



## wwPDB EM Validation Summary Report ⓘ

Dec 10, 2022 – 10:32 am GMT

PDB ID : 4USN  
EMDB ID : EMD-2706  
Title : The structure of the immature HIV-1 capsid in intact virus particles at sub-nm resolution  
Authors : Schur, F.K.M.; Hagen, W.J.H.; Rumlova, M.; Ruml, T.; Mueller, B.; Kraeuslich, H.-G.; Briggs, J.A.G.  
Deposited on : 2014-07-11  
Resolution : 8.80 Å (reported)  
Based on initial models : 1L6N, 3DS2

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)

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>.

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

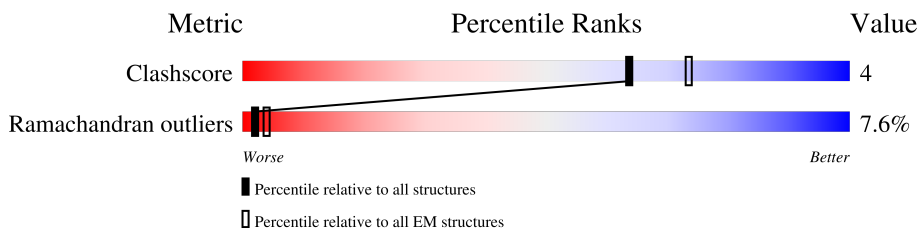
EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

# 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 8.80 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

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	210	15% 75% 22% .
1	B	210	14% 81% 18% .
1	C	210	15% 86% 13% .
1	D	210	15% 76% 23% .
1	E	210	16% 78% 21% .
1	F	210	16% 84% 14% .
1	G	210	17% 85% 14%
1	H	210	18% 79% 19% .
1	I	210	17% 85% 14% .

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Mol	Chain	Length	Quality of chain
1	J	210	
1	K	210	
1	L	210	
1	M	210	
1	N	210	
1	O	210	
1	P	210	
1	Q	210	
1	R	210	

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 22662 atoms, of which 7542 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 P24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
1	A	210	1259	420	419	210	210	0	0
1	B	210	1259	420	419	210	210	0	0
1	C	210	1259	420	419	210	210	0	0
1	D	210	1259	420	419	210	210	0	0
1	E	210	1259	420	419	210	210	0	0
1	F	210	1259	420	419	210	210	0	0
1	G	210	1259	420	419	210	210	0	0
1	H	210	1259	420	419	210	210	0	0
1	I	210	1259	420	419	210	210	0	0
1	J	210	1259	420	419	210	210	0	0
1	K	210	1259	420	419	210	210	0	0
1	L	210	1259	420	419	210	210	0	0
1	M	210	1259	420	419	210	210	0	0
1	N	210	1259	420	419	210	210	0	0
1	O	210	1259	420	419	210	210	0	0
1	P	210	1259	420	419	210	210	0	0
1	Q	210	1259	420	419	210	210	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
1	R	210	1259	420	419	210	210	0	0

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	207	GLU	ASP	conflict	UNP Q9IVM8
A	301	ALA	TYR	conflict	UNP Q9IVM8
A	340	GLY	ALA	conflict	UNP Q9IVM8
B	207	GLU	ASP	conflict	UNP Q9IVM8
B	301	ALA	TYR	conflict	UNP Q9IVM8
B	340	GLY	ALA	conflict	UNP Q9IVM8
C	207	GLU	ASP	conflict	UNP Q9IVM8
C	301	ALA	TYR	conflict	UNP Q9IVM8
C	340	GLY	ALA	conflict	UNP Q9IVM8
D	207	GLU	ASP	conflict	UNP Q9IVM8
D	301	ALA	TYR	conflict	UNP Q9IVM8
D	340	GLY	ALA	conflict	UNP Q9IVM8
E	207	GLU	ASP	conflict	UNP Q9IVM8
E	301	ALA	TYR	conflict	UNP Q9IVM8
E	340	GLY	ALA	conflict	UNP Q9IVM8
F	207	GLU	ASP	conflict	UNP Q9IVM8
F	301	ALA	TYR	conflict	UNP Q9IVM8
F	340	GLY	ALA	conflict	UNP Q9IVM8
G	207	GLU	ASP	conflict	UNP Q9IVM8
G	301	ALA	TYR	conflict	UNP Q9IVM8
G	340	GLY	ALA	conflict	UNP Q9IVM8
H	207	GLU	ASP	conflict	UNP Q9IVM8
H	301	ALA	TYR	conflict	UNP Q9IVM8
H	340	GLY	ALA	conflict	UNP Q9IVM8
I	207	GLU	ASP	conflict	UNP Q9IVM8
I	301	ALA	TYR	conflict	UNP Q9IVM8
I	340	GLY	ALA	conflict	UNP Q9IVM8
J	207	GLU	ASP	conflict	UNP Q9IVM8
J	301	ALA	TYR	conflict	UNP Q9IVM8
J	340	GLY	ALA	conflict	UNP Q9IVM8
K	207	GLU	ASP	conflict	UNP Q9IVM8
K	301	ALA	TYR	conflict	UNP Q9IVM8
K	340	GLY	ALA	conflict	UNP Q9IVM8
L	207	GLU	ASP	conflict	UNP Q9IVM8
L	301	ALA	TYR	conflict	UNP Q9IVM8
L	340	GLY	ALA	conflict	UNP Q9IVM8

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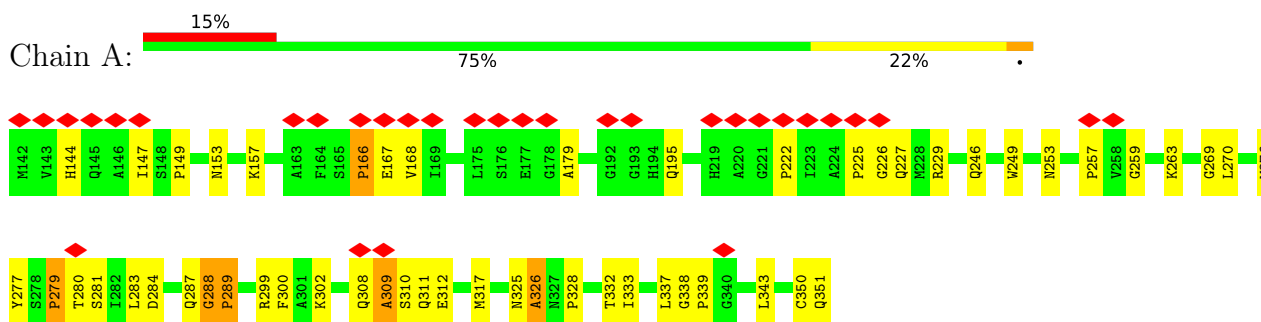
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Chain	Residue	Modelled	Actual	Comment	Reference
M	207	GLU	ASP	conflict	UNP Q9IVM8
M	301	ALA	TYR	conflict	UNP Q9IVM8
M	340	GLY	ALA	conflict	UNP Q9IVM8
N	207	GLU	ASP	conflict	UNP Q9IVM8
N	301	ALA	TYR	conflict	UNP Q9IVM8
N	340	GLY	ALA	conflict	UNP Q9IVM8
O	207	GLU	ASP	conflict	UNP Q9IVM8
O	301	ALA	TYR	conflict	UNP Q9IVM8
O	340	GLY	ALA	conflict	UNP Q9IVM8
P	207	GLU	ASP	conflict	UNP Q9IVM8
P	301	ALA	TYR	conflict	UNP Q9IVM8
P	340	GLY	ALA	conflict	UNP Q9IVM8
Q	207	GLU	ASP	conflict	UNP Q9IVM8
Q	301	ALA	TYR	conflict	UNP Q9IVM8
Q	340	GLY	ALA	conflict	UNP Q9IVM8
R	207	GLU	ASP	conflict	UNP Q9IVM8
R	301	ALA	TYR	conflict	UNP Q9IVM8
R	340	GLY	ALA	conflict	UNP Q9IVM8

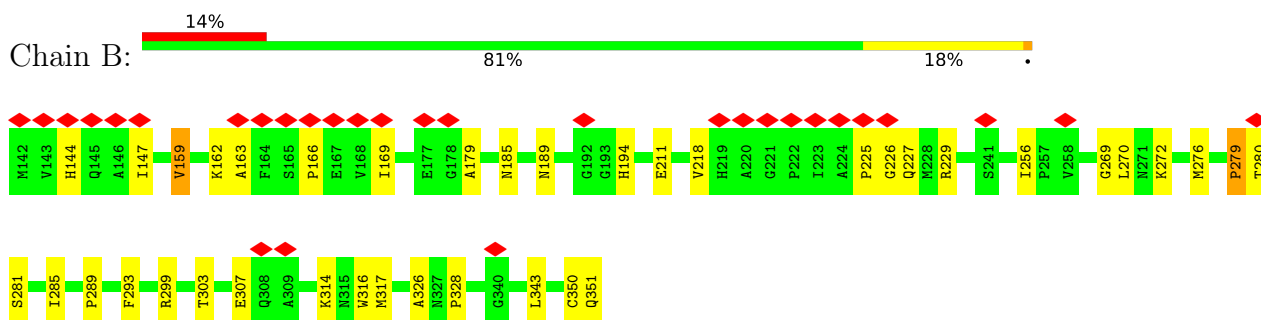
### 3 Residue-property plots [i](#)

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.

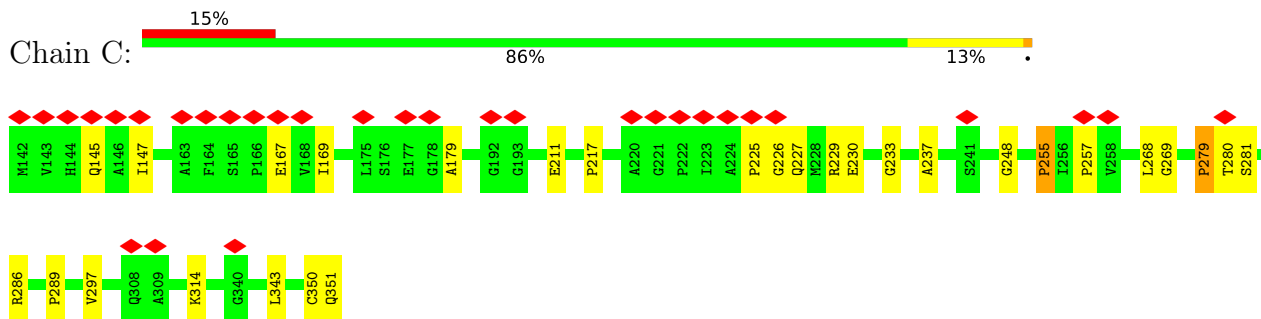
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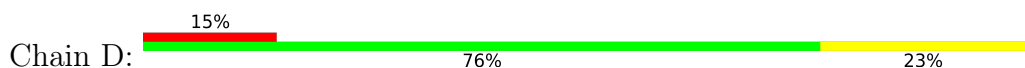
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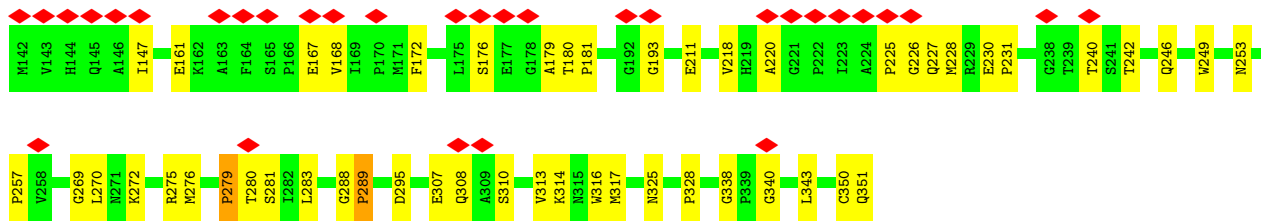


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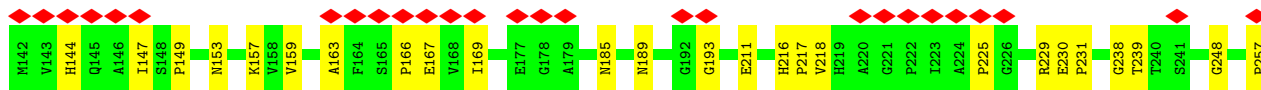
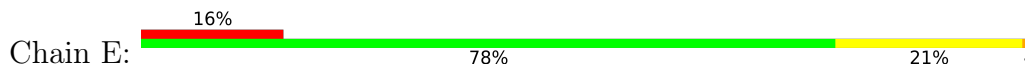


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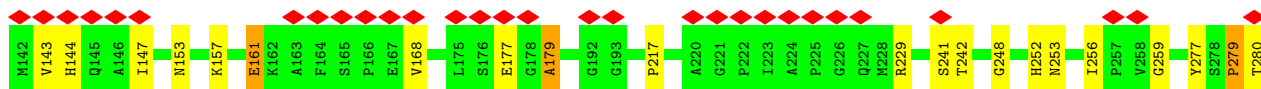
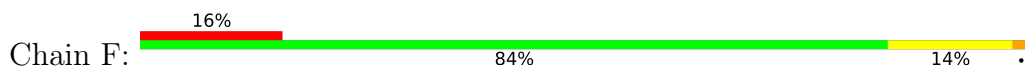




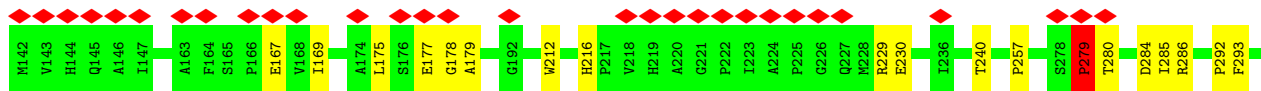
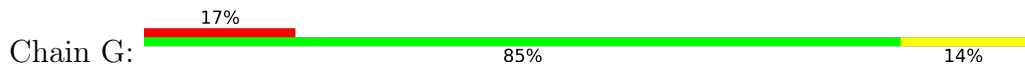
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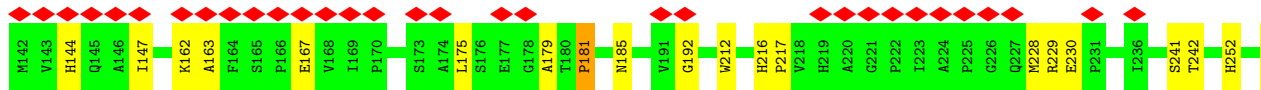
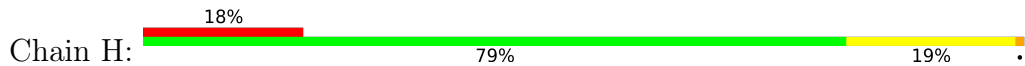
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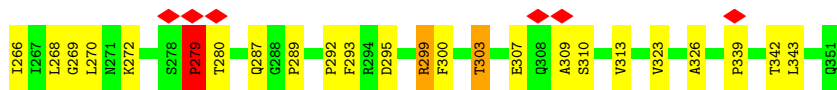
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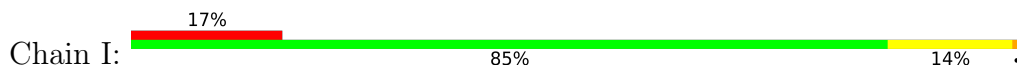
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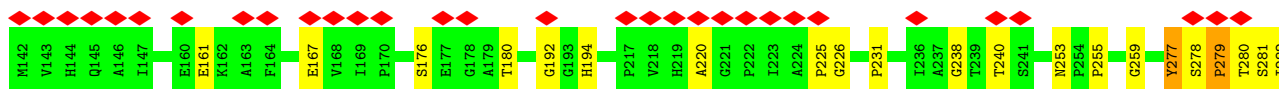




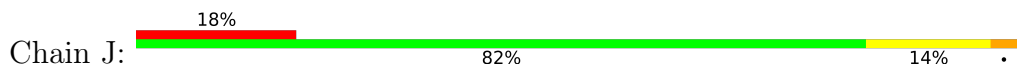
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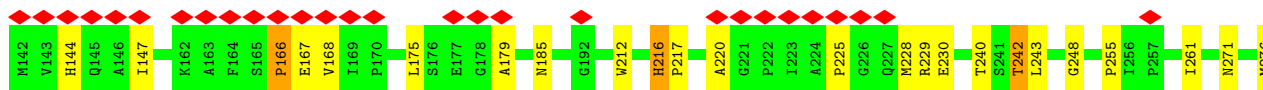
Chain I:



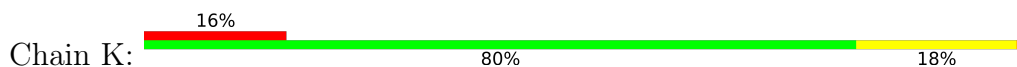
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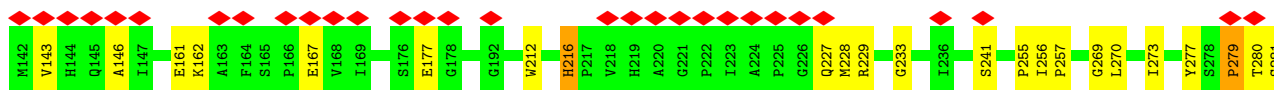
Chain J:



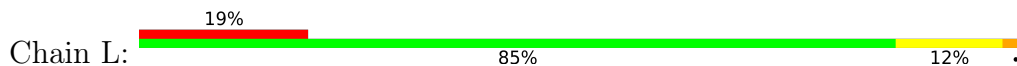
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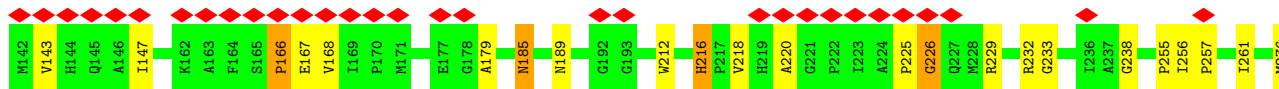
Chain K:



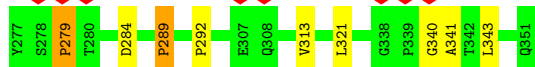
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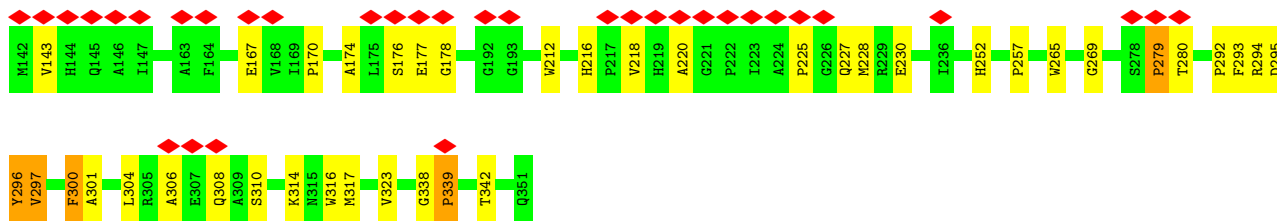
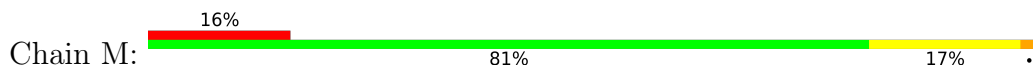


Chain L:

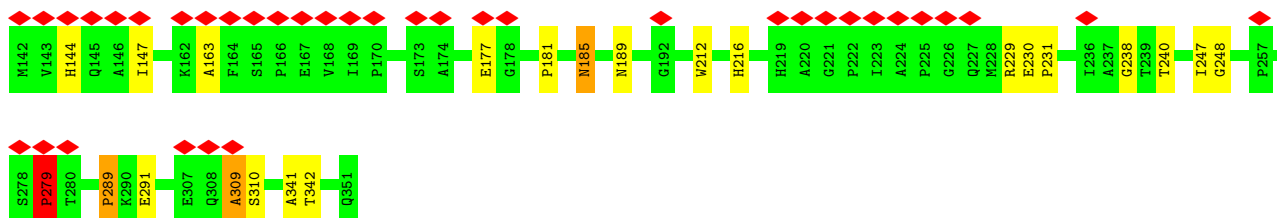
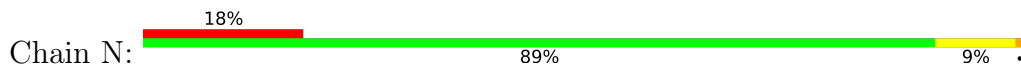


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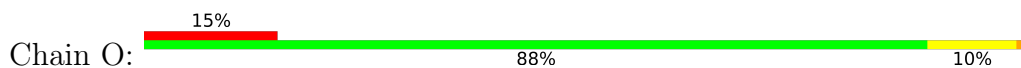




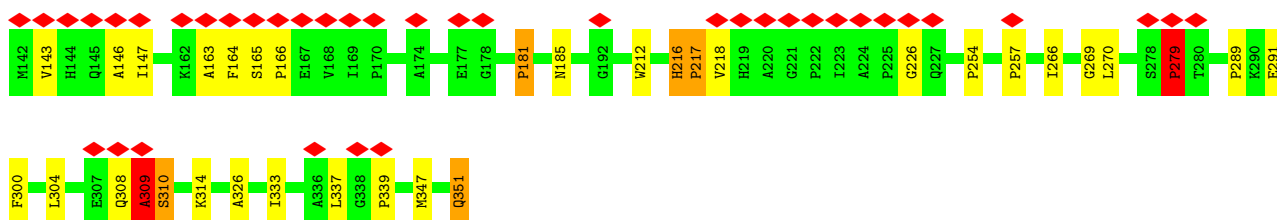
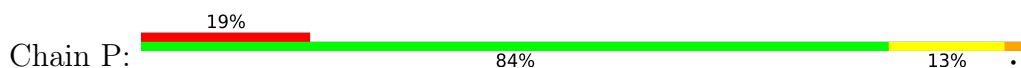
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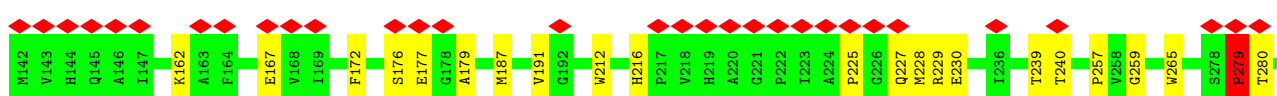
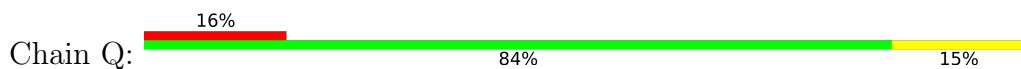
• Molecule 1: P24



• Molecule 1: P24

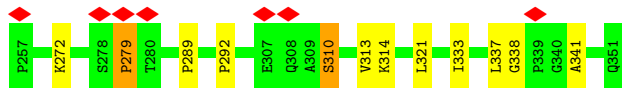
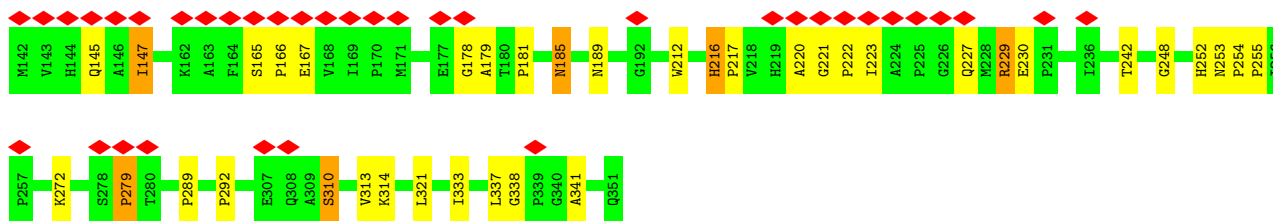
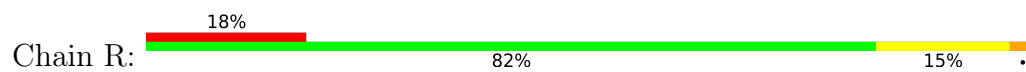


• Molecule 1: P24





- Molecule 1: P24



## 4 Experimental information

Property	Value	Source
EM reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of tilted images used	Not provided	
Resolution determination method	Not provided	
CTF correction method	PHASE FLIPPING OF INDIVIDUAL TILTS	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	42000	Depositor
Image detector	GATAN MULTISCAN	Depositor
Maximum voxel value	0.870	Depositor
Minimum voxel value	-0.726	Depositor
Average voxel value	-0.004	Depositor
Voxel value standard deviation	0.098	Depositor
Recommended contour level	0.27	Depositor
Tomogram size ( $\text{\AA}$ )	283.5, 283.5, 283.5	wwPDB
Tomogram dimensions	140, 140, 140	wwPDB
Tomogram angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Grid spacing ( $\text{\AA}$ )	2.025, 2.025, 2.025	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	A	1.98	7/839 (0.8%)	1.74	9/1047 (0.9%)
1	B	1.96	3/839 (0.4%)	1.73	9/1047 (0.9%)
1	C	1.95	3/839 (0.4%)	1.67	4/1047 (0.4%)
1	D	1.95	4/839 (0.5%)	1.67	11/1047 (1.1%)
1	E	1.98	11/839 (1.3%)	1.66	8/1047 (0.8%)
1	F	1.98	6/839 (0.7%)	1.64	6/1047 (0.6%)
1	G	1.91	5/839 (0.6%)	1.63	4/1047 (0.4%)
1	H	1.91	6/839 (0.7%)	1.71	9/1047 (0.9%)
1	I	1.89	2/839 (0.2%)	1.67	7/1047 (0.7%)
1	J	1.84	4/839 (0.5%)	1.71	11/1047 (1.1%)
1	K	1.84	5/839 (0.6%)	1.66	5/1047 (0.5%)
1	L	1.83	4/839 (0.5%)	1.68	10/1047 (1.0%)
1	M	1.94	7/839 (0.8%)	1.65	8/1047 (0.8%)
1	N	1.91	3/839 (0.4%)	1.71	8/1047 (0.8%)
1	O	1.91	2/839 (0.2%)	1.66	5/1047 (0.5%)
1	P	1.90	2/839 (0.2%)	1.68	8/1047 (0.8%)
1	Q	1.91	6/839 (0.7%)	1.61	4/1047 (0.4%)
1	R	1.94	5/839 (0.6%)	1.69	5/1047 (0.5%)
All	All	1.92	85/15102 (0.6%)	1.68	131/18846 (0.7%)

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
1	A	0	9
1	B	0	6
1	C	0	6
1	D	0	12
1	E	0	2
1	F	0	9
1	G	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	14
1	I	0	5
1	J	0	12
1	K	0	5
1	L	0	6
1	M	0	5
1	N	0	5
1	O	0	6
1	P	0	5
1	Q	0	2
1	R	0	6
All	All	0	118

The worst 5 of 85 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	185	ASN	CA-C	-6.31	1.36	1.52
1	F	295	ASP	CA-C	-6.24	1.36	1.52
1	D	328	PRO	CA-C	-6.23	1.40	1.52
1	L	238	GLY	CA-C	-6.18	1.42	1.51
1	A	328	PRO	CA-C	-6.15	1.40	1.52

The worst 5 of 131 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	242	THR	CA-C-N	-8.27	99.01	117.20
1	A	289	PRO	N-CA-C	-7.78	91.86	112.10
1	J	166	PRO	N-CA-C	7.57	131.77	112.10
1	L	166	PRO	N-CA-C	7.45	131.46	112.10
1	D	351	GLN	N-CA-C	-7.17	91.64	111.00

There are no chirality outliers.

5 of 118 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	269	GLY	Mainchain
1	A	277	TYR	Mainchain
1	A	279	PRO	Peptide
1	A	284	ASP	Mainchain
1	A	288	GLY	Mainchain

## 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	840	419	218	8	0
1	B	840	419	218	5	0
1	C	840	419	219	1	0
1	D	840	419	217	4	0
1	E	840	419	218	7	0
1	F	840	419	219	3	0
1	G	840	419	219	6	0
1	H	840	419	218	4	0
1	I	840	419	219	4	0
1	J	840	419	219	3	0
1	K	840	419	217	6	0
1	L	840	419	219	2	0
1	M	840	419	218	6	0
1	N	840	419	219	3	0
1	O	840	419	219	3	0
1	P	840	419	218	5	0
1	Q	840	419	219	6	0
1	R	840	419	219	5	0
All	All	15120	7542	3932	81	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 4.

The worst 5 of 81 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:F:179:ALA:O	1:F:259:GLY:HA3	2.08	0.54
1:Q:179:ALA:O	1:Q:259:GLY:HA2	2.10	0.52
1:R:181:PRO:O	1:R:185:ASN:N	2.45	0.50
1:G:175:LEU:C	1:G:177:GLU:H	2.17	0.48
1:H:303:THR:O	1:H:307:GLU:N	2.46	0.48

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	208/210 (99%)	168 (81%)	20 (10%)	20 (10%)	0	10
1	B	208/210 (99%)	170 (82%)	23 (11%)	15 (7%)	1	14
1	C	208/210 (99%)	167 (80%)	24 (12%)	17 (8%)	1	12
1	D	208/210 (99%)	169 (81%)	19 (9%)	20 (10%)	0	10
1	E	208/210 (99%)	169 (81%)	22 (11%)	17 (8%)	1	12
1	F	208/210 (99%)	170 (82%)	25 (12%)	13 (6%)	1	17
1	G	208/210 (99%)	176 (85%)	21 (10%)	11 (5%)	2	19
1	H	208/210 (99%)	174 (84%)	17 (8%)	17 (8%)	1	12
1	I	208/210 (99%)	169 (81%)	24 (12%)	15 (7%)	1	14
1	J	208/210 (99%)	173 (83%)	17 (8%)	18 (9%)	1	11
1	K	208/210 (99%)	171 (82%)	18 (9%)	19 (9%)	1	11
1	L	208/210 (99%)	173 (83%)	20 (10%)	15 (7%)	1	14
1	M	208/210 (99%)	176 (85%)	17 (8%)	15 (7%)	1	14
1	N	208/210 (99%)	179 (86%)	20 (10%)	9 (4%)	2	22
1	O	208/210 (99%)	168 (81%)	28 (14%)	12 (6%)	1	18
1	P	208/210 (99%)	177 (85%)	13 (6%)	18 (9%)	1	11
1	Q	208/210 (99%)	178 (86%)	15 (7%)	15 (7%)	1	14
1	R	208/210 (99%)	177 (85%)	11 (5%)	20 (10%)	0	10
All	All	3744/3780 (99%)	3104 (83%)	354 (10%)	286 (8%)	2	13

5 of 286 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	HIS
1	A	147	ILE
1	A	167	GLU
1	A	179	ALA

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	225	PRO

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 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.

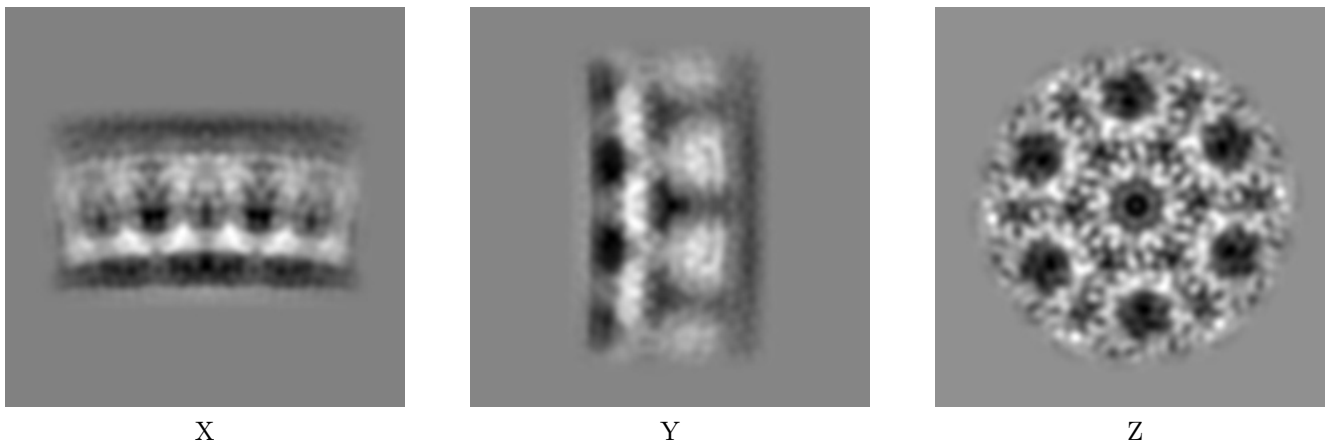
### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Tomogram visualisation [i](#)

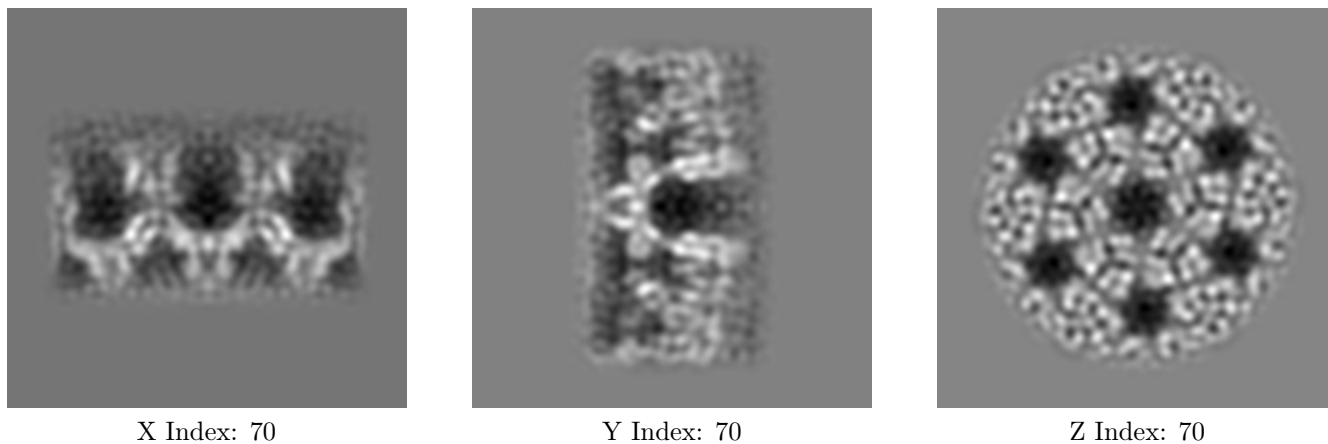
This section contains visualisations of the EMDB entry EMD-2706. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

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



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

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



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

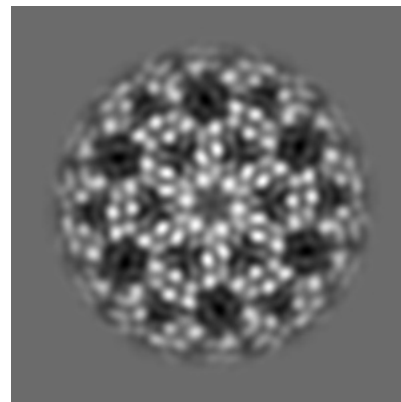
### 6.3 Largest variance slices [i](#)



X Index: 69



Y Index: 52



Z Index: 62

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

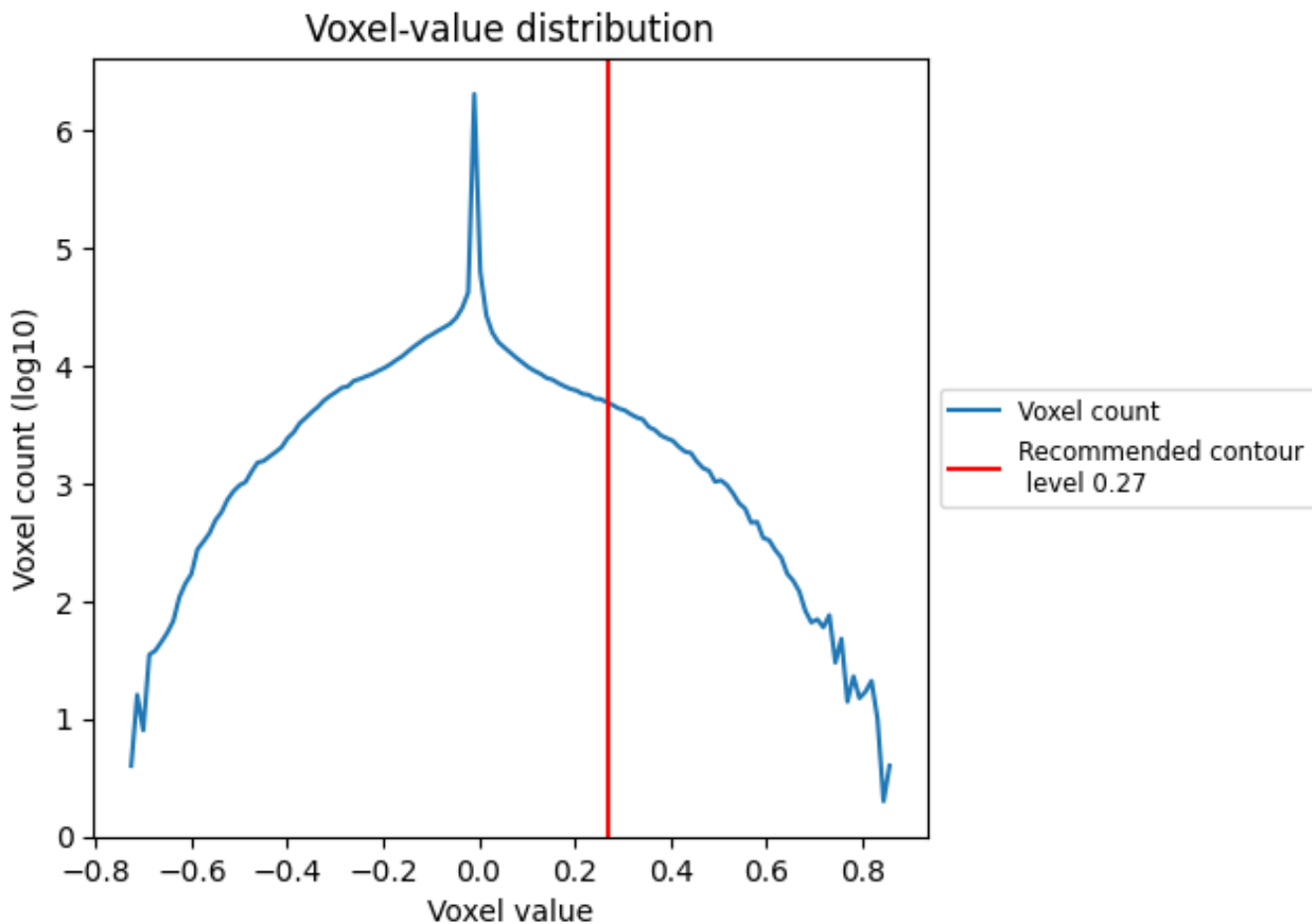
### 6.4 Mask visualisation [i](#)

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

## 7 Tomogram analysis [i](#)

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

### 7.1 Voxel-value distribution [i](#)



The voxel-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic.

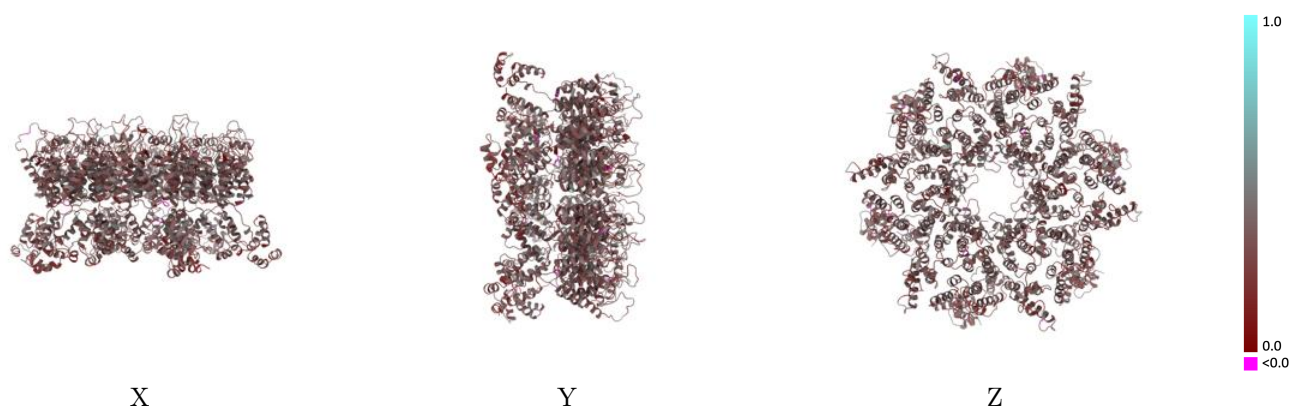
## 8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-2706 and PDB model 4USN. Per-residue inclusion information can be found in section 3 on page 7.

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

This section was not generated.

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

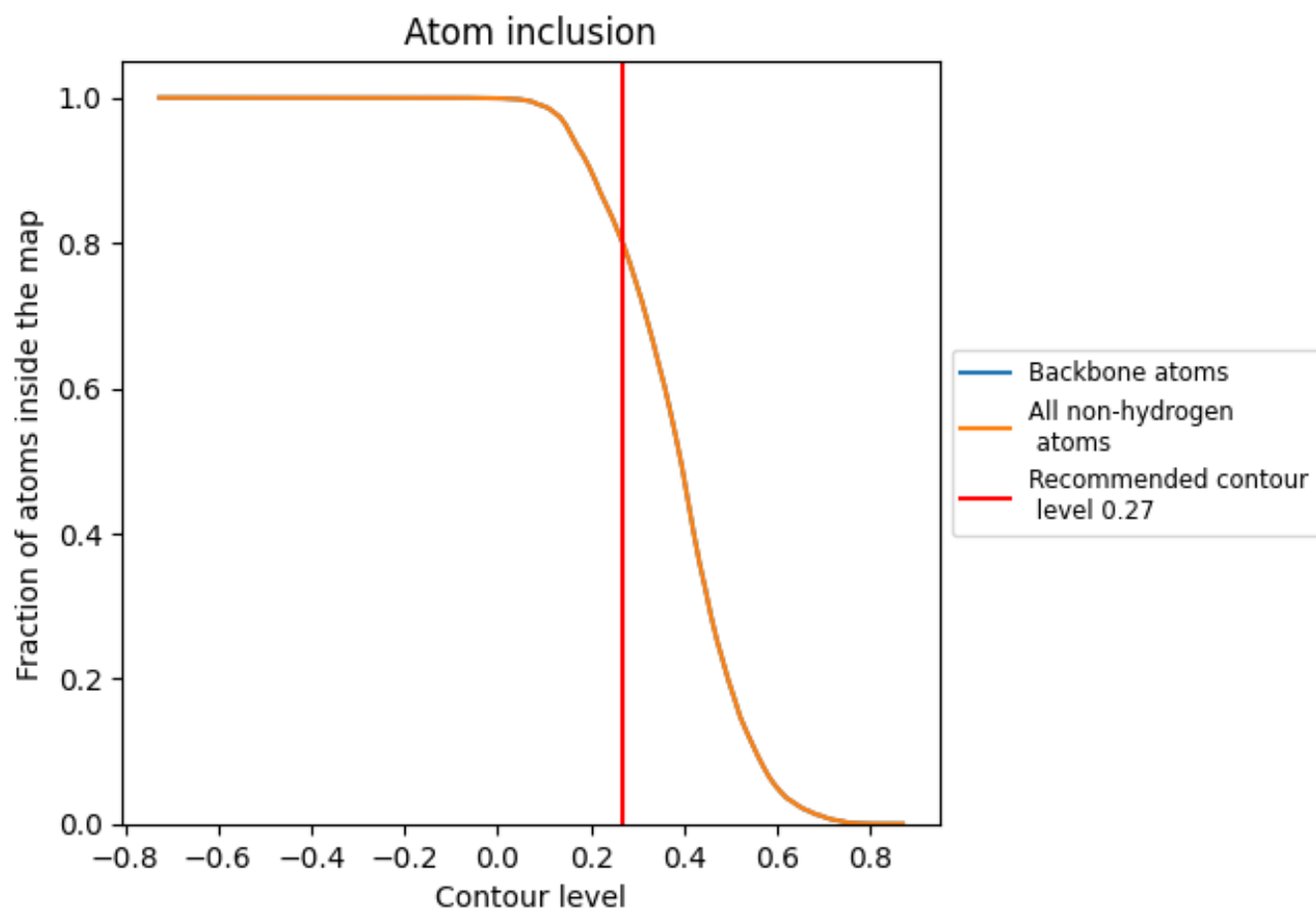


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

### 8.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.







































## 8.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

## 8.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.27) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7979	 0.3140
A	 0.8107	 0.3180
B	 0.8036	 0.3190
C	 0.8083	 0.3240
D	 0.7988	 0.3240
E	 0.8155	 0.3200
F	 0.8012	 0.3220
G	 0.8119	 0.3180
H	 0.7786	 0.3070
I	 0.8024	 0.3130
J	 0.7810	 0.3080
K	 0.8012	 0.3150
L	 0.7738	 0.2990
M	 0.8095	 0.3230
N	 0.7881	 0.3080
O	 0.8083	 0.3120
P	 0.7798	 0.3020
Q	 0.7940	 0.3140
R	 0.7833	 0.3050

