conflict	UNP P0DTC2
A	681	HIS	PRO	conflict	UNP P0DTC2
A	764	LYS	ASN	conflict	UNP P0DTC2
A	796	TYR	ASP	conflict	UNP P0DTC2
A	954	HIS	GLN	conflict	UNP P0DTC2
A	969	LYS	ASN	conflict	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
A	1274	GLY	-	expression tag	UNP P0DTC2
A	1275	GLY	-	expression tag	UNP P0DTC2
A	1276	GLY	-	expression tag	UNP P0DTC2
A	1277	GLY	-	expression tag	UNP P0DTC2
A	1278	SER	-	expression tag	UNP P0DTC2
A	1279	GLY	-	expression tag	UNP P0DTC2
A	1280	GLY	-	expression tag	UNP P0DTC2
A	1281	GLY	-	expression tag	UNP P0DTC2
A	1282	GLY	-	expression tag	UNP P0DTC2
A	1283	SER	-	expression tag	UNP P0DTC2
A	1284	TRP	-	expression tag	UNP P0DTC2
A	1285	SER	-	expression tag	UNP P0DTC2
A	1286	HIS	-	expression tag	UNP P0DTC2
A	1287	PRO	-	expression tag	UNP P0DTC2
A	1288	GLN	-	expression tag	UNP P0DTC2
A	1289	PHE	-	expression tag	UNP P0DTC2
A	1290	GLU	-	expression tag	UNP P0DTC2
A	1291	LYS	-	expression tag	UNP P0DTC2
A	1292	GLY	-	expression tag	UNP P0DTC2
A	1293	GLY	-	expression tag	UNP P0DTC2
A	1294	GLY	-	expression tag	UNP P0DTC2
A	1295	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1296	SER	-	expression tag	UNP P0DTC2
A	1297	GLY	-	expression tag	UNP P0DTC2
A	1298	GLY	-	expression tag	UNP P0DTC2
A	1299	GLY	-	expression tag	UNP P0DTC2
A	1300	GLY	-	expression tag	UNP P0DTC2
A	1301	SER	-	expression tag	UNP P0DTC2
A	1302	TRP	-	expression tag	UNP P0DTC2
A	1303	SER	-	expression tag	UNP P0DTC2
A	1304	HIS	-	expression tag	UNP P0DTC2
A	1305	PRO	-	expression tag	UNP P0DTC2
A	1306	GLN	-	expression tag	UNP P0DTC2
A	1307	PHE	-	expression tag	UNP P0DTC2
A	1308	GLU	-	expression tag	UNP P0DTC2
A	1309	LYS	-	expression tag	UNP P0DTC2
B	22	ILE	THR	conflict	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	27	SER	ALA	conflict	UNP P0DTC2
B	83	ALA	VAL	conflict	UNP P0DTC2
B	143	ASP	GLY	conflict	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	146	GLN	HIS	conflict	UNP P0DTC2
B	183	GLU	GLN	conflict	UNP P0DTC2
B	213	GLU	VAL	conflict	UNP P0DTC2
B	252	VAL	GLY	conflict	UNP P0DTC2
B	339	HIS	GLY	conflict	UNP P0DTC2
B	346	THR	ARG	conflict	UNP P0DTC2
B	368	ILE	LEU	conflict	UNP P0DTC2
B	371	PHE	SER	conflict	UNP P0DTC2
B	373	PRO	SER	conflict	UNP P0DTC2
B	375	PHE	SER	conflict	UNP P0DTC2
B	376	ALA	THR	conflict	UNP P0DTC2
B	405	ASN	ASP	conflict	UNP P0DTC2
B	408	SER	ARG	conflict	UNP P0DTC2
B	417	ASN	LYS	conflict	UNP P0DTC2
B	440	LYS	ASN	conflict	UNP P0DTC2
B	445	PRO	VAL	conflict	UNP P0DTC2
B	446	SER	GLY	conflict	UNP P0DTC2
B	460	LYS	ASN	conflict	UNP P0DTC2
B	477	ASN	SER	conflict	UNP P0DTC2
B	478	LYS	THR	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	484	ALA	GLU	conflict	UNP P0DTC2
B	486	PRO	PHE	conflict	UNP P0DTC2
B	490	SER	PHE	conflict	UNP P0DTC2
B	498	ARG	GLN	conflict	UNP P0DTC2
B	501	TYR	ASN	conflict	UNP P0DTC2
B	505	HIS	TYR	conflict	UNP P0DTC2
B	614	GLY	ASP	conflict	UNP P0DTC2
B	655	TYR	HIS	conflict	UNP P0DTC2
B	679	LYS	ASN	conflict	UNP P0DTC2
B	681	HIS	PRO	conflict	UNP P0DTC2
B	764	LYS	ASN	conflict	UNP P0DTC2
B	796	TYR	ASP	conflict	UNP P0DTC2
B	954	HIS	GLN	conflict	UNP P0DTC2
B	969	LYS	ASN	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
B	1274	GLY	-	expression tag	UNP P0DTC2
B	1275	GLY	-	expression tag	UNP P0DTC2
B	1276	GLY	-	expression tag	UNP P0DTC2
B	1277	GLY	-	expression tag	UNP P0DTC2
B	1278	SER	-	expression tag	UNP P0DTC2
B	1279	GLY	-	expression tag	UNP P0DTC2
B	1280	GLY	-	expression tag	UNP P0DTC2
B	1281	GLY	-	expression tag	UNP P0DTC2
B	1282	GLY	-	expression tag	UNP P0DTC2
B	1283	SER	-	expression tag	UNP P0DTC2
B	1284	TRP	-	expression tag	UNP P0DTC2
B	1285	SER	-	expression tag	UNP P0DTC2
B	1286	HIS	-	expression tag	UNP P0DTC2
B	1287	PRO	-	expression tag	UNP P0DTC2
B	1288	GLN	-	expression tag	UNP P0DTC2
B	1289	PHE	-	expression tag	UNP P0DTC2
B	1290	GLU	-	expression tag	UNP P0DTC2
B	1291	LYS	-	expression tag	UNP P0DTC2
B	1292	GLY	-	expression tag	UNP P0DTC2
B	1293	GLY	-	expression tag	UNP P0DTC2
B	1294	GLY	-	expression tag	UNP P0DTC2
B	1295	GLY	-	expression tag	UNP P0DTC2
B	1296	SER	-	expression tag	UNP P0DTC2
B	1297	GLY	-	expression tag	UNP P0DTC2
B	1298	GLY	-	expression tag	UNP P0DTC2
B	1299	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1300	GLY	-	expression tag	UNP P0DTC2
B	1301	SER	-	expression tag	UNP P0DTC2
B	1302	TRP	-	expression tag	UNP P0DTC2
B	1303	SER	-	expression tag	UNP P0DTC2
B	1304	HIS	-	expression tag	UNP P0DTC2
B	1305	PRO	-	expression tag	UNP P0DTC2
B	1306	GLN	-	expression tag	UNP P0DTC2
B	1307	PHE	-	expression tag	UNP P0DTC2
B	1308	GLU	-	expression tag	UNP P0DTC2
B	1309	LYS	-	expression tag	UNP P0DTC2
C	22	ILE	THR	conflict	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	27	SER	ALA	conflict	UNP P0DTC2
C	83	ALA	VAL	conflict	UNP P0DTC2
C	143	ASP	GLY	conflict	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	146	GLN	HIS	conflict	UNP P0DTC2
C	183	GLU	GLN	conflict	UNP P0DTC2
C	213	GLU	VAL	conflict	UNP P0DTC2
C	252	VAL	GLY	conflict	UNP P0DTC2
C	339	HIS	GLY	conflict	UNP P0DTC2
C	346	THR	ARG	conflict	UNP P0DTC2
C	368	ILE	LEU	conflict	UNP P0DTC2
C	371	PHE	SER	conflict	UNP P0DTC2
C	373	PRO	SER	conflict	UNP P0DTC2
C	375	PHE	SER	conflict	UNP P0DTC2
C	376	ALA	THR	conflict	UNP P0DTC2
C	405	ASN	ASP	conflict	UNP P0DTC2
C	408	SER	ARG	conflict	UNP P0DTC2
C	417	ASN	LYS	conflict	UNP P0DTC2
C	440	LYS	ASN	conflict	UNP P0DTC2
C	445	PRO	VAL	conflict	UNP P0DTC2
C	446	SER	GLY	conflict	UNP P0DTC2
C	460	LYS	ASN	conflict	UNP P0DTC2
C	477	ASN	SER	conflict	UNP P0DTC2
C	478	LYS	THR	conflict	UNP P0DTC2
C	484	ALA	GLU	conflict	UNP P0DTC2
C	486	PRO	PHE	conflict	UNP P0DTC2
C	490	SER	PHE	conflict	UNP P0DTC2
C	498	ARG	GLN	conflict	UNP P0DTC2

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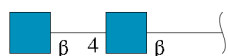
Chain	Residue	Modelled	Actual	Comment	Reference
C	501	TYR	ASN	conflict	UNP P0DTC2
C	505	HIS	TYR	conflict	UNP P0DTC2
C	614	GLY	ASP	conflict	UNP P0DTC2
C	655	TYR	HIS	conflict	UNP P0DTC2
C	679	LYS	ASN	conflict	UNP P0DTC2
C	681	HIS	PRO	conflict	UNP P0DTC2
C	764	LYS	ASN	conflict	UNP P0DTC2
C	796	TYR	ASP	conflict	UNP P0DTC2
C	954	HIS	GLN	conflict	UNP P0DTC2
C	969	LYS	ASN	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2
C	1274	GLY	-	expression tag	UNP P0DTC2
C	1275	GLY	-	expression tag	UNP P0DTC2
C	1276	GLY	-	expression tag	UNP P0DTC2
C	1277	GLY	-	expression tag	UNP P0DTC2
C	1278	SER	-	expression tag	UNP P0DTC2
C	1279	GLY	-	expression tag	UNP P0DTC2
C	1280	GLY	-	expression tag	UNP P0DTC2
C	1281	GLY	-	expression tag	UNP P0DTC2
C	1282	GLY	-	expression tag	UNP P0DTC2
C	1283	SER	-	expression tag	UNP P0DTC2
C	1284	TRP	-	expression tag	UNP P0DTC2
C	1285	SER	-	expression tag	UNP P0DTC2
C	1286	HIS	-	expression tag	UNP P0DTC2
C	1287	PRO	-	expression tag	UNP P0DTC2
C	1288	GLN	-	expression tag	UNP P0DTC2
C	1289	PHE	-	expression tag	UNP P0DTC2
C	1290	GLU	-	expression tag	UNP P0DTC2
C	1291	LYS	-	expression tag	UNP P0DTC2
C	1292	GLY	-	expression tag	UNP P0DTC2
C	1293	GLY	-	expression tag	UNP P0DTC2
C	1294	GLY	-	expression tag	UNP P0DTC2
C	1295	GLY	-	expression tag	UNP P0DTC2
C	1296	SER	-	expression tag	UNP P0DTC2
C	1297	GLY	-	expression tag	UNP P0DTC2
C	1298	GLY	-	expression tag	UNP P0DTC2
C	1299	GLY	-	expression tag	UNP P0DTC2
C	1300	GLY	-	expression tag	UNP P0DTC2
C	1301	SER	-	expression tag	UNP P0DTC2
C	1302	TRP	-	expression tag	UNP P0DTC2
C	1303	SER	-	expression tag	UNP P0DTC2

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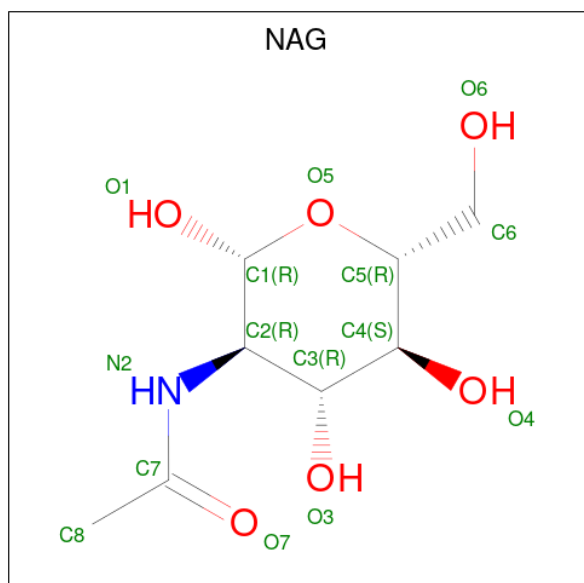
Chain	Residue	Modelled	Actual	Comment	Reference
C	1304	HIS	-	expression tag	UNP P0DTC2
C	1305	PRO	-	expression tag	UNP P0DTC2
C	1306	GLN	-	expression tag	UNP P0DTC2
C	1307	PHE	-	expression tag	UNP P0DTC2
C	1308	GLU	-	expression tag	UNP P0DTC2
C	1309	LYS	-	expression tag	UNP P0DTC2

- Molecule 2 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
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

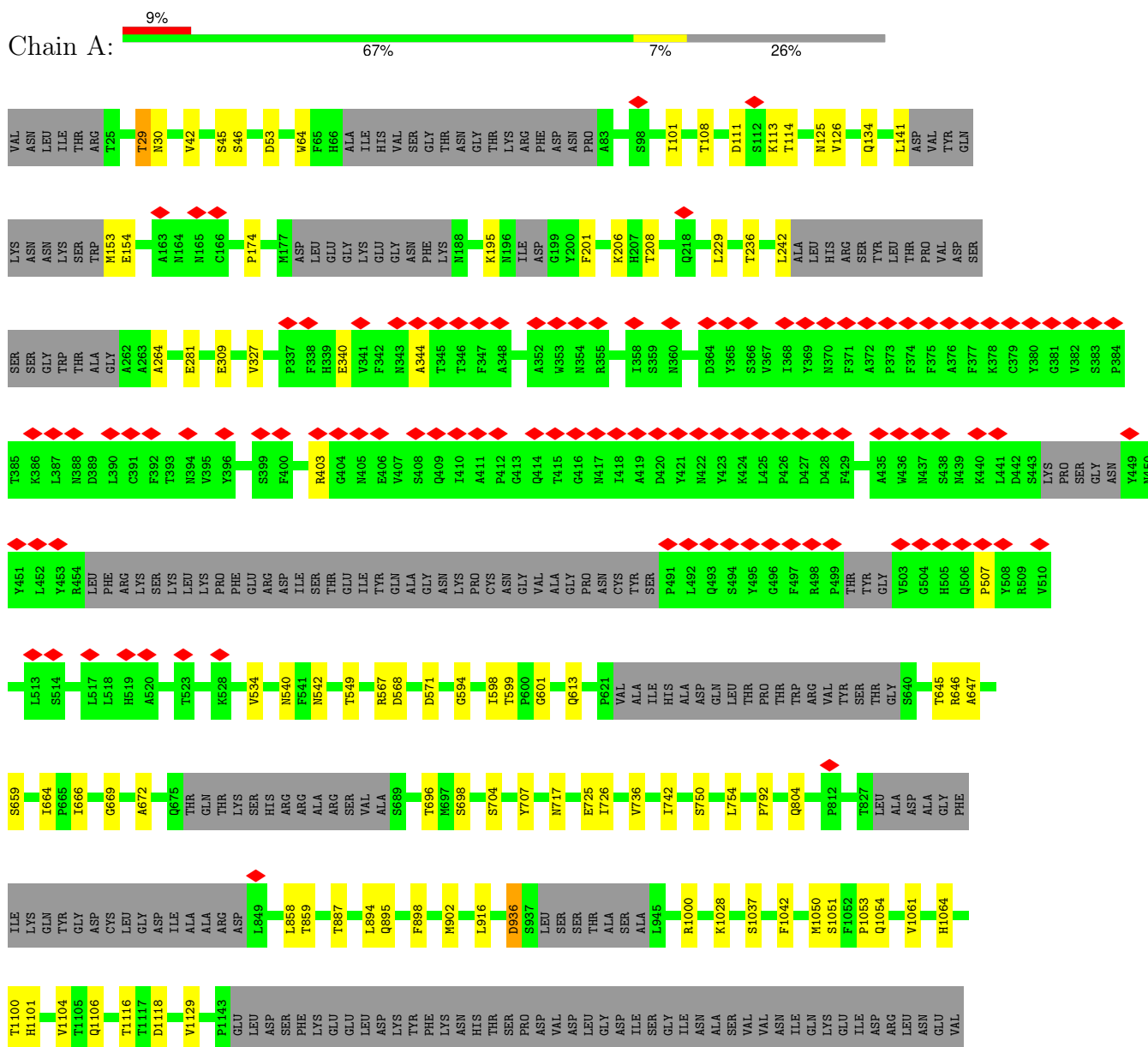


Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3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

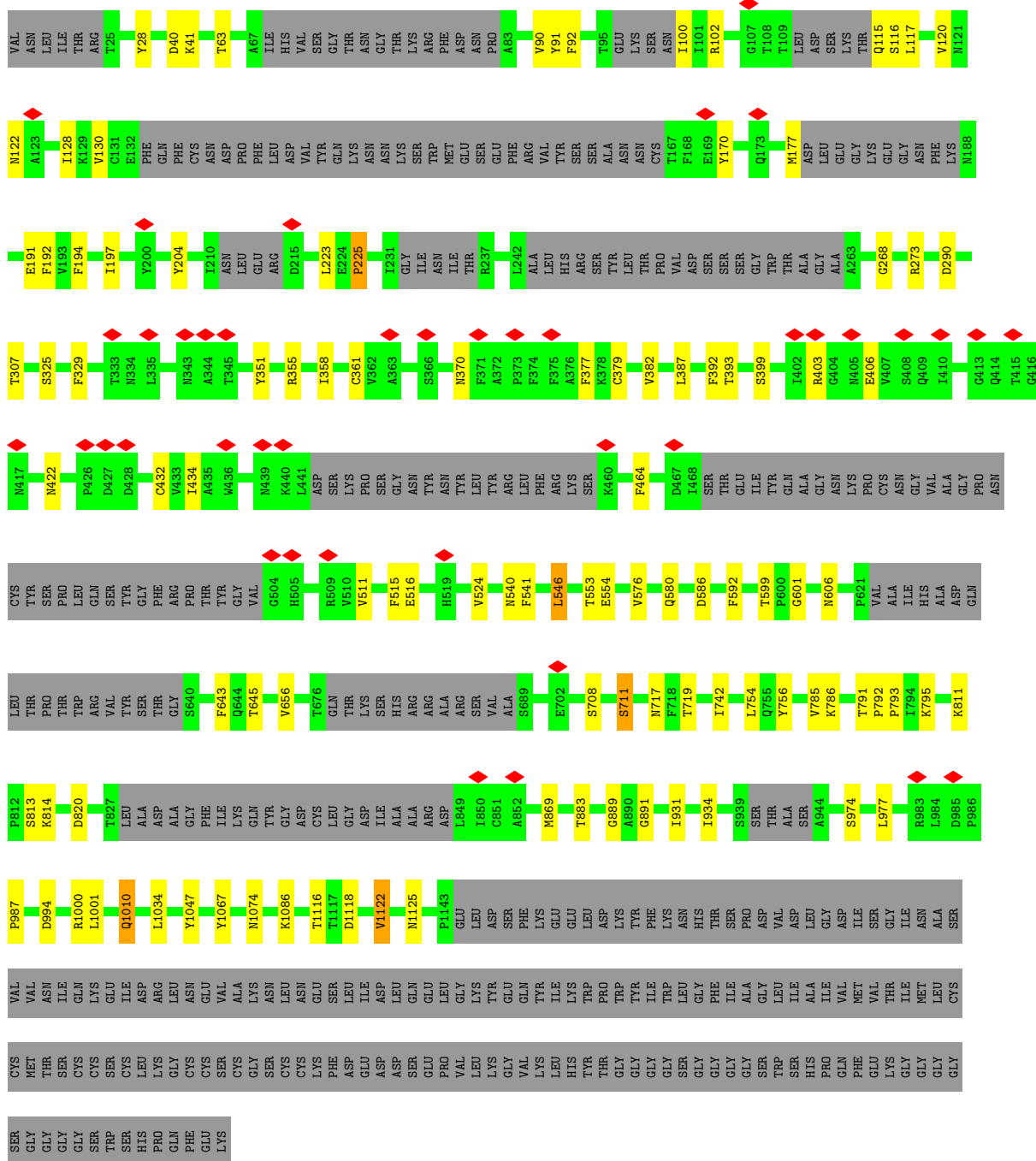
3 Residue-property plots

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



- Molecule 1: Spike glycoprotein



- Molecule 1: Spike glycoprotein



Chain E:  50% 50%

MAG1
MAG2

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

Chain F:  50% 50%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	91663	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.0	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.913	Depositor
Minimum map value	-0.558	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.07	Depositor
Map size (\AA)	405.0, 405.0, 405.0	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.75, 0.75, 0.75	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.20	0/7116	0.42	0/9700
1	B	0.20	0/7126	0.44	2/9704 (0.0%)
1	C	0.22	2/7007 (0.0%)	0.41	2/9530 (0.0%)
All	All	0.21	2/21249 (0.0%)	0.43	4/28934 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	817	PHE	CA-C	-5.15	1.46	1.52
1	C	817	PHE	N-CA	-5.05	1.40	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	987	PRO	CA-N-CD	-12.49	94.52	112.00
1	B	225	PRO	CA-N-CD	-11.80	95.48	112.00
1	B	987	PRO	CA-N-CD	-6.06	103.51	112.00
1	C	987	PRO	N-CD-CG	-5.15	95.48	103.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6989	0	6461	51	0
1	B	6981	0	6776	61	0
1	C	6859	0	6698	61	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
3	A	98	0	91	0	0
3	B	84	0	78	1	0
3	C	84	0	78	1	0
All	All	21179	0	20257	165	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 4.

All (165) 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:120:VAL:HG12	1:B:122:ASN:OD1	1.44	1.16
1:A:898:PHE:CZ	1:A:1050:MET:HE1	1.85	1.11
1:B:120:VAL:CG1	1:B:122:ASN:OD1	2.00	1.10
1:A:895:GLN:NE2	1:C:706:ALA:O	1.94	1.01
1:B:392:PHE:CE1	1:B:515:PHE:CE1	2.56	0.94
1:C:817:PHE:CE2	1:C:821:LEU:HD11	2.24	0.73
1:A:902:MET:HG2	1:A:916:LEU:HD21	1.70	0.72
1:B:392:PHE:HE1	1:B:515:PHE:CE1	2.08	0.69
1:A:206:LYS:HE3	1:A:208:THR:OG1	1.93	0.68
1:A:898:PHE:HZ	1:A:1050:MET:HE1	1.58	0.67
1:A:645:THR:HG22	1:A:647:ALA:H	1.60	0.66
1:C:1116:THR:HG22	1:C:1118:ASP:H	1.59	0.66
1:C:740:MET:HG3	1:C:744:GLY:HA2	1.78	0.65
1:B:791:THR:HG21	1:B:795:LYS:HZ3	1.62	0.63
1:A:895:GLN:OE1	1:C:711:SER:OG	2.09	0.63
1:A:1100:THR:HG1	1:A:1101:HIS:HD1	1.45	0.62
1:B:643:PHE:CE2	1:B:645:THR:OG1	2.53	0.62
1:B:811:LYS:HE2	1:B:813:SER:HB2	1.82	0.61
1:B:120:VAL:HG11	1:B:122:ASN:OD1	1.98	0.61
1:A:599:THR:HG22	1:A:601:GLY:H	1.64	0.61
1:B:128:ILE:HB	1:B:170:TYR:HB3	1.82	0.60
1:B:1116:THR:HG22	1:B:1118:ASP:H	1.67	0.59
1:A:707:TYR:HB3	1:B:792:PRO:HG3	1.84	0.58
1:B:120:VAL:HG12	1:B:122:ASN:CG	2.27	0.58
1:B:599:THR:HG22	1:B:601:GLY:H	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:902:MET:CG	1:A:916:LEU:HD21	2.34	0.57
1:B:811:LYS:NZ	1:B:820:ASP:OD1	2.38	0.57
1:B:1047:TYR:HB2	1:B:1067:TYR:HB3	1.87	0.56
1:A:108:THR:HG1	1:A:114:THR:HG1	1.52	0.56
1:A:725:GLU:OE2	1:A:1064:HIS:NE2	2.38	0.55
1:A:669:GLY:HA3	1:B:869:MET:HE1	1.88	0.55
1:C:716:THR:HG22	1:C:716:THR:O	2.06	0.54
1:B:177:MET:SD	1:B:177:MET:N	2.81	0.54
1:B:273:ARG:NH1	1:B:290:ASP:OD2	2.41	0.54
1:C:550:GLY:HA2	1:C:589:PRO:HA	1.90	0.54
1:A:726:ILE:HG13	1:A:1061:VAL:HG22	1.90	0.53
1:B:1086:LYS:HA	1:B:1125:ASN:HA	1.91	0.53
1:A:792:PRO:HG2	1:C:707:TYR:HB3	1.91	0.52
1:B:355:ARG:HH12	1:B:464:PHE:HB3	1.74	0.52
1:C:92:PHE:HB3	1:C:192:PHE:HB2	1.90	0.52
1:B:115:GLN:HE22	1:B:117:LEU:HD12	1.75	0.52
1:B:120:VAL:CG1	1:B:122:ASN:CG	2.81	0.52
1:C:979:ASP:OD2	1:C:983:ARG:NH2	2.42	0.52
1:C:455:LEU:HD13	1:C:491:PRO:HB2	1.92	0.52
1:A:53:ASP:OD2	1:A:195:LYS:NZ	2.42	0.52
1:C:214:ARG:NH1	1:C:215:ASP:O	2.43	0.52
1:B:191:GLU:HB3	1:B:223:LEU:HD21	1.92	0.52
1:A:64:TRP:HE1	1:A:264:ALA:HB1	1.75	0.51
1:B:325:SER:HA	1:B:540:ASN:HB2	1.92	0.51
1:C:770:ILE:HD11	1:C:1012:LEU:HD23	1.91	0.51
1:A:201:PHE:HB3	1:A:229:LEU:HB2	1.92	0.51
1:A:659:SER:HB3	1:A:698:SER:HB3	1.93	0.51
1:A:126:VAL:HG23	1:A:174:PRO:HA	1.91	0.51
1:A:113:LYS:HG3	1:A:114:THR:HG23	1.93	0.51
1:B:742:ILE:O	1:B:1000:ARG:NH1	2.42	0.51
1:C:815:ARG:NH1	1:C:820:ASP:OD1	2.44	0.51
1:C:803:SER:HB2	3:C:2004:NAG:H82	1.94	0.50
1:C:817:PHE:O	1:C:820:ASP:N	2.44	0.50
1:C:985:ASP:OD1	1:C:985:ASP:N	2.41	0.50
1:A:567:ARG:HD3	1:A:571:ASP:HA	1.93	0.50
1:B:643:PHE:CD2	1:B:645:THR:OG1	2.64	0.50
1:C:786:LYS:NZ	1:C:891:GLY:O	2.44	0.50
1:A:1028:LYS:NZ	1:A:1042:PHE:O	2.43	0.50
1:C:1001:LEU:O	1:C:1005:GLN:HG3	2.12	0.50
1:B:392:PHE:CE1	1:B:515:PHE:CZ	2.99	0.49
1:C:817:PHE:CZ	1:C:821:LEU:HD11	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:PHE:HB3	1:B:192:PHE:HB2	1.95	0.49
1:C:577:ARG:HH21	1:C:582:LEU:HB3	1.77	0.49
1:C:605:SER:OG	1:C:606:ASN:N	2.44	0.49
1:B:786:LYS:NZ	1:B:891:GLY:O	2.46	0.49
1:A:540:ASN:OD1	1:A:549:THR:OG1	2.30	0.49
1:A:742:ILE:O	1:A:1000:ARG:NH1	2.44	0.48
1:A:42:VAL:HG11	1:C:567:ARG:HD2	1.94	0.48
1:A:898:PHE:CE1	1:A:1050:MET:HE1	2.44	0.48
1:C:1091:ARG:NH1	1:C:1118:ASP:O	2.47	0.48
1:B:708:SER:HB3	1:B:711:SER:HB2	1.94	0.48
1:A:45:SER:OG	1:A:46:SER:N	2.44	0.47
1:A:887:THR:HB	1:A:894:LEU:HD23	1.96	0.47
1:C:887:THR:HB	1:C:894:LEU:HD23	1.96	0.47
1:C:1028:LYS:NZ	1:C:1042:PHE:O	2.47	0.47
1:C:1047:TYR:HB2	1:C:1067:TYR:HB3	1.95	0.47
1:B:379:CYS:HA	1:B:432:CYS:HA	1.97	0.47
1:B:541:PHE:HE1	1:B:546:LEU:HD23	1.79	0.47
1:B:553:THR:HG23	1:B:586:ASP:HB2	1.97	0.47
1:A:936:ASP:OD1	1:A:936:ASP:N	2.46	0.47
1:B:392:PHE:CE1	1:B:515:PHE:CD1	3.00	0.47
1:C:605:SER:OG	1:C:607:GLN:OE1	2.32	0.47
1:B:1074:ASN:HD21	3:B:2005:NAG:H2	1.80	0.47
1:C:357:ARG:HG3	1:C:397:ALA:HB3	1.97	0.46
1:B:791:THR:HG21	1:B:795:LYS:NZ	2.30	0.46
1:C:374:PHE:HD1	1:C:434:ILE:HG21	1.80	0.46
1:C:763:LEU:HB3	1:C:1008:VAL:HG21	1.96	0.46
1:C:858:LEU:HD13	1:C:959:LEU:HD22	1.98	0.46
1:A:108:THR:HG22	1:A:236:THR:HG23	1.97	0.46
1:C:559:PHE:HB2	1:C:584:ILE:HD11	1.97	0.46
1:B:361:CYS:H	1:B:524:VAL:HG22	1.80	0.46
1:C:817:PHE:CE2	1:C:821:LEU:CD1	2.96	0.46
1:C:391:CYS:HA	1:C:525:CYS:HA	1.98	0.45
1:B:553:THR:OG1	1:B:554:GLU:N	2.49	0.45
1:C:535:LYS:NZ	1:C:554:GLU:OE2	2.41	0.45
1:C:819:GLU:OE1	1:C:1055:SER:OG	2.33	0.45
1:A:29:THR:OG1	1:A:30:ASN:N	2.48	0.45
1:C:395:VAL:HG22	1:C:515:PHE:HE1	1.81	0.45
1:A:327:VAL:HA	1:A:542:ASN:HB3	1.97	0.45
1:A:1116:THR:HG22	1:A:1118:ASP:H	1.81	0.45
1:B:351:TYR:HB3	1:B:422:ASN:HD22	1.81	0.45
1:C:902:MET:HE1	1:C:1049:LEU:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:811:LYS:HG3	1:B:814:LYS:H	1.81	0.45
1:C:349:SER:HA	1:C:401:VAL:HG12	1.98	0.45
1:A:141:LEU:HB3	1:A:242:LEU:HD12	1.98	0.45
1:B:100:ILE:HD12	1:B:102:ARG:HE	1.81	0.45
1:C:34:ARG:NH1	1:C:191:GLU:OE2	2.44	0.45
1:C:742:ILE:O	1:C:1000:ARG:NH1	2.49	0.45
1:B:204:TYR:HD2	1:B:225:PRO:HD3	1.81	0.44
1:C:276:LEU:HB3	1:C:289:VAL:HG22	1.99	0.44
1:A:153:MET:HG2	1:A:154:GLU:N	2.32	0.44
1:A:1053:PRO:O	1:A:1054:GLN:NE2	2.48	0.44
1:B:592:PHE:HZ	1:C:855:PHE:HA	1.83	0.43
1:B:90:VAL:HB	1:B:194:PHE:HD2	1.83	0.43
1:C:273:ARG:NH2	1:C:290:ASP:OD2	2.51	0.43
1:A:594:GLY:HA3	1:A:613:GLN:HE21	1.83	0.43
1:C:403:ARG:HH11	1:C:405:ASN:HB3	1.83	0.43
1:C:1086:LYS:HA	1:C:1125:ASN:HA	2.01	0.43
1:C:598:ILE:HG23	1:C:664:ILE:HG21	2.01	0.43
1:C:1115:ILE:HD13	1:C:1115:ILE:HA	1.92	0.43
1:B:403:ARG:HB3	1:B:406:GLU:HB3	2.00	0.42
1:C:64:TRP:HE1	1:C:264:ALA:HB1	1.84	0.42
1:C:879:ALA:O	1:C:883:THR:OG1	2.32	0.42
1:A:598:ILE:HG23	1:A:664:ILE:HG21	2.02	0.42
1:C:1108:ASN:OD1	1:C:1108:ASN:N	2.52	0.42
1:B:889:GLY:HA3	1:B:1034:LEU:HD23	2.01	0.42
1:A:403:ARG:HA	1:A:507:PRO:HA	2.02	0.42
1:B:393:THR:OG1	1:B:516:GLU:O	2.36	0.42
1:C:661:GLU:O	1:C:695:TYR:OH	2.29	0.42
1:B:91:TYR:HB3	1:B:268:GLY:HA3	2.02	0.42
1:C:599:THR:HG22	1:C:601:GLY:H	1.85	0.41
1:C:333:THR:O	1:C:333:THR:OG1	2.37	0.41
1:A:125:ASN:OD1	1:A:125:ASN:N	2.54	0.41
1:A:666:ILE:HD11	1:A:672:ALA:HB2	2.03	0.41
1:A:902:MET:CG	1:A:916:LEU:CD2	2.98	0.41
1:B:40:ASP:OD1	1:B:40:ASP:N	2.52	0.41
1:B:541:PHE:CE1	1:B:546:LEU:HD23	2.54	0.41
1:B:792:PRO:HA	1:B:793:PRO:HD3	1.92	0.41
1:A:281:GLU:H	1:A:281:GLU:HG3	1.67	0.41
1:B:399:SER:HB3	1:B:511:VAL:HG23	2.03	0.41
1:A:645:THR:HG22	1:A:646:ARG:N	2.36	0.41
1:C:716:THR:O	1:C:716:THR:CG2	2.69	0.41
1:C:886:TRP:HB3	1:C:1035:GLY:HA2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1051:SER:OG	1:A:1064:HIS:ND1	2.50	0.41
1:B:116:SER:OG	1:B:130:VAL:O	2.34	0.41
1:A:111:ASP:HA	1:A:134:GLN:HA	2.01	0.41
1:A:568:ASP:OD1	1:A:568:ASP:N	2.53	0.41
1:B:1010:GLN:NE2	1:C:762:GLN:OE1	2.54	0.41
1:C:393:THR:OG1	1:C:516:GLU:O	2.34	0.41
1:A:340:GLU:HA	1:A:344:ALA:HB2	2.03	0.40
1:B:756:TYR:OH	1:B:994:ASP:OD1	2.34	0.40
1:B:1086:LYS:HD2	1:B:1122:VAL:HG21	2.03	0.40
1:A:736:VAL:HG22	1:A:858:LEU:HD23	2.03	0.40
1:B:434:ILE:HB	1:B:511:VAL:HG12	2.03	0.40
1:C:84:LEU:HD22	1:C:267:VAL:HG21	2.02	0.40
1:C:853:GLN:HG2	1:C:963:VAL:HG21	2.03	0.40
1:B:28:TYR:HE1	1:B:63:THR:HG22	1.87	0.40
1:B:370:ASN:HA	1:B:377:PHE:HZ	1.86	0.40
1:B:931:ILE:HD12	1:B:934:ILE:HG13	2.02	0.40
1:B:329:PHE:O	1:B:580:GLN:NE2	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	932/1290 (72%)	877 (94%)	55 (6%)	0	100	100
1	B	885/1290 (69%)	841 (95%)	44 (5%)	0	100	100
1	C	855/1290 (66%)	815 (95%)	40 (5%)	0	100	100
All	All	2672/3870 (69%)	2533 (95%)	139 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	697/1114 (63%)	681 (98%)	16 (2%)	45	73
1	B	762/1114 (68%)	741 (97%)	21 (3%)	38	69
1	C	754/1114 (68%)	749 (99%)	5 (1%)	81	91
All	All	2213/3342 (66%)	2171 (98%)	42 (2%)	52	77

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	THR
1	A	101	ILE
1	A	309	GLU
1	A	534	VAL
1	A	696	THR
1	A	704	SER
1	A	717	ASN
1	A	750	SER
1	A	754	LEU
1	A	804	GLN
1	A	859	THR
1	A	936	ASP
1	A	1037	SER
1	A	1104	VAL
1	A	1106	GLN
1	A	1129	VAL
1	B	41	LYS
1	B	197	ILE
1	B	307	THR
1	B	358	ILE
1	B	382	VAL
1	B	387	LEU
1	B	546	LEU
1	B	576	VAL
1	B	606	ASN
1	B	656	VAL

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Mol	Chain	Res	Type
1	B	711	SER
1	B	717	ASN
1	B	719	THR
1	B	754	LEU
1	B	785	VAL
1	B	883	THR
1	B	974	SER
1	B	977	LEU
1	B	1001	LEU
1	B	1010	GLN
1	B	1122	VAL
1	C	510	VAL
1	C	512	VAL
1	C	534	VAL
1	C	723	THR
1	C	1129	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	ASN
1	A	314	GLN
1	A	613	GLN
1	A	644	GLN
1	A	907	ASN
1	A	949	GLN
1	A	1010	GLN
1	A	1134	ASN
1	B	417	ASN
1	B	644	GLN
1	B	762	GLN
1	B	935	GLN
1	B	955	ASN
1	B	1010	GLN
1	B	1088	HIS
1	C	26	GLN
1	C	196	ASN
1	C	536	ASN
1	C	540	ASN
1	C	606	ASN
1	C	762	GLN
1	C	774	GLN

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Mol	Chain	Res	Type
1	C	1083	HIS
1	C	1101	HIS
1	C	1142	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](#)

6 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	14,14,15	0.43	0	17,19,21	1.04	1 (5%)
2	NAG	D	2	2	14,14,15	0.91	1 (7%)	17,19,21	2.38	3 (17%)
2	NAG	E	1	2	14,14,15	0.35	0	17,19,21	0.70	0
2	NAG	E	2	2	14,14,15	0.92	1 (7%)	17,19,21	1.12	2 (11%)
2	NAG	F	1	2	14,14,15	0.43	0	17,19,21	1.04	1 (5%)
2	NAG	F	2	2	14,14,15	0.40	0	17,19,21	0.47	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
2	NAG	D	1	2	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	2	2	-	4/6/23/26	0/1/1/1
2	NAG	E	1	2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	2	-	4/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2	NAG	C1-C2	3.16	1.56	1.52
2	D	2	NAG	C1-C2	2.68	1.56	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	NAG	C2-N2-C7	8.29	134.01	122.90
2	D	2	NAG	C1-C2-N2	4.10	116.90	110.43
2	D	1	NAG	C2-N2-C7	3.27	127.29	122.90
2	F	1	NAG	C2-N2-C7	3.25	127.26	122.90
2	E	2	NAG	C2-N2-C7	3.19	127.18	122.90
2	E	2	NAG	C1-O5-C5	2.20	115.13	112.19
2	D	2	NAG	C8-C7-N2	2.13	119.64	116.12

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	NAG	O5-C5-C6-O6
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	F	1	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	D	1	NAG	C1-C2-N2-C7
2	D	2	NAG	C1-C2-N2-C7
2	E	2	NAG	C1-C2-N2-C7
2	F	1	NAG	C1-C2-N2-C7
2	D	1	NAG	C3-C2-N2-C7

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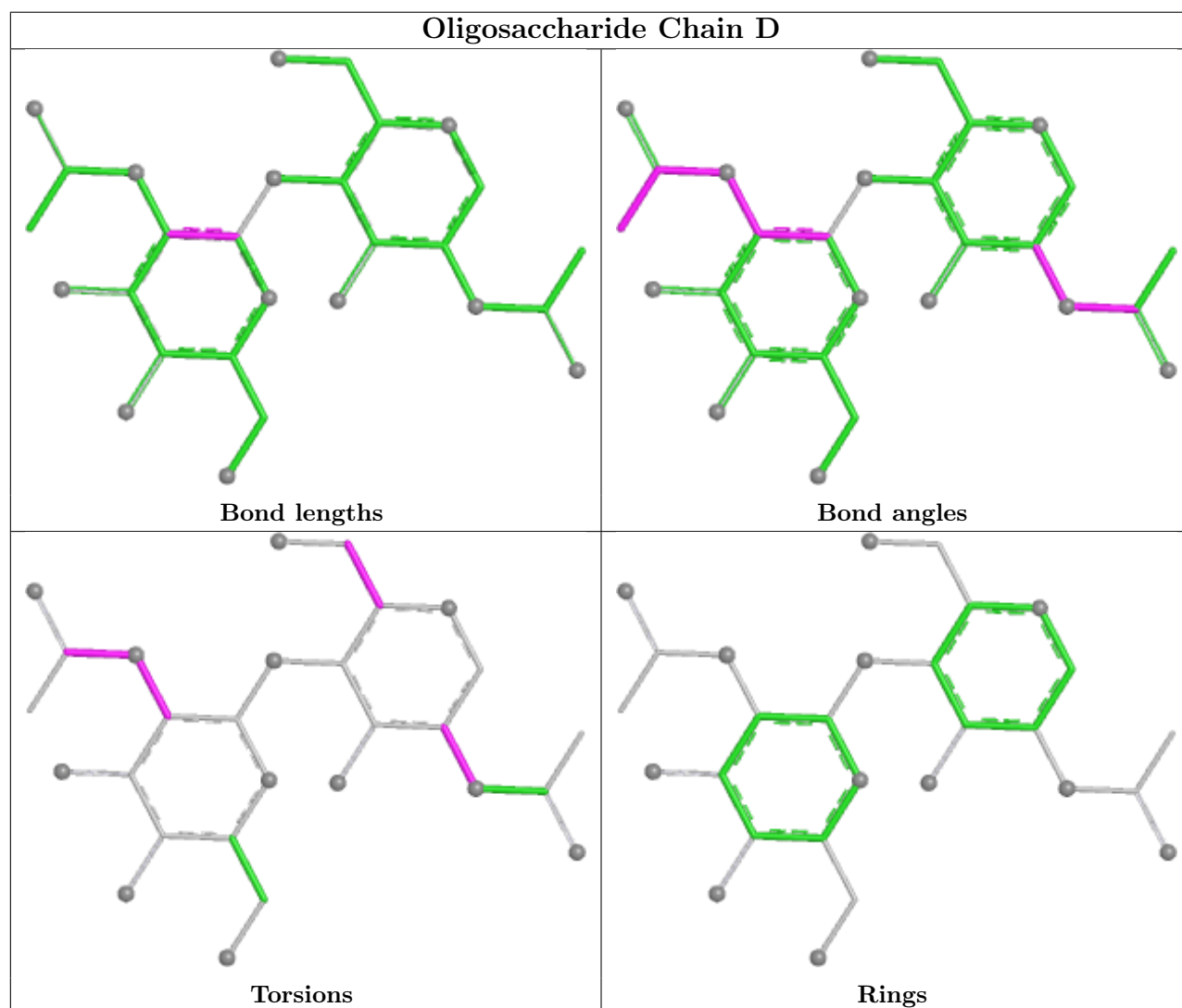
Continued from previous page...

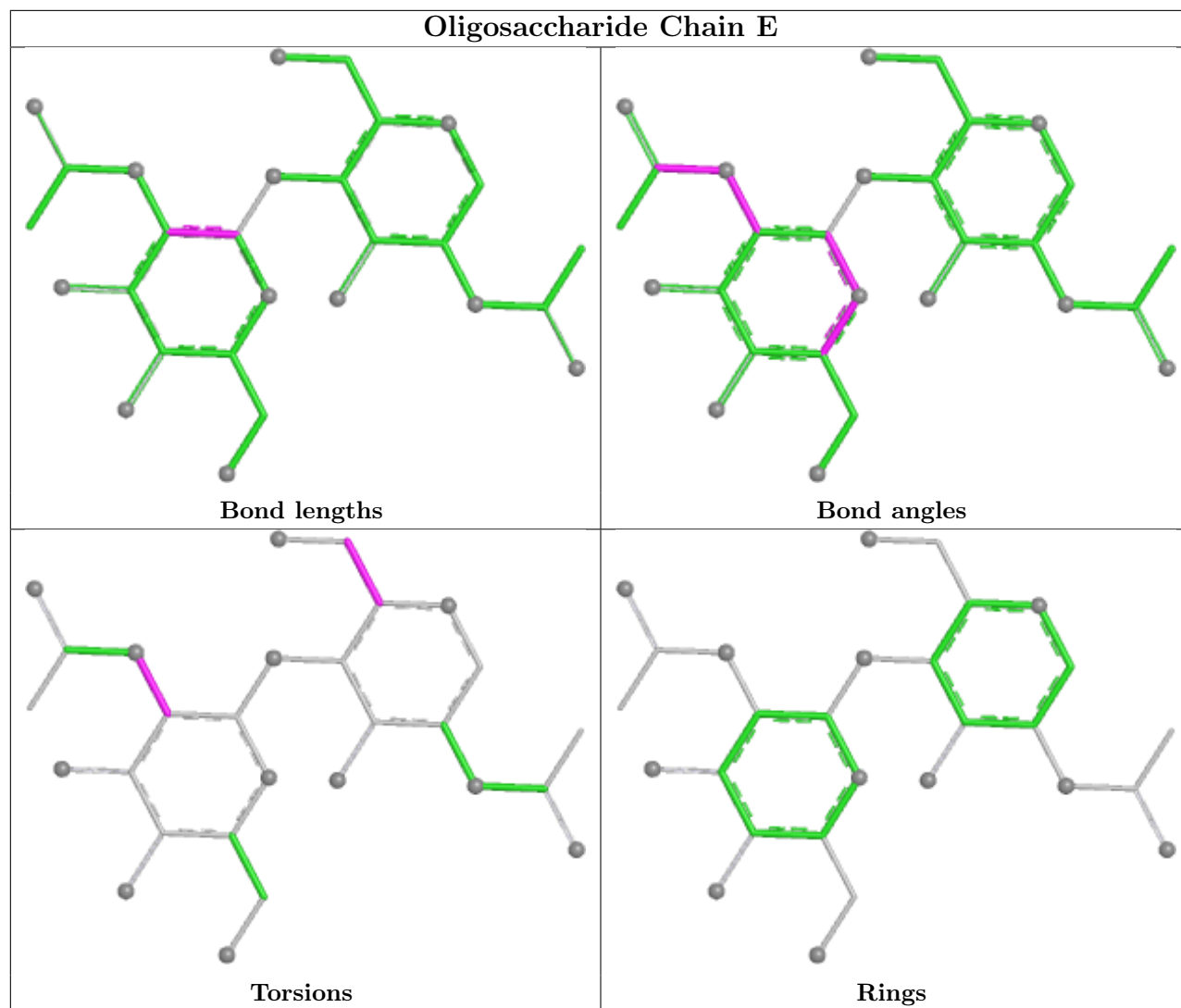
Mol	Chain	Res	Type	Atoms
2	D	2	NAG	C3-C2-N2-C7
2	E	2	NAG	C3-C2-N2-C7
2	F	1	NAG	C3-C2-N2-C7

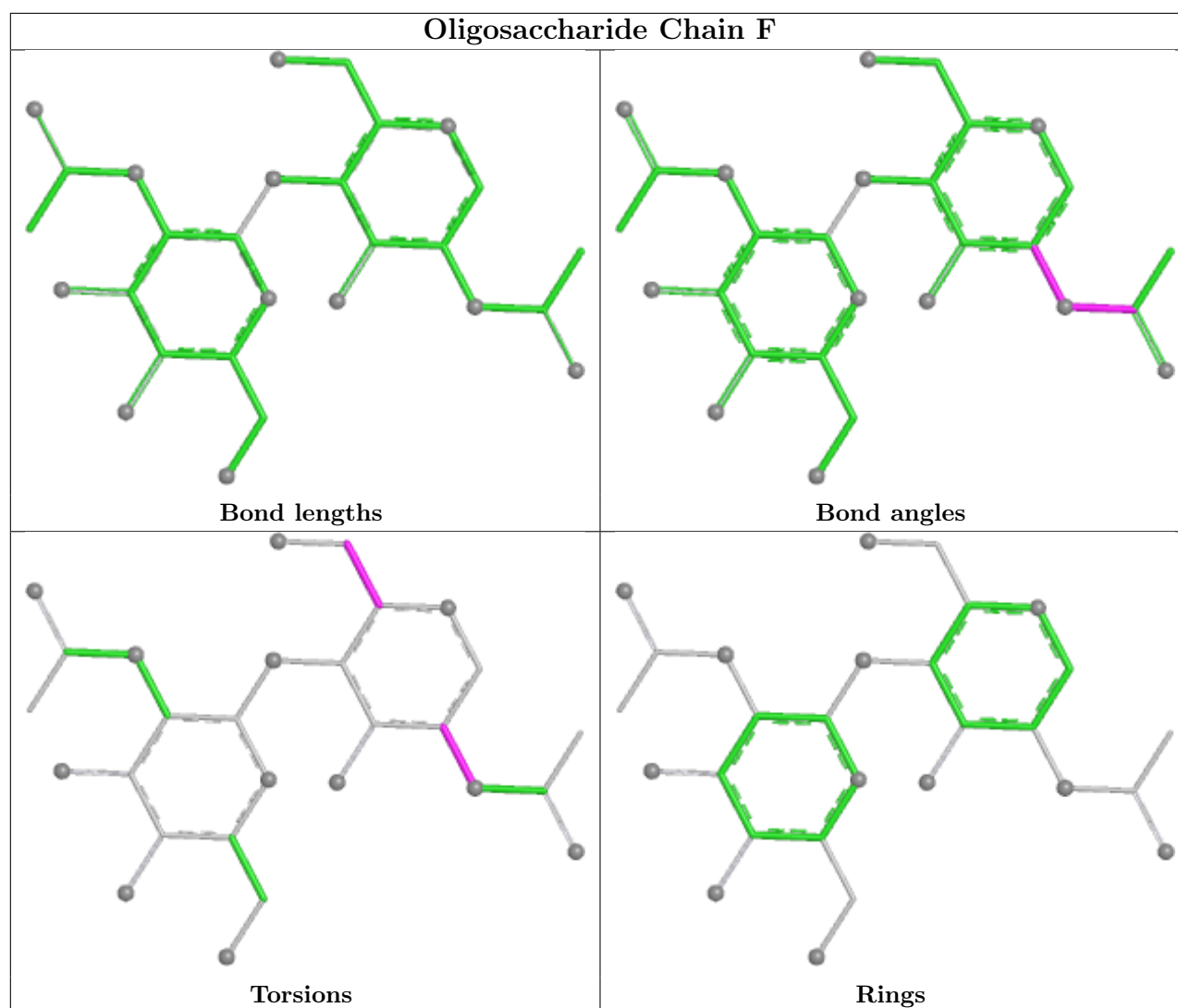
There are no ring outliers.

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](#)

19 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	B	2005	-	14,14,15	0.35	0	17,19,21	0.60	0
3	NAG	A	1402	-	14,14,15	0.32	0	17,19,21	0.51	0
3	NAG	B	2004	1	14,14,15	0.41	0	17,19,21	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	C	2005	-	14,14,15	0.44	0	17,19,21	1.05	1 (5%)
3	NAG	B	2002	1	14,14,15	0.40	0	17,19,21	0.50	0
3	NAG	A	1403	1	14,14,15	0.41	0	17,19,21	0.50	0
3	NAG	C	2006	-	14,14,15	0.31	0	17,19,21	0.52	0
3	NAG	C	2002	-	14,14,15	0.30	0	17,19,21	0.60	0
3	NAG	A	1406	1	14,14,15	0.45	0	17,19,21	0.60	1 (5%)
3	NAG	A	1401	1	14,14,15	1.61	2 (14%)	17,19,21	1.39	1 (5%)
3	NAG	C	2003	-	14,14,15	0.76	1 (7%)	17,19,21	2.38	3 (17%)
3	NAG	A	1407	-	14,14,15	0.30	0	17,19,21	0.50	0
3	NAG	B	2006	-	14,14,15	0.32	0	17,19,21	0.53	0
3	NAG	B	2003	-	14,14,15	0.24	0	17,19,21	0.61	0
3	NAG	C	2001	-	14,14,15	0.75	1 (7%)	17,19,21	1.90	4 (23%)
3	NAG	A	1404	1	14,14,15	0.35	0	17,19,21	0.51	0
3	NAG	A	1405	1	14,14,15	0.40	0	17,19,21	0.44	0
3	NAG	B	2001	1	14,14,15	0.48	0	17,19,21	0.40	0
3	NAG	C	2004	1	14,14,15	0.47	0	17,19,21	0.50	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
3	NAG	B	2005	-	-	3/6/23/26	0/1/1/1
3	NAG	A	1402	-	-	1/6/23/26	0/1/1/1
3	NAG	B	2004	1	-	2/6/23/26	0/1/1/1
3	NAG	C	2005	-	-	4/6/23/26	0/1/1/1
3	NAG	B	2002	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1403	1	-	4/6/23/26	0/1/1/1
3	NAG	C	2006	-	-	0/6/23/26	0/1/1/1
3	NAG	C	2002	-	-	4/6/23/26	0/1/1/1
3	NAG	A	1406	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1401	1	-	4/6/23/26	0/1/1/1
3	NAG	C	2003	-	-	6/6/23/26	0/1/1/1
3	NAG	A	1407	-	-	0/6/23/26	0/1/1/1
3	NAG	B	2006	-	-	0/6/23/26	0/1/1/1
3	NAG	B	2003	-	-	4/6/23/26	0/1/1/1
3	NAG	C	2001	-	-	3/6/23/26	0/1/1/1
3	NAG	A	1404	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1405	1	-	2/6/23/26	0/1/1/1
3	NAG	B	2001	1	-	2/6/23/26	0/1/1/1
3	NAG	C	2004	1	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1401	NAG	O5-C1	4.80	1.51	1.43
3	A	1401	NAG	C1-C2	3.40	1.57	1.52
3	C	2001	NAG	O5-C1	-2.24	1.39	1.43
3	C	2003	NAG	C1-C2	2.18	1.55	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2003	NAG	C2-N2-C7	8.33	134.07	122.90
3	A	1401	NAG	C1-O5-C5	5.17	119.12	112.19
3	C	2001	NAG	C1-O5-C5	4.49	118.21	112.19
3	C	2003	NAG	C1-C2-N2	4.00	116.73	110.43
3	C	2001	NAG	C3-C4-C5	3.94	117.37	110.23
3	C	2001	NAG	C2-N2-C7	3.38	127.43	122.90
3	C	2005	NAG	C2-N2-C7	3.28	127.29	122.90
3	C	2003	NAG	C8-C7-N2	2.16	119.70	116.12
3	A	1406	NAG	C1-O5-C5	2.10	115.00	112.19
3	C	2001	NAG	O5-C5-C4	2.08	115.88	110.83

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	2005	NAG	C4-C5-C6-O6
3	B	2003	NAG	O5-C5-C6-O6
3	B	2004	NAG	O5-C5-C6-O6
3	C	2002	NAG	O5-C5-C6-O6
3	A	1401	NAG	O5-C5-C6-O6
3	B	2001	NAG	O5-C5-C6-O6
3	A	1404	NAG	O5-C5-C6-O6
3	A	1405	NAG	O5-C5-C6-O6
3	C	2005	NAG	O5-C5-C6-O6
3	B	2001	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	A	1405	NAG	C4-C5-C6-O6
3	B	2003	NAG	C4-C5-C6-O6
3	C	2002	NAG	C4-C5-C6-O6
3	A	1403	NAG	O5-C5-C6-O6
3	A	1404	NAG	C4-C5-C6-O6
3	B	2004	NAG	C4-C5-C6-O6
3	A	1403	NAG	C4-C5-C6-O6
3	A	1401	NAG	C8-C7-N2-C2
3	A	1401	NAG	O7-C7-N2-C2
3	A	1403	NAG	C8-C7-N2-C2
3	A	1403	NAG	O7-C7-N2-C2
3	B	2003	NAG	C8-C7-N2-C2
3	B	2003	NAG	O7-C7-N2-C2
3	B	2005	NAG	C8-C7-N2-C2
3	B	2005	NAG	O7-C7-N2-C2
3	C	2002	NAG	C8-C7-N2-C2
3	C	2002	NAG	O7-C7-N2-C2
3	C	2003	NAG	C8-C7-N2-C2
3	C	2003	NAG	O7-C7-N2-C2
3	C	2004	NAG	C8-C7-N2-C2
3	C	2004	NAG	O7-C7-N2-C2
3	B	2002	NAG	O5-C5-C6-O6
3	A	1401	NAG	C4-C5-C6-O6
3	C	2003	NAG	C4-C5-C6-O6
3	C	2003	NAG	O5-C5-C6-O6
3	C	2001	NAG	O5-C5-C6-O6
3	A	1402	NAG	O5-C5-C6-O6
3	B	2005	NAG	O5-C5-C6-O6
3	B	2002	NAG	C4-C5-C6-O6
3	C	2001	NAG	C1-C2-N2-C7
3	C	2003	NAG	C1-C2-N2-C7
3	C	2005	NAG	C1-C2-N2-C7
3	C	2001	NAG	C3-C2-N2-C7
3	C	2003	NAG	C3-C2-N2-C7
3	C	2005	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2005	NAG	1	0
3	C	2004	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.

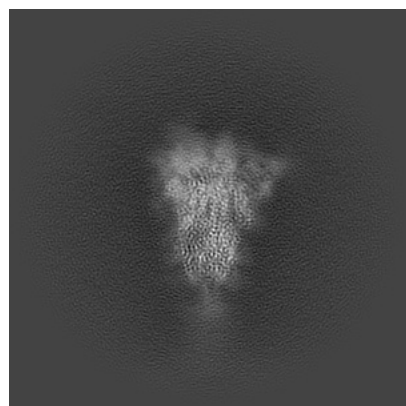
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42524. These allow visual inspection of the internal detail of the map and identification of artifacts.

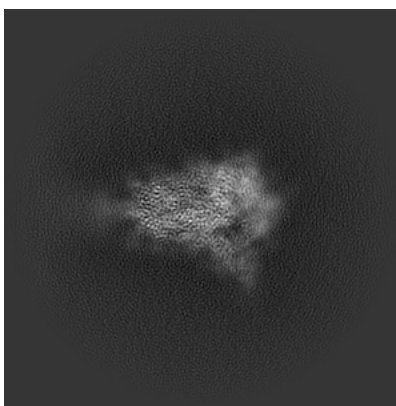
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

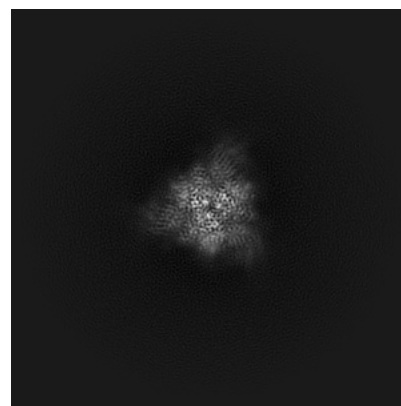
6.1.1 Primary map



X

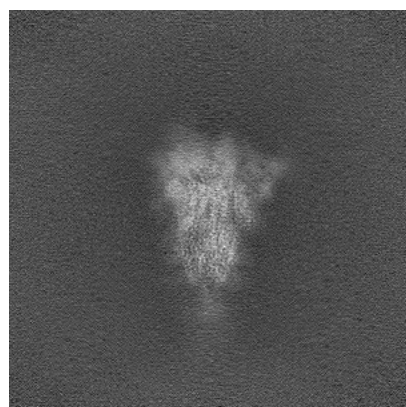


Y

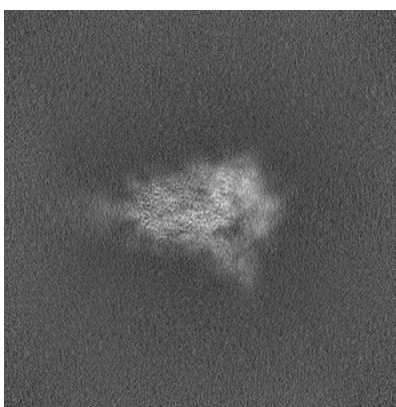


Z

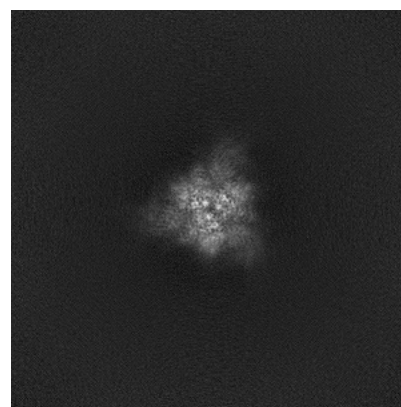
6.1.2 Raw map



X



Y

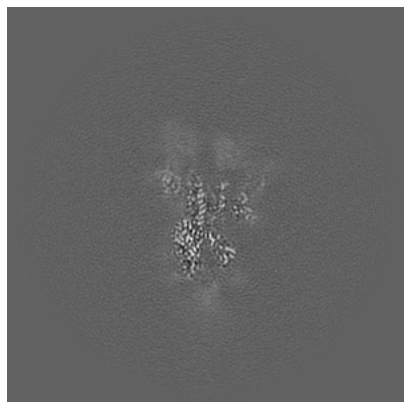


Z

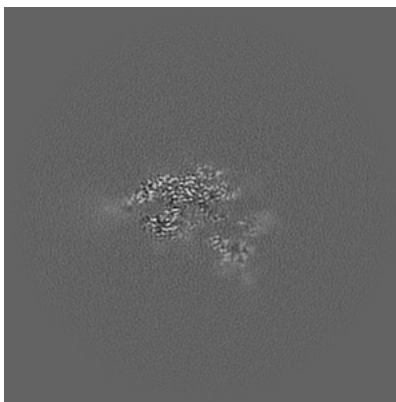
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

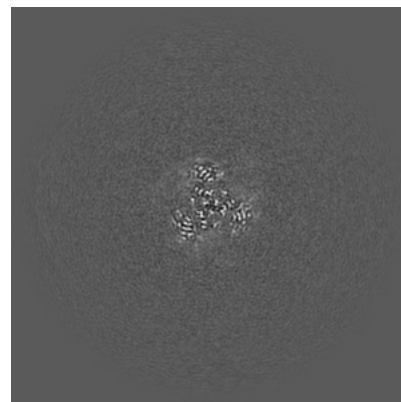
6.2.1 Primary map



X Index: 270

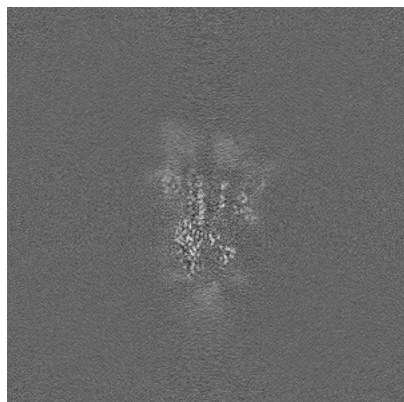


Y Index: 270

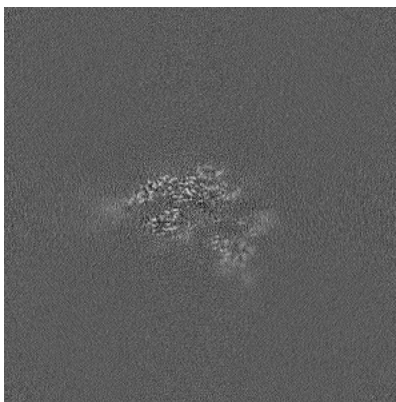


Z Index: 270

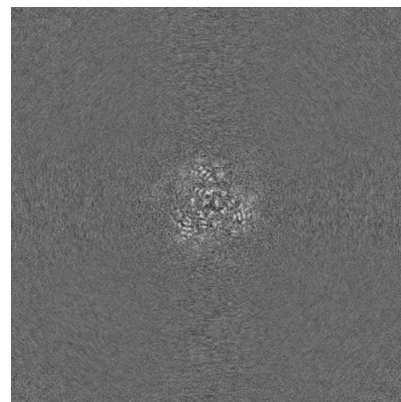
6.2.2 Raw map



X Index: 270



Y Index: 270

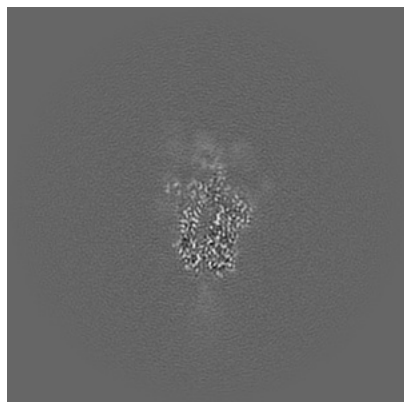


Z Index: 270

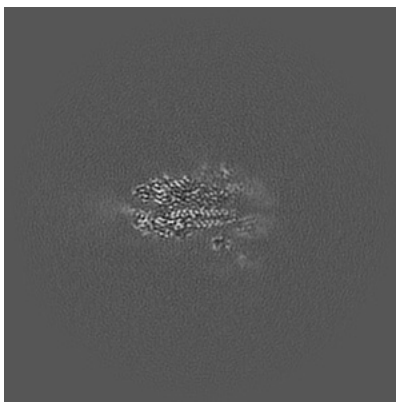
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

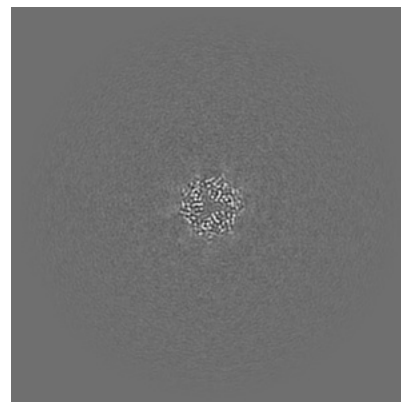
6.3.1 Primary map



X Index: 254

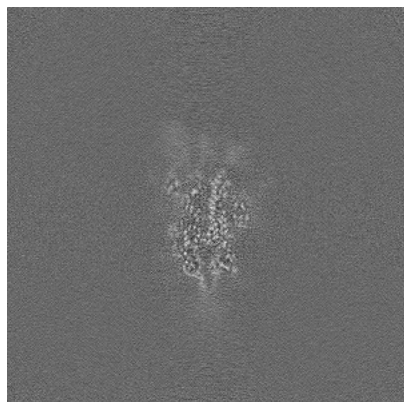


Y Index: 279

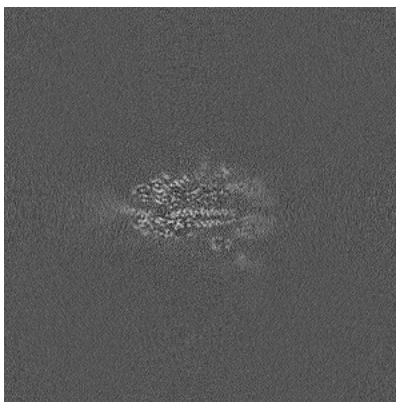


Z Index: 208

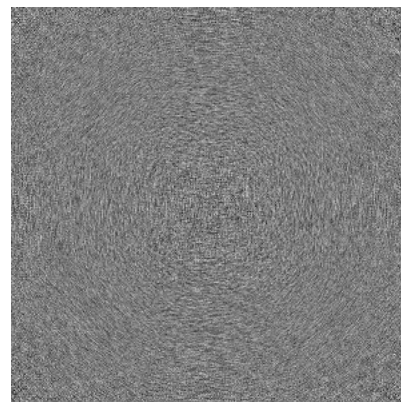
6.3.2 Raw map



X Index: 261



Y Index: 279

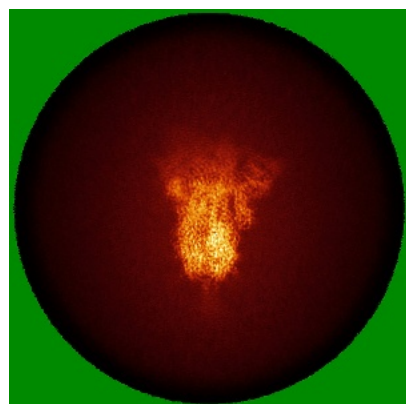


Z Index: 0

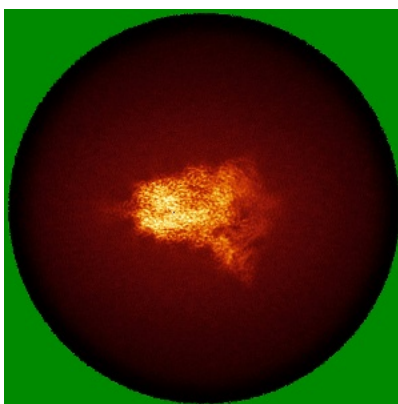
The images above show the largest variance slices of the map in three orthogonal directions.

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

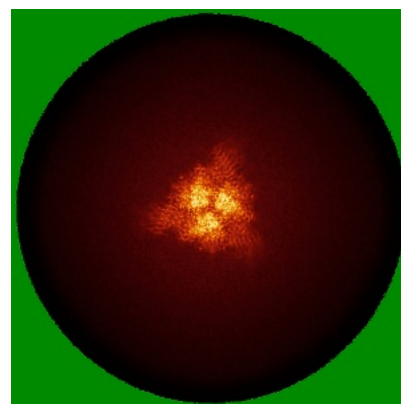
6.4.1 Primary map



X

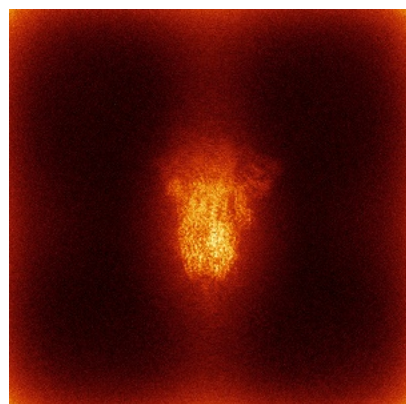


Y

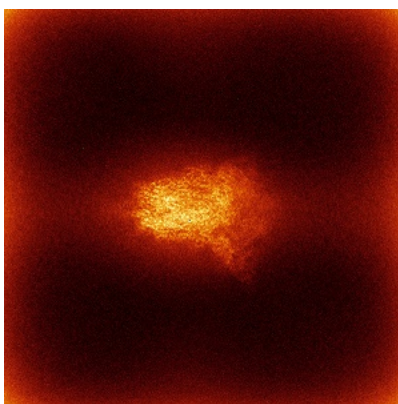


Z

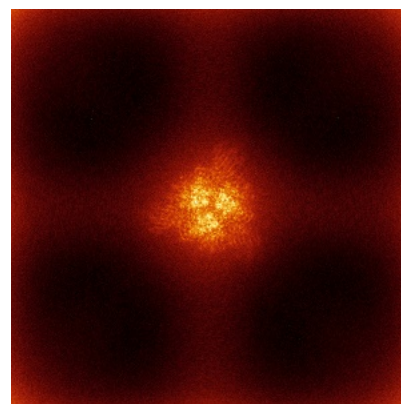
6.4.2 Raw map



X



Y

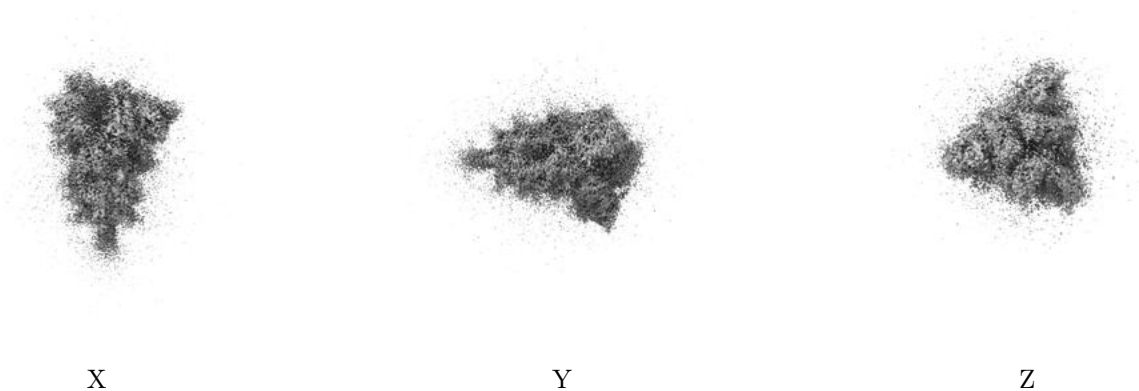


Z

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.

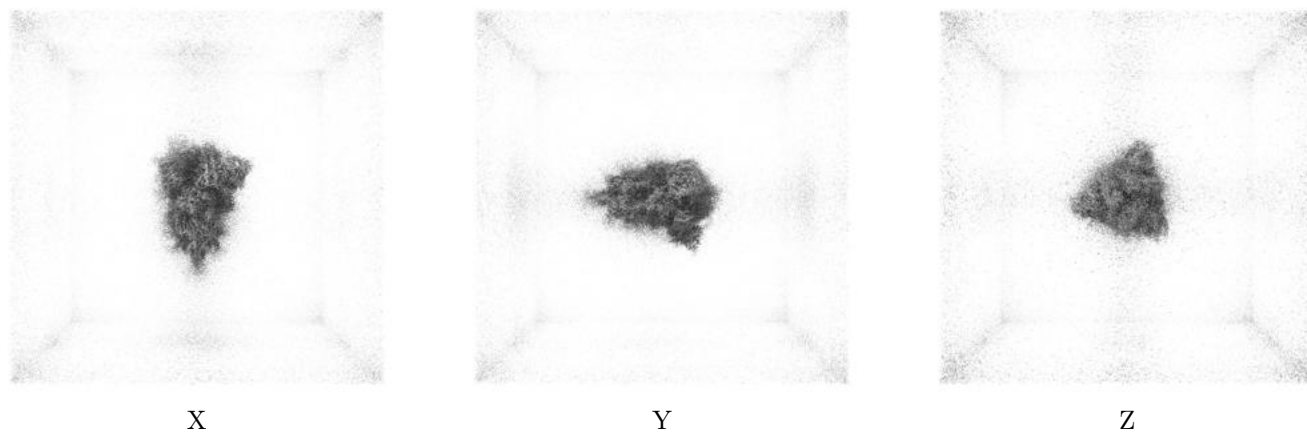
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.07. 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.

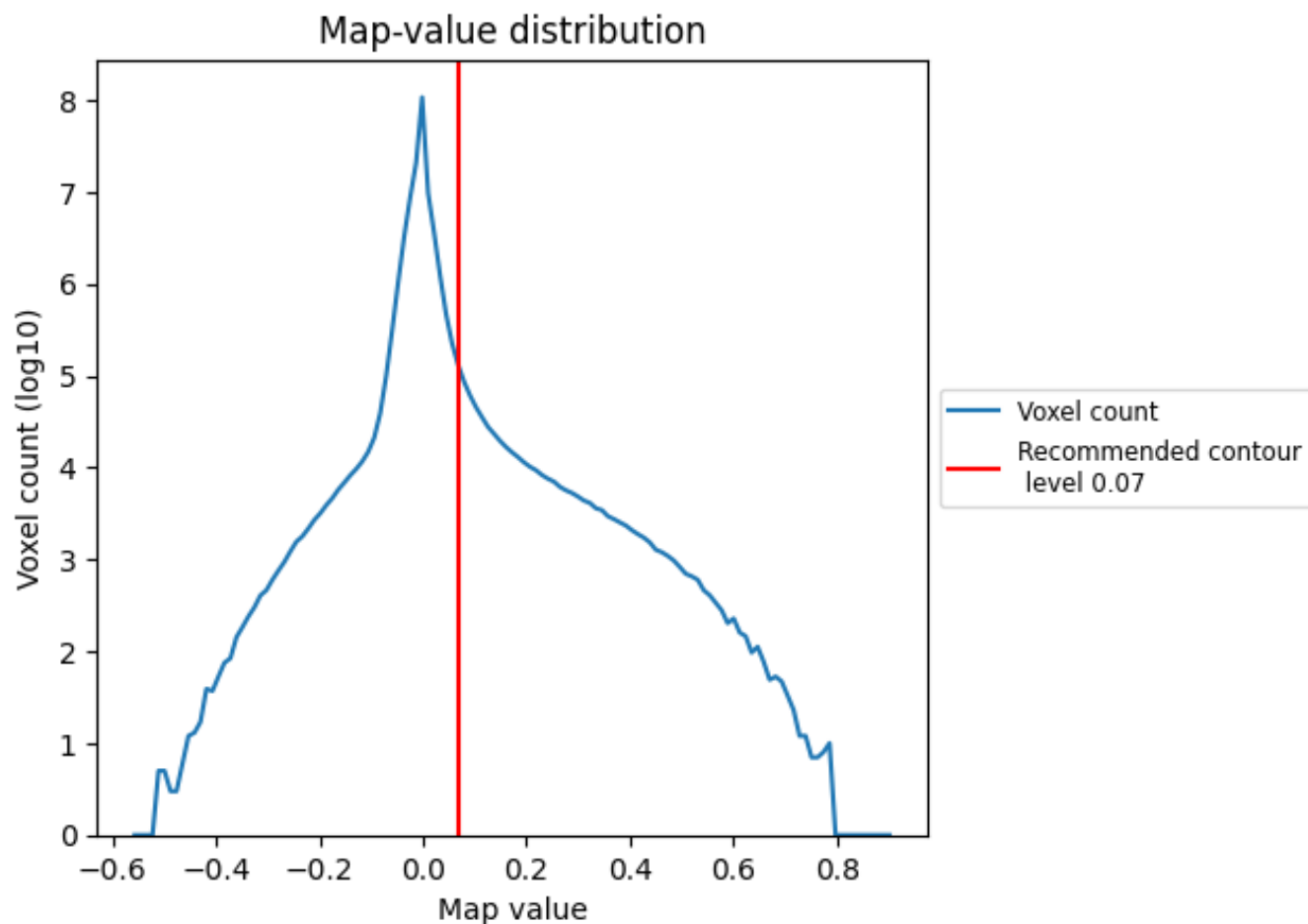
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

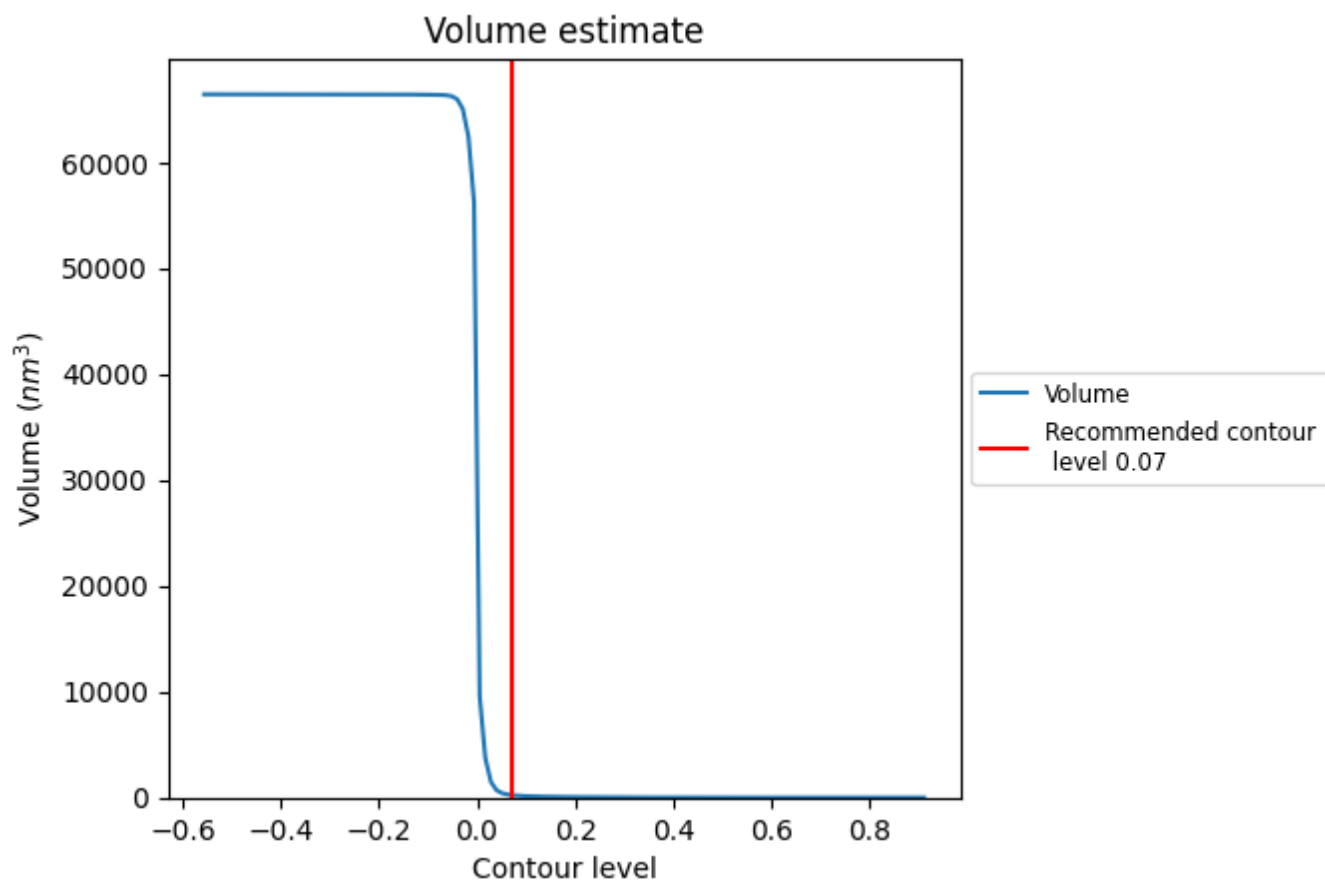
This section contains the results of statistical analysis of the map.

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.

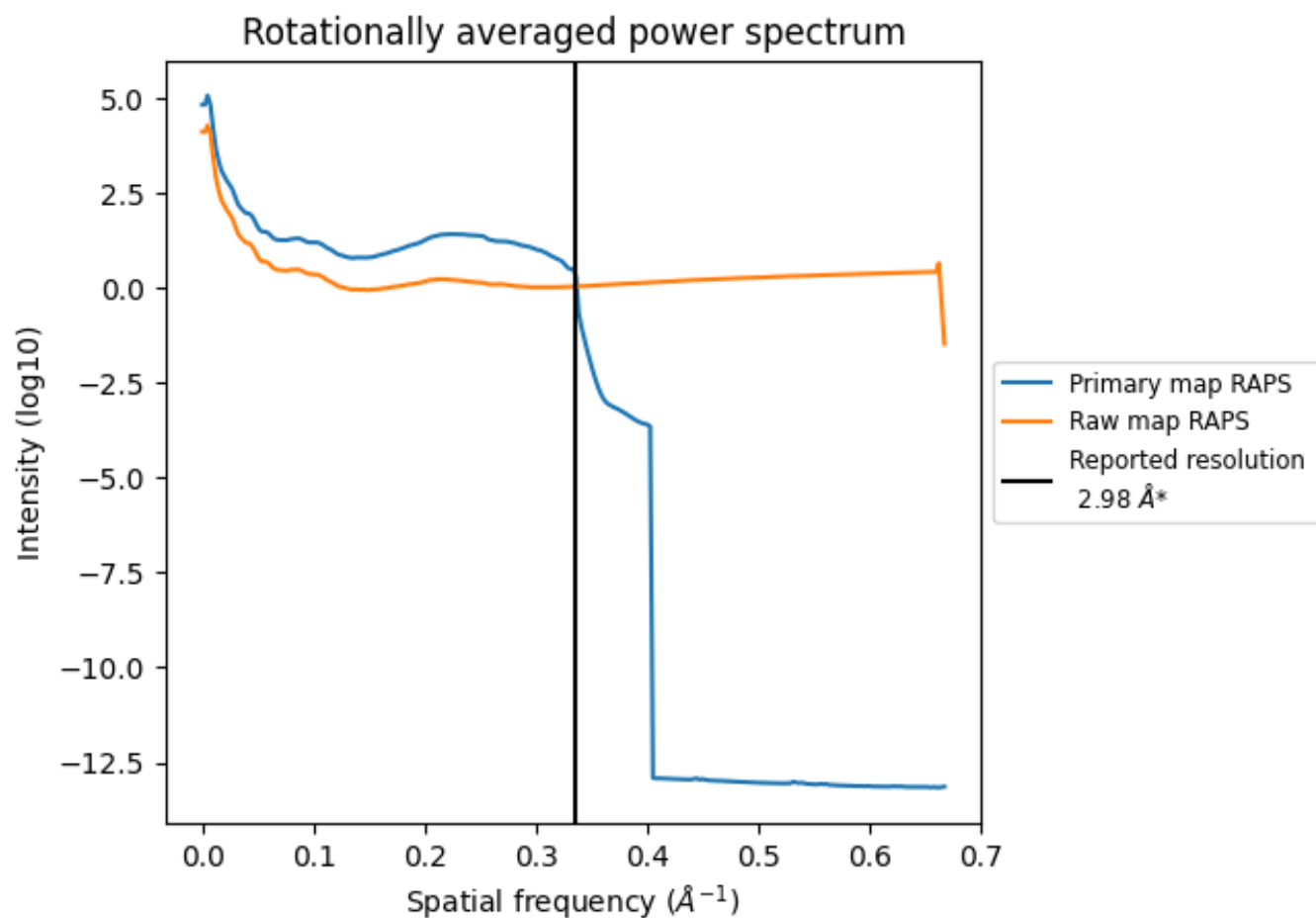
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 242 nm³; this corresponds to an approximate mass of 218 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 ⓘ

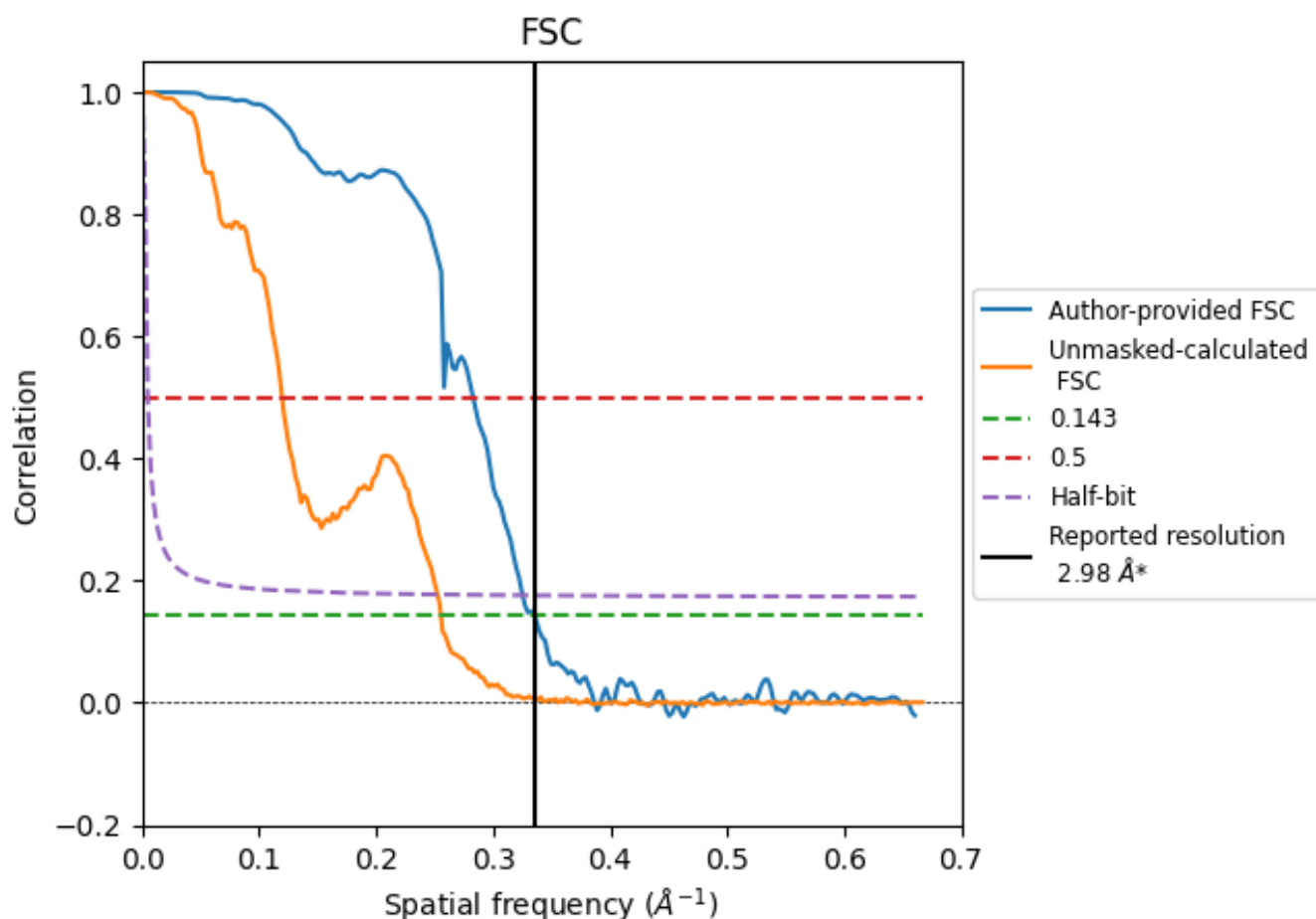


*Reported resolution corresponds to spatial frequency of 0.336 Å⁻¹

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 0.336 Å⁻¹

8.2 Resolution estimates [i](#)

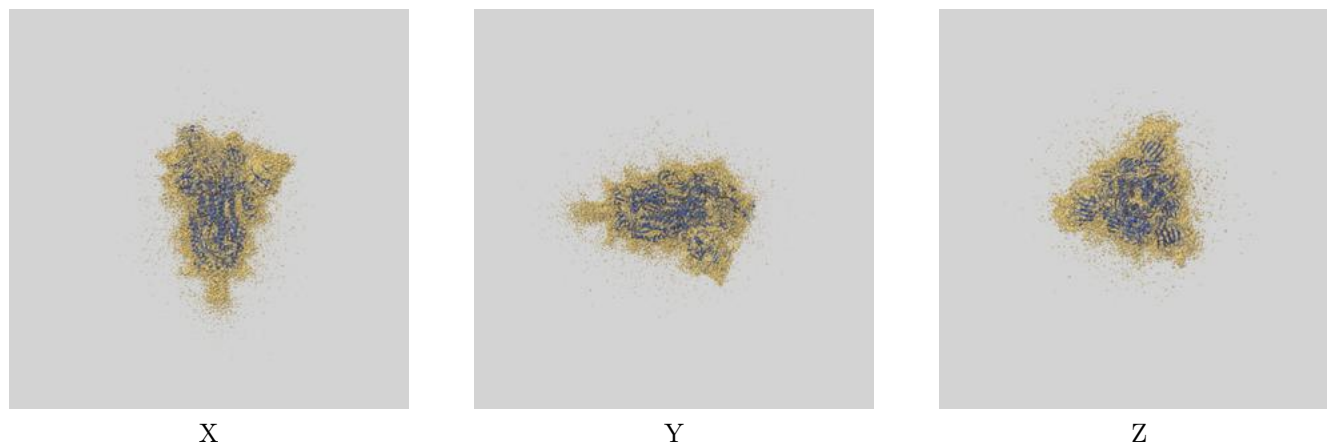
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.98	-	-
Author-provided FSC curve	2.98	3.53	3.08
Unmasked-calculated*	3.92	8.36	3.96

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.92 differs from the reported value 2.98 by more than 10 %

9 Map-model fit [i](#)

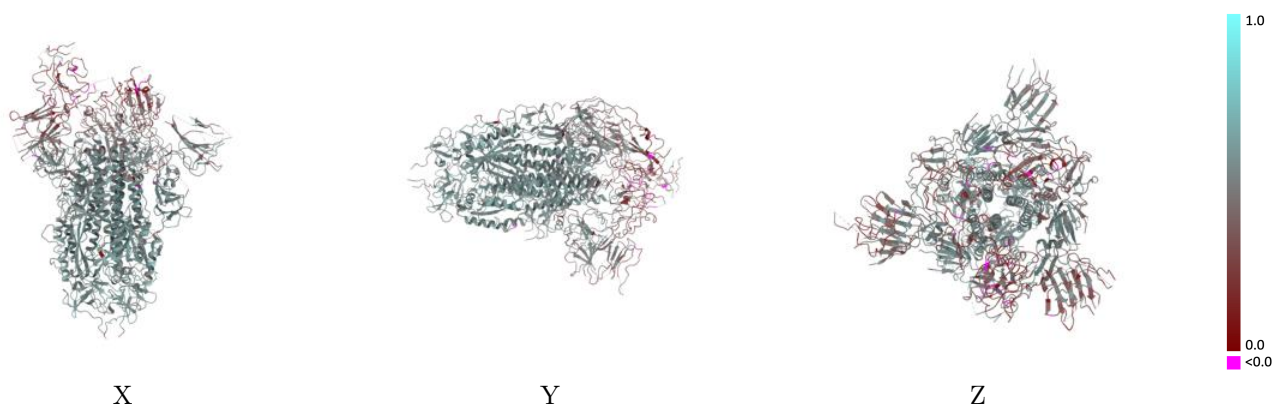
This section contains information regarding the fit between EMDB map EMD-42524 and PDB model 8USZ. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



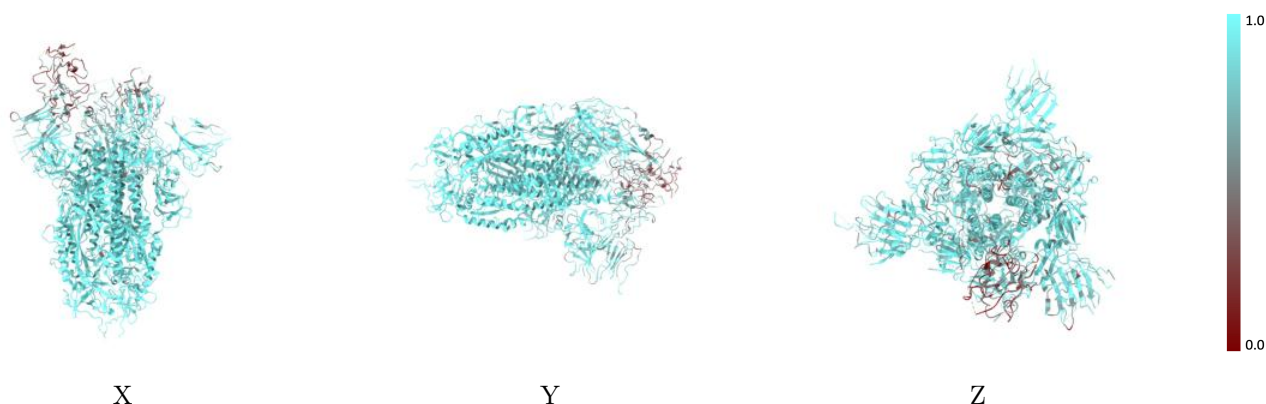
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



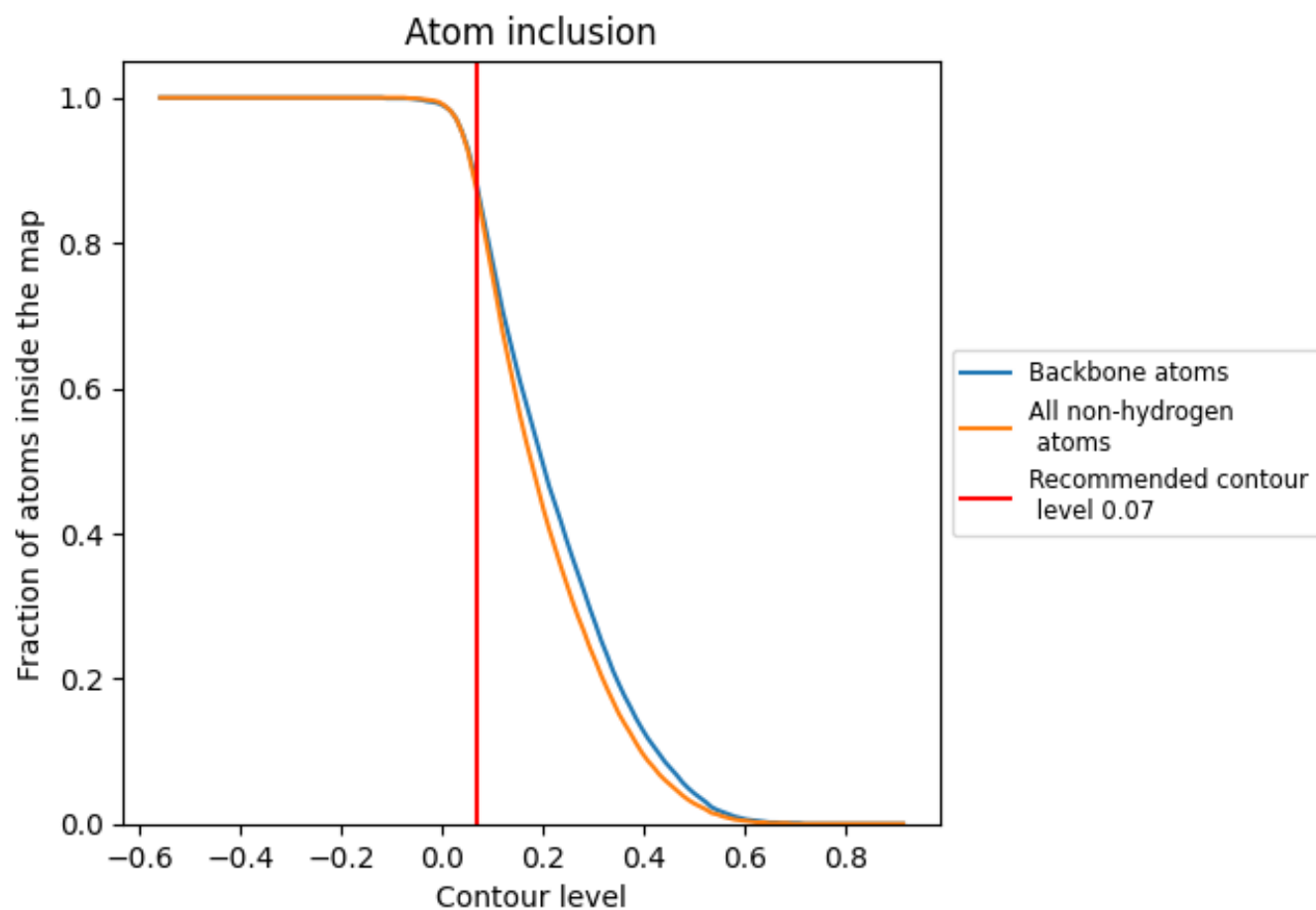
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 87% 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	<div><div></div></div> 0.8690	<div><div></div></div> 0.4830
A	<div><div></div></div> 0.8580	<div><div></div></div> 0.4860
B	<div><div></div></div> 0.8690	<div><div></div></div> 0.4730
C	<div><div></div></div> 0.8830	<div><div></div></div> 0.4910
D	<div><div></div></div> 0.9290	<div><div></div></div> 0.4720
E	<div><div></div></div> 0.8210	<div><div></div></div> 0.4530
F	<div><div></div></div> 0.7860	<div><div></div></div> 0.4510

1.0

0.0

<0.0