Integrative Structure Validation Report

October 09, 2025 - 04:49 PM PDT

The following software was used in the production of this report:

IHMValidation Version 3.0
Python-IHM Version 2.5
MolProbity Version 4.5.2
EMDB validation analysis Version 0.0.1.dev127
ChimeraX Version 1.9
Chimera Version 1.19
MapQ Version 1.8.1

PDB ID	9A86 | pdb_00009a86
PDB-Dev ID	PDBDEV_00000371
Structure Title	Elliptical 52-mer bacterial gasdermin pore model from Vitiosangium sp.
Structure Authors	Johnson, A.G.; Mayer, M.L.; Schaefer, S.L.; McNamara-Bordewick, N.K.; Hummer, G.; Kranzusch, P.J.
Deposited on	2024-01-25

This is a PDB-IHM Structure Validation Report.

We welcome your comments at helpdesk@pdb-ihm.org

A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

List of references used to build this report is available here.

1. Overview

1.1. Summary

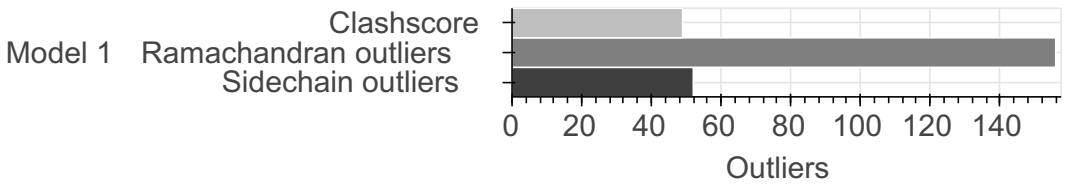
This entry consists of 1 model(s). A total of 3 dataset(s) were used to build this entry.

Name	Type	Count
2DEM class average	Experimental data	1
3DEM volume	Experimental data	1
Experimental model	Starting model	1

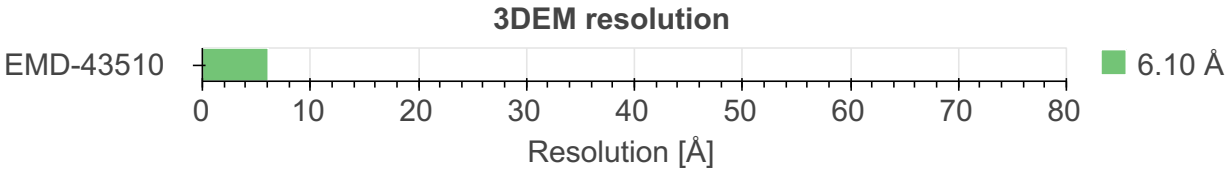
1.2. Overall quality

This validation report contains model quality assessments for all structures, data quality and fit to model assessments for SAS and crosslinking-MS datasets. Data quality and fit to model assessments for other datasets and model uncertainty are under development. Number of plots is limited to 256.

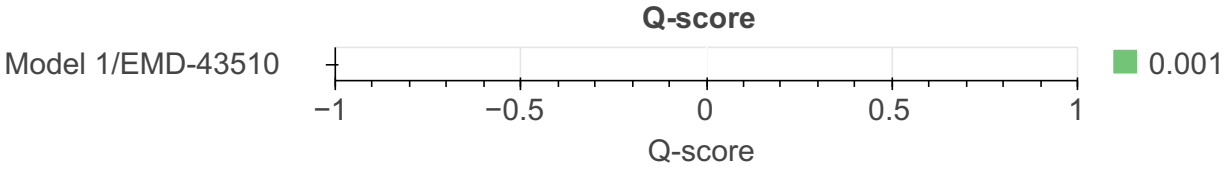
Model Quality: MolProbity Analysis



Data Quality



Fit to Data Used for Modeling



2. Model Details

2.1. Ensemble information

This entry consists of 0 distinct ensemble(s).

2.2. Representation

This entry has 1 representation(s).

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
1	1	1	Gasdermin bGSDM	A	234	-	1-234	100.00 / 100.00	Atomic
				B					
				C					
				D					
				E					
				F					
				G					
				H					
				I					
				J					
				K					
				L					
				M					
				N					
				O					
				P					
				Q					
				R					
				S					
				T					
				U					
				V					
				W					
				X					
				Y					
				Z					
				AA [a]					
				BA [b]					
				CA [c]					
				DA [d]					
				EA [e]					
				FA [f]					
				GA [g]					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				HA [h]					
				IA [i]					
				JA [j]					
				KA [k]					
				LA [l]					
				MA [m]					
				NA [n]					
				OA [o]					
				PA [p]					
				QA [q]					
				RA [r]					
				SA [s]					
				TA [t]					
				UA [u]					
				VA [v]					
				WA [w]					
				XA [x]					
				YA [y]					
				ZA [z]					

2.3. Datasets used for modeling

There are 3 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Experimental model	PDB	pdb_00008sl0
2	3DEM volume	EMDB	EMD-43510
3	2DEM class average	Zenodo	10.5281/zenodo.10570209

2.4. Methodology and software

This entry is a result of 1 distinct protocol(s).

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
1	1	Not available	Not available	To make the 52-mer pore model, protomer models (PDB 8SL0) were realigned using a custom script and a geometric model based on the number of protomers observed in the major 2D classes (52) and the eccentricity of a cryo-EM map of an oval pore (0.86, EMD-43510). Protomers were realigned to preserve the inter-subunit hydrogen bonding pattern observed in the slinky-like oligomer.	Not available	False	False

There are 2 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	Python	v3.9.7	model building	https://www.python.org/
2	MDAnalysis	v2.4.2	model building	https://www.mdanalysis.org/

3. Data quality

3.3. 3DEM

This section describes quality of the 3DEM datasets

EMD-43510

3.3.1. Experimental information

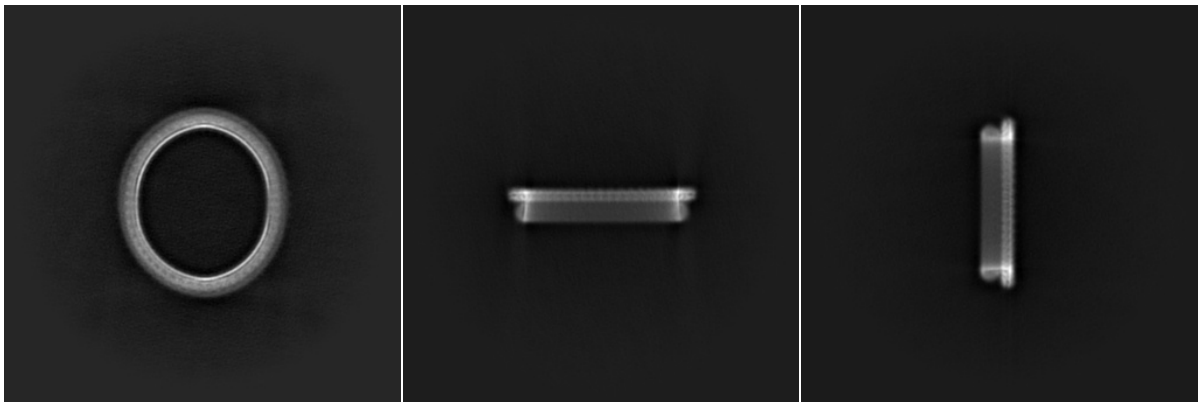
EM reconstruction method:	SINGLE PARTICLE
Resolution:	6.10 Å
Recommended level:	0.600
Estimated volume:	1788.87 nm³
Specimen preparation:	Preparation ID 1 Vitrification
Map-only validation report:	wwPDB validation report

3.3.2. Map visualisation

This section contains visualisations of the EMDB entry EMD-43510. 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.

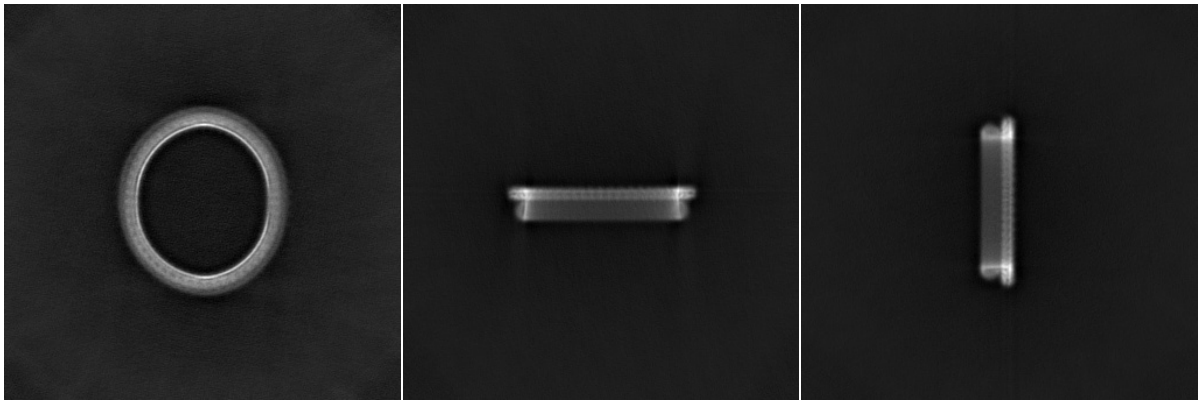
3.3.2.1. Orthogonal projections

Primary map



X **Y** **Z**

Raw map

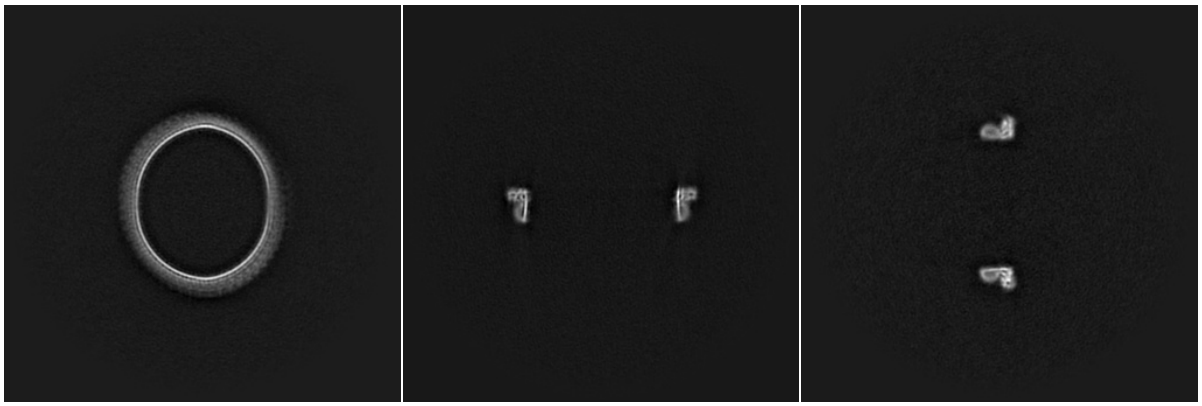


X **Y** **Z**

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

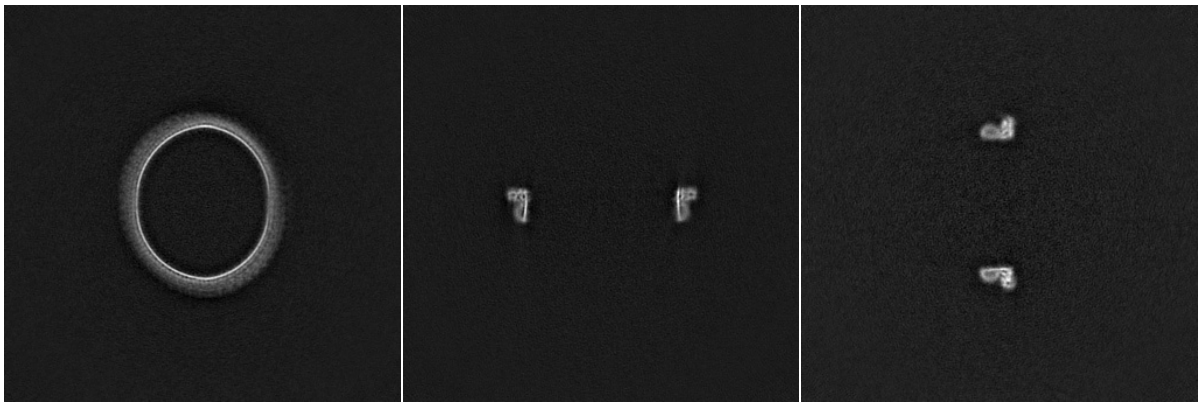
3.3.2.2. Central slices

Primary map



X Index: 170 **Y Index: 170** **Z Index: 170**

Raw map

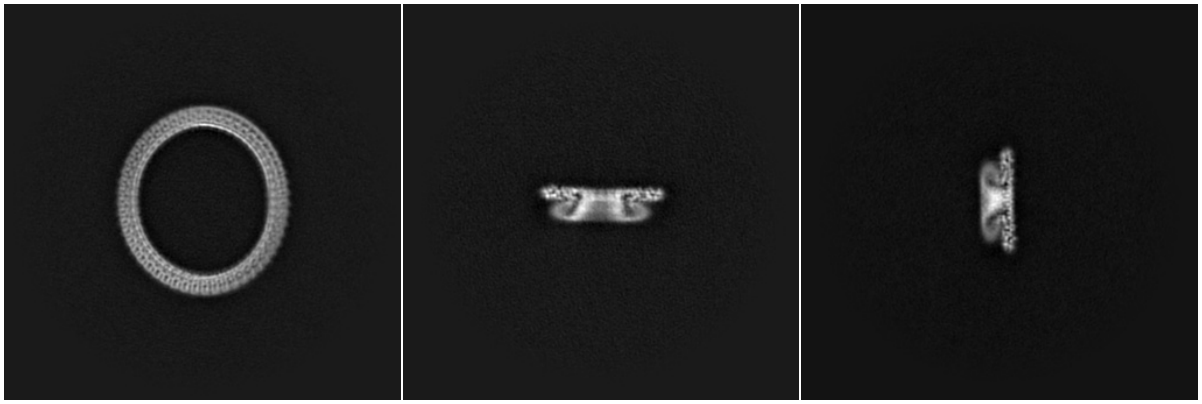


X Index: 170 **Y Index: 170** **Z Index: 170**

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

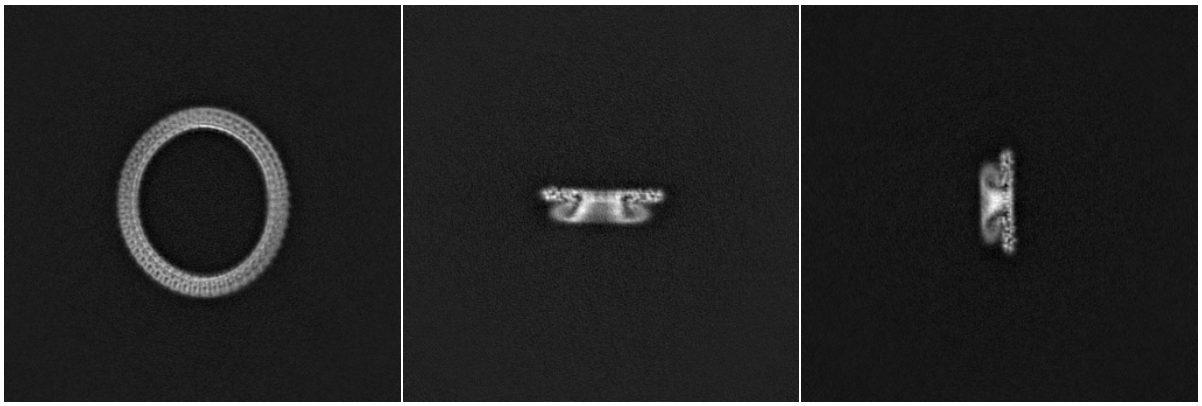
3.3.2.3. Largest variance slices

Primary map



X Index: 179 **Y Index: 114** **Z Index: 105**

Raw map

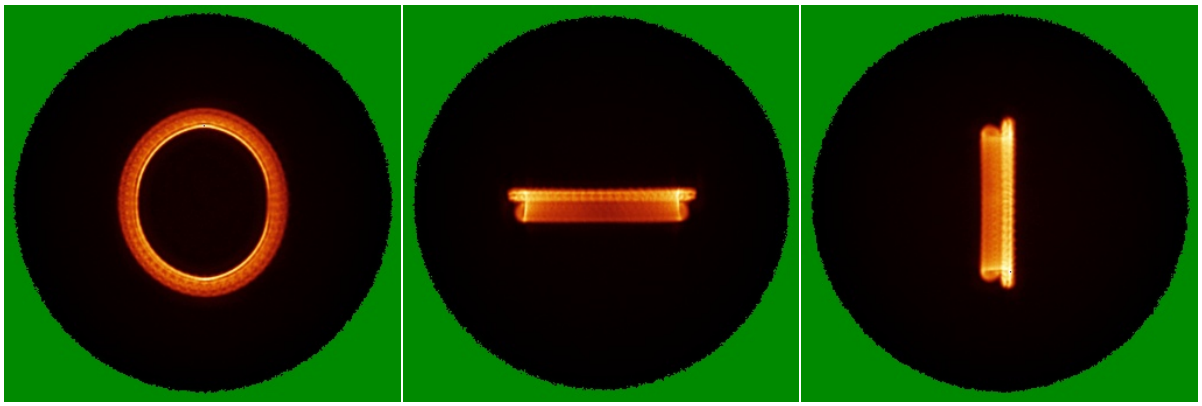


X Index: 179 **Y Index: 114** **Z Index: 105**

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

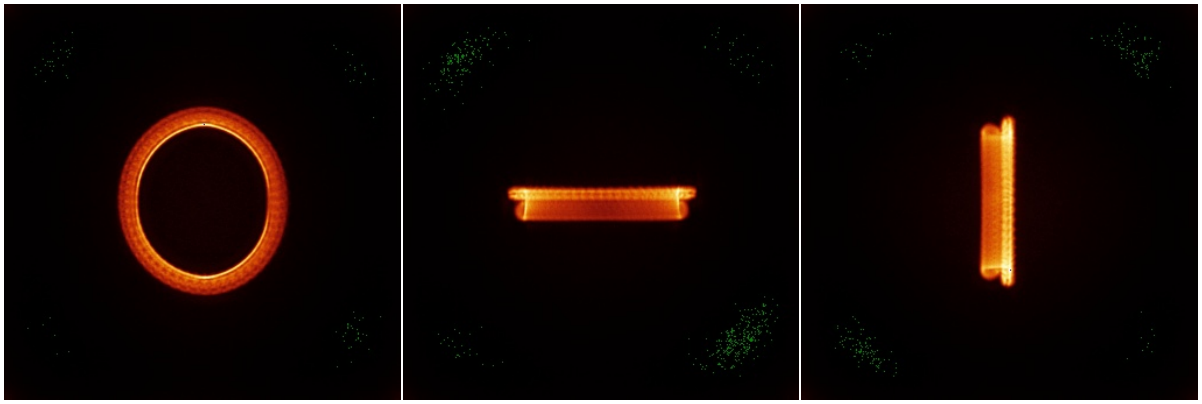
3.3.2.4 Orthogonal standard-deviation projections (false-color)

Primary map



X **Y** **Z**

Raw map

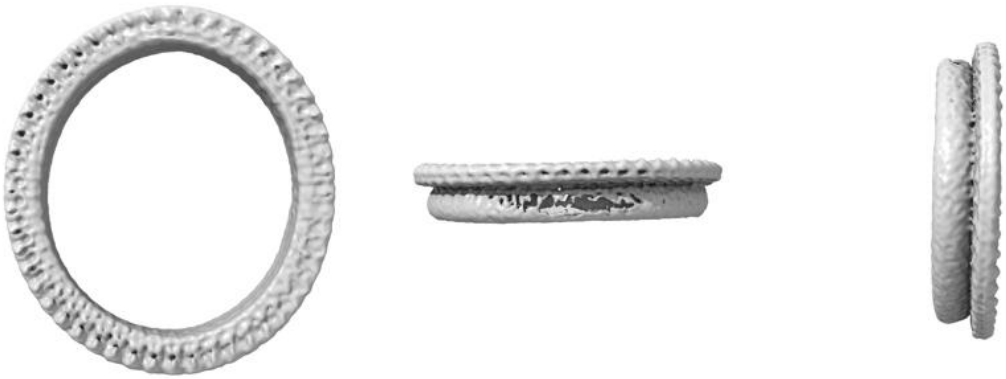


X **Y** **Z**

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.

3.3.2.5. Orthogonal surface views

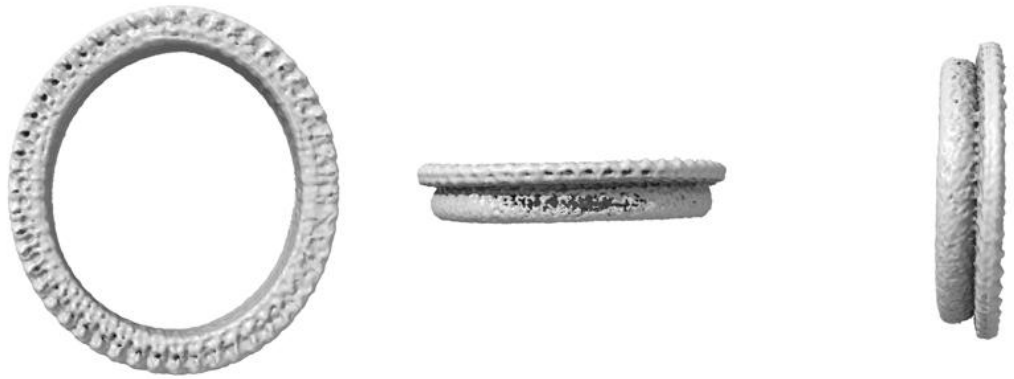
Primary map



X **Y** **Z**

The images above show the 3D surface view of the map at the recommended contour level 0.600 . These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

Raw map



X **Y** **Z**

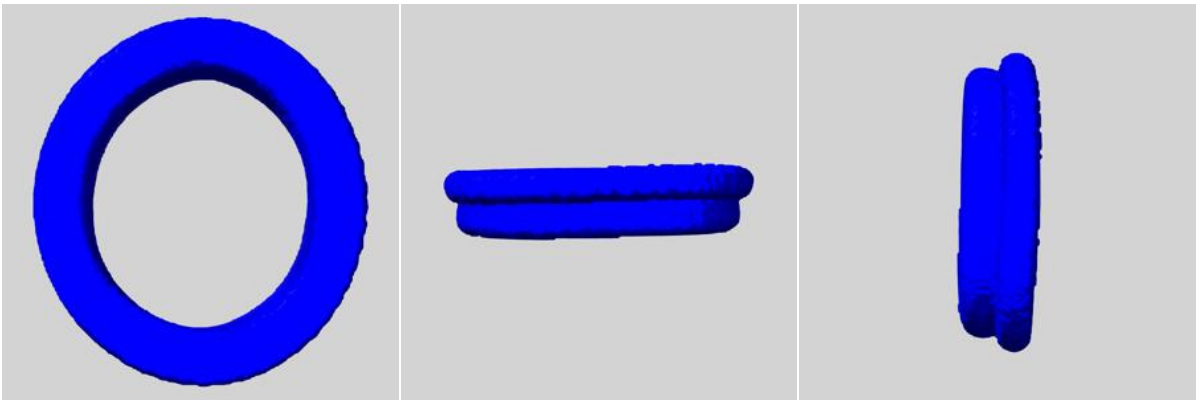
These images show the 3D surface of the raw map. The raw map's contour level 0.530 was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

3.3.2.6. Mask visualisation

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_43510_msk_1.map

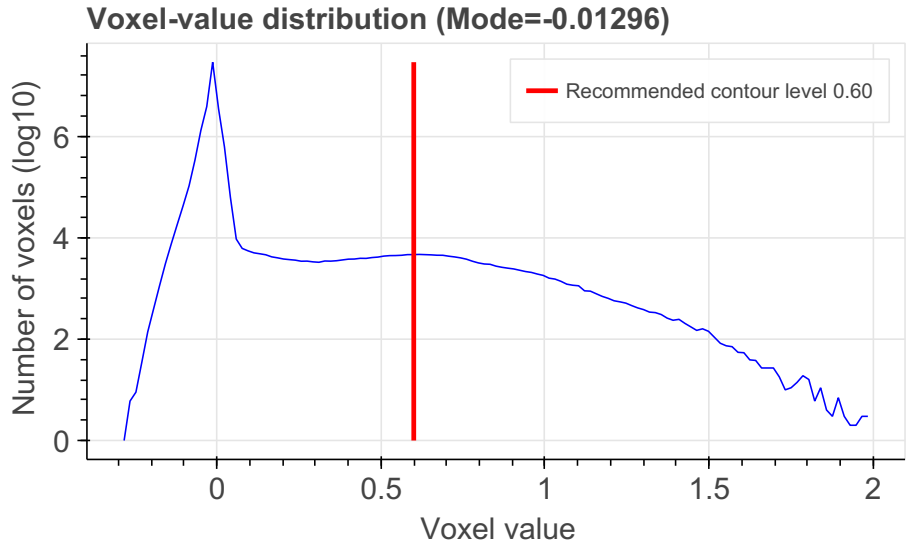


X **Y** **Z**

3.3.3. Map analysis

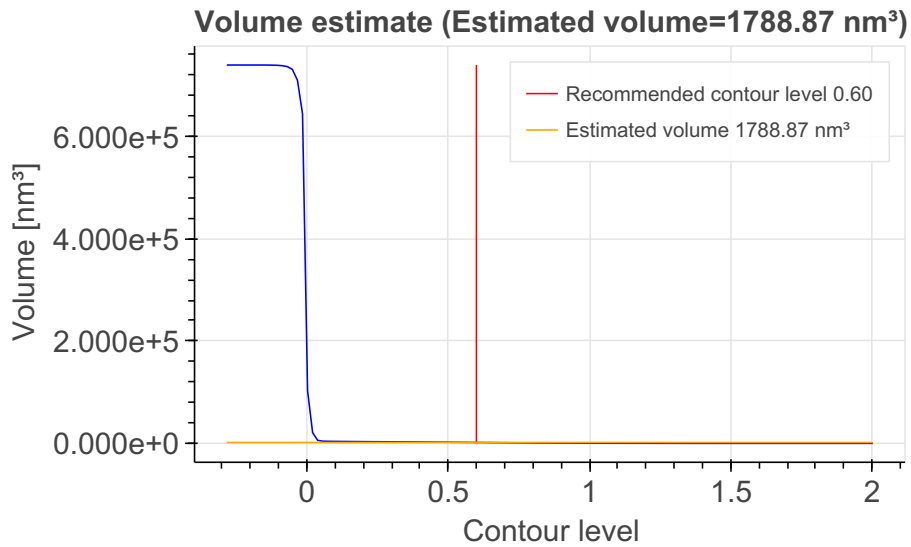
This section contains the results of statistical analysis of the map.

3.3.3.1. Map-value distribution



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

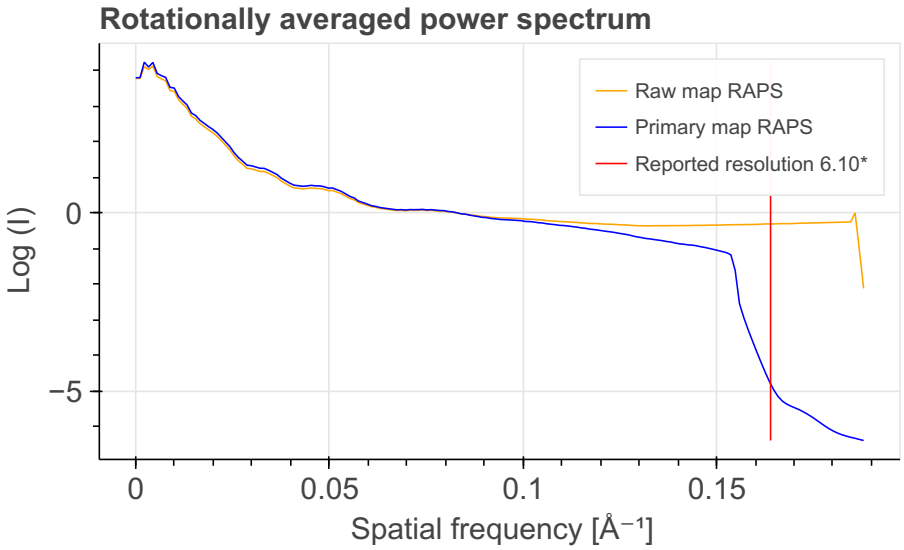
3.3.3.2. Volume estimate



The volume at the recommended contour level is 1788.87 nm³.

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.

3.3.3.3. Rotationally averaged power spectrum

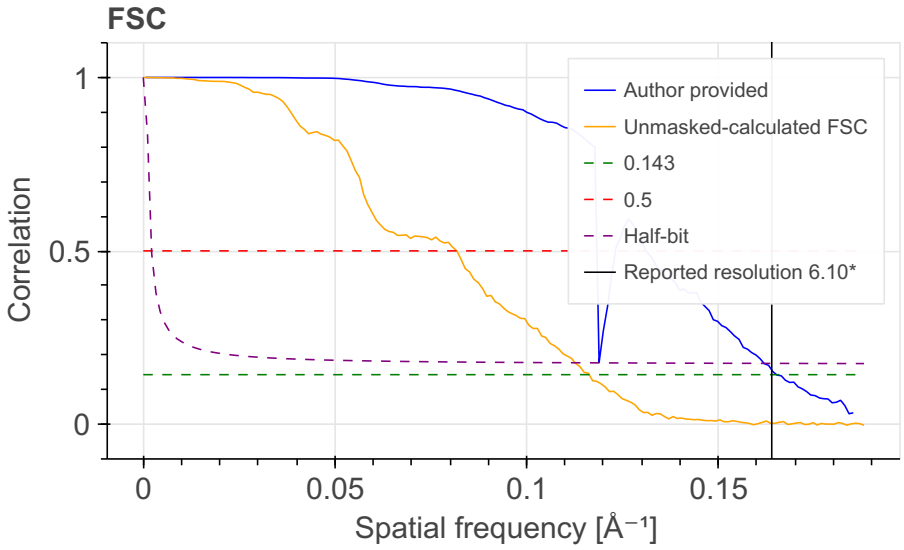


*Reported resolution corresponds to spatial frequency of 0.164 Å⁻¹

3.3.4. Fourier-Shell correlation

3.3.4.1. FSC

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.



*Reported resolution corresponds to spatial frequency of 0.164 Å⁻¹

3.3.4.2. Resolution estimates

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	**0.5**	**Half-bit**
Reported by author	6.10	-	-
Author-provided FSC curve	6.05	8.45	6.18
Unmasked-calculated*	8.60	12.22	8.88

*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 8.60 differs from the reported value 6.10 by more than 10%.

3.4. 2DEM class average

Validation for this section is under development.

4. Model quality

For models with atomic structures, MolProbity analysis is performed. For models with coarse-grained or multi-scale structures, excluded volume analysis is performed.

4.1b. MolProbity Analysis

Excluded volume satisfaction for the models in the entry are listed below. The Analysed column shows the number of particle-partice or particle-atom pairs for which excluded volume was analysed.

Standard geometry: bond outliers

There are 52 bond length outliers in this entry (0.06% of 93860 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
T	4	P1L	SG-C7	110.77	3.95	1.73	1	1
V	4	P1L	SG-C7	110.76	3.95	1.73	1	1
P	4	P1L	SG-C7	110.76	3.95	1.73	1	1
U	4	P1L	SG-C7	110.75	3.95	1.73	1	1
L	4	P1L	SG-C7	110.75	3.95	1.73	1	1
J	4	P1L	SG-C7	110.75	3.95	1.73	1	1
W	4	P1L	SG-C7	110.75	3.95	1.73	1	1
G	4	P1L	SG-C7	110.74	3.95	1.73	1	1
TA	4	P1L	SG-C7	110.74	3.95	1.73	1	1
LA	4	P1L	SG-C7	110.74	3.95	1.73	1	1
Y	4	P1L	SG-C7	110.74	3.95	1.73	1	1
YA	4	P1L	SG-C7	110.74	3.95	1.73	1	1
E	4	P1L	SG-C7	110.74	3.95	1.73	1	1
EA	4	P1L	SG-C7	110.74	3.95	1.73	1	1
R	4	P1L	SG-C7	110.74	3.95	1.73	1	1
RA	4	P1L	SG-C7	110.74	3.95	1.73	1	1
XA	4	P1L	SG-C7	110.73	3.95	1.73	1	1
K	4	P1L	SG-C7	110.73	3.95	1.73	1	1
Q	4	P1L	SG-C7	110.73	3.95	1.73	1	1
QA	4	P1L	SG-C7	110.73	3.95	1.73	1	1
DA	4	P1L	SG-C7	110.73	3.95	1.73	1	1
S	4	P1L	SG-C7	110.73	3.95	1.73	1	1
FA	4	P1L	SG-C7	110.73	3.95	1.73	1	1

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
SA	4	P1L	SG-C7	110.73	3.95	1.73	1	1
I	4	P1L	SG-C7	110.73	3.95	1.73	1	1
IA	4	P1L	SG-C7	110.73	3.95	1.73	1	1
NA	4	P1L	SG-C7	110.73	3.95	1.73	1	1
A	4	P1L	SG-C7	110.73	3.95	1.73	1	1
AA	4	P1L	SG-C7	110.73	3.95	1.73	1	1
N	4	P1L	SG-C7	110.73	3.95	1.73	1	1
ZA	4	P1L	SG-C7	110.73	3.95	1.73	1	1
H	4	P1L	SG-C7	110.72	3.95	1.73	1	1
HA	4	P1L	SG-C7	110.72	3.95	1.73	1	1
UA	4	P1L	SG-C7	110.72	3.95	1.73	1	1
PA	4	P1L	SG-C7	110.72	3.95	1.73	1	1
CA	4	P1L	SG-C7	110.72	3.95	1.73	1	1
D	4	P1L	SG-C7	110.72	3.95	1.73	1	1
MA	4	P1L	SG-C7	110.72	3.95	1.73	1	1
Z	4	P1L	SG-C7	110.72	3.95	1.73	1	1
M	4	P1L	SG-C7	110.72	3.95	1.73	1	1
C	4	P1L	SG-C7	110.72	3.95	1.73	1	1
GA	4	P1L	SG-C7	110.72	3.95	1.73	1	1
KA	4	P1L	SG-C7	110.71	3.95	1.73	1	1
X	4	P1L	SG-C7	110.71	3.95	1.73	1	1
BA	4	P1L	SG-C7	110.71	3.95	1.73	1	1
O	4	P1L	SG-C7	110.71	3.95	1.73	1	1
OA	4	P1L	SG-C7	110.71	3.95	1.73	1	1
F	4	P1L	SG-C7	110.71	3.95	1.73	1	1
B	4	P1L	SG-C7	110.71	3.95	1.73	1	1
VA	4	P1L	SG-C7	110.70	3.95	1.73	1	1
JA	4	P1L	SG-C7	110.69	3.95	1.73	1	1
WA	4	P1L	SG-C7	110.69	3.95	1.73	1	1

Standard geometry: angle outliers

There are 174 bond angle outliers in this entry (0.14% of 126672 assessed bonds). A summary is provided below. The output is limited to 100 rows.

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
N	4	P1L	SG-C7-C8	6.87	88.62	109.23	1	1
J	4	P1L	SG-C7-C8	6.87	88.62	109.23	1	1

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
T	4	P1L	SG-C7-C8	6.87	88.63	109.23	1	1
Y	4	P1L	SG-C7-C8	6.87	88.63	109.23	1	1
P	4	P1L	SG-C7-C8	6.87	88.63	109.23	1	1
XA	4	P1L	SG-C7-C8	6.86	88.64	109.23	1	1
K	4	P1L	SG-C7-C8	6.86	88.64	109.23	1	1
S	4	P1L	SG-C7-C8	6.86	88.64	109.23	1	1
C	4	P1L	SG-C7-C8	6.86	88.64	109.23	1	1
H	4	P1L	SG-C7-C8	6.86	88.64	109.23	1	1
HA	4	P1L	SG-C7-C8	6.86	88.64	109.23	1	1
UA	4	P1L	SG-C7-C8	6.86	88.64	109.23	1	1
D	4	P1L	SG-C7-C8	6.86	88.64	109.23	1	1
B	4	P1L	SG-C7-C8	6.86	88.64	109.23	1	1
IA	4	P1L	SG-C7-C8	6.86	88.64	109.23	1	1
F	4	P1L	SG-C7-C8	6.86	88.64	109.23	1	1
ZA	4	P1L	SG-C7-C8	6.86	88.64	109.23	1	1
GA	4	P1L	SG-C7-C8	6.86	88.64	109.23	1	1
Q	4	P1L	SG-C7-C8	6.86	88.64	109.23	1	1
L	4	P1L	SG-C7-C8	6.86	88.64	109.23	1	1
W	4	P1L	SG-C7-C8	6.86	88.64	109.23	1	1
PA	4	P1L	SG-C7-C8	6.86	88.64	109.23	1	1
CA	4	P1L	SG-C7-C8	6.86	88.64	109.23	1	1
I	4	P1L	SG-C7-C8	6.86	88.65	109.23	1	1
VA	4	P1L	SG-C7-C8	6.86	88.65	109.23	1	1
NA	4	P1L	SG-C7-C8	6.86	88.65	109.23	1	1
AA	4	P1L	SG-C7-C8	6.86	88.65	109.23	1	1
A	4	P1L	SG-C7-C8	6.86	88.65	109.23	1	1
U	4	P1L	SG-C7-C8	6.86	88.65	109.23	1	1
BA	4	P1L	SG-C7-C8	6.86	88.65	109.23	1	1
OA	4	P1L	SG-C7-C8	6.86	88.65	109.23	1	1
V	4	P1L	SG-C7-C8	6.86	88.65	109.23	1	1
QA	4	P1L	SG-C7-C8	6.86	88.65	109.23	1	1
DA	4	P1L	SG-C7-C8	6.86	88.65	109.23	1	1
M	4	P1L	SG-C7-C8	6.86	88.65	109.23	1	1
MA	4	P1L	SG-C7-C8	6.86	88.65	109.23	1	1
Z	4	P1L	SG-C7-C8	6.86	88.65	109.23	1	1

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
O	4	P1L	SG-C7-C8	6.86	88.65	109.23	1	1
FA	4	P1L	SG-C7-C8	6.86	88.65	109.23	1	1
E	4	P1L	SG-C7-C8	6.86	88.65	109.23	1	1
RA	4	P1L	SG-C7-C8	6.86	88.65	109.23	1	1
EA	4	P1L	SG-C7-C8	6.86	88.65	109.23	1	1
R	4	P1L	SG-C7-C8	6.86	88.65	109.23	1	1
LA	4	P1L	SG-C7-C8	6.86	88.65	109.23	1	1
YA	4	P1L	SG-C7-C8	6.86	88.65	109.23	1	1
G	4	P1L	SG-C7-C8	6.86	88.65	109.23	1	1
TA	4	P1L	SG-C7-C8	6.86	88.65	109.23	1	1
JA	4	P1L	SG-C7-C8	6.86	88.66	109.23	1	1
WA	4	P1L	SG-C7-C8	6.86	88.66	109.23	1	1
KA	4	P1L	SG-C7-C8	6.86	88.66	109.23	1	1
X	4	P1L	SG-C7-C8	6.86	88.66	109.23	1	1
SA	4	P1L	SG-C7-C8	6.85	88.68	109.23	1	1
ZA	119	ASP	CA-CB-CG	5.25	117.85	112.60	1	1
JA	119	ASP	CA-CB-CG	5.25	117.85	112.60	1	1
F	119	ASP	CA-CB-CG	5.25	117.85	112.60	1	1
WA	119	ASP	CA-CB-CG	5.24	117.84	112.60	1	1
TA	119	ASP	CA-CB-CG	5.24	117.84	112.60	1	1
KA	119	ASP	CA-CB-CG	5.24	117.84	112.60	1	1
AA	119	ASP	CA-CB-CG	5.24	117.84	112.60	1	1
NA	119	ASP	CA-CB-CG	5.24	117.84	112.60	1	1
CA	119	ASP	CA-CB-CG	5.23	117.83	112.60	1	1
PA	119	ASP	CA-CB-CG	5.23	117.83	112.60	1	1
SA	119	ASP	CA-CB-CG	5.23	117.83	112.60	1	1
R	119	ASP	CA-CB-CG	5.23	117.83	112.60	1	1
EA	119	ASP	CA-CB-CG	5.23	117.83	112.60	1	1
RA	119	ASP	CA-CB-CG	5.23	117.83	112.60	1	1
UA	119	ASP	CA-CB-CG	5.23	117.83	112.60	1	1
HA	119	ASP	CA-CB-CG	5.23	117.83	112.60	1	1
C	119	ASP	CA-CB-CG	5.23	117.83	112.60	1	1
G	119	ASP	CA-CB-CG	5.22	117.82	112.60	1	1
V	119	ASP	CA-CB-CG	5.22	117.82	112.60	1	1
VA	119	ASP	CA-CB-CG	5.22	117.82	112.60	1	1

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
IA	119	ASP	CA-CB-CG	5.22	117.82	112.60	1	1
YA	119	ASP	CA-CB-CG	5.22	117.82	112.60	1	1
Y	119	ASP	CA-CB-CG	5.22	117.82	112.60	1	1
LA	119	ASP	CA-CB-CG	5.22	117.82	112.60	1	1
S	119	ASP	CA-CB-CG	5.22	117.82	112.60	1	1
A	119	ASP	CA-CB-CG	5.22	117.82	112.60	1	1
Z	119	ASP	CA-CB-CG	5.22	117.82	112.60	1	1
MA	119	ASP	CA-CB-CG	5.22	117.82	112.60	1	1
XA	119	ASP	CA-CB-CG	5.22	117.82	112.60	1	1
OA	119	ASP	CA-CB-CG	5.22	117.82	112.60	1	1
BA	119	ASP	CA-CB-CG	5.21	117.81	112.60	1	1
O	119	ASP	CA-CB-CG	5.21	117.81	112.60	1	1
B	119	ASP	CA-CB-CG	5.21	117.81	112.60	1	1
Q	119	ASP	CA-CB-CG	5.21	117.81	112.60	1	1
QA	119	ASP	CA-CB-CG	5.21	117.81	112.60	1	1
DA	119	ASP	CA-CB-CG	5.21	117.81	112.60	1	1
D	119	ASP	CA-CB-CG	5.21	117.81	112.60	1	1
W	119	ASP	CA-CB-CG	5.21	117.81	112.60	1	1
P	119	ASP	CA-CB-CG	5.21	117.81	112.60	1	1
X	119	ASP	CA-CB-CG	5.21	117.81	112.60	1	1
H	119	ASP	CA-CB-CG	5.21	117.81	112.60	1	1
FA	119	ASP	CA-CB-CG	5.21	117.81	112.60	1	1
N	119	ASP	CA-CB-CG	5.21	117.81	112.60	1	1
U	119	ASP	CA-CB-CG	5.20	117.80	112.60	1	1
T	119	ASP	CA-CB-CG	5.20	117.80	112.60	1	1
GA	119	ASP	CA-CB-CG	5.20	117.80	112.60	1	1
L	119	ASP	CA-CB-CG	5.20	117.80	112.60	1	1
I	119	ASP	CA-CB-CG	5.20	117.80	112.60	1	1

Too-close contacts

The following all-atom clashscore is based on a MolProbity analysis. All-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The table below contains clashscores for all atomic models in this entry.

Model ID	Clash score	Number of clashes
1	48.93	8973

There are 8973 clashes. The table below contains the detailed list of all clashes based on a MolProbity analysis. Bad clashes are >= 0.4 Angstrom. The output is limited to 100 rows.

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
OA:230:PHE:CE1	PA:141:VAL:HG12	1.71	1	1
A:230:PHE:CE1	B:141:VAL:HG12	1.70	1	1
P:15:LEU:HG	Q:203:VAL:CG2	1.69	1	1
QA:230:PHE:CE1	RA:141:VAL:HG12	1.68	1	1
O:230:PHE:CE1	P:141:VAL:HG12	1.67	1	1
YA:230:PHE:CE1	ZA:141:VAL:HG12	1.67	1	1
N:230:PHE:CE1	O:141:VAL:HG12	1.66	1	1
V:87:LYS:HD2	W:186:VAL:CB	1.66	1	1
EA:15:LEU:HD11	FA:203:VAL:CG2	1.66	1	1
P:230:PHE:CE1	Q:141:VAL:HG12	1.66	1	1
EA:124:LEU:HD21	FA:45:SER:CB	1.65	1	1
V:89:VAL:HB	W:187:VAL:CG1	1.65	1	1
SA:230:PHE:CE1	TA:141:VAL:HG12	1.65	1	1
AA:218:PHE:CE2	BA:42:TYR:CD2	1.65	1	1
PA:230:PHE:CE1	QA:141:VAL:HG12	1.65	1	1
WA:230:PHE:CE1	XA:141:VAL:HG12	1.65	1	1
U:218:PHE:CE2	V:42:TYR:CD2	1.64	1	1
JA:67:ALA:HB3	KA:205:TYR:CE1	1.64	1	1
D:15:LEU:CD1	E:203:VAL:HG21	1.64	1	1
AA:230:PHE:CE1	BA:141:VAL:HG12	1.64	1	1
UA:230:PHE:CE1	VA:141:VAL:HG12	1.64	1	1
SA:89:VAL:HB	TA:187:VAL:CG1	1.64	1	1
NA:230:PHE:CE1	OA:141:VAL:HG12	1.64	1	1
V:230:PHE:CZ	W:141:VAL:HG12	1.64	1	1
Q:230:PHE:CE1	R:141:VAL:HG12	1.63	1	1
RA:230:PHE:CE1	SA:141:VAL:HG12	1.63	1	1
A:141:VAL:HG12	ZA:230:PHE:CE1	1.63	1	1
C:69:ILE:CD	D:204:THR:H	1.62	1	1
R:86:LEU:HD21	S:188:GLY:CA	1.62	1	1
J:228:THR:HG21	K:140:PRO:CG	1.62	1	1
Z:230:PHE:CZ	AA:141:VAL:HG12	1.62	1	1
EA:124:LEU:CD2	FA:45:SER:HB3	1.62	1	1
UA:230:PHE:CZ	VA:141:VAL:HG12	1.62	1	1
R:230:PHE:CE1	S:141:VAL:HG12	1.62	1	1
U:87:LYS:CE	V:186:VAL:HG13	1.62	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
VA:89:VAL:CG1	WA:187:VAL:HG11	1.61	1	1
Y:230:PHE:CE1	Z:141:VAL:HG12	1.61	1	1
V:87:LYS:CE	W:186:VAL:HG13	1.61	1	1
AA:230:PHE:CE1	BA:141:VAL:CG1	1.61	1	1
PA:15:LEU:HG	QA:203:VAL:CG2	1.61	1	1
SA:14:ARG:HG3	TA:203:VAL:CG1	1.61	1	1
CA:69:ILE:CD	DA:204:THR:H	1.61	1	1
TA:89:VAL:CB	UA:187:VAL:CG1	1.61	1	1
VA:230:PHE:CZ	WA:141:VAL:HG12	1.61	1	1
E:124:LEU:CD2	F:45:SER:HB3	1.61	1	1
U:230:PHE:CZ	V:141:VAL:HG12	1.61	1	1
E:124:LEU:CD1	F:45:SER:HB2	1.61	1	1
S:230:PHE:CE1	T:141:VAL:HG12	1.61	1	1
A:141:VAL:HG12	ZA:230:PHE:CZ	1.60	1	1
X:89:VAL:CG1	Y:187:VAL:HG11	1.60	1	1
NA:230:PHE:CE1	OA:141:VAL:CG1	1.60	1	1
A:230:PHE:CE1	B:141:VAL:CB	1.60	1	1
TA:230:PHE:CE1	UA:141:VAL:HG12	1.60	1	1
A:218:PHE:CE2	B:42:TYR:CD2	1.60	1	1
A:230:PHE:CZ	B:141:VAL:HG12	1.60	1	1
W:230:PHE:CE1	X:141:VAL:HG12	1.60	1	1
N:86:LEU:CD2	O:188:GLY:H	1.60	1	1
S:86:LEU:HD21	T:188:GLY:CA	1.60	1	1
XA:230:PHE:CE1	YA:141:VAL:HG12	1.60	1	1
U:230:PHE:CE1	V:141:VAL:HG12	1.60	1	1
LA:67:ALA:HB2	MA:207:GLY:CA	1.60	1	1
A:218:PHE:HE2	B:42:TYR:CD2	1.60	1	1
NA:230:PHE:HE1	OA:141:VAL:CG1	1.60	1	1
J:67:ALA:HB3	K:205:TYR:CE1	1.59	1	1
W:89:VAL:CG1	X:187:VAL:HG11	1.59	1	1
UA:218:PHE:CE2	VA:42:TYR:CD2	1.59	1	1
N:230:PHE:HE1	O:141:VAL:CG1	1.59	1	1
QA:15:LEU:CG	RA:203:VAL:HG23	1.59	1	1
QA:86:LEU:HD21	RA:188:GLY:CA	1.59	1	1
S:14:ARG:HG3	T:203:VAL:CG1	1.59	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
UA:87:LYS:HD2	VA:186:VAL:CB	1.59	1	1
F:124:LEU:HD21	G:45:SER:CB	1.59	1	1
VA:89:VAL:HB	WA:187:VAL:CG1	1.59	1	1
P:86:LEU:HD21	Q:188:GLY:CA	1.59	1	1
DA:15:LEU:CD1	EA:203:VAL:HG21	1.59	1	1
Z:230:PHE:CE1	AA:141:VAL:HG12	1.58	1	1
IA:86:LEU:HD21	JA:187:VAL:C	1.58	1	1
A:230:PHE:CE1	B:141:VAL:CG1	1.58	1	1
OA:230:PHE:HE1	PA:141:VAL:CG1	1.58	1	1
W:230:PHE:CZ	X:141:VAL:HG12	1.58	1	1
T:230:PHE:CE1	U:141:VAL:HG12	1.58	1	1
RA:124:LEU:CD2	SA:45:SER:HB2	1.58	1	1
E:15:LEU:HD11	F:203:VAL:CG2	1.58	1	1
GA:124:LEU:HD21	HA:45:SER:CB	1.58	1	1
VA:230:PHE:CE1	WA:141:VAL:HG12	1.58	1	1
AA:230:PHE:CE1	BA:141:VAL:CB	1.58	1	1
TA:124:LEU:CD2	UA:45:SER:CB	1.58	1	1
YA:65:ALA:CB	ZA:208:GLU:CD	1.58	1	1
AA:218:PHE:HE2	BA:42:TYR:CD2	1.58	1	1
T:89:VAL:CB	U:187:VAL:CG1	1.57	1	1
RA:86:LEU:CD2	SA:188:GLY:HA3	1.57	1	1
Y:230:PHE:CZ	Z:141:VAL:HG12	1.57	1	1
U:87:LYS:HD2	V:186:VAL:CB	1.57	1	1
FA:124:LEU:HD21	GA:45:SER:CB	1.57	1	1
SA:86:LEU:HD21	TA:188:GLY:CA	1.57	1	1
K:228:THR:HG21	L:140:PRO:CG	1.57	1	1
IA:228:THR:CG2	JA:140:PRO:CD	1.57	1	1
XA:89:VAL:CG1	YA:187:VAL:HG11	1.57	1	1
S:89:VAL:HB	T:187:VAL:CG1	1.57	1	1
VA:87:LYS:HD2	WA:186:VAL:CB	1.57	1	1

Torsion angles: Protein backbone

In the following table, Ramachandran outliers are listed. The Analysed column shows the number of residues for which the backbone conformation was analysed.

Model ID	Analysed	Favored	Allowed	Outliers
1	11856	10608	1092	156

There are 156 unique backbone outliers. Detailed list of outliers are tabulated below. The output is limited to 100 rows.

Chain	Res	Type	Models (Total)
A	182	GLU	1
A	183	ILE	1
A	223	LYS	1
AA	182	GLU	1
AA	183	ILE	1
AA	223	LYS	1
B	182	GLU	1
B	183	ILE	1
B	223	LYS	1
BA	182	GLU	1
BA	183	ILE	1
BA	223	LYS	1
C	182	GLU	1
C	183	ILE	1
C	223	LYS	1
CA	182	GLU	1
CA	183	ILE	1
CA	223	LYS	1
D	182	GLU	1
D	183	ILE	1
D	223	LYS	1
DA	182	GLU	1
DA	183	ILE	1
DA	223	LYS	1
E	182	GLU	1
E	183	ILE	1
E	223	LYS	1
EA	182	GLU	1
EA	183	ILE	1
EA	223	LYS	1
F	182	GLU	1
F	183	ILE	1
F	223	LYS	1
FA	182	GLU	1

Chain	Res	Type	Models (Total)
FA	183	ILE	1
FA	223	LYS	1
G	182	GLU	1
G	183	ILE	1
G	223	LYS	1
GA	182	GLU	1
GA	183	ILE	1
GA	223	LYS	1
H	182	GLU	1
H	183	ILE	1
H	223	LYS	1
HA	182	GLU	1
HA	183	ILE	1
HA	223	LYS	1
I	182	GLU	1
I	183	ILE	1
I	223	LYS	1
IA	182	GLU	1
IA	183	ILE	1
IA	223	LYS	1
J	182	GLU	1
J	183	ILE	1
J	223	LYS	1
JA	182	GLU	1
JA	183	ILE	1
JA	223	LYS	1
K	182	GLU	1
K	183	ILE	1
K	223	LYS	1
KA	182	GLU	1
KA	183	ILE	1
KA	223	LYS	1
L	182	GLU	1
L	183	ILE	1
L	223	LYS	1

Chain	Res	Type	Models (Total)
LA	182	GLU	1
LA	183	ILE	1
LA	223	LYS	1
M	182	GLU	1
M	183	ILE	1
M	223	LYS	1
MA	182	GLU	1
MA	183	ILE	1
MA	223	LYS	1
N	182	GLU	1
N	183	ILE	1
N	223	LYS	1
NA	182	GLU	1
NA	183	ILE	1
NA	223	LYS	1
O	182	GLU	1
O	183	ILE	1
O	223	LYS	1
OA	182	GLU	1
OA	183	ILE	1
OA	223	LYS	1
P	182	GLU	1
P	183	ILE	1
P	223	LYS	1
PA	182	GLU	1
PA	183	ILE	1
PA	223	LYS	1
Q	182	GLU	1
Q	183	ILE	1
Q	223	LYS	1
QA	182	GLU	1

Torsion angles : Protein sidechains

In the following table, sidechain rotameric outliers are listed. The Analysed column shows the number of residues for which the sidechain conformation was analysed.

Model ID	Analysed	Favored	Allowed	Outliers
1	9100	7904	1144	52

There are 52 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	119	ASP	1
AA	119	ASP	1
B	119	ASP	1
BA	119	ASP	1
C	119	ASP	1
CA	119	ASP	1
D	119	ASP	1
DA	119	ASP	1
E	119	ASP	1
EA	119	ASP	1
F	119	ASP	1
FA	119	ASP	1
G	119	ASP	1
GA	119	ASP	1
H	119	ASP	1
HA	119	ASP	1
I	119	ASP	1
IA	119	ASP	1
J	119	ASP	1
JA	119	ASP	1
K	119	ASP	1
KA	119	ASP	1
L	119	ASP	1
LA	119	ASP	1
M	119	ASP	1
MA	119	ASP	1
N	119	ASP	1
NA	119	ASP	1
O	119	ASP	1
OA	119	ASP	1
P	119	ASP	1

Chain	Res	Type	Models (Total)
PA	119	ASP	1
Q	119	ASP	1
QA	119	ASP	1
R	119	ASP	1
RA	119	ASP	1
S	119	ASP	1
SA	119	ASP	1
T	119	ASP	1
TA	119	ASP	1
U	119	ASP	1
UA	119	ASP	1
V	119	ASP	1
VA	119	ASP	1
W	119	ASP	1
WA	119	ASP	1
X	119	ASP	1
XA	119	ASP	1
Y	119	ASP	1
YA	119	ASP	1
Z	119	ASP	1
ZA	119	ASP	1

5. Fit to Data Used for Modeling Assessment

5.3. 3DEM

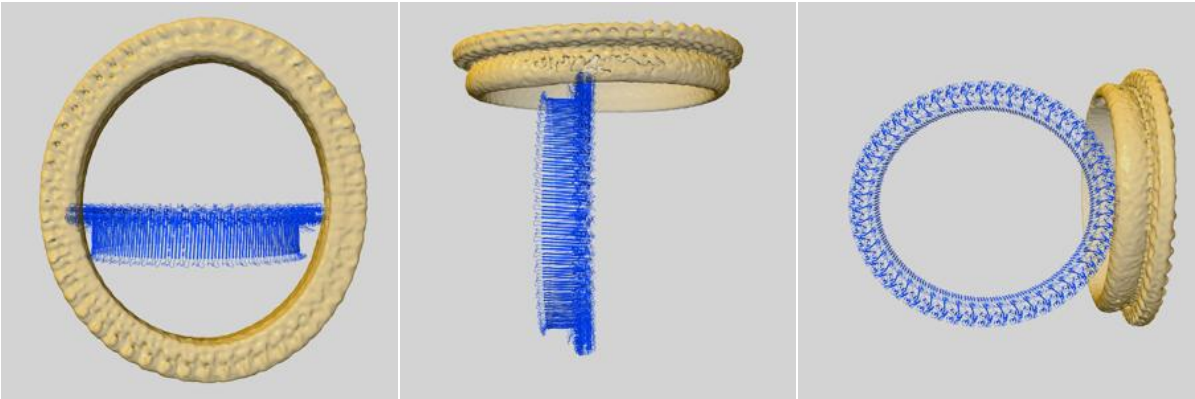
This section describes fit of models to the 3DEM data. Only results for the representative model, selected as a first model with the largest number of asymmetric units.

EMD-43510

5.3.1. Map-model fit

Only results for the representative Model 1 are shown.

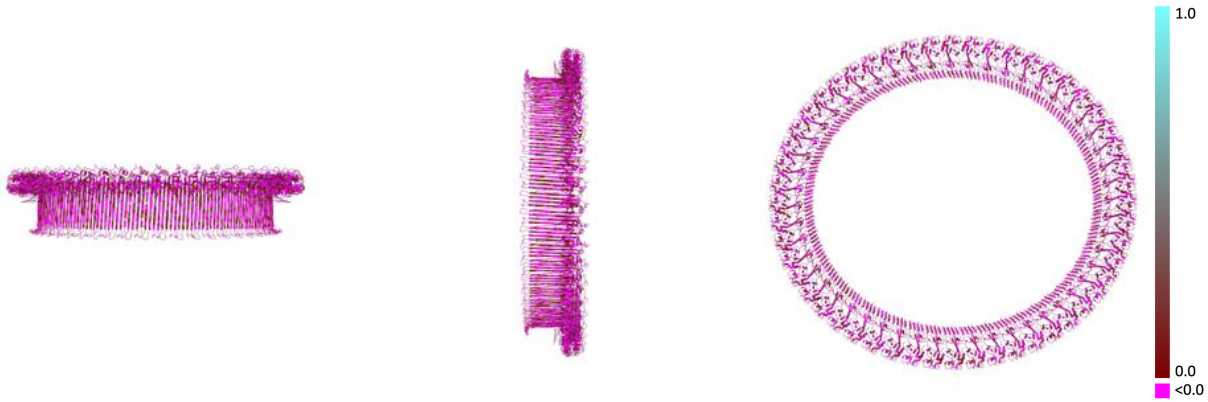
5.3.1.1 Map-model overlay



X **Y** **Z**

The images above show the 3D surface view of the map at the recommended contour level 0.600 at 50% transparency in yellow overlaid with a ribbon representation of the model colored in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

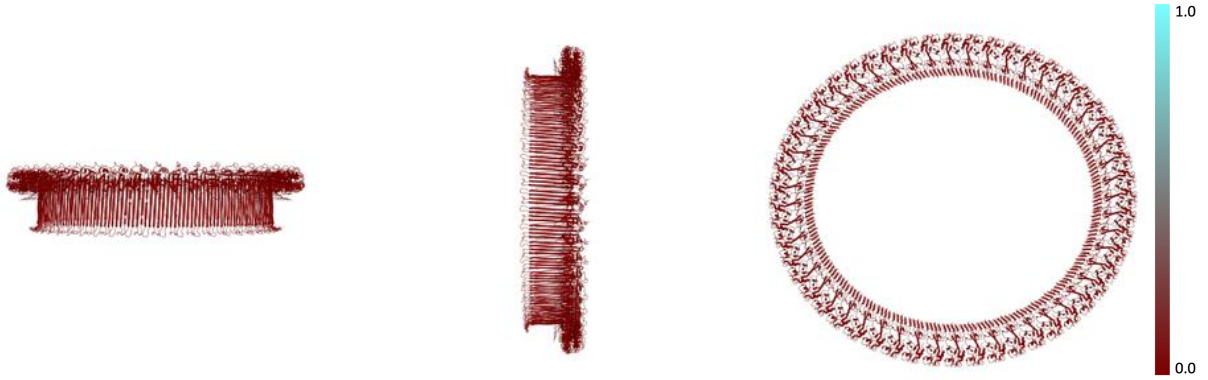
5.3.1.2. Q-score mapped to coordinate model



X **Y** **Z**

The images above show the model with each residue colored according to 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.

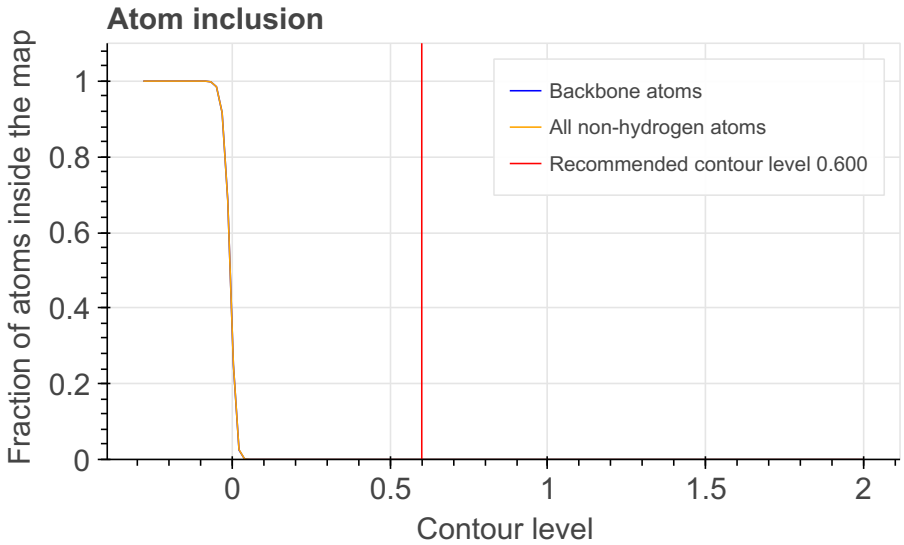
5.3.1.3. Atom inclusion mapped to coordinate model



X **Y** **Z**

The images above show the model with each residue colored according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level 0.600 .

5.3.1.4. Atom inclusion



At the recommended contour level, 0% of all backbone atoms, 0% of all non-hydrogen atoms, are inside the map.

5.3.1.5. Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.600) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.000	0.001
A	0.000	0.002
B	0.000	-0.004
C	0.000	0.007
D	0.000	-0.005
E	0.000	-0.010
F	0.000	-0.010
G	0.000	-0.001
H	0.000	-0.002
I	0.000	-0.007
J	0.000	-0.012
K	0.000	0.003
L	0.000	-0.006
M	0.000	0.005
N	0.000	0.020
O	0.000	0.015
P	0.000	-0.008
Q	0.000	-0.008
R	0.000	0.008
S	0.000	-0.003
T	0.000	-0.001

Chain	Atom inclusion	Q-score
U	0.000	0.000
V	0.000	-0.010
W	0.000	0.011
X	0.000	-0.002
Y	0.000	0.004
Z	0.000	-0.006
AA	0.000	0.021
BA	0.000	-0.001
CA	0.000	0.000
DA	0.000	0.012
EA	0.000	-0.005
FA	0.000	0.014
GA	0.000	0.013
HA	0.000	0.018
IA	0.000	0.013
JA	0.000	0.001
KA	0.000	-0.002
LA	0.000	-0.009
MA	0.000	0.008
NA	0.000	-0.007
OA	0.000	0.001
PA	0.000	0.004
QA	0.000	-0.022
RA	0.000	-0.004
SA	0.000	0.004
TA	0.000	-0.012
UA	0.000	0.002
VA	0.000	-0.003
WA	0.000	0.011
XA	0.000	0.001
YA	0.000	-0.001
ZA	0.000	0.004

5.4. 2DEM class average

Validation for this section is under development.

6. Fit to Data Used for Validation Assessment

Validation for this section is under development.

Acknowledgments

The development of integrative model validation metrics, implementation of a model validation pipeline, and creation of a validation report for integrative structures are funded by NSF awards to the PDB-IHM team (DBI-1756248, DBI-2112966, DBI-2112967, DBI-2112968, and DBI-1756250) and awards from NSF, NIH, and DOE to the RCSB PDB (DBI-2321666, R01GM157729, and DE-SC0019749). The PDB-IHM team and members of the Sali lab contributed model validation metrics and software packages.

Dr. Jill Trewhella, Dr. Dina Schneidman, and members of the SASBDB repository are acknowledged for their advice and support in implementing SAS validation methods. Team members from the labs of Dr. Juri Rappsilber, Dr. Alexander Leitner, Dr. Andrea Graziadei, and members of PRIDE database are acknowledged for their advice and support in implementing crosslinking-MS validation methods. We are grateful to Dr. Shruthi Viswanath for discussions about uncertainty assessment of integrative structural models.

Members of the wwPDB Integrative/Hybrid Methods Task Force provided recommendations and community support for the project.