

wwPDB EM Validation Summary Report (i)

Mar 6, 2023 – 12:33 pm GMT

PDB ID : 7ZN7

EMDB ID : EMD-14802

Title : Cryo-EM structure of RCMV-E E27 bound to human DDB1 (deltaBPB) and

rat STAT2 CCD

Authors: Lauer, S.; Spahn, C.M.T.; Schwefel, D.

Deposited on : 2022-04-20

Resolution: 3.78 Å(reported)

Based on initial model : 6ZUE

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

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 (1)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev43

MolProbity : 4.02b-467

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

MapQ : 1.9.9

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

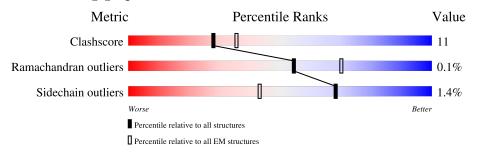
Validation Pipeline (wwPDB-VP) : 2.32.1

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 3.78 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 $(\# \mathrm{Entries})$	${ m EM\ structures} \ (\#{ m Entries})$
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 >=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	840	•	71	%	22%	7%								
2	В	659	7%	47%	14%	39%									
3	D	845	7% 10%	5%	85%										



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10497 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 DNA damage-binding protein 1.

Mo	l Chain	Residues		A	AltConf	Trace			
1	A	783	Total 6179	C 3927	N 1042	O 1176	S 34	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q16531
A	-1	PRO	-	expression tag	UNP Q16531
A	0	GLY	-	expression tag	UNP Q16531
A	700	GLY	-	linker	UNP Q16531
A	701	ASN	-	linker	UNP Q16531
A	702	GLY	-	linker	UNP Q16531
A	703	ASN	-	linker	UNP Q16531
A	704	SER	-	linker	UNP Q16531
A	705	GLY	-	linker	UNP Q16531

• Molecule 2 is a protein called B27a.

Mol	Chain	Residues		At	AltConf	Trace			
2	В	400	Total 3272	C 2074	N 586	O 590	S 22	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	-2	GLY	-	expression tag	UNP K7Y9Z1
В	-1	PRO	-	expression tag	UNP K7Y9Z1
В	0	GLY	-	expression tag	UNP K7Y9Z1

• Molecule 3 is a protein called Signal transducer and activator of transcription.



\mathbf{Mol}	Chain	Residues		At	oms	AltConf	Trace		
9	D	128	Total	С	N	О	S	0	0
3	D	120	1045	665	188	188	4	U	

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	GLY	-	expression tag	UNP Q5XI26
D	-1	PRO	-	expression tag	UNP Q5XI26
D	0	GLY	-	expression tag	UNP Q5XI26

• Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
4	В	1	Total Zn 1 1	0

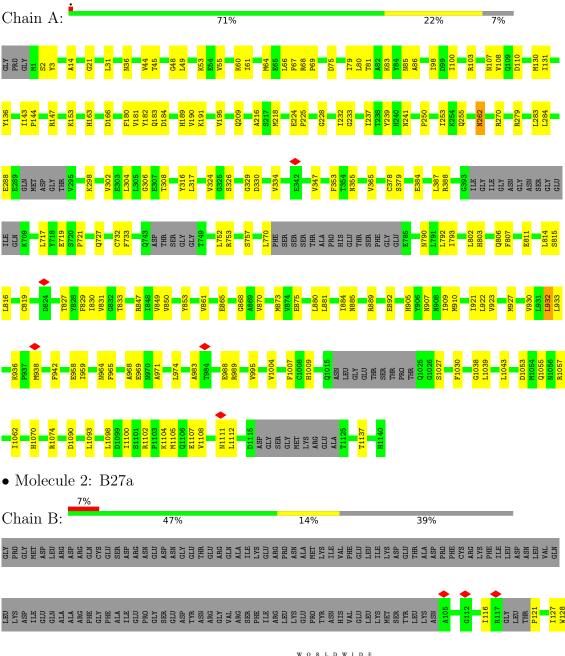


EMD-14802, 7ZN7

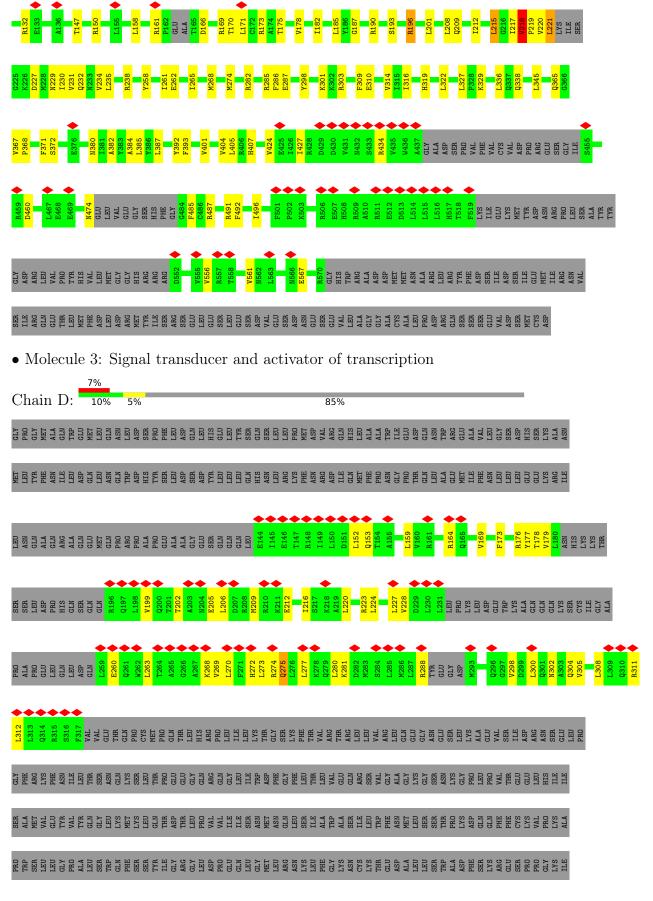
3 Residue-property plots (i)

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: DNA damage-binding protein 1









PRO PHE TRP	THR	ASP	TEG	LEU VAL	HIS	HIS	LYS	LEU	TRP	ASP	ARG	ILE	GLY	VAL	SER	SER	GLU	ARG	LEU	LYS	MET	VAL	GLY	THR	LEU	ARG	SER	GLU	SER	GLU	GLY	THR
CYS SER TRP	VAL	GLN	ASP ASP	VAL	TAR	SER	GEN	TYR	THR	GLU	LEU	GLN	LEU	FEG	AE DIS	IE	ARG	HIS	GLN	E E	GLU	GLU	ALA	GLU	ASN		ARG	LEU	PRO	ARG	PRO	ASP
GLU ALA PHE	GLY CYS TYB	TYR	CLU	ASN	den Gen	ARG	LYS	LEU	LYS	ARG	ILE	VAL	SER	ARG	GLN	ASP	LEU	GLN	PRO	GLU	LEO	GLN	PRO	SER	LEU	LEU	ASP	GLU	MET	SER	MET	LEU
ALA ARG ASP	GLU	GLN	LEU LEU	VAL	LEU	LEU	VAL	PRO	LYS	ASP	THR	LEU	PRO	PRO	GLN	LEU	GLU	PRO ASP	PRO AT A	ARG	ALA	ASN	LEU	PRO	GLU	ASP	LEU	GLN	LEU	GLN	LEU	THR
GLY GLU MET	GLU	ARG	ASN	ILE	ASP	MET	TYR	ASP	PRO	LEU	GLY	GLN	ILE	GLU	GLU	TYR	SER	CYS	SER	PHE :	VAL	ASP	PRO	LEO	PRO	GLU	ASP					



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	389784	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	62	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	31000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.694	Depositor
Minimum map value	-2.391	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.077	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	270.0, 270.0, 270.0	wwPDB
Map dimensions	216, 216, 216	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.25, 1.25, 1.25	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: ZN

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					
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5				
1	A	0.33	0/6286	0.57	0/8494				
2	В	0.34	0/3334	0.55	0/4499				
3	D	0.34	0/1050	0.65	0/1408				
All	All	0.34	0/10670	0.57	0/14401				

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	6179	0	6179	125	0
2	В	3272	0	3245	67	0
3	D	1045	0	1111	34	0
4	В	1	0	0	0	0
All	All	10497	0	10535	222	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 11.

The worst 5 of 222 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
2:B:487:ARG:O	2:B:491:ARG:HG3	1.86	0.76
1:A:103:ARG:NH1	1:A:147:ARG:HH12	1.84	0.75
1:A:830:ILE:HG12	1:A:850:VAL:HG23	1.69	0.73
1:A:182:TYR:HE1	1:A:191:LYS:HG3	1.54	0.72
1:A:1104:LYS:HA	1:A:1107:GLU:HG3	1.75	0.69

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	Perce	ntiles
1	A	769/840 (92%)	714 (93%)	55 (7%)	0	100	100
2	В	386/659 (59%)	373 (97%)	12 (3%)	1 (0%)	41	74
3	D	120/845 (14%)	115 (96%)	5 (4%)	0	100	100
All	All	1275/2344 (54%)	1202 (94%)	72 (6%)	1 (0%)	54	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	В	218	VAL

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	686/729 (94%)	682 (99%)	4 (1%)	86 92
2	В	351/579 (61%)	342 (97%)	9 (3%)	46 70
3	D	117/764 (15%)	114 (97%)	3 (3%)	46 70
All	All	1154/2072 (56%)	1138 (99%)	16 (1%)	68 82

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

Mol	Chain	Res	Type
3	D	220	LEU
3	D	159	LEU
2	В	215	LEU
2	В	336	LEU
2	В	208	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1034	ASN
2	В	209	GLN
2	В	508	HIS
2	В	319	HIS
1	A	262	ASN

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)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 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.



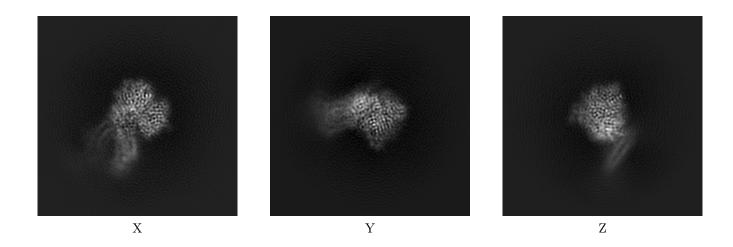
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-14802. These allow visual inspection of the internal detail of the map and identification of artifacts.

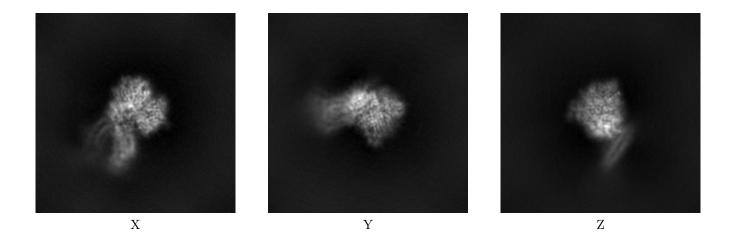
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

6.1.1 Primary map



6.1.2 Raw map

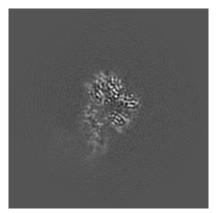


The images above show the map projected in three orthogonal directions.

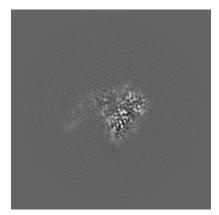


6.2 Central slices (i)

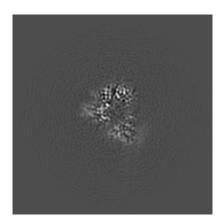
6.2.1 Primary map





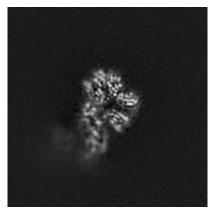


Y Index: 108

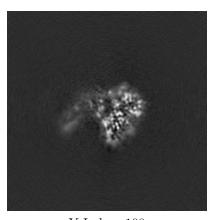


Z Index: 108

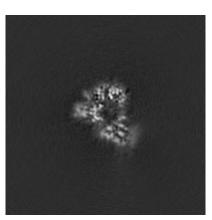
6.2.2 Raw map



X Index: 108



Y Index: 108



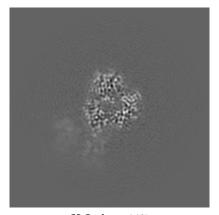
Z Index: 108

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

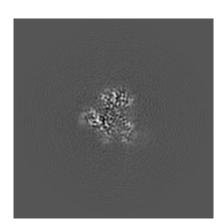


6.3 Largest variance slices (i)

6.3.1 Primary map





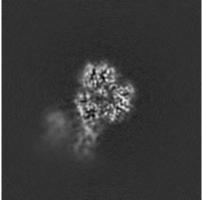


X Index: 117

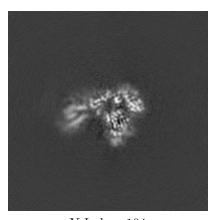
Y Index: 113

Z Index: 115

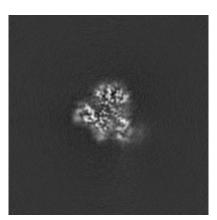
6.3.2 Raw map







Y Index: 104



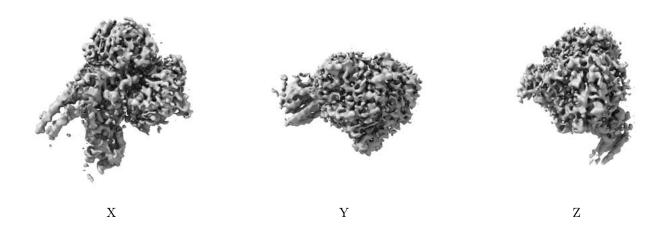
Z Index: 115

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



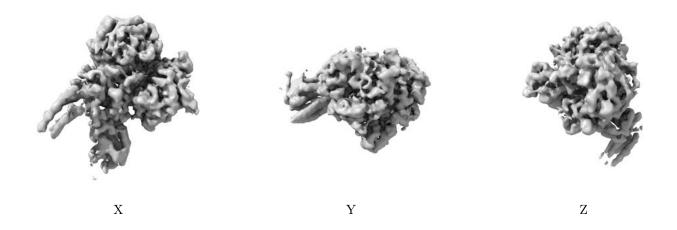
6.4 Orthogonal surface views (i)

6.4.1 Primary map



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.

6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.5 Mask visualisation (i)

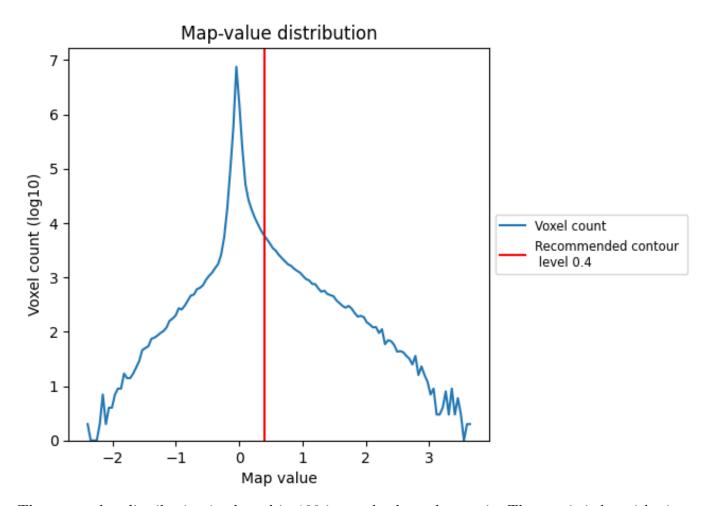
This section was not generated. No masks/segmentation were deposited.



7 Map analysis (i)

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

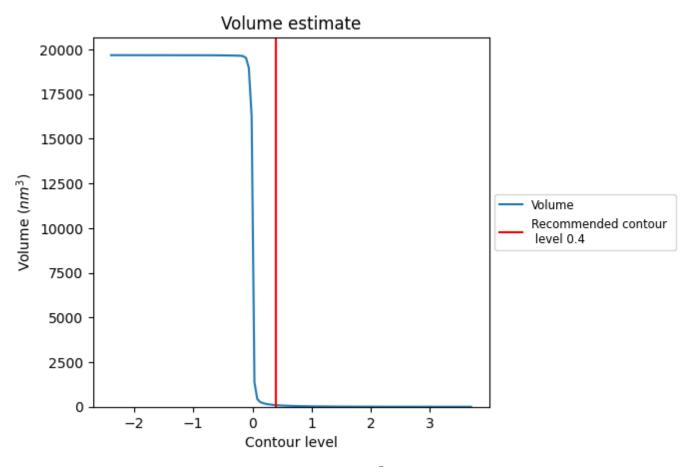
7.1 Map-value distribution (i)



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



7.2 Volume estimate (i)

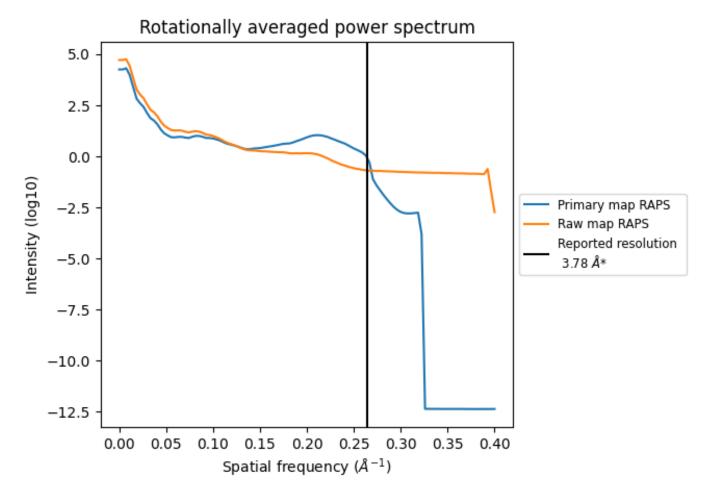


The volume at the recommended contour level is $90~\mathrm{nm^3}$; this corresponds to an approximate mass of $82~\mathrm{kDa}$.

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)



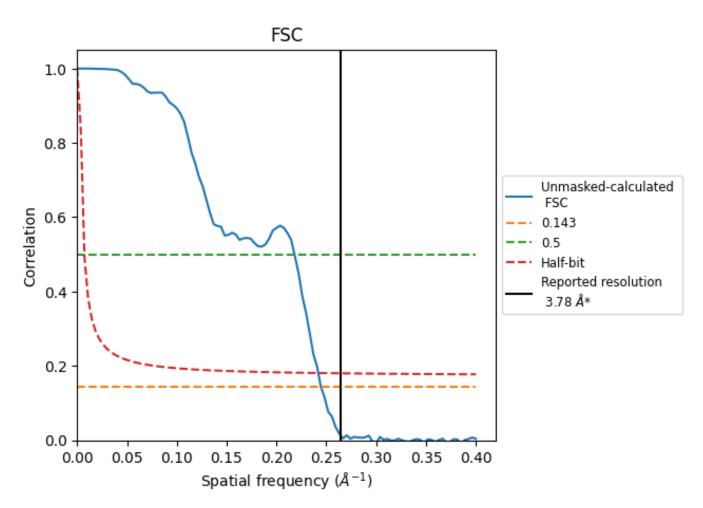
^{*}Reported resolution corresponds to spatial frequency of 0.265 $\mbox{Å}^{-1}$



8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



^{*}Reported resolution corresponds to spatial frequency of 0.265 $\rm \mathring{A}^{-1}$



8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)			
resolution estimate (A)	0.143	0.5	Half-bit	
Reported by author	3.78	-	-	
Author-provided FSC curve	-	-	-	
Unmasked-calculated*	4.09	4.59	4.13	

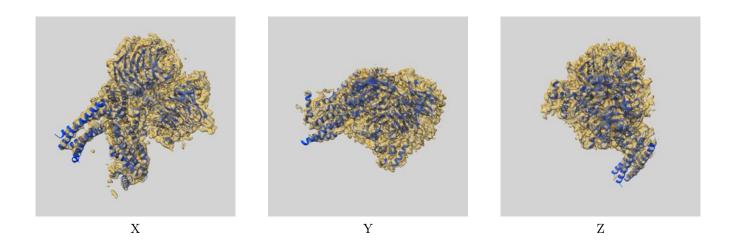
^{*}Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-14802 and PDB model 7ZN7. Per-residue inclusion information can be found in section 3 on page 5.

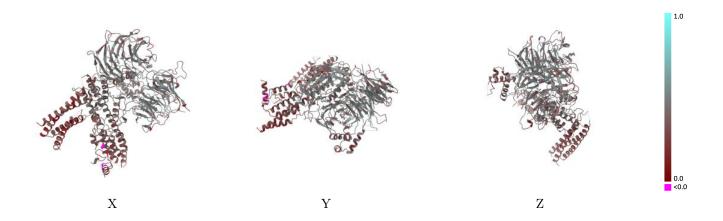
9.1 Map-model overlay (i)



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

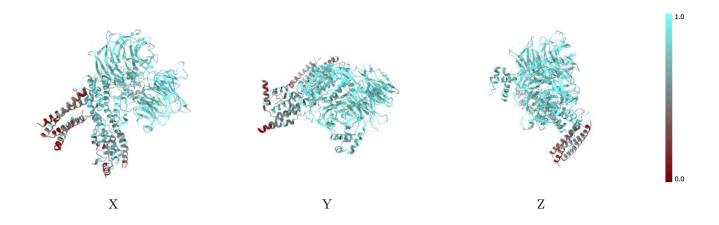


9.2 Q-score mapped to coordinate model (i)



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.

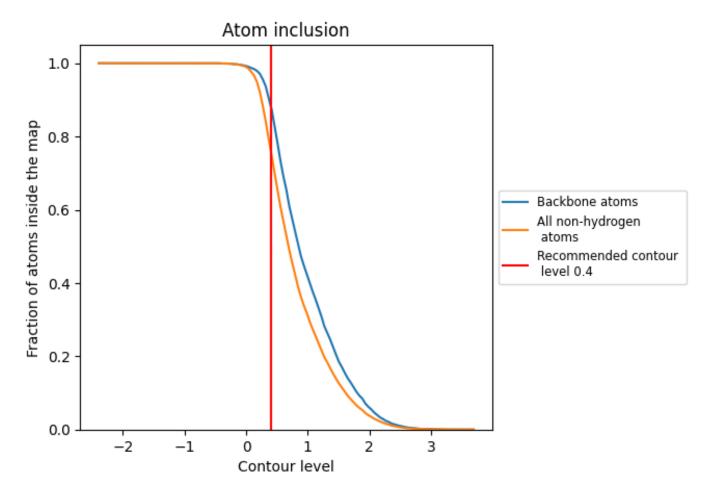
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.4).



9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.



9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7600	0.3950
A	0.8487	0.4400
В	0.7138	0.3530
D	0.3739	0.2650



