



wwPDB EM Validation Summary Report ⓘ

Mar 12, 2026 – 04:12 PM UTC

PDB ID : 7CRB / pdb_00007crb
EMDB ID : EMD-30449
Title : Cryo-EM structure of plant NLR RPP1 LRR-ID domain in complex with ATR1
Authors : Ma, S.C.; Lapin, D.; Liu, L.; Sun, Y.; Song, W.; Zhang, X.X.; Logemann, E.; Yu, D.L.; Wang, J.; Jirschitzka, J.; Han, Z.F.; SchulzeLefert, P.; Parker, J.E.; Chai, J.J.
Deposited on : 2020-08-13
Resolution : 3.16 Å(reported)

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

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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>.

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

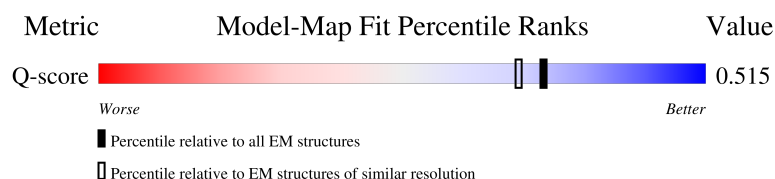
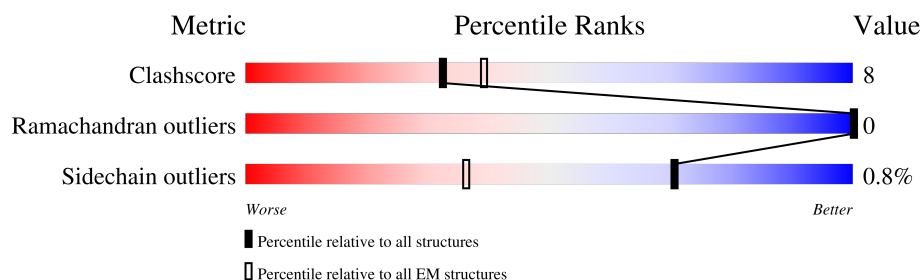
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.16 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14474 (2.66 - 3.66)

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 $\leq 5\%$. 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	J	311	
2	A	1221	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6806 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 Avirulence protein ATR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	J	235	Total	C	N	O	S	0	0
			1880	1190	323	362	5		

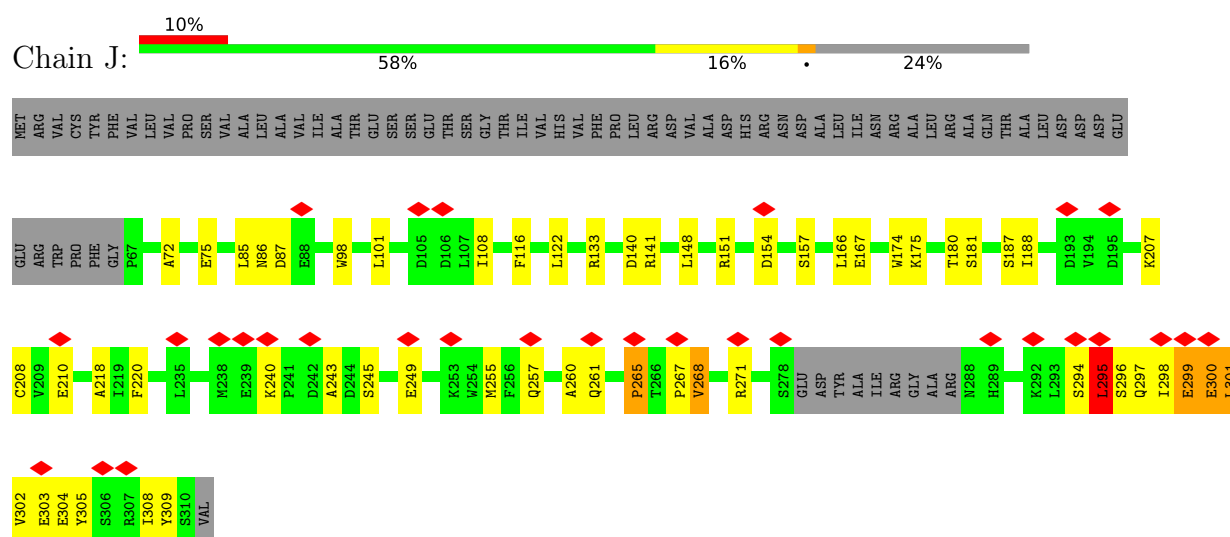
- Molecule 2 is a protein called NAD⁺ hydrolase (NADase).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	616	Total	C	N	O	S	0	0
			4926	3128	832	932	34		

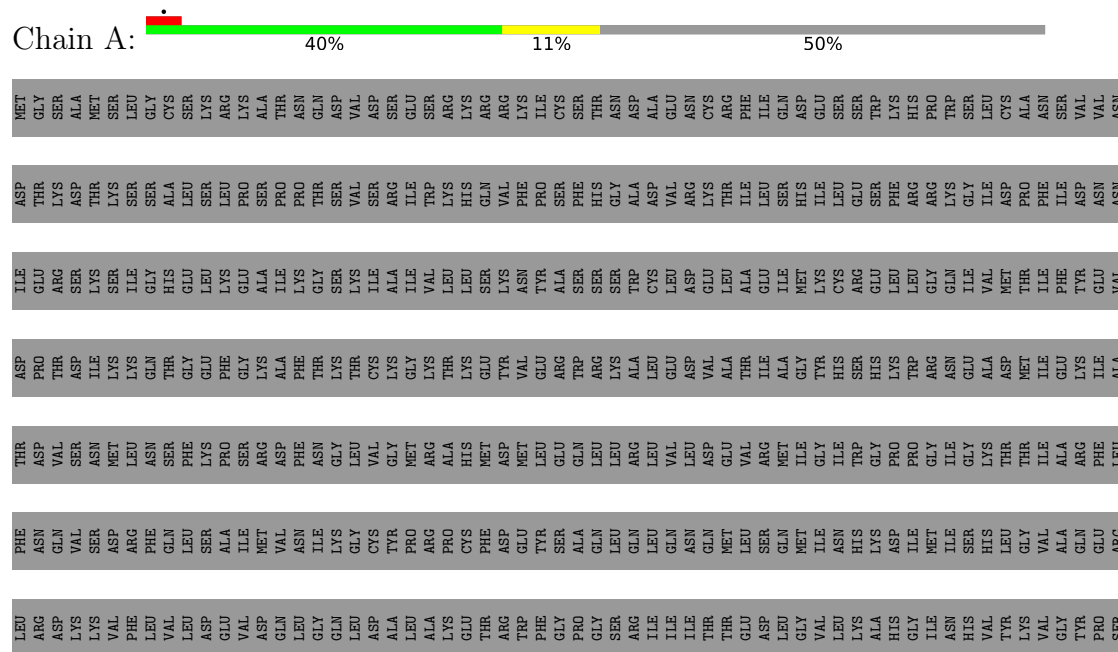
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Avirulence protein ATR1



• Molecule 2: NAD⁺ hydrolase (NADase)



E1172	L1173	M1071	P927	L776	K612	LEU
M1181	P1073	L1072	S930	E777	N613	ALA
I1184	V1077	T931	L782	L785	V614	LYS
I1187	H1083	R937	P786	L786	E615	SER
I1192	R1084	L938	N790	I619	E616	LEU
R1195	S1087	V946	A791	S620	I619	ILE
GLU	G1088	P947	N792	E621	S620	SER
THR	D1089	L948	N793	K622	K622	ILE
ARG	I1093	S949	L794	V633	V633	ASN
SER	K1094	S952	L799	R634	R634	ILE
LEU	L1095	I961	L808	K638	K638	GLN
ARG	K1096	P809	P809	N639	N639	LYS
SER	E1097	I811	A810	H640	H640	THR
SER	S1098	A814	L817	H643	H643	ASP
PRO	P1099	E979	L823	E644	E644	LEU
ASP	L1100	P995	P832	R645	R645	GLN
LEU	P1101	V989	A838	L646	L646	GLY
SER	T1102	V992	L844	Q647	Q647	ARG
PRO	T1103	R995	R847	K662	K662	GLU
GLU	F1106	A1001	N864	G663	G663	THR
SER	K1107	L1002	F868	Y664	Y664	ARG
ARG	A1108	R1003	N884	Q665	Q665	LEU
VAL	C1109	N1008	L886	N666	N666	GLN
SER	I1110	H1009	R887	L669	L669	ILE
CYS	E1115	L1013	K888	M683	M683	ALA
ASP	E1116	L1016	L893	K690	K690	LEU
HIS	M1117	S1030	L903	L691	L691	ALA
CYS	S1118	L1031	P904	W692	W692	GLY
ASP	Y1119	E1032	T905	E693	E693	GLY
HIS	D1120	C1036	N906	R699	R699	LEU
CYS	L1121	C1037	I907	L715	L715	LEU
ASP	I1128	P1048	L907	P716	P716	GLY
GLU	Q1134	L1053	T914	L729	L729	SER
THR	N1135	L1060	L915	R730	R730	ALA
ASP	D1136	M1061	N916	E591	E591	ARG
GLU	Q1140	M1062	L917	N594	N594	LYS
LEU	C1141	H1063	L917	D595	D595	LYS
LEU	T1142	E1165	L917	D596	D596	PHE
LEU	P1143	E1166	L917	T597	T597	LYS
LEU	L1163	E1167	L917	I598	I598	ASP
LEU	E1168	V1168	L917	D599	D599	VAL
LEU	S1170	T1169	L917	S600	S600	ARG
LEU	T1171	L917	L917	R601	R601	THR
LEU	L917	L917	L917	R602	R602	GLY
LEU	L917	L917	L917	D609	D609	GLN
LEU	L917	L917	L917	L610	L610	LEU
LEU	L917	L917	L917	Y611	Y611	HIS
LEU	L917	L917	L917	L917	L917	LEU
LEU	L917	L917	L917	L917	L917	THR
LEU	L917	L917	L917	L917	L917	PRO
LEU	L917	L917	L917	L917	L917	ILE

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	222015	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 ($e^-/\text{\AA}^2$)	23.542	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	101.269	Depositor
Minimum map value	-67.279	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	18	Depositor
Map size (Å)	395.24402, 395.24402, 395.24402	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0979, 1.0979, 1.0979	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	J	0.32	0/1924	0.65	8/2603 (0.3%)
2	A	0.27	0/5016	0.44	1/6798 (0.0%)
All	All	0.28	0/6940	0.51	9/9401 (0.1%)

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	294	SER	N-CA-C	-9.05	102.25	113.38
2	A	947	PRO	CB-CA-C	-5.93	103.18	110.95
1	J	300	GLU	N-CA-C	-5.59	105.10	111.14
1	J	301	LEU	N-CA-C	-5.45	106.21	112.92
1	J	265	PRO	CA-N-CD	-5.33	104.54	112.00

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	J	1880	0	1824	37	0
2	A	4926	0	5010	82	0
All	All	6806	0	6834	116	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 8.

The worst 5 of 116 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:A:1128:ILE:HD13	2:A:1163:LEU:HD21	1.73	0.70
2:A:1140:GLN:HE21	2:A:1166:GLU:HB3	1.59	0.66
2:A:1036:CYS:SG	2:A:1037:CYS:N	2.69	0.66
2:A:1142:THR:HB	2:A:1164:GLU:HB3	1.79	0.64
2:A:690:LYS:NZ	2:A:693:GLU:OE2	2.30	0.63

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	J	231/311 (74%)	219 (95%)	12 (5%)	0	100	100
2	A	614/1221 (50%)	552 (90%)	62 (10%)	0	100	100
All	All	845/1532 (55%)	771 (91%)	74 (9%)	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	J	202/265 (76%)	199 (98%)	3 (2%)	57	72

Continued on next page...

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	581/1114 (52%)	578 (100%)	3 (0%)	81	82
All	All	783/1379 (57%)	777 (99%)	6 (1%)	70	78

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

Mol	Chain	Res	Type
2	A	1103	THR
2	A	1116	GLU
2	A	1117	MET
1	J	295	LEU
1	J	268	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	801	ASN
2	A	824	ASN
2	A	1140	GLN
2	A	960	GLN
2	A	665	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](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

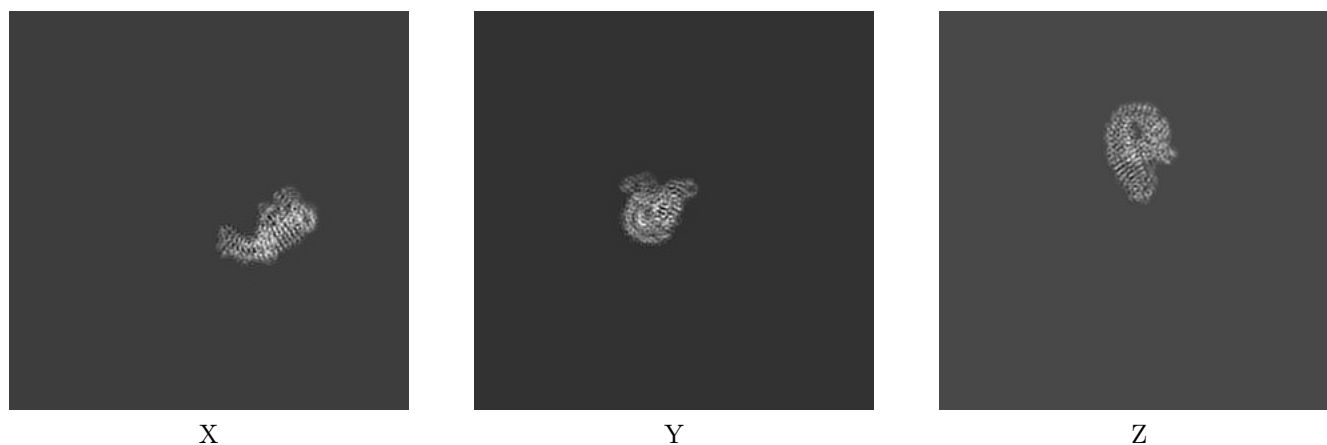
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30449. 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](#)

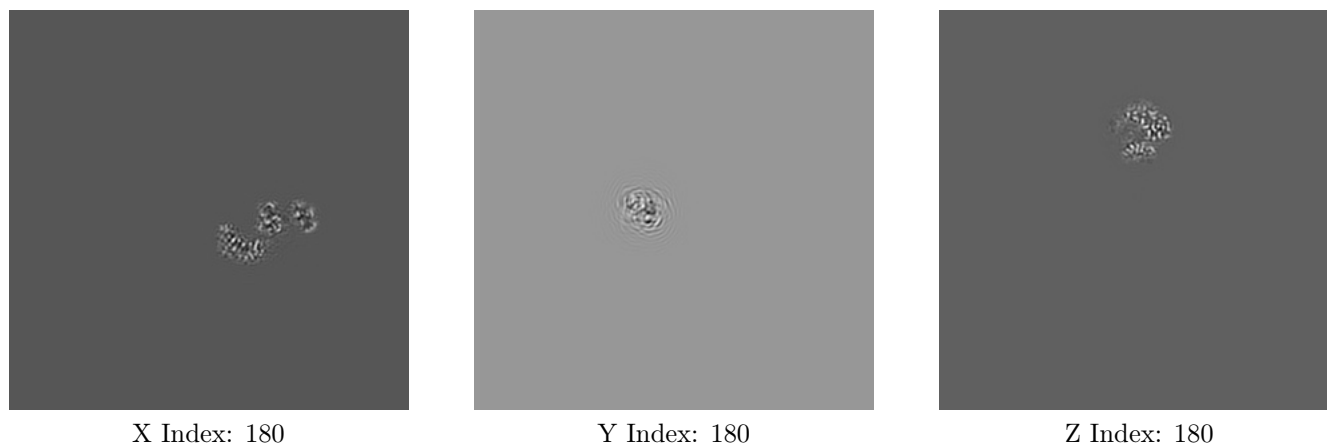
6.1.1 Primary map



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: 170



Y Index: 230

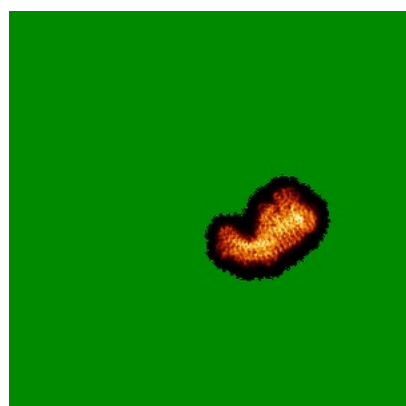


Z Index: 150

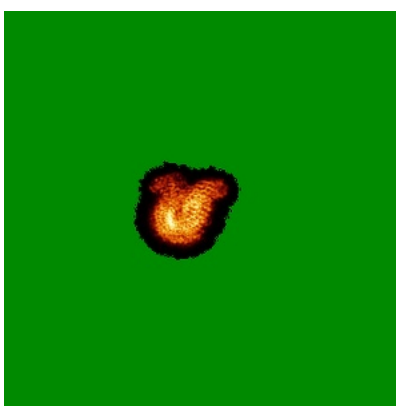
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

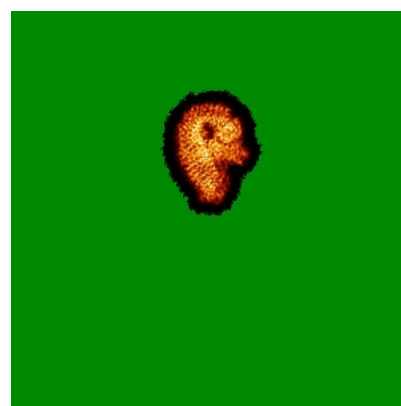
6.4.1 Primary map



X



Y

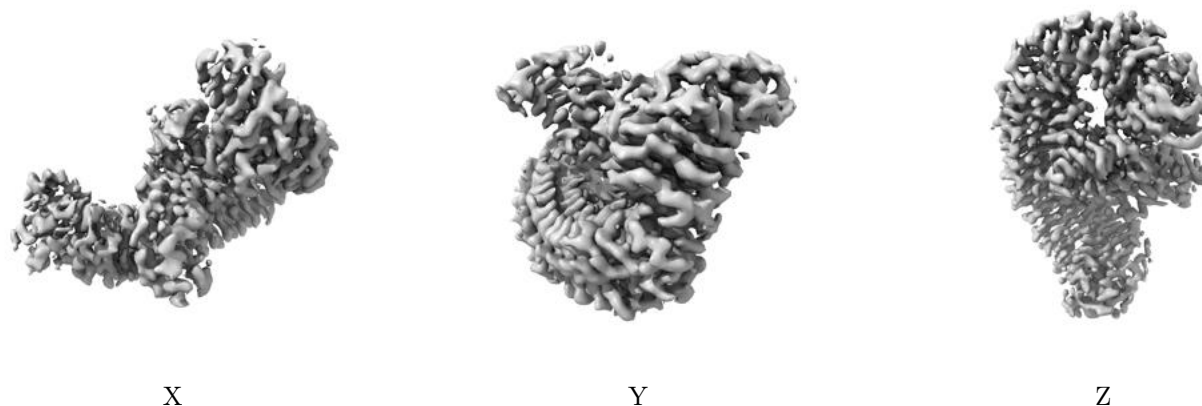


Z

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.

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 18.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

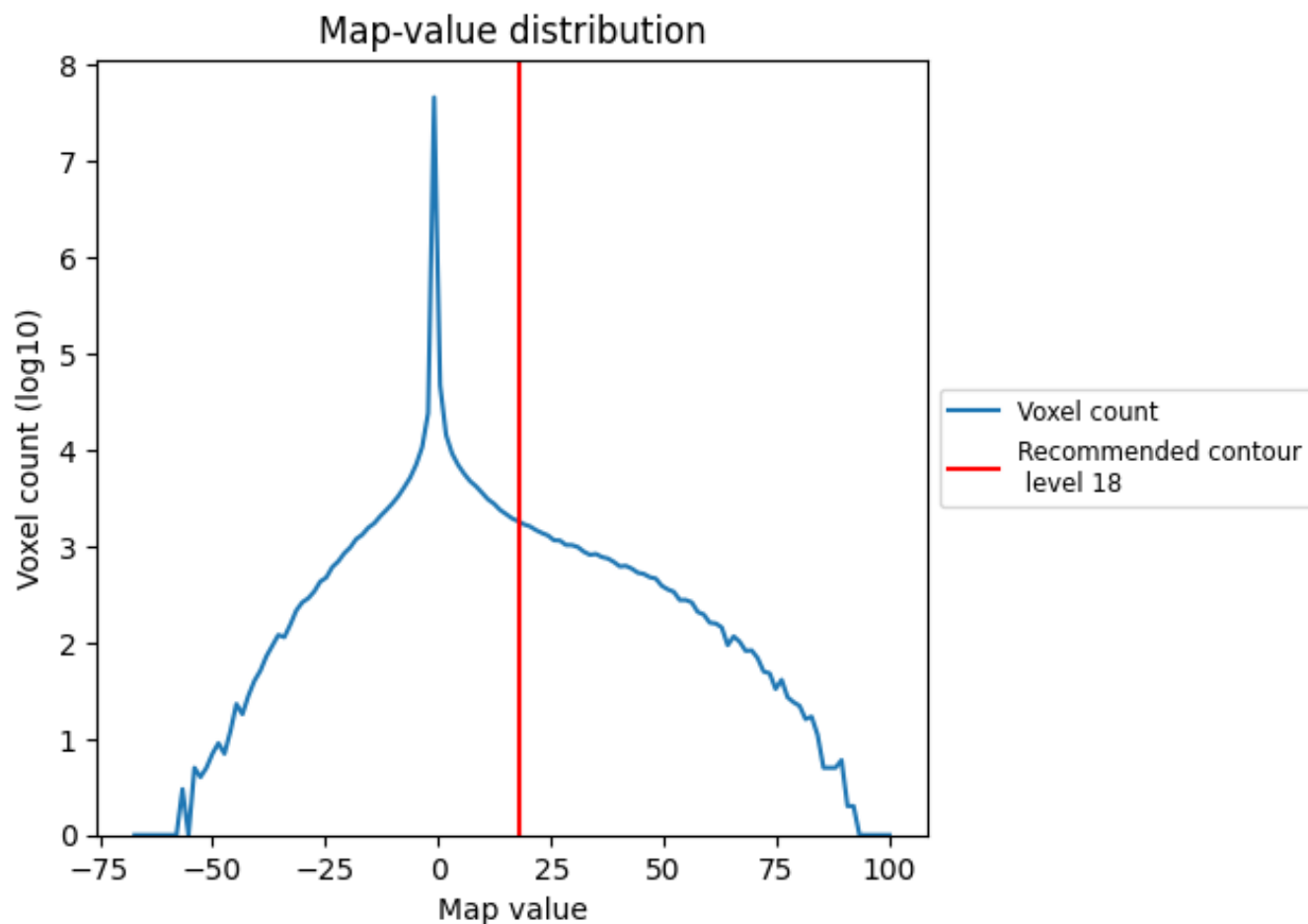
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

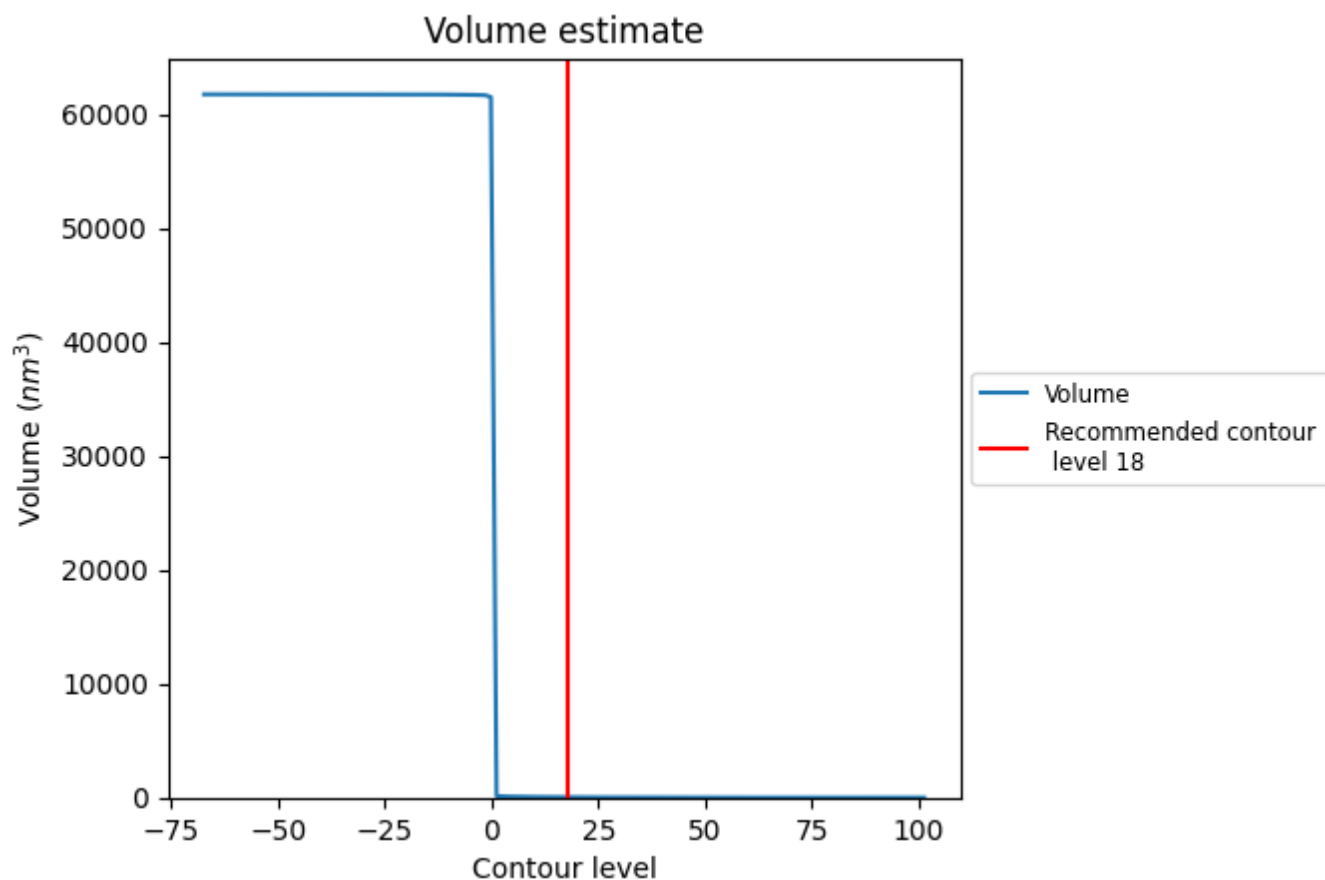
This section contains the results of statistical analysis of the map.

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.

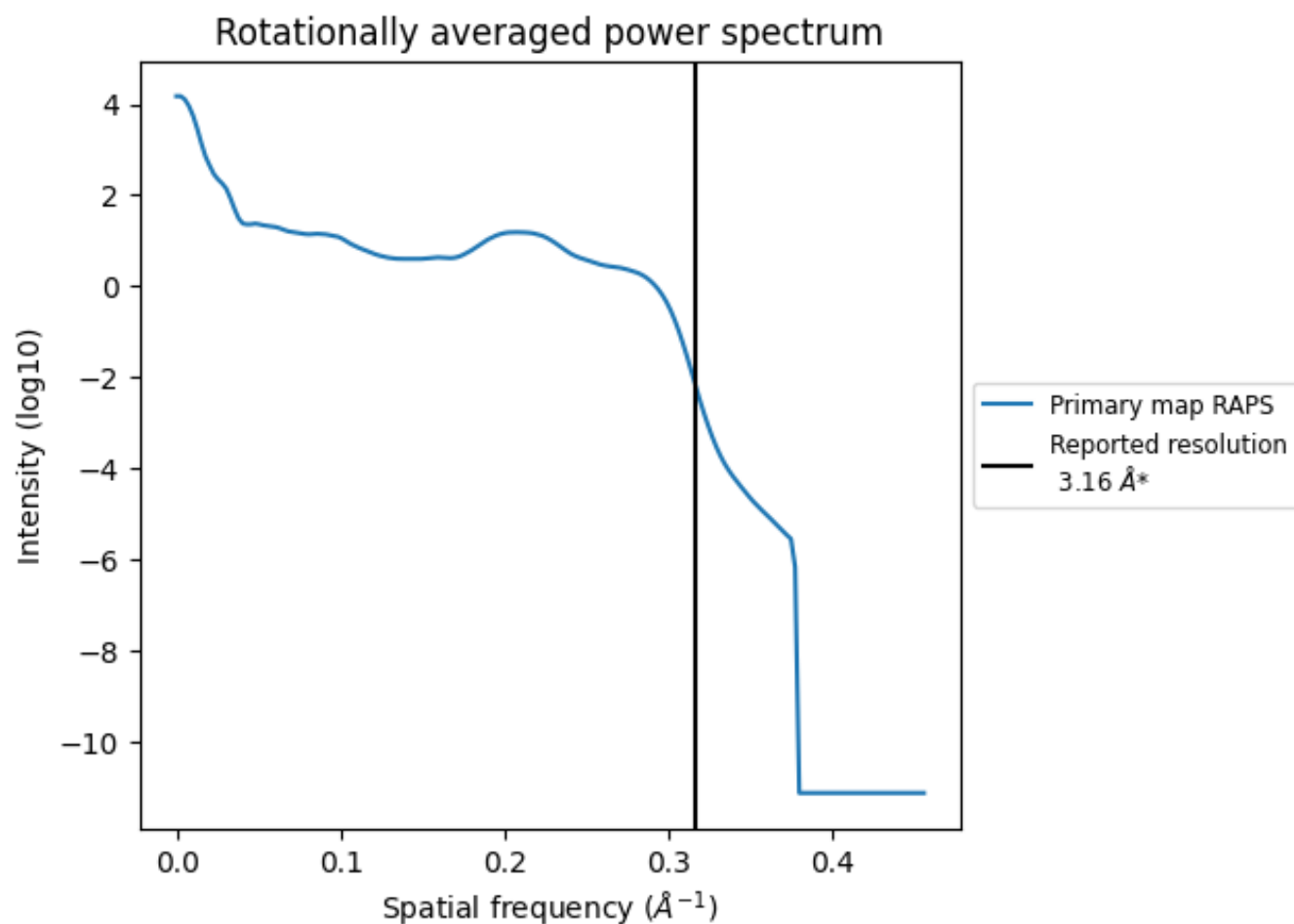
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 35 nm³; this corresponds to an approximate mass of 32 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.316 $\text{\AA}^{-1}$

8 Fourier-Shell correlation

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

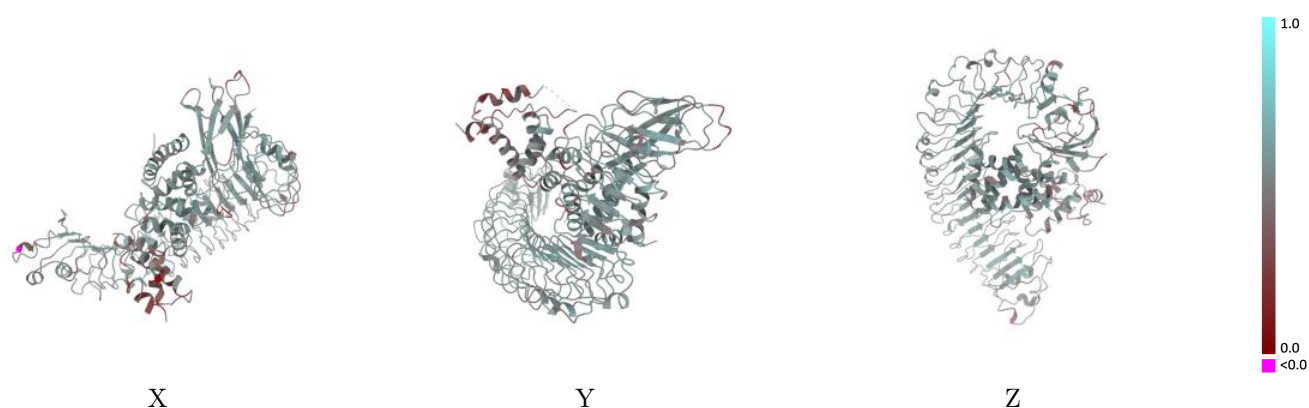
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30449 and PDB model 7CRB. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay [i](#)

This section was not generated.

9.2 Q-score mapped to coordinate model [i](#)



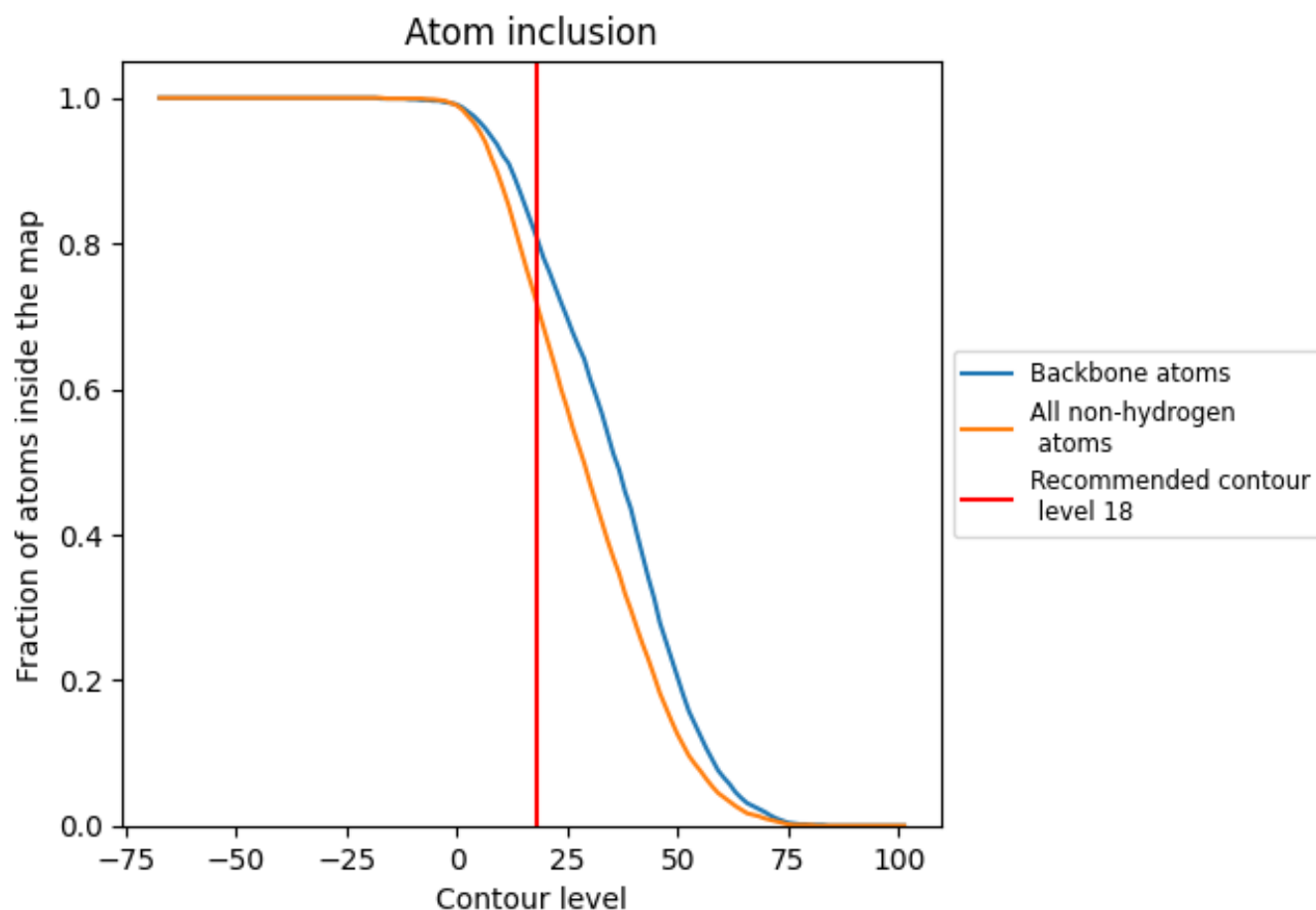
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

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 (18).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7200	0.5150
A	0.7340	0.5230
J	0.6820	0.4940

