



## wwPDB EM Validation Summary Report ⓘ

May 27, 2024 – 01:45 PM JST

PDB ID : 7ELE  
EMDB ID : EMD-31182  
Title : Cryo-EM structure of Arabidopsis DCL1 in complex with pre-miRNA 166f  
Authors : Wei, X.; Ke, H.; Feng, Y.  
Deposited on : 2021-04-09  
Resolution : 4.90 Å(reported)

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

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

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<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev92  
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

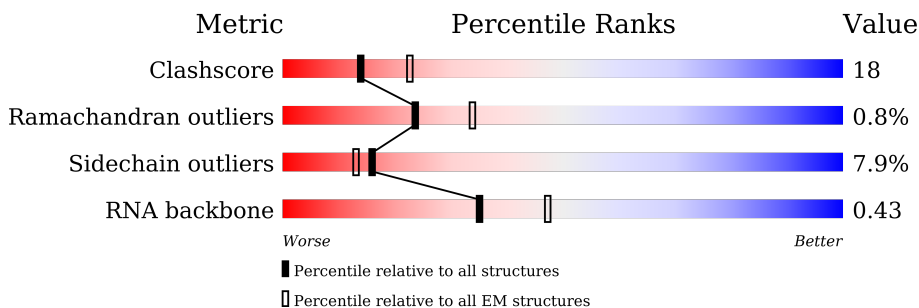
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1909	
2	G	89	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10733 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 Endoribonuclease Dicer homolog 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1137	Total	C	N	O	S	0	0
			8976	5726	1548	1642	60		

- Molecule 2 is a RNA chain called pre-miRNA 166f.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	83	Total	C	N	O	P	0	0
			1757	786	303	585	83		



CYS	LYS	ALA	PRO	K1689	V1690	L1691	L1694	V1695	E1696	S1697	I1698	I1702	S1706	D1709	T1710	A1713	W1714	A1717	F1717	L1721	W1725	L1730	P1731	M1732	H1733	P1734	V1735	R1736	E1737	R1741	C1742	Q1743	Q1744	Q1745	A1746	E1747	G1748	L1749	E1750	Y1751	K1752	A1753	S1754	R1755	S1756	G1757	N1758	A1760	L1761							
H1611	L1612	F1613	F1614	T1615	L1619	L1619	R1623	L1624	T1625	D1626	L1627	R1628	N1633	N1634	E1635	N1636	F1637	A1638	R1639	V1640	A1641	H1644	K1645	L1646	H1647	L1648	Y1649	L1650	R1651	L1657	E1658	K1659	R1662	V1665	K1666	Q1669	THR	GLU	SER	SER	SER	SER	LYS	PRO	GLY	PHE	ASN	SER	PHE	GLY	LEU	ASP				
M1526	K1527	W1528	I1529	G1530	I1531	HIS	VAL	GLU	ASP	PRO	PRO	VAL	ASP	GLY	THR	LYS	ASN	VAL	GLY	VAL	PRO	GLU	SER	VAL	LEU	LEU	LYS	ILE	D1558	L1562	A1565	K1571	E1572	K1573	L1576	I1580	T1581	H1582	R1585	S1591	C1592	Y1593	Q1594	R1595	L1596	E1597	F1598	L1607								
GLY	SER	SER	PHE	ASP	GLU	GLU	GLN	LYS	PRO	VAL	SER	GLU	ASN	SER	ASP	VAL	PHE	GLU	GLY	GLY	PRO	GLU	GLY	GLY	GLY	GLY	GLY	ASP	LEU	SER	TYR	R1495	V1496	L1497	S1498	K1499	T1500	L1502	A1503	D1504	V1505	V1506	E1507	A1508	L1509	I1510	Y1513	A1522	T1523	H1524	L1525					
S1390	L1393	K1396	Y1397	P1398	Q1399	K1400	H1401	Q1404	L1405	T1406	R1407	Q1411	M1412	V1413	S1414	M1416	V1417	L1418	Y1419	K1425	G1426	L1427	Q1428	S1429	ILE	GLN	ALA	ASP	ARG	PHE	PRO	SER	ARG	TRP	SER	ALA	PRO	ARG	ARG	PRO	ARG	PHE	GLY	GLY	THR	V1300	L1301	D1302	F1303	T1304						
L1309	P1310	P1311	E1312	L1313	C1314	H1317	P1318	L1319	G1320	G1321	L1322	I1324	R1325	G1326	A1327	L1330	P1331	S1332	I1333	M1334	R1335	R1336	V1337	L1338	S1339	M1340	A1343	K1347	N1348	L1349	T1350	S1351	Y1352	T1356	T1359	C1368	Q1369	E1370	T1371	F1372	C1373	Y1374	E1375	L1378	L1379	L1380	L1385	W1387								
F1225	D1228	S1229	I1230	C1231	Y1232	D1233	Y1246	L1247	G1248	Y1252	H1253	T1254	D1257	Y1258	Q1261	K1262	Y1263	L1267	M1268	K1269	P1270	Q1271	Q1272	I1275	K1276	G1277	R1278	Y1282	CYS	LYS	ASN	LEU	LEU	SER	PRO	ARG	ARG	PRO	ARG	PHE	GLY	GLY	THR	V1300	L1301	D1302	F1303	T1304								
SER	HIS	THR	PRO	TYR	GLY	ILE	ARG	GLY	ALA	VAL	SER	PHE	ASP	VAL	VAL	ARG	ALA	SER	GLY	LEU	LEU	PRO	VAL	ARG	ASP	ALA	PHE	GLU	LYS	GLY	LYS	L1199	M1200	E1209	D1210	L1211	I1212	G1213	K1214	ILE	VAL	THR	ALA	ALA	SER	GLY	GLY	R1224								
E1016	L1017	E1020	L1021	S1023	M1024	S1025	D1027	L1028	Y1029	V1030	R1032	K1037	A1038	S1039	L1040	K1043	G1044	S1045	L1046	D1047	N1051	L1056	F1069	D1069	VAL	ASP	VAL	GLU	SER	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR								
ARG	GLU	PHE	TYR	PRO	GLU	GLY	VAL	ALA	ASP	VAL	LYS	GLY	GLY	TRP	VAL	E975	V976	C977	E978	K981	H984	TYR	MET	TYR	ASN	VAL	ARG	CYS	VAL	ASP	PHE	GLY	SER	SER	LYS	LYS	ALA	ALA	ASP	PRO	PHE	GLN	ASP	ASP	GLY	GLY	VAL	S1007	E1008	F1009	A1010	L1012	F1013	G1014	N1015	
Q882	L883	P884	N885	A887	P888	F889	E890	I891	L892	P895	V896	C897	S898	S899	L902	Q905	A906	V907	K914	A920	PHE	THR	ASP	MET	LEU	PRO	ASP	LYS	GLY	GLY	GLY	GLY	ASP	ALA	GLU	LYS	LYS	ALA	ALA	ASP	PRO	PHE	GLN	ASP	ASP	GLY	GLY	VAL	S1007	E1008	F1009	A1010	L1012	F1013	G1014	N1015
E802	R803	T804	N805	L806	K810	D811	R814	L815	I816	S817	I818	D819	A820	V821	P822	G823	T824	V825	Y826	M834	L837	N838	H845	F846	S849	Q850	L851	P852	G853	R854	R855	Y856	A857	I858	L859	R860	F863	S864	M865	E866	K867	H868	E869	K870	T875	S878	C879	L881								



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	300148	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 ( $e^-/\text{\AA}^2$ )	64	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.028	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	202.80002, 202.80002, 202.80002	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.014, 1.014, 1.014	Depositor

## 5 Model quality

### 5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.40	0/9133	0.59	0/12319
2	G	0.57	0/1958	1.13	0/3039
All	All	0.44	0/11091	0.73	0/15358

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

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	8976	0	9149	315	0
2	G	1757	0	893	57	0
All	All	10733	0	10042	361	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 18.

The worst 5 of 361 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)
1:A:670:PHE:HB2	1:A:747:ARG:HA	1.53	0.91
2:G:28:A:H62	2:G:59:G:N2	1.70	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1009:PHE:HA	1:A:1088:VAL:O	1.72	0.88
1:A:424:GLN:HG2	1:A:429:ILE:HB	1.63	0.81
2:G:28:A:H62	2:G:59:G:H21	1.24	0.81

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1111/1909 (58%)	1001 (90%)	101 (9%)	9 (1%)	19 60

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	367	ILE
1	A	663	ALA
1	A	728	VAL
1	A	817	SER
1	A	419	LYS

### 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	983/1639 (60%)	905 (92%)	78 (8%)	12 38

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1224	ARG
1	A	1524	HIS
1	A	1257	ASP
1	A	1369	GLN
1	A	1743	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1523	ASN
1	A	1633	ASN
1	A	1789	ASN
1	A	1758	ASN
1	A	1775	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	G	79/89 (88%)	33 (41%)	2 (2%)

5 of 33 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	G	3	A
2	G	9	G
2	G	10	C
2	G	14	G
2	G	16	U

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	G	13	G
2	G	25	U

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

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.

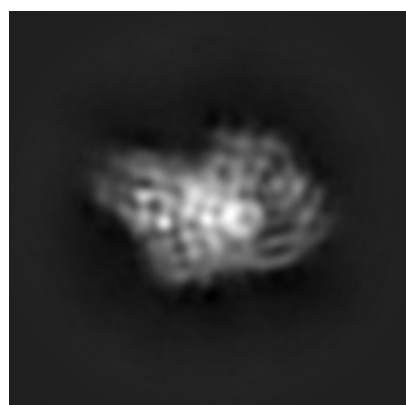
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31182. These allow visual inspection of the internal detail of the map and identification of artifacts.

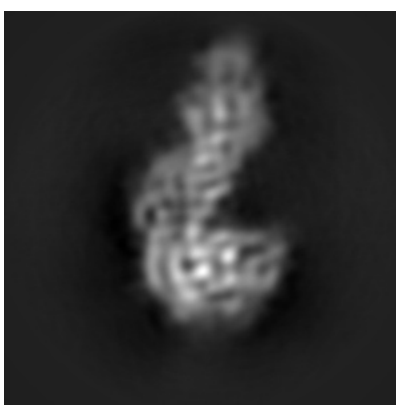
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

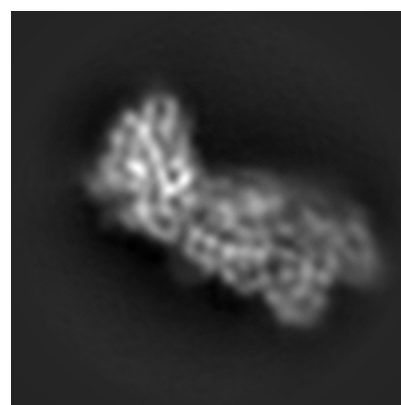
#### 6.1.1 Primary map



X



Y

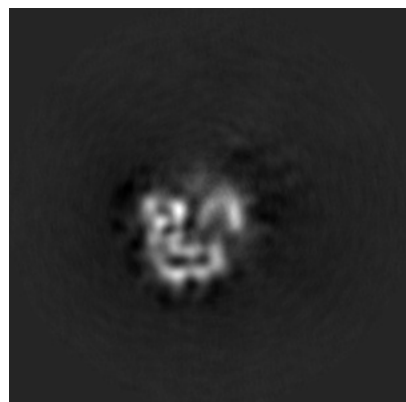


Z

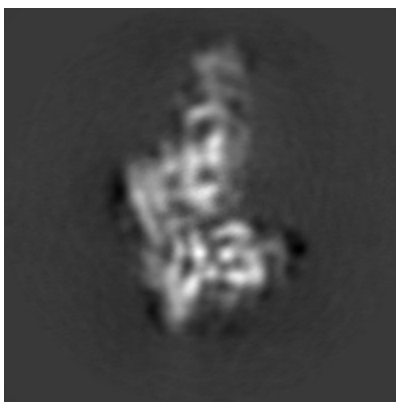
The images above show the map projected in three orthogonal directions.

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

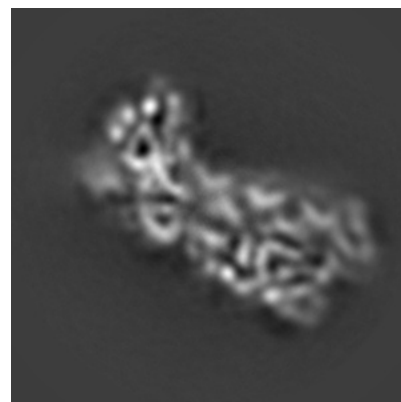
#### 6.2.1 Primary map



X Index: 100



Y Index: 100

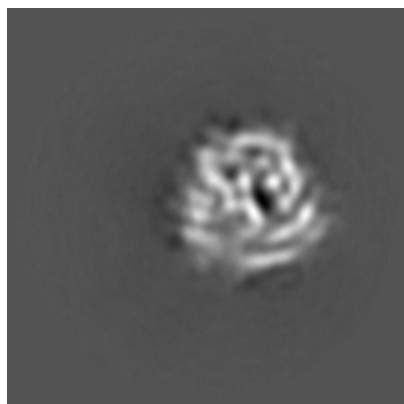


Z Index: 100

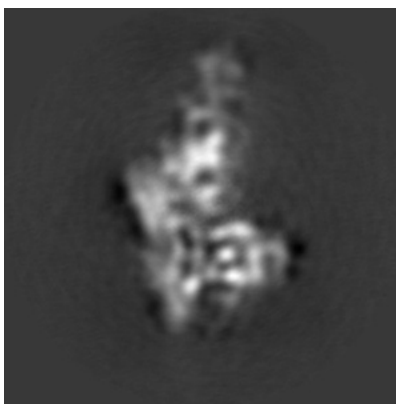
The images above show central slices of the map in three orthogonal directions.

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

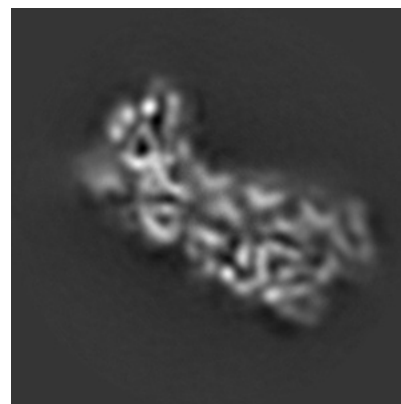
### 6.3.1 Primary map



X Index: 66



Y Index: 102



Z Index: 99

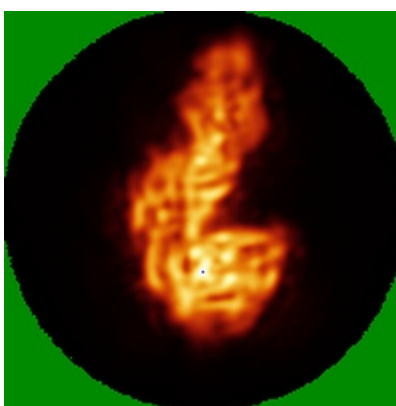
The images above show the largest variance slices of the map in three orthogonal directions.

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

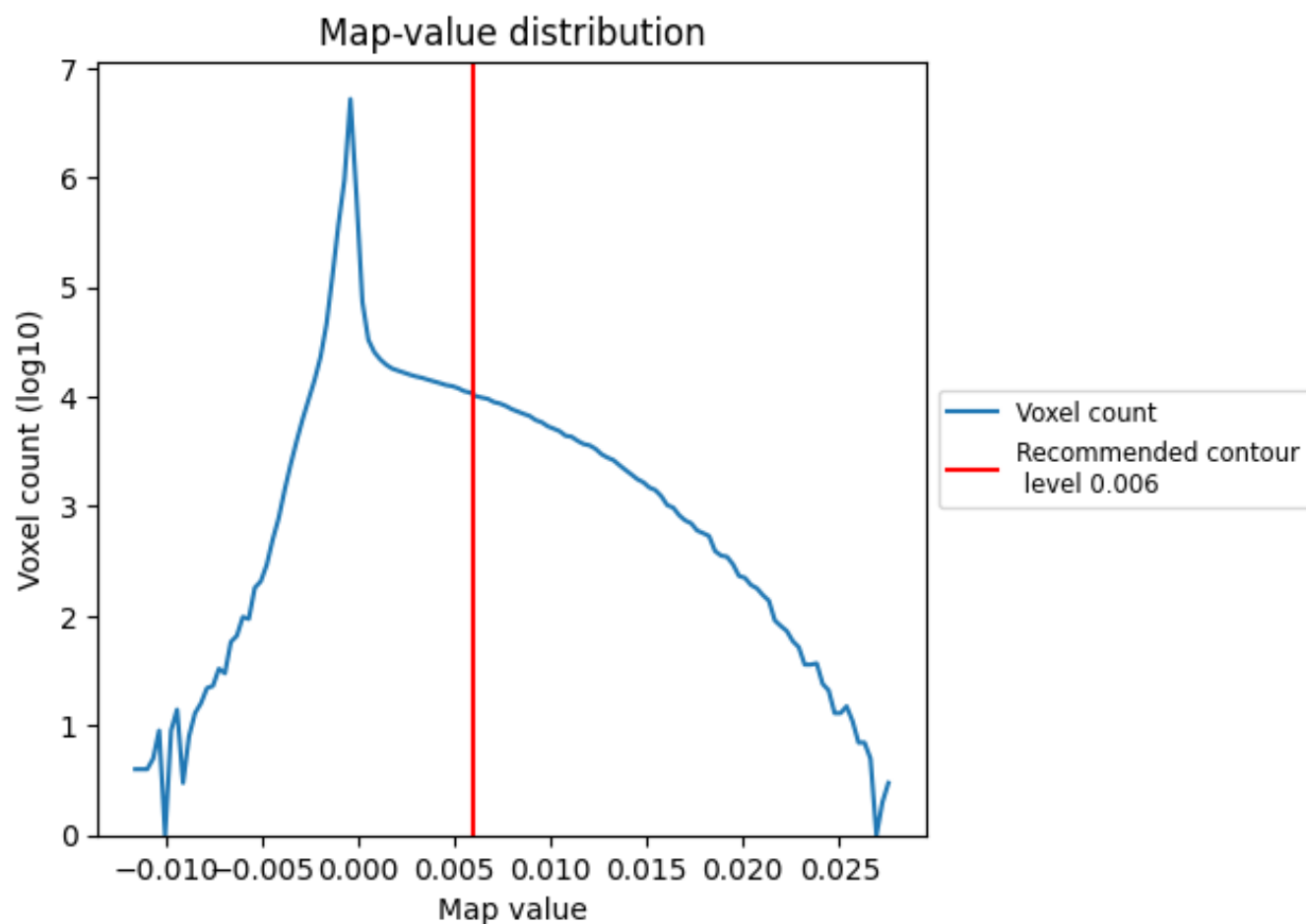
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

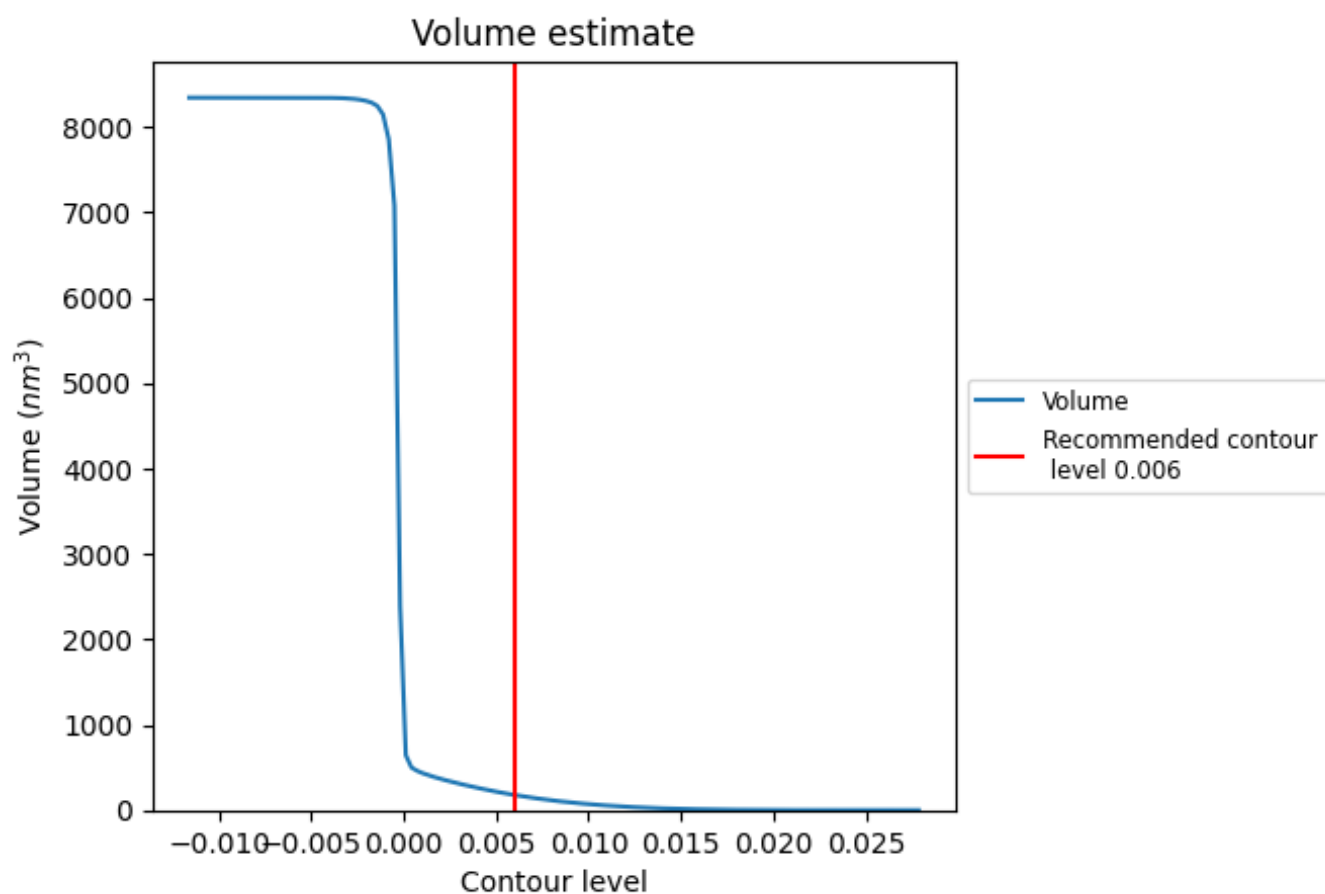
This section contains the results of statistical analysis of the map.

### 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](#)

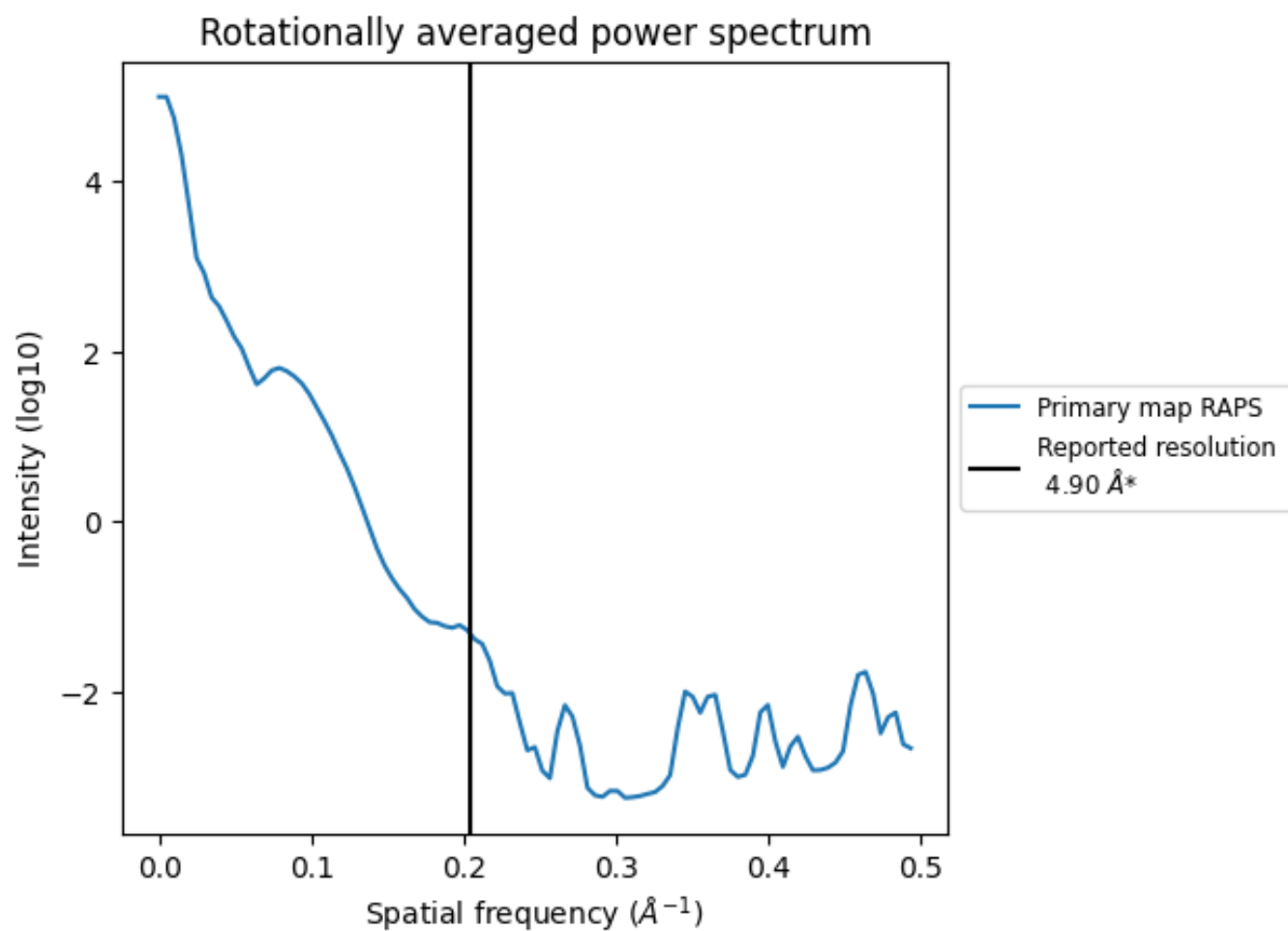


The volume at the recommended contour level is 177  $\text{nm}^3$ ; this corresponds to an approximate mass of 160 kDa.

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 0.204 Å<sup>-1</sup>

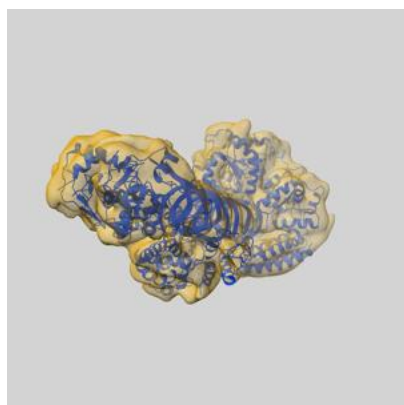
## 8 Fourier-Shell correlation

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

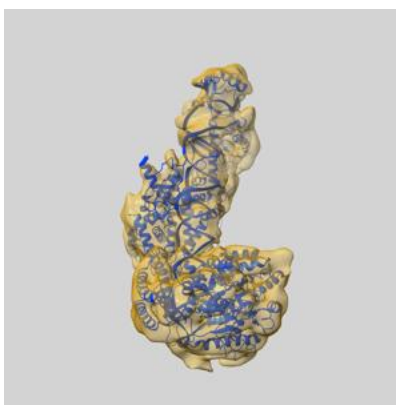
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31182 and PDB model 7ELE. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

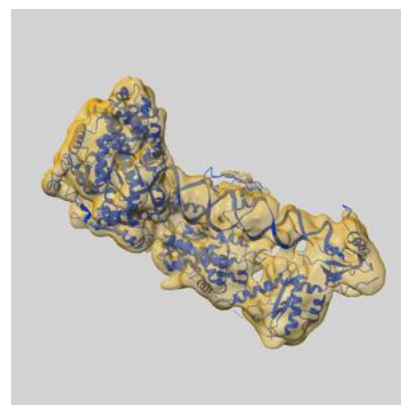
### 9.1 Map-model overlay [i](#)



X



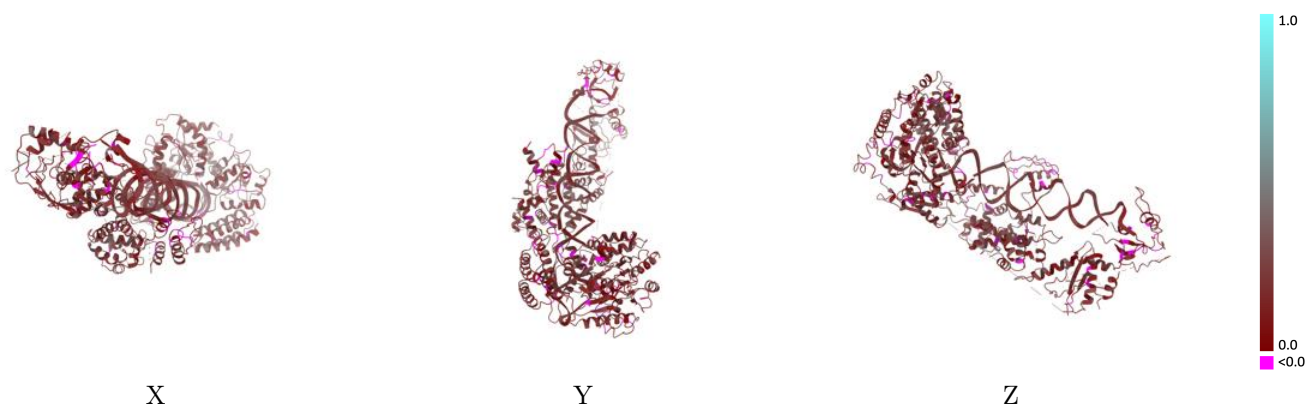
Y



Z

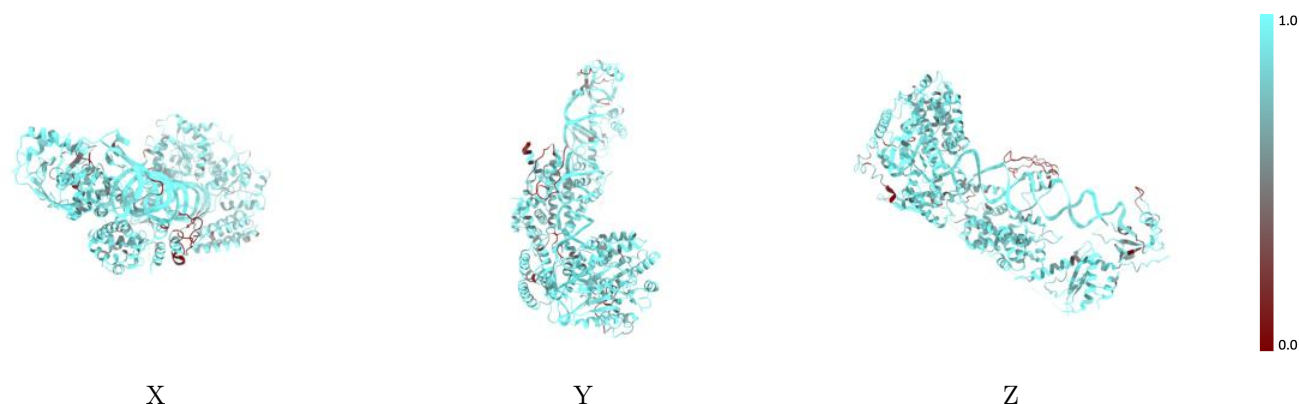
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



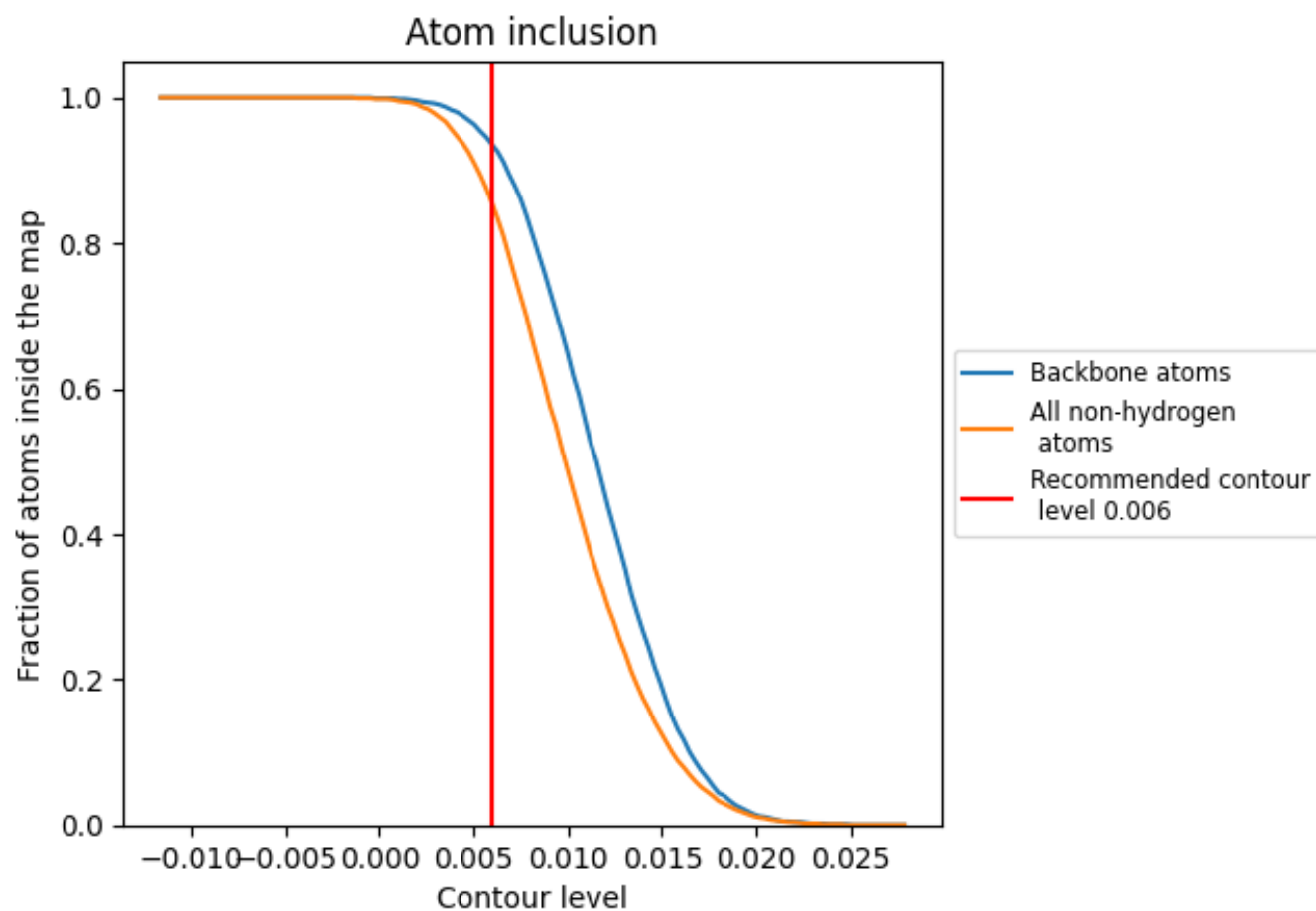
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.006).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 94% of all backbone atoms, 85% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8540	<div></div> 0.1860
A	<div></div> 0.8360	<div></div> 0.1790
G	<div></div> 0.9440	<div></div> 0.2200

