



wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 09:16 am GMT

PDB ID : 6HXX
EMDB ID : EMD-0297
Title : Potato virus Y
Authors : Podobnik, M.; Kezar, A.; Novacek, J.; Polak, M.
Deposited on : 2018-10-18
Resolution : 3.40 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 ⓘ 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:

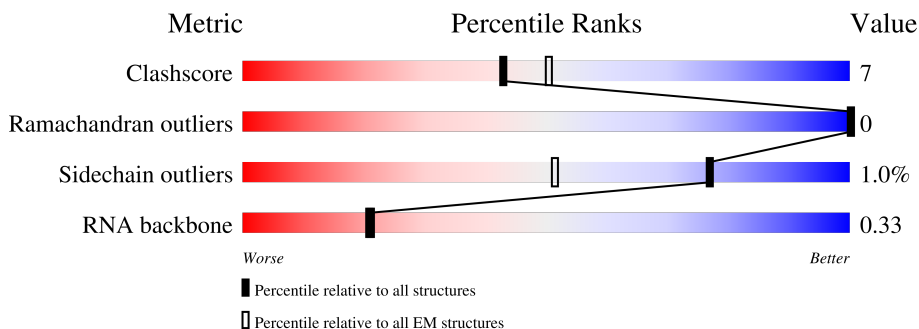
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

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 3.40 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 ≥ 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	AA	267	
1	AB	267	
1	AC	267	
1	AD	267	
1	AE	267	
1	AF	267	
1	AG	267	

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Mol	Chain	Length	Quality of chain			
1	AH	267	21%	70%	14%	16%
1	AI	267	20%	69%	14%	16%
1	AJ	267	22%	69%	15%	16%
1	AK	267	20%	69%	15%	16%
1	AL	267	21%	69%	14%	16%
1	AM	267	20%	69%	15%	16%
1	AN	267	21%	69%	15%	16%
1	AO	267	20%	69%	15%	16%
1	AP	267	21%	67%	16%	16%
1	AQ	267	21%	68%	15%	16%
1	AR	267	20%	68%	15%	16%
1	AS	267	21%	69%	15%	16%
1	AT	267	21%	68%	16%	16%
1	AU	267	21%	69%	15%	16%
1	AV	267	21%	68%	16%	16%
1	AW	267	21%	68%	16%	16%
1	AX	267	21%	67%	17%	16%
1	AY	267	19%	67%	16%	16%
1	AZ	267	21%	67%	16%	16%
1	BA	267	20%	70%	14%	16%
1	BB	267	21%	69%	15%	16%
1	BC	267	21%	69%	15%	16%
1	BD	267	20%	70%	14%	16%
1	BE	267	21%	69%	15%	16%
1	BF	267	22%	69%	15%	16%

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Mol	Chain	Length	Quality of chain
1	BG	267	 21% 68% 16% 16%
1	BH	267	 21% 69% 15% 16%
1	BI	267	 21% 70% 14% 16%
2	Aa	5	100%
2	Ab	5	100%
2	Ac	5	100%
2	Ad	5	100%
2	Ae	5	100%
2	Af	5	100%
2	Ag	5	100%
2	Ah	5	100%
2	Ai	5	100%
2	Aj	5	100%
2	Ak	5	100%
2	Al	5	100%
2	Am	5	100%
2	An	5	100%
2	Ao	5	100%
2	Ap	5	100%
2	Aq	5	100%
2	Ar	5	100%
2	As	5	100%
2	At	5	100%
2	Au	5	100%
2	Av	5	100%

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Mol	Chain	Length	Quality of chain
2	Aw	5	 100%
2	Ax	5	 100%
2	Ay	5	 100%
2	Az	5	 100%
2	Ba	5	 100%
2	Bb	5	 100%
2	Bc	5	 100%
2	Bd	5	 100%
2	Be	5	 100%
2	Bf	5	 100%
2	Bg	5	 100%
2	Bh	5	 100%
2	Bi	5	 100%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 65765 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 Coat protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	AA	224	1779	1115	311	339	14	0	0
1	AB	224	1779	1115	311	339	14	0	0
1	AC	224	1779	1115	311	339	14	0	0
1	AD	224	1779	1115	311	339	14	0	0
1	AE	224	1779	1115	311	339	14	0	0
1	AF	224	1779	1115	311	339	14	0	0
1	AG	224	1779	1115	311	339	14	0	0
1	AH	224	1779	1115	311	339	14	0	0
1	AI	224	1779	1115	311	339	14	0	0
1	AJ	224	1779	1115	311	339	14	0	0
1	AK	224	1779	1115	311	339	14	0	0
1	AL	224	1779	1115	311	339	14	0	0
1	AM	224	1779	1115	311	339	14	0	0
1	AN	224	1779	1115	311	339	14	0	0
1	AO	224	1779	1115	311	339	14	0	0
1	AP	224	1779	1115	311	339	14	0	0
1	AQ	224	1779	1115	311	339	14	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	AR	224	Total	C	N	O	S	0	0
			1779	1115	311	339	14		
1	AS	224	Total	C	N	O	S	0	0
			1779	1115	311	339	14		
1	AT	224	Total	C	N	O	S	0	0
			1779	1115	311	339	14		
1	AU	224	Total	C	N	O	S	0	0
			1779	1115	311	339	14		
1	AV	224	Total	C	N	O	S	0	0
			1779	1115	311	339	14		
1	AW	224	Total	C	N	O	S	0	0
			1779	1115	311	339	14		
1	AX	224	Total	C	N	O	S	0	0
			1779	1115	311	339	14		
1	AY	224	Total	C	N	O	S	0	0
			1779	1115	311	339	14		
1	AZ	224	Total	C	N	O	S	0	0
			1779	1115	311	339	14		
1	BA	224	Total	C	N	O	S	0	0
			1779	1115	311	339	14		
1	BB	224	Total	C	N	O	S	0	0
			1779	1115	311	339	14		
1	BC	224	Total	C	N	O	S	0	0
			1779	1115	311	339	14		
1	BD	224	Total	C	N	O	S	0	0
			1779	1115	311	339	14		
1	BE	224	Total	C	N	O	S	0	0
			1779	1115	311	339	14		
1	BF	224	Total	C	N	O	S	0	0
			1779	1115	311	339	14		
1	BG	224	Total	C	N	O	S	0	0
			1779	1115	311	339	14		
1	BH	224	Total	C	N	O	S	0	0
			1779	1115	311	339	14		
1	BI	224	Total	C	N	O	S	0	0
			1779	1115	311	339	14		

- Molecule 2 is a RNA chain called RNA (5'-R(P*UP*UP*UP*UP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Aa	5	Total	C	N	O	P	0	0
			100	45	10	40	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	Ab	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Ac	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Ad	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Ae	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Af	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Ag	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Ah	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Ai	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Aj	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Ak	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Al	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Am	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	An	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Ao	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Ap	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Aq	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Ar	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	As	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	At	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Au	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Av	5	Total 100	C 45	N 10	O 40	P 5	0	0

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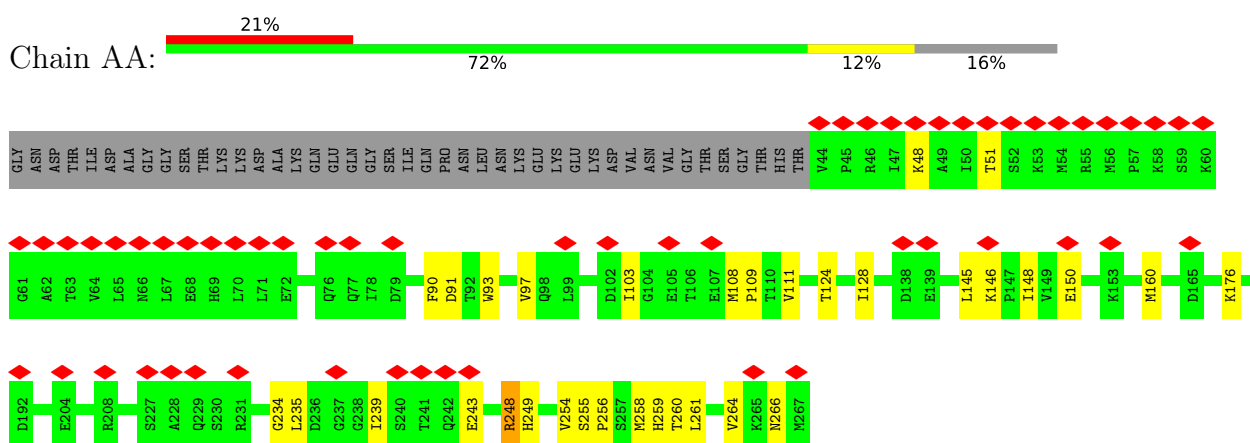
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Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	N	O			P
2	Aw	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Ax	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Ay	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Az	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Ba	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Bb	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Bc	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Bd	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Be	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Bf	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Bg	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Bh	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Bi	5	Total 100	C 45	N 10	O 40	P 5	0	0

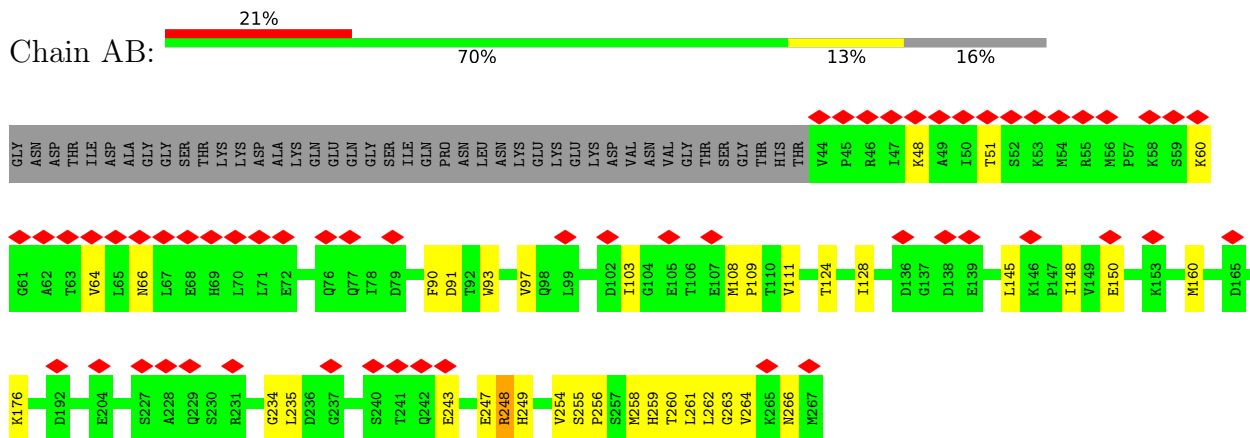
3 Residue-property plots [i](#)

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.

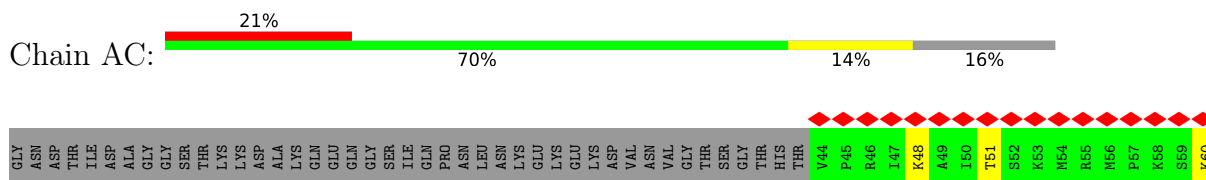
- Molecule 1: Coat protein

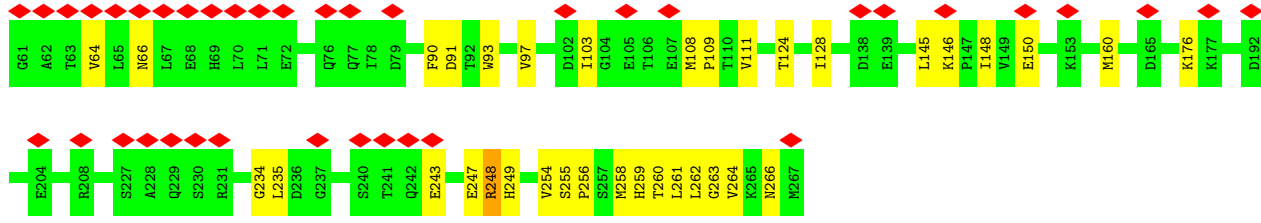


- Molecule 1: Coat protein

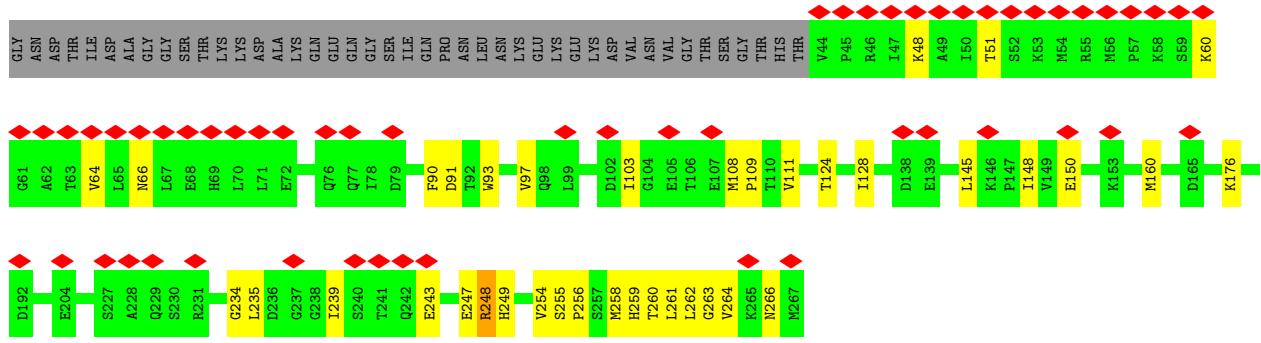


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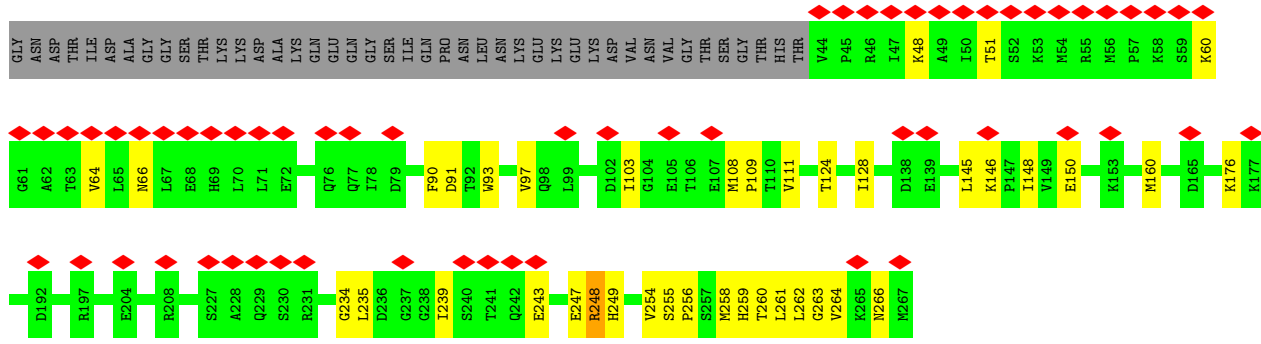




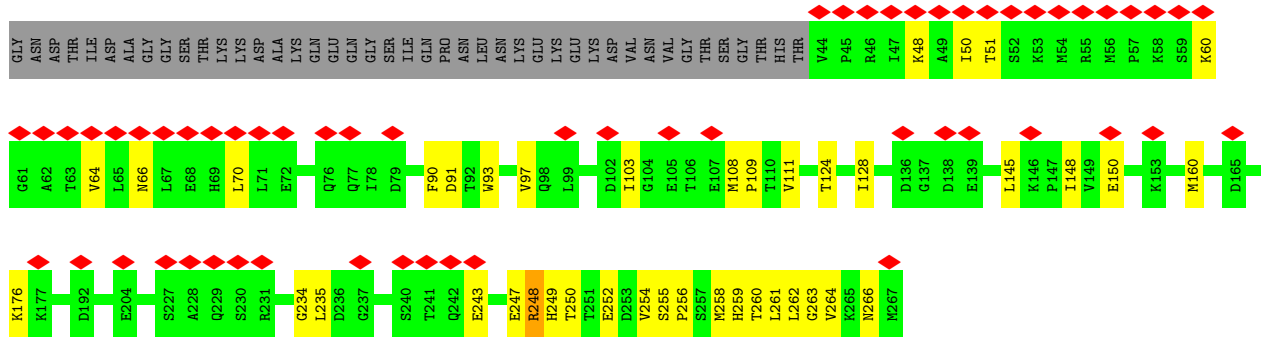
• Molecule 1: Coat protein



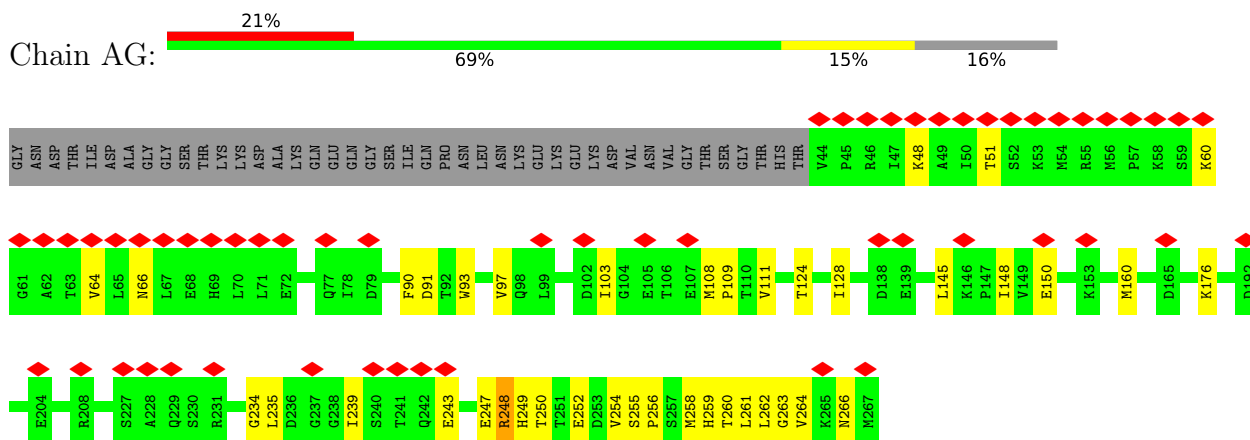
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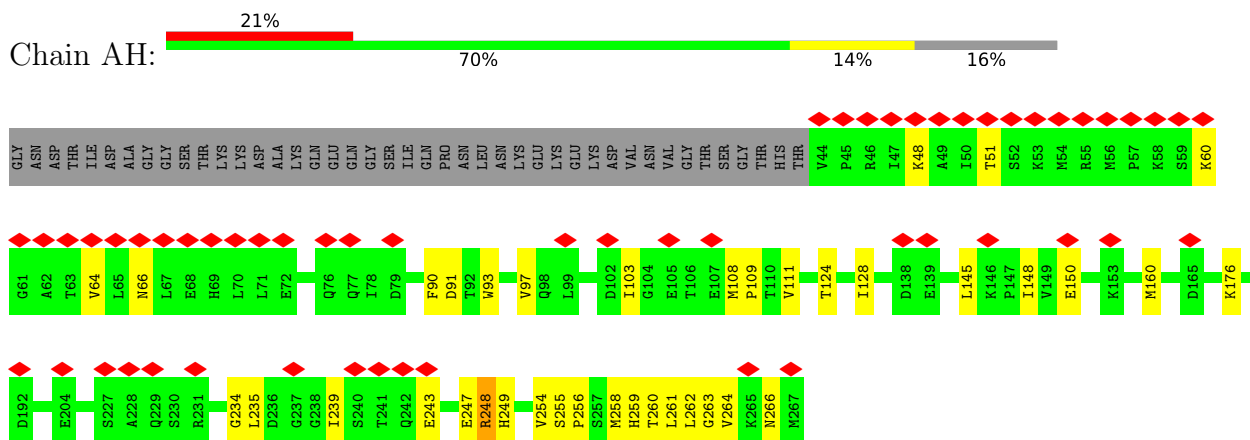
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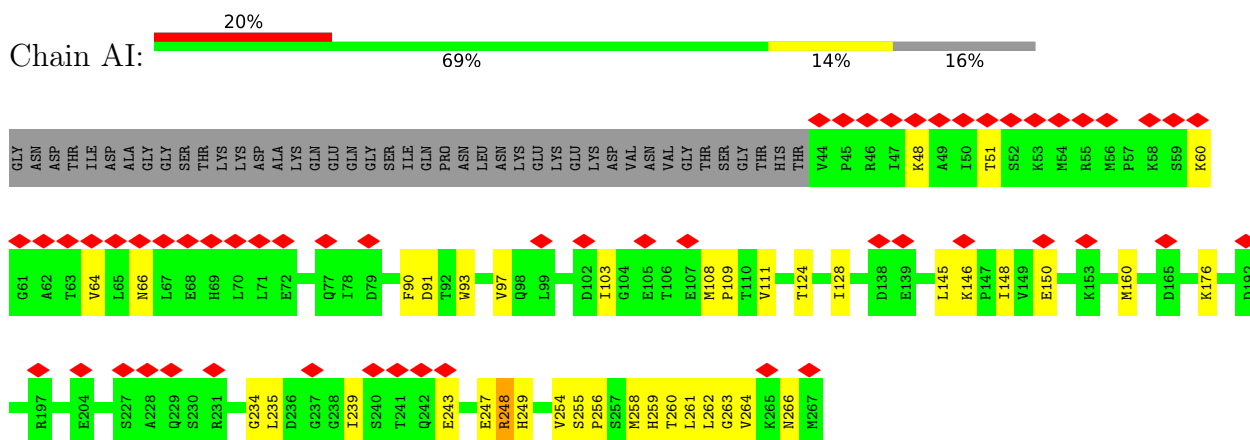
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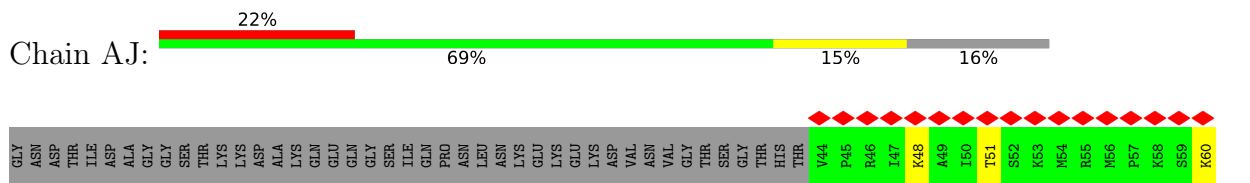
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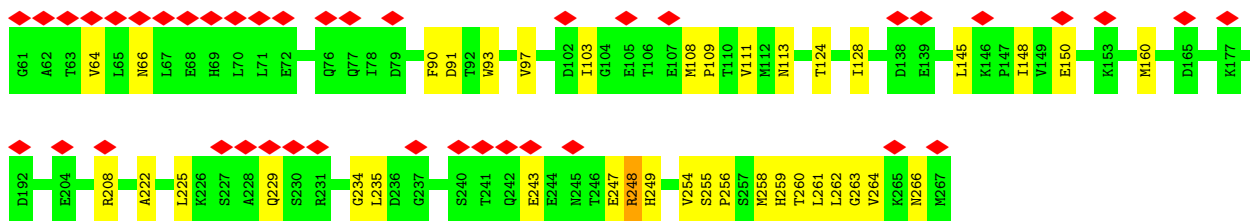


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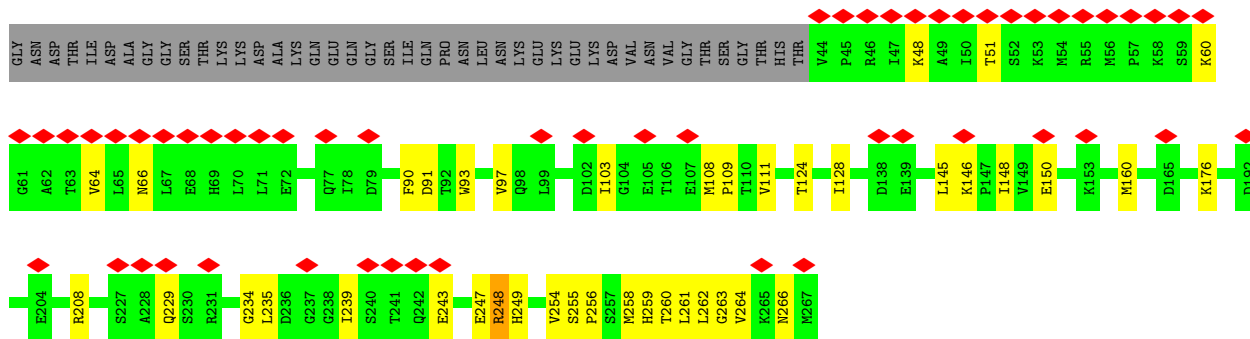


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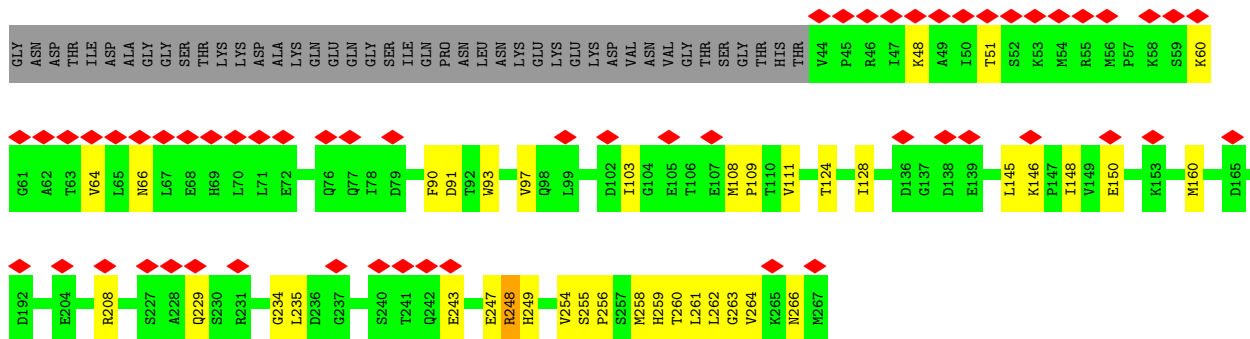




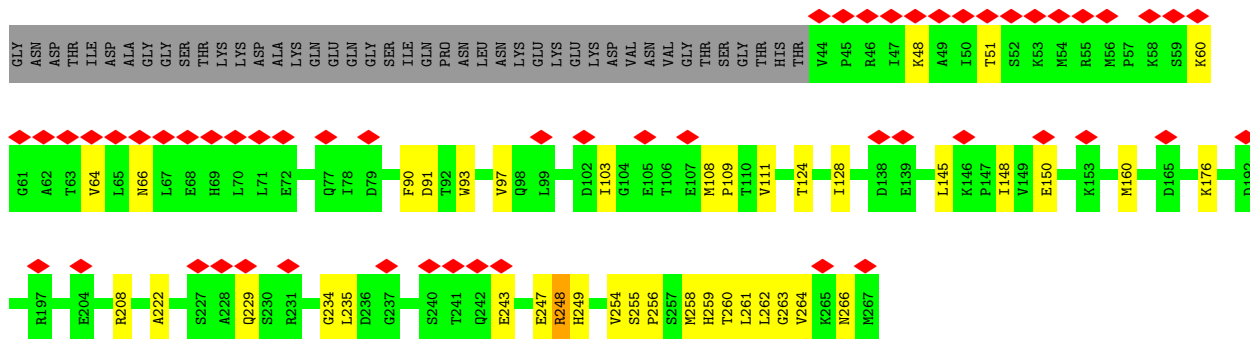
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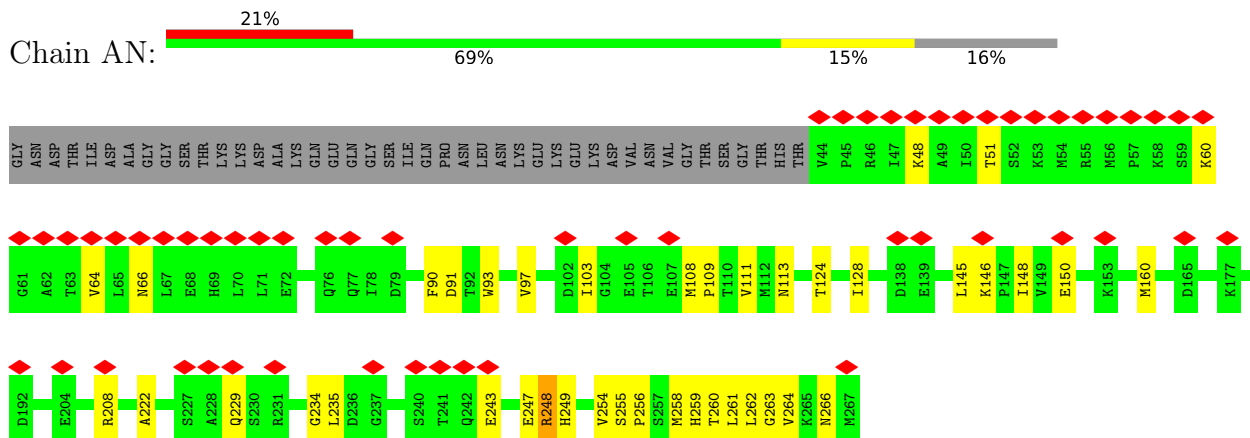
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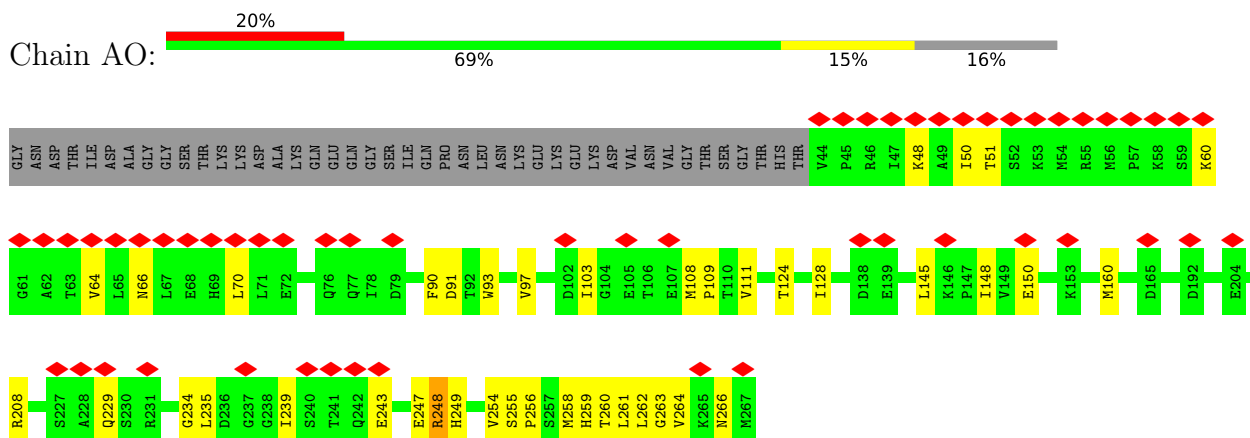
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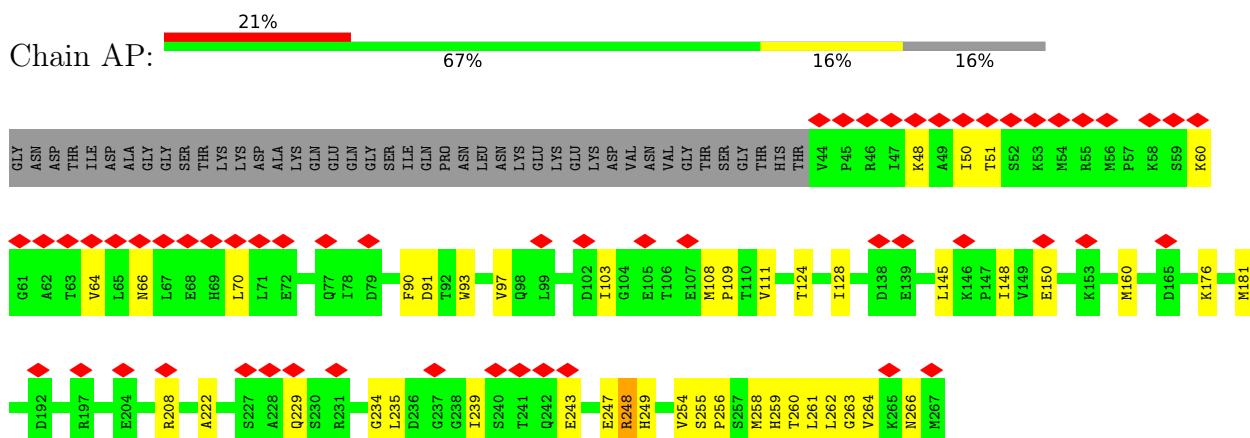
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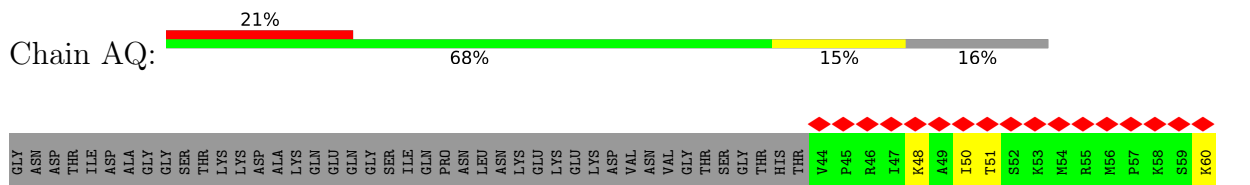
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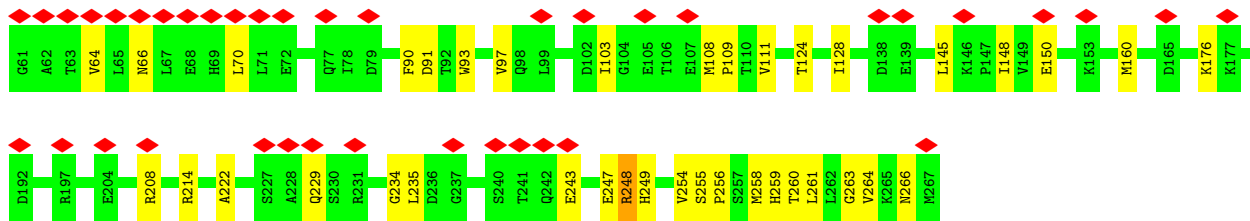


• Molecule 1: Coat protein



• Molecule 1: Coat protein

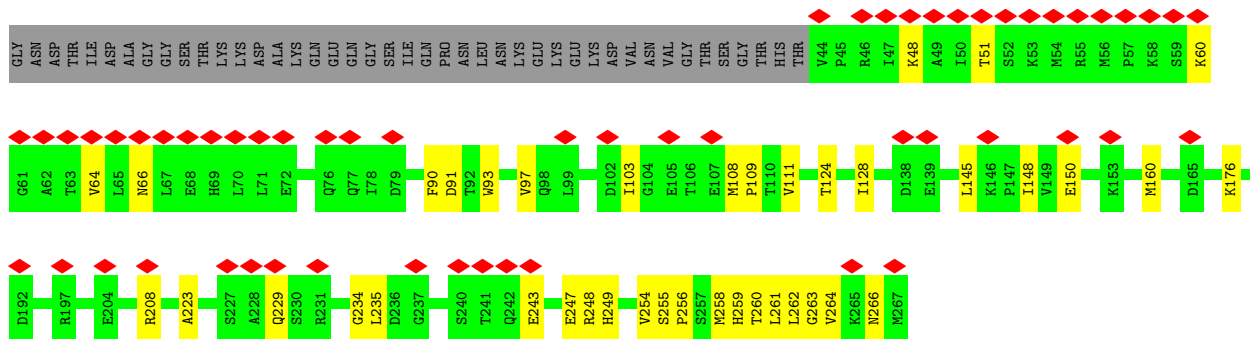




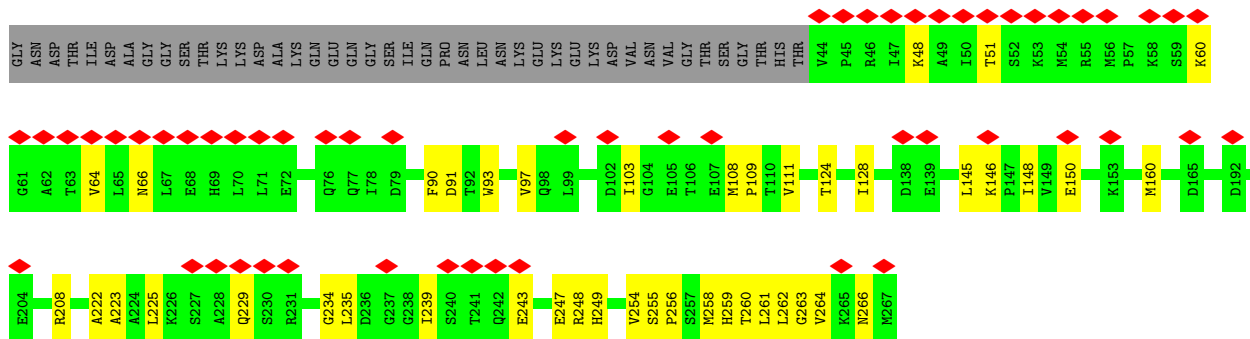
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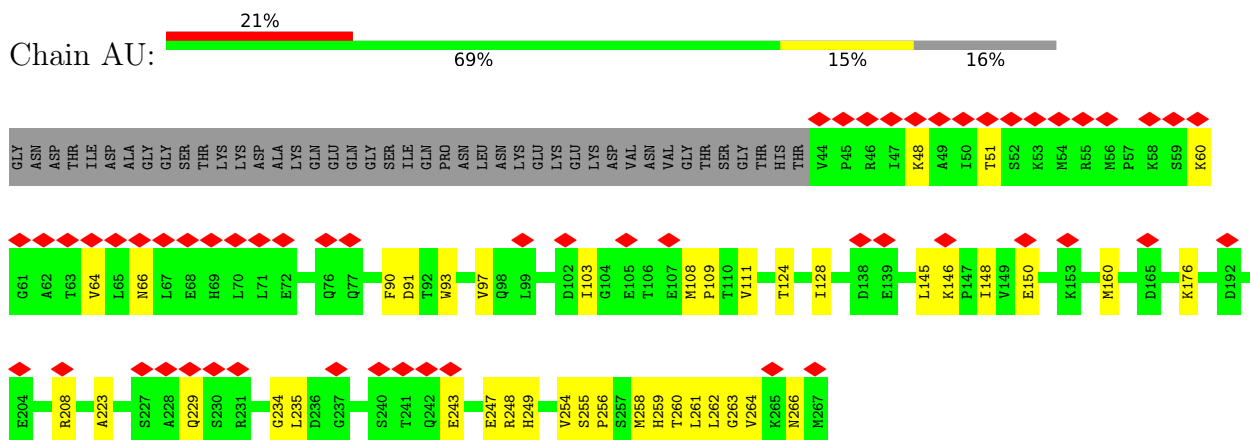
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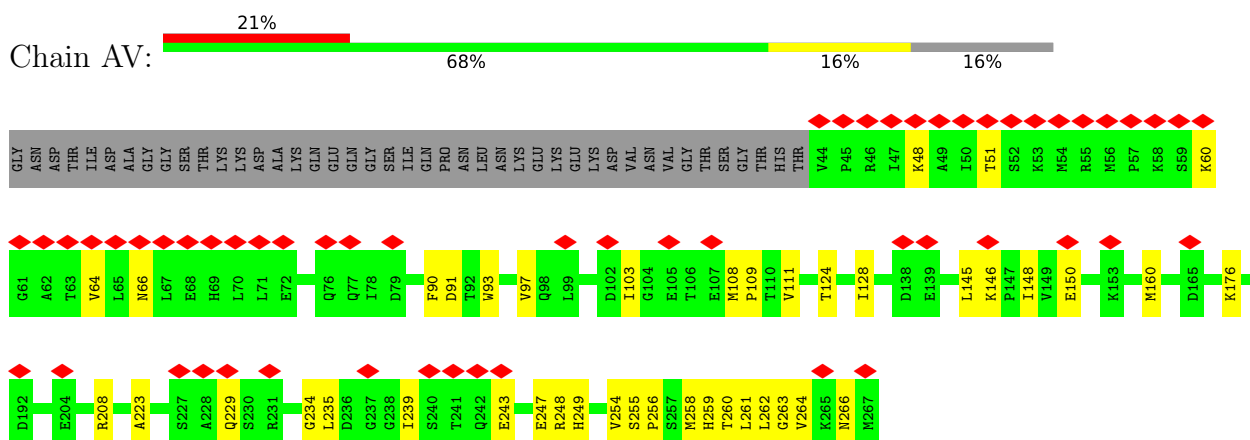
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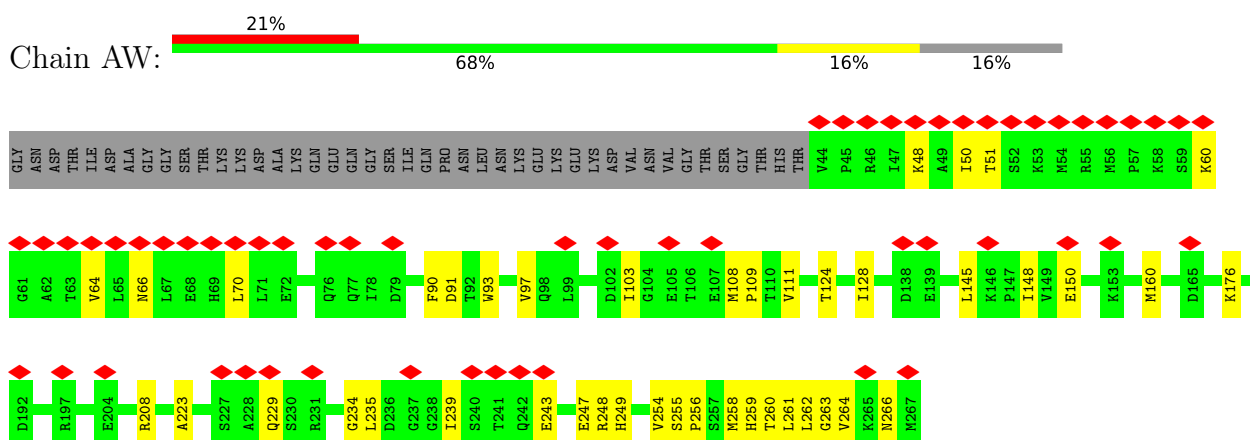
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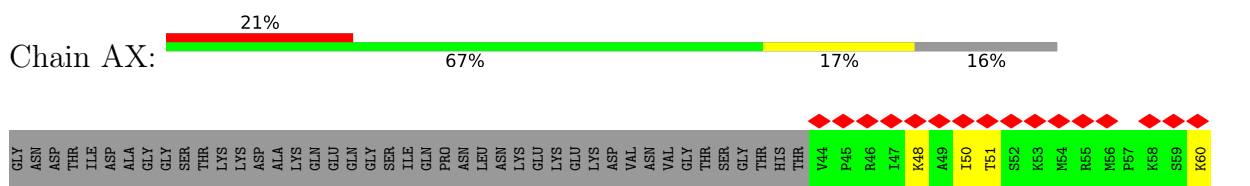
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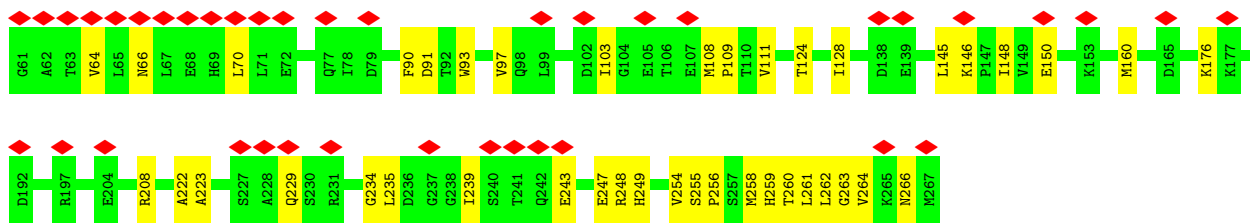


• Molecule 1: Coat protein

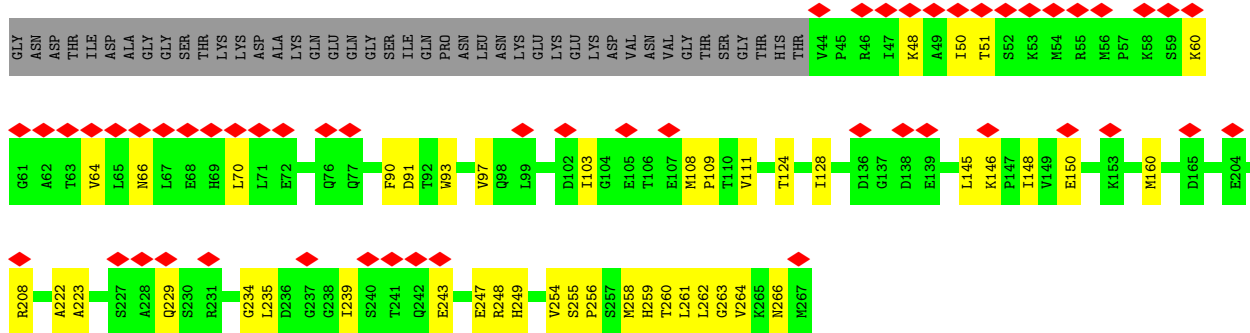


• Molecule 1: Coat protein

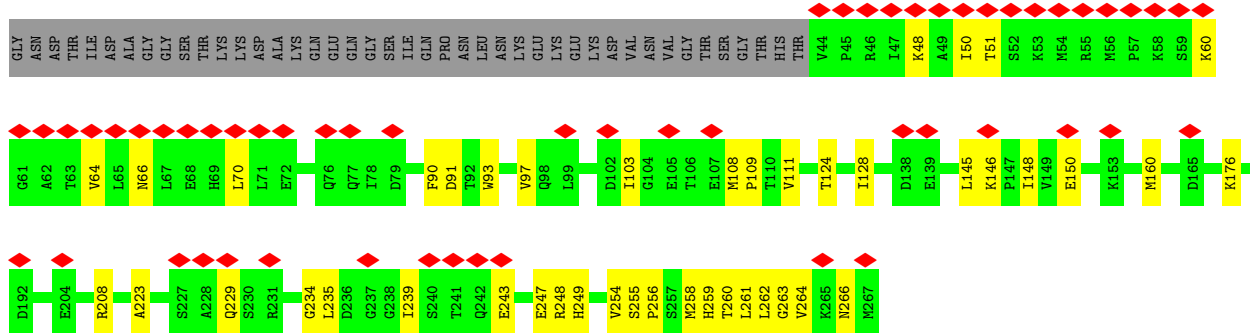




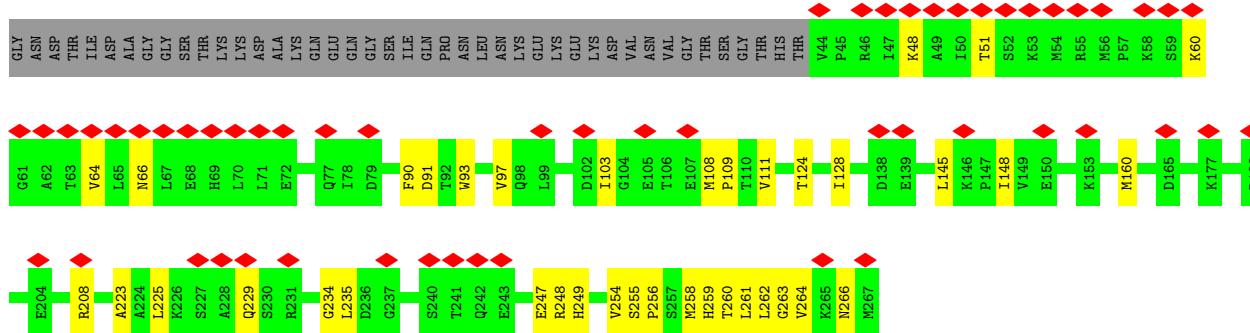
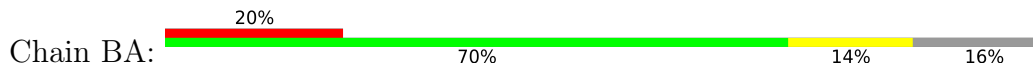
• Molecule 1: Coat protein



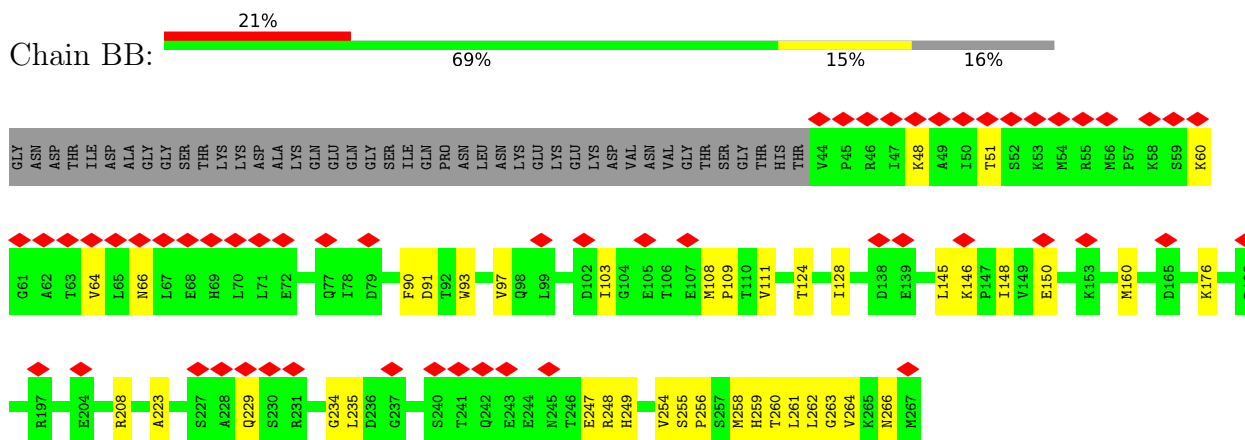
• Molecule 1: Coat protein



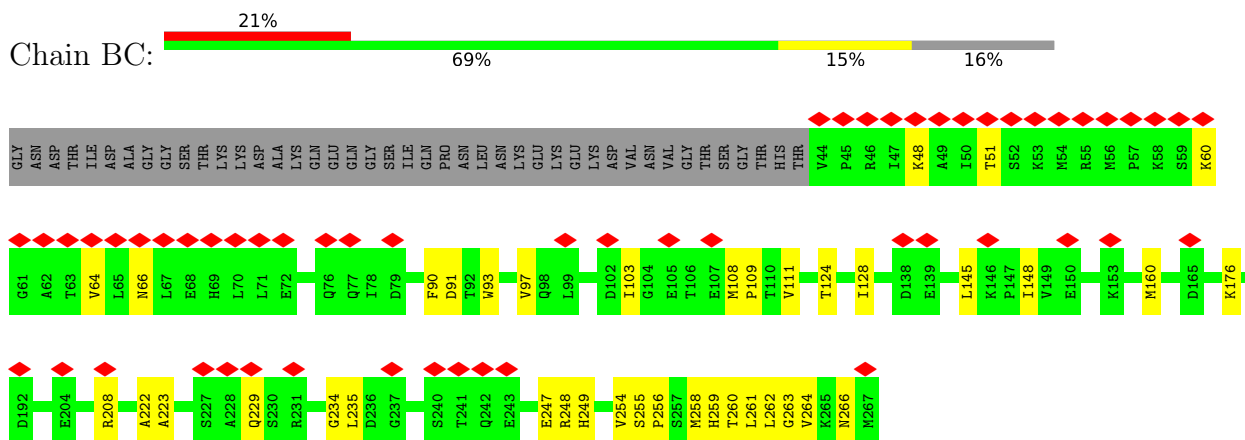
• Molecule 1: Coat protein



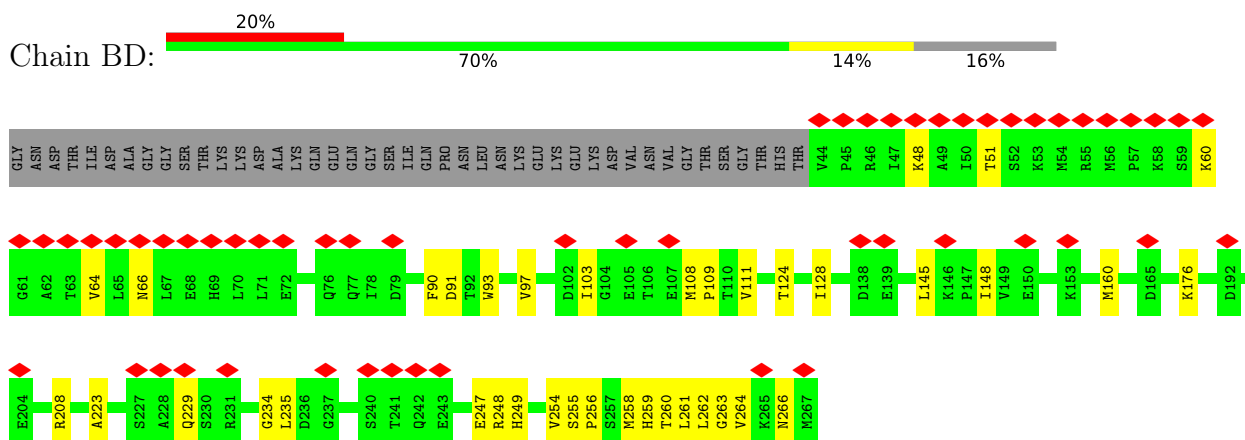
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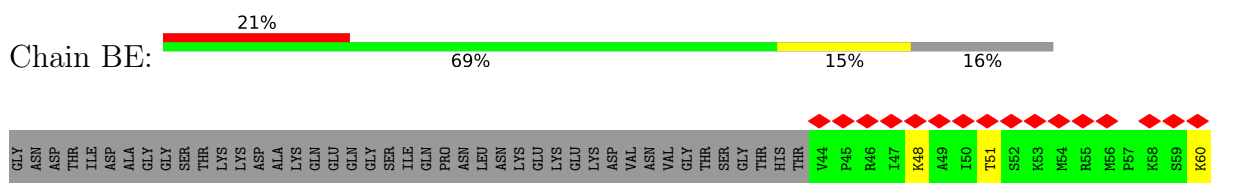
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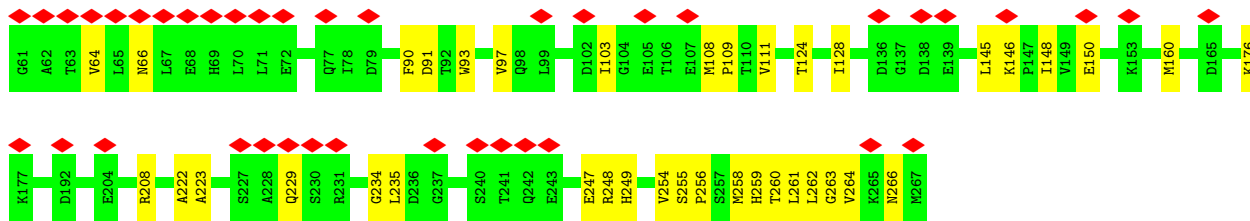


• Molecule 1: Coat protein

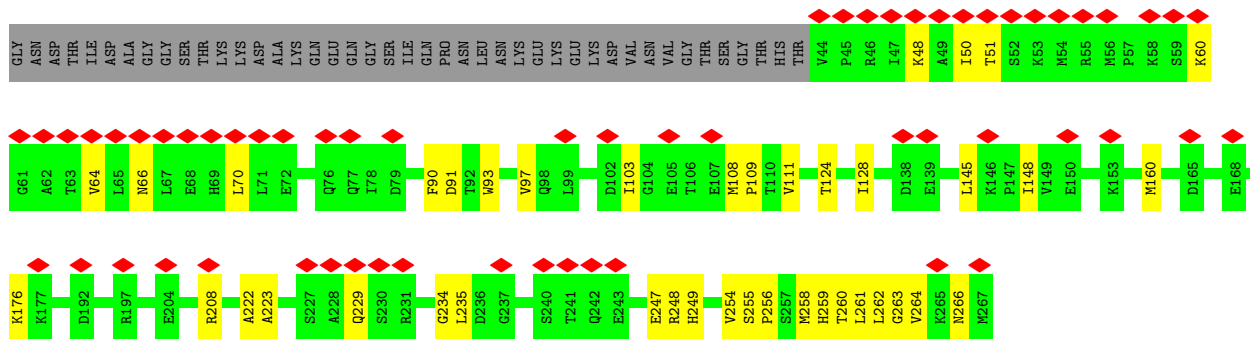


• Molecule 1: Coat protein

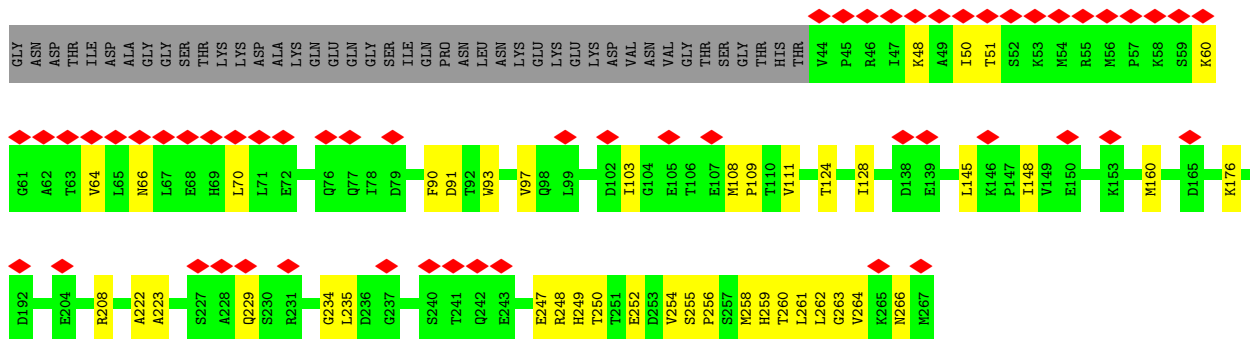




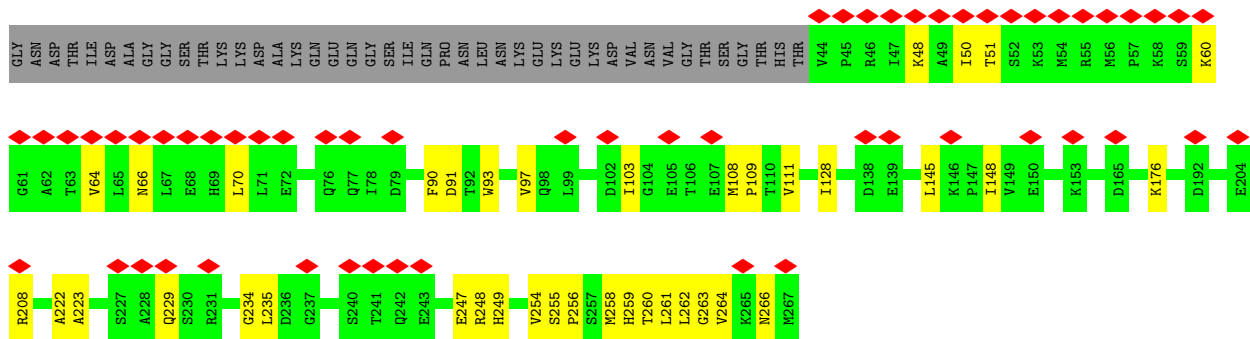
• Molecule 1: Coat protein



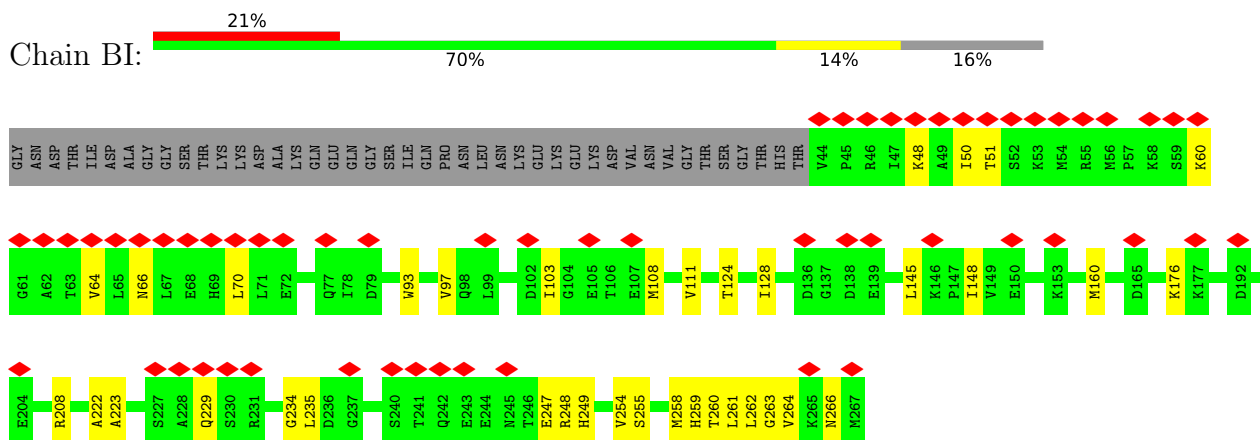
• Molecule 1: Coat protein



• Molecule 1: Coat protein



- Molecule 1: Coat protein



- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Aa:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Ab:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Ac:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Ad:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Ae:  100%


There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Af:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Ag:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Ah:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Ai:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Aj:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Ak:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Al:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Am:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain An:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Ao:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Ap:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Aq:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Ar:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain As:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain At:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Au:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Av:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Aw:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Ax:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Ay:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Az:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Ba:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Bb:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Bc:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Bd:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Be:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Bf:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Bg:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Bh:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Bi:  100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-40.95°, rise=3.95 Å, axial sym=C1	Depositor
Number of segments used	162213	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 ($e^-/\text{Å}^2$)	48.6	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.435	Depositor
Minimum map value	-0.249	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.132	Depositor
Map size (Å)	381.96, 381.96, 381.96	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.061, 1.061, 1.061	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	AA	0.38	0/1815	0.62	0/2457
1	AB	0.38	0/1815	0.62	0/2457
1	AC	0.38	0/1815	0.62	0/2457
1	AD	0.38	0/1815	0.62	0/2457
1	AE	0.38	0/1815	0.62	0/2457
1	AF	0.38	0/1815	0.62	0/2457
1	AG	0.38	0/1815	0.62	0/2457
1	AH	0.38	0/1815	0.62	0/2457
1	AI	0.38	0/1815	0.62	0/2457
1	AJ	0.38	0/1815	0.62	0/2457
1	AK	0.38	0/1815	0.62	0/2457
1	AL	0.38	0/1815	0.62	0/2457
1	AM	0.38	0/1815	0.62	0/2457
1	AN	0.38	0/1815	0.62	0/2457
1	AO	0.38	0/1815	0.62	0/2457
1	AP	0.38	0/1815	0.62	0/2457
1	AQ	0.38	0/1815	0.62	0/2457
1	AR	0.38	0/1815	0.62	0/2457
1	AS	0.38	0/1815	0.62	0/2457
1	AT	0.38	0/1815	0.62	0/2457
1	AU	0.38	0/1815	0.63	0/2457
1	AV	0.38	0/1815	0.63	0/2457
1	AW	0.38	0/1815	0.62	0/2457
1	AX	0.38	0/1815	0.62	0/2457
1	AY	0.38	0/1815	0.62	0/2457
1	AZ	0.38	0/1815	0.62	0/2457
1	BA	0.38	0/1815	0.62	0/2457
1	BB	0.38	0/1815	0.62	0/2457
1	BC	0.38	0/1815	0.62	0/2457
1	BD	0.38	0/1815	0.62	0/2457
1	BE	0.38	0/1815	0.62	0/2457
1	BF	0.38	0/1815	0.62	0/2457
1	BG	0.38	0/1815	0.62	0/2457
1	BH	0.38	0/1815	0.62	0/2457

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	BI	0.38	0/1815	0.62	0/2457
2	Aa	0.25	0/109	0.71	0/166
2	Ab	0.25	0/109	0.71	0/166
2	Ac	0.26	0/109	0.71	0/166
2	Ad	0.25	0/109	0.71	0/166
2	Ae	0.25	0/109	0.71	0/166
2	Af	0.25	0/109	0.71	0/166
2	Ag	0.25	0/109	0.71	0/166
2	Ah	0.25	0/109	0.71	0/166
2	Ai	0.26	0/109	0.71	0/166
2	Aj	0.25	0/109	0.71	0/166
2	Ak	0.25	0/109	0.71	0/166
2	Al	0.25	0/109	0.71	0/166
2	Am	0.25	0/109	0.71	0/166
2	An	0.26	0/109	0.72	0/166
2	Ao	0.26	0/109	0.71	0/166
2	Ap	0.25	0/109	0.71	0/166
2	Aq	0.25	0/109	0.71	0/166
2	Ar	0.26	0/109	0.71	0/166
2	As	0.25	0/109	0.71	0/166
2	At	0.26	0/109	0.72	0/166
2	Au	0.26	0/109	0.71	0/166
2	Av	0.25	0/109	0.71	0/166
2	Aw	0.26	0/109	0.71	0/166
2	Ax	0.26	0/109	0.71	0/166
2	Ay	0.26	0/109	0.71	0/166
2	Az	0.25	0/109	0.71	0/166
2	Ba	0.25	0/109	0.71	0/166
2	Bb	0.25	0/109	0.71	0/166
2	Bc	0.26	0/109	0.71	0/166
2	Bd	0.26	0/109	0.71	0/166
2	Be	0.25	0/109	0.71	0/166
2	Bf	0.25	0/109	0.71	0/166
2	Bg	0.26	0/109	0.71	0/166
2	Bh	0.25	0/109	0.71	0/166
2	Bi	0.25	0/109	0.71	0/166
All	All	0.38	0/67340	0.63	0/91805

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	AA	1779	0	1761	24	0
1	AB	1779	0	1761	29	0
1	AC	1779	0	1761	33	0
1	AD	1779	0	1761	32	0
1	AE	1779	0	1761	33	0
1	AF	1779	0	1761	33	0
1	AG	1779	0	1761	33	0
1	AH	1779	0	1761	33	0
1	AI	1779	0	1761	33	0
1	AJ	1779	0	1761	33	0
1	AK	1779	0	1761	34	0
1	AL	1779	0	1761	32	0
1	AM	1779	0	1761	34	0
1	AN	1779	0	1761	34	0
1	AO	1779	0	1761	34	0
1	AP	1779	0	1761	35	0
1	AQ	1779	0	1761	34	0
1	AR	1779	0	1761	35	0
1	AS	1779	0	1761	33	0
1	AT	1779	0	1761	38	0
1	AU	1779	0	1761	33	0
1	AV	1779	0	1761	34	0
1	AW	1779	0	1761	34	0
1	AX	1779	0	1761	36	0
1	AY	1779	0	1761	35	0
1	AZ	1779	0	1761	34	0
1	BA	1779	0	1761	29	0
1	BB	1779	0	1761	30	0
1	BC	1779	0	1761	31	0
1	BD	1779	0	1761	30	0
1	BE	1779	0	1761	33	0
1	BF	1779	0	1761	34	0
1	BG	1779	0	1761	33	0
1	BH	1779	0	1761	31	0
1	BI	1779	0	1761	25	0
2	Aa	100	0	50	0	0
2	Ab	100	0	50	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Ac	100	0	50	0	0
2	Ad	100	0	50	0	0
2	Ae	100	0	50	0	0
2	Af	100	0	50	0	0
2	Ag	100	0	50	0	0
2	Ah	100	0	50	0	0
2	Ai	100	0	50	0	0
2	Aj	100	0	50	0	0
2	Ak	100	0	50	0	0
2	Al	100	0	50	0	0
2	Am	100	0	50	0	0
2	An	100	0	50	0	0
2	Ao	100	0	50	0	0
2	Ap	100	0	50	0	0
2	Aq	100	0	50	0	0
2	Ar	100	0	50	0	0
2	As	100	0	50	0	0
2	At	100	0	50	0	0
2	Au	100	0	50	0	0
2	Av	100	0	50	0	0
2	Aw	100	0	50	0	0
2	Ax	100	0	50	0	0
2	Ay	100	0	50	0	0
2	Az	100	0	50	0	0
2	Ba	100	0	50	0	0
2	Bb	100	0	50	0	0
2	Bc	100	0	50	0	0
2	Bd	100	0	50	0	0
2	Be	100	0	50	0	0
2	Bf	100	0	50	0	0
2	Bg	100	0	50	0	0
2	Bh	100	0	50	0	0
2	Bi	100	0	51	0	0
All	All	65765	0	63386	796	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 7.

The worst 5 of 796 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:AM:260:THR:O	1:AM:261:LEU:C	2.44	0.56
1:AV:260:THR:O	1:AV:261:LEU:C	2.44	0.56
1:AE:260:THR:O	1:AE:261:LEU:C	2.44	0.56
1:AN:260:THR:O	1:AN:261:LEU:C	2.44	0.56
1:AU:260:THR:O	1:AU:261:LEU:C	2.44	0.56

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	AA	222/267 (83%)	204 (92%)	18 (8%)	0	100	100
1	AB	222/267 (83%)	204 (92%)	18 (8%)	0	100	100
1	AC	222/267 (83%)	204 (92%)	18 (8%)	0	100	100
1	AD	222/267 (83%)	204 (92%)	18 (8%)	0	100	100
1	AE	222/267 (83%)	204 (92%)	18 (8%)	0	100	100
1	AF	222/267 (83%)	204 (92%)	18 (8%)	0	100	100
1	AG	222/267 (83%)	204 (92%)	18 (8%)	0	100	100
1	AH	222/267 (83%)	204 (92%)	18 (8%)	0	100	100
1	AI	222/267 (83%)	204 (92%)	18 (8%)	0	100	100
1	AJ	222/267 (83%)	204 (92%)	18 (8%)	0	100	100
1	AK	222/267 (83%)	204 (92%)	18 (8%)	0	100	100
1	AL	222/267 (83%)	204 (92%)	18 (8%)	0	100	100
1	AM	222/267 (83%)	204 (92%)	18 (8%)	0	100	100
1	AN	222/267 (83%)	204 (92%)	18 (8%)	0	100	100
1	AO	222/267 (83%)	204 (92%)	18 (8%)	0	100	100
1	AP	222/267 (83%)	204 (92%)	18 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AQ	222/267 (83%)	204 (92%)	18 (8%)	0	100	100
1	AR	222/267 (83%)	204 (92%)	18 (8%)	0	100	100
1	AS	222/267 (83%)	204 (92%)	18 (8%)	0	100	100
1	AT	222/267 (83%)	204 (92%)	18 (8%)	0	100	100
1	AU	222/267 (83%)	204 (92%)	18 (8%)	0	100	100
1	AV	222/267 (83%)	204 (92%)	18 (8%)	0	100	100
1	AW	222/267 (83%)	204 (92%)	18 (8%)	0	100	100
1	AX	222/267 (83%)	204 (92%)	18 (8%)	0	100	100
1	AY	222/267 (83%)	204 (92%)	18 (8%)	0	100	100
1	AZ	222/267 (83%)	204 (92%)	18 (8%)	0	100	100
1	BA	222/267 (83%)	204 (92%)	18 (8%)	0	100	100
1	BB	222/267 (83%)	204 (92%)	18 (8%)	0	100	100
1	BC	222/267 (83%)	204 (92%)	18 (8%)	0	100	100
1	BD	222/267 (83%)	204 (92%)	18 (8%)	0	100	100
1	BE	222/267 (83%)	204 (92%)	18 (8%)	0	100	100
1	BF	222/267 (83%)	204 (92%)	18 (8%)	0	100	100
1	BG	222/267 (83%)	204 (92%)	18 (8%)	0	100	100
1	BH	222/267 (83%)	204 (92%)	18 (8%)	0	100	100
1	BI	222/267 (83%)	204 (92%)	18 (8%)	0	100	100
All	All	7770/9345 (83%)	7140 (92%)	630 (8%)	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	AA	194/229 (85%)	192 (99%)	2 (1%)	76	88
1	AB	194/229 (85%)	192 (99%)	2 (1%)	76	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AC	194/229 (85%)	192 (99%)	2 (1%)	76	88
1	AD	194/229 (85%)	192 (99%)	2 (1%)	76	88
1	AE	194/229 (85%)	192 (99%)	2 (1%)	76	88
1	AF	194/229 (85%)	192 (99%)	2 (1%)	76	88
1	AG	194/229 (85%)	192 (99%)	2 (1%)	76	88
1	AH	194/229 (85%)	192 (99%)	2 (1%)	76	88
1	AI	194/229 (85%)	192 (99%)	2 (1%)	76	88
1	AJ	194/229 (85%)	192 (99%)	2 (1%)	76	88
1	AK	194/229 (85%)	192 (99%)	2 (1%)	76	88
1	AL	194/229 (85%)	192 (99%)	2 (1%)	76	88
1	AM	194/229 (85%)	192 (99%)	2 (1%)	76	88
1	AN	194/229 (85%)	192 (99%)	2 (1%)	76	88
1	AO	194/229 (85%)	192 (99%)	2 (1%)	76	88
1	AP	194/229 (85%)	192 (99%)	2 (1%)	76	88
1	AQ	194/229 (85%)	192 (99%)	2 (1%)	76	88
1	AR	194/229 (85%)	192 (99%)	2 (1%)	76	88
1	AS	194/229 (85%)	192 (99%)	2 (1%)	76	88
1	AT	194/229 (85%)	192 (99%)	2 (1%)	76	88
1	AU	194/229 (85%)	192 (99%)	2 (1%)	76	88
1	AV	194/229 (85%)	192 (99%)	2 (1%)	76	88
1	AW	194/229 (85%)	192 (99%)	2 (1%)	76	88
1	AX	194/229 (85%)	192 (99%)	2 (1%)	76	88
1	AY	194/229 (85%)	192 (99%)	2 (1%)	76	88
1	AZ	194/229 (85%)	192 (99%)	2 (1%)	76	88
1	BA	194/229 (85%)	192 (99%)	2 (1%)	76	88
1	BB	194/229 (85%)	192 (99%)	2 (1%)	76	88
1	BC	194/229 (85%)	192 (99%)	2 (1%)	76	88
1	BD	194/229 (85%)	192 (99%)	2 (1%)	76	88
1	BE	194/229 (85%)	192 (99%)	2 (1%)	76	88
1	BF	194/229 (85%)	192 (99%)	2 (1%)	76	88
1	BG	194/229 (85%)	192 (99%)	2 (1%)	76	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BH	194/229 (85%)	192 (99%)	2 (1%)	76	88
1	BI	194/229 (85%)	192 (99%)	2 (1%)	76	88
All	All	6790/8015 (85%)	6720 (99%)	70 (1%)	77	88

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BC	249	HIS
1	BD	249	HIS
1	BG	249	HIS
1	AM	248	ARG
1	AL	249	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	Aa	4/5 (80%)	0	0
2	Ab	4/5 (80%)	0	0
2	Ac	4/5 (80%)	0	0
2	Ad	4/5 (80%)	0	0
2	Ae	4/5 (80%)	0	0
2	Af	4/5 (80%)	0	0
2	Ag	4/5 (80%)	0	0
2	Ah	4/5 (80%)	0	0
2	Ai	4/5 (80%)	0	0
2	Aj	4/5 (80%)	0	0
2	Ak	4/5 (80%)	0	0
2	Al	4/5 (80%)	0	0
2	Am	4/5 (80%)	0	0
2	An	4/5 (80%)	0	0
2	Ao	4/5 (80%)	0	0
2	Ap	4/5 (80%)	0	0
2	Aq	4/5 (80%)	0	0
2	Ar	4/5 (80%)	0	0
2	As	4/5 (80%)	0	0
2	At	4/5 (80%)	0	0
2	Au	4/5 (80%)	0	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	Av	4/5 (80%)	0	0
2	Aw	4/5 (80%)	0	0
2	Ax	4/5 (80%)	0	0
2	Ay	4/5 (80%)	0	0
2	Az	4/5 (80%)	0	0
2	Ba	4/5 (80%)	0	0
2	Bb	4/5 (80%)	0	0
2	Bc	4/5 (80%)	0	0
2	Bd	4/5 (80%)	0	0
2	Be	4/5 (80%)	0	0
2	Bf	4/5 (80%)	0	0
2	Bg	4/5 (80%)	0	0
2	Bh	4/5 (80%)	0	0
2	Bi	4/5 (80%)	0	0
All	All	140/175 (80%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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.

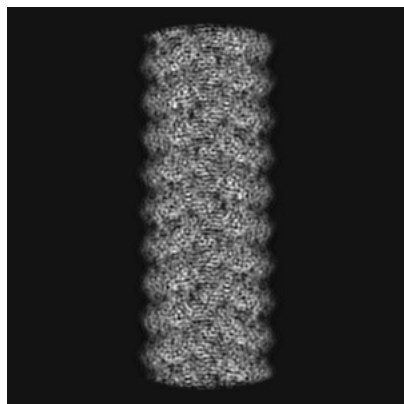
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0297. These allow visual inspection of the internal detail of the map and identification of artifacts.

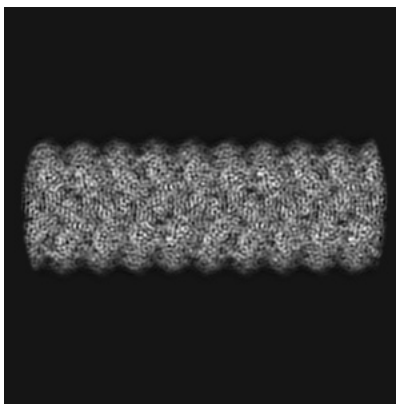
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

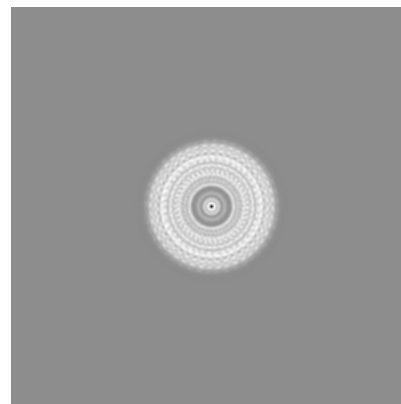
6.1.1 Primary map



X

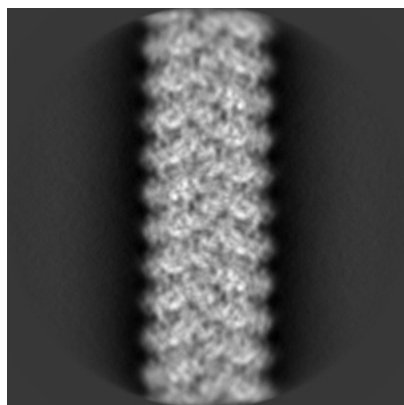


Y

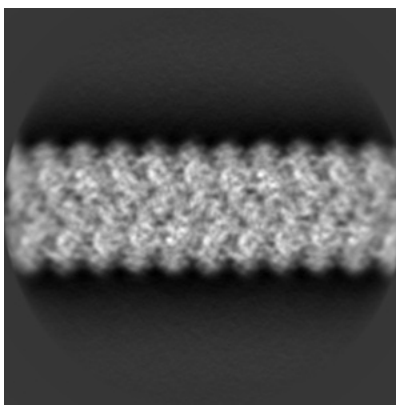


Z

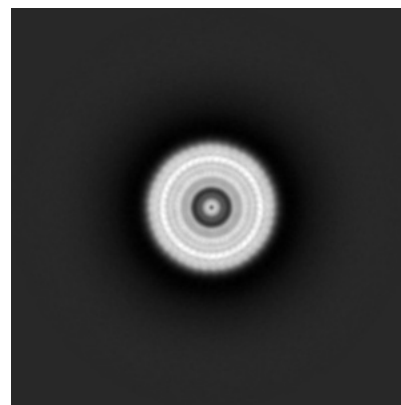
6.1.2 Raw map



X



Y

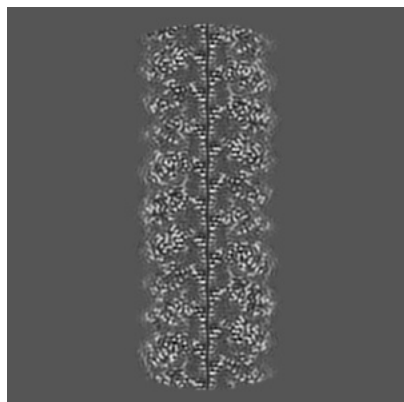


Z

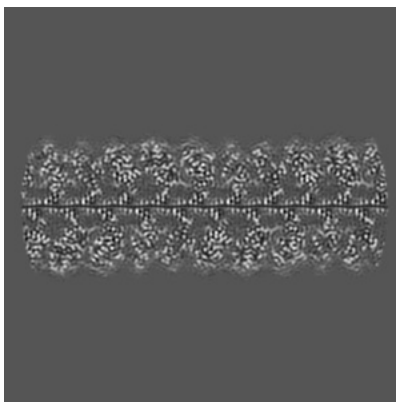
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

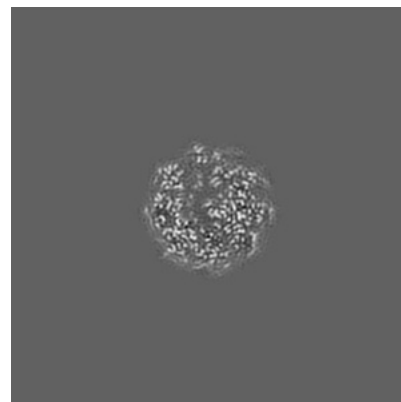
6.2.1 Primary map



X Index: 180

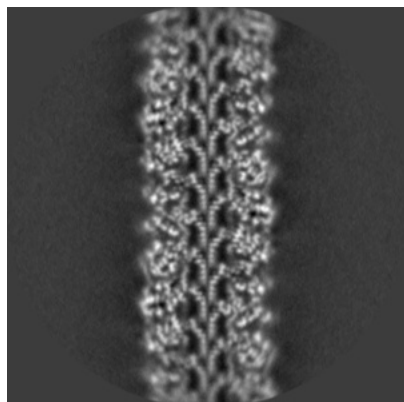


Y Index: 180

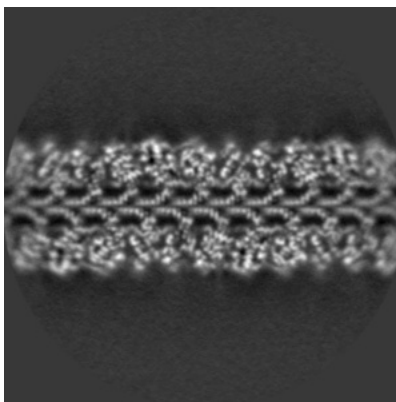


Z Index: 180

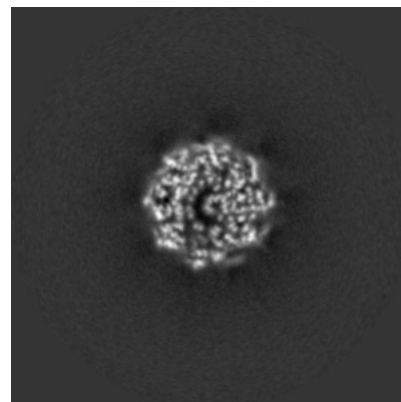
6.2.2 Raw map



X Index: 180



Y Index: 180

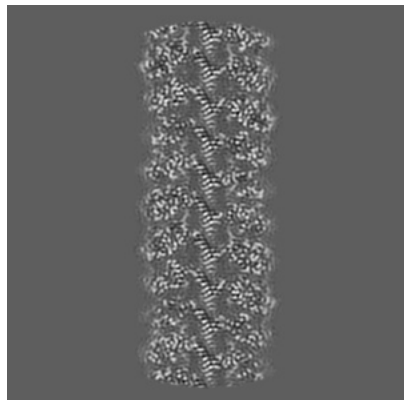


Z Index: 180

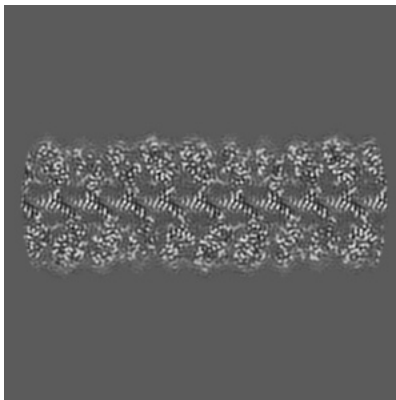
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

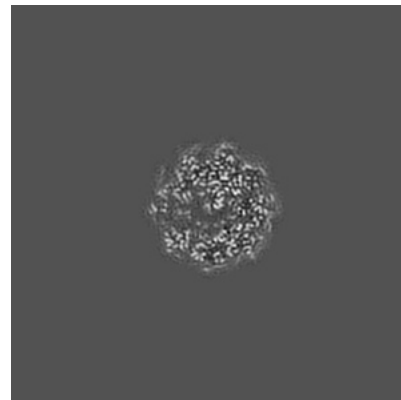
6.3.1 Primary map



X Index: 183

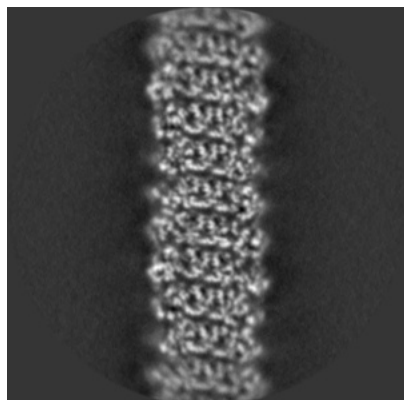


Y Index: 177

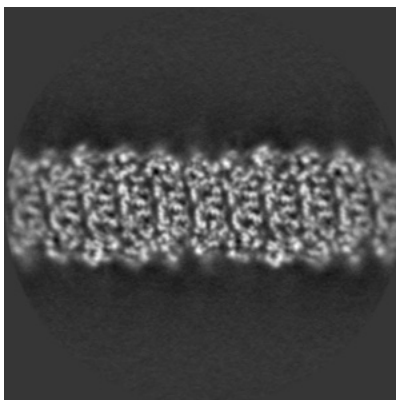


Z Index: 172

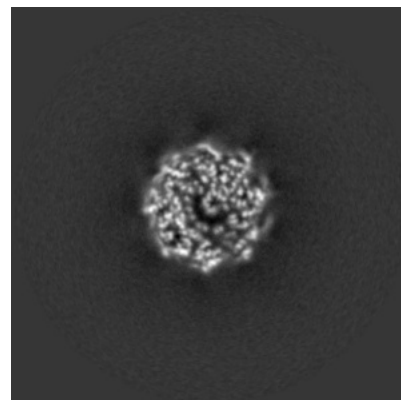
6.3.2 Raw map



X Index: 152



Y Index: 208

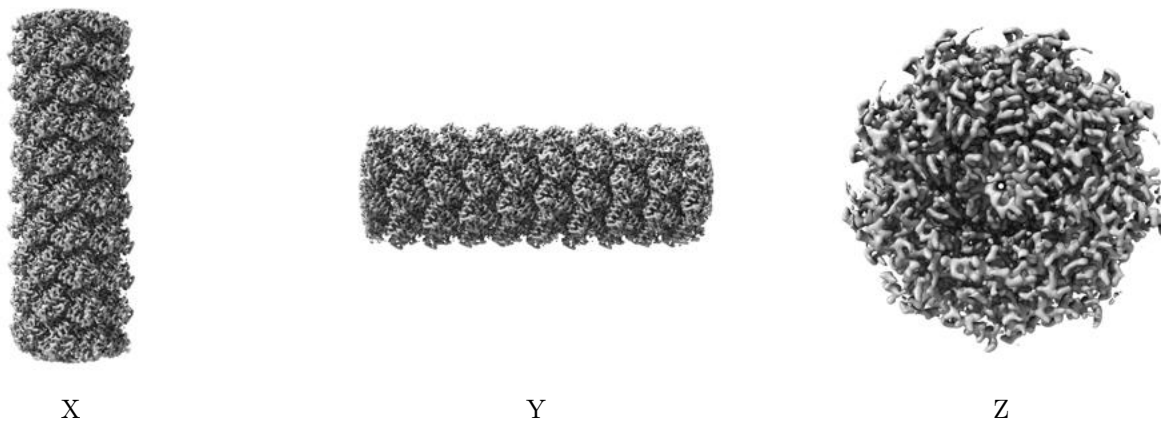


Z Index: 217

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

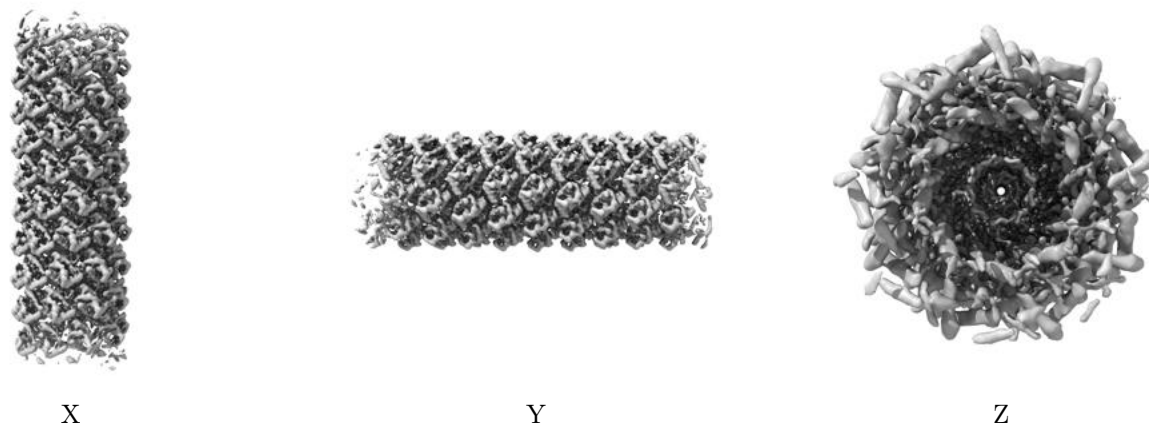
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.132. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

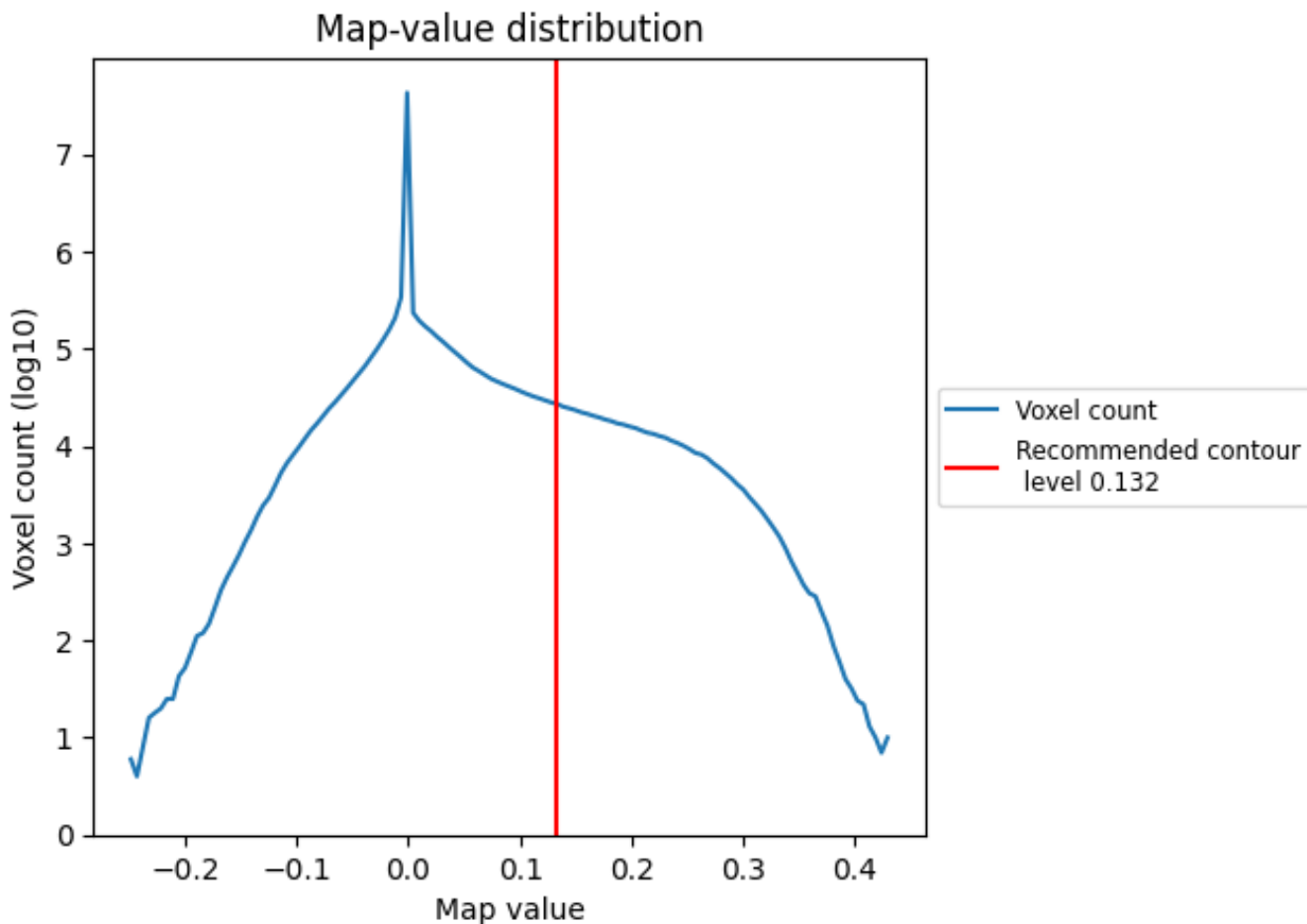
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

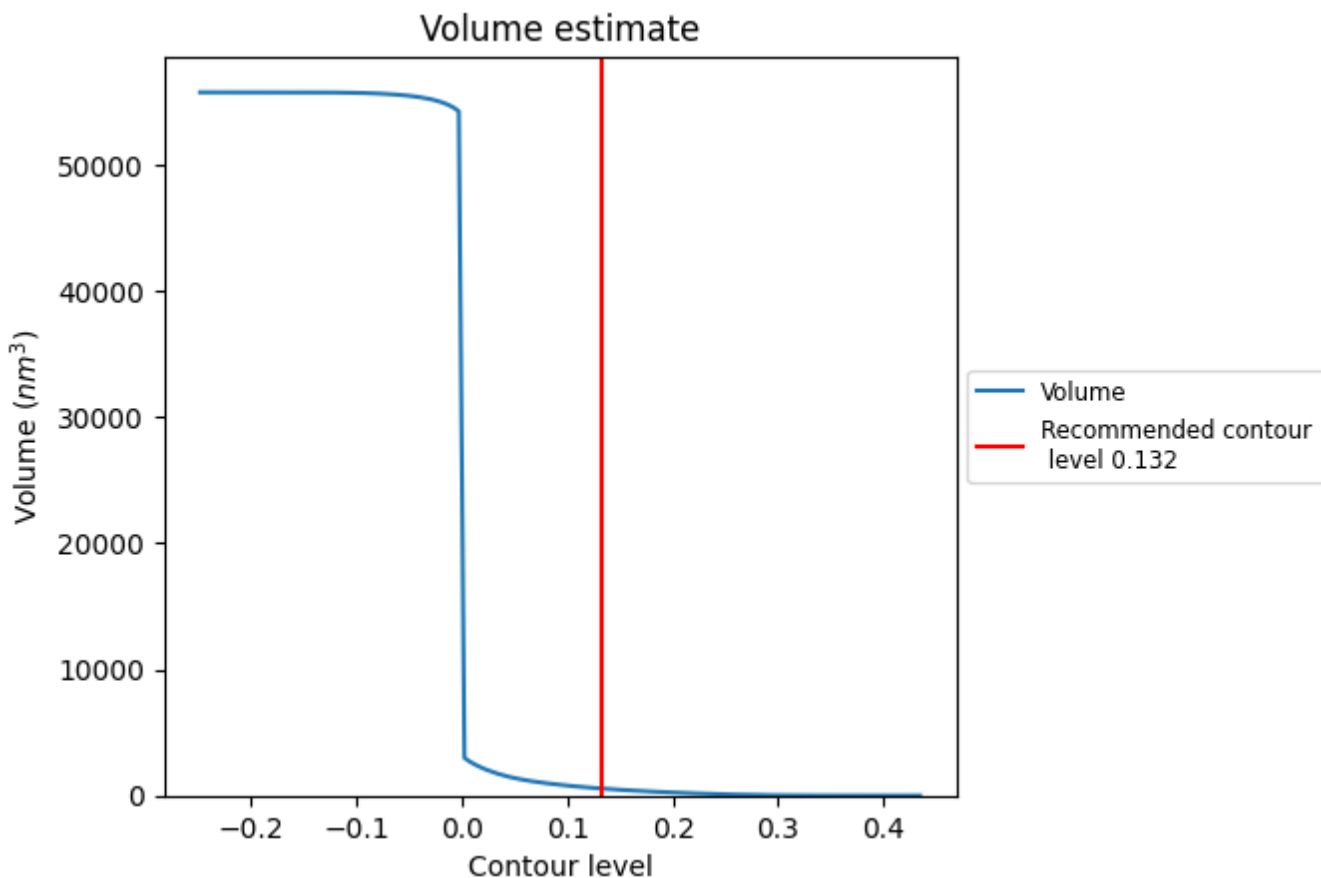
This section contains the results of statistical analysis of the map.

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.

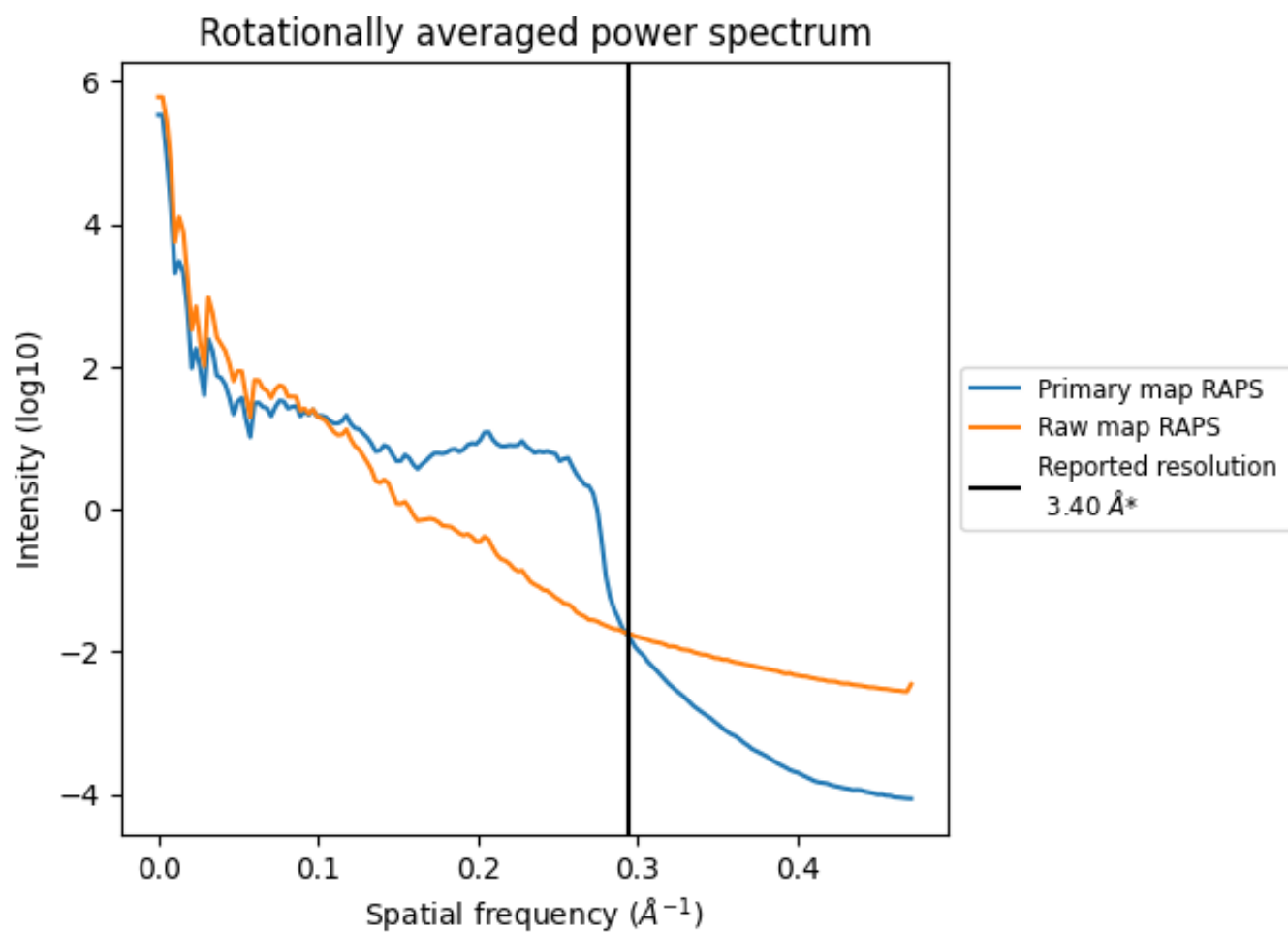
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 560 nm³; this corresponds to an approximate mass of 506 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](#)

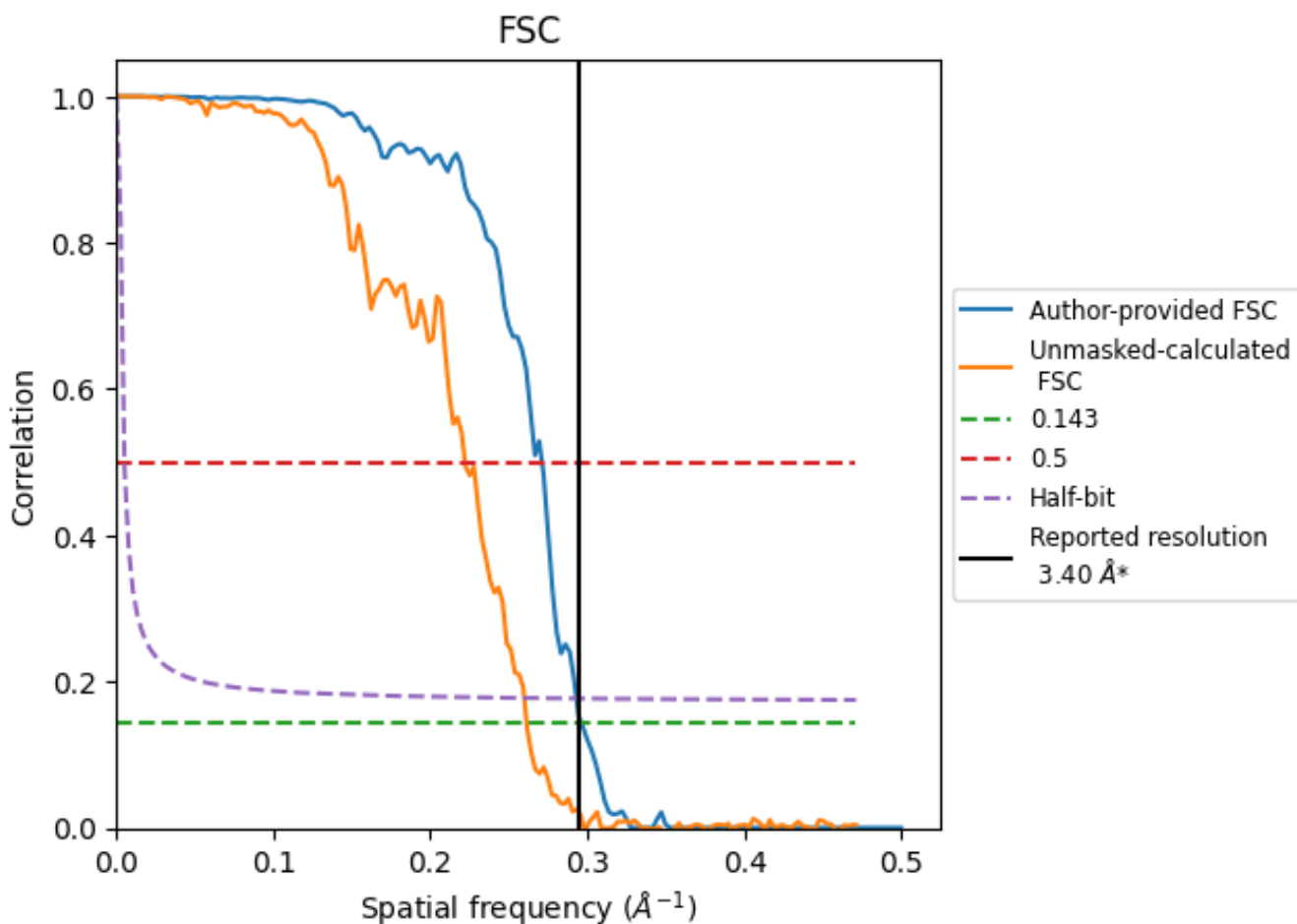


*Reported resolution corresponds to spatial frequency of 0.294 \AA^{-1}

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 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

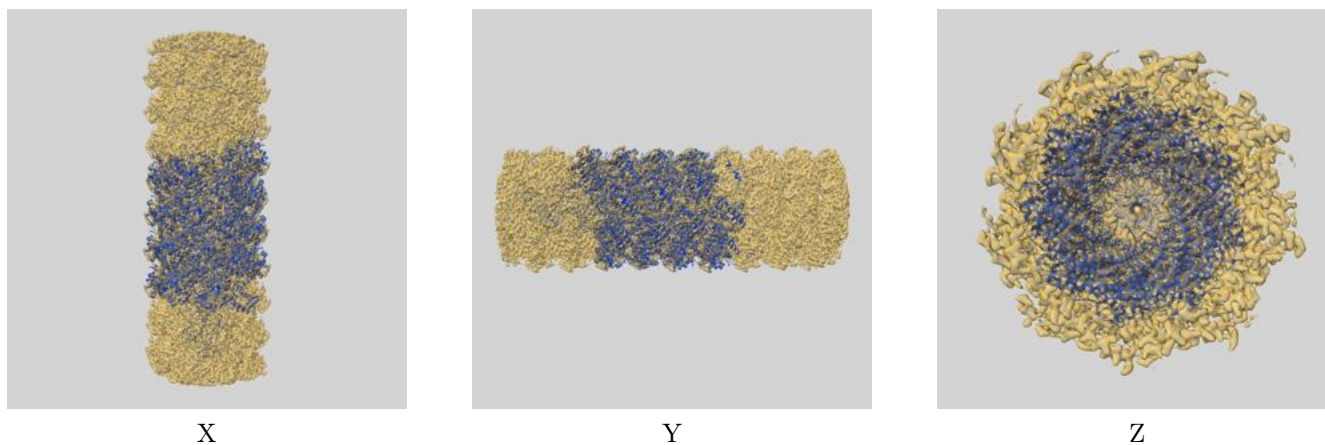
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.37	3.69	3.41
Unmasked-calculated*	3.83	4.50	3.85

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.83 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

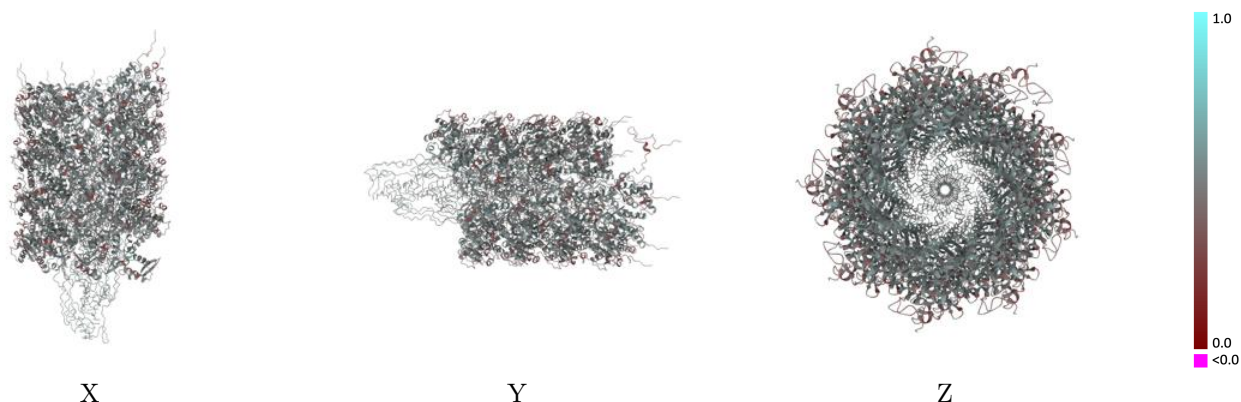
This section contains information regarding the fit between EMDB map EMD-0297 and PDB model 6HXX. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



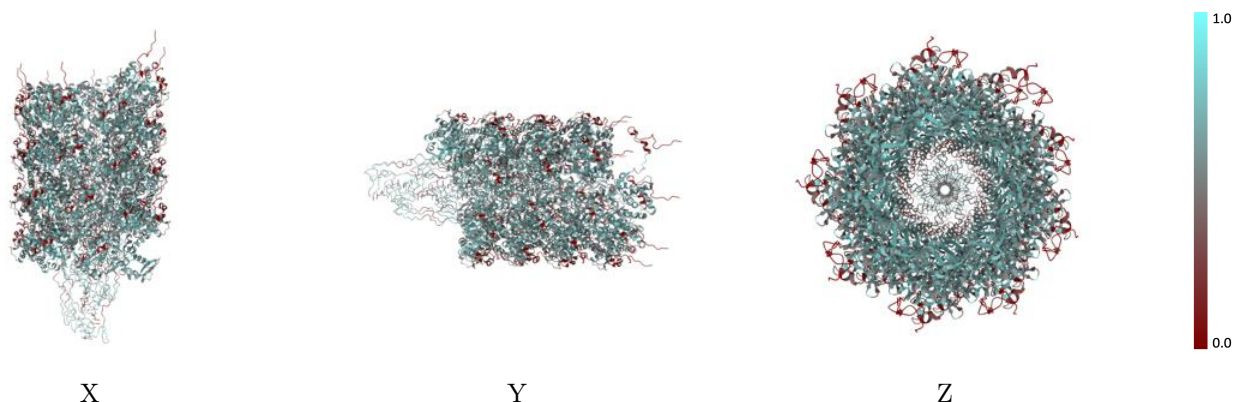
The images above show the 3D surface view of the map at the recommended contour level 0.132 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



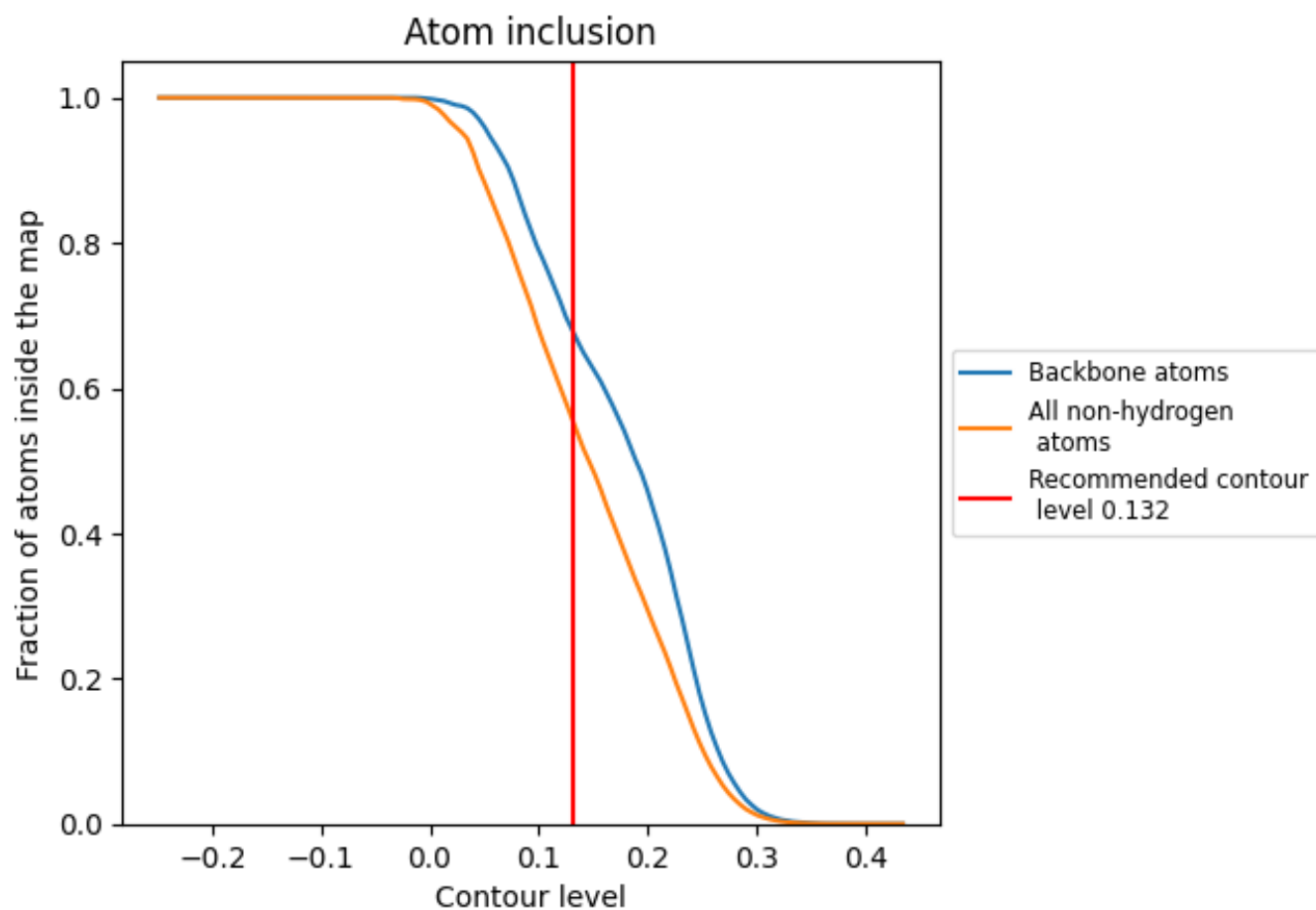
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.132).

9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 55% 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 (0.132) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5524	0.4820
AA	0.5394	0.4810
AB	0.5377	0.4810
AC	0.5365	0.4810
AD	0.5382	0.4810
AE	0.5348	0.4820
AF	0.5354	0.4790
AG	0.5400	0.4800
AH	0.5405	0.4780
AI	0.5388	0.4810
AJ	0.5365	0.4800
AK	0.5377	0.4810
AL	0.5359	0.4810
AM	0.5382	0.4810
AN	0.5359	0.4790
AO	0.5423	0.4800
AP	0.5377	0.4790
AQ	0.5342	0.4780
AR	0.5377	0.4800
AS	0.5377	0.4810
AT	0.5388	0.4810
AU	0.5377	0.4810
AV	0.5411	0.4800
AW	0.5394	0.4780
AX	0.5394	0.4780
AY	0.5400	0.4790
AZ	0.5365	0.4790
Aa	0.8100	0.5100
Ab	0.8000	0.5140
Ac	0.8100	0.5140
Ad	0.8100	0.5080
Ae	0.8100	0.5010
Af	0.8100	0.5060
Ag	0.8100	0.5130
Ah	0.8200	0.5080



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Chain	Atom inclusion	Q-score
Ai	 0.8000	 0.5130
Aj	 0.8100	 0.5150
Ak	 0.8100	 0.5120
Al	 0.8100	 0.5100
Am	 0.8000	 0.5010
An	 0.8100	 0.5050
Ao	 0.8000	 0.5090
Ap	 0.8000	 0.5050
Aq	 0.8100	 0.5120
Ar	 0.8100	 0.5180
As	 0.8200	 0.5150
At	 0.8100	 0.5160
Au	 0.8100	 0.5100
Av	 0.8100	 0.5050
Aw	 0.8100	 0.5010
Ax	 0.8000	 0.5050
Ay	 0.8300	 0.5130
Az	 0.8000	 0.5150
BA	 0.5377	 0.4800
BB	 0.5342	 0.4810
BC	 0.5365	 0.4810
BD	 0.5365	 0.4820
BE	 0.5388	 0.4810
BF	 0.5359	 0.4790
BG	 0.5371	 0.4770
BH	 0.5377	 0.4790
BI	 0.5354	 0.4800
Ba	 0.8200	 0.5130
Bb	 0.8100	 0.5170
Bc	 0.8100	 0.5120
Bd	 0.8100	 0.5060
Be	 0.8200	 0.5040
Bf	 0.8100	 0.5050
Bg	 0.8100	 0.5110
Bh	 0.8000	 0.5040
Bi	 0.8200	 0.5150