

wwPDB EM Validation Summary Report (i)

Jun 8, 2024 – 09:24 PM EDT

PDB ID	:	8SX3
EMDB ID	:	EMD-40825
Title	:	10E8-GT10.2 immunogen in complex with human Fab 10E8 and mouse Fab
		W6-10
Authors	:	Huang, J.; Ozorowski, G.; Ward, A.B.
Deposited on		
Resolution	:	4.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/EMValidationReportHelp with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

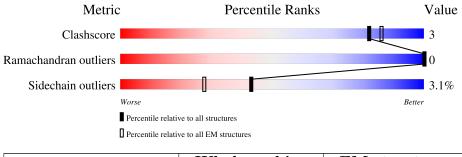
EMDB validation analysis	:	0.0.1. dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 4.00 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	EM structures
Metric	$(\# {\rm Entries})$	$(\# { m Entries})$
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	Δ	224	8%						
	A	224	13%	46%	5%	48%			
2	В	214		46%	•	50%			
3	С	187	17%	729	6	10% • 18%			
4	Н	234	10%	50%	5%	45%			
5	L	215	6%	45%	5%	50%			
6	D	2		50%	100%				



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 4816 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 W6-10 mouse Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	А	117	Total 913	C 588	N 148	0 174	${ m S} { m 3}$	0	0

• Molecule 2 is a protein called W6-10 mouse light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	В	107	Total	С	Ν	0	\mathbf{S}	0	0
	D	107	821	518	138	162	3	0	0

• Molecule 3 is a protein called 10E8-GT10.2 immunogen.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	С	154	Total 1236	C 791	N 212	0 229	S 4	0	0

• Molecule 4 is a protein called 10E8 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Н	129	Total 1016	C 652	N 170	0 189	${f S}{5}$	0	0

• Molecule 5 is a protein called 10E8 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	107	Total 802	C 494	N 146	O 160	${S \over 2}$	0	0

• Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.





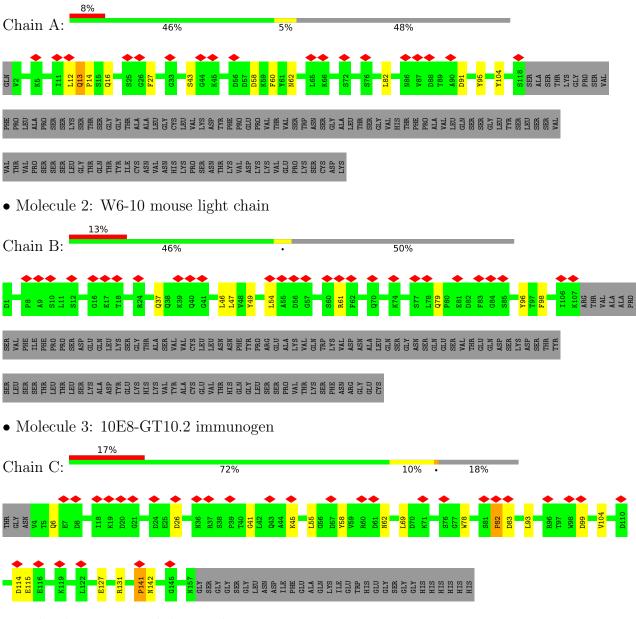
Mol	Chain	Residues	Atoms				AltConf	Trace
6	D	2	Total 28	C 16	N 2	O 10	0	0



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: W6-10 mouse Fab heavy chain



• Molecule 4: 10E8 Fab heavy chain



Chain H:	10%	50%	5%	45%	
GLU V2 E6 L11	S17 S23 A24 F27 F28 F28	D30 N31 R38 G45 E46 C45 C45 C45 C45 C49	G57 G68 N76 S77 T78 N79 B84	N87 L88 R89 M90 E91 A99 A99 D106	X111 E115 R123 C124 SER ALA
SER THR LYS GLY PRO SER VAL PHE	PRO LEU ALA PRO SER SER LYS SER SER SER	GLY GLY THR ALA ALA ALA CVS CVS CVS CVS CVS CVS CVS CVS CVS TYS TYR	PHE PRO GLU PRO PRO VAL VAL SER ASN SER SER GLY	ALA LEU THR SER GLY VAL HTS PHE PRO ALA VAL	GLN SER SER GLY
LEU TYR SER LEU SER SER VAL VAL	THR VAL PRO SER SER SER SER LEU GLY GLN	THR TYR TYR TYR CYS CYS CYS ASN VAL ASN FRO SER ASN THR	LYS VAL ASP LYS LYS LYS VAL GLU PRO LYS SER SER CYS		
	5: 10E8 light	chain			
Chain L:	% 45	5%	50	0%	
SER TYR E2 C14 C14 R15	T1 6 D2 4 H2 9 K3 6 G3 9	862 168 168 168 166 168 166 166 166 166 166	A77 A78 A78 B80 B80 B81 B81 B81 B81 B81 B81 B81 A81 A81 A81 A81 A81 A81 A81 A81 A81 A	ALLOS CLA CLA CLA CLA CLA CLA ALA ALA ALA ALA	PRO SER SER SLU GLU CLU CLU CLU
ALA ASN LYS LYS ALA THR LEU VAL CYS	LEU ILE SER ASP PHE PHE PRO GLY ALA VAL	THR VAL ALA TRP TRP LYS ALA SER SER PRO VAL VAL VAL	GLY VAL CLU CLU THR THR THR PRO SER CLY SER SER ASN	ASN LYS TYR ALA ALA ALA SER SER TYR LEU LEU SER LEU	GLU GLN TRP LYS
SER HIS ARG SER TYR SER CYS GLN	VAL THR HIS GLU GLY SER THR VAL GLU LYS	THR VAL ALA PRO FRO GLU CYS SER			

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

50% Chain D: 100%



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	56628	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose $(e^-/\text{\AA}^2)$	53	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.403	Depositor
Minimum map value	-0.274	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	301.6, 301.6, 301.6	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles $(^{\circ})$	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.725, 0.725, 0.725	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

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	Bo	nd lengths	Bond angles		
			# Z > 5	RMSZ	# Z > 5	
1	А	0.36	0/937	0.80	2/1274~(0.2%)	
2	В	0.39	0/842	0.82	2/1143~(0.2%)	
3	С	0.51	2/1262~(0.2%)	0.97	7/1714~(0.4%)	
4	Н	0.42	0/1048	0.88	0/1423	
5	L	0.37	0/816	0.90	1/1101~(0.1%)	
All	All	0.42	2/4905~(0.0%)	0.88	12/6655~(0.2%)	

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	С	141	PRO	CG-CD	-11.24	1.13	1.50
3	С	141	PRO	N-CD	5.72	1.55	1.47

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	С	141	PRO	CA-N-CD	-12.00	94.70	111.50
3	С	141	PRO	N-CD-CG	-11.08	86.58	103.20
3	С	82	PRO	CA-N-CD	-8.90	99.04	111.50
3	С	141	PRO	CA-CB-CG	-7.09	90.52	104.00
1	А	60	PHE	CB-CG-CD2	5.89	124.92	120.80

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	913	0	891	4	0
2	В	821	0	783	3	0
3	С	1236	0	1240	9	0
4	Н	1016	0	952	7	0
5	L	802	0	783	5	0
6	D	28	0	25	0	0
All	All	4816	0	4674	24	0

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.

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 24 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)
5:L:75:GLY:O	5:L:77:GLN:NE2	2.14	0.78
1:A:13:GLN:NE2	1:A:14:PRO:O	2.20	0.74
1:A:13:GLN:NE2	1:A:16:GLN:OE1	2.24	0.70
1:A:104:TYR:OH	3:C:131:ARG:NH1	2.26	0.68
1:A:91:ASP:OD1	1:A:95:TYR:OH	2.16	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	А	115/224~(51%)	111 (96%)	4 (4%)	0	100 100
2	В	105/214~(49%)	103~(98%)	2(2%)	0	100 100
3	С	152/187~(81%)	150 (99%)	2(1%)	0	100 100

Continued on next page...



001000	continued from proto do pagom										
Mol	Chain	Analysed Favoured Allowed		Allowed	Outliers Percent						
4	Н	127/234~(54%)	127 (100%)	0	0	100 100					
5	L	105/215~(49%)	102 (97%)	3(3%)	0	100 100					
All	All	604/1074~(56%)	593~(98%)	11 (2%)	0	100 100					

Continued from previous page...

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	Analysed Rotameric Outl		Percentiles
1	А	100/193~(52%)	94~(94%)	6~(6%)	19 47
2	В	89/185~(48%)	87~(98%)	2(2%)	52 71
3	С	136/160~(85%)	132 (97%)	4 (3%)	42 65
4	Н	105/196~(54%)	103~(98%)	2(2%)	57 75
5	L	86/179~(48%)	84 (98%)	2(2%)	50 70
All	All	516/913~(56%)	500~(97%)	16 (3%)	43 63

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	L	29	HIS
4	Н	105	TYR
3	С	6	GLN
4	Н	28	ASP
2	В	54	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

2 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	Dec	Link	Bo	Bond lengths		Bond angles		
IVIOI	туре	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
6	NAG	D	1	3,6	14,14,15	0.18	0	17,19,21	0.51	0
6	NAG	D	2	6	14,14,15	0.21	0	17,19,21	0.55	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
6	NAG	D	1	3,6	-	0/6/23/26	0/1/1/1
6	NAG	D	2	6	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

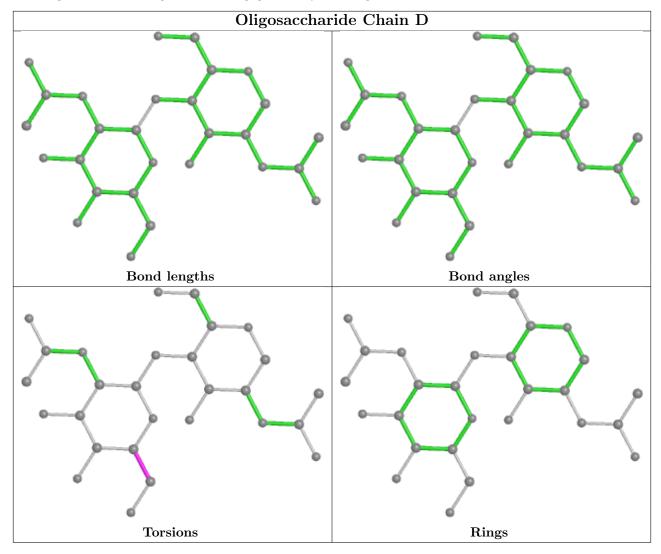
Mol	Chain	Res	Type	Atoms
6	D	2	NAG	C4-C5-C6-O6
6	D	2	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,





bond angles, torsion angles, and ring geometry for oligosaccharide.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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.



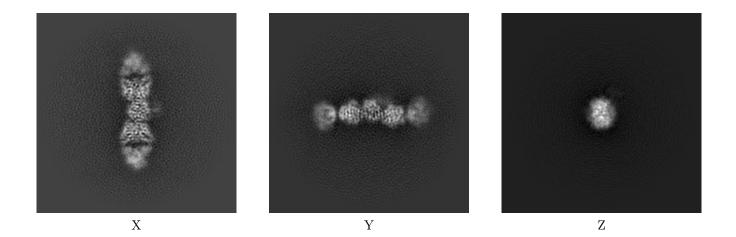
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-40825. These allow visual inspection of the internal detail of the map and identification of artifacts.

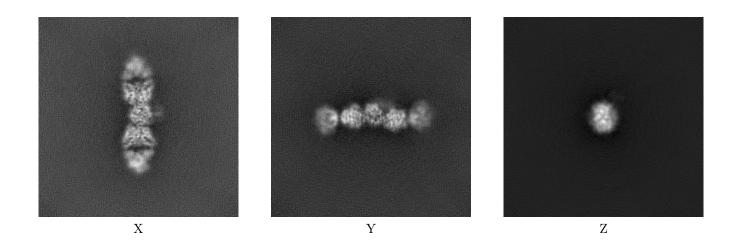
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

6.1.1 Primary map



6.1.2 Raw map

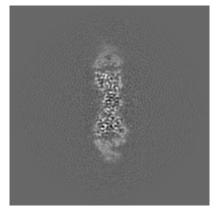


The images above show the map projected in three orthogonal directions.

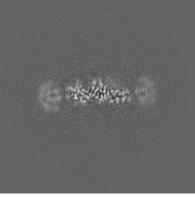


6.2 Central slices (i)

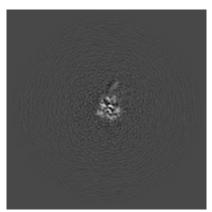
6.2.1 Primary map



X Index: 208

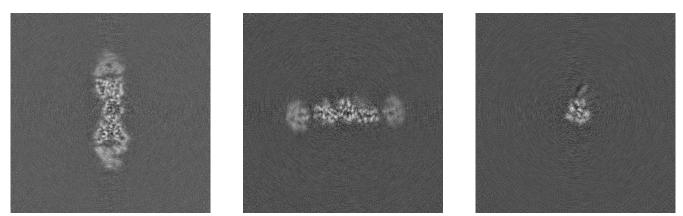


Y Index: 208



Z Index: 208

6.2.2 Raw map



X Index: 208

Y Index: 208

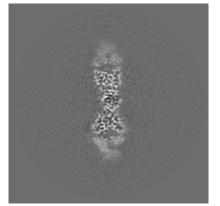
Z Index: 208

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

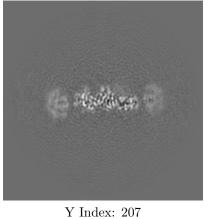


6.3 Largest variance slices (i)

6.3.1 Primary map



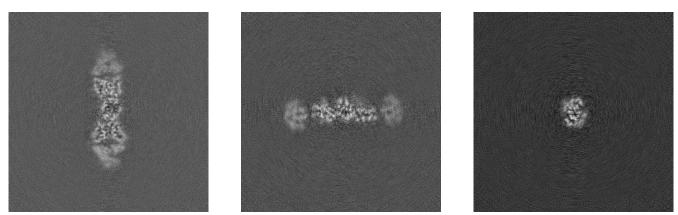
X Index: 206





Z Index: 167

6.3.2 Raw map



X Index: 207

Y Index: 208

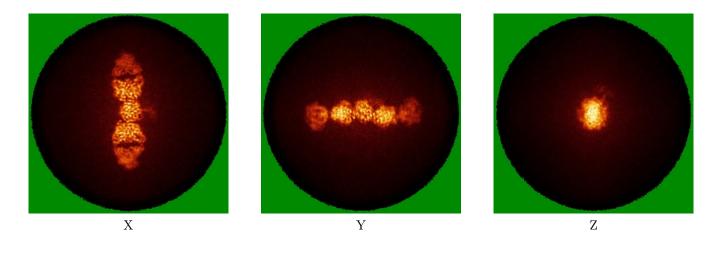
Z Index: 168

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

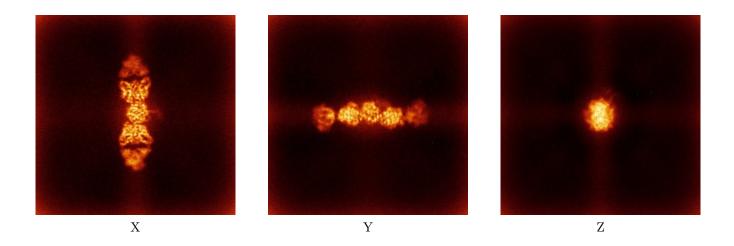


6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



6.4.2 Raw map

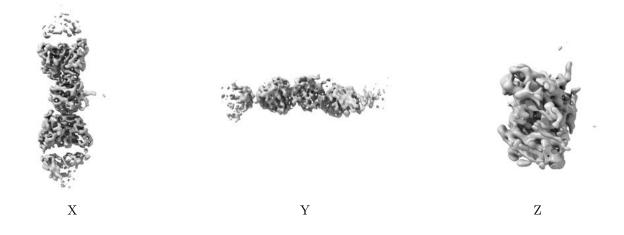


The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



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 0.1. 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.



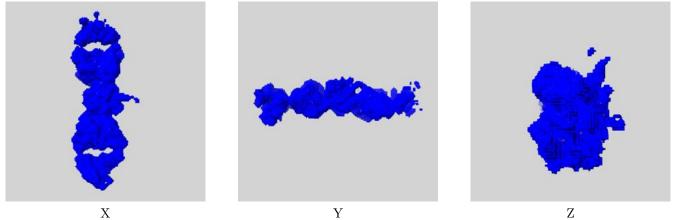
Mask visualisation (i) 6.6

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

A mask typically either:

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

$emd_{40825}msk_{1.map}$ (i) 6.6.1

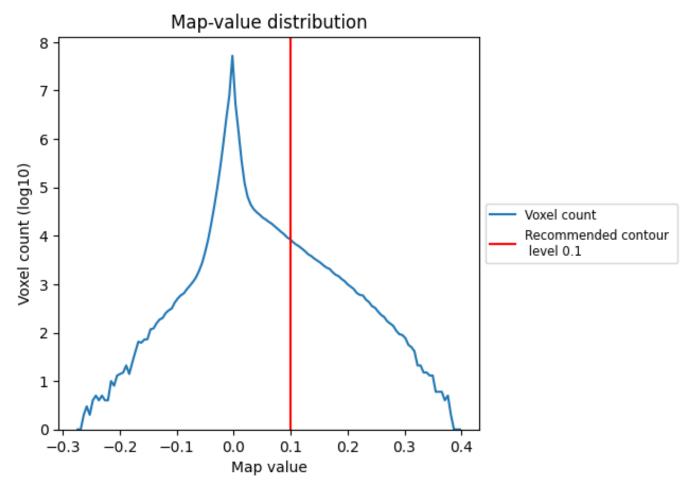




7 Map analysis (i)

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

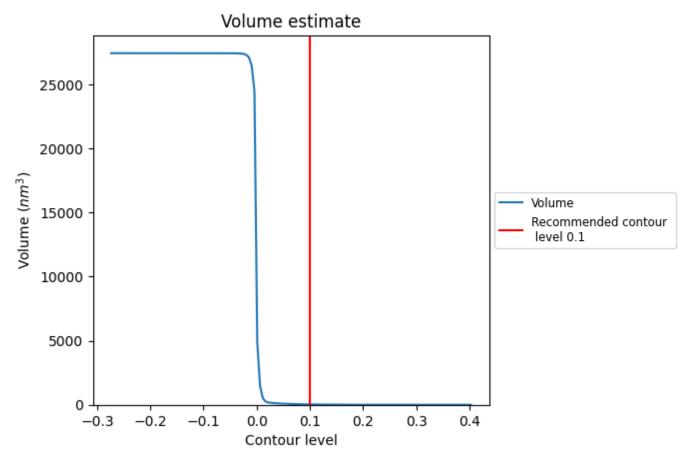
7.1 Map-value distribution (i)



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)

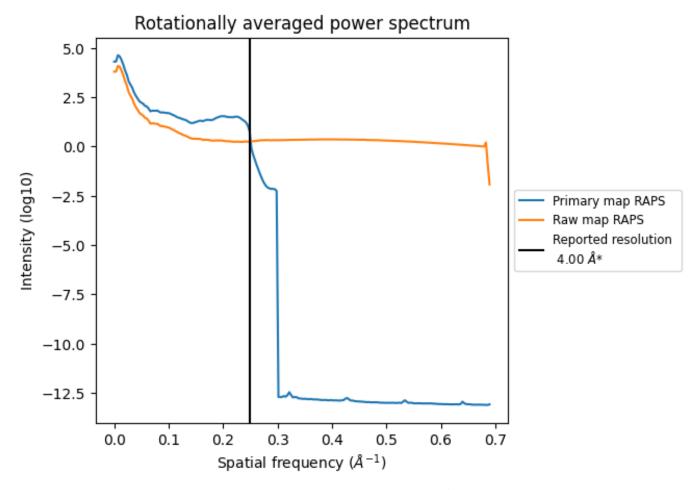


The volume at the recommended contour level is 29 $\rm nm^3;$ this corresponds to an approximate mass of 26 kDa.

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)



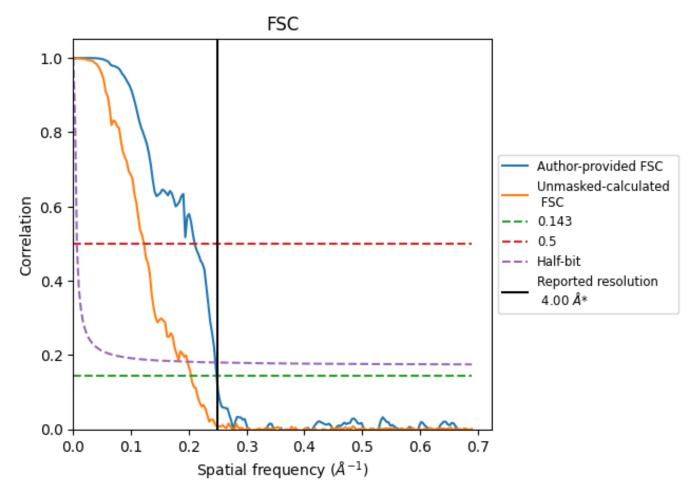
*Reported resolution corresponds to spatial frequency of 0.250 \AA^{-1}



8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.250 ${\rm \AA^{-1}}$



8.2 Resolution estimates (i)

Resolution estimate (Å)	$\operatorname{estimato}(\lambda)$ Estimation criterion (FSC cut-	criterion (FSC cut-off)	
Resolution estimate (A)	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	4.03	4.76	4.06
Unmasked-calculated*	4.90	8.17	5.05

*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 4.90 differs from the reported value 4.0 by more than 10 %



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-40825 and PDB model 8SX3. Per-residue inclusion information can be found in section 3 on page 5.

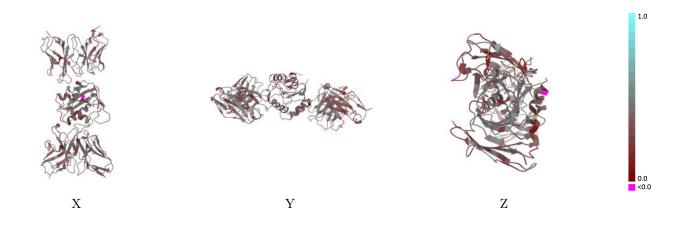
9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

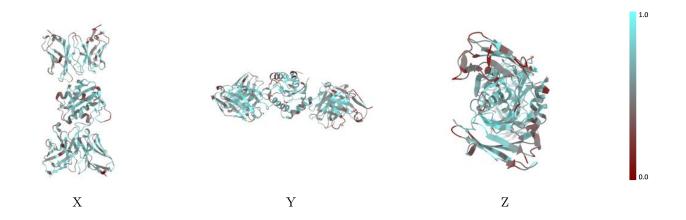


9.2 Q-score mapped to coordinate model (i)



The images above show the model with each residue coloured according 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.

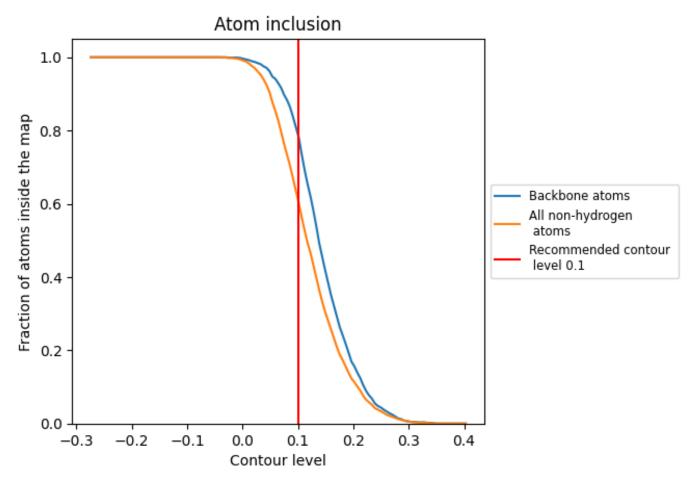
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.1).



9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.



1.0

0.0 <0.0

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6120	0.3780
А	0.6180	0.3760
В	0.5560	0.3630
С	0.6160	0.3820
D	0.4640	0.3530
Н	0.6410	0.3870
L	0.6270	0.3810

