wwPDB EM Validation Summary Report

May 25, 2024 – 03:11 PM EDT

PDB ID	:	7N84
EMDB ID	:	EMD-24231
Title	:	Double nuclear outer ring from the isolated yeast NPC
Authors	:	Akey, C.W.; Rout, M.P.; Ouch, C.; Echevarria, I.; Fernandez-Martinez, J.; Nudelman, I.
Deposited on	:	2021-06-13
Resolution	:	11.60 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:

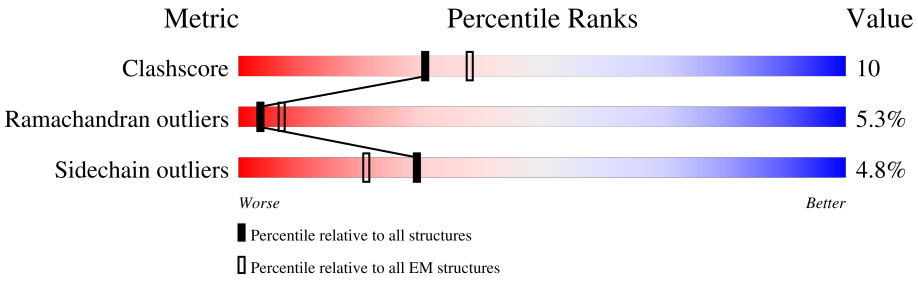
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 11.60 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

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	X	1655	6% 44% 18% 6% • 31%
2	Y	63	100%
2	Z	63	100%
3	a	1037	66% 25% 5% • •
3	l	1037	68% 24% 5% •
4	b	744	64% 23% • 9%
4	m	744	62% 22% 6% 10%
5	c	712	56% 19% • 21%

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Mol	Chain	Length	Quality of chain
5	n	712	
6	d	297	
6	o	297	
7	e	349	
7	p	349	
8	f	726	
8	q	726	
9	g	1157	
9	r	1157	

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 83142 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 Nucleoporin NUP188.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	X	1137	Total	C	N	O	S	0	0
			9208	6035	1455	1700	18		

- Molecule 2 is a protein called unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	Y	63	Total	C	N	O	0	0
			315	189	63	63		
2	Z	63	Total	C	N	O	0	0
			315	189	63	63		

- Molecule 3 is a protein called Nucleoporin NUP120.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	a	1006	Total	C	N	O	S	0	0
			8279	5346	1334	1566	33		
3	l	1006	Total	C	N	O	S	0	0
			8279	5346	1334	1566	33		

- Molecule 4 is a protein called Nucleoporin NUP85.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	b	675	Total	C	N	O	S	0	0
			5424	3493	863	1038	30		
4	m	670	Total	C	N	O	S	0	0
			5384	3468	857	1031	28		

- Molecule 5 is a protein called Nucleoporin 145c.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	c	559	Total	C	N	O	S	0	0
			4520	2884	750	869	17		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	n	557	Total 4505	C 2873	N 748	O 867	S 17	0	0

- Molecule 6 is a protein called Protein transport protein SEC13.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	d	274	Total 2160	C 1379	N 369	O 409	S 3	0	0
6	o	274	Total 2160	C 1379	N 369	O 409	S 3	0	0

- Molecule 7 is a protein called Nucleoporin SEH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	e	307	Total 2438	C 1543	N 422	O 462	S 11	0	0
7	p	307	Total 2438	C 1543	N 422	O 462	S 11	0	0

- Molecule 8 is a protein called Nucleoporin NUP84.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	f	649	Total 5261	C 3370	N 866	O 1011	S 14	0	0
8	q	648	Total 5254	C 3365	N 865	O 1010	S 14	0	0

- Molecule 9 is a protein called Nucleoporin NUP133.

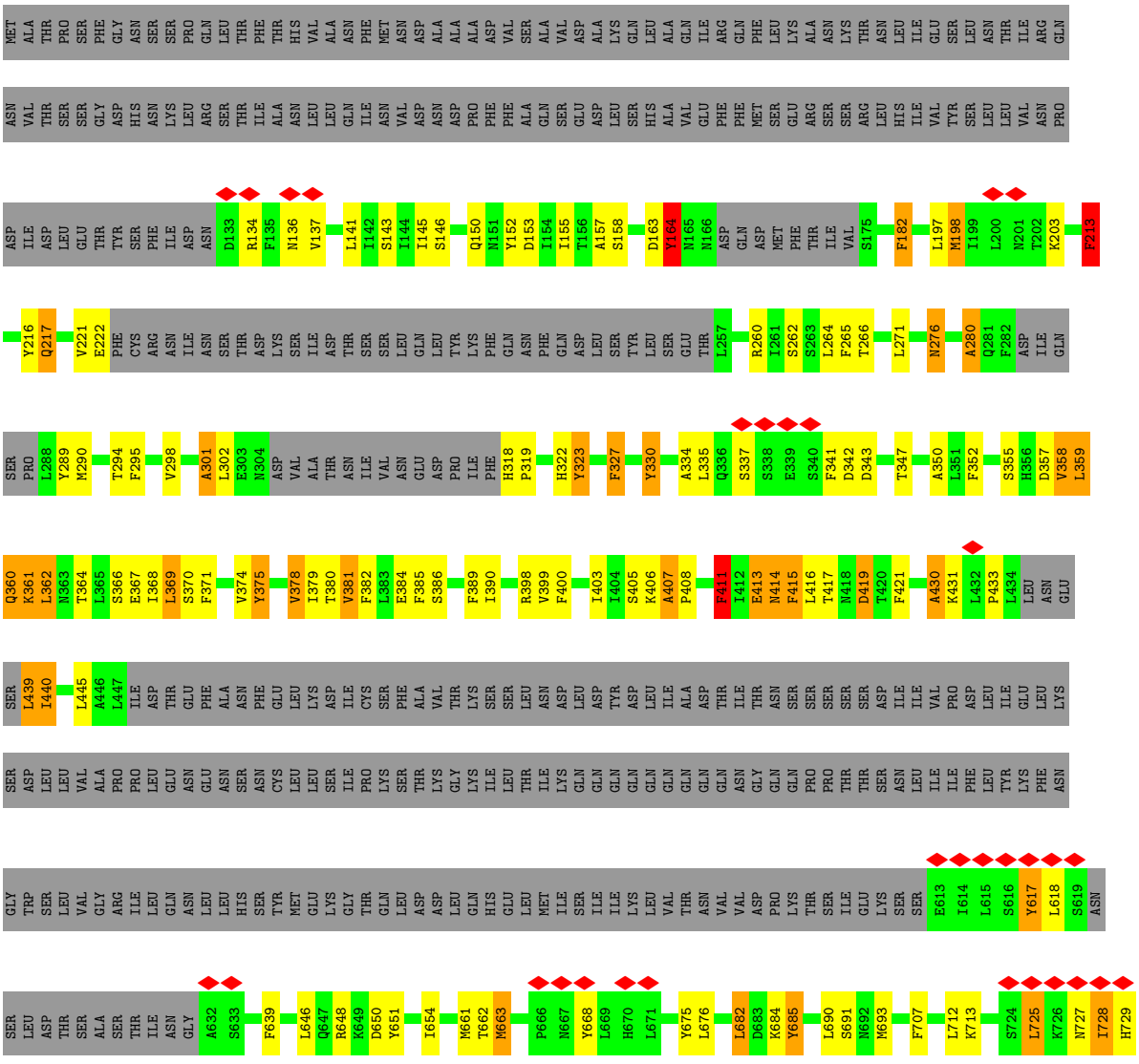
Mol	Chain	Residues	Atoms					AltConf	Trace
9	g	1062	Total 8627	C 5541	N 1393	O 1664	S 29	0	0
9	r	1056	Total 8575	C 5511	N 1381	O 1654	S 29	0	0

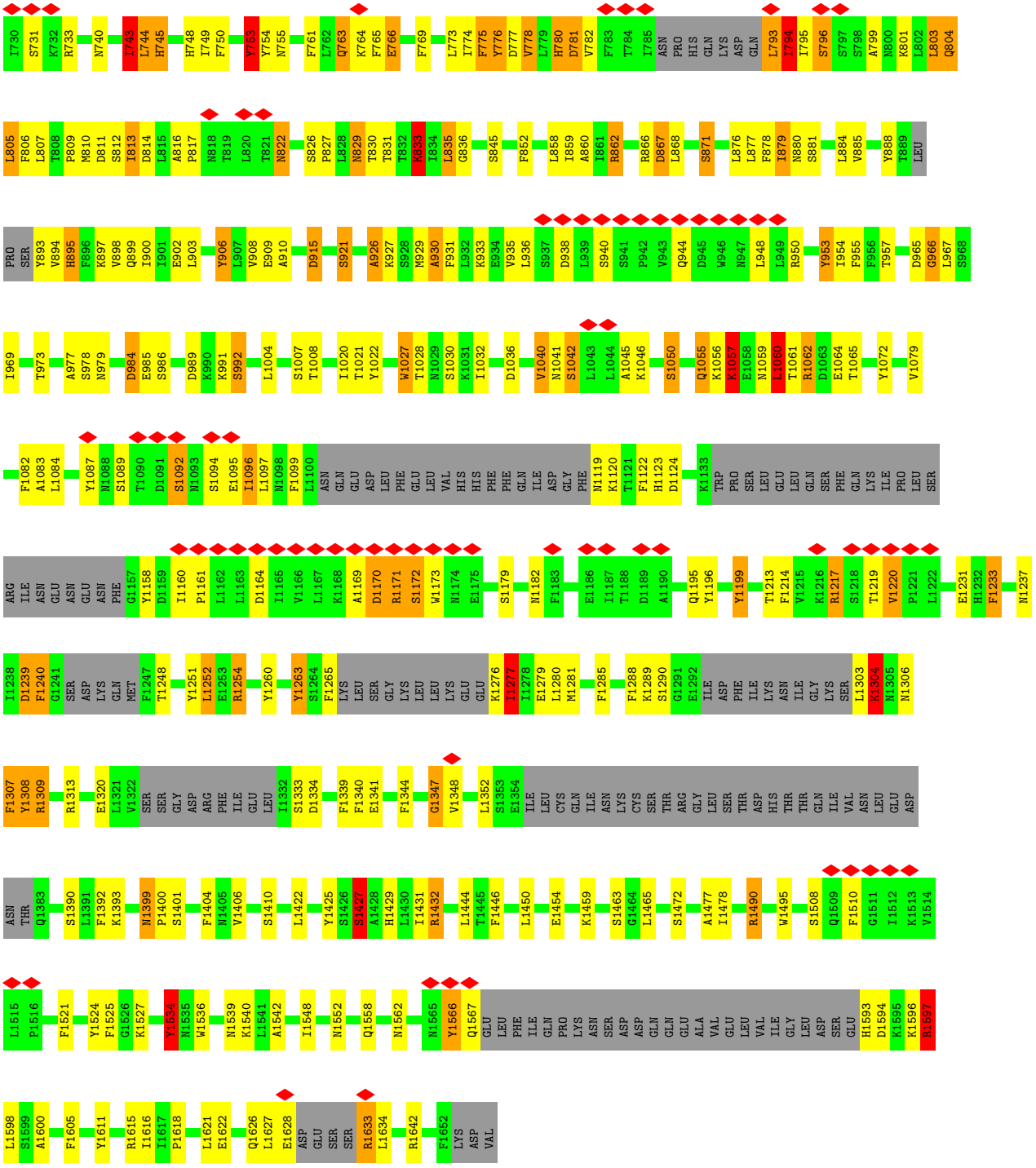
3 Residue-property plots (i)

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: Nucleoporin NUP188

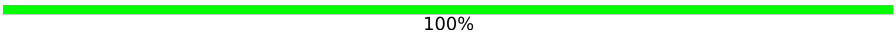
Chain X:





- Molecule 2: unknown

Chain Y:



There are no outlier residues recorded for this chain.

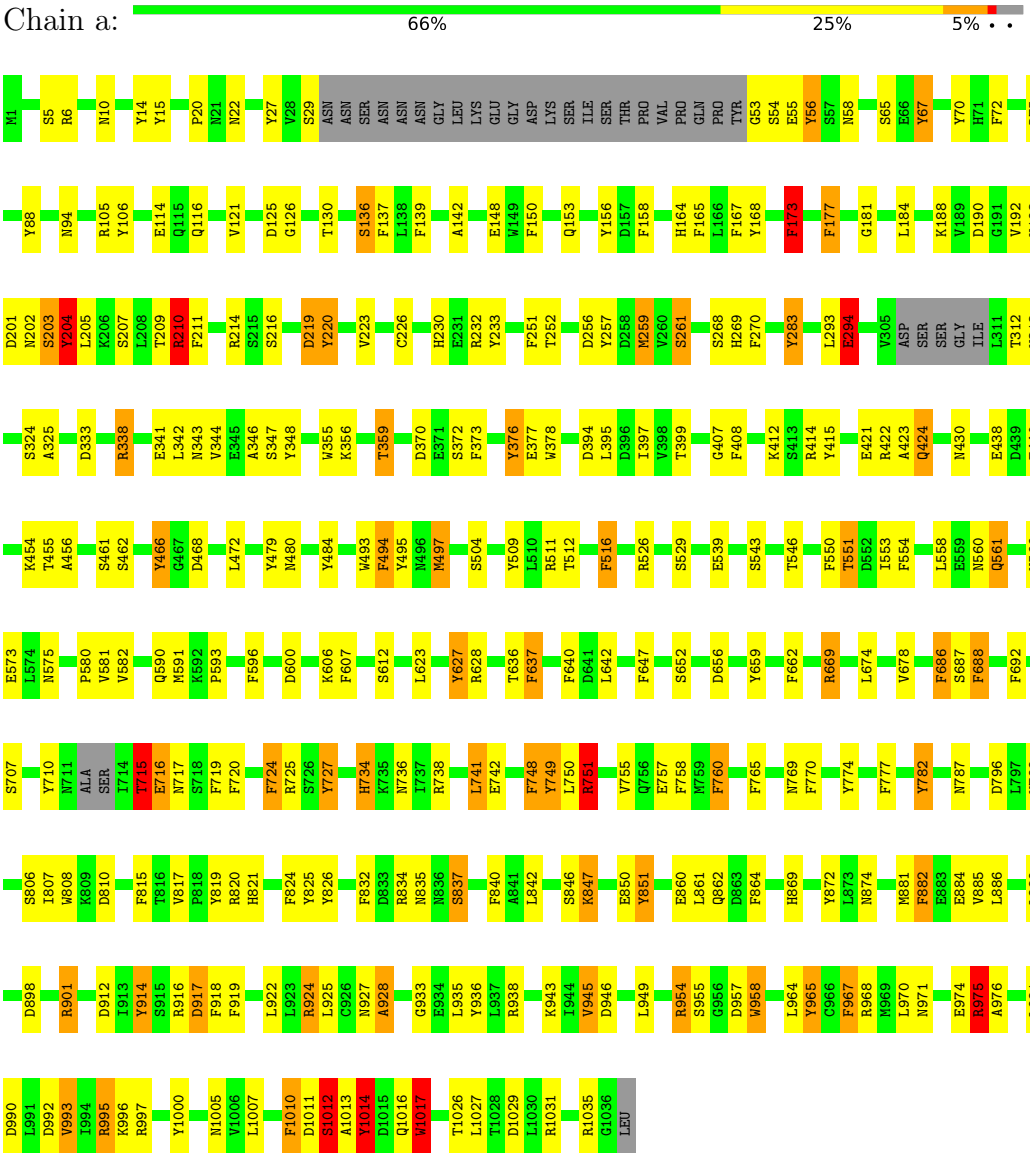
- Molecule 2: unknown

Chain Z:

There are no outlier residues recorded for this chain.

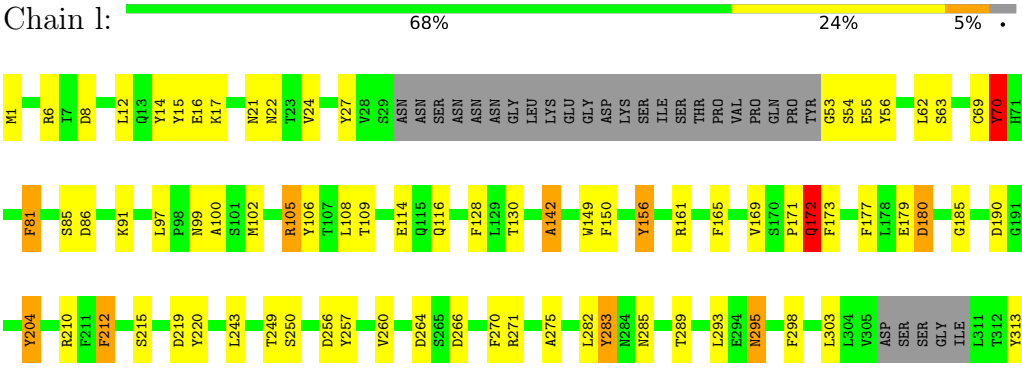
• Molecule 3: Nucleoporin NUP120

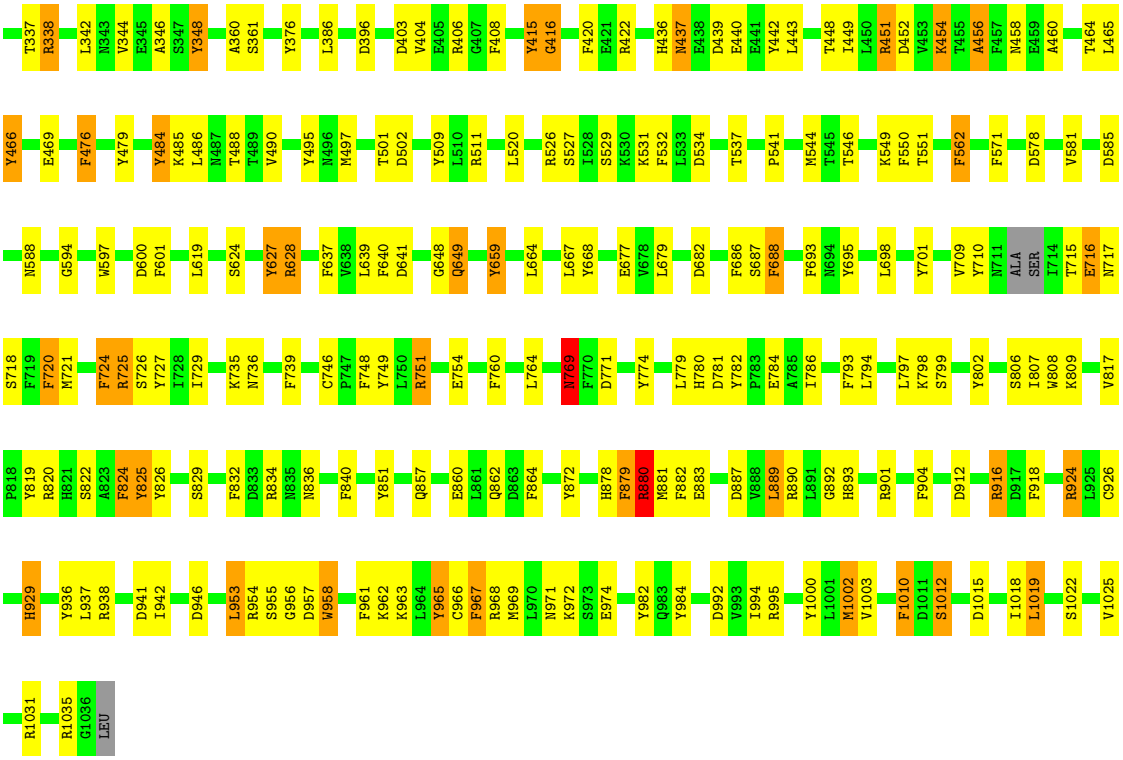
Chain a:



• Molecule 3: Nucleoporin NUP120

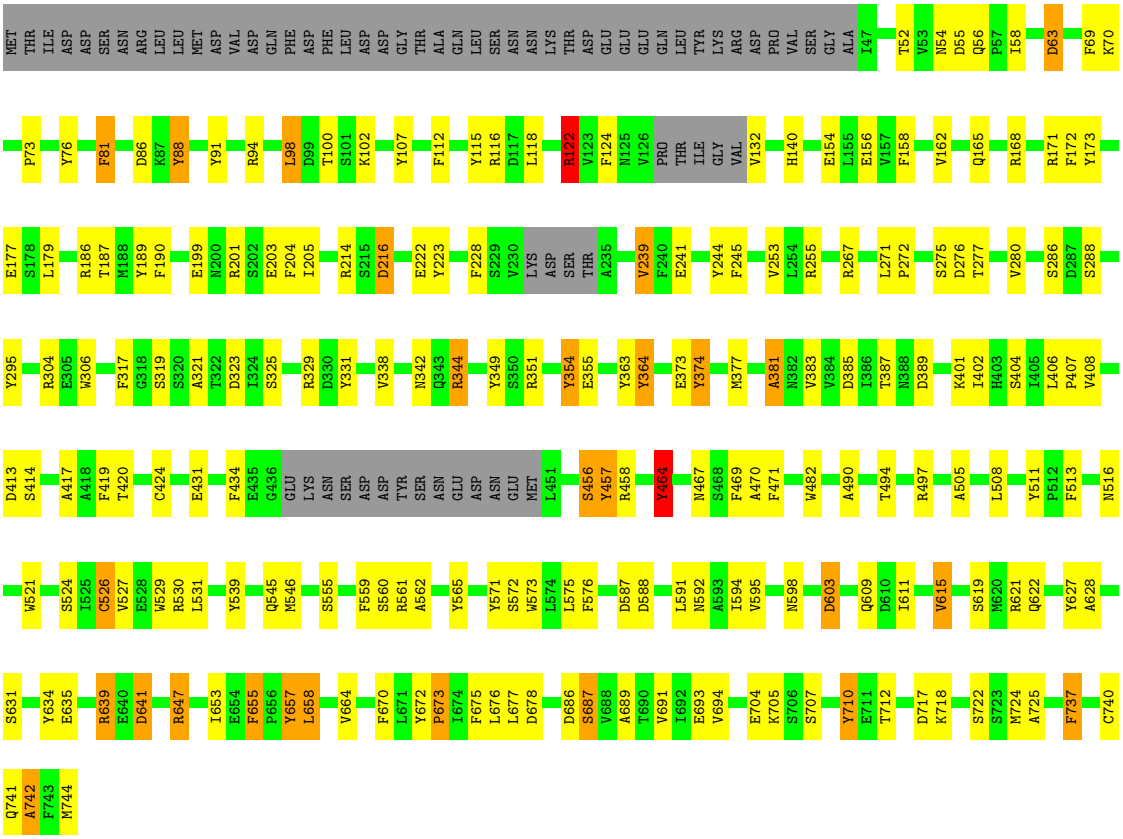
Chain l:





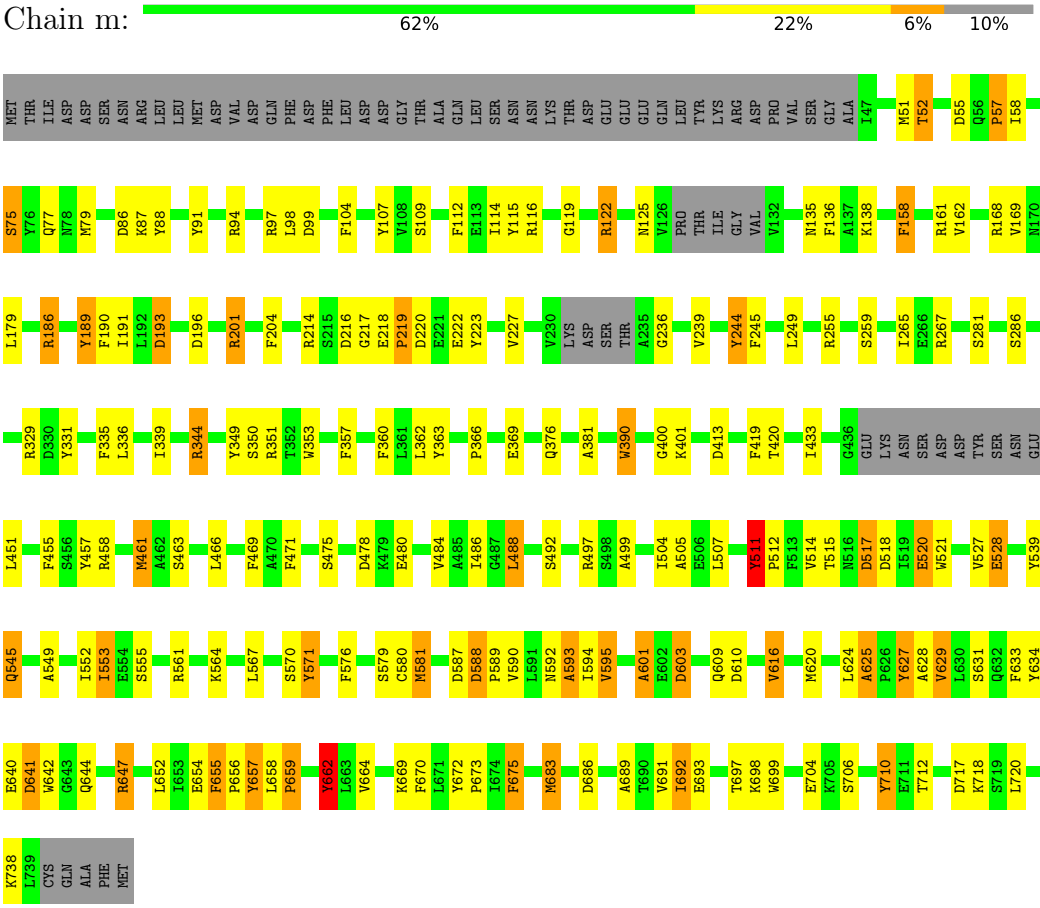
• Molecule 4: Nucleoporin NUP85

Chain b:



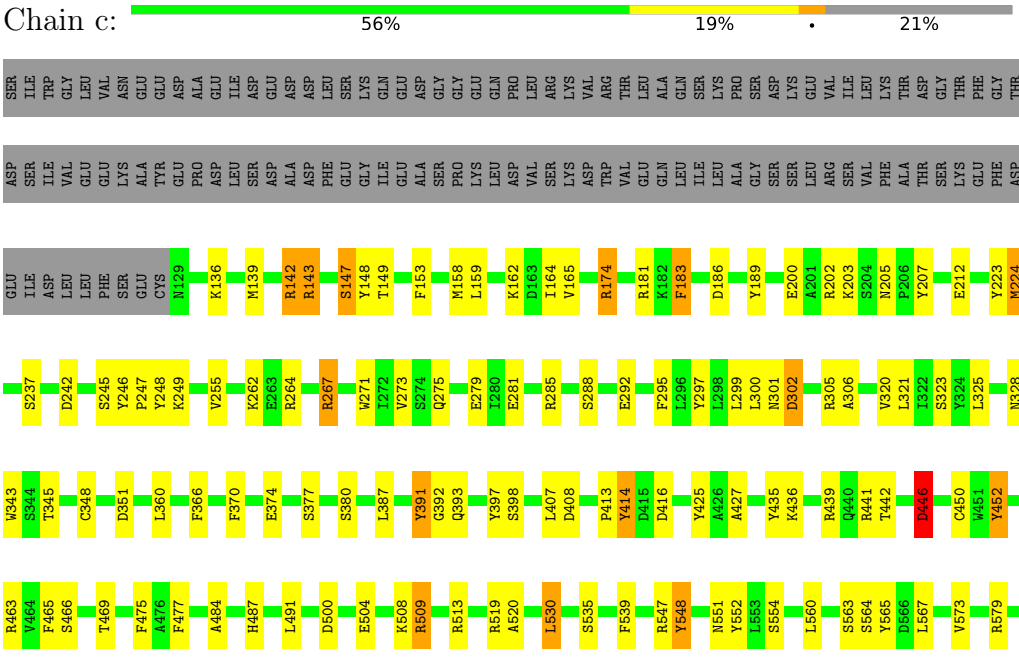
• Molecule 4: Nucleoporin NUP85

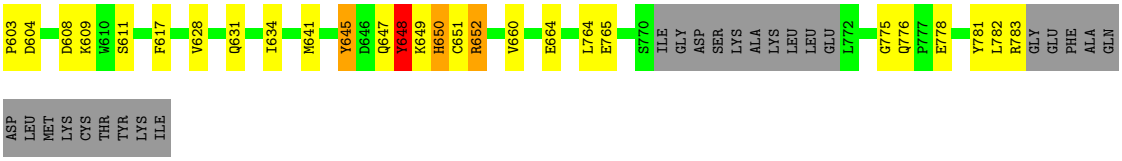
Chain m:



• Molecule 5: Nucleoporin 145c

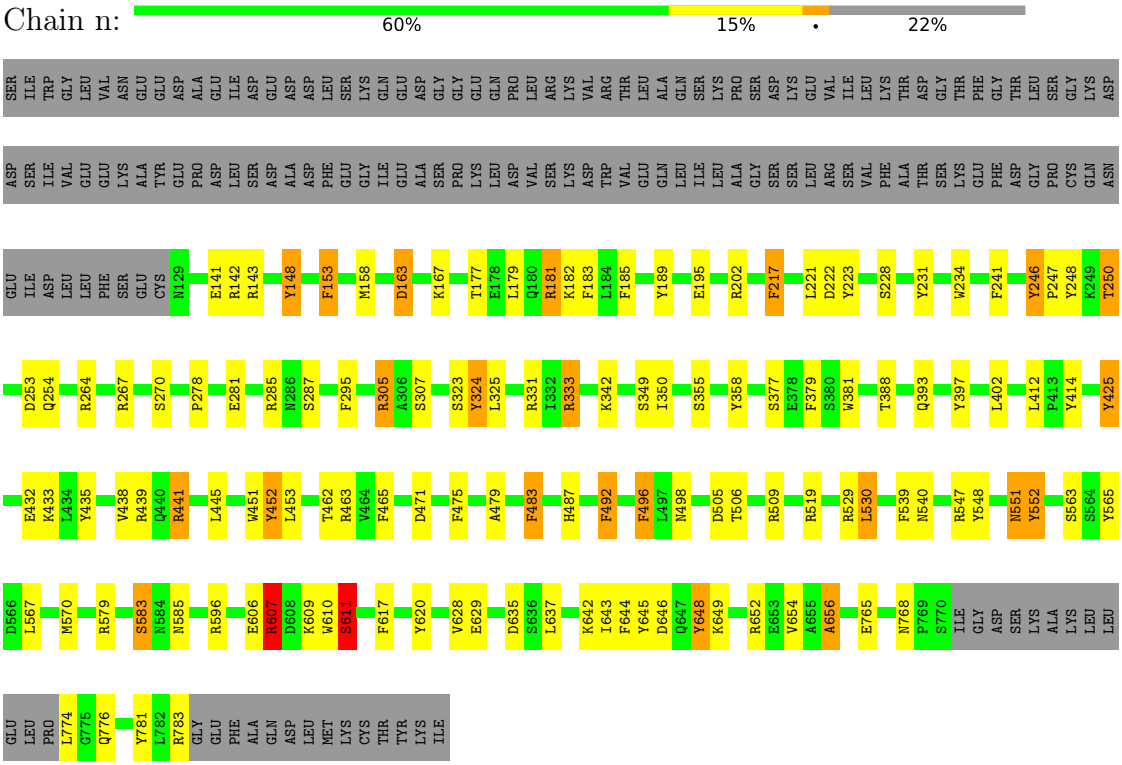
Chain c:





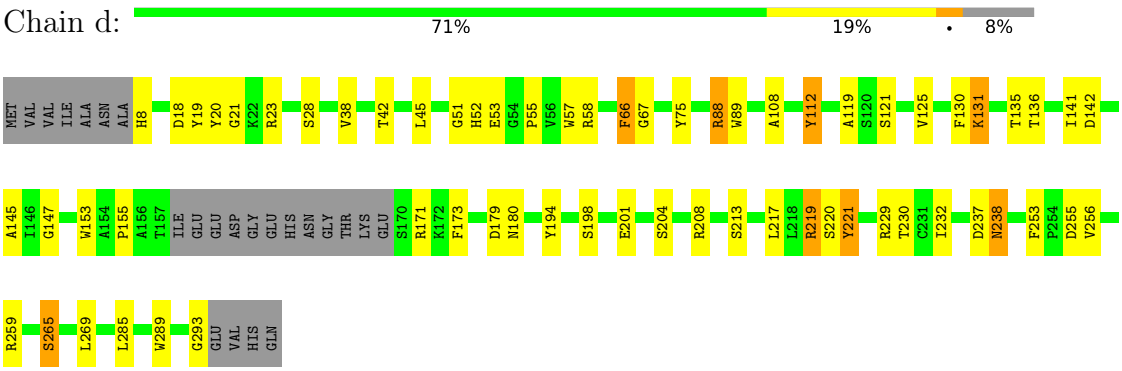
• Molecule 5: Nucleoporin 145c

Chain n:



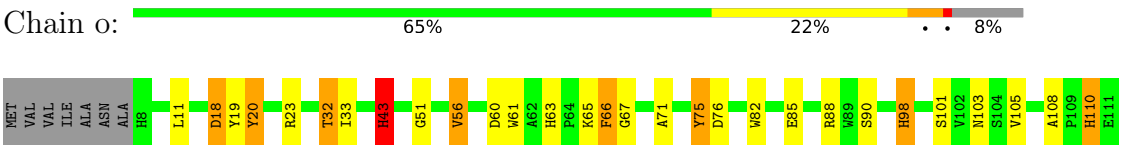
• Molecule 6: Protein transport protein SEC13

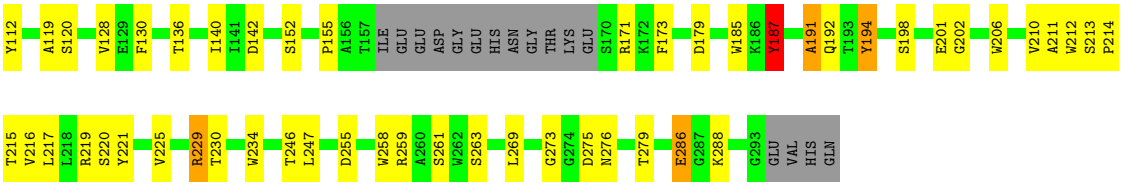
Chain d:



• Molecule 6: Protein transport protein SEC13

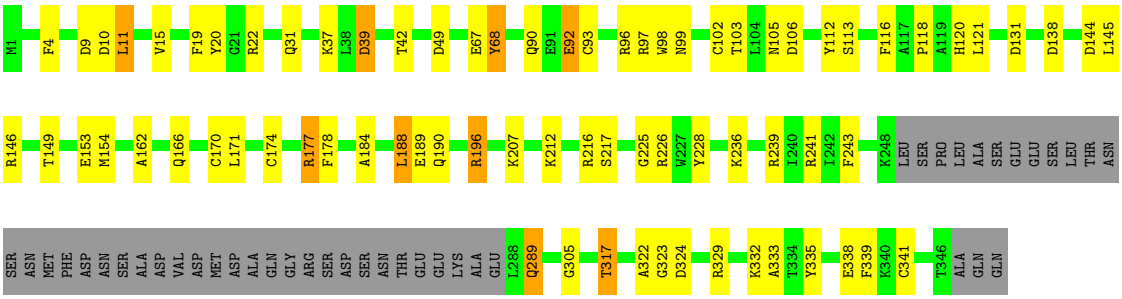
Chain o:





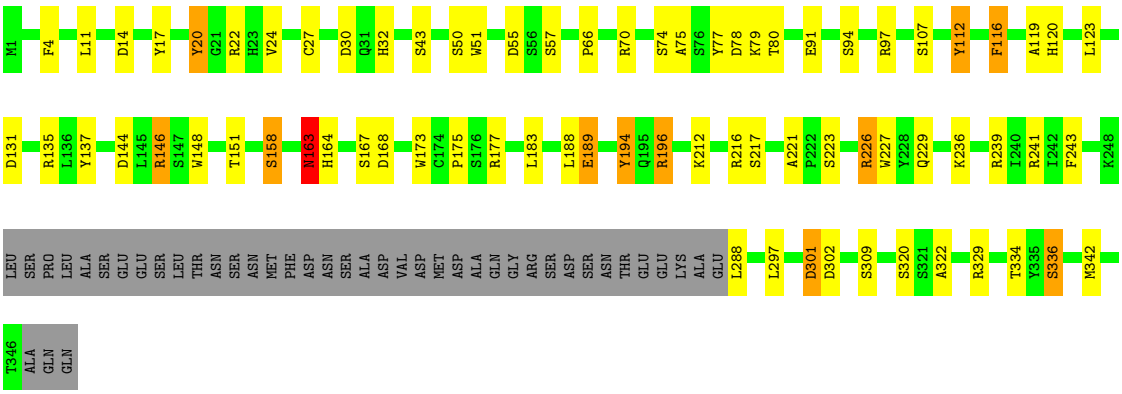
• Molecule 7: Nucleoporin SEH1

Chain e:



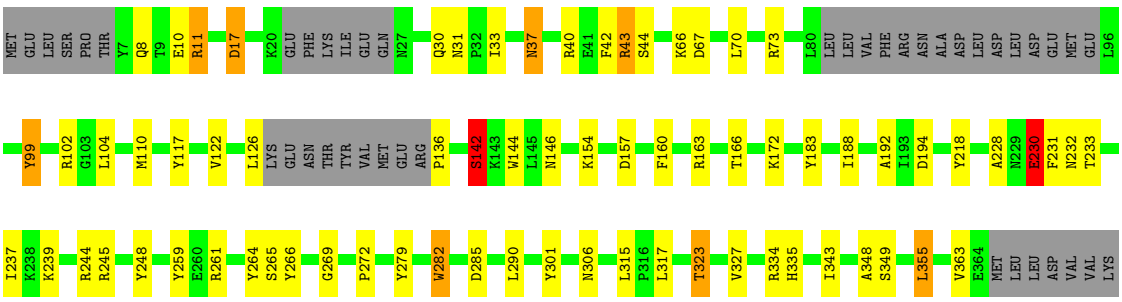
• Molecule 7: Nucleoporin SEH1

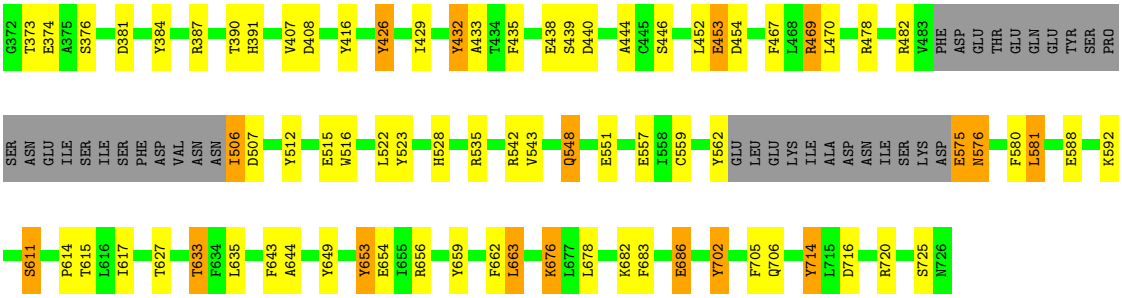
Chain p:



• Molecule 8: Nucleoporin NUP84

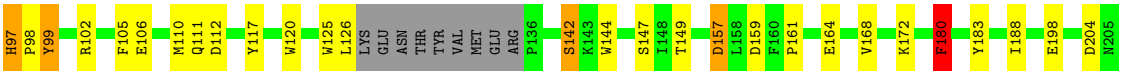
Chain f:

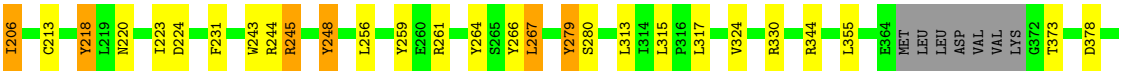


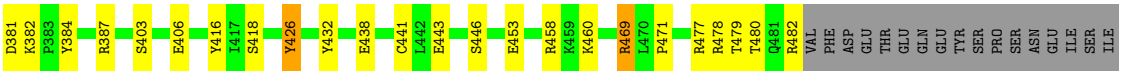


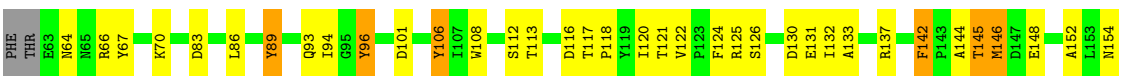
• Molecule 8: Nucleoporin NUP84

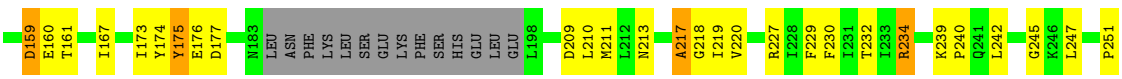
Chain q:





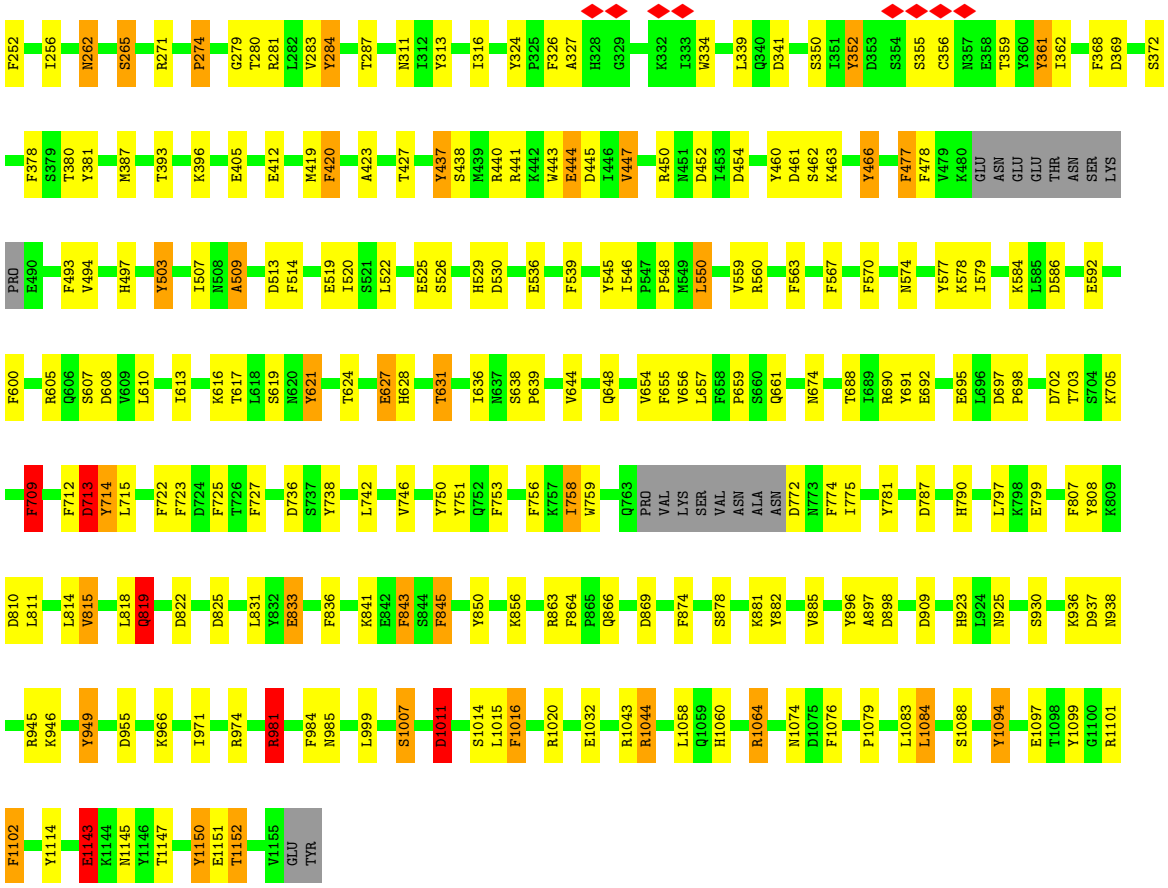






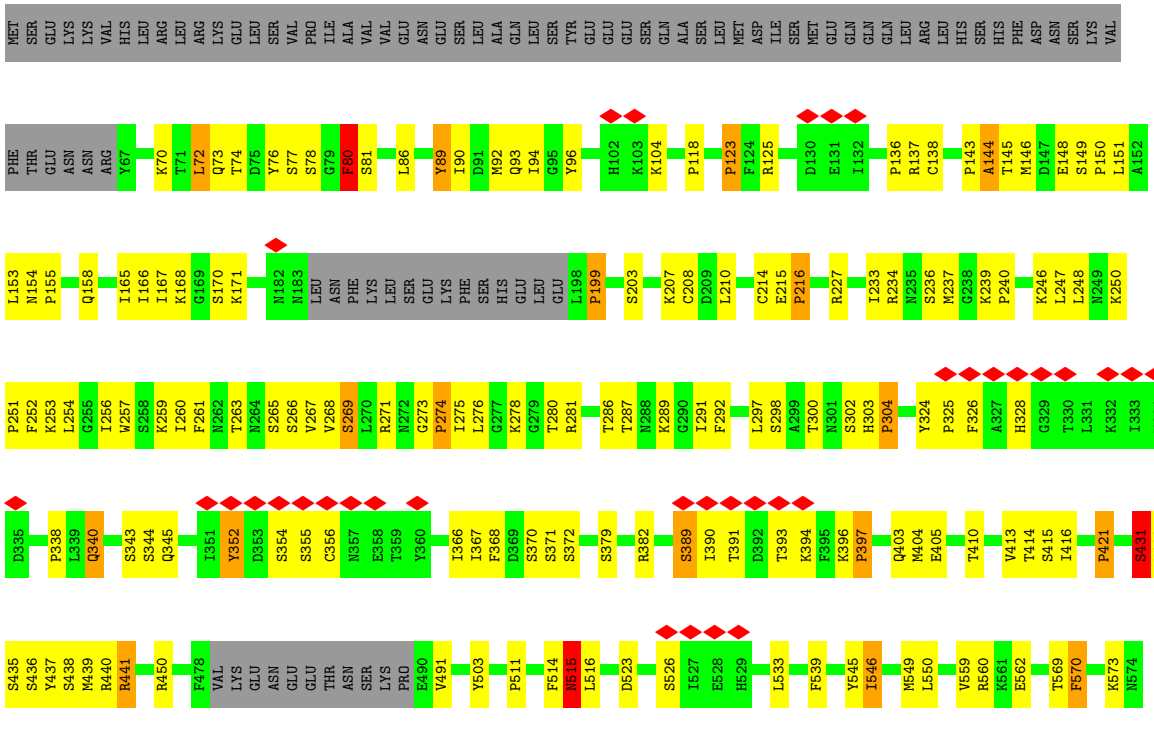
• Molecule 9: Nucleoporin NUP133

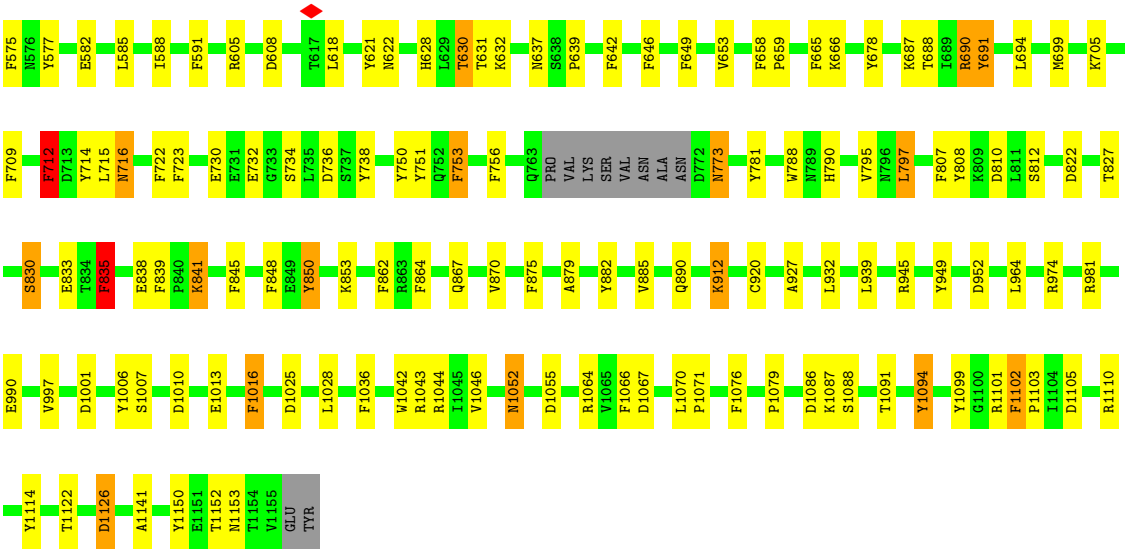
Chain g:



• Molecule 9: Nucleoporin NUP133

Chain r:




F575 N576 Y577 E582 L585 I588 F591 R605 D608 T617 L618 Y621 N622 H628 L629 T630 T631 K632 N637 S638 P639 F642 F646 F649 V653 F658 P659 F665 K666 Y678 K687 T688 I689 R690 Y691 L694 M699 K705
F709 F712 D713 Y714 L715 N716 F722 F723 E730 E731 E732 G733 S734 L735 D736 S737 Y738 Y750 Y751 Q752 F753 F756 Q763 PRO VAL LYS SER VAL ASN ALA ASN D772 N773 Y781 W788 N789 H790 V795 N796 L797 F807 Y808 K809 D810 L811 S812 D822 T827
S830 E833 T834 F835 E838 F839 P840 K841 F845 F848 E849 Y850 K853 F862 R863 F864 Q867 V870 F875 A879 Y882 V885 Q890 K912 C920 A927 L932 L939 R945 Y949 D962 L964 R974 R981
E990 V997 D1001 Y1006 S1007 D1010 E1013 F1016 D1025 L1028 F1036 W1042 R1043 R1044 I1045 V1046 N1052 D1055 R1064 V1065 F1066 D1067 L1070 P1071 F1076 P1079 D1086 K1087 S1088 T1091 Y1094 Y1099 G1100 R1101 F1102 P1103 I1104 D1105 R1110
Y1114 T1122 D1126 A1141 Y1150 E1151 T1152 N1153 T1154 V1155 GLU TYR

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	45000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3800	Depositor
Magnification	37651	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.130	Depositor
Minimum map value	-0.019	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	1276.8, 1276.8, 1276.8	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.66, 2.66, 2.66	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	X	1.68	65/9370 (0.7%)	2.00	242/12670 (1.9%)
3	a	1.73	82/8464 (1.0%)	2.03	250/11469 (2.2%)
3	l	1.75	82/8461 (1.0%)	2.03	235/11460 (2.1%)
4	b	1.71	48/5533 (0.9%)	2.00	149/7493 (2.0%)
4	m	1.73	42/5492 (0.8%)	1.97	149/7440 (2.0%)
5	c	1.72	40/4600 (0.9%)	1.95	107/6211 (1.7%)
5	n	1.70	30/4584 (0.7%)	1.93	95/6188 (1.5%)
6	d	1.75	22/2220 (1.0%)	1.91	46/3028 (1.5%)
6	o	1.72	16/2220 (0.7%)	2.04	73/3028 (2.4%)
7	e	1.71	19/2499 (0.8%)	2.01	70/3388 (2.1%)
7	p	1.66	14/2499 (0.6%)	1.95	60/3388 (1.8%)
8	f	1.64	22/5359 (0.4%)	1.90	115/7258 (1.6%)
8	q	1.69	39/5352 (0.7%)	1.92	139/7248 (1.9%)
9	g	1.69	58/8806 (0.7%)	1.97	210/11936 (1.8%)
9	r	3.94	53/8755 (0.6%)	2.91	392/11870 (3.3%)
All	All	2.05	632/84214 (0.8%)	2.09	2332/114075 (2.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	X	7	51
3	a	0	71
3	l	1	50
4	b	0	30
4	m	0	29
5	c	0	27
5	n	0	28
6	d	0	5
6	o	0	11
7	e	0	9

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	p	0	12
8	f	1	15
8	q	1	19
9	g	0	54
9	r	0	33
All	All	10	444

The worst 5 of 632 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	r	251	PRO	N-CD	123.85	3.21	1.47
9	r	150	PRO	N-CD	123.31	3.20	1.47
9	r	155	PRO	N-CD	122.44	3.19	1.47
9	r	325	PRO	N-CD	121.60	3.18	1.47
9	r	304	PRO	N-CD	119.21	3.14	1.47

The worst 5 of 2332 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	r	72	LEU	O-C-N	-62.08	23.37	122.70
9	r	431	SER	O-C-N	-49.50	43.50	122.70
9	r	215	GLU	C-N-CD	-43.53	24.84	120.60
9	r	274	PRO	N-CA-CB	38.04	148.95	103.30
9	r	150	PRO	N-CA-CB	37.90	148.78	103.30

5 of 10 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	X	793	LEU	CA
1	X	794	ILE	CA
1	X	1060	LEU	CA
1	X	1276	LYS	CA
1	X	1277	ILE	CA

5 of 444 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	150	GLN	Peptide
1	X	164	TYR	Sidechain
1	X	182	PHE	Sidechain
1	X	213	PHE	Peptide
1	X	322	HIS	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	X	9208	0	9538	148	0
2	Y	315	0	65	0	0
2	Z	315	0	65	0	0
3	a	8279	0	8125	0	0
3	l	8279	0	8121	0	0
4	b	5424	0	5397	0	0
4	m	5384	0	5361	0	0
5	c	4520	0	4539	0	0
5	n	4505	0	4521	0	0
6	d	2160	0	2096	0	0
6	o	2160	0	2096	0	0
7	e	2438	0	2378	0	0
7	p	2438	0	2378	0	0
8	f	5261	0	5261	0	0
8	q	5254	0	5252	0	0
9	g	8627	0	8539	0	0
9	r	8575	0	8469	0	0
All	All	83142	0	82201	148	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 10.

The worst 5 of 148 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:X:745:HIS:CE1	1:X:749:ILE:HG22	1.41	1.50
1:X:319:PRO:HD2	1:X:357:ASP:OD2	1.22	1.32
1:X:775:PHE:CE2	1:X:811:ASP:O	1.88	1.26
1:X:745:HIS:CE1	1:X:749:ILE:CG2	2.32	1.13
1:X:813:ILE:HG23	1:X:816:ALA:HB3	1.14	1.12

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	X	1099/1655 (66%)	839 (76%)	171 (16%)	89 (8%)	1	12
3	a	996/1037 (96%)	825 (83%)	114 (11%)	57 (6%)	1	18
3	l	991/1037 (96%)	809 (82%)	115 (12%)	67 (7%)	1	15
4	b	667/744 (90%)	545 (82%)	80 (12%)	42 (6%)	1	17
4	m	662/744 (89%)	531 (80%)	81 (12%)	50 (8%)	1	13
5	c	551/712 (77%)	474 (86%)	53 (10%)	24 (4%)	2	22
5	n	549/712 (77%)	488 (89%)	48 (9%)	13 (2%)	6	33
6	d	270/297 (91%)	229 (85%)	35 (13%)	6 (2%)	6	35
6	o	270/297 (91%)	231 (86%)	28 (10%)	11 (4%)	3	23
7	e	303/349 (87%)	263 (87%)	30 (10%)	10 (3%)	4	26
7	p	303/349 (87%)	265 (88%)	30 (10%)	8 (3%)	5	31
8	f	635/726 (88%)	554 (87%)	55 (9%)	26 (4%)	3	23
8	q	634/726 (87%)	546 (86%)	66 (10%)	22 (4%)	3	25
9	g	1052/1157 (91%)	847 (80%)	137 (13%)	68 (6%)	1	16
9	r	1048/1157 (91%)	917 (88%)	88 (8%)	43 (4%)	3	23
All	All	10030/11699 (86%)	8363 (83%)	1131 (11%)	536 (5%)	3	19

5 of 536 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	136	ASN
1	X	217	GLN
1	X	370	SER
1	X	408	PRO
1	X	430	ALA

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	X	1072/1557 (69%)	990 (92%)	82 (8%)	13	37
3	a	945/972 (97%)	897 (95%)	48 (5%)	24	48
3	l	945/972 (97%)	908 (96%)	37 (4%)	32	56
4	b	606/670 (90%)	579 (96%)	27 (4%)	27	52
4	m	602/670 (90%)	572 (95%)	30 (5%)	24	49
5	c	513/646 (79%)	487 (95%)	26 (5%)	24	48
5	n	511/646 (79%)	497 (97%)	14 (3%)	44	65
6	d	233/252 (92%)	223 (96%)	10 (4%)	29	53
6	o	233/252 (92%)	219 (94%)	14 (6%)	19	44
7	e	269/305 (88%)	261 (97%)	8 (3%)	41	63
7	p	269/305 (88%)	258 (96%)	11 (4%)	30	55
8	f	594/669 (89%)	549 (92%)	45 (8%)	13	37
8	q	593/669 (89%)	566 (95%)	27 (5%)	27	52
9	g	997/1088 (92%)	949 (95%)	48 (5%)	25	51
9	r	991/1088 (91%)	971 (98%)	20 (2%)	55	74
All	All	9373/10761 (87%)	8926 (95%)	447 (5%)	29	51

5 of 447 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	f	408	ASP
9	r	848	PHE
9	g	1058	LEU
9	r	632	LYS
7	p	342	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 137 such sidechains are listed below:

Mol	Chain	Res	Type
9	r	428	GLN
9	r	510	ASN
9	r	796	ASN
6	d	192	GLN
6	d	144	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	l	4
5	c	2
5	n	2
9	r	1
3	a	1
9	g	1

The worst 5 of 11 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	r	877:GLU	C	878:SER	N	16.07
1	l	207:SER	C	208:LEU	N	14.63
1	l	206:LYS	C	207:SER	N	13.72
1	a	486:LEU	C	487:ASN	N	6.43
1	c	533:PRO	C	535:SER	N	5.54

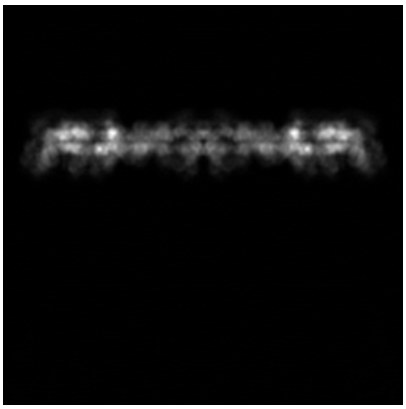
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24231. These allow visual inspection of the internal detail of the map and identification of artifacts.

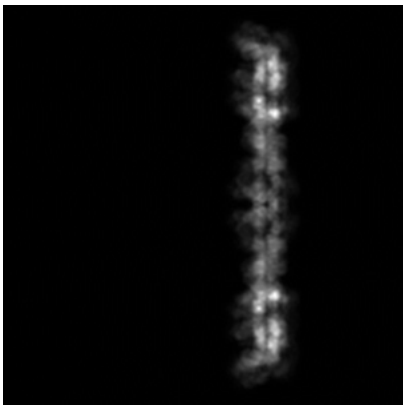
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

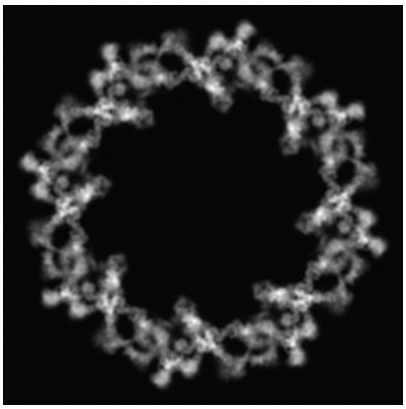
6.1.1 Primary map



X

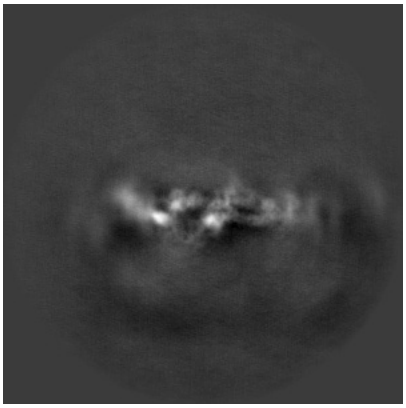


Y

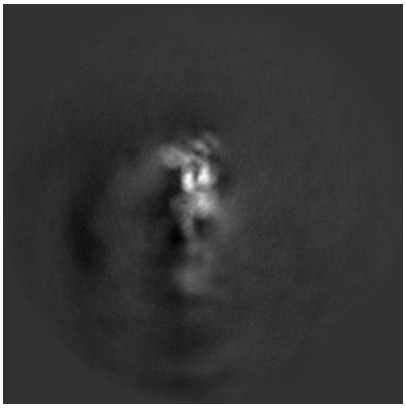


Z

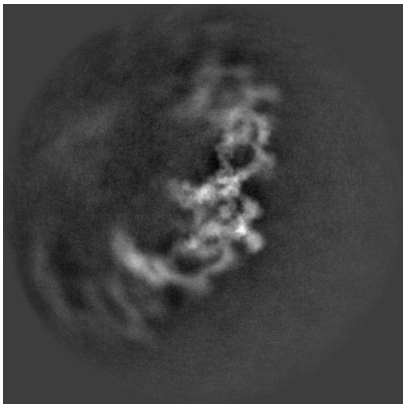
6.1.2 Raw map



X



Y



Z

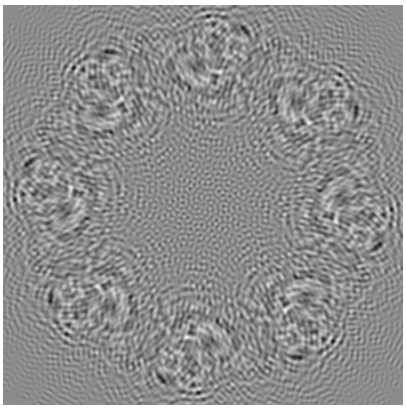
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map

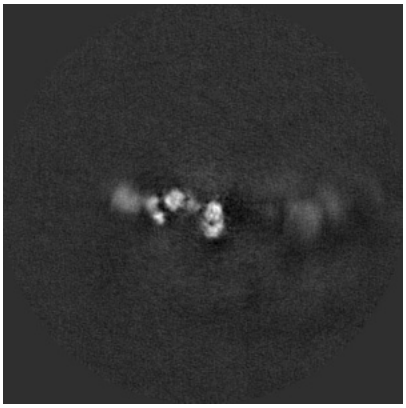
X Index: 240

Y Index: 240

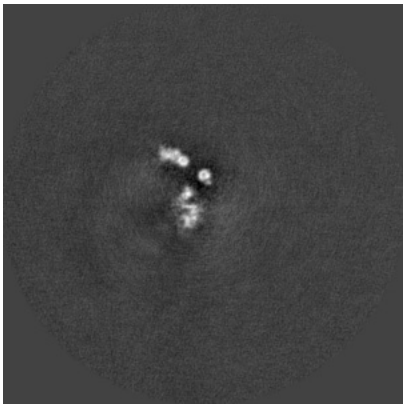


Z Index: 240

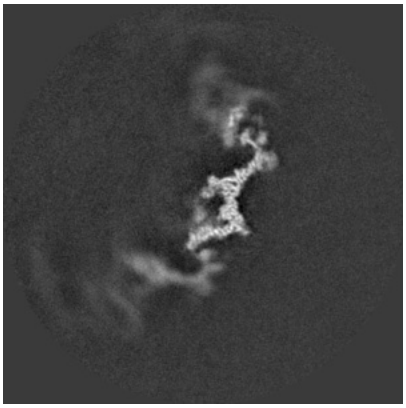
6.2.2 Raw map



X Index: 150



Y Index: 150

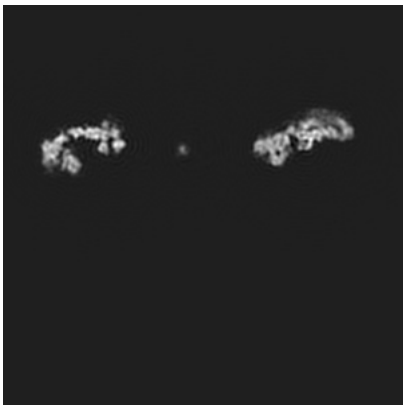


Z Index: 150

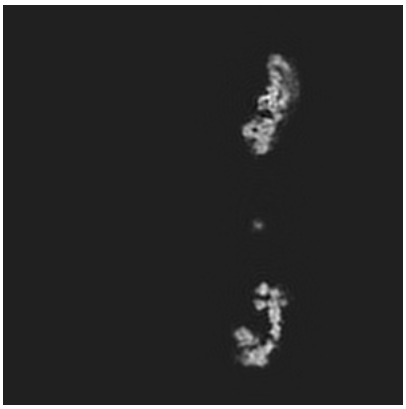
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

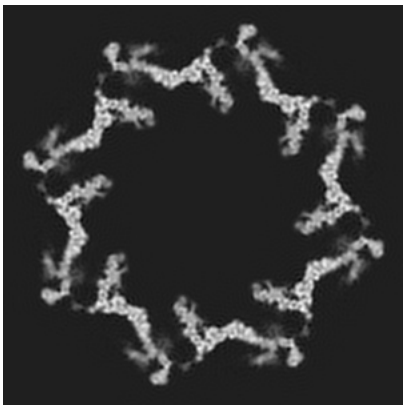
6.3.1 Primary map



X Index: 351

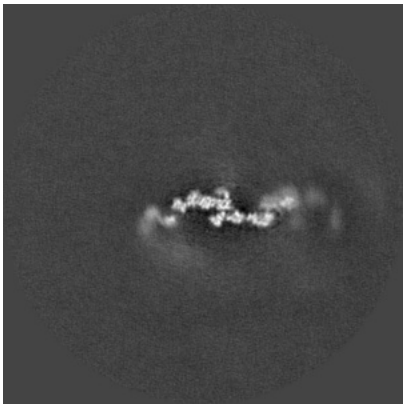


Y Index: 129

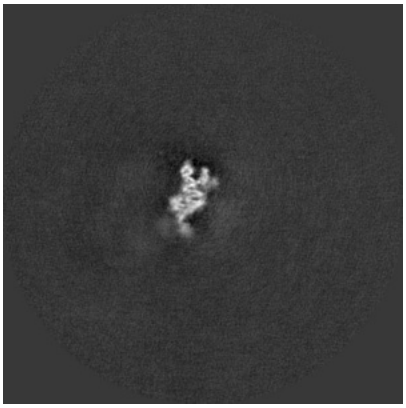


Z Index: 309

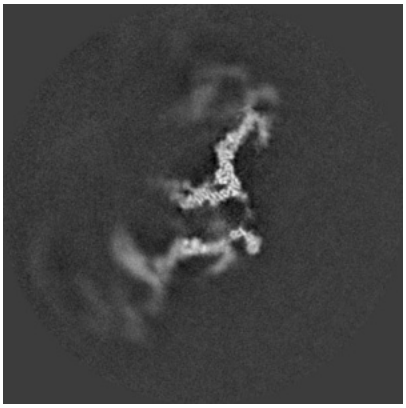
6.3.2 Raw map



X Index: 170



Y Index: 158

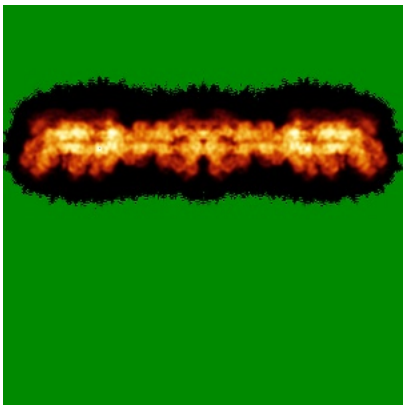


Z Index: 140

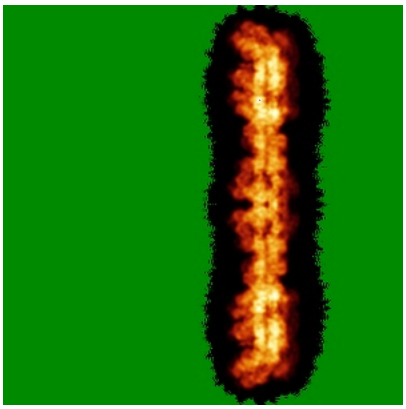
The images above show the largest variance slices of the map in three orthogonal directions.

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

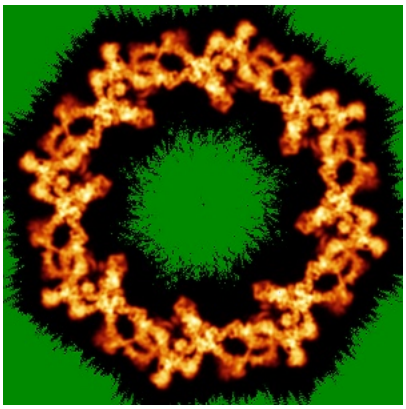
6.4.1 Primary map



X

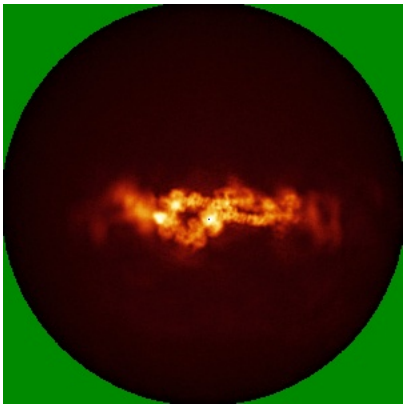


Y

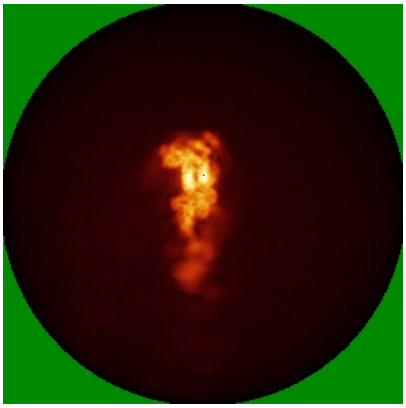


Z

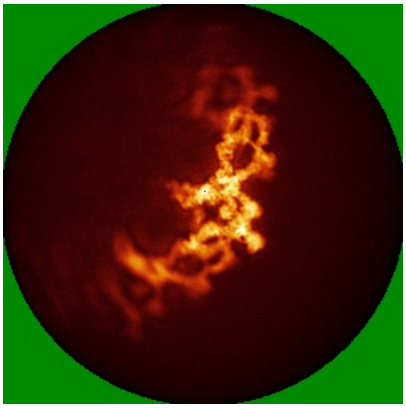
6.4.2 Raw map



X



Y

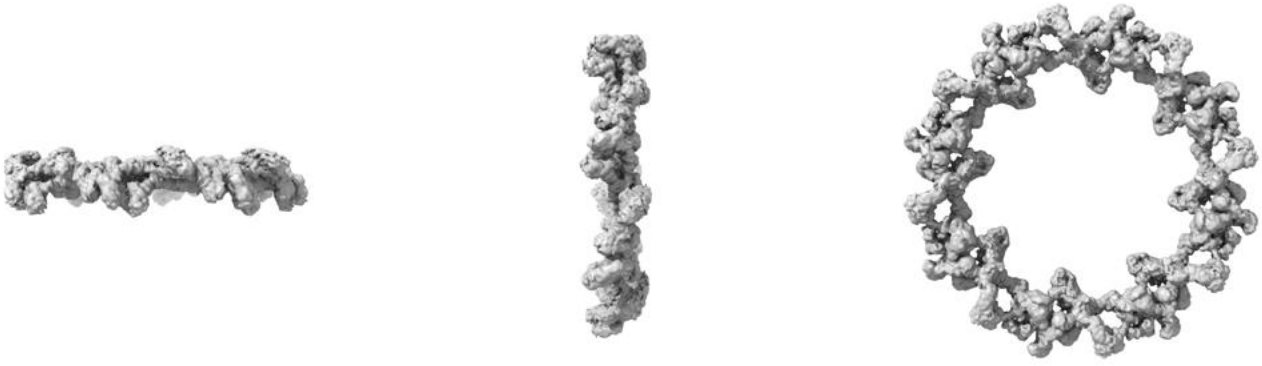


Z

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)

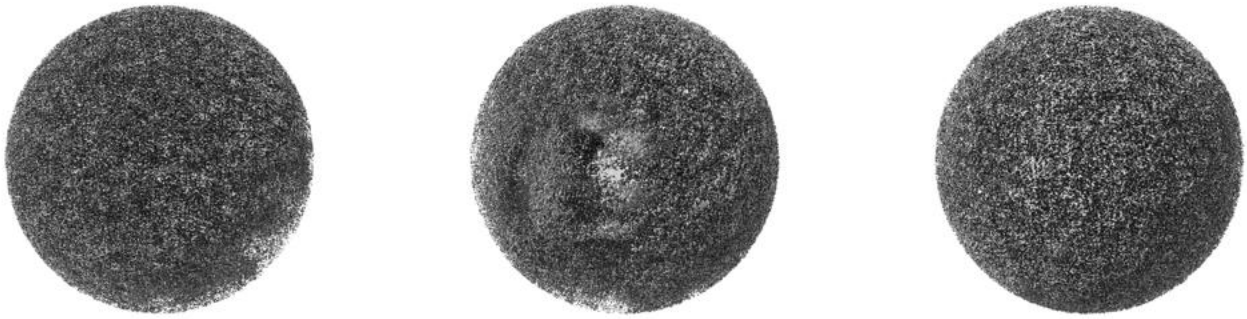
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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.

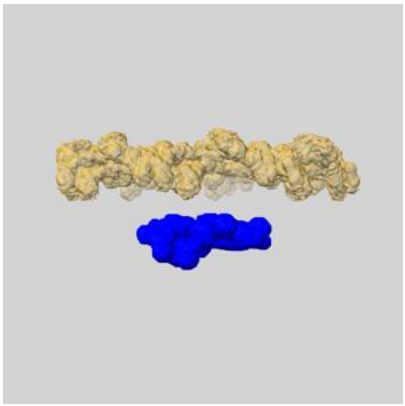
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

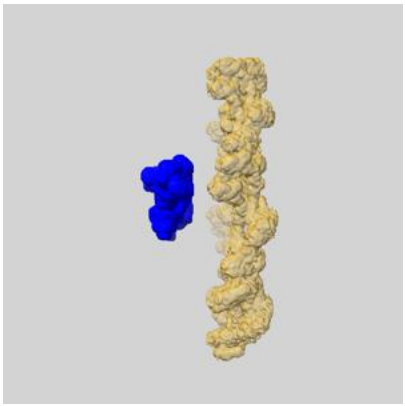
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

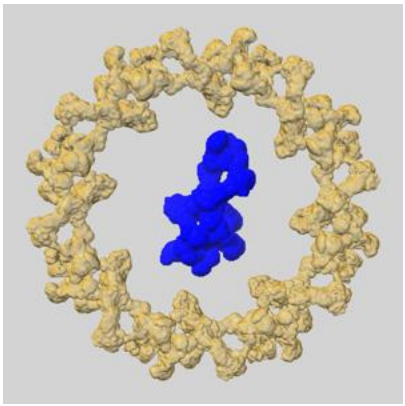
6.6.1 emd_24231_msk_1.map (i)



X



Y

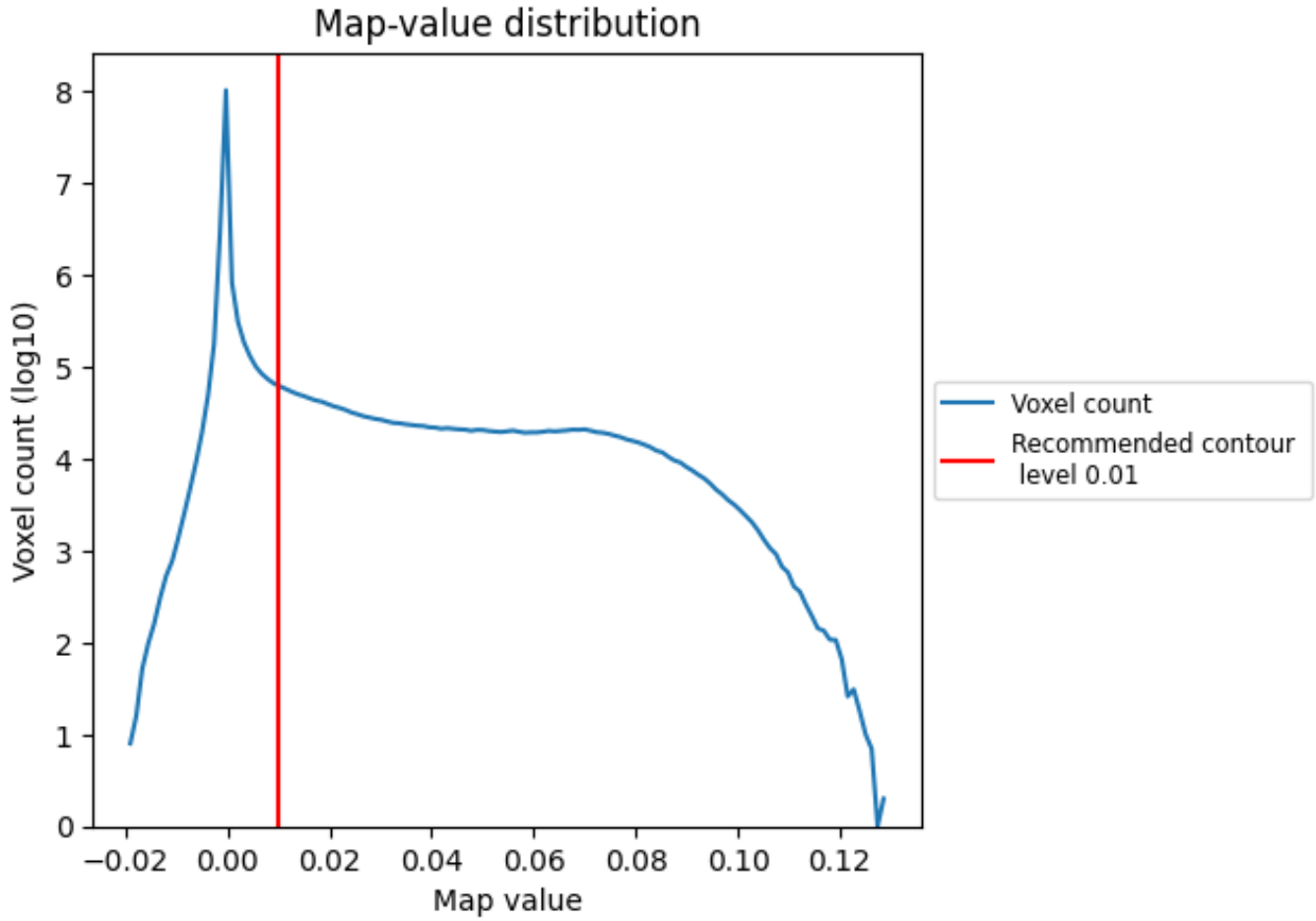


Z

7 Map analysis

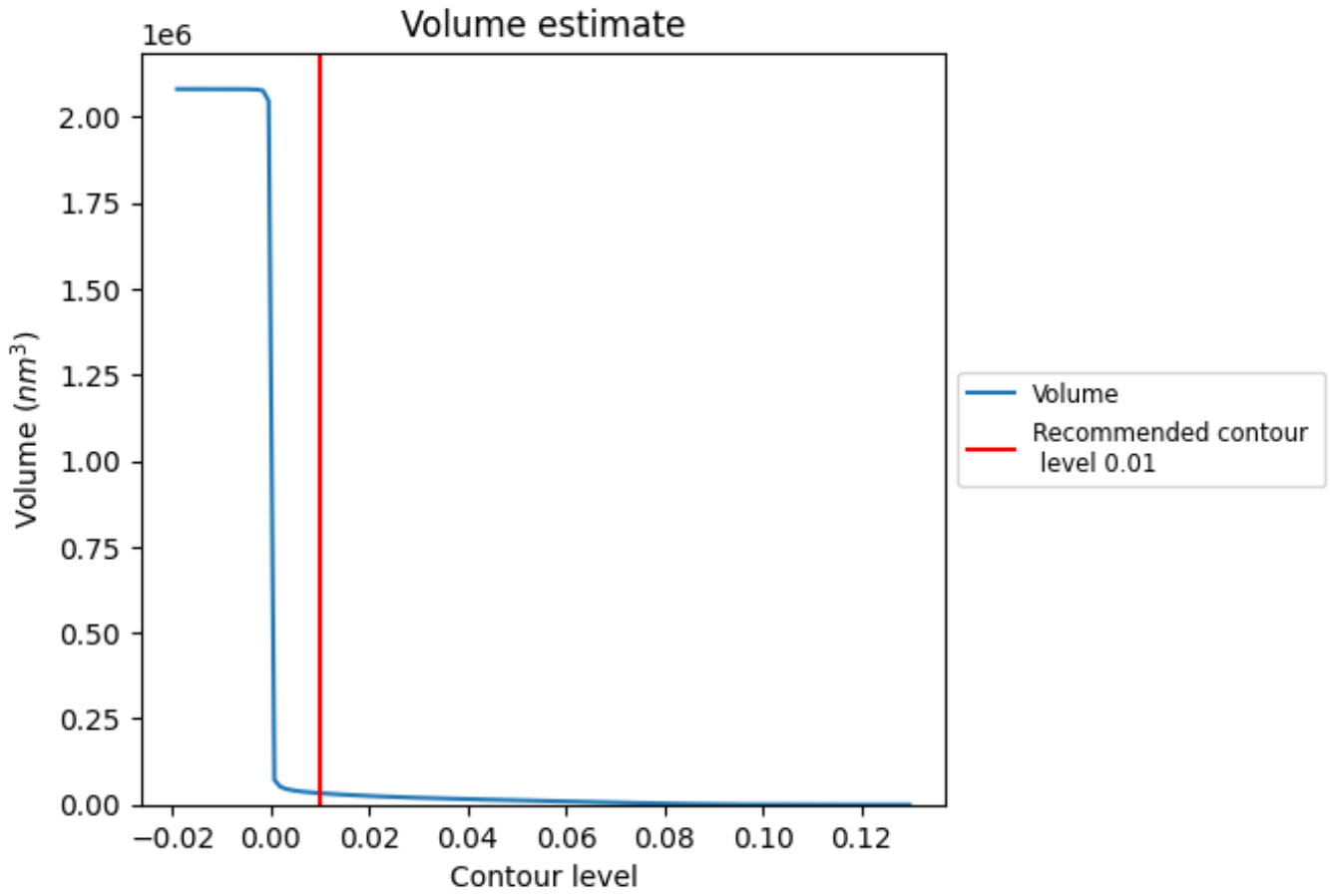
This section contains the results of statistical analysis of the map.

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.

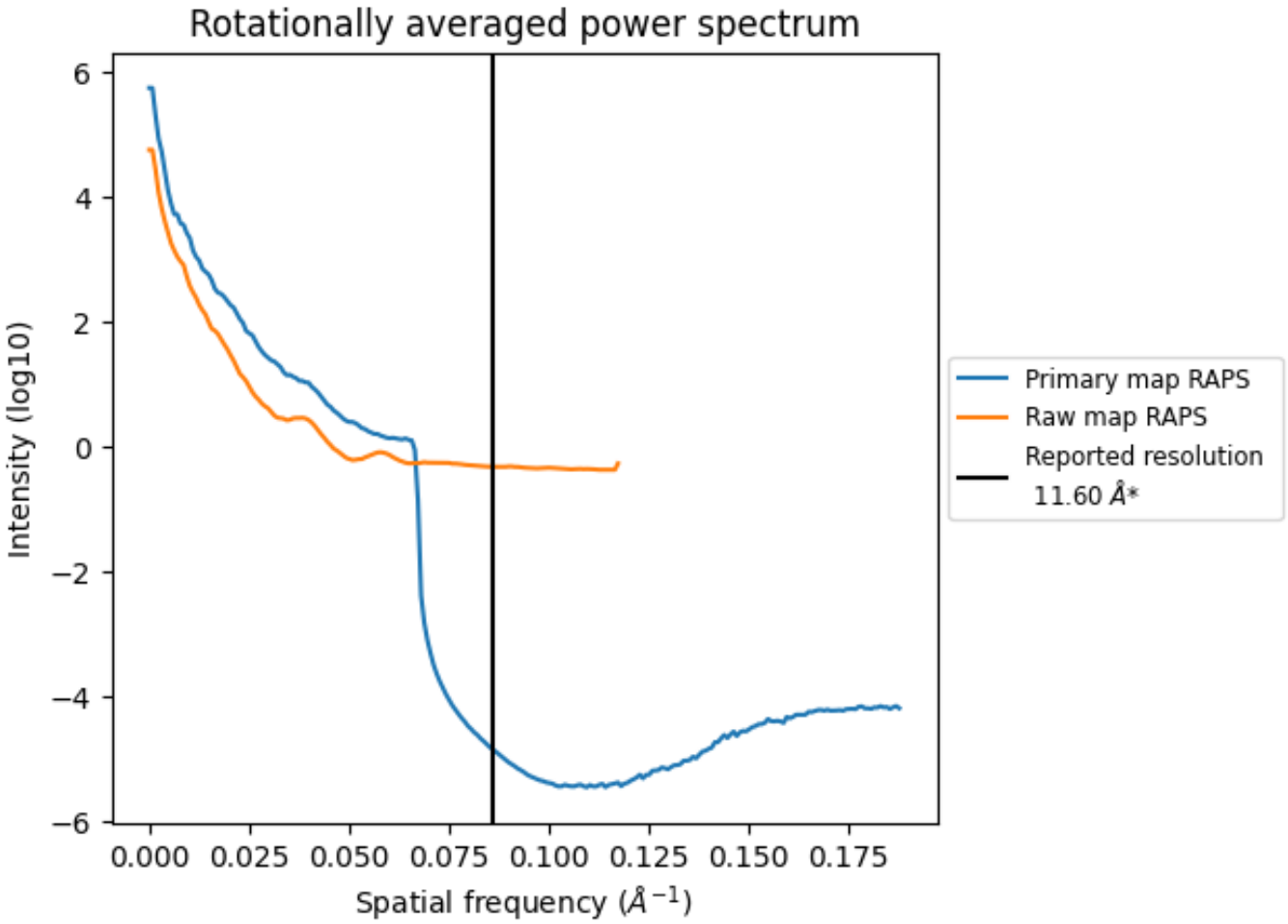
7.2 Volume estimate (i)



The volume at the recommended contour level is 33303 nm^3; this corresponds to an approximate mass of 30083 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)

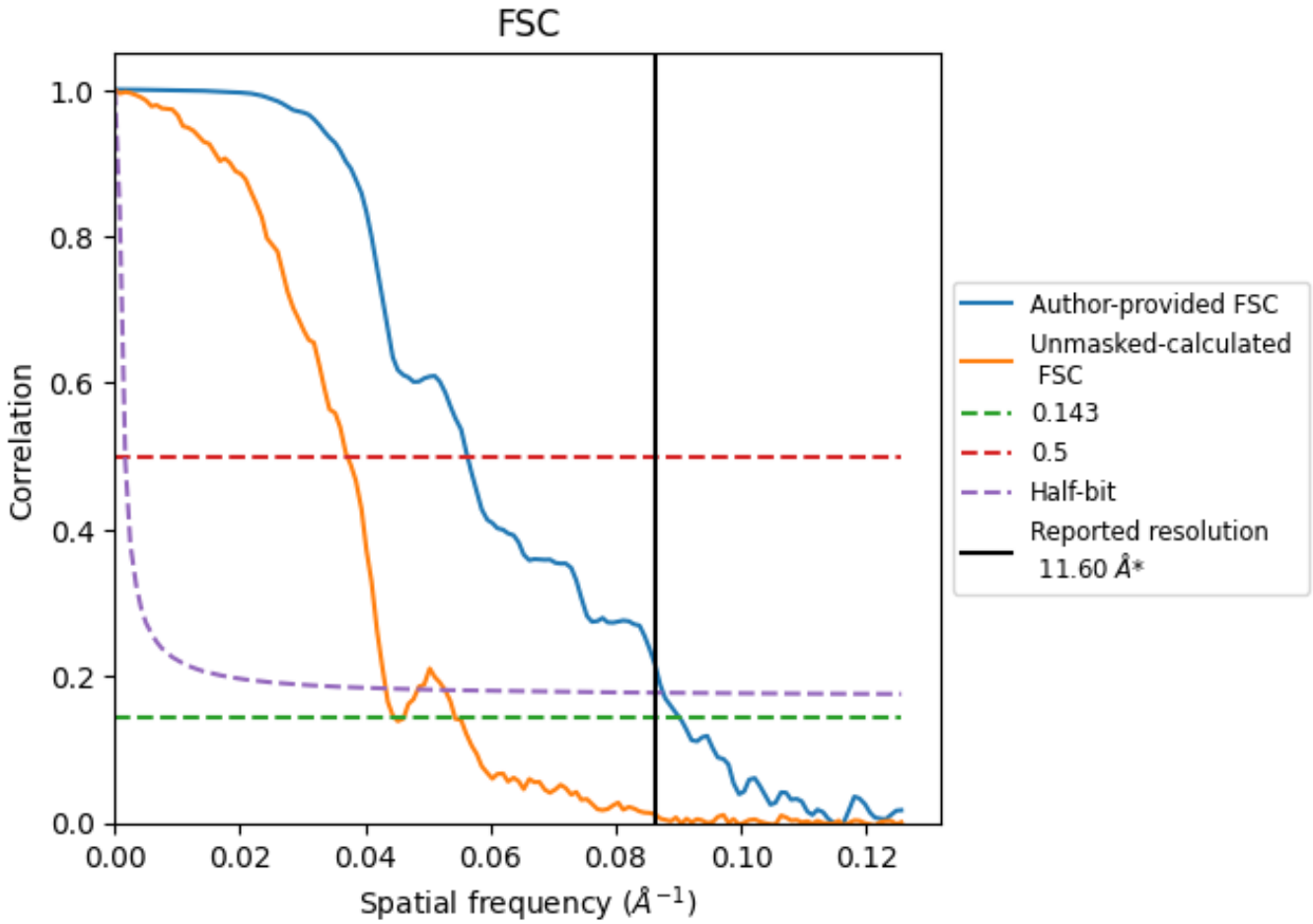


*Reported resolution corresponds to spatial frequency of 0.086 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.086 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	11.60	-	-
Author-provided FSC curve	11.09	17.76	11.42
Unmasked-calculated*	22.37	26.95	23.15

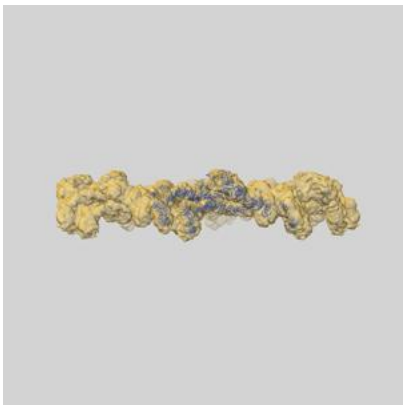
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 22.37 differs from the reported value 11.6 by more than 10 %

9 Map-model fit

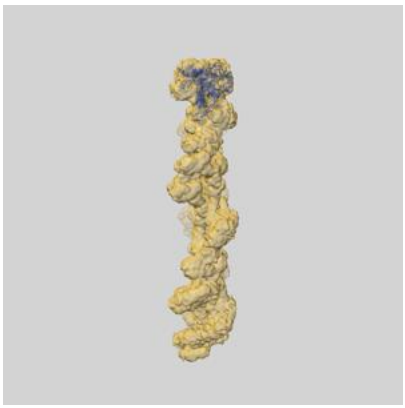
This section contains information regarding the fit between EMDB map EMD-24231 and PDB model 7N84. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

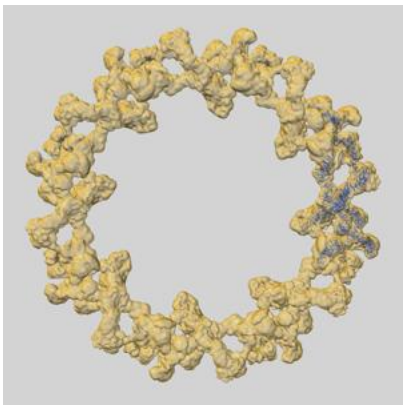
9.1.1 Map-model overlay



X

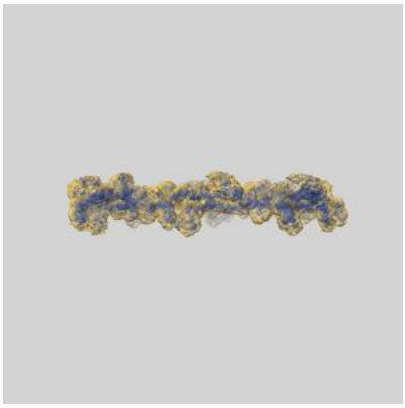


Y

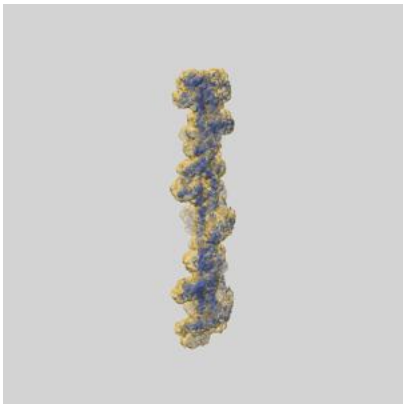


Z

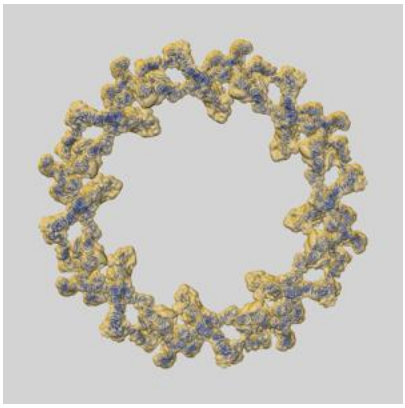
9.1.2 Map-model assembly overlay



X



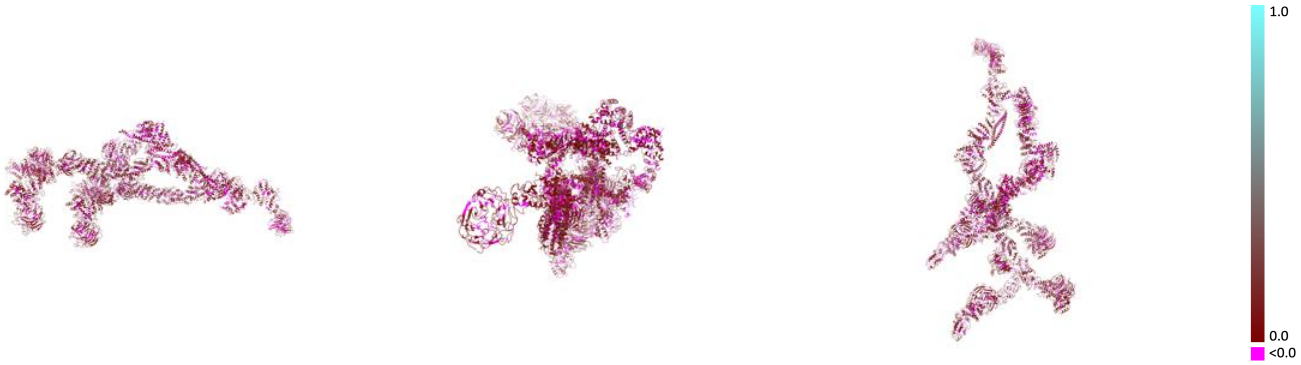
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 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.

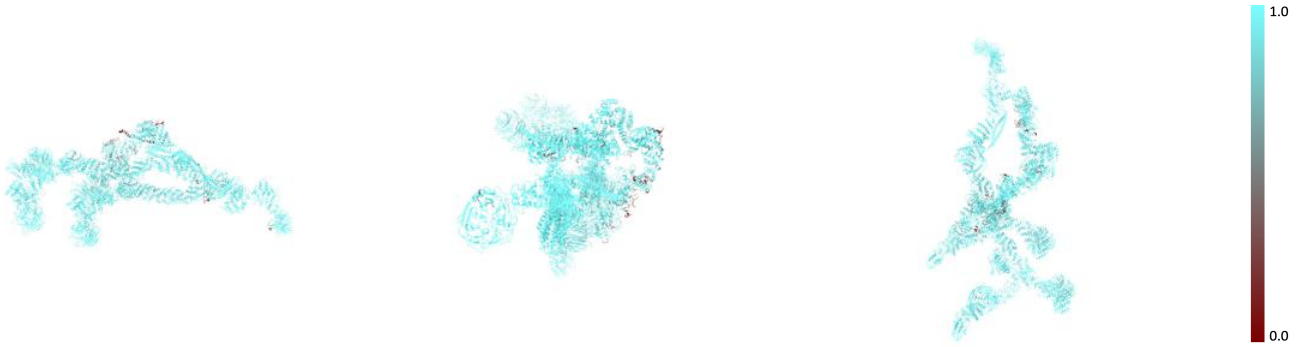
9.2 Q-score mapped to coordinate model



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.

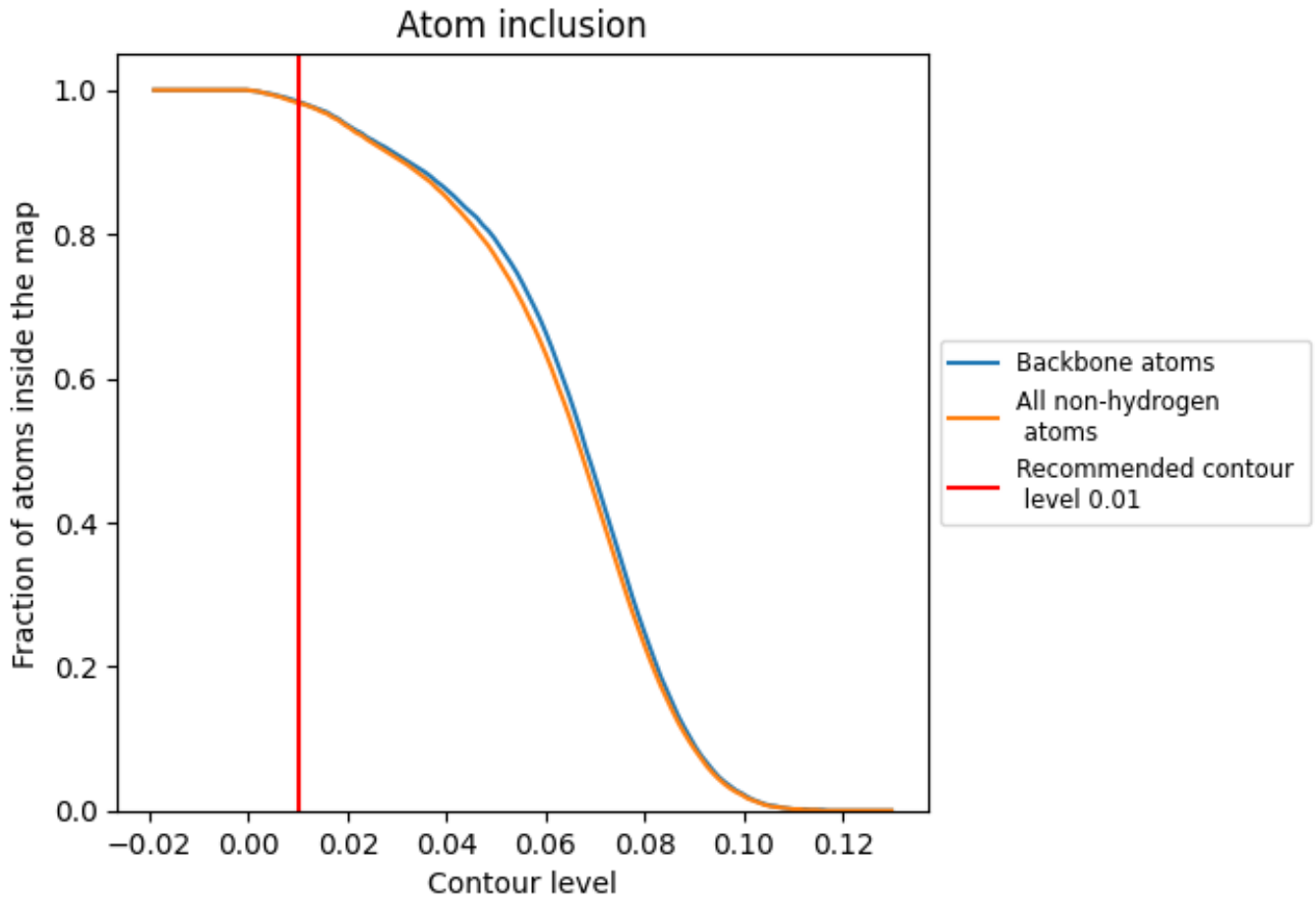
9.3 Atom inclusion mapped to coordinate model



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 (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 98% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9820	0.0630
X	0.8870	0.0340
Y	0.9870	0.0690
Z	1.0000	0.0680
a	1.0000	0.0700
b	1.0000	0.0610
c	1.0000	0.0820
d	1.0000	0.0660
e	1.0000	0.0680
f	1.0000	0.0760
g	0.9910	0.0490
l	1.0000	0.0700
m	1.0000	0.0700
n	1.0000	0.0860
o	1.0000	0.0690
p	1.0000	0.0620
q	1.0000	0.0770
r	0.9610	0.0520