

# wwPDB EM Validation Summary Report (i)

#### Mar 20, 2024 – 07:29 AM JST

PDB ID	:	7BW4
EMDB ID	:	EMD-30226
Title	:	Structure of the RNA-dependent RNA polymerase from SARS-CoV-2
Authors	:	Peng, Q.; Peng, R.; Shi, Y.
Deposited on	:	2020-04-13
Resolution	:	3.70 Å(reported)

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

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

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

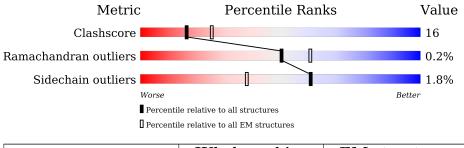
:	0.0.1.dev70
:	4.02b-467
:	20191225.v01 (using entries in the PDB archive December 25th 2019)
:	1.9.13
:	Engh & Huber $(2001)$
:	Parkinson et al. (1996)
:	2.36
	: : : :

# 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 3.70 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM} {f structures} \ (\#{f Entries})$
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	А	923	•		59%		27%	• 12%	
2	В	198			47%	11%	42%		
2	D	198	5%	25%	19%		56%		
3	С	83	•		61%		17%	22%	



# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8605 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 RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	А	811	Total 6541	C 4198	N 1087	0 1211	S 45	0	0

• Molecule 2 is a protein called Non-structural protein 8.

Mol	Chain	Residues	Atoms				AltConf	Trace	
9	В	115	Total	С	Ν	0	S	0	0
	D	115	890	561	150	172	7	0	0
0	л	87	Total	С	Ν	0	S	0	0
		01	676	431	111	128	6		0

• Molecule 3 is a protein called Non-structural protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	С	65	Total 496	C 313	N 82	O 96	${ m S}{ m 5}$	0	0

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

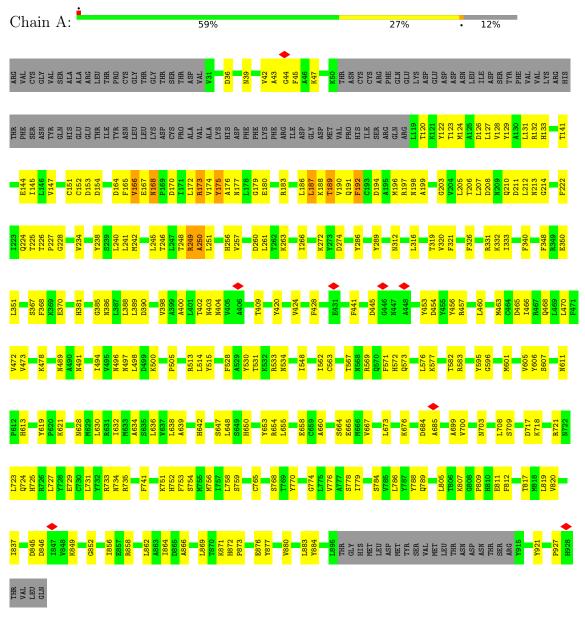
Mo	Chain	Residues	Atoms	AltConf
4	А	2	Total Zn 2 2	0



# 3 Residue-property plots (i)

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

• Molecule 1: RNA-directed RNA polymerase



• Molecule 2: Non-structural protein 8



Chain	B:	47%	1	.1%	42%		
ALA TLE ALA SER GITI	PHE SER SER LEU PRO SER	TYR ALA ALA ALA ALA ALA GLN GLN GLU CI U	GLN GLN ALA ALA ASN GLY SER SER	VAL VAL VAL LEU LYS LYS LYS LYS LYS LYS	SER LEU ASN VAL ALA LYS SER GLU	PHE ASP ASP ASP ALA ALA MET MET GLN	ARG LYS LEU GLU
LYS MET ALA ASP CI M	ALA MET THR GLN MET TYR	LYS GLN ALA ALA ALA ALA ALA ALA CLU CLU S85 S85	M94 L98 L103 N104 N105	N109 D112 1120 T124	K127 V130 V130 1132 P133 D134	T137 Y138 S173 M174 D175	P183 N192 SER
ALA VAL LYS LEU CIN	WITD						
• Mole		Non-structural p	rotein 8				
Chain	D:	25%	19%		56%		
ALA ILE ALA SER SER	PHE SER SER LEU PRO	TYR ALA ALA ALA ALA ALA GLU GLU GLU CTYR	GLN ALA VAL ALA ALA ASN GLY SER SER	VAL VAL VAL LEU LYS LYS LYS LYS LYS	SER LEU ASN VAL ALA LYS SER GLU	PHE ASP ASP ASP ALA ALA MET GLN	ARG LYS LEU GLU
LYS MET ALA ASP CI N	ALLA MET THR GLN MET TYR	LYS GLN ALA ARG SER GLU GLU ASP ASP ALA ALA ALA	1841 885 193 193 193 193 193 193 193	R96 R96 L98 N00 N100 L103 N100	N108 N109 A110 A110 A111 B112 G113 C114	V115 P116 L117 N118 T119 T120 P121	L1 22 THR THR ALA ALA
K127 L128 M129 V130	D134 Y135 N136 T137	N140 F147 A150 A150 SER ALA L153 L153 Q157	V160 V160 D161 A162 A162 S164 K165	V167 V167 CLN LEU SER CLU CLU SER SER MET	ASP ASN SER PRO ASN LEU ALA TRP	P183 L184 1185 V186 A187 A188 L189 R190	A191 ASN SER ALA VAL LYS
GLN							
• Mole	ecule 3: 1	Non-structural p	orotein 7				
Chain	C:	61%	2	1	7%	22%	
S1 K2 D5	T9 V12 L13 L14 S15	V16 V22 W29 H36 F49 F49 V53 S54	V58 V58 VAL VAL VAL	LLE ASN LYS CYS GLU GLU GLU MET LEU	ASP ASN ARG ALA THR LEU GLN		



# 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	101646	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose $(e^-/\text{\AA}^2)$	60	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	0.079	Depositor
Minimum map value	-0.044	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	204.8, 204.8, 204.8	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles $(^{\circ})$	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8, 0.8, 0.8	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		
	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.30	0/6709	0.44	0/9106	
2	В	0.24	0/903	0.45	0/1232	
2	D	0.24	0/683	0.45	0/928	
3	С	0.23	0/499	0.40	0/672	
All	All	0.28	0/8794	0.44	0/11938	

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	А	6541	0	6323	211	0
2	В	890	0	906	18	0
2	D	676	0	687	35	0
3	С	496	0	528	10	0
4	А	2	0	0	0	0
All	All	8605	0	8444	268	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 16.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:162:ALA:HB2	2:D:183:PRO:HG2	1.17	1.11
2:D:183:PRO:O	2:D:184:LEU:HD22	1.50	1.10
2:D:162:ALA:HB2	2:D:183:PRO:CG	1.87	1.04
1:A:187:LEU:HD21	1:A:286:TYR:CE1	2.01	0.94
1:A:402:THR:HG22	1:A:404:ASN:H	1.32	0.94

The worst 5 of 268 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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	entiles
1	А	805/923~(87%)	763~(95%)	40 (5%)	2~(0%)	47	78
2	В	113/198~(57%)	112 (99%)	1 (1%)	0	100	100
2	D	79/198~(40%)	76~(96%)	3~(4%)	0	100	100
3	$\mathbf{C}$	63/83~(76%)	61~(97%)	2(3%)	0	100	100
All	All	1060/1402~(76%)	1012 (96%)	46 (4%)	2~(0%)	50	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	175	TYR
1	А	250	ALA

#### 5.3.2 Protein sidechains (i)

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



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	713/816~(87%)	696~(98%)	17~(2%)	49 71
2	В	101/167~(60%)	101 (100%)	0	100 100
2	D	77/167~(46%)	77~(100%)	0	100 100
3	С	60/77~(78%)	60 (100%)	0	100 100
All	All	951/1227~(78%)	934~(98%)	17~(2%)	61 77

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

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	$\operatorname{Res}$	Type
1	А	456	TYR
1	А	734	ASN
1	А	189	THR
1	А	190	VAL
1	А	191	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
3	С	36	HIS
2	D	109	ASN
1	А	650	HIS
1	А	703	ASN
1	А	722	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 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.
There are no bond length 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-30226. 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)

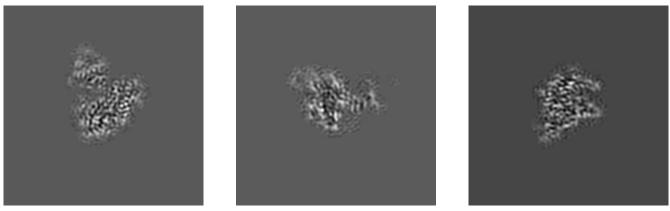
#### 6.1.1 Primary map



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

### 6.2 Central slices (i)

#### 6.2.1 Primary map



X Index: 128

Y Index: 128

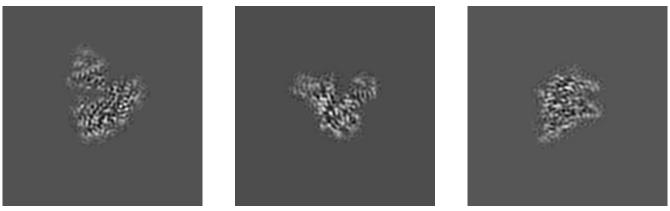


Z Index: 128

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: 127

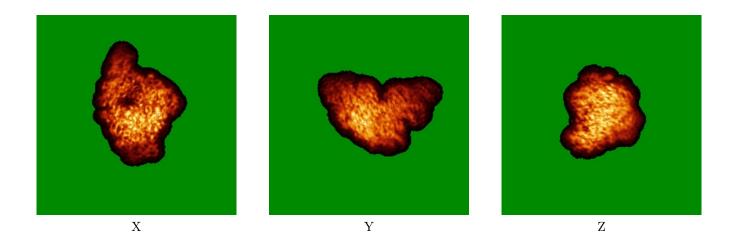
Y Index: 145

Z Index: 127

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

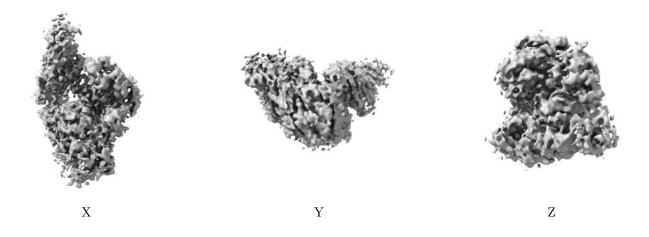


The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



### 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 0.01. 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)

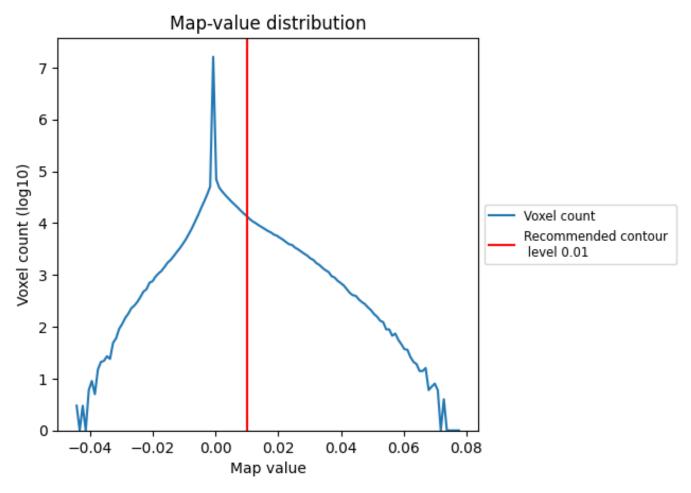
This section was not generated. No masks/segmentation were deposited.



# 7 Map analysis (i)

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

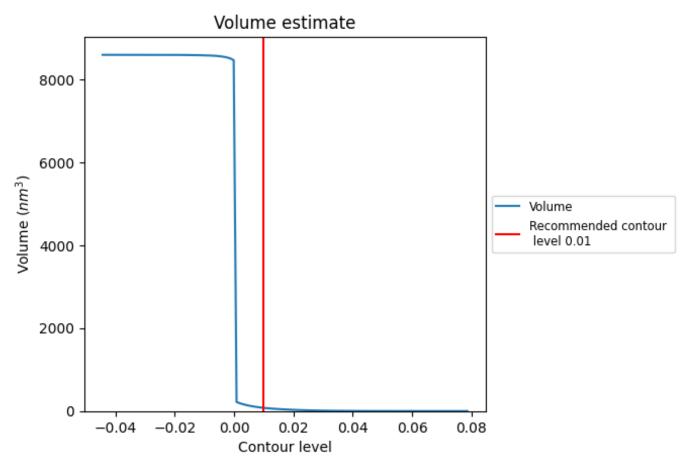
## 7.1 Map-value distribution (i)



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)

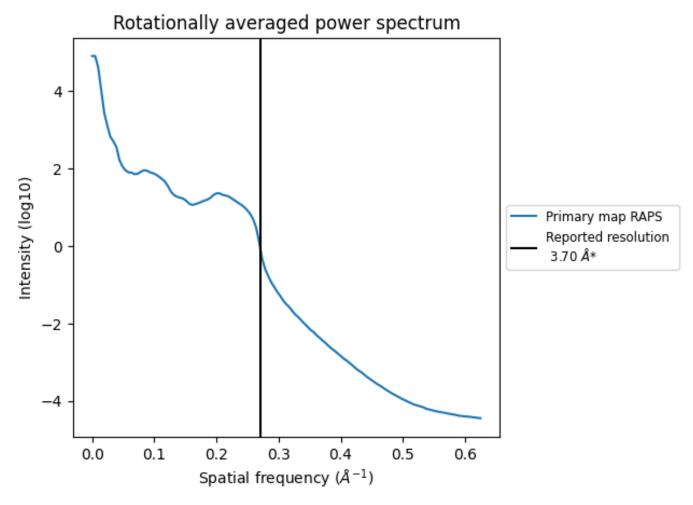


The volume at the recommended contour level is 77  $\text{nm}^3$ ; this corresponds to an approximate mass of 70 kDa.

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)



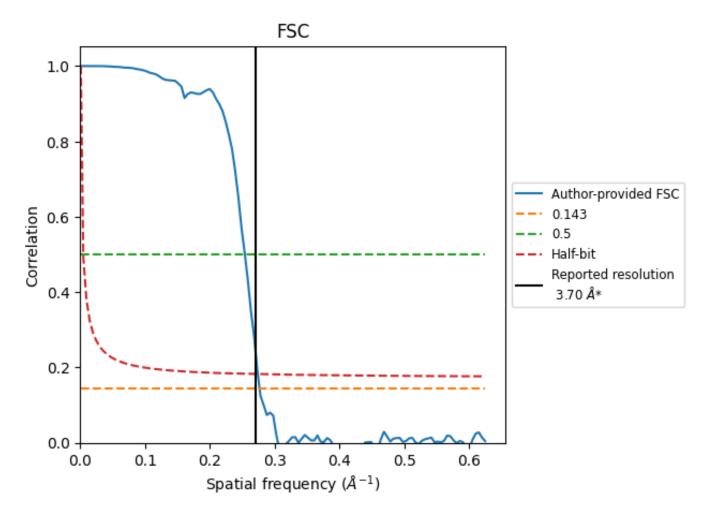
\*Reported resolution corresponds to spatial frequency of 0.270  ${\rm \AA^{-1}}$ 



# 8 Fourier-Shell correlation (i)

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

#### 8.1 FSC (i)



\*Reported resolution corresponds to spatial frequency of 0.270  $\text{\AA}^{-1}$ 



# 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	3.70	-	-
Author-provided FSC curve	3.61	3.93	3.65
Unmasked-calculated*	-	-	-

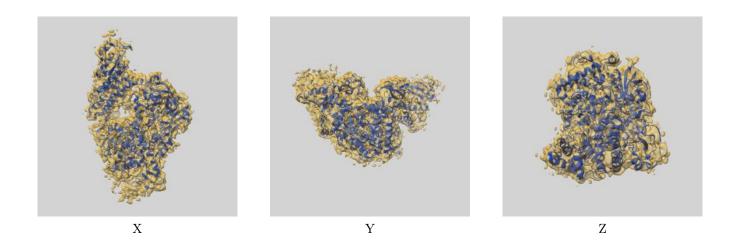
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.



# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-30226 and PDB model 7BW4. Per-residue inclusion information can be found in section 3 on page 4.

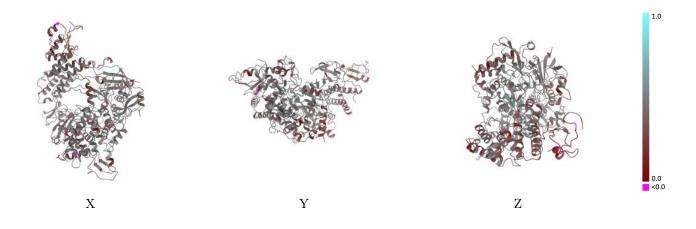
## 9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.01 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.

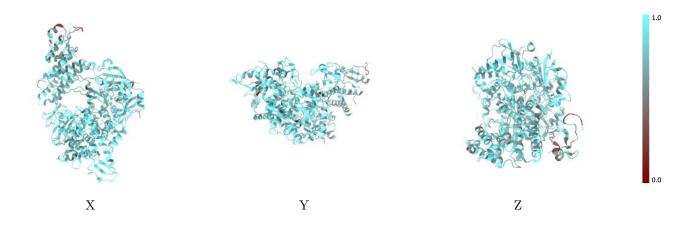


### 9.2 Q-score mapped to coordinate model (i)



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.

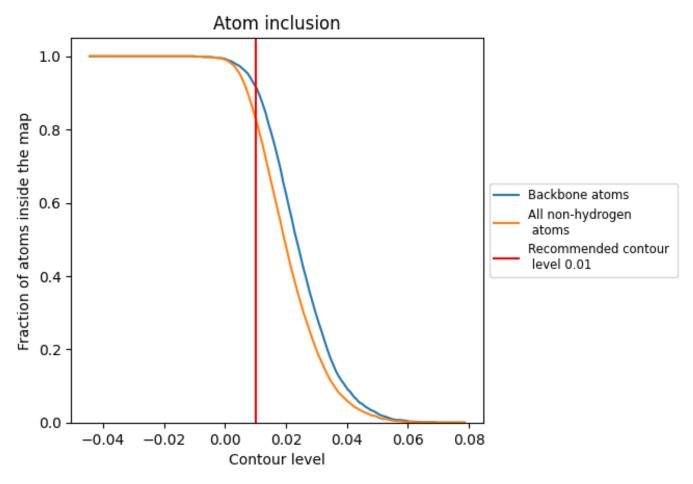
#### 9.3 Atom inclusion mapped to coordinate model (i)



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 (0.01).



### 9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.



1.0

0.0 <0.0

### 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8310	0.4170
А	0.8560	0.4280
В	0.8210	0.4200
С	0.7830	0.4070
D	0.6410	0.3050

