wwPDB EM Validation Summary Report

Nov 28, 2022 – 03:02 PM EST

PDB ID	:	7TBI
EMDB ID	:	EMD-10198
Title	:	Composite structure of the S. cerevisiae nuclear pore complex (NPC)
Authors	:	Petrovic, S.; Samanta, D.; Perriches, T.; Bley, C.J.; Thierbach, K.; Brown, B.; Nie, S.; Mobbs, G.W.; Stevens, T.A.; Liu, X.; Tomaleri, G.P.; Schaus, L.; Hoelz, A.
Deposited on	:	2021-12-22
Resolution	:	25.00 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

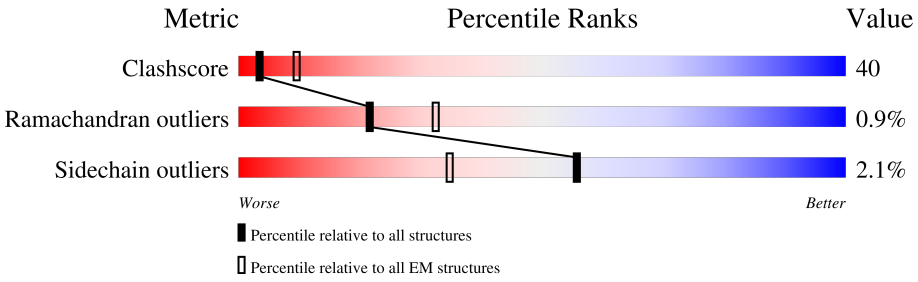
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 25.00 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.



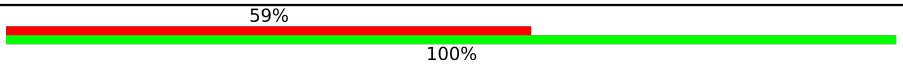
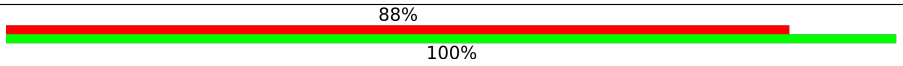
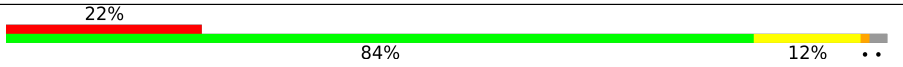
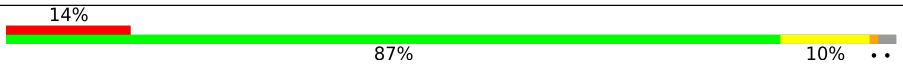
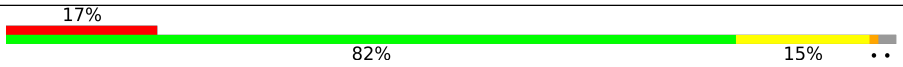
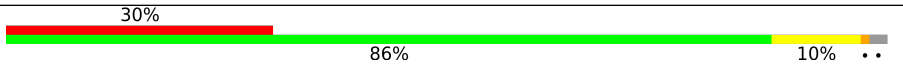
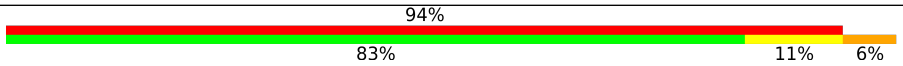
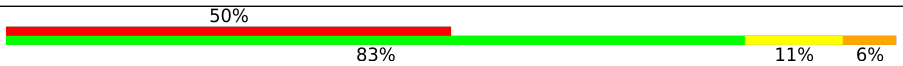
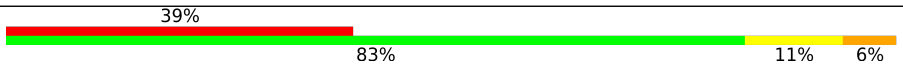
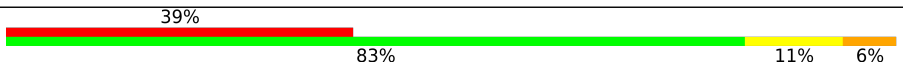
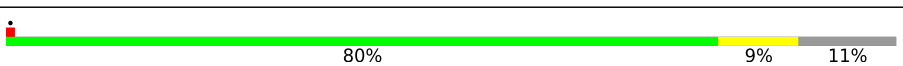
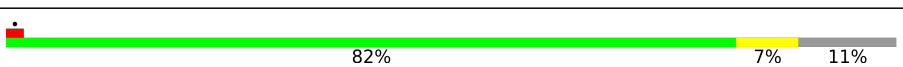
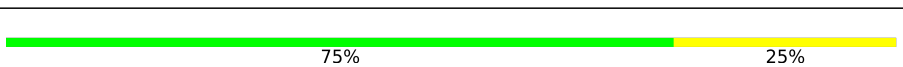
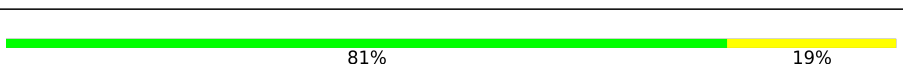
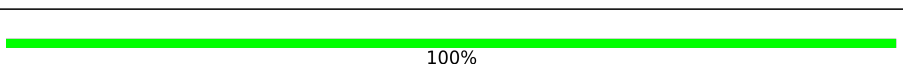
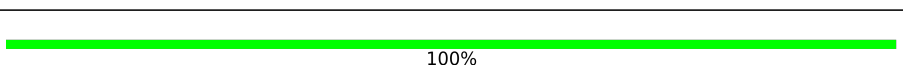
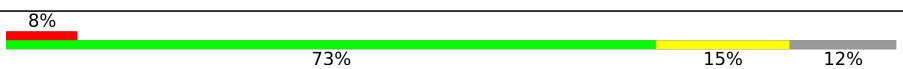
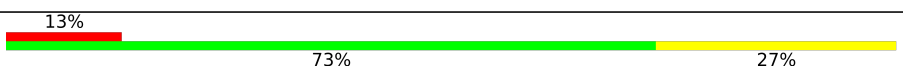
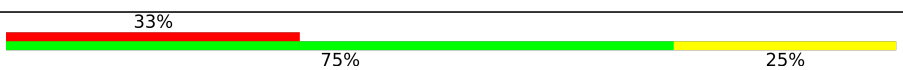
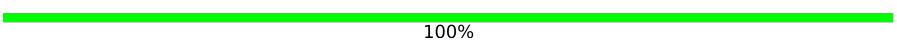
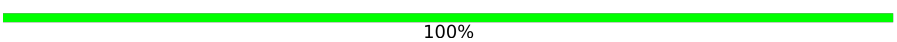
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	A1	1316	11% 87% 6% 7%
1	A2	1316	17% 87% 6% 6%
1	A3	1316	17% 87% 6% 6%
1	A4	1316	10% 87% 6% 7%
2	B1	14	57% 93% 7%
2	B2	14	93% 7%
2	B3	14	93% 7%
2	B4	14	36% 93% 7%

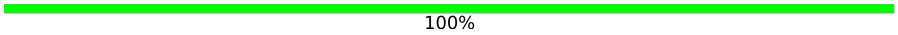
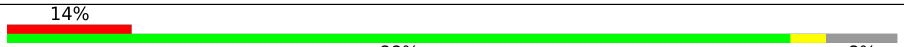
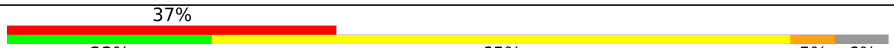
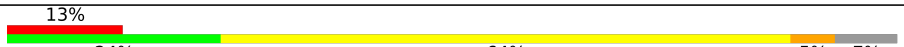
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C1	17	
3	C2	17	
3	C3	17	
3	C4	17	
4	D1	720	
4	D2	720	
4	D3	720	
4	D4	720	
5	E1	18	
5	E2	18	
5	E3	18	
5	E4	18	
6	F1	1848	
6	F2	1848	
7	G1	53	
7	G2	53	
8	H1	13	
8	H2	13	
9	I1	1756	
9	I2	1756	
10	J1	63	
10	J2	63	
11	K1	9	
11	K2	9	
12	L1	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
12	L2	2	
13	M1	183	
13	M2	183	
13	M3	183	
13	M4	183	
14	N1	222	
14	N2	222	
14	N3	222	
14	N4	222	
15	O1	241	
15	O2	241	
15	O3	241	
15	O4	241	
16	P1	40	
16	P2	40	
16	P3	40	
16	P4	40	
17	Q1	1100	
17	Q2	1100	
18	R1	720	
19	R2	726	
20	S1	621	
20	S2	621	
21	T1	286	
21	T2	286	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
22	U1	346	54% 34% 11%
22	U2	346	62% 26% 11%
23	V1	698	10% 68% 20% 11%
23	V2	698	67% 20% 11%
24	W1	1037	5% 69% 16% 14%
24	W2	1037	17% 71% 14% 14%
25	X1	187	40% 22% 51% 10% 12%
25	X2	187	10% 22% 51% 11% 12%
26	Y1	340	22% 14% 27% 13% 43%
26	Y2	340	9% 11% 30% 11% 5% 43%
27	Z1	713	8% 12% 40% 26% 7% 14%
27	Z2	713	10% 13% 39% 27% 7% 14%
28	a1	146	87% 94% 6%
28	a2	146	71% 94% 6%
29	b1	86	13% 53% 35% 9%
29	b2	86	7% 53% 35% 10%

2 Entry composition (i)

There are 29 unique types of molecules in this entry. The entry contains 221308 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 Nup157/Nup170.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A2	1231	Total	C	N	O	S	1	0
			9730	6152	1707	1843	28		
1	A3	1231	Total	C	N	O	S	1	0
			9730	6152	1707	1843	28		
1	A4	1227	Total	C	N	O	S	1	0
			9703	6135	1703	1838	27		
1	A1	1227	Total	C	N	O	S	1	0
			9703	6135	1703	1838	27		

- Molecule 2 is a protein called Nup53/Nup59 R3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B1	14	Total	C	N	O	S	0	0
			111	73	19	18	1		
2	B2	14	Total	C	N	O	S	0	0
			111	73	19	18	1		
2	B3	14	Total	C	N	O	S	0	0
			111	73	19	18	1		
2	B4	14	Total	C	N	O	S	0	0
			111	73	19	18	1		

- Molecule 3 is a protein called Nup145N/Nup100/Nup116 R3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C2	17	Total	C	N	O	S	0	0
			138	88	24	25	1		
3	C3	17	Total	C	N	O	S	0	0
			138	88	24	25	1		
3	C1	17	Total	C	N	O	S	0	0
			138	88	24	25	1		
3	C4	17	Total	C	N	O	S	0	0
			138	88	24	25	1		

- Molecule 4 is a protein called Nic96 SOL.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D1	703	Total	C	N	O	S	1	0
			5589	3520	999	1036	34		
4	D2	703	Total	C	N	O	S	1	0
			5589	3520	999	1036	34		
4	D3	703	Total	C	N	O	S	1	0
			5589	3520	999	1036	34		
4	D4	703	Total	C	N	O	S	1	0
			5589	3520	999	1036	34		

- Molecule 5 is a protein called Nup53/Nup59 R2.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E1	18	Total	C	N	O	0	0
			137	88	22	27		
5	E2	18	Total	C	N	O	0	0
			137	88	22	27		
5	E3	18	Total	C	N	O	0	0
			137	88	22	27		
5	E4	18	Total	C	N	O	0	0
			137	88	22	27		

- Molecule 6 is a protein called Nup188.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F1	1641	Total	C	N	O	S	0	0
			12779	8190	2201	2333	55		
6	F2	1641	Total	C	N	O	S	0	0
			12779	8190	2201	2333	55		

- Molecule 7 is a protein called Nic96 R2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G1	53	Total	C	N	O	S	0	0
			438	274	75	88	1		
7	G2	53	Total	C	N	O	S	0	0
			438	274	75	88	1		

- Molecule 8 is a protein called Nup145N/Nup100/Nup116 R2.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	H1	13	Total	C	N	O	0	0
			94	58	15	21		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
8	H2	13	Total 94	C 58	N 15	O 21	0	0

- Molecule 9 is a protein called Nup192.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I1	1542	Total 12307	C 7880	N 2084	O 2278	S 65	0	0
9	I2	1542	Total 12307	C 7880	N 2084	O 2278	S 65	0	0

- Molecule 10 is a protein called Nic96 R2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J1	63	Total 504	C 315	N 86	O 102	S 1	0	0
10	J2	63	Total 504	C 315	N 86	O 102	S 1	0	0

- Molecule 11 is a protein called Nup145N/Nup100/Nup116 R1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K1	9	Total 73	C 51	N 10	O 11	S 1	0	0
11	K2	9	Total 73	C 51	N 10	O 11	S 1	0	0

- Molecule 12 is a protein called Nup53/Nup59 R1.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	L1	2	Total 15	C 11	N 2	O 2	0	0
12	L2	2	Total 15	C 11	N 2	O 2	0	0

- Molecule 13 is a protein called Nsp1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M1	169	Total 1372	C 855	N 235	O 276	S 6	0	0
13	M2	169	Total 1372	C 855	N 235	O 276	S 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M3	169	Total	C	N	O	S	0	0
			1372	855	235	276	6		
13	M4	169	Total	C	N	O	S	0	0
			1372	855	235	276	6		

- Molecule 14 is a protein called Nup57.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N1	180	Total	C	N	O	S	0	0
			1401	876	236	282	7		
14	N2	180	Total	C	N	O	S	0	0
			1401	876	236	282	7		
14	N3	180	Total	C	N	O	S	0	0
			1401	876	236	282	7		
14	N4	180	Total	C	N	O	S	0	0
			1401	876	236	282	7		

- Molecule 15 is a protein called Nup49.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O1	241	Total	C	N	O	S	0	0
			1971	1239	360	368	4		
15	O2	241	Total	C	N	O	S	0	0
			1971	1239	360	368	4		
15	O3	241	Total	C	N	O	S	0	0
			1971	1239	360	368	4		
15	O4	241	Total	C	N	O	S	0	0
			1971	1239	360	368	4		

- Molecule 16 is a protein called Nic96 R1.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	P1	40	Total	C	N	O	0	0
			311	195	59	57		
16	P2	40	Total	C	N	O	0	0
			311	195	59	57		
16	P3	40	Total	C	N	O	0	0
			311	195	59	57		
16	P4	40	Total	C	N	O	0	0
			311	195	59	57		

- Molecule 17 is a protein called Nup133.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q1	1031	Total 8392	C 5405	N 1357	O 1606	S 24	0	0
17	Q2	1027	Total 8359	C 5382	N 1352	O 1601	S 24	0	0

- Molecule 18 is a protein called Nup84.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R1	669	Total 5448	C 3496	N 892	O 1043	S 17	0	0

- Molecule 19 is a protein called Nup84.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R2	622	Total 5069	C 3262	N 822	O 970	S 15	0	0

- Molecule 20 is a protein called Nup145C.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S1	511	Total 3805	C 2417	N 648	O 730	S 10	0	0
20	S2	511	Total 3805	C 2417	N 648	O 730	S 10	0	0

- Molecule 21 is a protein called Sec13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T1	274	Total 2160	C 1379	N 369	O 409	S 3	0	0
21	T2	274	Total 2160	C 1379	N 369	O 409	S 3	0	0

- Molecule 22 is a protein called Seh1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U1	307	Total 2438	C 1543	N 422	O 462	S 11	0	0
22	U2	307	Total 2438	C 1543	N 422	O 462	S 11	0	0

- Molecule 23 is a protein called Nup85.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V1	620	Total	C	N	O	S	0	0
			4535	2884	753	877	21		
23	V2	620	Total	C	N	O	S	0	0
			4535	2884	753	877	21		

- Molecule 24 is a protein called Nup120.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W1	896	Total	C	N	O	S	0	0
			6622	4232	1099	1275	16		
24	W2	896	Total	C	N	O	S	0	0
			6622	4232	1099	1275	16		

- Molecule 25 is a protein called Nsp1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X1	164	Total	C	N	O	S	0	0
			1321	817	221	282	1		
25	X2	164	Total	C	N	O	S	0	0
			1321	817	221	282	1		

- Molecule 26 is a protein called Nup159.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y1	195	Total	C	N	O	S	0	0
			1590	1013	269	300	8		
26	Y2	195	Total	C	N	O	S	0	0
			1590	1013	269	300	8		

- Molecule 27 is a protein called Nup82.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z1	610	Total	C	N	O	S	0	0
			4990	3182	826	965	17		
27	Z2	610	Total	C	N	O	S	0	0
			4990	3182	826	965	17		

- Molecule 28 is a protein called Nup116 CTD.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	a1	146	Total	C	N	O	S	Se	0	0
			1165	745	204	212	3	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf	Trace
28	a2	146	Total 1165	C 745	N 204	O 212	S 3	Se 1	0	0

- Molecule 29 is a protein called Dyn2.

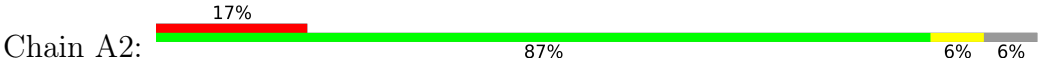
Mol	Chain	Residues	Atoms				AltConf	Trace
29	b1	86	Total 691	C 453	N 111	O 127	0	0
29	b2	86	Total 691	C 453	N 111	O 127	0	0

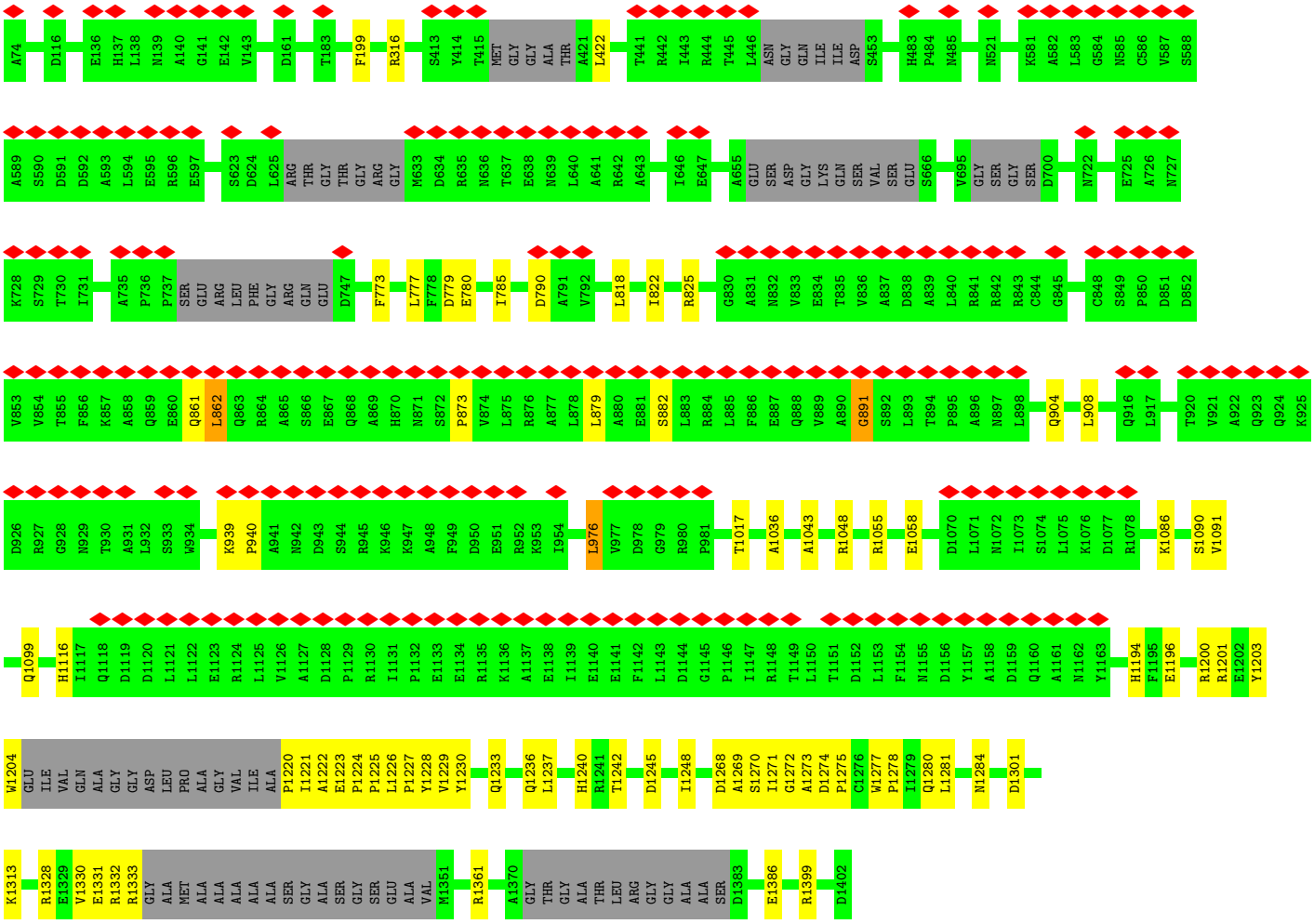
3 Residue-property plots (i)

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

• Molecule 1: Nup157/Nup170

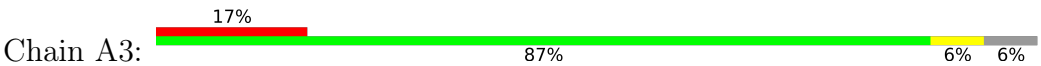
Chain A2:

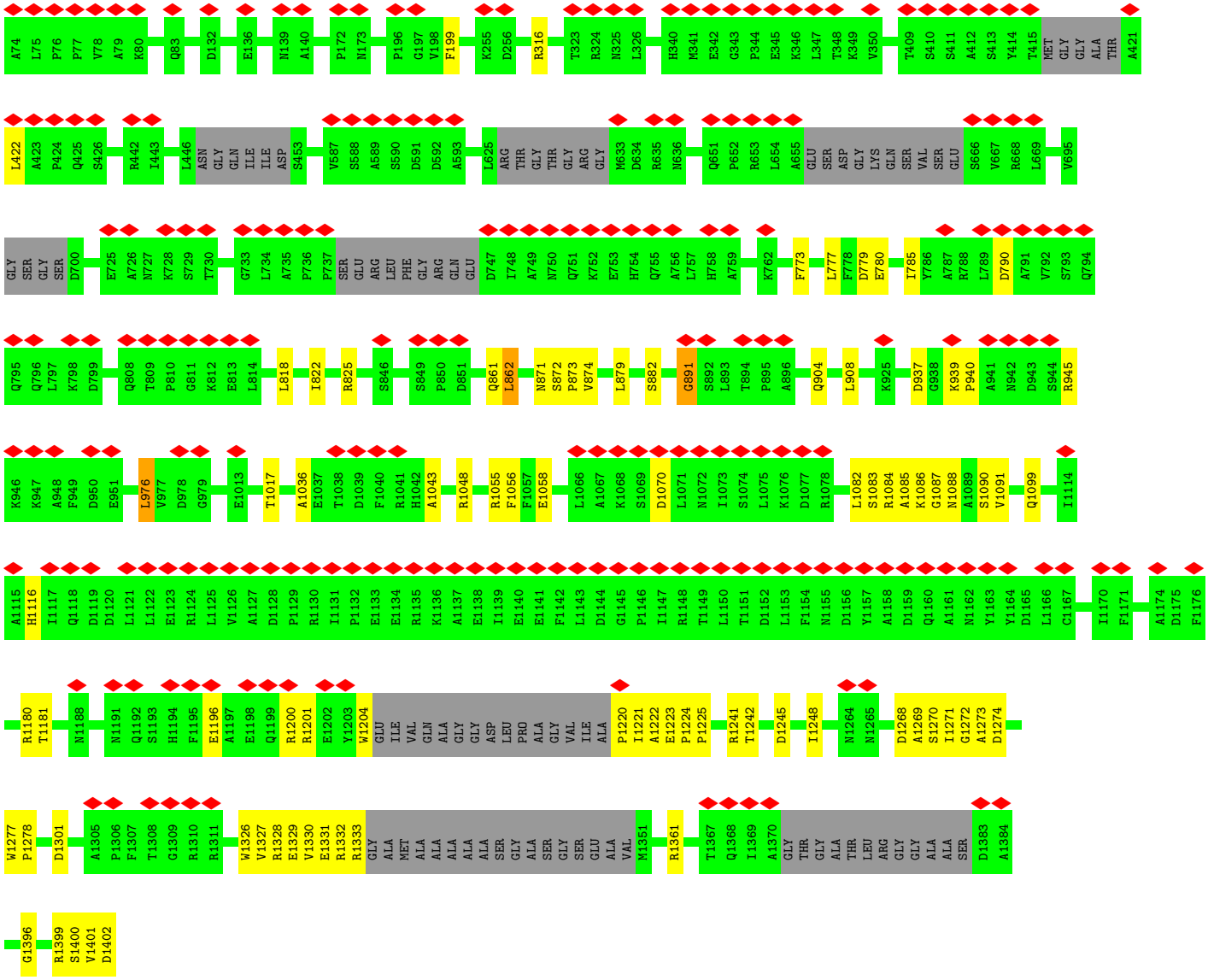




• Molecule 1: Nup157/Nup170

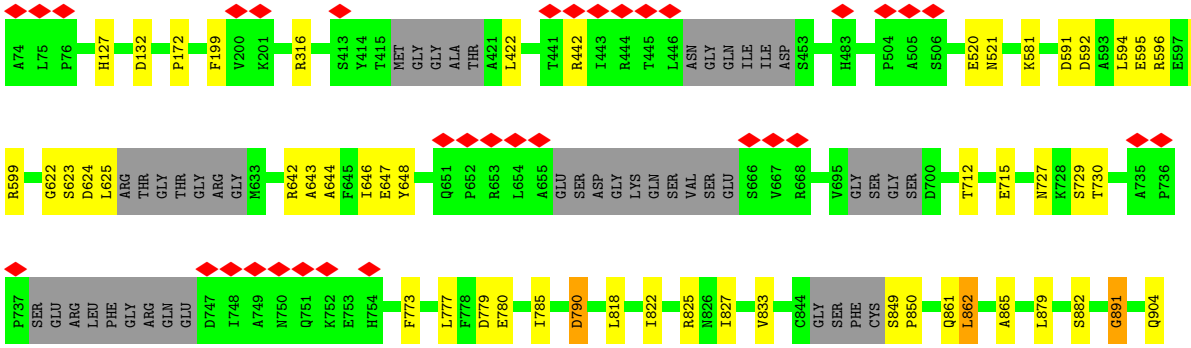
Chain A3:

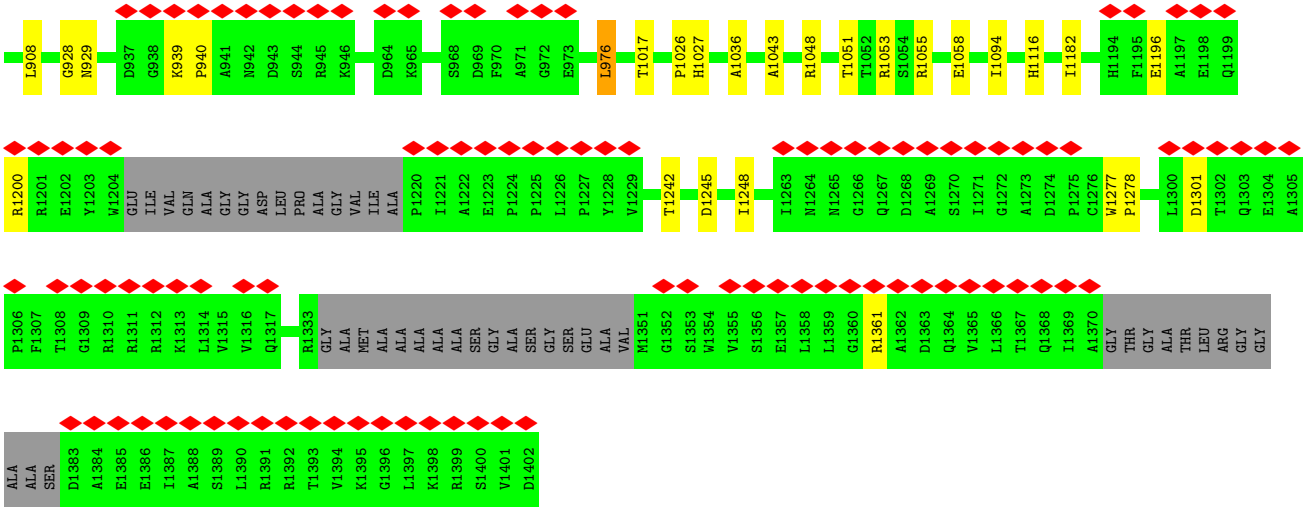




- Molecule 1: Nup157/Nup170

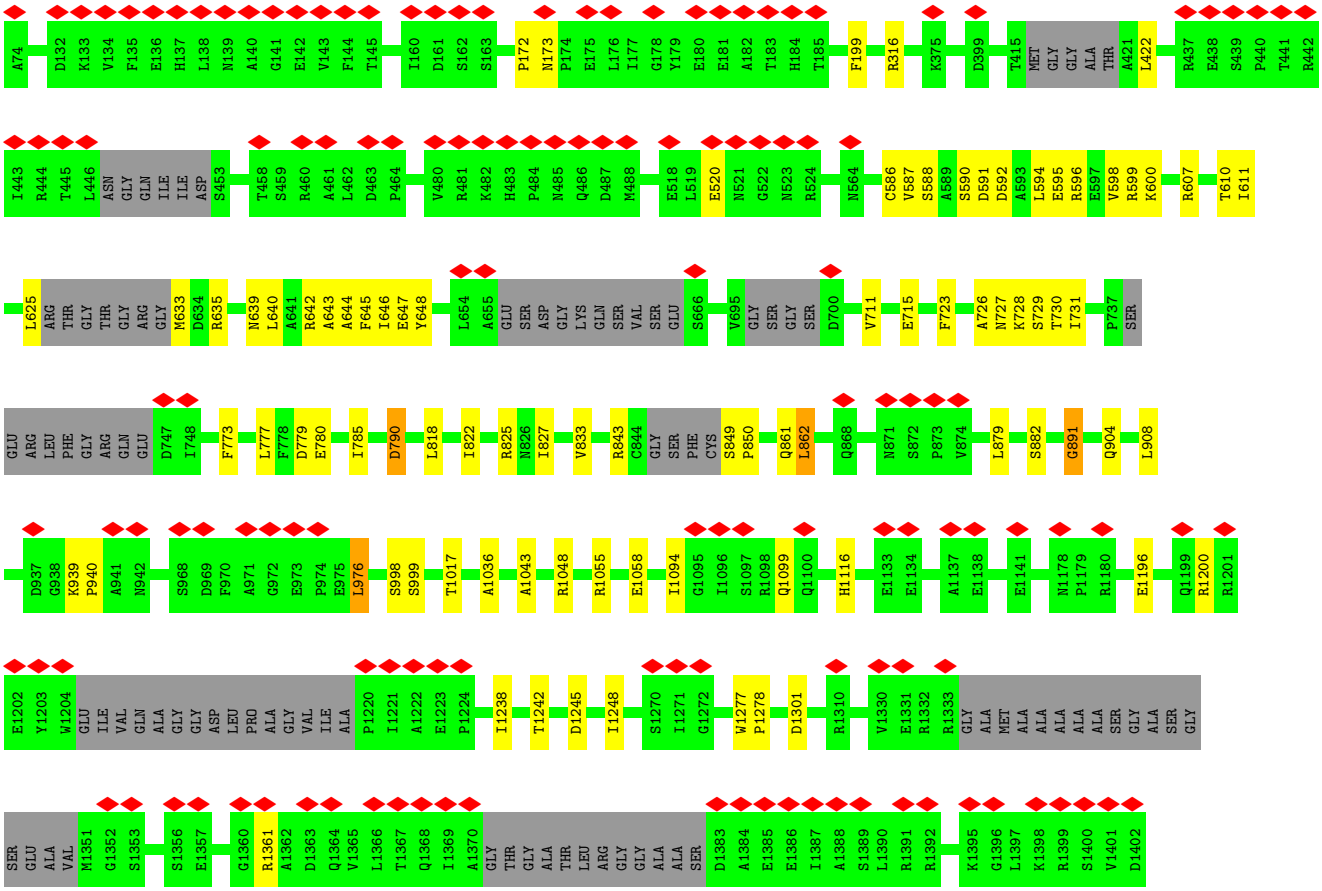
Chain A4:





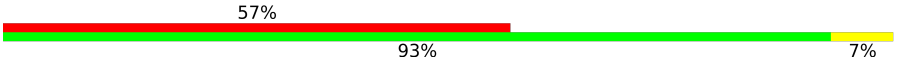
• Molecule 1: Nup157/Nup170

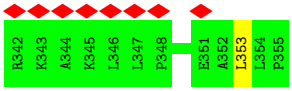
Chain A1:



• Molecule 2: Nup53/Nup59 R3

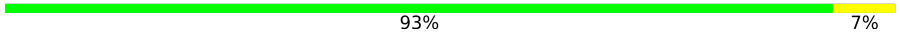
Chain B1:





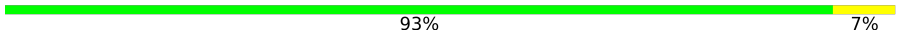
• Molecule 2: Nup53/Nup59 R3

Chain B2:



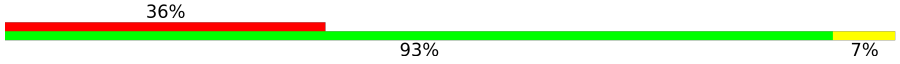
• Molecule 2: Nup53/Nup59 R3

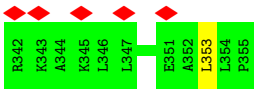
Chain B3:



• Molecule 2: Nup53/Nup59 R3

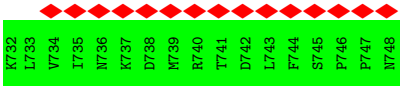
Chain B4:





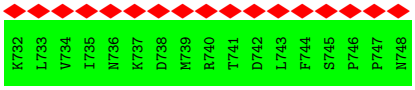
• Molecule 3: Nup145N/Nup100/Nup116 R3

Chain C2:



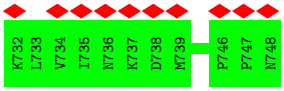
• Molecule 3: Nup145N/Nup100/Nup116 R3

Chain C3:



• Molecule 3: Nup145N/Nup100/Nup116 R3

Chain C1:



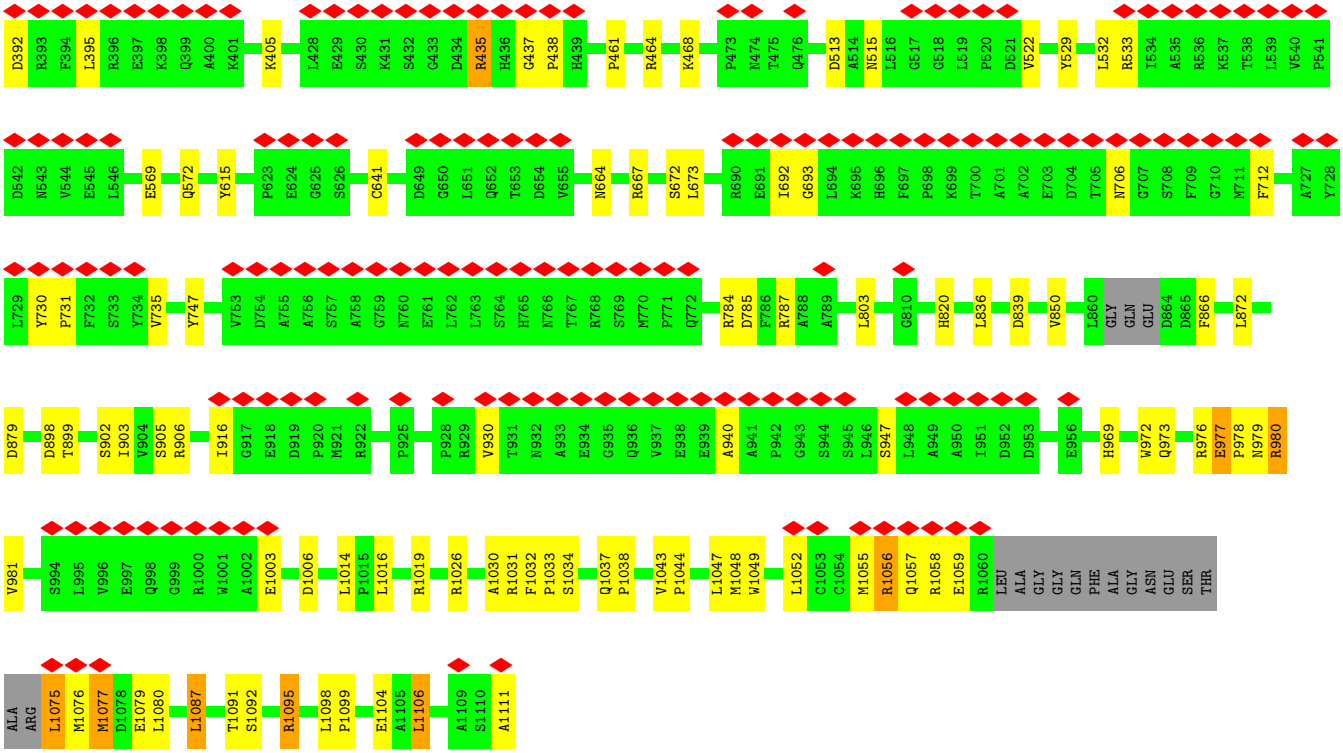
• Molecule 3: Nup145N/Nup100/Nup116 R3

Chain C4:

There are no outlier residues recorded for this chain.

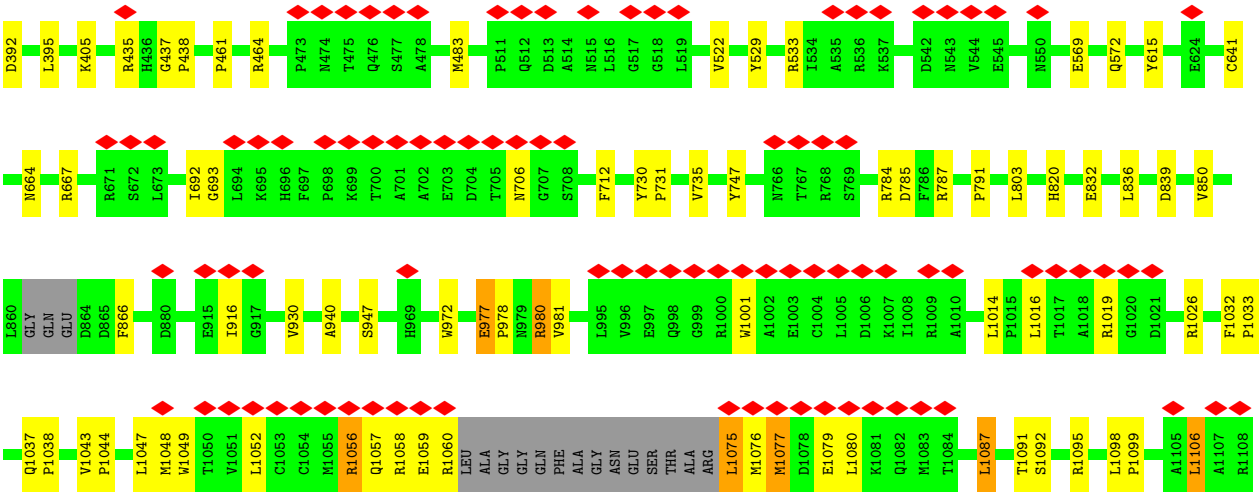
• Molecule 4: Nic96 SOL

Chain D1:



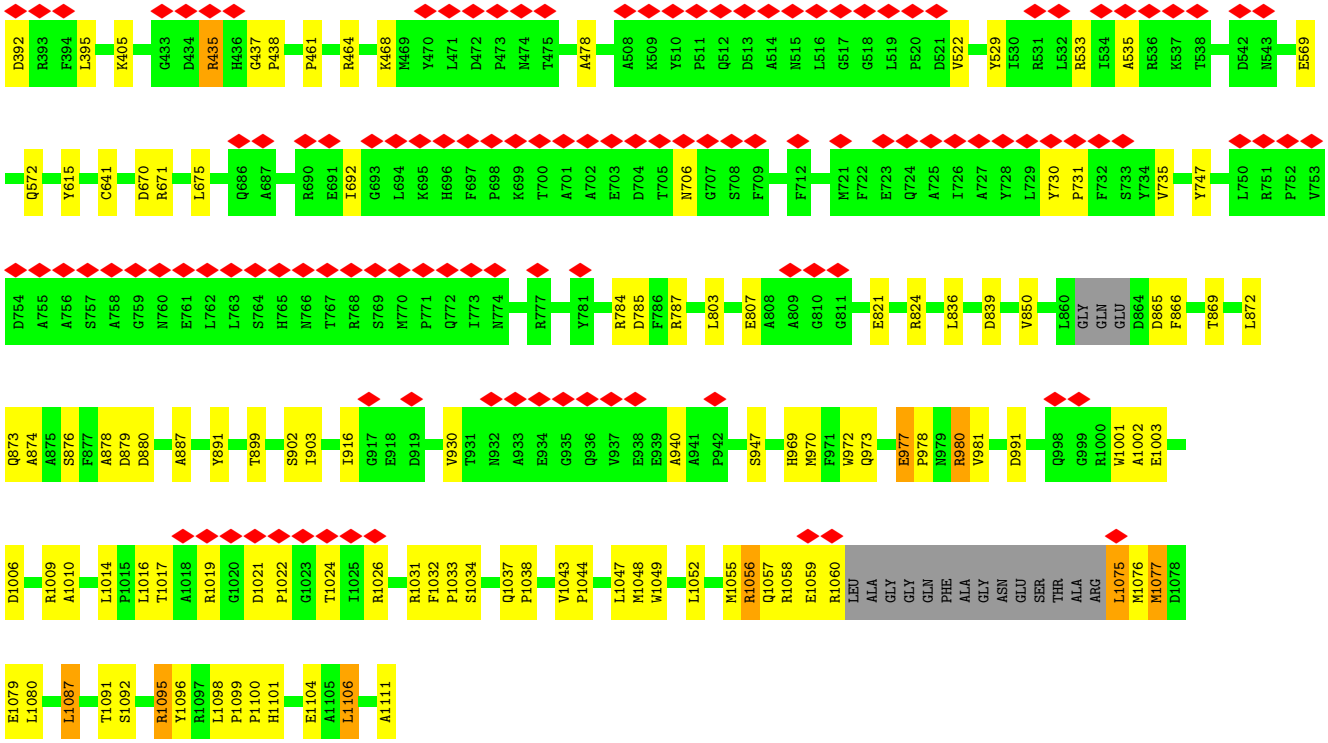
• Molecule 4: Nic96 SOL

Chain D2:



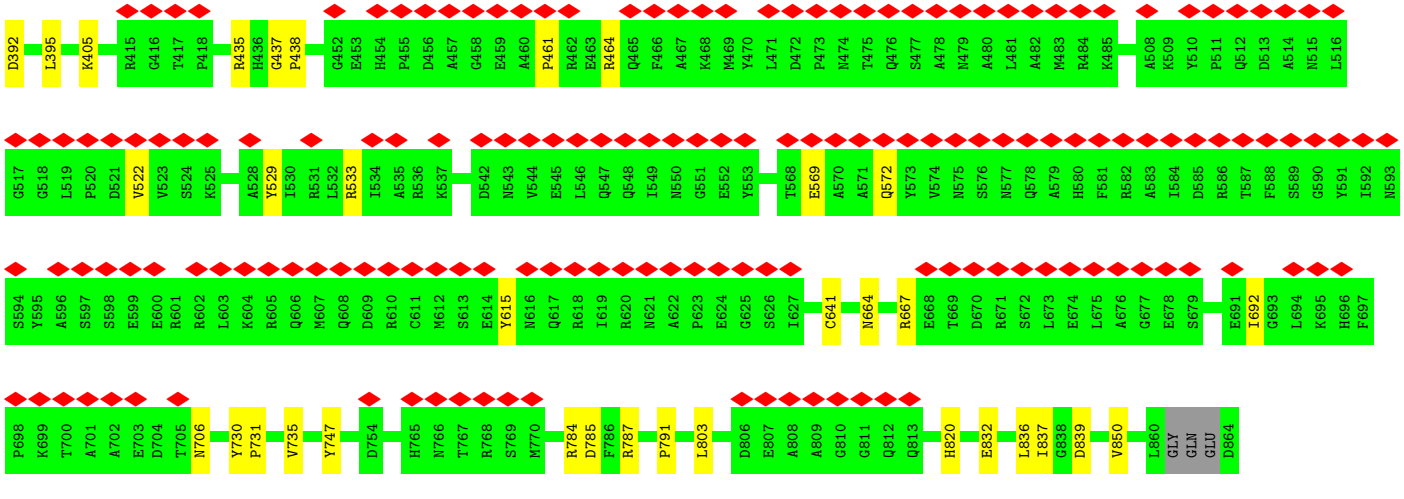
• Molecule 4: Nic96 SOL

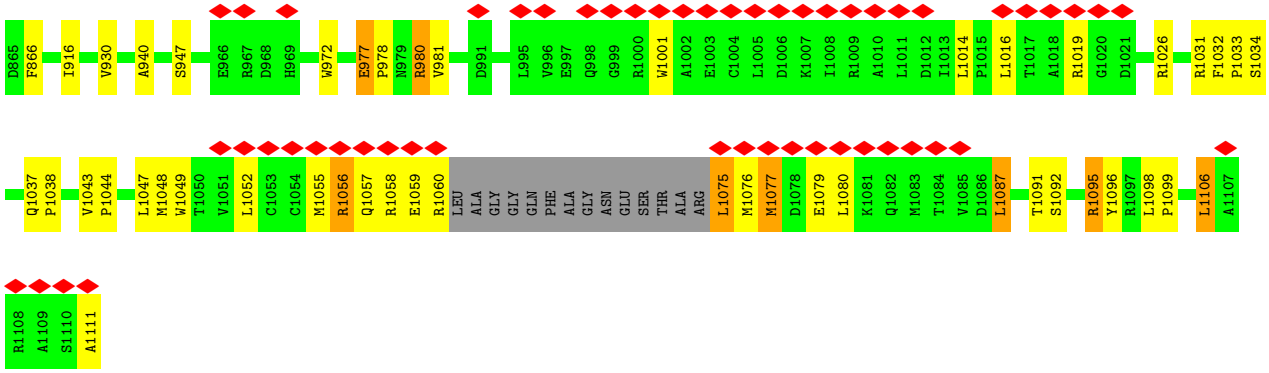
Chain D3:



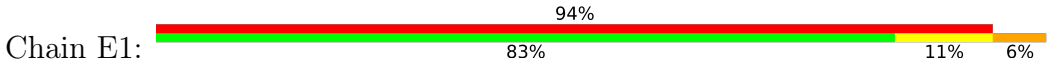
• Molecule 4: Nic96 SOL

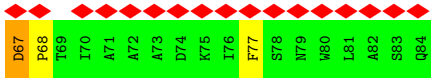
Chain D4:



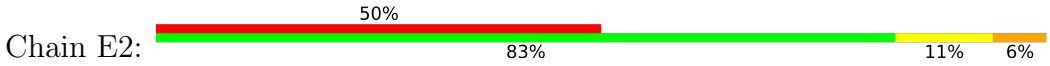


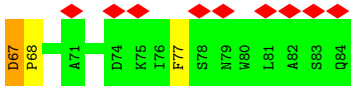
• Molecule 5: Nup53/Nup59 R2



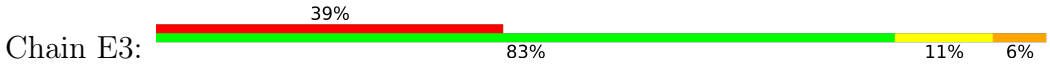


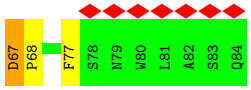
• Molecule 5: Nup53/Nup59 R2



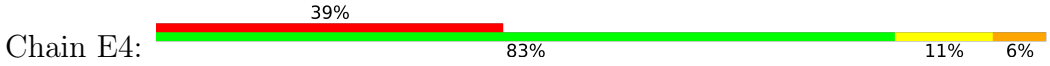


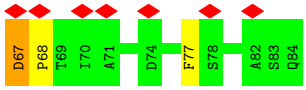
• Molecule 5: Nup53/Nup59 R2



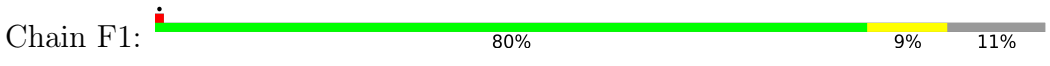


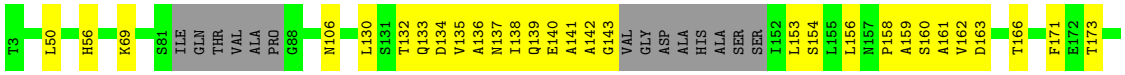
• Molecule 5: Nup53/Nup59 R2

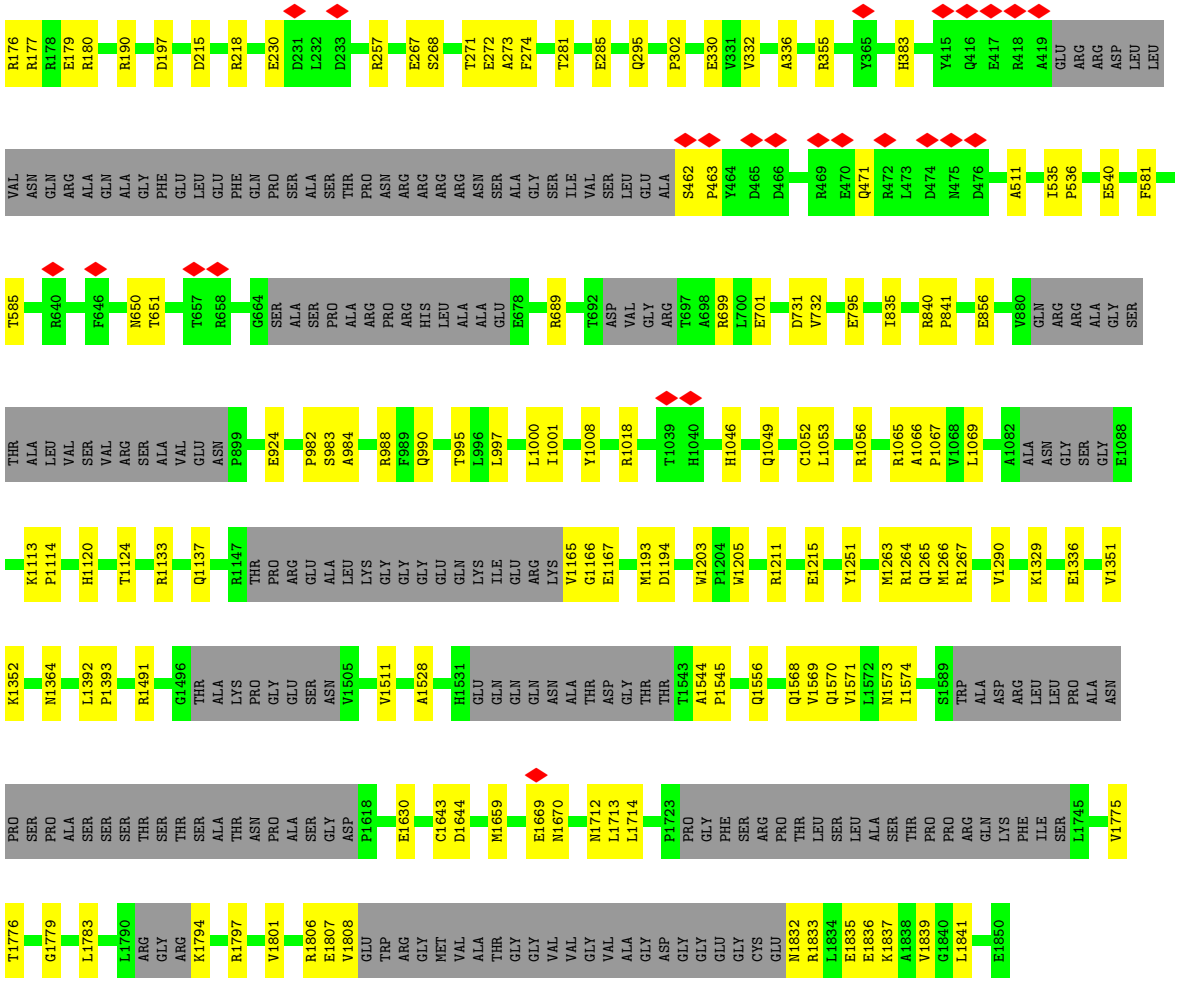




• Molecule 6: Nup188

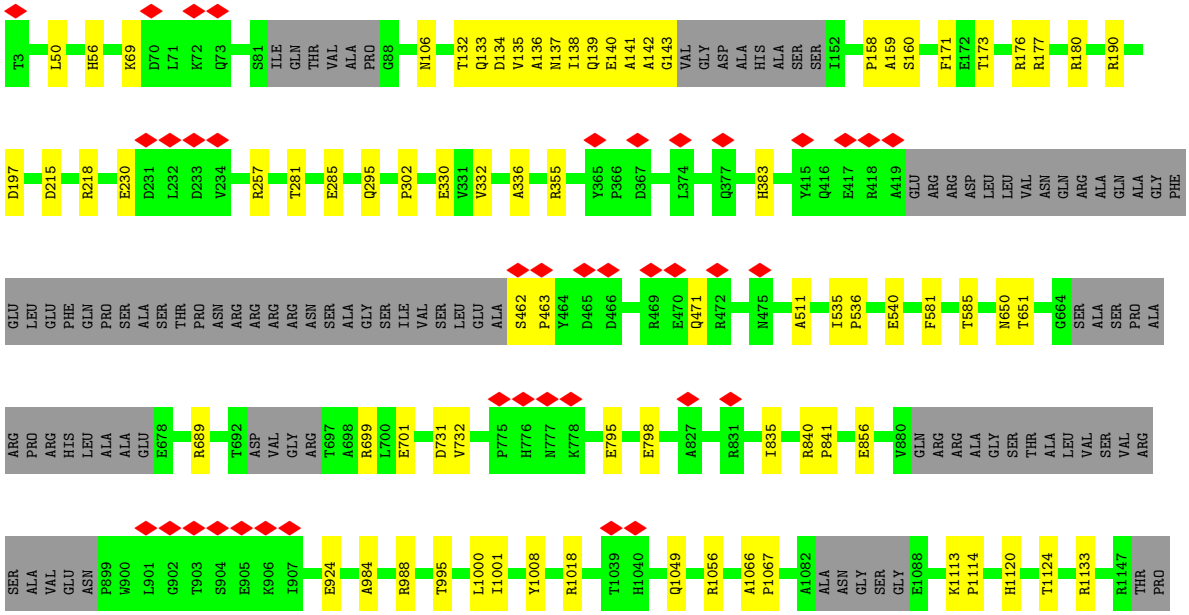


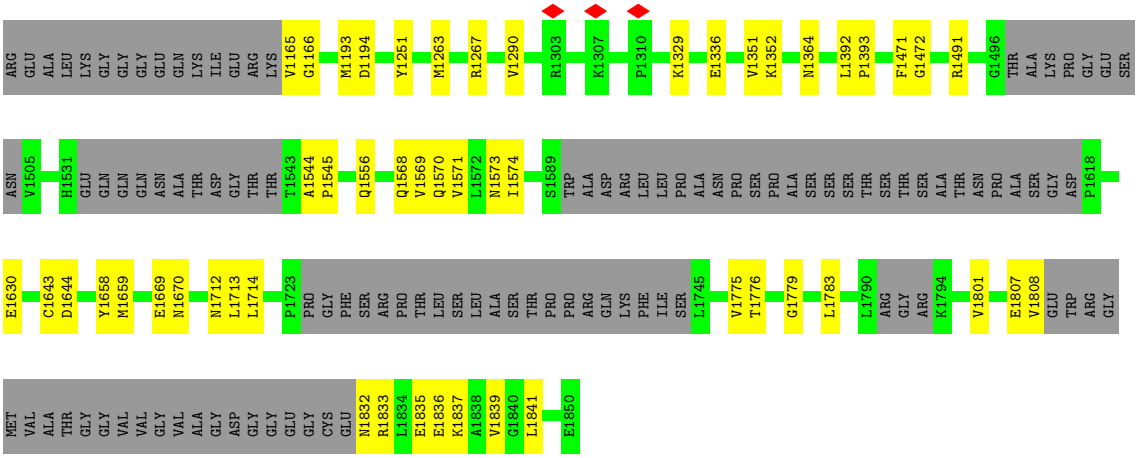




• Molecule 6: Nup188

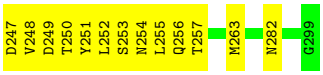
Chain F2:





• Molecule 7: Nic96 R2

Chain G1:

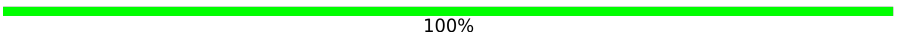


• Molecule 7: Nic96 R2

Chain G2:

• Molecule 8: Nup145N/Nup100/Nup116 R2

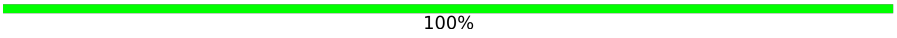
Chain H1:



There are no outlier residues recorded for this chain.

• Molecule 8: Nup145N/Nup100/Nup116 R2

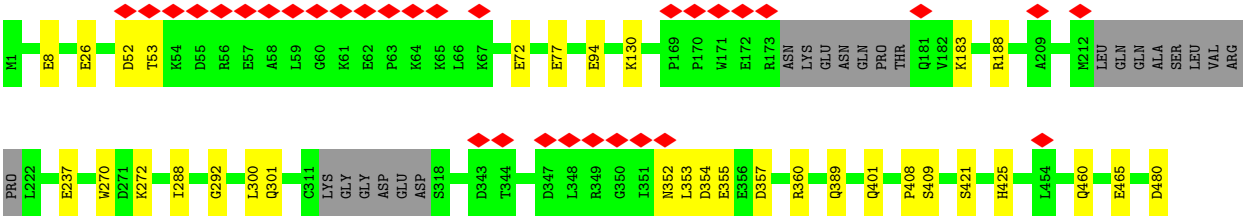
Chain H2:

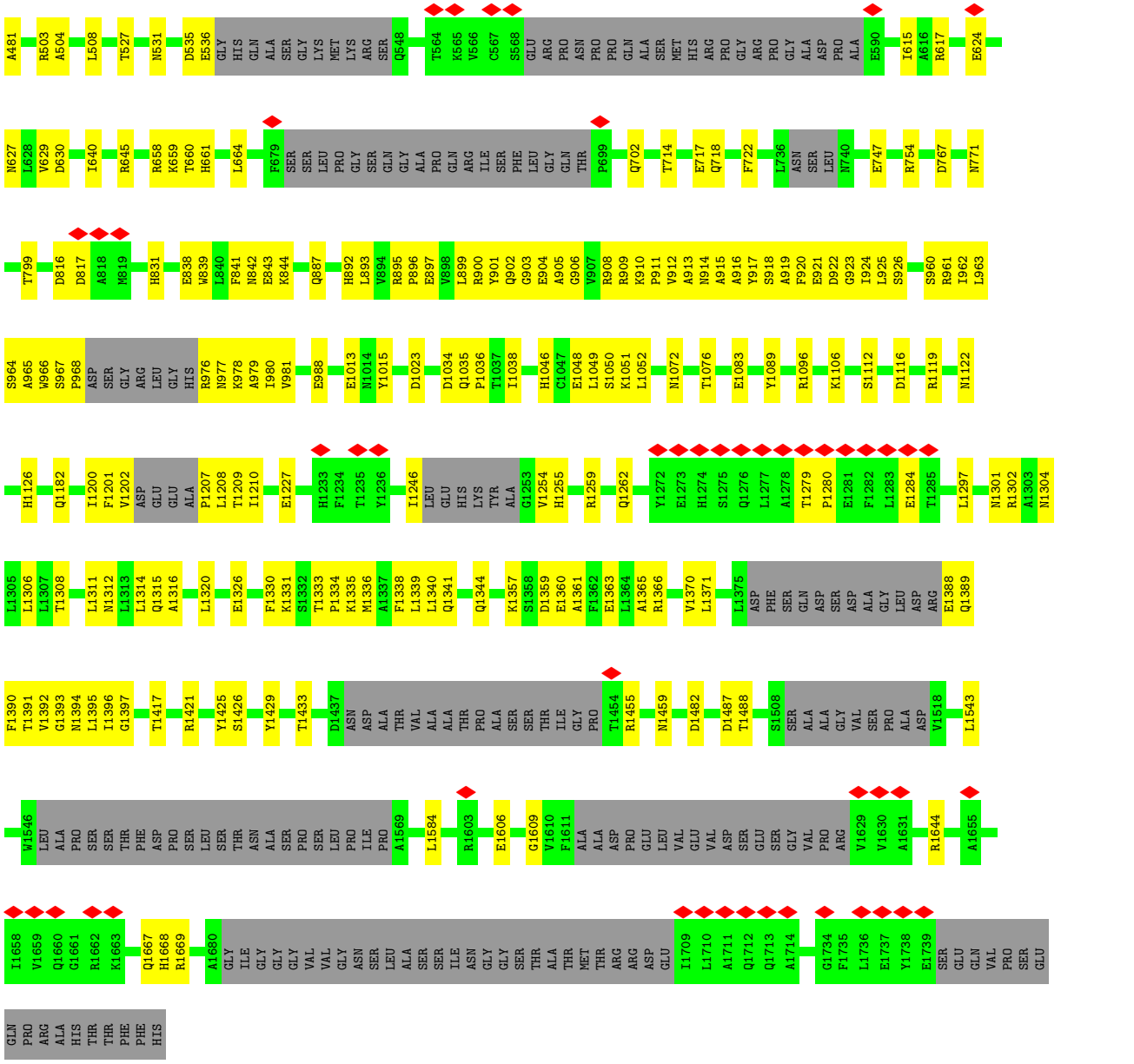


There are no outlier residues recorded for this chain.

• Molecule 9: Nup192

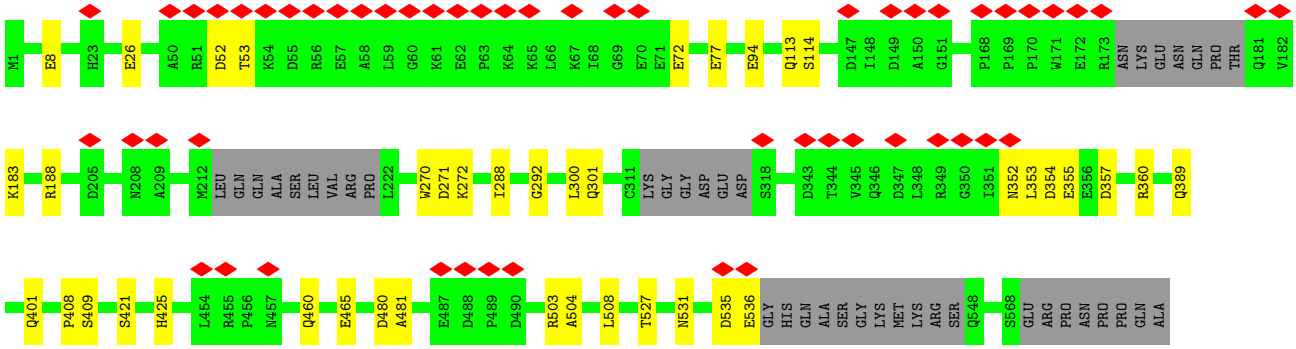
Chain I1:

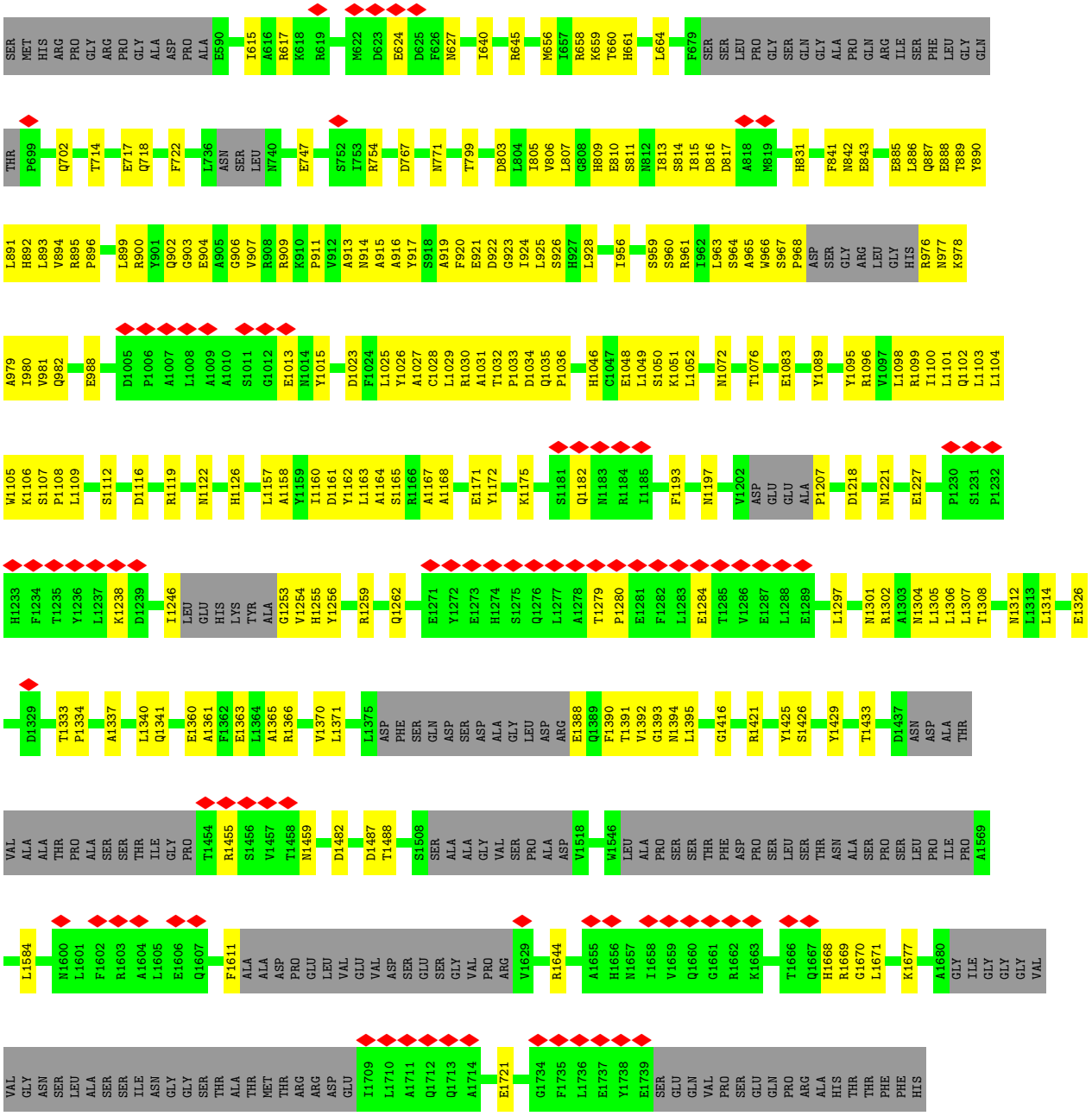




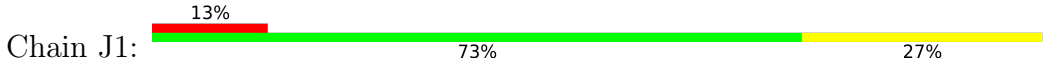
• Molecule 9: Nup192

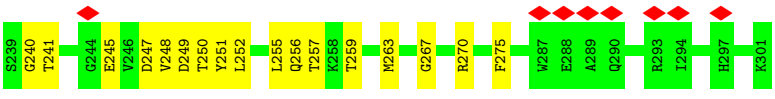
Chain I2:



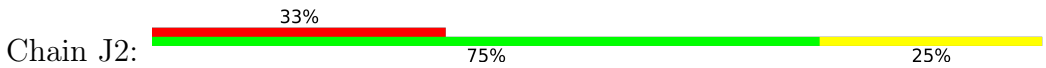


• Molecule 10: Nic96 R2

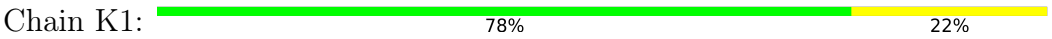




• Molecule 10: Nic96 R2



• Molecule 11: Nup145N/Nup100/Nup116 R1



• Molecule 11: Nup145N/Nup100/Nup116 R1

There are no outlier residues recorded for this chain.

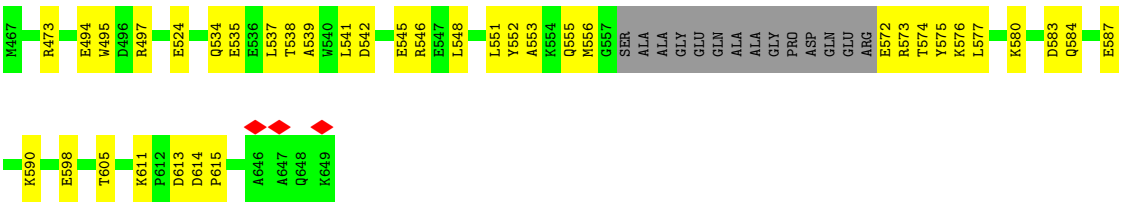
• Molecule 12: Nup53/Nup59 R1

There are no outlier residues recorded for this chain.

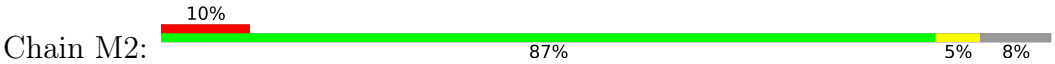
• Molecule 12: Nup53/Nup59 R1

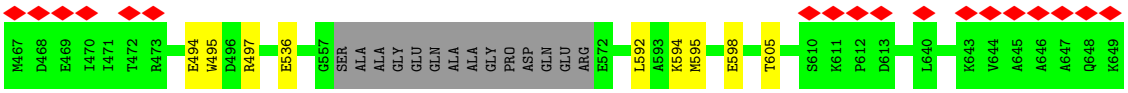
There are no outlier residues recorded for this chain.

• Molecule 13: Nsp1

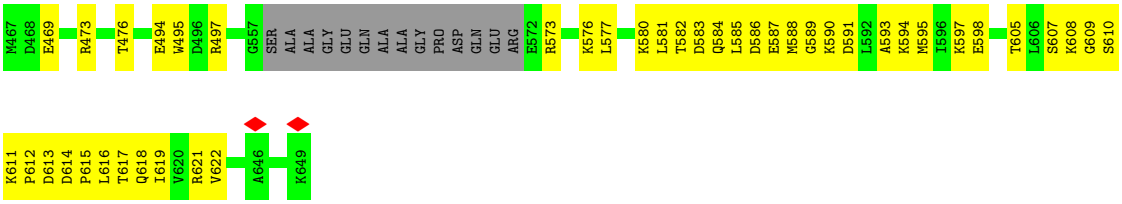


• Molecule 13: Nsp1



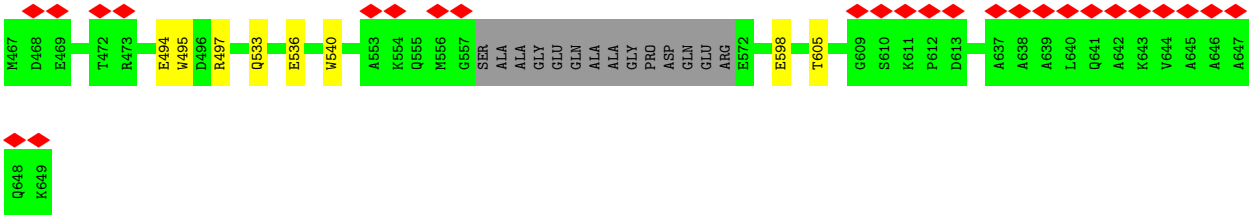


• Molecule 13: Nsp1



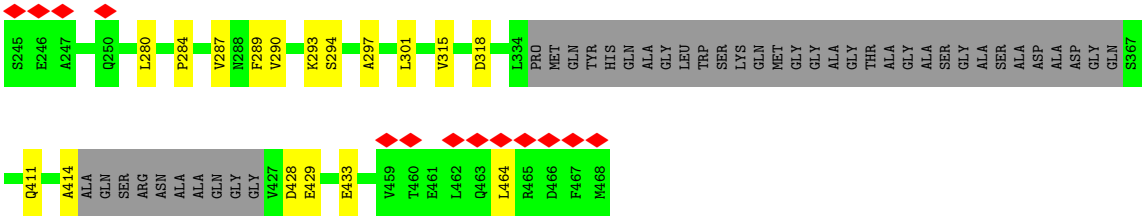
• Molecule 13: Nsp1

Chain M4:



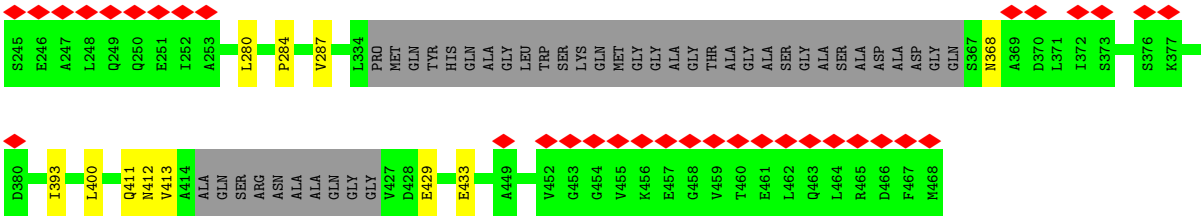
• Molecule 14: Nup57

Chain N1:



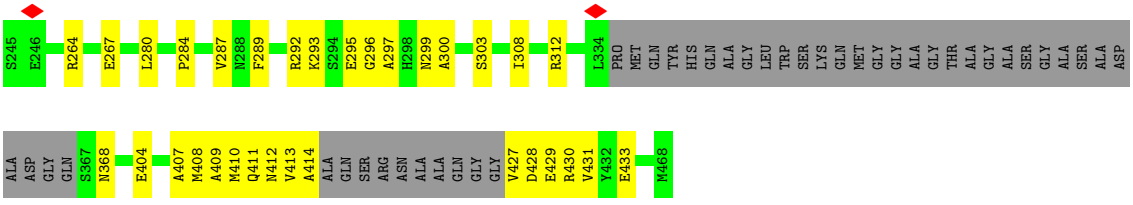
• Molecule 14: Nup57

Chain N2:



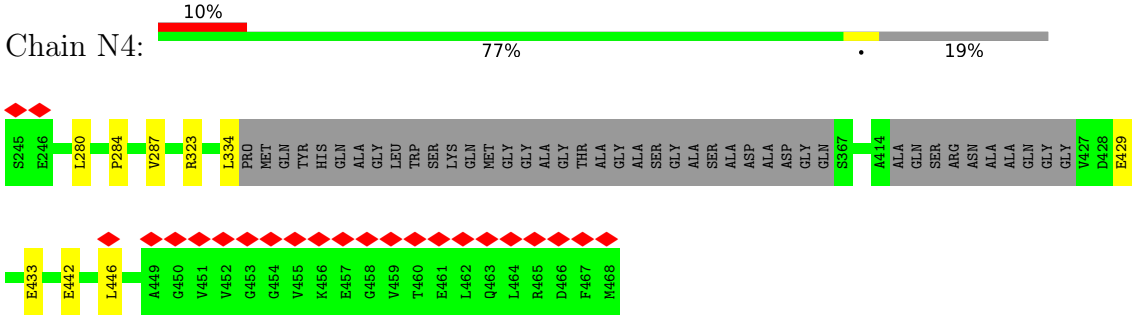
• Molecule 14: Nup57

Chain N3:



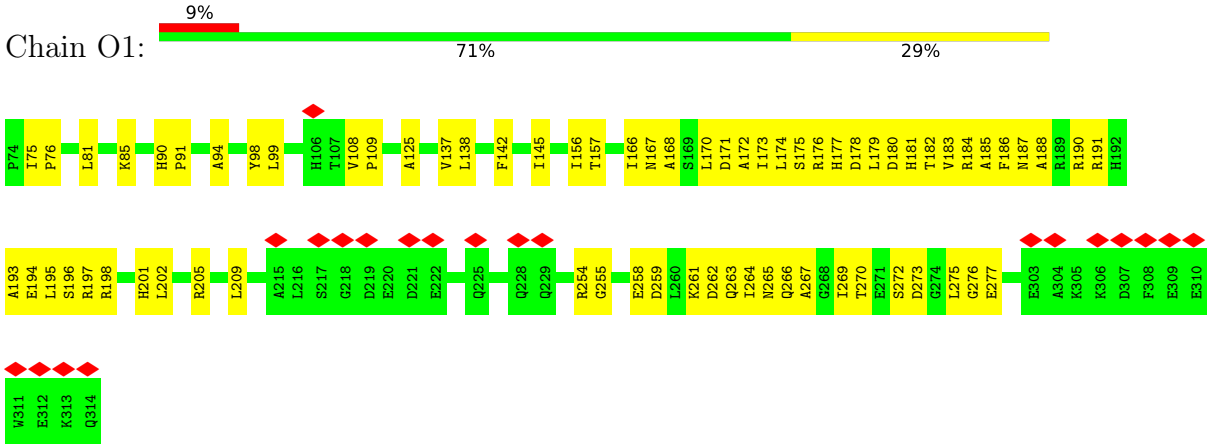
• Molecule 14: Nup57

Chain N4:



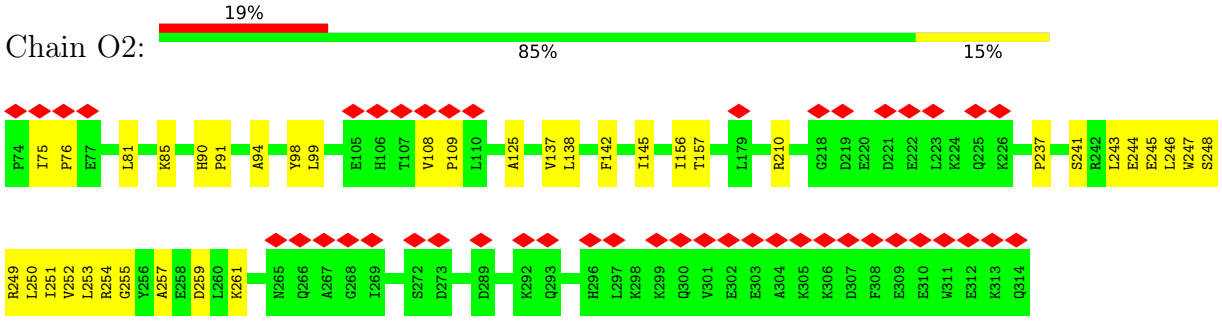
• Molecule 15: Nup49

Chain O1:



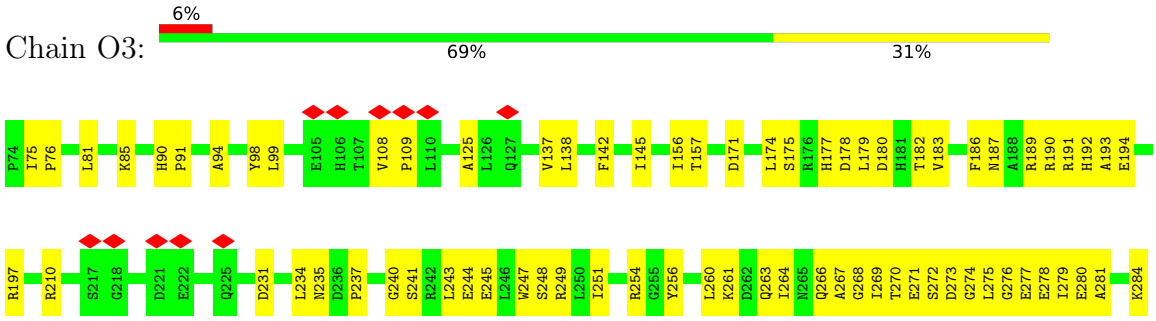
• Molecule 15: Nup49

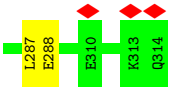
Chain O2:



• Molecule 15: Nup49

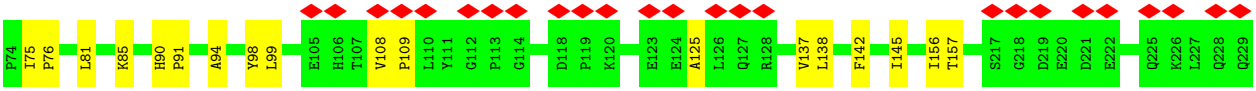
Chain O3:

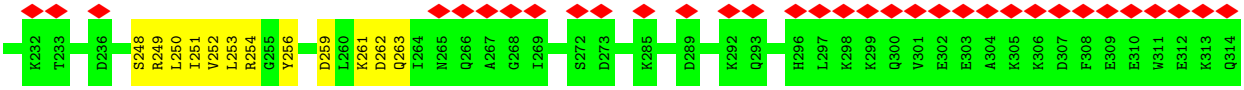




• Molecule 15: Nup49

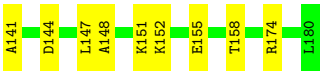
Chain O4:





• Molecule 16: Nic96 R1

Chain P1:



• Molecule 16: Nic96 R1

Chain P2:

• Molecule 16: Nic96 R1

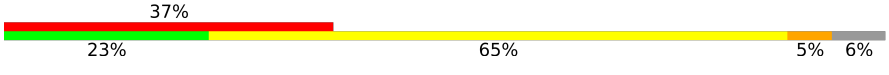
Chain P3:

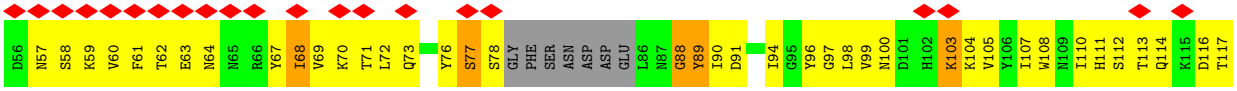
• Molecule 16: Nic96 R1

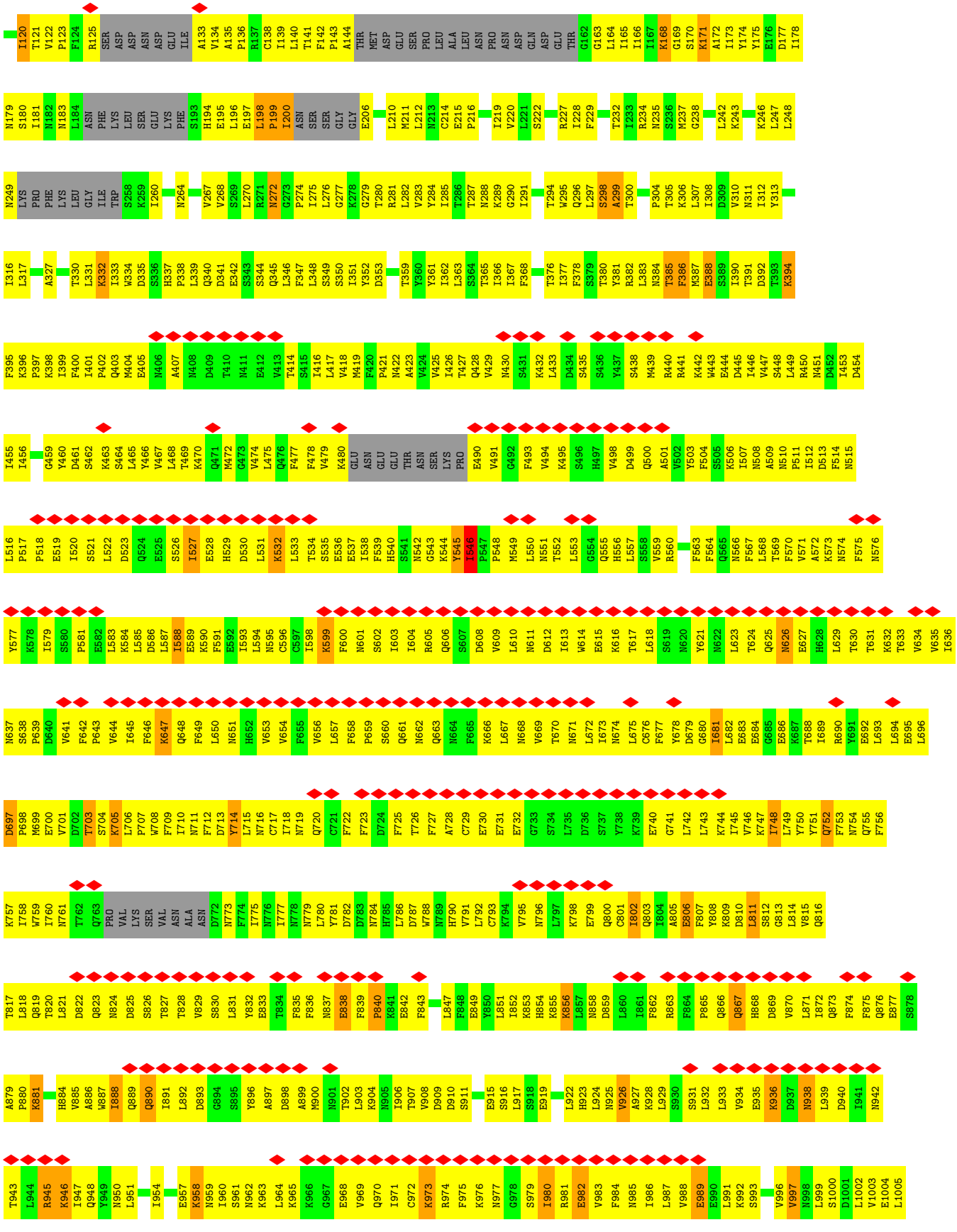
Chain P4:

• Molecule 17: Nup133

Chain Q1:

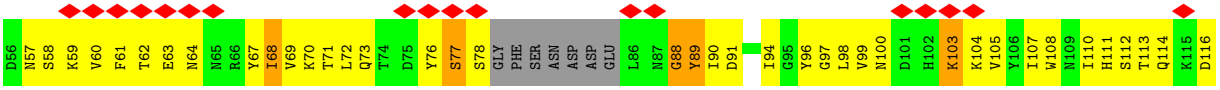


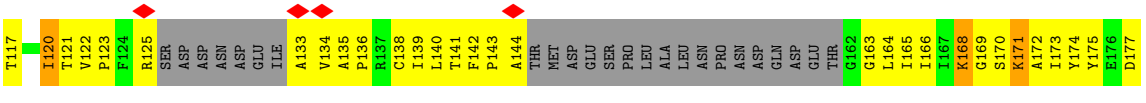


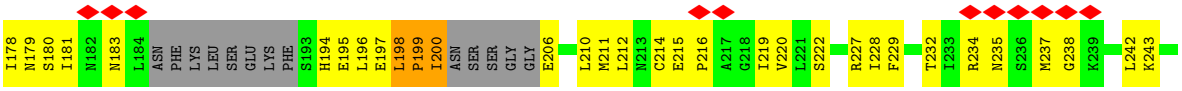


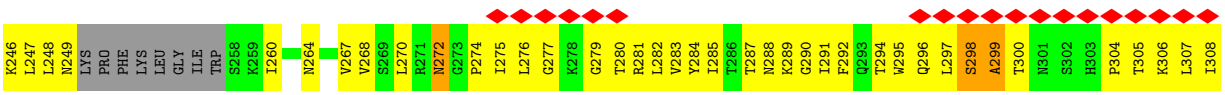
• Molecule 17: Nup133

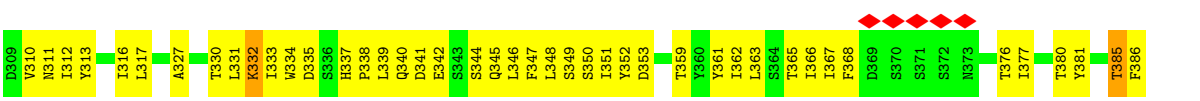
Chain Q2:

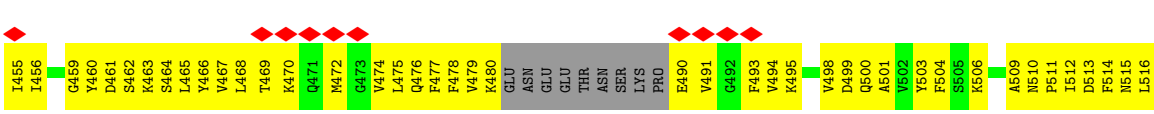


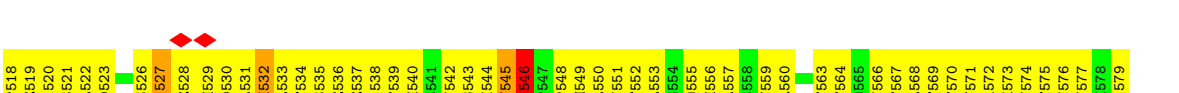


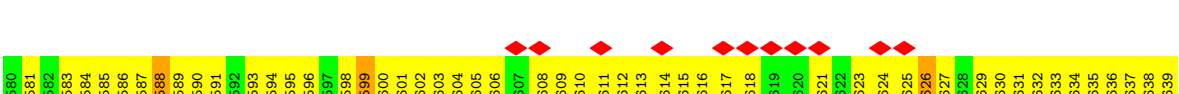


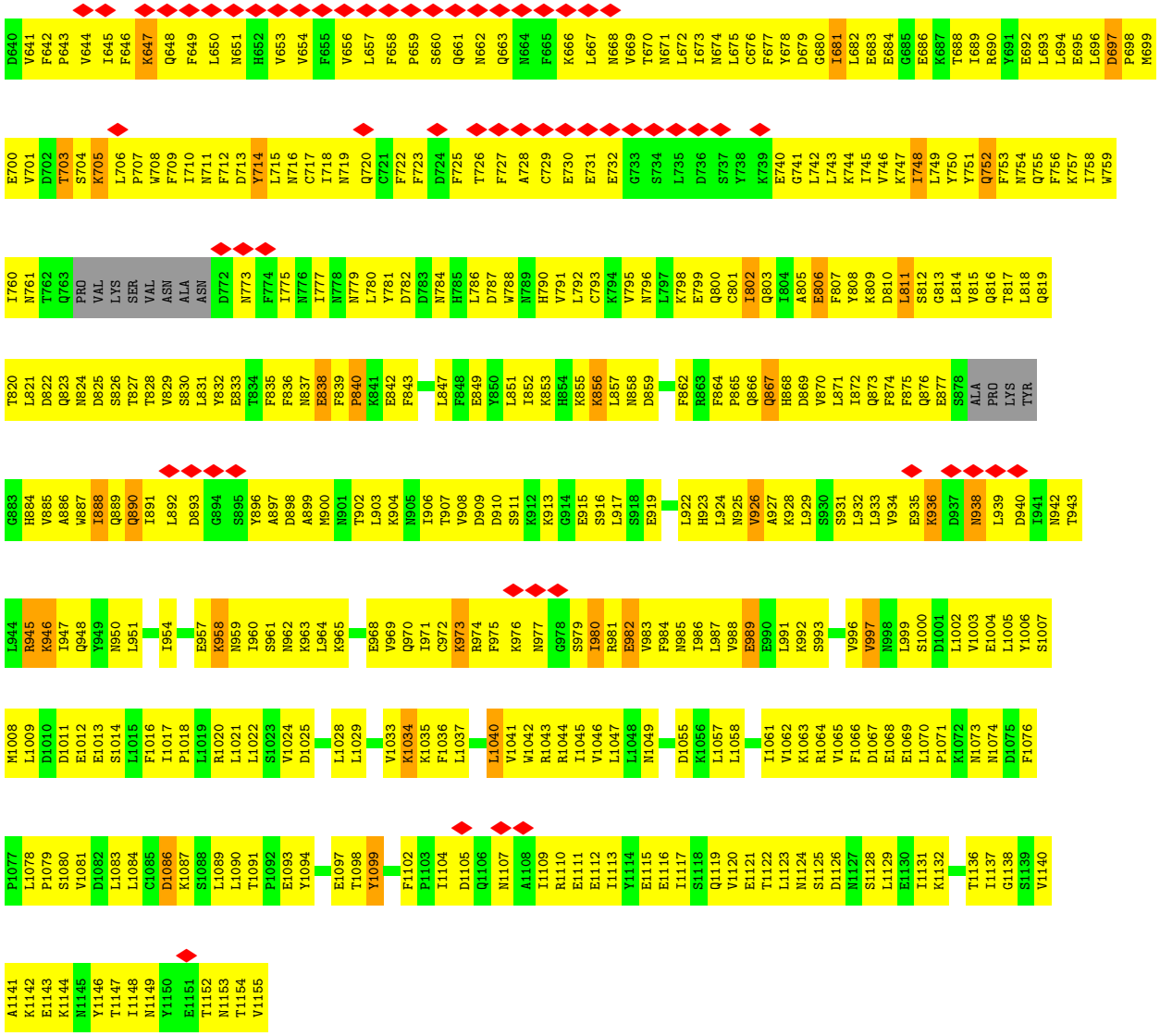






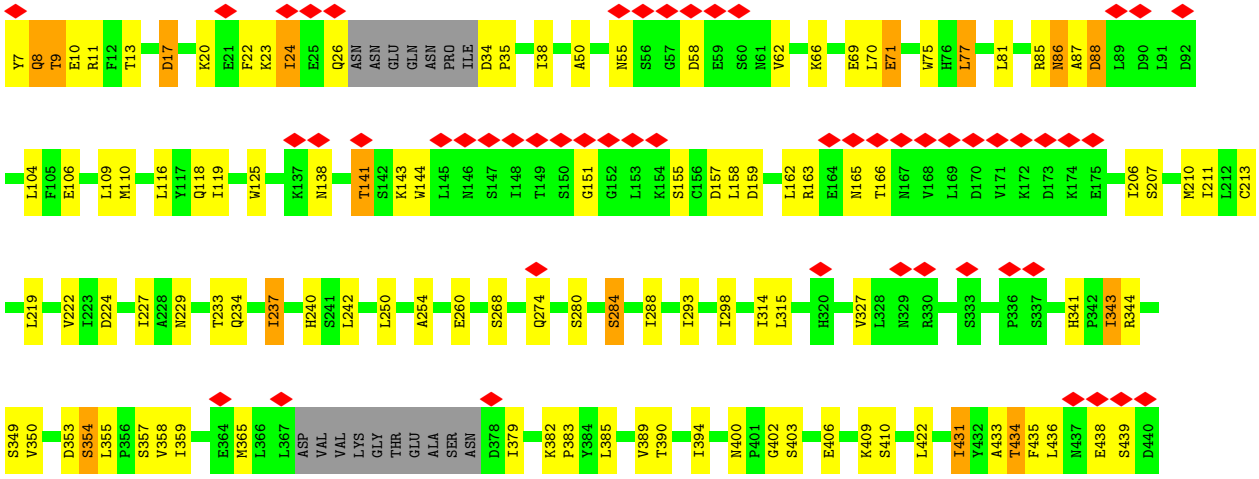


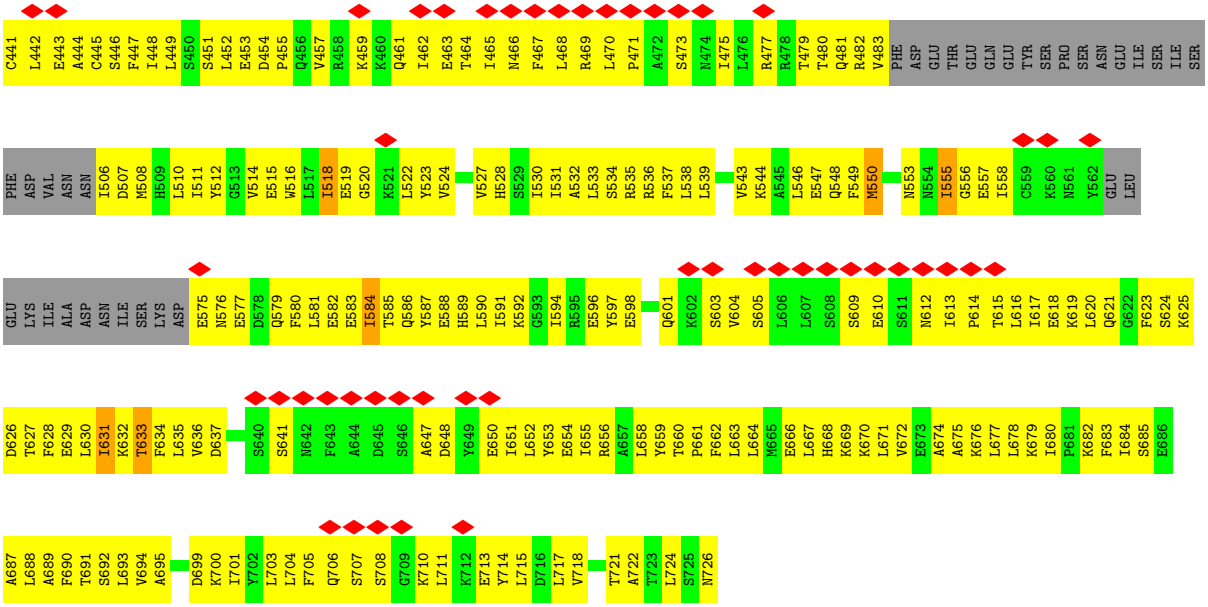




• Molecule 18: Nup84

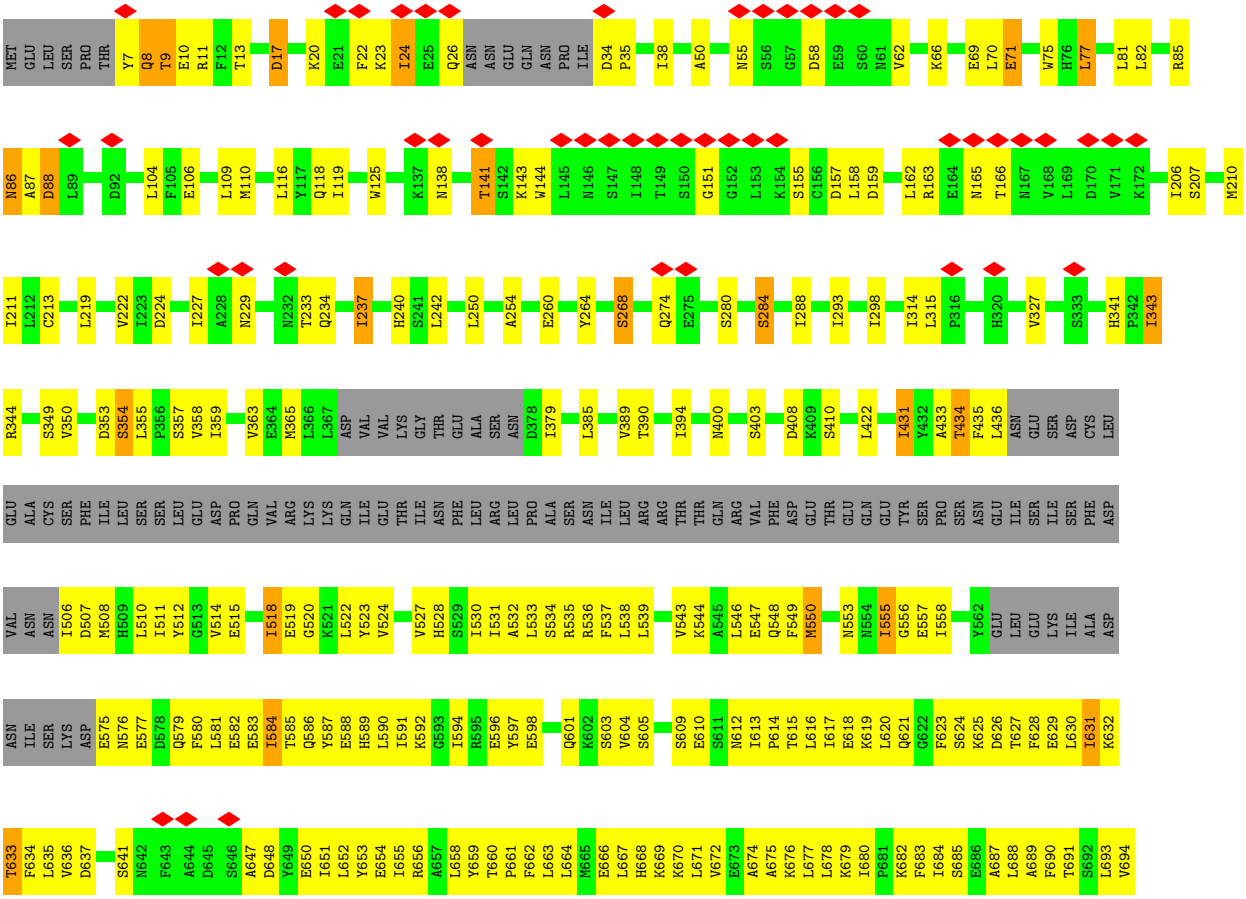
Chain R1:

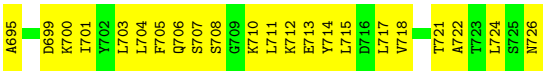




• Molecule 19: Nup84

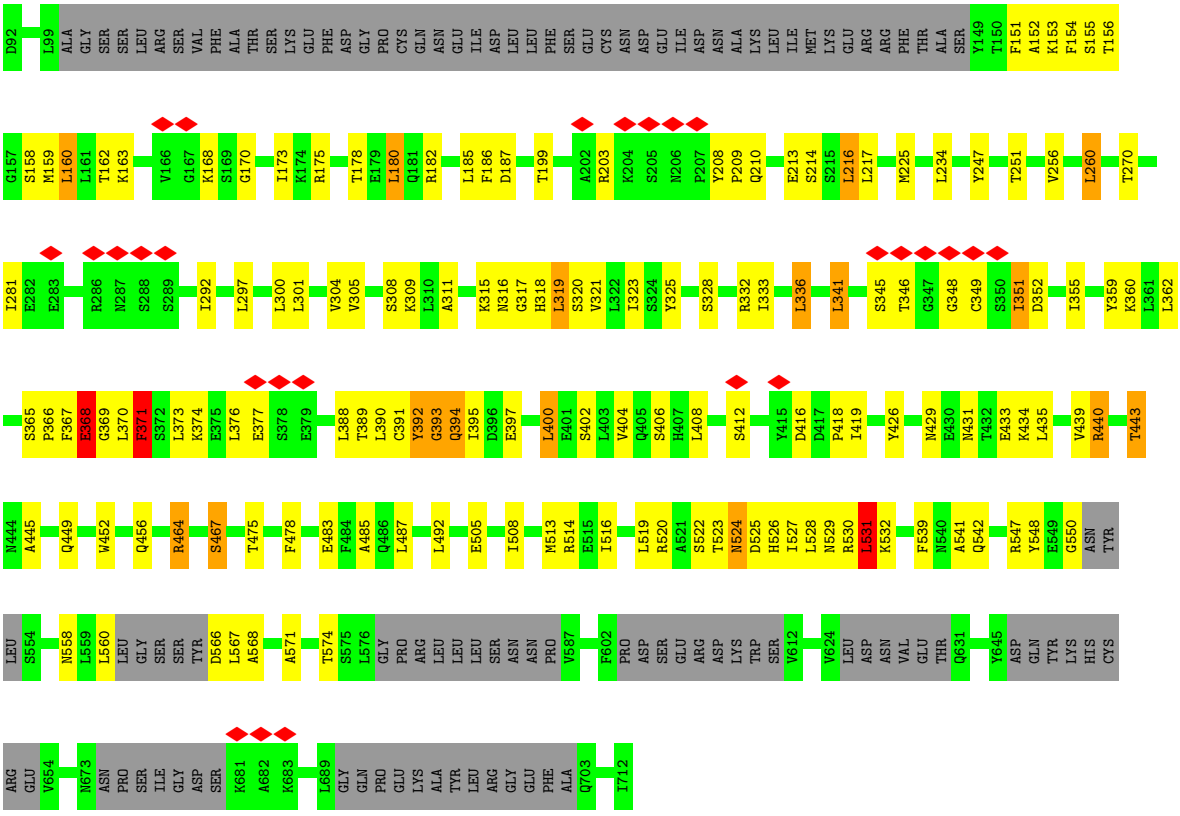
Chain R2:





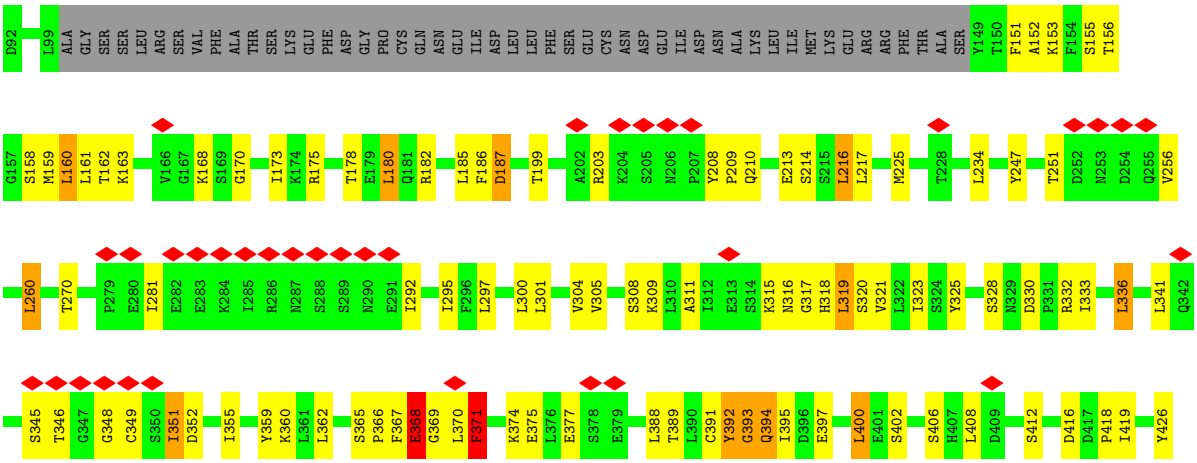
• Molecule 20: Nup145C

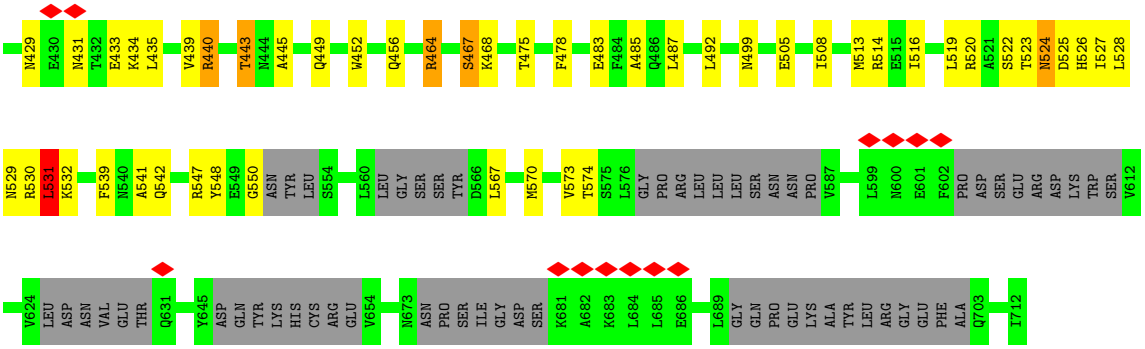
Chain S1:



• Molecule 20: Nup145C

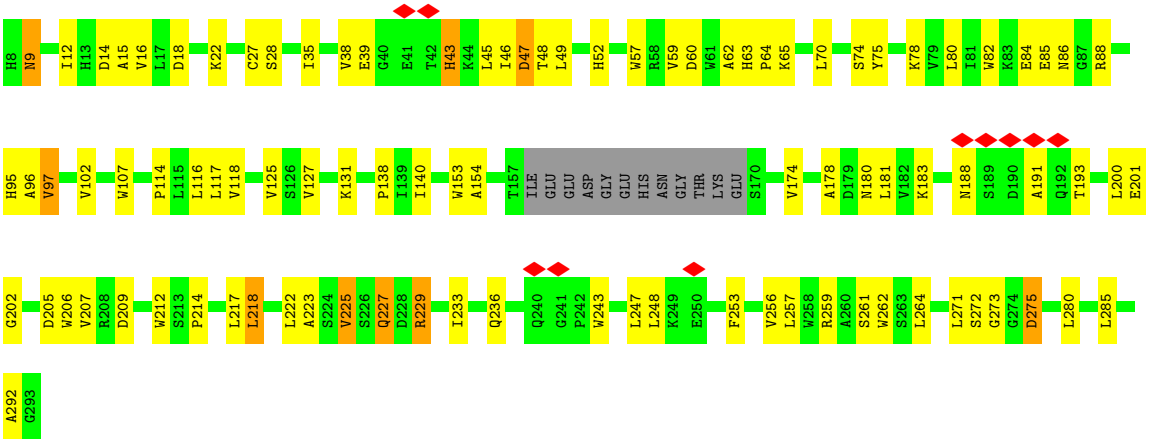
Chain S2:





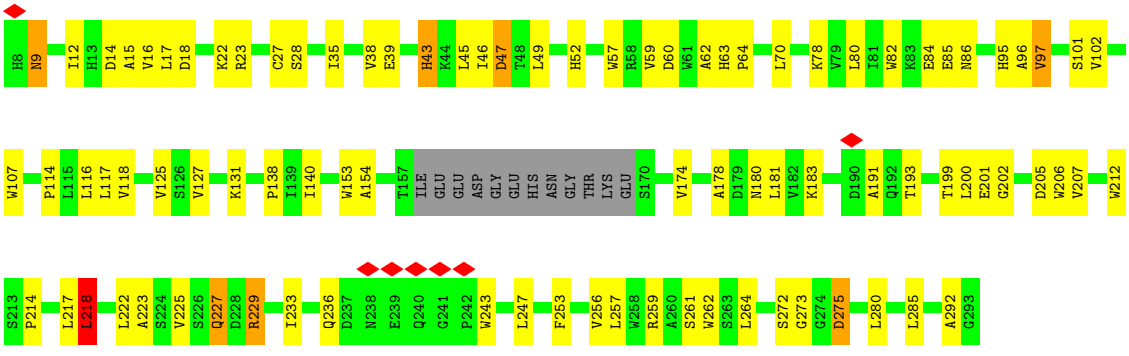
• Molecule 21: Sec13

Chain T1:



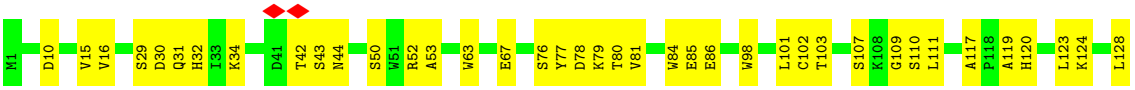
• Molecule 21: Sec13

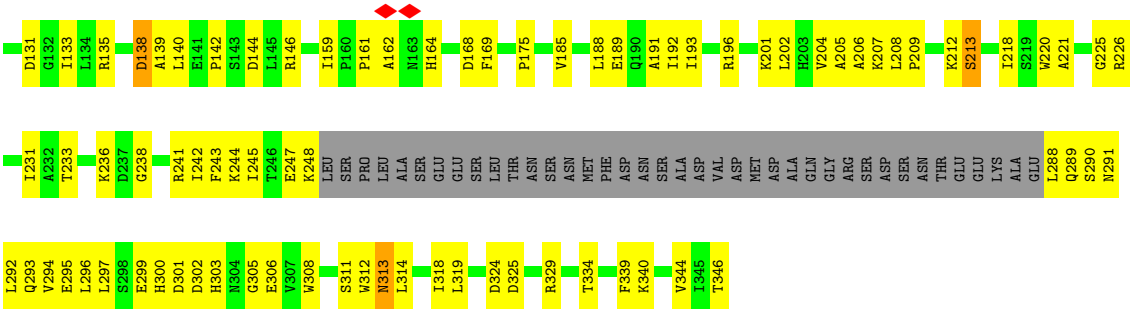
Chain T2:



• Molecule 22: Seh1

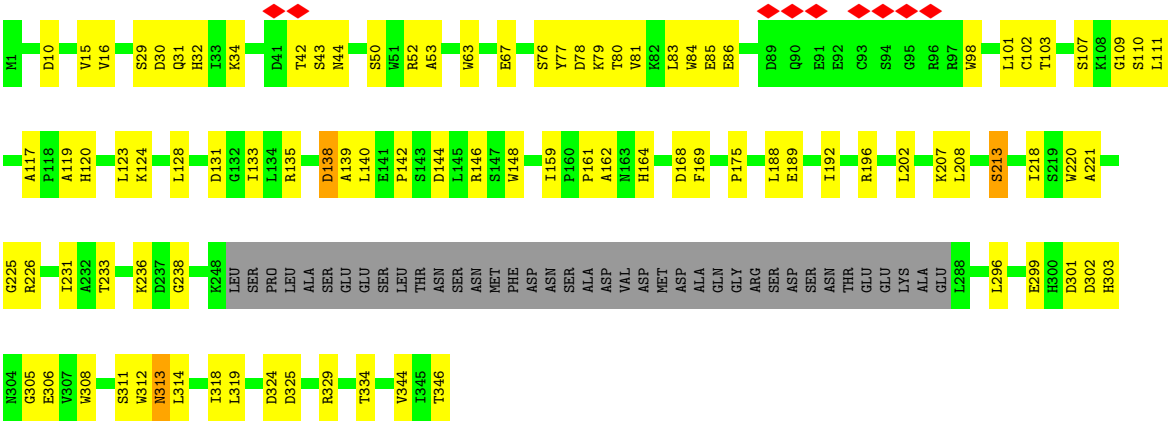
Chain U1:





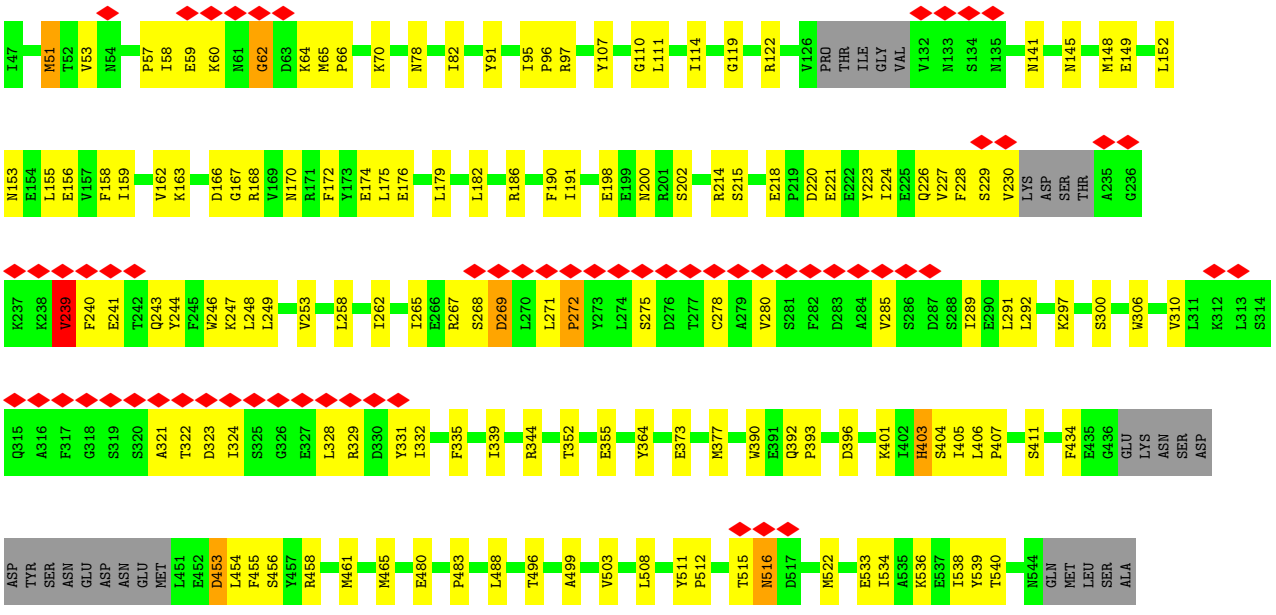
• Molecule 22: Seh1

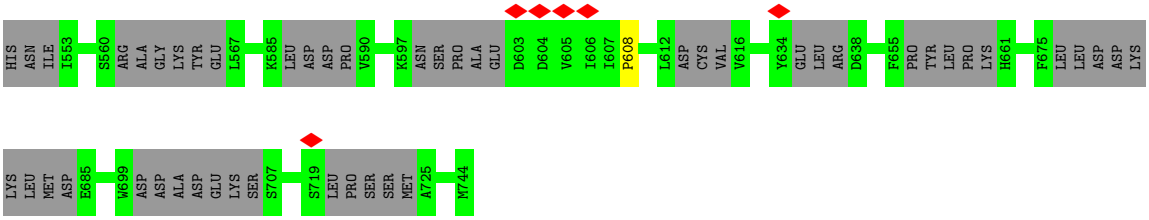
Chain U2:



• Molecule 23: Nup85

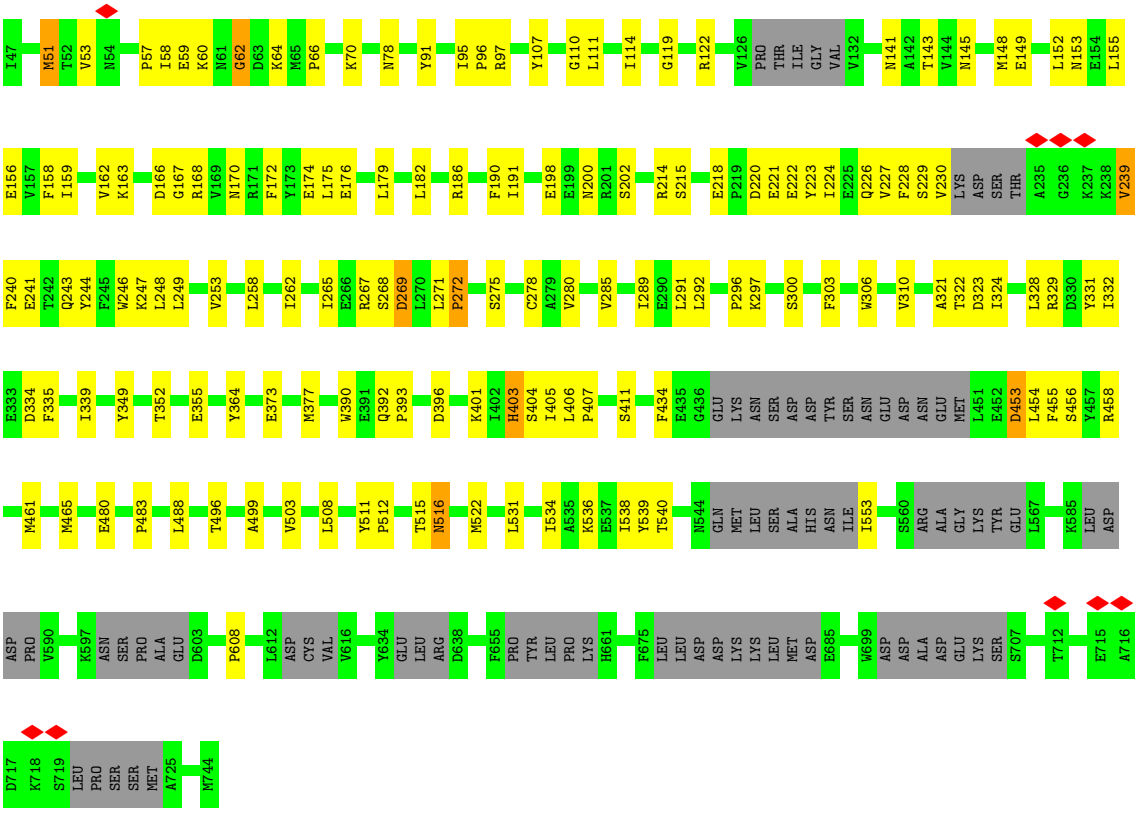
Chain V1:





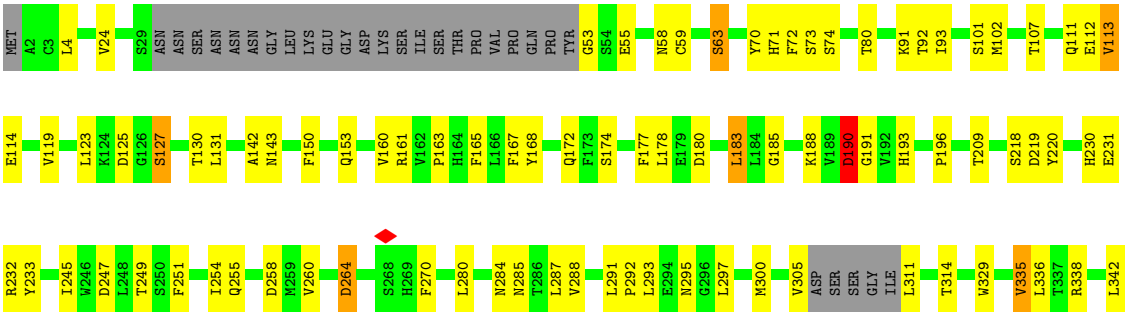
• Molecule 23: Nup85

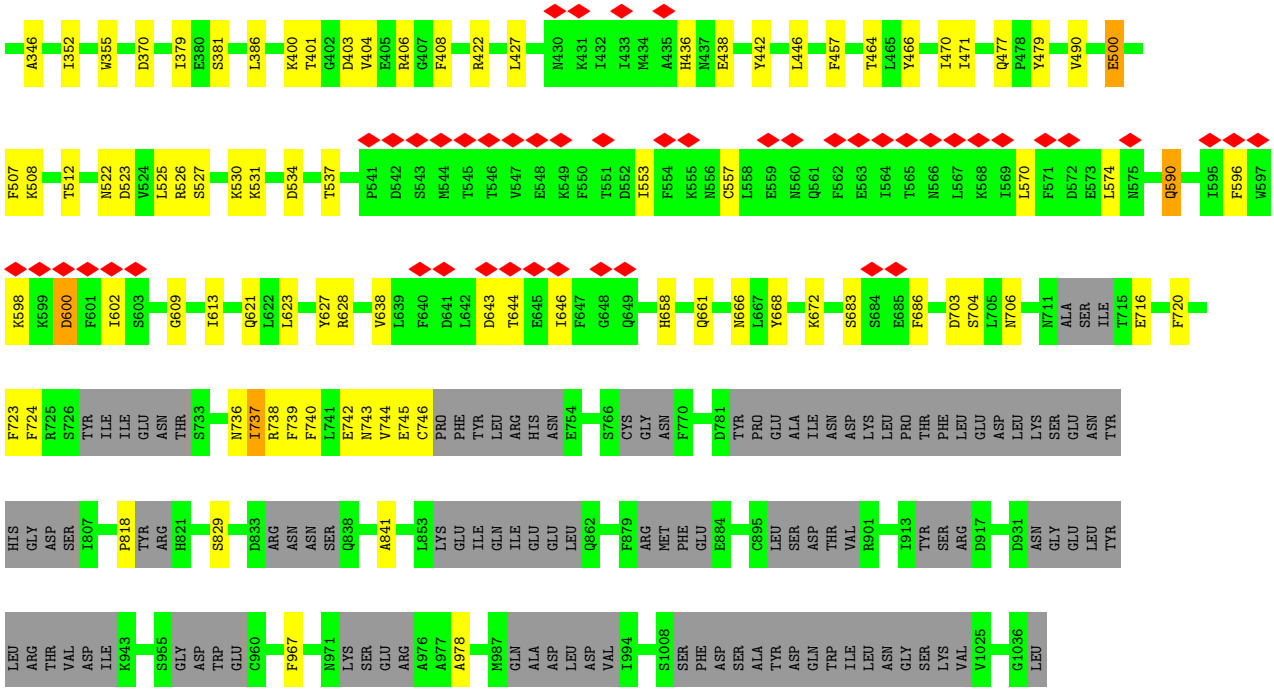
Chain V2:



• Molecule 24: Nup120

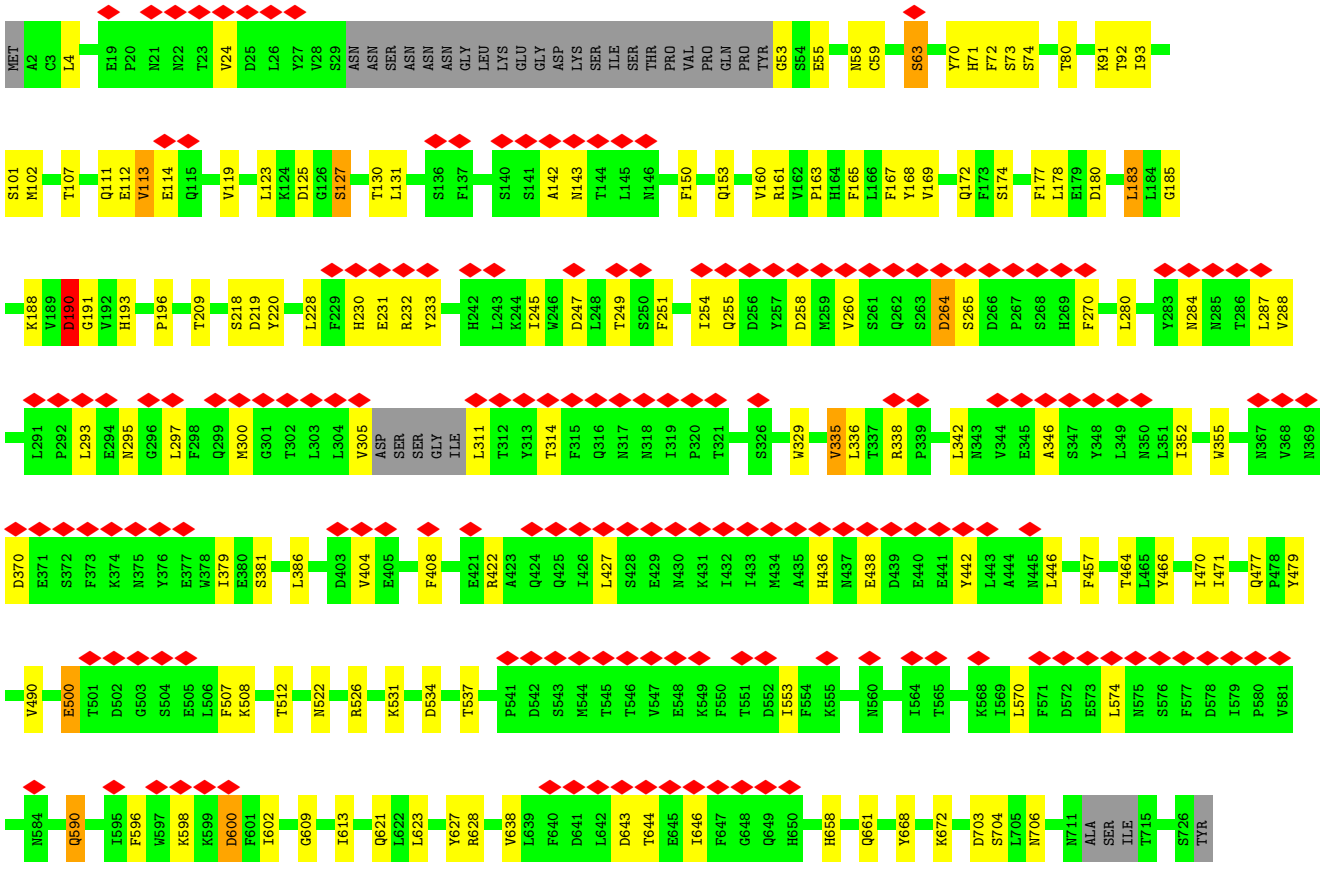
Chain W1:

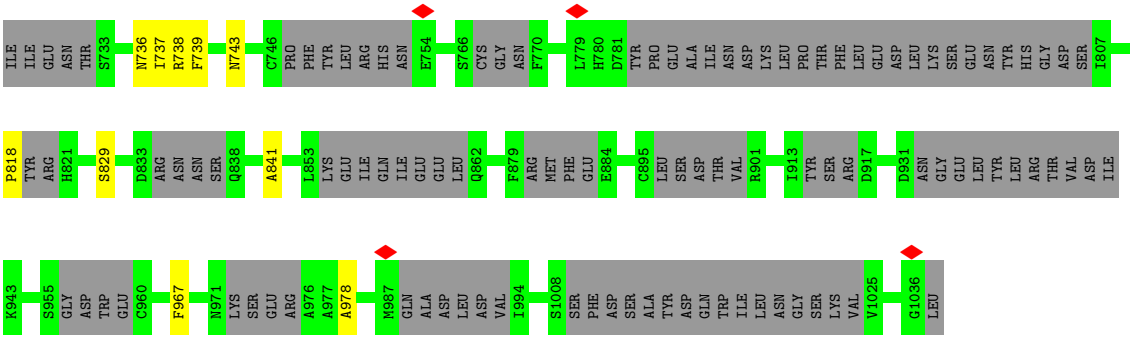




• Molecule 24: Nup120

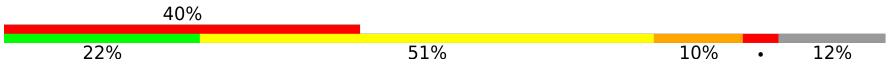
Chain W2:

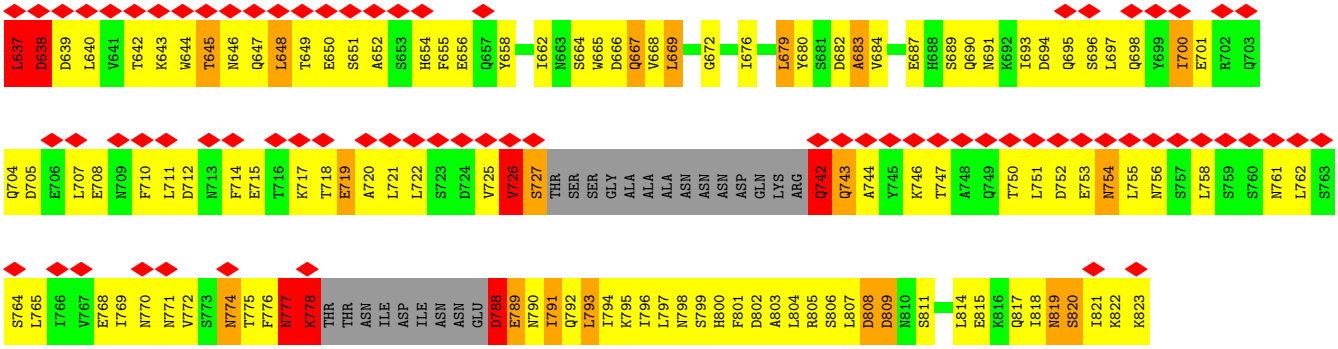




• Molecule 25: Nsp1

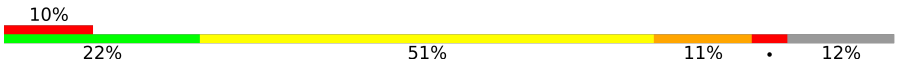
Chain X1:

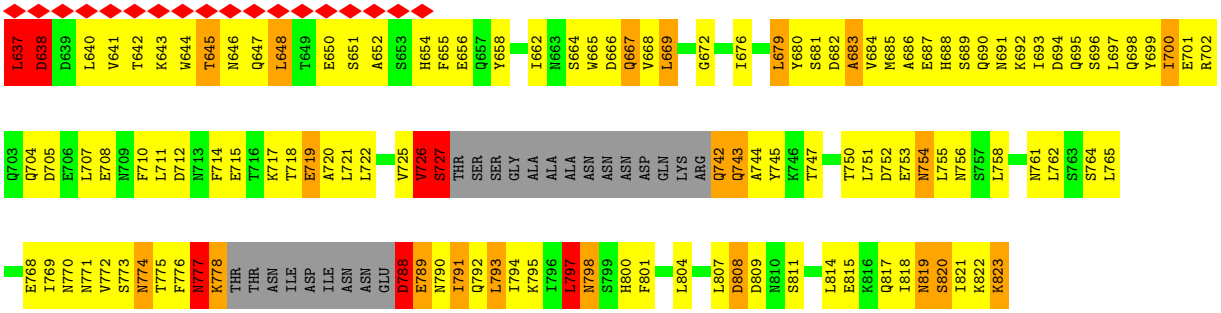




• Molecule 25: Nsp1

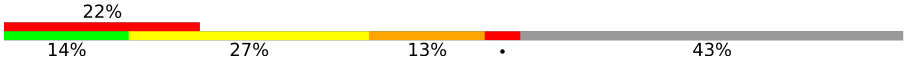
Chain X2:

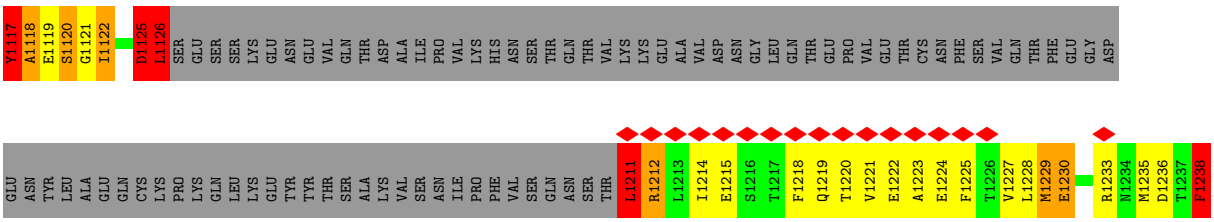


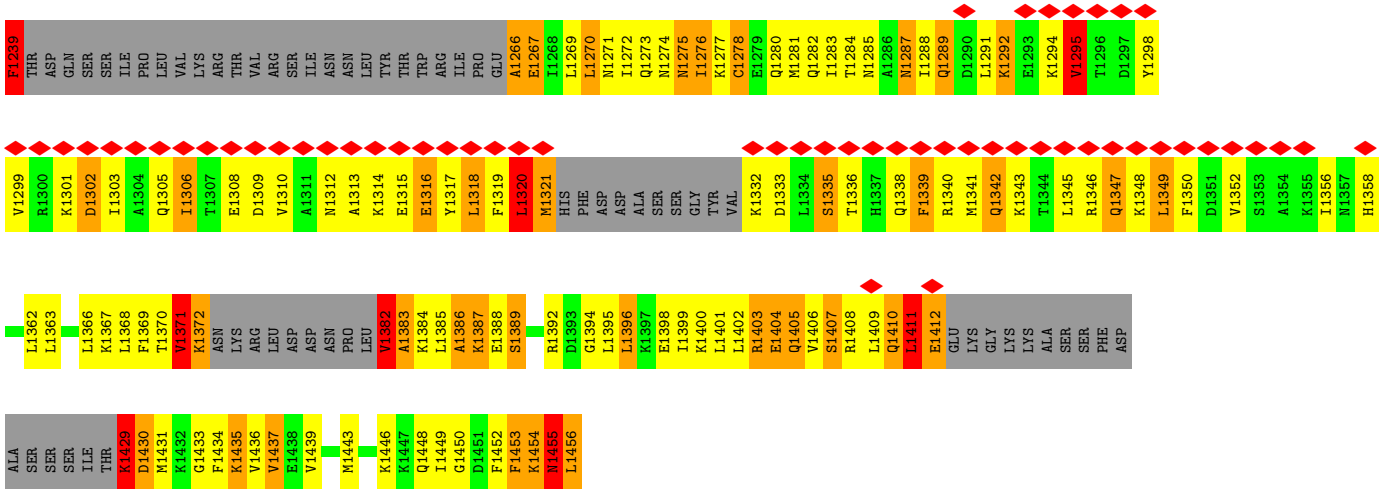


• Molecule 26: Nup159

Chain Y1:

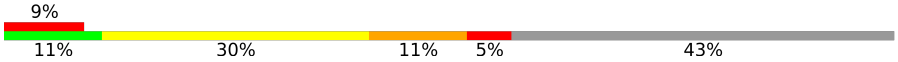


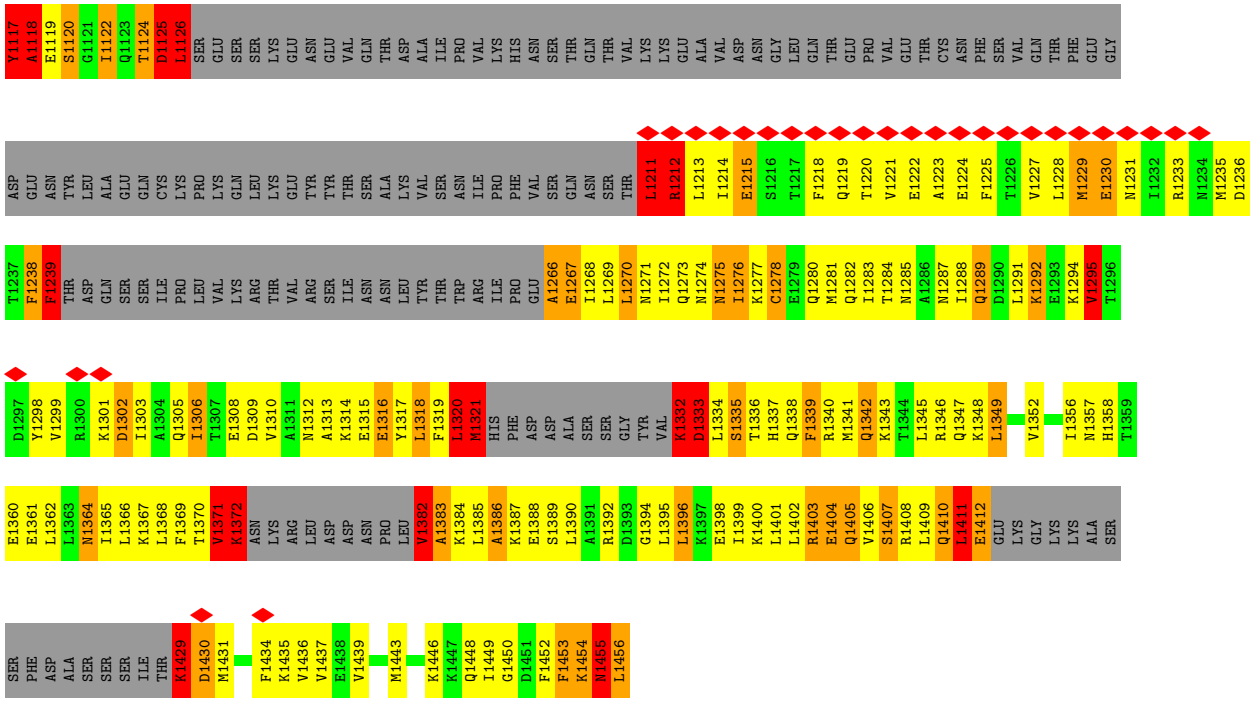




• Molecule 26: Nup159

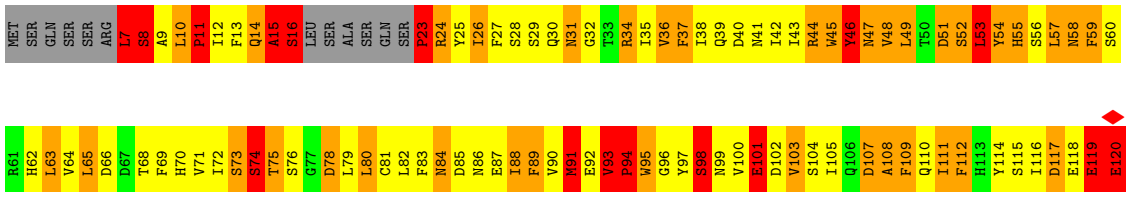
Chain Y2:

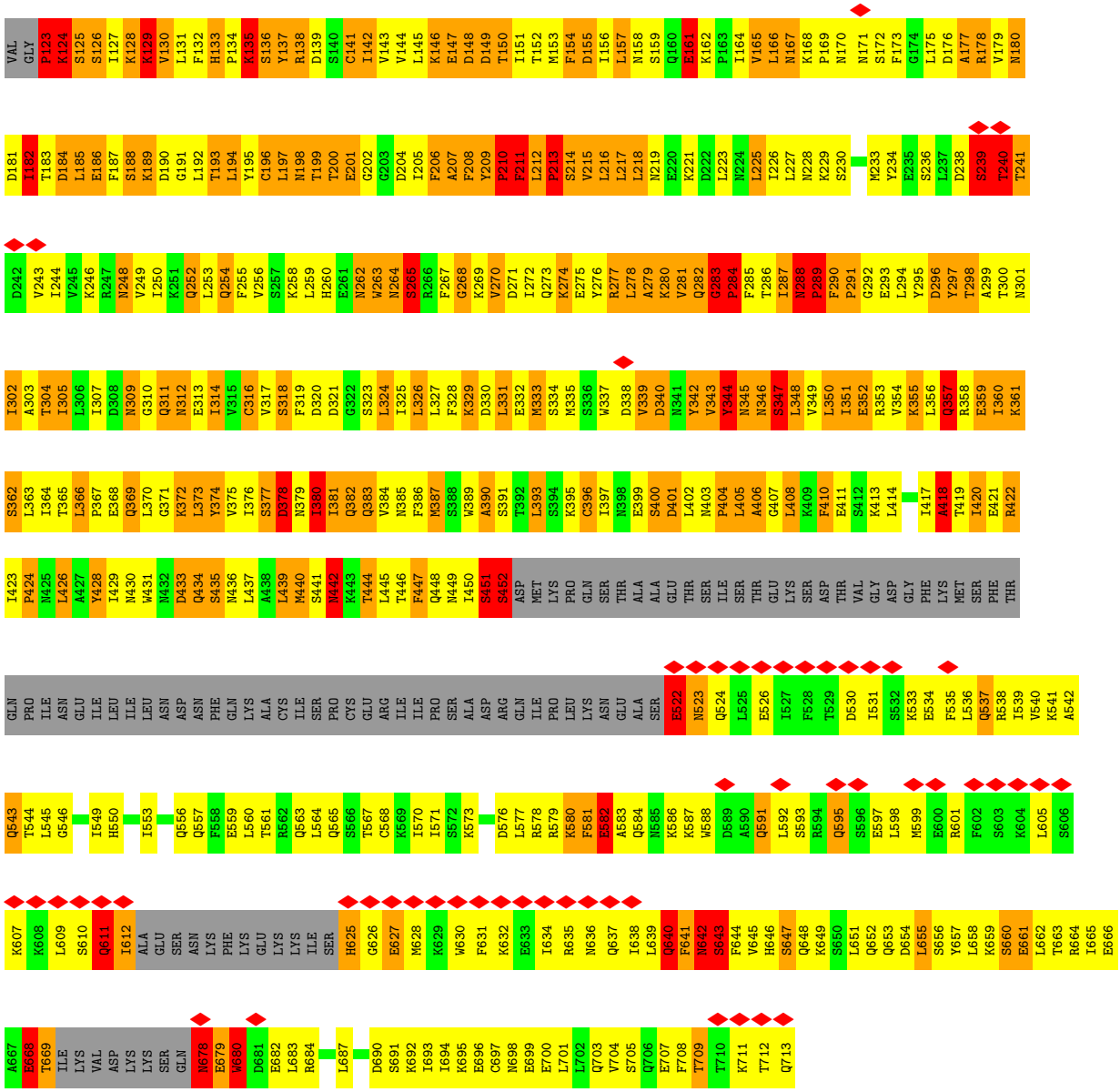




• Molecule 27: Nup82

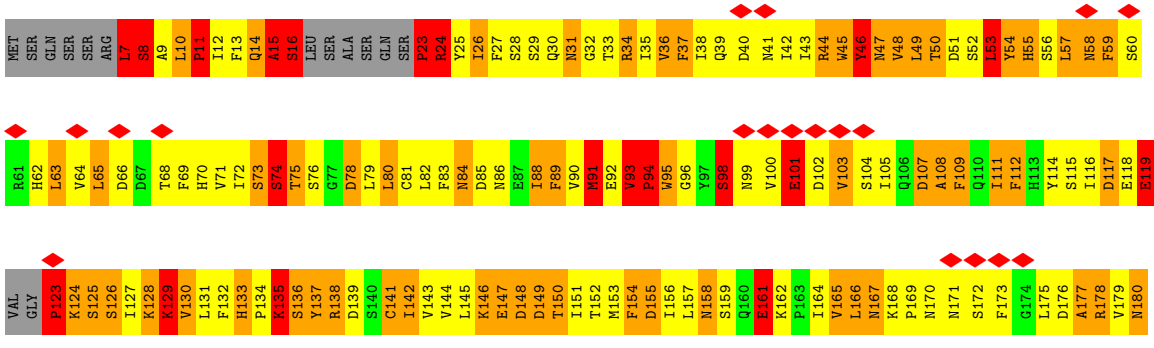
Chain Z1:

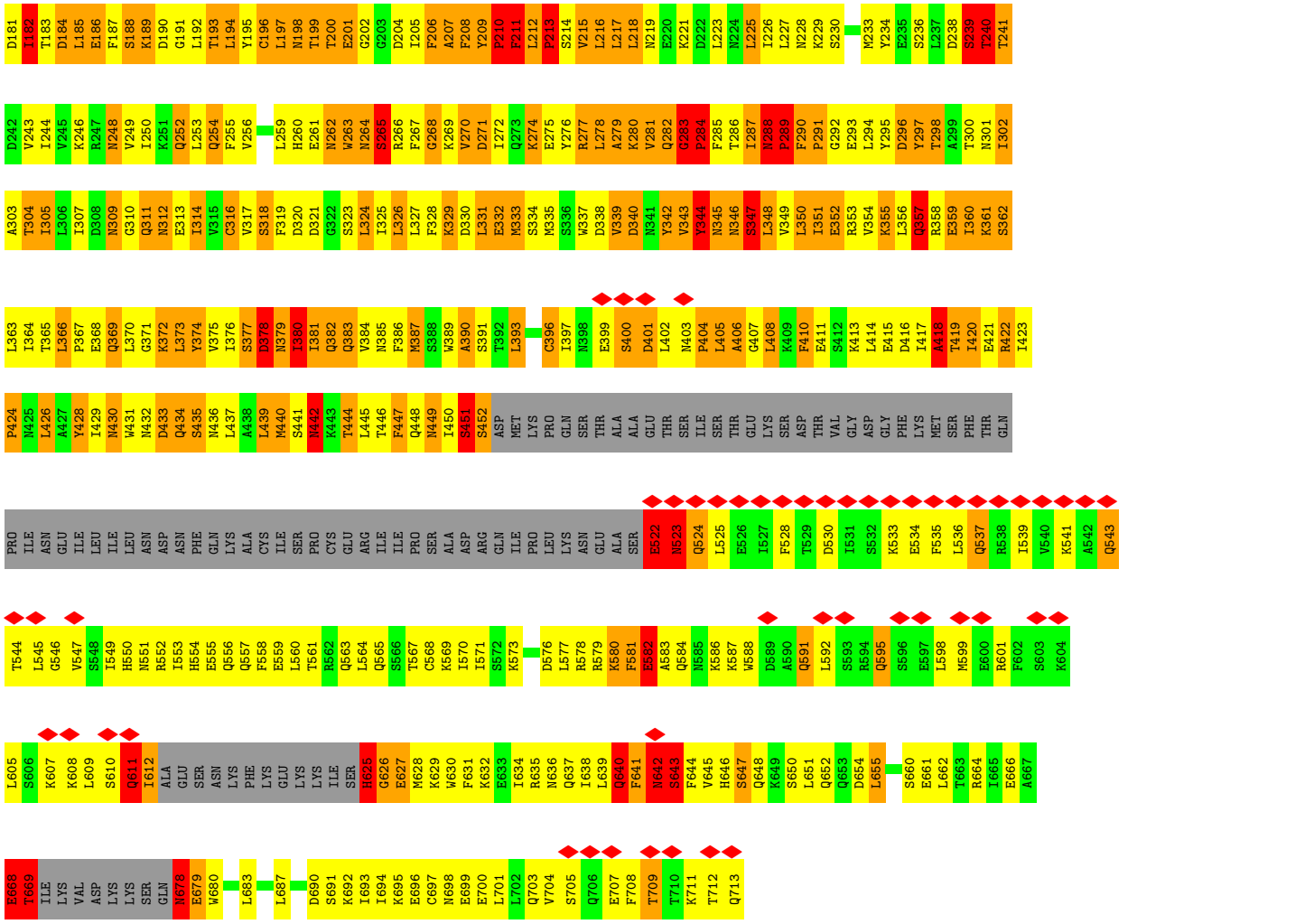




• Molecule 27: Nup82

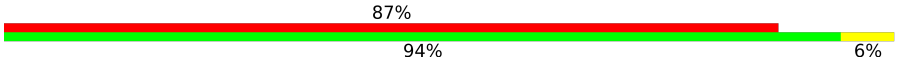
Chain Z2:

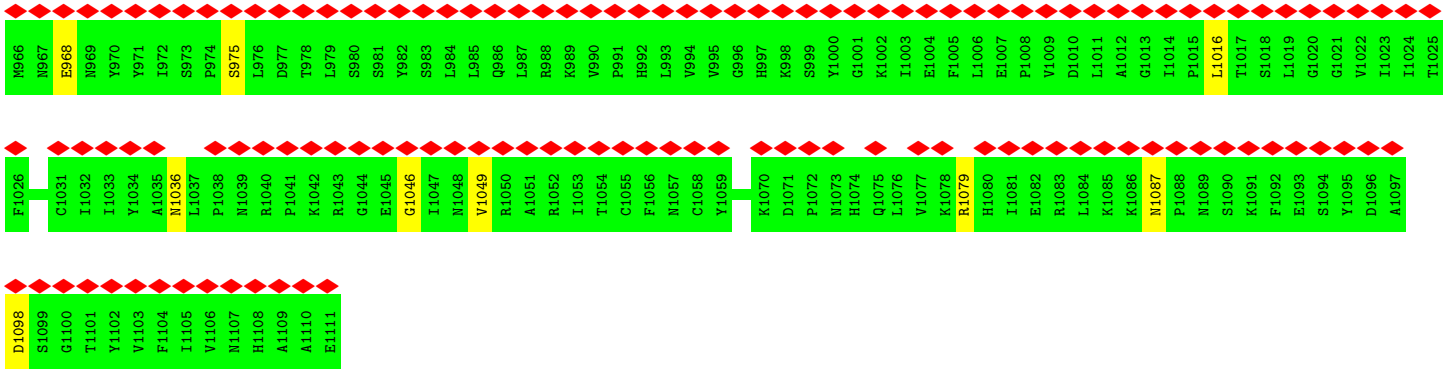




• Molecule 28: Nup116 CTD

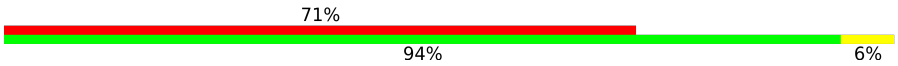
Chain a1:

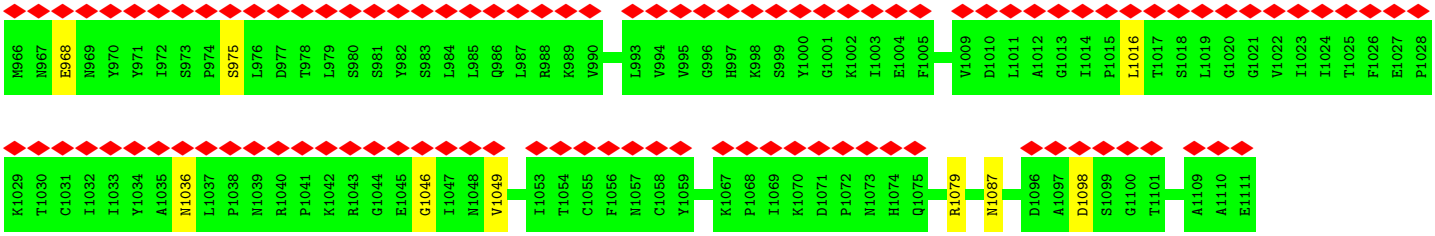




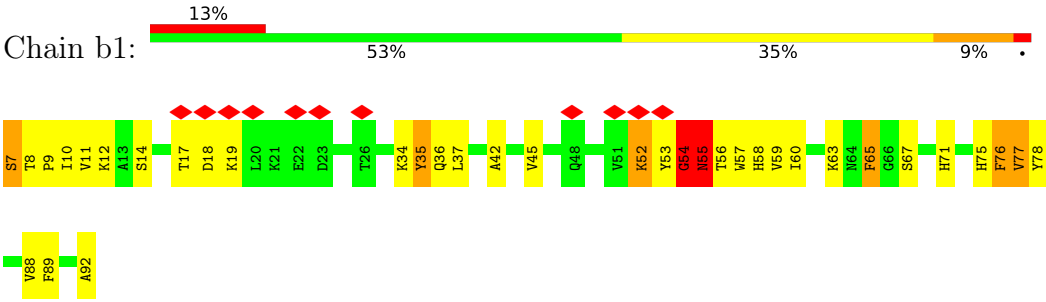
• Molecule 28: Nup116 CTD

Chain a2:

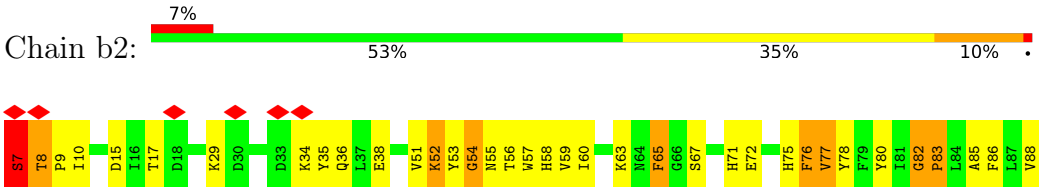




• Molecule 29: Dyn2



• Molecule 29: Dyn2



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, Not provided	
Number of subtomograms used	4000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	140	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.515	Depositor
Minimum map value	-0.337	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.0606	Depositor
Map size (Å)	1941.1199, 1941.1199, 1941.1199	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	6.74, 6.74, 6.74	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	A1	0.29	1/9897 (0.0%)	0.44	0/13434
1	A2	0.28	1/9926 (0.0%)	0.44	0/13474
1	A3	0.28	1/9926 (0.0%)	0.44	0/13474
1	A4	0.29	1/9897 (0.0%)	0.44	0/13434
2	B1	0.25	0/112	0.48	0/149
2	B2	0.25	0/112	0.48	0/149
2	B3	0.26	0/112	0.48	0/149
2	B4	0.25	0/112	0.48	0/149
3	C1	0.39	0/140	0.50	0/188
3	C2	0.39	0/140	0.50	0/188
3	C3	0.39	0/140	0.50	0/188
3	C4	0.39	0/140	0.50	0/188
4	D1	0.22	0/5696	0.38	0/7702
4	D2	0.22	0/5696	0.38	0/7702
4	D3	0.22	0/5696	0.38	0/7702
4	D4	0.22	0/5696	0.38	0/7702
5	E1	0.20	0/140	0.32	0/191
5	E2	0.20	0/140	0.32	0/191
5	E3	0.20	0/140	0.32	0/191
5	E4	0.20	0/140	0.33	0/191
6	F1	0.24	0/13031	0.39	0/17717
6	F2	0.24	0/13031	0.39	0/17717
7	G1	0.23	0/445	0.39	0/600
7	G2	0.23	0/445	0.38	0/600
8	H1	0.25	0/95	0.37	0/128
8	H2	0.25	0/95	0.37	0/128
9	I1	0.23	0/12541	0.36	0/16980
9	I2	0.23	0/12541	0.36	0/16980
10	J1	0.23	0/511	0.37	0/688
10	J2	0.23	0/511	0.37	0/688
11	K1	0.23	0/75	0.40	0/101
11	K2	0.24	0/75	0.39	0/101
12	L1	0.29	0/15	0.18	0/18
12	L2	0.29	0/15	0.18	0/18

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
13	M1	0.26	0/1388	0.39	0/1866
13	M2	0.26	0/1388	0.40	0/1866
13	M3	0.26	0/1388	0.40	0/1866
13	M4	0.26	0/1388	0.40	0/1866
14	N1	0.24	0/1413	0.38	0/1898
14	N2	0.25	0/1413	0.38	0/1898
14	N3	0.25	0/1413	0.38	0/1898
14	N4	0.25	0/1413	0.38	0/1898
15	O1	0.26	0/2011	0.41	0/2715
15	O2	0.26	0/2011	0.41	0/2715
15	O3	0.26	0/2011	0.41	0/2715
15	O4	0.27	0/2011	0.41	0/2715
16	P1	0.23	0/312	0.38	0/416
16	P2	0.24	0/312	0.38	0/416
16	P3	0.23	0/312	0.38	0/416
16	P4	0.23	0/312	0.38	0/416
17	Q1	0.90	0/8558	1.17	14/11594 (0.1%)
17	Q2	0.90	0/8522	1.17	14/11543 (0.1%)
18	R1	0.64	0/5549	0.83	3/7512 (0.0%)
19	R2	0.60	0/5167	0.81	3/6998 (0.0%)
20	S1	0.37	0/3860	0.66	2/5224 (0.0%)
20	S2	0.37	0/3860	0.66	2/5224 (0.0%)
21	T1	0.32	0/2220	0.62	0/3028
21	T2	0.32	0/2220	0.62	1/3028 (0.0%)
22	U1	0.28	0/2499	0.64	0/3388
22	U2	0.28	0/2499	0.64	0/3388
23	V1	0.31	0/4602	0.58	2/6246 (0.0%)
23	V2	0.31	0/4602	0.58	2/6246 (0.0%)
24	W1	0.33	0/6730	0.55	1/9158 (0.0%)
24	W2	0.33	0/6730	0.55	1/9158 (0.0%)
25	X1	13.08	17/1334 (1.3%)	3.38	56/1799 (3.1%)
25	X2	13.35	17/1334 (1.3%)	3.45	56/1799 (3.1%)
26	Y1	18.10	39/1600 (2.4%)	4.40	111/2135 (5.2%)
26	Y2	19.43	42/1600 (2.6%)	4.44	123/2135 (5.8%)
27	Z1	10.50	150/5078 (3.0%)	3.50	427/6856 (6.2%)
27	Z2	10.27	154/5078 (3.0%)	3.59	430/6856 (6.3%)
28	a1	0.35	0/1193	0.64	0/1617
28	a2	0.35	0/1193	0.64	0/1617
29	b1	4.70	21/707 (3.0%)	3.27	67/954 (7.0%)
29	b2	3.69	25/707 (3.5%)	3.29	68/954 (7.1%)
All	All	3.49	469/225362 (0.2%)	1.16	1383/305237 (0.5%)

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	A1	0	2
1	A2	0	2
1	A3	0	2
1	A4	0	2
17	Q1	0	1
17	Q2	0	1
18	R1	0	1
19	R2	0	1
20	S1	0	2
20	S2	0	2
24	W1	0	2
24	W2	0	2
25	X1	1	5
25	X2	1	9
26	Y1	2	16
26	Y2	3	15
27	Z1	9	24
27	Z2	9	25
29	b1	0	4
29	b2	1	4
All	All	26	122

The worst 5 of 469 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	Z2	522	GLU	N-CA	437.41	10.21	1.46
26	Y2	1429	LYS	N-CA	312.18	7.70	1.46
25	X2	637	LEU	N-CA	298.89	7.44	1.46
26	Y2	1126	LEU	CA-C	292.74	9.14	1.52
25	X1	637	LEU	N-CA	285.24	7.16	1.46

The worst 5 of 1383 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	Z1	123	PRO	CA-N-CD	-66.84	17.93	111.50
27	Z2	15	ALA	N-CA-CB	-56.85	30.51	110.10
27	Z1	23	PRO	CA-N-CD	-54.13	35.72	111.50
27	Z2	23	PRO	CA-N-CD	-50.65	40.59	111.50
26	Y2	1117	TYR	CA-C-N	-49.82	7.60	117.20

5 of 26 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	X1	742	GLN	CA
25	X2	788	ASP	CA
26	Y1	1266	ALA	CA
26	Y1	1333	ASP	CA
26	Y2	1212	ARG	CA

5 of 122 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A2	891	GLY	Mainchain
1	A2	976	LEU	Peptide
1	A3	891	GLY	Mainchain
1	A3	976	LEU	Peptide
1	A4	891	GLY	Mainchain

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	A1	9703	0	9614	513	0
1	A2	9730	0	9635	503	0
1	A3	9730	0	9637	432	0
1	A4	9703	0	9619	329	0
2	B1	111	0	127	1	0
2	B2	111	0	127	1	0
2	B3	111	0	127	1	0
2	B4	111	0	127	1	0
3	C1	138	0	144	0	0
3	C2	138	0	144	0	0
3	C3	138	0	144	0	0
3	C4	138	0	144	0	0
4	D1	5589	0	5542	199	0
4	D2	5589	0	5549	44	0
4	D3	5589	0	5536	365	0
4	D4	5589	0	5548	57	0
5	E1	137	0	130	2	0
5	E2	137	0	130	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E3	137	0	130	5	0
5	E4	137	0	130	2	0
6	F1	12779	0	12903	498	0
6	F2	12779	0	12920	194	0
7	G1	438	0	411	127	0
7	G2	438	0	413	84	0
8	H1	94	0	84	0	0
8	H2	94	0	84	0	0
9	I1	12307	0	12324	1356	0
9	I2	12307	0	12316	1831	0
10	J1	504	0	485	96	0
10	J2	504	0	487	50	0
11	K1	73	0	82	11	0
11	K2	73	0	82	0	0
12	L1	15	0	11	0	0
12	L2	15	0	11	0	0
13	M1	1372	0	1353	248	0
13	M2	1372	0	1363	29	0
13	M3	1372	0	1341	458	0
13	M4	1372	0	1363	18	0
14	N1	1401	0	1398	117	0
14	N2	1401	0	1397	40	0
14	N3	1401	0	1393	297	0
14	N4	1401	0	1393	21	0
15	O1	1971	0	1943	586	0
15	O2	1971	0	1966	166	0
15	O3	1971	0	1954	662	0
15	O4	1971	0	1966	111	0
16	P1	311	0	334	23	0
16	P2	311	0	334	2	0
16	P3	311	0	323	205	0
16	P4	311	0	334	2	0
17	Q1	8392	0	8304	1810	0
17	Q2	8359	0	8285	1714	0
18	R1	5448	0	5455	611	0
19	R2	5069	0	5067	518	0
20	S1	3805	0	3498	138	0
20	S2	3805	0	3499	118	0
21	T1	2160	0	2096	95	0
21	T2	2160	0	2095	73	0
22	U1	2438	0	2368	384	0
22	U2	2438	0	2378	56	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	V1	4535	0	4073	101	0
23	V2	4535	0	4073	102	0
24	W1	6622	0	5897	174	0
24	W2	6622	0	5907	75	0
25	X1	1321	0	1273	698	0
25	X2	1321	0	1271	910	0
26	Y1	1590	0	1630	776	0
26	Y2	1590	0	1621	1072	0
27	Z1	4990	0	4921	2638	0
27	Z2	4990	0	4936	2480	0
28	a1	1165	0	1181	0	0
28	a2	1165	0	1181	0	0
29	b1	691	0	696	0	0
29	b2	691	0	693	0	0
All	All	221308	0	217450	17039	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 40.

The worst 5 of 17039 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)
27:Z1:45:TRP:CZ2	27:Z1:95:TRP:CZ3	1.76	1.74
26:Y1:1236:ASP:HA	26:Y1:1239:PHE:CE2	1.19	1.68
27:Z2:45:TRP:CZ2	27:Z2:95:TRP:CZ3	1.76	1.68
25:X2:815:GLU:CG	26:Y2:1402:LEU:HD21	1.20	1.68
26:Y2:1339:PHE:CD2	27:Z2:630:TRP:CE3	1.81	1.68

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	A1	1205/1316 (92%)	1167 (97%)	38 (3%)	0	100	100
1	A2	1211/1316 (92%)	1172 (97%)	39 (3%)	0	100	100
1	A3	1211/1316 (92%)	1172 (97%)	39 (3%)	0	100	100
1	A4	1205/1316 (92%)	1167 (97%)	38 (3%)	0	100	100
2	B1	12/14 (86%)	11 (92%)	1 (8%)	0	100	100
2	B2	12/14 (86%)	11 (92%)	1 (8%)	0	100	100
2	B3	12/14 (86%)	11 (92%)	1 (8%)	0	100	100
2	B4	12/14 (86%)	11 (92%)	1 (8%)	0	100	100
3	C1	15/17 (88%)	11 (73%)	4 (27%)	0	100	100
3	C2	15/17 (88%)	11 (73%)	4 (27%)	0	100	100
3	C3	15/17 (88%)	11 (73%)	4 (27%)	0	100	100
3	C4	15/17 (88%)	11 (73%)	4 (27%)	0	100	100
4	D1	698/720 (97%)	668 (96%)	30 (4%)	0	100	100
4	D2	698/720 (97%)	668 (96%)	30 (4%)	0	100	100
4	D3	698/720 (97%)	668 (96%)	30 (4%)	0	100	100
4	D4	698/720 (97%)	668 (96%)	30 (4%)	0	100	100
5	E1	16/18 (89%)	16 (100%)	0	0	100	100
5	E2	16/18 (89%)	16 (100%)	0	0	100	100
5	E3	16/18 (89%)	16 (100%)	0	0	100	100
5	E4	16/18 (89%)	16 (100%)	0	0	100	100
6	F1	1611/1848 (87%)	1589 (99%)	22 (1%)	0	100	100
6	F2	1611/1848 (87%)	1589 (99%)	22 (1%)	0	100	100
7	G1	51/53 (96%)	51 (100%)	0	0	100	100
7	G2	51/53 (96%)	51 (100%)	0	0	100	100
8	H1	11/13 (85%)	7 (64%)	4 (36%)	0	100	100
8	H2	11/13 (85%)	7 (64%)	4 (36%)	0	100	100
9	I1	1508/1756 (86%)	1491 (99%)	17 (1%)	0	100	100
9	I2	1508/1756 (86%)	1491 (99%)	17 (1%)	0	100	100
10	J1	61/63 (97%)	61 (100%)	0	0	100	100
10	J2	61/63 (97%)	61 (100%)	0	0	100	100
11	K1	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
11	K2	7/9 (78%)	5 (71%)	2 (29%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	M1	165/183 (90%)	158 (96%)	7 (4%)	0	100	100
13	M2	165/183 (90%)	158 (96%)	7 (4%)	0	100	100
13	M3	165/183 (90%)	158 (96%)	7 (4%)	0	100	100
13	M4	165/183 (90%)	158 (96%)	7 (4%)	0	100	100
14	N1	174/222 (78%)	172 (99%)	2 (1%)	0	100	100
14	N2	174/222 (78%)	172 (99%)	2 (1%)	0	100	100
14	N3	174/222 (78%)	172 (99%)	2 (1%)	0	100	100
14	N4	174/222 (78%)	172 (99%)	2 (1%)	0	100	100
15	O1	239/241 (99%)	214 (90%)	25 (10%)	0	100	100
15	O2	239/241 (99%)	214 (90%)	25 (10%)	0	100	100
15	O3	239/241 (99%)	213 (89%)	26 (11%)	0	100	100
15	O4	239/241 (99%)	212 (89%)	27 (11%)	0	100	100
16	P1	38/40 (95%)	31 (82%)	7 (18%)	0	100	100
16	P2	38/40 (95%)	31 (82%)	7 (18%)	0	100	100
16	P3	38/40 (95%)	31 (82%)	7 (18%)	0	100	100
16	P4	38/40 (95%)	31 (82%)	7 (18%)	0	100	100
17	Q1	1013/1100 (92%)	946 (93%)	51 (5%)	16 (2%)	9	44
17	Q2	1007/1100 (92%)	940 (93%)	52 (5%)	15 (2%)	10	46
18	R1	657/720 (91%)	600 (91%)	45 (7%)	12 (2%)	8	40
19	R2	612/726 (84%)	560 (92%)	40 (6%)	12 (2%)	7	38
20	S1	491/621 (79%)	451 (92%)	30 (6%)	10 (2%)	7	38
20	S2	491/621 (79%)	451 (92%)	30 (6%)	10 (2%)	7	38
21	T1	270/286 (94%)	228 (84%)	36 (13%)	6 (2%)	6	35
21	T2	270/286 (94%)	228 (84%)	36 (13%)	6 (2%)	6	35
22	U1	303/346 (88%)	266 (88%)	31 (10%)	6 (2%)	7	38
22	U2	303/346 (88%)	266 (88%)	31 (10%)	6 (2%)	7	38
23	V1	592/698 (85%)	532 (90%)	50 (8%)	10 (2%)	9	42
23	V2	592/698 (85%)	532 (90%)	50 (8%)	10 (2%)	9	42
24	W1	858/1037 (83%)	798 (93%)	49 (6%)	11 (1%)	12	48
24	W2	858/1037 (83%)	798 (93%)	48 (6%)	12 (1%)	11	46
25	X1	158/187 (84%)	155 (98%)	2 (1%)	1 (1%)	25	66

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
25	X2	158/187 (84%)	156 (99%)	0	2 (1%)	12 48
26	Y1	183/340 (54%)	175 (96%)	6 (3%)	2 (1%)	14 52
26	Y2	183/340 (54%)	174 (95%)	7 (4%)	2 (1%)	14 52
27	Z1	598/713 (84%)	509 (85%)	51 (8%)	38 (6%)	1 16
27	Z2	598/713 (84%)	511 (86%)	50 (8%)	37 (6%)	1 17
28	a1	144/146 (99%)	120 (83%)	19 (13%)	5 (4%)	3 25
28	a2	144/146 (99%)	119 (83%)	20 (14%)	5 (4%)	3 25
29	b1	84/86 (98%)	73 (87%)	4 (5%)	7 (8%)	1 12
29	b2	84/86 (98%)	76 (90%)	4 (5%)	4 (5%)	2 21
All	All	27409/31134 (88%)	25871 (94%)	1293 (5%)	245 (1%)	21 57

5 of 245 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	Q1	168	LYS
17	Q1	199	PRO
17	Q1	386	PHE
17	Q1	545	TYR
17	Q1	546	ILE

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	A1	1058/1111 (95%)	1051 (99%)	7 (1%)	84 90
1	A2	1061/1111 (96%)	1054 (99%)	7 (1%)	84 90
1	A3	1061/1111 (96%)	1054 (99%)	7 (1%)	84 90
1	A4	1058/1111 (95%)	1051 (99%)	7 (1%)	84 90
2	B1	12/12 (100%)	12 (100%)	0	100 100
2	B2	12/12 (100%)	12 (100%)	0	100 100
2	B3	12/12 (100%)	12 (100%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B4	12/12 (100%)	12 (100%)	0	100	100
3	C1	17/17 (100%)	17 (100%)	0	100	100
3	C2	17/17 (100%)	17 (100%)	0	100	100
3	C3	17/17 (100%)	17 (100%)	0	100	100
3	C4	17/17 (100%)	17 (100%)	0	100	100
4	D1	584/593 (98%)	568 (97%)	16 (3%)	44	65
4	D2	584/593 (98%)	568 (97%)	16 (3%)	44	65
4	D3	584/593 (98%)	568 (97%)	16 (3%)	44	65
4	D4	584/593 (98%)	568 (97%)	16 (3%)	44	65
5	E1	14/14 (100%)	13 (93%)	1 (7%)	14	39
5	E2	14/14 (100%)	13 (93%)	1 (7%)	14	39
5	E3	14/14 (100%)	13 (93%)	1 (7%)	14	39
5	E4	14/14 (100%)	13 (93%)	1 (7%)	14	39
6	F1	1350/1507 (90%)	1350 (100%)	0	100	100
6	F2	1350/1507 (90%)	1350 (100%)	0	100	100
7	G1	47/47 (100%)	47 (100%)	0	100	100
7	G2	47/47 (100%)	47 (100%)	0	100	100
8	H1	10/10 (100%)	10 (100%)	0	100	100
8	H2	10/10 (100%)	10 (100%)	0	100	100
9	I1	1340/1509 (89%)	1339 (100%)	1 (0%)	93	97
9	I2	1340/1509 (89%)	1339 (100%)	1 (0%)	93	97
10	J1	54/54 (100%)	54 (100%)	0	100	100
10	J2	54/54 (100%)	54 (100%)	0	100	100
11	K1	9/9 (100%)	9 (100%)	0	100	100
11	K2	9/9 (100%)	9 (100%)	0	100	100
12	L1	1/1 (100%)	1 (100%)	0	100	100
12	L2	1/1 (100%)	1 (100%)	0	100	100
13	M1	146/154 (95%)	146 (100%)	0	100	100
13	M2	146/154 (95%)	146 (100%)	0	100	100
13	M3	146/154 (95%)	146 (100%)	0	100	100
13	M4	146/154 (95%)	146 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N1	150/173 (87%)	150 (100%)	0	100	100
14	N2	150/173 (87%)	150 (100%)	0	100	100
14	N3	150/173 (87%)	150 (100%)	0	100	100
14	N4	150/173 (87%)	150 (100%)	0	100	100
15	O1	213/213 (100%)	213 (100%)	0	100	100
15	O2	213/213 (100%)	213 (100%)	0	100	100
15	O3	213/213 (100%)	213 (100%)	0	100	100
15	O4	213/213 (100%)	213 (100%)	0	100	100
16	P1	32/32 (100%)	32 (100%)	0	100	100
16	P2	32/32 (100%)	32 (100%)	0	100	100
16	P3	32/32 (100%)	32 (100%)	0	100	100
16	P4	32/32 (100%)	32 (100%)	0	100	100
17	Q1	967/1034 (94%)	929 (96%)	38 (4%)	32	56
17	Q2	964/1034 (93%)	926 (96%)	38 (4%)	32	56
18	R1	615/663 (93%)	590 (96%)	25 (4%)	30	55
19	R2	570/669 (85%)	545 (96%)	25 (4%)	28	53
20	S1	367/567 (65%)	332 (90%)	35 (10%)	8	27
20	S2	367/567 (65%)	332 (90%)	35 (10%)	8	27
21	T1	233/243 (96%)	223 (96%)	10 (4%)	29	53
21	T2	233/243 (96%)	224 (96%)	9 (4%)	32	56
22	U1	269/303 (89%)	261 (97%)	8 (3%)	41	63
22	U2	269/303 (89%)	261 (97%)	8 (3%)	41	63
23	V1	424/628 (68%)	415 (98%)	9 (2%)	53	72
23	V2	424/628 (68%)	414 (98%)	10 (2%)	49	69
24	W1	639/972 (66%)	616 (96%)	23 (4%)	35	59
24	W2	639/972 (66%)	616 (96%)	23 (4%)	35	59
25	X1	155/174 (89%)	151 (97%)	4 (3%)	46	66
25	X2	155/174 (89%)	150 (97%)	5 (3%)	39	61
26	Y1	178/312 (57%)	170 (96%)	8 (4%)	27	52
26	Y2	178/312 (57%)	163 (92%)	15 (8%)	11	33
27	Z1	577/670 (86%)	544 (94%)	33 (6%)	20	45

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	Z2	577/670 (86%)	548 (95%)	29 (5%)	24	49
28	a1	132/131 (101%)	128 (97%)	4 (3%)	41	63
28	a2	132/131 (101%)	128 (97%)	4 (3%)	41	63
29	b1	75/75 (100%)	71 (95%)	4 (5%)	22	47
29	b2	75/75 (100%)	70 (93%)	5 (7%)	16	41
All	All	23746/27100 (88%)	23241 (98%)	505 (2%)	56	72

5 of 505 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	S1	351	ILE
27	Z1	582	GLU
20	S2	547	ARG
27	Z1	380	ILE
27	Z2	582	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 249 such sidechains are listed below:

Mol	Chain	Res	Type
17	Q2	938	ASN
27	Z2	260	HIS
22	U1	313	ASN
27	Z2	248	ASN
28	a1	969	ASN

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
18	R1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	R1	436:LEU	C	437:ASN	N	16.70

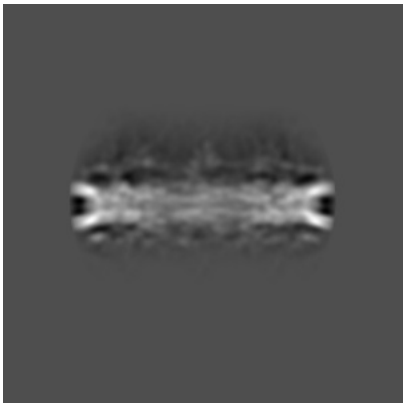
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10198. These allow visual inspection of the internal detail of the map and identification of artifacts.

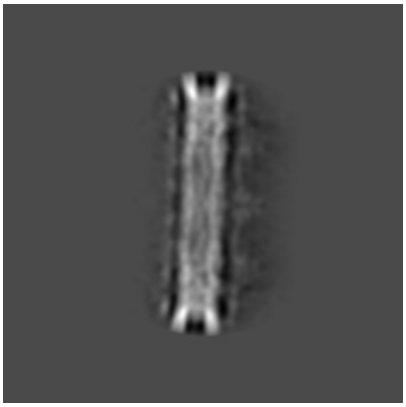
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

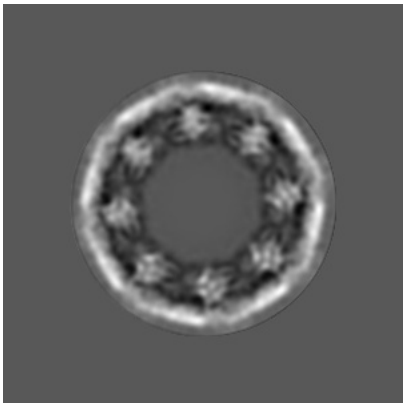
6.1.1 Primary map



X



Y



Z

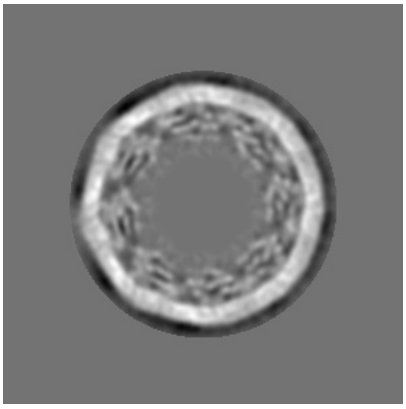
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map

X Index: 144

Y Index: 144



Z Index: 144

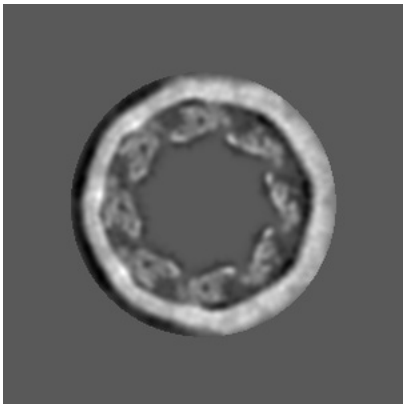
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 67

Y Index: 219



Z Index: 134

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.0606. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

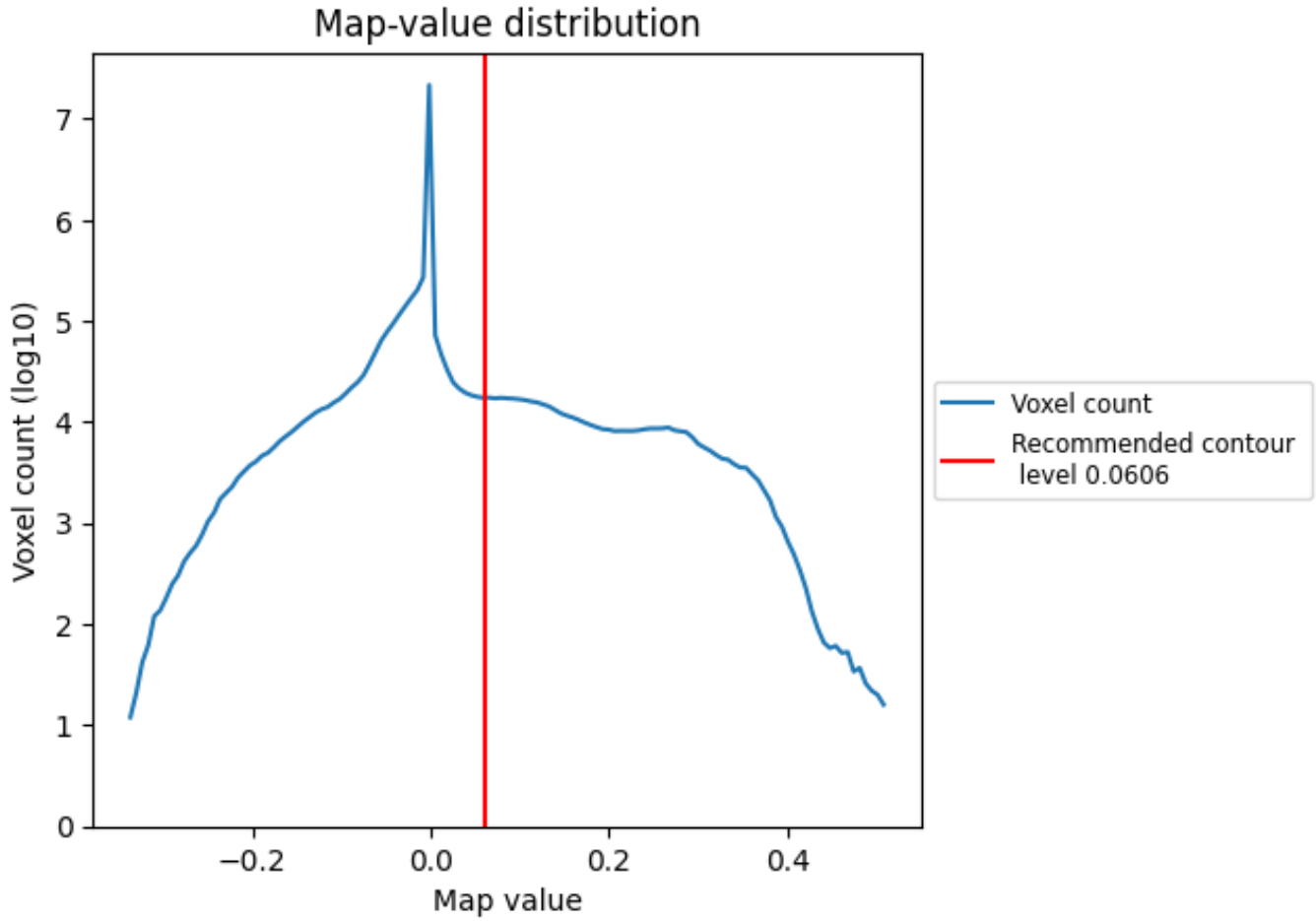
6.5 Mask visualisation (i)

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

7 Map analysis

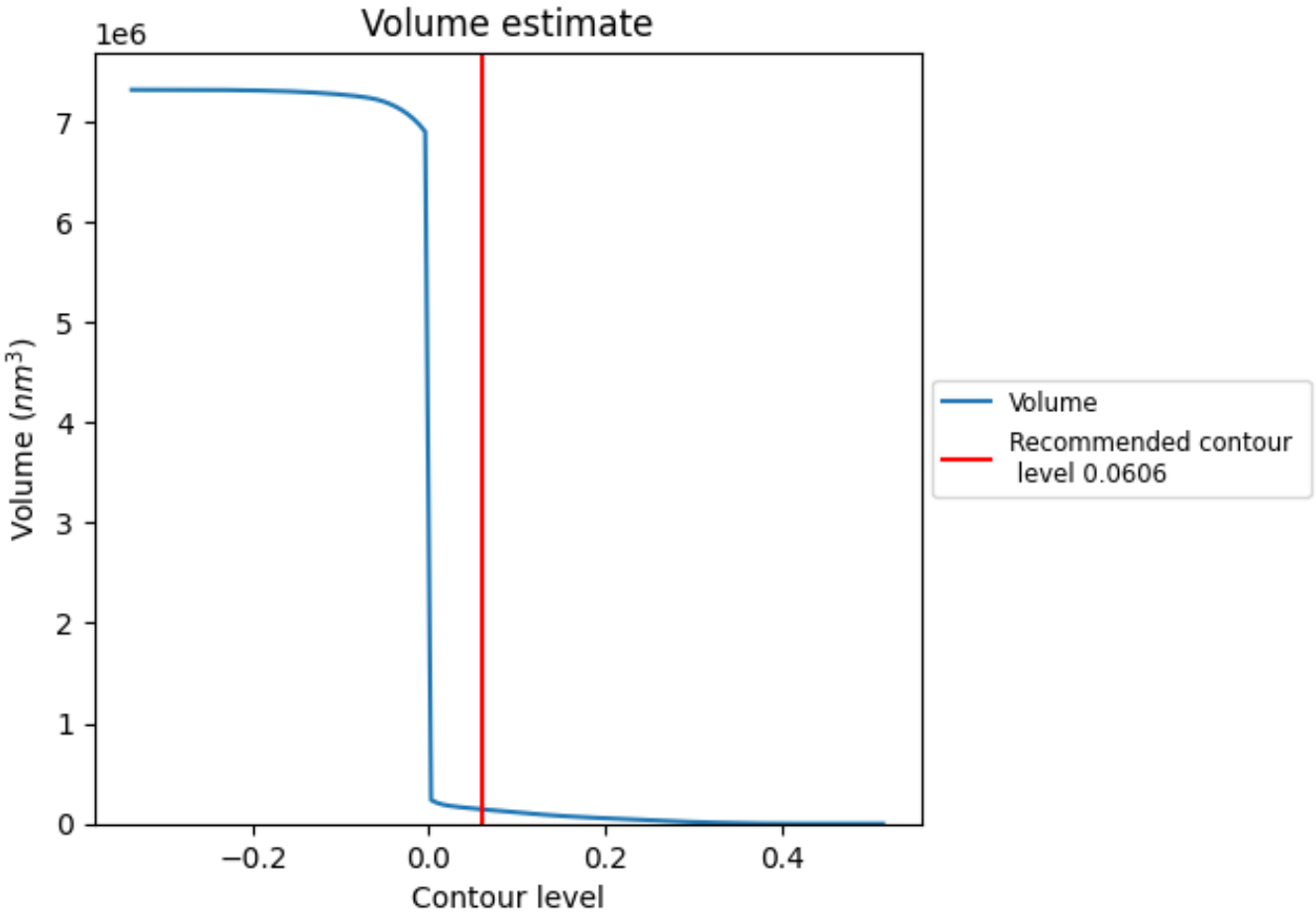
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

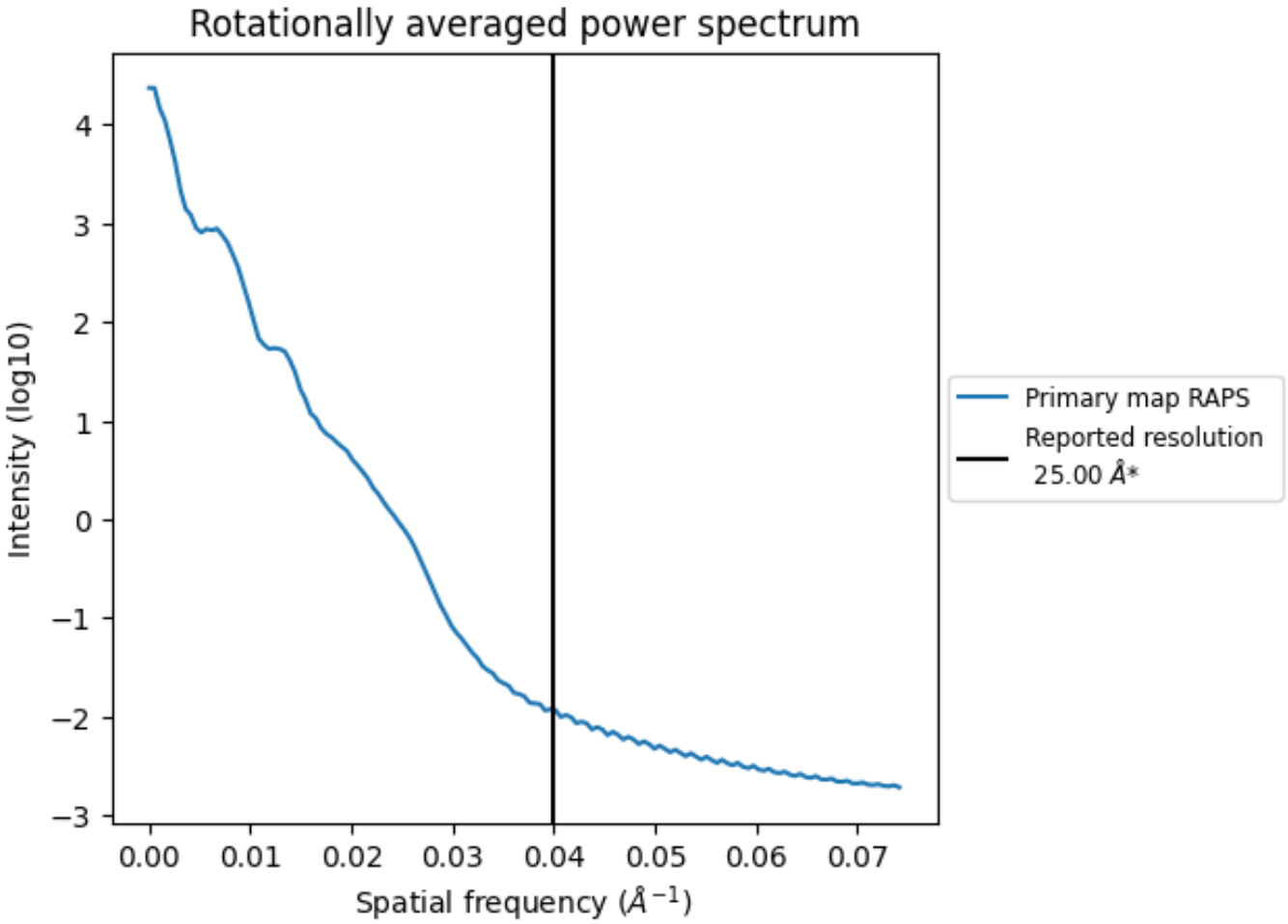
7.2 Volume estimate (i)



The volume at the recommended contour level is 143354 nm^3; this corresponds to an approximate mass of 129496 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 0.040 Å^{-1}

8 Fourier-Shell correlation (i)

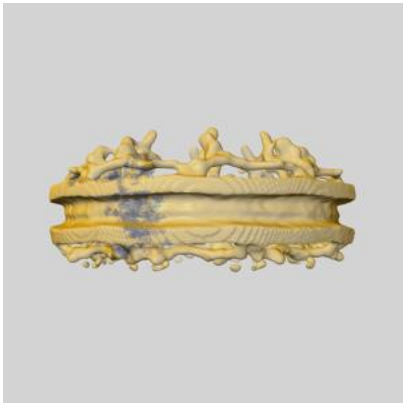
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

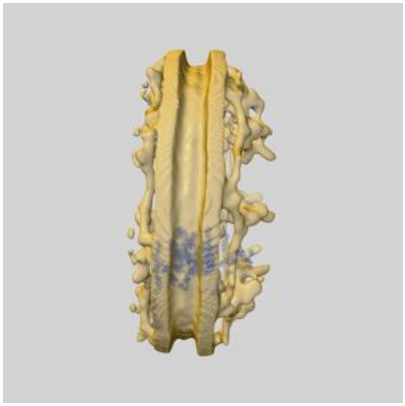
This section contains information regarding the fit between EMDB map EMD-10198 and PDB model 7TBI. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlays

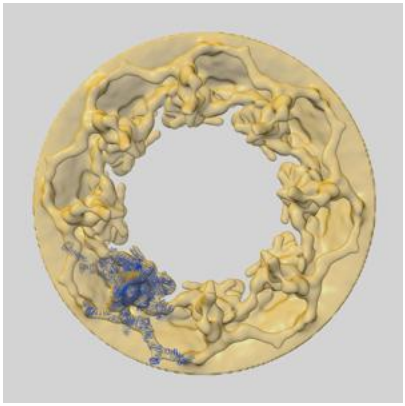
9.1.1 Map-model overlay



X

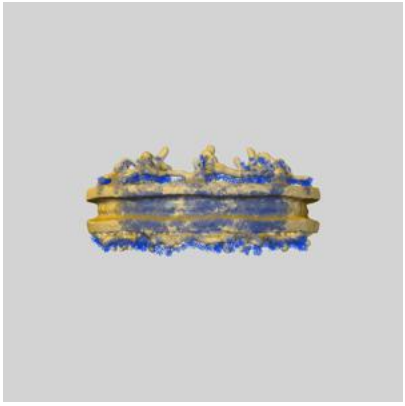


Y

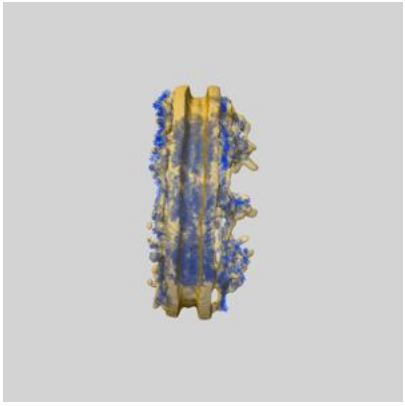


Z

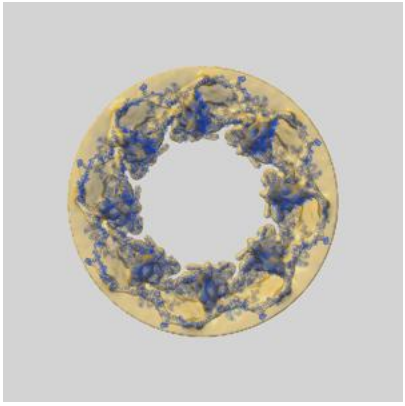
9.1.2 Map-model assembly overlay



X



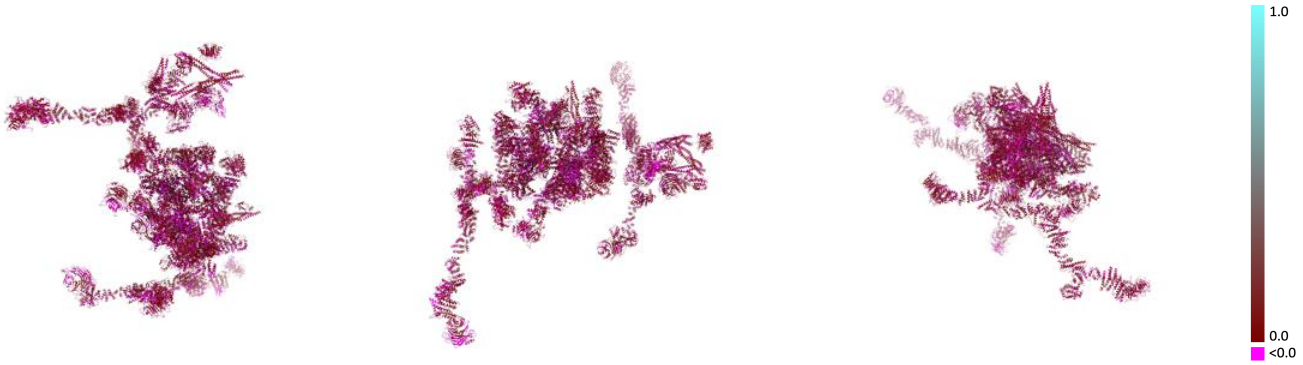
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0606 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.

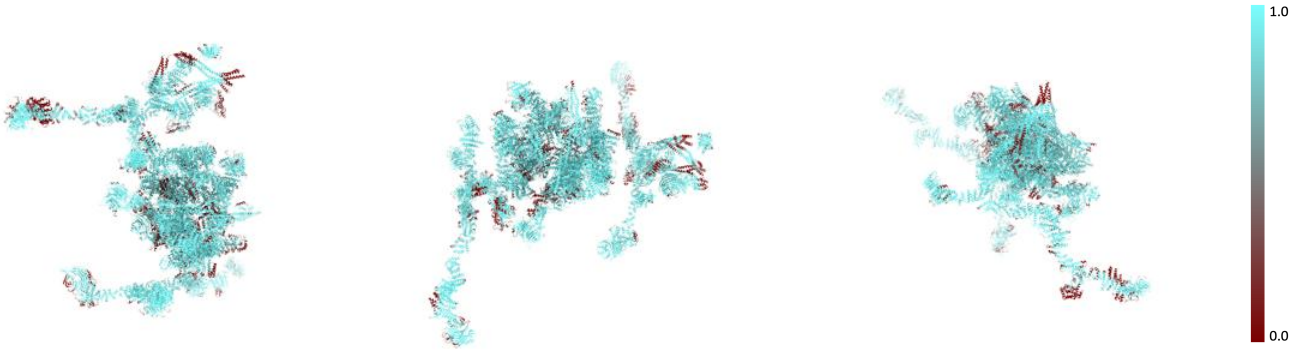
9.2 Q-score mapped to coordinate model



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.

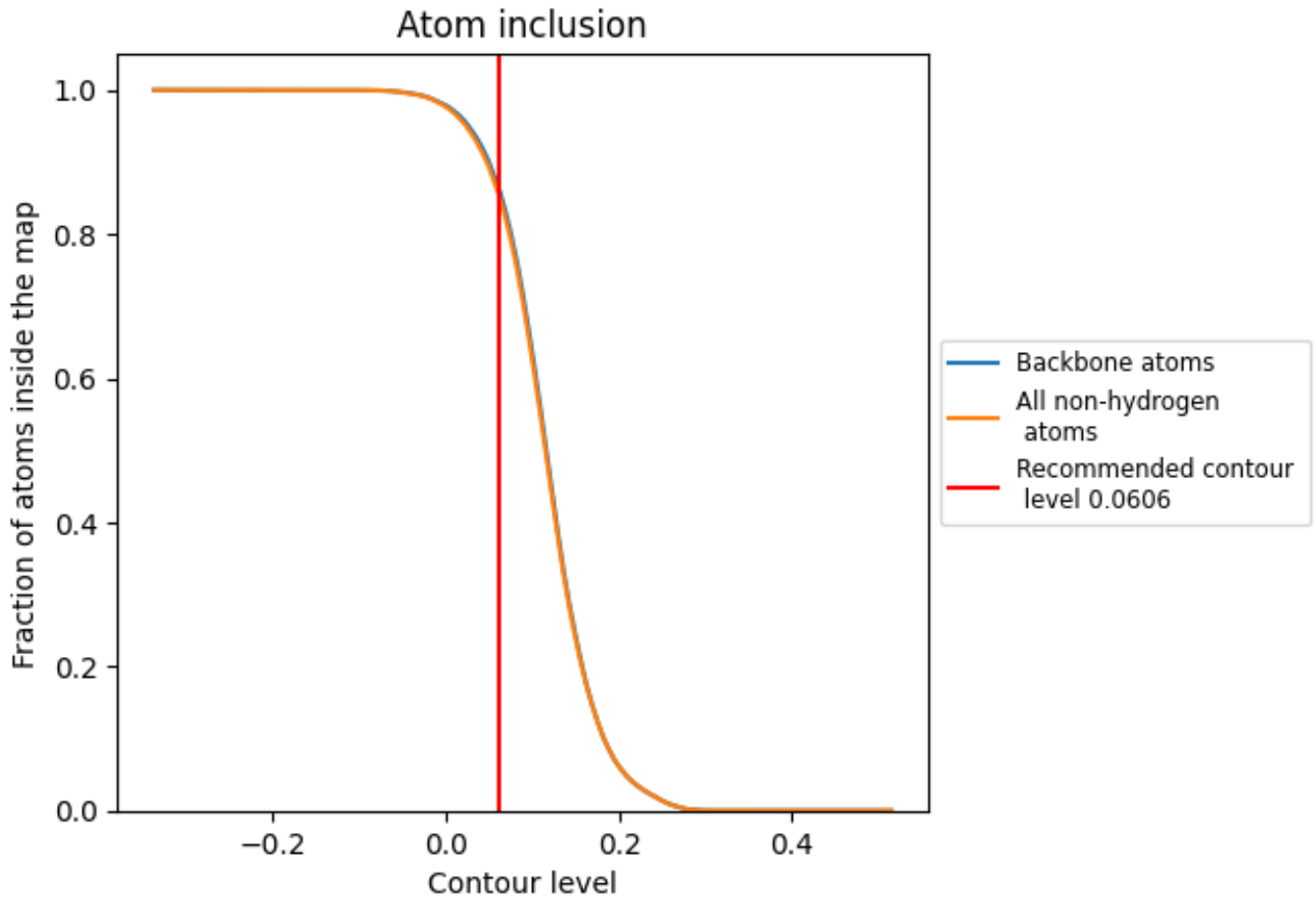
9.3 Atom inclusion mapped to coordinate model



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 (0.0606).

9.4 Atom inclusion (i)



At the recommended contour level, 87% 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 (0.0606) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8571	0.0390
A1	0.8768	0.0350
A2	0.8109	0.0310
A3	0.8042	0.0280
A4	0.8800	0.0400
B1	0.3761	-0.0070
B2	0.9817	-0.0050
B3	0.9450	0.0050
B4	0.5138	0.0150
C1	0.4338	0.0240
C2	0.1250	-0.0020
C3	0.0074	-0.0530
C4	1.0000	0.0600
D1	0.7618	0.0380
D2	0.8527	0.0480
D3	0.8241	0.0290
D4	0.6823	0.0380
E1	0.0662	-0.0330
E2	0.4706	-0.0120
E3	0.5515	0.0210
E4	0.6765	0.0440
F1	0.9806	0.0410
F2	0.9657	0.0410
G1	0.9813	0.0230
G2	0.9977	0.0280
H1	1.0000	0.0400
H2	1.0000	0.0300
I1	0.9384	0.0370
I2	0.8960	0.0340
J1	0.8540	0.0140
J2	0.6288	0.0080
K1	1.0000	0.0010
K2	1.0000	0.0450
L1	1.0000	0.0910
L2	1.0000	0.0070

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
M1	0.9889	0.0540
M2	0.8826	0.0570
M3	0.9799	0.0540
M4	0.8447	0.0490
N1	0.9235	0.0390
N2	0.8144	0.0360
N3	0.9755	0.0390
N4	0.8542	0.0530
O1	0.8947	0.0320
O2	0.7753	0.0340
O3	0.9310	0.0500
O4	0.7286	0.0400
P1	1.0000	0.0570
P2	1.0000	0.0950
P3	1.0000	-0.0310
P4	1.0000	0.1040
Q1	0.5909	0.0440
Q2	0.8523	0.0390
R1	0.8406	0.0590
R2	0.9020	0.0550
S1	0.9378	0.0560
S2	0.8858	0.0500
T1	0.9505	0.0470
T2	0.9618	0.0390
U1	0.9778	0.0500
U2	0.9586	0.0270
V1	0.8807	0.0490
V2	0.9832	0.0340
W1	0.9349	0.0440
W2	0.7669	0.0310
X1	0.5263	0.0350
X2	0.8764	0.0490
Y1	0.6060	0.0240
Y2	0.8351	0.0290
Z1	0.8904	0.0340
Z2	0.8783	0.0330
a1	0.1183	-0.0260
a2	0.2918	0.0050
b1	0.8419	0.0560
b2	0.9122	0.0540