wwPDB EM Validation Summary Report (i)

Feb 26, 2024 – 04:22 AM EST

PDB ID	:	6WLS
EMDB ID	:	EMD-21840
Title	:	Tetrahymena ribozyme models, 6.8 Angstrom resolution
Authors	:	Kappel, K.; Zhang, K.; Su, Z.; Watkins, A.M.; Kladwang, W.; Li, S.; Pintilie, G.; Topkar, V.V.; Rangan, R.; Zheludev, I.N.; Yesselman, J.D.; Chiu, W.; Das, R.
Deposited on	:	2020-04-20
Resolution	:	6.80 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 (i)) were used in the production of this report:

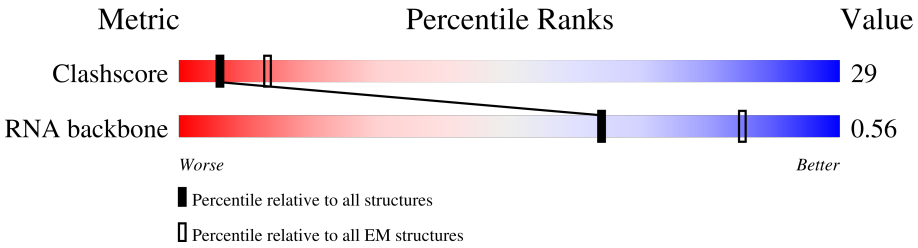
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 6.80 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
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 <=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	1-A	388	10% 40% 35% 24% ·
1	10-A	388	38% 39% 22% ·
1	11-A	388	36% 40% 23% ·
1	12-A	388	38% 38% 23% ·
1	13-A	388	36% 37% 25% ·
1	14-A	388	40% 36% 23% ·
1	15-A	388	37% 38% 23% ·
1	16-A	388	40% 38% 21% ·
1	17-A	388	37% 38% 24% ·

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Mol	Chain	Length	Quality of chain
1	18-A	388	37% 35% 27%
1	19-A	388	35% 38% 26%
1	2-A	388	39% 37% 22%
1	20-A	388	38% 37% 23%
1	3-A	388	39% 37% 23%
1	4-A	388	40% 37% 21%
1	5-A	388	38% 39% 21%
1	6-A	388	37% 38% 23%
1	7-A	388	36% 38% 24%
1	8-A	388	37% 38% 21%
1	9-A	388	37% 39% 22%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 249340 atoms, of which 83360 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 RNA chain called RNA (388-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
1	1-A	388	Total	C	H	N	O	P	0	0
			12467	3711	4168	1504	2697	387		
1	2-A	388	Total	C	H	N	O	P	0	0
			12467	3711	4168	1504	2697	387		
1	3-A	388	Total	C	H	N	O	P	0	0
			12467	3711	4168	1504	2697	387		
1	4-A	388	Total	C	H	N	O	P	0	0
			12467	3711	4168	1504	2697	387		
1	5-A	388	Total	C	H	N	O	P	0	0
			12467	3711	4168	1504	2697	387		
1	6-A	388	Total	C	H	N	O	P	0	0
			12467	3711	4168	1504	2697	387		
1	7-A	388	Total	C	H	N	O	P	0	0
			12467	3711	4168	1504	2697	387		
1	8-A	388	Total	C	H	N	O	P	0	0
			12467	3711	4168	1504	2697	387		
1	9-A	388	Total	C	H	N	O	P	0	0
			12467	3711	4168	1504	2697	387		
1	10-A	388	Total	C	H	N	O	P	0	0
			12467	3711	4168	1504	2697	387		
1	11-A	388	Total	C	H	N	O	P	0	0
			12467	3711	4168	1504	2697	387		
1	12-A	388	Total	C	H	N	O	P	0	0
			12467	3711	4168	1504	2697	387		
1	13-A	388	Total	C	H	N	O	P	0	0
			12467	3711	4168	1504	2697	387		
1	14-A	388	Total	C	H	N	O	P	0	0
			12467	3711	4168	1504	2697	387		
1	15-A	388	Total	C	H	N	O	P	0	0
			12467	3711	4168	1504	2697	387		
1	16-A	388	Total	C	H	N	O	P	0	0
			12467	3711	4168	1504	2697	387		
1	17-A	388	Total	C	H	N	O	P	0	0
			12467	3711	4168	1504	2697	387		

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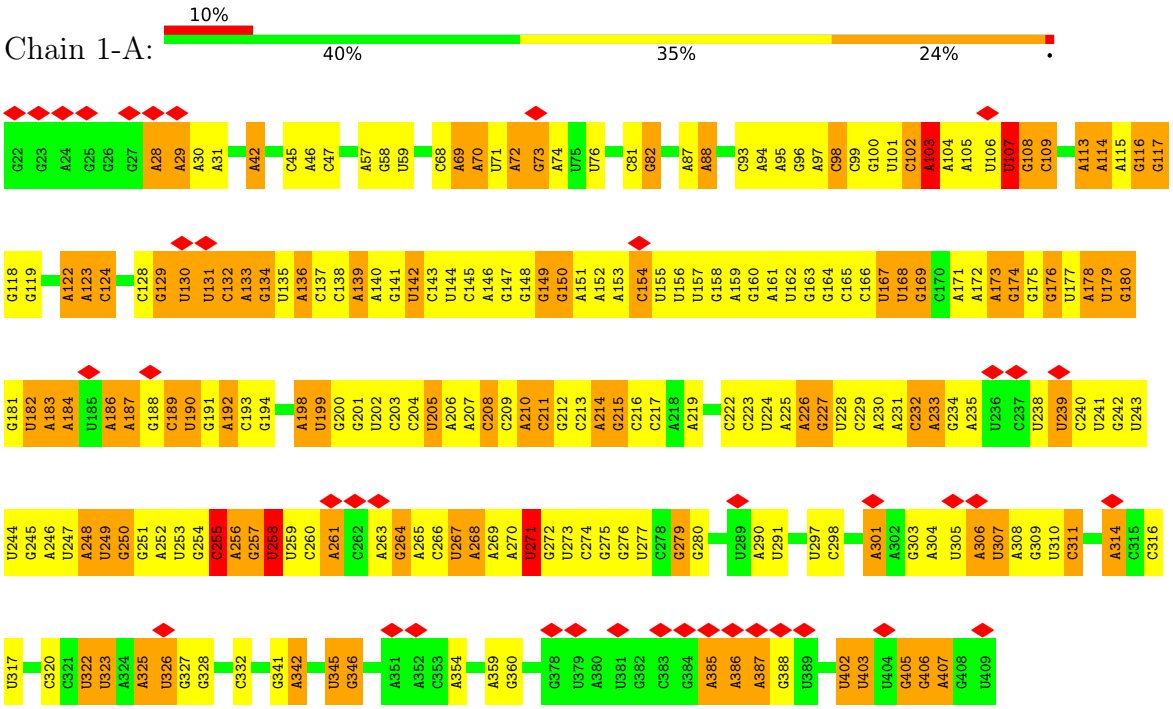
Mol	Chain	Residues	Atoms						AltConf	Trace
1	18-A	388	Total	C	H	N	O	P	0	0
			12467	3711	4168	1504	2697	387		
1	19-A	388	Total	C	H	N	O	P	0	0
			12467	3711	4168	1504	2697	387		
1	20-A	388	Total	C	H	N	O	P	0	0
			12467	3711	4168	1504	2697	387		

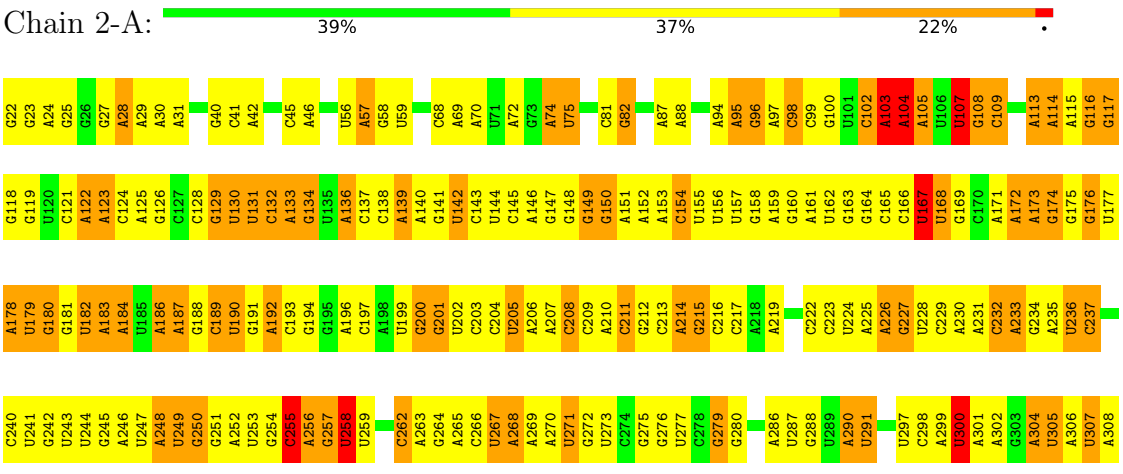
3 Residue-property plots (i)

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

• Molecule 1: RNA (388-MER)

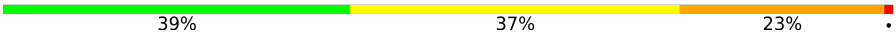


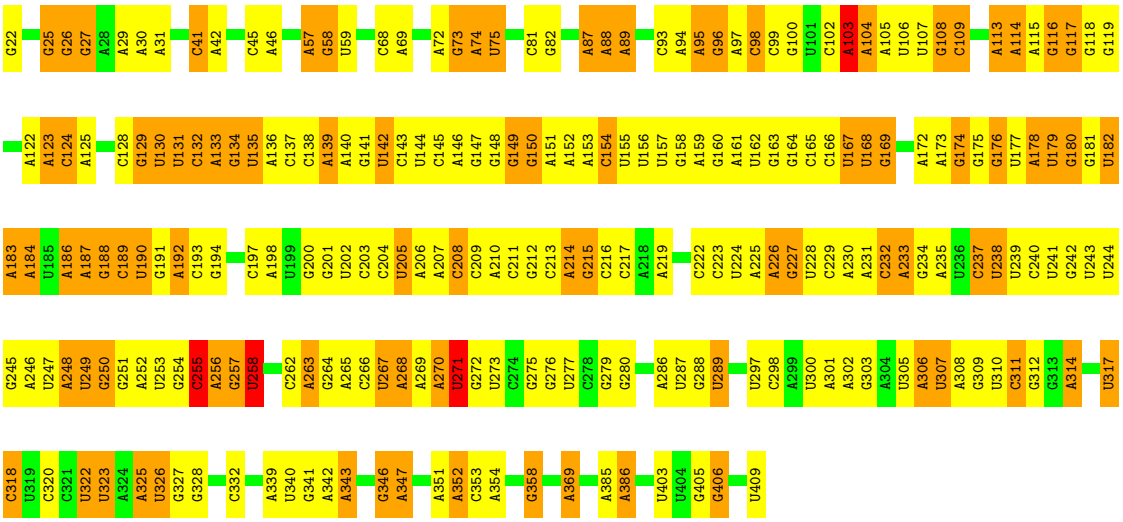
• Molecule 1: RNA (388-MER)



• Molecule 1: RNA (388-MER)

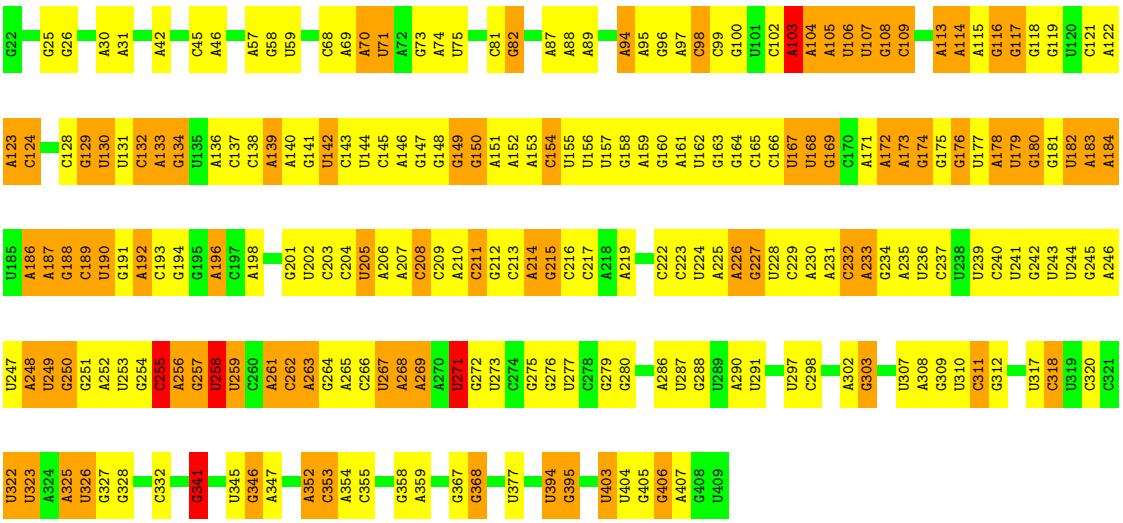
Chain 3-A:





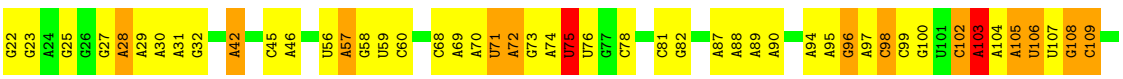
• Molecule 1: RNA (388-MER)

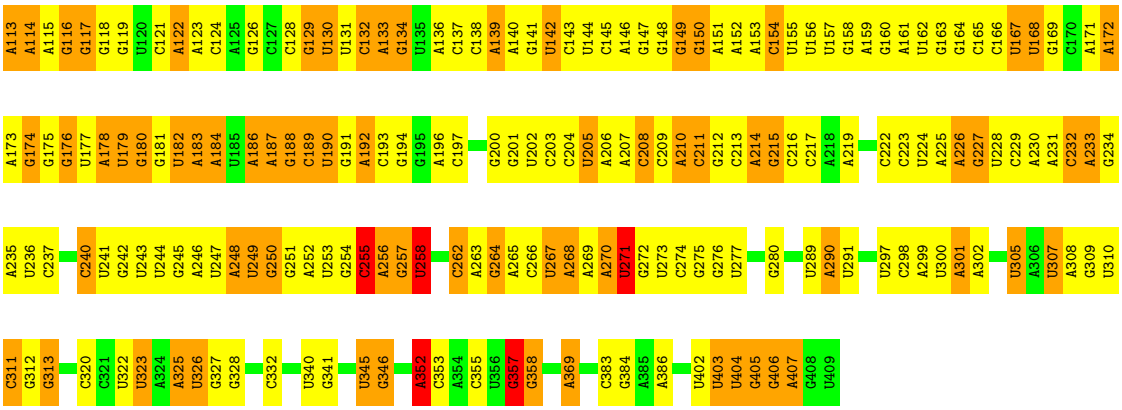
Chain 4-A:



• Molecule 1: RNA (388-MER)

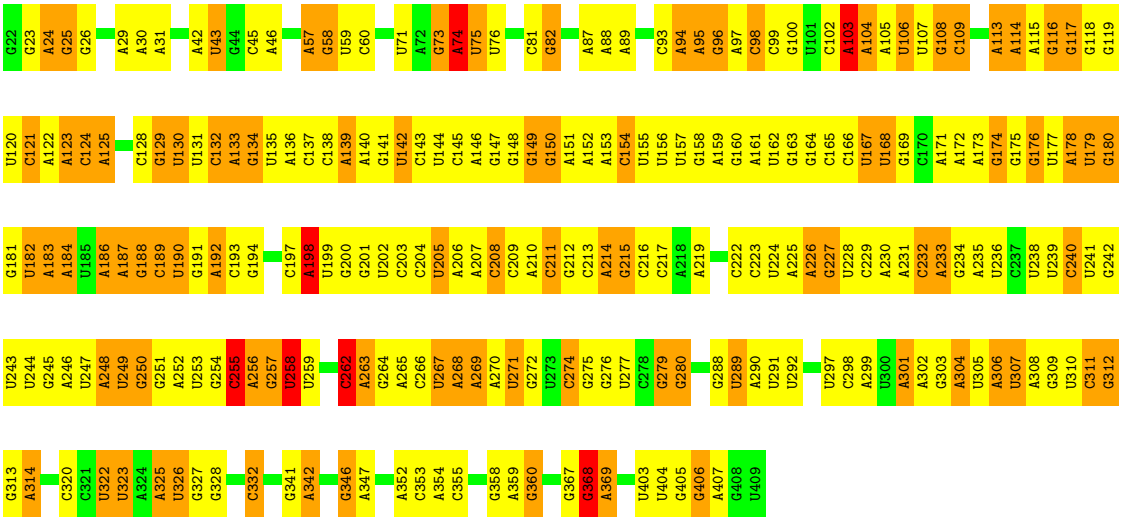
Chain 5-A:





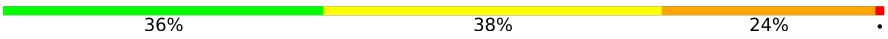
• Molecule 1: RNA (388-MER)

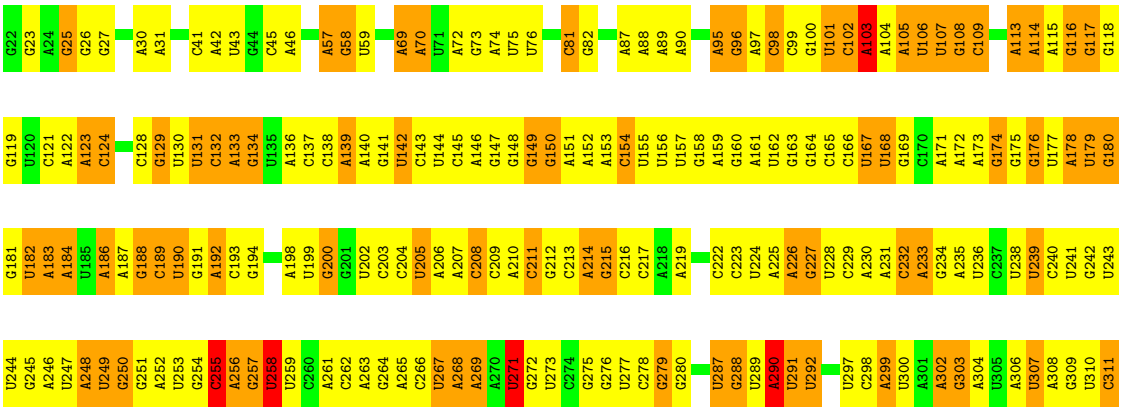
Chain 6-A:



• Molecule 1: RNA (388-MER)

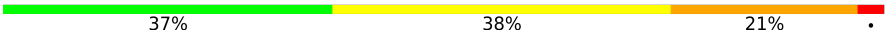
Chain 7-A:

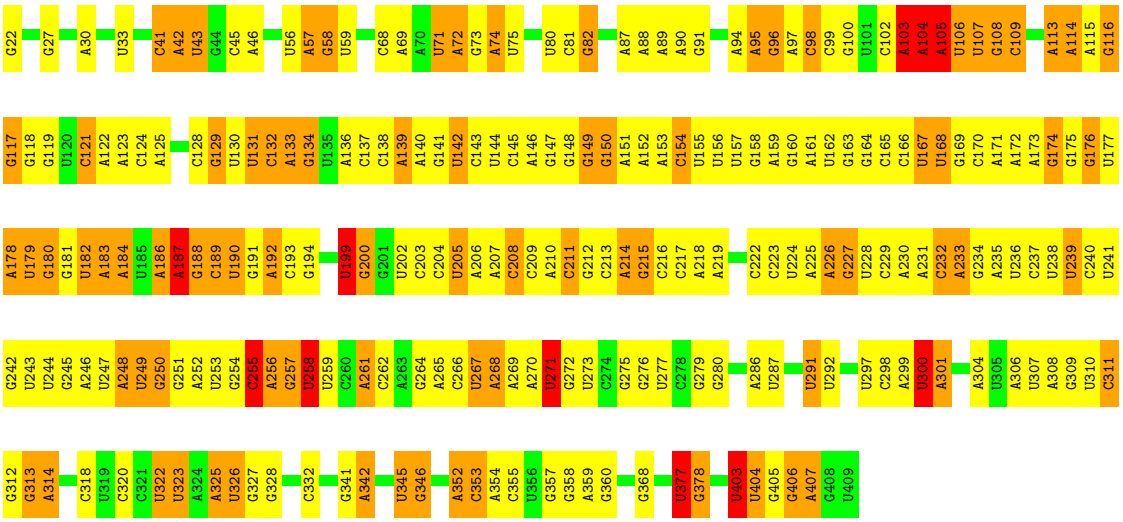




• Molecule 1: RNA (388-MER)

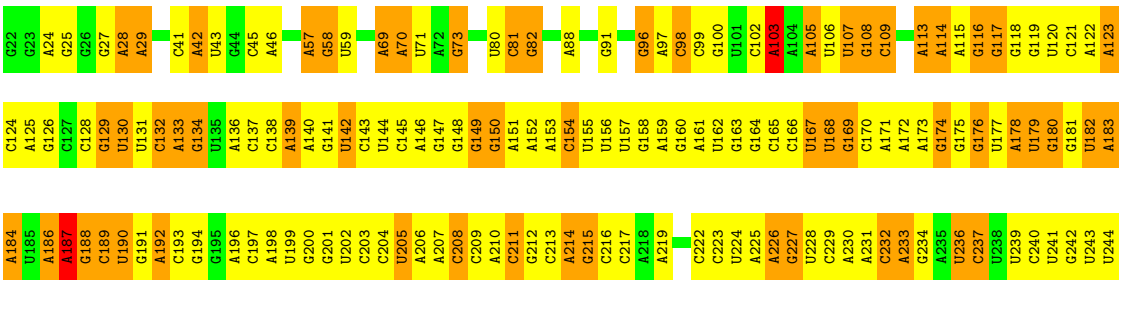
Chain 8-A:

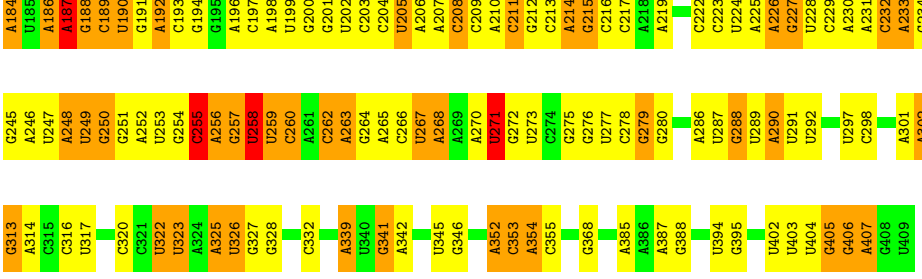




• Molecule 1: RNA (388-MER)

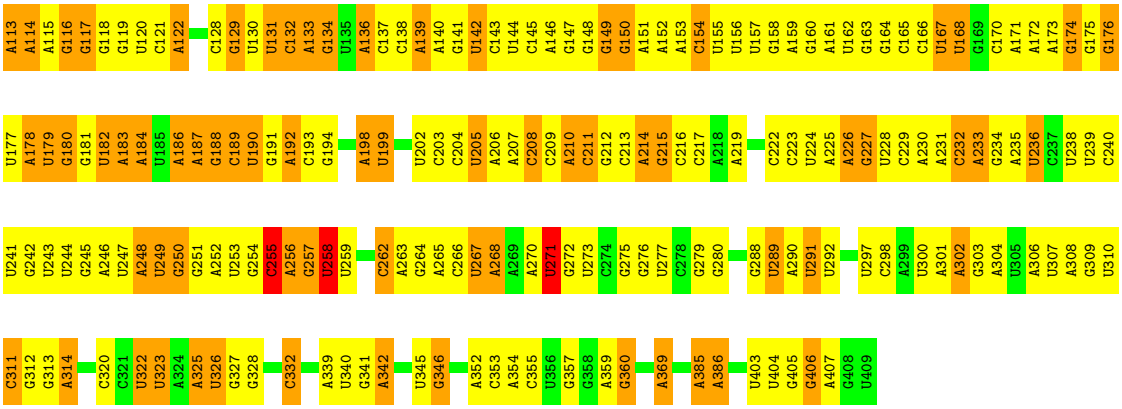
Chain 9-A:





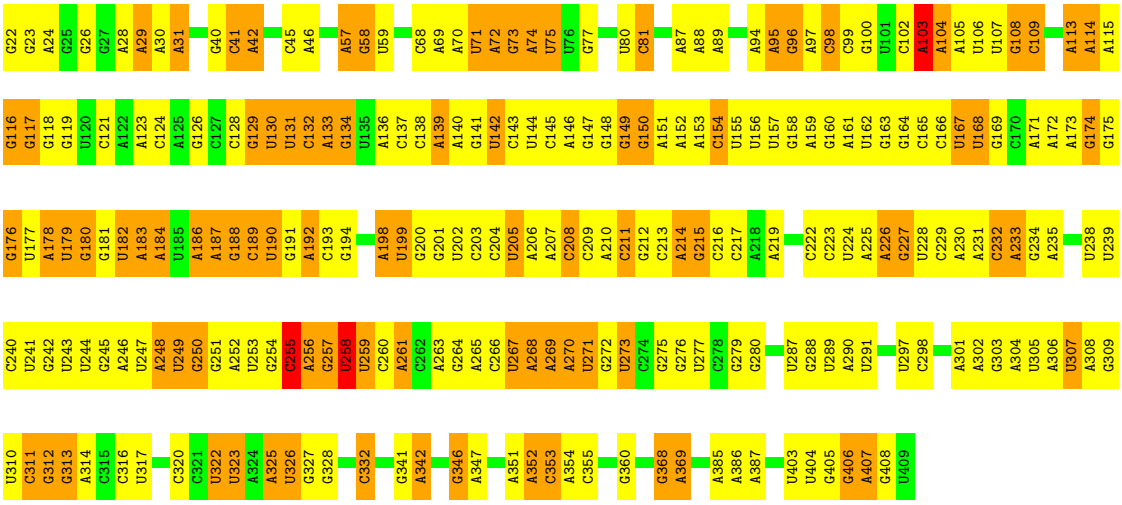
• Molecule 1: RNA (388-MER)

Chain 10-A:



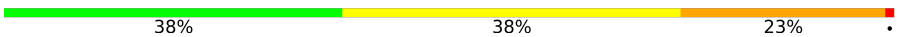
• Molecule 1: RNA (388-MER)

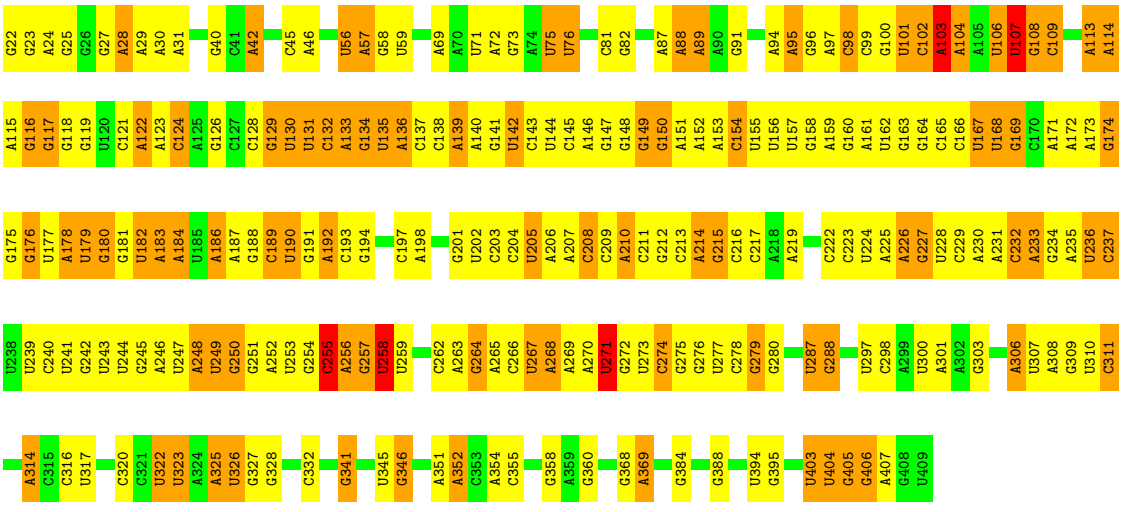
Chain 11-A:



• Molecule 1: RNA (388-MER)

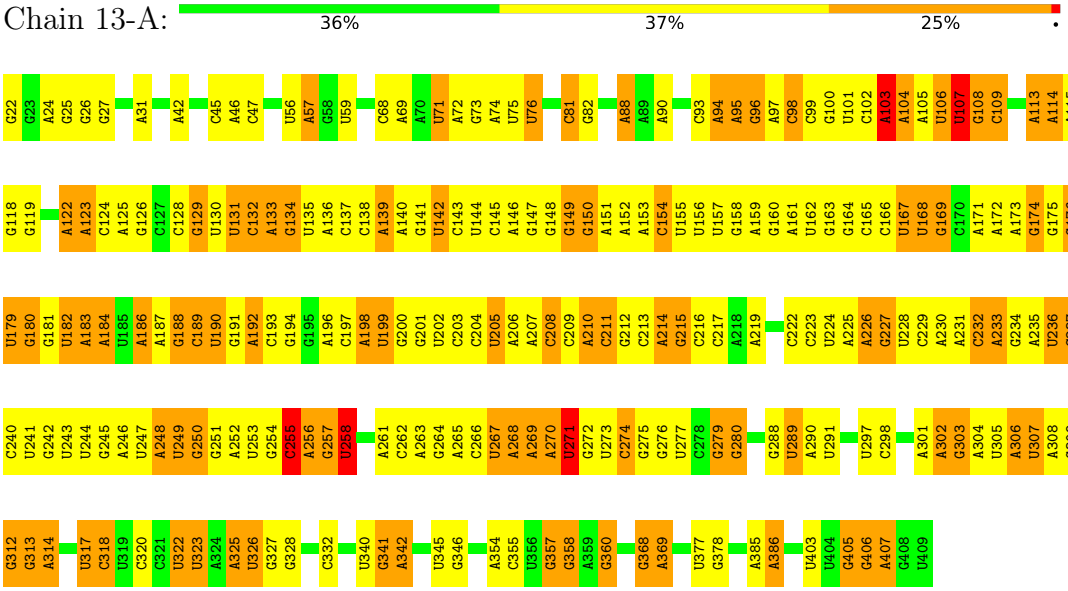
Chain 12-A:





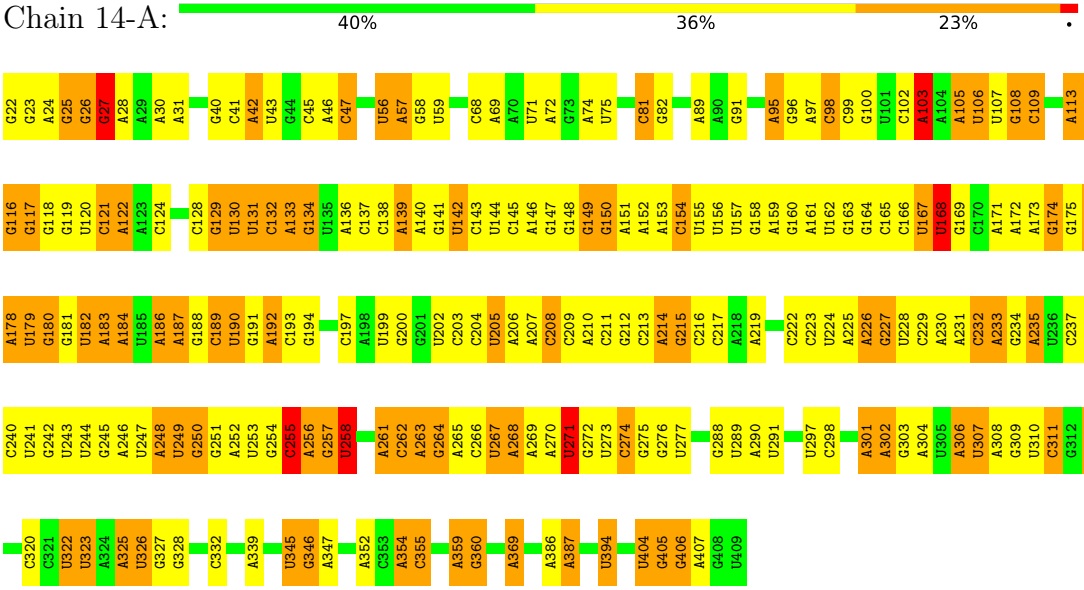
• Molecule 1: RNA (388-MER)

Chain 13-A:



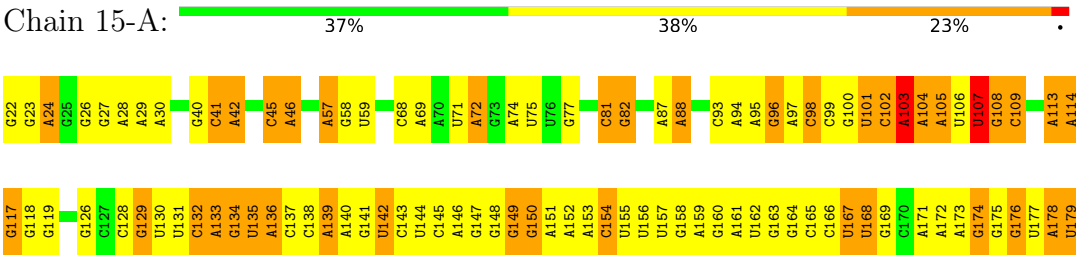
• Molecule 1: RNA (388-MER)

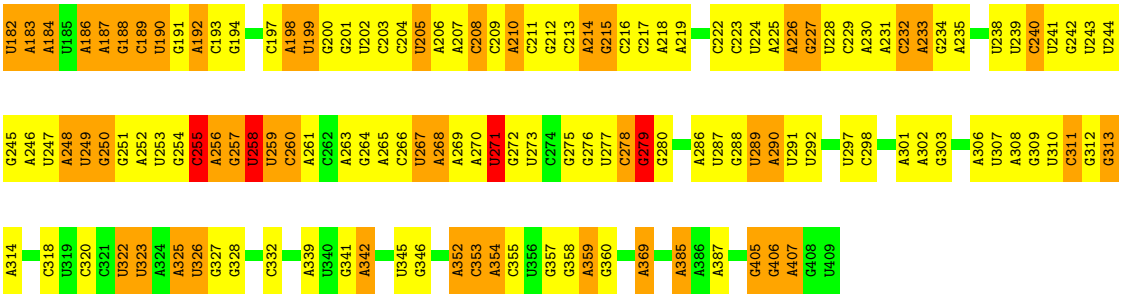
Chain 14-A:



• Molecule 1: RNA (388-MER)

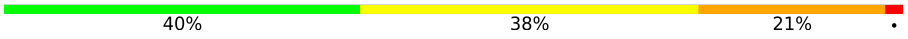
Chain 15-A:

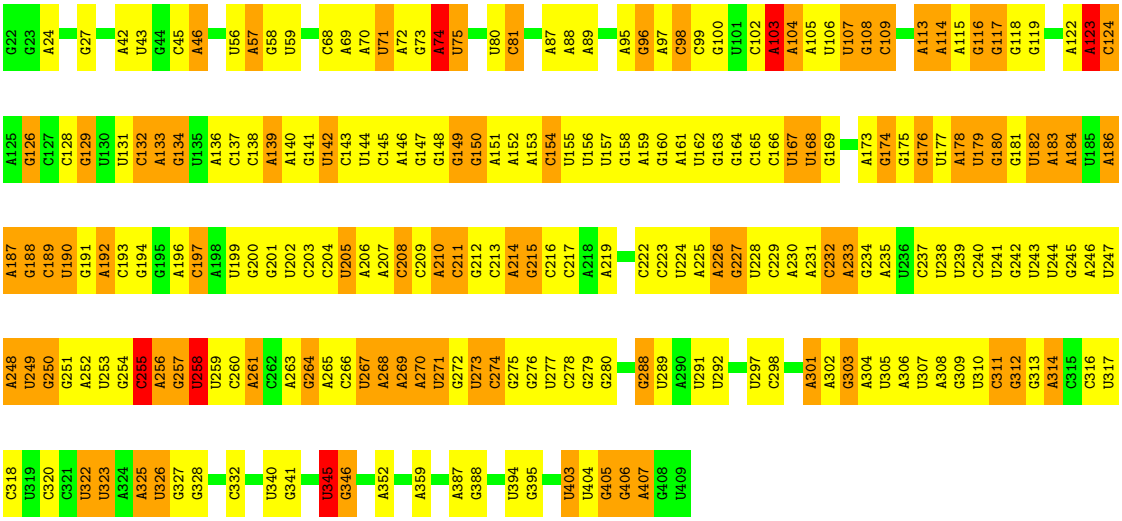




• Molecule 1: RNA (388-MER)

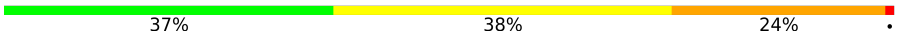
Chain 16-A:

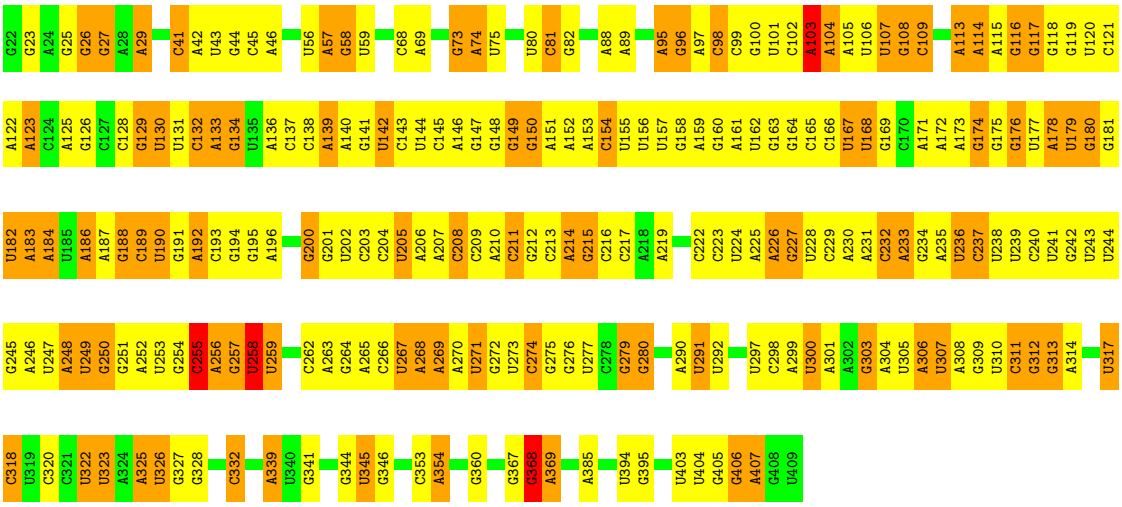




• Molecule 1: RNA (388-MER)

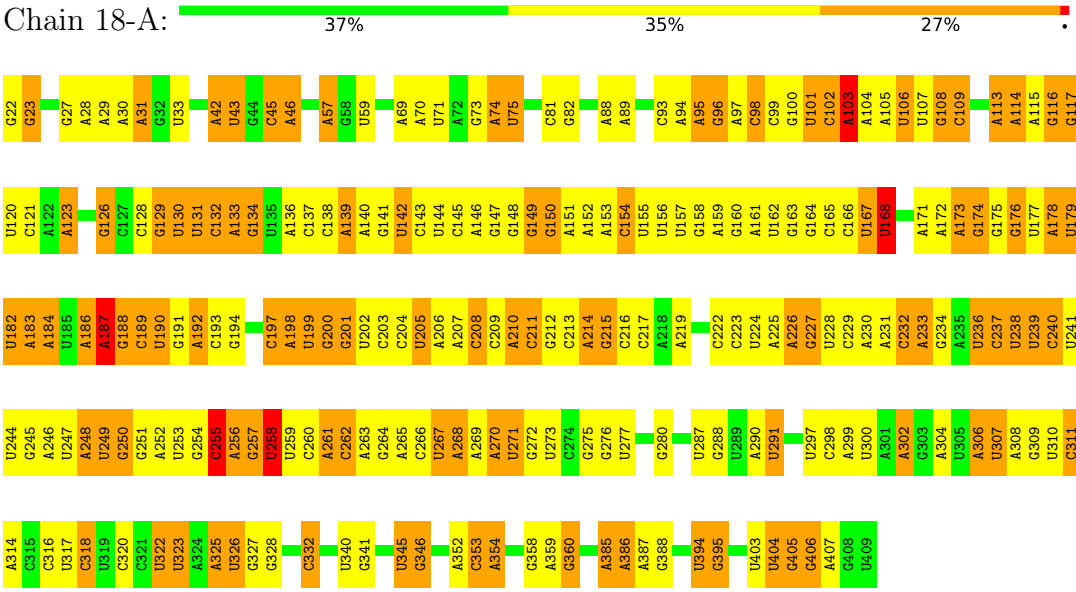
Chain 17-A:





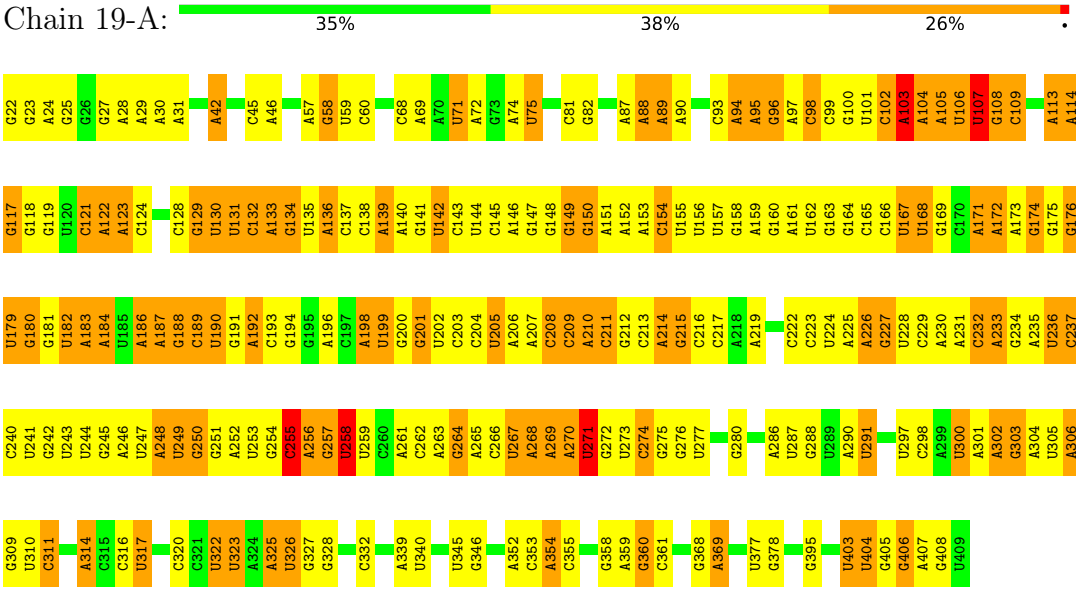
• Molecule 1: RNA (388-MER)

Chain 18-A:



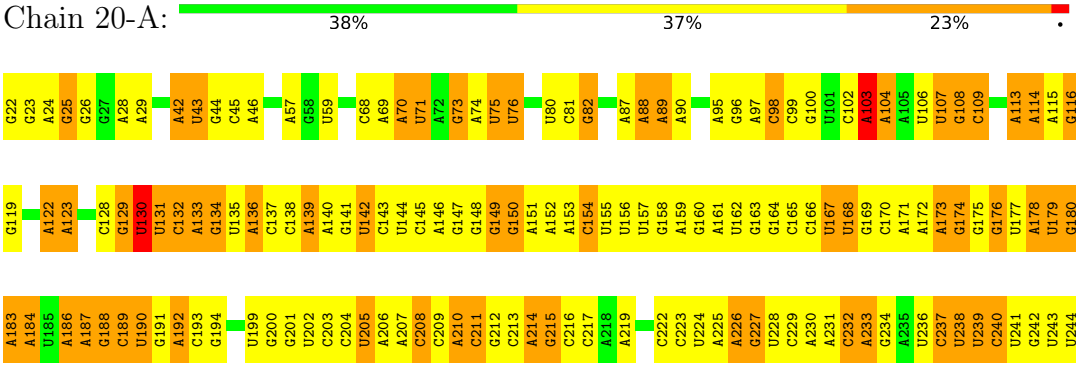
• Molecule 1: RNA (388-MER)

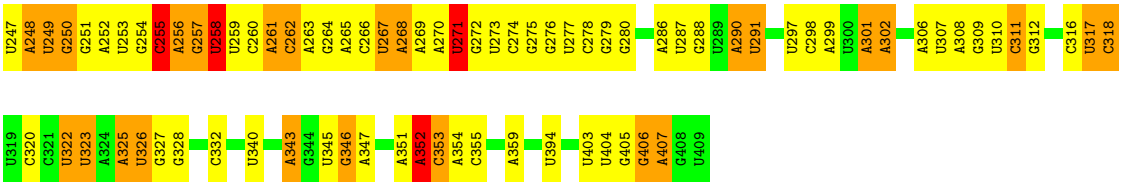
Chain 19-A:



• Molecule 1: RNA (388-MER)

Chain 20-A:




U247 A248 U249 G250 G251 A252 U253 G254 C255 A256 G257 U258 U259 C260 A261 C262 A263 G264 A265 C266 U267 A268 A269 A270 U271 G272 U273 C274 G275 G276 U277 C278 G279 G280 A286 U287 G288 U289 A290 U291 U297 C298 A299 U300 A301 A302 A306 U307 A308 G309 U310 C311 G312 C316 U317 C318
U319 C320 C321 U322 U323 A324 A325 U326 G327 G328 C332 U340 A343 G344 U345 G346 A347 A351 A352 C353 A354 C355 A359 U394 U403 U404 G405 G406 A407 G408 U409

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	74621	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	30	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	0.136	Depositor
Minimum map value	-0.063	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	205.44, 205.44, 205.44	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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	1-A	0.49	0/9293	0.86	7/14488 (0.0%)
1	2-A	0.50	1/9293 (0.0%)	0.87	9/14488 (0.1%)
1	3-A	0.49	0/9293	0.86	5/14488 (0.0%)
1	4-A	0.50	1/9293 (0.0%)	0.86	5/14488 (0.0%)
1	5-A	0.50	1/9293 (0.0%)	0.87	6/14488 (0.0%)
1	6-A	0.50	1/9293 (0.0%)	0.87	10/14488 (0.1%)
1	7-A	0.50	0/9293	0.87	8/14488 (0.1%)
1	8-A	0.50	1/9293 (0.0%)	0.88	13/14488 (0.1%)
1	9-A	0.50	0/9293	0.86	6/14488 (0.0%)
1	10-A	0.50	1/9293 (0.0%)	0.86	6/14488 (0.0%)
1	11-A	0.50	0/9293	0.86	5/14488 (0.0%)
1	12-A	0.50	0/9293	0.87	7/14488 (0.0%)
1	13-A	0.50	0/9293	0.87	7/14488 (0.0%)
1	14-A	0.49	1/9293 (0.0%)	0.87	8/14488 (0.1%)
1	15-A	0.49	1/9293 (0.0%)	0.86	7/14488 (0.0%)
1	16-A	0.50	2/9293 (0.0%)	0.87	11/14488 (0.1%)
1	17-A	0.49	1/9293 (0.0%)	0.86	6/14488 (0.0%)
1	18-A	0.50	1/9293 (0.0%)	0.87	7/14488 (0.0%)
1	19-A	0.49	0/9293	0.86	5/14488 (0.0%)
1	20-A	0.50	0/9293	0.88	8/14488 (0.1%)
All	All	0.50	12/185860 (0.0%)	0.87	146/289760 (0.1%)

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	1-A	0	4
1	2-A	0	4
1	3-A	0	4
1	4-A	0	4
1	5-A	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	6-A	0	4
1	7-A	0	4
1	8-A	0	4
1	9-A	0	4
1	10-A	0	4
1	11-A	0	4
1	12-A	0	4
1	13-A	0	4
1	14-A	0	4
1	15-A	0	4
1	16-A	0	4
1	17-A	0	4
1	18-A	0	4
1	19-A	0	4
1	20-A	0	4
All	All	0	80

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	10-A	56	U	O3'-P	8.03	1.70	1.61
1	6-A	368	G	O3'-P	-7.33	1.52	1.61
1	17-A	368	G	O3'-P	-6.75	1.53	1.61
1	16-A	273	U	C2'-C1'	-6.45	1.46	1.53
1	15-A	278	C	O3'-P	6.32	1.68	1.61

The worst 5 of 146 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	20-A	130	U	P-O3'-C3'	16.57	139.59	119.70
1	7-A	290	A	C2'-C3'-O3'	12.14	136.20	109.50
1	6-A	198	A	C2'-C3'-O3'	12.12	136.15	109.50
1	16-A	74	A	P-O3'-C3'	10.94	132.82	119.70
1	20-A	73	G	C5'-C4'-O4'	-8.56	98.82	109.10

There are no chirality outliers.

5 of 80 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-A	107	U	Sidechain
1	1-A	142	U	Sidechain

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Mol	Chain	Res	Type	Group
1	1-A	255	C	Sidechain
1	1-A	258	U	Sidechain
1	2-A	107	U	Sidechain

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	1-A	8299	4168	4169	343	0
1	2-A	8299	4168	4169	343	0
1	3-A	8299	4168	4169	384	0
1	4-A	8299	4168	4169	324	0
1	5-A	8299	4168	4169	369	0
1	6-A	8299	4168	4169	366	0
1	7-A	8299	4168	4169	347	0
1	8-A	8299	4168	4169	363	0
1	9-A	8299	4168	4169	355	0
1	10-A	8299	4168	4169	353	0
1	11-A	8299	4168	4169	347	0
1	12-A	8299	4168	4169	382	0
1	13-A	8299	4168	4169	385	0
1	14-A	8299	4168	4169	360	0
1	15-A	8299	4168	4169	379	0
1	16-A	8299	4168	4169	340	0
1	17-A	8299	4168	4169	361	0
1	18-A	8299	4168	4169	373	0
1	19-A	8299	4168	4169	380	0
1	20-A	8299	4168	4169	344	0
All	All	165980	83360	83380	7198	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 29.

The worst 5 of 7198 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:G:C8	1:A:405:G:OP1	1.63	1.49
1:A:88:A:OP1	1:A:88:A:C8	1.66	1.48
1:A:314:A:C8	1:A:314:A:OP2	1.78	1.36
1:A:235:A:C8	1:A:235:A:OP2	1.82	1.32
1:A:314:A:OP2	1:A:314:A:H8	1.08	1.29

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein molecules in this entry.

5.3.2 Protein sidechains (i)

There are no protein molecules in this entry.

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1-A	387/388 (99%)	94 (24%)	23 (5%)
1	10-A	387/388 (99%)	94 (24%)	20 (5%)
1	11-A	387/388 (99%)	97 (25%)	20 (5%)
1	12-A	387/388 (99%)	97 (25%)	23 (5%)
1	13-A	387/388 (99%)	102 (26%)	27 (6%)
1	14-A	387/388 (99%)	101 (26%)	23 (5%)
1	15-A	387/388 (99%)	94 (24%)	22 (5%)
1	16-A	387/388 (99%)	90 (23%)	22 (5%)
1	17-A	387/388 (99%)	96 (24%)	24 (6%)
1	18-A	387/388 (99%)	96 (24%)	30 (7%)
1	19-A	387/388 (99%)	100 (25%)	29 (7%)
1	2-A	387/388 (99%)	96 (24%)	22 (5%)
1	20-A	387/388 (99%)	102 (26%)	23 (5%)
1	3-A	387/388 (99%)	96 (24%)	28 (7%)
1	4-A	387/388 (99%)	95 (24%)	20 (5%)
1	5-A	387/388 (99%)	92 (23%)	20 (5%)
1	6-A	387/388 (99%)	93 (24%)	26 (6%)
1	7-A	387/388 (99%)	105 (27%)	21 (5%)
1	8-A	387/388 (99%)	97 (25%)	24 (6%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	9-A	387/388 (99%)	91 (23%)	21 (5%)
All	All	7740/7760 (99%)	1928 (24%)	468 (6%)

5 of 1928 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1-A	28	A
1	1-A	29	A
1	1-A	31	A
1	1-A	42	A
1	1-A	57	A

5 of 468 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	11-A	178	A
1	19-A	353	C
1	13-A	267	U
1	19-A	267	U
1	18-A	199	U

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

This section contains visualisations of the EMDB entry EMD-21840. 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

6.1.1 Primary map

X

Y

Z

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

6.2 Central slices

6.2.1 Primary map

X Index: 96

Y Index: 96

Z Index: 96

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: 101

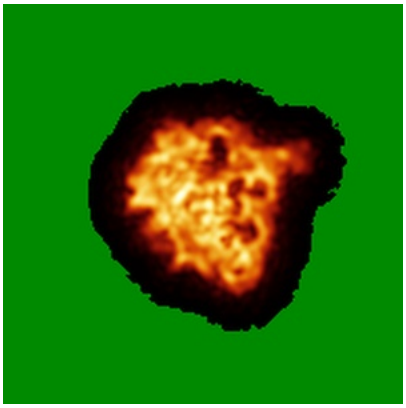
Y Index: 85

Z Index: 96

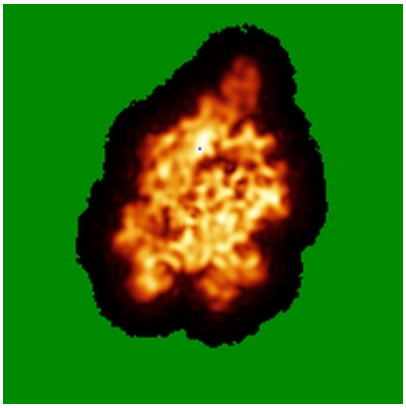
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



X



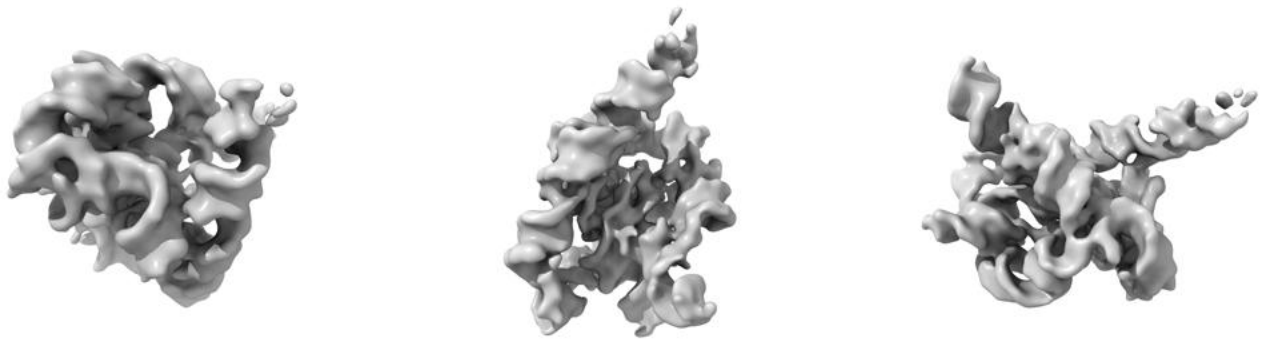
Y

Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

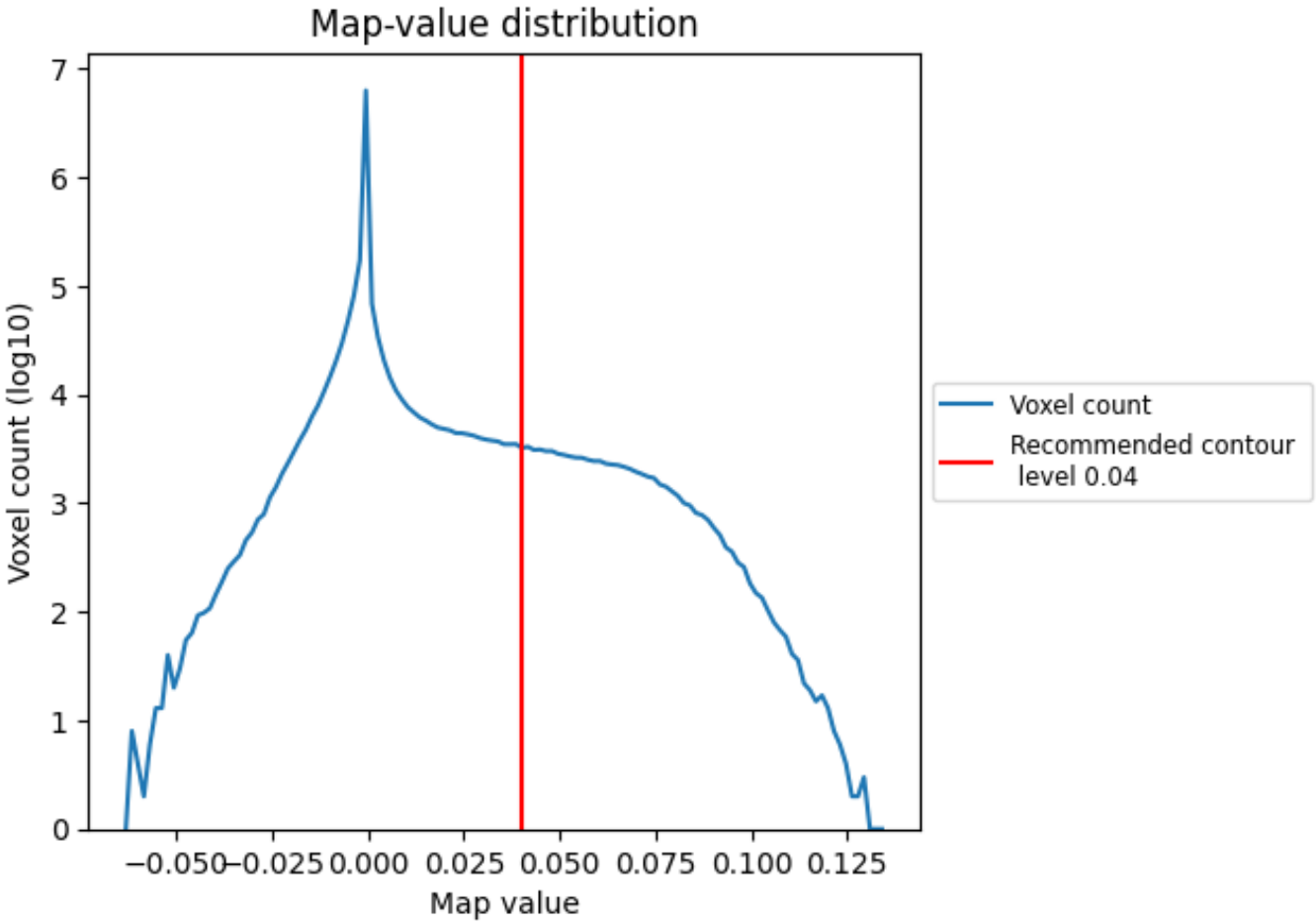
6.6 Mask visualisation (i)

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

7 Map analysis

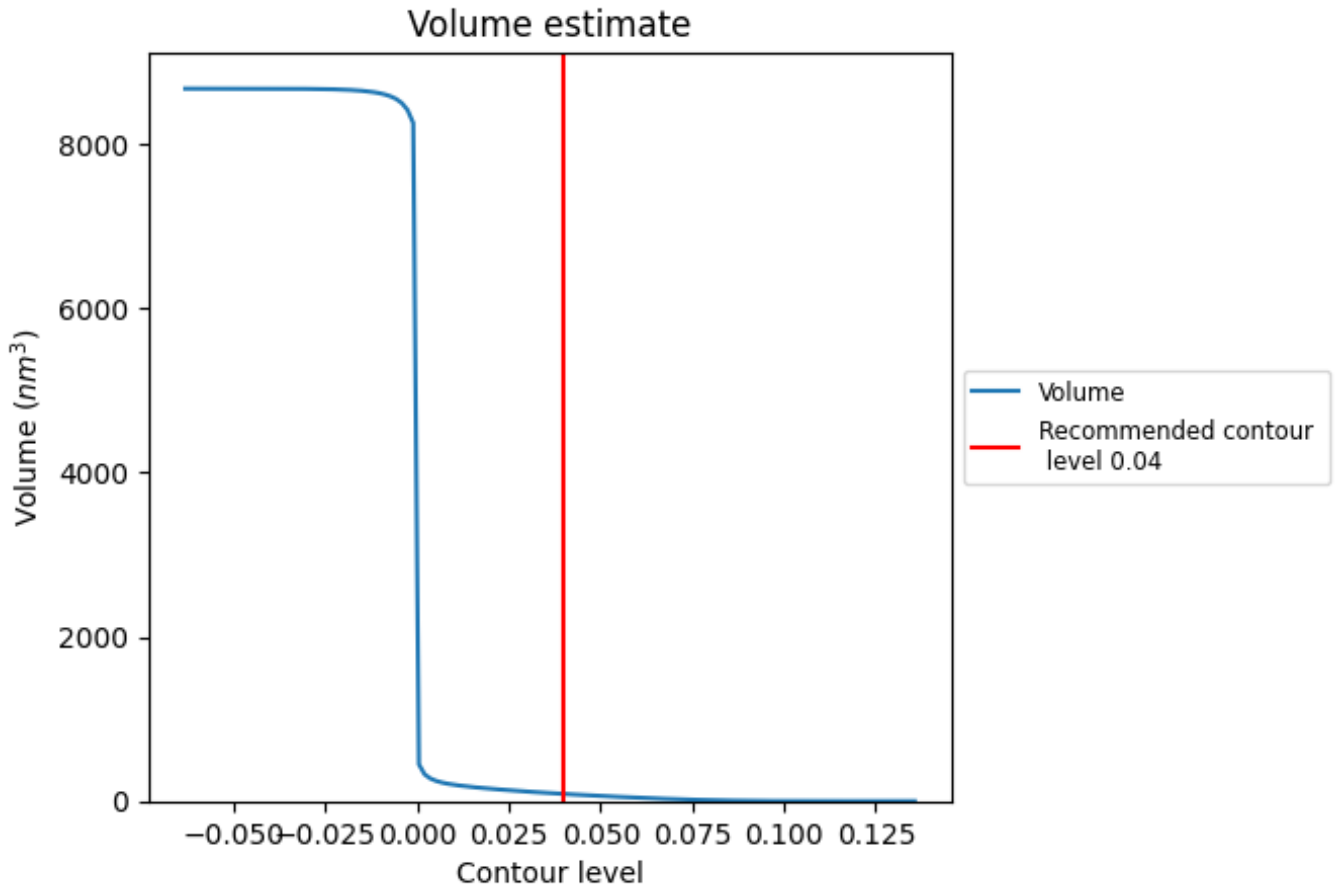
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

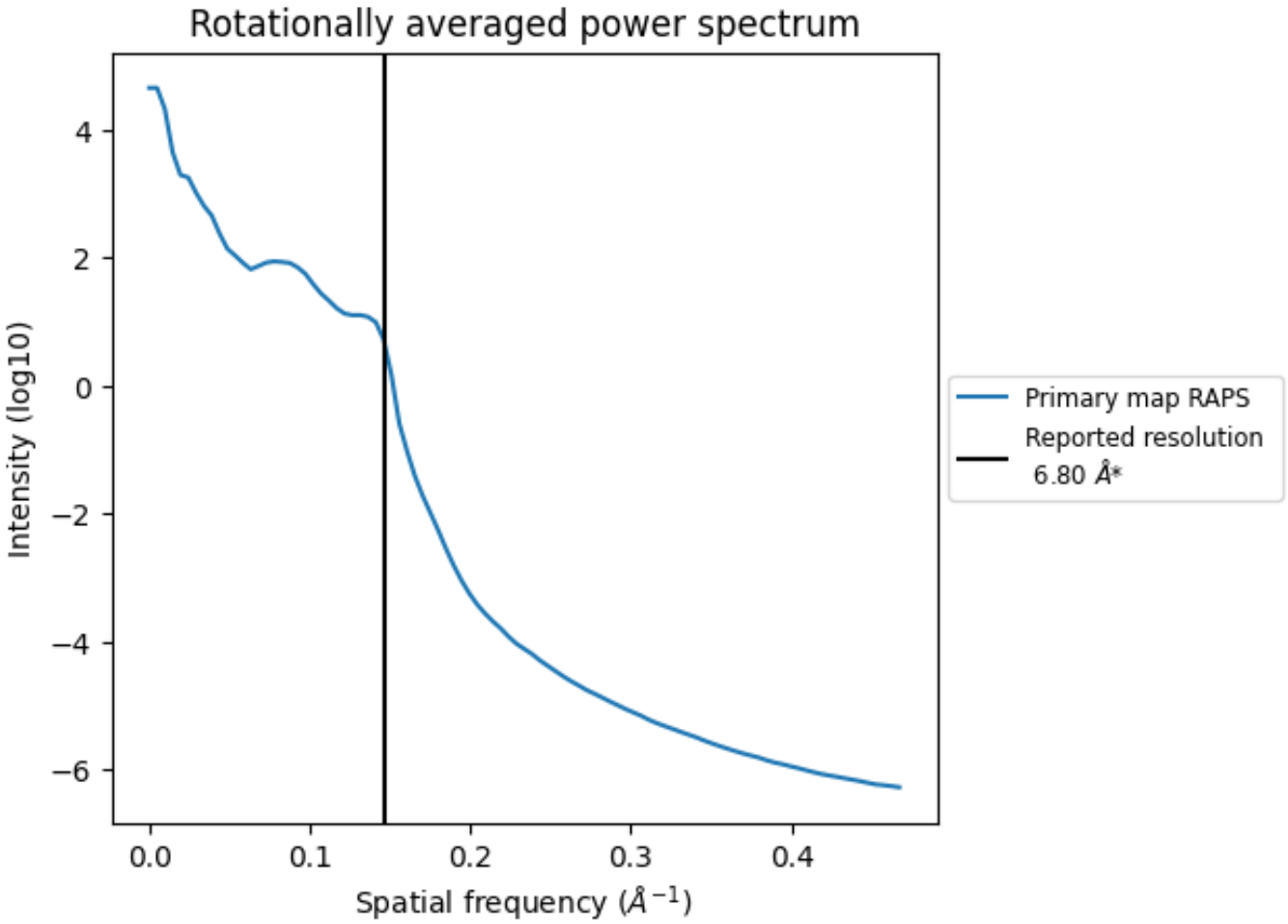
7.2 Volume estimate (i)



The volume at the recommended contour level is 88 nm^3; this corresponds to an approximate mass of 79 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 0.147 Å^{-1}

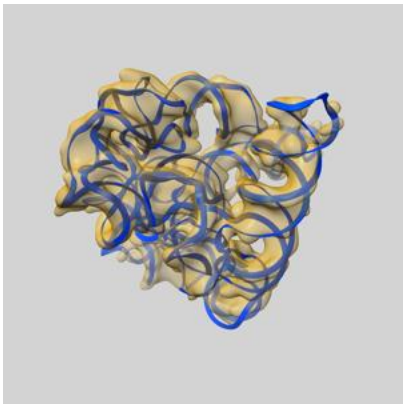
8 Fourier-Shell correlation (i)

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

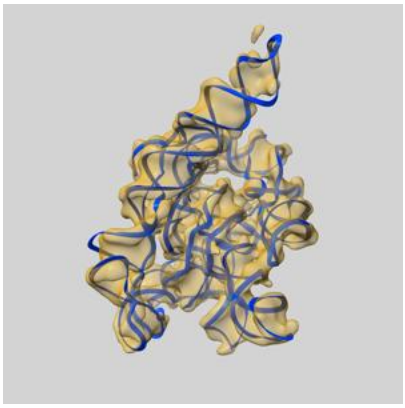
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-21840 and PDB model 6WLS. Per-residue inclusion information can be found in section 3 on page 6.

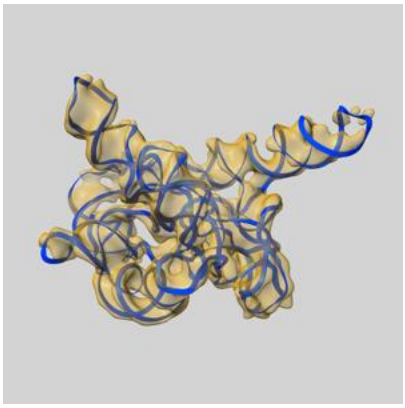
9.1 Map-model overlay



X



Y



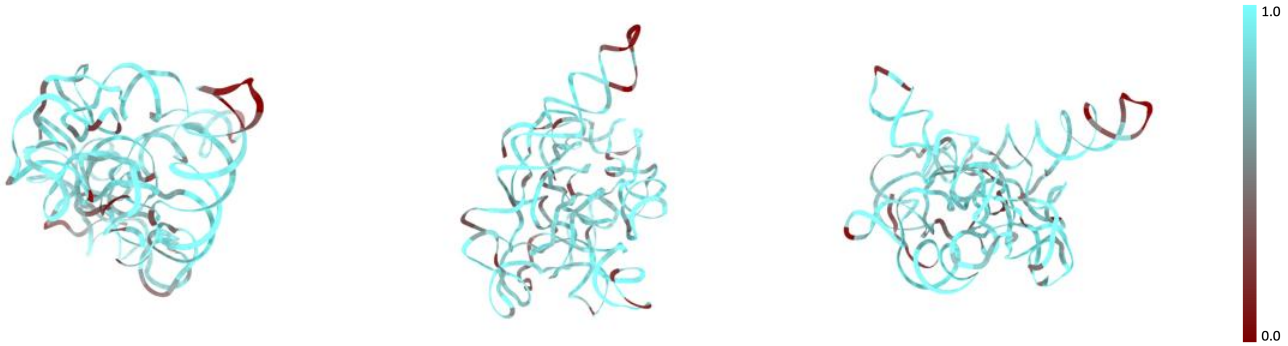
Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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)

This section was not generated.

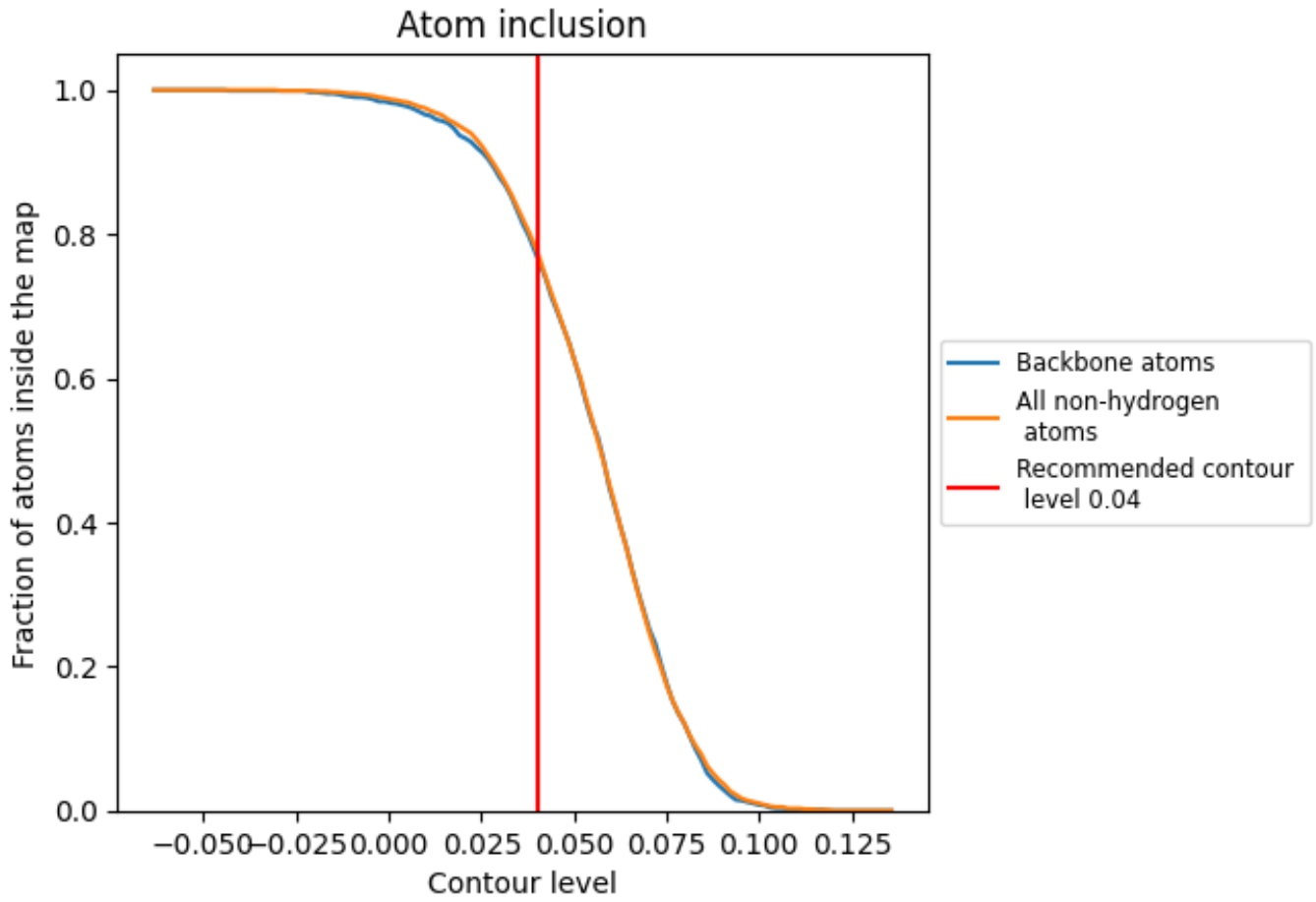
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 78% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	0.7770
A	0.7740