



## wwPDB EM Validation Summary Report ⓘ

Jun 22, 2022 – 07:15 am BST

PDB ID : 7OIX  
EMDB ID : EMD-12935  
Title : Structure of thermostable human MFSD2A in complex with thermostable human Sync2  
Authors : Martinez-Molledo, M.; Reyes, N.  
Deposited on : 2021-05-12  
Resolution : 3.60 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev8  
Mogul : 1.8.4, 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) : 2.29

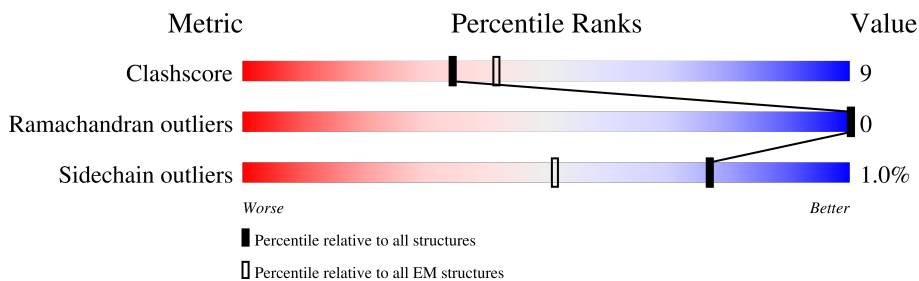
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.60 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  $\geq 3$ , 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	538	
2	B	530	
3	C	5	
4	D	7	

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 5869 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 Syncytin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	265	2097	1335	364	385	13	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	128	THR	MET	conflict	UNP P60508
A	153	PRO	SER	conflict	UNP P60508
A	190	THR	SER	conflict	UNP P60508
A	486	PHE	LEU	conflict	UNP P60508
A	487	ILE	THR	conflict	UNP P60508

- Molecule 2 is a protein called Isoform 2 of Sodium-dependent lysophosphatidylcholine symporter 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	451	3558	2359	564	614	21	0	0

There are 22 discrepancies between the modelled and reference sequences:

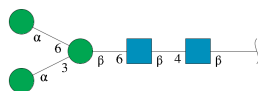
Chain	Residue	Modelled	Actual	Comment	Reference
B	43	ILE	VAL	conflict	UNP Q8NA29
B	51	VAL	LEU	conflict	UNP Q8NA29
B	102	PHE	LEU	conflict	UNP Q8NA29
B	108	SER	PRO	conflict	UNP Q8NA29
B	111	ARG	CYS	conflict	UNP Q8NA29
B	157	LEU	MET	conflict	UNP Q8NA29
B	177	SER	THR	conflict	UNP Q8NA29
B	240	ASN	LYS	conflict	UNP Q8NA29
B	250	ALA	VAL	conflict	UNP Q8NA29
B	251	SER	CYS	conflict	UNP Q8NA29
B	254	VAL	ILE	conflict	UNP Q8NA29

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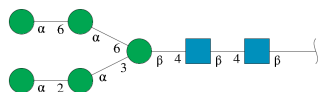
Chain	Residue	Modelled	Actual	Comment	Reference
B	261	THR	ILE	conflict	UNP Q8NA29
B	279	MET	ILE	conflict	UNP Q8NA29
B	280	SER	ALA	conflict	UNP Q8NA29
B	281	PHE	TYR	conflict	UNP Q8NA29
B	299	ALA	THR	conflict	UNP Q8NA29
B	316	ALA	VAL	conflict	UNP Q8NA29
B	383	VAL	ILE	conflict	UNP Q8NA29
B	386	VAL	ALA	conflict	UNP Q8NA29
B	420	SER	PHE	conflict	UNP Q8NA29
B	471	LYS	ASN	conflict	UNP Q8NA29
B	491	LEU	MET	conflict	UNP Q8NA29

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	C	5	61	34	2	25	0	0

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



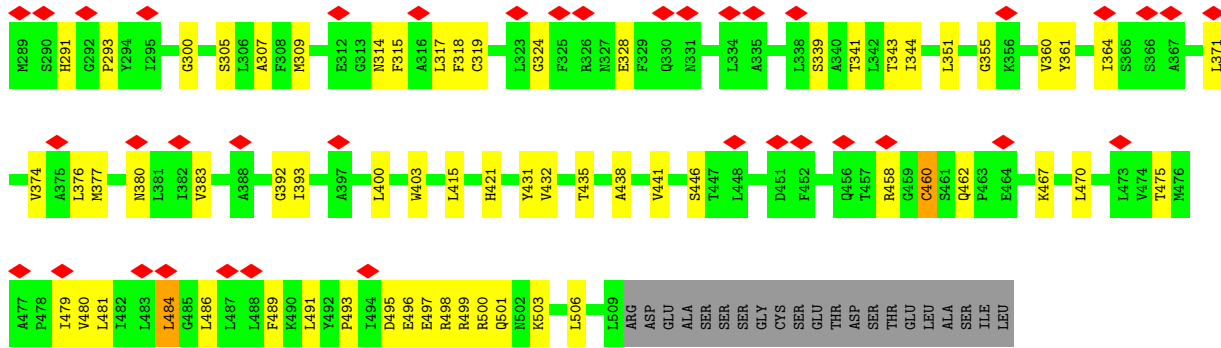
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	7	83	46	2	35	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms			AltConf	
			Total	C	N		O
5	A	1	Total	C	N	O	0
			70	40	5	25	
5	A	1	Total	C	N	O	0
			70	40	5	25	
5	A	1	Total	C	N	O	0
			70	40	5	25	
5	A	1	Total	C	N	O	0
			70	40	5	25	





- Molecule 3:  $\alpha$ -D-mannopyranose-(1-3)-[ $\alpha$ -D-mannopyranose-(1-6)] $\beta$ -D-mannopyranose-(1-6)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose

Chain C: 80% 20%



- Molecule 4:  $\alpha$ -D-mannopyranose-(1-2)- $\alpha$ -D-mannopyranose-(1-3)-[ $\alpha$ -D-mannopyranose-(1-6)- $\alpha$ -D-mannopyranose-(1-6)] $\beta$ -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose

Chain D: 14% 100%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	94703	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	47.1	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.224	Depositor
Minimum map value	-0.608	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.14	Depositor
Map size (Å)	341.88, 341.88, 341.88	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.814, 0.814, 0.814	Depositor



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, MAN, 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	0.40	0/2159	0.52	0/2948
2	B	0.37	0/3656	0.61	0/4981
All	All	0.38	0/5815	0.58	0/7929

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	2097	0	2035	28	0
2	B	3558	0	3603	78	0
3	C	61	0	52	2	0
4	D	83	0	70	0	0
5	A	70	0	65	1	0
All	All	5869	0	5825	103	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 9.

The worst 5 of 103 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)
2:B:351:LEU:HA	2:B:355:GLY:HA3	1.55	0.86
2:B:491:LEU:HG	2:B:493:PRO:HD2	1.61	0.83
2:B:344:ILE:HG23	2:B:400:LEU:HD22	1.72	0.70
2:B:70:TYR:OH	2:B:134:TRP:O	2.13	0.65
2:B:93:ASP:HB2	2:B:155:GLU:HG2	1.78	0.64

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	263/538 (49%)	252 (96%)	11 (4%)	0	100	100
2	B	447/530 (84%)	433 (97%)	14 (3%)	0	100	100
All	All	710/1068 (66%)	685 (96%)	25 (4%)	0	100	100

There are no Ramachandran outliers to report.

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	238/469 (51%)	238 (100%)	0	100	100
2	B	383/447 (86%)	377 (98%)	6 (2%)	62	83
All	All	621/916 (68%)	615 (99%)	6 (1%)	77	88

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	317	LEU
2	B	460	CYS
2	B	484	LEU
2	B	136	VAL
2	B	114	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	414	HIS
2	B	419	HIS
2	B	462	GLN
2	B	201	GLN
2	B	214	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](#)

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	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	NAG	C	1	1,3	14,14,15	0.54	0	17,19,21	0.42	0
3	NAG	C	2	3	14,14,15	1.22	1 (7%)	17,19,21	2.03	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	BMA	C	3	3	11,11,12	0.67	0	15,15,17	1.41	3 (20%)
3	MAN	C	4	3	11,11,12	0.57	0	15,15,17	1.39	2 (13%)
3	MAN	C	5	3	11,11,12	1.04	1 (9%)	15,15,17	1.09	2 (13%)
4	NAG	D	1	1,4	14,14,15	0.61	0	17,19,21	0.77	1 (5%)
4	NAG	D	2	4	14,14,15	0.57	1 (7%)	17,19,21	0.44	0
4	BMA	D	3	4	11,11,12	1.12	1 (9%)	15,15,17	1.13	2 (13%)
4	MAN	D	4	4	11,11,12	0.73	0	15,15,17	1.21	2 (13%)
4	MAN	D	5	4	11,11,12	0.93	1 (9%)	15,15,17	1.71	4 (26%)
4	MAN	D	6	4	11,11,12	1.23	2 (18%)	15,15,17	1.23	3 (20%)
4	MAN	D	7	4	11,11,12	0.79	0	15,15,17	1.17	2 (13%)

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	C	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	BMA	C	3	3	-	2/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1
3	MAN	C	5	3	-	2/2/19/22	0/1/1/1
4	NAG	D	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	3/6/23/26	0/1/1/1
4	BMA	D	3	4	-	2/2/19/22	0/1/1/1
4	MAN	D	4	4	-	2/2/19/22	0/1/1/1
4	MAN	D	5	4	-	2/2/19/22	0/1/1/1
4	MAN	D	6	4	-	2/2/19/22	0/1/1/1
4	MAN	D	7	4	-	2/2/19/22	1/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	NAG	O5-C1	4.03	1.50	1.43
4	D	6	MAN	O5-C1	-3.14	1.38	1.43
3	C	5	MAN	O5-C1	-2.89	1.39	1.43
4	D	3	BMA	O5-C1	-2.88	1.39	1.43
4	D	5	MAN	C1-C2	2.77	1.58	1.52

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	NAG	C1-O5-C5	8.22	123.32	112.19
3	C	4	MAN	C1-O5-C5	4.21	117.90	112.19
4	D	5	MAN	C1-C2-C3	3.77	114.30	109.67
4	D	4	MAN	C1-O5-C5	3.61	117.09	112.19
4	D	5	MAN	C1-O5-C5	3.41	116.81	112.19

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	3	BMA	C4-C5-C6-O6
3	C	5	MAN	O5-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
3	C	5	MAN	C4-C5-C6-O6
3	C	3	BMA	O5-C5-C6-O6

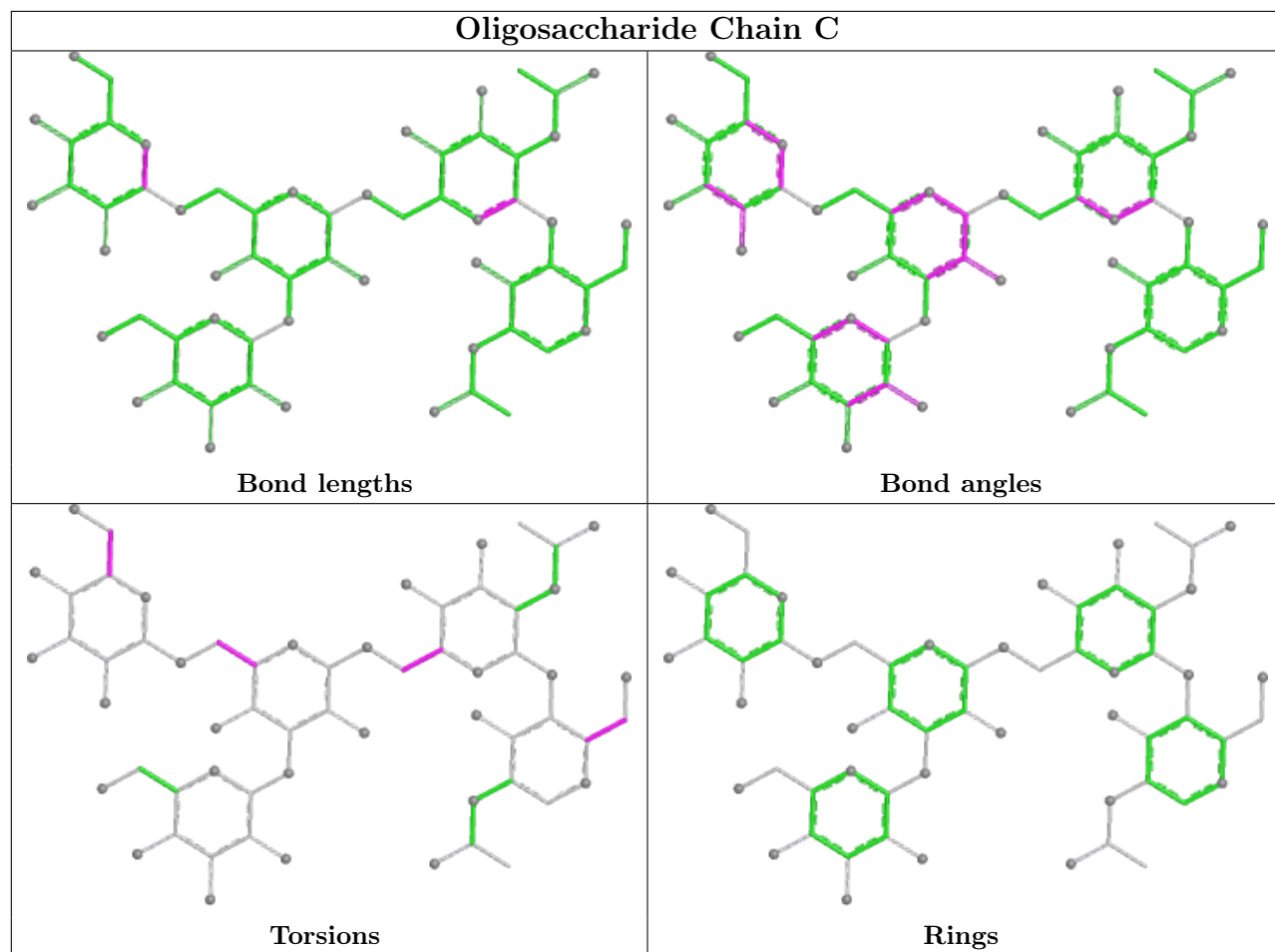
All (1) ring outliers are listed below:

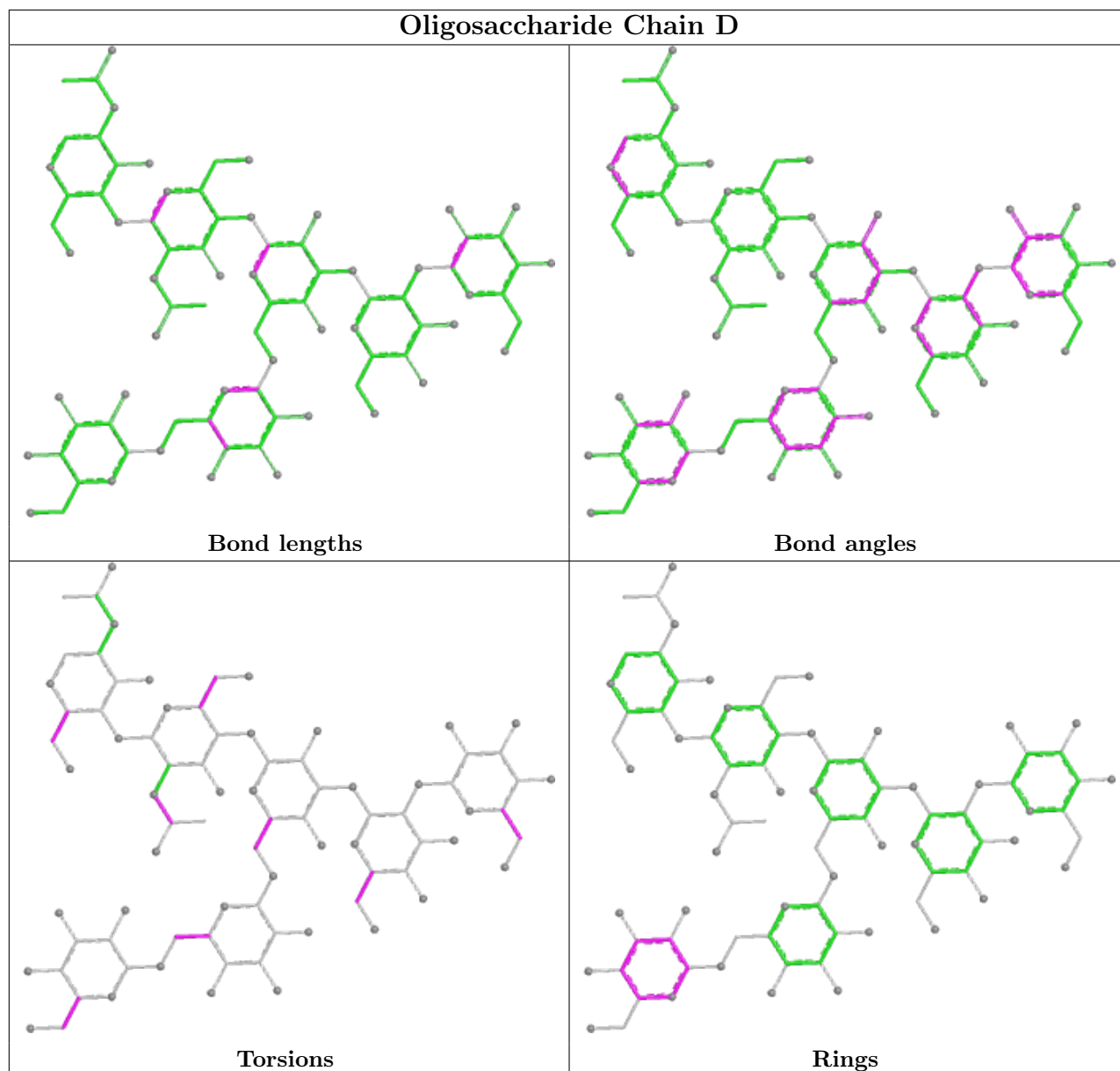
Mol	Chain	Res	Type	Atoms
4	D	7	MAN	C1-C2-C3-C4-C5-O5

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	NAG	1	0
3	C	2	NAG	1	0

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](#)

5 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
5	NAG	A	602	1	14,14,15	0.47	0	17,19,21	1.09	1 (5%)
5	NAG	A	601	1	14,14,15	0.45	0	17,19,21	0.45	0
5	NAG	A	604	1	14,14,15	0.49	0	17,19,21	1.08	1 (5%)
5	NAG	A	605	1	14,14,15	0.31	0	17,19,21	0.67	0
5	NAG	A	603	1	14,14,15	0.68	0	17,19,21	0.80	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
5	NAG	A	602	1	-	2/6/23/26	0/1/1/1
5	NAG	A	601	1	-	1/6/23/26	0/1/1/1
5	NAG	A	604	1	-	2/6/23/26	0/1/1/1
5	NAG	A	605	1	-	2/6/23/26	0/1/1/1
5	NAG	A	603	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	602	NAG	C1-O5-C5	4.13	117.78	112.19
5	A	604	NAG	C1-O5-C5	3.75	117.28	112.19

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	604	NAG	C4-C5-C6-O6
5	A	605	NAG	O5-C5-C6-O6
5	A	603	NAG	O5-C5-C6-O6
5	A	602	NAG	C8-C7-N2-C2
5	A	602	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	605	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.

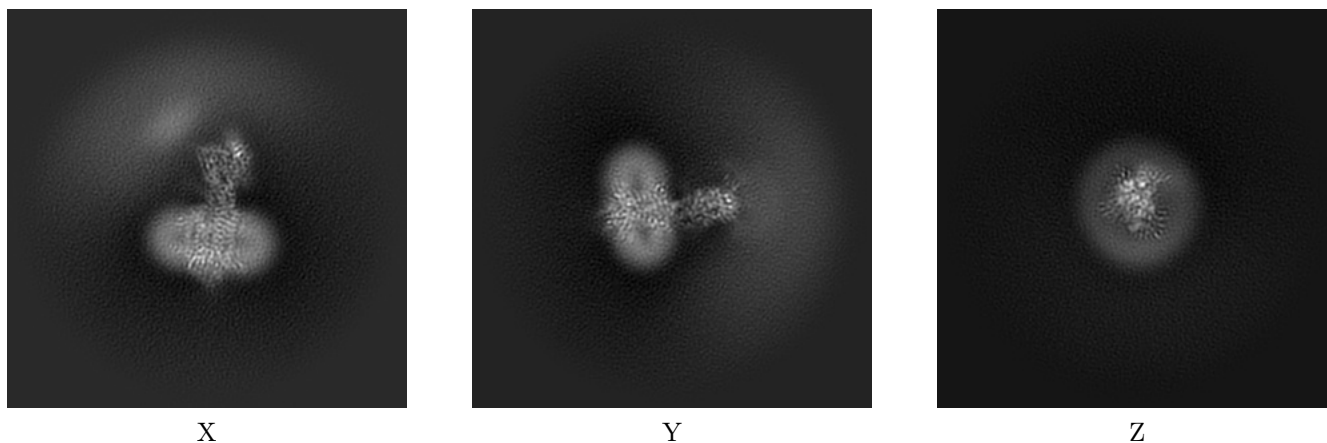
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12935. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

### 6.1 Orthogonal projections [i](#)

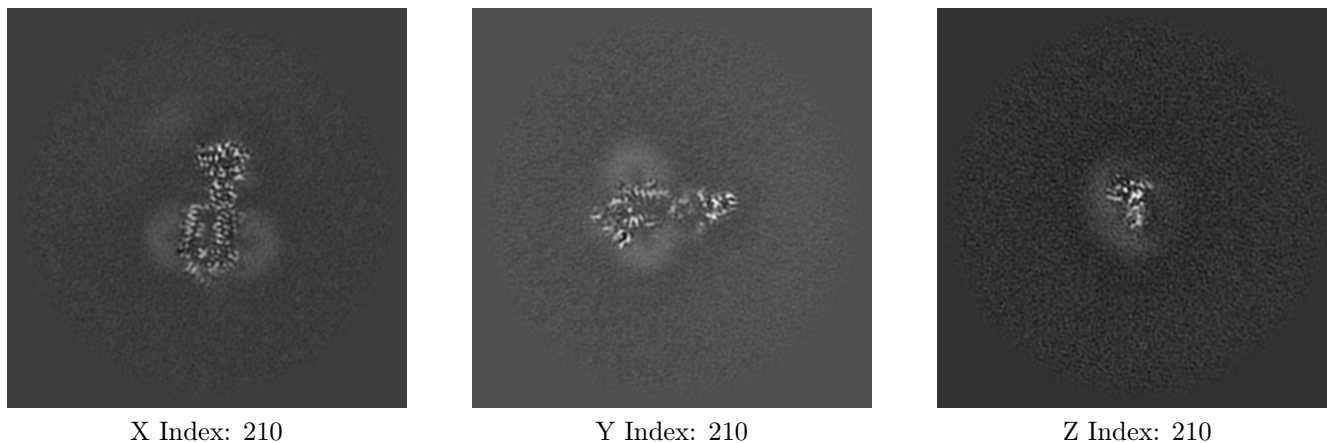
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

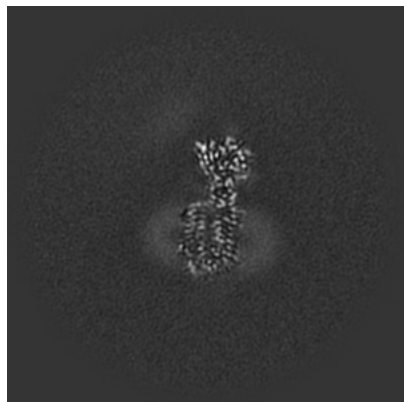
#### 6.2.1 Primary map



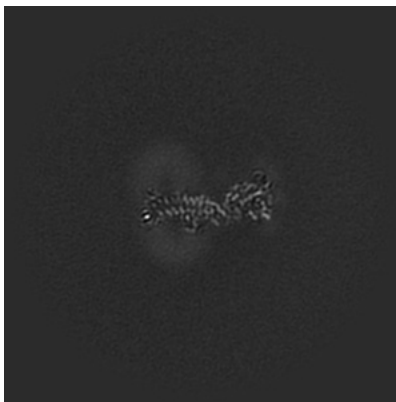
The images above show central slices of the map in three orthogonal directions.

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

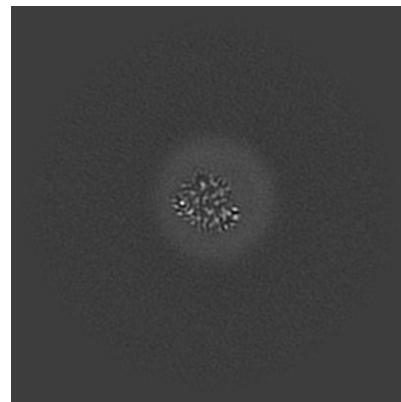
### 6.3.1 Primary map



X Index: 212



Y Index: 237



Z Index: 158

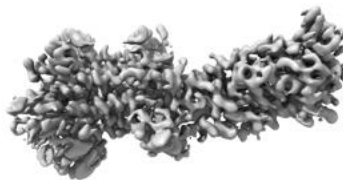
The images above show the largest variance slices of the map in three orthogonal directions.

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

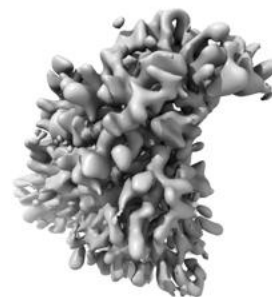
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.14. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

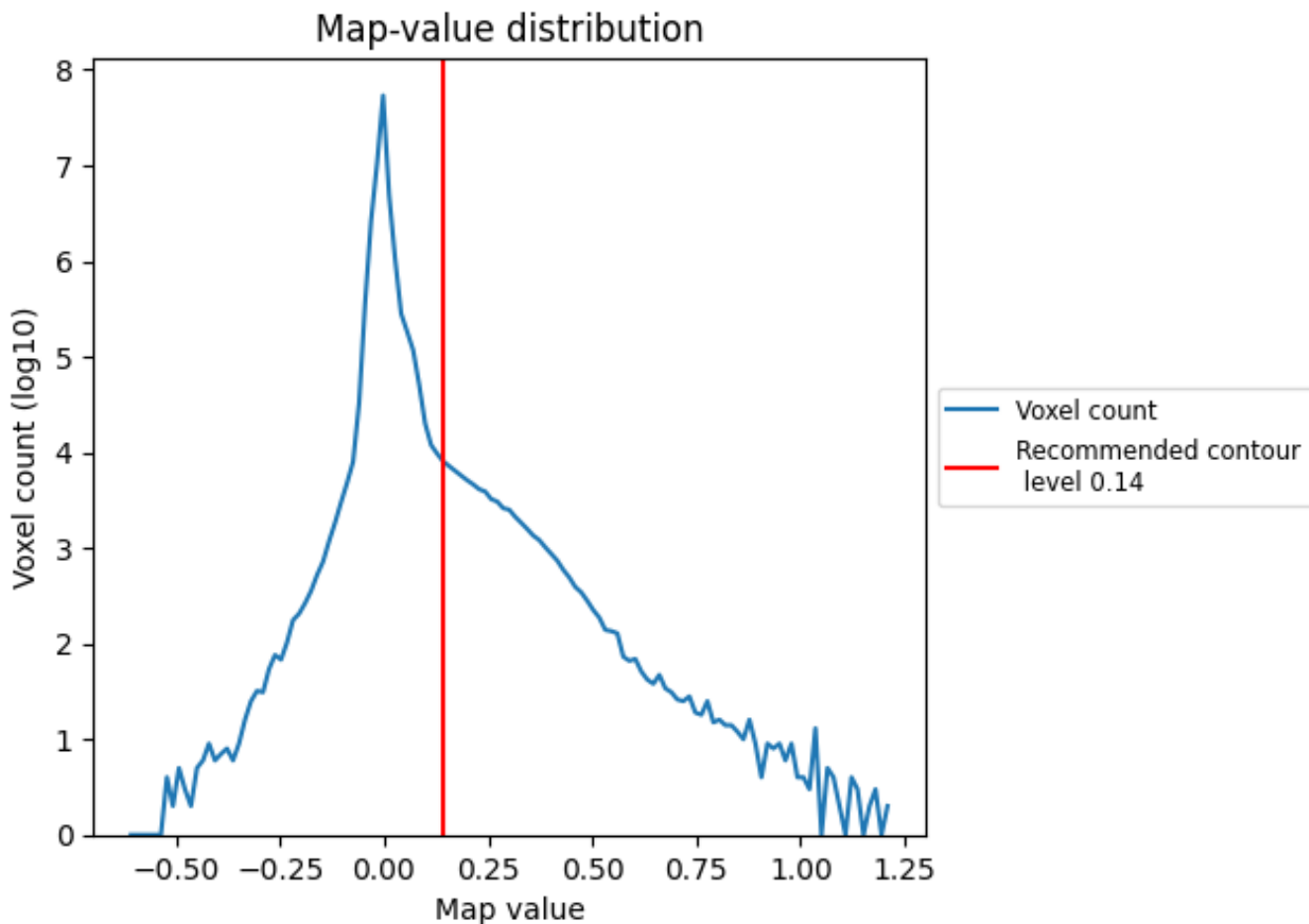
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

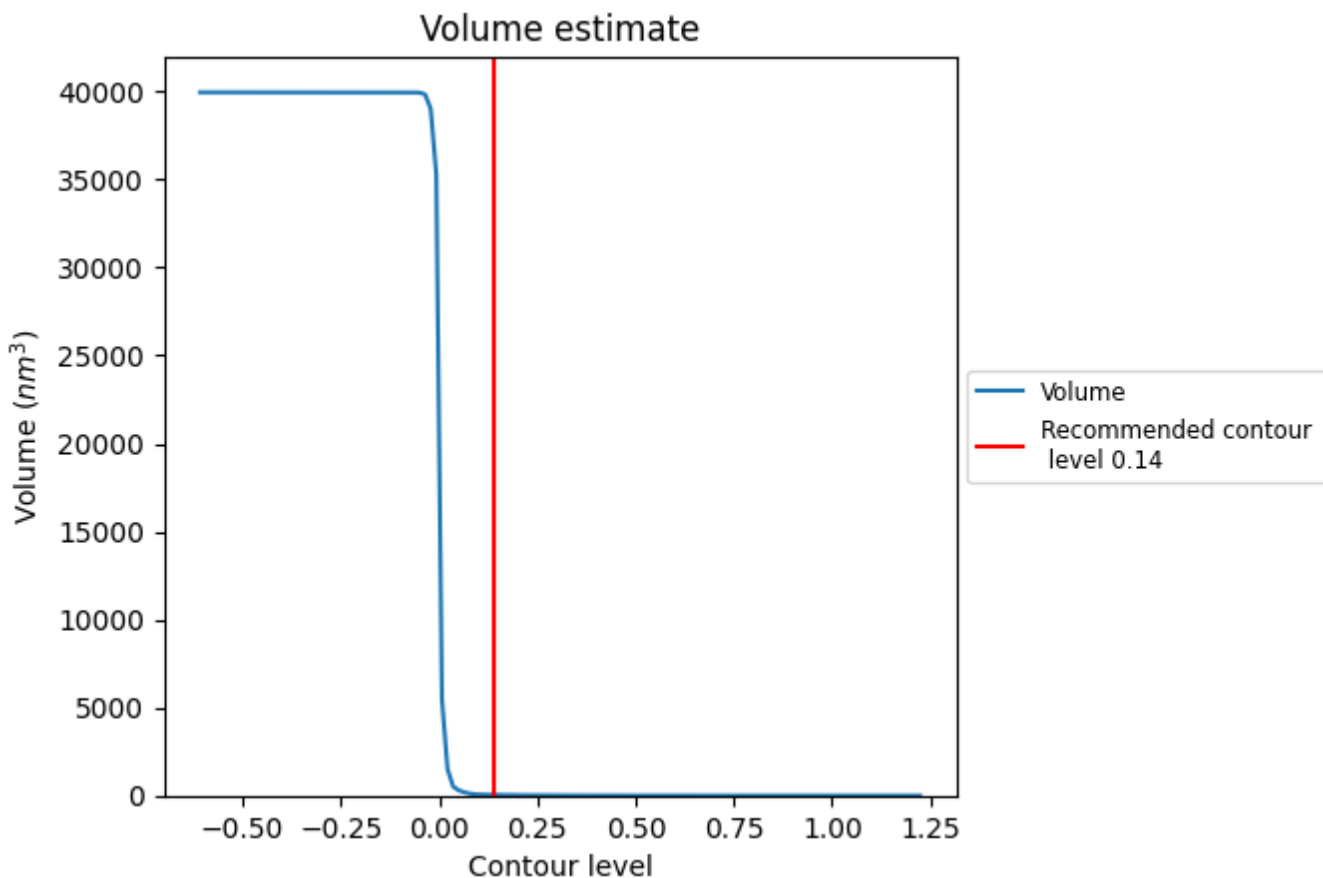
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

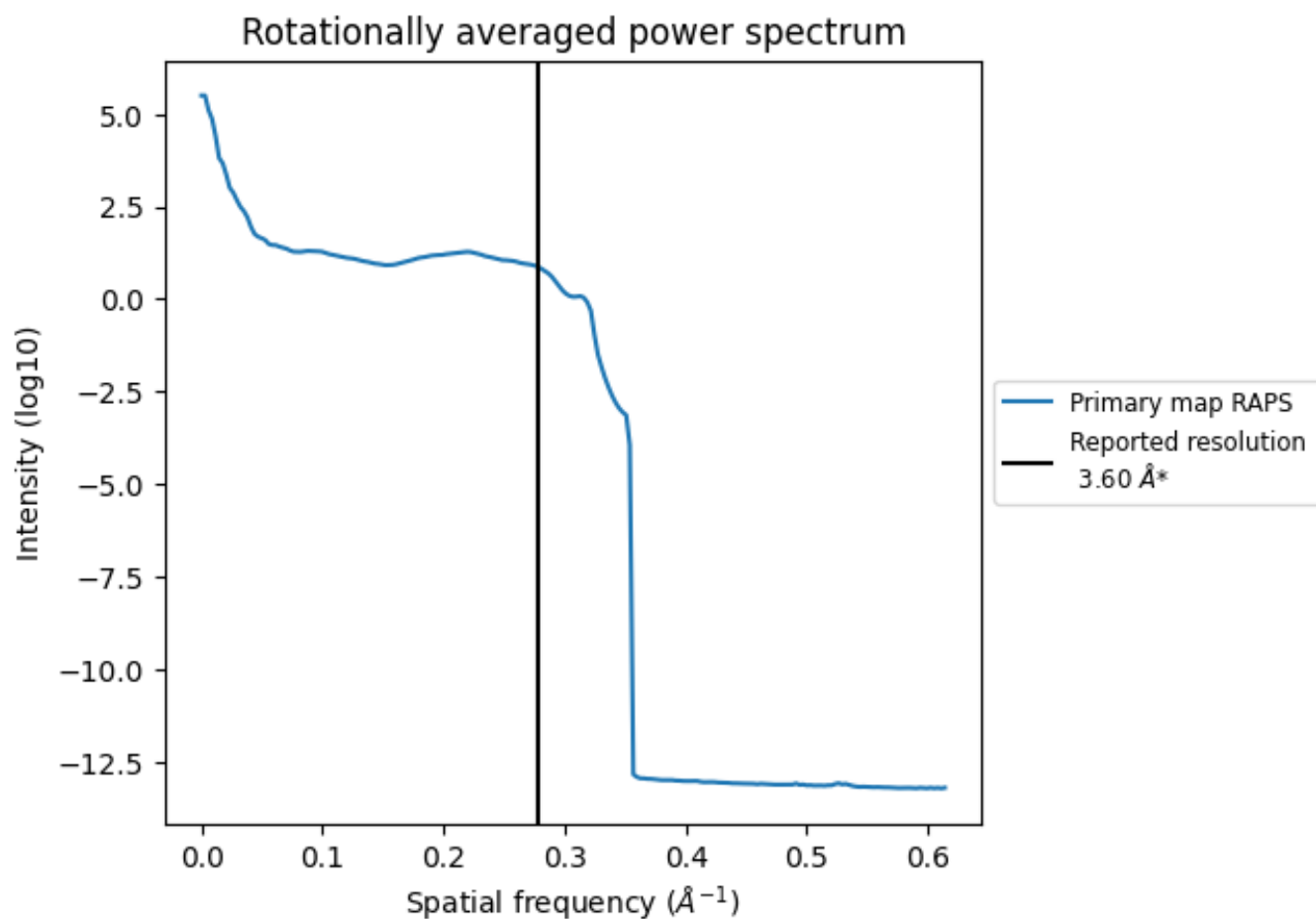
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 39 nm<sup>3</sup>; this corresponds to an approximate mass of 35 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  $0.278 \text{\AA}^{-1}$

## 8 Fourier-Shell correlation

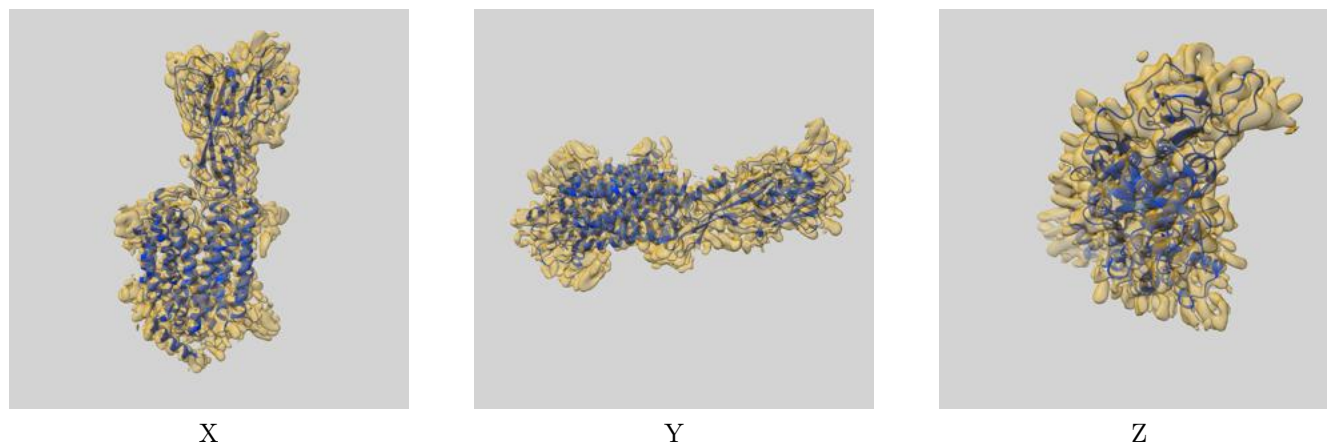
This section was not generated. No FSC curve or half-maps provided.



## 9 Map-model fit [i](#)

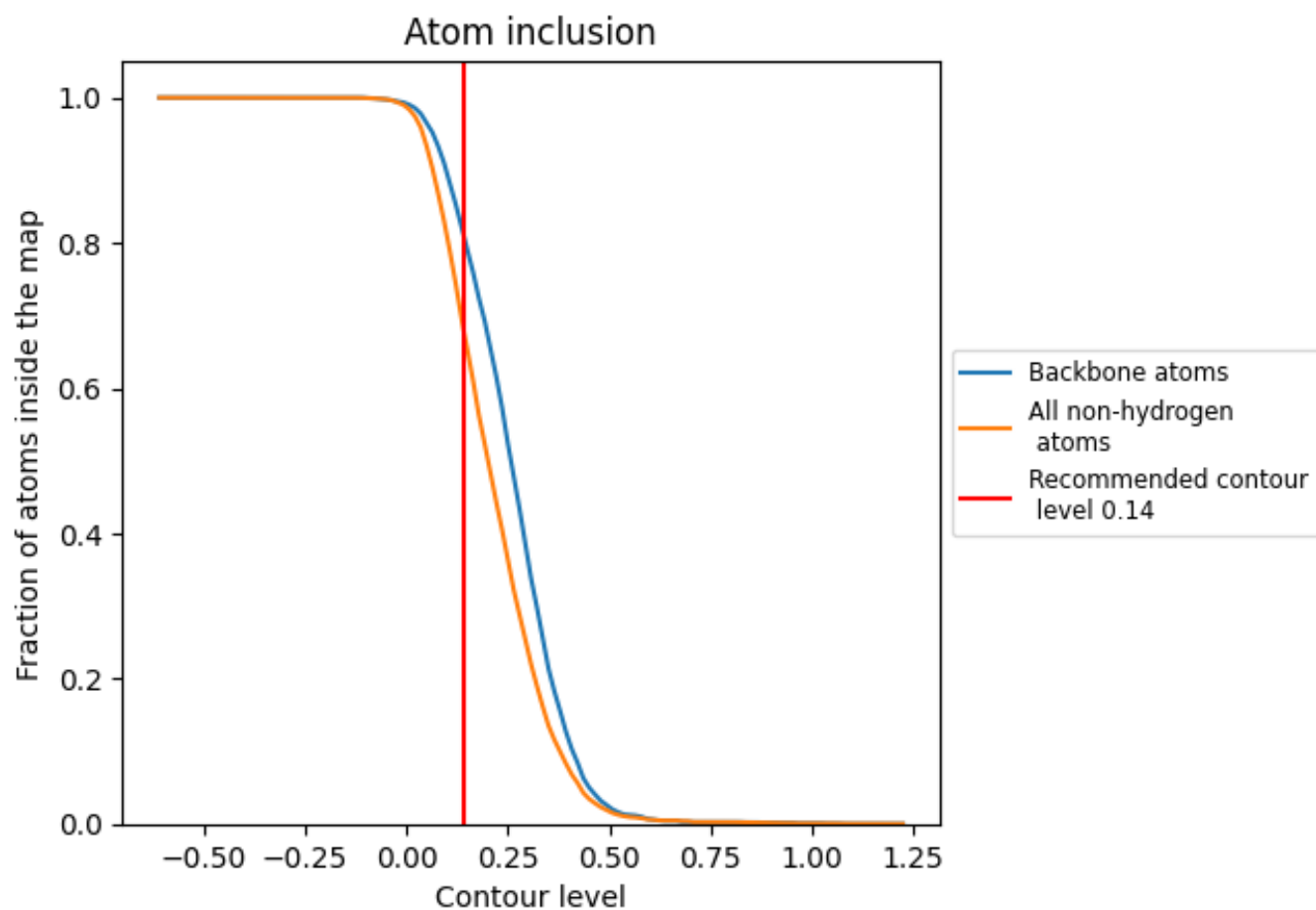
This section contains information regarding the fit between EMDB map EMD-12935 and PDB model 7OIX. Per-residue inclusion information can be found in section 3 on page 6.

### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.14 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, 81% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.