wwPDB EM Validation Summary Report (i)

Dec 12, 2022 – 07:29 am GMT

PDB ID	:	6Y50
EMDB ID	:	EMD-10688
Title	:	5'domain of human 17S U2 snRNP
Authors	:	Zhang, Z.; Will, C.L.; Bertram, K.; Luehrmann, R.; Stark, H.
Deposited on	:	2020-02-24
Resolution	:	4.10 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:

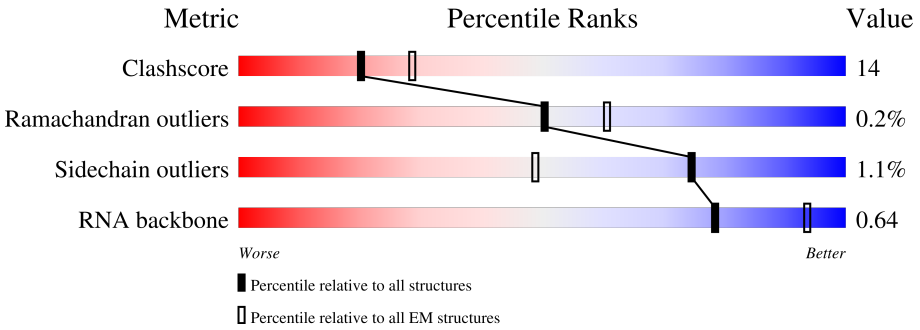
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 4.10 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.



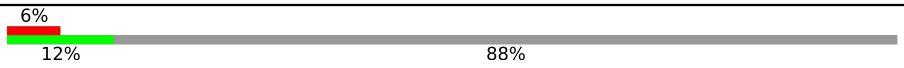
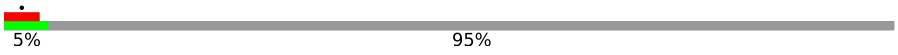
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 <=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	9	501	10% 20% 79%
2	y	110	14% 85% 15%
3	x	86	77% 23%
4	8	895	11% 88%
5	v	1217	10% 97%
6	u	1304	6% 64% 35%
7	2	188	14% 14% 10% 73%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	q	755	
9	p	1031	

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 14916 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 Splicing factor 3A subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	9	107	537	323	107	107	0	0

- Molecule 2 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	y	93	554	341	112	99	2	0	0

- Molecule 3 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	x	66	540	343	94	98	5	0	0

- Molecule 4 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	8	107	552	336	109	107	0	0

- Molecule 5 is a protein called Splicing factor 3B subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	v	1177	6500	4042	1237	1218	3	0	0

- Molecule 6 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	u	842	4500	2758	873	865	4	0	0

- Molecule 7 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	2	50	Total	C	N	O	P	0	0
			1056	473	177	356	50		

- Molecule 8 is a protein called HIV Tat-specific factor 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	q	94	Total	C	N	O	0	0
			470	282	94	94		

- Molecule 9 is a protein called Probable ATP-dependent RNA helicase DDX46.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	p	51	Total	C	N	O	0	0
			204	102	51	51		

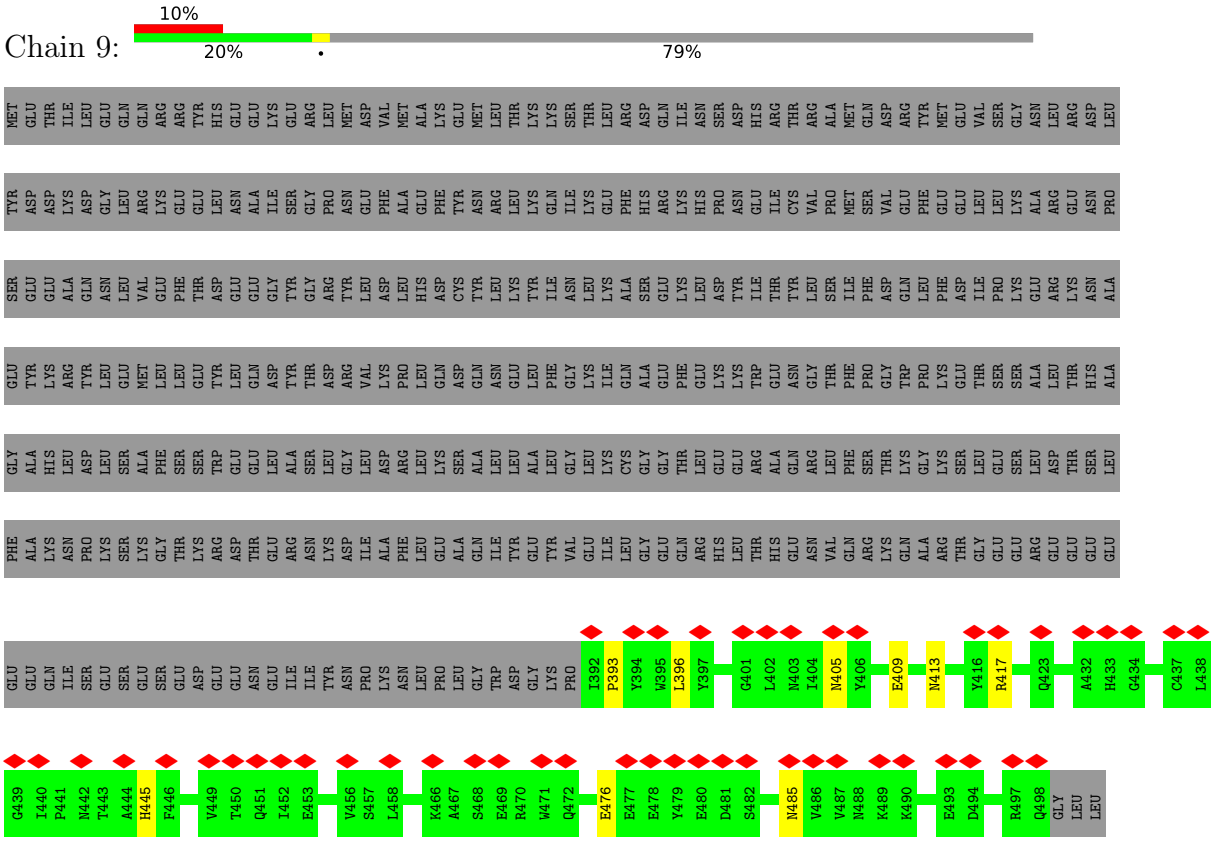
- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
10	y	3	Total	Zn	0
			3	3	

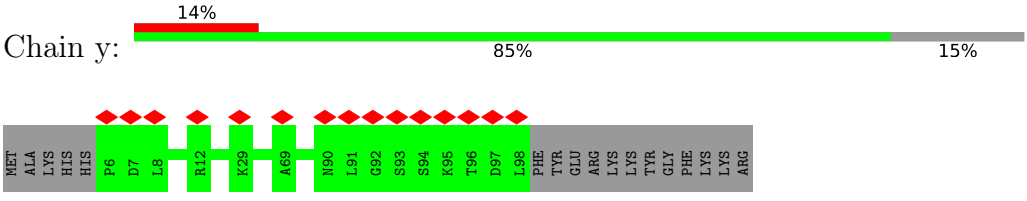
3 Residue-property plots (i)

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.

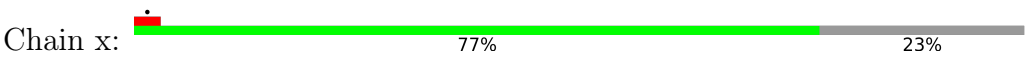
• Molecule 1: Splicing factor 3A subunit 3

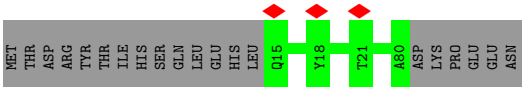


• Molecule 2: PHD finger-like domain-containing protein 5A



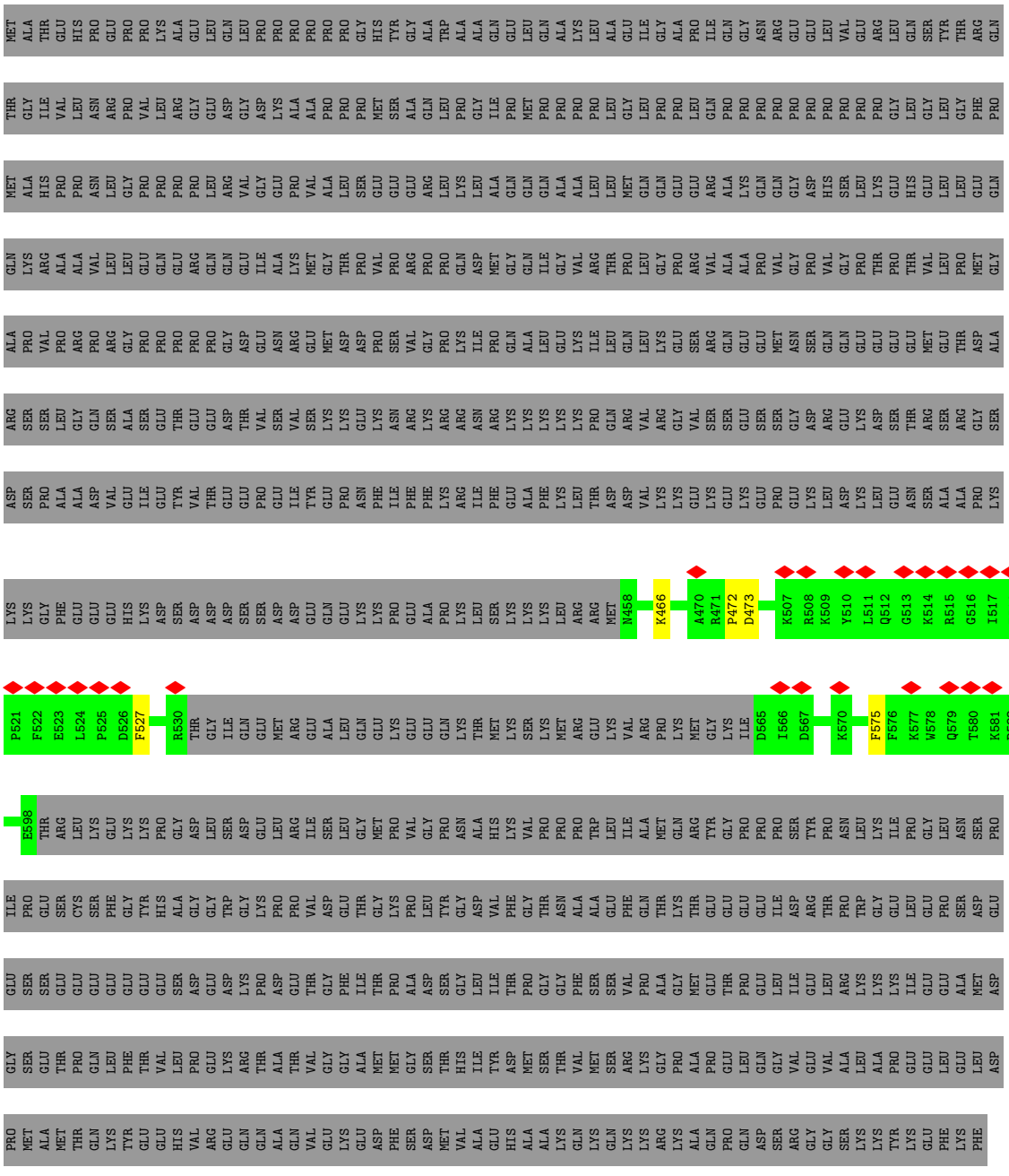
• Molecule 3: Splicing factor 3B subunit 5





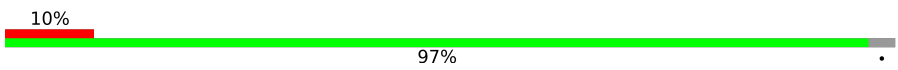
• Molecule 4: Splicing factor 3B subunit 2

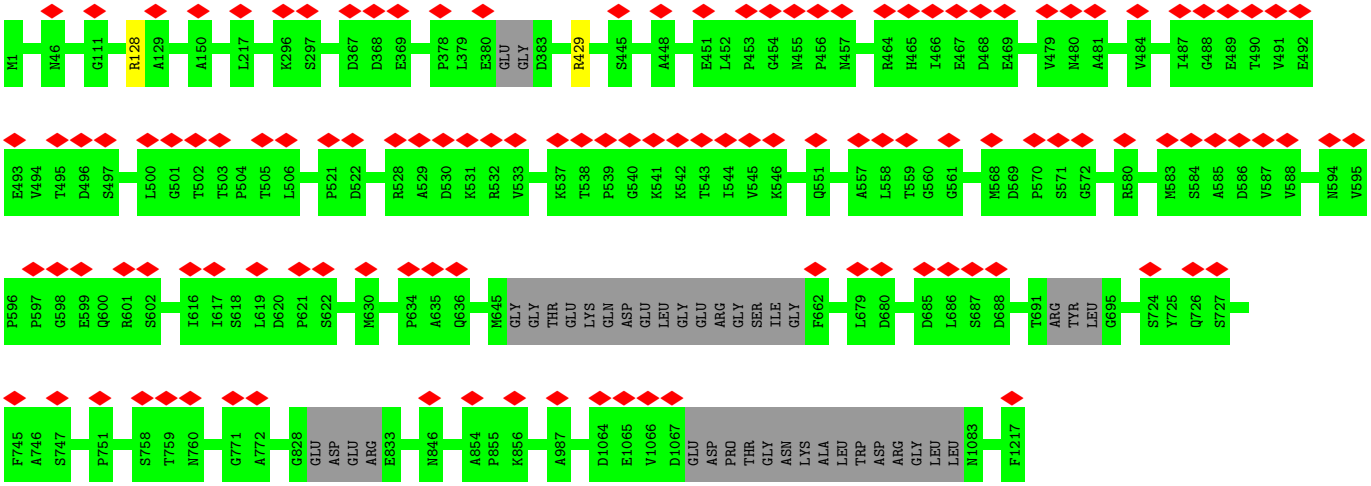
Chain 8:



• Molecule 5: Splicing factor 3B subunit 3

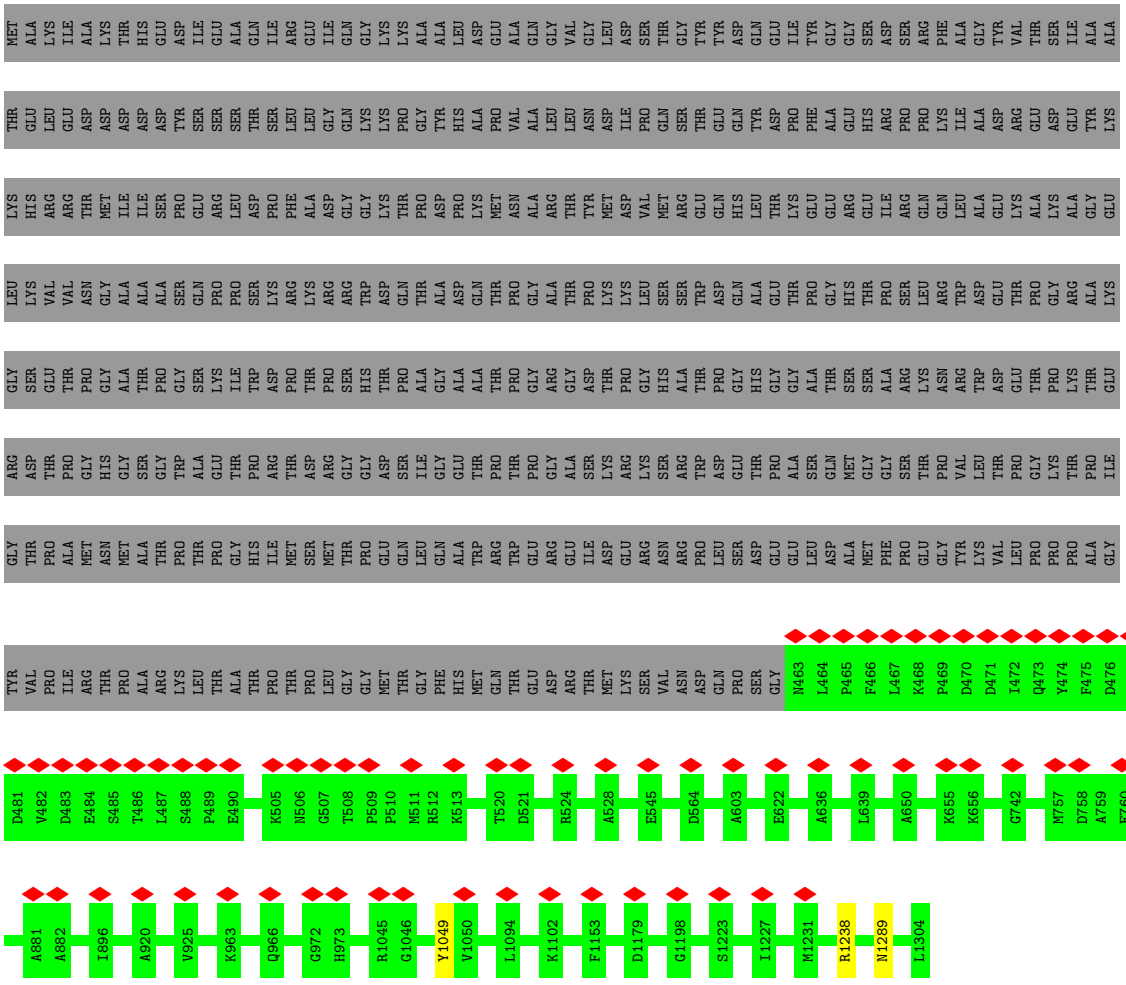
Chain v:





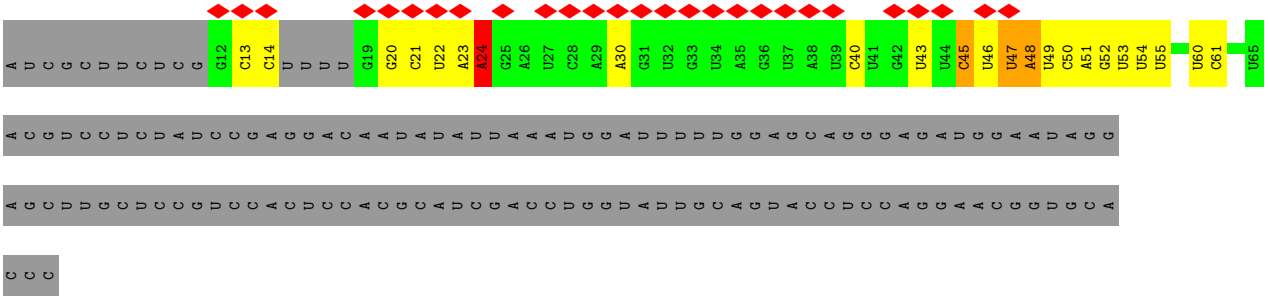
• Molecule 6: Splicing factor 3B subunit 1

Chain u:

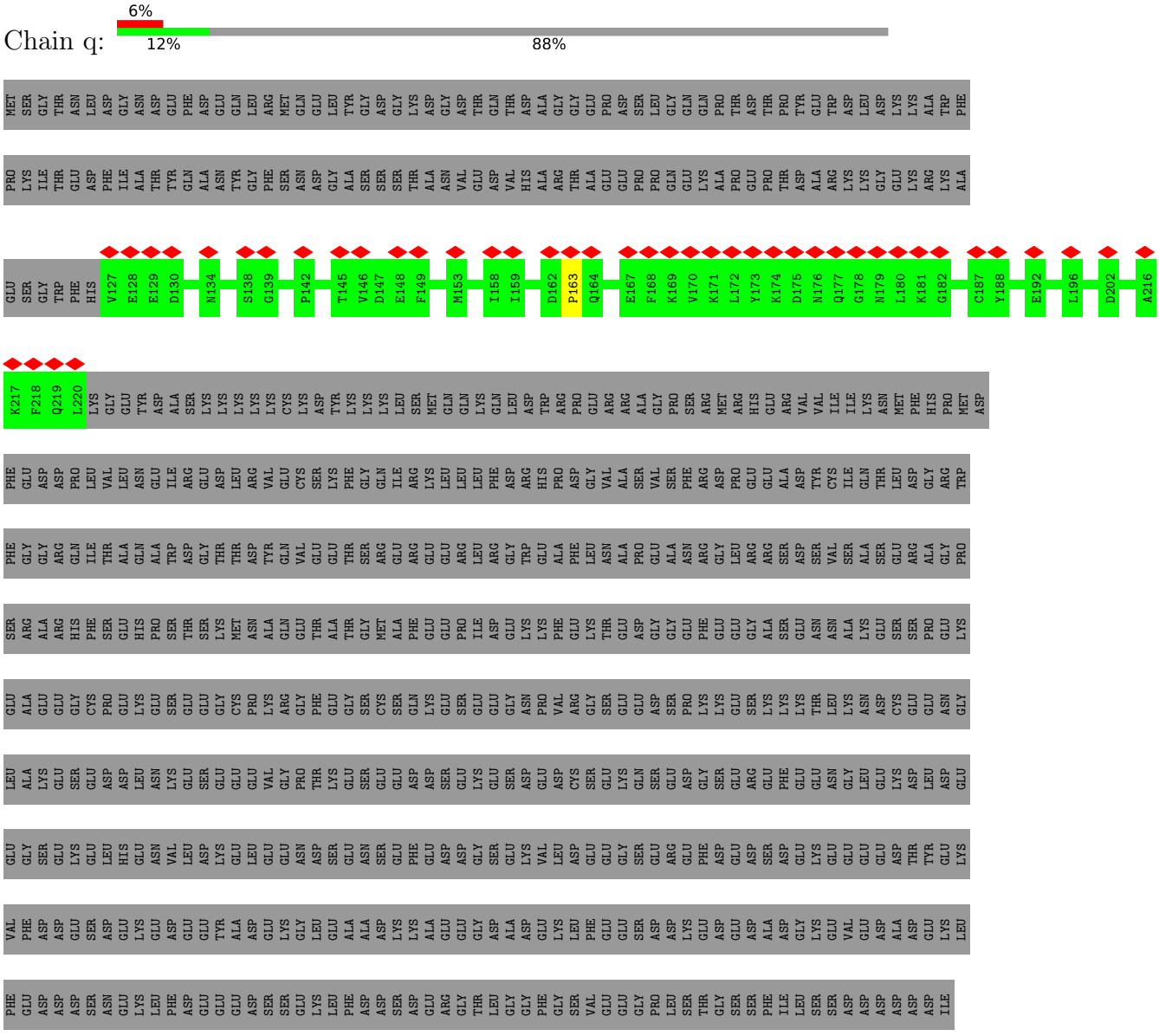


• Molecule 7: U2 snRNA

Chain 2:



• Molecule 8: HIV Tat-specific factor 1



• Molecule 9: Probable ATP-dependent RNA helicase DDX46

MET GLY ARG GLU SER ARG HIS TYR ARG LYS ARG SER ALA SER ARG GLY ARG SER GLY SER ARG SER ARG SER ARG SER PRO SER ASP LYS ARG SER LYS ARG GLY ASP ASP ARG ARG SER ARG SER ARG ASP ARG ASP ARG ARG ARG GLU ARG SER ARG SER ARG ASP LYS ARG ARG SER

ARG SER ARG ASP ARG LYS ARG LEU ARG ARG SER ARG SER ARG GLU ARG ASP ARG SER ARG GLU ARG ARG ARG SER ARG SER ARG ASP ARG ARG ARG SER ARG SER ARG SER ARG GLY ARG ARG SER ARG SER SER SER PRO GLY ASN LYS SER LYS LYS THR GLU ASN ARG SER ARG SER

LYS GLU LYS THR ASP GLY GLY GLU SER SER LYS GLU LYS LYS LYS ASP LYS ASP ASP LYS GLU ASP GLU LYS GLU K146 D147 A148 G149 N150 F151 D152 Q153 N154 K155 L156 E159 M160 R161 R166 K169 W170 R171 E172 E173 Q174 R175 K176 K177 A178 M179 E180 N181 I182 G183 E184 L185

K186 K187 E188 I189 E190 E191 M192 K193 Q194 G195 K196 LYS TRP SER LEU GLU ASP ASP ASP ASP ASP GLU ASP ASP PRO ALA GLU ALA GLU LYS GLU GLY ASN GLU MET GLU GLY GLU GLU LEU ASP PRO LEU ASP ALA TYR MET GLU GLU VAL LYS GLU GLU VAL LYS LYS PHE ASN MET ARG

SER VAL LYS GLY GLY GLY GLY ASN GLU LYS LYS SER GLY PRO THR VAL THR LYS VAL VAL THR VAL VAL THR THR LYS LYS ALA VAL VAL ASP SER ASP LYS LYS LYS GLY GLU LEU MET GLU ASN ASP GLN ASP ALA MET GLU TYR SER SER GLU GLU GLU GLU VAL ASP LEU GLN THR

ALA LEU THR GLY TYR GLN THR LYS GLN ARG LYS LEU LEU GLU PRO VAL ASP HIS GLY LYS ILE GLU TYR GLU PRO PHE ARG LYS ASN PHE TYR VAL GLU VAL PRO GLU LEU ALA LYS MET SER GLN GLU GLU VAL ASN VAL PHE ARG LEU GLU MET GLU GLY ILE THR VAL LYS GLY LYS

GLY CYS PRO LYS PRO ILE LYS SER TRP VAL GLN CYS GLY ILE SER MET LYS ILE LEU ASN SER LEU LYS LYS HIS GLY TYR GLU LYS PRO THR PRO ILE GLN THR GLN ALA ILE PRO ALA ILE MET SER GLY ARG ASP LEU ILE GLY ILE ALA LYS THR GLY SER GLY LYS THR ILE ALA

PHE LEU LEU PRO MET PHE ARG HIS ILE MET ASP GLN ARG SER LEU GLU GLU GLY GLU GLY PRO ILE ALA VAL ILE MET THR PRO THR ARG GLU LEU ALA LEU GLN ILE THR LYS GLU CYS LYS LYS PHE SER LYS THR LEU GLY LEU ARG VAL VAL CYS VAL TYR GLY GLY THR GLY ILE

SER GLU GLN ILE ALA GLU LEU LYS ARG GLY ALA GLU ILE ILE VAL CYS THR PRO GLY ARG MET ILE ASP MET LEU ALA ALA ASN SER GLY ARG VAL THR ASN LEU ARG ARG VAL THR TYR VAL VAL LEU ASP GLU ALA ASP ARG MET PHE ASP MET GLY PHE GLU PRO GLN VAL MET ARG

ILE VAL ASP ASN VAL ARG PRO ASP ARG GLN THR VAL MET PHE SER ALA THR PHE PRO ARG ALA MET GLU ALA LEU ALA ARG ARG ILE LEU SER LYS PRO ILE GLU VAL GLN VAL GLY GLY ARG SER VAL VAL CYS SER ASP VAL GLU GLN GLN VAL ILE VAL ILE GLU GLU LYS LYS

PHE LEU LYS LEU LEU GLU LEU LEU GLY HIS TYR GLN GLU SER GLY SER VAL ILE ILE PHE VAL ASP LYS GLN GLU HIS ALA ASP GLY LEU LEU LYS ASP LEU MET ARG ALA SER TYR PRO CYS MET SER LEU HIS GLY GLY ILE ASP GLN TYR ASP ARG ASP SER ILE ILE ASN ASP PHE

LYS ASN GLY THR CYS LYS LEU LEU VAL ALA THR SER VAL ALA ALA ARG GLY LEU ASP VAL LYS HIS LEU ILE LEU VAL VAL ASN TYR SER CYS PRO ASN HIS TYR GLU ASP TYR VAL HIS ARG ALA GLY ARG THR GLY ARG ALA GLY ASN LYS GLY TYR ALA TYR THR PHE ILE THR GLU

ASP GLN ALA ARG TYR ALA GLY ASP ILE ILE LYS ALA LEU GLU LEU SER GLY THR ALA VAL PRO PRO ASP LEU GLU LYS LEU TRP SER ASP PHE LYS ASP GLN GLN LYS ALA GLU GLY LYS ILE ILE LYS LYS SER SER GLY PHE SER GLY LYS GLY PHE LYS PHE ASP GLU THR GLU GLN

ALA LEU ALA ASN GLU ARG LYS LYS LEU GLN LYS ALA ALA LEU GLY LEU GLN ASP SER ASP ASP GLU ASP ALA ALA VAL ASP ILE ASP GLU GLN ILE GLU SER MET PHE ASN SER LYS LYS ARG VAL LYS ASP MET ALA ALA PRO GLY THR SER SER VAL PRO ALA PRO THR ALA GLY ASN

ALA GLU LYS LEU GLU ILE ALA LYS ARG LEU ALA LEU ARG ILE ASN ALA GLN LYS ASN LEU GLY ILE GLU SER GLN ASP VAL MET GLN GLN ALA THR ASN ALA ILE LEU ARG GLY GLY THR ILE LEU ALA PRO THR VAL SER ALA LYS THR ILE ALA GLU GLN LEU ALA GLU LYS ILE ASN

ALA LYS LEU ASN TYR VAL PRO LEU GLU LYS GLN GLU GLU GLU ARG GLN ASP GLY GLY GLN ASN GLU SER PHE LYS ARG TYR GLU GLU GLU LEU GLU ILE ASN ASP PHE PRO GLN THR ALA ARG TRP LYS VAL THR SER LYS GLU ALA LEU GLN ARG ILE SER GLU TYR SER GLU ALA ALA

ILE THR ILE ARG GLY THR TYR PHE PRO PRO GLY LYS GLU PRO LYS GLU GLY GLU ARG LYS ILE TYR LEU ALA ILE GLU SER ALA ASN GLU LEU ALA VAL GLN LYS ALA LYS ALA GLU ILE THR ARG LEU ILE LYS GLU GLU LEU ILE ARG LEU GLN ASN SER TYR GLN PRO THR ASN LYS

GLY ARG TYR LYS VAL LEU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	120070	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 ($e^-/Å^2$)	72	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.156	Depositor
Minimum map value	-0.088	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.038	Depositor
Map size (Å)	348.0, 348.0, 348.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.16, 1.16, 1.16	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	9	0.34	0/540	0.45	0/754
2	y	0.23	0/563	0.41	0/768
3	x	0.24	0/556	0.38	0/751
4	8	0.23	0/559	0.43	0/783
5	v	0.25	0/6605	0.45	0/9180
6	u	0.24	0/4559	0.39	0/6358
7	2	0.38	1/1177 (0.1%)	0.75	1/1827 (0.1%)
8	q	0.23	0/472	0.41	0/658
9	p	0.61	0/203	0.58	0/252
All	All	0.27	1/15234 (0.0%)	0.46	1/21331 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	2	45	C	O3'-P	-11.52	1.47	1.61

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	2	24	A	O3'-P-O5'	5.56	114.57	104.00

There are no chirality outliers.

There are no planarity outliers.

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	9	537	0	263	8	0
2	y	554	0	373	0	0
3	x	540	0	509	0	0
4	8	552	0	276	4	0
5	v	6500	0	3917	0	0
6	u	4500	0	2532	0	0
7	2	1056	0	533	15	0
8	q	470	0	214	0	0
9	p	204	0	56	0	0
10	y	3	0	0	0	0
All	All	14916	0	8673	24	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 14.

The worst 5 of 24 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)
1:9:405:ASN:HA	1:9:417:ARG:O	1.84	0.78
7:2:47:U:H3'	7:2:48:A:H5'	1.70	0.73
7:2:54:U:H2'	7:2:55:U:C6	2.37	0.59
7:2:20:G:H2'	7:2:21:C:C6	2.38	0.59
7:2:45:C:H5"	7:2:46:U:H5'	1.89	0.54

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	9	105/501 (21%)	91 (87%)	14 (13%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	y	91/110 (83%)	83 (91%)	8 (9%)	0	100 100
3	x	64/86 (74%)	58 (91%)	6 (9%)	0	100 100
4	8	103/895 (12%)	91 (88%)	12 (12%)	0	100 100
5	v	1165/1217 (96%)	1096 (94%)	69 (6%)	0	100 100
6	u	840/1304 (64%)	815 (97%)	24 (3%)	1 (0%)	51 84
8	q	92/755 (12%)	84 (91%)	7 (8%)	1 (1%)	14 50
9	p	49/1031 (5%)	39 (80%)	8 (16%)	2 (4%)	3 25
All	All	2509/5899 (42%)	2357 (94%)	148 (6%)	4 (0%)	50 80

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	p	185	LEU
6	u	1049	TYR
9	p	184	GLU
8	q	163	PRO

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	9	4/446 (1%)	4 (100%)	0	100 100
2	y	22/95 (23%)	22 (100%)	0	100 100
3	x	57/77 (74%)	57 (100%)	0	100 100
4	8	9/776 (1%)	9 (100%)	0	100 100
5	v	188/1051 (18%)	186 (99%)	2 (1%)	73 84
6	u	94/1104 (8%)	92 (98%)	2 (2%)	53 72
8	q	3/661 (0%)	3 (100%)	0	100 100
All	All	377/4210 (9%)	373 (99%)	4 (1%)	74 84

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	v	128	ARG
5	v	429	ARG
6	u	1238	ARG
6	u	1289	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
6	u	1289	ASN
6	u	1256	HIS
6	u	1186	GLN
5	v	1096	HIS
6	u	1213	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
7	2	48/188 (25%)	6 (12%)	0

5 of 6 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	2	22	U
7	2	23	A
7	2	24	A
7	2	43	U
7	2	47	U

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

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

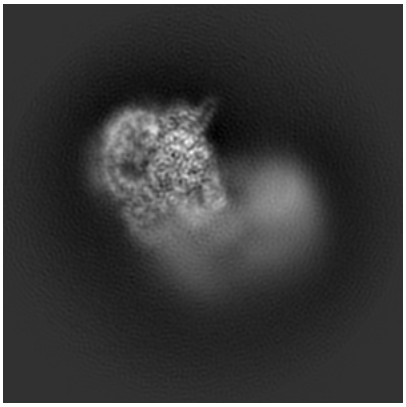
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10688. These allow visual inspection of the internal detail of the map and identification of artifacts.

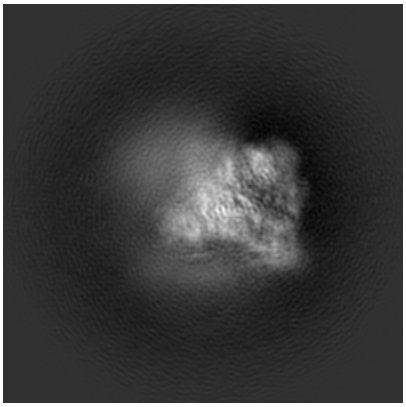
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

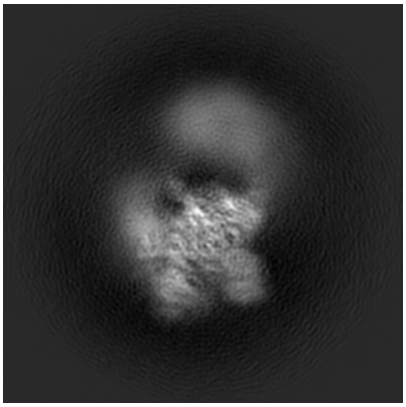
6.1.1 Primary map



X



Y

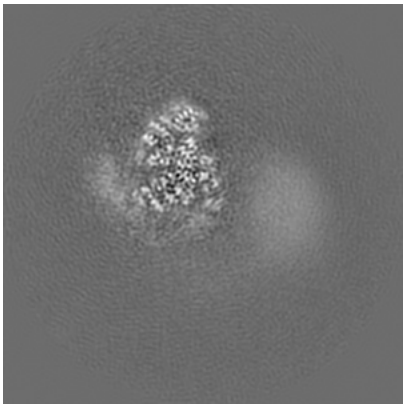


Z

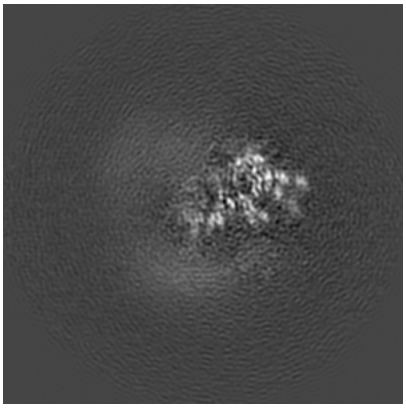
The images above show the map projected in three orthogonal directions.

6.2 Central slices

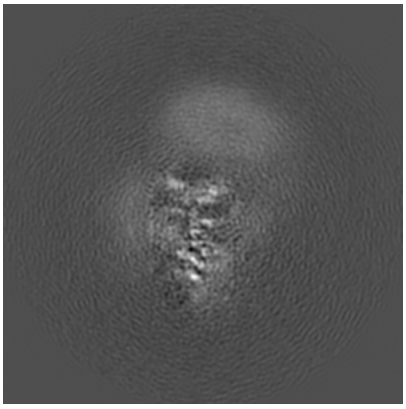
6.2.1 Primary map



X Index: 150



Y Index: 150

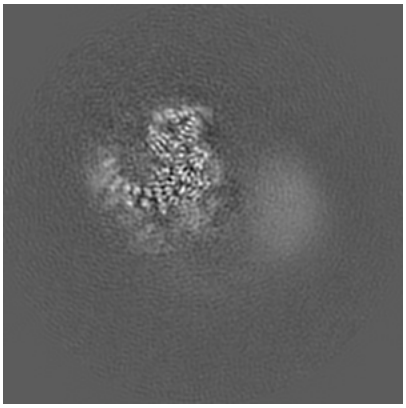


Z Index: 150

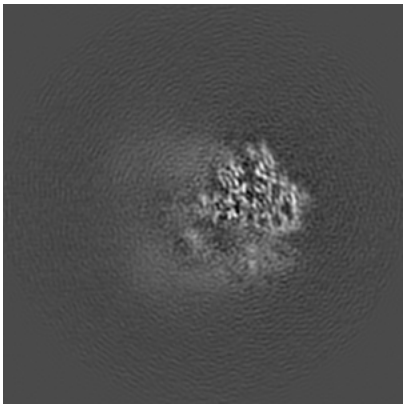
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

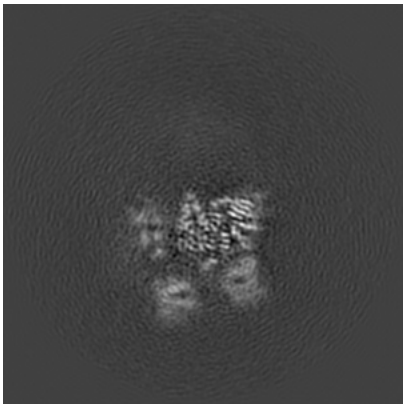
6.3.1 Primary map



X Index: 144



Y Index: 136



Z Index: 189

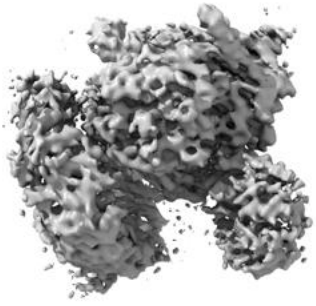
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.038. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

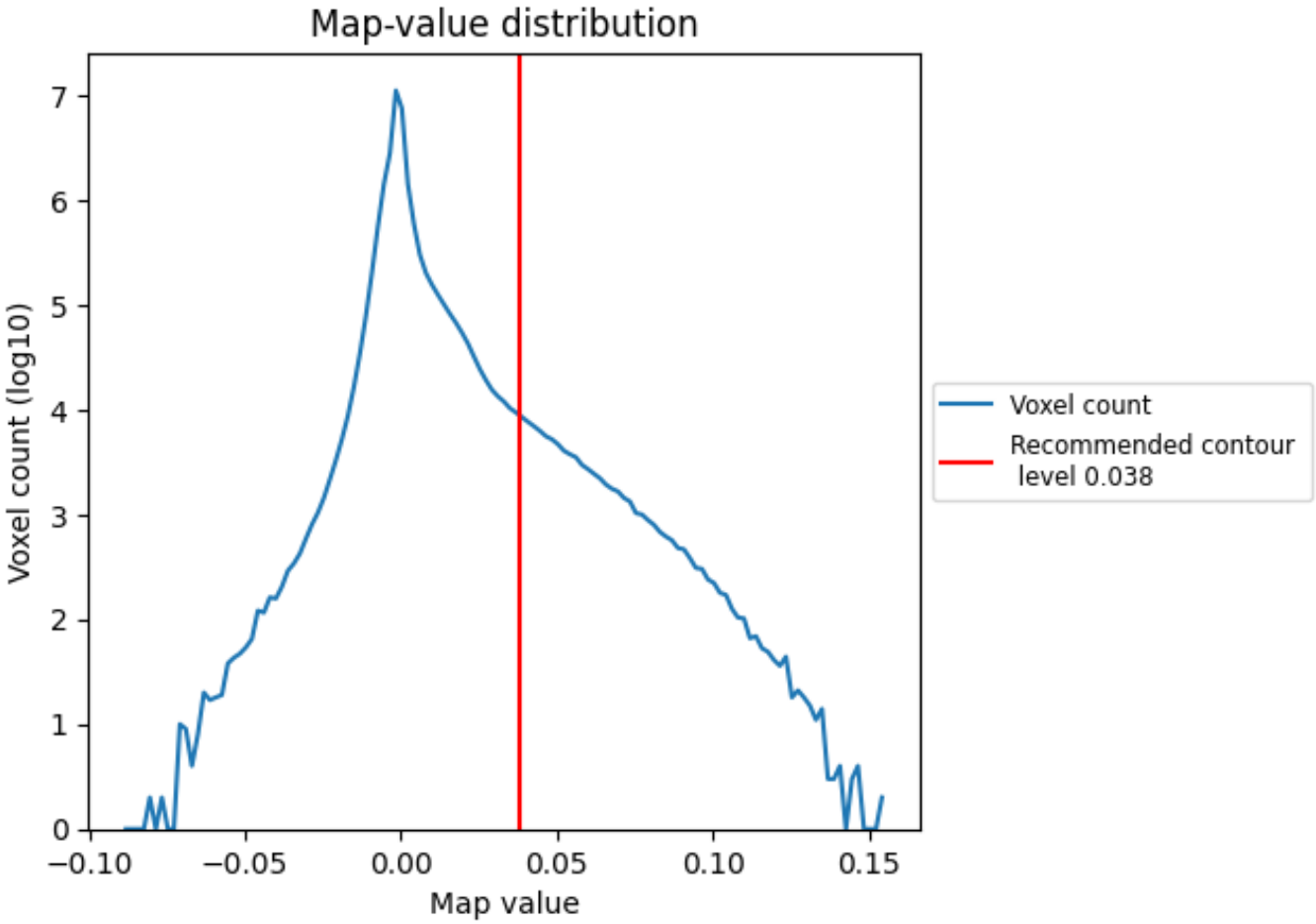
6.5 Mask visualisation (i)

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

7 Map analysis

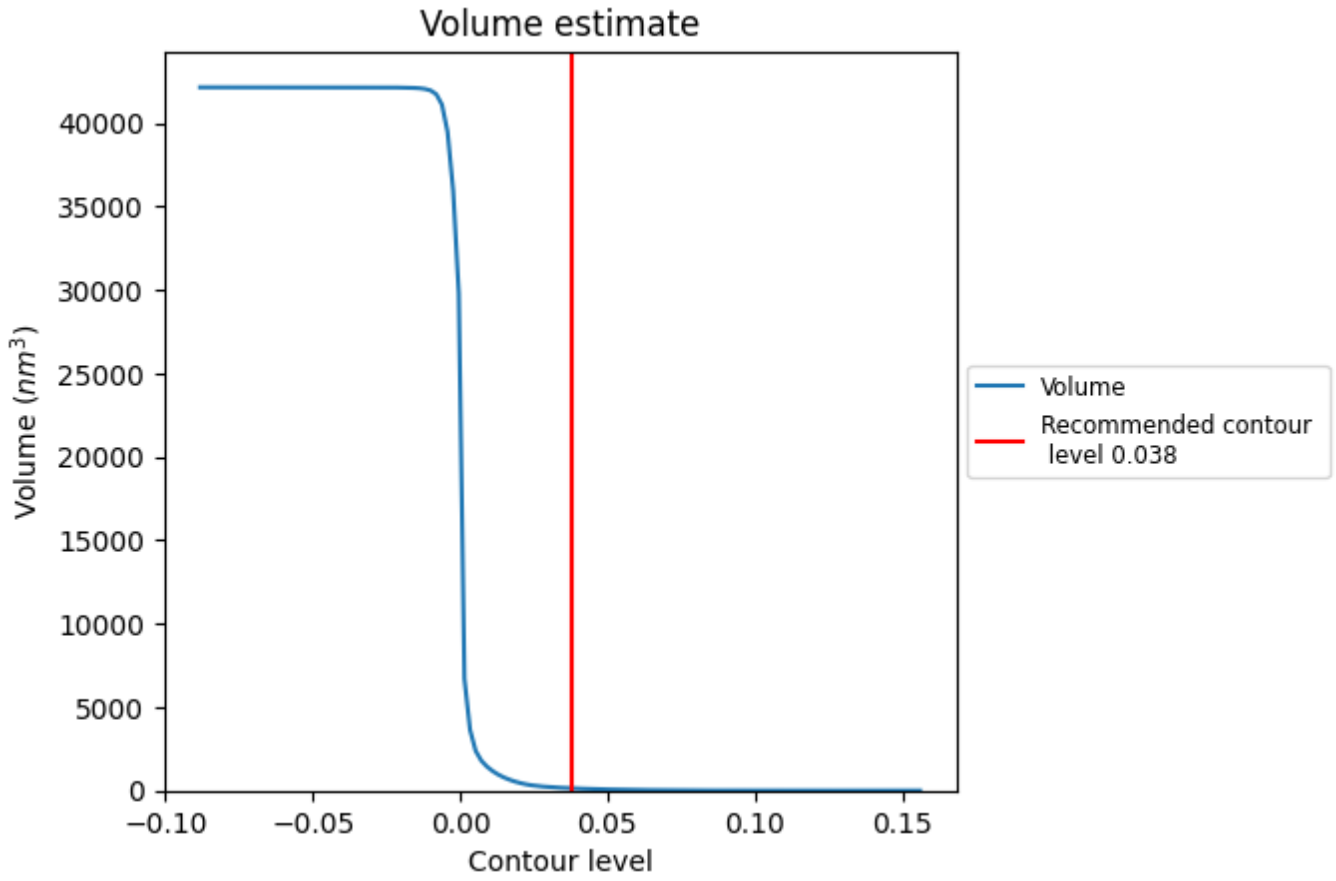
This section contains the results of statistical analysis of the map.

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.

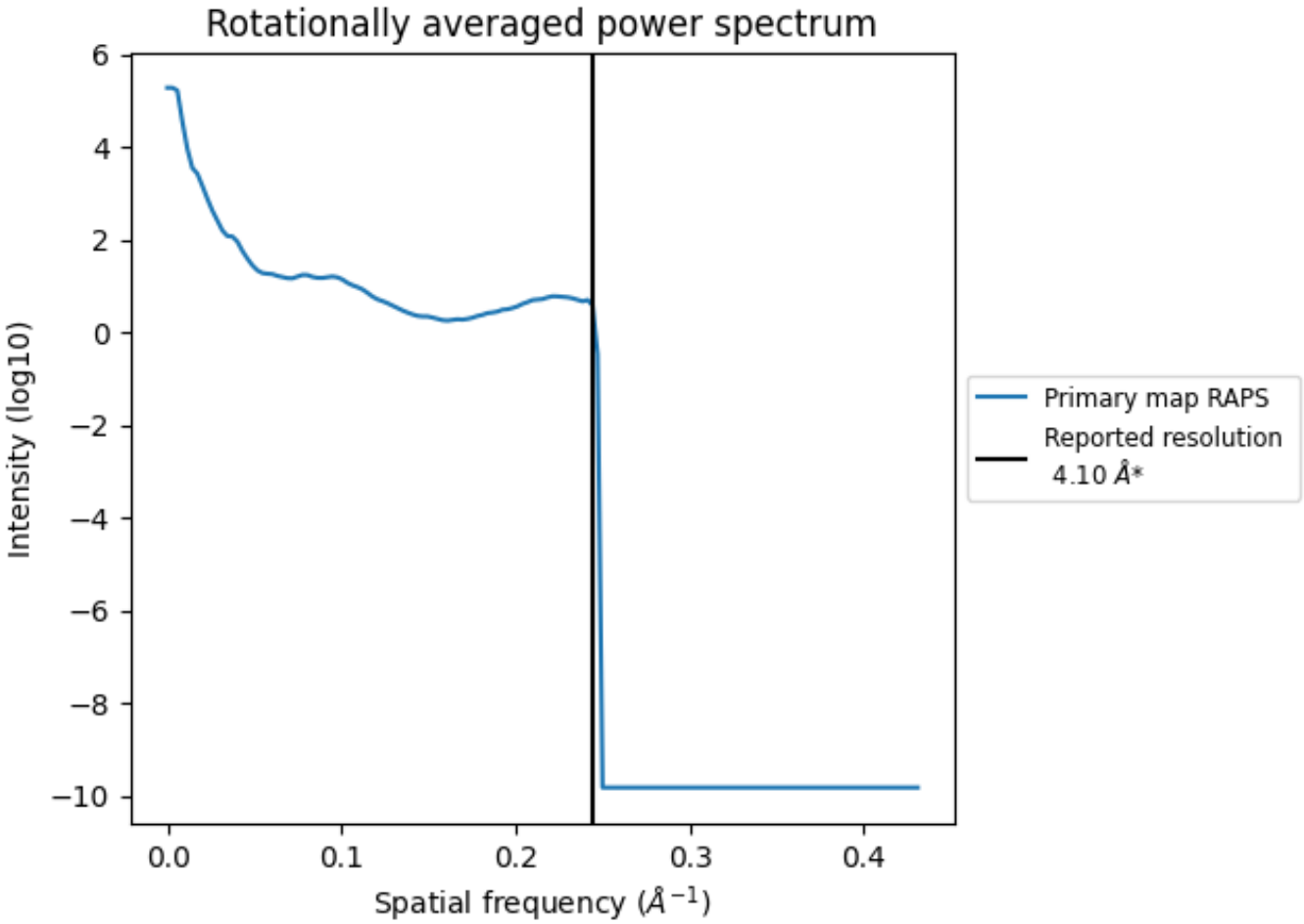
7.2 Volume estimate (i)



The volume at the recommended contour level is 136 nm^3; this corresponds to an approximate mass of 123 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 0.244 Å^{-1}

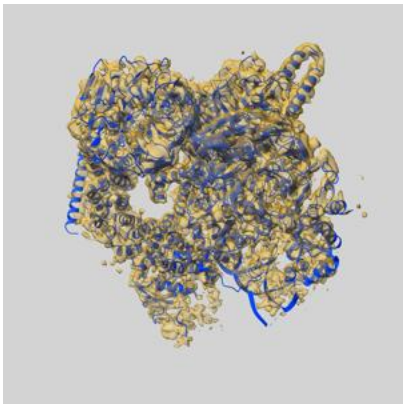
8 Fourier-Shell correlation

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

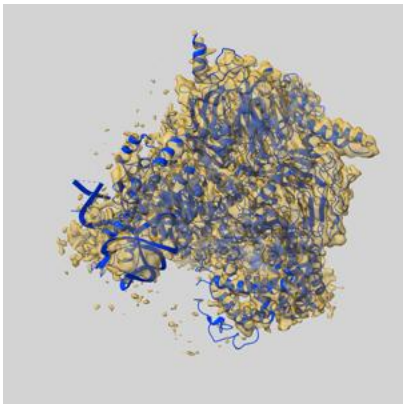
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10688 and PDB model 6Y50. Per-residue inclusion information can be found in section 3 on page 6.

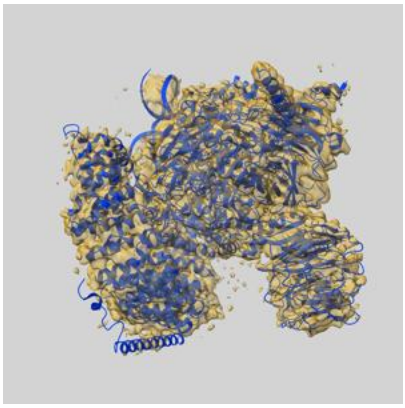
9.1 Map-model overlay



X



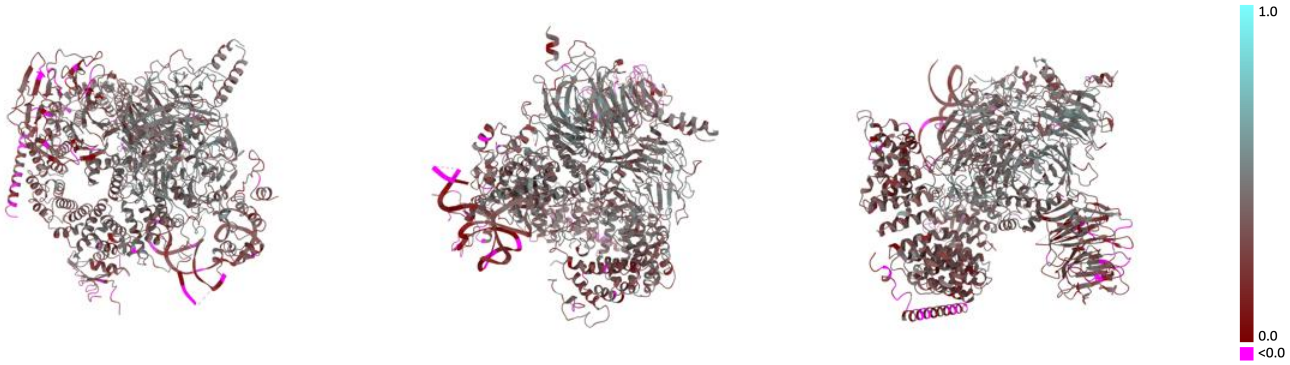
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.038 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.

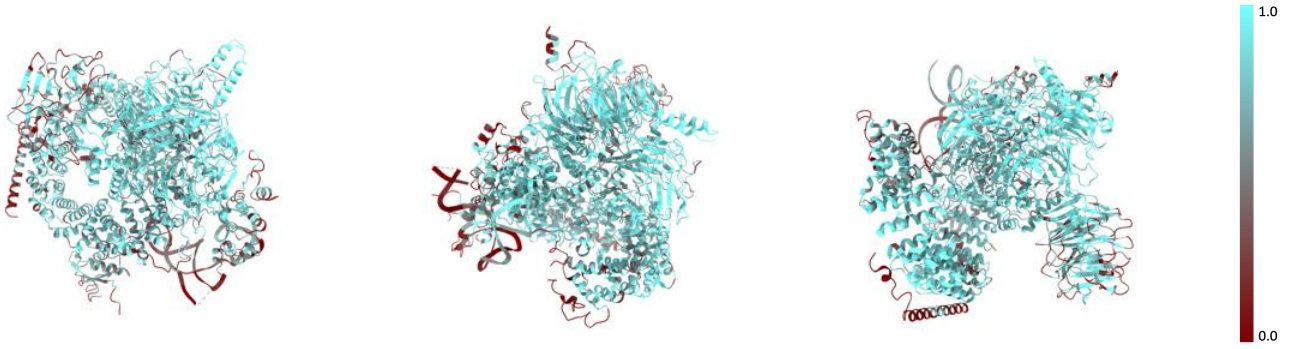
9.2 Q-score mapped to coordinate model



X Y Z

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

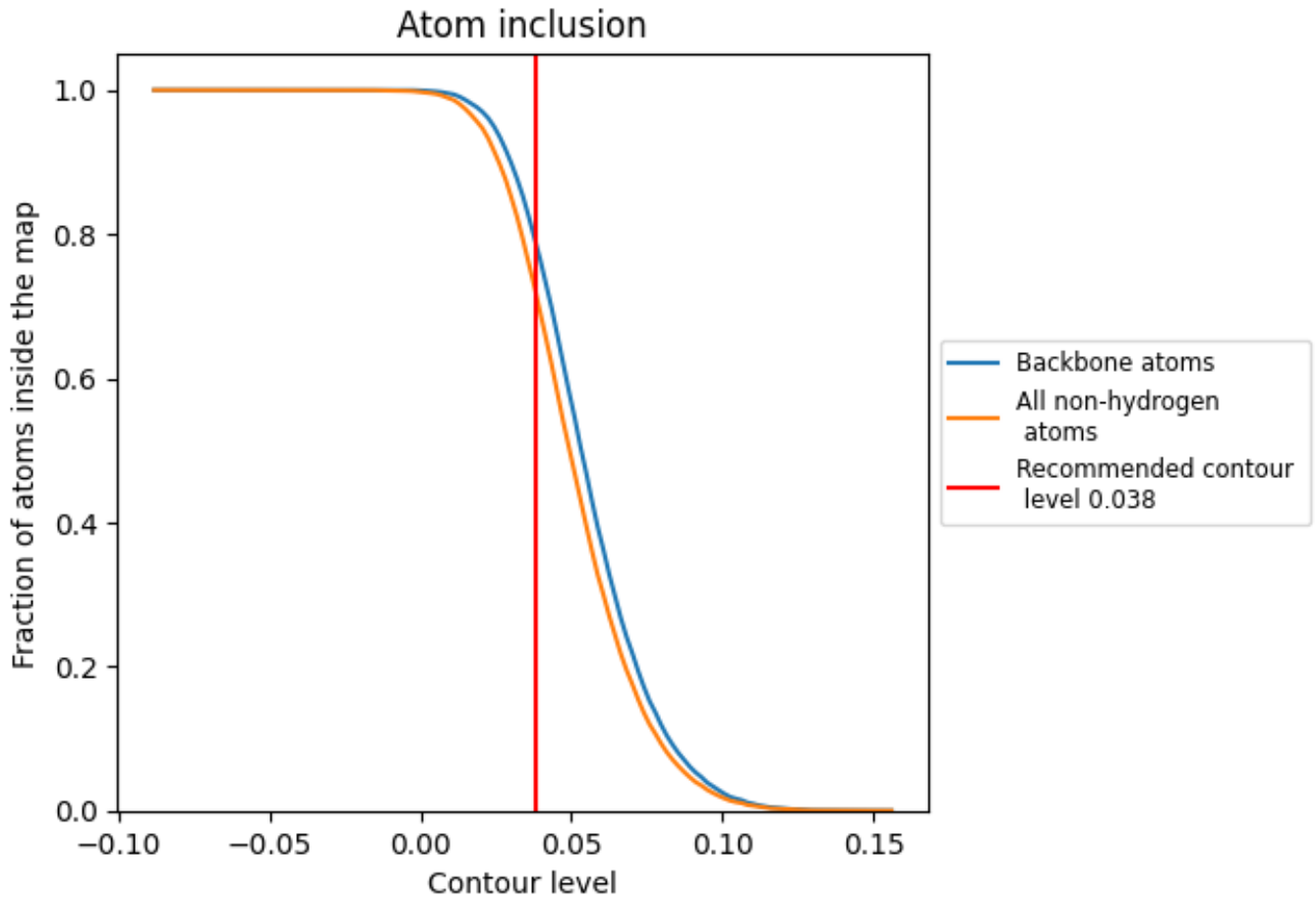
9.3 Atom inclusion mapped to coordinate model



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 (0.038).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.038) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7232	0.3510
2	0.3608	0.1290
8	0.6322	0.4010
9	0.4916	0.3180
p	0.1324	0.0800
q	0.4915	0.2290
u	0.7882	0.3480
v	0.7995	0.3970
x	0.7102	0.3830
y	0.7399	0.4190