wwPDB EM Validation Summary Report

May 25, 2024 – 04:05 PM EDT

PDB ID	:	7N85
EMDB ID	:	EMD-24232
Title	:	Inner ring spoke 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	:	7.60 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:

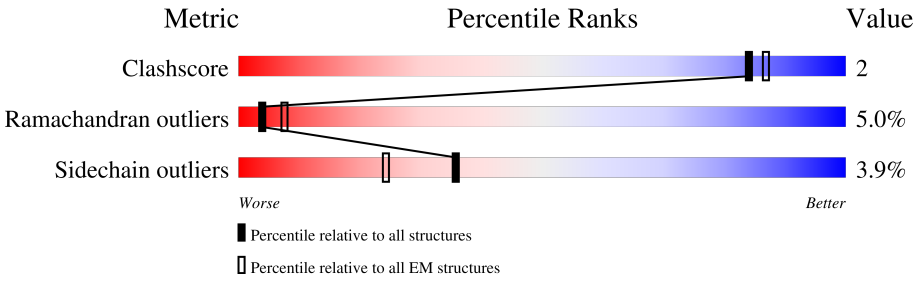
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 7.60 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	0	1502	65% 7% 27%
1	Y	1502	64% 6% 28%
2	1	1391	25% 71% 7% 20%
2	Z	1391	25% 72% 6% 20%
3	5	36	94% 6%
3	6	36	100%
4	A	823	19% 80%
4	D	823	19% 80%

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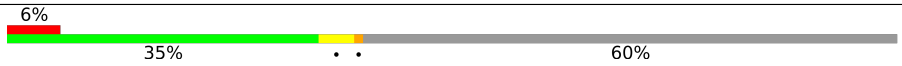
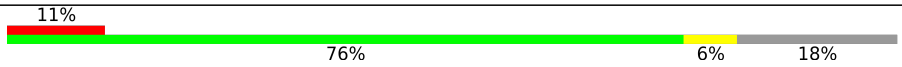
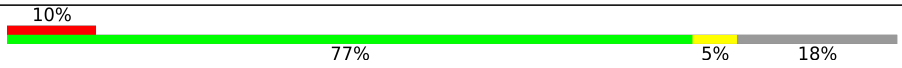
Mol	Chain	Length	Quality of chain
4	G	823	
4	J	823	
5	B	541	
5	E	541	
5	H	541	
5	K	541	
6	C	472	
6	F	472	
6	I	472	
6	L	472	
7	M	1683	
7	O	1683	
8	N	1655	
8	P	1655	
9	Q	839	
9	R	839	
9	S	839	
9	T	839	
10	U	475	
10	W	475	
11	V	528	
11	X	528	

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 123117 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 NUP170.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	1102	Total	C	N	O	S	0	0
			8890	5753	1449	1659	29		
1	Y	1084	Total	C	N	O	S	0	0
			8747	5663	1422	1632	30		

- Molecule 2 is a protein called Nucleoporin NUP157.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	1111	Total	C	N	O	S	0	0
			8903	5707	1477	1691	28		
2	Z	1108	Total	C	N	O	S	0	0
			8883	5695	1474	1686	28		

- Molecule 3 is a protein called Unknown connectors.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	5	36	Total	C	N	O	0	0
			181	108	36	37		
3	6	36	Total	C	N	O	0	0
			181	108	36	37		

- Molecule 4 is a protein called Nucleoporin NSP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	163	Total	C	N	O	S	0	0
			1315	814	220	280	1		
4	D	163	Total	C	N	O	S	0	0
			1315	814	220	280	1		
4	G	164	Total	C	N	O	S	0	0
			1321	817	221	282	1		
4	J	163	Total	C	N	O	S	0	0
			1315	814	220	280	1		

- Molecule 5 is a protein called Nucleoporin NUP57.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	217	Total	C	N	O	S	0	0
			1771	1115	317	336	3		
5	E	217	Total	C	N	O	S	0	0
			1771	1115	317	336	3		
5	H	217	Total	C	N	O	S	0	0
			1771	1115	317	336	3		
5	K	217	Total	C	N	O	S	0	0
			1771	1115	317	336	3		

- Molecule 6 is a protein called Nucleoporin NUP49/NSP49.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	166	Total	C	N	O	S	0	0
			1347	863	217	265	2		
6	F	167	Total	C	N	O	S	0	0
			1351	865	218	266	2		
6	I	166	Total	C	N	O	S	0	0
			1347	863	217	265	2		
6	L	167	Total	C	N	O	S	0	0
			1351	865	218	266	2		

- Molecule 7 is a protein called Nucleoporin NUP192.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	1520	Total	C	N	O	S	0	0
			11905	7692	1942	2240	31		
7	O	1521	Total	C	N	O	S	0	0
			11909	7694	1943	2241	31		

- Molecule 8 is a protein called Nucleoporin NUP188.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	1358	Total	C	N	O	S	0	0
			10955	7154	1742	2034	25		
8	P	1358	Total	C	N	O	S	0	0
			10955	7153	1743	2035	24		

- Molecule 9 is a protein called Nucleoporin NIC96.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Q	689	Total	C	N	O	S	0	0
			5192	3300	895	980	17		
9	R	707	Total	C	N	O	S	0	0
			5279	3351	913	998	17		
9	S	689	Total	C	N	O	S	0	0
			5189	3297	895	980	17		
9	T	707	Total	C	N	O	S	0	0
			5279	3351	913	998	17		

- Molecule 10 is a protein called Nucleoporin NUP53.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	U	93	Total	C	N	O	S	0	0
			736	480	118	136	2		
10	W	93	Total	C	N	O	S	0	0
			736	480	118	136	2		

- Molecule 11 is a protein called Nucleoporin ASM4.

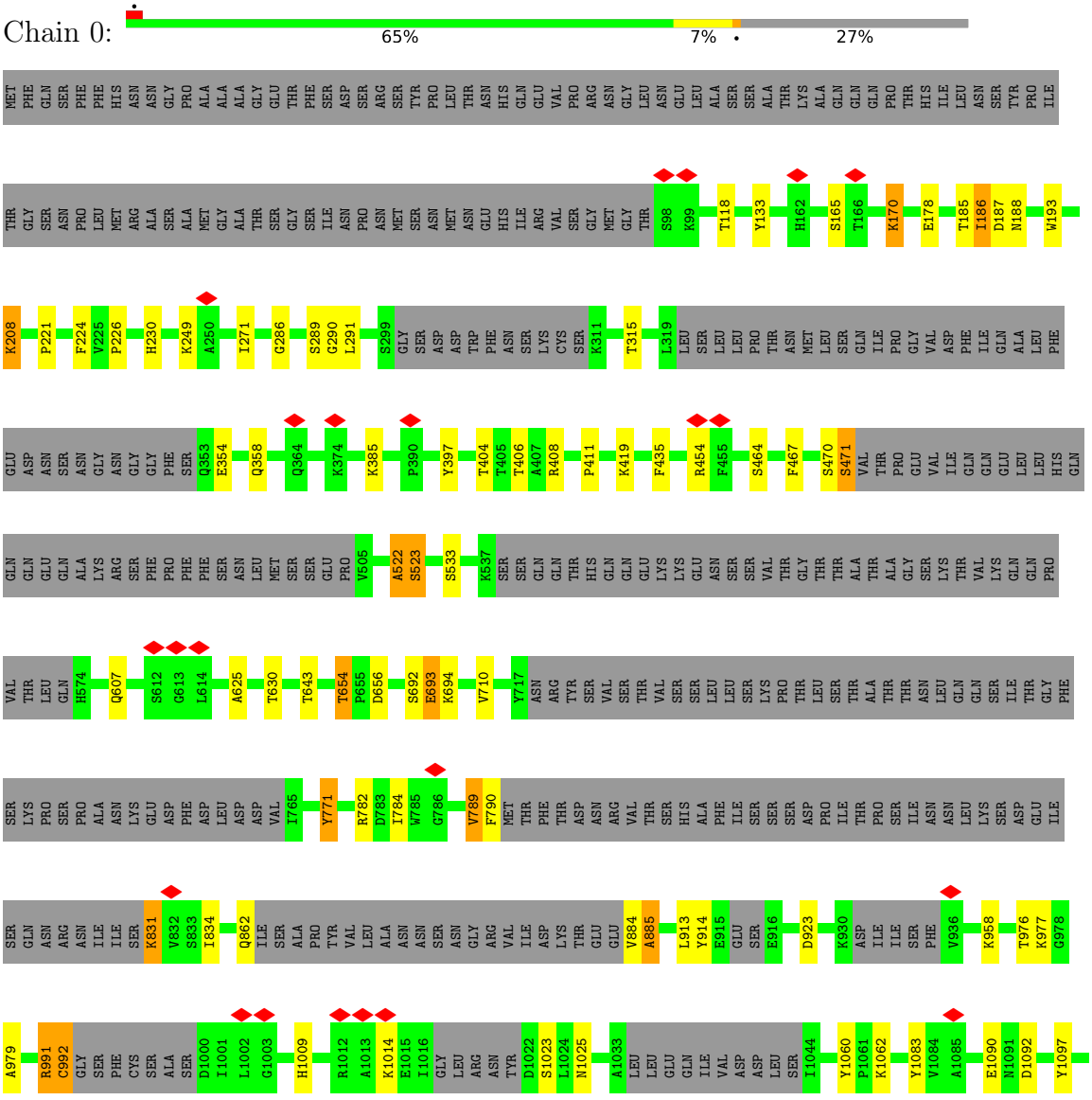
Mol	Chain	Residues	Atoms					AltConf	Trace
11	V	92	Total	C	N	O	S	0	0
			720	465	116	136	3		
11	X	93	Total	C	N	O	S	0	0
			731	471	120	137	3		

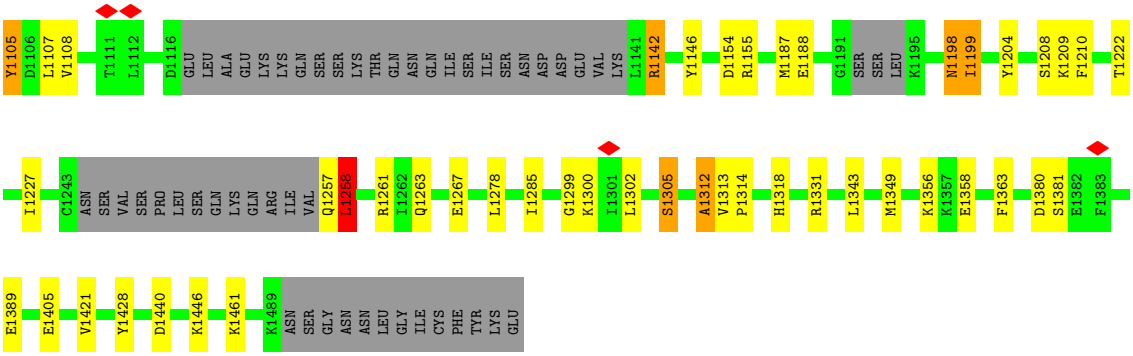
3 Residue-property plots (i)

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.

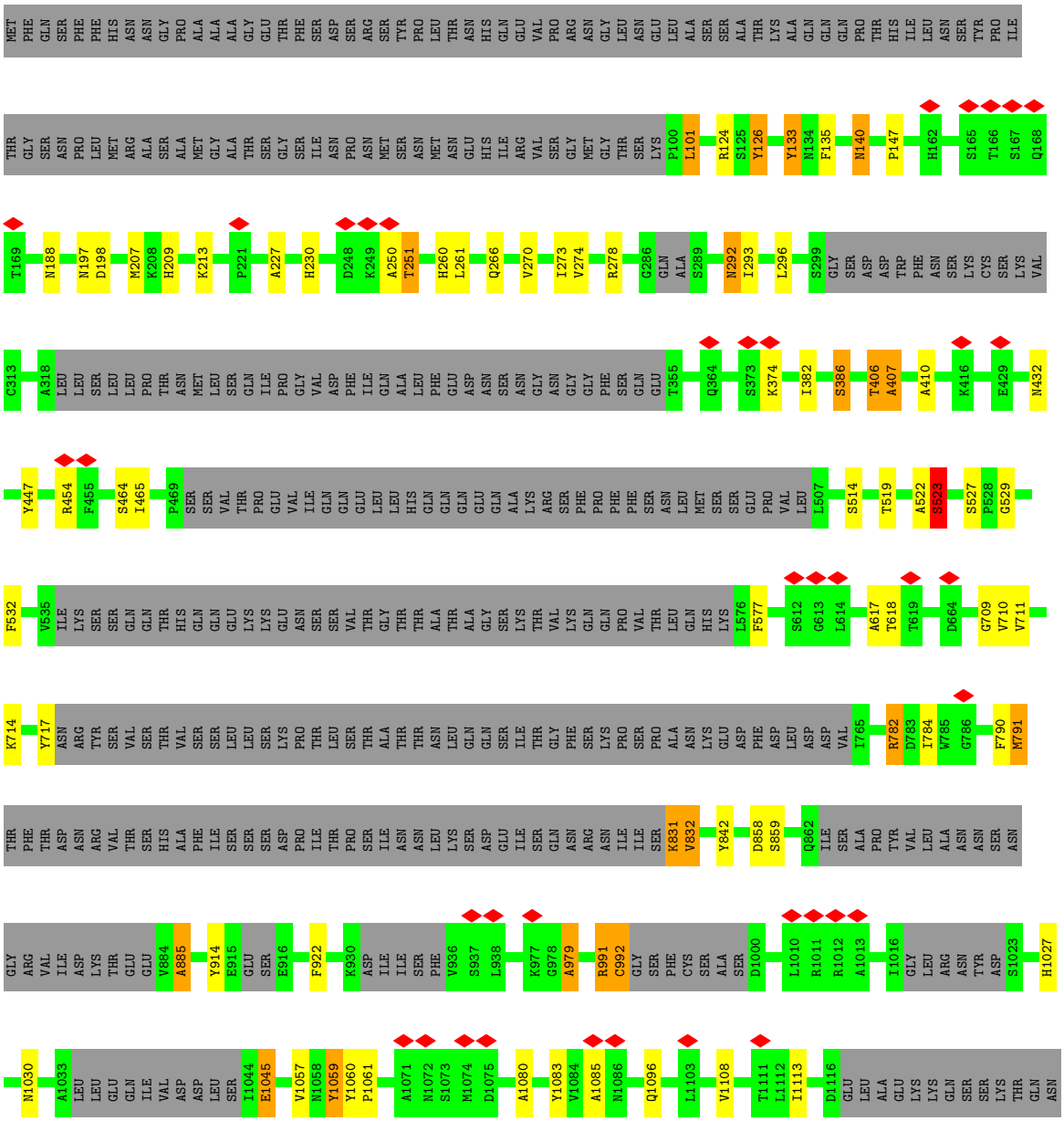
- Molecule 1: Nucleoporin NUP170

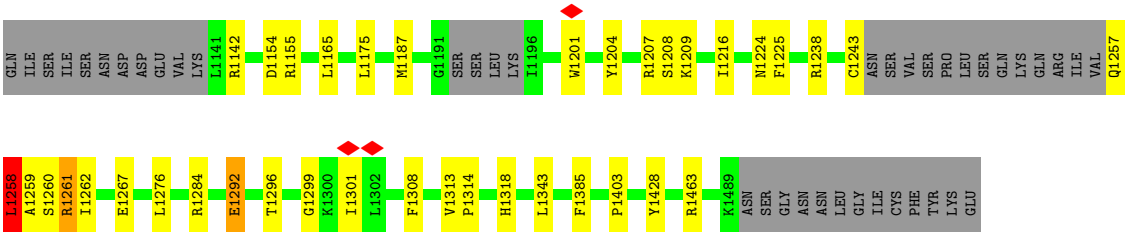
Chain 0:





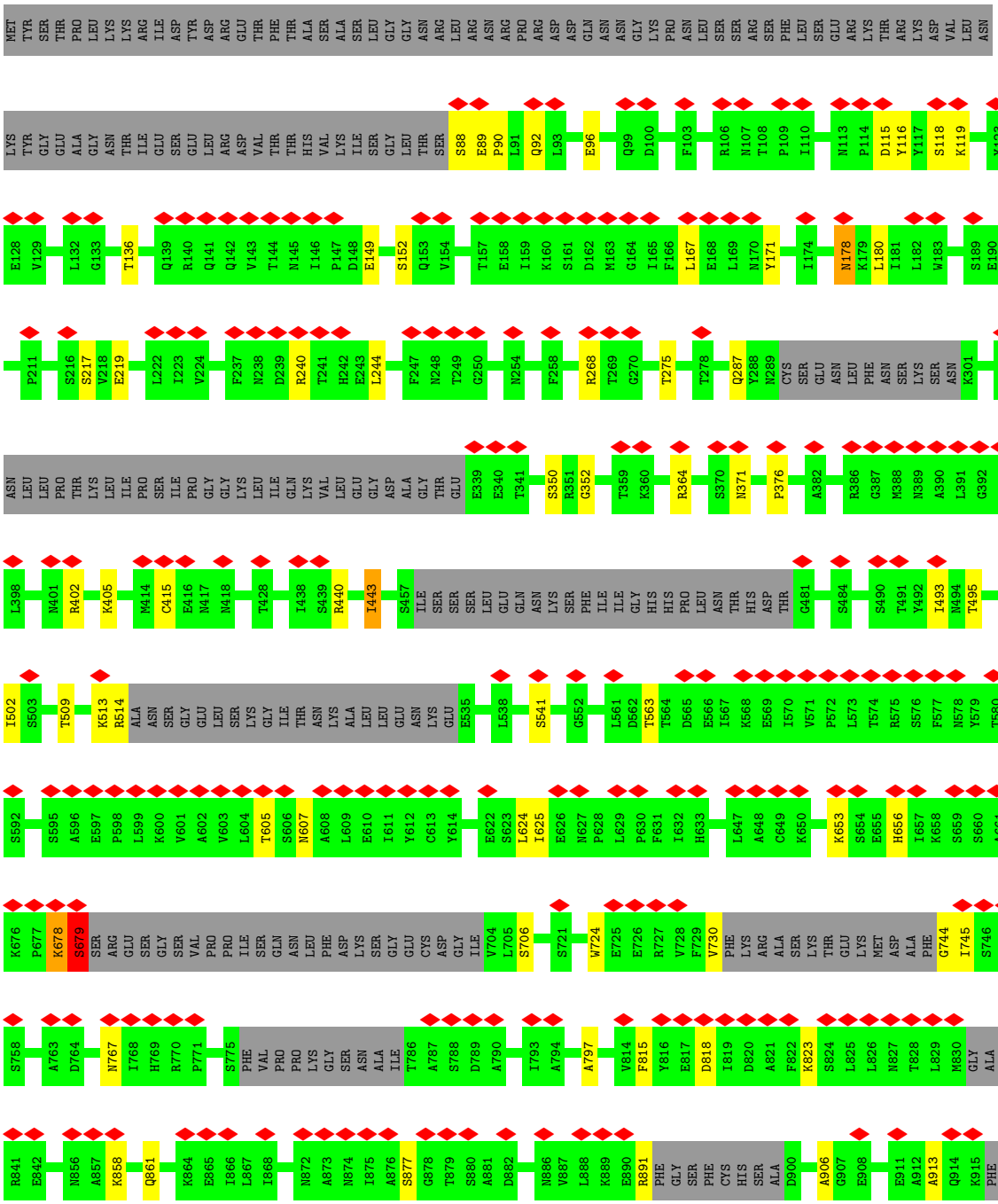
• Molecule 1: Nucleoporin NUP170

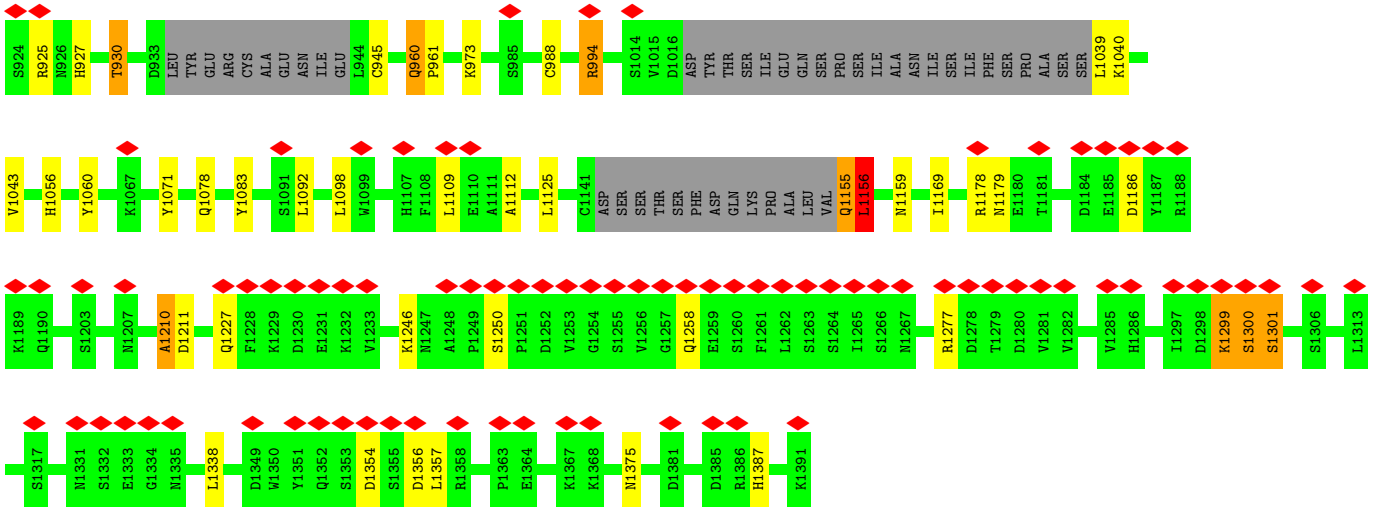




• Molecule 2: Nucleoporin NUP157

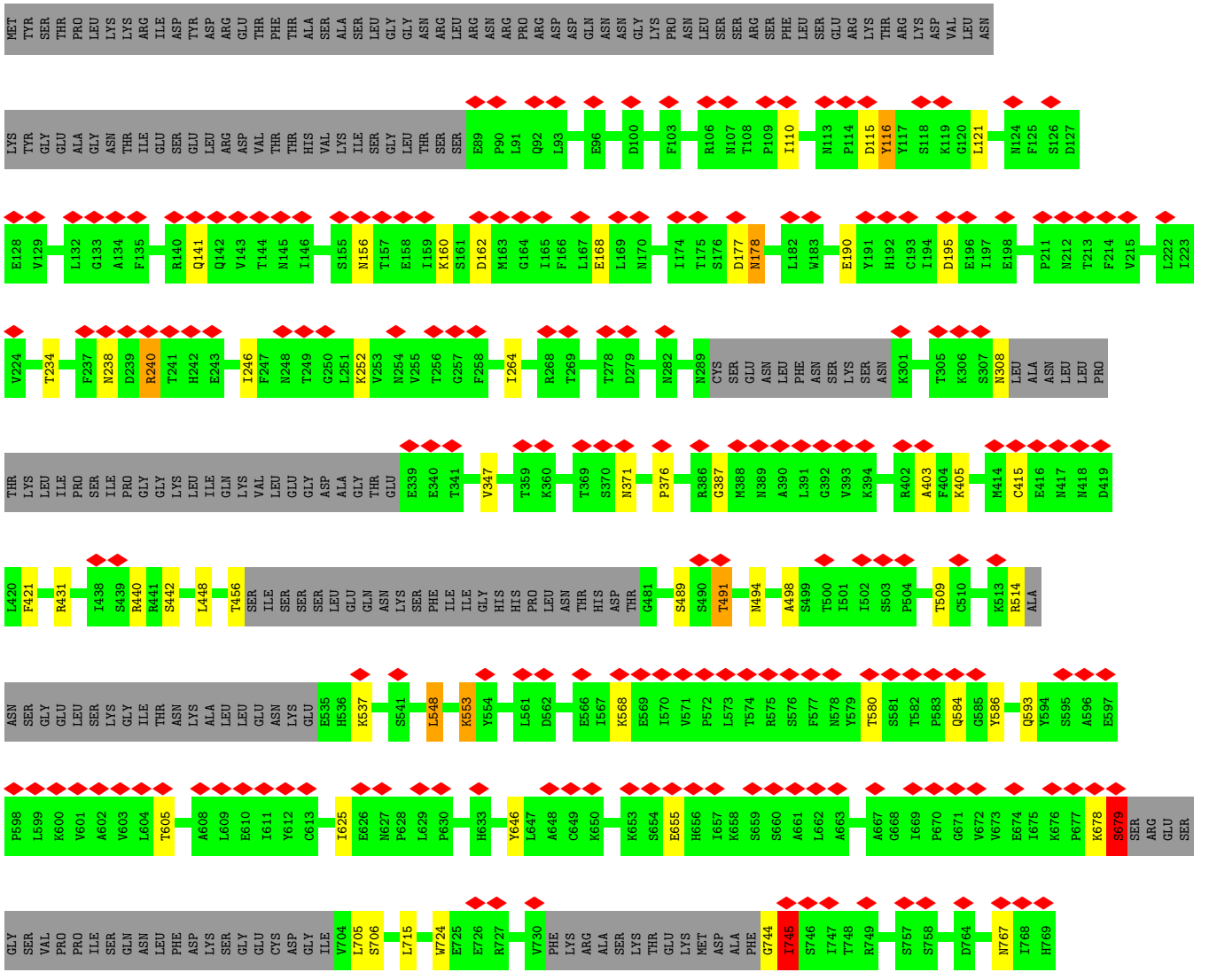
Chain 1:

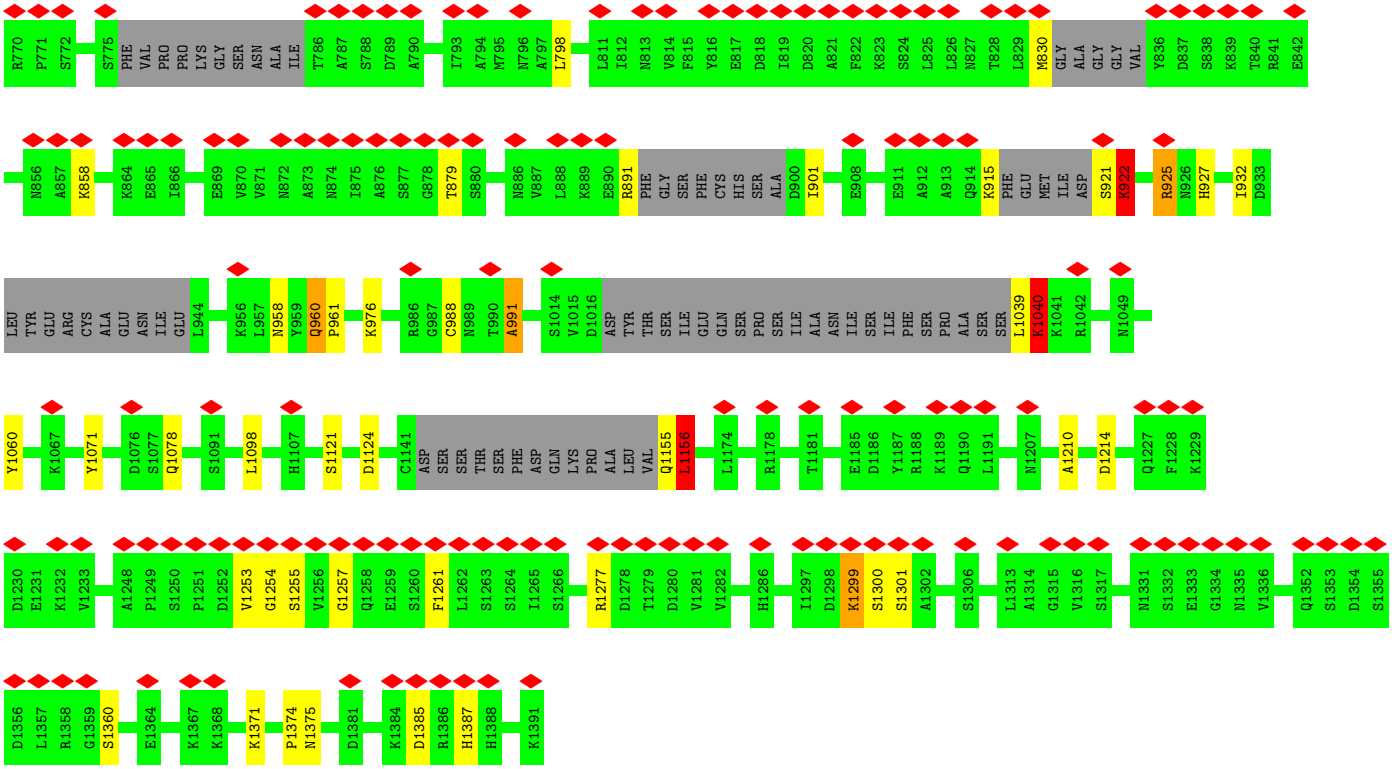




• Molecule 2: Nucleoporin NUP157

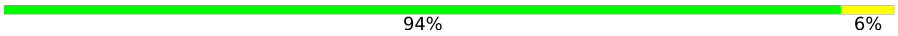
Chain Z:

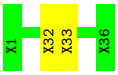




• Molecule 3: Unknown connectors

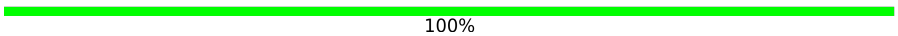
Chain 5:





• Molecule 3: Unknown connectors

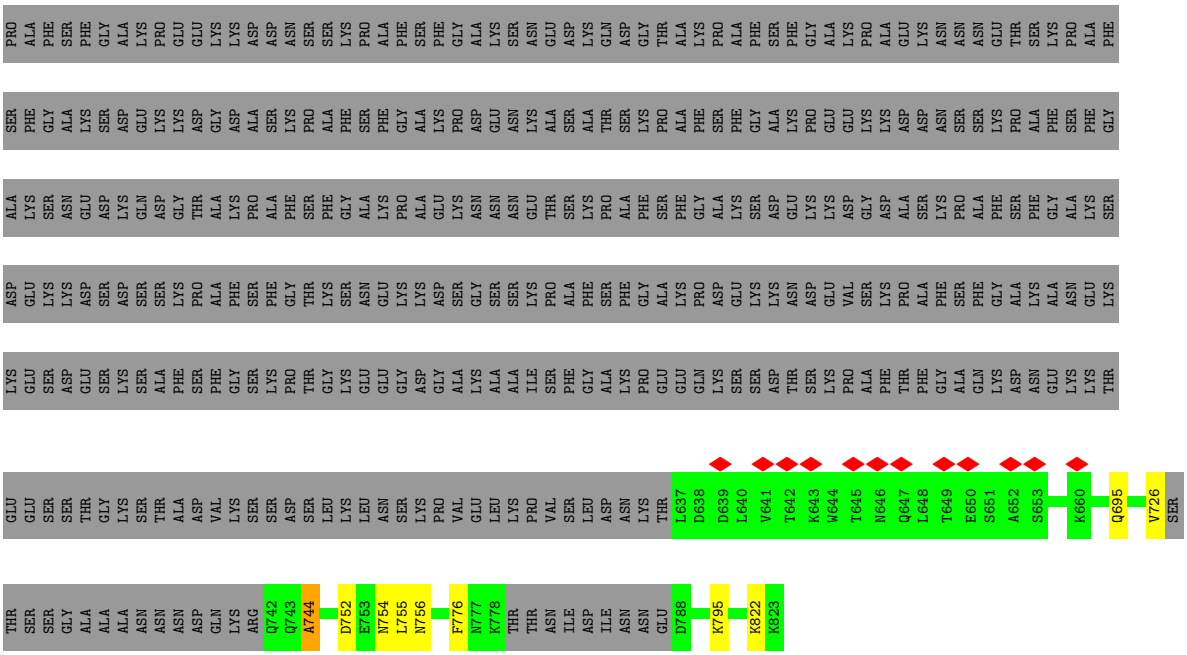
Chain 6:



There are no outlier residues recorded for this chain.

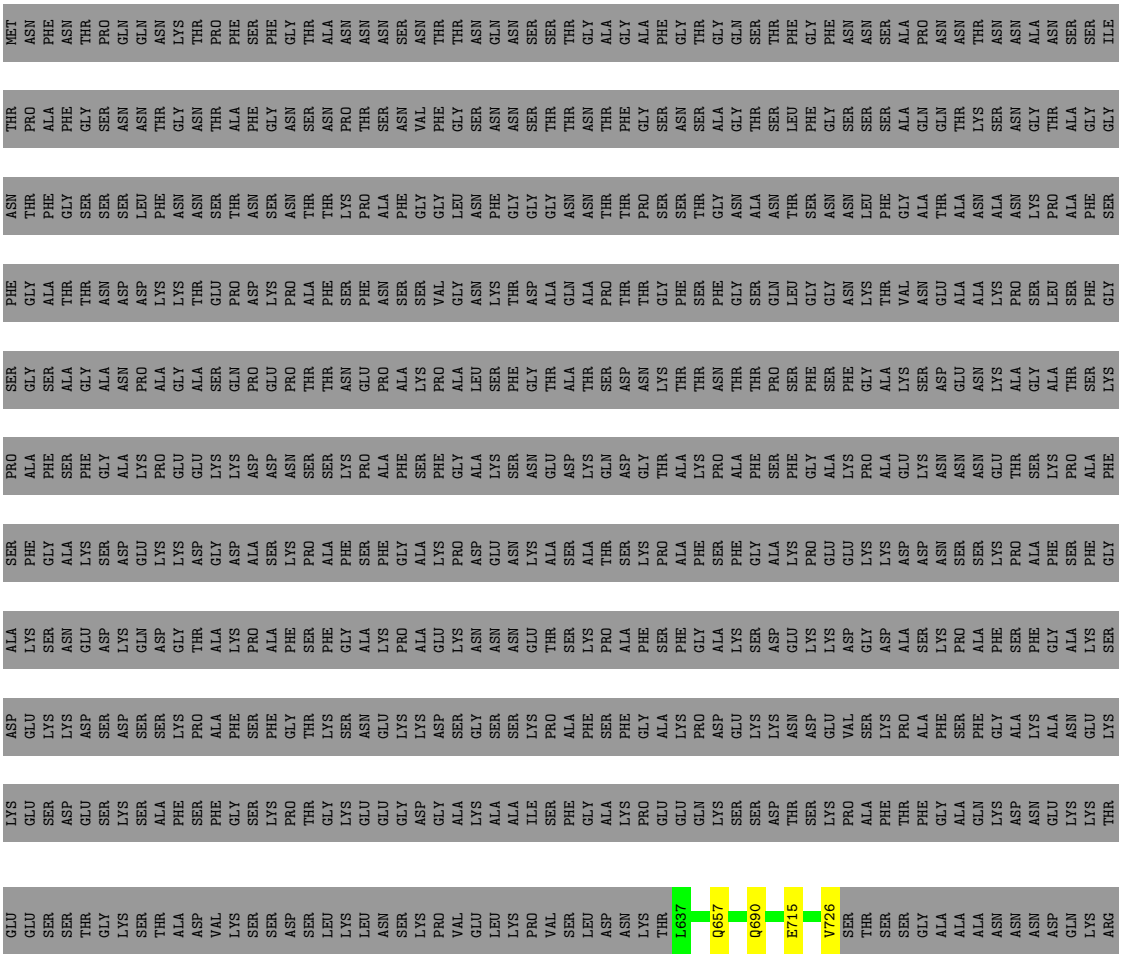
• Molecule 4: Nucleoporin NSP1

Chain A:



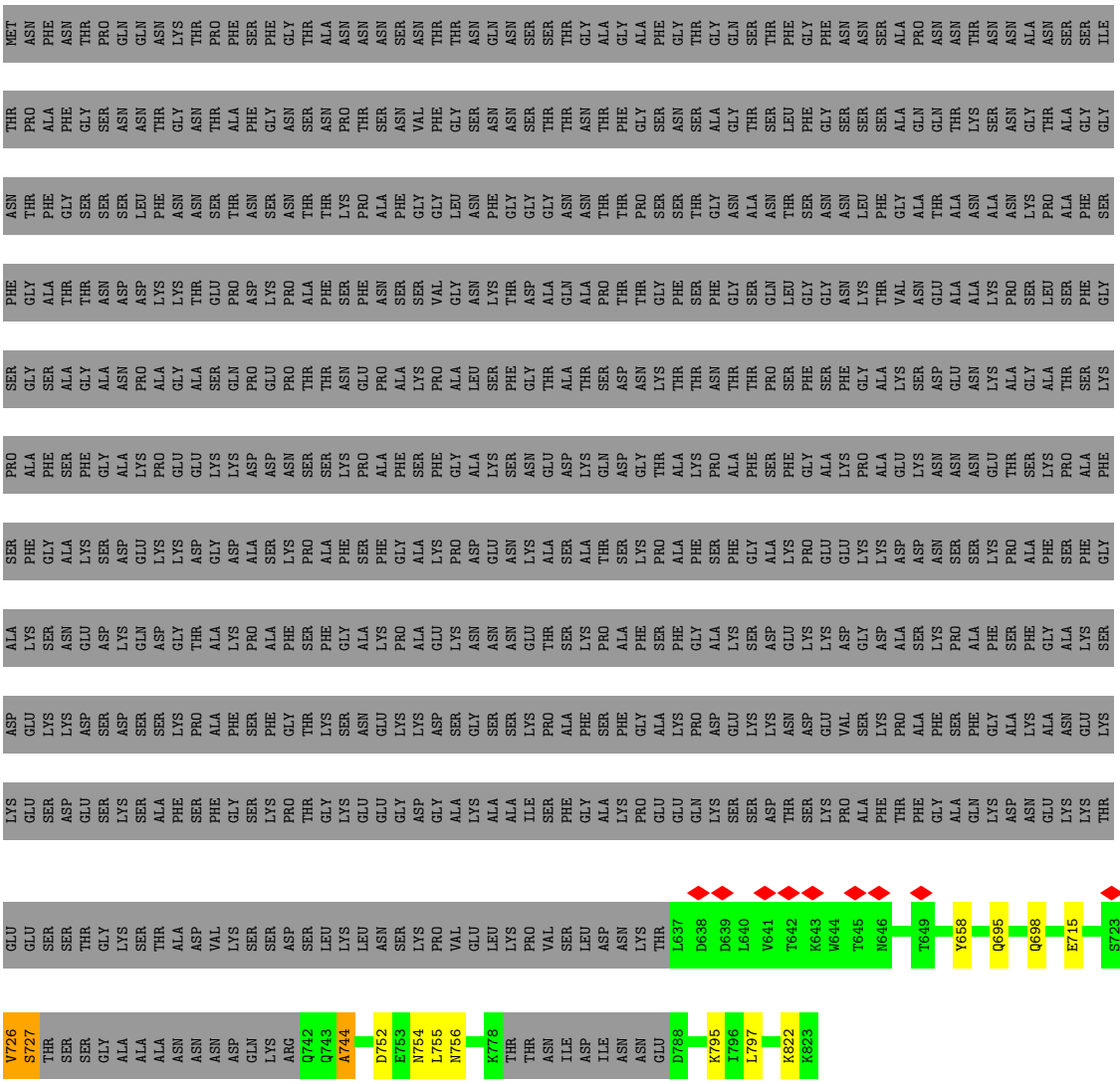
• Molecule 4: Nucleoporin NSP1

Chain D:



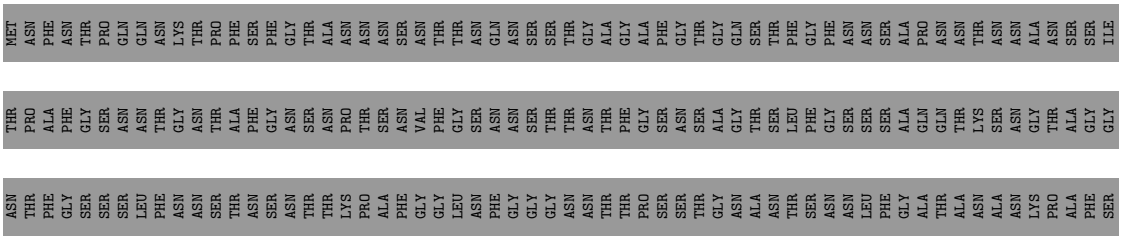
• Molecule 4: Nucleoporin NSP1

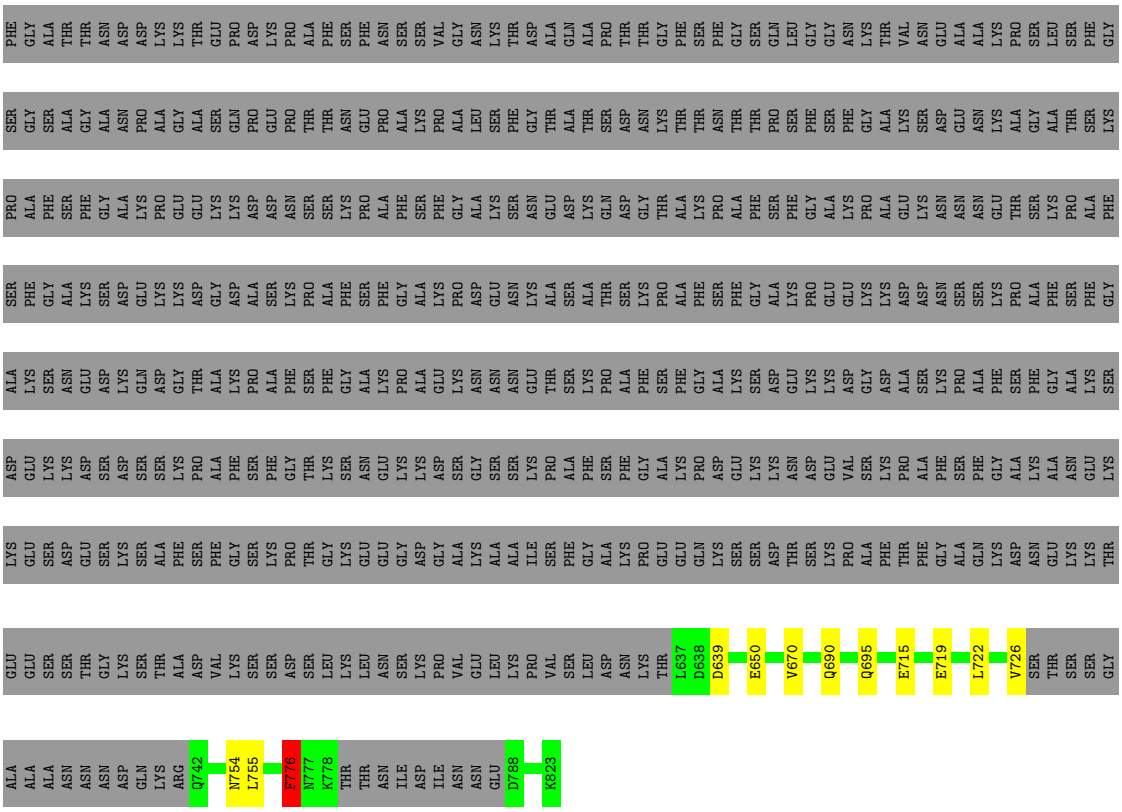
Chain G:



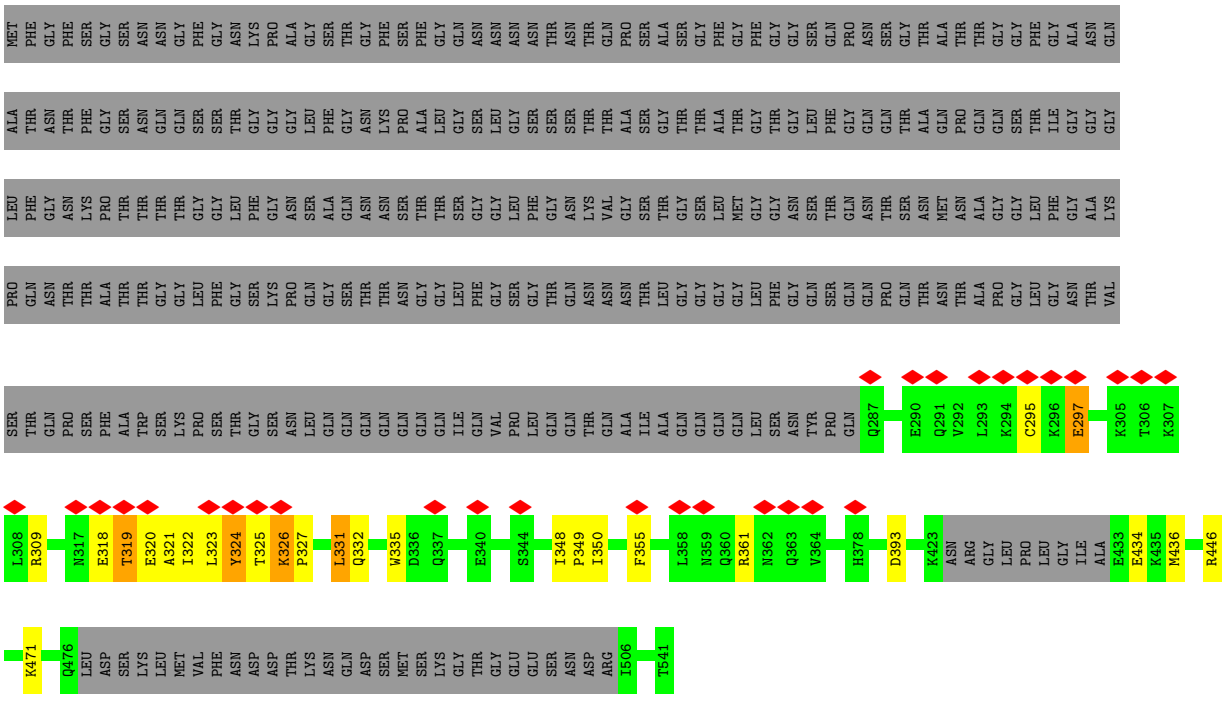
• Molecule 4: Nucleoporin NSP1

Chain J:



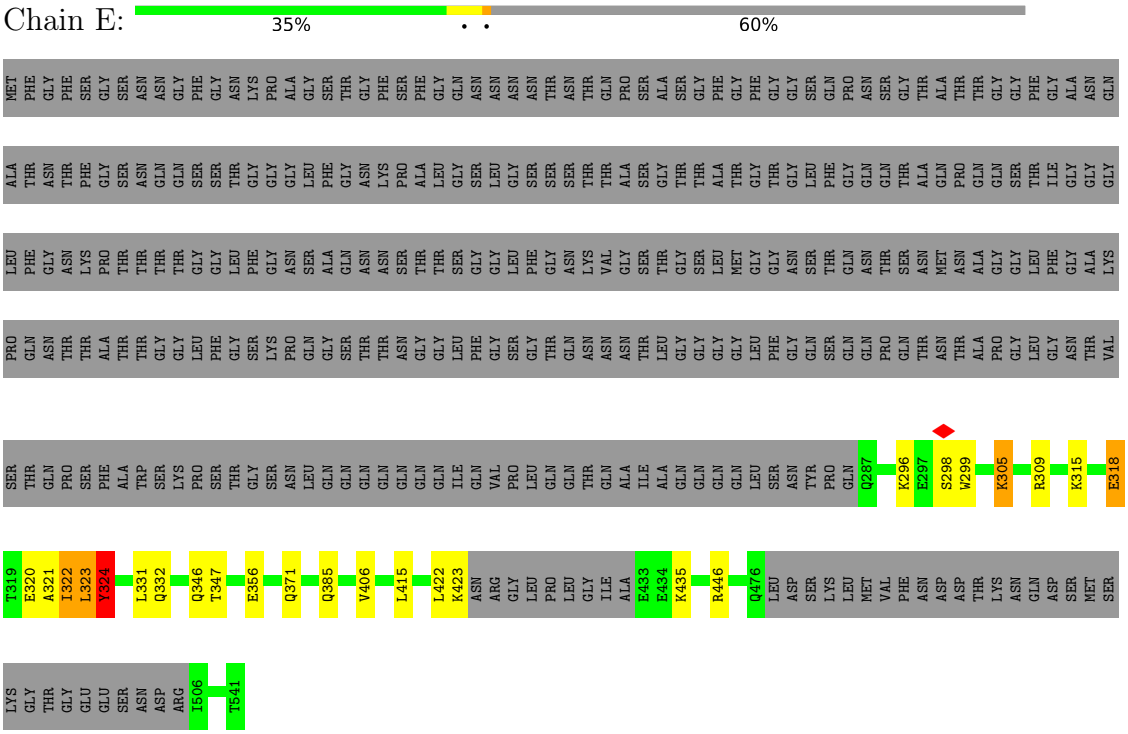


• Molecule 5: Nucleoporin NUP57



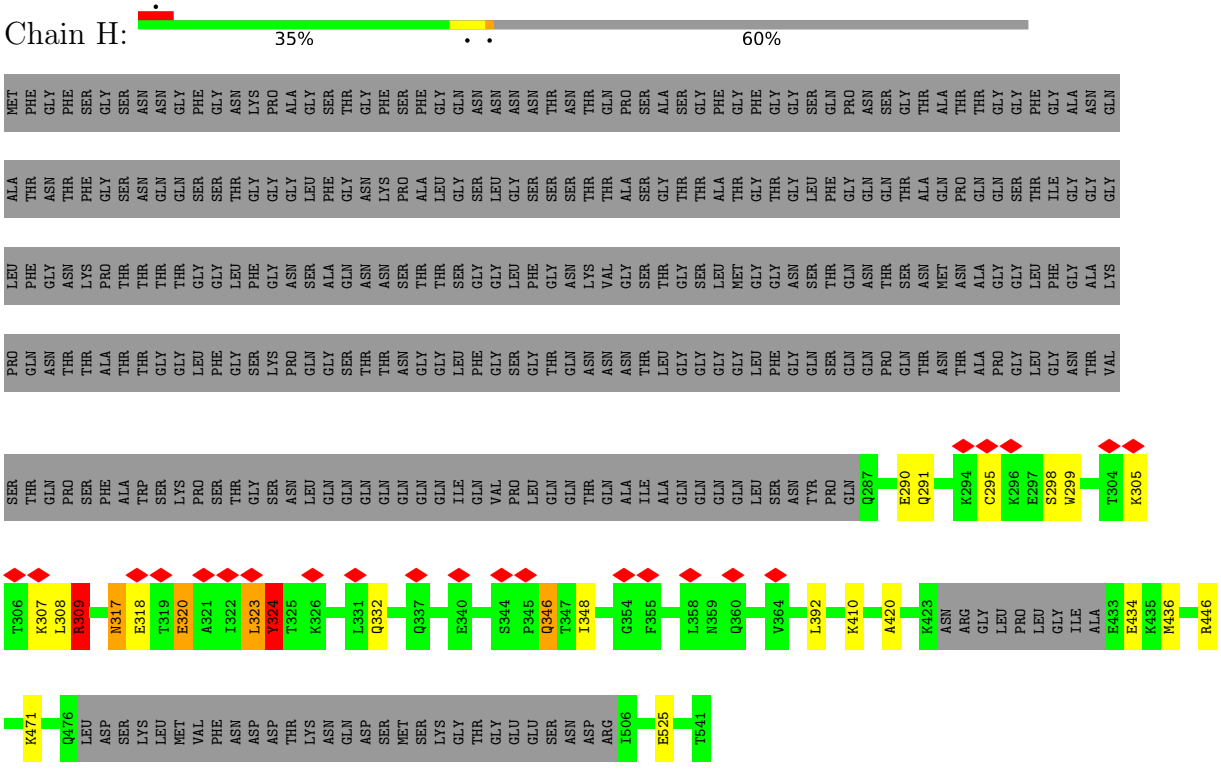
• Molecule 5: Nucleoporin NUP57

Chain E:



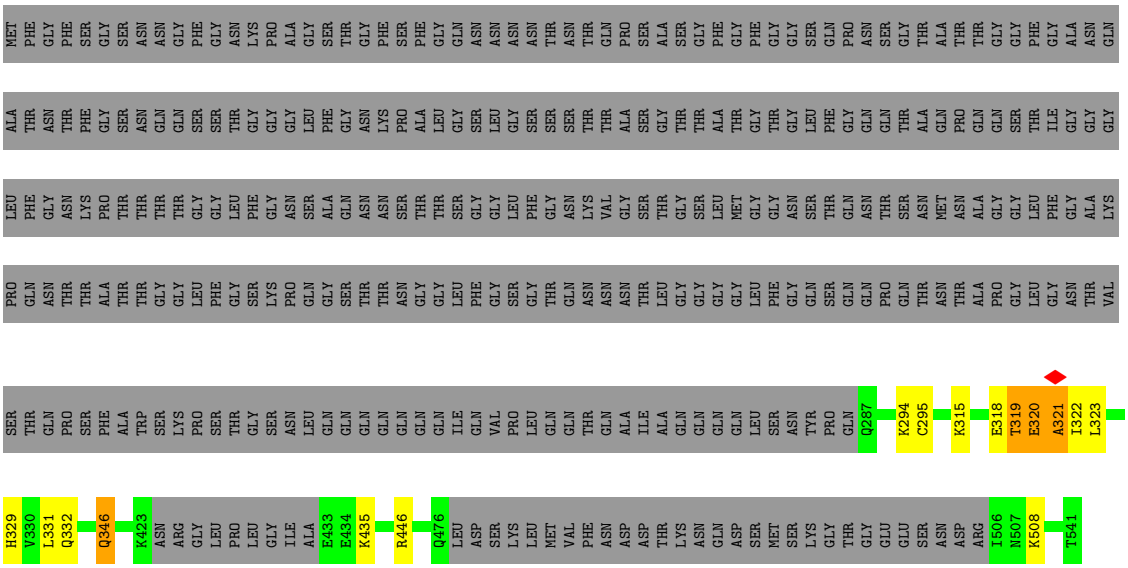
• Molecule 5: Nucleoporin NUP57

Chain H:

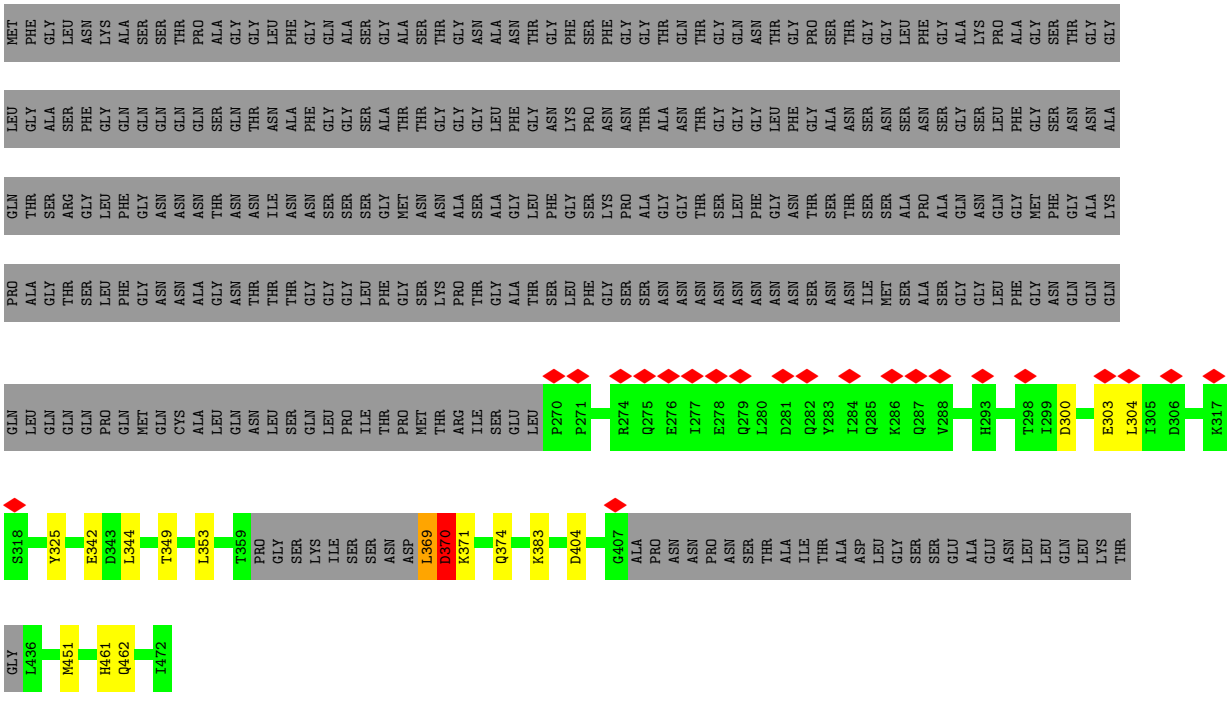


• Molecule 5: Nucleoporin NUP57

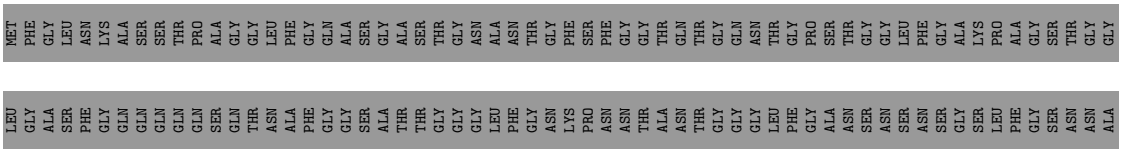
Chain K:

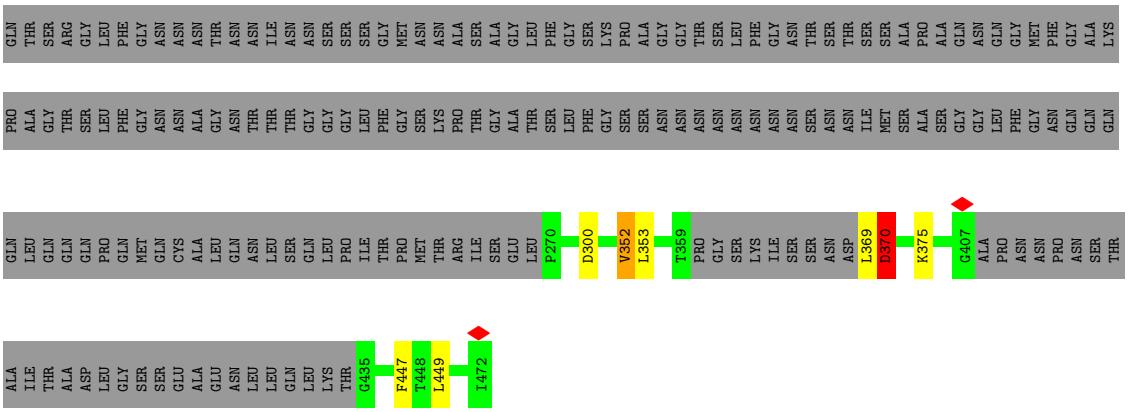


• Molecule 6: Nucleoporin NUP49/NSP49



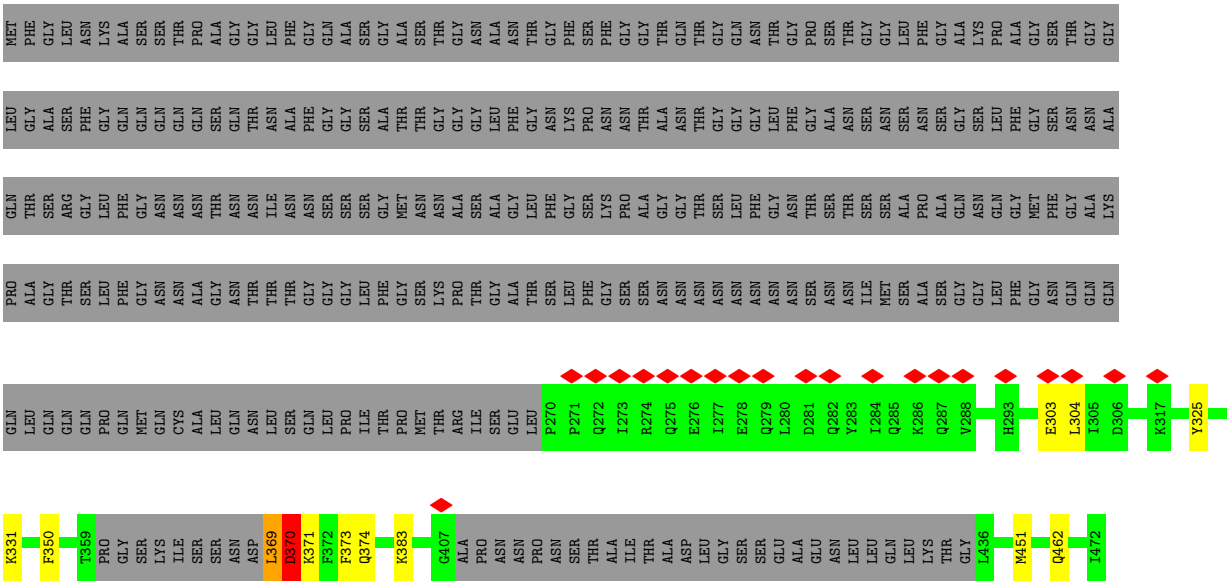
• Molecule 6: Nucleoporin NUP49/NSP49





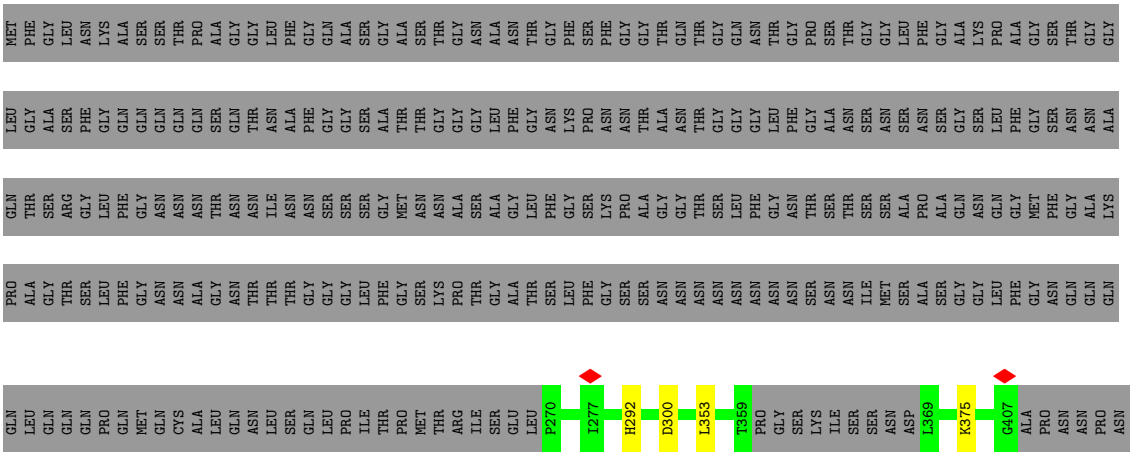
• Molecule 6: Nucleoporin NUP49/NSP49

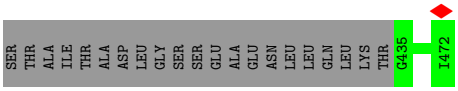
Chain I:



• Molecule 6: Nucleoporin NUP49/NSP49

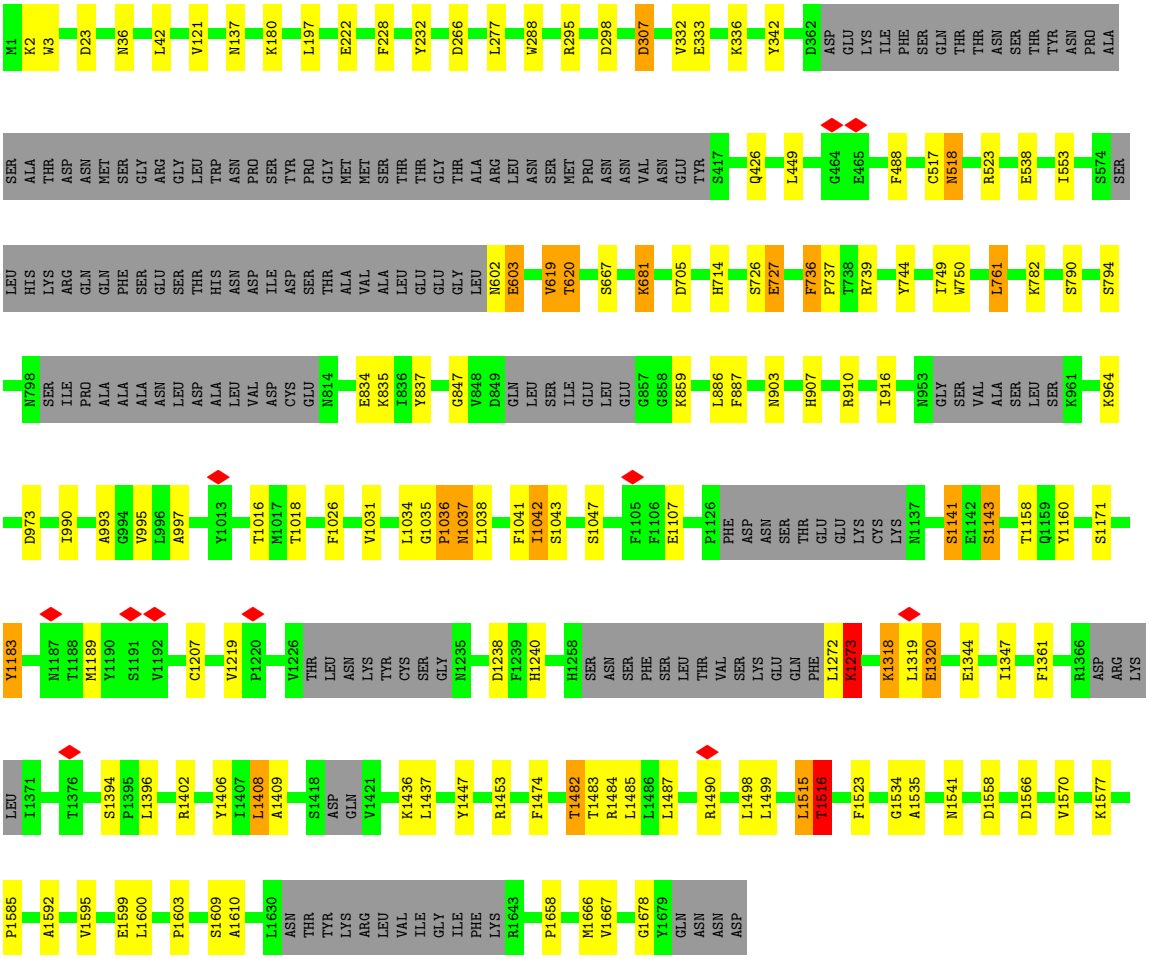
Chain L:





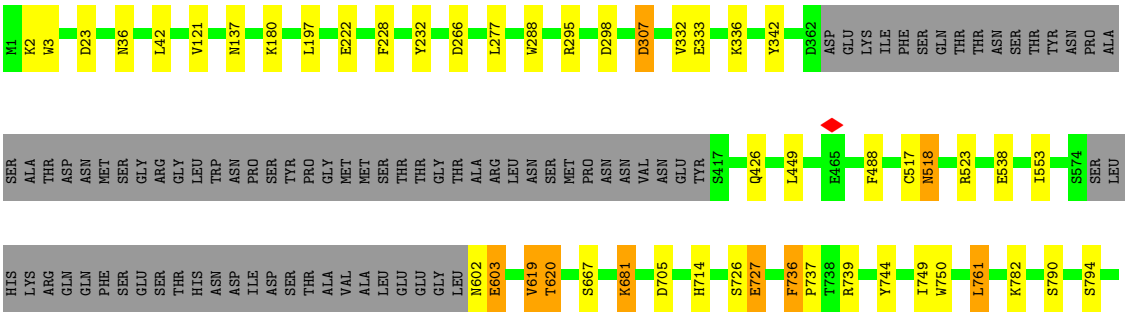
• Molecule 7: Nucleoporin NUP192

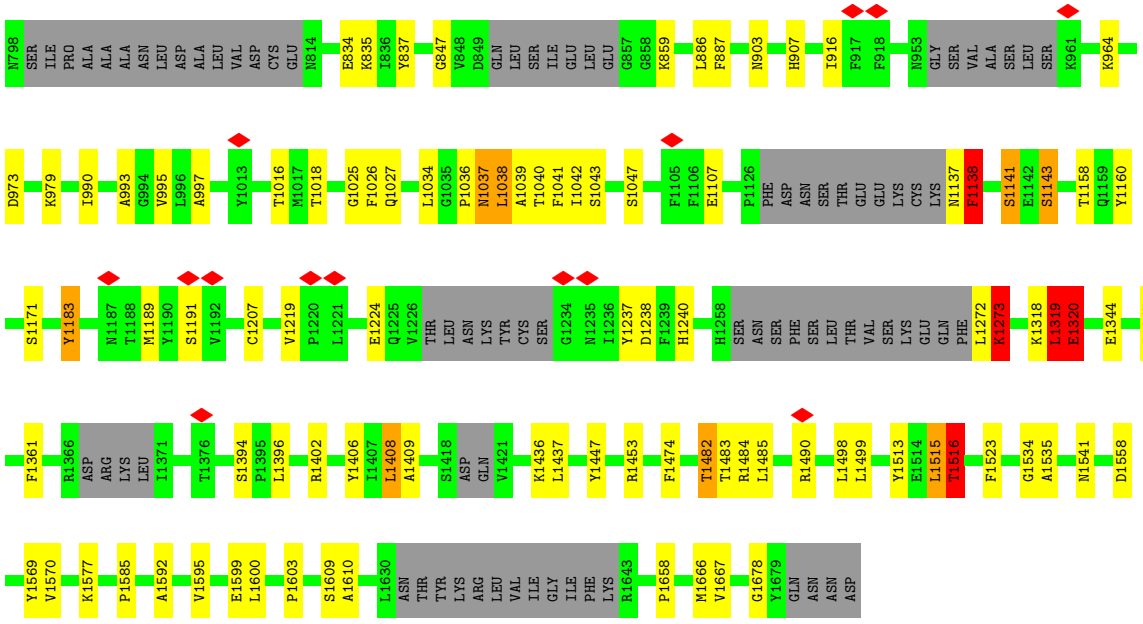
Chain M:



• Molecule 7: Nucleoporin NUP192

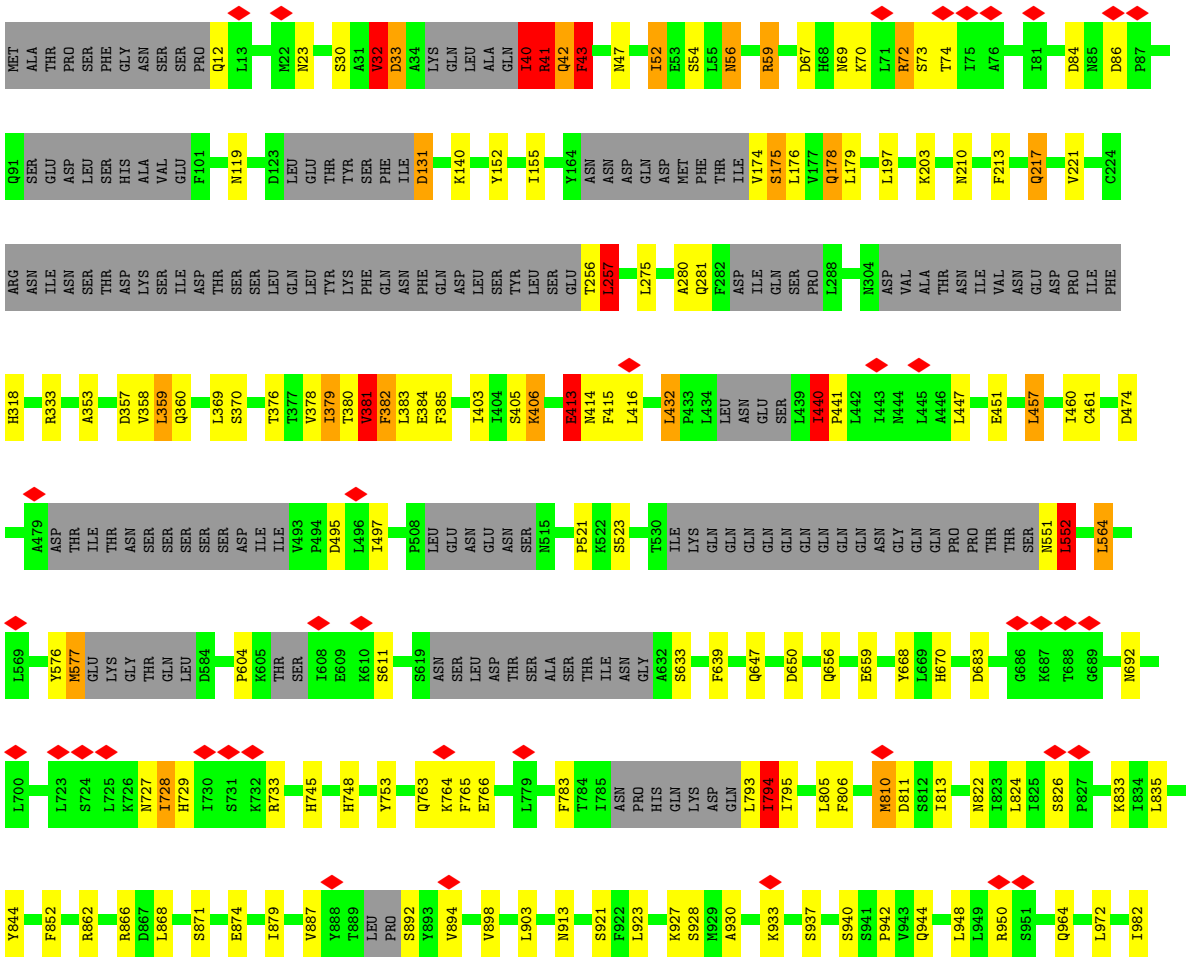
Chain O:

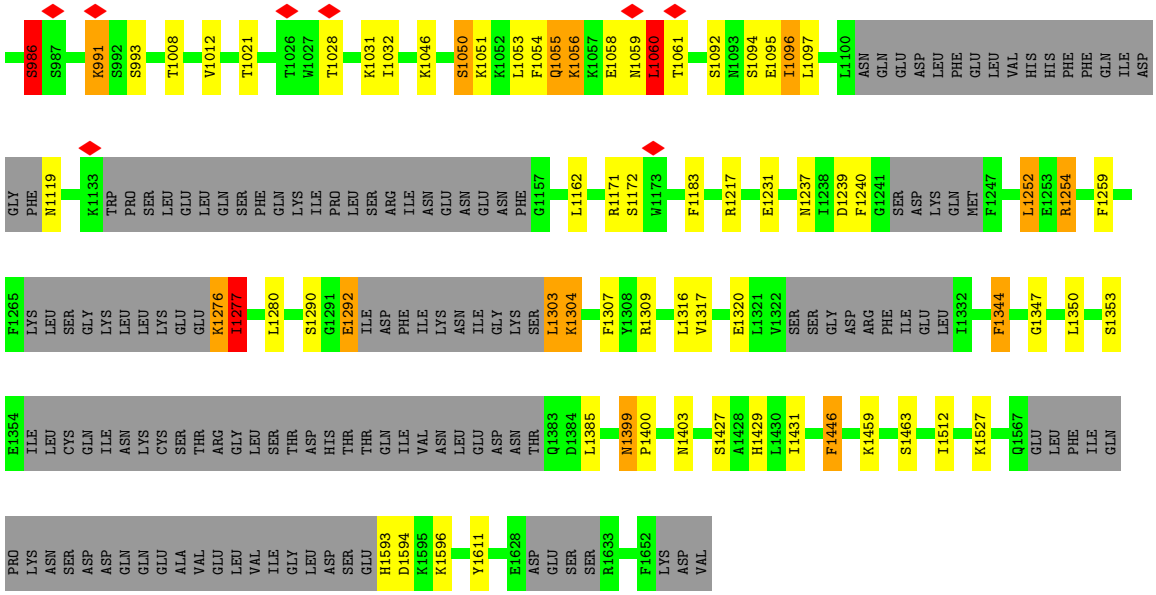




• Molecule 8: Nucleoporin NUP188

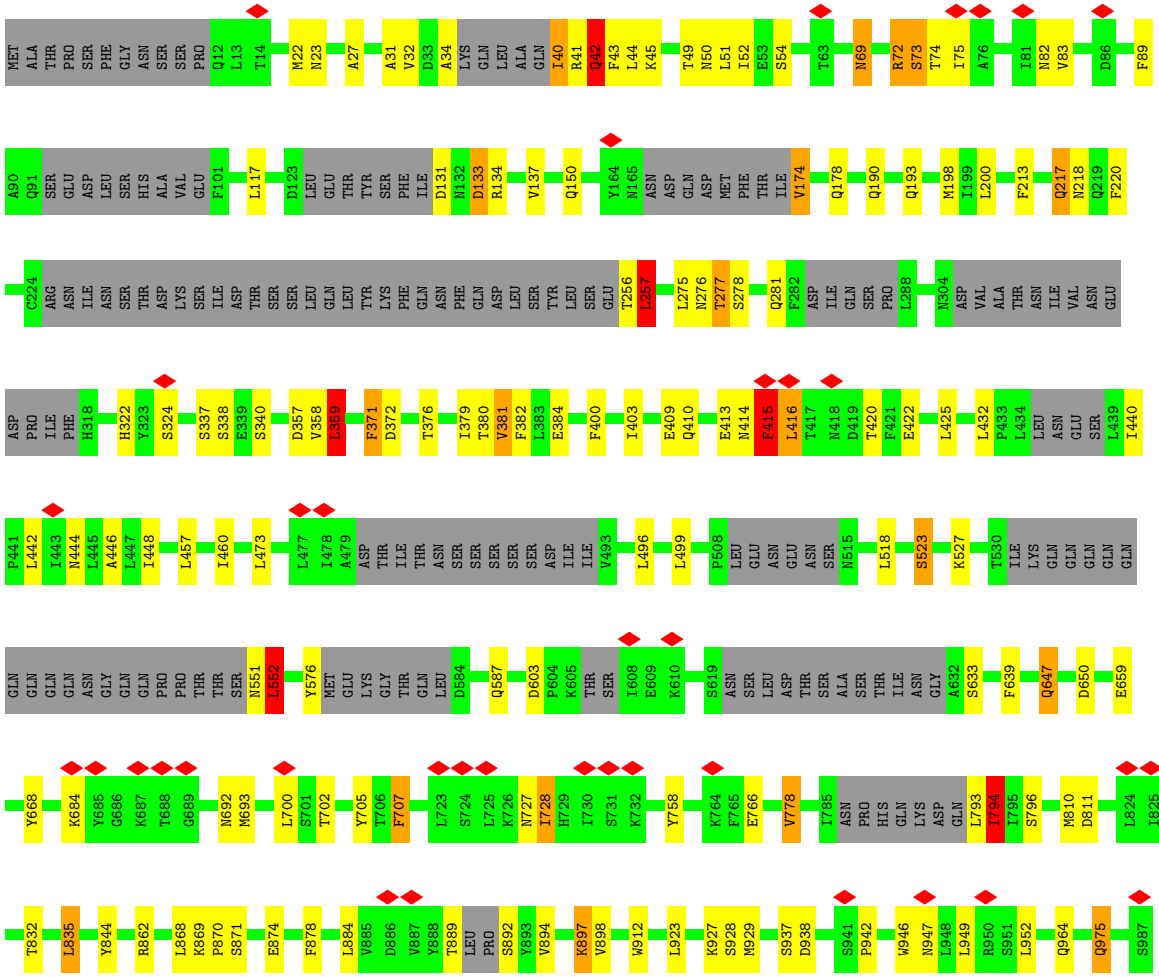
Chain N:

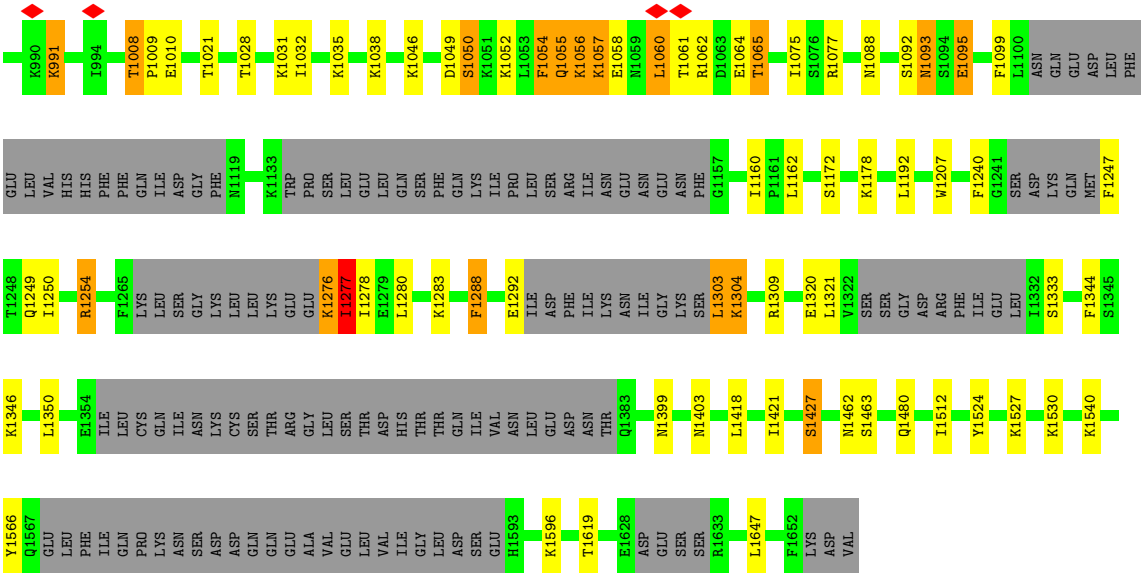




• Molecule 8: Nucleoporin NUP188

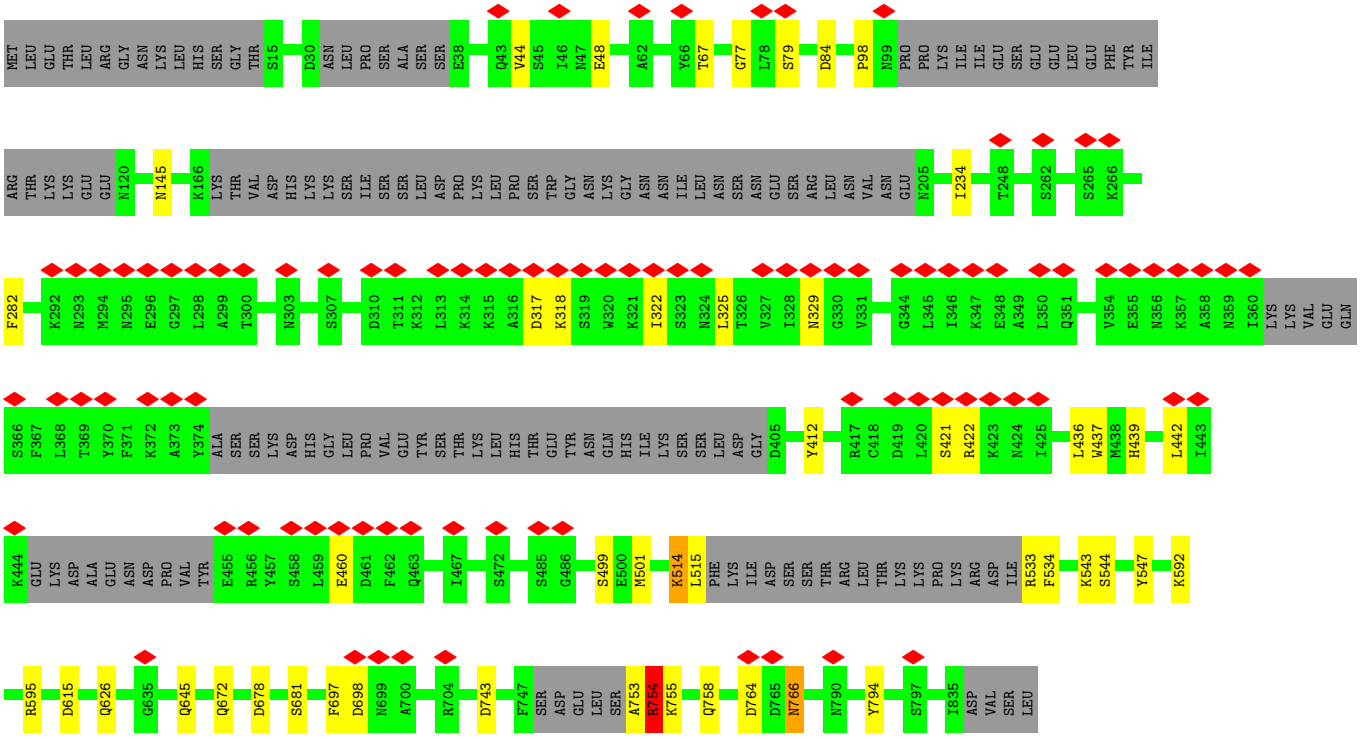
Chain P:





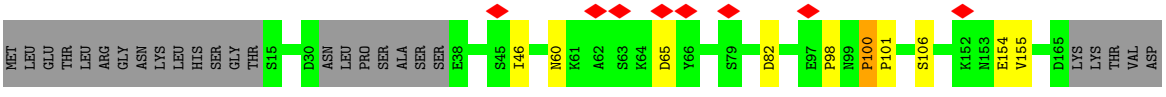
• Molecule 9: Nucleoporin NIC96

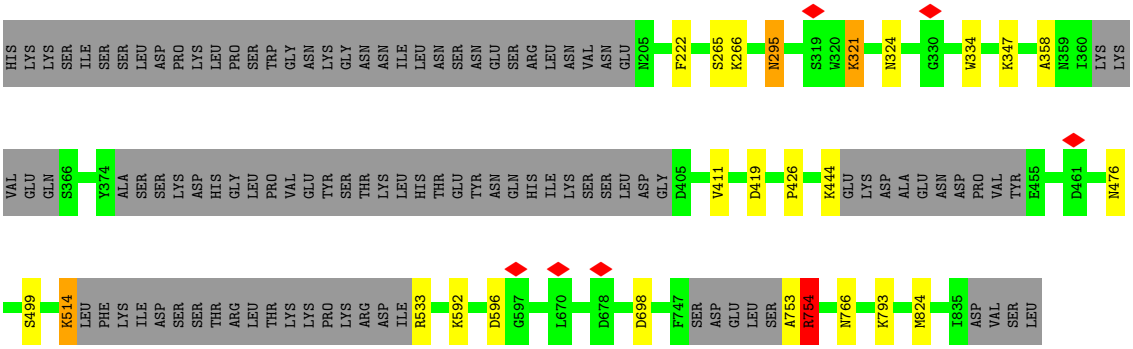
Chain Q:



• Molecule 9: Nucleoporin NIC96

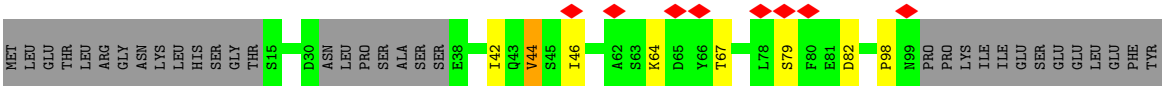
Chain R:

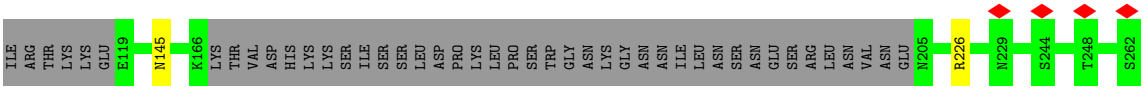


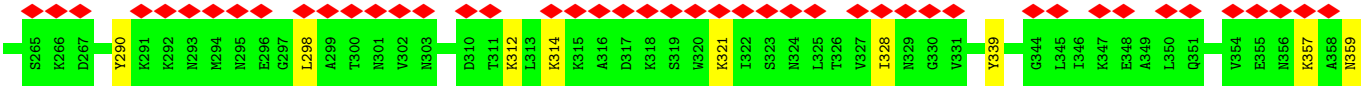


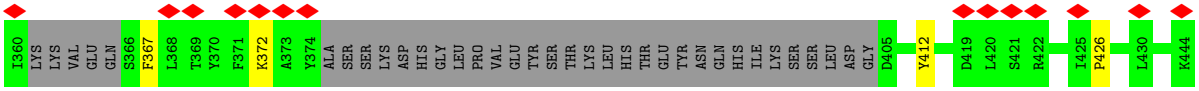
• Molecule 9: Nucleoporin NIC96

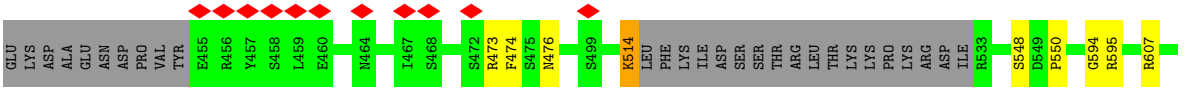
Chain S:

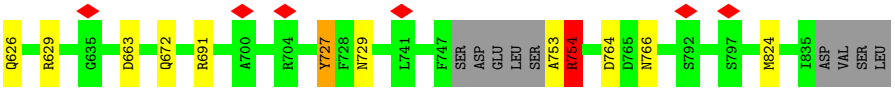






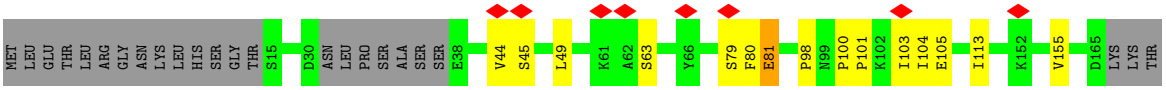


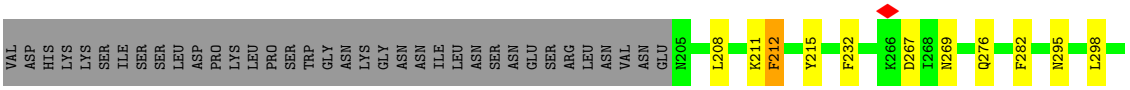


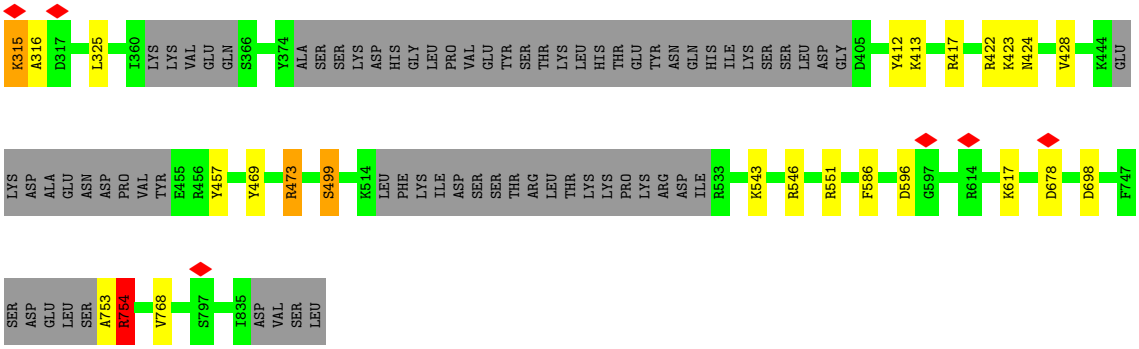


• Molecule 9: Nucleoporin NIC96

Chain T:

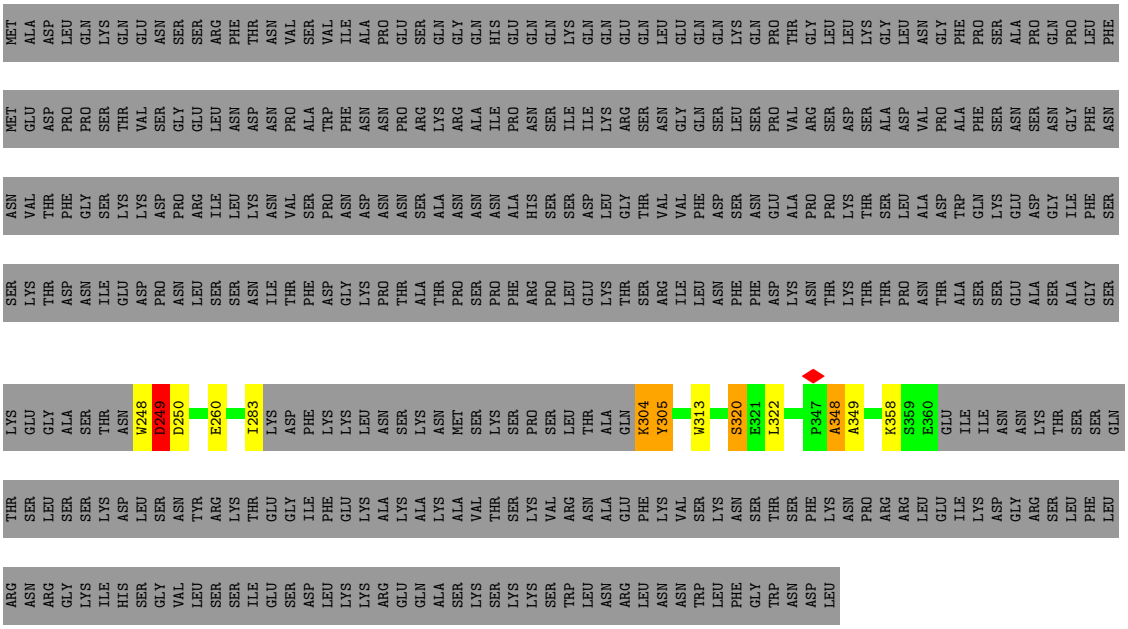






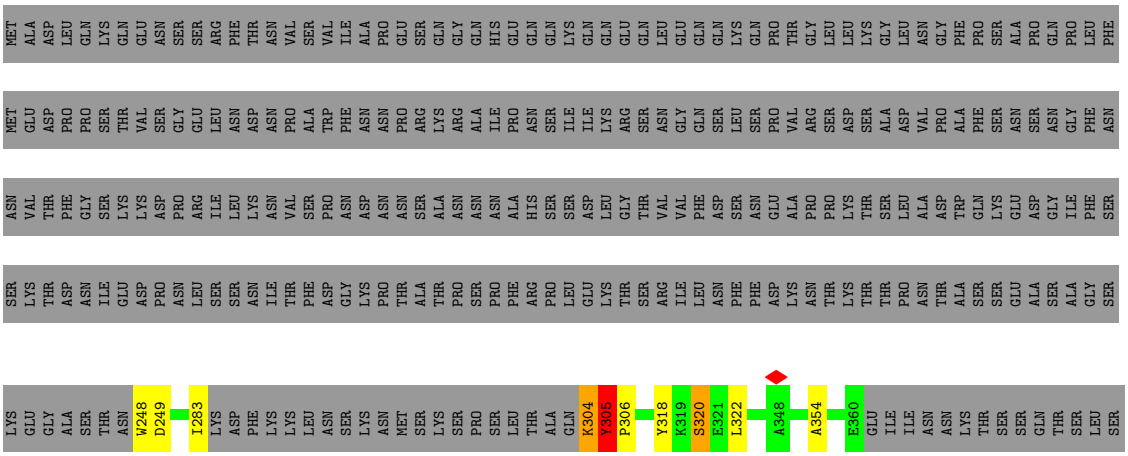
• Molecule 10: Nucleoporin NUP53

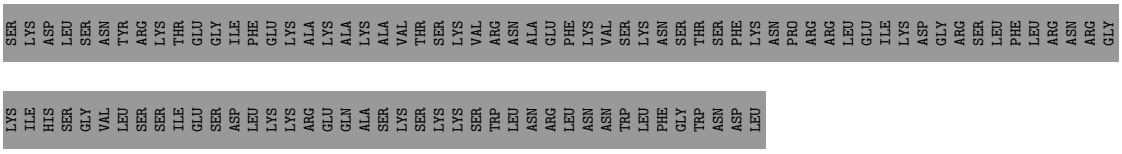
Chain U:



• Molecule 10: Nucleoporin NUP53

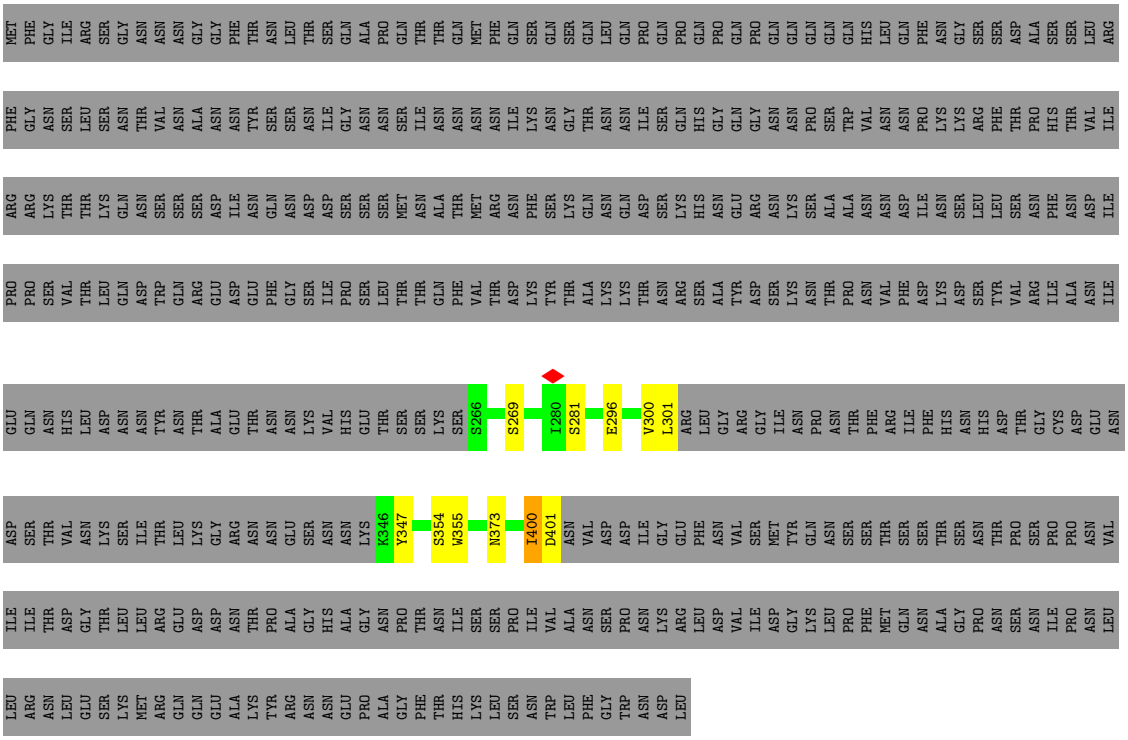
Chain W:





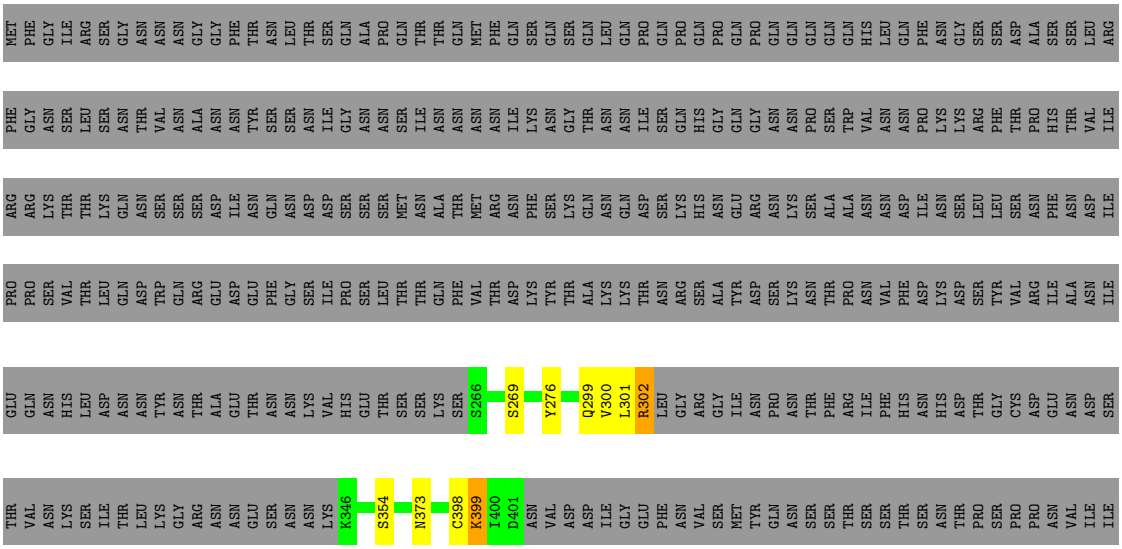
• Molecule 11: Nucleoporin ASM4

Chain V:



• Molecule 11: Nucleoporin ASM4

Chain X:



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

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

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	145000	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	4.327	Depositor
Minimum map value	0.000	Depositor
Average map value	0.019	Depositor
Map value standard deviation	0.121	Depositor
Recommended contour level	0.595	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

5.1 Standard geometry

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	0	1.00	11/9065 (0.1%)	1.16	45/12247 (0.4%)
1	Y	0.93	7/8920 (0.1%)	1.09	28/12052 (0.2%)
2	1	1.01	13/9072 (0.1%)	1.14	41/12276 (0.3%)
2	Z	1.09	18/9052 (0.2%)	1.24	52/12249 (0.4%)
4	A	0.91	2/1327 (0.2%)	0.92	3/1788 (0.2%)
4	D	0.91	2/1328 (0.2%)	0.89	2/1791 (0.1%)
4	G	1.15	2/1334 (0.1%)	1.21	9/1799 (0.5%)
4	J	0.92	2/1328 (0.2%)	0.92	4/1791 (0.2%)
5	B	0.86	0/1793	0.91	1/2411 (0.0%)
5	E	1.01	2/1793 (0.1%)	1.08	5/2411 (0.2%)
5	H	1.03	2/1793 (0.1%)	1.05	6/2411 (0.2%)
5	K	0.86	0/1793	0.89	0/2411
6	C	0.83	0/1364	0.90	2/1837 (0.1%)
6	F	0.99	2/1368 (0.1%)	1.14	8/1842 (0.4%)
6	I	0.84	0/1364	0.90	3/1837 (0.2%)
6	L	0.85	0/1368	0.89	0/1842
7	M	0.91	6/12128 (0.0%)	1.04	26/16436 (0.2%)
7	O	0.94	12/12132 (0.1%)	1.09	36/16441 (0.2%)
8	N	0.98	19/11142 (0.2%)	1.17	61/15068 (0.4%)
8	P	0.96	12/11142 (0.1%)	1.13	53/15069 (0.4%)
9	Q	0.98	5/5265 (0.1%)	1.08	21/7137 (0.3%)
9	R	0.94	3/5353 (0.1%)	1.02	12/7262 (0.2%)
9	S	0.94	3/5262 (0.1%)	1.04	22/7133 (0.3%)
9	T	0.93	2/5353 (0.0%)	1.05	21/7262 (0.3%)
10	U	1.44	6/752 (0.8%)	1.74	16/1016 (1.6%)
10	W	1.24	4/752 (0.5%)	1.33	9/1016 (0.9%)
11	V	1.14	2/737 (0.3%)	1.26	6/996 (0.6%)
11	X	1.22	2/748 (0.3%)	1.39	7/1010 (0.7%)
All	All	0.97	139/124828 (0.1%)	1.10	499/168841 (0.3%)

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	0	7	6
1	Y	4	8
2	1	8	1
2	Z	14	1
4	A	1	0
4	D	1	0
4	G	2	1
4	J	1	0
5	E	2	3
5	H	2	0
6	F	2	0
7	M	3	14
7	O	7	14
8	N	13	23
8	P	10	21
9	Q	4	0
9	R	3	1
9	S	3	1
9	T	2	0
10	U	5	1
10	W	3	2
11	V	2	0
11	X	2	0
All	All	101	97

The worst 5 of 139 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Z	744	GLY	N-CA	-23.98	1.10	1.46
2	Z	679	SER	CA-CB	-23.87	1.17	1.52
4	G	727	SER	CA-CB	-23.61	1.17	1.52
8	P	174	VAL	CA-CB	-19.97	1.12	1.54
2	1	679	SER	CA-CB	-19.22	1.24	1.52

The worst 5 of 499 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Z	1040	LYS	N-CA-CB	26.00	157.41	110.60
2	Z	1156	LEU	N-CA-CB	25.77	161.94	110.40
9	Q	753	ALA	CB-CA-C	25.56	148.44	110.10
10	U	249	ASP	N-CA-CB	22.28	150.70	110.60
2	Z	679	SER	N-CA-CB	22.12	143.69	110.50

5 of 101 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	471	SER	CA
1	0	884	VAL	CA
1	0	885	ALA	CA
1	0	991	ARG	CA
1	0	992	CYS	CA

5 of 97 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1208	SER	Peptide
1	0	1299	GLY	Peptide
1	0	186	ILE	Peptide
1	0	523	SER	Peptide
1	0	782	ARG	Peptide

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	0	8890	0	8960	8	0
1	Y	8747	0	8800	40	0
2	1	8903	0	8919	38	0
2	Z	8883	0	8898	31	0
3	5	181	0	37	3	0
3	6	181	0	38	0	0
4	A	1315	0	1274	0	0
4	D	1315	0	1275	0	0
4	G	1321	0	1280	1	0
4	J	1315	0	1275	8	0
5	B	1771	0	1832	29	0
5	E	1771	0	1832	14	0
5	H	1771	0	1832	5	0
5	K	1771	0	1831	29	0
6	C	1347	0	1376	8	0
6	F	1351	0	1379	1	0
6	I	1347	0	1376	5	0
6	L	1351	0	1379	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	M	11905	0	11614	30	0
7	O	11909	0	11617	46	0
8	N	10955	0	11304	95	0
8	P	10955	0	11301	137	0
9	Q	5192	0	4911	13	0
9	R	5279	0	4937	0	0
9	S	5189	0	4902	14	0
9	T	5279	0	4937	10	0
10	U	736	0	739	12	0
10	W	736	0	739	13	0
11	V	720	0	703	0	0
11	X	731	0	716	1	0
All	All	123117	0	122013	555	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 2.

The worst 5 of 555 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)
8:N:1277:ILE:HD11	8:N:1280:LEU:CG	1.25	1.65
2:1:745:ILE:HG21	2:1:815:PHE:CZ	1.22	1.61
8:P:1277:ILE:CD1	8:P:1280:LEU:HB2	1.22	1.61
2:1:745:ILE:CG2	2:1:815:PHE:CZ	1.82	1.57
2:1:745:ILE:HG22	2:1:815:PHE:CE2	1.36	1.56

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	1072/1502 (71%)	870 (81%)	139 (13%)	63 (6%)	1	17
1	Y	1052/1502 (70%)	876 (83%)	110 (10%)	66 (6%)	1	17
2	1	1085/1391 (78%)	934 (86%)	98 (9%)	53 (5%)	2	20
2	Z	1082/1391 (78%)	934 (86%)	94 (9%)	54 (5%)	2	20
4	A	156/823 (19%)	152 (97%)	2 (1%)	2 (1%)	12	48
4	D	157/823 (19%)	152 (97%)	2 (1%)	3 (2%)	8	38
4	G	158/823 (19%)	153 (97%)	2 (1%)	3 (2%)	8	38
4	J	157/823 (19%)	149 (95%)	4 (2%)	4 (2%)	5	32
5	B	211/541 (39%)	188 (89%)	16 (8%)	7 (3%)	4	26
5	E	211/541 (39%)	188 (89%)	13 (6%)	10 (5%)	2	21
5	H	211/541 (39%)	177 (84%)	20 (10%)	14 (7%)	1	15
5	K	211/541 (39%)	196 (93%)	10 (5%)	5 (2%)	6	33
6	C	160/472 (34%)	150 (94%)	5 (3%)	5 (3%)	4	27
6	F	161/472 (34%)	155 (96%)	3 (2%)	3 (2%)	8	38
6	I	160/472 (34%)	151 (94%)	7 (4%)	2 (1%)	12	48
6	L	161/472 (34%)	156 (97%)	4 (2%)	1 (1%)	25	66
7	M	1496/1683 (89%)	1266 (85%)	162 (11%)	68 (4%)	2	22
7	O	1497/1683 (89%)	1265 (84%)	164 (11%)	68 (4%)	2	22
8	N	1308/1655 (79%)	1018 (78%)	188 (14%)	102 (8%)	1	13
8	P	1308/1655 (79%)	1020 (78%)	186 (14%)	102 (8%)	1	13
9	Q	671/839 (80%)	593 (88%)	53 (8%)	25 (4%)	3	24
9	R	691/839 (82%)	595 (86%)	76 (11%)	20 (3%)	4	29
9	S	671/839 (80%)	589 (88%)	62 (9%)	20 (3%)	4	28
9	T	691/839 (82%)	595 (86%)	66 (10%)	30 (4%)	2	22
10	U	89/475 (19%)	77 (86%)	6 (7%)	6 (7%)	1	15
10	W	89/475 (19%)	77 (86%)	9 (10%)	3 (3%)	3	26
11	V	88/528 (17%)	71 (81%)	10 (11%)	7 (8%)	1	12
11	X	89/528 (17%)	72 (81%)	11 (12%)	6 (7%)	1	15
All	All	15093/25168 (60%)	12819 (85%)	1522 (10%)	752 (5%)	4	20

5 of 752 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	178	GLU
1	0	419	LYS
1	0	533	SER
1	0	693	GLU
1	0	694	LYS

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	0	994/1353 (74%)	952 (96%)	42 (4%)	30	54
1	Y	977/1353 (72%)	945 (97%)	32 (3%)	38	61
2	1	1007/1250 (81%)	962 (96%)	45 (4%)	27	52
2	Z	1004/1250 (80%)	974 (97%)	30 (3%)	41	63
4	A	154/674 (23%)	147 (96%)	7 (4%)	27	52
4	D	154/674 (23%)	151 (98%)	3 (2%)	57	75
4	G	155/674 (23%)	146 (94%)	9 (6%)	20	45
4	J	154/674 (23%)	147 (96%)	7 (4%)	27	52
5	B	196/439 (45%)	185 (94%)	11 (6%)	21	46
5	E	196/439 (45%)	187 (95%)	9 (5%)	27	52
5	H	196/439 (45%)	185 (94%)	11 (6%)	21	46
5	K	196/439 (45%)	189 (96%)	7 (4%)	35	59
6	C	155/377 (41%)	147 (95%)	8 (5%)	23	48
6	F	155/377 (41%)	151 (97%)	4 (3%)	46	66
6	I	155/377 (41%)	148 (96%)	7 (4%)	27	52
6	L	155/377 (41%)	152 (98%)	3 (2%)	57	75
7	M	1279/1538 (83%)	1235 (97%)	44 (3%)	37	60
7	O	1279/1538 (83%)	1233 (96%)	46 (4%)	35	59
8	N	1276/1557 (82%)	1204 (94%)	72 (6%)	21	46
8	P	1276/1557 (82%)	1215 (95%)	61 (5%)	25	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	Q	508/762 (67%)	493 (97%)	15 (3%)	41	63
9	R	507/762 (66%)	494 (97%)	13 (3%)	46	66
9	S	507/762 (66%)	496 (98%)	11 (2%)	52	71
9	T	507/762 (66%)	497 (98%)	10 (2%)	55	74
10	U	79/421 (19%)	76 (96%)	3 (4%)	33	57
10	W	79/421 (19%)	75 (95%)	4 (5%)	24	48
11	V	80/477 (17%)	78 (98%)	2 (2%)	47	68
11	X	81/477 (17%)	78 (96%)	3 (4%)	34	58
All	All	13461/22200 (61%)	12942 (96%)	519 (4%)	36	56

5 of 519 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Y	273	ILE
1	Y	831	LYS
1	Y	207	MET
7	M	1016	THR
7	M	727	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 93 such sidechains are listed below:

Mol	Chain	Res	Type
8	P	1249	GLN
9	S	812	GLN
9	Q	439	HIS
9	R	658	ASN
9	T	733	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	637:LEU	C	638:ASP	N	3.38

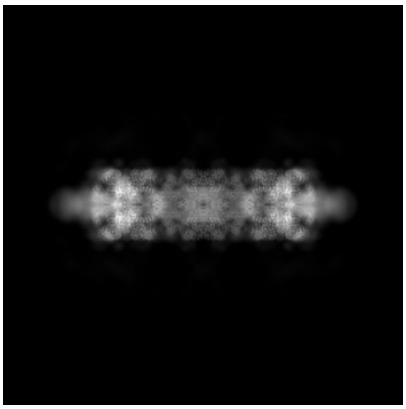
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24232. These allow visual inspection of the internal detail of the map and identification of artifacts.

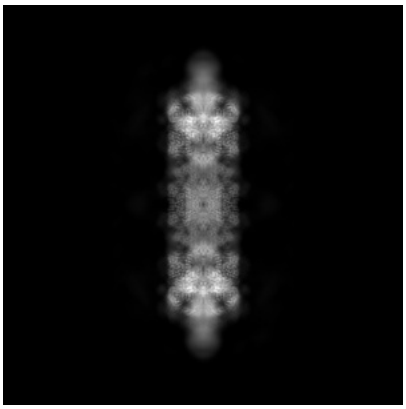
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

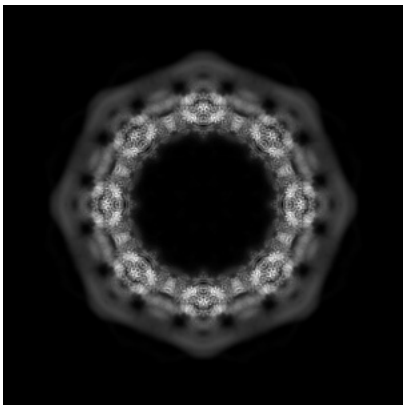
6.1.1 Primary map



X

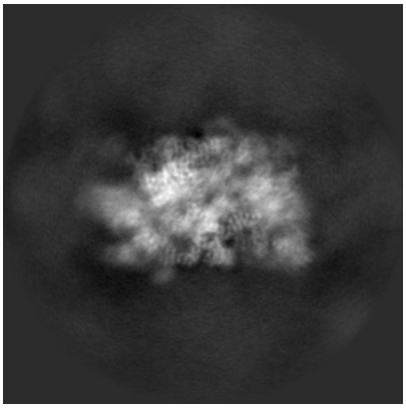


Y

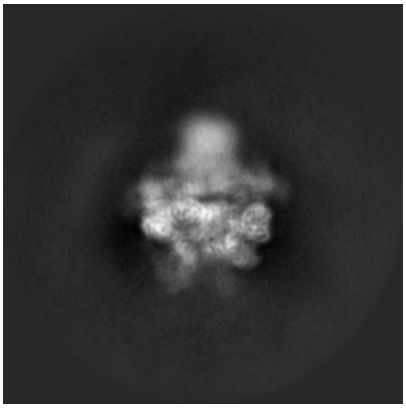


Z

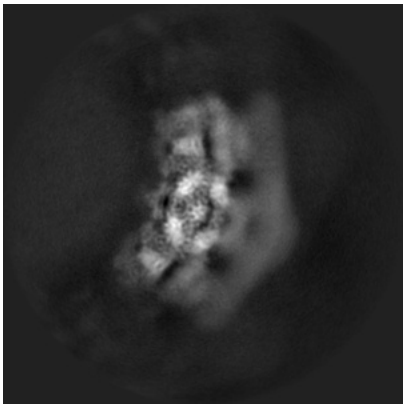
6.1.2 Raw map



X



Y

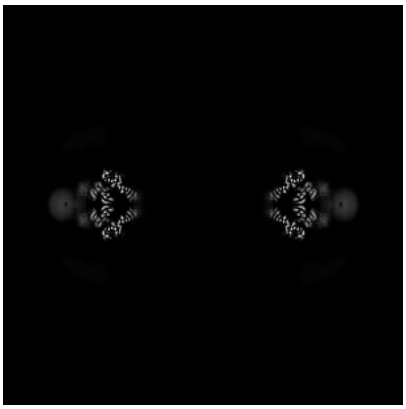


Z

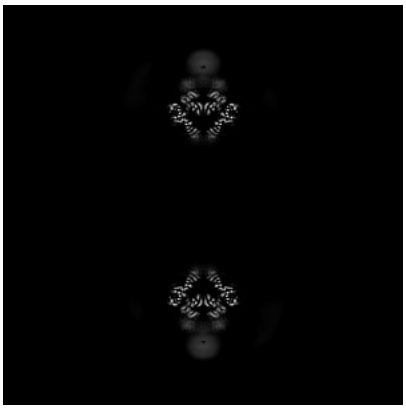
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

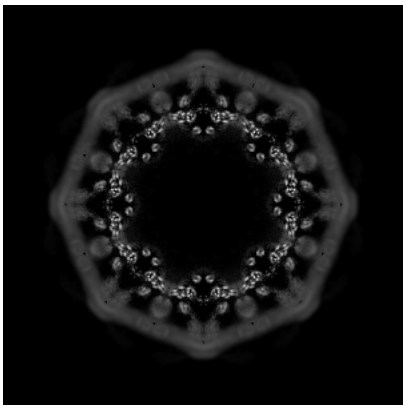
6.2.1 Primary map



X Index: 240

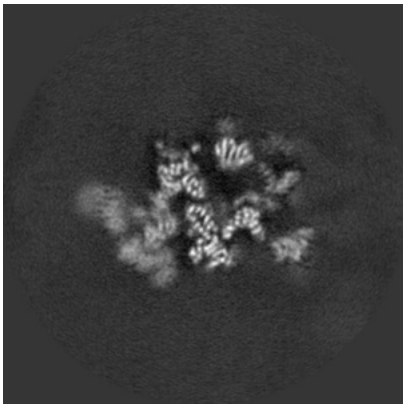


Y Index: 240

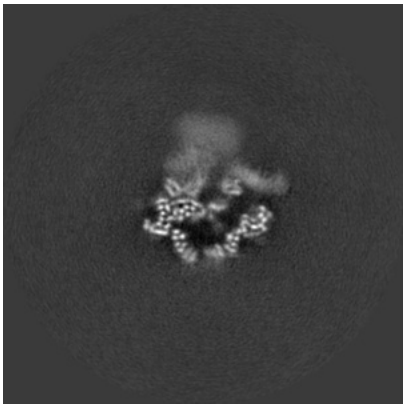


Z Index: 240

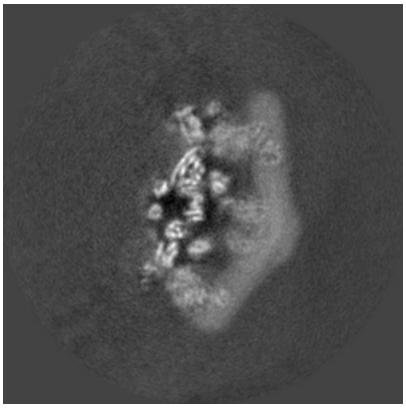
6.2.2 Raw map



X Index: 133



Y Index: 133

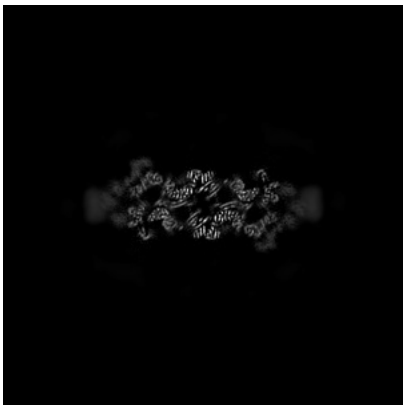


Z Index: 133

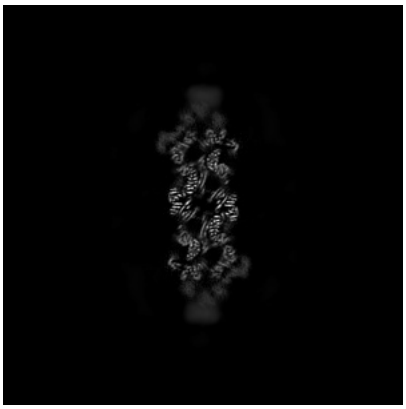
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

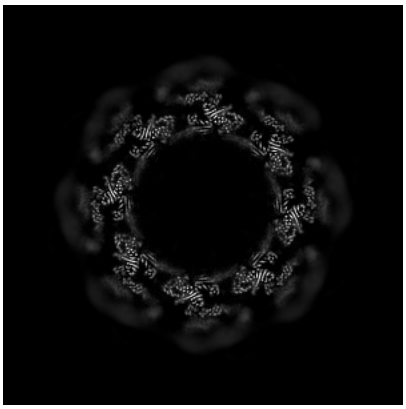
6.3.1 Primary map



X Index: 340

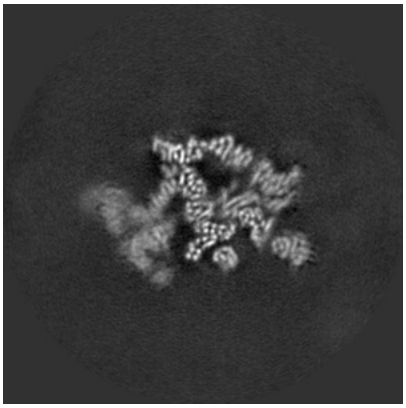


Y Index: 140

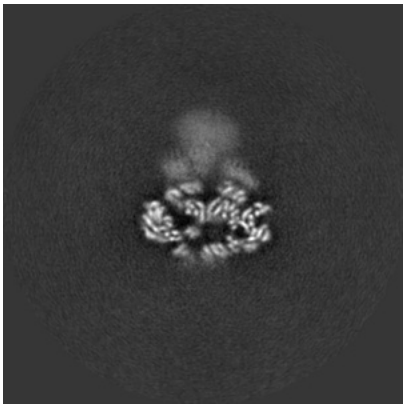


Z Index: 257

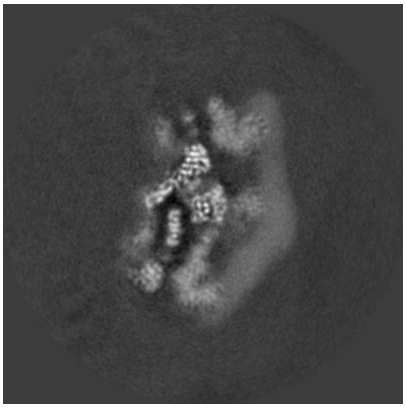
6.3.2 Raw map



X Index: 129



Y Index: 126

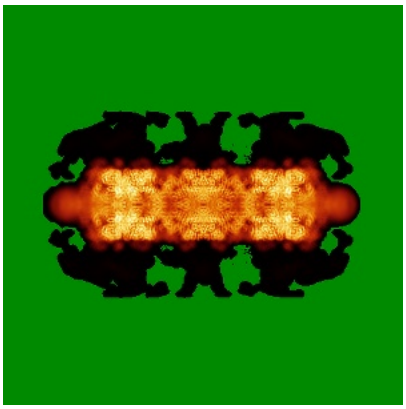


Z Index: 125

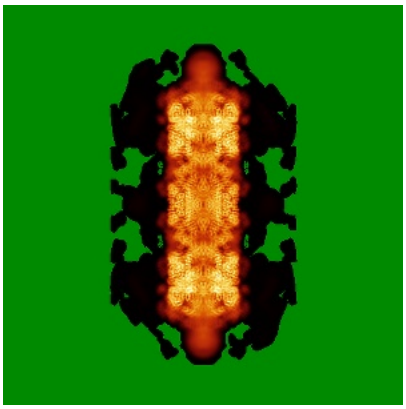
The images above show the largest variance slices of the map in three orthogonal directions.

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

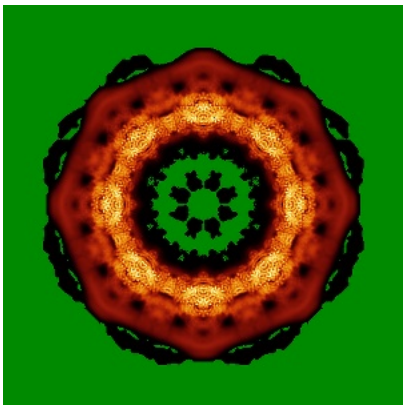
6.4.1 Primary map



X

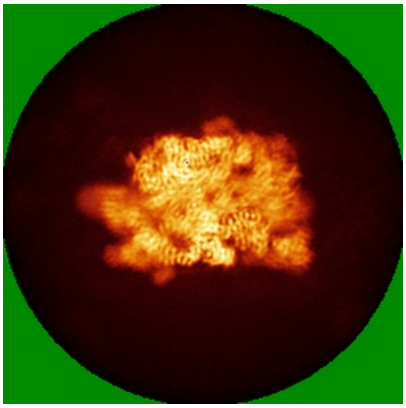


Y

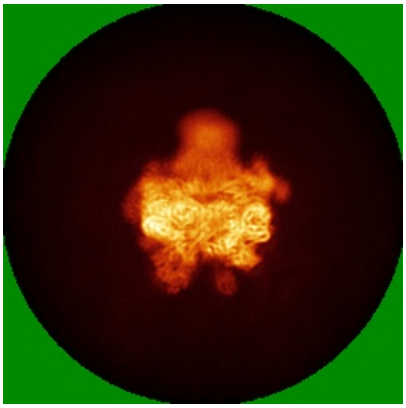


Z

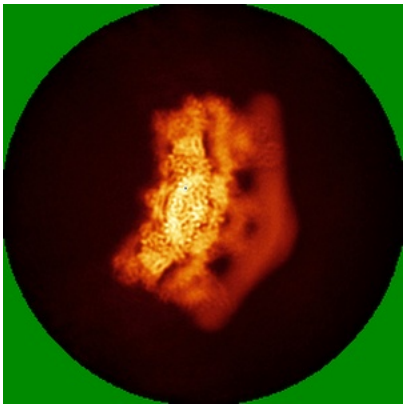
6.4.2 Raw map



X



Y

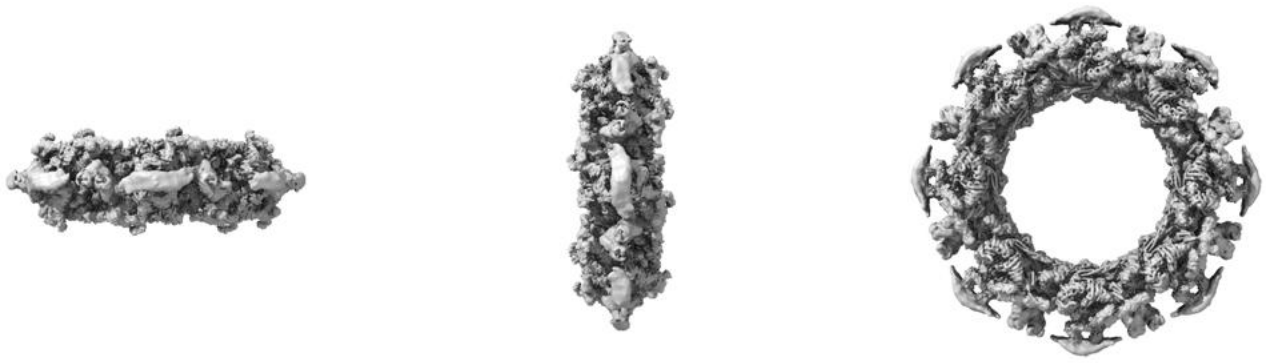


Z

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)

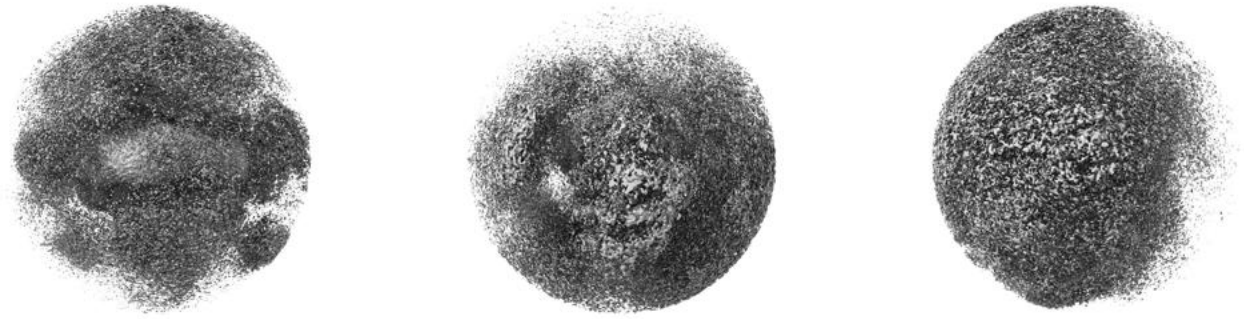
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.595. 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.

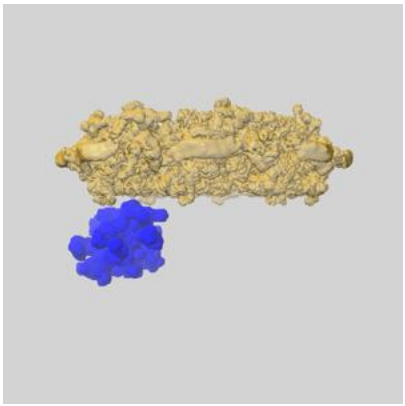
6.6 Mask visualisation (i)

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

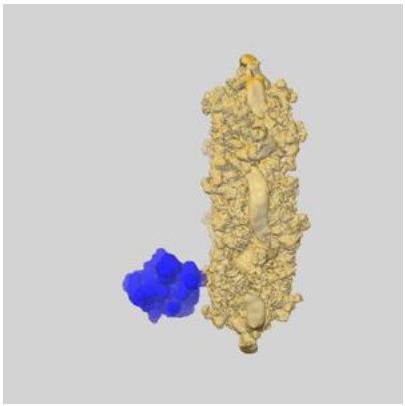
A mask typically either:

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

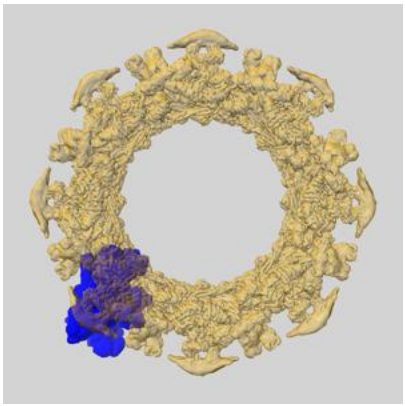
6.6.1 emd_24232_msk_1.map (i)



X



Y

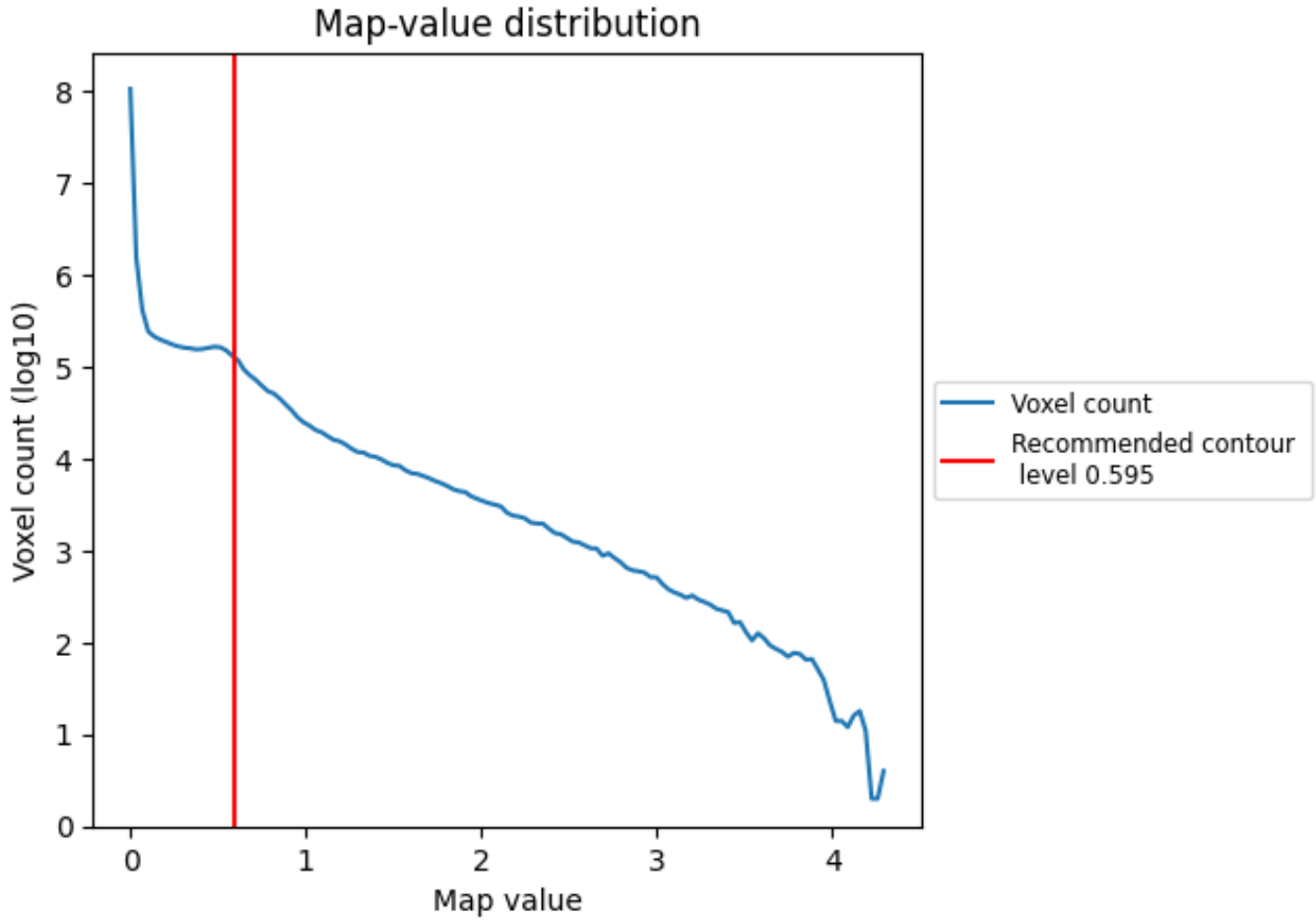


Z

7 Map analysis

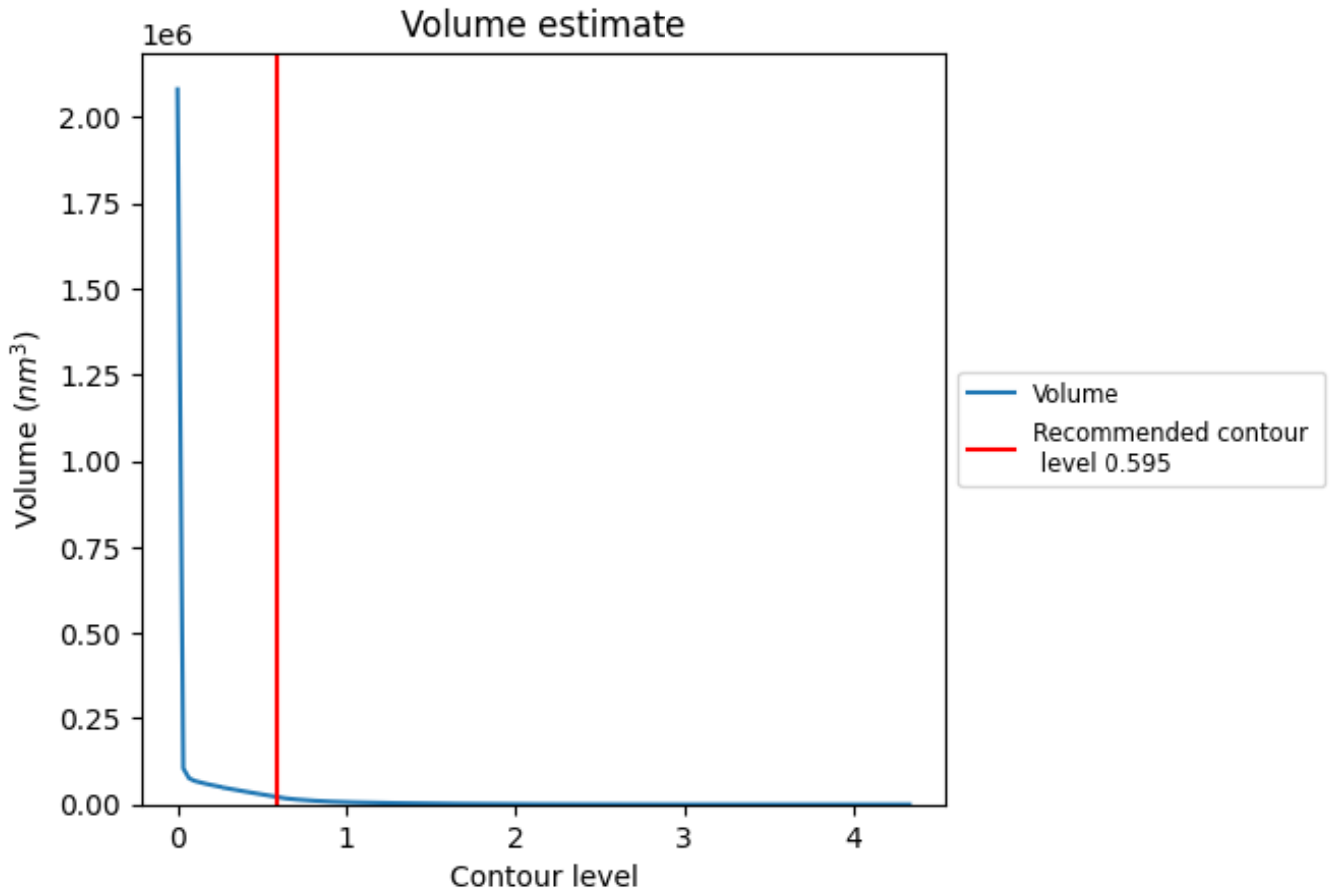
This section contains the results of statistical analysis of the map.

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.

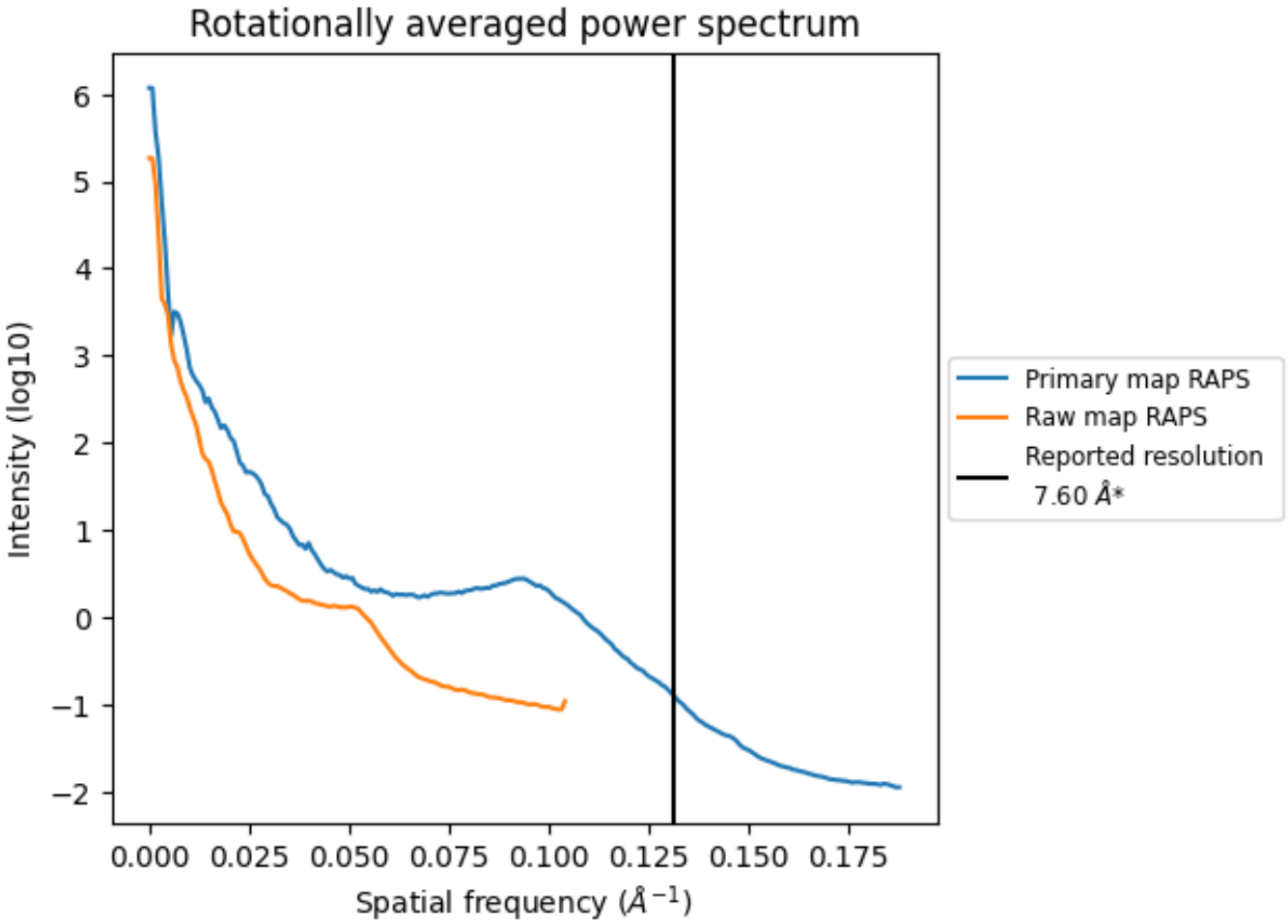
7.2 Volume estimate (i)



The volume at the recommended contour level is 20941 nm^3; this corresponds to an approximate mass of 18917 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)

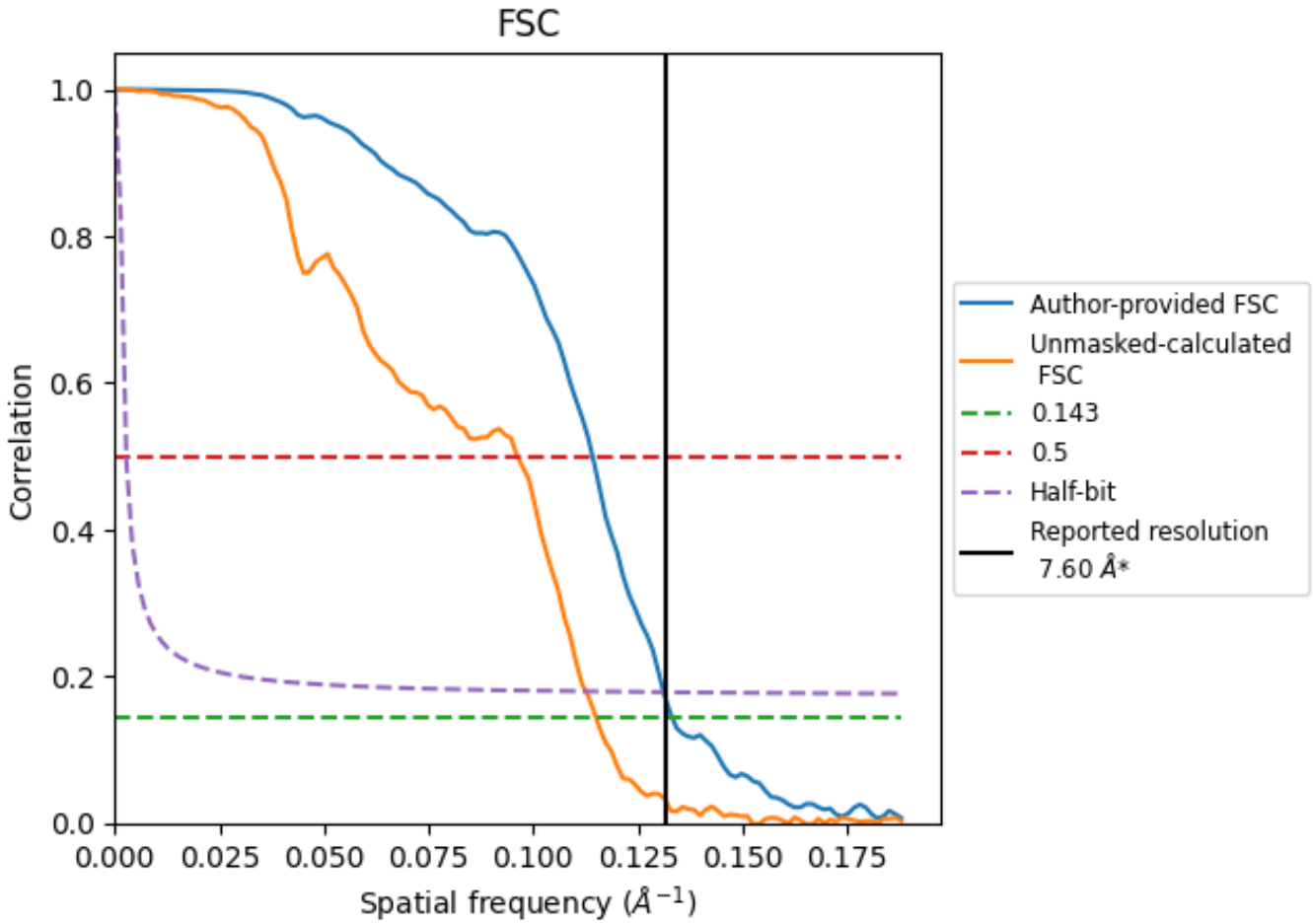


*Reported resolution corresponds to spatial frequency of 0.132 Å^{-1}

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 0.132 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.60	-	-
Author-provided FSC curve	7.51	8.76	7.62
Unmasked-calculated*	8.69	10.40	8.88

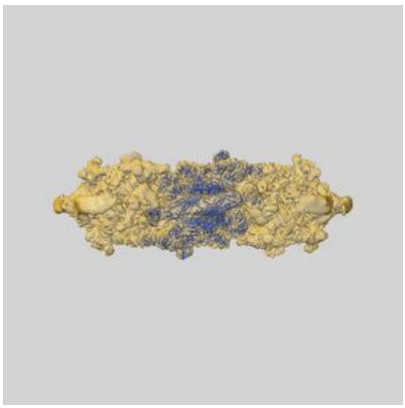
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.69 differs from the reported value 7.6 by more than 10 %

9 Map-model fit

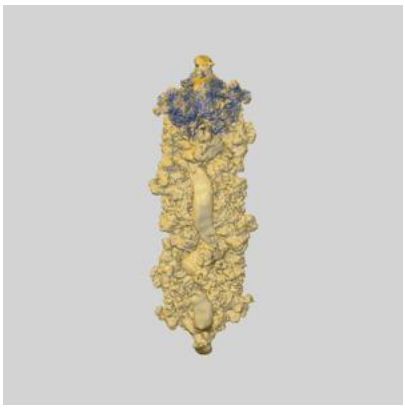
This section contains information regarding the fit between EMDB map EMD-24232 and PDB model 7N85. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlays

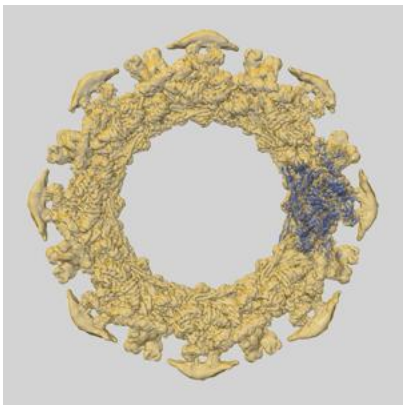
9.1.1 Map-model overlay



X

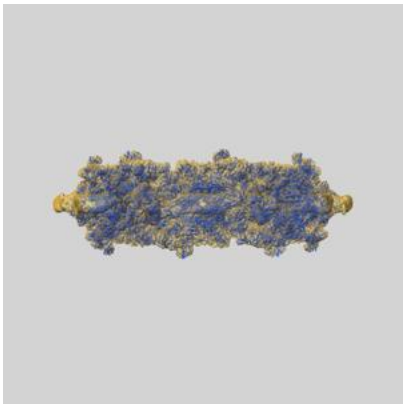


Y

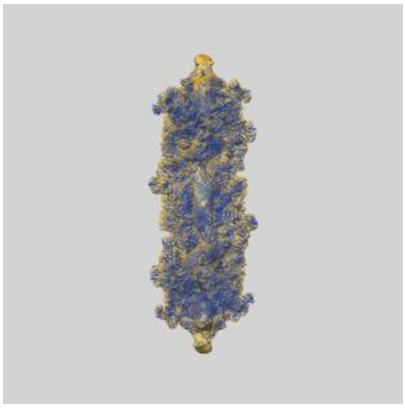


Z

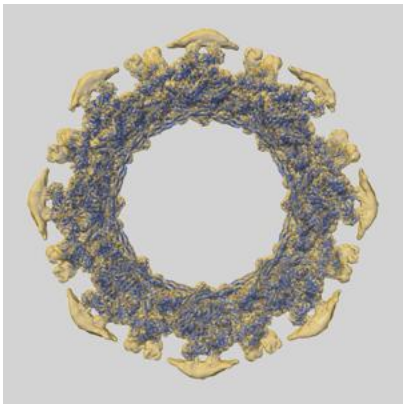
9.1.2 Map-model assembly overlay



X



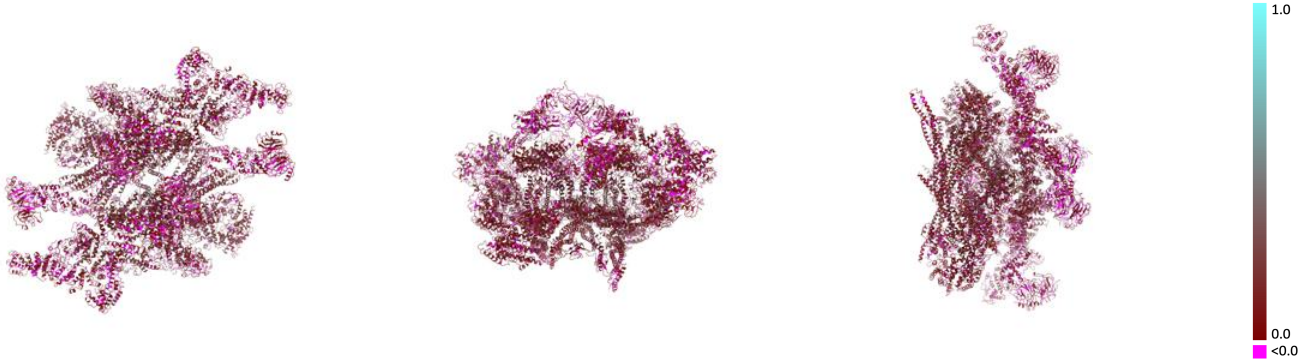
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.595 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.

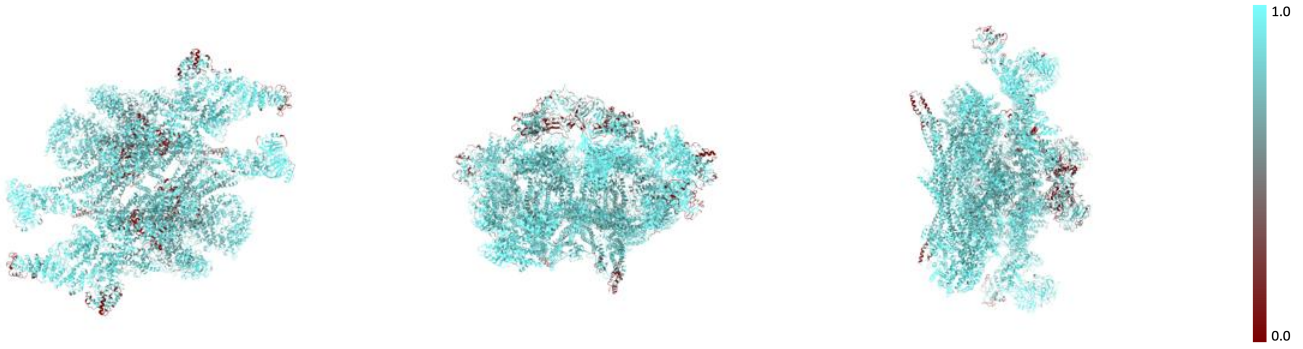
9.2 Q-score mapped to coordinate model



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.

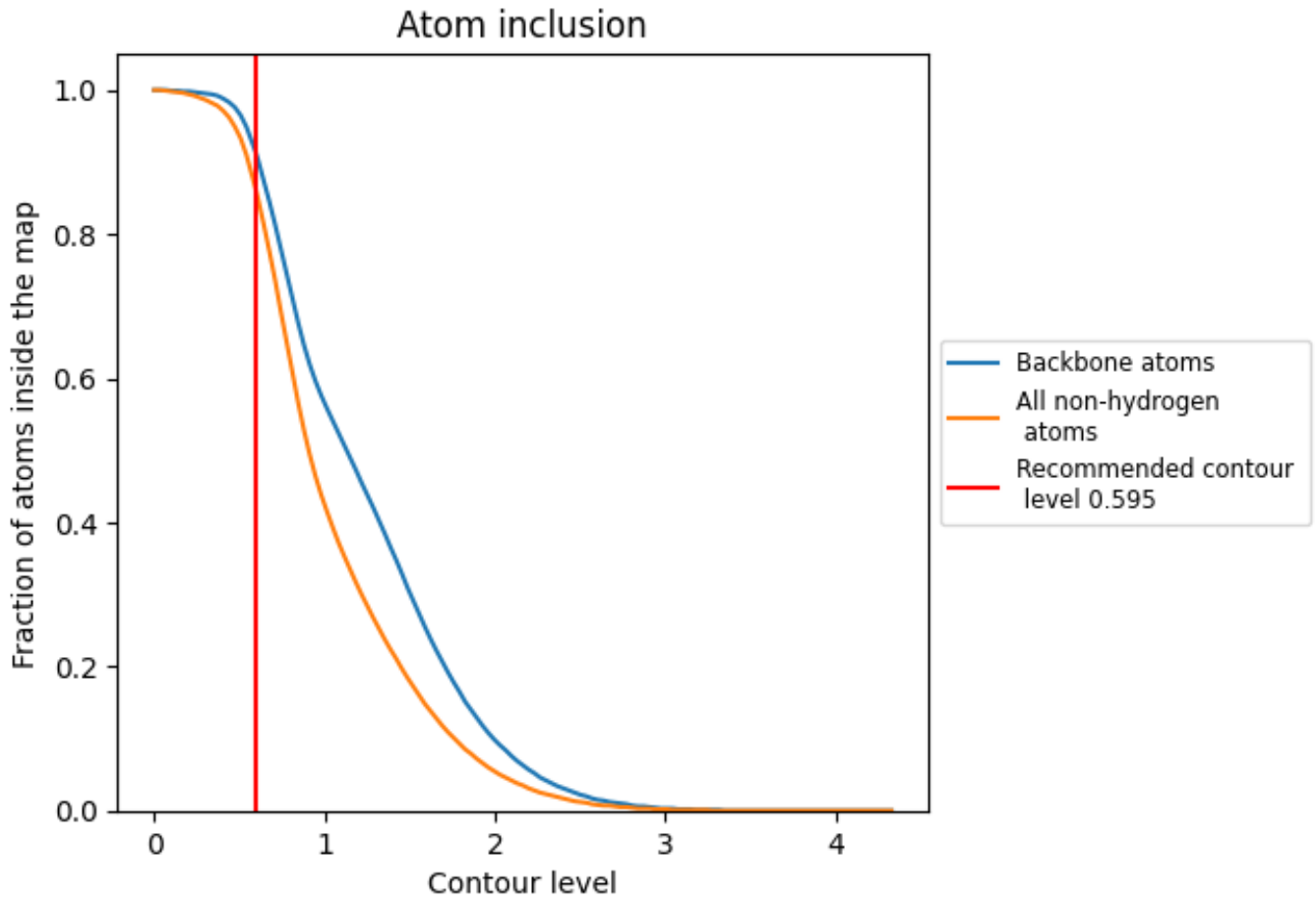
9.3 Atom inclusion mapped to coordinate model



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 (0.595).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 86% 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 (0.595) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8630	0.1130
0	0.9440	0.0850
1	0.6350	0.0560
5	0.9560	0.2120
6	0.9720	0.2110
A	0.8240	0.1360
B	0.7280	0.1140
C	0.7580	0.1240
D	0.9310	0.1530
E	0.9240	0.1480
F	0.9120	0.1380
G	0.8330	0.1380
H	0.7630	0.1140
I	0.7570	0.1250
J	0.9160	0.1540
K	0.9040	0.1380
L	0.8930	0.1440
M	0.9400	0.1340
N	0.8840	0.1320
O	0.9250	0.1360
P	0.8970	0.1310
Q	0.8360	0.1070
R	0.9210	0.1400
S	0.8470	0.1000
T	0.9380	0.1370
U	0.9810	0.0880
V	0.9710	0.0690
W	0.9890	0.0810
X	0.9940	0.0810
Y	0.9260	0.0850
Z	0.6360	0.0610