



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 07:49 AM UTC

PDB ID : 9SOB / pdb_00009sob
EMDB ID : EMD-54657
Title : Structural Model of the Nuclear Pore Complex in Arabidopsis thaliana
Authors : Obarska-Kosinska, A.; Sanchez Carrillo, I.B.; Hoffmann, P.C.; Fourcassie, V.; Beck, M.; Germain, H.
Deposited on : 2025-09-12
Resolution : 35.00 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:

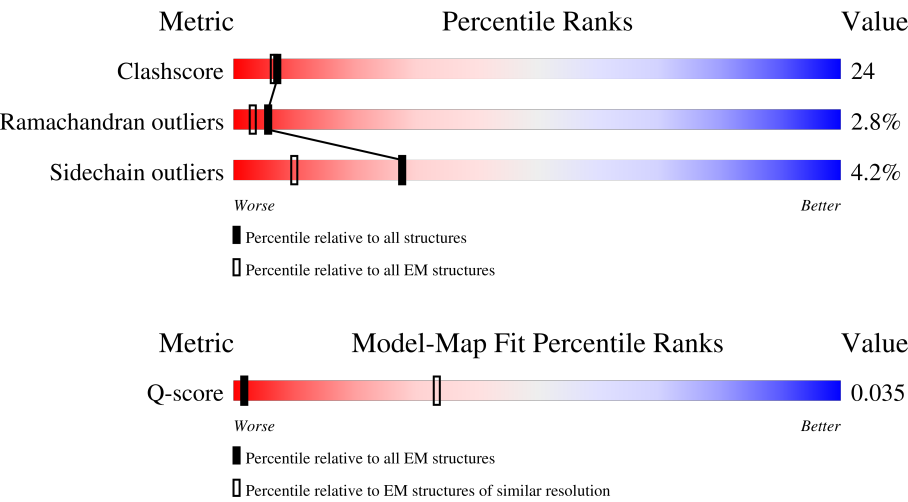
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 35.00 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3 (33.00 - 33.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	R	1495	
1	R16	1495	
1	R8	1495	
2	M	704	

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Mol	Chain	Length	Quality of chain
2	M16	704	
2	M8	704	
3	N	302	
3	N16	302	
3	N8	302	
4	T	684	
4	T16	684	
4	T8	684	
5	P	716	
5	P16	716	
5	P8	716	
6	O	326	
6	O16	326	
6	O8	326	
7	Q	361	
7	Q16	361	
7	Q8	361	
8	L	977	
8	L16	977	
8	L8	977	
9	K	709	
9	K16	709	
9	K8	709	
10	C	1838	
10	C16	1838	

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Mol	Chain	Length	Quality of chain
10	C24	1838	
10	C32	1838	
10	C8	1838	
11	A16	860	
11	A24	860	
11	A32	860	
11	A40	860	
12	A	763	
12	A48	763	
13	V	196	
14	W	810	
15	J	185	
16	A8	63	
17	F	28	
17	F16	28	
17	F24	28	
17	F8	28	
18	B	1965	
18	B8	1965	
19	4	447	
19	48	447	
20	E	519	
20	E8	519	
21	H	254	
21	H16	254	

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Mol	Chain	Length	Quality of chain
21	H24	254	
21	H8	254	
22	I	237	
22	I16	237	
22	I24	237	
22	I8	237	
23	J16	197	
23	J24	197	
23	J32	197	
23	J8	197	
24	D	1464	
24	D16	1464	
24	D24	1464	
24	D32	1464	
24	D40	1464	
24	D8	1464	

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 402561 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 Nuclear pore complex protein NUP160.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	1464	Total	C	N	O	S	0	0
			11593	7388	1952	2188	65		
1	R8	1464	Total	C	N	O	S	0	0
			11593	7388	1952	2188	65		
1	R16	1464	Total	C	N	O	S	0	0
			11593	7388	1952	2188	65		

- Molecule 2 is a protein called Nuclear pore complex protein NUP96.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	696	Total	C	N	O	S	0	0
			5598	3577	939	1054	28		
2	M8	696	Total	C	N	O	S	0	0
			5598	3577	939	1054	28		
2	M16	696	Total	C	N	O	S	0	0
			5598	3577	939	1054	28		

- Molecule 3 is a protein called Protein transport protein SEC13 homolog B.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	302	Total	C	N	O	S	0	0
			2302	1451	398	444	9		
3	N8	302	Total	C	N	O	S	0	0
			2302	1451	398	444	9		
3	N16	302	Total	C	N	O	S	0	0
			2302	1451	398	444	9		

- Molecule 4 is a protein called E3 ubiquitin-protein ligase HOS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	T	684	Total	C	N	O	S	0	0
			5498	3453	960	1049	36		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	T8	684	Total	C	N	O	S	0	0
			5498	3453	960	1049	36		
4	T16	684	Total	C	N	O	S	0	0
			5498	3453	960	1049	36		

- Molecule 5 is a protein called Nuclear pore complex protein NUP85.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	P	708	Total	C	N	O	S	0	0
			5620	3572	974	1041	33		
5	P8	708	Total	C	N	O	S	0	0
			5620	3572	974	1041	33		
5	P16	708	Total	C	N	O	S	0	0
			5620	3572	974	1041	33		

- Molecule 6 is a protein called Protein SEH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	O	303	Total	C	N	O	S	0	0
			2336	1467	387	468	14		
6	O8	303	Total	C	N	O	S	0	0
			2336	1467	387	468	14		
6	O16	303	Total	C	N	O	S	0	0
			2336	1467	387	468	14		

- Molecule 7 is a protein called Nuclear pore complex protein NUP43.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Q	361	Total	C	N	O	S	0	0
			2770	1732	480	546	12		
7	Q8	361	Total	C	N	O	S	0	0
			2770	1732	480	546	12		
7	Q16	361	Total	C	N	O	S	0	0
			2770	1732	480	546	12		

- Molecule 8 is a protein called Nuclear pore complex protein NUP107.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	974	Total	C	N	O	S	0	0
			7770	4912	1322	1481	55		
8	L8	974	Total	C	N	O	S	0	0
			7770	4912	1322	1481	55		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	L16	974	Total	C	N	O	S	0	0
			7770	4912	1322	1481	55		

- Molecule 9 is a protein called Nuclear pore complex protein NUP133.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	705	Total	C	N	O	S	0	0
			5695	3569	992	1104	30		
9	K8	705	Total	C	N	O	S	0	0
			5695	3569	992	1104	30		
9	K16	705	Total	C	N	O	S	0	0
			5696	3569	992	1105	30		

- Molecule 10 is a protein called Nuclear pore complex protein NUP205.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C16	1838	Total	C	N	O	S	0	0
			14529	9239	2457	2763	70		
10	C24	1838	Total	C	N	O	S	0	0
			14529	9239	2457	2763	70		
10	C	1824	Total	C	N	O	S	0	0
			14402	9155	2437	2740	70		
10	C8	1793	Total	C	N	O	S	0	0
			14177	9023	2397	2687	70		
10	C32	1838	Total	C	N	O	S	0	0
			14529	9239	2457	2763	70		

- Molecule 11 is a protein called Nuclear pore complex protein NUP93A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A24	818	Total	C	N	O	S	0	0
			6472	4058	1154	1227	33		
11	A40	818	Total	C	N	O	S	0	0
			6472	4058	1154	1227	33		
11	A16	818	Total	C	N	O	S	0	0
			6472	4058	1154	1227	33		
11	A32	818	Total	C	N	O	S	0	0
			6472	4058	1154	1227	33		

- Molecule 12 is a protein called Nuclear pore complex protein NUP93A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A	723	Total	C	N	O	S	0	0
			5726	3594	1023	1078	31		
12	A48	726	Total	C	N	O	S	0	0
			5752	3612	1026	1083	31		

- Molecule 13 is a protein called Nuclear pore complex protein NUP214.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	V	196	Total	C	N	O	S	0	0
			1590	987	289	304	10		

- Molecule 14 is a protein called Nuclear pore complex protein NUP88.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	W	787	Total	C	N	O	S	0	0
			6141	3886	1047	1185	23		

- Molecule 15 is a protein called Nuclear pore complex protein NUP62.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	185	Total	C	N	O	S	0	0
			1504	923	266	310	5		

- Molecule 16 is a protein called Nuclear pore complex protein NUP93A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	A8	63	Total	C	N	O	S	0	0
			523	326	90	102	5		

- Molecule 17 is a protein called Nuclear pore complex protein NUP35.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	F8	28	Total	C	N	O	S	0	0
			213	133	31	48	1		
17	F	28	Total	C	N	O	S	0	0
			213	133	31	48	1		
17	F24	28	Total	C	N	O	S	0	0
			213	133	31	48	1		
17	F16	28	Total	C	N	O	S	0	0
			213	133	31	48	1		

- Molecule 18 is a protein called Nucleoporin (DUF3414).

Mol	Chain	Residues	Atoms					AltConf	Trace
18	B	1965	Total	C	N	O	S	0	0
			15417	9887	2528	2913	89		
18	B8	1965	Total	C	N	O	S	0	0
			15417	9887	2528	2913	89		

- Molecule 19 is a protein called Aladin.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	4	447	Total	C	N	O	S	0	0
			3413	2155	583	659	16		
19	48	447	Total	C	N	O	S	0	0
			3413	2155	583	659	16		

- Molecule 20 is a protein called Nucleoporin protein Ndc1-Nup protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	E	519	Total	C	N	O	S	0	0
			4057	2648	667	727	15		
20	E8	519	Total	C	N	O	S	0	0
			4057	2648	667	727	15		

- Molecule 21 is a protein called Nuclear pore complex protein NUP54.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	H	254	Total	C	N	O	S	0	0
			2023	1254	366	392	11		
21	H8	254	Total	C	N	O	S	0	0
			2023	1254	366	392	11		
21	H24	254	Total	C	N	O	S	0	0
			2023	1254	366	392	11		
21	H16	254	Total	C	N	O	S	0	0
			2023	1254	366	392	11		

- Molecule 22 is a protein called NUP58.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	I	237	Total	C	N	O	S	0	0
			1939	1219	351	359	10		
22	I8	237	Total	C	N	O	S	0	0
			1939	1219	351	359	10		
22	I24	237	Total	C	N	O	S	0	0
			1939	1219	351	359	10		

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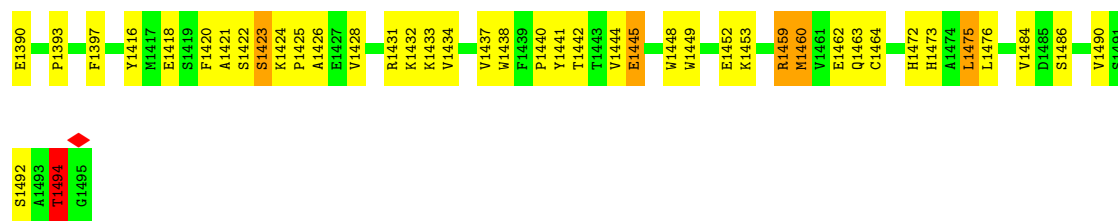
Mol	Chain	Residues	Atoms					AltConf	Trace
22	I16	237	Total	C	N	O	S	0	0
			1939	1219	351	359	10		

- Molecule 23 is a protein called Nuclear pore complex protein NUP62.

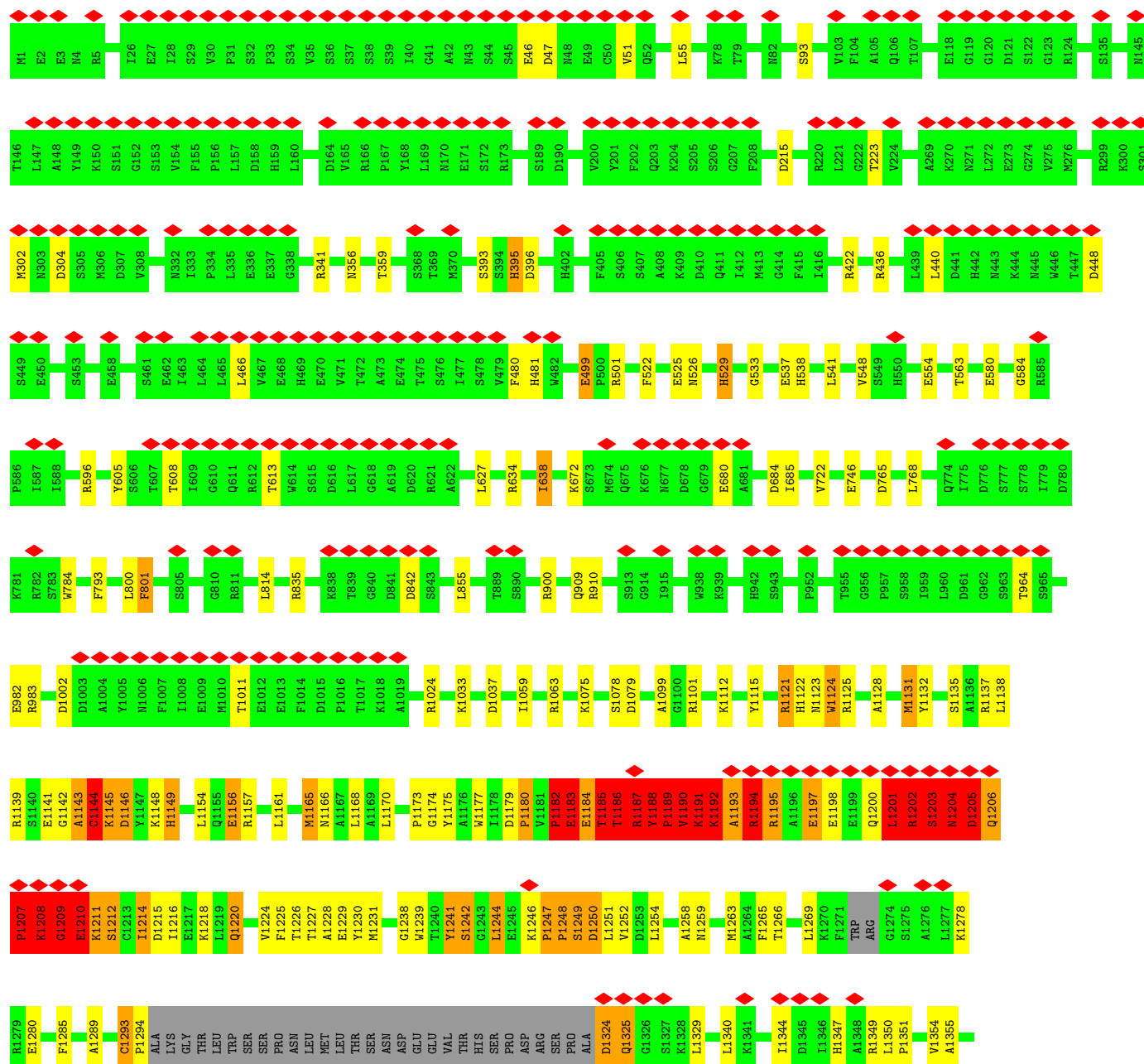
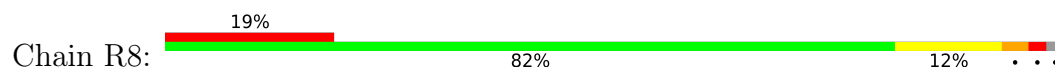
Mol	Chain	Residues	Atoms					AltConf	Trace
23	J32	197	Total	C	N	O	S	0	0
			1601	983	284	327	7		
23	J8	197	Total	C	N	O	S	0	0
			1601	983	284	327	7		
23	J24	197	Total	C	N	O	S	0	0
			1601	983	284	327	7		
23	J16	197	Total	C	N	O	S	0	0
			1601	983	284	327	7		

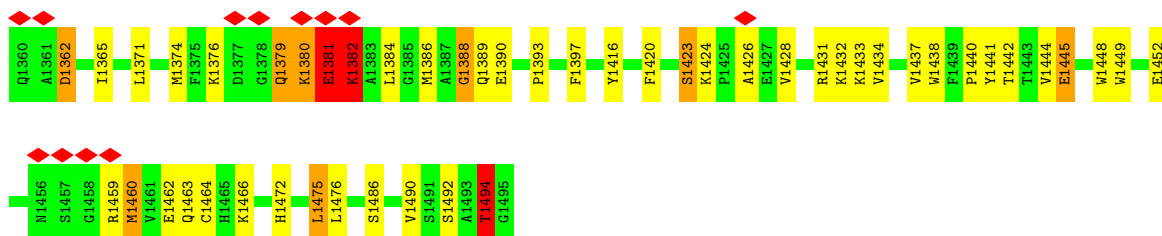
- Molecule 24 is a protein called Nuclear pore complex protein NUP155.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	D	1453	Total	C	N	O	S	0	0
			11141	6950	1960	2168	63		
24	D8	1453	Total	C	N	O	S	0	0
			11141	6950	1960	2168	63		
24	D16	1453	Total	C	N	O	S	0	0
			11141	6950	1960	2168	63		
24	D24	1453	Total	C	N	O	S	0	0
			11141	6950	1960	2168	63		
24	D32	1453	Total	C	N	O	S	0	0
			11141	6950	1960	2168	63		
24	D40	1453	Total	C	N	O	S	0	0
			11141	6950	1960	2168	63		

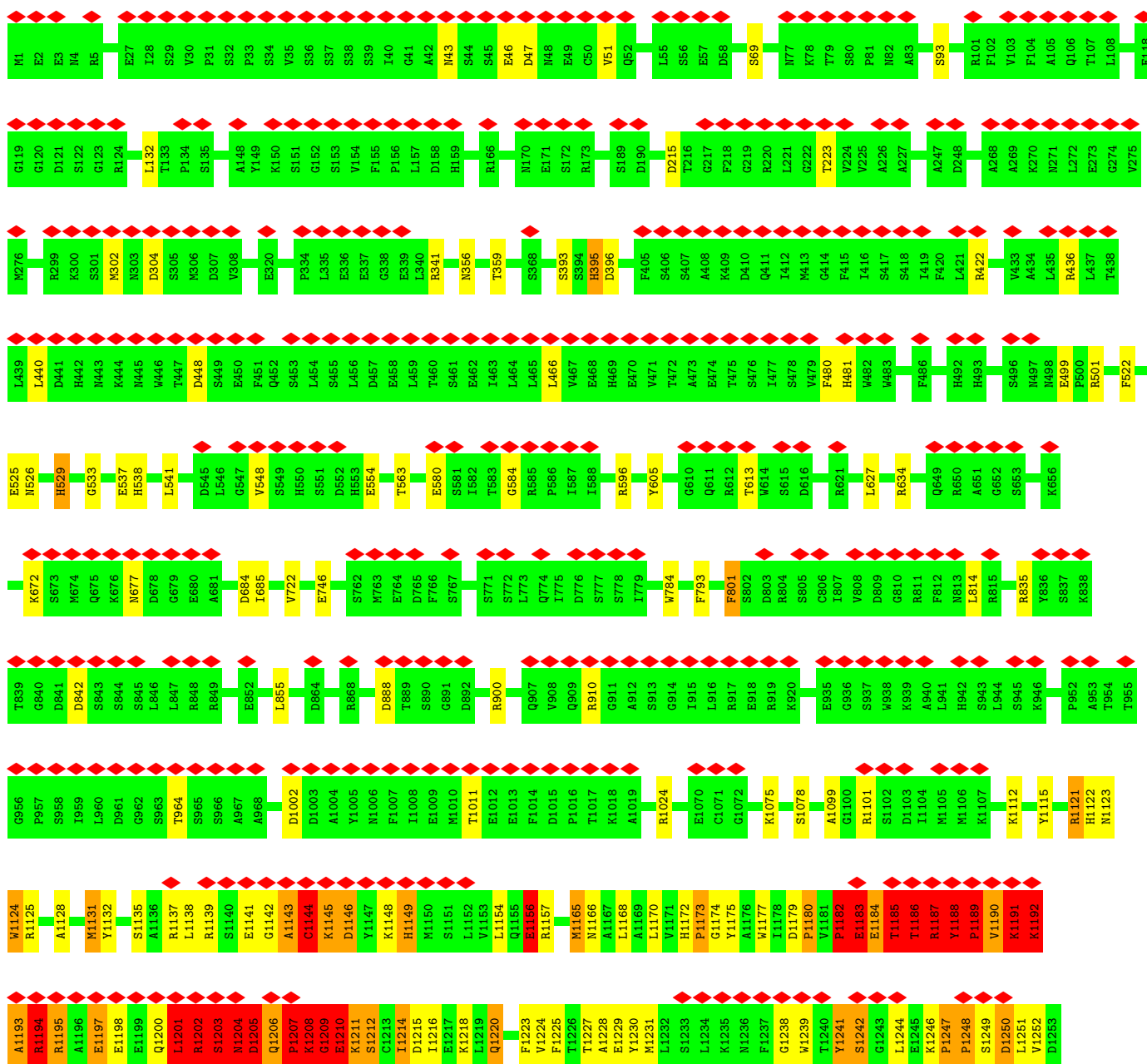
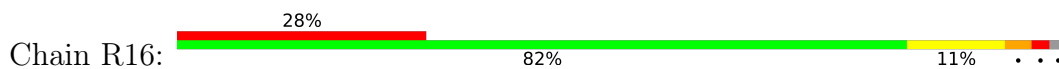


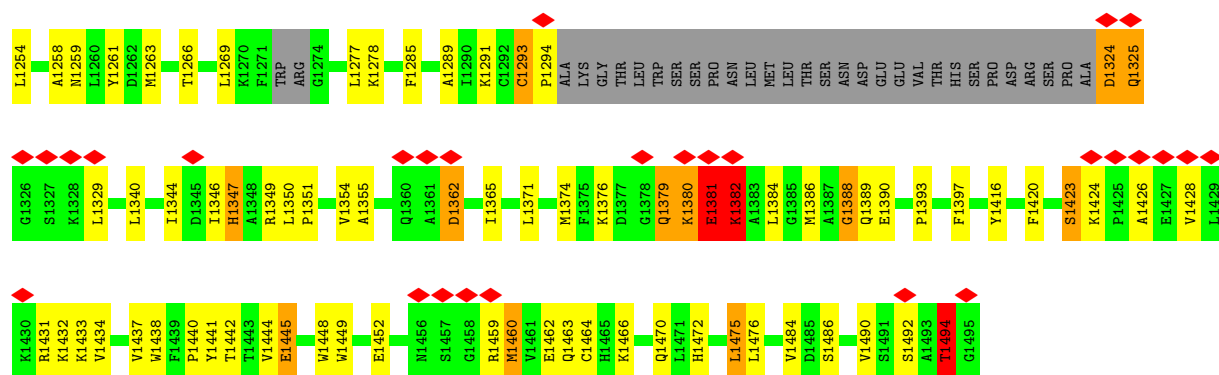
• Molecule 1: Nuclear pore complex protein NUP160



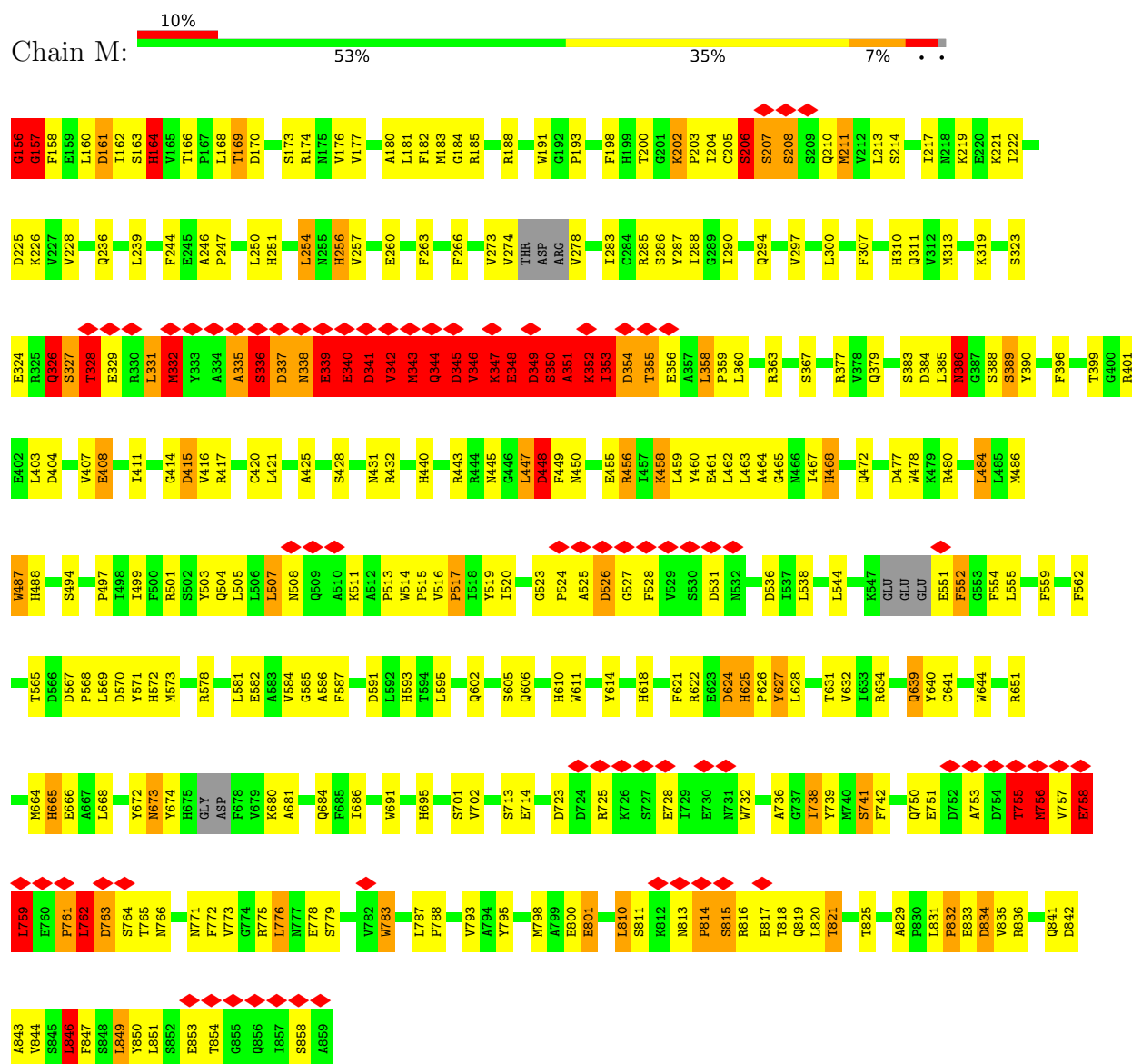


• Molecule 1: Nuclear pore complex protein NUP160



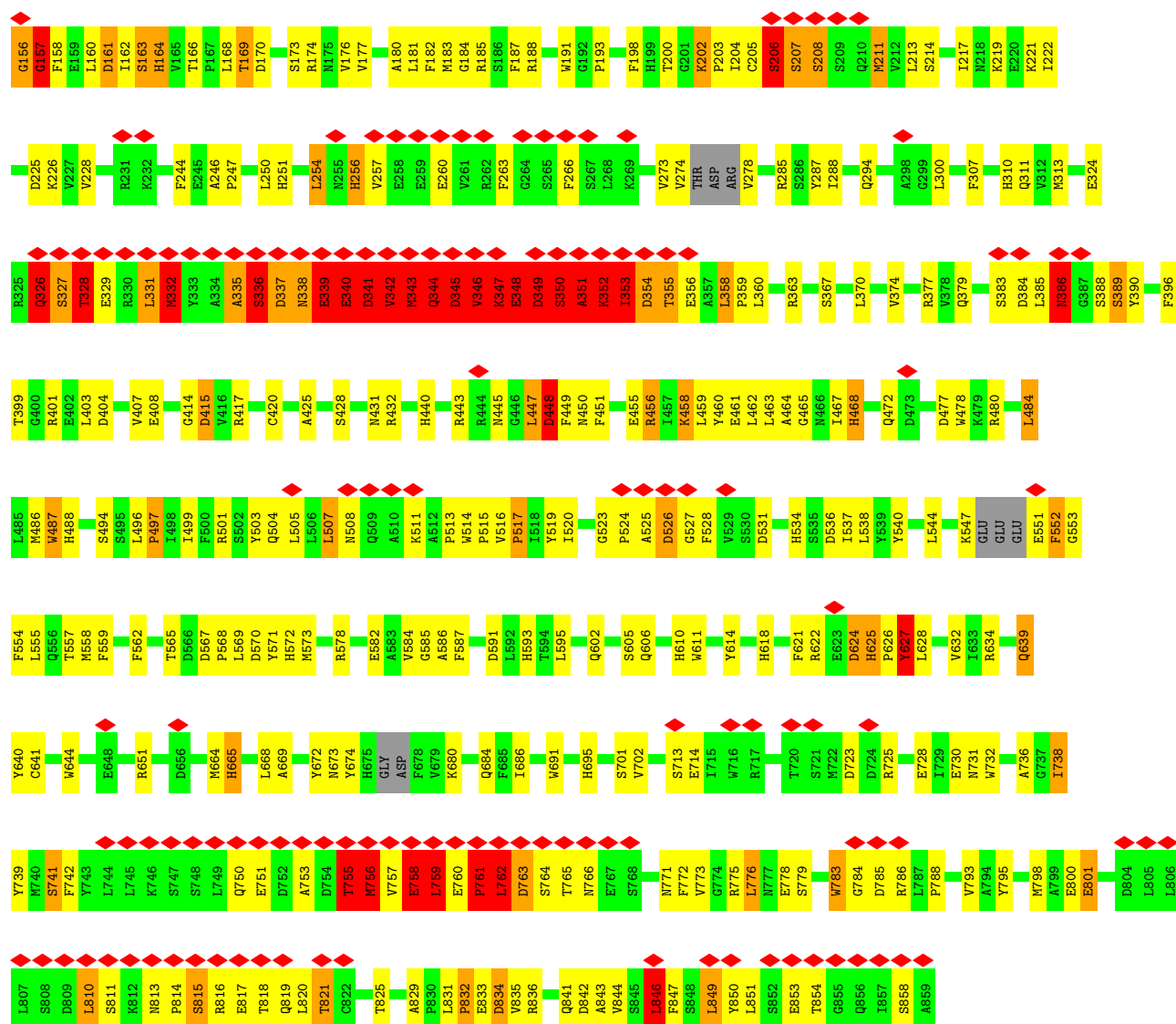


• Molecule 2: Nuclear pore complex protein NUP96



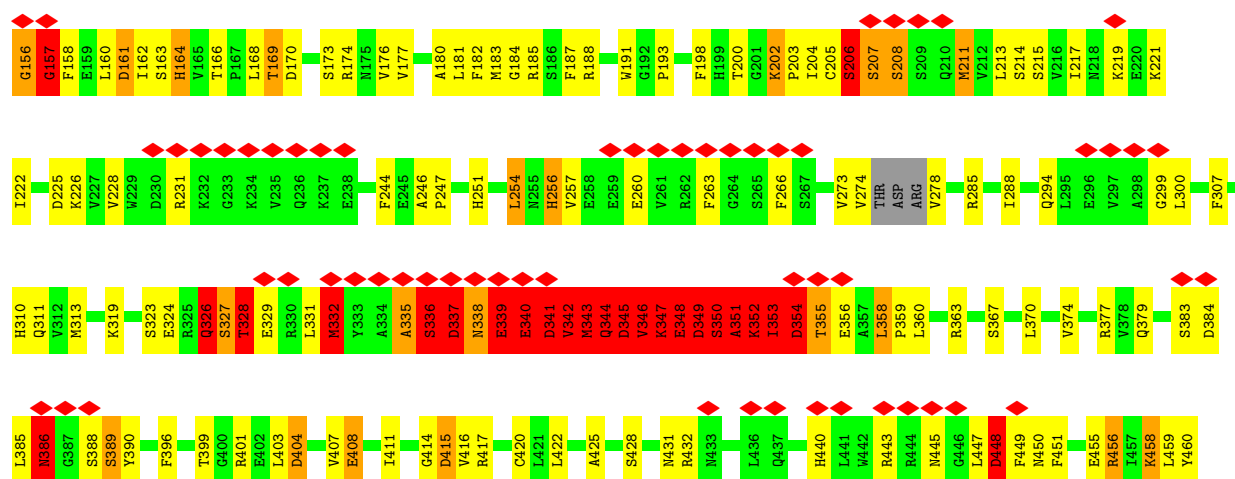
• Molecule 2: Nuclear pore complex protein NUP96

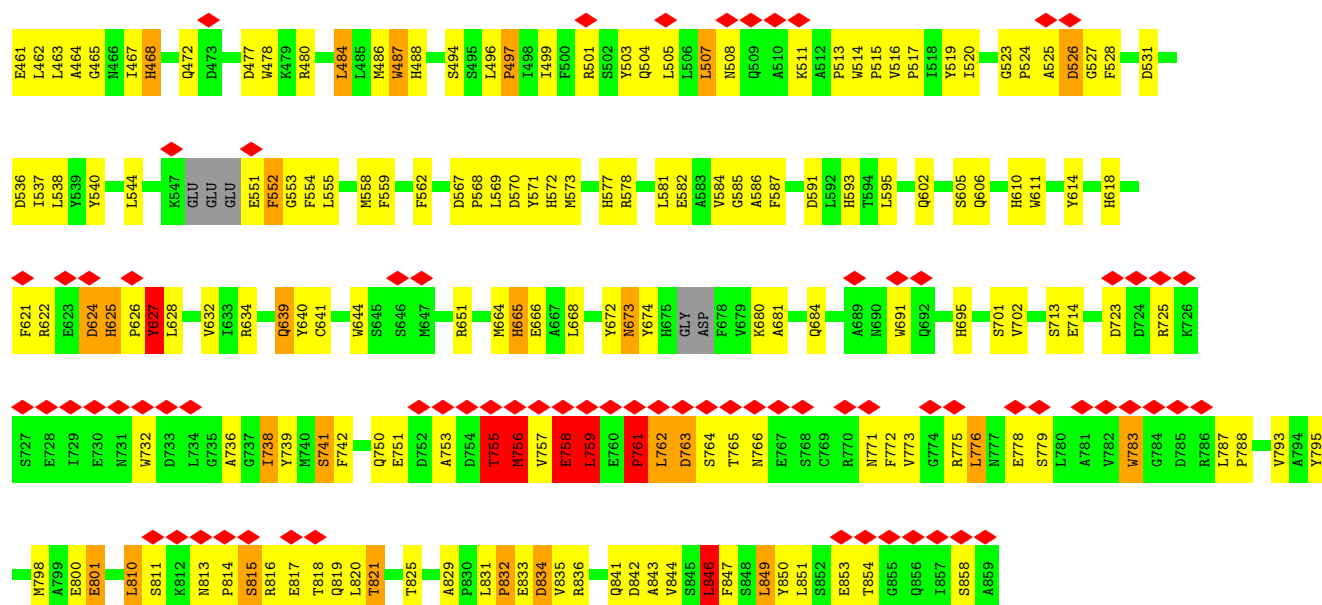




● Molecule 2: Nuclear pore complex protein NUP96

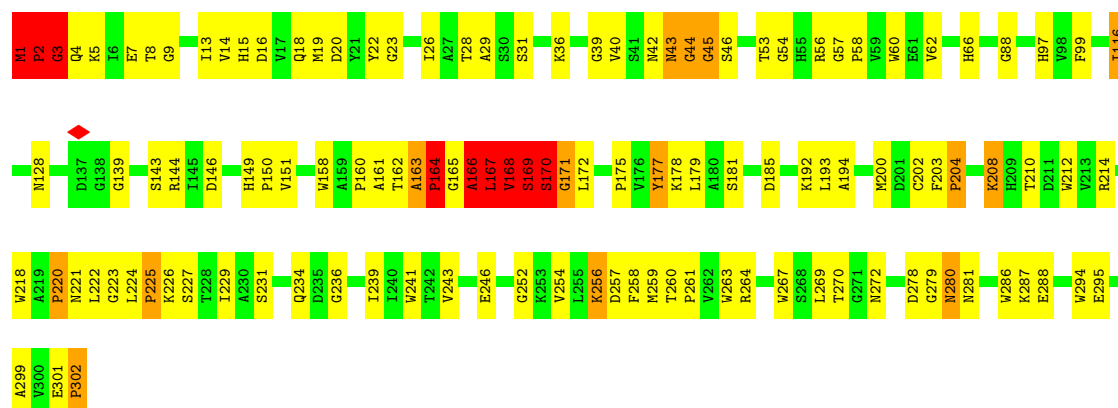
Chain M16: 19% 53% 35% 7% 5%





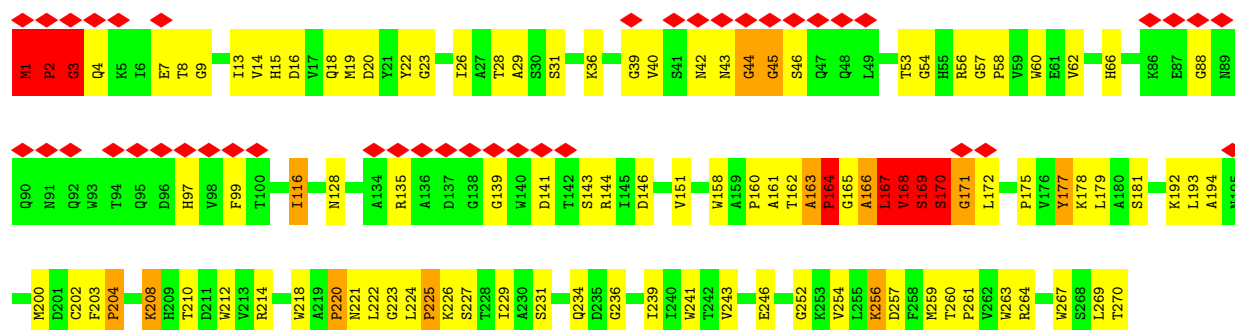
• Molecule 3: Protein transport protein SEC13 homolog B

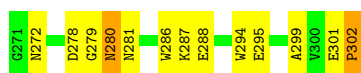
Chain N: 59% 33% 5%



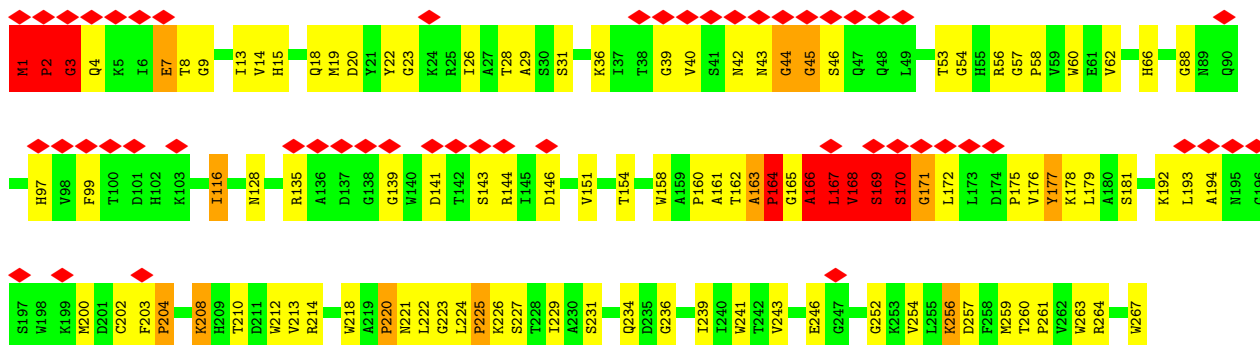
• Molecule 3: Protein transport protein SEC13 homolog B

Chain N8: 14% 60% 32% 5%

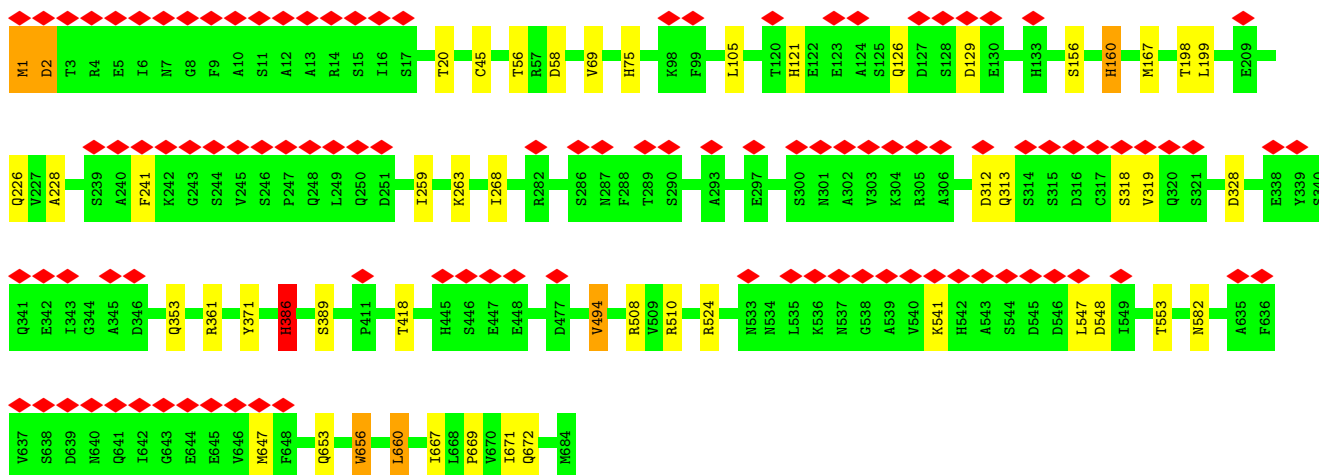




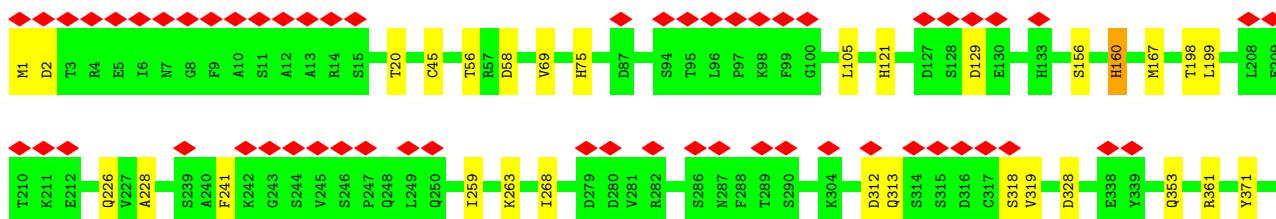
• Molecule 3: Protein transport protein SEC13 homolog B

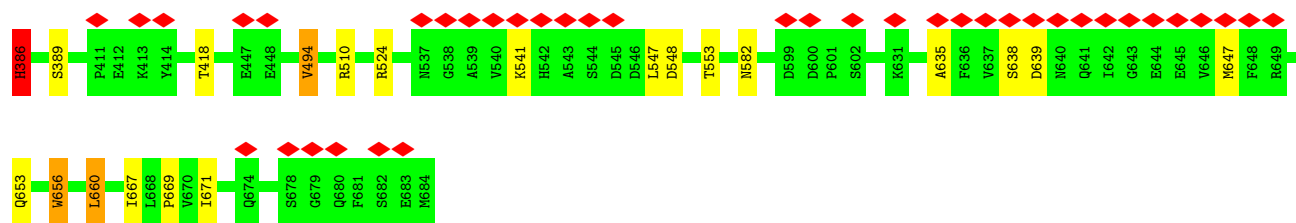


• Molecule 4: E3 ubiquitin-protein ligase HOS1

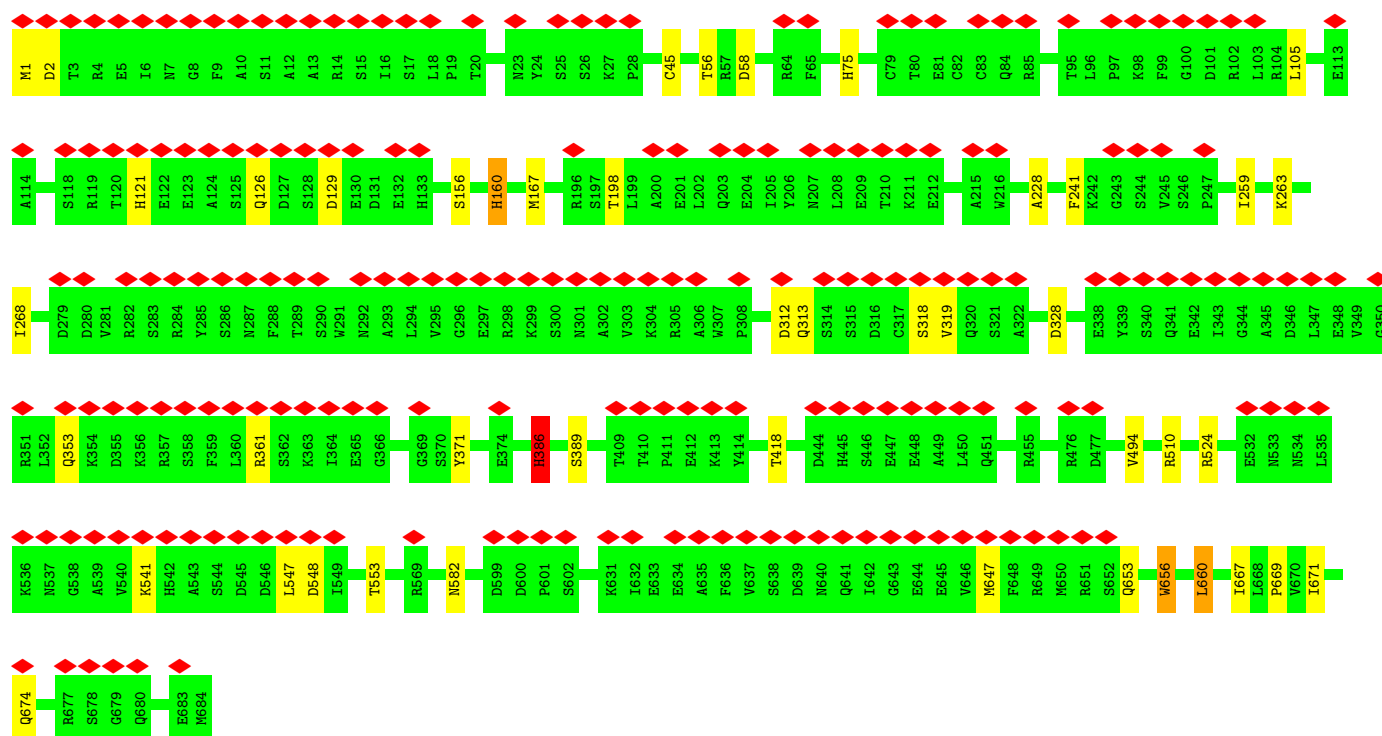


• Molecule 4: E3 ubiquitin-protein ligase HOS1

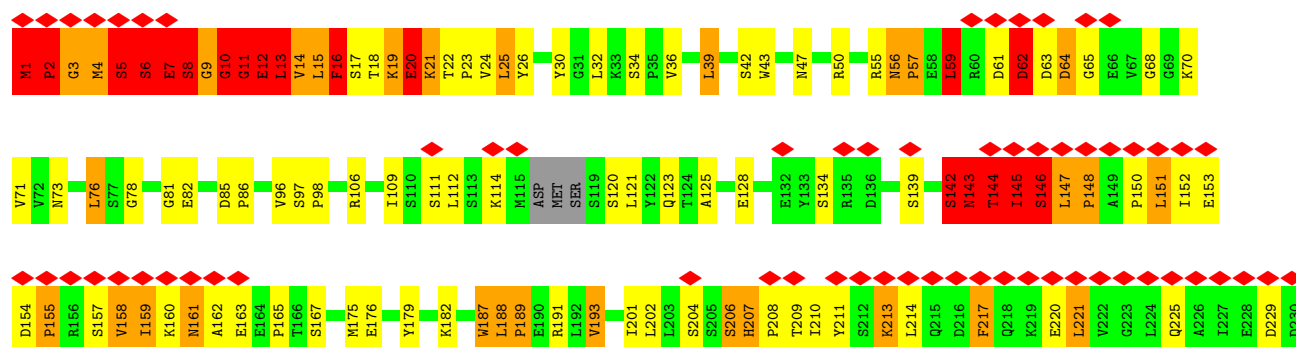


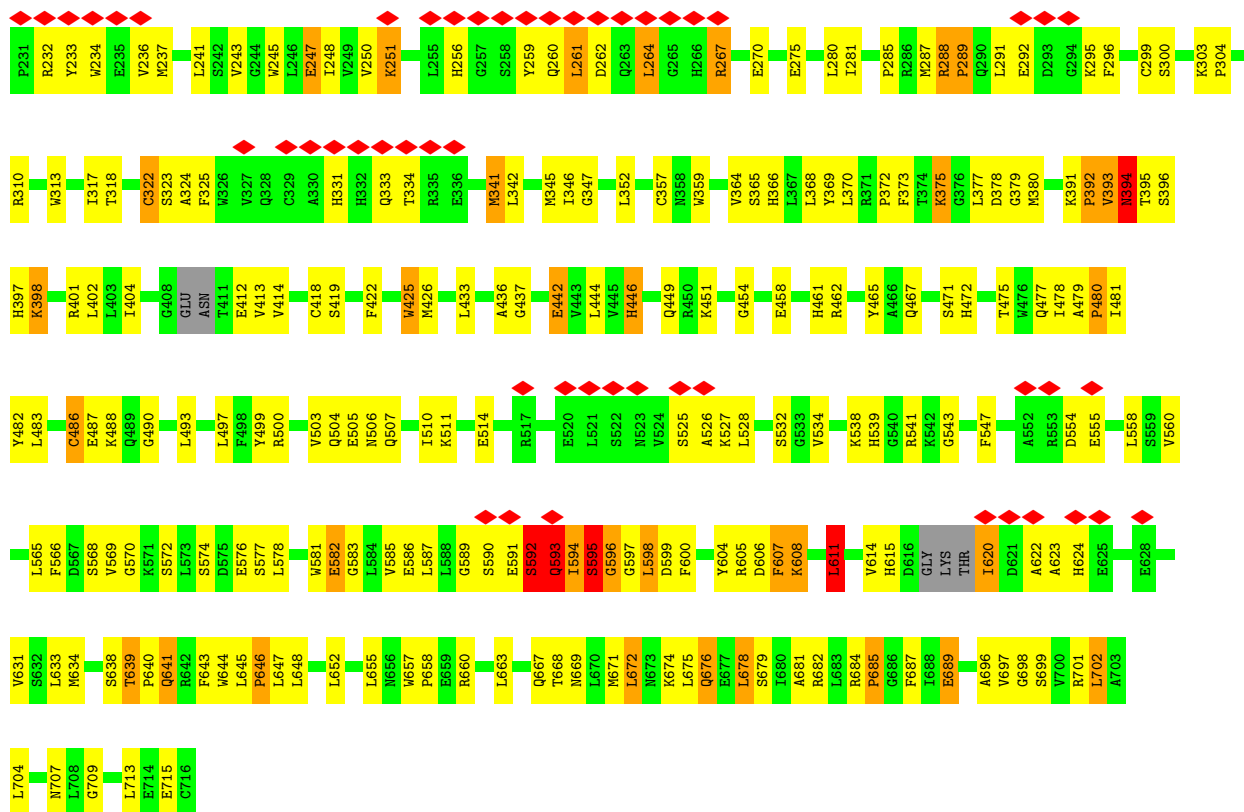


• Molecule 4: E3 ubiquitin-protein ligase HOS1

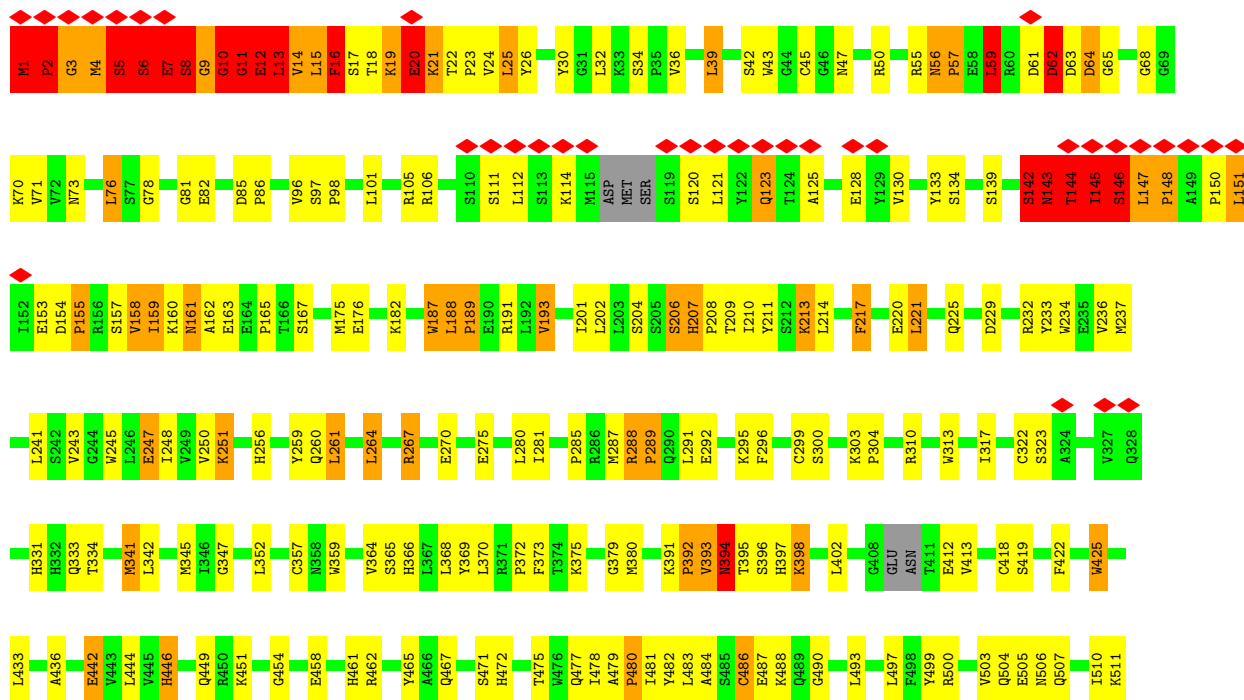


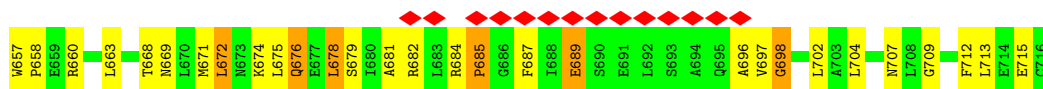
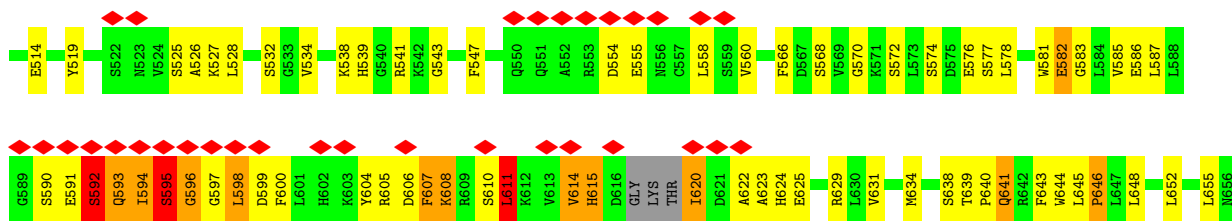
• Molecule 5: Nuclear pore complex protein NUP85



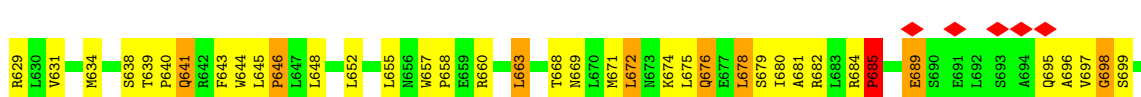
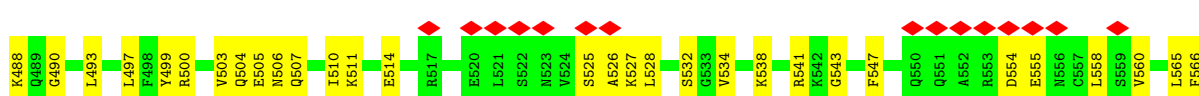
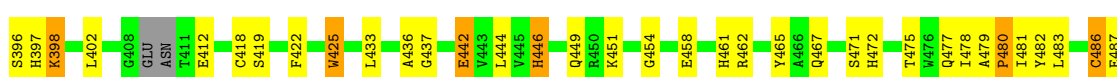
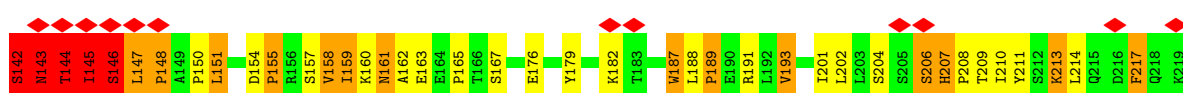
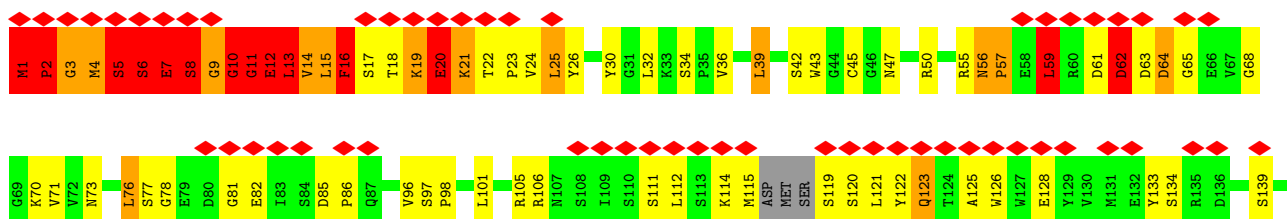


• Molecule 5: Nuclear pore complex protein NUP85

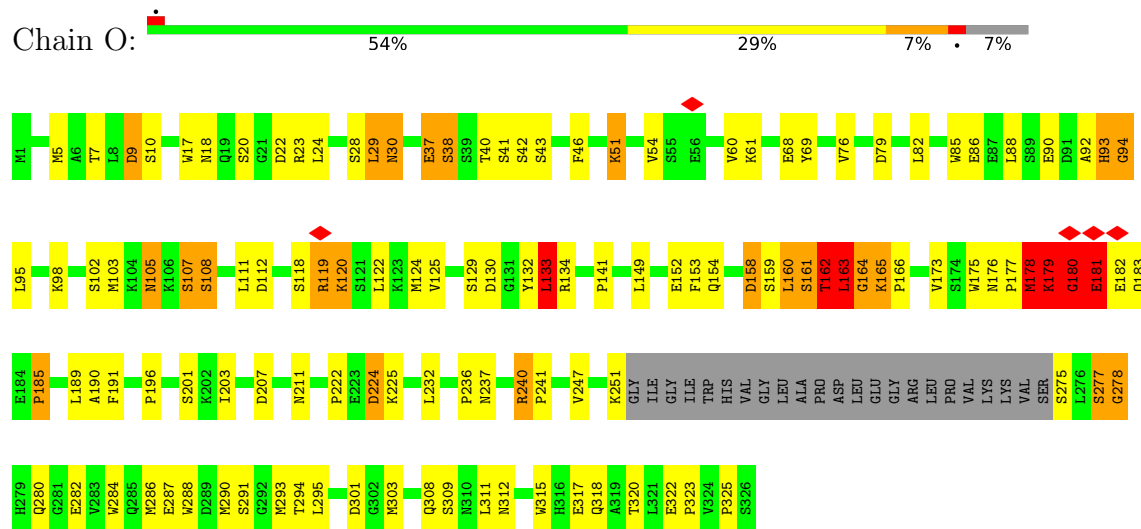




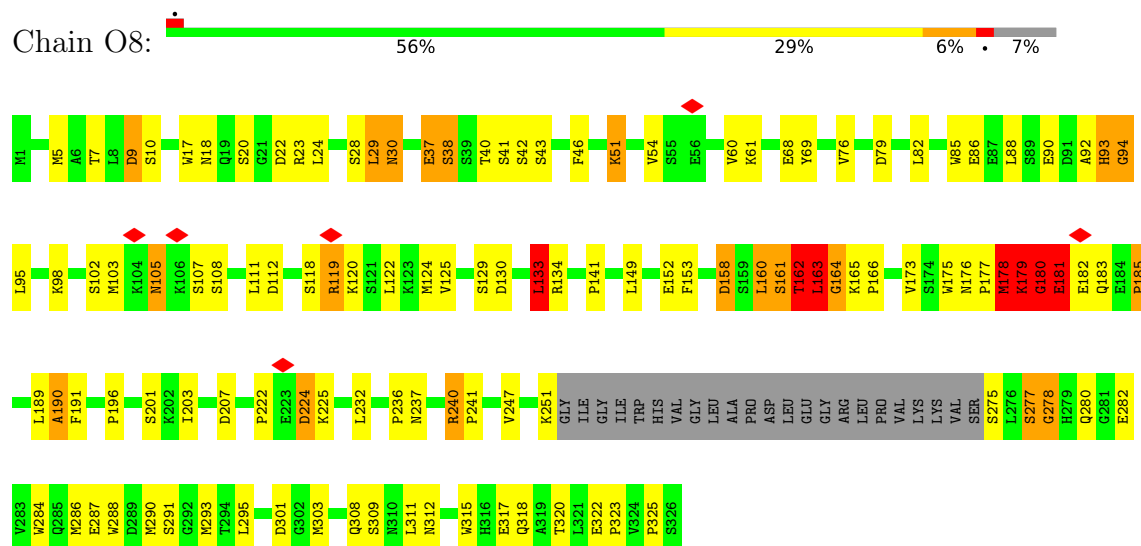
• Molecule 5: Nuclear pore complex protein NUP85



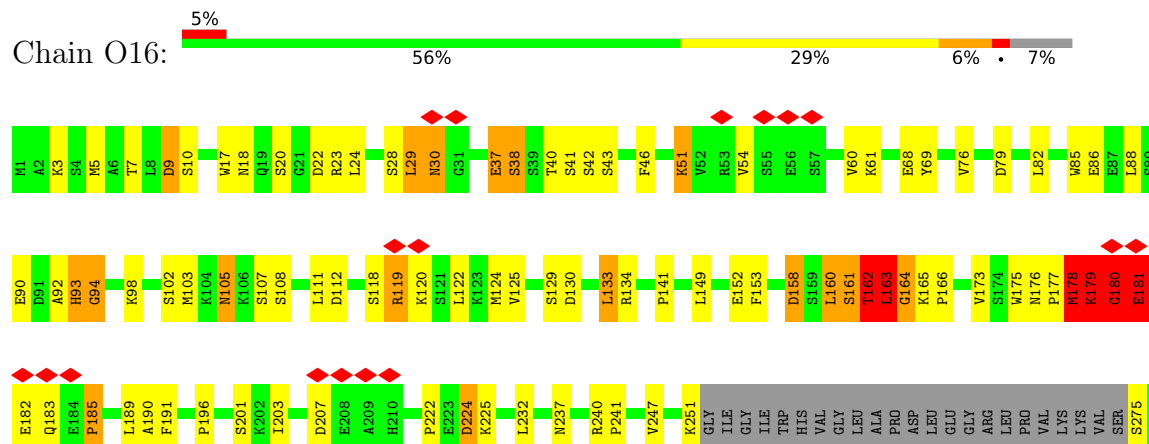
• Molecule 6: Protein SEH1

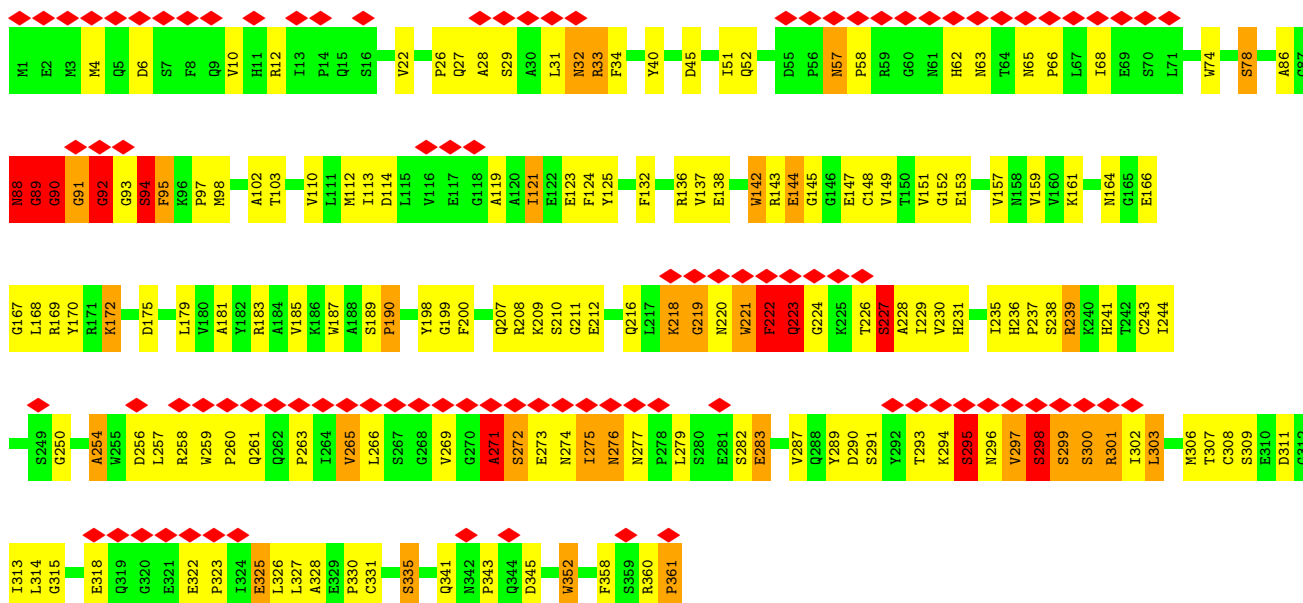


• Molecule 6: Protein SEH1

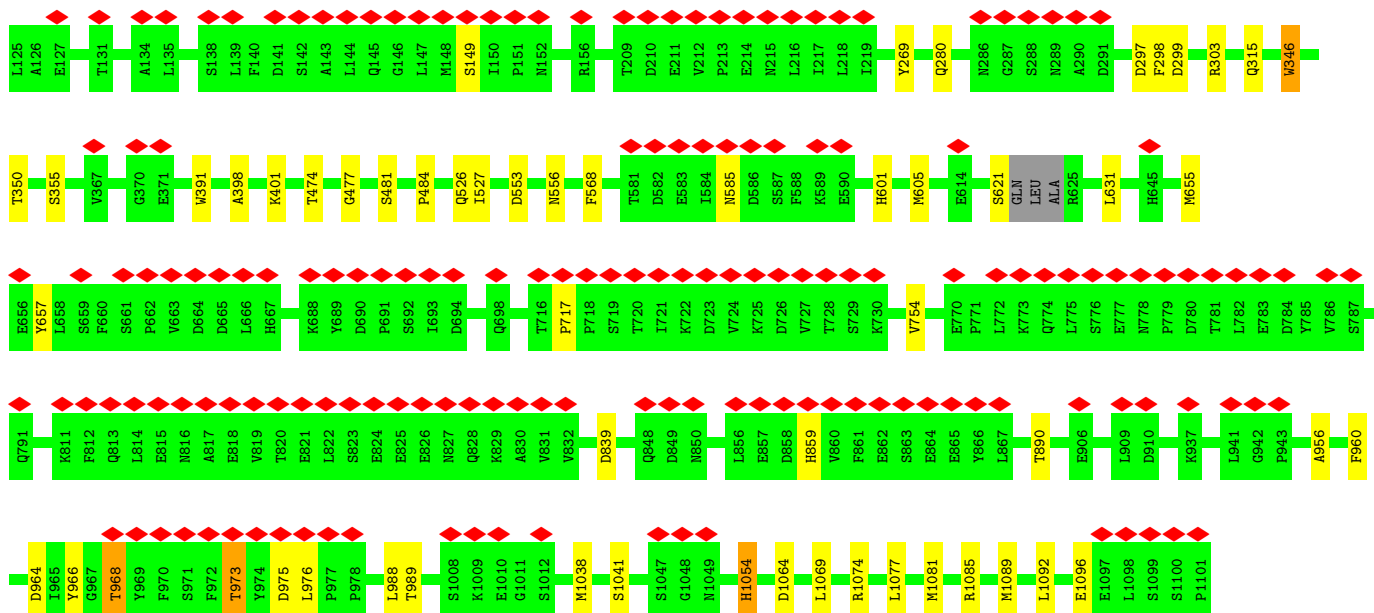


• Molecule 6: Protein SEH1

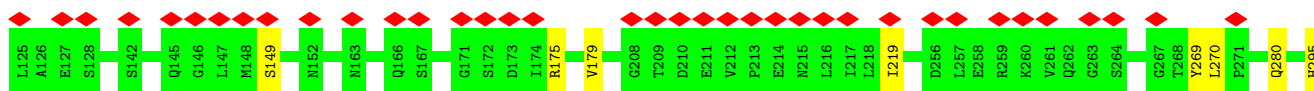


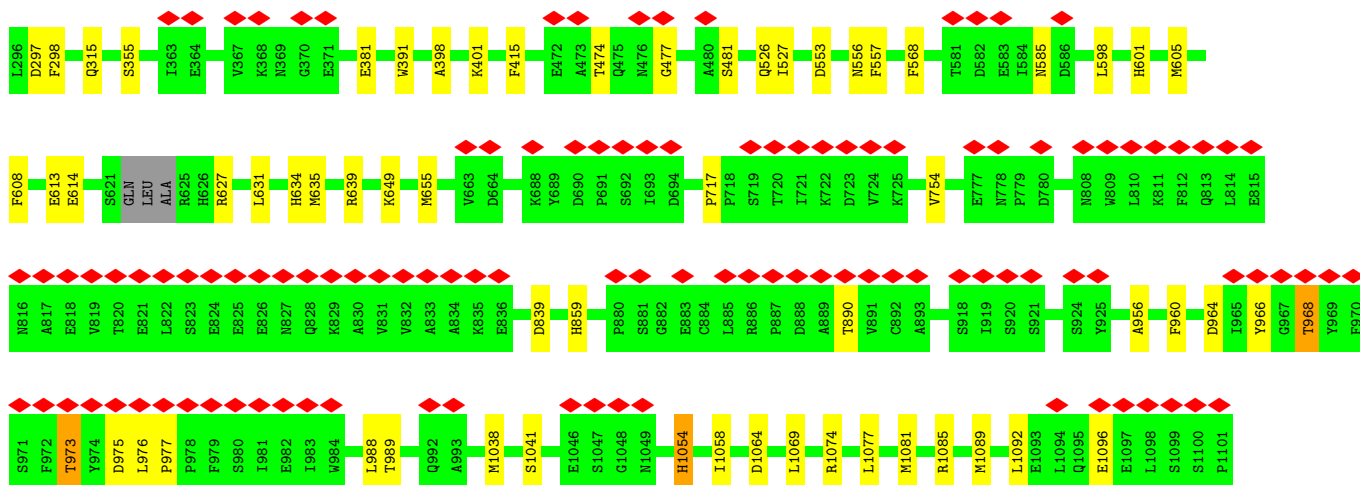


• Molecule 8: Nuclear pore complex protein NUP107

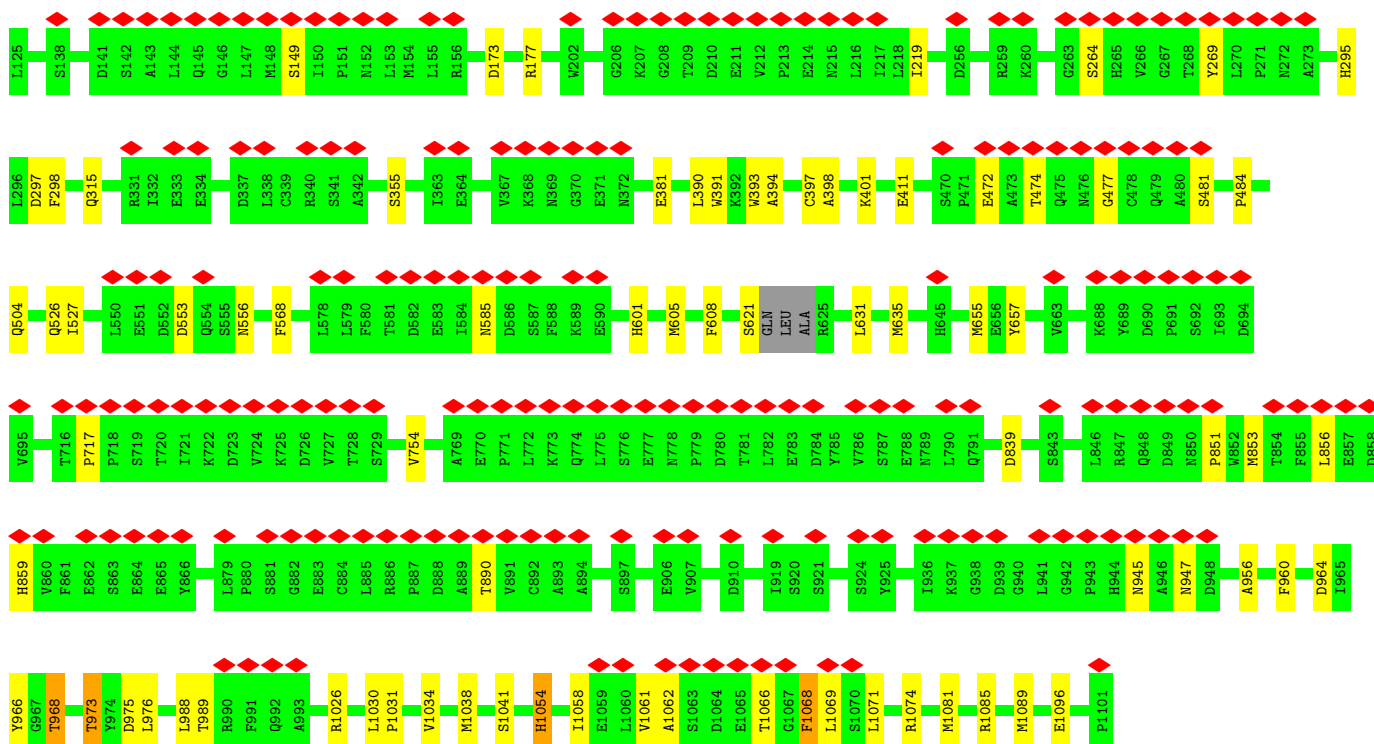


• Molecule 8: Nuclear pore complex protein NUP107

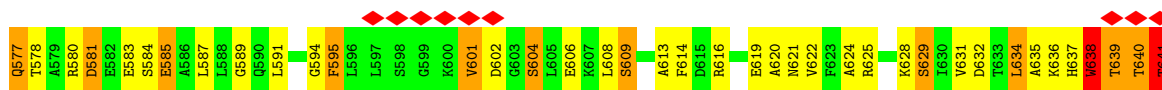




• Molecule 8: Nuclear pore complex protein NUP107

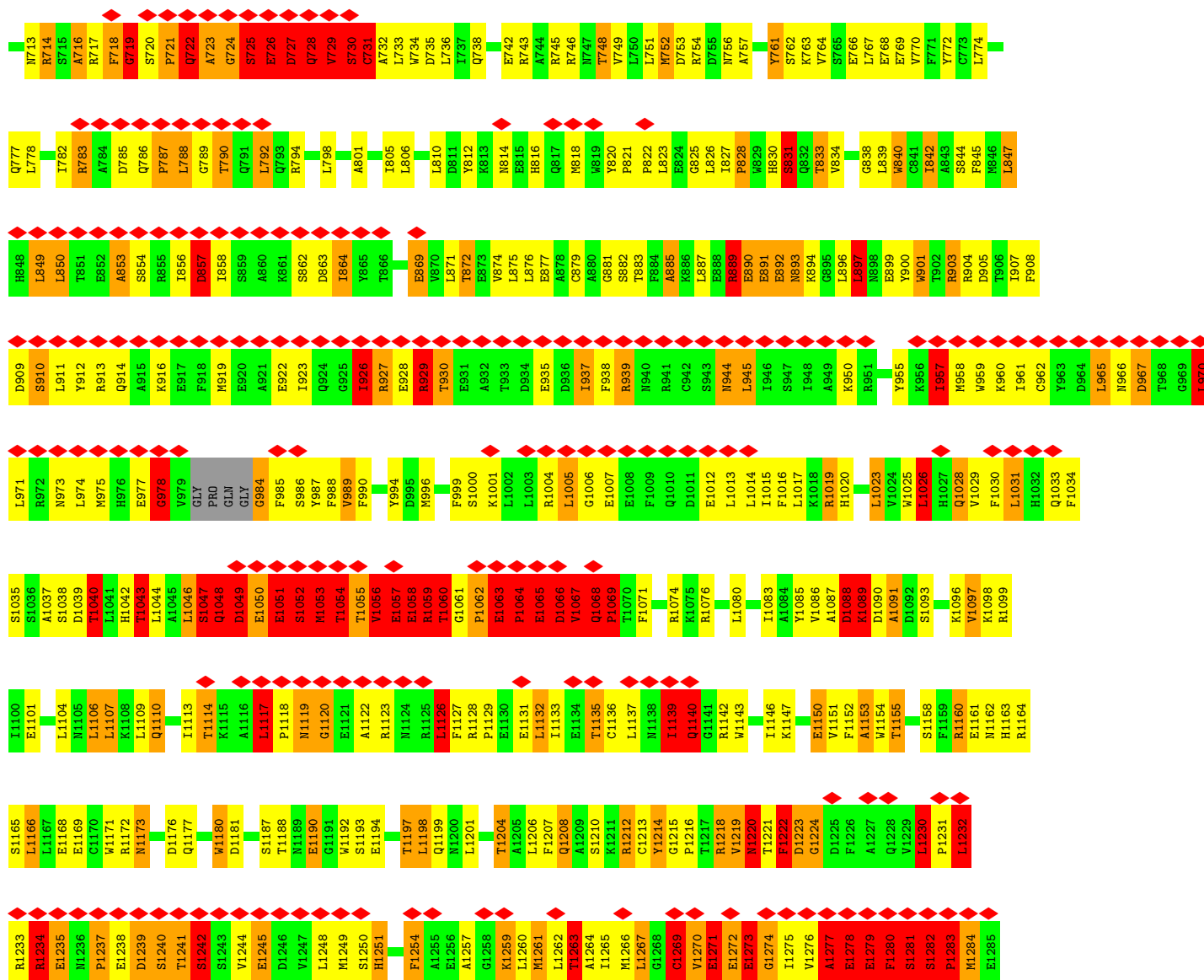


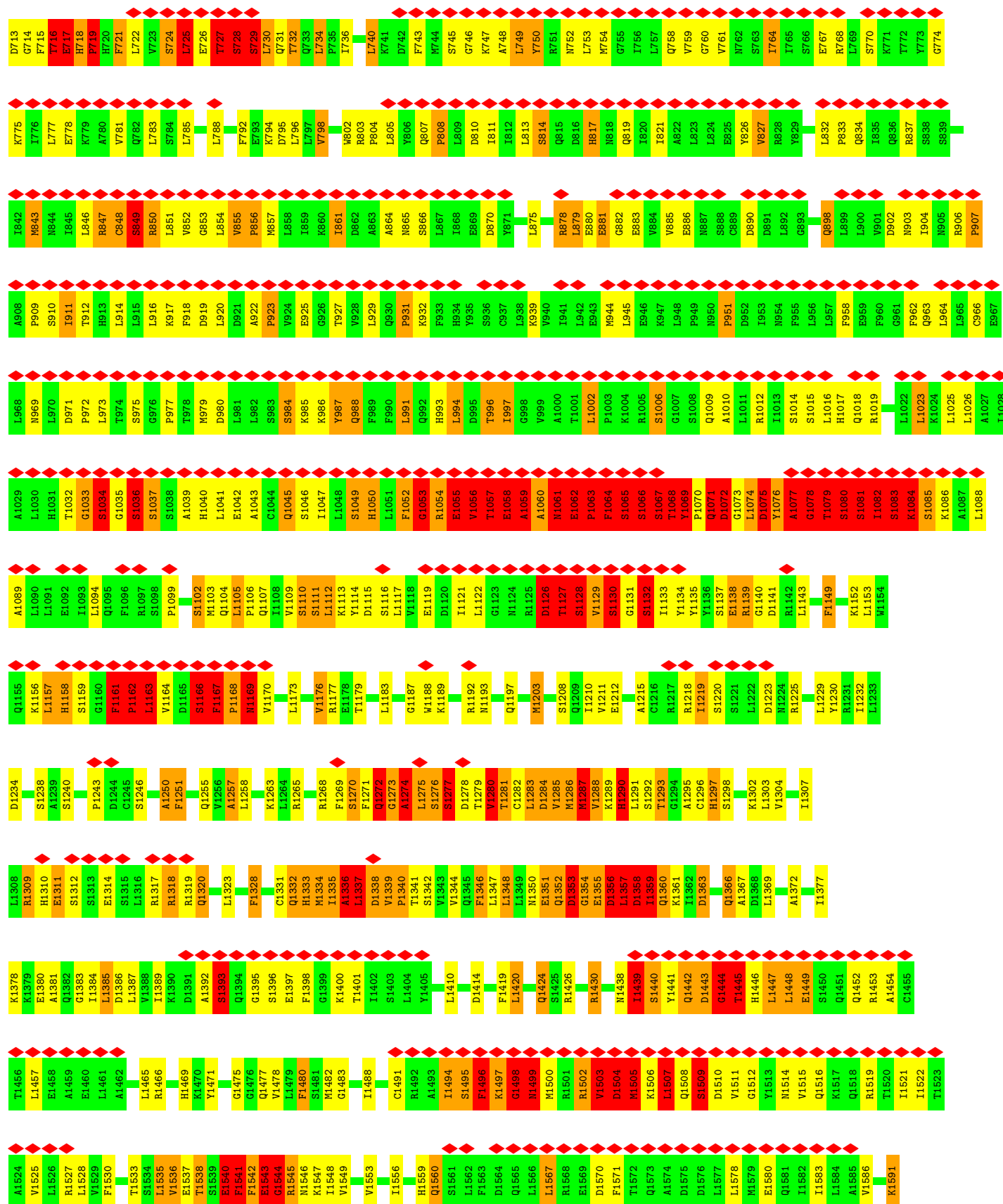
• Molecule 9: Nuclear pore complex protein NUP133



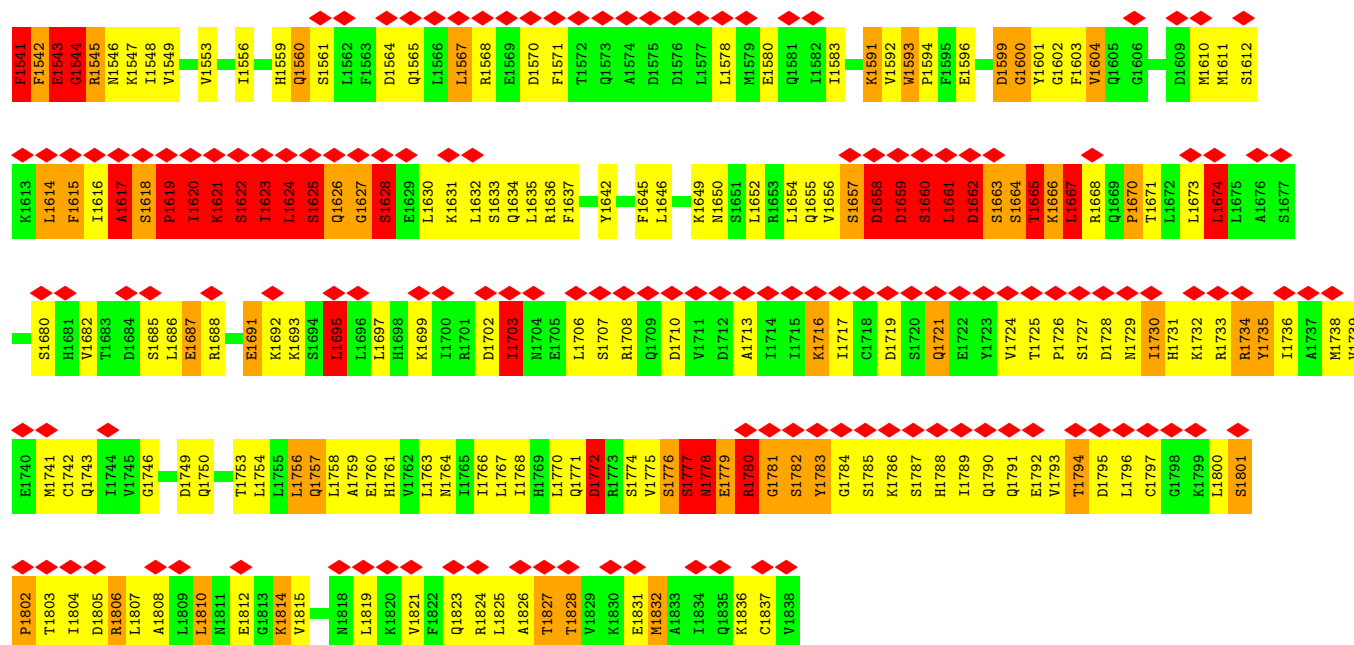


T640	T641	R642	G643	A644	E645	V646	V647	A648	M649	T650	V651	I652	Q655	L656	V657	V658	K659	Q660	E664	I665	F666	L667	H668	F669	L670	A671	L672	S673	K674	C675	H676	E677	E678	L679	C680	S681	Q683	S686	L691	E695	K696	L697	M700	R703	L704	E705	L706	Q707	M708	M709	Q577	I578	S580	D581	E582	E583	S584	E585	A586	L587	L588	G589	Q590	F592	E593	G594	F595	L596	L597	S598	G599	K600	V601	D602	G603	S604	L605	E606	K607	L608	S609	D610	A613	F614	D615	R616	E619	A620	I621	V622	F623	A624	R625	K628	S629	L630	V631	D632	T633	A635	K636	H637	V638	T639
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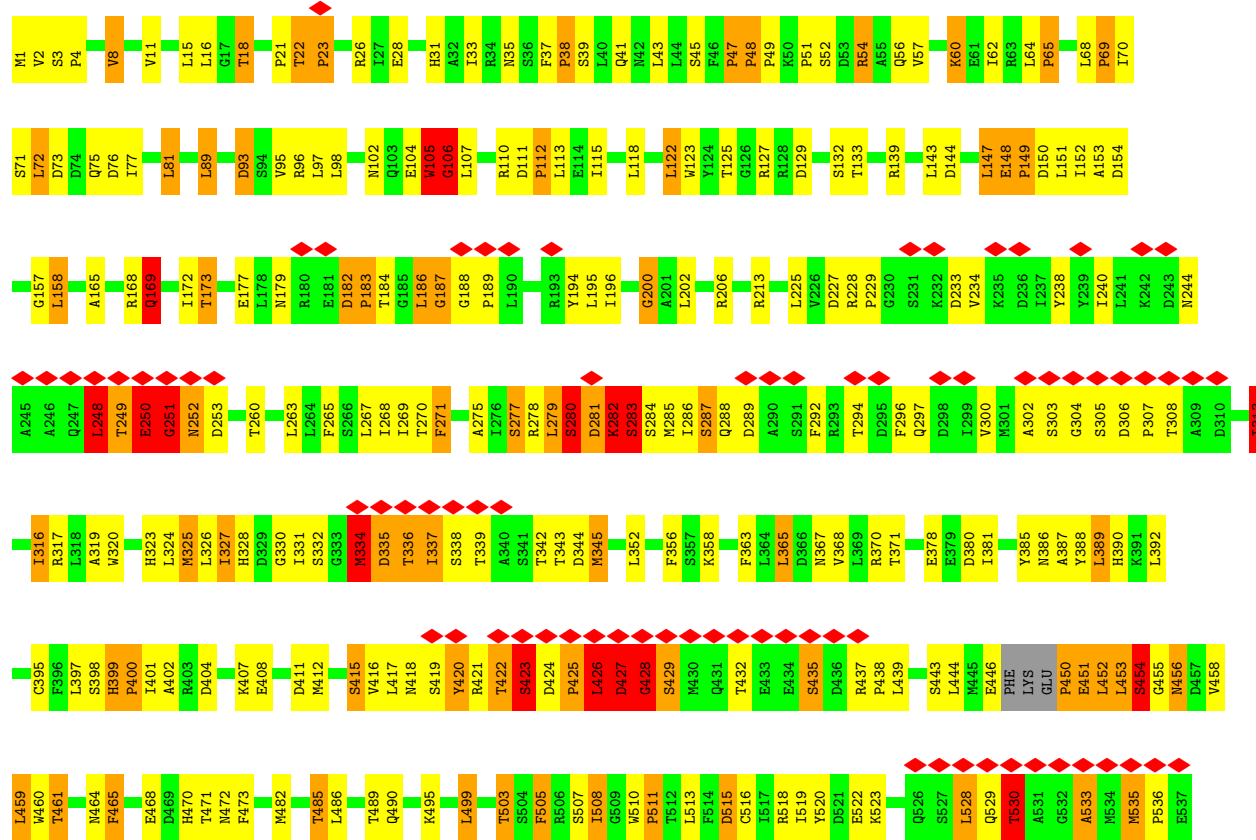








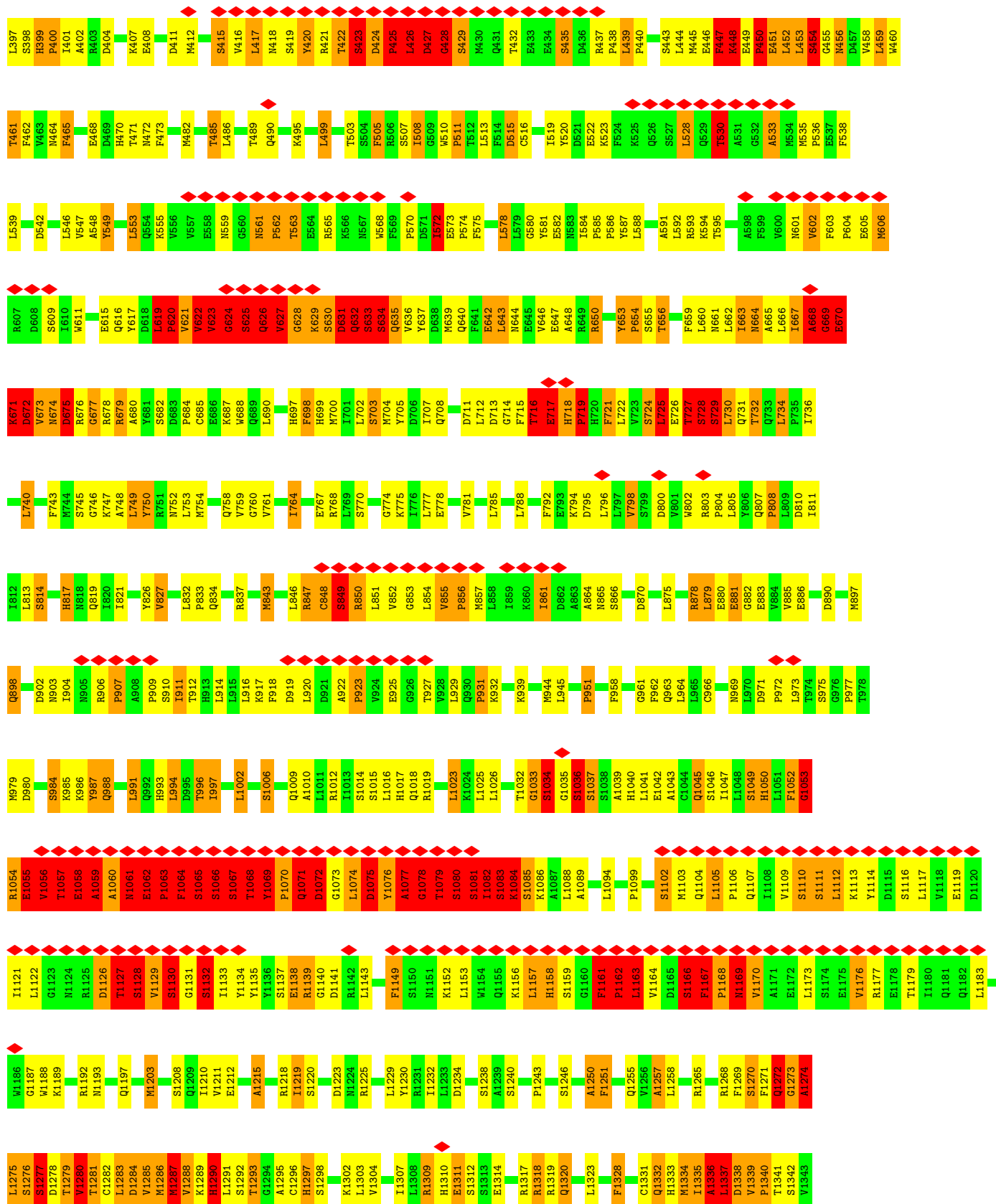
• Molecule 10: Nuclear pore complex protein NUP205

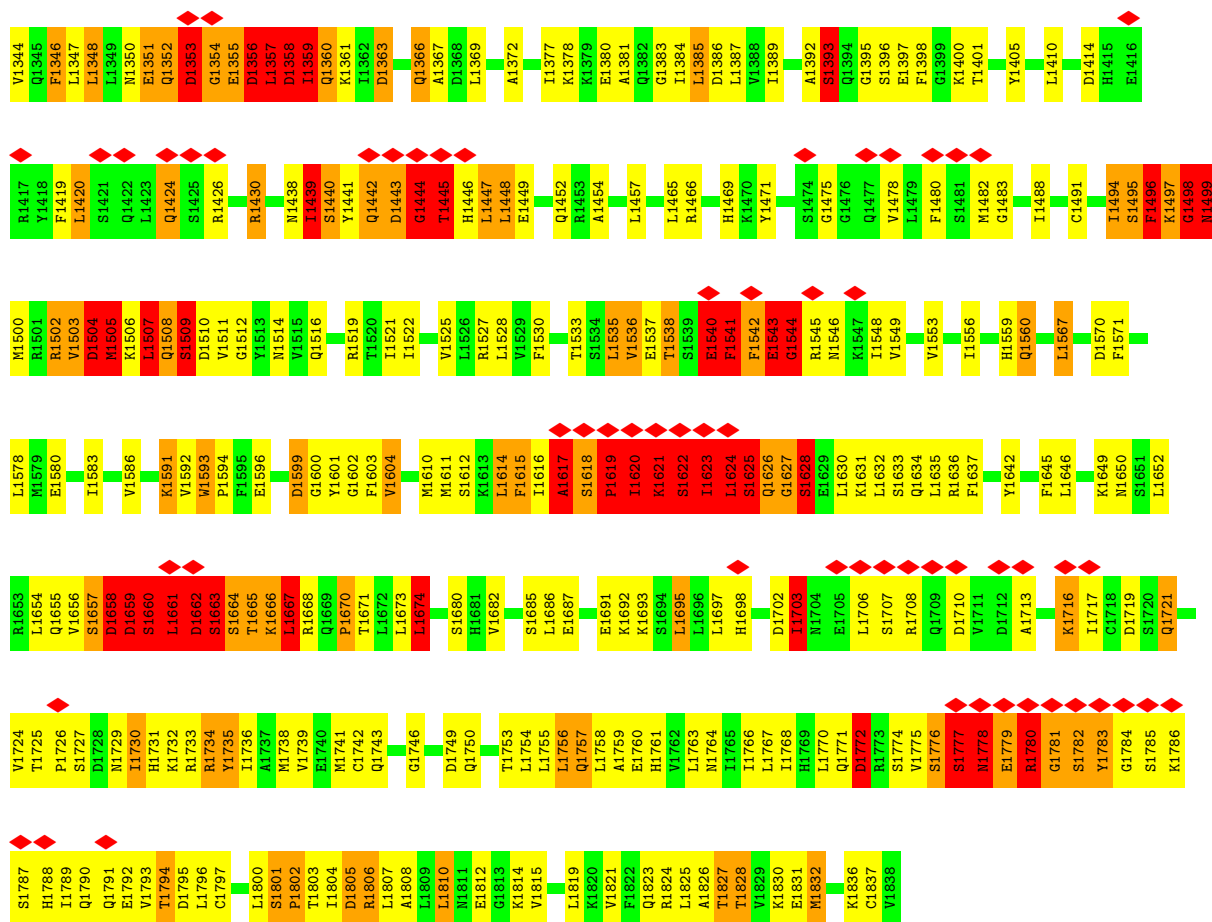




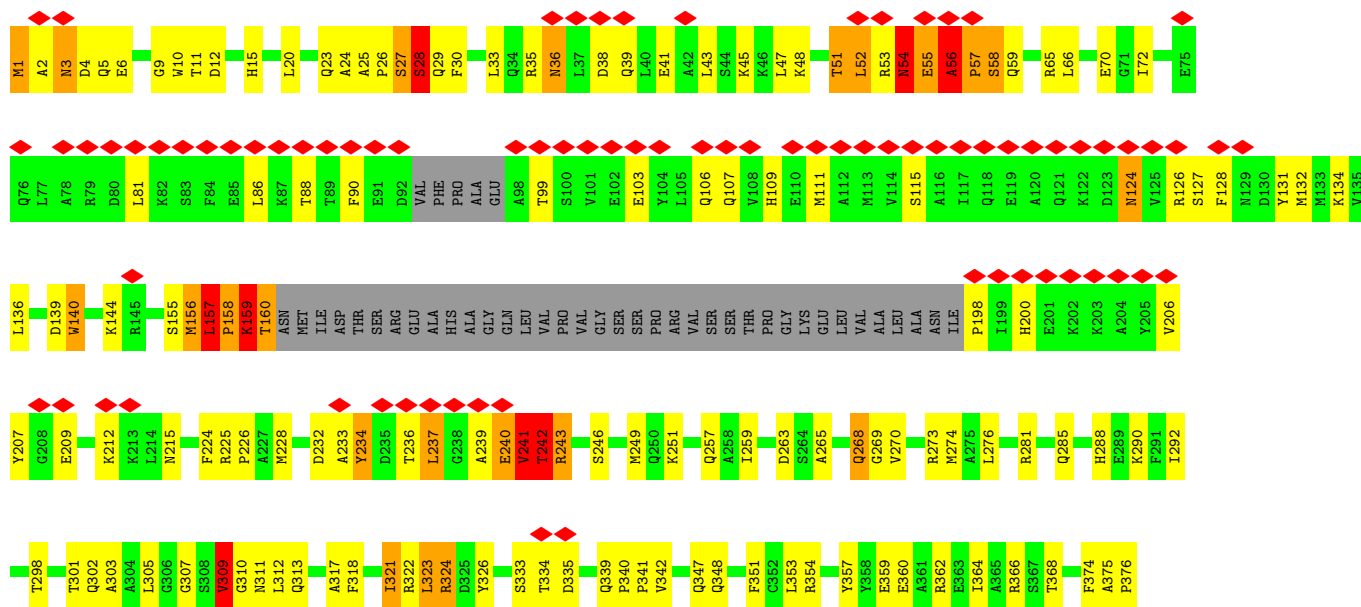


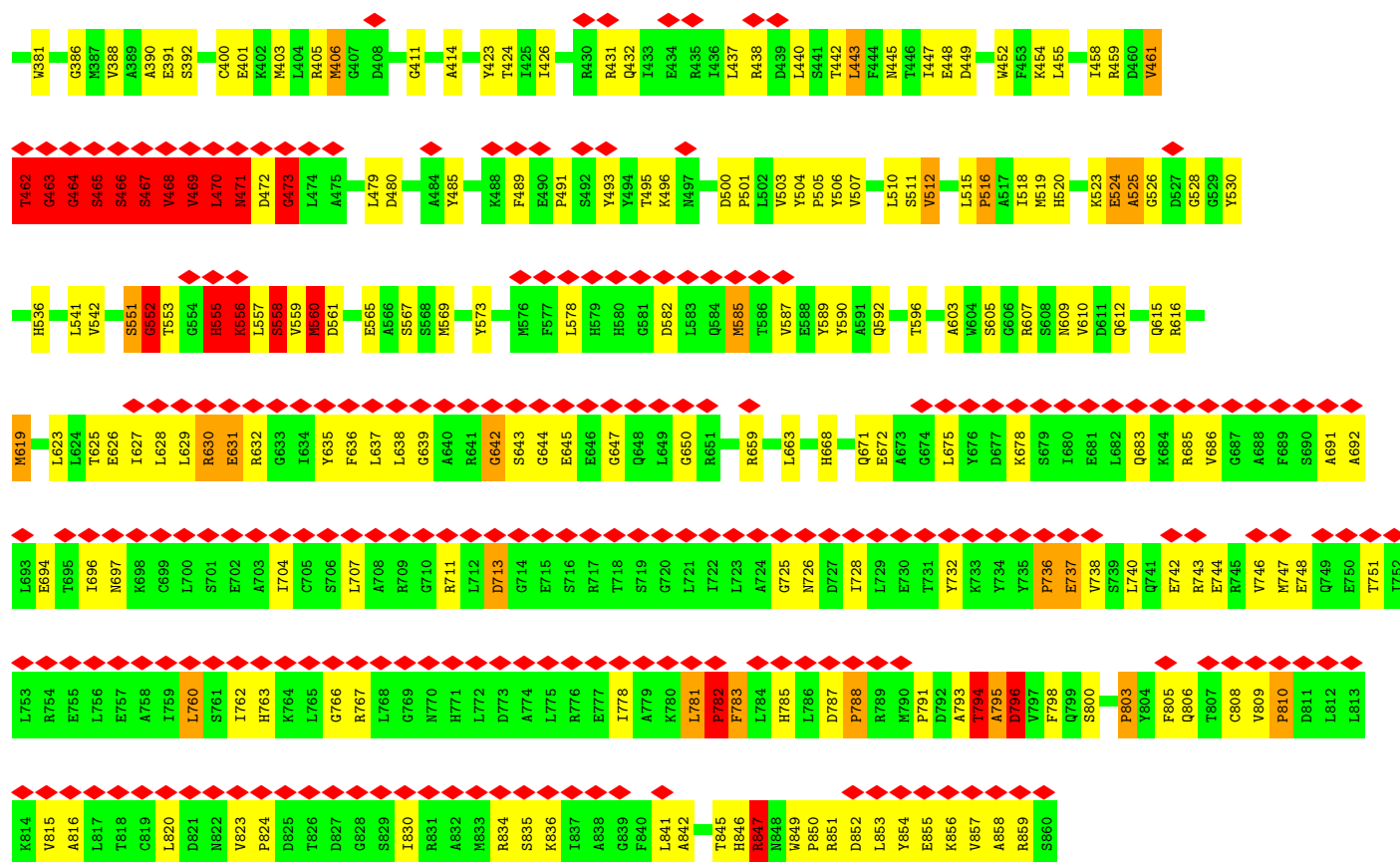




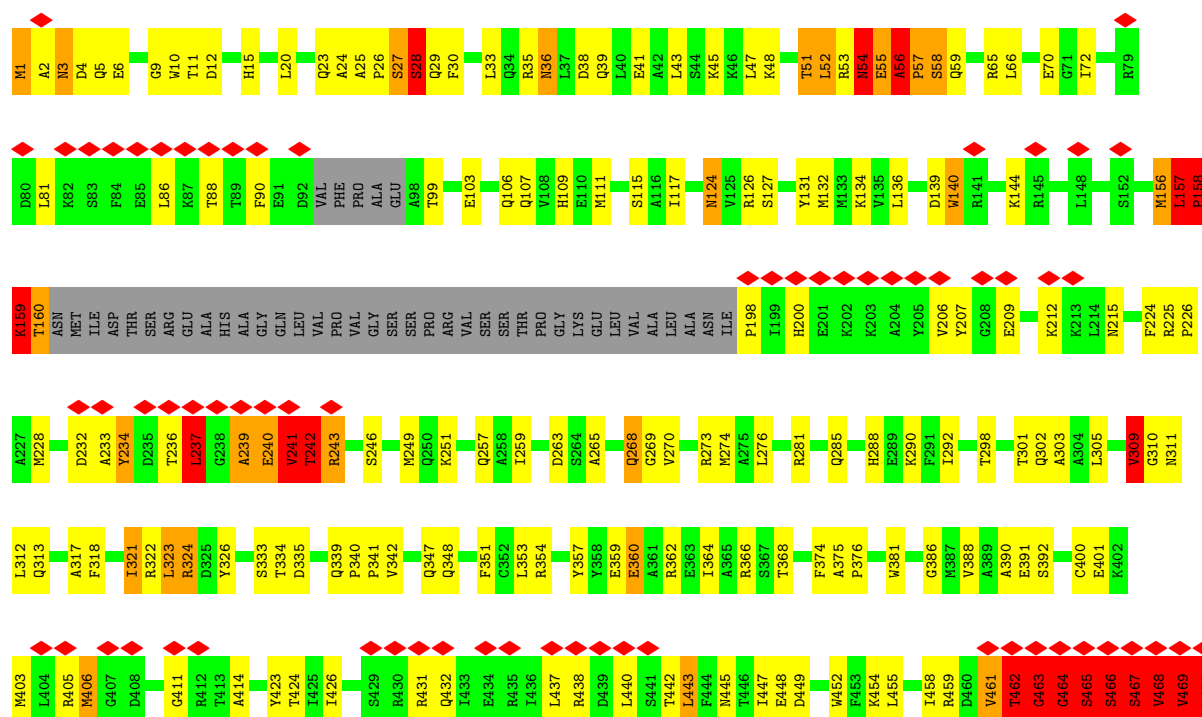


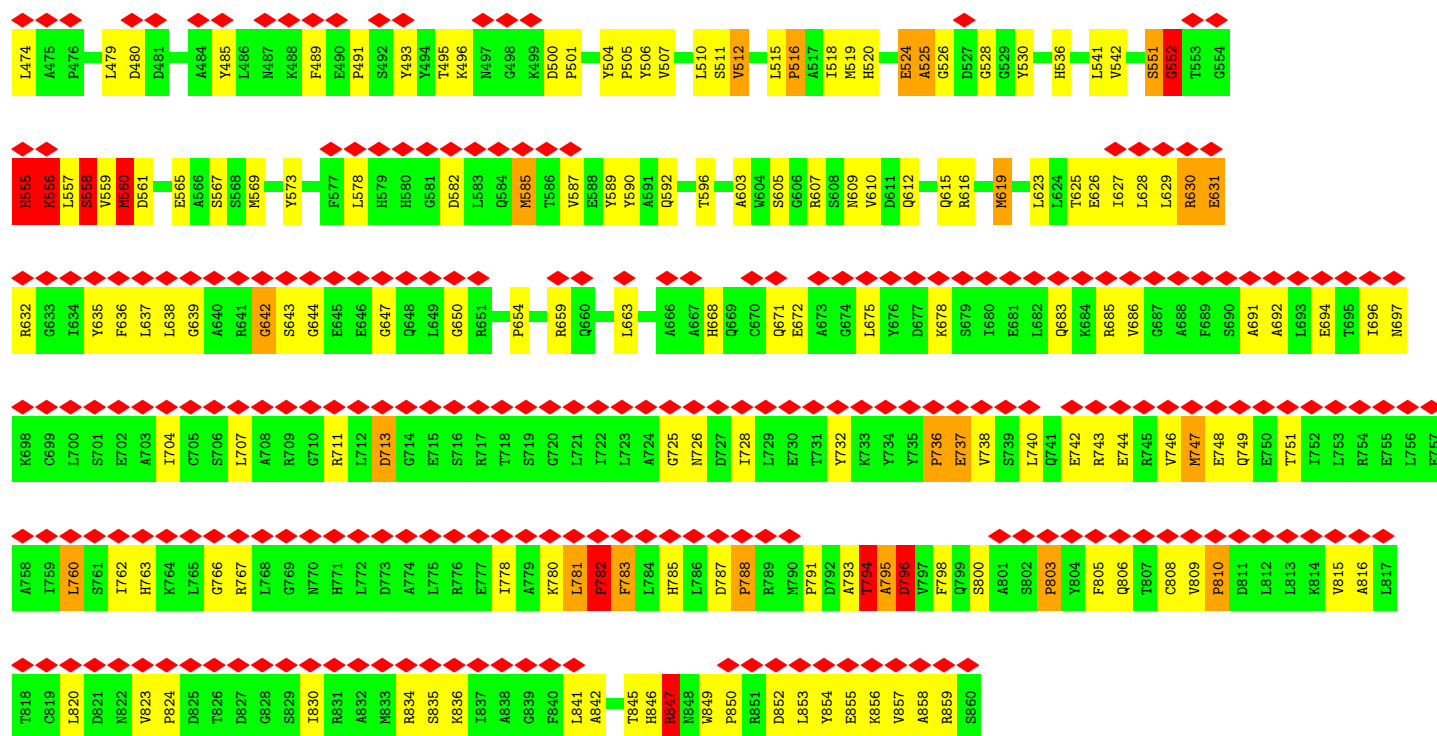
• Molecule 11: Nuclear pore complex protein NUP93A



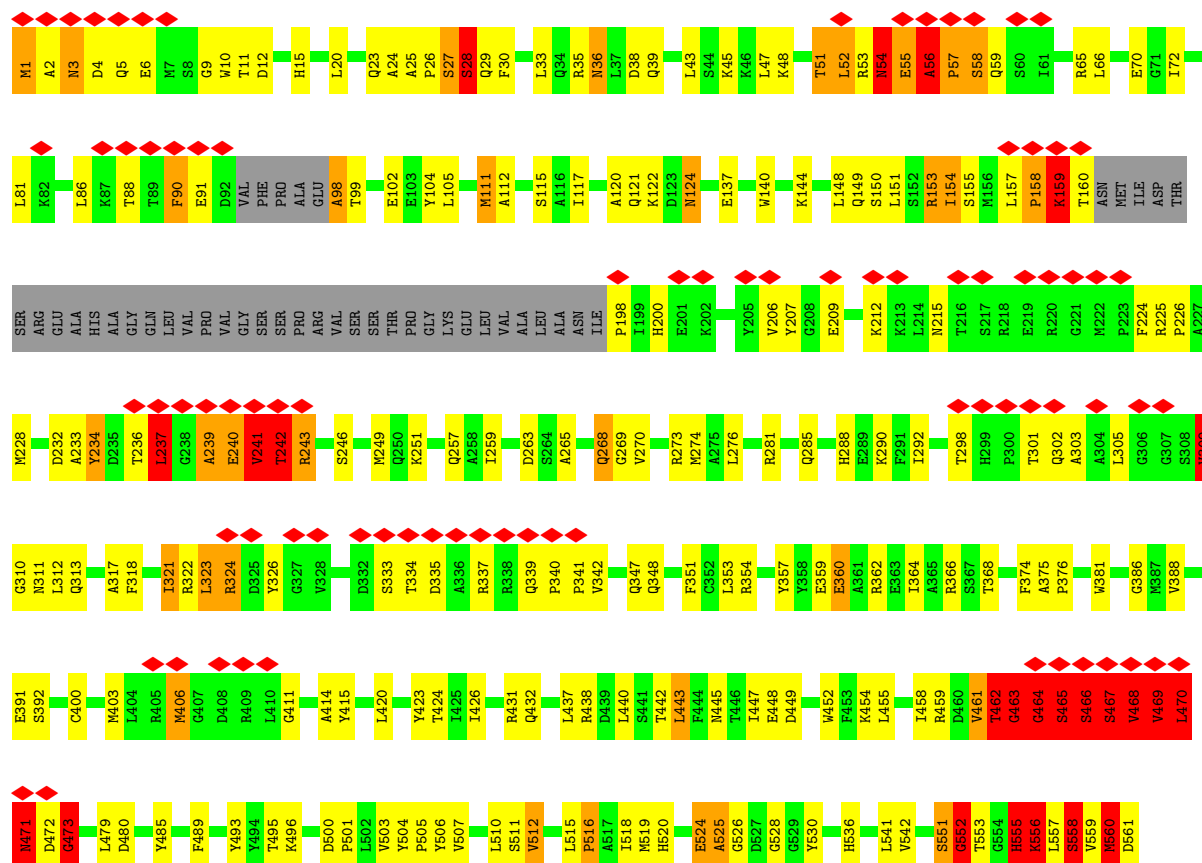


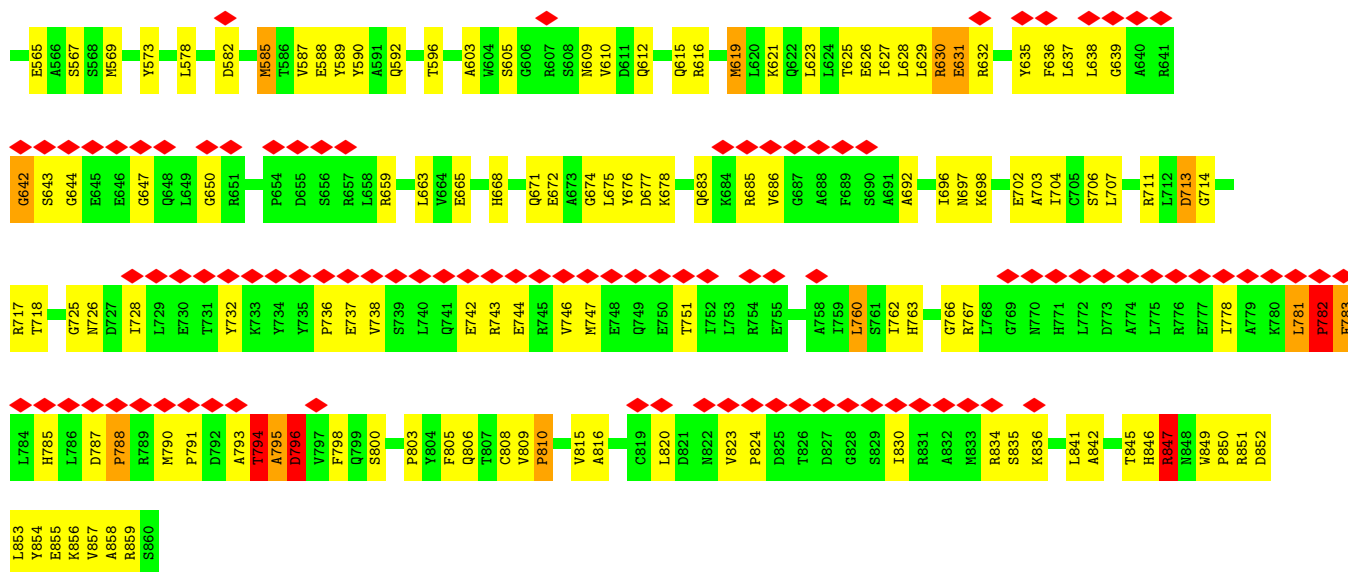
• Molecule 11: Nuclear pore complex protein NUP93A



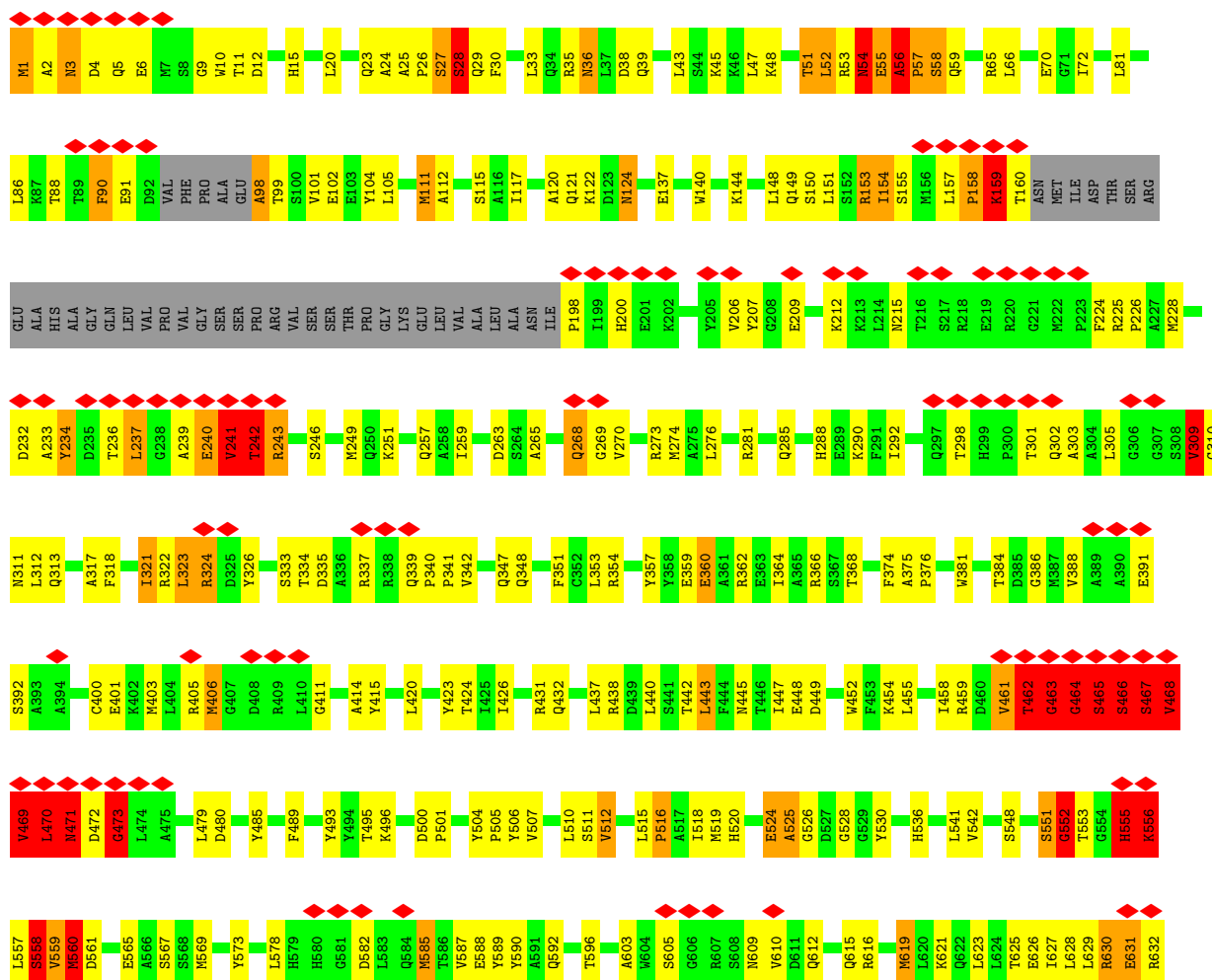


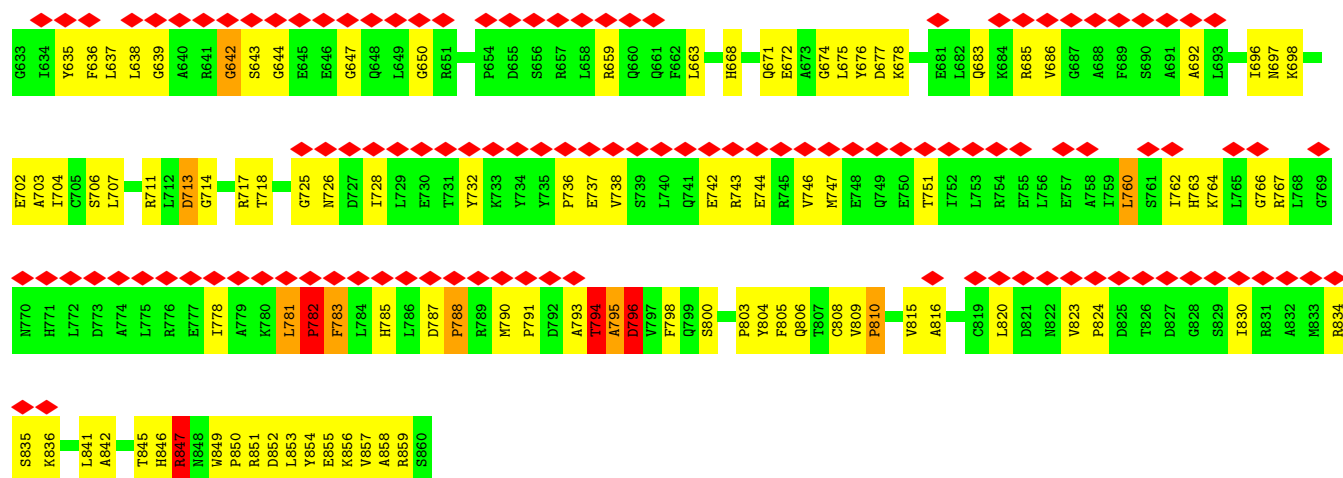
• Molecule 11: Nuclear pore complex protein NUP93A



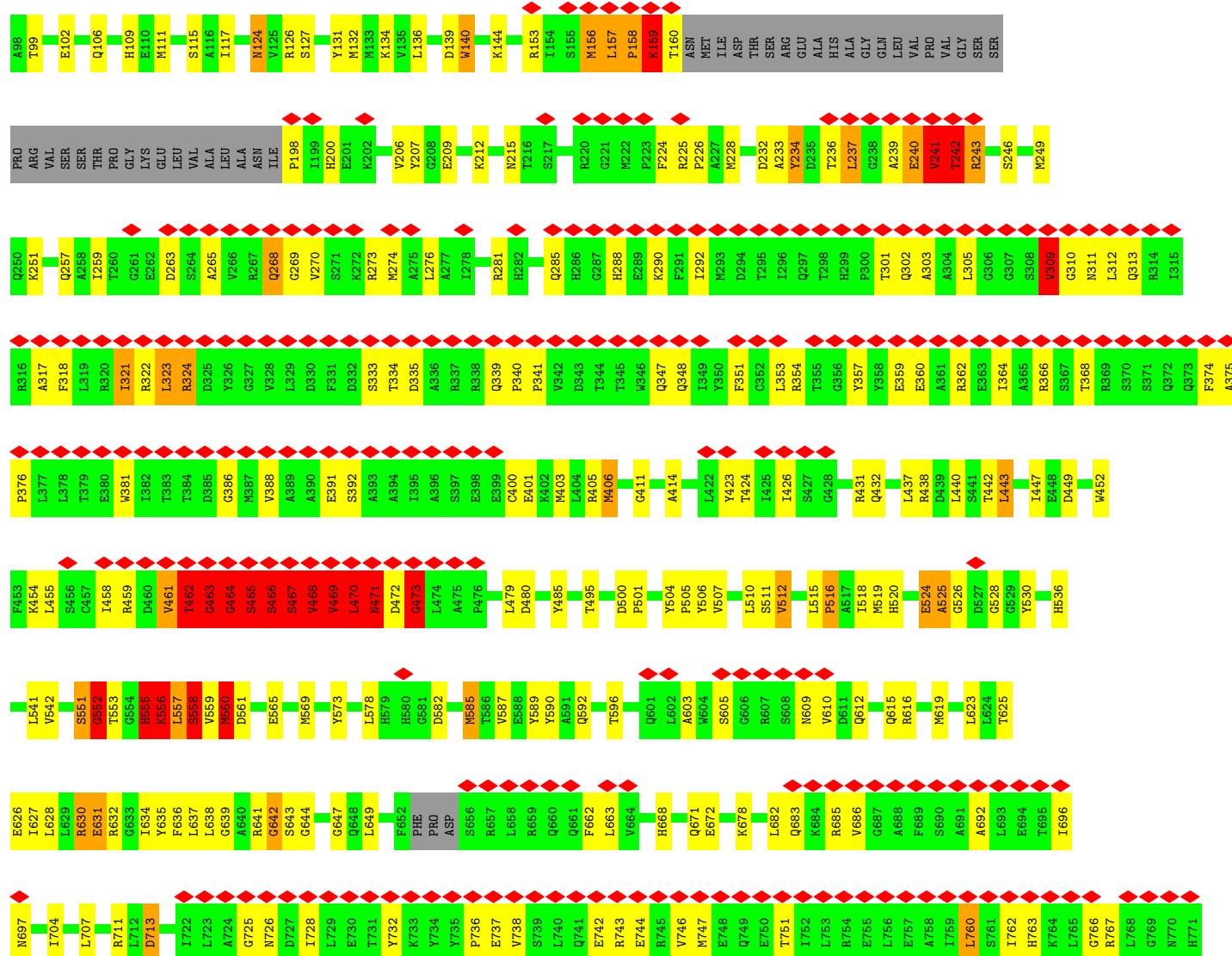


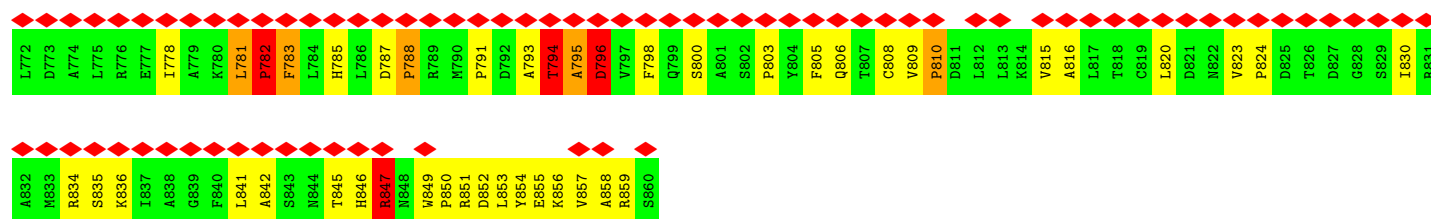
• Molecule 11: Nuclear pore complex protein NUP93A





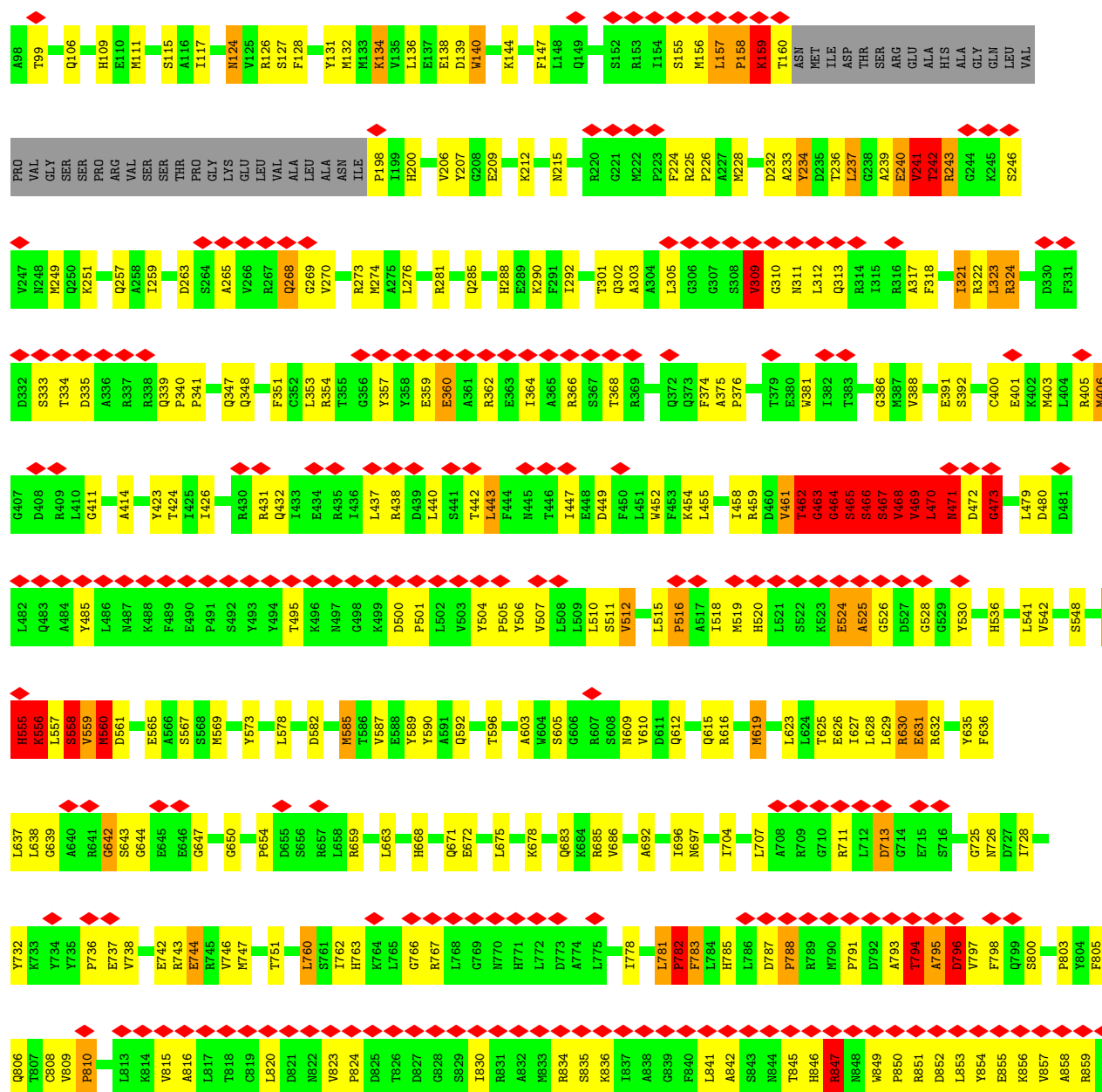
• Molecule 12: Nuclear pore complex protein NUP93A

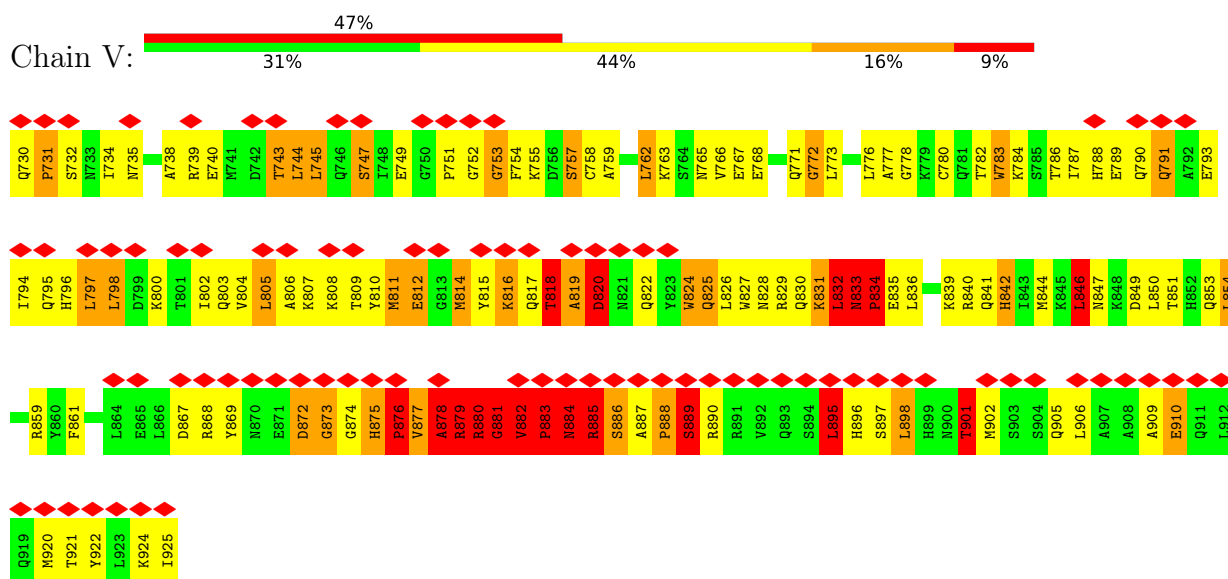




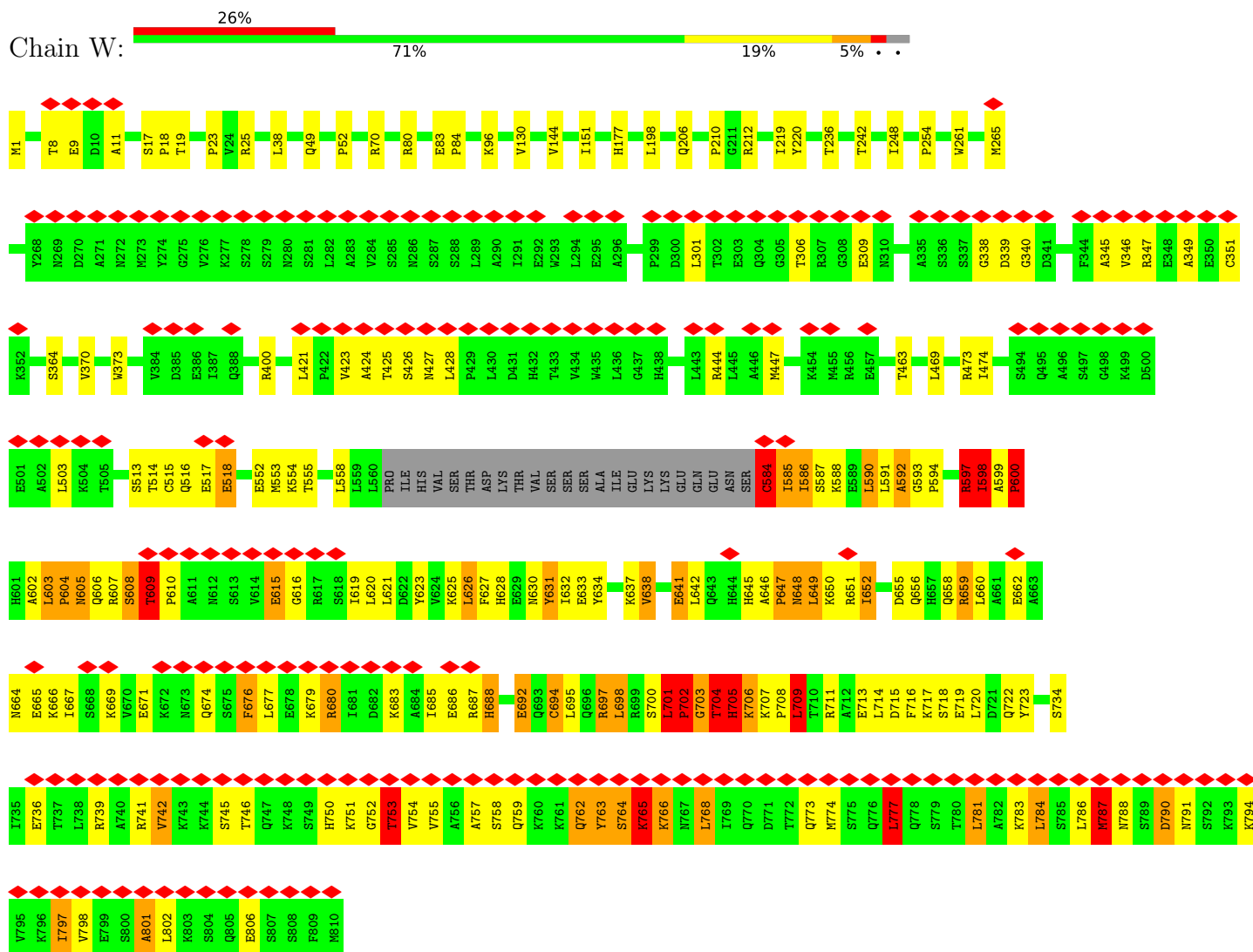
• Molecule 12: Nuclear pore complex protein NUP93A

Chain A48: 28% 56% 31% 5% 5%

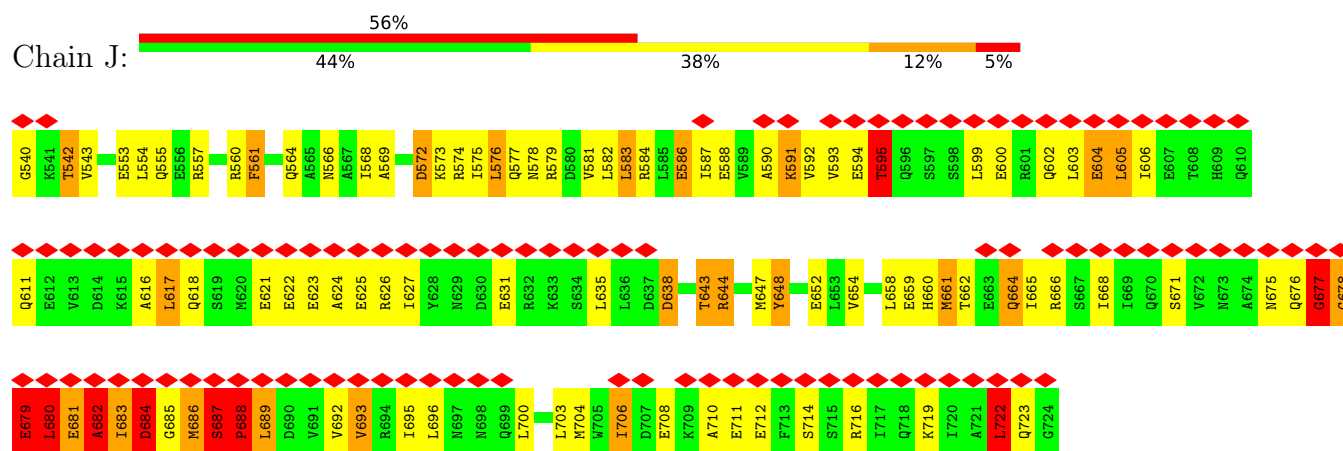




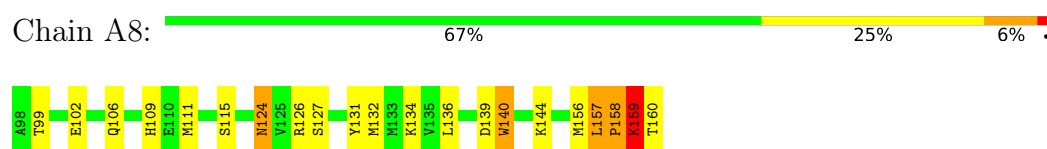
• Molecule 14: Nuclear pore complex protein NUP88



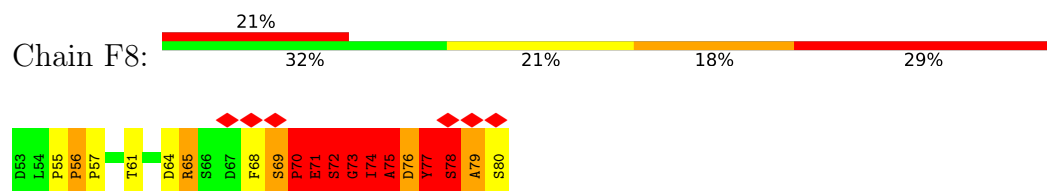
- Molecule 15: Nuclear pore complex protein NUP62



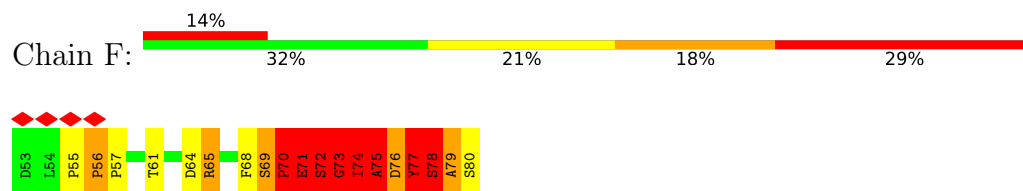
- Molecule 16: Nuclear pore complex protein NUP93A



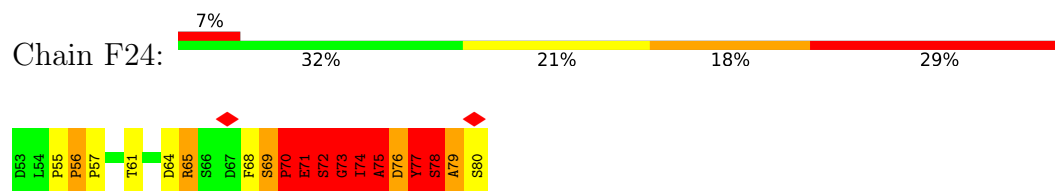
- Molecule 17: Nuclear pore complex protein NUP35



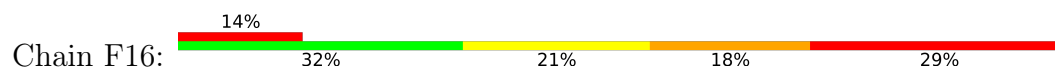
- Molecule 17: Nuclear pore complex protein NUP35

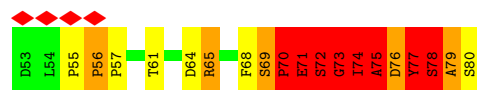


- Molecule 17: Nuclear pore complex protein NUP35

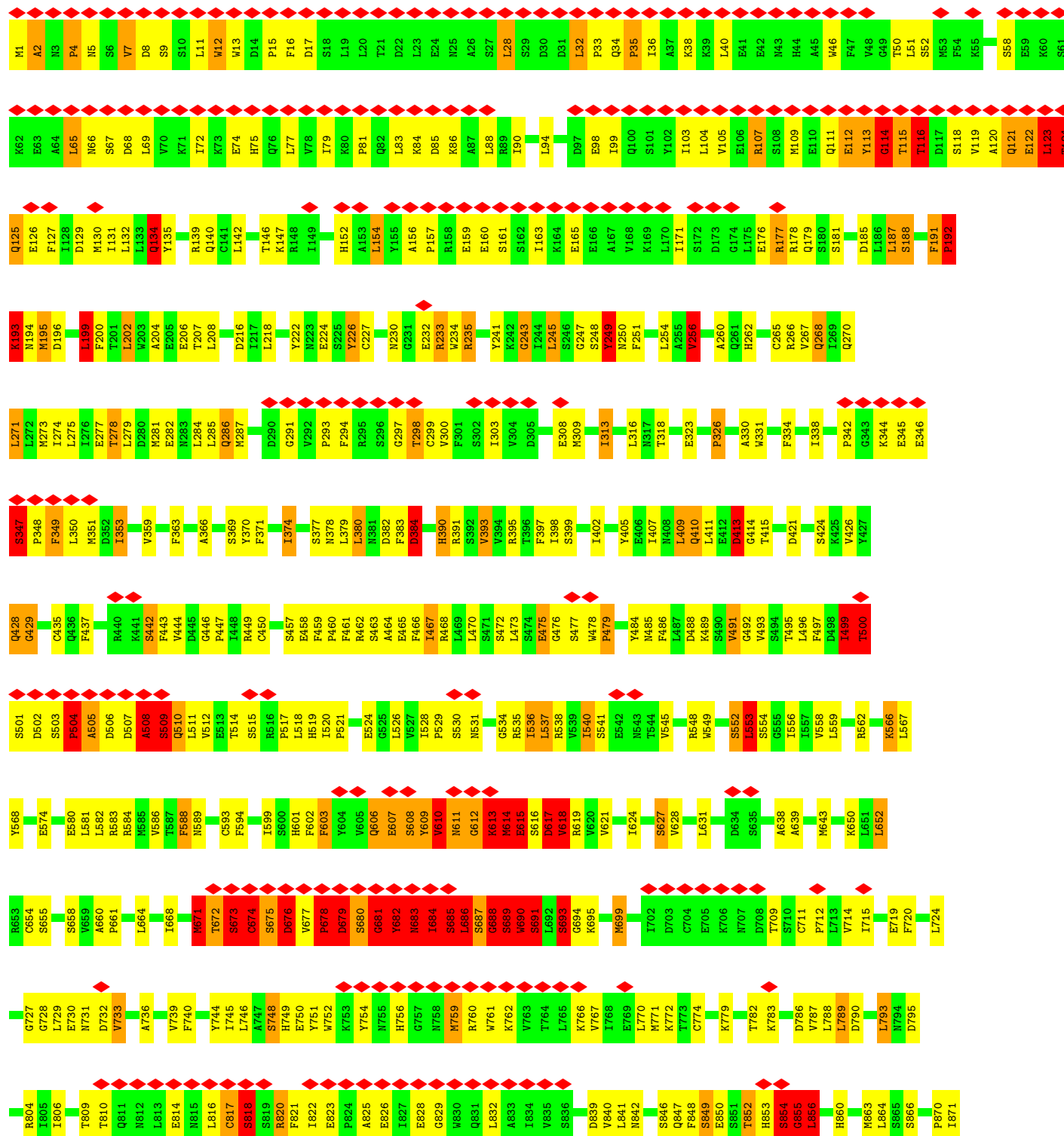


- Molecule 17: Nuclear pore complex protein NUP35

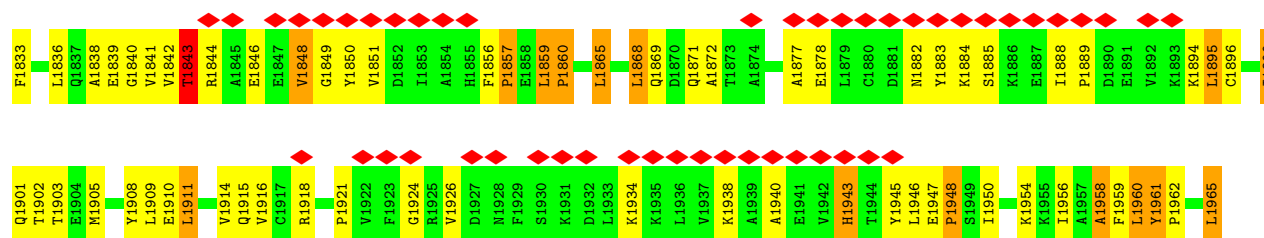




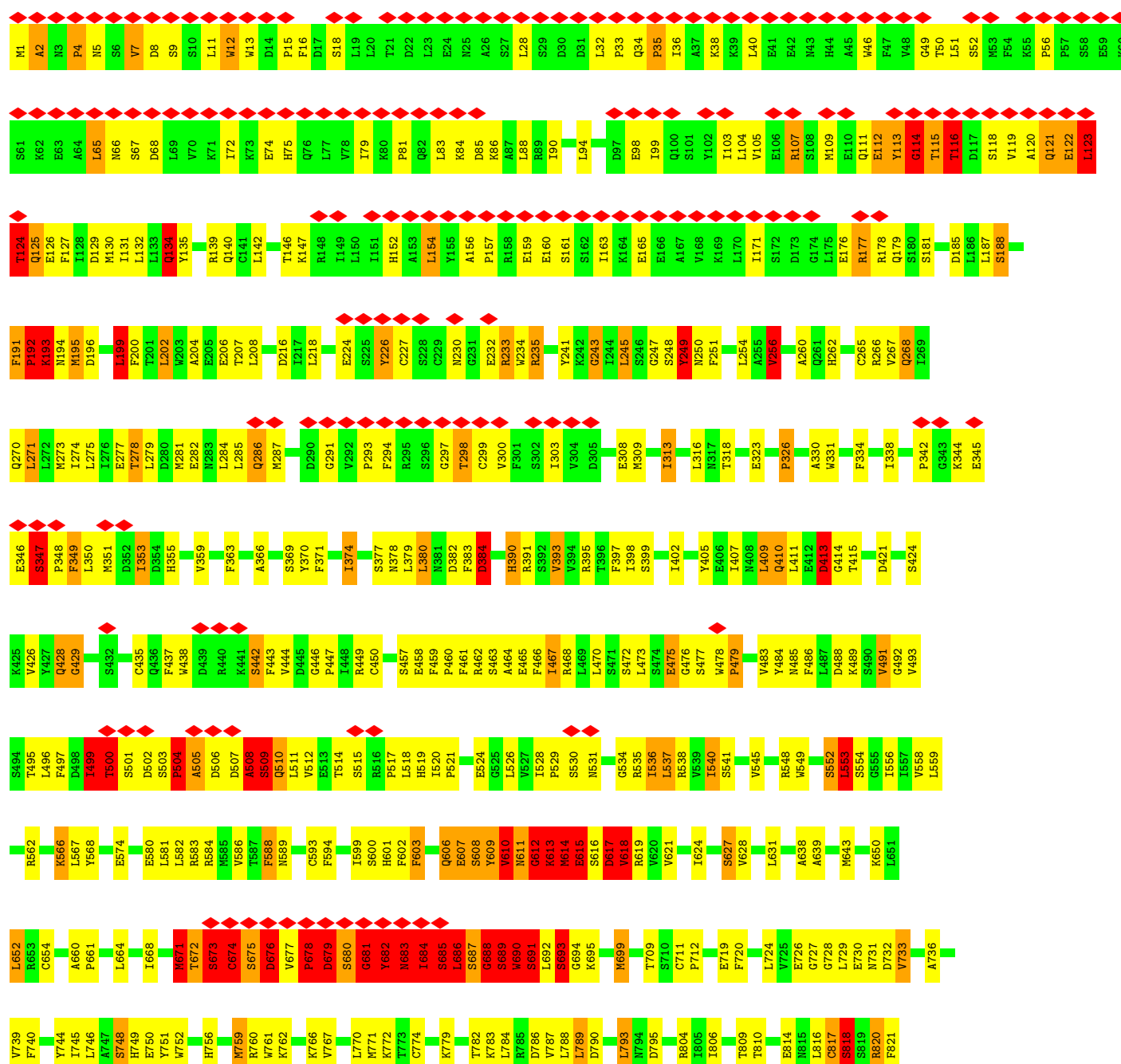
• Molecule 18: Nucleoporin (DUF3414)



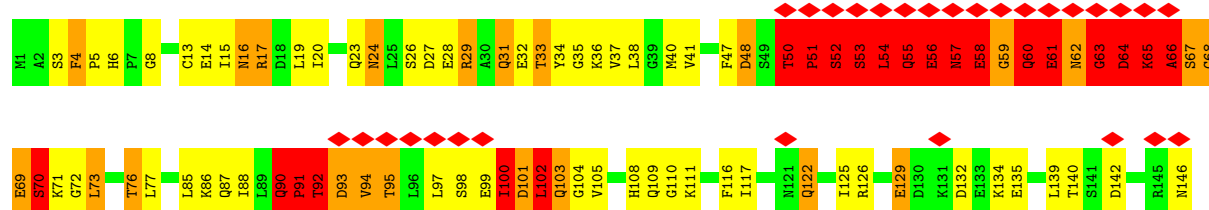


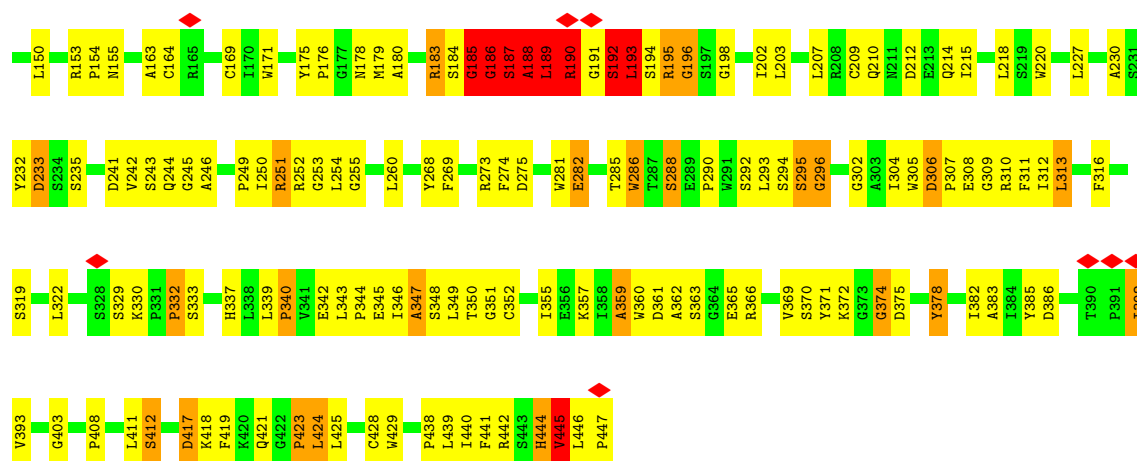


• Molecule 18: Nucleoporin (DUF3414)

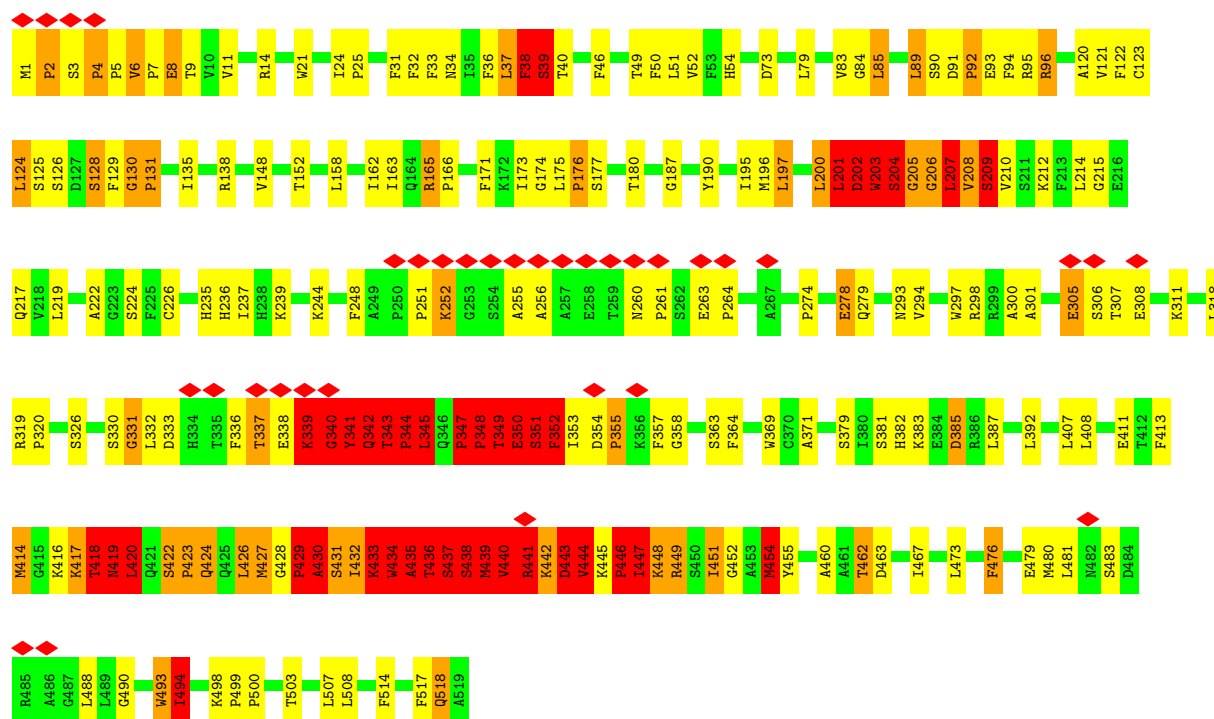




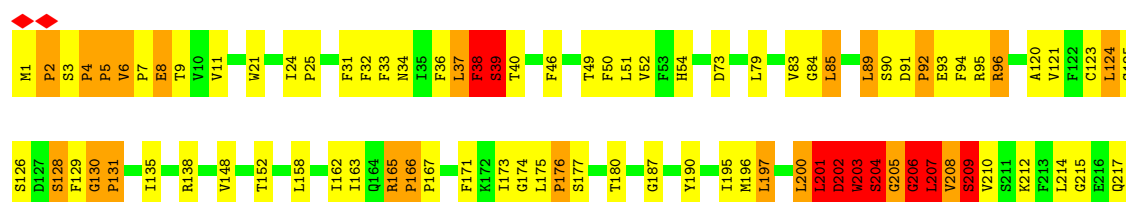


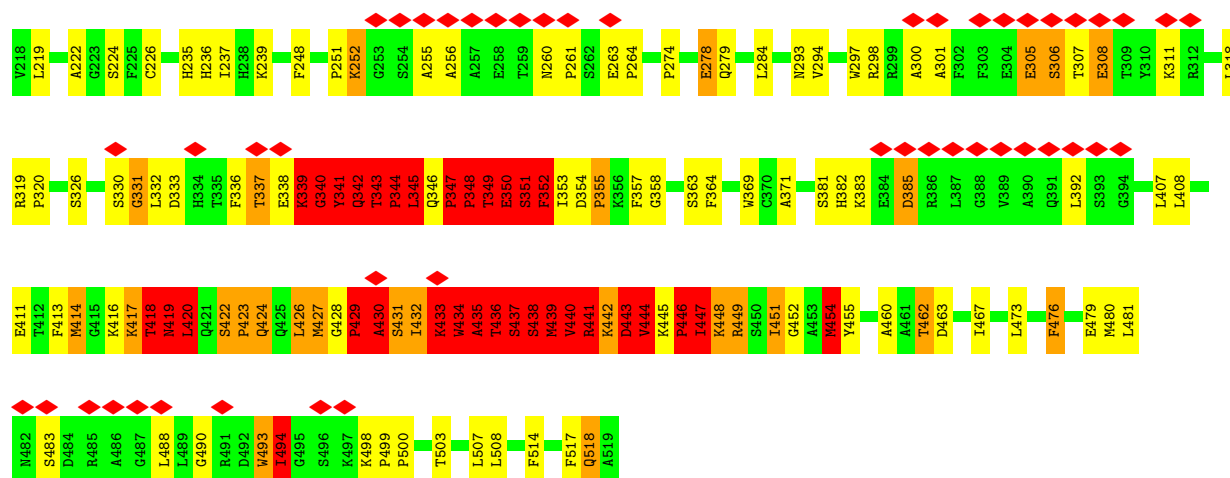


• Molecule 20: Nucleoporin protein Ndc1-Nup protein

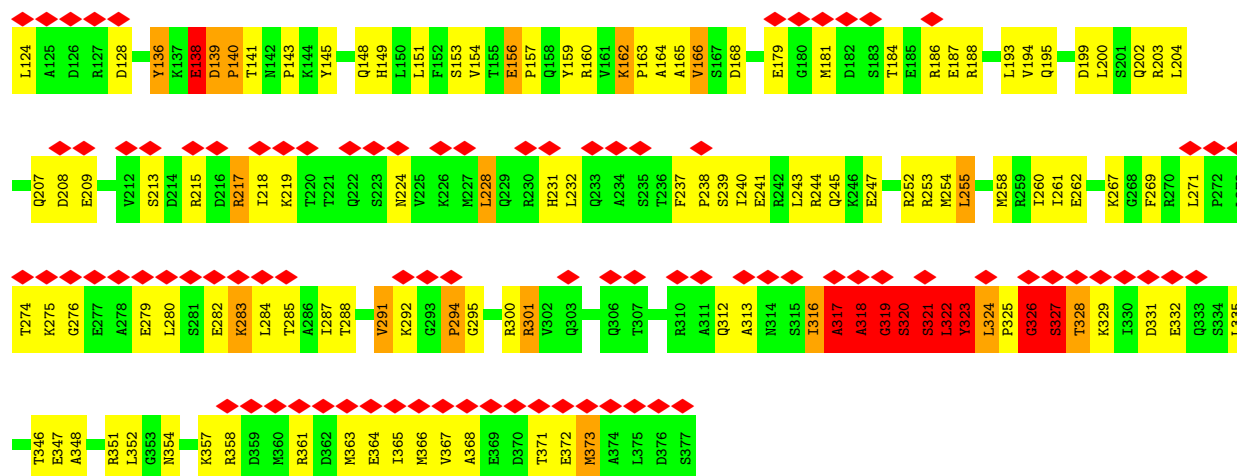


• Molecule 20: Nucleoporin protein Ndc1-Nup protein

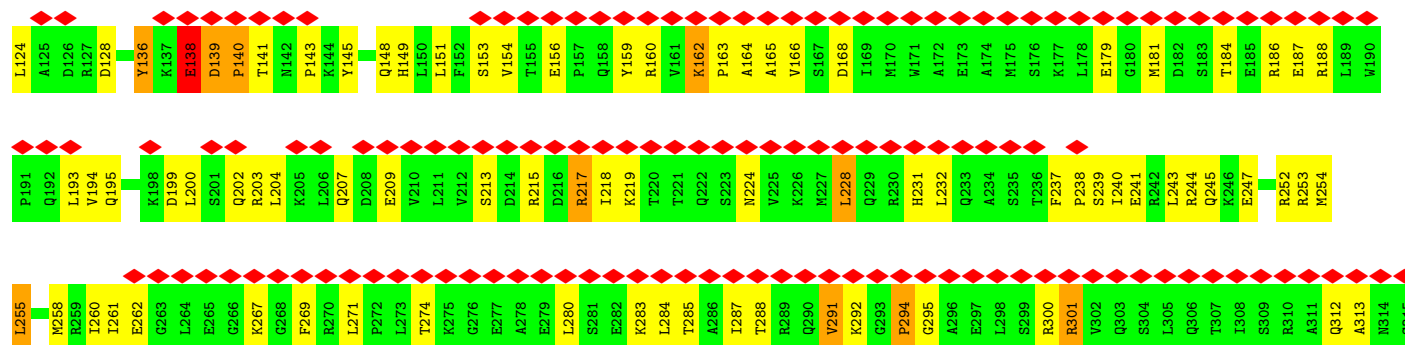


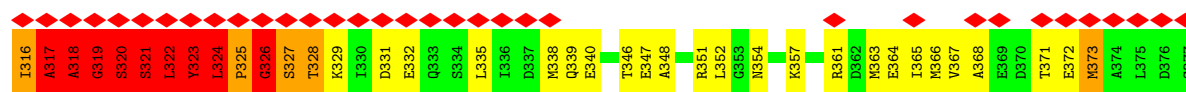


• Molecule 21: Nuclear pore complex protein NUP54

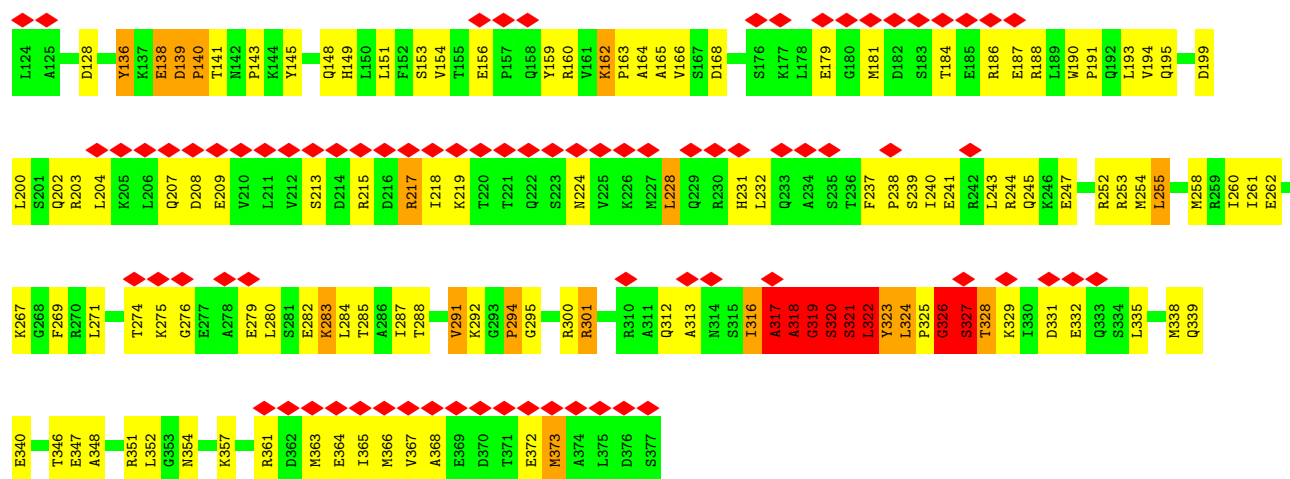


• Molecule 21: Nuclear pore complex protein NUP54

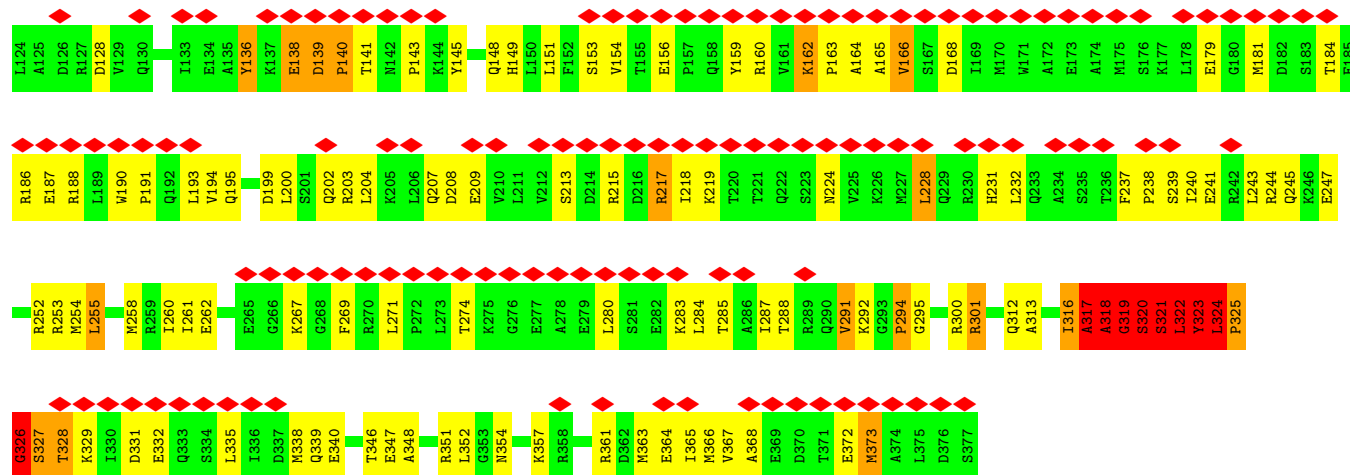




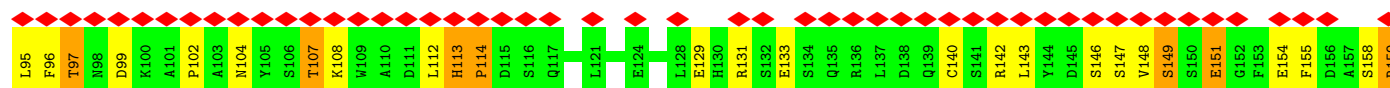
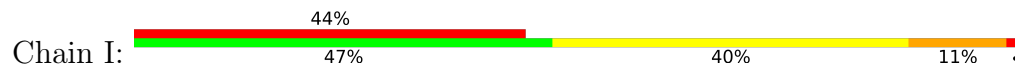
• Molecule 21: Nuclear pore complex protein NUP54

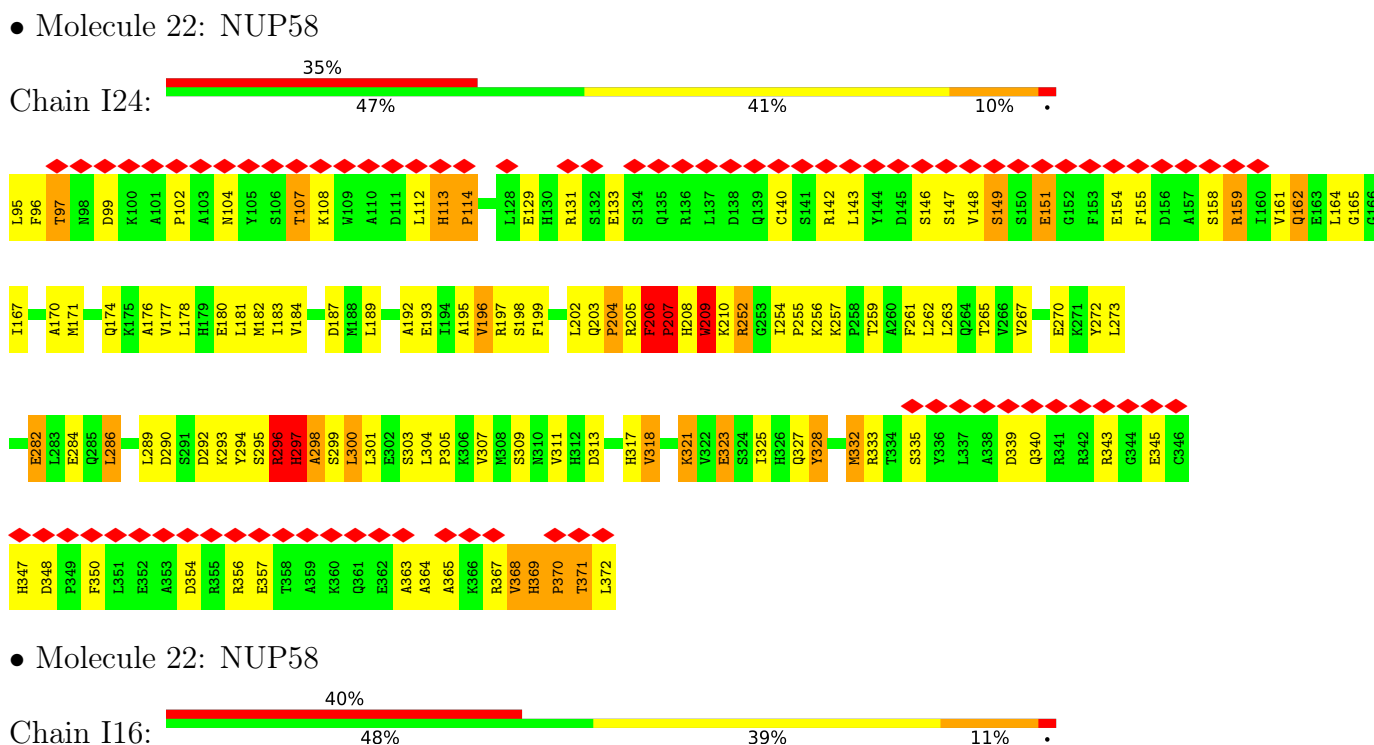
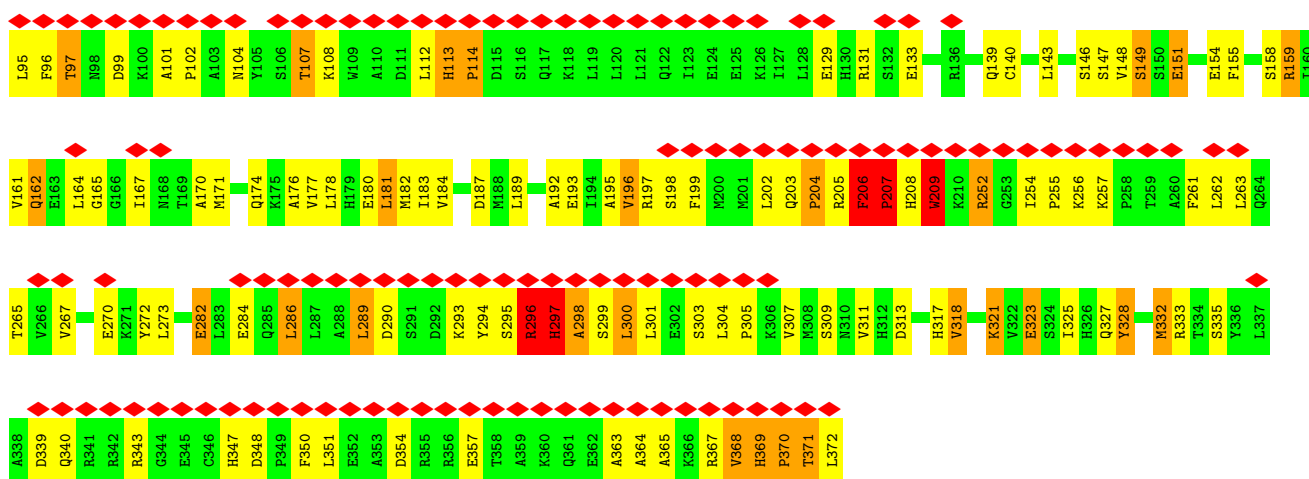
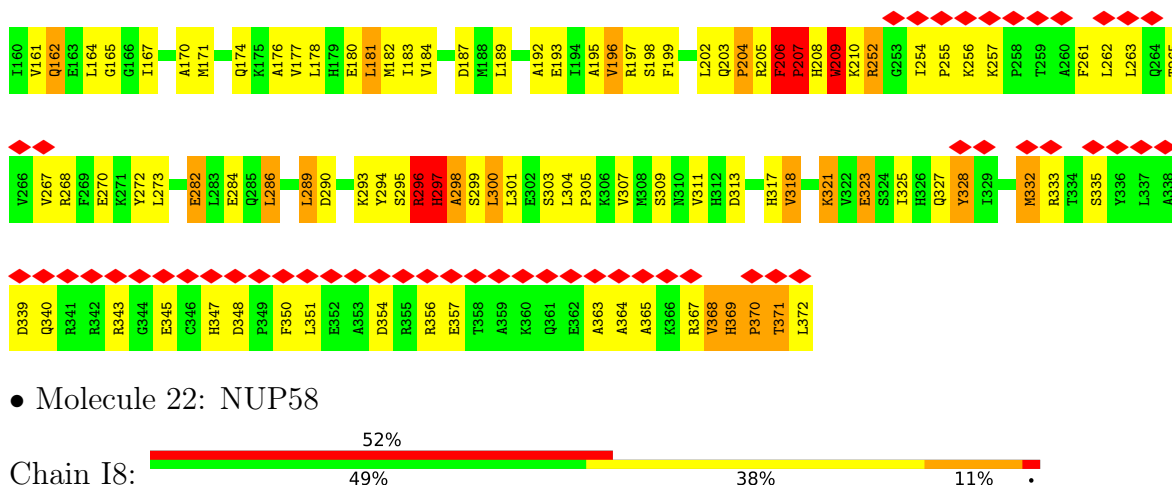


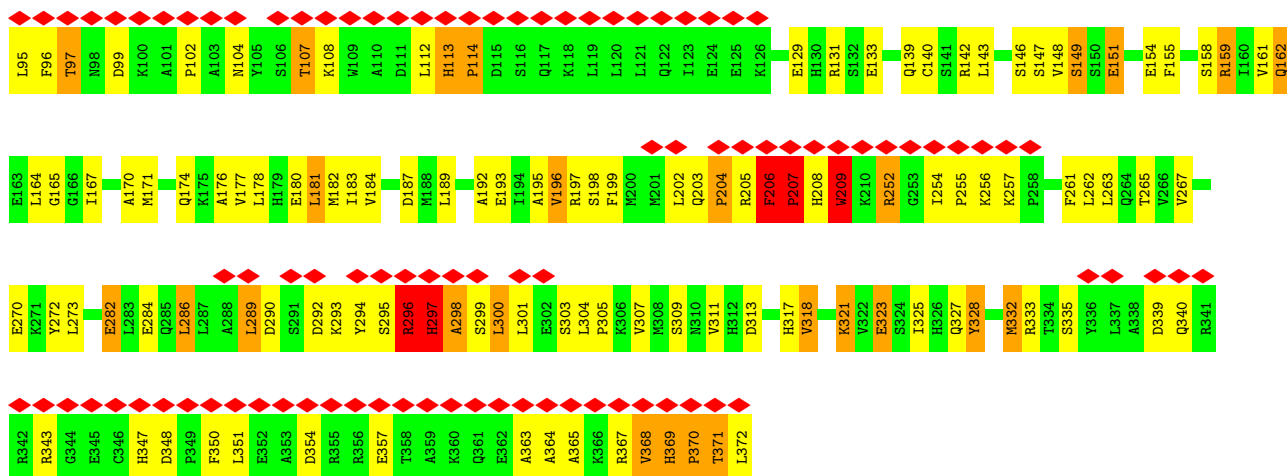
• Molecule 21: Nuclear pore complex protein NUP54



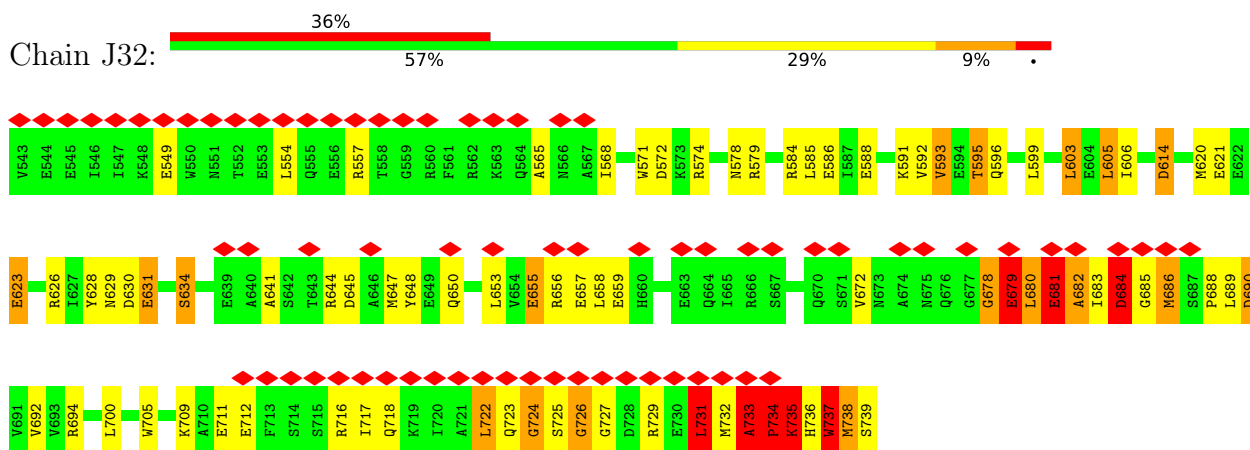
• Molecule 22: NUP58

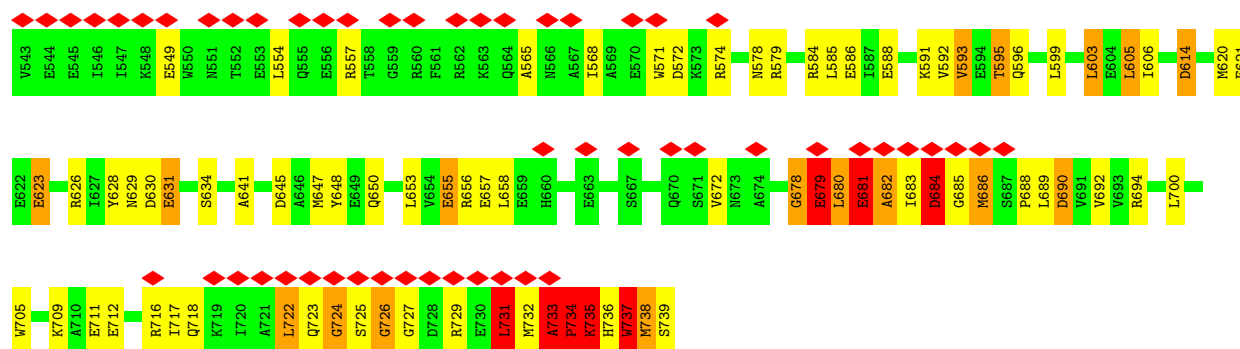




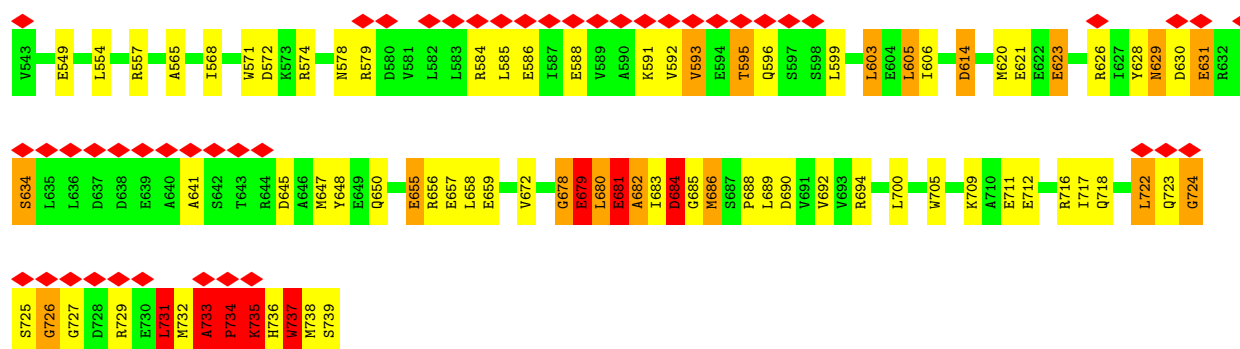


• Molecule 23: Nuclear pore complex protein NUP62

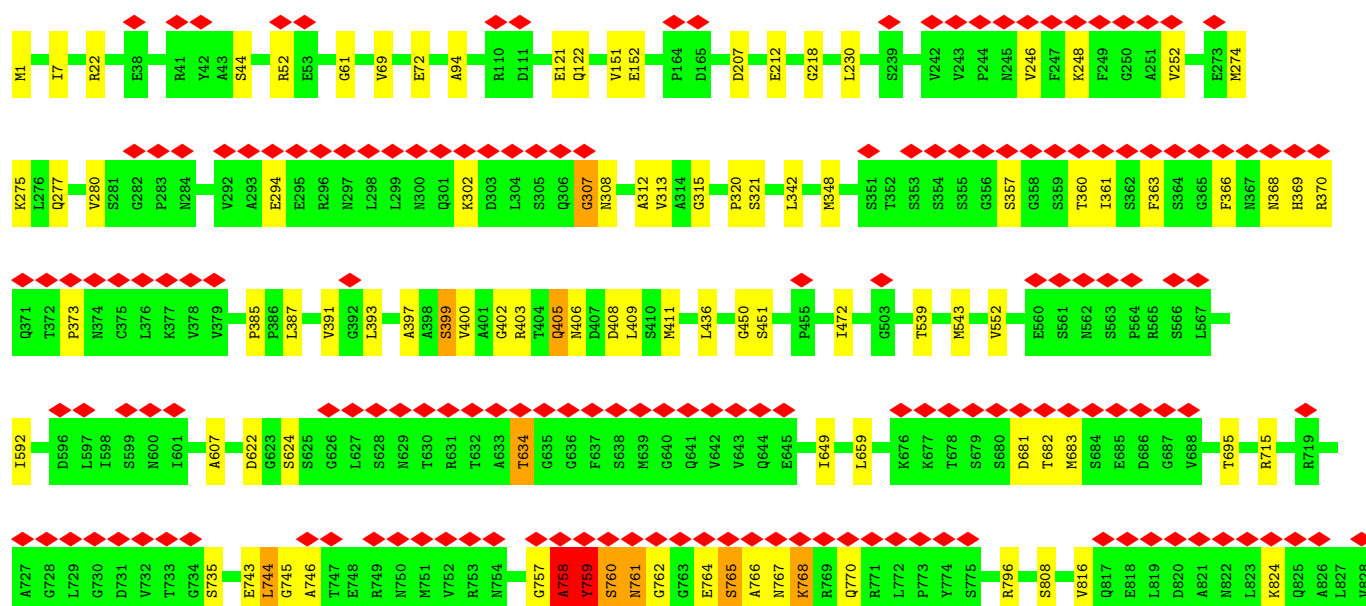
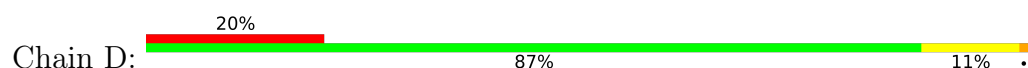


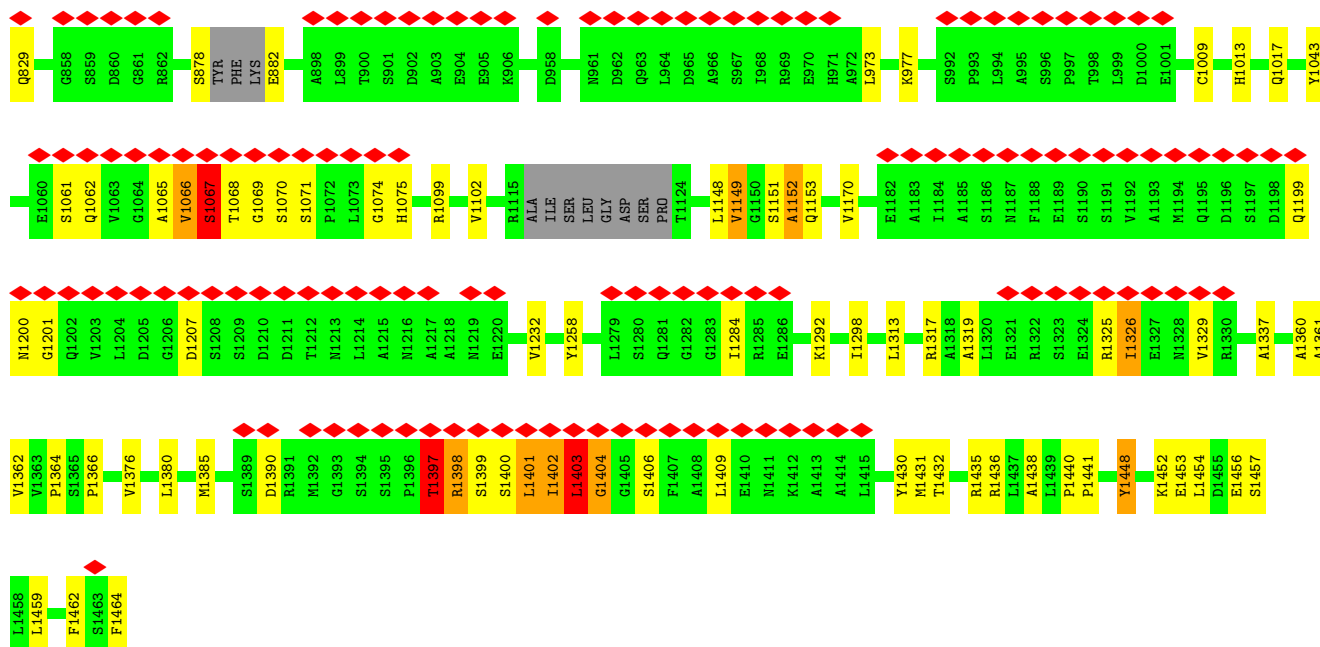


• Molecule 23: Nuclear pore complex protein NUP62

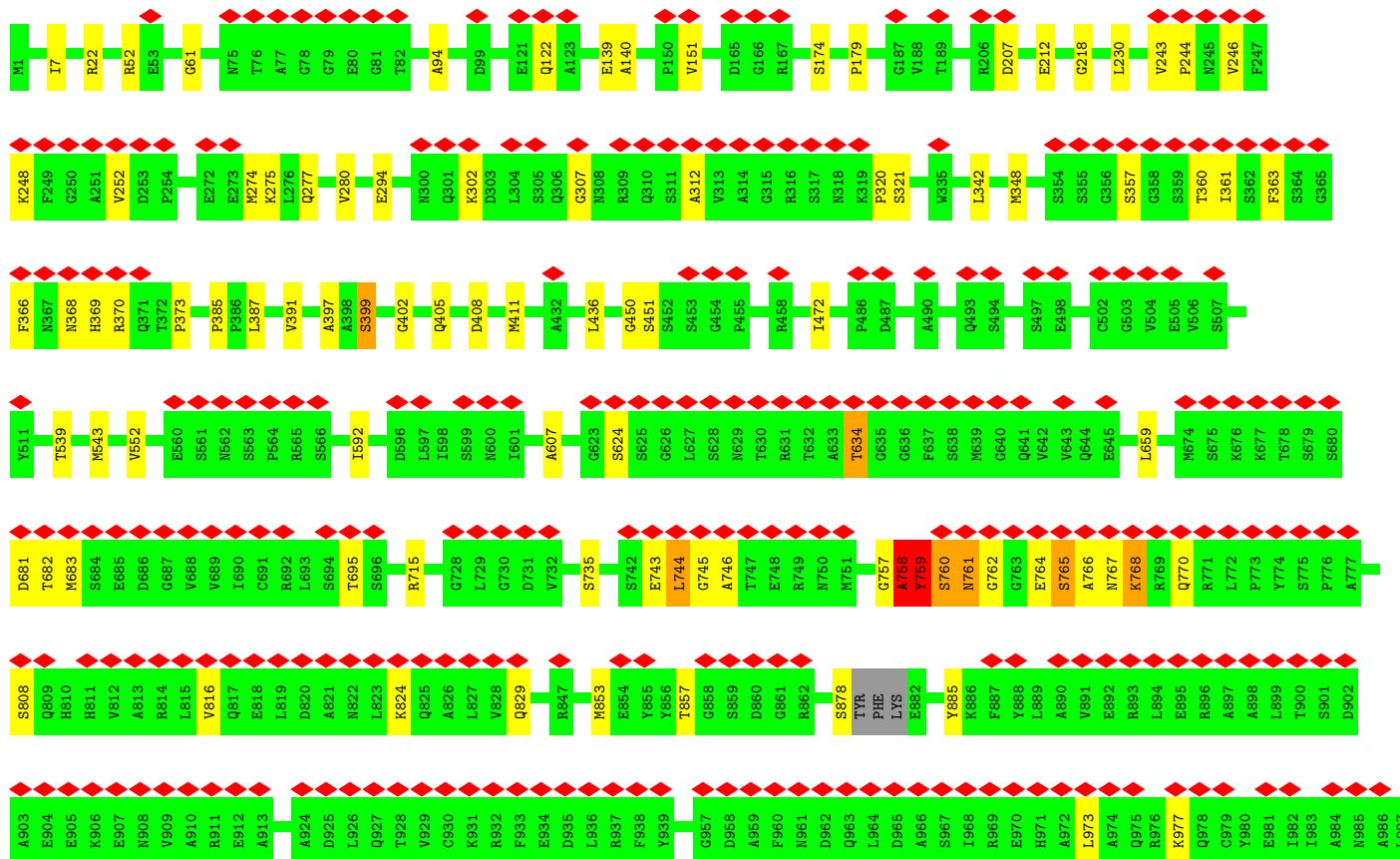
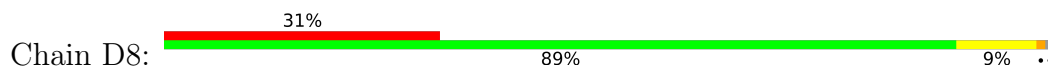


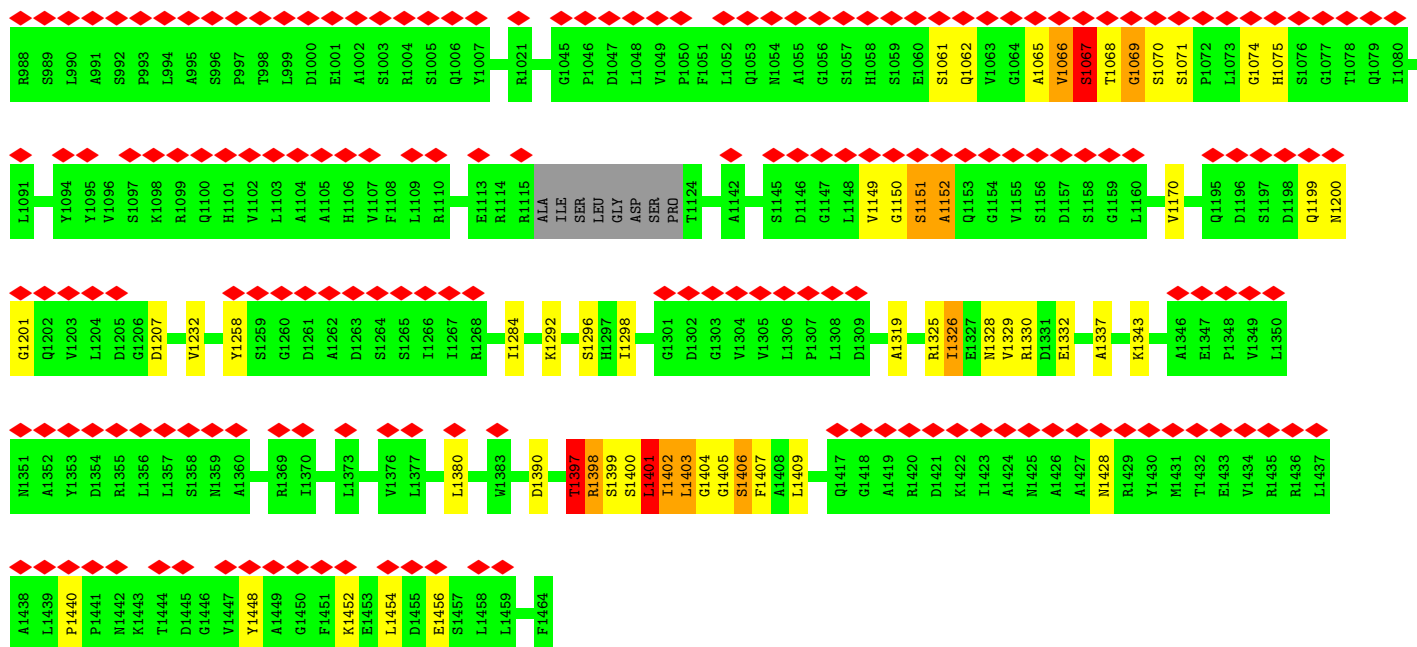
• Molecule 24: Nuclear pore complex protein NUP155



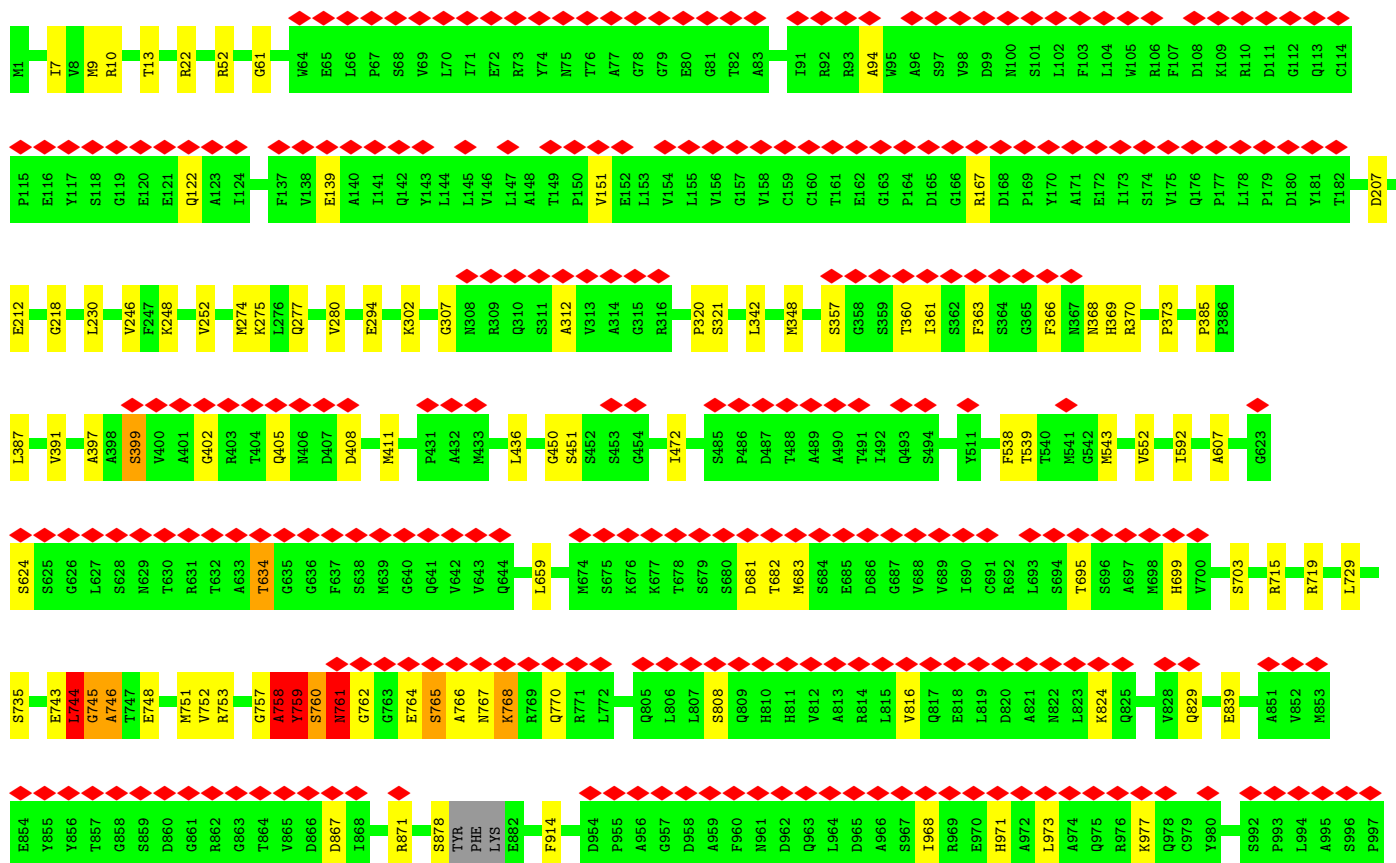
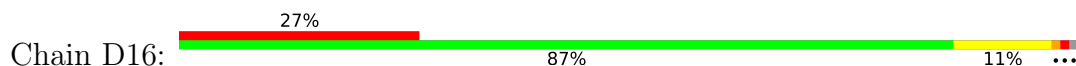


● Molecule 24: Nuclear pore complex protein NUP155

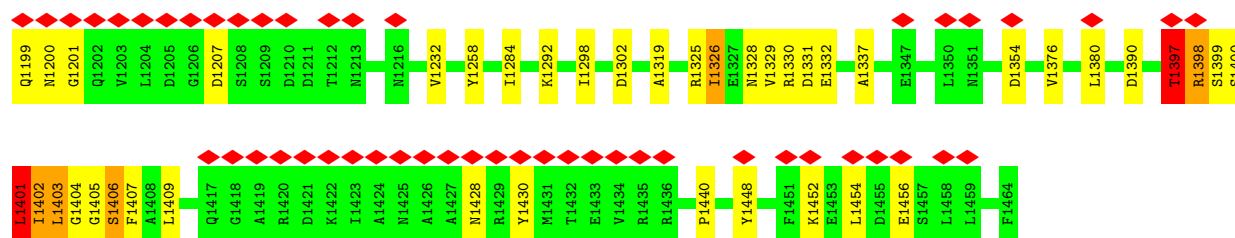




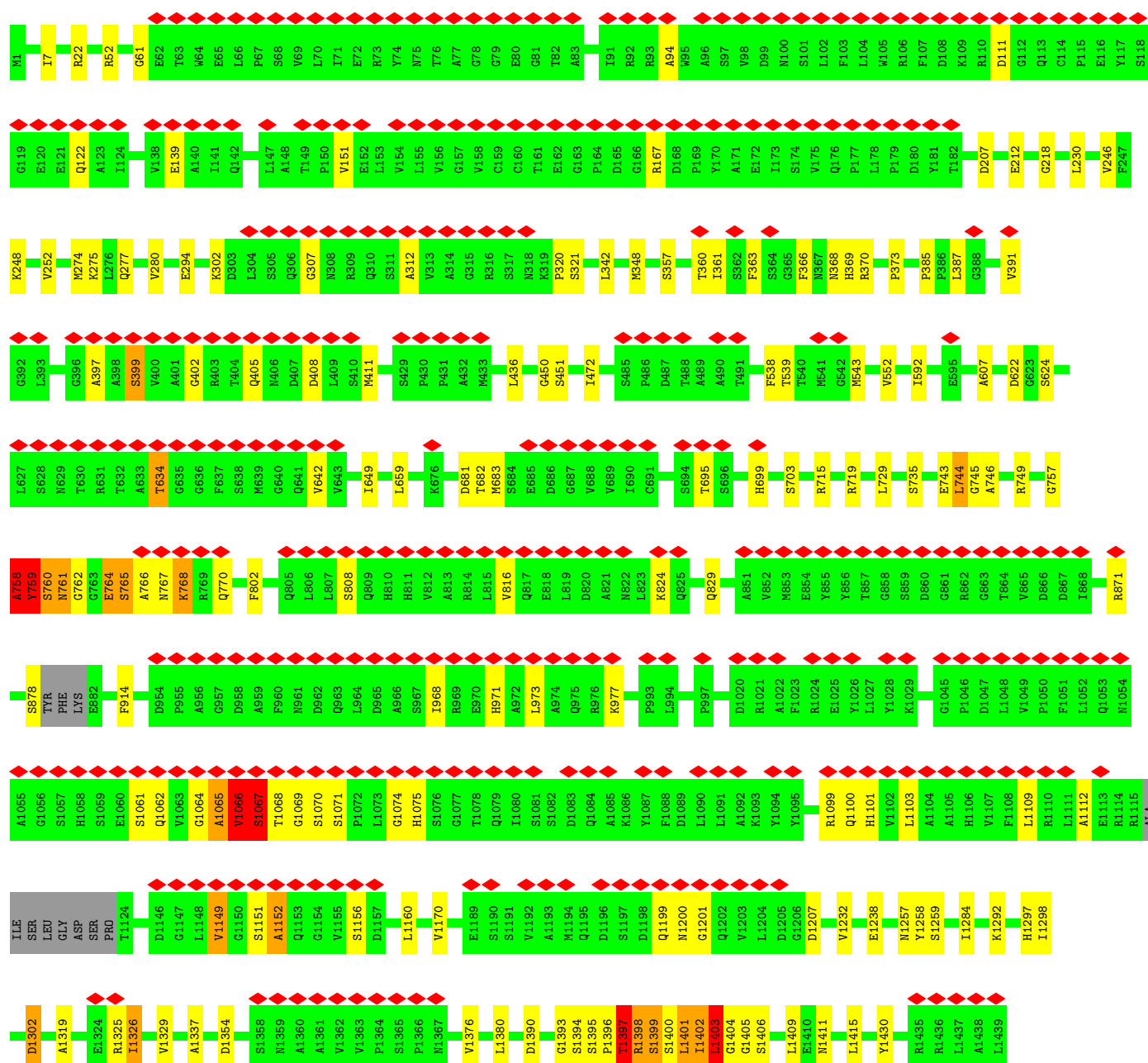
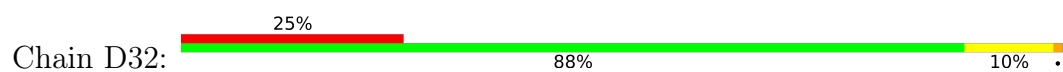
• Molecule 24: Nuclear pore complex protein NUP155

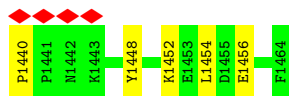






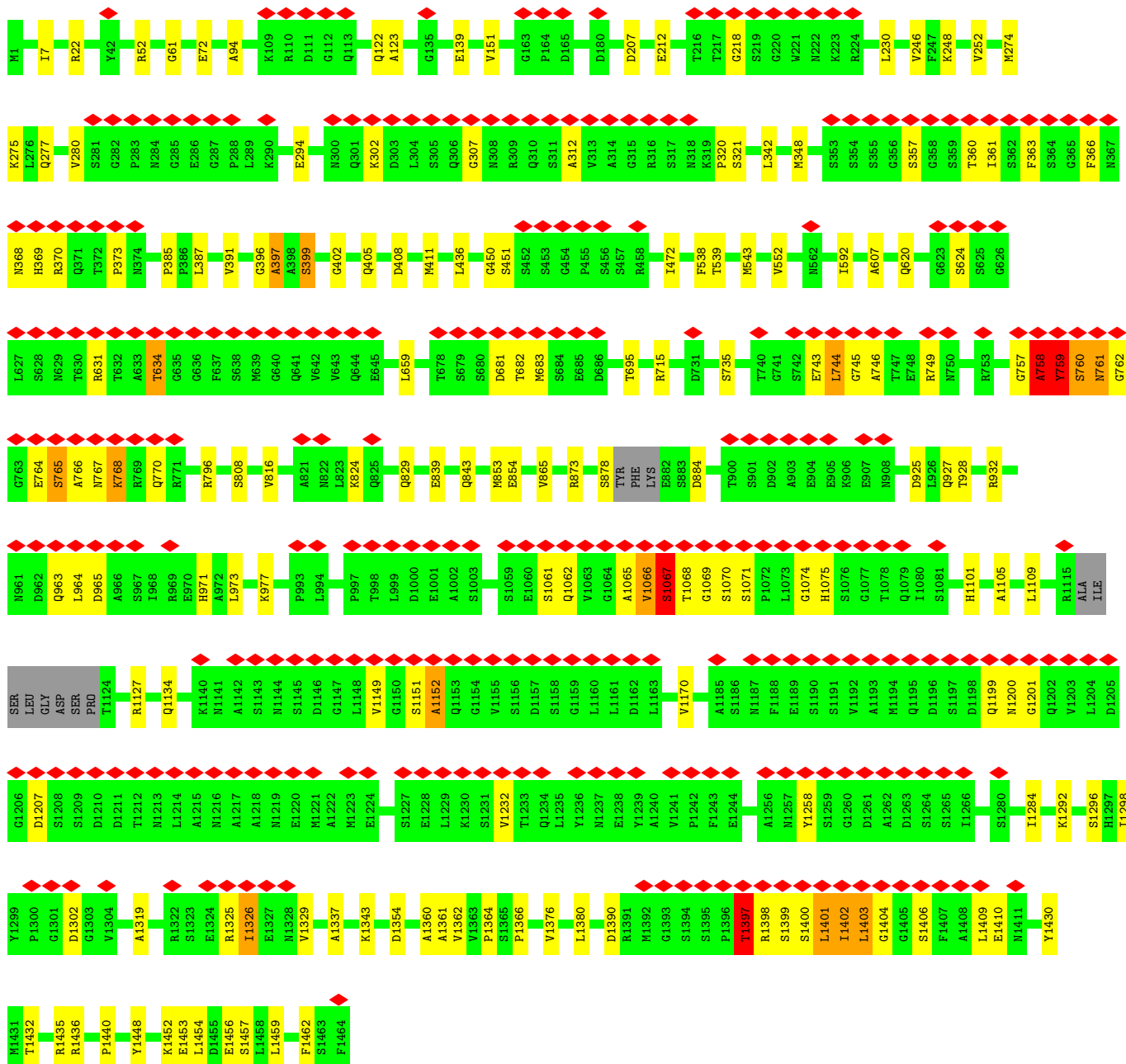
• Molecule 24: Nuclear pore complex protein NUP155





● Molecule 24: Nuclear pore complex protein NUP155

Chain D40: 21% 87% 11% ..



4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C8	Depositor
Number of subtomograms used	75	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	130	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.380	Depositor
Minimum map value	-0.333	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.07	Depositor
Map size (\AA)	1740.8, 1740.8, 1740.8	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	8.704, 8.704, 8.704	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	R	2.22	73/11843 (0.6%)	1.56	85/16033 (0.5%)
1	R16	2.21	73/11843 (0.6%)	1.56	84/16033 (0.5%)
1	R8	2.22	73/11843 (0.6%)	1.56	81/16033 (0.5%)
2	M	1.26	111/5730 (1.9%)	1.42	99/7766 (1.3%)
2	M16	1.26	114/5730 (2.0%)	1.42	97/7766 (1.2%)
2	M8	1.26	111/5730 (1.9%)	1.42	97/7766 (1.2%)
3	N	1.24	41/2366 (1.7%)	1.32	25/3234 (0.8%)
3	N16	1.24	39/2366 (1.6%)	1.32	25/3234 (0.8%)
3	N8	1.24	40/2366 (1.7%)	1.32	25/3234 (0.8%)
4	T	3.67	6/5605 (0.1%)	1.68	19/7591 (0.3%)
4	T16	3.67	6/5605 (0.1%)	1.68	17/7591 (0.2%)
4	T8	3.67	6/5605 (0.1%)	1.68	17/7591 (0.2%)
5	P	1.26	106/5736 (1.8%)	1.29	85/7754 (1.1%)
5	P16	1.26	105/5736 (1.8%)	1.29	85/7754 (1.1%)
5	P8	1.26	107/5736 (1.9%)	1.29	85/7754 (1.1%)
6	O	1.17	33/2391 (1.4%)	1.30	34/3246 (1.0%)
6	O16	1.16	33/2391 (1.4%)	1.30	34/3246 (1.0%)
6	O8	1.17	33/2391 (1.4%)	1.30	34/3246 (1.0%)
7	Q	1.29	51/2834 (1.8%)	1.48	53/3849 (1.4%)
7	Q16	1.29	51/2834 (1.8%)	1.48	53/3849 (1.4%)
7	Q8	1.28	48/2834 (1.7%)	1.48	53/3849 (1.4%)
8	L	2.52	4/7942 (0.1%)	1.52	13/10761 (0.1%)
8	L16	2.52	3/7942 (0.0%)	1.52	13/10761 (0.1%)
8	L8	2.52	3/7942 (0.0%)	1.52	13/10761 (0.1%)
9	K	1.77	213/5800 (3.7%)	1.91	212/7828 (2.7%)
9	K16	0.77	0/5801	1.25	6/7828 (0.1%)
9	K8	1.77	215/5800 (3.7%)	1.91	211/7828 (2.7%)
10	C	1.59	399/14649 (2.7%)	1.80	503/19823 (2.5%)
10	C16	1.59	409/14783 (2.8%)	1.82	520/20005 (2.6%)
10	C24	1.59	410/14783 (2.8%)	1.82	526/20005 (2.6%)
10	C32	1.59	413/14783 (2.8%)	1.82	525/20005 (2.6%)
10	C8	1.58	381/14420 (2.6%)	1.73	454/19508 (2.3%)
11	A16	1.24	107/6584 (1.6%)	1.21	61/8878 (0.7%)
11	A24	1.24	99/6584 (1.5%)	1.23	68/8878 (0.8%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
11	A32	1.24	108/6584 (1.6%)	1.21	61/8878 (0.7%)
11	A40	1.24	99/6584 (1.5%)	1.23	68/8878 (0.8%)
12	A	1.23	84/5826 (1.4%)	1.21	58/7855 (0.7%)
12	A48	1.23	86/5855 (1.5%)	1.21	58/7897 (0.7%)
13	V	1.78	67/1617 (4.1%)	1.71	42/2175 (1.9%)
14	W	1.13	65/6274 (1.0%)	1.36	70/8517 (0.8%)
15	J	1.49	50/1516 (3.3%)	1.41	26/2038 (1.3%)
16	A8	1.16	5/530 (0.9%)	1.38	10/709 (1.4%)
17	F	1.44	6/220 (2.7%)	2.85	17/302 (5.6%)
17	F16	1.45	6/220 (2.7%)	2.88	17/302 (5.6%)
17	F24	1.45	6/220 (2.7%)	2.88	17/302 (5.6%)
17	F8	1.44	6/220 (2.7%)	2.87	17/302 (5.6%)
18	B	1.42	356/15710 (2.3%)	1.68	461/21300 (2.2%)
18	B8	1.42	356/15710 (2.3%)	1.68	467/21300 (2.2%)
19	4	1.53	98/3497 (2.8%)	1.74	92/4746 (1.9%)
19	48	1.53	98/3497 (2.8%)	1.74	89/4746 (1.9%)
20	E	1.51	95/4165 (2.3%)	1.56	92/5657 (1.6%)
20	E8	1.51	95/4165 (2.3%)	1.56	91/5657 (1.6%)
21	H	1.31	46/2046 (2.2%)	1.31	24/2749 (0.9%)
21	H16	1.32	45/2046 (2.2%)	1.31	24/2749 (0.9%)
21	H24	1.31	45/2046 (2.2%)	1.31	24/2749 (0.9%)
21	H8	1.31	45/2046 (2.2%)	1.31	24/2749 (0.9%)
22	I	1.45	50/1978 (2.5%)	1.35	33/2664 (1.2%)
22	I16	1.45	50/1978 (2.5%)	1.34	32/2664 (1.2%)
22	I24	1.45	48/1978 (2.4%)	1.34	33/2664 (1.2%)
22	I8	1.45	51/1978 (2.6%)	1.34	31/2664 (1.2%)
23	J16	1.30	30/1617 (1.9%)	1.42	39/2174 (1.8%)
23	J24	1.30	29/1617 (1.8%)	1.42	39/2174 (1.8%)
23	J32	1.30	31/1617 (1.9%)	1.41	39/2174 (1.8%)
23	J8	1.30	31/1617 (1.9%)	1.42	39/2174 (1.8%)
24	D	0.76	2/11328 (0.0%)	1.25	27/15333 (0.2%)
24	D16	0.76	2/11328 (0.0%)	1.25	26/15333 (0.2%)
24	D24	0.76	2/11328 (0.0%)	1.25	24/15333 (0.2%)
24	D32	0.76	2/11328 (0.0%)	1.25	26/15333 (0.2%)
24	D40	0.76	2/11328 (0.0%)	1.25	27/15333 (0.2%)
24	D8	0.76	2/11328 (0.0%)	1.25	26/15333 (0.2%)
All	All	1.65	6115/410270 (1.5%)	1.52	6602/555195 (1.2%)

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	R	0	45
1	R16	0	45
1	R8	0	45
2	M	0	33
2	M16	0	34
2	M8	0	33
3	N	0	14
3	N16	0	14
3	N8	0	14
4	T	0	7
4	T16	0	7
4	T8	0	7
5	P	0	33
5	P16	0	33
5	P8	0	33
6	O	0	9
6	O16	0	9
6	O8	0	9
7	Q	0	17
7	Q16	0	17
7	Q8	0	17
8	L	0	3
8	L16	0	3
8	L8	0	3
9	K	0	84
9	K16	0	6
9	K8	0	84
10	C	0	171
10	C16	0	178
10	C24	0	178
10	C32	0	178
10	C8	0	146
11	A16	0	38
11	A24	0	40
11	A32	0	38
11	A40	0	40
12	A	0	36
12	A48	0	36
13	V	0	24
14	W	0	22
15	J	0	7
16	A8	0	3
17	F	0	10

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Mol	Chain	#Chirality outliers	#Planarity outliers
17	F16	0	10
17	F24	0	10
17	F8	0	10
18	B	0	196
18	B8	0	198
19	4	0	43
19	48	0	43
20	E	0	51
20	E8	0	51
21	H	0	8
21	H16	0	8
21	H24	0	8
21	H8	0	8
22	I	0	12
22	I16	0	12
22	I24	0	12
22	I8	0	12
23	J16	0	9
23	J24	0	9
23	J32	0	9
23	J8	0	9
24	D	0	29
24	D16	0	29
24	D24	0	29
24	D32	0	29
24	D40	0	29
24	D8	0	29
All	All	0	2705

The worst 5 of 6115 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	529	HIS	CD2-NE2	170.27	3.25	1.37
1	R8	529	HIS	CD2-NE2	170.21	3.25	1.37
1	R16	529	HIS	CD2-NE2	170.14	3.25	1.37
4	T	160	HIS	CD2-NE2	169.95	3.24	1.37
4	T8	160	HIS	CD2-NE2	169.94	3.24	1.37

The worst 5 of 6602 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L8	1054	HIS	ND1-CE1-NE2	-53.29	55.11	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	1054	HIS	ND1-CE1-NE2	-53.27	55.12	108.40
8	L16	1054	HIS	ND1-CE1-NE2	-53.26	55.14	108.40
1	R16	529	HIS	ND1-CE1-NE2	-52.76	55.64	108.40
1	R	529	HIS	ND1-CE1-NE2	-52.75	55.65	108.40

There are no chirality outliers.

5 of 2705 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	R	436	ARG	Sidechain
1	R	47	ASP	Peptide
1	R	480	PHE	Sidechain
1	R	501	ARG	Sidechain
1	R	596	ARG	Sidechain

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	R	11593	0	11503	425	0
1	R16	11593	0	11502	207	0
1	R8	11593	0	11503	298	0
2	M	5598	0	5453	470	0
2	M16	5598	0	5451	523	0
2	M8	5598	0	5449	487	0
3	N	2302	0	2202	186	0
3	N16	2302	0	2202	192	0
3	N8	2302	0	2202	185	0
4	T	5498	0	5401	66	0
4	T16	5498	0	5401	68	0
4	T8	5498	0	5401	68	0
5	P	5620	0	5646	488	0
5	P16	5620	0	5647	375	0
5	P8	5620	0	5647	389	0
6	O	2336	0	2241	218	0
6	O16	2336	0	2243	164	0
6	O8	2336	0	2243	181	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	Q	2770	0	2651	175	0
7	Q16	2770	0	2651	163	0
7	Q8	2770	0	2651	167	0
8	L	7770	0	7584	103	0
8	L16	7770	0	7579	207	0
8	L8	7770	0	7583	161	0
9	K	5695	0	5537	500	0
9	K16	5696	0	5544	128	0
9	K8	5695	0	5537	493	0
10	C	14402	0	14575	1157	0
10	C16	14529	0	14695	1187	0
10	C24	14529	0	14696	1208	0
10	C32	14529	0	14697	1031	0
10	C8	14177	0	14346	1063	0
11	A16	6472	0	6473	547	0
11	A24	6472	0	6474	496	0
11	A32	6472	0	6472	530	0
11	A40	6472	0	6474	503	0
12	A	5726	0	5723	313	0
12	A48	5752	0	5745	317	0
13	V	1590	0	1576	201	0
14	W	6141	0	6109	391	0
15	J	1504	0	1487	188	0
16	A8	523	0	517	33	0
17	F	213	0	187	41	0
17	F16	213	0	187	40	0
17	F24	213	0	187	39	0
17	F8	213	0	187	40	0
18	B	15417	0	15672	1142	0
18	B8	15417	0	15674	1132	0
19	4	3413	0	3328	200	0
19	48	3413	0	3328	214	0
20	E	4057	0	4120	256	0
20	E8	4057	0	4120	272	0
21	H	2023	0	2068	226	0
21	H16	2023	0	2066	194	0
21	H24	2023	0	2066	231	0
21	H8	2023	0	2066	189	0
22	I	1939	0	1924	202	0
22	I16	1939	0	1924	206	0
22	I24	1939	0	1924	200	0
22	I8	1939	0	1923	189	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	J16	1601	0	1575	175	0
23	J24	1601	0	1575	203	0
23	J32	1601	0	1575	201	0
23	J8	1601	0	1575	173	0
24	D	11141	0	11068	316	0
24	D16	11141	0	11074	343	0
24	D24	11141	0	11072	147	0
24	D32	11141	0	11074	263	0
24	D40	11141	0	11072	230	0
24	D8	11141	0	11075	152	0
All	All	402561	0	400399	18966	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 24.

The worst 5 of 18966 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)
18:B8:1210:CYS:SG	18:B8:1234:MET:HE1	1.23	1.74
2:M:847:PHE:HB2	4:T:656:TRP:CZ3	1.17	1.70
9:K8:1085:TYR:CE1	9:K8:1093:SER:HB2	1.24	1.68
10:C:345:MET:HE1	10:C:401:ILE:CD1	1.19	1.67
18:B:1210:CYS:SG	18:B:1234:MET:HE1	1.23	1.67

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	R	1458/1495 (98%)	1379 (95%)	60 (4%)	19 (1%)	9	42
1	R16	1458/1495 (98%)	1379 (95%)	59 (4%)	20 (1%)	9	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R8	1458/1495 (98%)	1379 (95%)	59 (4%)	20 (1%)	9	40
2	M	688/704 (98%)	650 (94%)	19 (3%)	19 (3%)	4	24
2	M16	688/704 (98%)	650 (94%)	19 (3%)	19 (3%)	4	24
2	M8	688/704 (98%)	650 (94%)	19 (3%)	19 (3%)	4	24
3	N	300/302 (99%)	285 (95%)	12 (4%)	3 (1%)	12	49
3	N16	300/302 (99%)	285 (95%)	12 (4%)	3 (1%)	12	49
3	N8	300/302 (99%)	285 (95%)	12 (4%)	3 (1%)	12	49
4	T	682/684 (100%)	647 (95%)	29 (4%)	6 (1%)	14	51
4	T16	682/684 (100%)	647 (95%)	29 (4%)	6 (1%)	14	51
4	T8	682/684 (100%)	647 (95%)	29 (4%)	6 (1%)	14	51
5	P	700/716 (98%)	668 (95%)	15 (2%)	17 (2%)	4	27
5	P16	700/716 (98%)	668 (95%)	16 (2%)	16 (2%)	5	28
5	P8	700/716 (98%)	668 (95%)	16 (2%)	16 (2%)	5	28
6	O	299/326 (92%)	286 (96%)	5 (2%)	8 (3%)	4	25
6	O16	299/326 (92%)	287 (96%)	4 (1%)	8 (3%)	4	25
6	O8	299/326 (92%)	286 (96%)	5 (2%)	8 (3%)	4	25
7	Q	359/361 (99%)	335 (93%)	15 (4%)	9 (2%)	4	26
7	Q16	359/361 (99%)	335 (93%)	15 (4%)	9 (2%)	4	26
7	Q8	359/361 (99%)	335 (93%)	15 (4%)	9 (2%)	4	26
8	L	970/977 (99%)	925 (95%)	34 (4%)	11 (1%)	11	46
8	L16	970/977 (99%)	925 (95%)	34 (4%)	11 (1%)	11	46
8	L8	970/977 (99%)	925 (95%)	34 (4%)	11 (1%)	11	46
9	K	701/709 (99%)	638 (91%)	29 (4%)	34 (5%)	1	16
9	K16	701/709 (99%)	663 (95%)	24 (3%)	14 (2%)	6	31
9	K8	701/709 (99%)	638 (91%)	29 (4%)	34 (5%)	1	16
10	C	1816/1838 (99%)	1681 (93%)	64 (4%)	71 (4%)	2	19
10	C16	1836/1838 (100%)	1693 (92%)	69 (4%)	74 (4%)	2	18
10	C24	1836/1838 (100%)	1693 (92%)	69 (4%)	74 (4%)	2	18
10	C32	1836/1838 (100%)	1693 (92%)	68 (4%)	75 (4%)	2	18
10	C8	1781/1838 (97%)	1667 (94%)	56 (3%)	58 (3%)	3	21
11	A16	812/860 (94%)	779 (96%)	17 (2%)	16 (2%)	6	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	A24	812/860 (94%)	778 (96%)	17 (2%)	17 (2%)	5	30
11	A32	812/860 (94%)	779 (96%)	17 (2%)	16 (2%)	6	31
11	A40	812/860 (94%)	778 (96%)	17 (2%)	17 (2%)	5	30
12	A	717/763 (94%)	688 (96%)	15 (2%)	14 (2%)	6	31
12	A48	722/763 (95%)	693 (96%)	15 (2%)	14 (2%)	6	32
13	V	194/196 (99%)	175 (90%)	8 (4%)	11 (6%)	1	14
14	W	783/810 (97%)	737 (94%)	30 (4%)	16 (2%)	6	31
15	J	183/185 (99%)	175 (96%)	3 (2%)	5 (3%)	4	25
16	A8	61/63 (97%)	60 (98%)	0	1 (2%)	7	38
17	F	26/28 (93%)	18 (69%)	3 (12%)	5 (19%)	0	2
17	F16	26/28 (93%)	18 (69%)	3 (12%)	5 (19%)	0	2
17	F24	26/28 (93%)	18 (69%)	3 (12%)	5 (19%)	0	2
17	F8	26/28 (93%)	18 (69%)	3 (12%)	5 (19%)	0	2
18	B	1963/1965 (100%)	1806 (92%)	79 (4%)	78 (4%)	2	18
18	B8	1963/1965 (100%)	1807 (92%)	78 (4%)	78 (4%)	2	18
19	4	445/447 (100%)	403 (91%)	16 (4%)	26 (6%)	1	14
19	48	445/447 (100%)	403 (91%)	16 (4%)	26 (6%)	1	14
20	E	517/519 (100%)	471 (91%)	19 (4%)	27 (5%)	1	15
20	E8	517/519 (100%)	471 (91%)	18 (4%)	28 (5%)	1	15
21	H	252/254 (99%)	245 (97%)	1 (0%)	6 (2%)	4	27
21	H16	252/254 (99%)	245 (97%)	1 (0%)	6 (2%)	4	27
21	H24	252/254 (99%)	245 (97%)	1 (0%)	6 (2%)	4	27
21	H8	252/254 (99%)	245 (97%)	1 (0%)	6 (2%)	4	27
22	I	233/237 (98%)	224 (96%)	7 (3%)	2 (1%)	14	51
22	I16	233/237 (98%)	224 (96%)	7 (3%)	2 (1%)	14	51
22	I24	233/237 (98%)	224 (96%)	7 (3%)	2 (1%)	14	51
22	I8	233/237 (98%)	224 (96%)	7 (3%)	2 (1%)	14	51
23	J16	195/197 (99%)	188 (96%)	5 (3%)	2 (1%)	12	49
23	J24	195/197 (99%)	188 (96%)	5 (3%)	2 (1%)	12	49
23	J32	195/197 (99%)	188 (96%)	5 (3%)	2 (1%)	12	49
23	J8	195/197 (99%)	188 (96%)	5 (3%)	2 (1%)	12	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	D	1447/1464 (99%)	1335 (92%)	70 (5%)	42 (3%)	3	23
24	D16	1447/1464 (99%)	1336 (92%)	69 (5%)	42 (3%)	3	23
24	D24	1447/1464 (99%)	1334 (92%)	71 (5%)	42 (3%)	3	23
24	D32	1447/1464 (99%)	1334 (92%)	71 (5%)	42 (3%)	3	23
24	D40	1447/1464 (99%)	1336 (92%)	69 (5%)	42 (3%)	3	23
24	D8	1447/1464 (99%)	1336 (92%)	69 (5%)	42 (3%)	3	23
All	All	50840/51742 (98%)	47606 (94%)	1822 (4%)	1412 (3%)	6	24

5 of 1412 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	R	302	MET
1	R	1183	GLU
1	R	1185	THR
1	R	1186	THR
1	R	1192	LYS

5.3.2 Protein sidechains ⓘ

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	R	1286/1314 (98%)	1245 (97%)	41 (3%)	34	56
1	R16	1286/1314 (98%)	1247 (97%)	39 (3%)	36	57
1	R8	1286/1314 (98%)	1246 (97%)	40 (3%)	35	56
2	M	619/626 (99%)	598 (97%)	21 (3%)	32	54
2	M16	619/626 (99%)	599 (97%)	20 (3%)	34	56
2	M8	619/626 (99%)	597 (96%)	22 (4%)	31	52
3	N	246/246 (100%)	243 (99%)	3 (1%)	63	75
3	N16	246/246 (100%)	242 (98%)	4 (2%)	55	70
3	N8	246/246 (100%)	244 (99%)	2 (1%)	73	80
4	T	611/611 (100%)	590 (97%)	21 (3%)	32	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	T16	611/611 (100%)	596 (98%)	15 (2%)	42	63
4	T8	611/611 (100%)	592 (97%)	19 (3%)	35	56
5	P	622/629 (99%)	603 (97%)	19 (3%)	35	56
5	P16	622/629 (99%)	606 (97%)	16 (3%)	40	62
5	P8	622/629 (99%)	604 (97%)	18 (3%)	37	58
6	O	262/280 (94%)	257 (98%)	5 (2%)	50	67
6	O16	262/280 (94%)	257 (98%)	5 (2%)	50	67
6	O8	262/280 (94%)	257 (98%)	5 (2%)	50	67
7	Q	302/302 (100%)	297 (98%)	5 (2%)	53	69
7	Q16	302/302 (100%)	298 (99%)	4 (1%)	61	74
7	Q8	302/302 (100%)	299 (99%)	3 (1%)	68	78
8	L	859/861 (100%)	853 (99%)	6 (1%)	76	81
8	L16	859/861 (100%)	851 (99%)	8 (1%)	70	79
8	L8	859/861 (100%)	853 (99%)	6 (1%)	76	81
9	K	621/623 (100%)	569 (92%)	52 (8%)	10	30
9	K16	621/623 (100%)	616 (99%)	5 (1%)	73	80
9	K8	621/623 (100%)	570 (92%)	51 (8%)	10	31
10	C	1628/1641 (99%)	1473 (90%)	155 (10%)	8	25
10	C16	1641/1641 (100%)	1488 (91%)	153 (9%)	8	26
10	C24	1641/1641 (100%)	1498 (91%)	143 (9%)	9	29
10	C32	1641/1641 (100%)	1499 (91%)	142 (9%)	9	29
10	C8	1598/1641 (97%)	1451 (91%)	147 (9%)	8	27
11	A16	696/730 (95%)	676 (97%)	20 (3%)	37	58
11	A24	696/730 (95%)	678 (97%)	18 (3%)	40	62
11	A32	696/730 (95%)	676 (97%)	20 (3%)	37	58
11	A40	696/730 (95%)	678 (97%)	18 (3%)	40	62
12	A	614/647 (95%)	597 (97%)	17 (3%)	38	60
12	A48	617/647 (95%)	602 (98%)	15 (2%)	43	64
13	V	175/175 (100%)	154 (88%)	21 (12%)	5	17
14	W	693/715 (97%)	665 (96%)	28 (4%)	28	49
15	J	166/166 (100%)	156 (94%)	10 (6%)	17	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	A8	59/59 (100%)	55 (93%)	4 (7%)	14	36
17	F	25/25 (100%)	22 (88%)	3 (12%)	5	17
17	F16	25/25 (100%)	22 (88%)	3 (12%)	5	17
17	F24	25/25 (100%)	22 (88%)	3 (12%)	5	17
17	F8	25/25 (100%)	22 (88%)	3 (12%)	5	17
18	B	1759/1759 (100%)	1652 (94%)	107 (6%)	17	38
18	B8	1759/1759 (100%)	1654 (94%)	105 (6%)	17	39
19	4	374/374 (100%)	356 (95%)	18 (5%)	23	44
19	48	374/374 (100%)	355 (95%)	19 (5%)	21	42
20	E	450/450 (100%)	425 (94%)	25 (6%)	19	40
20	E8	450/450 (100%)	423 (94%)	27 (6%)	17	39
21	H	223/223 (100%)	217 (97%)	6 (3%)	39	61
21	H16	223/223 (100%)	220 (99%)	3 (1%)	61	74
21	H24	223/223 (100%)	220 (99%)	3 (1%)	61	74
21	H8	223/223 (100%)	217 (97%)	6 (3%)	39	61
22	I	212/212 (100%)	204 (96%)	8 (4%)	29	50
22	I16	212/212 (100%)	202 (95%)	10 (5%)	23	45
22	I24	212/212 (100%)	202 (95%)	10 (5%)	23	45
22	I8	212/212 (100%)	203 (96%)	9 (4%)	26	48
23	J16	176/176 (100%)	168 (96%)	8 (4%)	24	46
23	J24	176/176 (100%)	168 (96%)	8 (4%)	24	46
23	J32	176/176 (100%)	168 (96%)	8 (4%)	24	46
23	J8	176/176 (100%)	168 (96%)	8 (4%)	24	46
24	D	1214/1223 (99%)	1201 (99%)	13 (1%)	65	76
24	D16	1214/1223 (99%)	1197 (99%)	17 (1%)	59	72
24	D24	1214/1223 (99%)	1196 (98%)	18 (2%)	57	72
24	D32	1214/1223 (99%)	1197 (99%)	17 (1%)	59	72
24	D40	1214/1223 (99%)	1197 (99%)	17 (1%)	59	72
24	D8	1214/1223 (99%)	1201 (99%)	13 (1%)	65	76
All	All	44535/45058 (99%)	42674 (96%)	1861 (4%)	28	48

5 of 1861 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	C	718	HIS
10	C32	805	LEU
10	C8	1614	LEU
10	C32	634	SER
22	I16	371	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 312 such sidechains are listed below:

Mol	Chain	Res	Type
18	B	1032	GLN
21	H8	312	GLN
18	B	1745	HIS
18	B8	1748	HIS
24	D	654	HIS

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 oligosaccharides 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
10	C16	17
10	C24	17
10	C	17
10	C32	17
10	C8	15
9	K	9
9	K8	9
18	B8	7
18	B	6
11	A24	5
11	A40	5
11	A16	5
11	A32	5
19	4	5
19	48	5
1	R	4
1	R8	4
1	R16	4
14	W	4
12	A	4
12	A48	4
20	E	3
20	E8	3
5	P	3
5	P8	3
5	P16	3
13	V	3
22	I	2
22	I8	2
22	I24	2
22	I16	2
7	Q	2
7	Q8	2
7	Q16	2
3	N	2
3	N8	2
3	N16	2
15	J	1
23	J32	1
23	J8	1
23	J24	1
23	J16	1

The worst 5 of 211 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	210:LYS	C	252:ARG	N	22.49
1	I8	210:LYS	C	252:ARG	N	22.49
1	I24	210:LYS	C	252:ARG	N	22.49
1	I16	210:LYS	C	252:ARG	N	22.49
1	R	1121:ARG	C	1122:HIS	N	1.87

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54657. These allow visual inspection of the internal detail of the map and identification of artifacts.

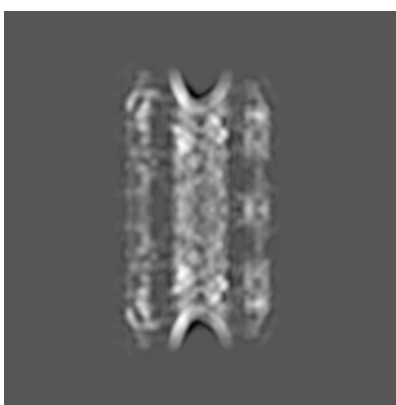
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

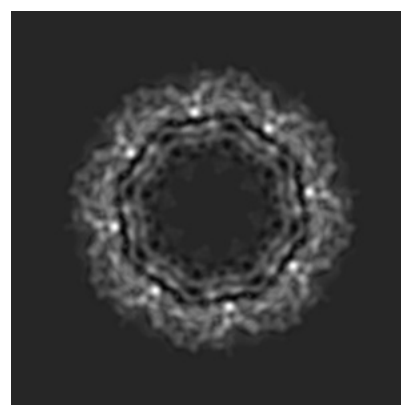
6.1.1 Primary map



X



Y



Z

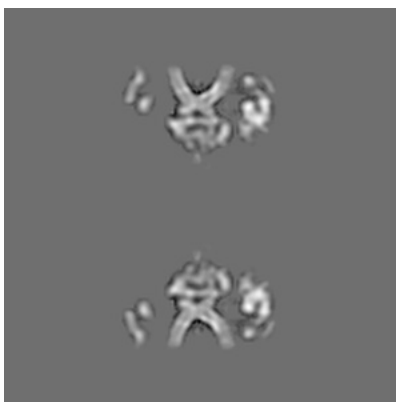
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

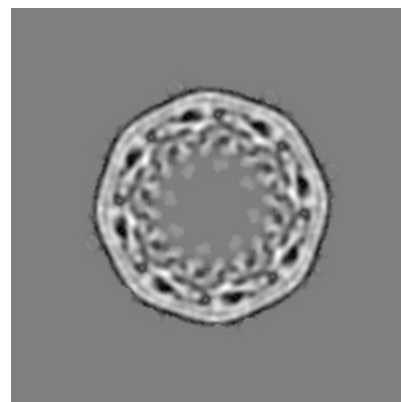
6.2.1 Primary map



X Index: 100



Y Index: 100



Z Index: 100

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

6.3 Largest variance slices [i](#)

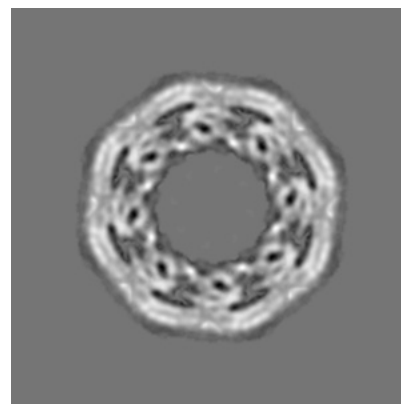
6.3.1 Primary map



X Index: 140



Y Index: 140

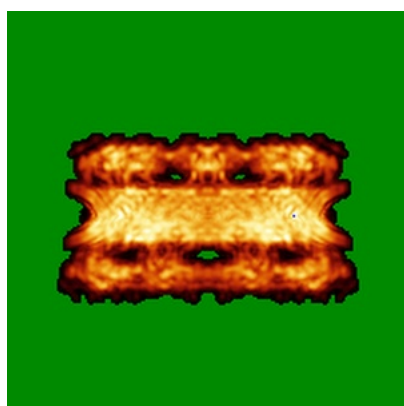


Z Index: 90

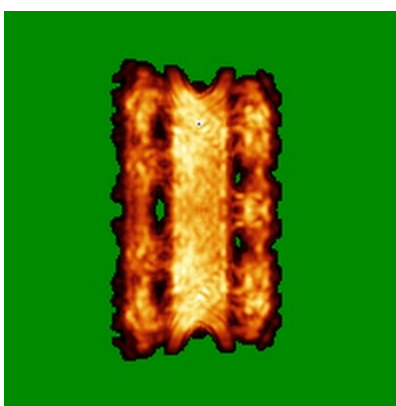
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

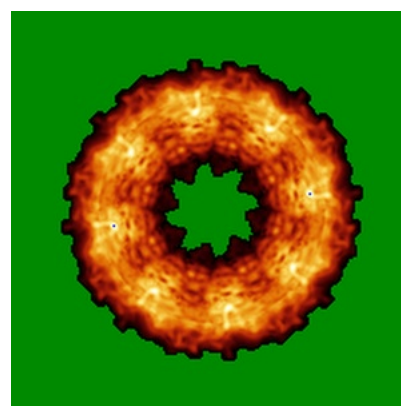
6.4.1 Primary map



X



Y

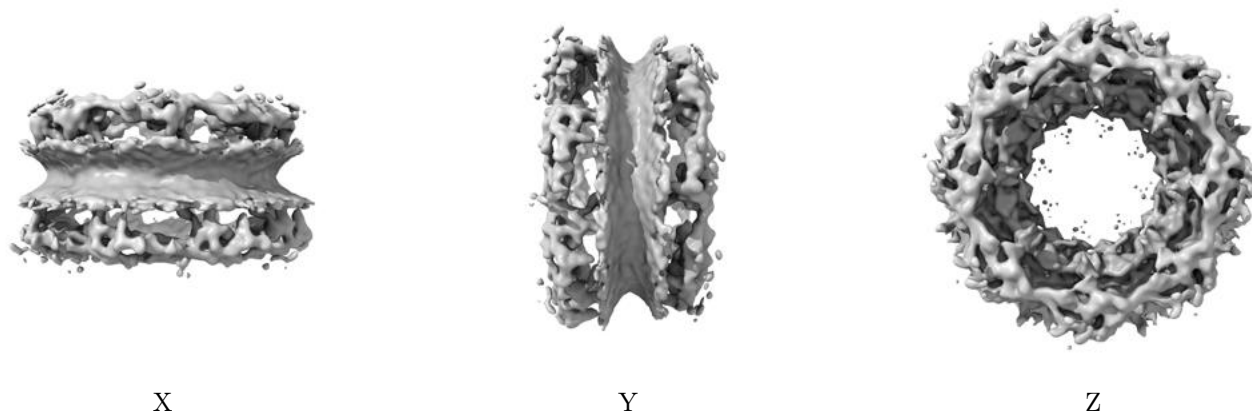


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

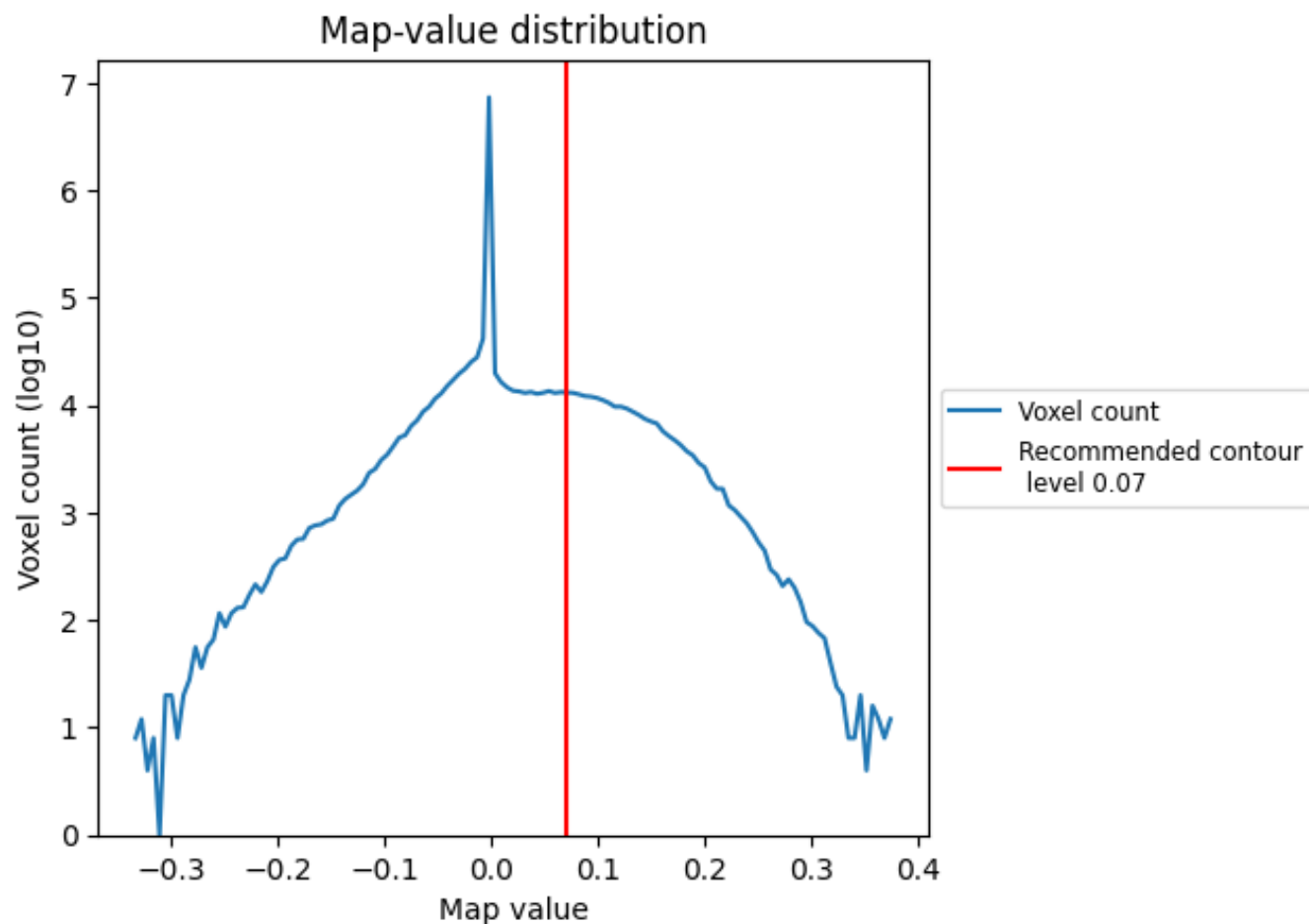
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

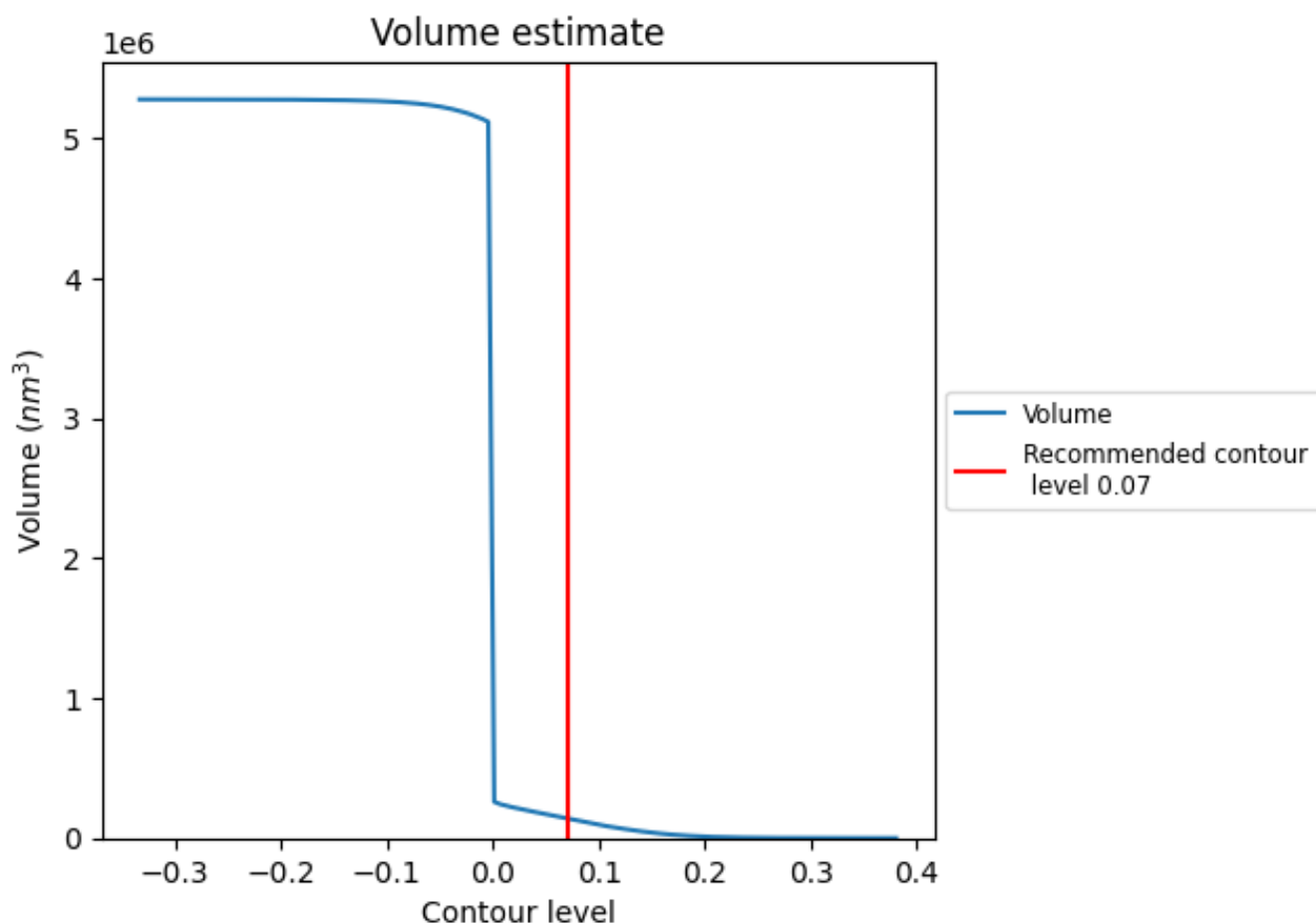
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

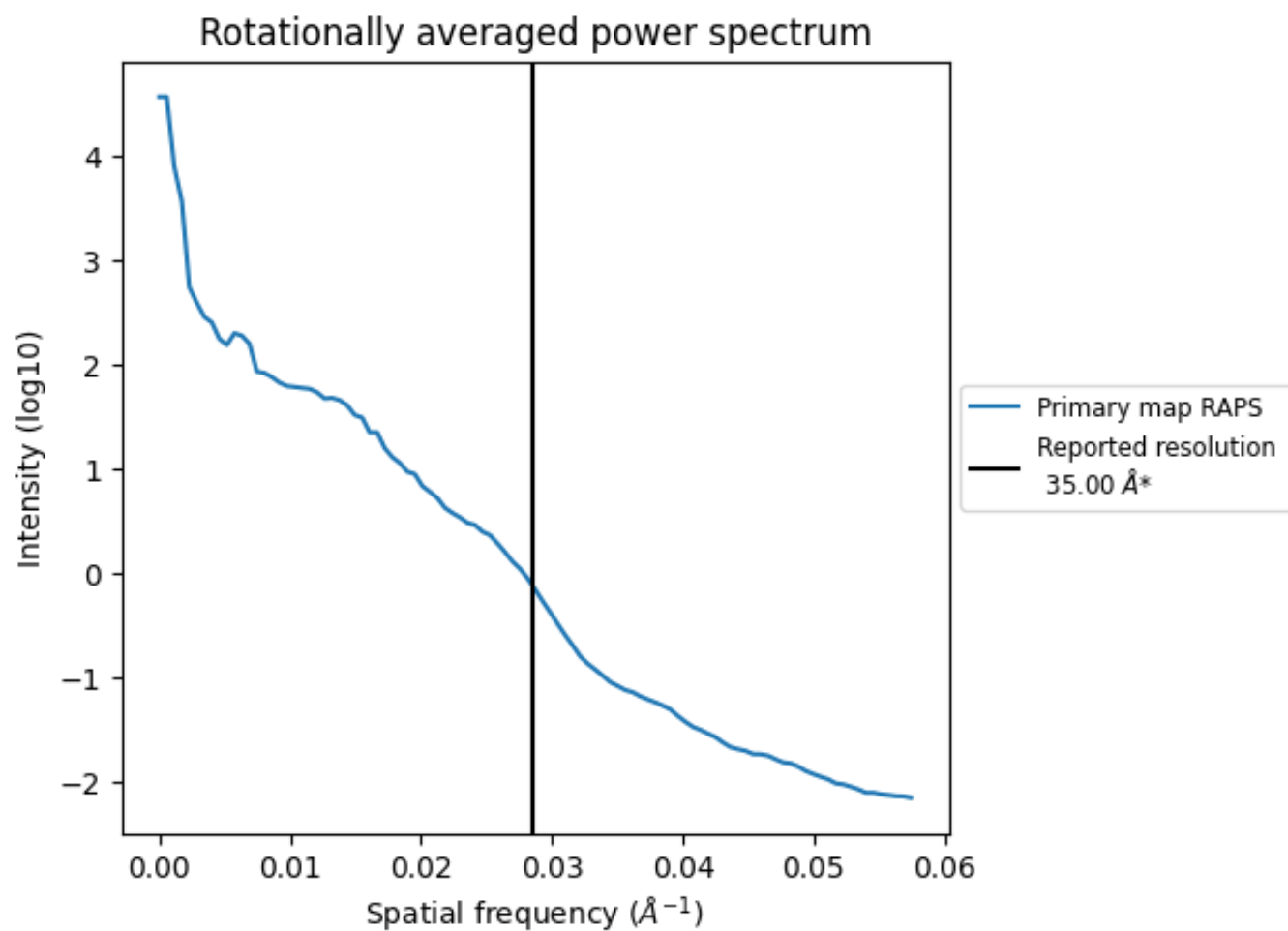
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 139608 nm³; this corresponds to an approximate mass of 126112 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.029 Å⁻¹

8 Fourier-Shell correlation

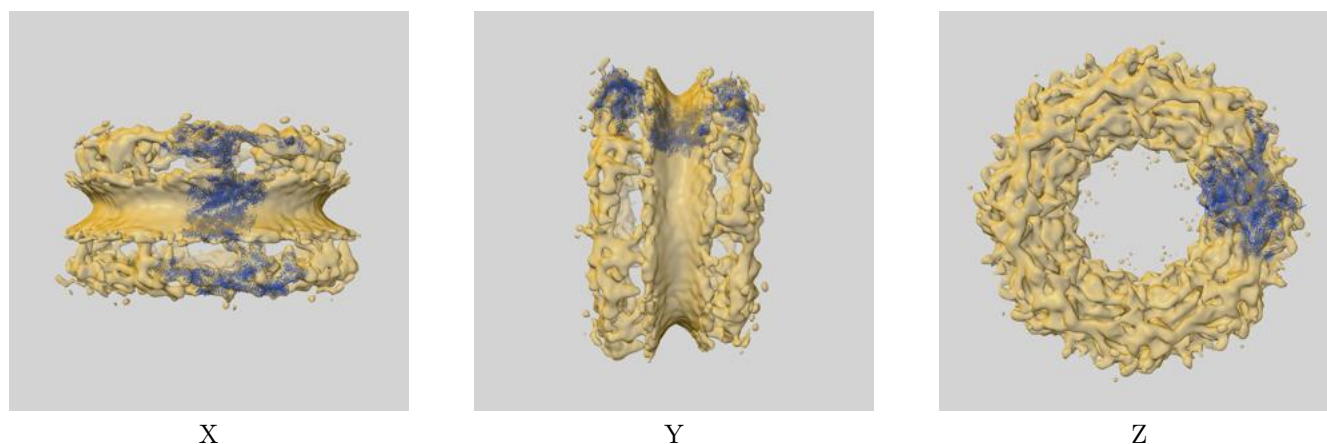
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit ⓘ

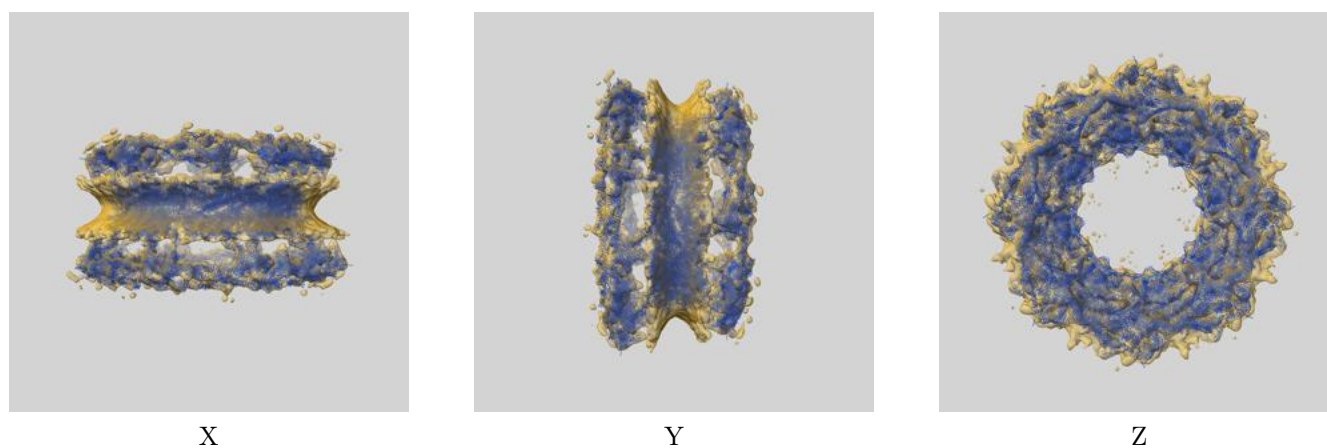
This section contains information regarding the fit between EMDB map EMD-54657 and PDB model 9SOB. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlays

9.1.1 Map-model overlay ⓘ

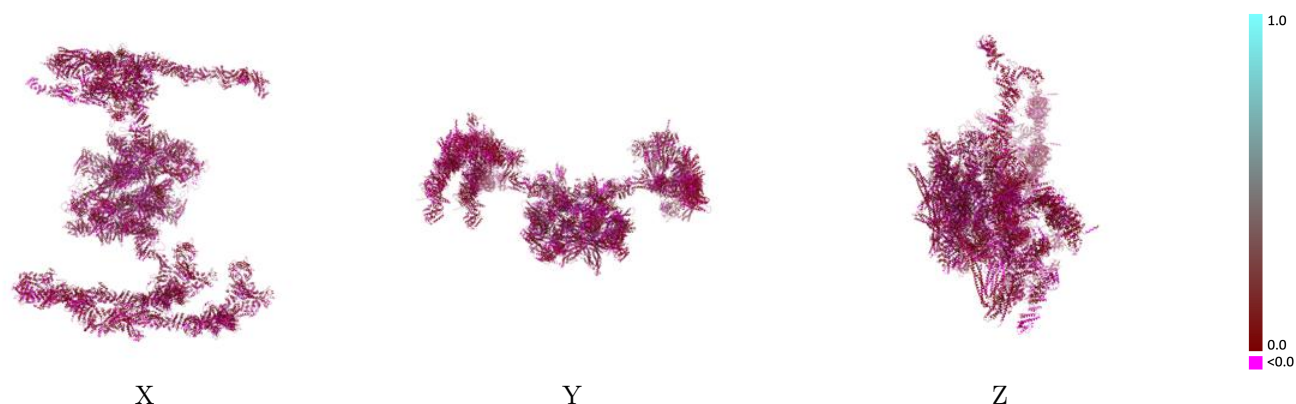


9.1.2 Map-model assembly overlay ⓘ



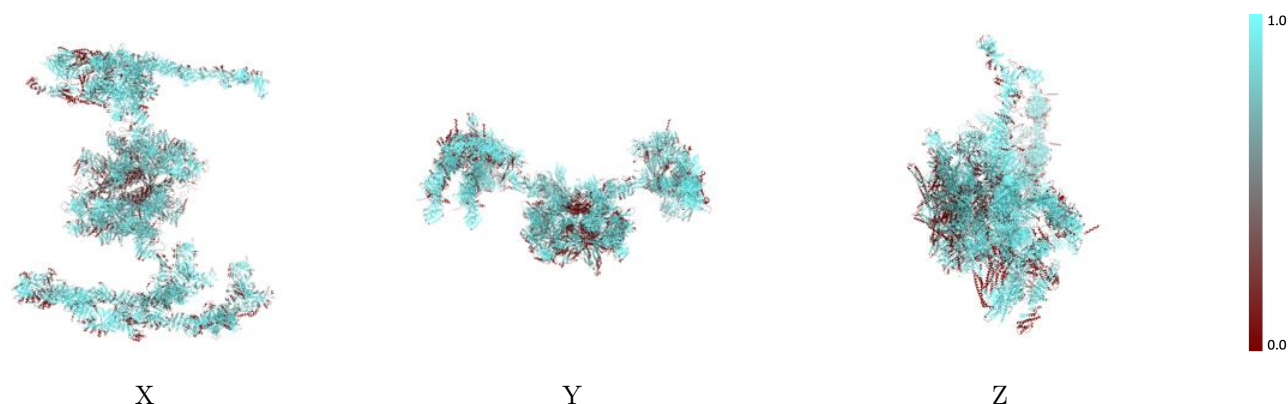
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



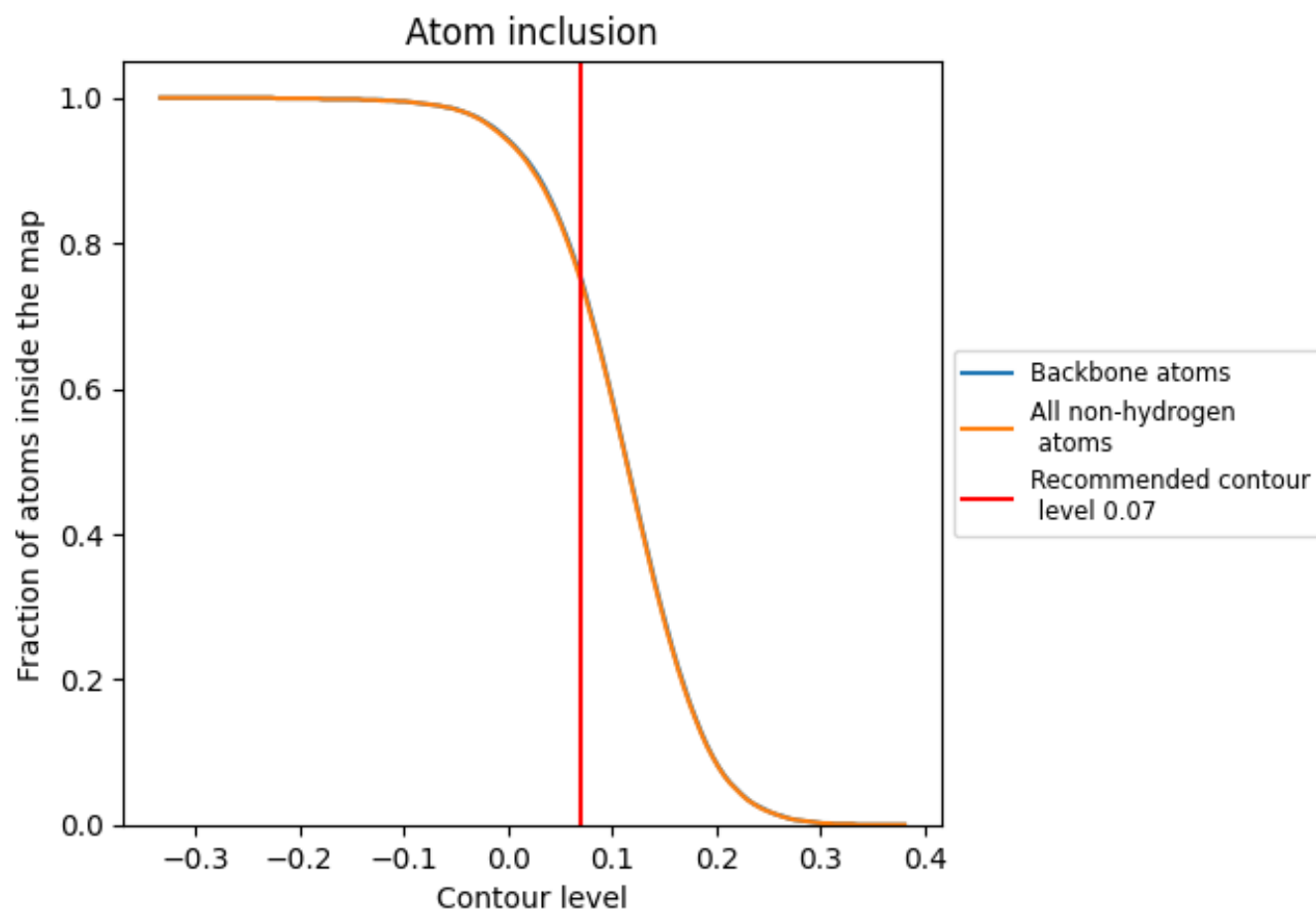
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.07).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 75% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7480	 0.0350
4	 0.8420	 0.0370
48	 0.8910	 0.0370
A	 0.5230	 0.0170
A16	 0.7680	 0.0370
A24	 0.6180	 0.0180
A32	 0.7450	 0.0350
A40	 0.6230	 0.0290
A48	 0.6960	 0.0400
A8	 0.9810	 0.0440
B	 0.6910	 0.0340
B8	 0.7400	 0.0350
C	 0.8060	 0.0340
C16	 0.5100	 0.0280
C24	 0.6970	 0.0300
C32	 0.8040	 0.0410
C8	 0.7490	 0.0370
D	 0.7880	 0.0320
D16	 0.7260	 0.0290
D24	 0.7400	 0.0260
D32	 0.7440	 0.0330
D40	 0.7880	 0.0360
D8	 0.6770	 0.0300
E	 0.9250	 0.0420
E8	 0.8990	 0.0260
F	 0.8570	 0.0250
F16	 0.8330	 0.0500
F24	 0.9230	 0.0260
F8	 0.8090	 -0.0060
H	 0.6330	 0.0390
H16	 0.4710	 0.0260
H24	 0.6750	 0.0350
H8	 0.3240	 0.0310
I	 0.5440	 0.0370
I16	 0.5770	 0.0310



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Chain	Atom inclusion	Q-score
I24	 0.6450	 0.0470
I8	 0.4490	 0.0230
J	 0.4350	 0.0320
J16	 0.7560	 0.0700
J24	 0.7140	 0.0420
J32	 0.6230	 0.0560
J8	 0.6470	 0.0580
K	 0.7940	 0.0400
K16	 0.8170	 0.0520
K8	 0.6200	 0.0310
L	 0.8160	 0.0450
L16	 0.7840	 0.0370
L8	 0.8380	 0.0370
M	 0.8920	 0.0450
M16	 0.7960	 0.0360
M8	 0.7930	 0.0400
N	 0.9880	 0.0350
N16	 0.8080	 0.0320
N8	 0.8520	 0.0260
O	 0.9760	 0.0380
O16	 0.9240	 0.0430
O8	 0.9770	 0.0460
P	 0.8200	 0.0340
P16	 0.8000	 0.0410
P8	 0.8740	 0.0440
Q	 0.8400	 0.0300
Q16	 0.7150	 0.0410
Q8	 0.8080	 0.0370
R	 0.8590	 0.0300
R16	 0.7130	 0.0360
R8	 0.8030	 0.0380
T	 0.8390	 0.0470
T16	 0.6860	 0.0300
T8	 0.8460	 0.0400
V	 0.5360	 0.0540
W	 0.7110	 0.0310