wwPDB EM Validation Summary Report

Nov 8, 2021 – 09:28 pm GMT

PDB ID	:	7NYC
EMDB ID	:	EMD-12650
Title	:	cryoEM structure of 3C9-sMAC
Authors	:	Menny, A.; Couves, E.C.; Bubeck, D.
Deposited on	:	2021-03-22
Resolution	:	3.50 Å(reported)
Based on initial models	:	6CXO, 2WCY, 6H03, 4A5W, 6H04

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

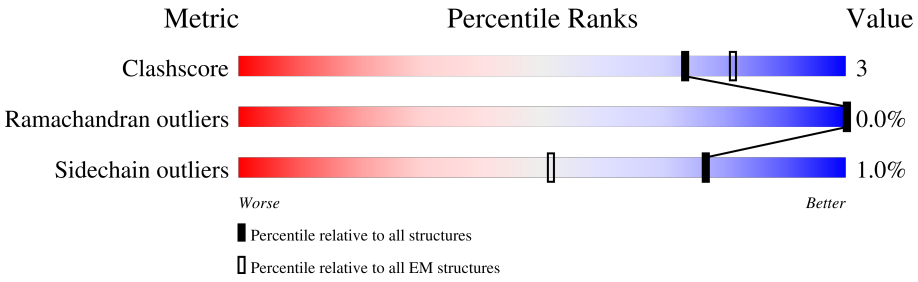
EMDB validation analysis	:	0.0.0.dev97
Mogul	:	1.8.4 (270009), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

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)
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.

Mol	Chain	Length	Quality of chain
1	C	821	21% 92% 6%
2	D	537	82% 9% 9%
3	E	554	6% 79% 8% 13%
4	G	538	8% 68% 27%
4	H	538	14% 69% 5% 25%
4	I	538	9% 54% 43%
5	B	913	7% 72% 6% 21%
6	A	1658	8% 89% 7%

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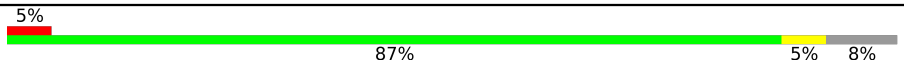
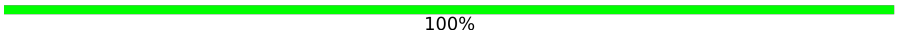
Mol	Chain	Length	Quality of chain
7	F	182	
8	K	2	
9	J	3	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	BMA	C	901	-	-	X	-
10	BMA	D	602	-	-	X	-
10	BMA	E	603	-	-	X	-
12	NAG	E	604	-	-	X	-
12	NAG	G	702	-	-	X	-
13	FUC	B	1001	-	-	X	-

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 41307 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 Complement component C7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	C	809	5977	3696	1054	1179	48	0	0

- Molecule 2 is a protein called Complement component C8 beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	487	3914	2434	702	743	35	0	0

- Molecule 3 is a protein called Complement component C8 alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	482	3805	2354	671	743	37	0	0

- Molecule 4 is a protein called Complement component C9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	G	393	3079	1919	527	604	29	0	0
4	H	404	Total	C	N	O	S	0	0
			3192	1990	553	620	29		
4	I	309	Total	C	N	O	S	0	0
			2433	1523	414	480	16		

- Molecule 5 is a protein called Complement component C6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B	718	5631	3479	993	1109	50	0	0

- Molecule 6 is a protein called Complement C5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	1542	Total	C	N	O	S	0	0
			11744	7507	1949	2251	37		

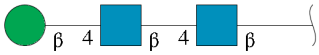
- Molecule 7 is a protein called Complement component C8 gamma chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	168	Total	C	N	O	S	0	0
			1319	841	230	244	4		

- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

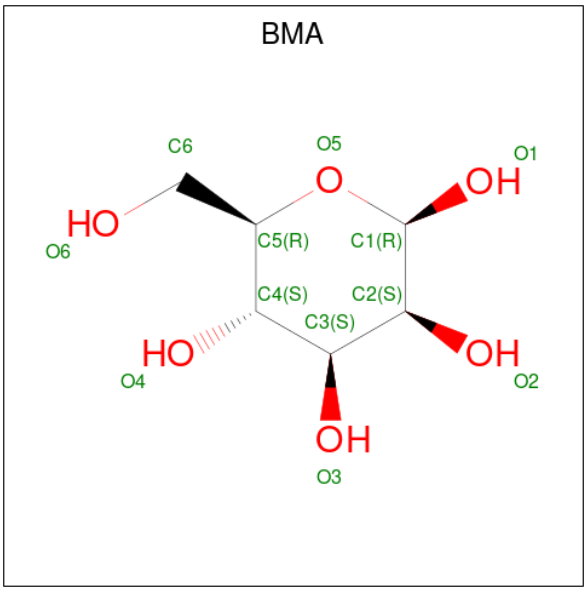
Mol	Chain	Residues	Atoms				AltConf	Trace
8	K	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 9 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
9	J	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 10 is beta-D-mannopyranose (three-letter code: BMA) (formula: $C_6H_{12}O_6$).

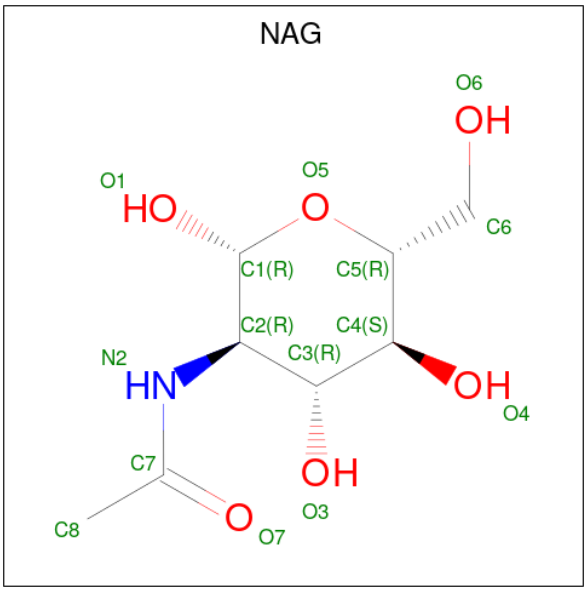


Mol	Chain	Residues	Atoms	AltConf
10	C	1	Total C O 11 6 5	0
10	D	1	Total C O 22 12 10	0
10	D	1	Total C O 22 12 10	0
10	E	1	Total C O 33 18 15	0
10	E	1	Total C O 33 18 15	0
10	E	1	Total C O 33 18 15	0
10	G	1	Total C O 11 6 5	0

- Molecule 11 is CALCIUM ION (three-letter code: CA) (formula: Ca).

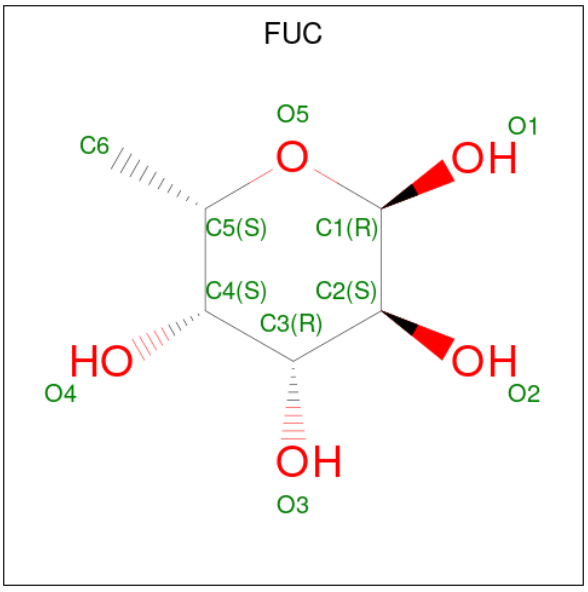
Mol	Chain	Residues	Atoms	AltConf
11	D	1	Total Ca 1 1	0
11	E	1	Total Ca 1 1	0
11	H	1	Total Ca 1 1	0

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
12	E	1	Total	C	N	O	0
			14	8	1	5	
12	G	1	Total	C	N	O	0
			14	8	1	5	
12	B	1	Total	C	N	O	0
			14	8	1	5	
12	H	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 13 is alpha-L-fucopyranose (three-letter code: FUC) (formula: $C_6H_{12}O_5$).

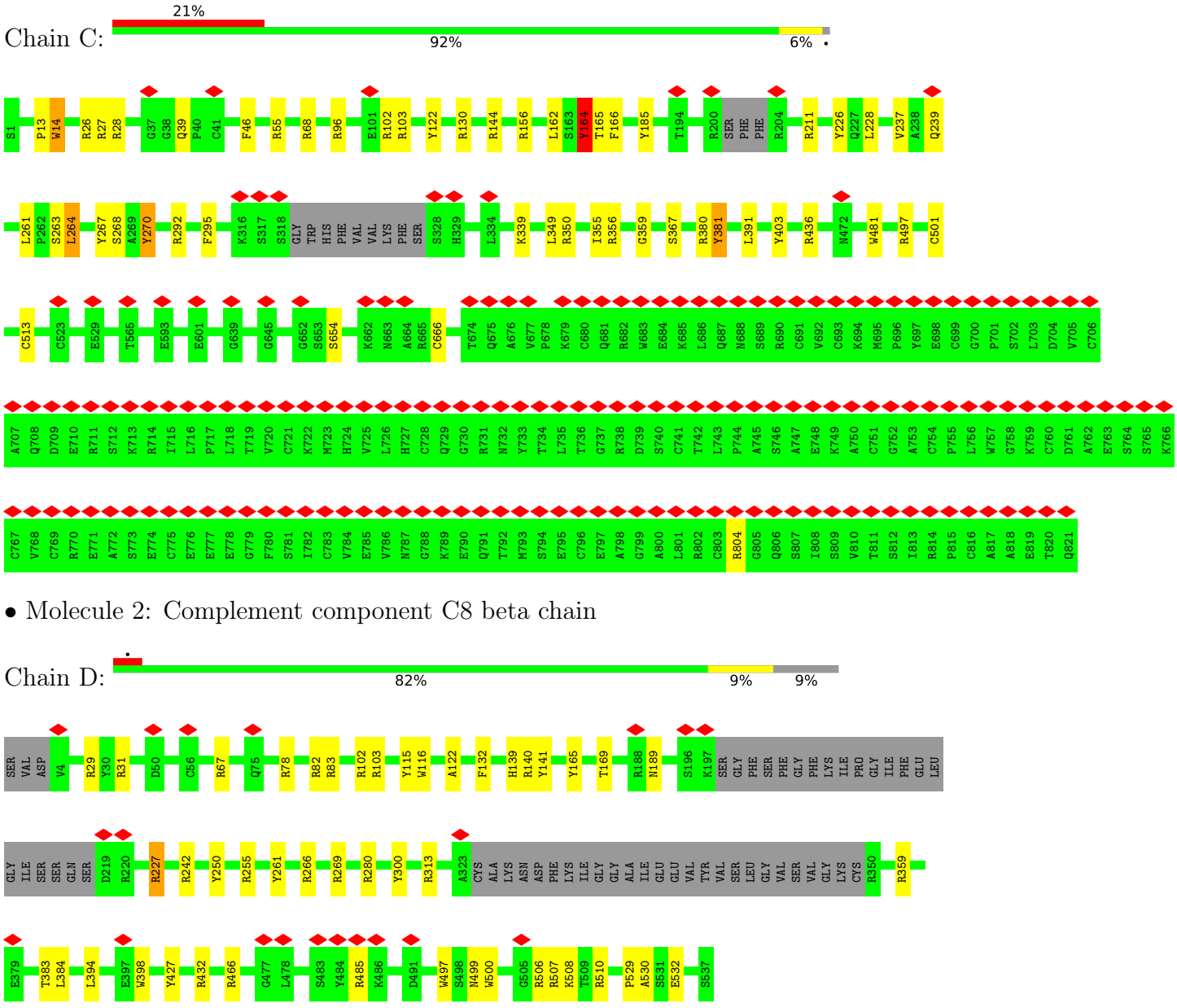


Mol	Chain	Residues	Atoms			AltConf
13	B	1	Total	C	O	0
			10	6	4	

3 Residue-property plots (i)

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.

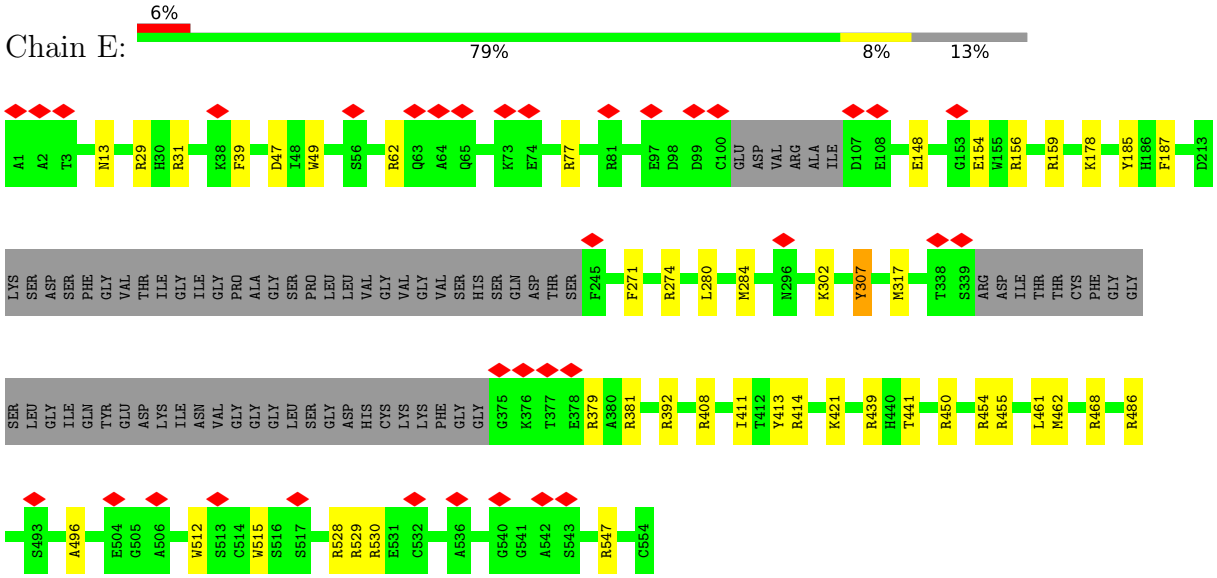
• Molecule 1: Complement component C7



• Molecule 2: Complement component C8 beta chain

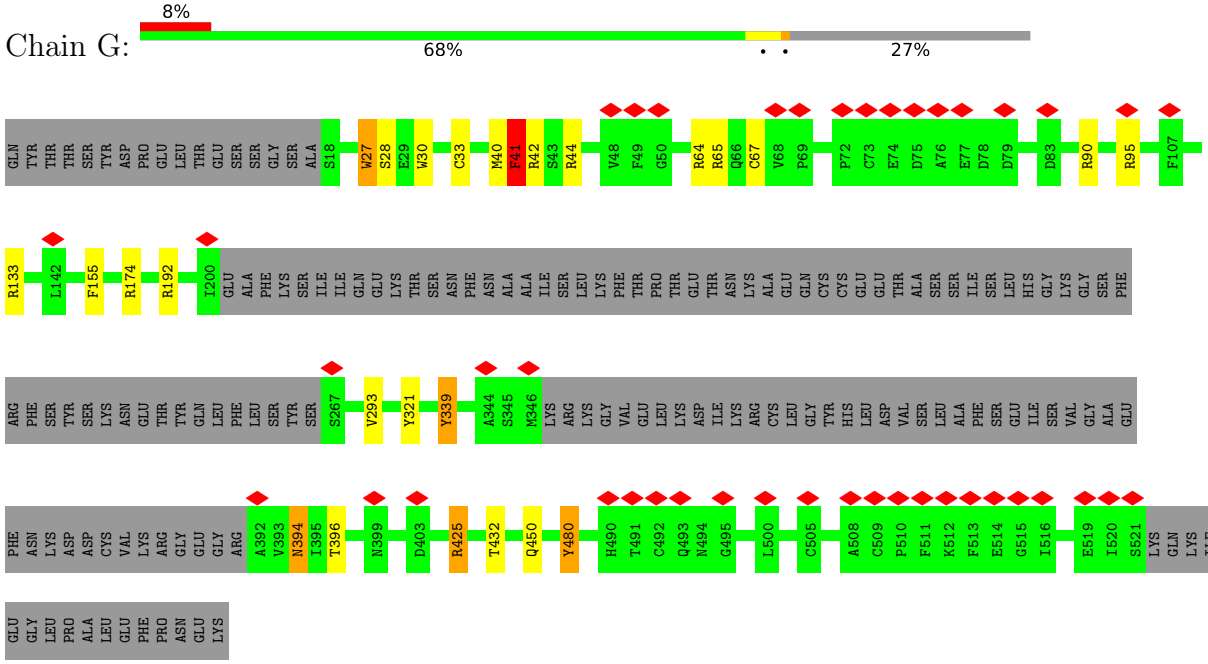
• Molecule 3: Complement component C8 alpha chain

Chain E:



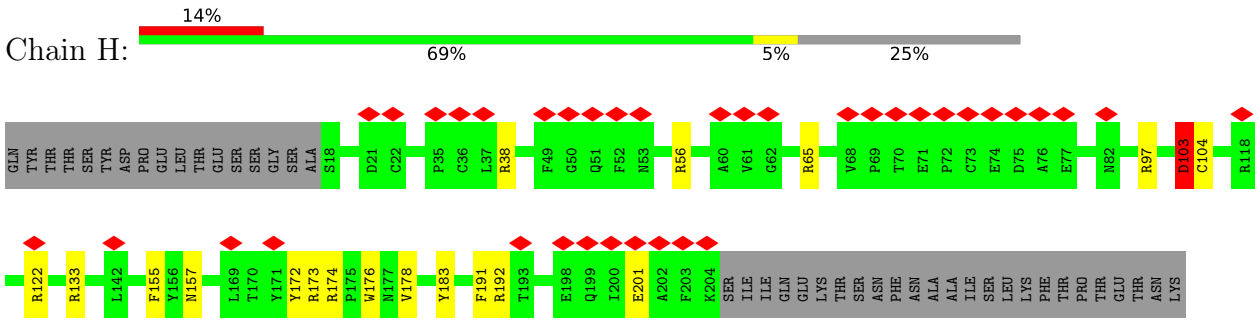
• Molecule 4: Complement component C9

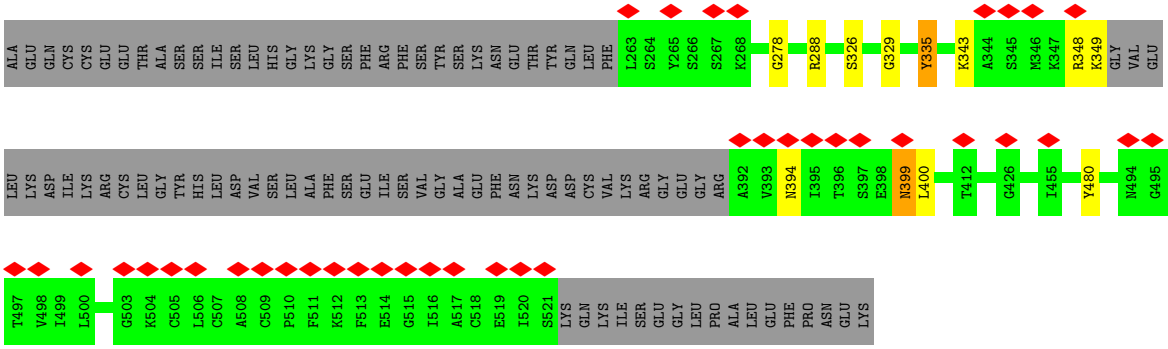
Chain G:



• Molecule 4: Complement component C9

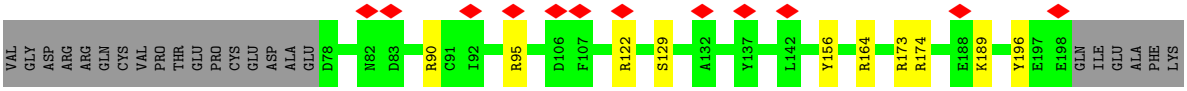
Chain H:

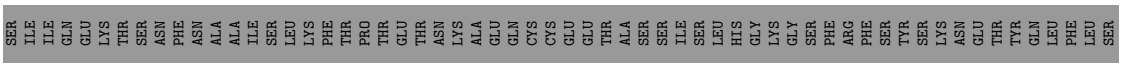


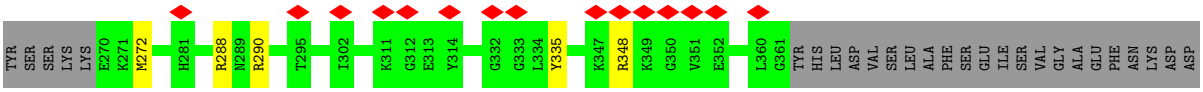


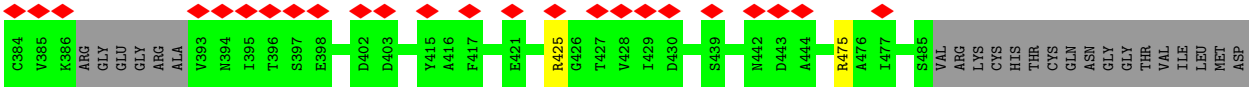
• Molecule 4: Complement component C9

Chain I:



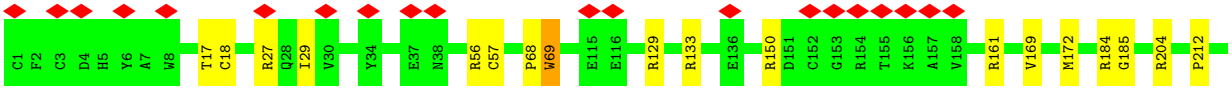


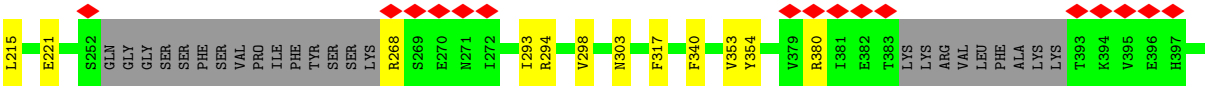


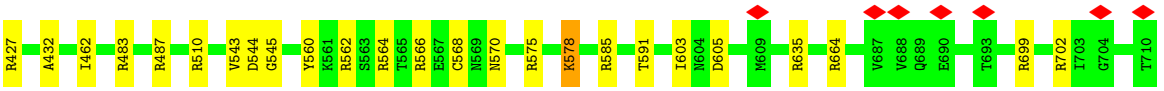


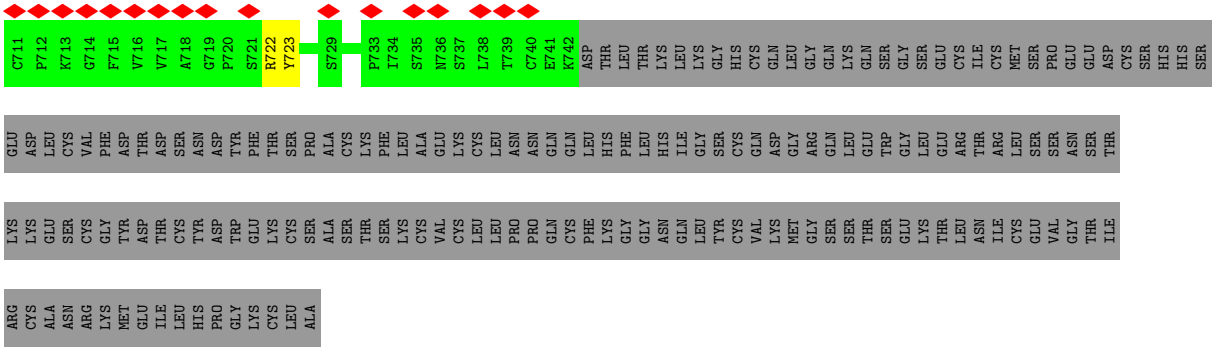
• Molecule 5: Complement component C6

Chain B:

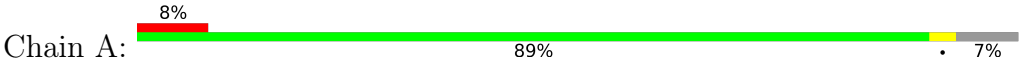


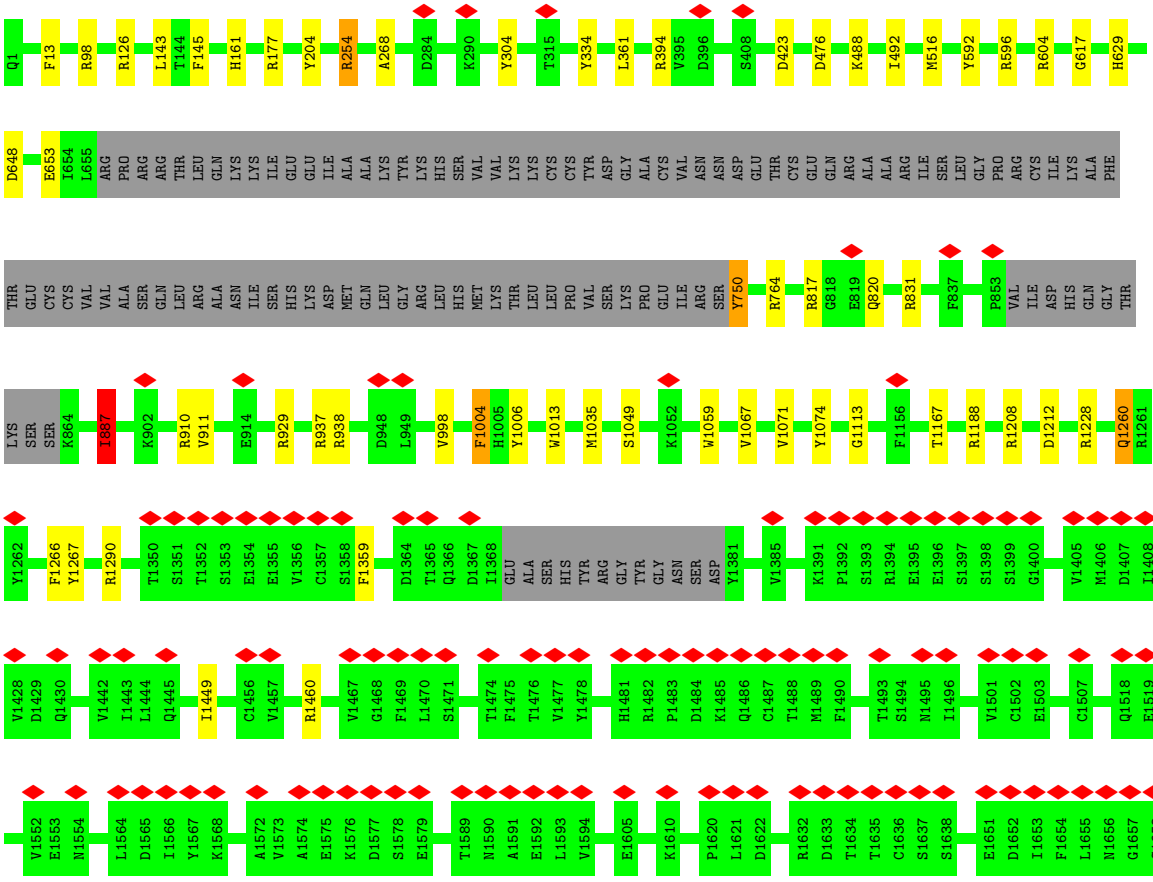




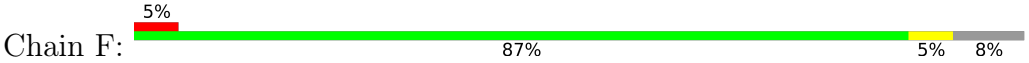


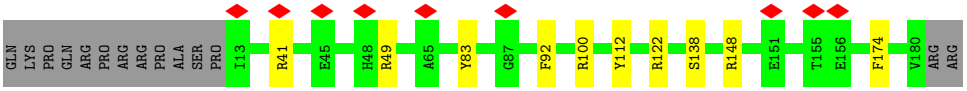
• Molecule 6: Complement C5





• Molecule 7: Complement component C8 gamma chain



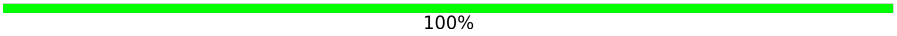


• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

• Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	85151	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	2.230	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.007	Depositor
Map size (Å)	418.80002, 418.80002, 418.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.047, 1.047, 1.047	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, FUC, BMA, CA

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	C	0.67	0/6109	1.01	22/8290 (0.3%)
2	D	0.71	0/4004	1.10	25/5409 (0.5%)
3	E	0.70	0/3882	1.07	17/5230 (0.3%)
4	G	0.72	2/3138 (0.1%)	1.09	18/4241 (0.4%)
4	H	0.72	1/3253 (0.0%)	1.04	12/4389 (0.3%)
4	I	0.71	0/2476	1.02	11/3343 (0.3%)
5	B	0.70	2/5750 (0.0%)	1.05	26/7770 (0.3%)
6	A	0.66	0/11993	0.99	19/16320 (0.1%)
7	F	0.72	1/1348 (0.1%)	1.04	7/1829 (0.4%)
All	All	0.69	6/41953 (0.0%)	1.04	157/56821 (0.3%)

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	C	0	7
2	D	0	6
3	E	0	3
4	G	0	3
4	H	0	5
4	I	0	3
5	B	0	4
6	A	0	12
All	All	0	43

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	27	TRP	CG-CD1	10.45	1.51	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	201	GLU	CD-OE2	8.22	1.34	1.25
7	F	138	SER	CB-OG	-6.50	1.33	1.42
5	B	268	ARG	N-CA	-5.75	1.34	1.46
4	G	27	TRP	CD1-NE1	5.54	1.47	1.38

The worst 5 of 157 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	27	TRP	CG-CD1-NE1	-13.59	96.51	110.10
5	B	483	ARG	NE-CZ-NH1	10.26	125.43	120.30
3	E	77	ARG	NE-CZ-NH1	9.59	125.10	120.30
4	G	90	ARG	NE-CZ-NH2	9.15	124.88	120.30
3	E	159	ARG	NE-CZ-NH1	9.10	124.85	120.30

There are no chirality outliers.

5 of 43 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	122	TYR	Sidechain
1	C	164	TYR	Sidechain
1	C	239	GLN	Peptide
1	C	267	TYR	Sidechain
1	C	28	ARG	Sidechain

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	C	5977	0	5400	30	0
2	D	3914	0	3736	56	0
3	E	3805	0	3588	58	0
4	G	3079	0	2910	35	0
4	H	3192	0	3044	12	0
4	I	2433	0	2302	4	0
5	B	5631	0	5332	54	0
6	A	11744	0	11282	25	0
7	F	1319	0	1282	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	K	28	0	25	5	0
9	J	39	0	34	0	0
10	C	11	0	10	6	0
10	D	22	0	20	25	0
10	E	33	0	30	27	0
10	G	11	0	10	0	0
11	D	1	0	0	0	0
11	E	1	0	0	0	0
11	H	1	0	0	0	0
12	B	14	0	13	4	0
12	E	14	0	13	8	0
12	G	14	0	13	7	0
12	H	14	0	13	1	0
13	B	10	0	10	11	0
All	All	41307	0	39067	267	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 3.

The worst 5 of 267 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)
4:G:30:TRP:HH2	4:G:65:ARG:CB	1.31	1.43
4:H:399:ASN:HB2	4:I:196:TYR:CE1	1.64	1.31
4:G:30:TRP:CH2	4:G:65:ARG:CB	2.16	1.28
5:B:543:VAL:HB	5:B:578:LYS:CE	1.65	1.25
5:B:221:GLU:HG3	12:B:1002:NAG:O6	1.09	1.24

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	C	803/821 (98%)	778 (97%)	25 (3%)	0	100	100
2	D	481/537 (90%)	465 (97%)	15 (3%)	1 (0%)	47	81
3	E	474/554 (86%)	457 (96%)	17 (4%)	0	100	100
4	G	387/538 (72%)	367 (95%)	20 (5%)	0	100	100
4	H	398/538 (74%)	386 (97%)	12 (3%)	0	100	100
4	I	301/538 (56%)	286 (95%)	15 (5%)	0	100	100
5	B	712/913 (78%)	667 (94%)	45 (6%)	0	100	100
6	A	1534/1658 (92%)	1430 (93%)	103 (7%)	1 (0%)	51	84
7	F	166/182 (91%)	161 (97%)	5 (3%)	0	100	100
All	All	5256/6279 (84%)	4997 (95%)	257 (5%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	530	ALA
6	A	887	ILE

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	C	615/714 (86%)	609 (99%)	6 (1%)	76	88
2	D	433/473 (92%)	431 (100%)	2 (0%)	88	94
3	E	410/466 (88%)	409 (100%)	1 (0%)	93	98
4	G	340/477 (71%)	332 (98%)	8 (2%)	49	76
4	H	353/477 (74%)	347 (98%)	6 (2%)	60	82
4	I	264/477 (55%)	260 (98%)	4 (2%)	65	84
5	B	630/810 (78%)	624 (99%)	6 (1%)	76	88
6	A	1234/1470 (84%)	1225 (99%)	9 (1%)	84	93
7	F	136/149 (91%)	135 (99%)	1 (1%)	84	93

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4415/5513 (80%)	4372 (99%)	43 (1%)	77 88

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	H	480	TYR
6	A	1013	TRP
6	A	423	ASP
6	A	750	TYR
6	A	1260	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
6	A	1260	GLN
6	A	629	HIS
3	E	305	ASN
3	E	24	GLN
4	H	471	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)

5 monosaccharides are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

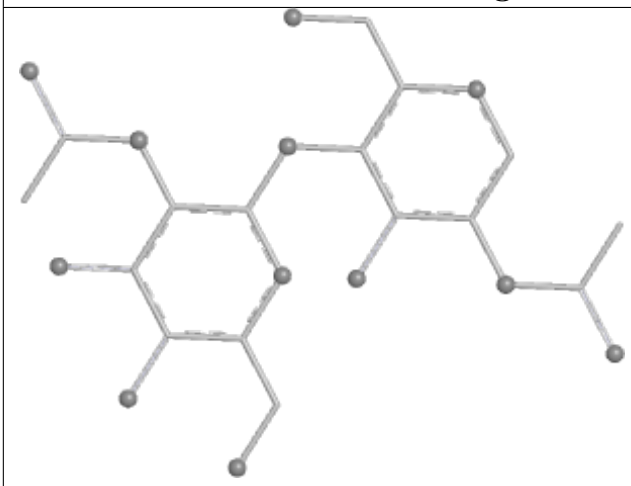
There are no torsion outliers.

There are no ring outliers.

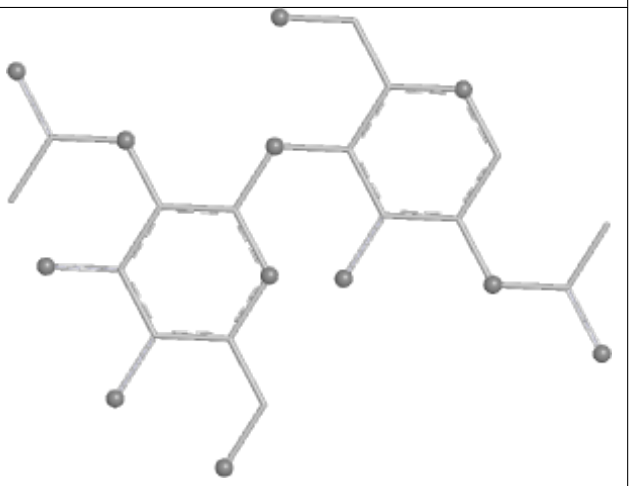
No monomer is involved in short contacts.

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

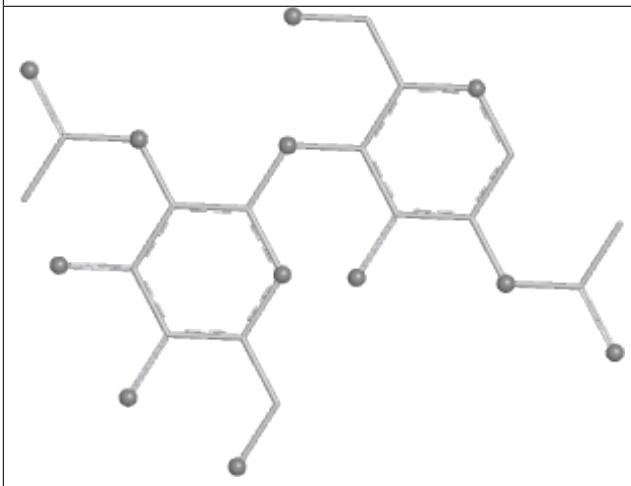
Oligosaccharide Chain K



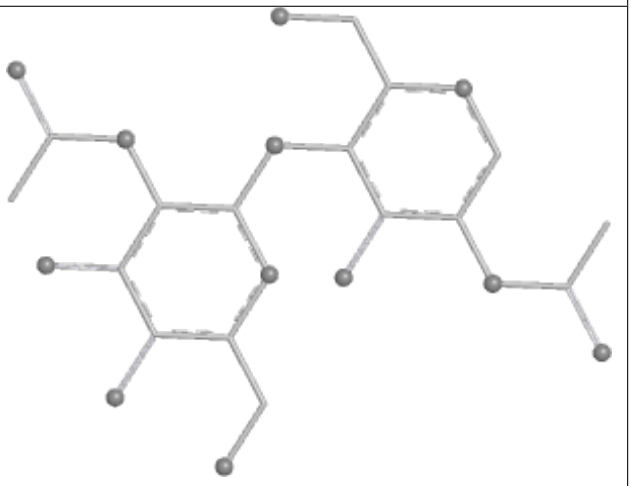
Bond lengths



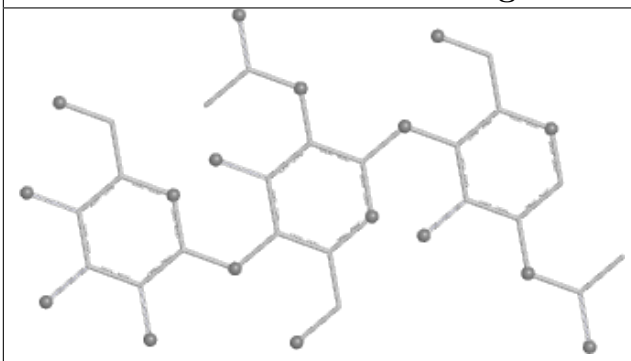
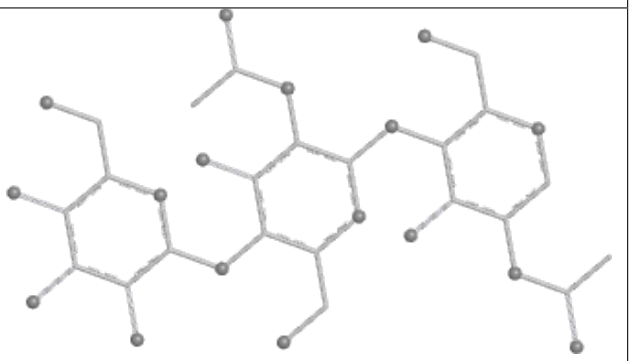
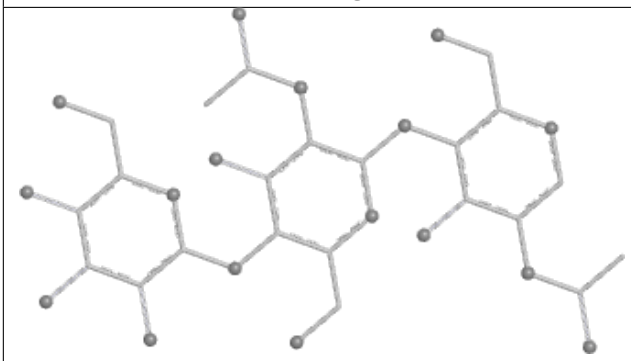
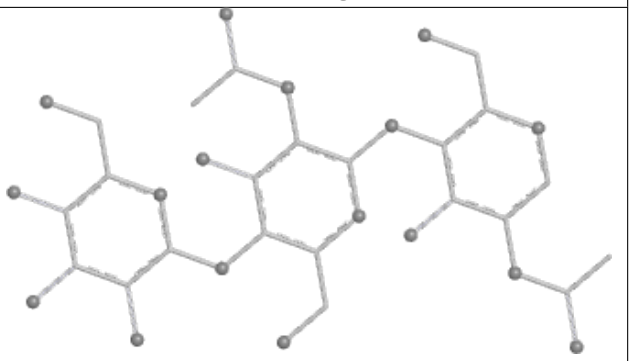
Bond angles



Torsions



Rings

Oligosaccharide Chain J	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 3 are monoatomic - leaving 12 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

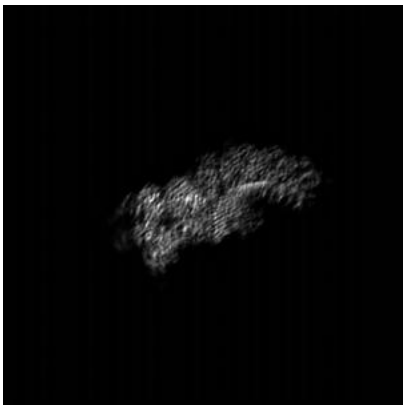
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12650. These allow visual inspection of the internal detail of the map and identification of artifacts.

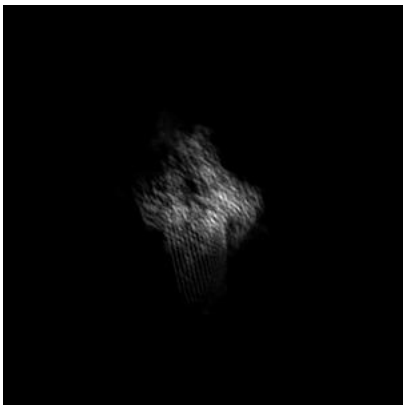
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

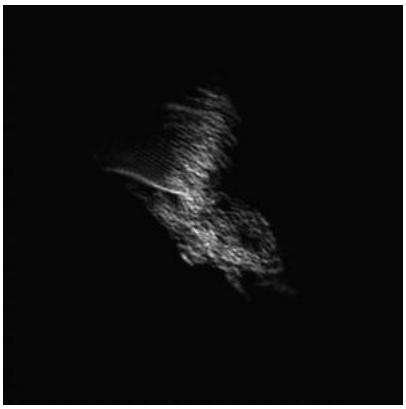
6.1.1 Primary map



X

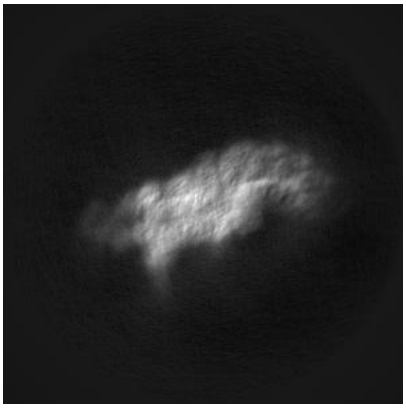


Y

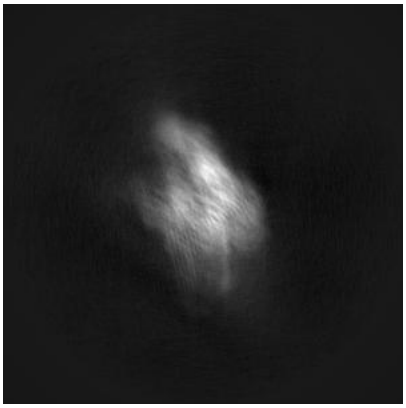


Z

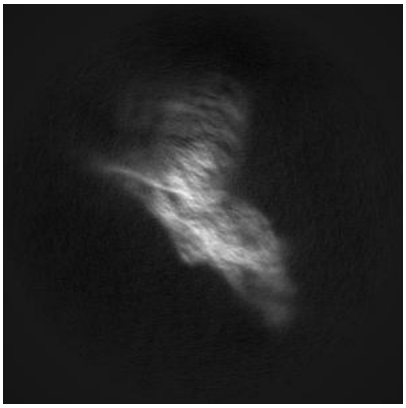
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices (i)

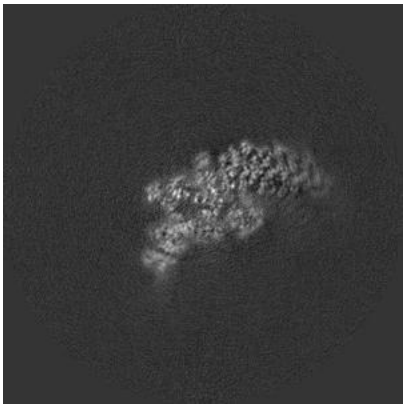
6.2.1 Primary map

X Index: 200

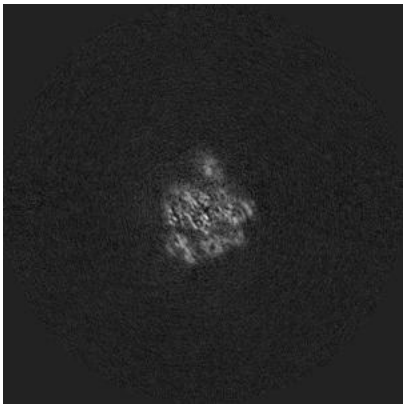
Y Index: 200

Z Index: 200

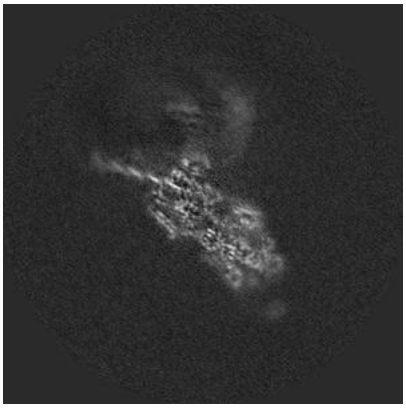
6.2.2 Raw map



X Index: 200



Y Index: 200



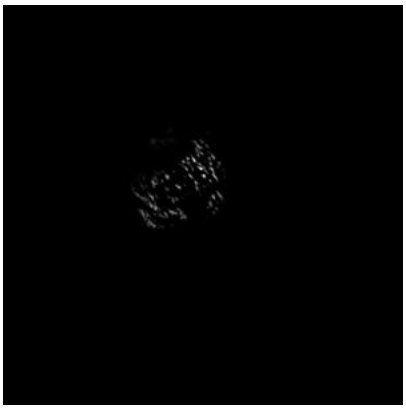
Z Index: 200

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

6.3 Largest variance slices (i)

6.3.1 Primary map

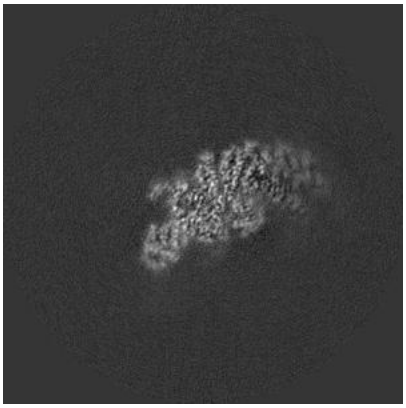
X Index: 194



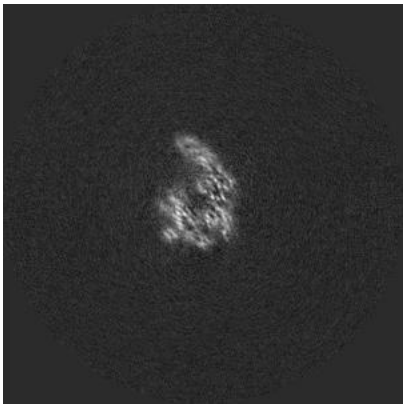
Y Index: 151

Z Index: 205

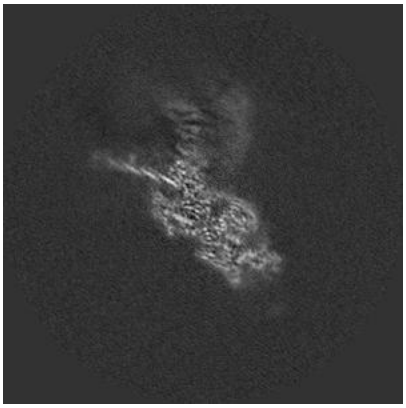
6.3.2 Raw map



X Index: 194



Y Index: 181

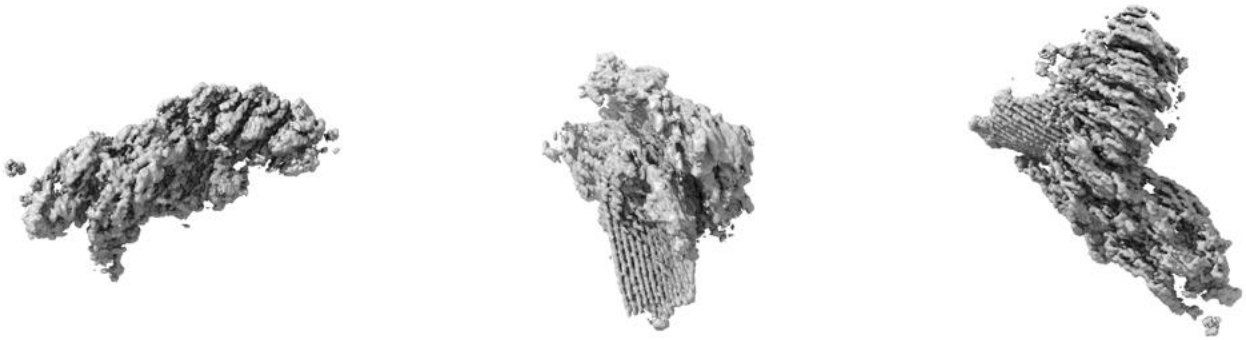


Z Index: 205

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

6.4 Orthogonal surface views (i)

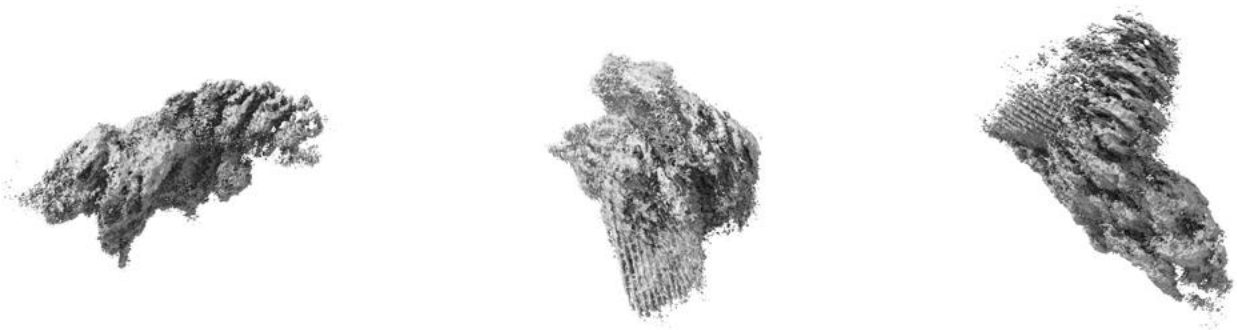
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.007. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

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.

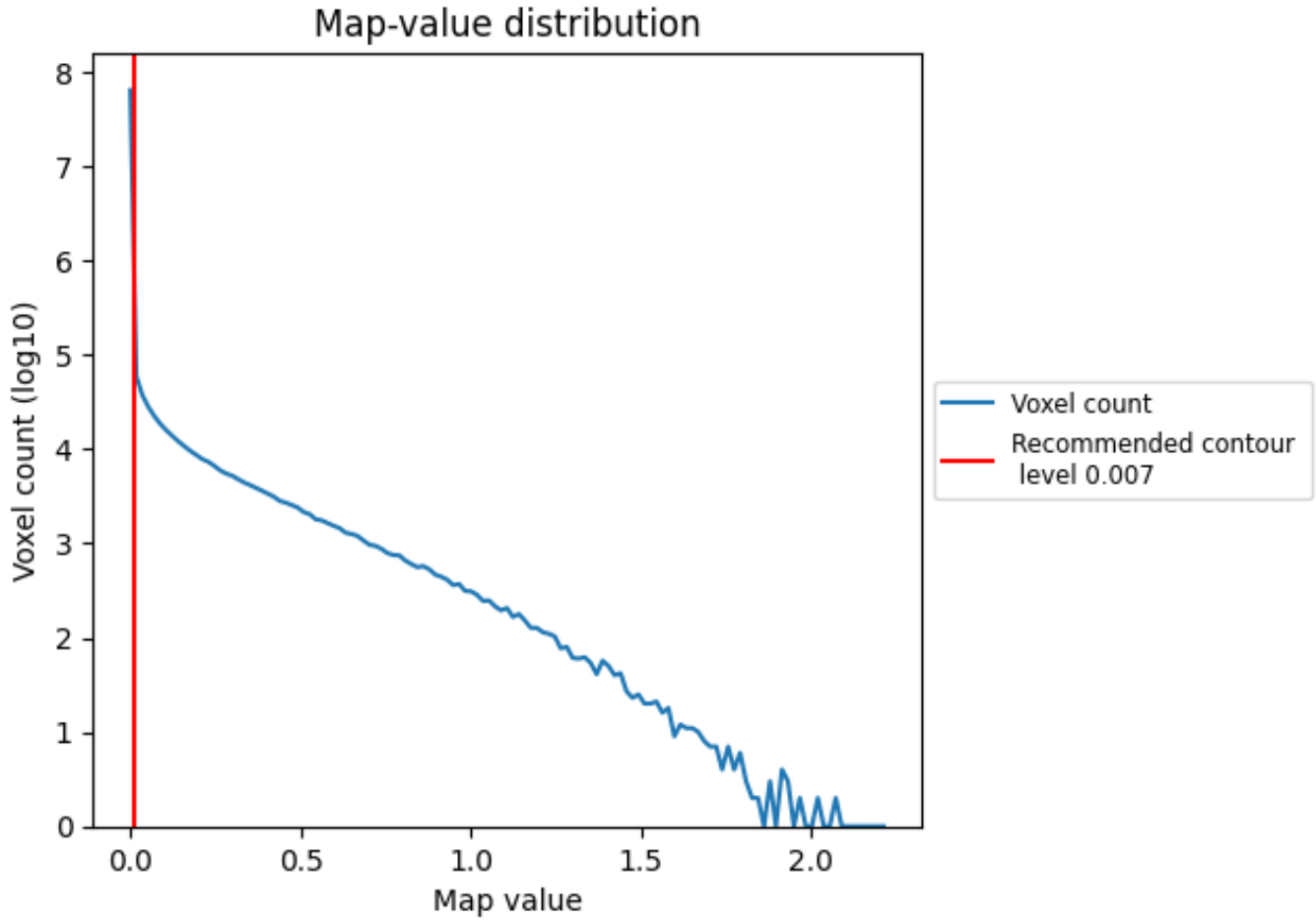
6.5 Mask visualisation (i)

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

7 Map analysis

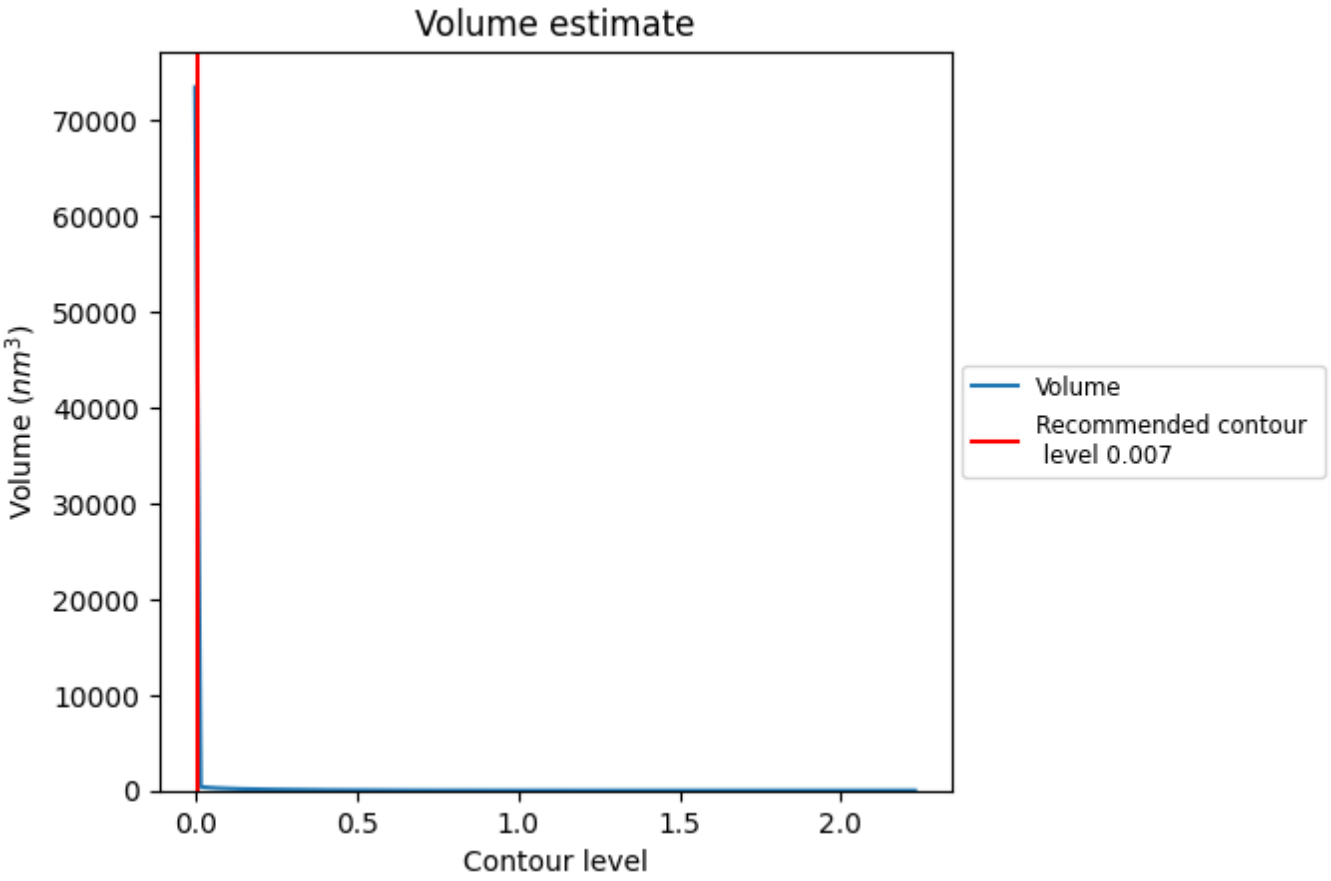
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

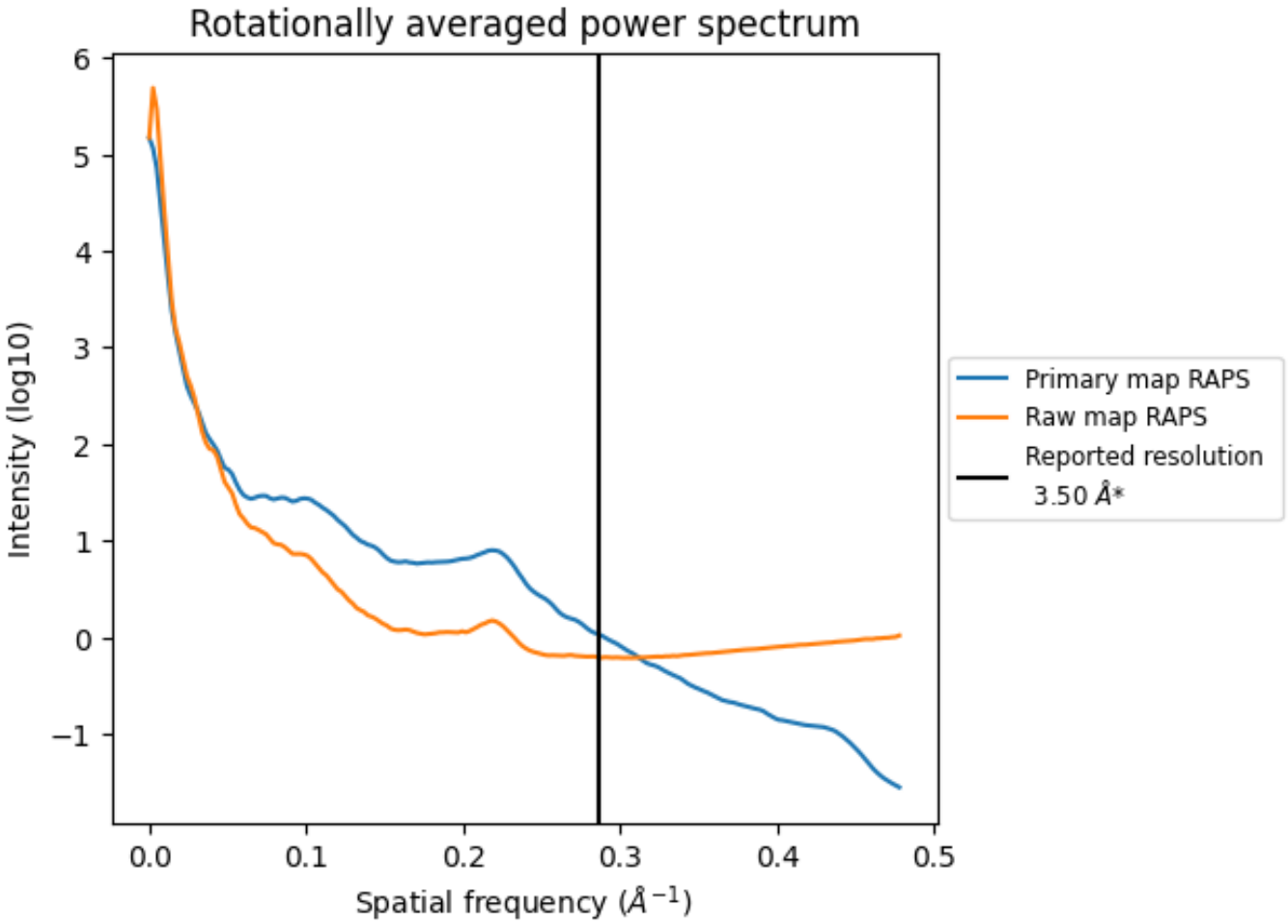
7.2 Volume estimate (i)



The volume at the recommended contour level is 36597 nm^3; this corresponds to an approximate mass of 33059 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)

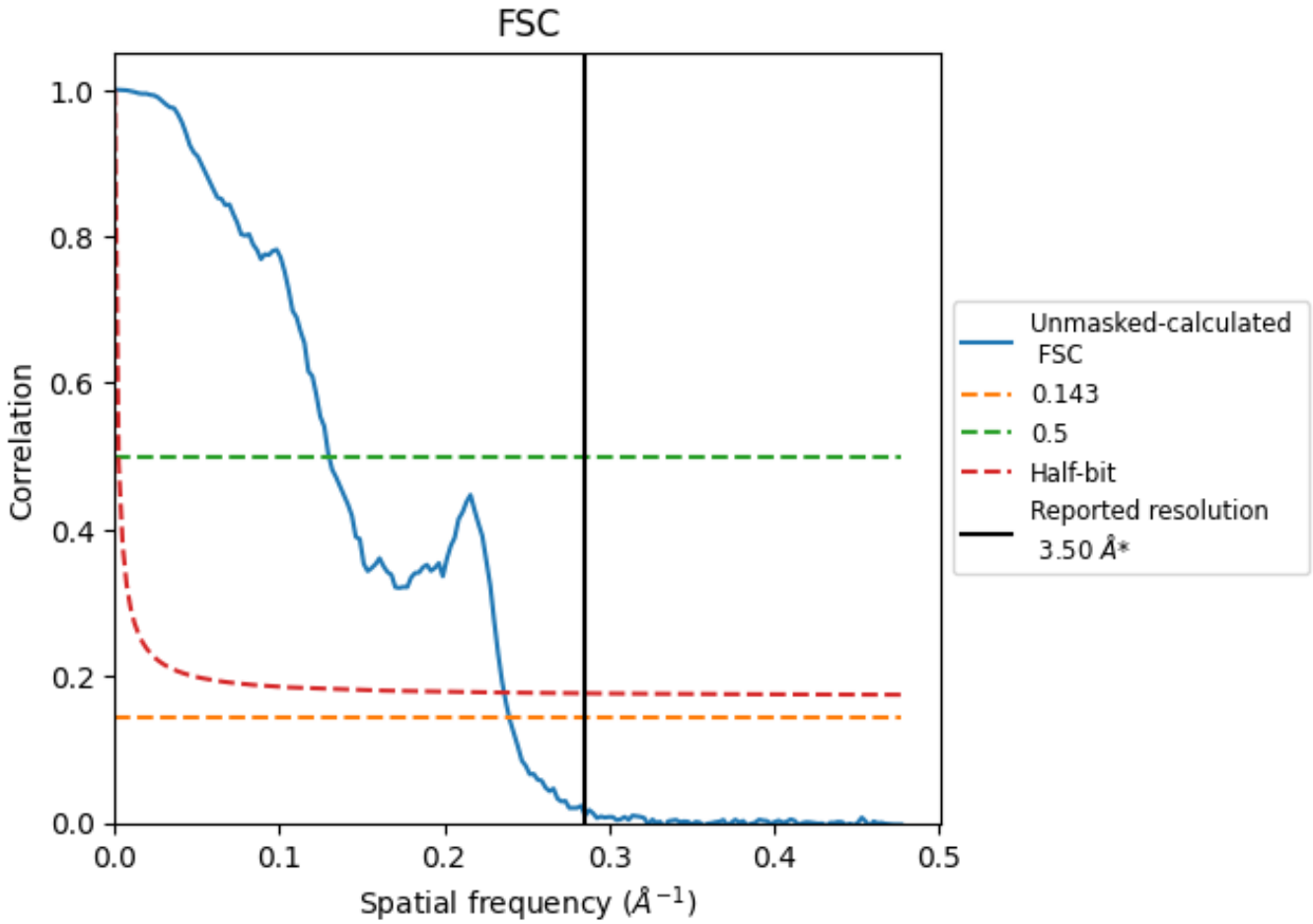


*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8 Fourier-Shell correlation

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



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

8.2 Resolution estimates (i)

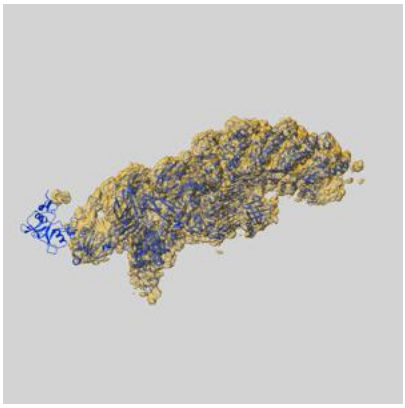
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.17	7.69	4.23

*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 4.17 differs from the reported value 3.5 by more than 10 %

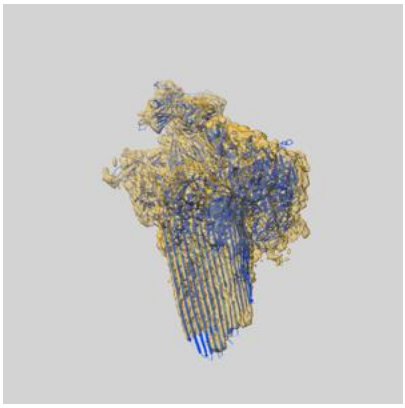
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12650 and PDB model 7NYC. Per-residue inclusion information can be found in section 3 on page 9.

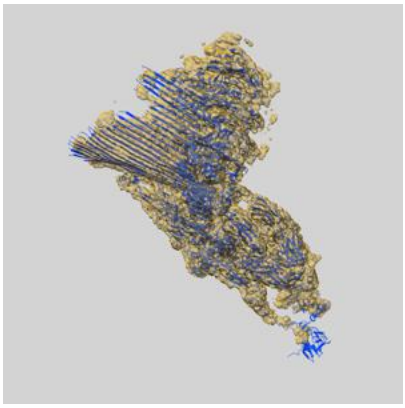
9.1 Map-model overlay



X



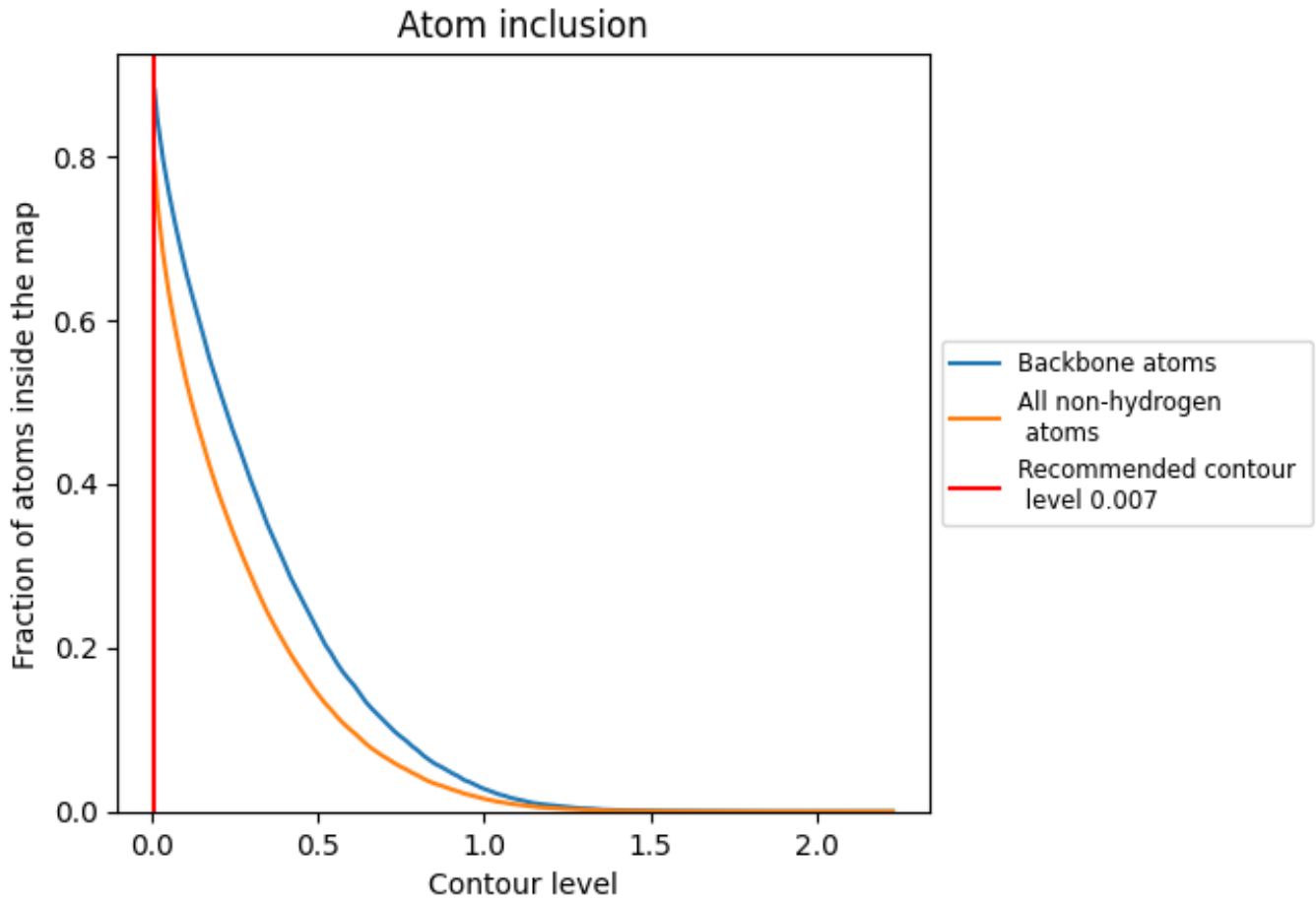
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.007 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 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.