Preliminary Full wwPDB EM Validation Report ⓘ

Mar 5, 2021 – 11:24 AM JST

Deposition ID : D_1300021032

This is a Preliminary Full wwPDB EM Validation Report.

This report is produced by the wwPDB Deposition System during initial deposition but before annotation of the structure.

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:

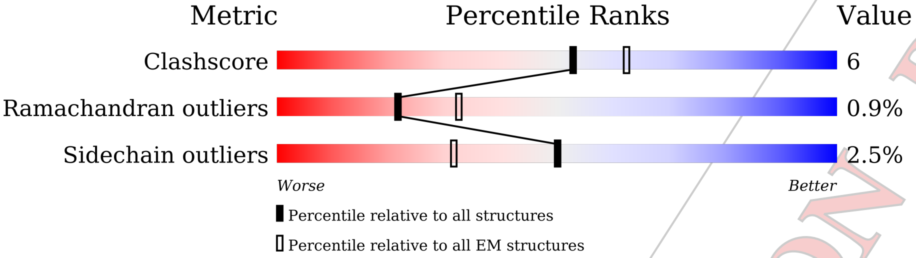
EMDB validation analysis	:	0.0.0.dev61
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.17.1

1 Overall quality at a glance

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

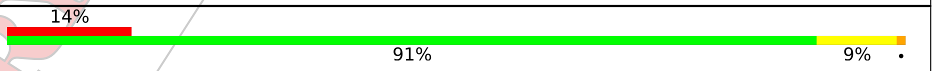
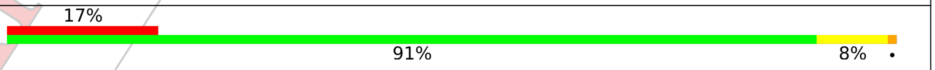
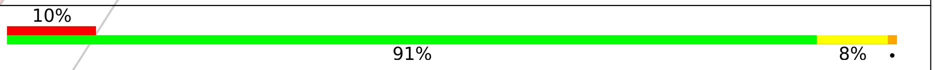
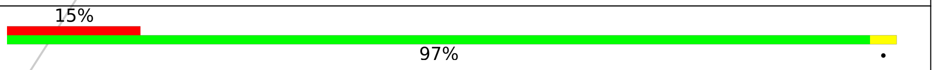
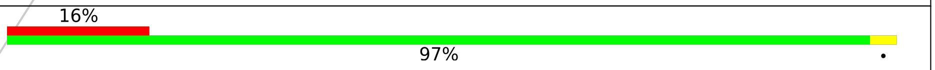
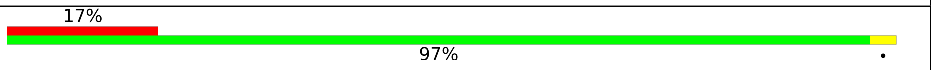
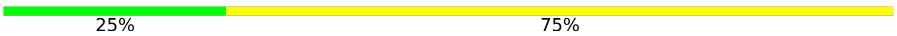
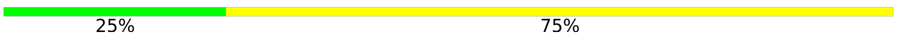
The reported resolution of this entry is unknown.

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	A	116	 14% 91% 9% •
1	B	116	 17% 91% 8% •
1	C	116	 10% 91% 8% •
2	a	340	 15% 97% •
2	b	340	 16% 97% •
2	c	340	 17% 97% •
3	D	4	 25% 75%
3	E	4	 25% 75%

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Mol	Chain	Length	Quality of chain
3	F	4	

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 10989 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.

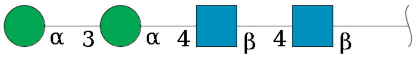
- Molecule 1 is a protein.

Mol	Chain	Residues	Atoms	AltConf	Trace
1	A	116	Total C N O S 883 556 143 178 6	0	0
1	B	116	Total C N O S 883 556 143 178 6	0	0
1	C	116	Total C N O S 883 556 143 178 6	0	0

- Molecule 2 is a protein.

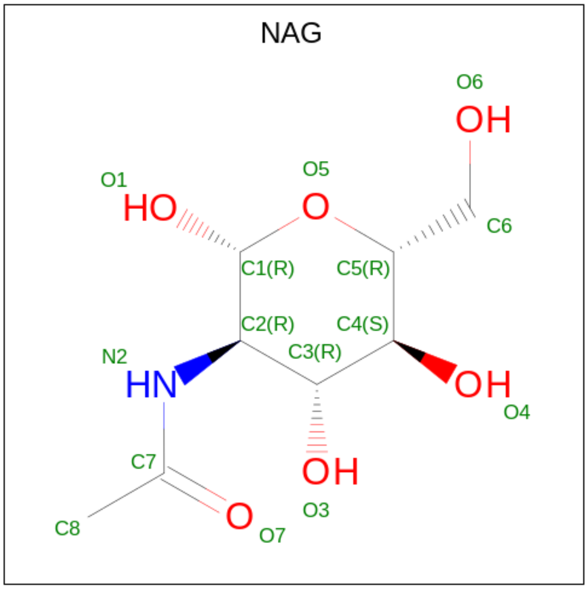
Mol	Chain	Residues	Atoms	AltConf	Trace
2	a	340	Total C N O S 2664 1698 449 510 7	0	0
2	b	340	Total C N O S 2664 1698 449 510 7	0	0
2	c	340	Total C N O S 2664 1698 449 510 7	0	0

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



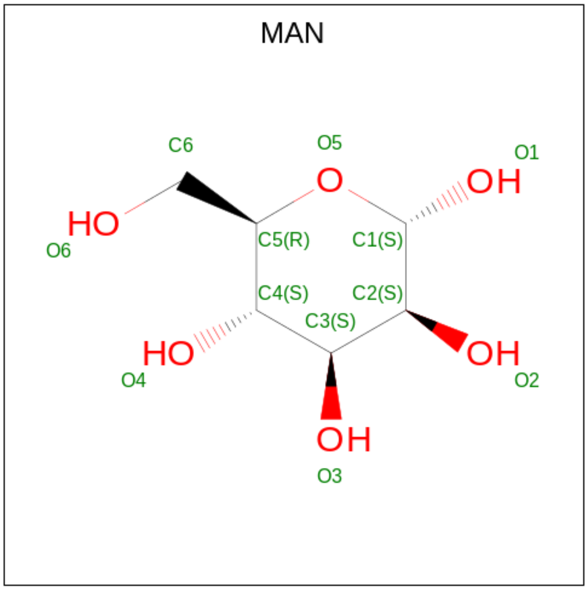
Mol	Chain	Residues	Atoms	AltConf	Trace
3	D	4	Total C N O 50 28 2 20	0	0
3	E	4	Total C N O 50 28 2 20	0	0
3	F	4	Total C N O 50 28 2 20	0	0

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



Mol	Chain	Residues	Atoms	AltConf
4	D	1	Total C N O 42 24 3 15	0
4	D	1	Total C N O 42 24 3 15	0
4	D	1	Total C N O 42 24 3 15	0
4	E	1	Total C N O 42 24 3 15	0
4	E	1	Total C N O 42 24 3 15	0
4	E	1	Total C N O 42 24 3 15	0
4	F	1	Total C N O 42 24 3 15	0
4	F	1	Total C N O 42 24 3 15	0
4	F	1	Total C N O 42 24 3 15	0

- Molecule 5 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



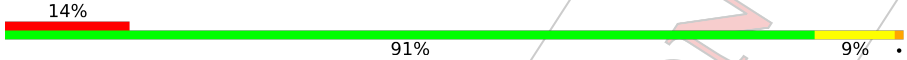
Mol	Chain	Residues	Atoms	AltConf
5	D	1	Total C O 24 12 12	0
5	D	1	Total C O 24 12 12	0
5	E	1	Total C O 24 12 12	0
5	E	1	Total C O 24 12 12	0
5	F	1	Total C O 24 12 12	0
5	F	1	Total C O 24 12 12	0

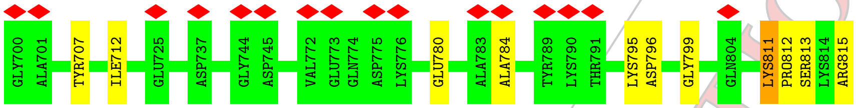
3 Residue-property plots ⓘ

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:

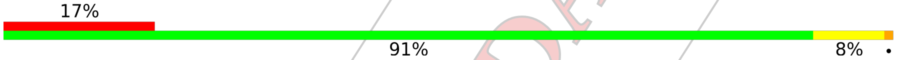
Chain A:

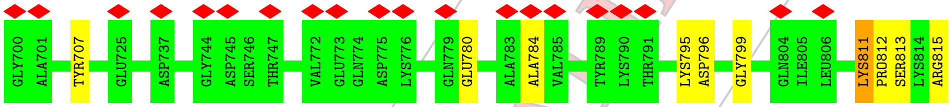




- Molecule 1:

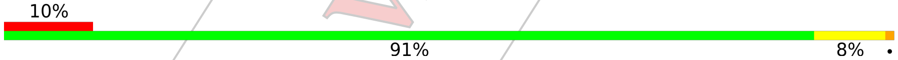
Chain B:

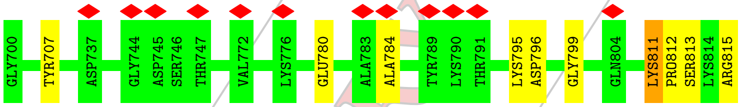




- Molecule 1:

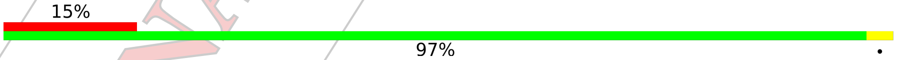
Chain C:

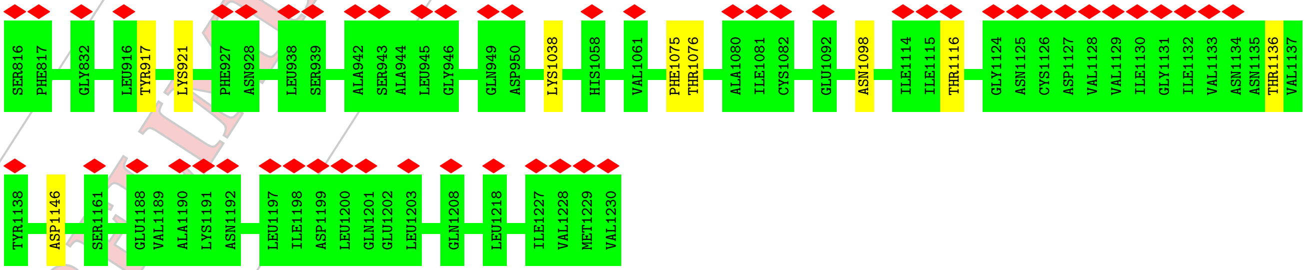




- Molecule 2:

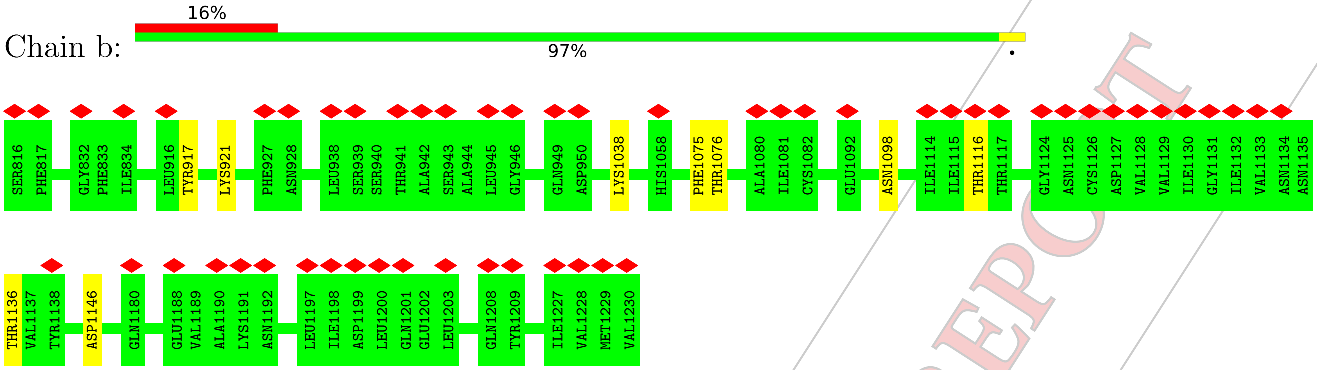
Chain a:





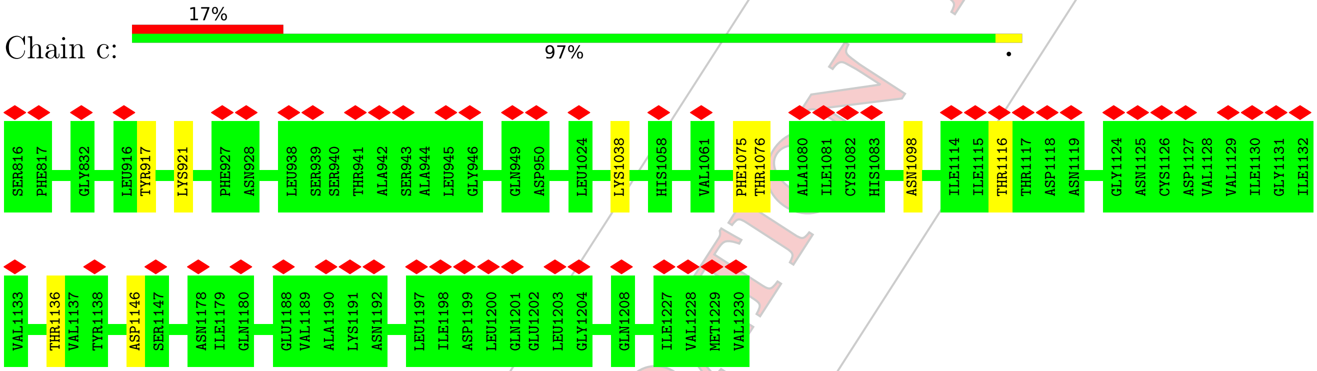
- Molecule 2:

Chain b:



- Molecule 2:

Chain c:

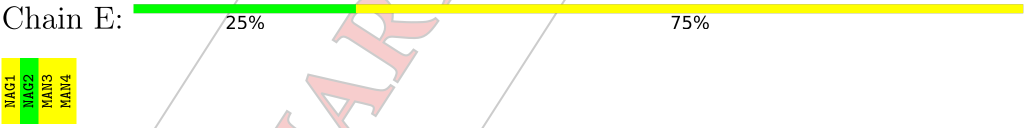


- Molecule 3: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

- Molecule 3: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



- Molecule 3: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, Not provided	
Number of subtomograms used	Not provided	
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	Not provided	
Voltage (kV)	Not provided	
Electron dose $(e^-/\text{Å}^2)$	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	Not provided	
Maximum map value	1.750	Depositor
Minimum map value	-1.754	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.052	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	391.68, 391.68, 391.68	wwPDB
Map dimensions	144, 144, 144	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.72, 2.72, 2.72	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, MAN

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	0.24	0/899	0.39	0/1222
1	B	0.25	0/899	0.39	0/1222
1	C	0.24	0/899	0.39	0/1222
2	a	0.24	0/2714	0.37	0/3686
2	b	0.24	0/2714	0.37	0/3686
2	c	0.24	0/2714	0.37	0/3686
All	All	0.24	0/10839	0.37	0/14724

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	883	0	874	4	0
1	B	883	0	874	3	0
1	C	883	0	874	3	0
2	a	2664	0	2643	0	0
2	b	2664	0	2643	0	0
2	c	2664	0	2643	0	0
3	D	50	0	43	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	50	0	43	0	0
3	F	50	0	43	0	0
4	D	42	0	39	0	0
4	E	42	0	39	0	0
4	F	42	0	39	0	0
5	D	24	0	24	0	0
5	E	24	0	24	0	0
5	F	24	0	24	0	0
All	All	10989	0	10869	10	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 6.

All (10) 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:813:SER:OG	1:A:815:ARG:NH1	2.18	0.77
1:B:813:SER:OG	1:B:815:ARG:NH1	2.18	0.76
1:C:813:SER:OG	1:C:815:ARG:NH1	2.18	0.75
1:A:811:LYS:H	1:A:812:PRO:HD2	1.73	0.53
1:C:811:LYS:H	1:C:812:PRO:HD2	1.73	0.52
1:B:811:LYS:H	1:B:812:PRO:HD2	1.73	0.52
1:B:780:GLU:HA	1:B:784:ALA:HB3	1.93	0.51
1:C:780:GLU:HA	1:C:784:ALA:HB3	1.93	0.51
1:A:780:GLU:HA	1:A:784:ALA:HB3	1.93	0.51
1:A:712:ILE:HD12	1:A:712:ILE:HA	1.93	0.41

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	114/116 (98%)	95 (83%)	16 (14%)	3 (3%)	5	5
1	B	114/116 (98%)	95 (83%)	16 (14%)	3 (3%)	5	5
1	C	114/116 (98%)	95 (83%)	16 (14%)	3 (3%)	5	5
2	a	336/340 (99%)	292 (87%)	43 (13%)	1 (0%)	41	41
2	b	336/340 (99%)	292 (87%)	43 (13%)	1 (0%)	41	41
2	c	336/340 (99%)	292 (87%)	43 (13%)	1 (0%)	41	41
All	All	1350/1368 (99%)	1161 (86%)	177 (13%)	12 (1%)	21	17

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	799	GLY
1	A	811	LYS
1	B	799	GLY
1	B	811	LYS
1	C	799	GLY
1	C	811	LYS
2	a	1146	ASP
2	b	1146	ASP
2	c	1146	ASP
1	A	795	LYS
1	B	795	LYS
1	C	795	LYS

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	103/103 (100%)	101 (98%)	2 (2%)	57	57
1	B	103/103 (100%)	101 (98%)	2 (2%)	57	57
1	C	103/103 (100%)	101 (98%)	2 (2%)	57	57
2	a	295/295 (100%)	287 (97%)	8 (3%)	44	44
2	b	295/295 (100%)	287 (97%)	8 (3%)	44	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	c	295/295 (100%)	287 (97%)	8 (3%)	44	44
All	All	1194/1194 (100%)	1164 (98%)	30 (2%)	50	47

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	707	TYR
1	A	796	ASP
1	B	707	TYR
1	B	796	ASP
1	C	707	TYR
1	C	796	ASP
2	a	917	TYR
2	a	921	LYS
2	a	1038	LYS
2	a	1075	PHE
2	a	1076	THR
2	a	1098	ASN
2	a	1116	THR
2	a	1136	THR
2	b	917	TYR
2	b	921	LYS
2	b	1038	LYS
2	b	1075	PHE
2	b	1076	THR
2	b	1098	ASN
2	b	1116	THR
2	b	1136	THR
2	c	917	TYR
2	c	921	LYS
2	c	1038	LYS
2	c	1075	PHE
2	c	1076	THR
2	c	1098	ASN
2	c	1116	THR
2	c	1136	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	751	ASN

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Mol	Chain	Res	Type
1	A	774	GLN
1	B	751	ASN
1	B	762	GLN
1	B	774	GLN
1	C	717	ASN
1	C	751	ASN
1	C	762	GLN
1	C	774	GLN
2	a	925	ASN
2	a	953	ASN
2	a	1048	HIS
2	a	1098	ASN
2	a	1113	GLN
2	a	1142	GLN
2	b	925	ASN
2	b	953	ASN
2	b	1048	HIS
2	b	1098	ASN
2	b	1113	GLN
2	b	1135	ASN
2	b	1142	GLN
2	c	925	ASN
2	c	953	ASN
2	c	1048	HIS
2	c	1098	ASN
2	c	1113	GLN
2	c	1142	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

12 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	$\#\lvert Z\rvert > 2$	Counts	RMSZ	$\#\lvert Z\rvert > 2$
3	NAG	D	1	3,2	14,14,15	0.95	2 (14%)	17,19,21	0.88	1 (5%)
3	NAG	D	2	3	14,14,15	0.21	0	17,19,21	0.42	0
3	MAN	D	3	3	11,11,12	0.78	0	15,15,17	1.34	2 (13%)
3	MAN	D	4	3	11,11,12	0.81	0	15,15,17	1.40	3 (20%)
3	NAG	E	1	3,2	14,14,15	0.95	1 (7%)	17,19,21	0.88	1 (5%)
3	NAG	E	2	3	14,14,15	0.20	0	17,19,21	0.42	0
3	MAN	E	3	3	11,11,12	0.80	0	15,15,17	1.34	2 (13%)
3	MAN	E	4	3	11,11,12	0.81	0	15,15,17	1.40	3 (20%)
3	NAG	F	1	3,2	14,14,15	0.94	1 (7%)	17,19,21	0.88	1 (5%)
3	NAG	F	2	3	14,14,15	0.19	0	17,19,21	0.41	0
3	MAN	F	3	3	11,11,12	0.79	0	15,15,17	1.33	2 (13%)
3	MAN	F	4	3	11,11,12	0.81	0	15,15,17	1.40	3 (20%)

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	D	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	MAN	D	3	3	-	0/2/19/22	1/1/1/1
3	MAN	D	4	3	-	0/2/19/22	0/1/1/1
3	NAG	E	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	MAN	E	3	3	-	0/2/19/22	1/1/1/1
3	MAN	E	4	3	-	0/2/19/22	0/1/1/1
3	NAG	F	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	MAN	F	3	3	-	0/2/19/22	1/1/1/1
3	MAN	F	4	3	-	0/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1	NAG	O5-C1	2.83	1.48	1.43
3	D	1	NAG	O5-C1	2.81	1.48	1.43
3	F	1	NAG	O5-C1	2.78	1.48	1.43
3	D	1	NAG	C1-C2	2.01	1.55	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	3	MAN	C1-O5-C5	3.79	117.33	112.19
3	D	3	MAN	C1-O5-C5	3.78	117.31	112.19
3	E	3	MAN	C1-O5-C5	3.77	117.30	112.19
3	E	4	MAN	C1-O5-C5	3.43	116.85	112.19
3	F	4	MAN	C1-O5-C5	3.41	116.81	112.19
3	D	4	MAN	C1-O5-C5	3.41	116.81	112.19
3	D	1	NAG	C1-O5-C5	3.40	116.79	112.19
3	E	1	NAG	C1-O5-C5	3.38	116.77	112.19
3	F	1	NAG	C1-O5-C5	3.38	116.77	112.19
3	D	4	MAN	O5-C1-C2	2.45	114.56	110.77
3	F	4	MAN	O5-C1-C2	2.44	114.54	110.77
3	E	4	MAN	O5-C1-C2	2.44	114.54	110.77
3	F	4	MAN	O2-C2-C3	-2.26	105.61	110.14
3	D	3	MAN	O2-C2-C3	-2.24	105.66	110.14
3	E	3	MAN	O2-C2-C3	-2.23	105.67	110.14
3	E	4	MAN	O2-C2-C3	-2.23	105.67	110.14
3	D	4	MAN	O2-C2-C3	-2.22	105.70	110.14
3	F	3	MAN	O2-C2-C3	-2.21	105.71	110.14

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6

All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	3	MAN	C1-C2-C3-C4-C5-O5

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Mol	Chain	Res	Type	Atoms
3	D	3	MAN	C1-C2-C3-C4-C5-O5
3	F	3	MAN	C1-C2-C3-C4-C5-O5

No monomer is involved in short contacts.

5.6 Ligand geometry

15 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	E	41	2	14,14,15	0.22	0	17,19,21	0.42	0
4	NAG	D	21	1	14,14,15	0.21	0	17,19,21	0.42	0
4	NAG	D	41	2	14,14,15	0.22	0	17,19,21	0.43	0
5	MAN	D	36	-	12,12,12	0.50	0	17,17,17	0.84	1 (5%)
5	MAN	E	36	-	12,12,12	0.50	0	17,17,17	0.84	1 (5%)
4	NAG	F	21	1	14,14,15	0.22	0	17,19,21	0.42	0
5	MAN	F	36	-	12,12,12	0.49	0	17,17,17	0.84	1 (5%)
5	MAN	F	38	-	12,12,12	0.50	0	17,17,17	0.84	1 (5%)
4	NAG	E	26	2	14,14,15	0.25	0	17,19,21	0.43	0
4	NAG	D	26	2	14,14,15	0.26	0	17,19,21	0.43	0
4	NAG	F	26	2	14,14,15	0.26	0	17,19,21	0.41	0
5	MAN	D	38	-	12,12,12	0.50	0	17,17,17	0.84	1 (5%)
5	MAN	E	38	-	12,12,12	0.48	0	17,17,17	0.85	1 (5%)
4	NAG	E	21	1	14,14,15	0.22	0	17,19,21	0.42	0
4	NAG	F	41	2	14,14,15	0.23	0	17,19,21	0.42	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	E	41	2	-	2/6/23/26	0/1/1/1
4	NAG	D	21	1	-	0/6/23/26	0/1/1/1
4	NAG	D	41	2	-	2/6/23/26	0/1/1/1
5	MAN	D	36	-	-	1/2/22/22	0/1/1/1
5	MAN	E	36	-	-	1/2/22/22	0/1/1/1
4	NAG	F	21	1	-	0/6/23/26	0/1/1/1
5	MAN	F	36	-	-	1/2/22/22	0/1/1/1
5	MAN	F	38	-	-	0/2/22/22	0/1/1/1
4	NAG	E	26	2	-	2/6/23/26	0/1/1/1
4	NAG	D	26	2	-	2/6/23/26	0/1/1/1
4	NAG	F	26	2	-	2/6/23/26	0/1/1/1
5	MAN	D	38	-	-	0/2/22/22	0/1/1/1
5	MAN	E	38	-	-	0/2/22/22	0/1/1/1
4	NAG	E	21	1	-	0/6/23/26	0/1/1/1
4	NAG	F	41	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	38	MAN	O2-C2-C3	-2.05	105.62	110.35
5	E	36	MAN	O2-C2-C3	-2.02	105.67	110.35
5	F	36	MAN	O2-C2-C3	-2.02	105.68	110.35
5	F	38	MAN	O2-C2-C3	-2.02	105.68	110.35
5	D	38	MAN	O2-C2-C3	-2.02	105.69	110.35
5	D	36	MAN	O2-C2-C3	-2.01	105.69	110.35

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	41	NAG	O5-C5-C6-O6
4	E	41	NAG	O5-C5-C6-O6
4	F	41	NAG	O5-C5-C6-O6
4	D	41	NAG	C4-C5-C6-O6
4	E	41	NAG	C4-C5-C6-O6
4	F	41	NAG	C4-C5-C6-O6
4	D	26	NAG	C4-C5-C6-O6
4	E	26	NAG	C4-C5-C6-O6
4	F	26	NAG	C4-C5-C6-O6
5	D	36	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	E	36	MAN	O5-C5-C6-O6
5	F	36	MAN	O5-C5-C6-O6
4	D	26	NAG	O5-C5-C6-O6
4	E	26	NAG	O5-C5-C6-O6
4	F	26	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	a	1
2	b	1
2	c	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	a	834:ILE	C	910:GLY	N	10.81
1	b	834:ILE	C	910:GLY	N	10.81
1	c	834:ILE	C	910:GLY	N	10.81

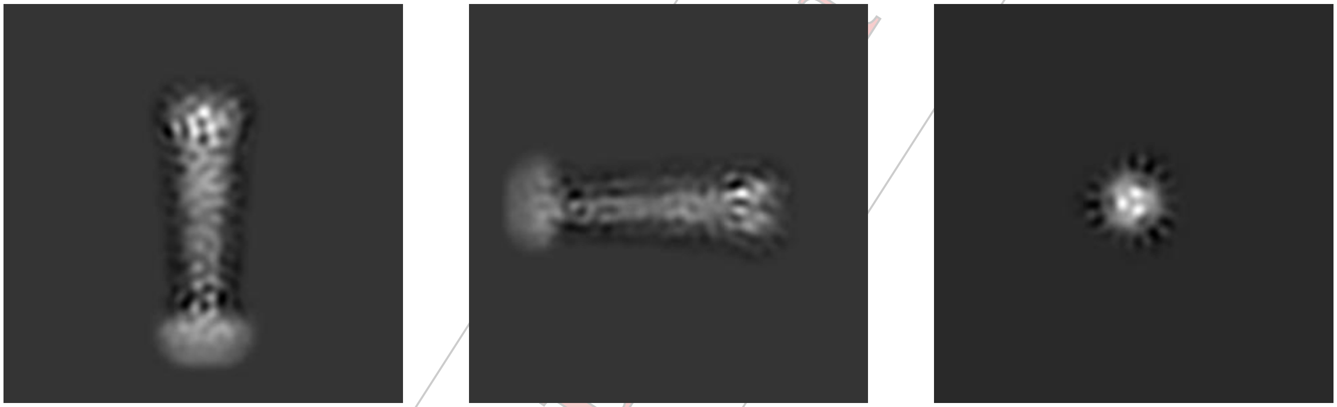
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry D_1300021032. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections ⓘ

6.1.1 Primary map



X Y Z

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

6.2 Central slices ⓘ

6.2.1 Primary map

X Index: 72 Y Index: 72 Z Index: 72

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map

X Index: 74 Y Index: 72 Z Index: 98

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

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

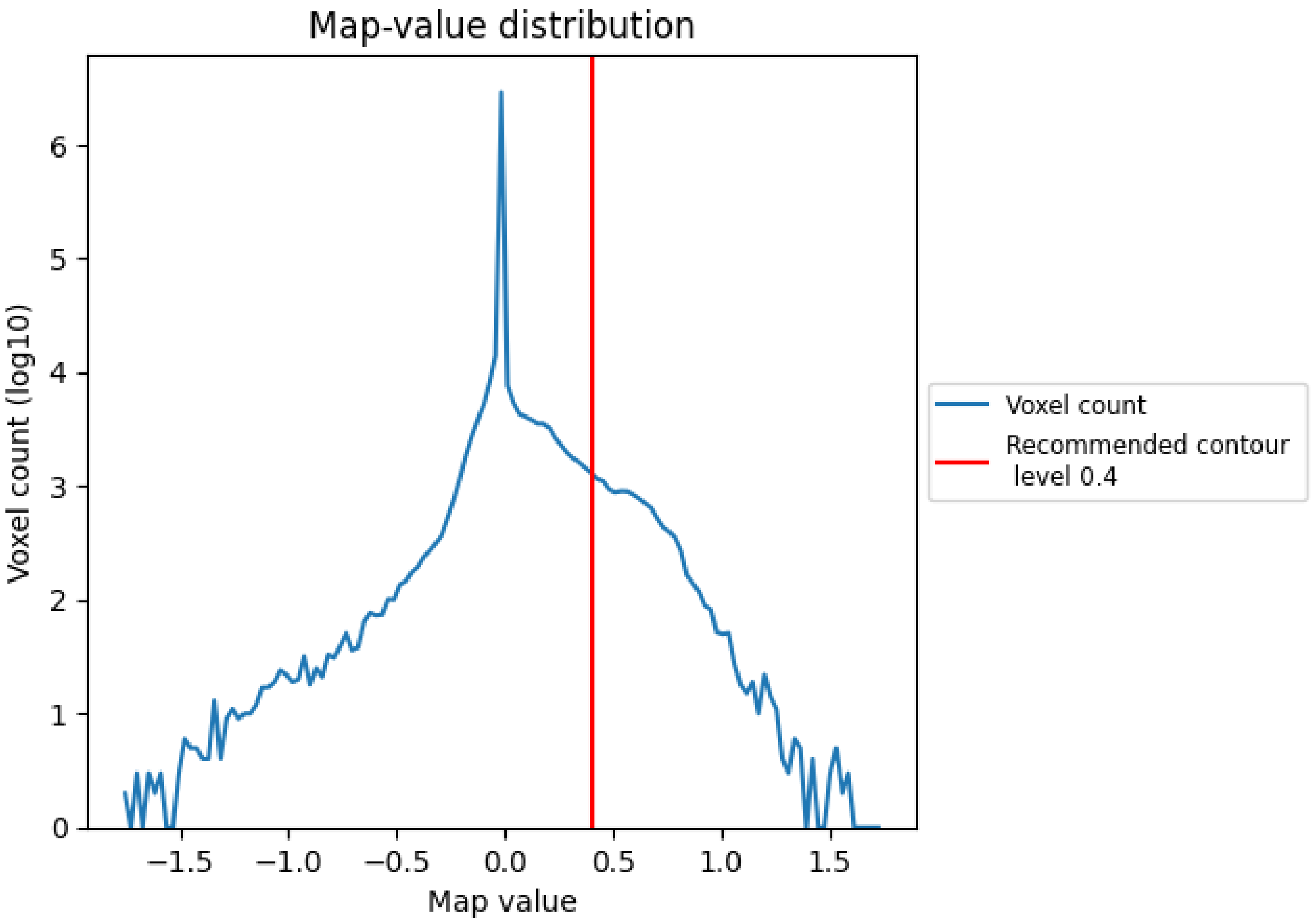
6.5 Mask visualisation ⓘ

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

7 Map analysis (i)

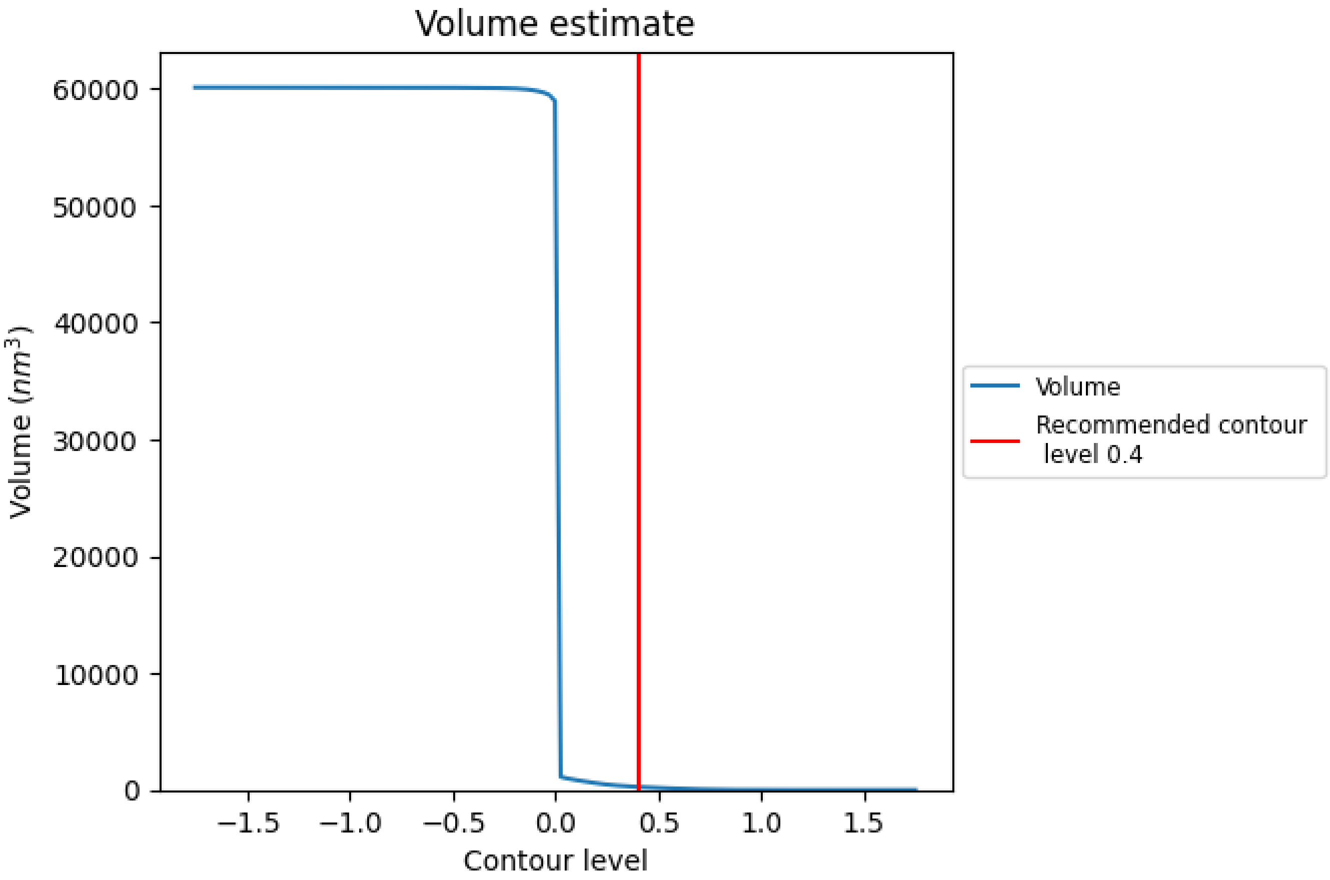
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

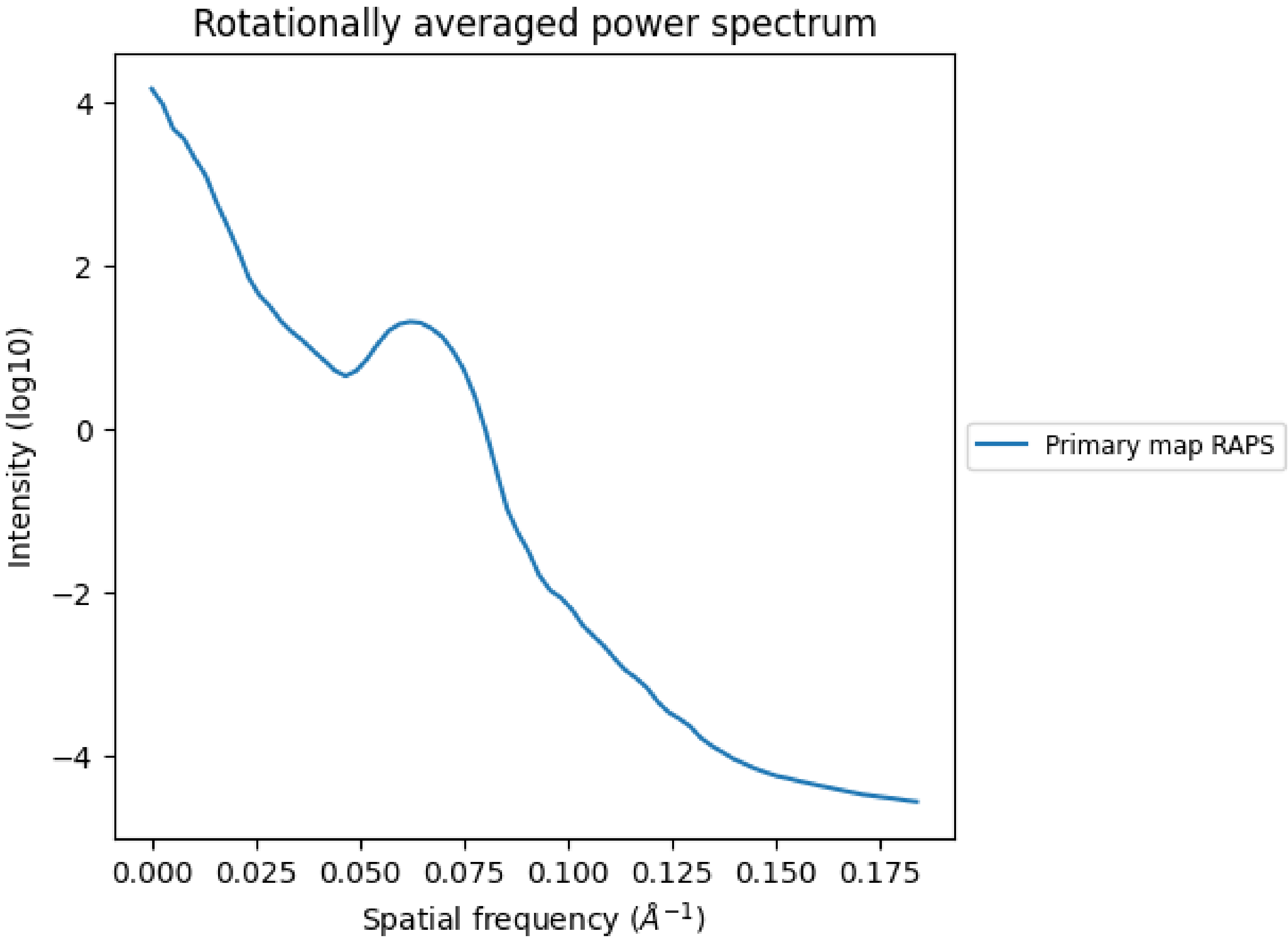
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 261 nm^3; this corresponds to an approximate mass of 236 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.

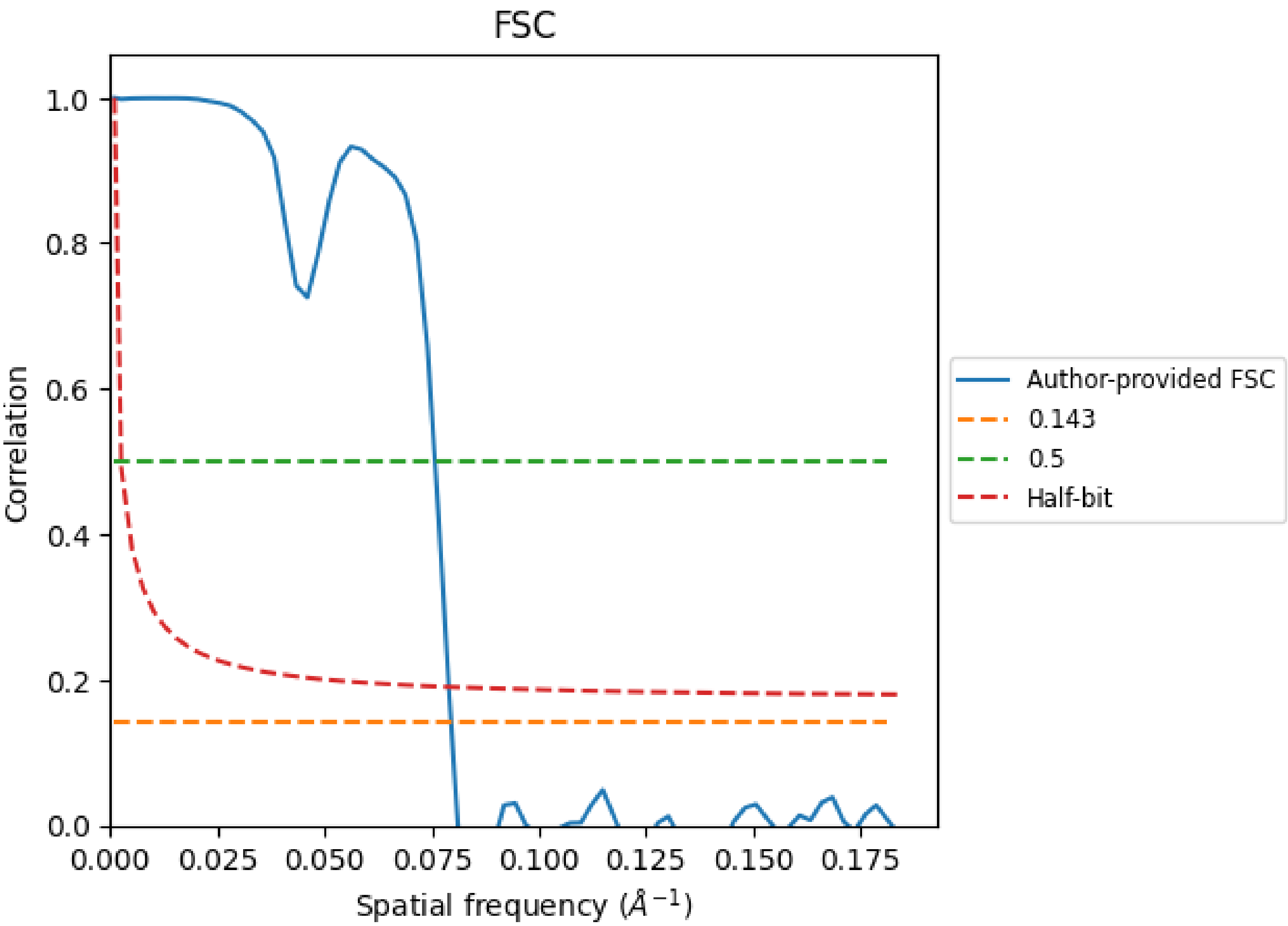
7.3 Rotationally averaged power spectrum ⓘ



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 ⓘ



8.2 Resolution estimates (i)

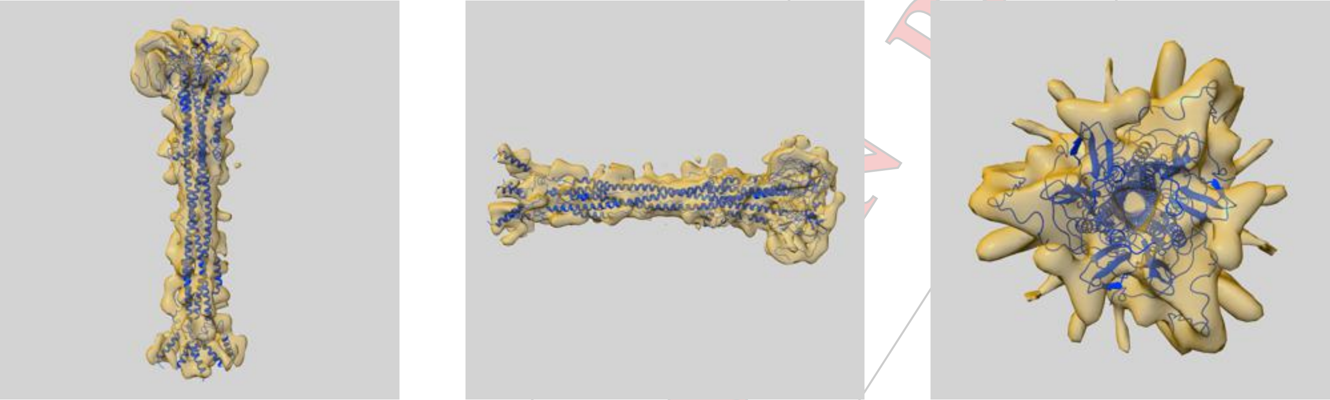
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	12.99	13.66	13.07
Calculated*	-	-	-

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

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map D_1300021032 and PDB model D_1300021032. Per-residue inclusion information can be found in section 3 on page 7.

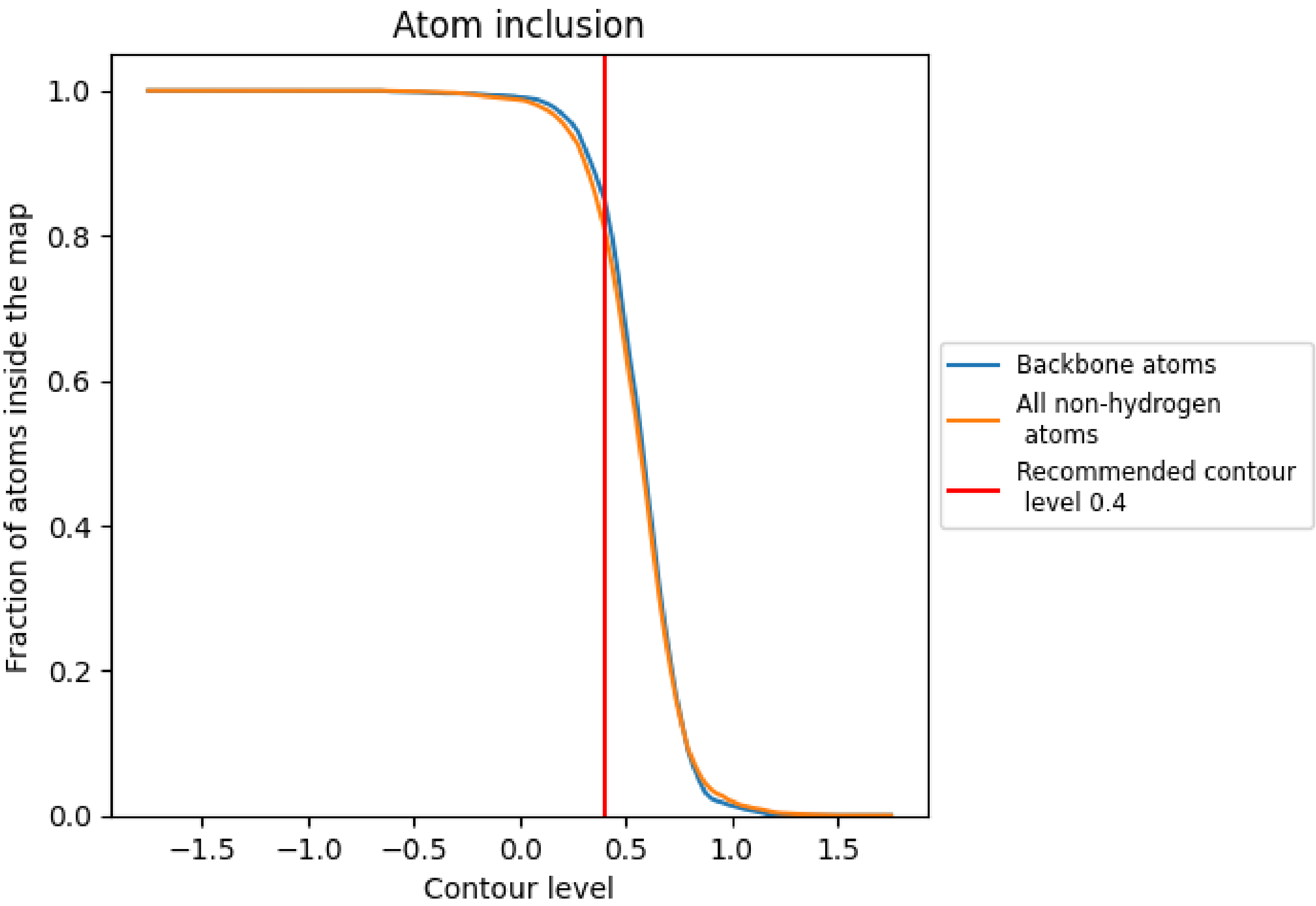
9.1 Map-model overlay ⓘ



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.4 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 ⓘ



At the recommended contour level, 85% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.