wwPDB EM Validation Summary Report (i)

Jul 8, 2024 – 01:35 pm BST

PDB ID	:	7PEQ
EMDB ID	:	EMD-12814
Title	:	Model of the outer rings of the human nuclear pore complex
Authors	:	Schuller, A.P.; Wojtynek, M.; Mankus, D.; Tatli, M.; Kronenberg-Tenga, R.; Regmi, S.G.; Dasso, M.; Weis, K.; Medalia, O.; Schwartz, T.U.
Deposited on	:	2021-08-11
Resolution	:	35.00 Å(reported)
Based on initial model	:	5A9Q

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:

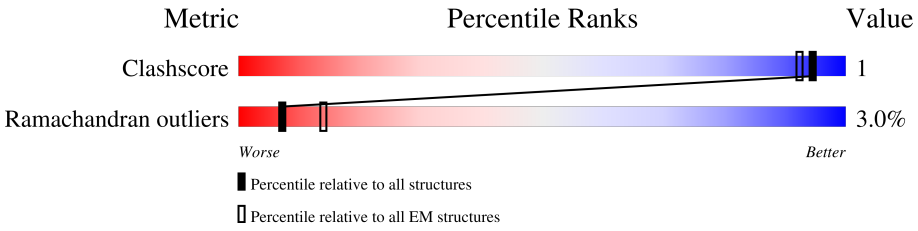
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance

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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023

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	AC	1156	45% 54%
1	BC	1156	45% 54%
1	CC	1156	6% 45% 54%
1	DC	1156	45% 54%
2	AD	925	70% 27%
2	BD	925	72% 27%
2	CD	925	72% 27%
2	DD	925	72% 27%
3	AE	937	54% 42%

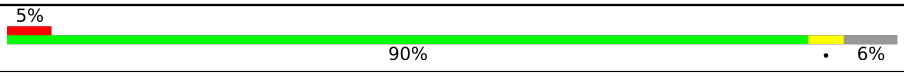
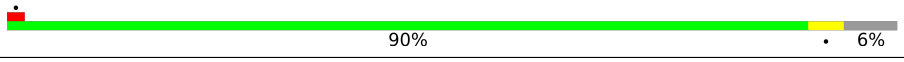
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	BE	937	11% 55% 42%
3	CE	937	55% 42%
3	DE	937	55% 42%
4	AF	322	87% 11%
4	BF	322	85% 11%
4	CF	322	86% 11%
4	DF	322	85% 11%
5	AG	360	18% 85% 12%
5	BG	360	10% 86% 12%
5	CG	360	15% 86% 12%
5	DG	360	86% 12%
6	AH	656	90% 6%
6	BH	656	6% 90% 6%
6	CH	656	90% 6%
6	DH	656	6% 90% 6%
7	AI	380	80% 17%
7	BI	380	80% 17%
7	CI	380	80% 17%
7	DI	380	80% 17%
8	AJ	1436	18% 66% 31%
8	BJ	1436	15% 65% 31%
8	CJ	1436	7% 65% 31%
8	DJ	1436	6% 65% 31%
9	AK	326	5% 91% 6%
9	BK	326	90% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	CK	326	
9	DK	326	

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 91352 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 Nup133.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	AC	528	Total 2629	C 1573	N 528	O 528	0	0
1	BC	528	Total 2629	C 1573	N 528	O 528	0	0
1	CC	528	Total 2629	C 1573	N 528	O 528	0	0
1	DC	528	Total 2629	C 1573	N 528	O 528	0	0

- Molecule 2 is a protein called Nuclear pore complex protein Nup107.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	AD	678	Total 3367	C 2011	N 678	O 678	0	0
2	BD	678	Total 3367	C 2011	N 678	O 678	0	0
2	CD	678	Total 3367	C 2011	N 678	O 678	0	0
2	DD	678	Total 3367	C 2011	N 678	O 678	0	0

- Molecule 3 is a protein called Nuclear pore complex protein Nup96.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	AE	543	Total 2700	C 1614	N 543	O 543	0	0
3	BE	543	Total 2700	C 1614	N 543	O 543	0	0
3	CE	543	Total 2700	C 1614	N 543	O 543	0	0
3	DE	543	Total 2700	C 1614	N 543	O 543	0	0

- Molecule 4 is a protein called Protein SEC13 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	AF	285	Total	C	N	O	0	0
			1402	832	285	285		
4	BF	285	Total	C	N	O	0	0
			1402	832	285	285		
4	CF	285	Total	C	N	O	0	0
			1402	832	285	285		
4	DF	285	Total	C	N	O	0	0
			1402	832	285	285		

- Molecule 5 is a protein called Nucleoporin SEH1.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	AG	316	Total	C	N	O	0	0
			1564	932	316	316		
5	BG	316	Total	C	N	O	0	0
			1564	932	316	316		
5	CG	316	Total	C	N	O	0	0
			1564	932	316	316		
5	DG	316	Total	C	N	O	0	0
			1564	932	316	316		

- Molecule 6 is a protein called Nuclear pore complex protein Nup85.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	AH	632	Total	C	N	O	0	0
			3134	1870	632	632		
6	BH	632	Total	C	N	O	0	0
			3134	1870	632	632		
6	CH	632	Total	C	N	O	0	0
			3134	1870	632	632		
6	DH	632	Total	C	N	O	0	0
			3134	1870	632	632		

- Molecule 7 is a protein called Nucleoporin Nup43.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	AI	316	Total	C	N	O	22	0
			1599	963	318	318		
7	BI	316	Total	C	N	O	22	0
			1599	963	318	318		
7	CI	316	Total	C	N	O	18	0
			1599	963	318	318		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
7	DI	316	Total 1599	C 963	N 318	O 318	18	0

- Molecule 8 is a protein called Nuclear pore complex protein Nup160.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	AJ	996	Total 4932	C 2940	N 996	O 996	0	0
8	BJ	996	Total 4932	C 2940	N 996	O 996	0	0
8	CJ	996	Total 4932	C 2940	N 996	O 996	0	0
8	DJ	996	Total 4932	C 2940	N 996	O 996	0	0

- Molecule 9 is a protein called Nucleoporin Nup37.

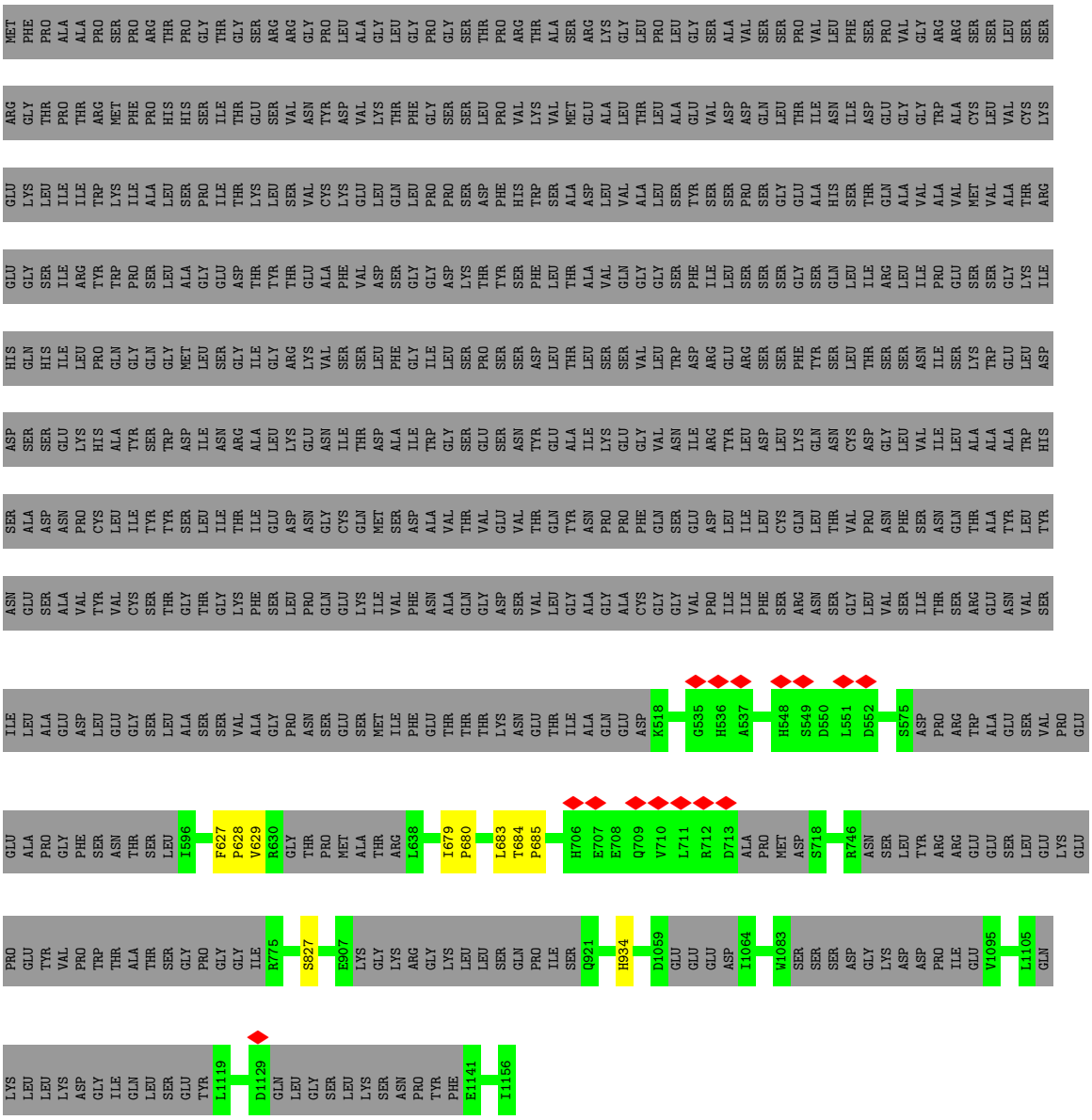
Mol	Chain	Residues	Atoms				AltConf	Trace
9	AK	307	Total 1511	C 897	N 307	O 307	0	0
9	BK	307	Total 1511	C 897	N 307	O 307	0	0
9	CK	307	Total 1511	C 897	N 307	O 307	0	0
9	DK	307	Total 1511	C 897	N 307	O 307	0	0

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.

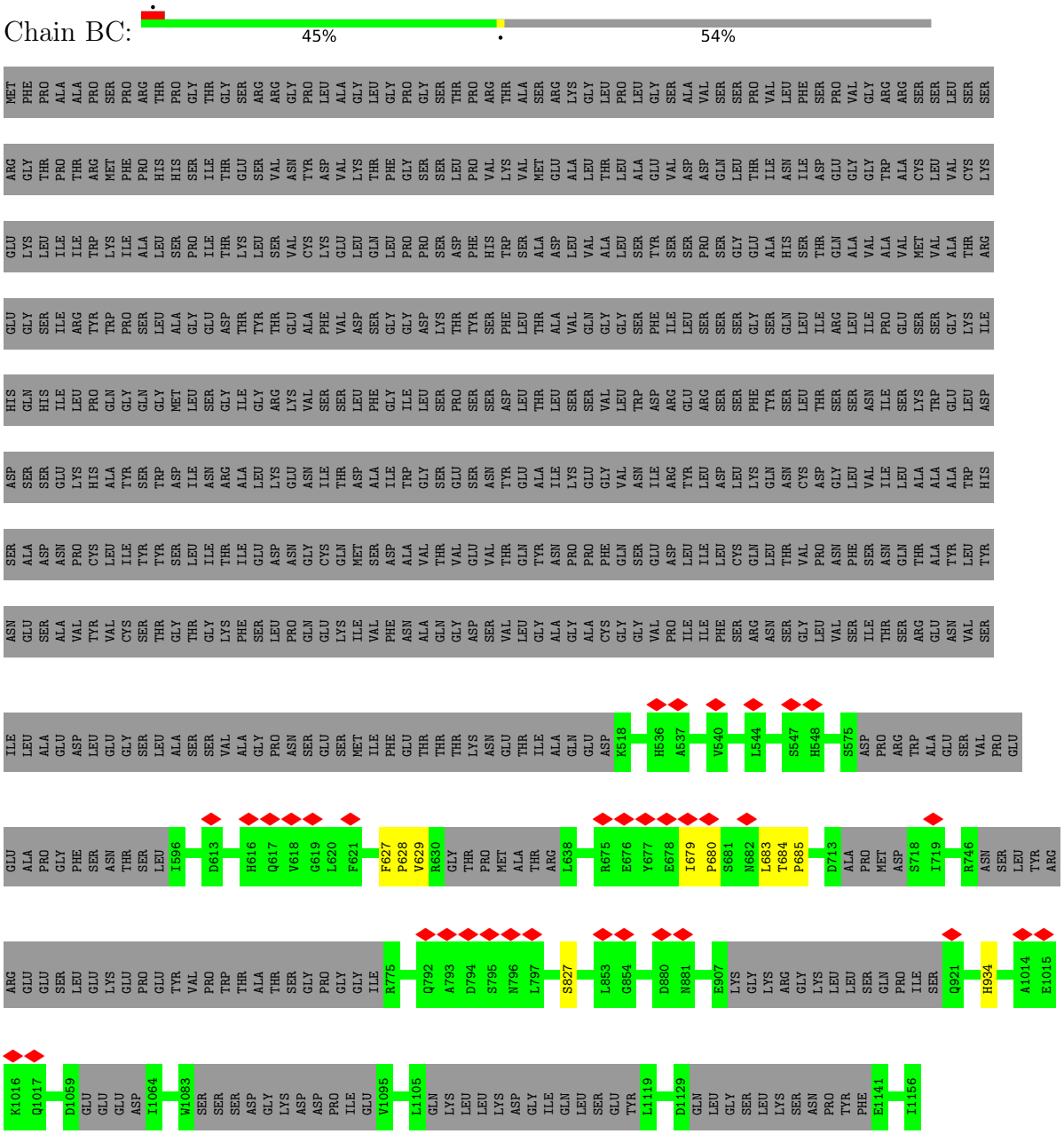
- Molecule 1: Nuclear pore complex protein Nup133

Chain AC:



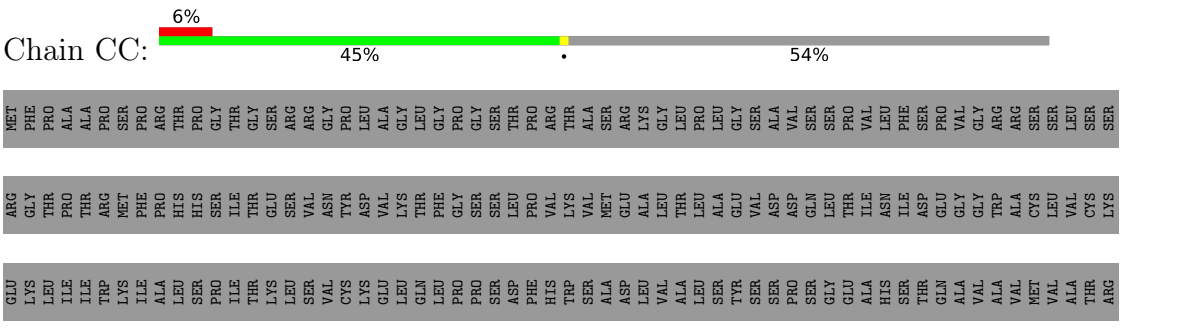
• Molecule 1: Nuclear pore complex protein Nup133

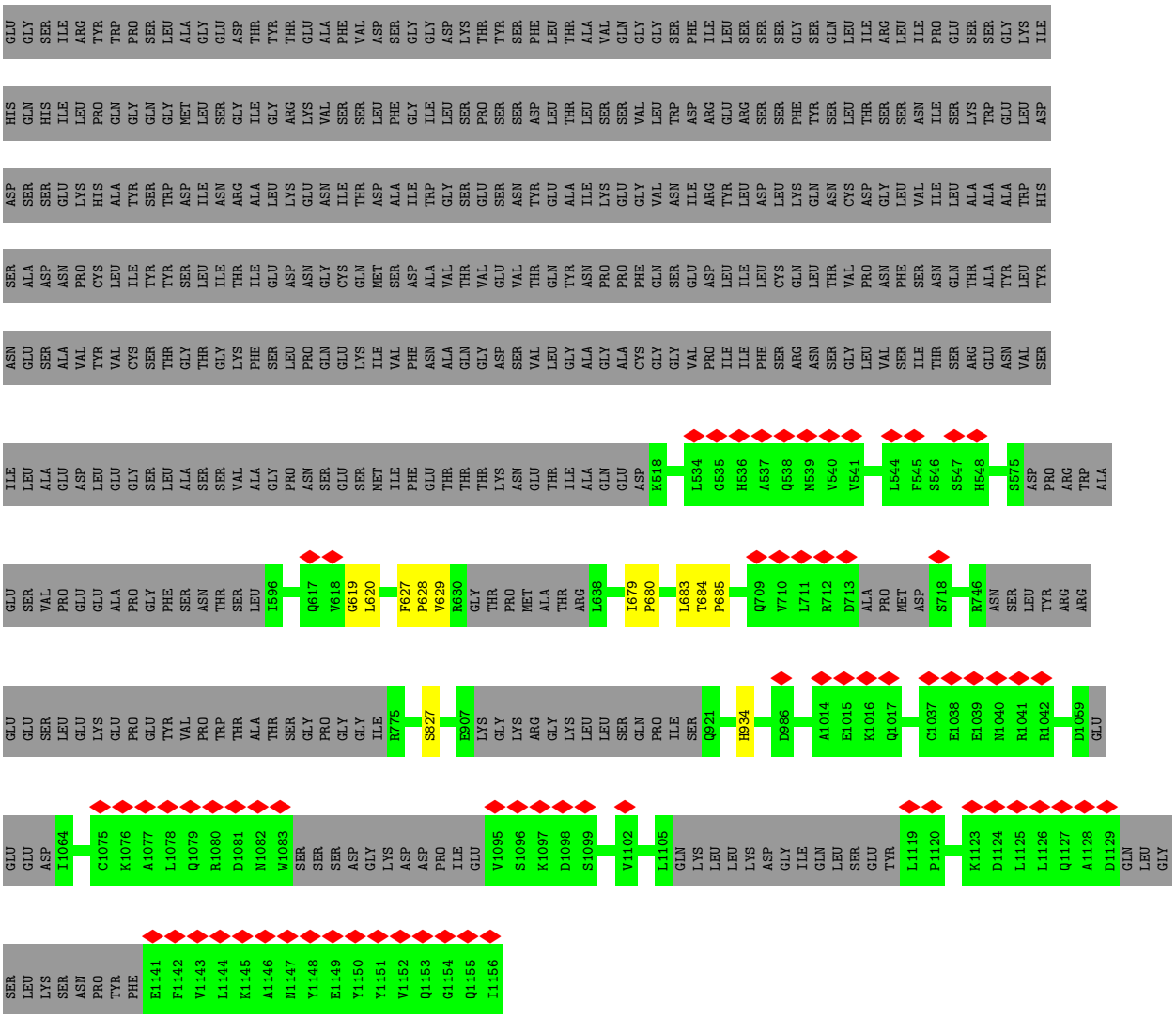
Chain BC:



• Molecule 1: Nuclear pore complex protein Nup133

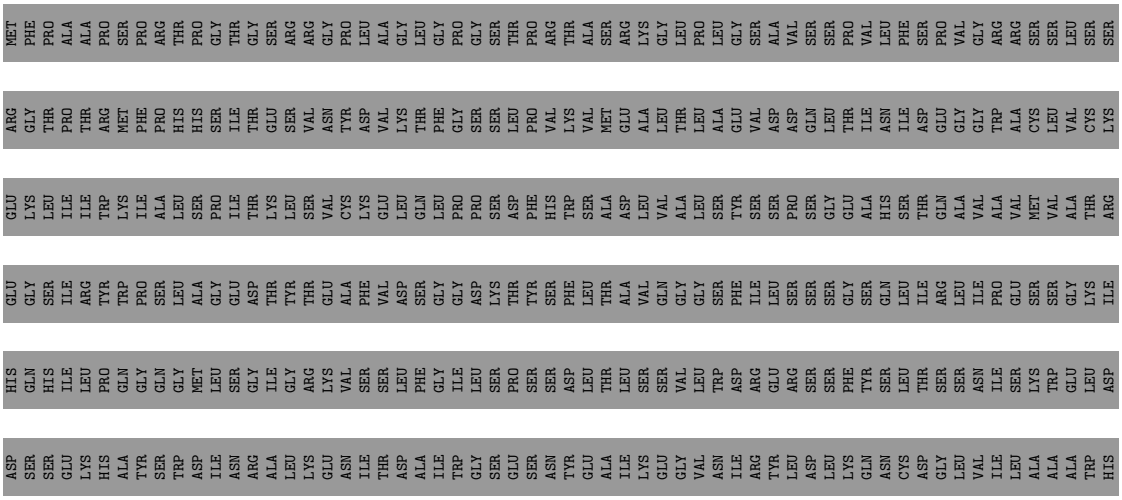
Chain CC:

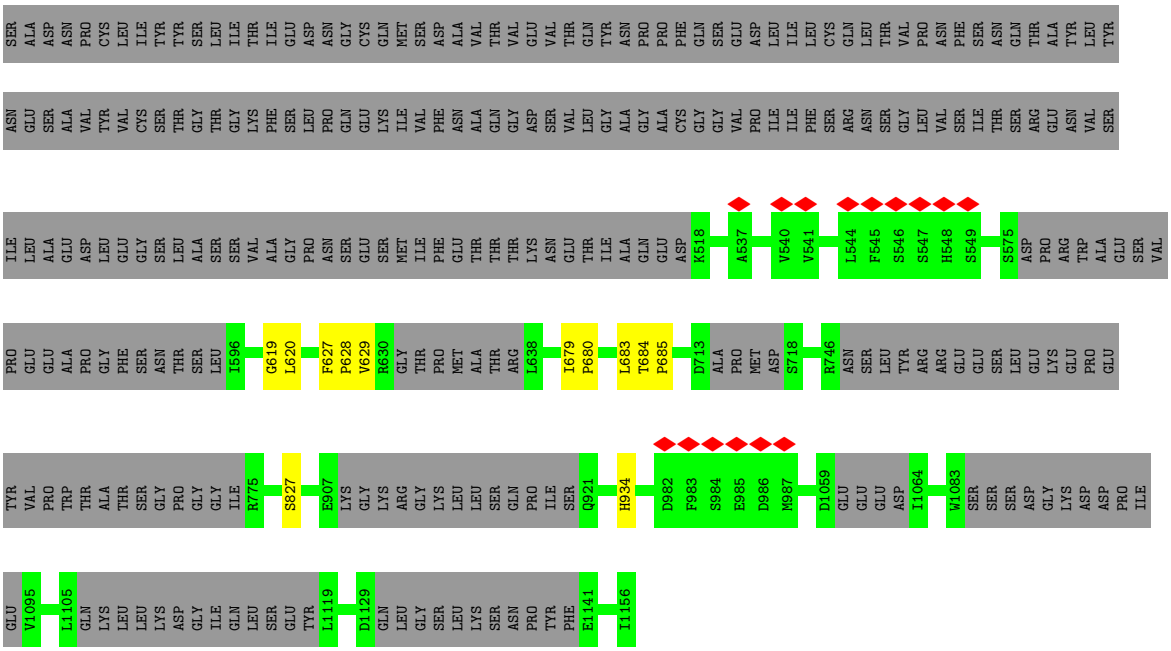




• Molecule 1: Nuclear pore complex protein Nup133

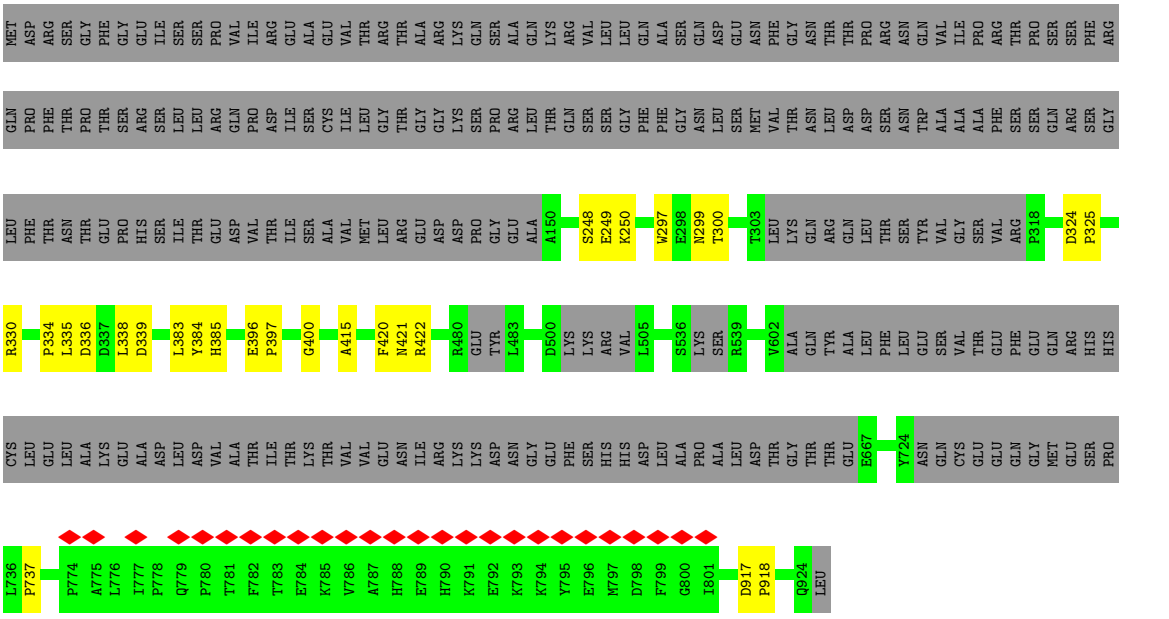
Chain DC:





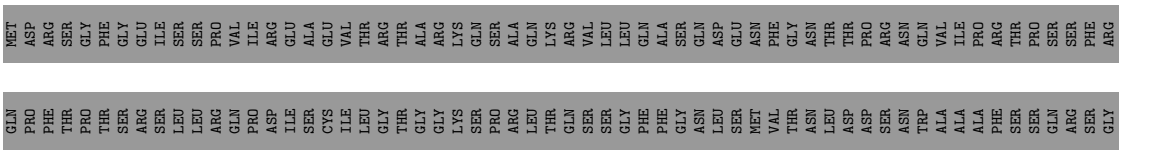
• Molecule 2: Nuclear pore complex protein Nup107

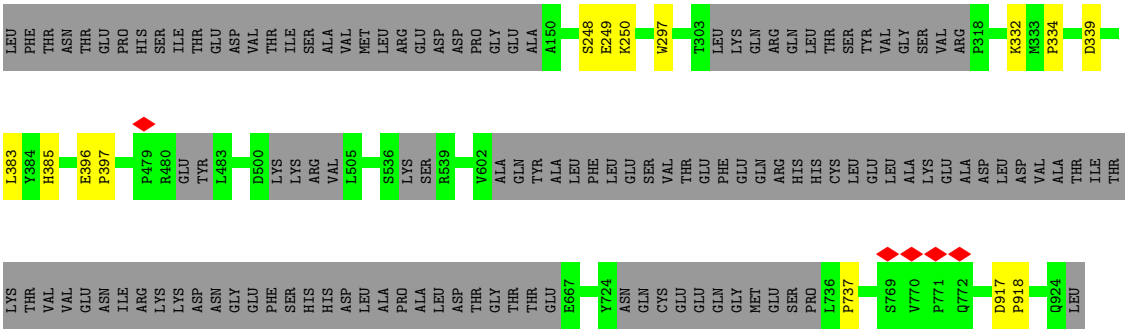
Chain AD:



• Molecule 2: Nuclear pore complex protein Nup107

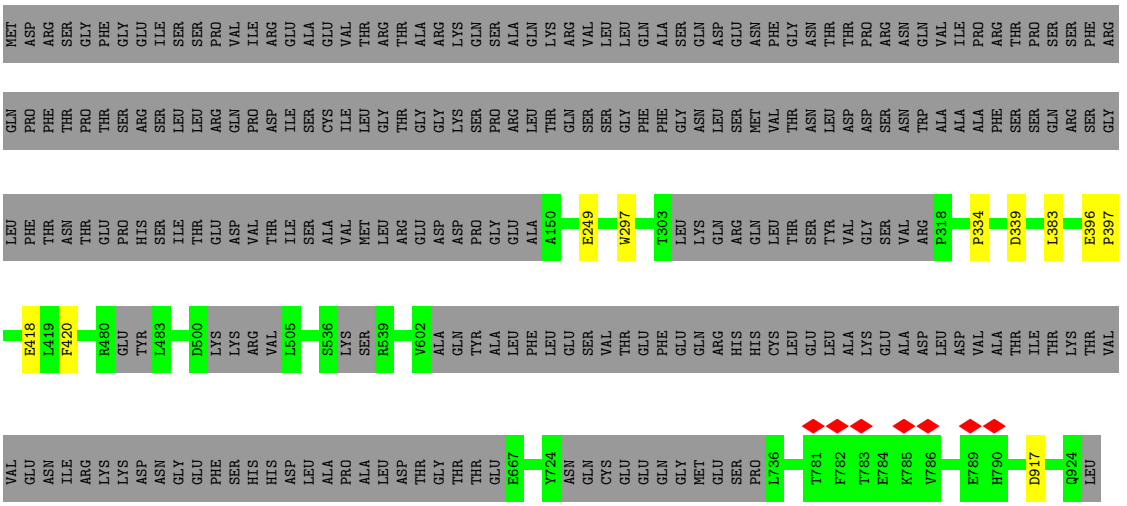
Chain BD:





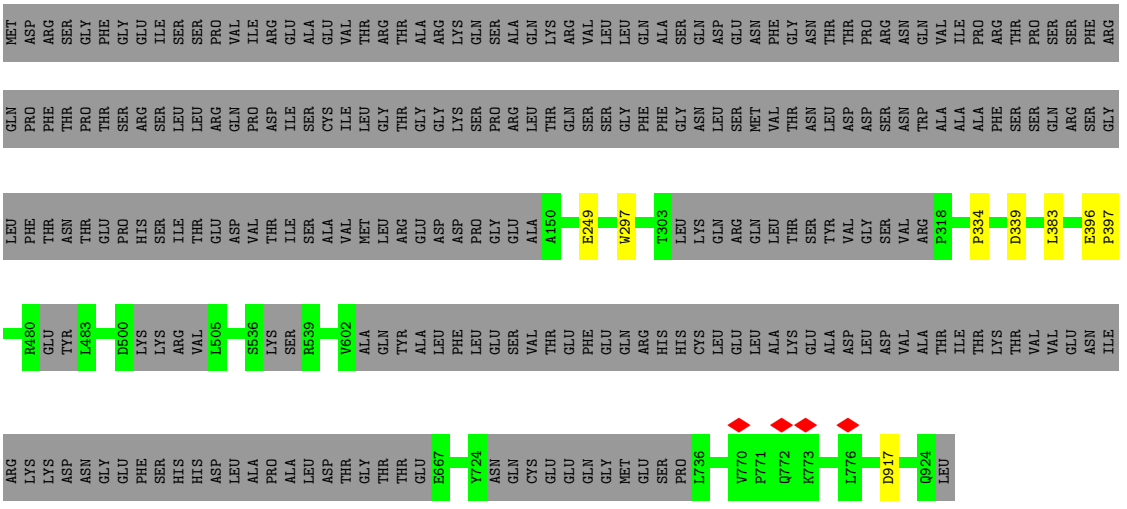
• Molecule 2: Nuclear pore complex protein Nup107

Chain CD:



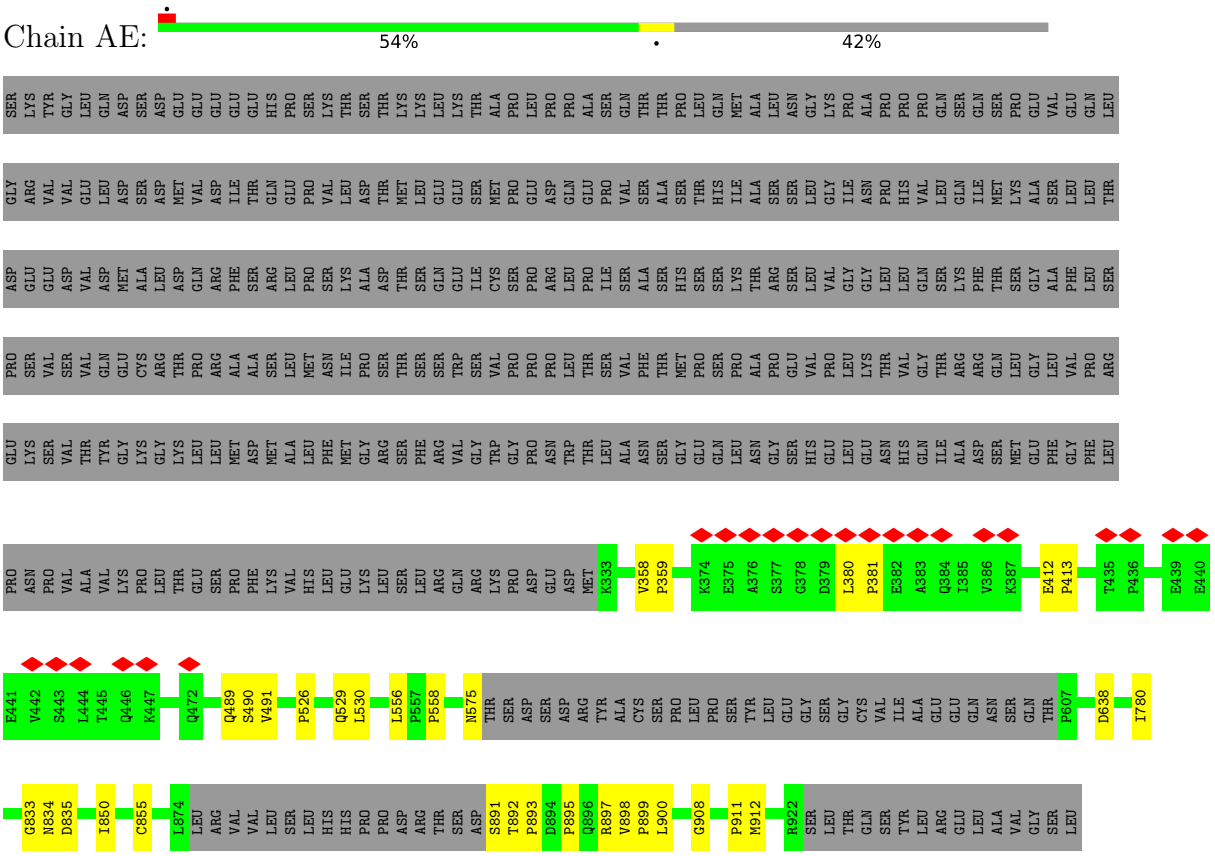
• Molecule 2: Nuclear pore complex protein Nup107

Chain DD:



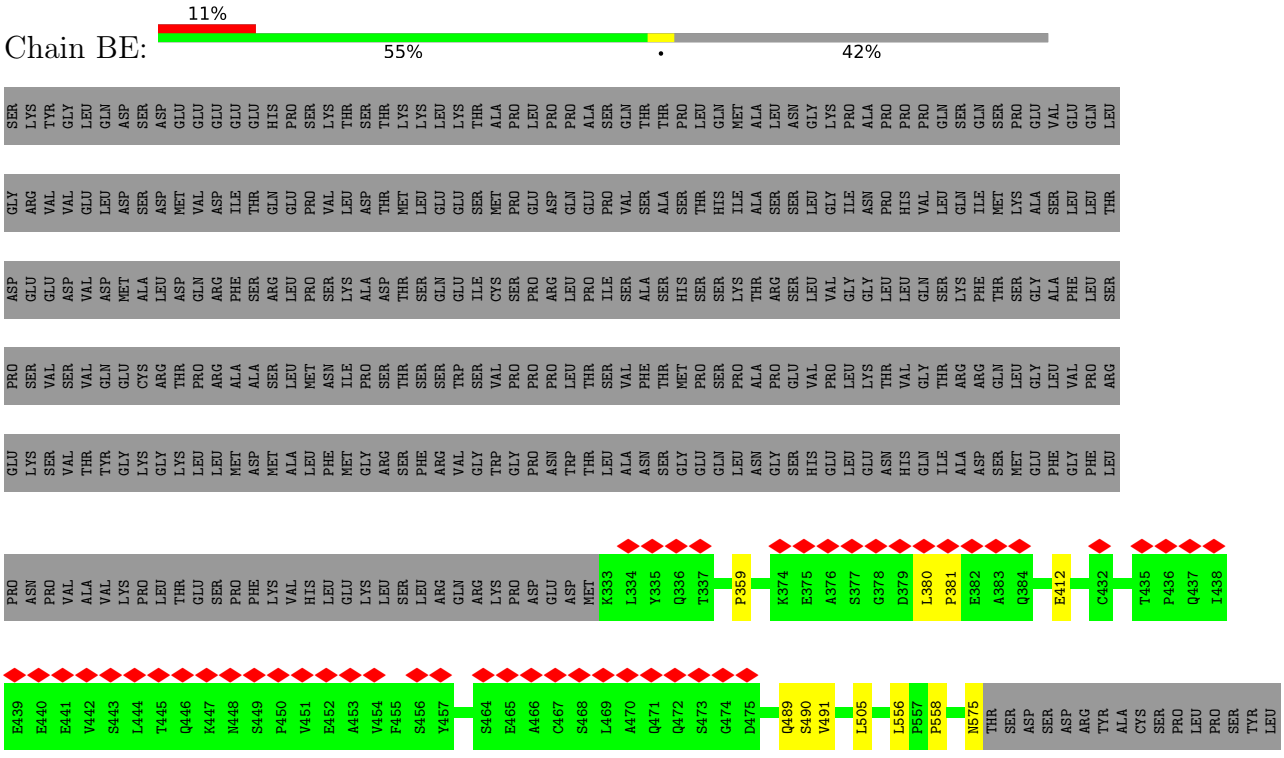
• Molecule 3: Nuclear pore complex protein Nup96

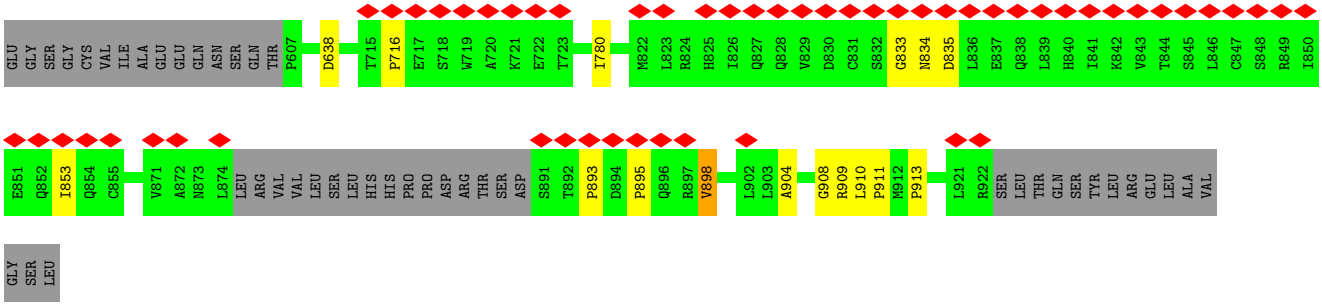
Chain AE:



• Molecule 3: Nuclear pore complex protein Nup96

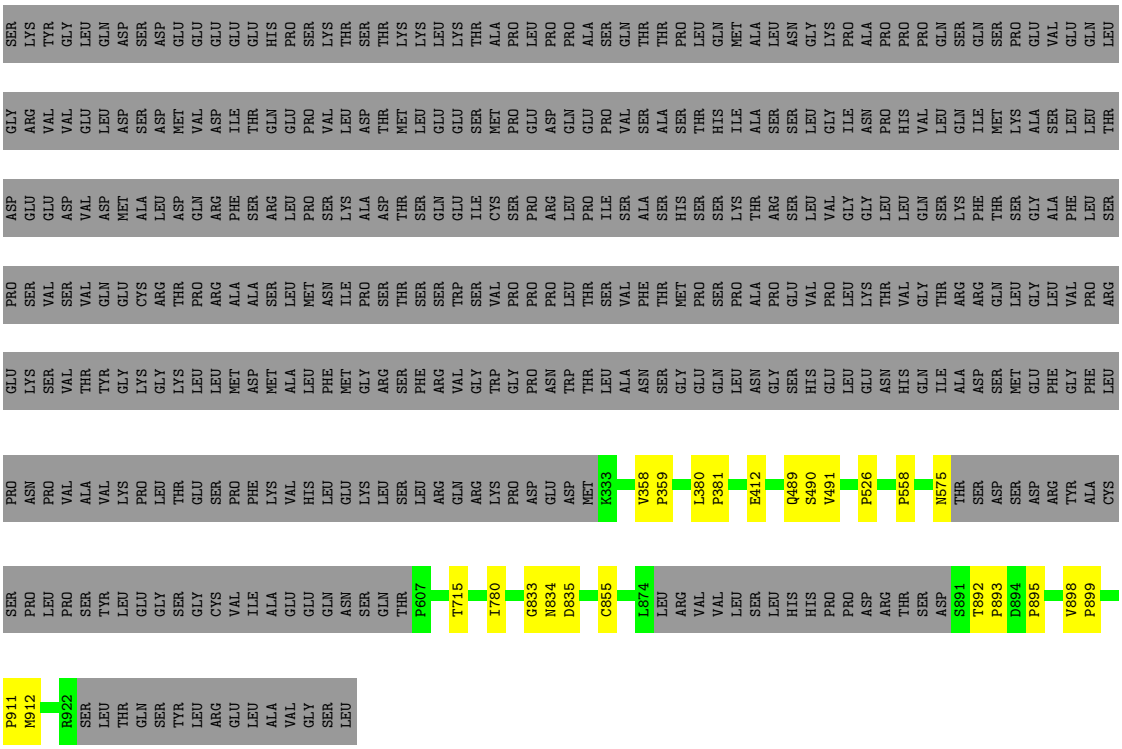
Chain BE:





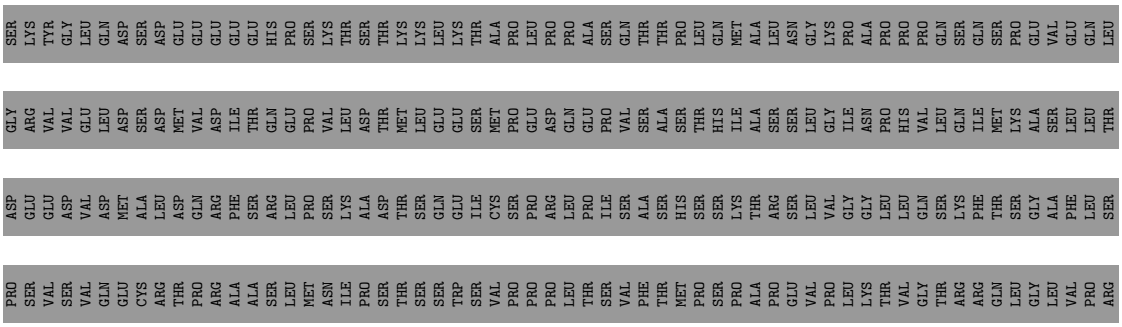
• Molecule 3: Nuclear pore complex protein Nup96

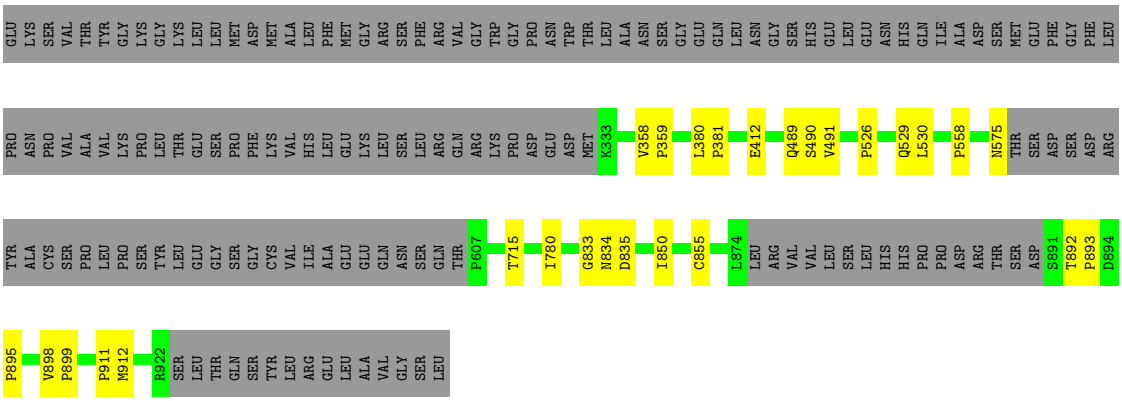
Chain CE:



• Molecule 3: Nuclear pore complex protein Nup96

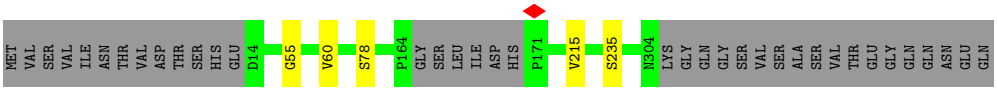
Chain DE:





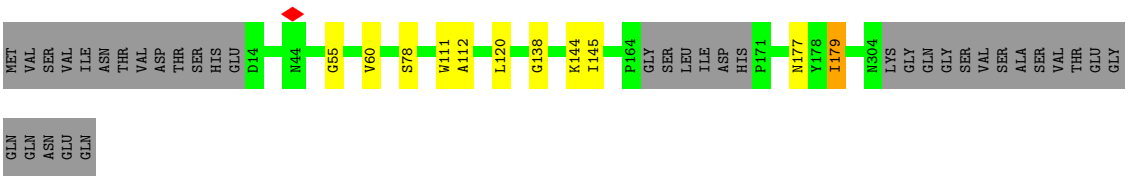
• Molecule 4: Protein SEC13 homolog

Chain AF:



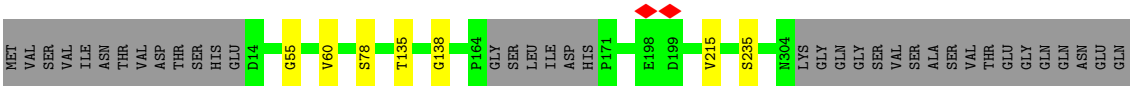
• Molecule 4: Protein SEC13 homolog

Chain BF:



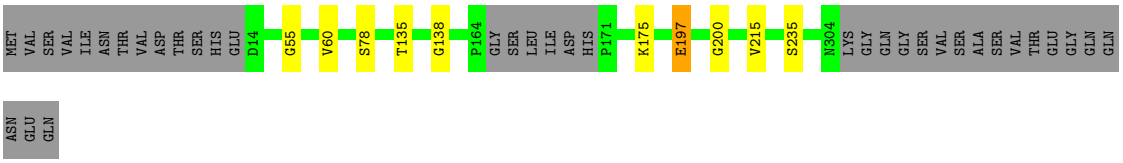
• Molecule 4: Protein SEC13 homolog

Chain CF:



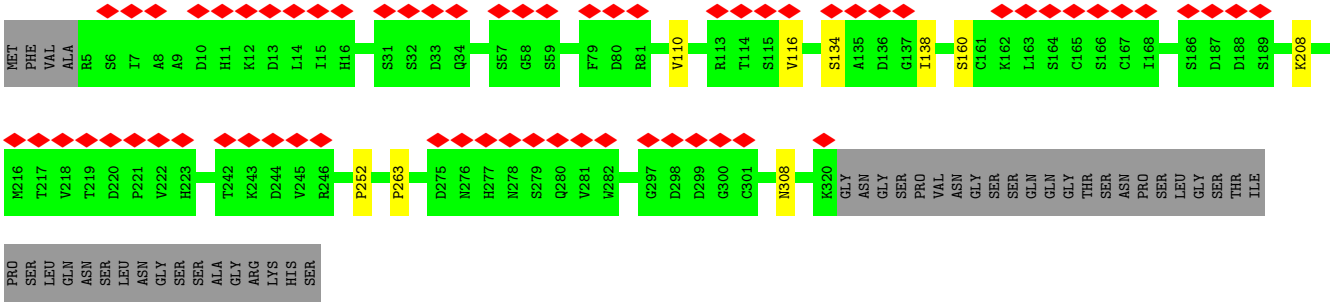
• Molecule 4: Protein SEC13 homolog

Chain DF:

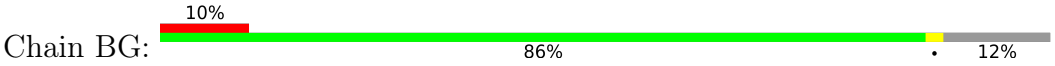


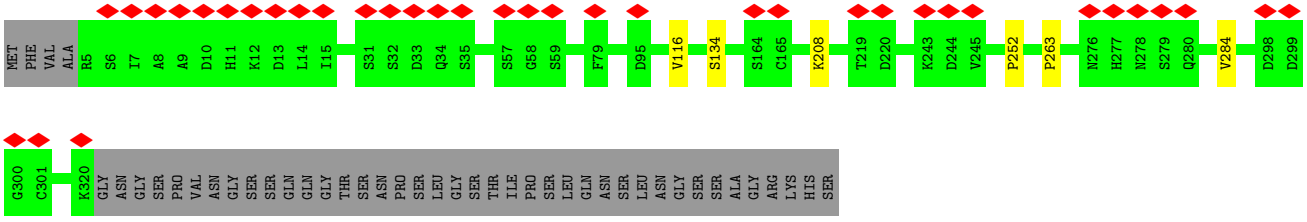
• Molecule 5: Nucleoporin SEH1

Chain AG:

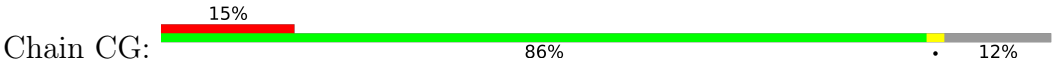


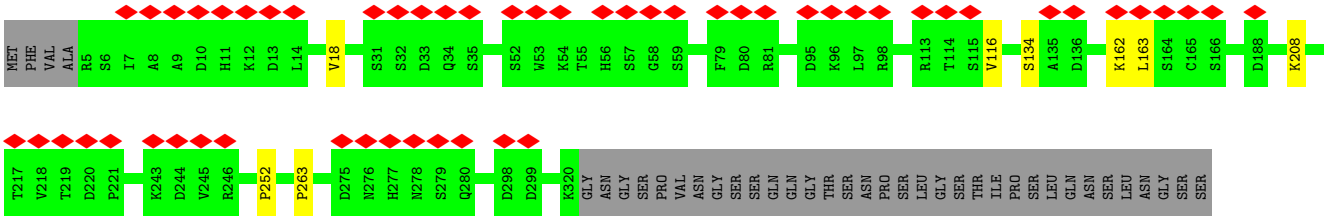
• Molecule 5: Nucleoporin SEH1



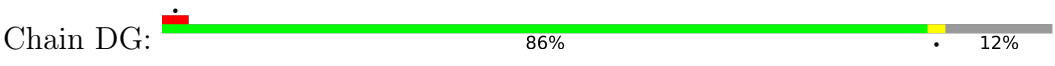


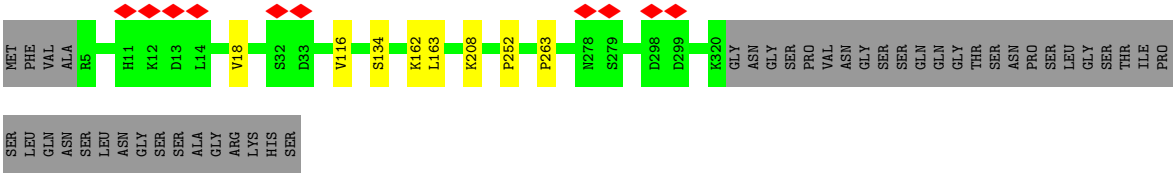
• Molecule 5: Nucleoporin SEH1



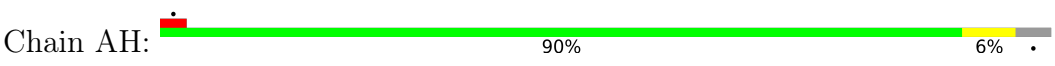


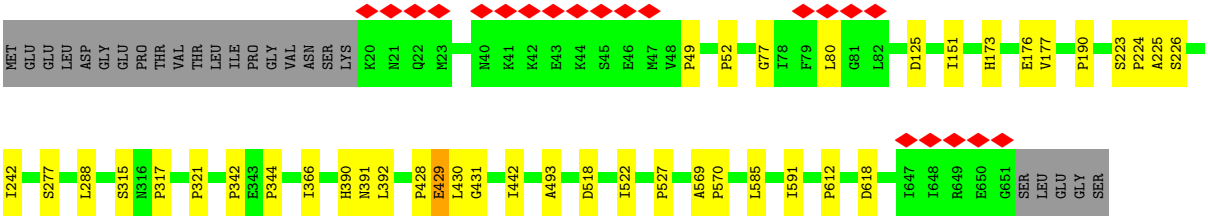
• Molecule 5: Nucleoporin SEH1



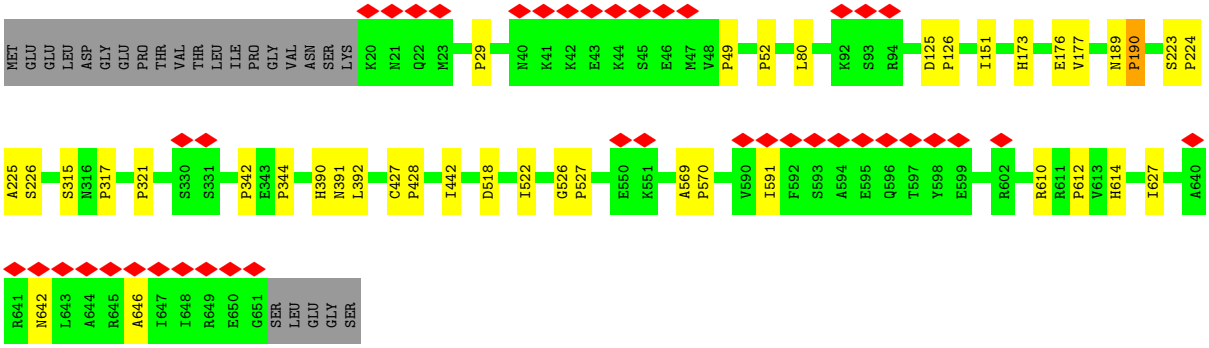


• Molecule 6: Nuclear pore complex protein Nup85

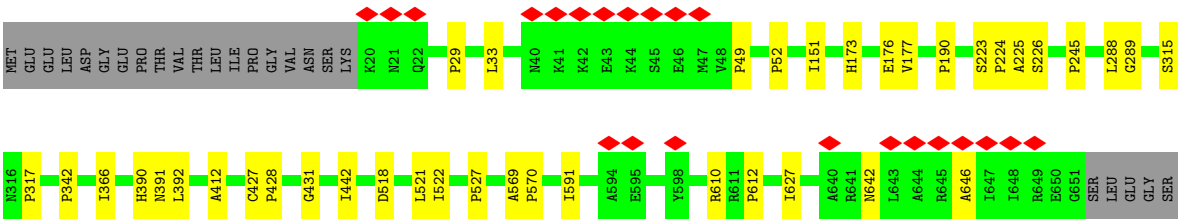




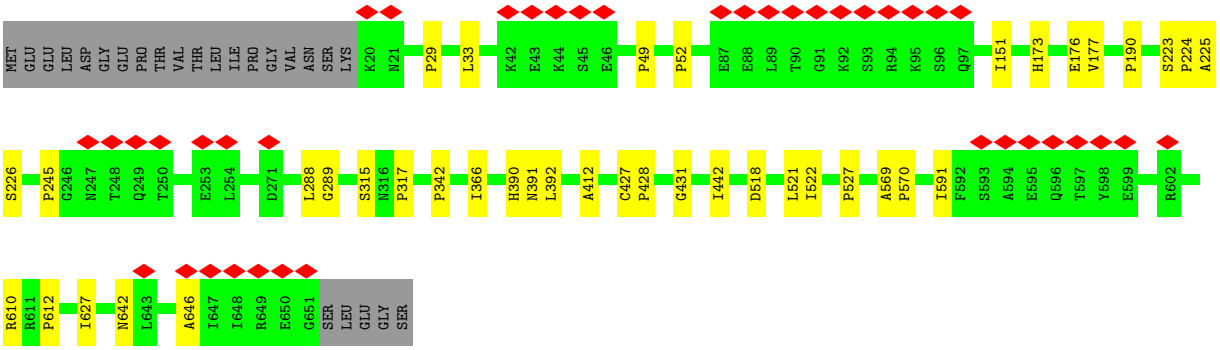
• Molecule 6: Nuclear pore complex protein Nup85



• Molecule 6: Nuclear pore complex protein Nup85

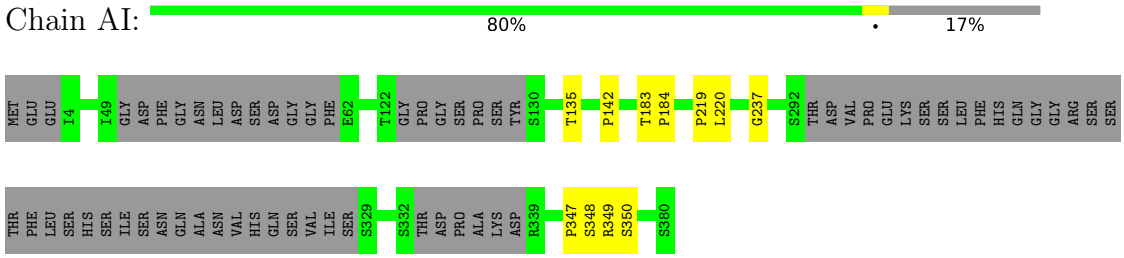


• Molecule 6: Nuclear pore complex protein Nup85



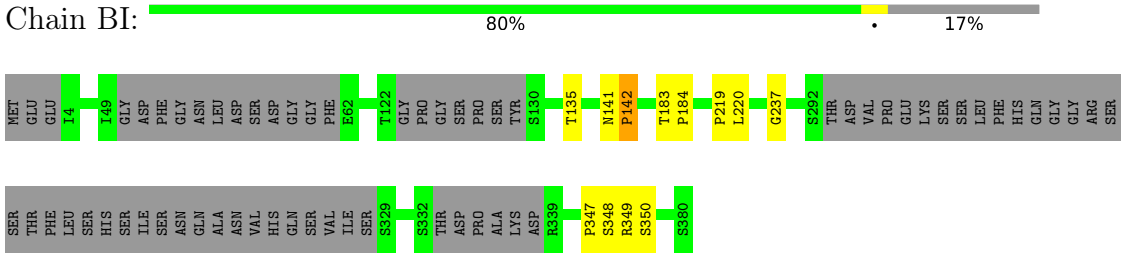
• Molecule 7: Nucleoporin Nup43

Chain AI:



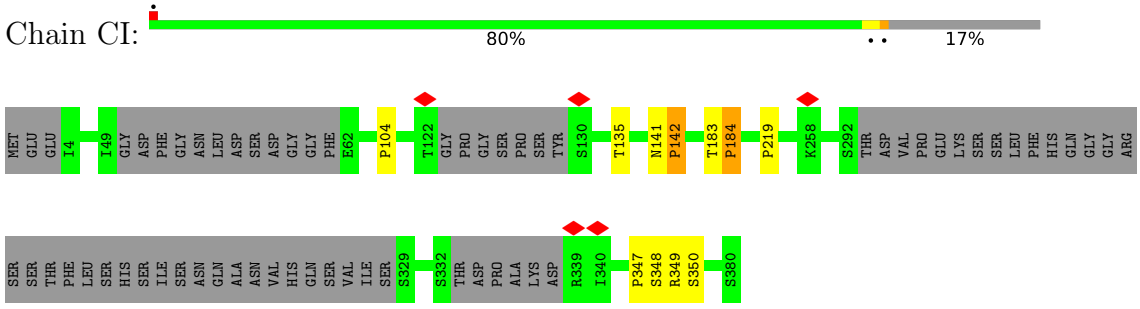
• Molecule 7: Nucleoporin Nup43

Chain BI:



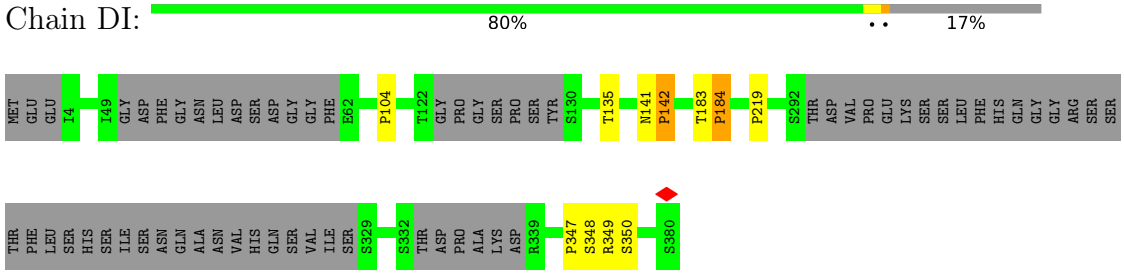
• Molecule 7: Nucleoporin Nup43

Chain CI:



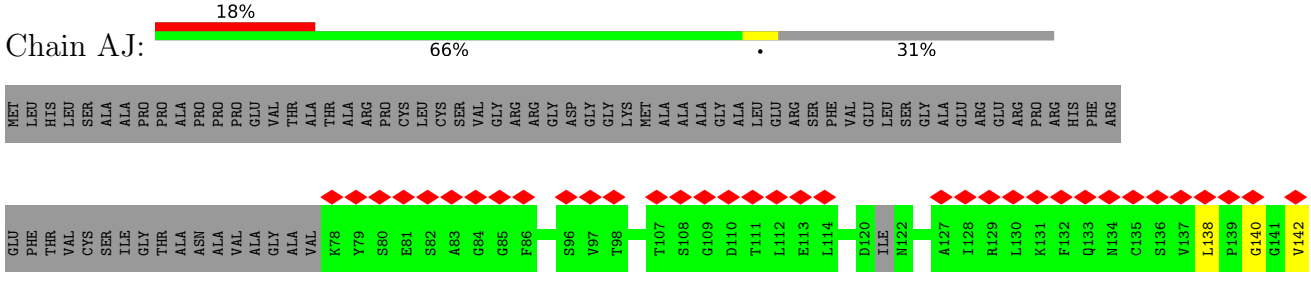
• Molecule 7: Nucleoporin Nup43

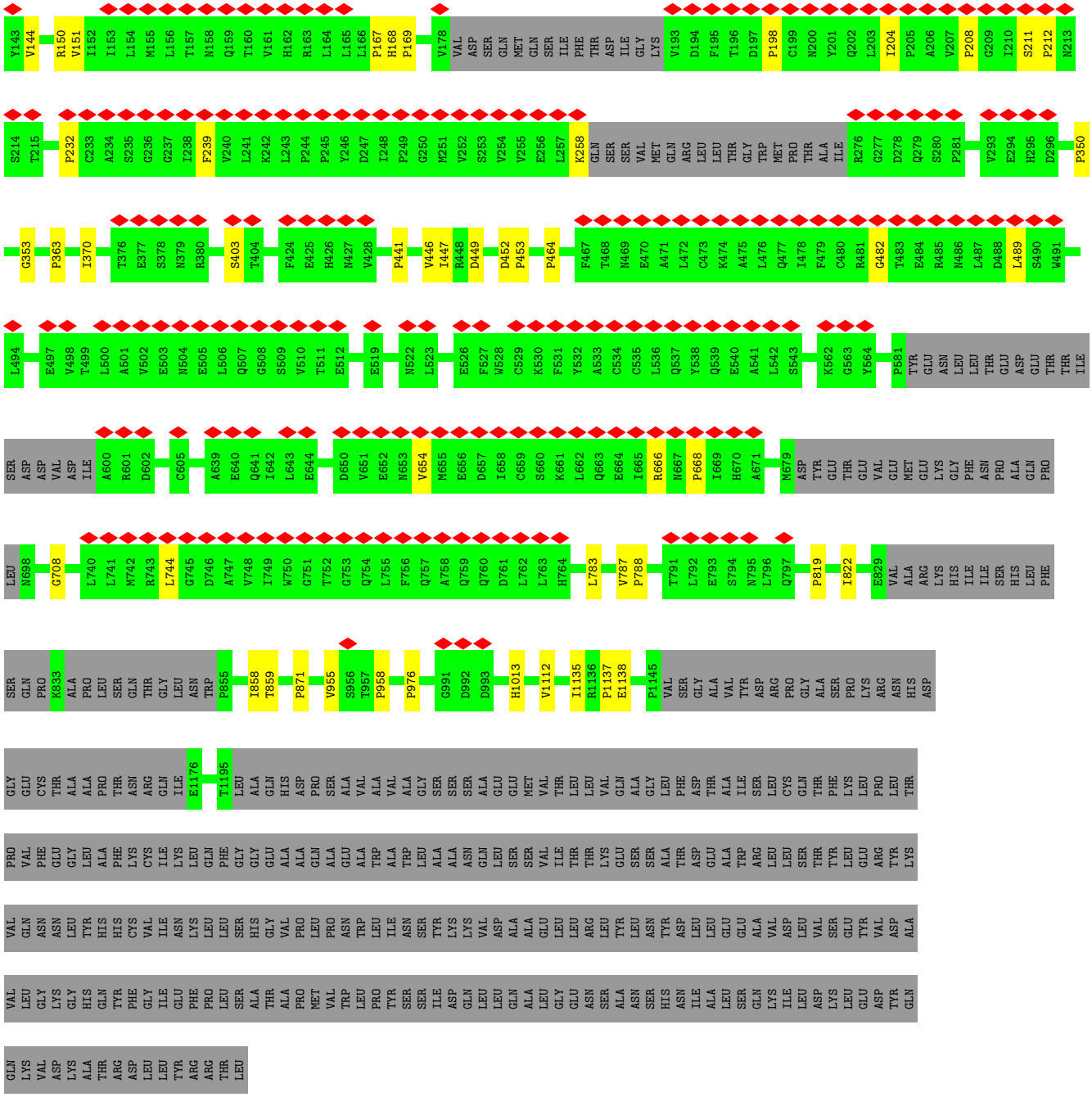
Chain DI:



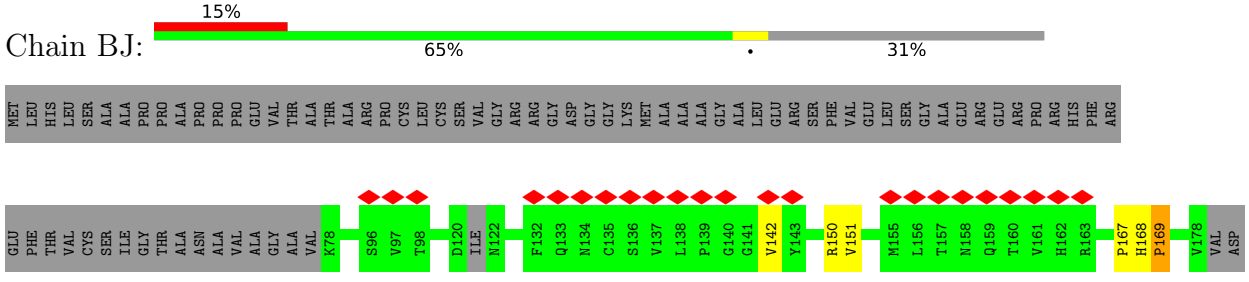
• Molecule 8: Nuclear pore complex protein Nup160

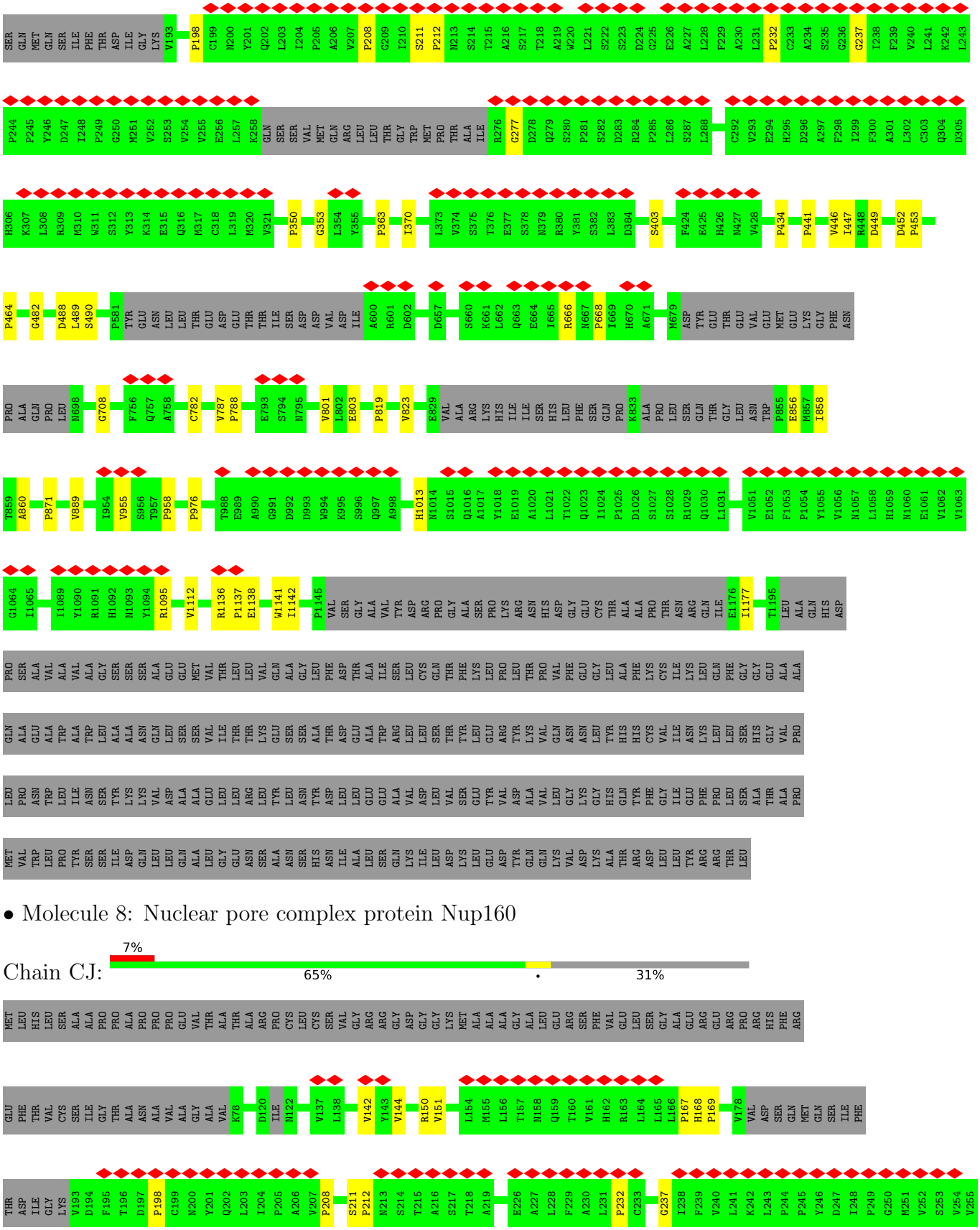
Chain AJ:





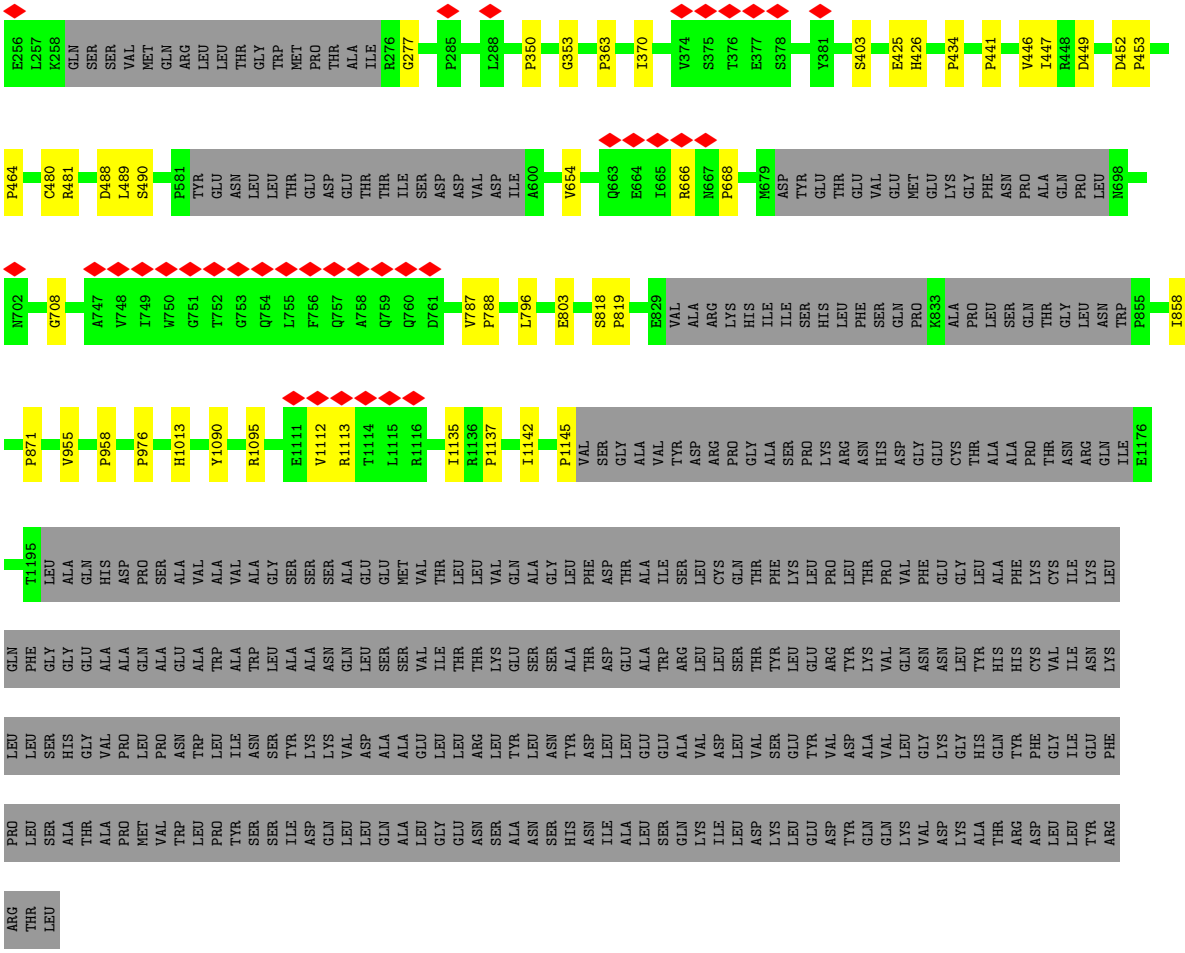
• Molecule 8: Nuclear pore complex protein Nup160





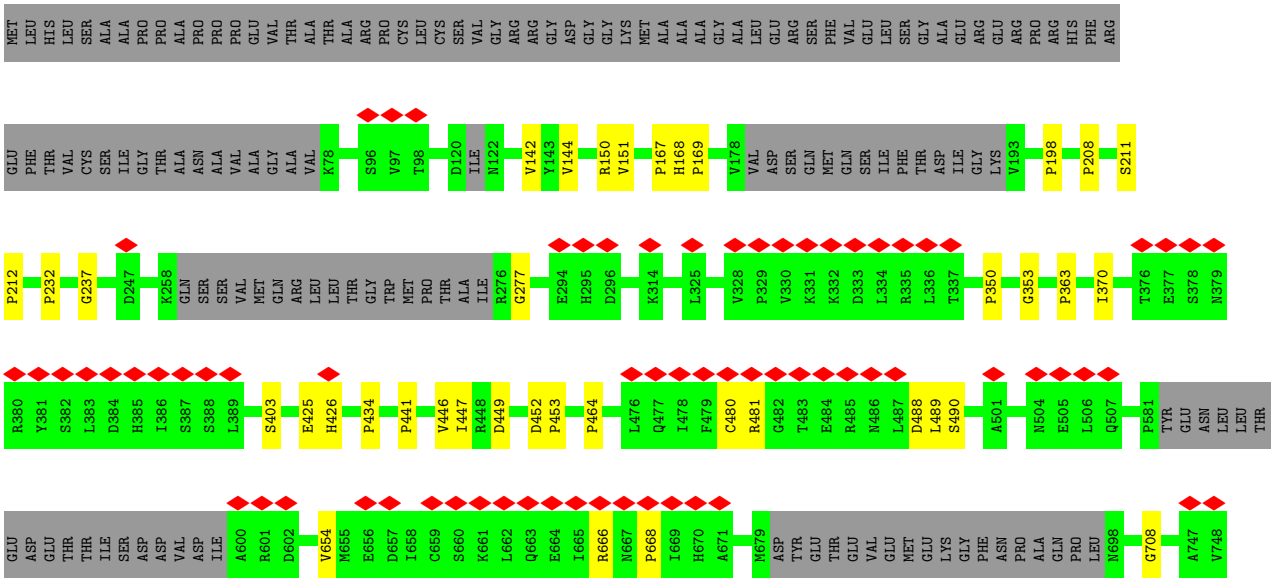
• Molecule 8: Nuclear pore complex protein Nup160

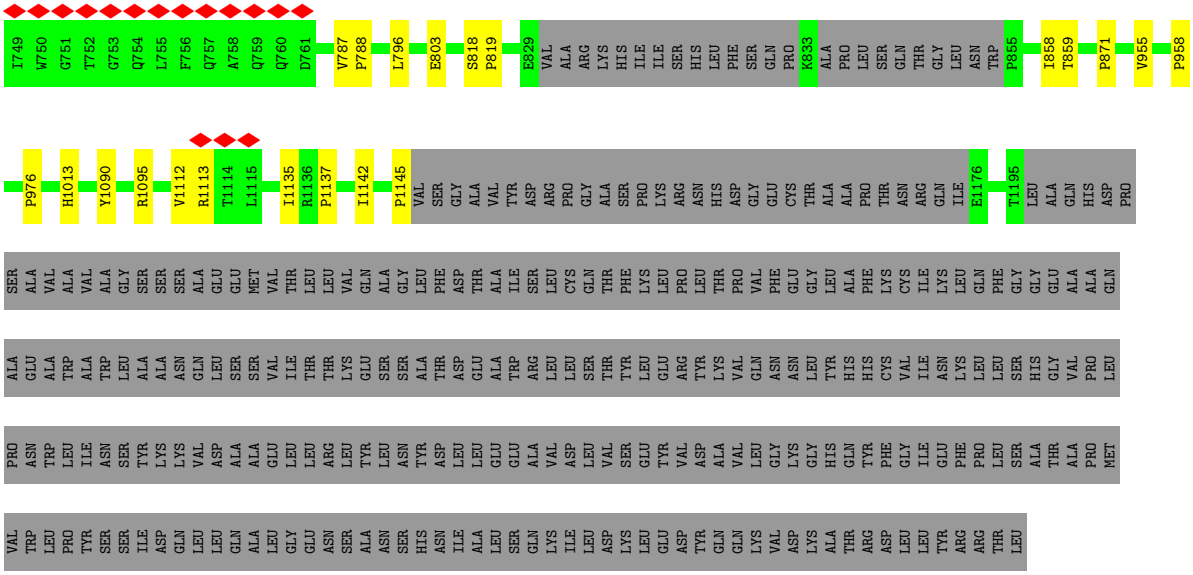
Chain CJ:



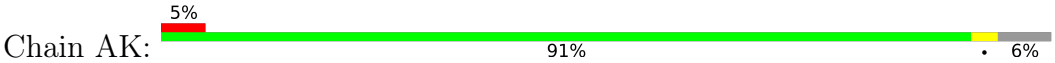
• Molecule 8: Nuclear pore complex protein Nup160

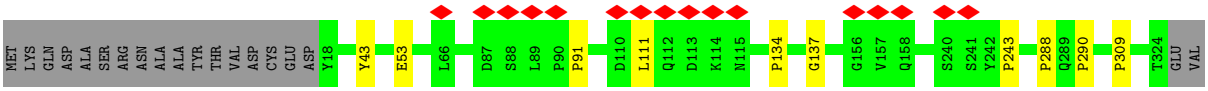
Chain DJ:



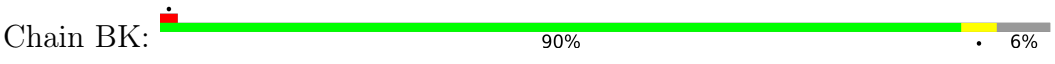


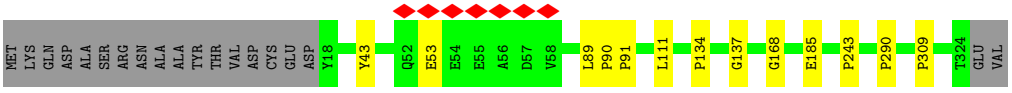
• Molecule 9: Nucleoporin Nup37



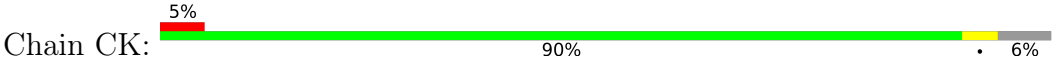


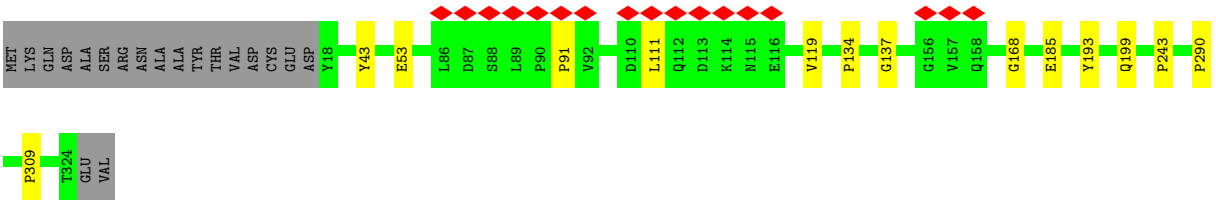
• Molecule 9: Nucleoporin Nup37



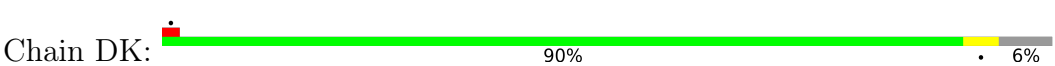


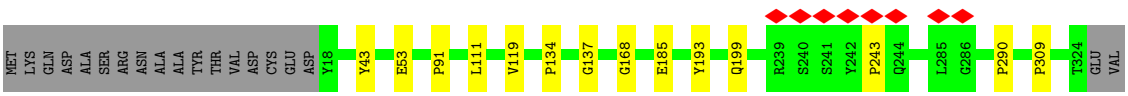
• Molecule 9: Nucleoporin Nup37





• Molecule 9: Nucleoporin Nup37





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C8	Depositor
Number of subtomograms used	1252	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	2.4	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	1.000	Depositor
Minimum map value	0.000	Depositor
Average map value	0.351	Depositor
Map value standard deviation	0.050	Depositor
Recommended contour level	0.44	Depositor
Map size (Å)	2188.8, 2188.8, 2188.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	6.84, 6.84, 6.84	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	AC	0.22	0/2619	0.37	0/3644
1	BC	0.22	0/2619	0.37	0/3644
1	CC	0.22	0/2619	0.37	0/3644
1	DC	0.22	0/2619	0.37	0/3644
2	AD	0.26	0/3362	0.44	0/4685
2	BD	0.26	0/3362	0.44	0/4685
2	CD	0.26	0/3362	0.44	0/4685
2	DD	0.26	0/3362	0.44	0/4685
3	AE	0.23	0/2699	0.38	0/3768
3	BE	0.23	0/2699	0.39	0/3768
3	CE	0.23	0/2698	0.38	0/3765
3	DE	0.23	0/2698	0.38	0/3765
4	AF	0.25	0/1400	0.45	0/1943
4	BF	0.25	0/1400	0.45	0/1943
4	CF	0.25	0/1400	0.45	0/1943
4	DF	0.25	0/1400	0.46	0/1943
5	AG	0.24	0/1563	0.46	0/2177
5	BG	0.24	0/1563	0.46	0/2177
5	CG	0.24	0/1563	0.46	0/2177
5	DG	0.24	0/1563	0.46	0/2177
6	AH	0.23	0/3133	0.39	0/4369
6	BH	0.23	0/3133	0.38	0/4369
6	CH	0.23	0/3130	0.38	0/4360
6	DH	0.23	0/3130	0.38	0/4360
7	AI	0.24	0/1647	0.44	0/2287
7	BI	0.24	0/1647	0.44	0/2287
7	CI	0.24	0/1647	0.45	0/2287
7	DI	0.24	0/1647	0.45	0/2287
8	AJ	0.23	0/4925	0.40	0/6855
8	BJ	0.23	0/4925	0.40	0/6855
8	CJ	0.23	0/4925	0.40	0/6855
8	DJ	0.23	0/4925	0.40	0/6855
9	AK	0.26	0/1510	0.49	0/2098
9	BK	0.26	0/1510	0.49	0/2098

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
9	CK	0.25	0/1509	0.48	0/2095
9	DK	0.25	0/1509	0.48	0/2095
All	All	0.24	0/91422	0.42	0/127274

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	AC	2629	0	1167	2	0
1	BC	2629	0	1167	2	0
1	CC	2629	0	1167	3	0
1	DC	2629	0	1167	3	0
2	AD	3367	0	1489	15	0
2	BD	3367	0	1489	4	0
2	CD	3367	0	1489	4	0
2	DD	3367	0	1489	2	0
3	AE	2700	0	1200	6	0
3	BE	2700	0	1200	4	0
3	CE	2700	0	1199	3	0
3	DE	2700	0	1199	5	0
4	AF	1402	0	648	2	0
4	BF	1402	0	648	6	0
4	CF	1402	0	648	3	0
4	DF	1402	0	648	4	0
5	AG	1564	0	712	2	0
5	BG	1564	0	712	1	0
5	CG	1564	0	712	2	0
5	DG	1564	0	712	3	0
6	AH	3134	0	1393	5	0
6	BH	3134	0	1393	6	0
6	CH	3134	0	1390	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	DH	3134	0	1390	6	0
7	AI	1599	0	706	4	0
7	BI	1599	0	706	5	0
7	CI	1599	0	707	4	0
7	DI	1599	0	707	4	0
8	AJ	4932	0	2159	5	0
8	BJ	4932	0	2159	6	0
8	CJ	4932	0	2158	9	0
8	DJ	4932	0	2158	9	0
9	AK	1511	0	674	0	0
9	BK	1511	0	674	1	0
9	CK	1511	0	673	2	0
9	DK	1511	0	673	2	0
All	All	91352	0	40582	140	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 1.

The worst 5 of 140 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)
2:AD:297:TRP:CB	2:AD:339:ASP:CB	2.28	1.12
2:AD:297:TRP:HA	2:AD:339:ASP:CB	2.00	0.92
2:AD:297:TRP:CA	2:AD:339:ASP:CB	2.51	0.88
2:AD:300:THR:CB	2:AD:336:ASP:N	2.43	0.80
2:DD:297:TRP:CB	2:DD:339:ASP:CB	2.64	0.75

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	AC	508/1156 (44%)	465 (92%)	35 (7%)	8 (2%)	9	44
1	BC	508/1156 (44%)	465 (92%)	35 (7%)	8 (2%)	9	44
1	CC	508/1156 (44%)	466 (92%)	34 (7%)	8 (2%)	9	44
1	DC	508/1156 (44%)	466 (92%)	34 (7%)	8 (2%)	9	44
2	AD	668/925 (72%)	618 (92%)	41 (6%)	9 (1%)	12	48
2	BD	668/925 (72%)	627 (94%)	34 (5%)	7 (1%)	15	55
2	CD	668/925 (72%)	622 (93%)	41 (6%)	5 (1%)	22	63
2	DD	668/925 (72%)	625 (94%)	39 (6%)	4 (1%)	25	66
3	AE	541/937 (58%)	451 (83%)	67 (12%)	23 (4%)	2	22
3	BE	541/937 (58%)	453 (84%)	67 (12%)	21 (4%)	3	23
3	CE	539/937 (58%)	453 (84%)	67 (12%)	19 (4%)	3	25
3	DE	539/937 (58%)	453 (84%)	67 (12%)	19 (4%)	3	25
4	AF	281/322 (87%)	245 (87%)	35 (12%)	1 (0%)	34	72
4	BF	281/322 (87%)	217 (77%)	59 (21%)	5 (2%)	8	40
4	CF	281/322 (87%)	246 (88%)	33 (12%)	2 (1%)	22	63
4	DF	281/322 (87%)	239 (85%)	37 (13%)	5 (2%)	8	40
5	AG	314/360 (87%)	266 (85%)	43 (14%)	5 (2%)	9	44
5	BG	314/360 (87%)	266 (85%)	44 (14%)	4 (1%)	12	48
5	CG	314/360 (87%)	272 (87%)	38 (12%)	4 (1%)	12	48
5	DG	314/360 (87%)	272 (87%)	38 (12%)	4 (1%)	12	48
6	AH	630/656 (96%)	516 (82%)	80 (13%)	34 (5%)	2	19
6	BH	630/656 (96%)	518 (82%)	81 (13%)	31 (5%)	2	20
6	CH	624/656 (95%)	518 (83%)	76 (12%)	30 (5%)	2	21
6	DH	624/656 (95%)	518 (83%)	76 (12%)	30 (5%)	2	21
7	AI	324/380 (85%)	274 (85%)	44 (14%)	6 (2%)	8	38
7	BI	324/380 (85%)	273 (84%)	45 (14%)	6 (2%)	8	38
7	CI	324/380 (85%)	282 (87%)	34 (10%)	8 (2%)	5	32
7	DI	324/380 (85%)	282 (87%)	34 (10%)	8 (2%)	5	32
8	AJ	983/1436 (68%)	804 (82%)	135 (14%)	44 (4%)	2	22
8	BJ	983/1436 (68%)	806 (82%)	130 (13%)	47 (5%)	2	21
8	CJ	982/1436 (68%)	809 (82%)	130 (13%)	43 (4%)	2	22
8	DJ	982/1436 (68%)	812 (83%)	127 (13%)	43 (4%)	2	22

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	AK	305/326 (94%)	246 (81%)	49 (16%)	10 (3%)	4	26
9	BK	305/326 (94%)	247 (81%)	47 (15%)	11 (4%)	3	25
9	CK	303/326 (93%)	249 (82%)	44 (14%)	10 (3%)	4	26
9	DK	303/326 (93%)	249 (82%)	44 (14%)	10 (3%)	4	26
All	All	18194/25992 (70%)	15590 (86%)	2064 (11%)	540 (3%)	7	28

5 of 540 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AC	627	PHE
1	AC	680	PRO
1	AC	685	PRO
2	AD	324	ASP
2	AD	325	PRO

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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
8	CJ	3
8	DJ	3
6	CH	3
6	DH	3
9	CK	1
9	DK	1
3	CE	1
3	DE	1

The worst 5 of 16 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	CJ	784:ALA	C	785:THR	N	25.54
1	DJ	784:ALA	C	785:THR	N	25.54
1	CH	613:VAL	C	614:HIS	N	24.84
1	DH	613:VAL	C	614:HIS	N	24.83
1	CH	525:LEU	C	526:GLY	N	22.68

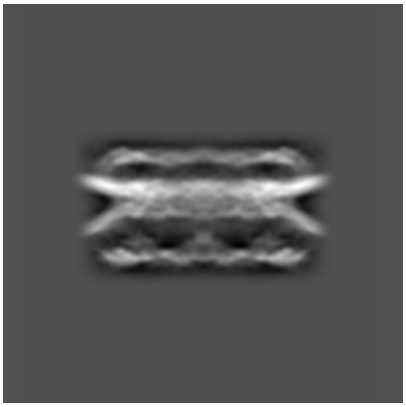
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12814. These allow visual inspection of the internal detail of the map and identification of artifacts.

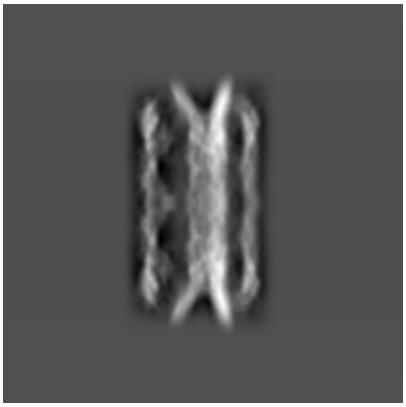
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

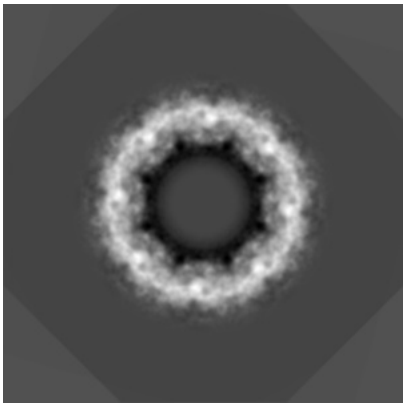
6.1.1 Primary map



X



Y



Z

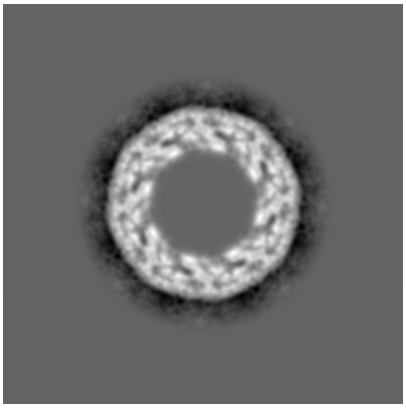
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map

X Index: 160

Y Index: 160



Z Index: 160

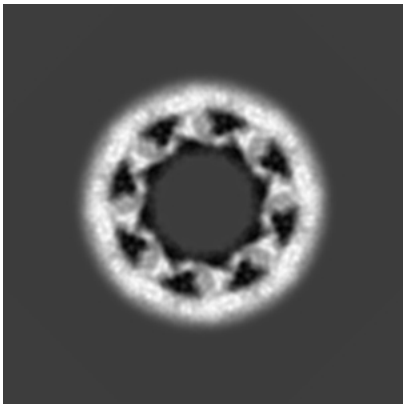
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 100

Y Index: 220

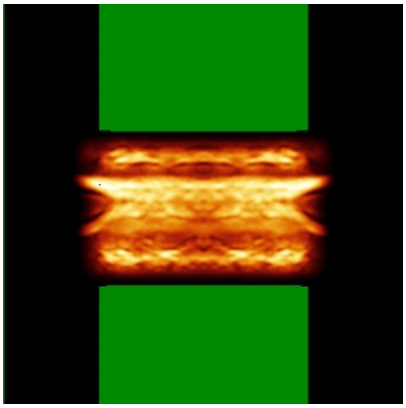


Z Index: 174

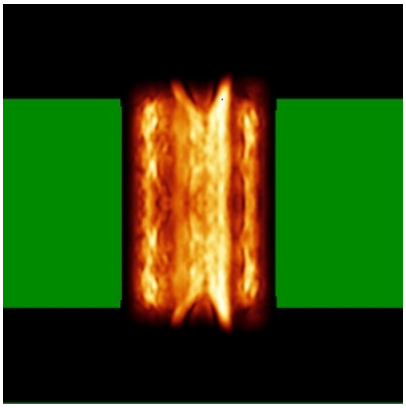
The images above show the largest variance slices of the map in three orthogonal directions.

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

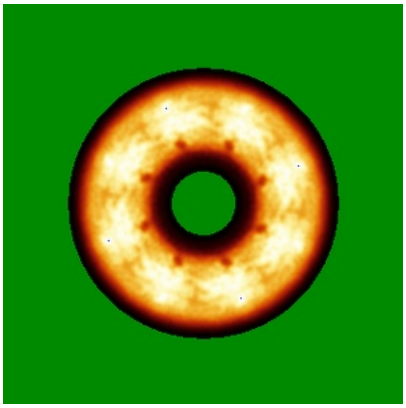
6.4.1 Primary map



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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.44. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

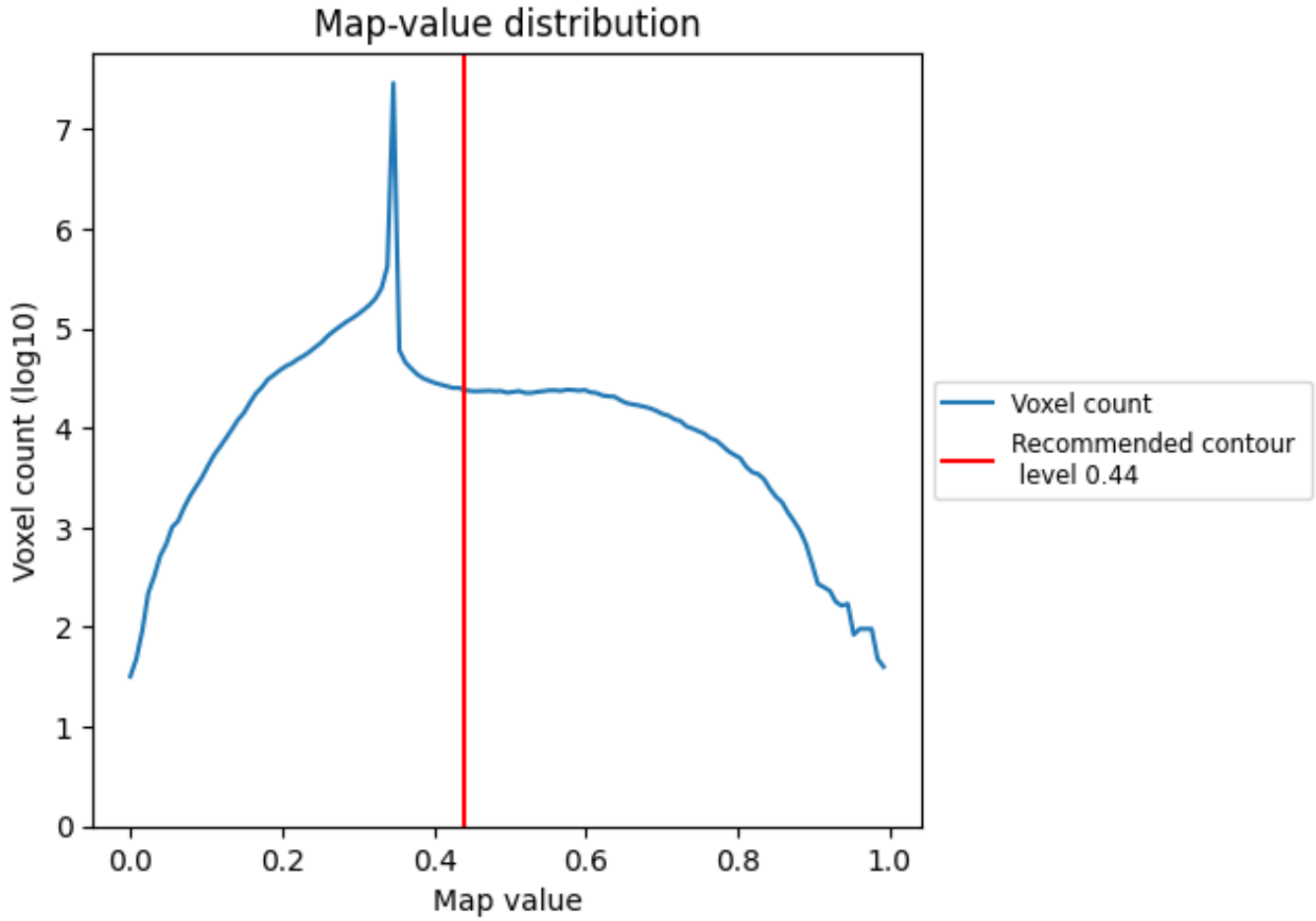
6.6 Mask visualisation (i)

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

7 Map analysis

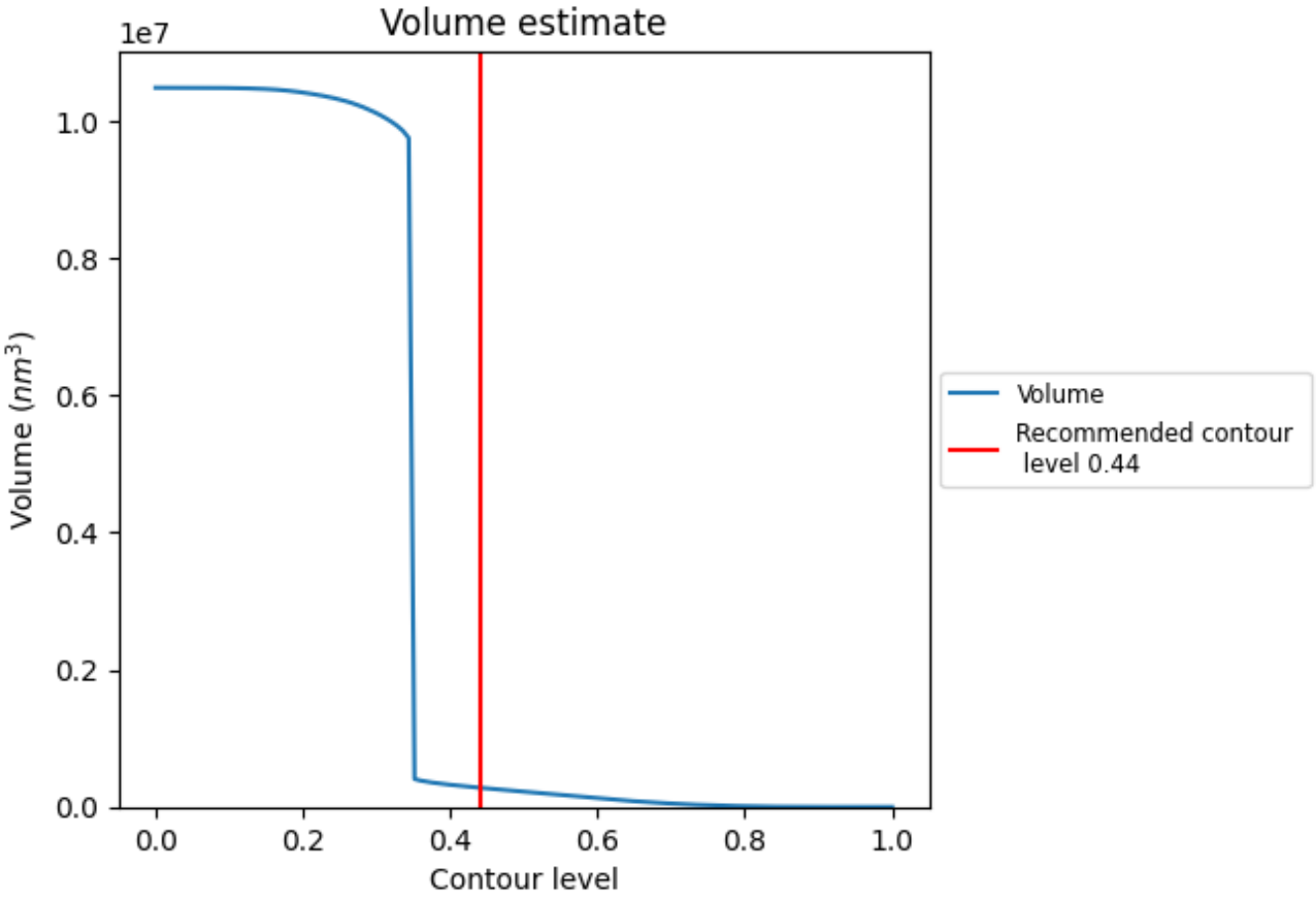
This section contains the results of statistical analysis of the map.

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.

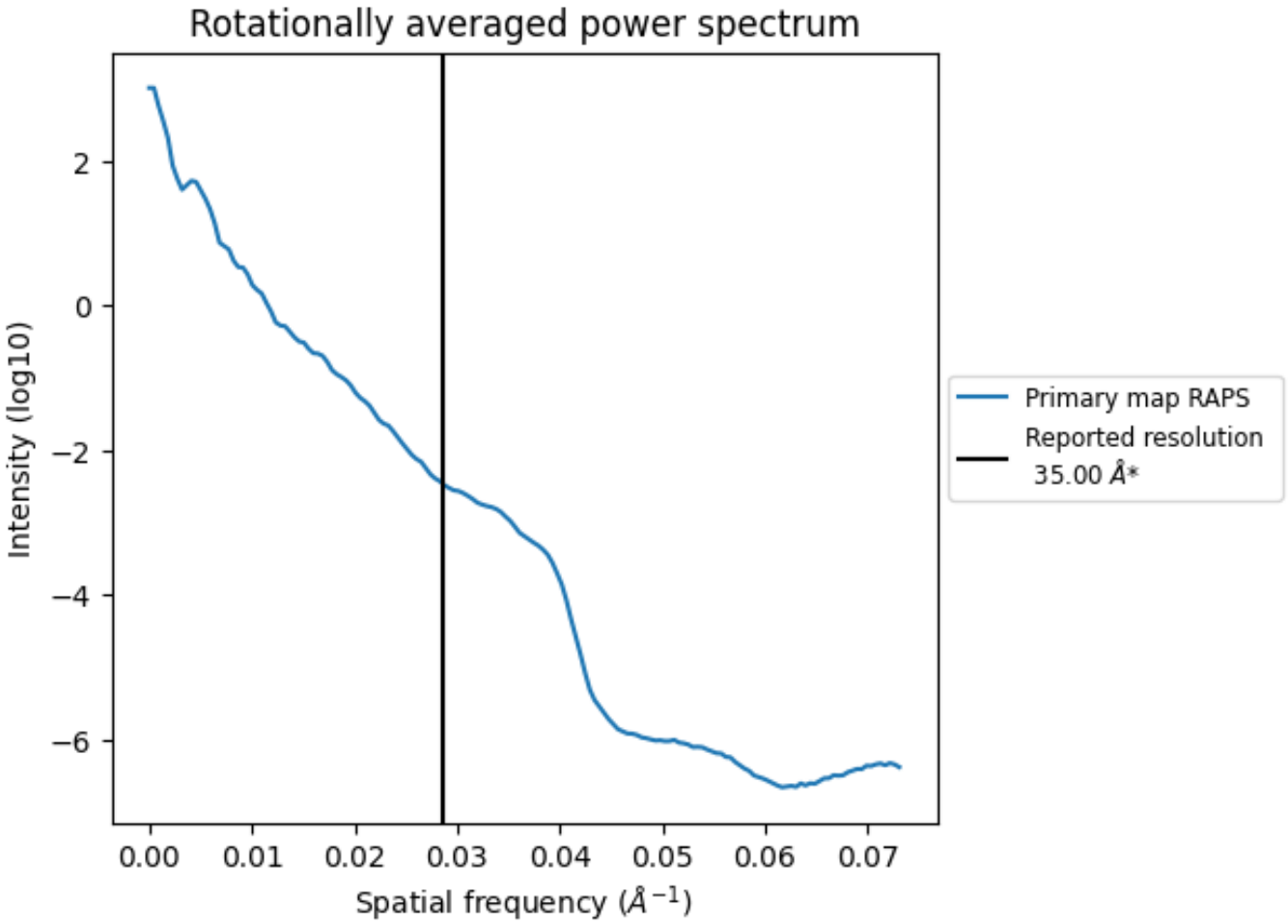
7.2 Volume estimate (i)



The volume at the recommended contour level is 280168 nm^3; this corresponds to an approximate mass of 253083 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 0.029 Å^{-1}

8 Fourier-Shell correlation (i)

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

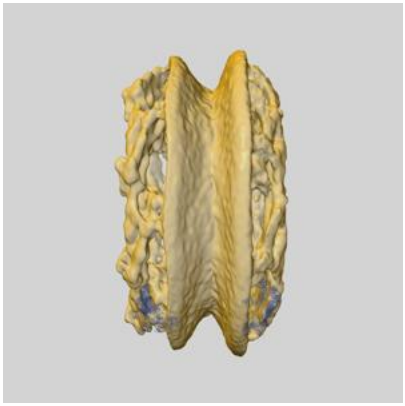
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12814 and PDB model 7PEQ. Per-residue inclusion information can be found in section 3 on page 8.

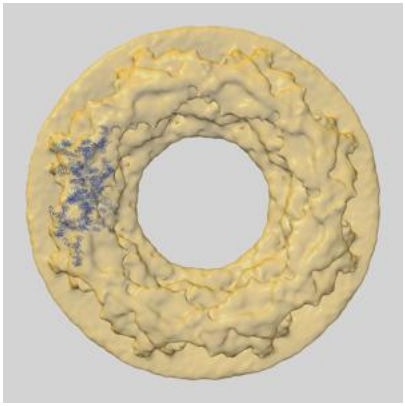
9.1 Map-model overlays

9.1.1 Map-model overlay

X

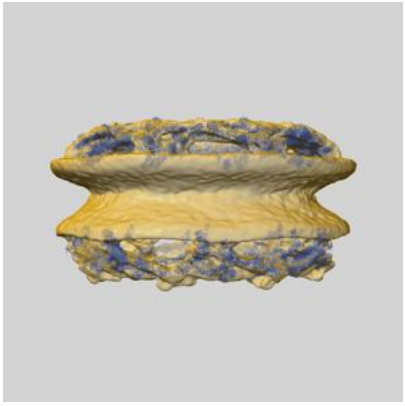


Y

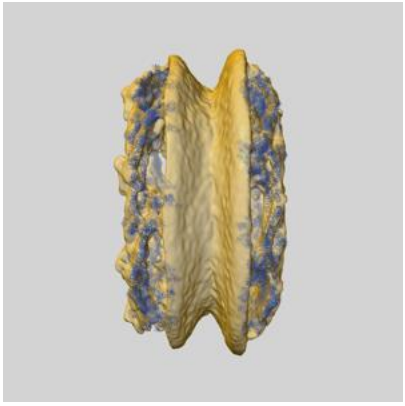


Z

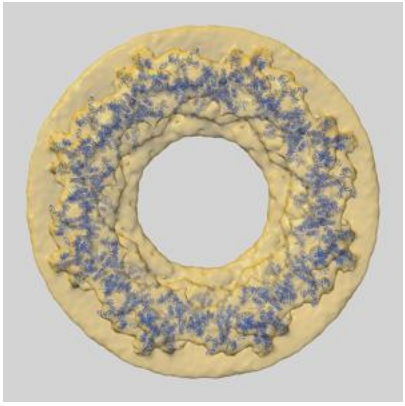
9.1.2 Map-model assembly overlay



X



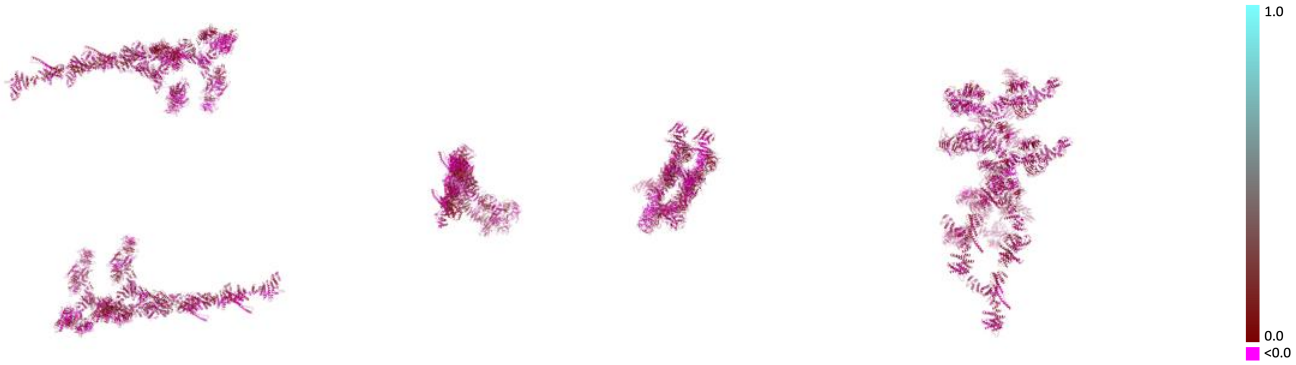
Y



Z

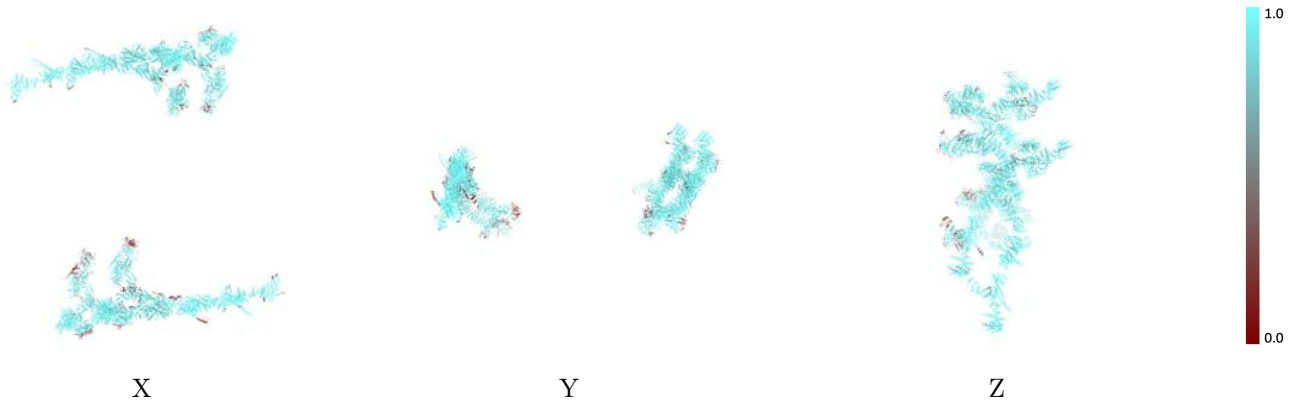
The images above show the 3D surface view of the map at the recommended contour level 0.44 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model



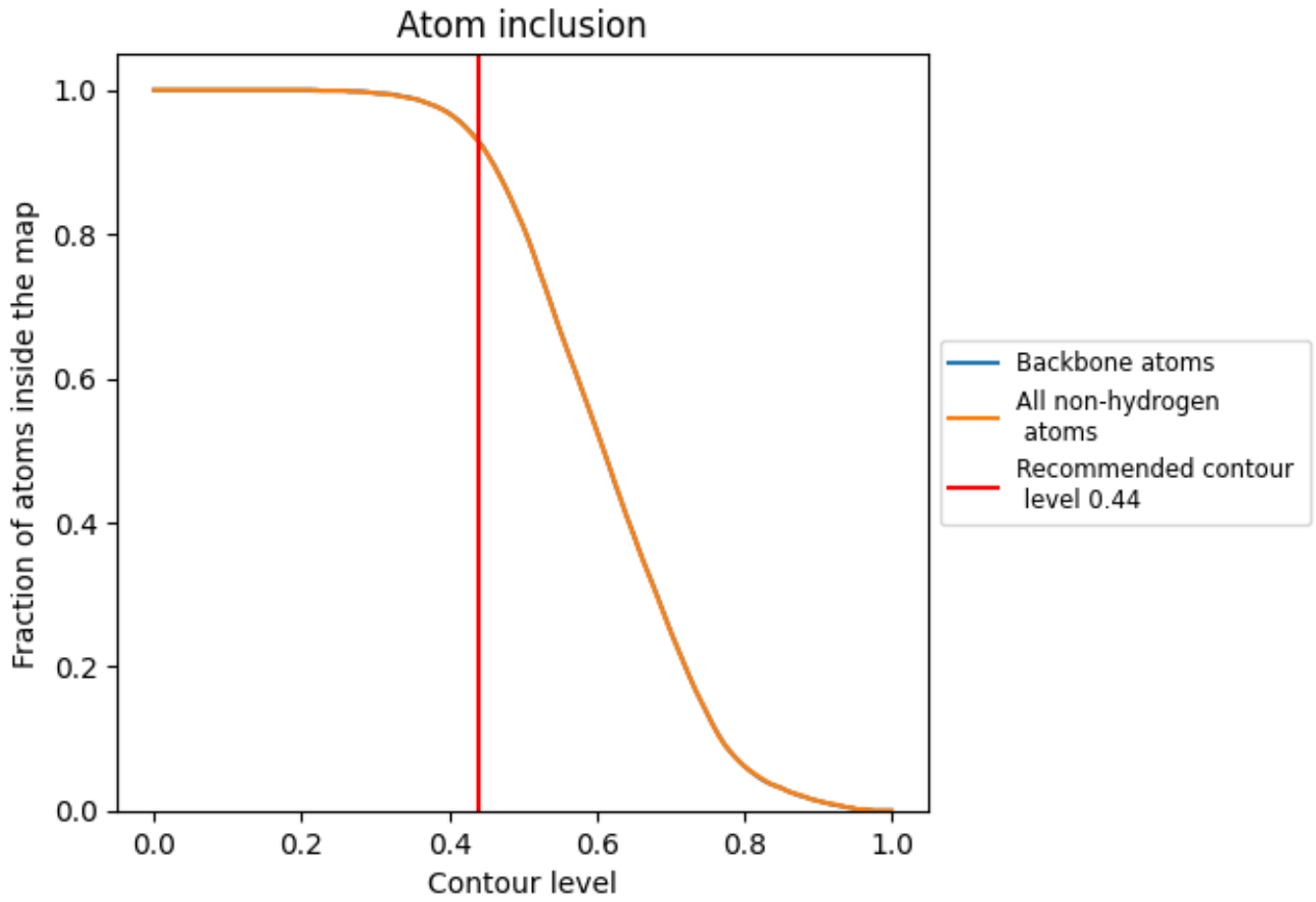
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.44).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 93% 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 (0.44) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9280	0.0370
AC	0.9610	0.0570
AD	0.9600	0.0370
AE	0.9590	0.0550
AF	0.9960	0.0350
AG	0.7880	0.0300
AH	0.9660	0.0330
AI	0.9980	0.0450
AJ	0.7450	0.0330
AK	0.9480	0.0310
BC	0.9310	0.0320
BD	0.9930	0.0460
BE	0.8140	0.0540
BF	0.9960	0.0390
BG	0.8840	0.0290
BH	0.9340	0.0480
BI	0.9990	0.0570
BJ	0.7820	0.0290
BK	0.9720	0.0280
CC	0.8650	0.0480
CD	0.9910	0.0530
CE	1.0000	0.0320
CF	0.9940	0.0460
CG	0.8360	0.0440
CH	0.9650	0.0100
CI	0.9840	0.0320
CJ	0.8970	0.0030
CK	0.9480	0.0430
DC	0.9710	0.0450
DD	0.9940	0.0560
DE	1.0000	0.0530
DF	1.0000	0.0300
DG	0.9680	0.0470
DH	0.9340	0.0240
DI	0.9970	0.0300

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
DJ	0.9140	0.0260
DK	0.9760	0.0100