

# wwPDB EM Validation Summary Report (i)

Feb 27, 2024 – 06:46 AM EST

PDB ID : 6UXV

EMDB ID : EMD-20933

Title : SWI/SNF Body Module

Authors : He, Y.; Han, Y. Deposited on : 2019-11-08

Resolution : 4.70 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:

EMDB validation analysis : 0.0.1.dev70

MolProbity : 4.02b-467

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

 $MapQ \quad : \quad 1.9.13$ 

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

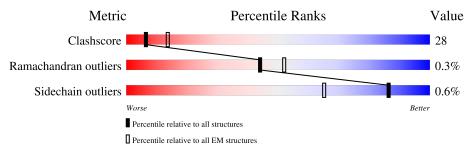
Validation Pipeline (wwPDB-VP) : 2.36

# 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 4.70 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	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	1703	• •	92%
2	В	1314	16% 21%	63%
3	С	905	10% 17%	73%
4	D	825	9% 11%	81%
4	Е	825	8% 9%	83%
4	F	825	16% 10%	73%
4	G	825	14% 9%	76%
5	Н	566	20% 259	55%

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Mol	Chain	Length		Quality of chair	in	
6	I	179	34%	26% •	39%	
7	J	67	60	0%	40%	
8	K	28	-	93%		7%
9	L	18	11%	100%		
9	О	18	44%	94%		6%
10	M	83	<u>·</u>	93%		7%
11	N	30	<u>-</u>	93%		7%



# 2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 16649 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 Transcription regulatory protein SNF2.

Mol	Chain	Residues		At	oms	AltConf	Trace		
1	A	140	Total 1133	C 715	N 196	O 220	S	0	0

• Molecule 2 is a protein called SWI/SNF chromatin-remodeling complex subunit SWI1.

Mol	Chain	Residues		At	AltConf	Trace			
2	В	482	Total 3890	C 2519	N 637	O 723	S 11	0	0

• Molecule 3 is a protein called SWI/SNF chromatin-remodeling complex subunit SNF5.

Mol	Chain	Residues	${f Atoms}$					AltConf	Trace
3	С	245	Total 2005	C 1256	N 346	O 395	S 8	0	0

• Molecule 4 is a protein called SWI/SNF complex subunit SWI3.

Mol	Chain	Residues		At	oms		AltConf	Trace	
4	D	159	Total	С	N	О	S	0	0
4	ע	159	1322	853	225	239	5	0	0
4	E	139	Total	С	N	О	S	0	0
4	<u> 1</u> 2	139	1152	746	198	205	3	U	U
4	F	221	Total	С	N	О	S	0	0
4	I'	221	1583	987	287	304	5		U
1	С	197	Total	С	N	О	S	0	0
4	G	197	1435	904	258	268	5	0	

• Molecule 5 is a protein called Transcription regulatory protein SNF12.

$\mathbf{N}$	/Iol	Chain	Residues	${f Atoms}$					AltConf	Trace
	5	Н	257	Total 2085	C 1323	N 355	O 400	S 7	0	0



• Molecule 6 is a protein called Transcription regulatory protein SNF6.

Mol	Chain	Residues		${f Atoms}$					Trace
6	Т	109	Total	С	N	О	S	0	0
	1	109	818	504	155	156	3	0	0

• Molecule 7 is a protein called Unknown protein.

Mol	Chain	Residues		Aton	ns	AltConf	Trace	
7	J	67	Total 336	C 201	N 67	O 68	0	0

• Molecule 8 is a protein called Unknown protein.

Mol	Chain	Residues	1	Atoms				Trace
8	K	28	Total	С	N	О	0	0
Ü			141	84	28	29		

• Molecule 9 is a protein called Unknown protein.

Mol	Chain	Residues	_	Ator	$\overline{\mathbf{n}}$ s	AltConf	Trace	
0	Т	10	Total	С	N	О	0	0
9	L	18	91	54	18	19	U	0
0	0	10	Total	С	N	О	0	0
9		18	91	54	18	19	U	U

 $\bullet$  Molecule 10 is a protein called SWI/SNF global transcription activator complex subunit SWP82.

Mol	Chain	Residues		Aton	ıs		AltConf	Trace
10	M	83	Total 416	C 249	N 83	O 84	0	0

• Molecule 11 is a protein called Unknown protein.

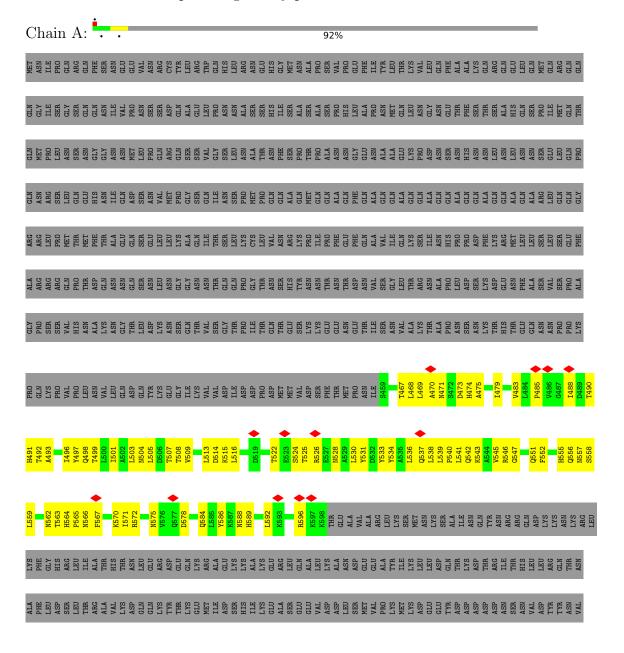
Mol	Chain	Residues		Ator	ns		AltConf	Trace
11	N	30	Total 151	C 90	N 30	O 31	0	0



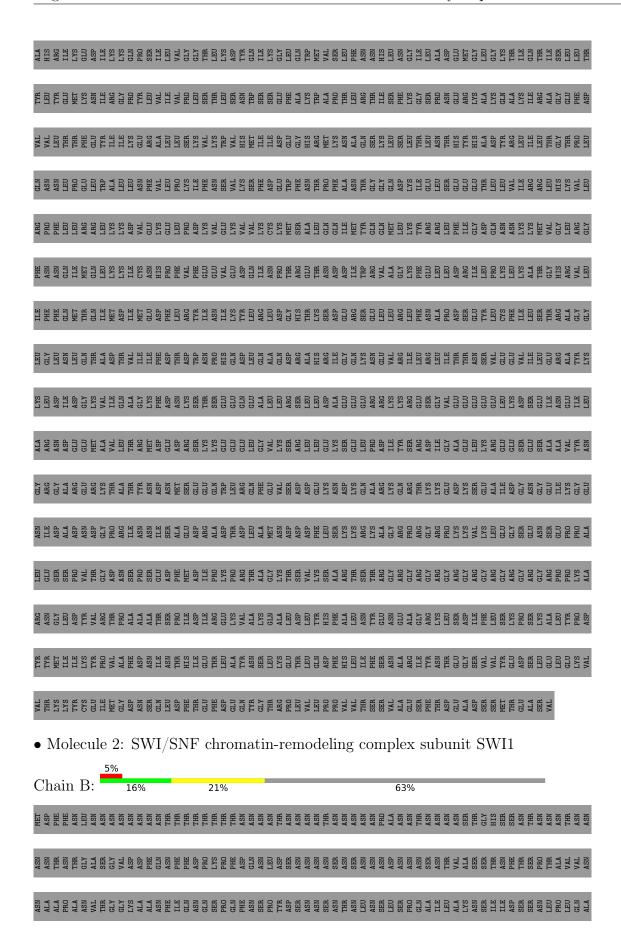
# 3 Residue-property plots (i)

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.

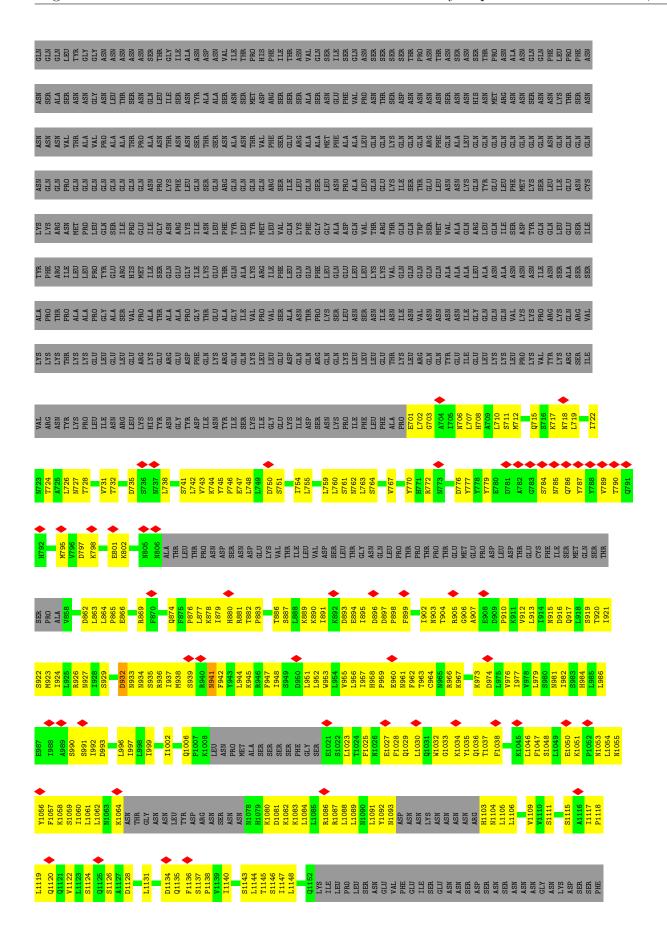
• Molecule 1: Transcription regulatory protein SNF2



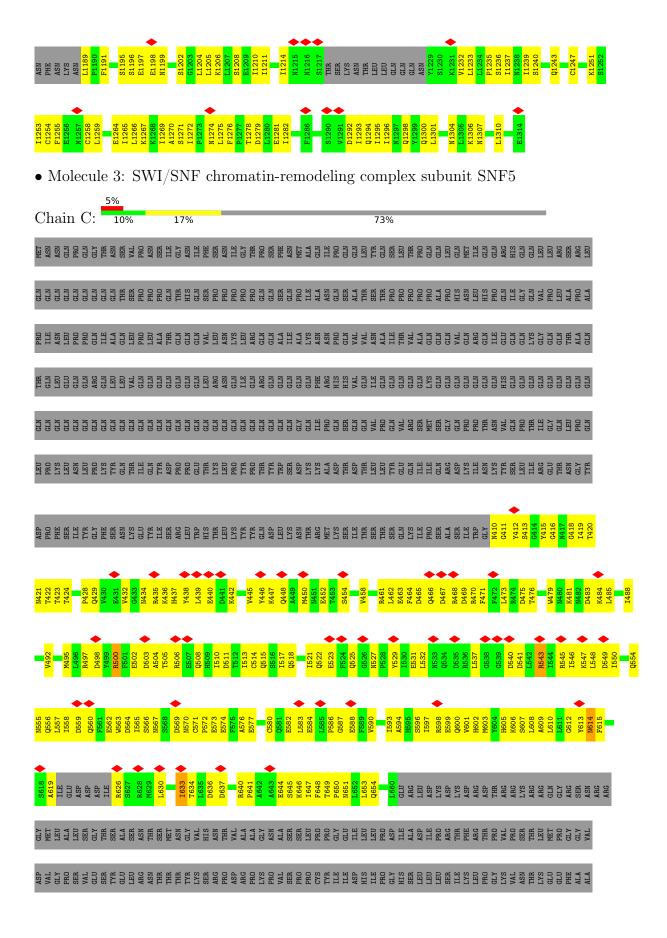




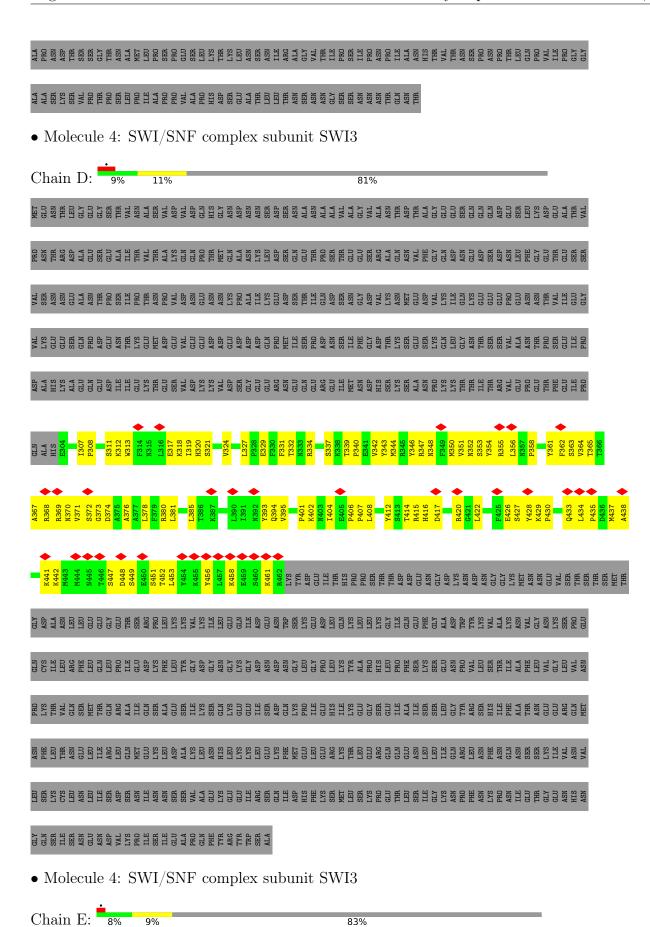




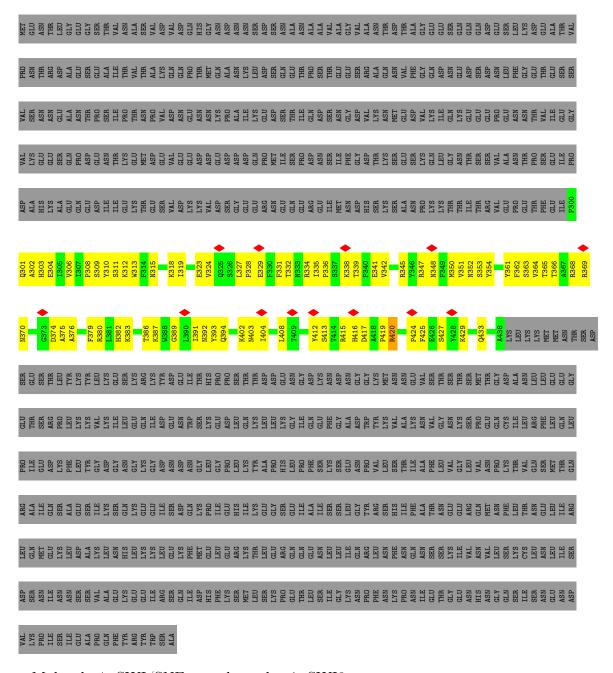








PDB



• Molecule 4: SWI/SNF complex subunit SWI3

Chain F: 16% 10% 73%

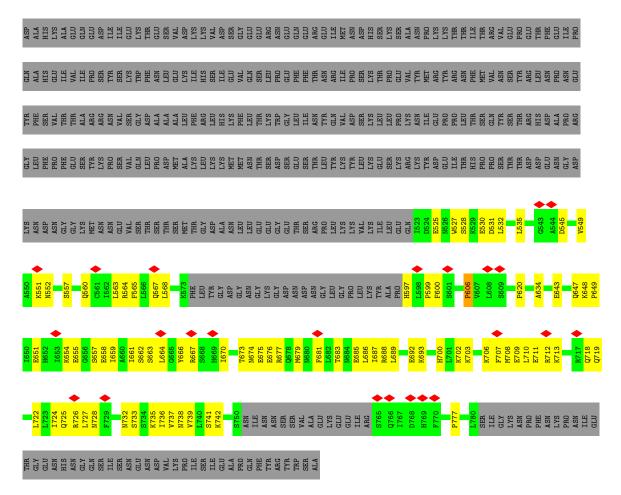
Chain F: 16% 10% 73%

Chain F: 16% 10% 73%

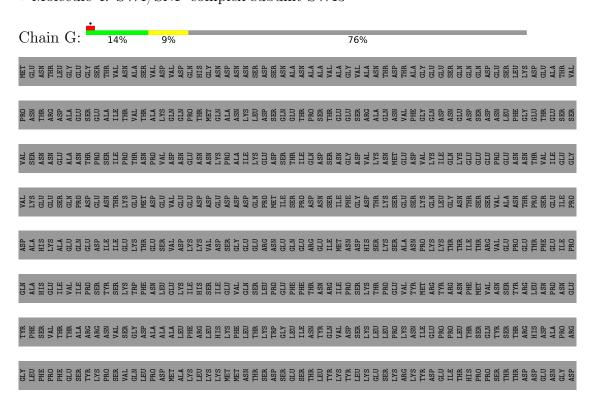
Chair F: 16% 10%

Chair F: 16%

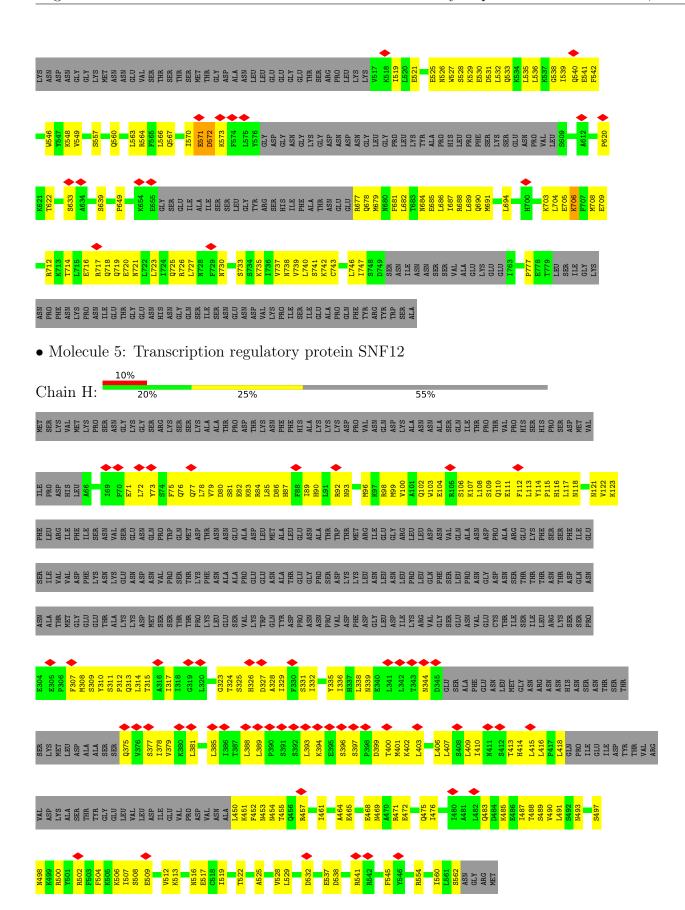




• Molecule 4: SWI/SNF complex subunit SWI3

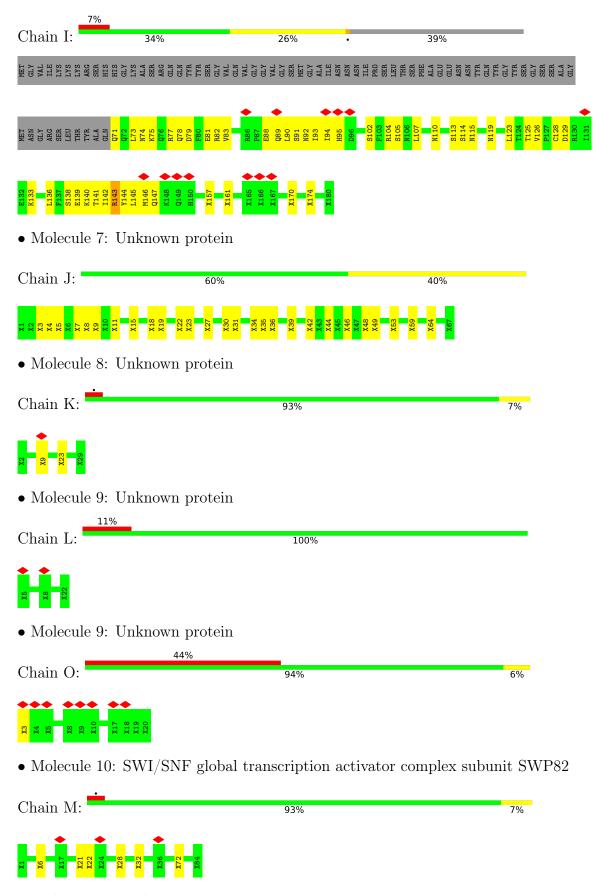






• Molecule 6: Transcription regulatory protein SNF6





• Molecule 11: Unknown protein









# 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	61518	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY; CTF amplitude	Depositor
	correction was performed following 3D auto	
	refinement in relion.	
Microscope	JEOL 3200FS	Depositor
Voltage (kV)	200	Depositor
Electron dose $(e^-/\text{Å}^2)$	76.5	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	0.093	Depositor
Minimum map value	-0.040	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	430.08002, 430.08002, 430.08002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.12, 1.12, 1.12	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	Во	ond angles
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	A	0.33	0/1154	0.47	0/1572
2	В	0.38	0/3958	0.52	0/5364
3	С	0.35	0/2040	0.54	0/2756
4	D	0.34	0/1359	0.47	0/1838
4	Е	0.40	0/1189	0.51	0/1616
4	F	0.32	0/1596	0.52	5/2154~(0.2%)
4	G	0.33	0/1446	0.51	3/1949~(0.2%)
5	Н	0.35	0/2119	0.47	0/2856
6	I	0.32	0/682	0.48	0/913
All	All	0.35	0/15543	0.50	8/21018~(0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	В	0	2

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$Ideal(^{o})$
4	F	606	PRO	N-CA-CB	6.95	111.64	103.30
4	G	620	PRO	N-CA-CB	6.10	110.62	103.30
4	F	649	PRO	N-CA-CB	6.07	110.58	103.30
4	F	599	PRO	N-CA-CB	5.89	110.36	103.30
4	F	777	PRO	N-CA-CB	5.72	110.16	103.30

There are no chirality outliers.

All (2) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
2	В	776	ASP	Peptide
2	В	932	ASP	Peptide

#### 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	1133	0	1122	86	0
2	В	3890	0	4008	250	0
3	С	2005	0	1939	164	0
4	D	1322	0	1325	97	0
4	Е	1152	0	1137	87	0
4	F	1583	0	1397	72	0
4	G	1435	0	1294	59	0
5	Н	2085	0	2104	139	0
6	I	818	0	708	67	0
7	J	336	0	70	19	0
8	K	141	0	33	3	0
9	L	91	0	21	0	0
9	O	91	0	21	2	0
10	M	416	0	92	4	0
11	N	151	0	41	3	0
All	All	16649	0	15312	902	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 28.

The worst 5 of 902 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
4:D:412:TYR:CD1	5:H:560:ILE:HG23	1.62	1.34
4:D:412:TYR:CD1	5:H:560:ILE:CG2	2.12	1.32
4:D:412:TYR:CG	5:H:560:ILE:HG21	1.93	1.02
1:A:570:LYS:HE2	6:I:90:LEU:H	1.25	0.98
4:D:412:TYR:HD1	5:H:560:ILE:HG23	1.16	0.95

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	A	138/1703 (8%)	118 (86%)	20 (14%)	0	100	100
2	В	468/1314 (36%)	364 (78%)	104 (22%)	0	100	100
3	С	241/905 (27%)	176 (73%)	63 (26%)	2 (1%)	19	60
4	D	157/825 (19%)	131 (83%)	26 (17%)	0	100	100
4	E	137/825 (17%)	113 (82%)	24 (18%)	0	100	100
4	F	215/825~(26%)	186 (86%)	27 (13%)	2 (1%)	17	56
4	G	189/825 (23%)	164 (87%)	24 (13%)	1 (0%)	29	68
5	Н	249/566 (44%)	217 (87%)	32 (13%)	0	100	100
6	I	78/179 (44%)	67 (86%)	11 (14%)	0	100	100
All	All	1872/7967 (24%)	1536 (82%)	331 (18%)	5 (0%)	44	76

#### All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	606	PRO
3	С	614	ASN
4	G	572	ASP
4	F	648	LYS
3	С	612	GLY

#### 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	Percei	ntiles
1	A	129/1520~(8%)	129 (100%)	0	100	100
2	В	460/1218 (38%)	458 (100%)	2 (0%)	91	94
3	С	222/823 (27%)	219 (99%)	3 (1%)	67	81
4	D	150/751 (20%)	150 (100%)	0	100	100
4	E	129/751 (17%)	128 (99%)	1 (1%)	81	89
4	F	138/751 (18%)	138 (100%)	0	100	100
4	G	127/751 (17%)	125 (98%)	2 (2%)	62	79
5	Н	239/517~(46%)	238 (100%)	1 (0%)	91	94
6	I	79/133 (59%)	78 (99%)	1 (1%)	69	82
All	All	1673/7215 (23%)	1663 (99%)	10 (1%)	86	92

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	G	706	LYS
5	Н	562	SER
6	I	143	ARG
3	С	543	ARG
3	С	633	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
3	С	614	ASN
5	Н	469	ASN
4	Е	411	GLN
5	Н	326	HIS
4	G	745	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)

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
6	I	1
10	M	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	150:HIS	С	152:UNK	N	20.17
1	M	22:UNK	С	24:UNK	N	7.86



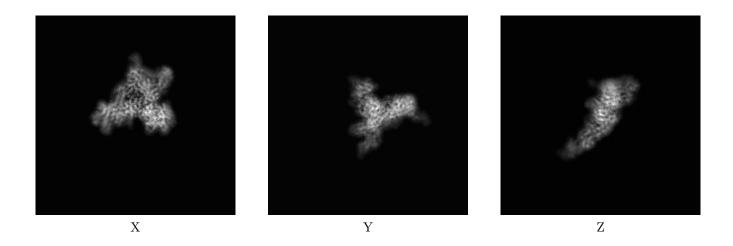
# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-20933. 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)

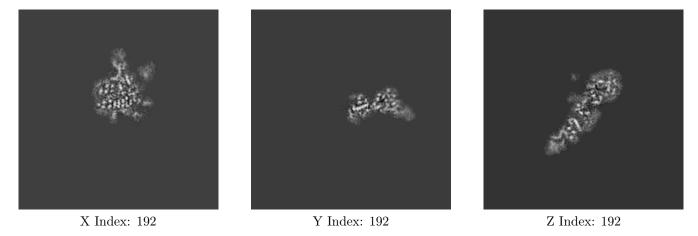
#### 6.1.1 Primary map



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

#### 6.2 Central slices (i)

#### 6.2.1 Primary map

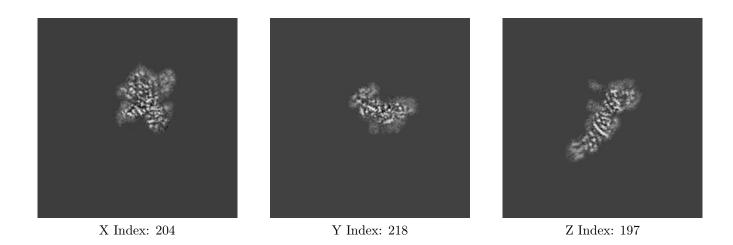




The images above show central slices of the map in three orthogonal directions.

### 6.3 Largest variance slices (i)

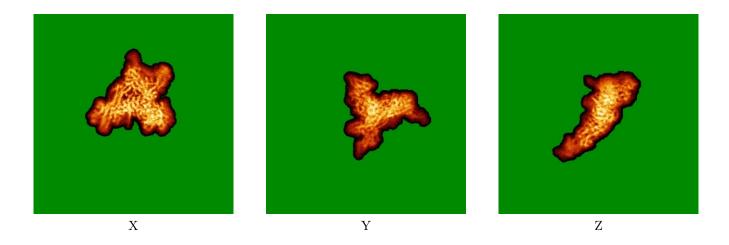
#### 6.3.1 Primary map



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 0.035. 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)

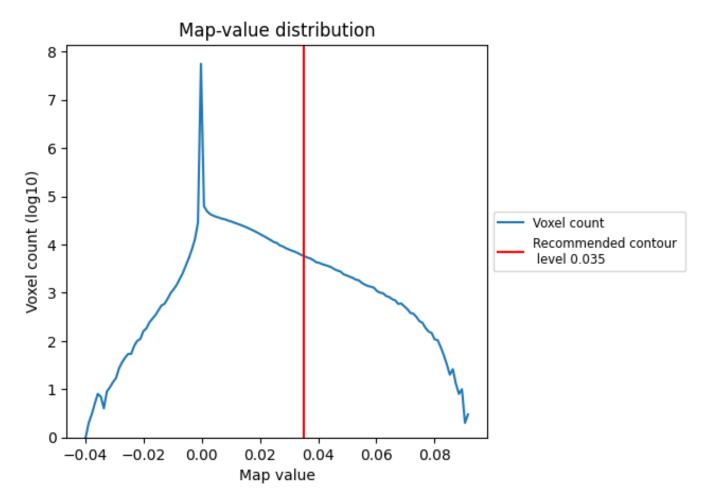
This section was not generated. No masks/segmentation were deposited.



# 7 Map analysis (i)

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

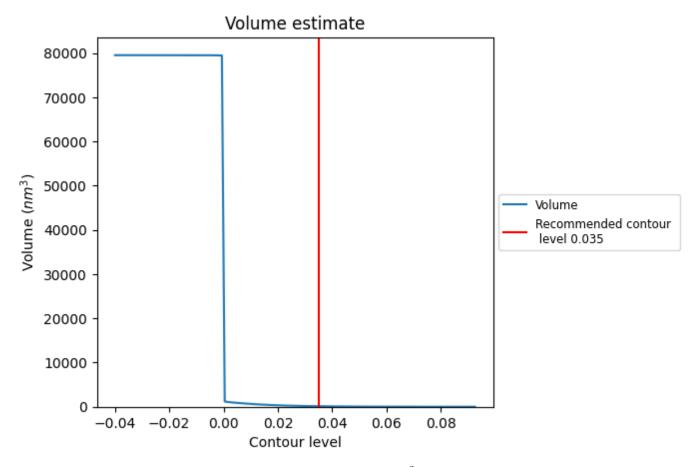
### 7.1 Map-value distribution (i)



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)

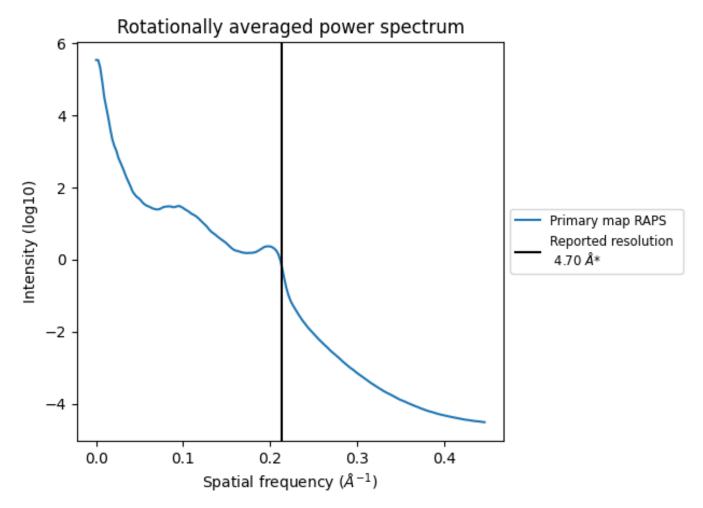


The volume at the recommended contour level is  $118~\mathrm{nm}^3$ ; this corresponds to an approximate mass of  $107~\mathrm{kDa}$ .

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)



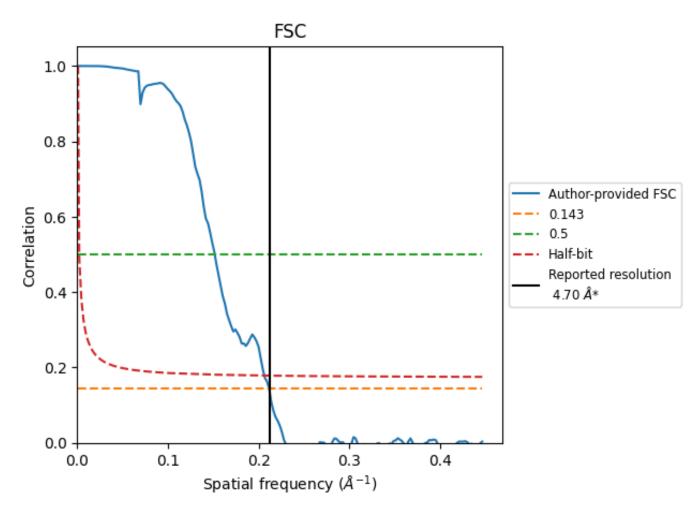
<sup>\*</sup>Reported resolution corresponds to spatial frequency of 0.213  ${\rm \AA}^{-1}$ 



# 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 0.213  $\rm \AA^{-1}$ 



# 8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
rtesolution estimate (A)	0.143	0.5	Half-bit
Reported by author	4.70	-	-
Author-provided FSC curve	4.73	6.60	4.85
Unmasked-calculated*	-	-	-

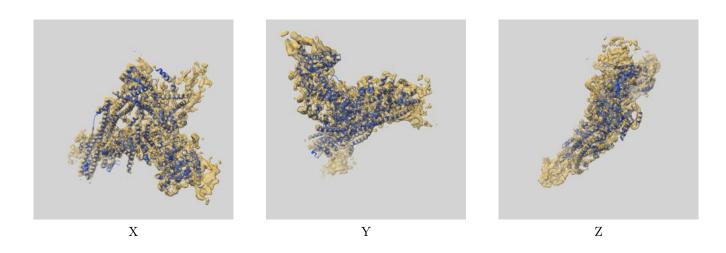
<sup>\*</sup>Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.



# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-20933 and PDB model 6UXV. Per-residue inclusion information can be found in section 3 on page 6.

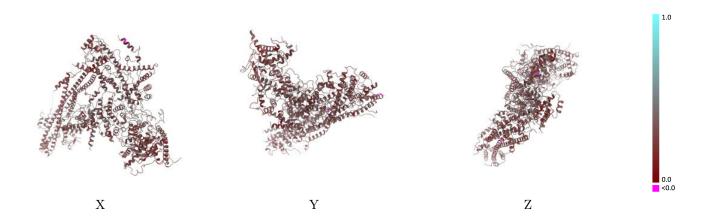
# 9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.035 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.

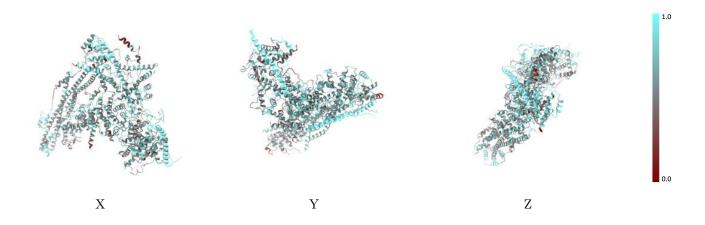


#### 9.2 Q-score mapped to coordinate model (i)



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.

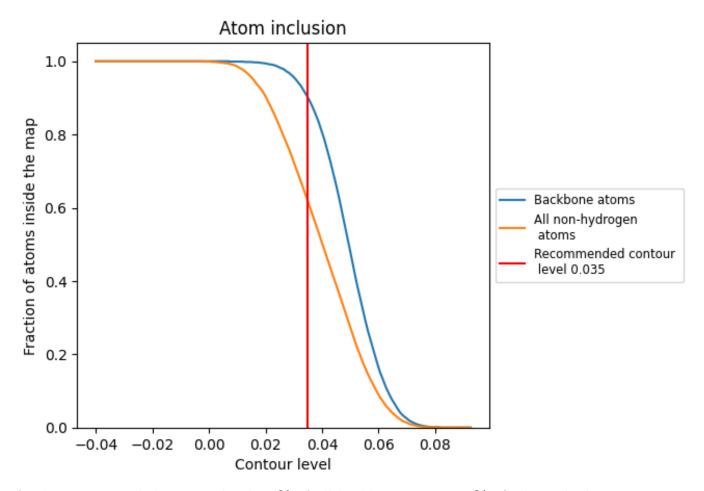
### 9.3 Atom inclusion mapped to coordinate model (i)



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 (0.035).



# 9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 62% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6170	0.3220
A	0.6270	0.3330
В	0.5990	0.3360
С	0.5540	0.3140
D	0.5780	0.3070
E	0.6410	0.3420
F	0.6220	0.2950
G	0.6530	0.3150
Н	0.5500	0.2930
I	0.6320	0.3310
J	0.9170	0.3710
K	0.8650	0.4030
L	0.7580	0.2930
M	0.8650	0.3650
N	0.8740	0.4630
О	0.4400	0.1680



