wwPDB EM Validation Summary Report (i)

Nov 19, 2022 – 02:19 pm GMT

PDB ID	:	5IJO
EMDB ID	:	EMD-8085
Title	:	Alternative composite structure of the inner ring of the human nuclear pore complex (16 copies of Nup188, 16 copies of Nup205)
Authors	:	Kosinski, J.; Mosalaganti, S.; von Appen, A.; Beck, M.
Deposited on	:	2016-03-02
Resolution	:	21.40 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:

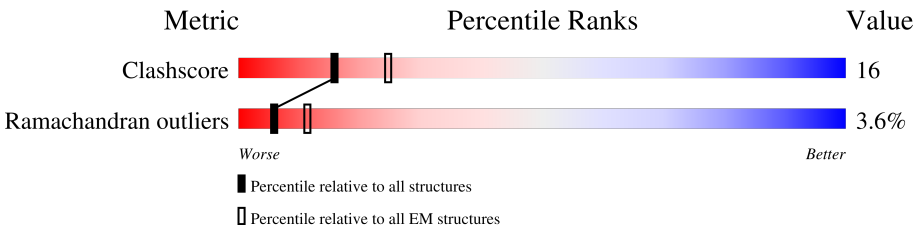
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 21.40 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	A	1391	• 43% • 53%
1	B	1391	5% 43% • 53%
1	E	1391	10% 73% • • 22%
1	K	1391	35% 73% 5% • 22%
1	Q	1391	9% 73% • 22%
1	W	1391	17% 73% 5% 22%
2	C	819	12% 64% 11% • 22%
2	I	819	14% 66% 10% • 22%
2	O	819	9% 65% 10% • 22%

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Mol	Chain	Length	Quality of chain
2	U	819	16% 66% 10% 22%
3	D	2012	5% 45% 49%
3	P	2012	5% 46% 49%
4	F	507	13% 35% 16% 9% 5% 34%
4	L	507	13% 35% 16% 9% 5% 34%
4	R	507	15% 35% 16% 9% 5% 34%
4	X	507	10% 36% 16% 9% 5% 34%
5	G	599	17% 7% 71%
5	M	599	17% 7% 71%
5	S	599	17% 7% 71%
5	Y	599	17% 7% 71%
6	H	522	6% 18% 11% 68%
6	N	522	18% 11% 68%
6	T	522	8% 18% 11% 68%
6	Z	522	5% 18% 11% 68%
7	J	1749	9% 63% 7% 28%
7	V	1749	7% 64% 7% 28%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 76526 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 Nup155.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	A	650	3214	1914	650	650	0	0
1	B	650	3214	1914	650	650	0	0
1	E	1083	5366	3200	1083	1083	0	0
1	K	1083	5366	3200	1083	1083	0	0
1	Q	1083	5366	3200	1083	1083	0	0
1	W	1083	5366	3200	1083	1083	0	0

- Molecule 2 is a protein called Nuclear pore complex protein Nup93.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	C	636	3152	1880	636	636	0	0
2	I	636	3152	1880	636	636	0	0
2	O	636	3152	1880	636	636	0	0
2	U	636	3152	1880	636	636	0	0

- Molecule 3 is a protein called Nuclear pore complex protein Nup205.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	D	1028	5094	3038	1028	1028	0	0
3	P	1028	5094	3038	1028	1028	0	0

- Molecule 4 is a protein called Nucleoporin p54.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	F	335	1658	988	335	335	0	0
4	L	335	1658	988	335	335	0	0
4	R	335	1658	988	335	335	0	0
4	X	335	1658	988	335	335	0	0

- Molecule 5 is a protein called Nucleoporin p58/p45.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	G	171	853	511	171	171	0	0
5	M	171	853	511	171	171	0	0
5	S	171	853	511	171	171	0	0
5	Y	171	853	511	171	171	0	0

- Molecule 6 is a protein called Nuclear pore glycoprotein p62.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	H	169	842	504	169	169	0	0
6	N	169	842	504	169	169	0	0
6	T	169	842	504	169	169	0	0
6	Z	169	842	504	169	169	0	0

- Molecule 7 is a protein called Nucleoporin NUP188 homolog.

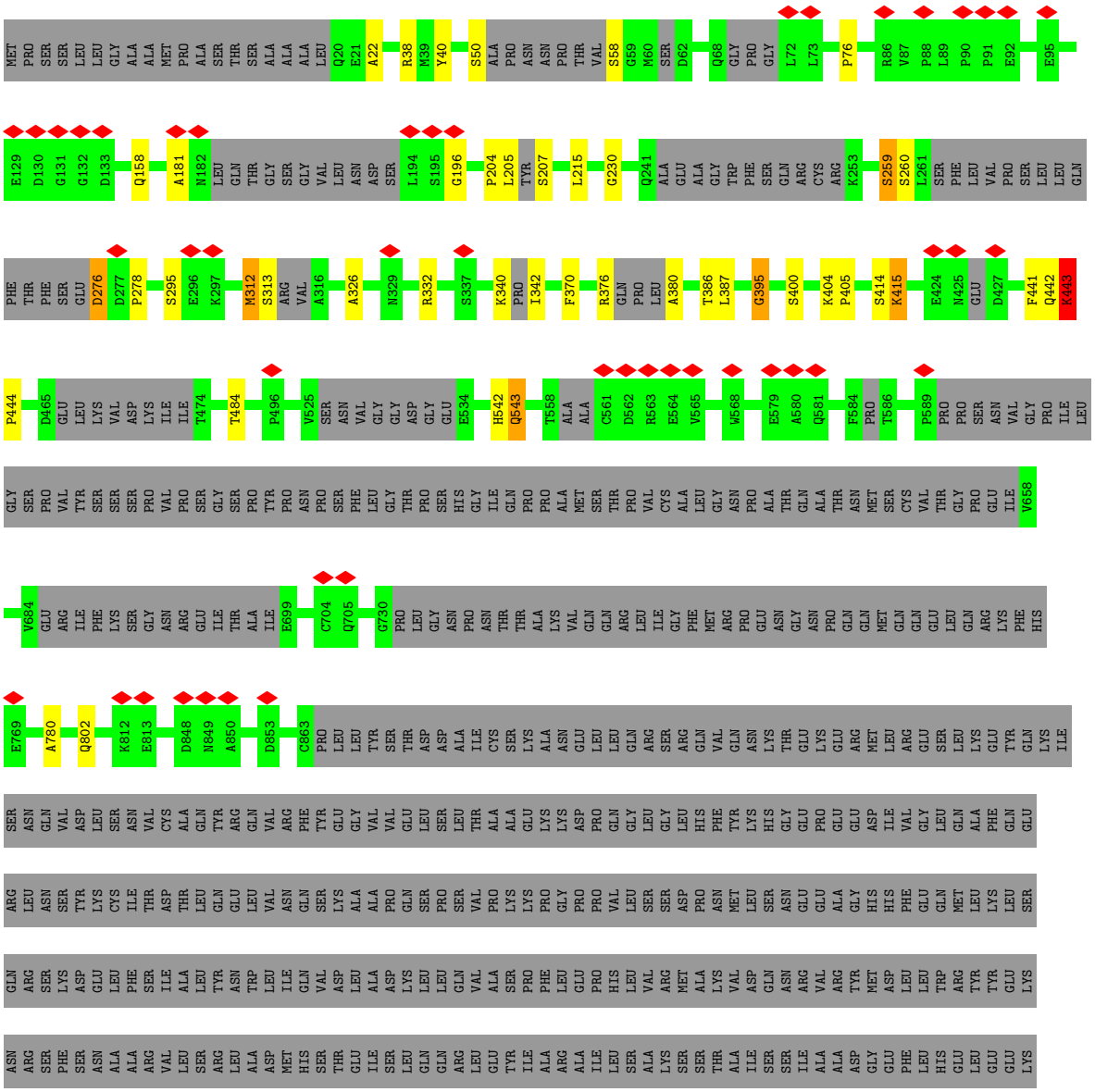
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	J	1256	6213	3701	1256	1256	0	0
7	V	1256	6213	3701	1256	1256	0	0

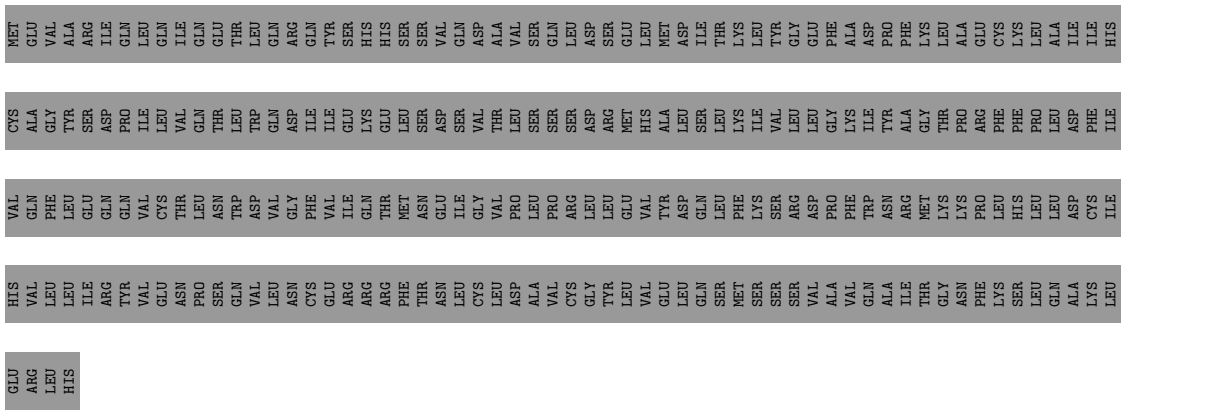
3 Residue-property plots (i)

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 Nup155

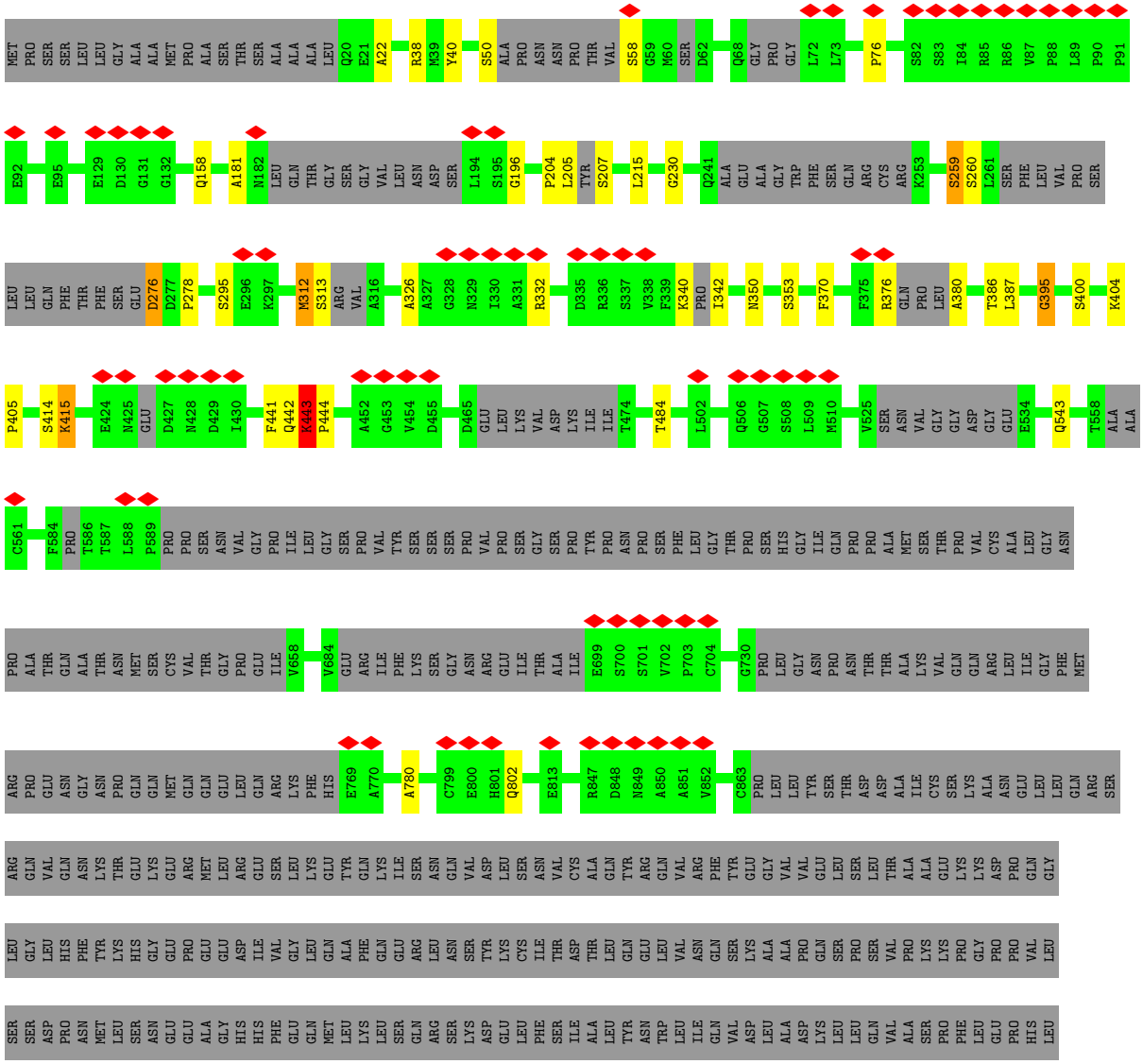
Chain A:

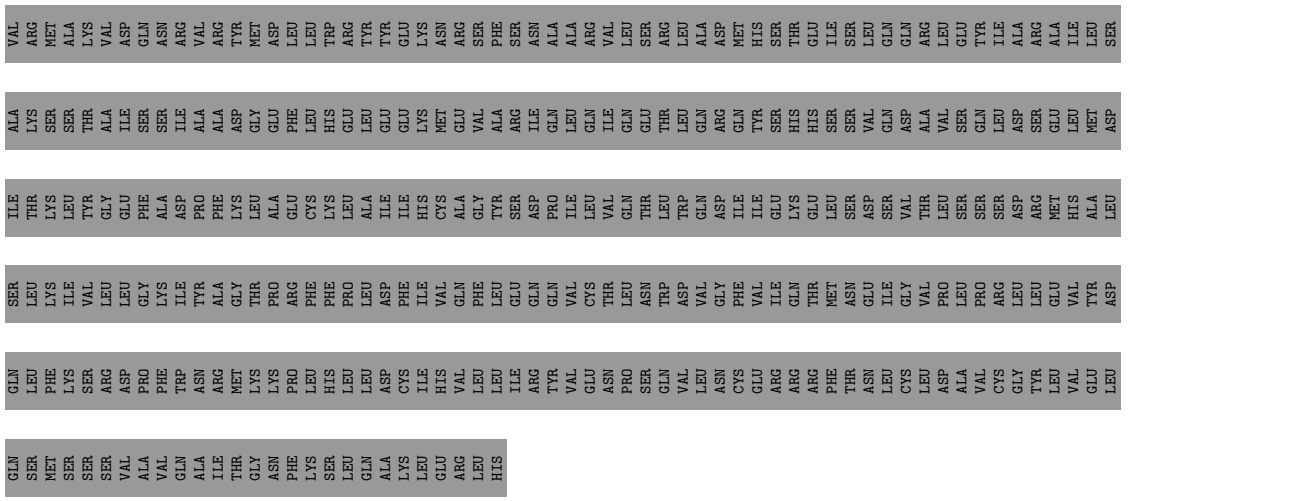




- Molecule 1: Nuclear pore complex protein Nup155

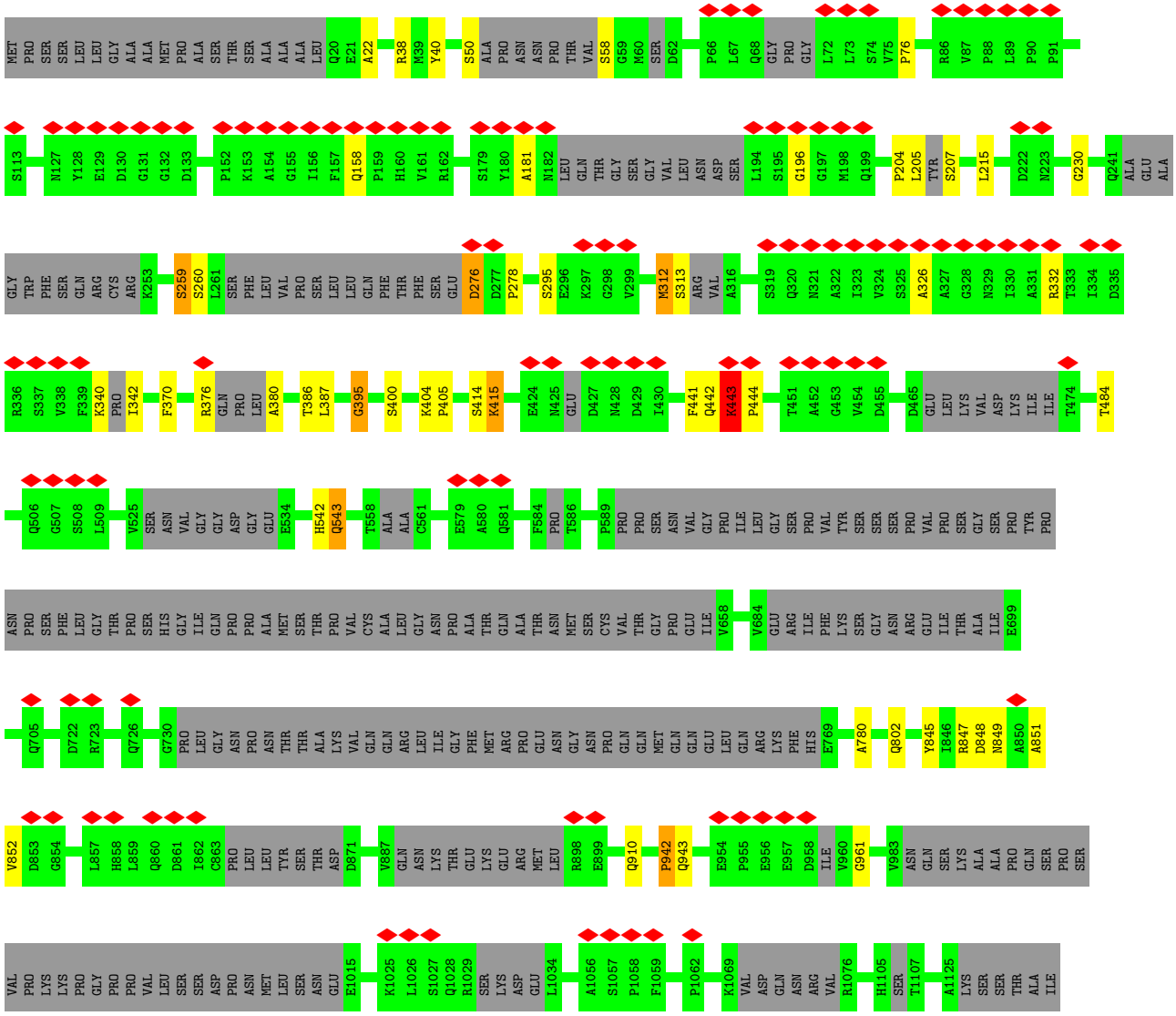
Chain B: 5% 43% • 53%

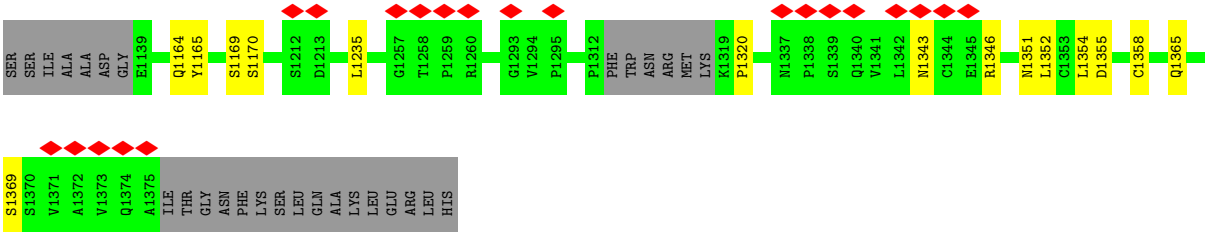




- Molecule 1: Nuclear pore complex protein Nup155

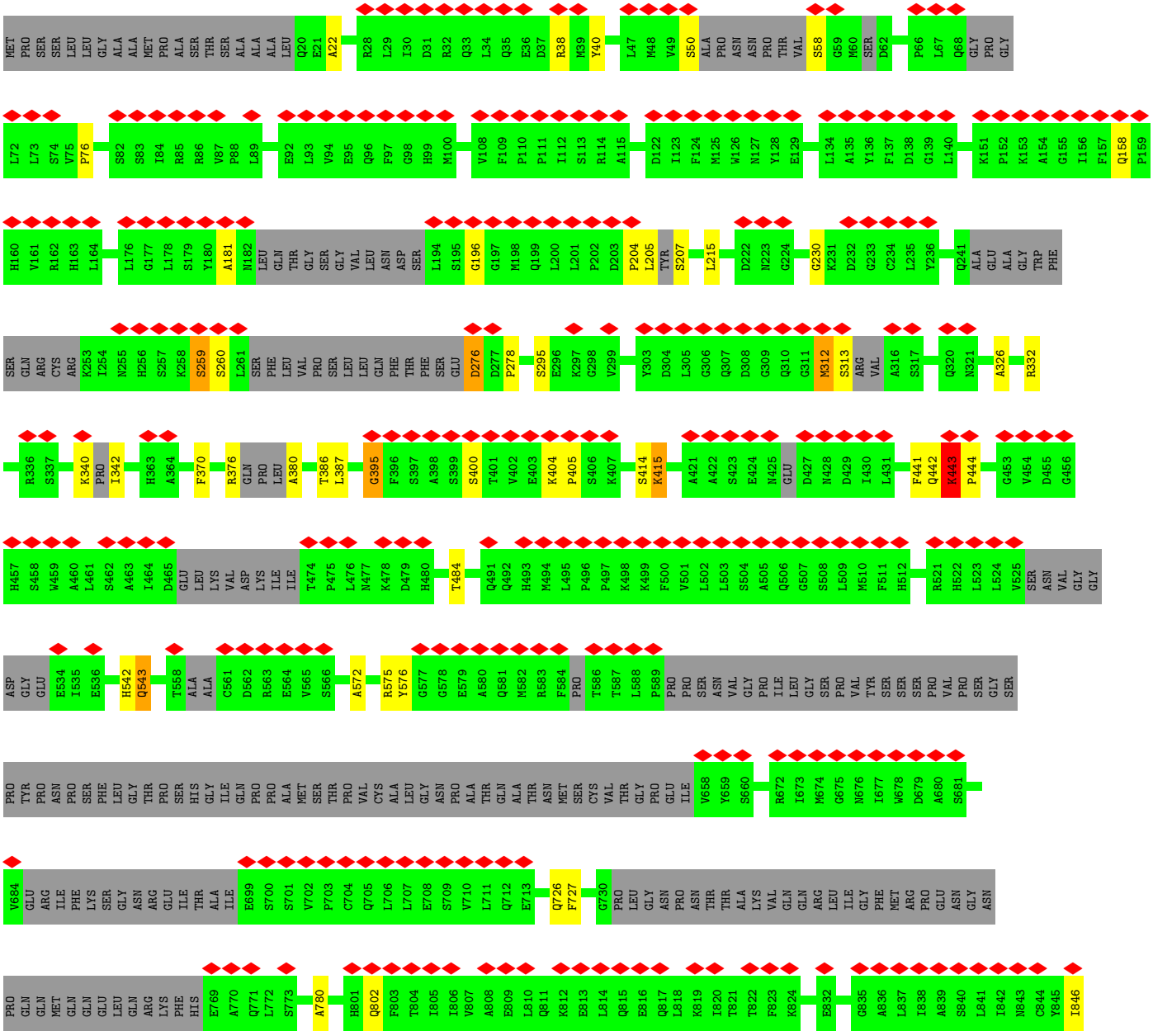
Chain E:

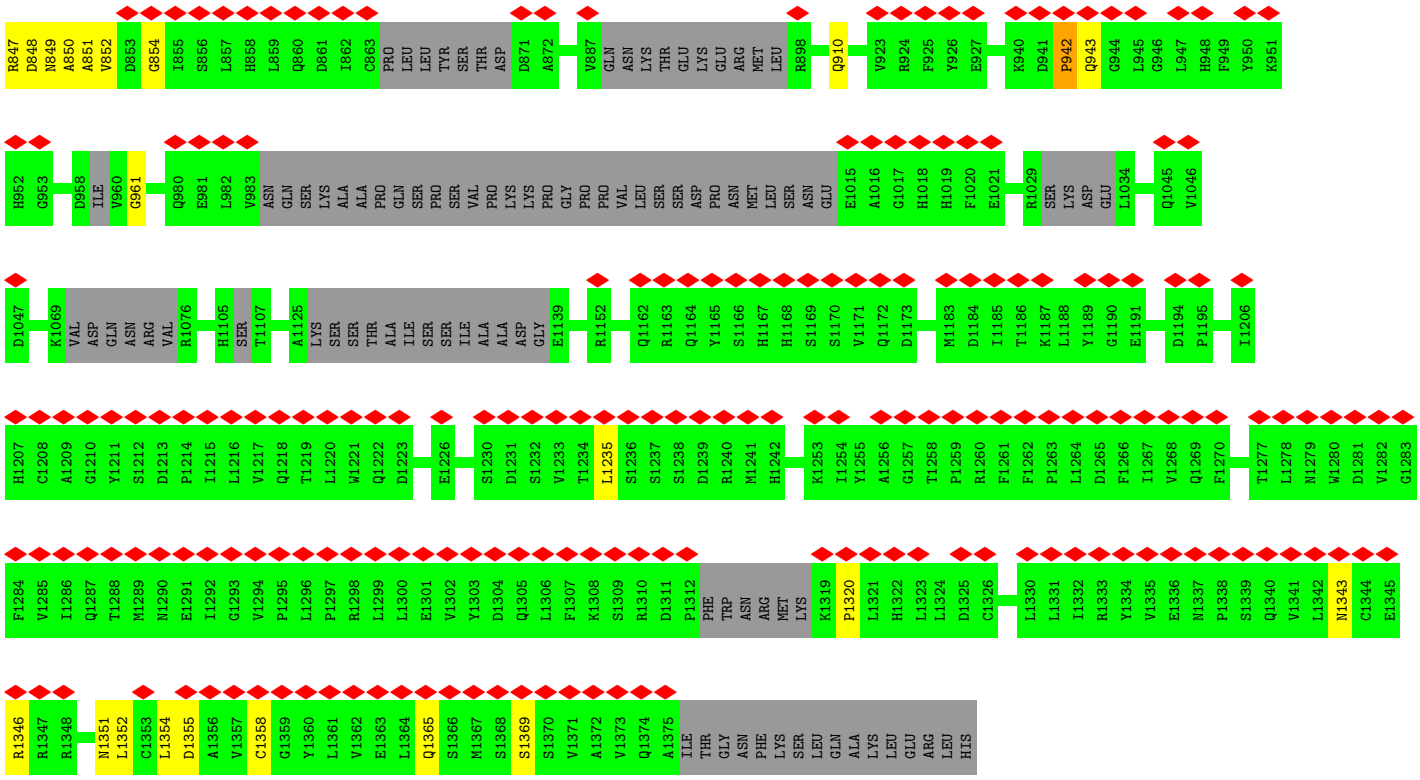




• Molecule 1: Nuclear pore complex protein Nup155

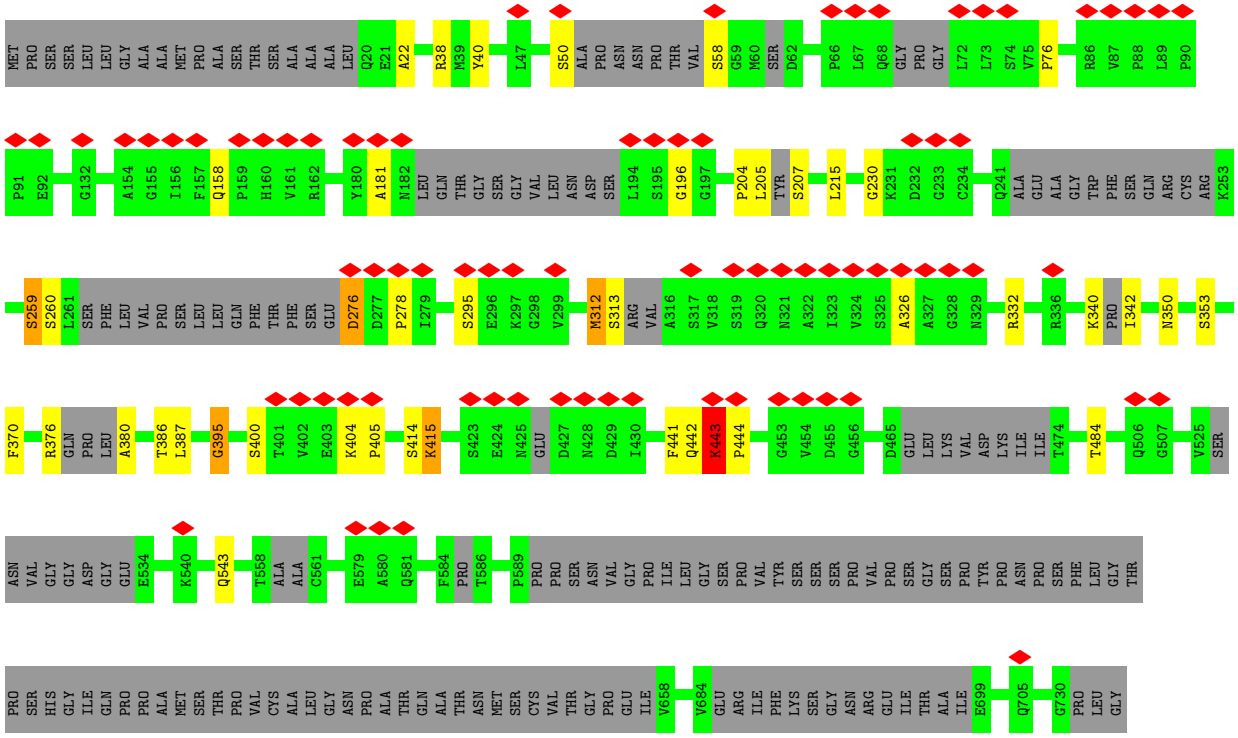
Chain K:

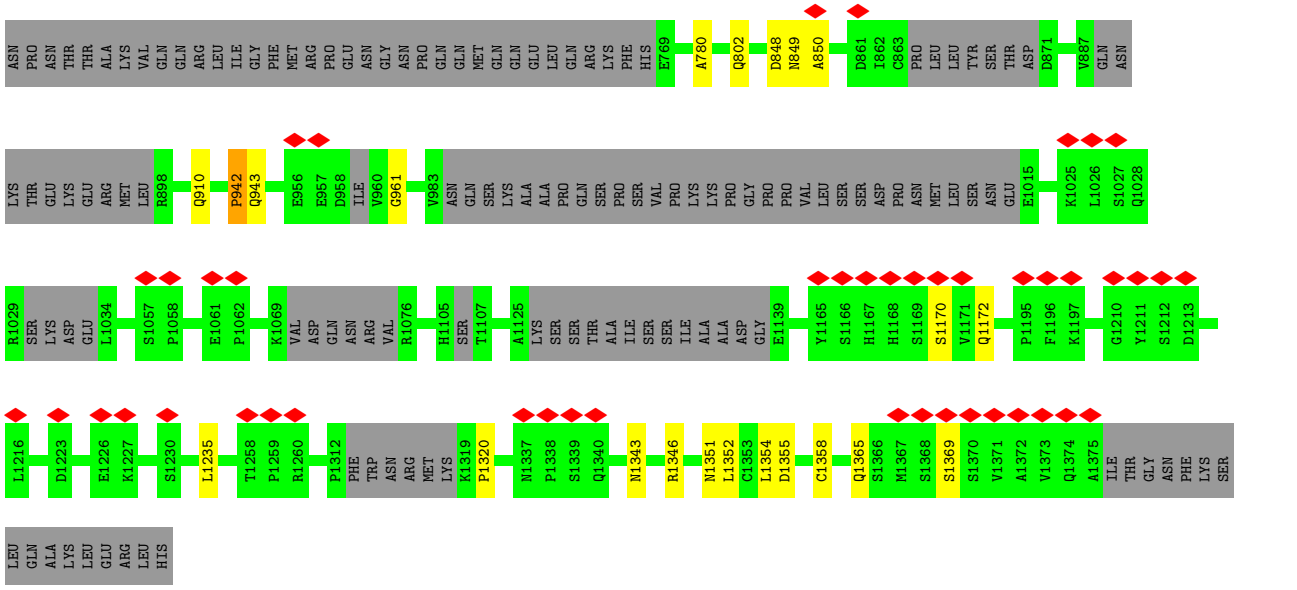




- Molecule 1: Nuclear pore complex protein Nup155

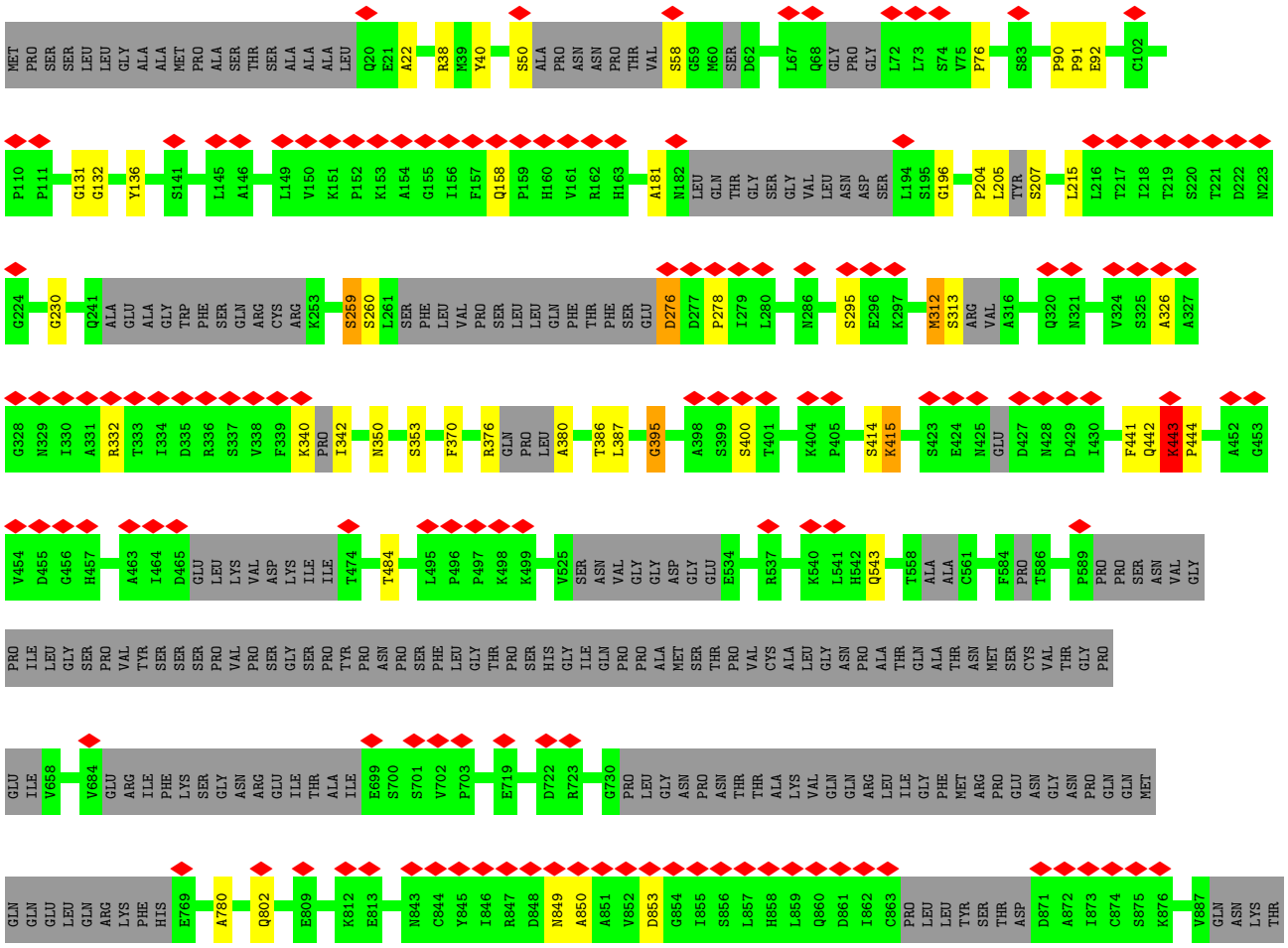
Chain Q:

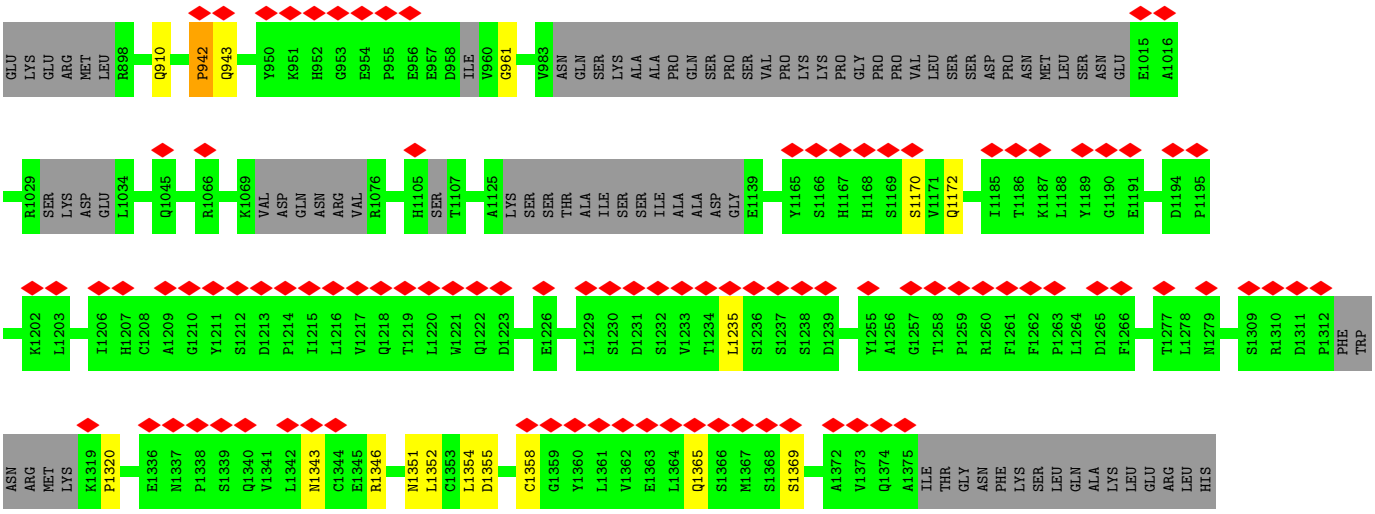




- Molecule 1: Nuclear pore complex protein Nup155

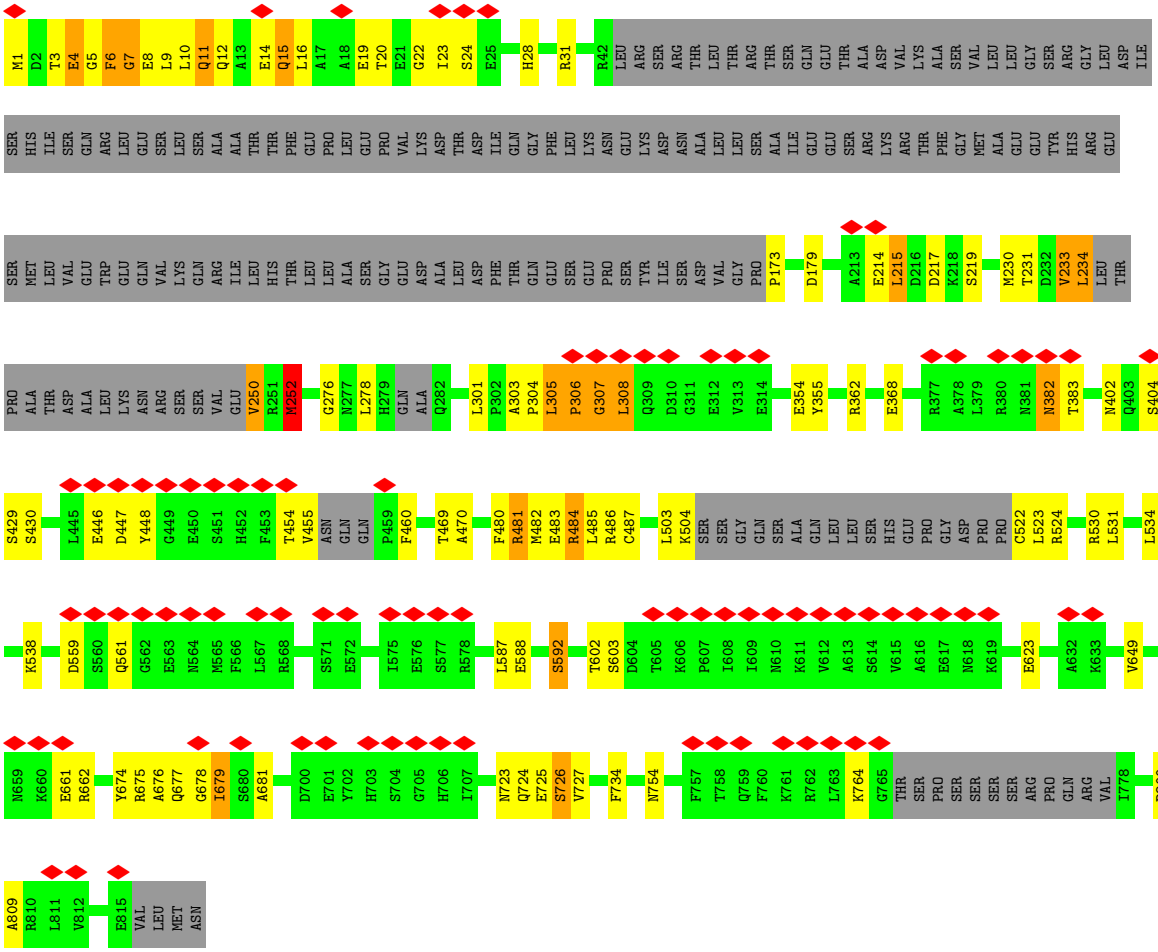
Chain W:





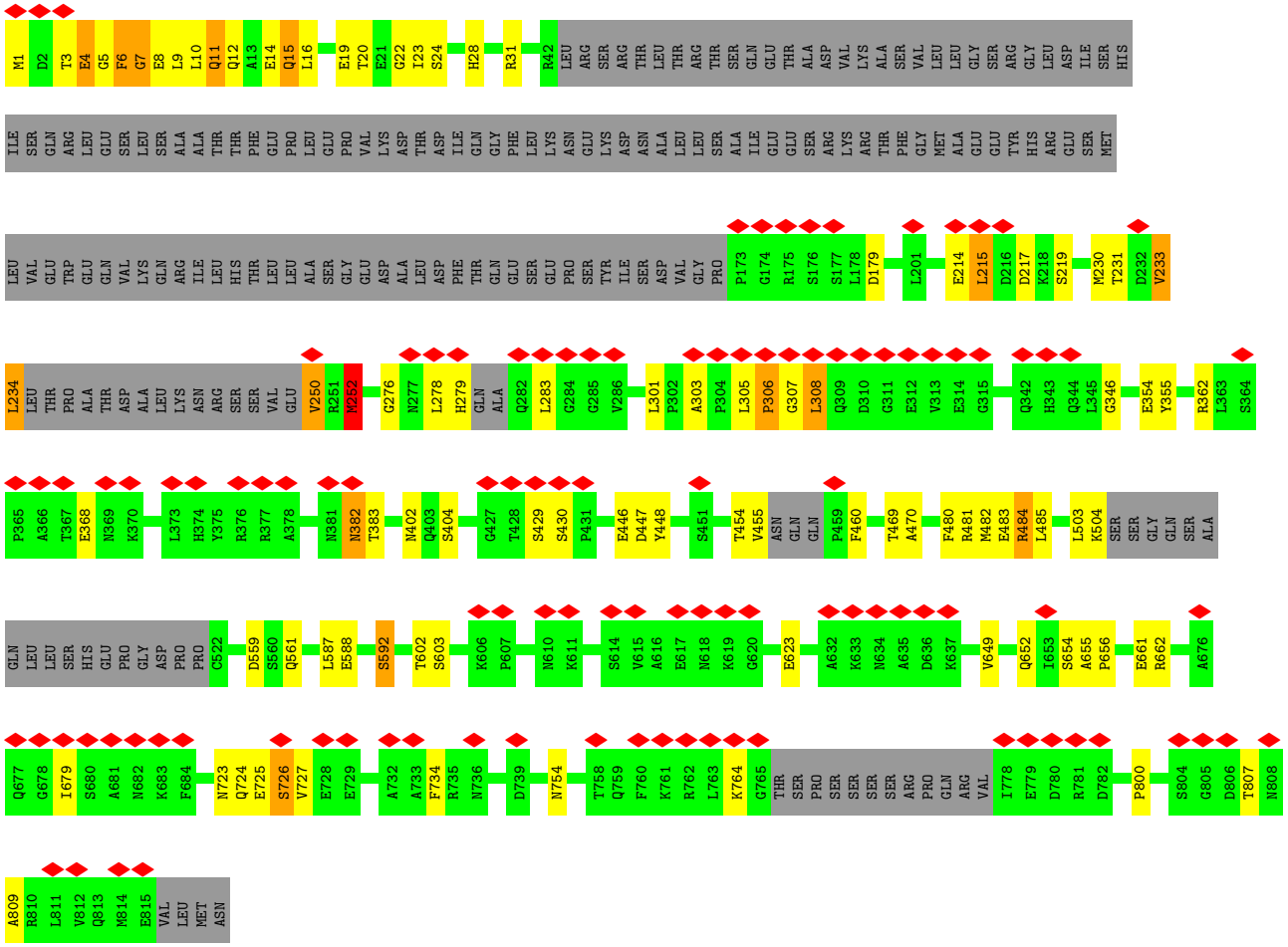
- Molecule 2: Nuclear pore complex protein Nup93

Chain C:



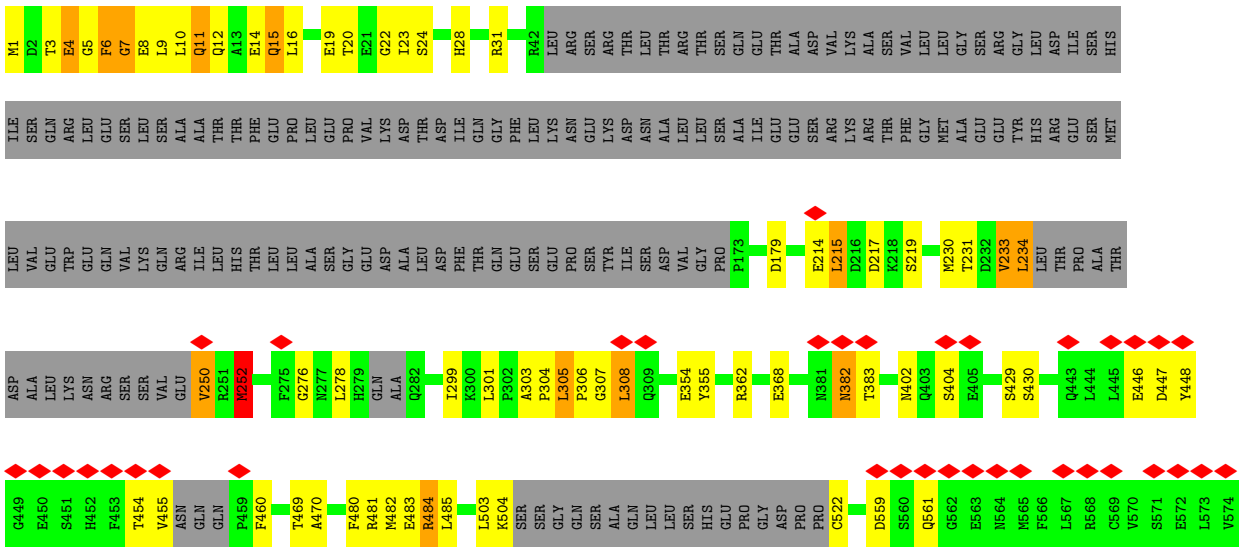
- Molecule 2: Nuclear pore complex protein Nup93

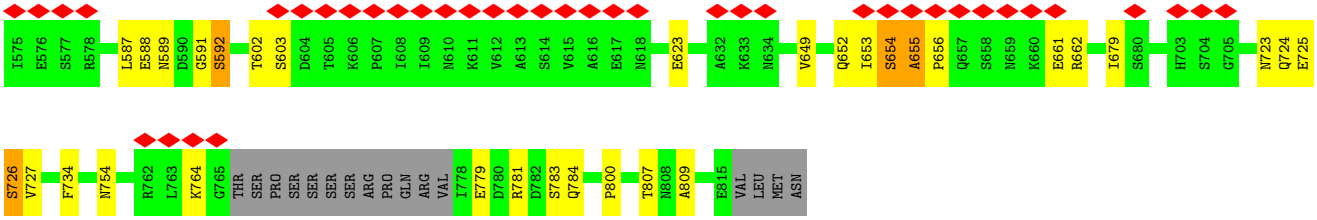
Chain I:



- Molecule 2: Nuclear pore complex protein Nup93

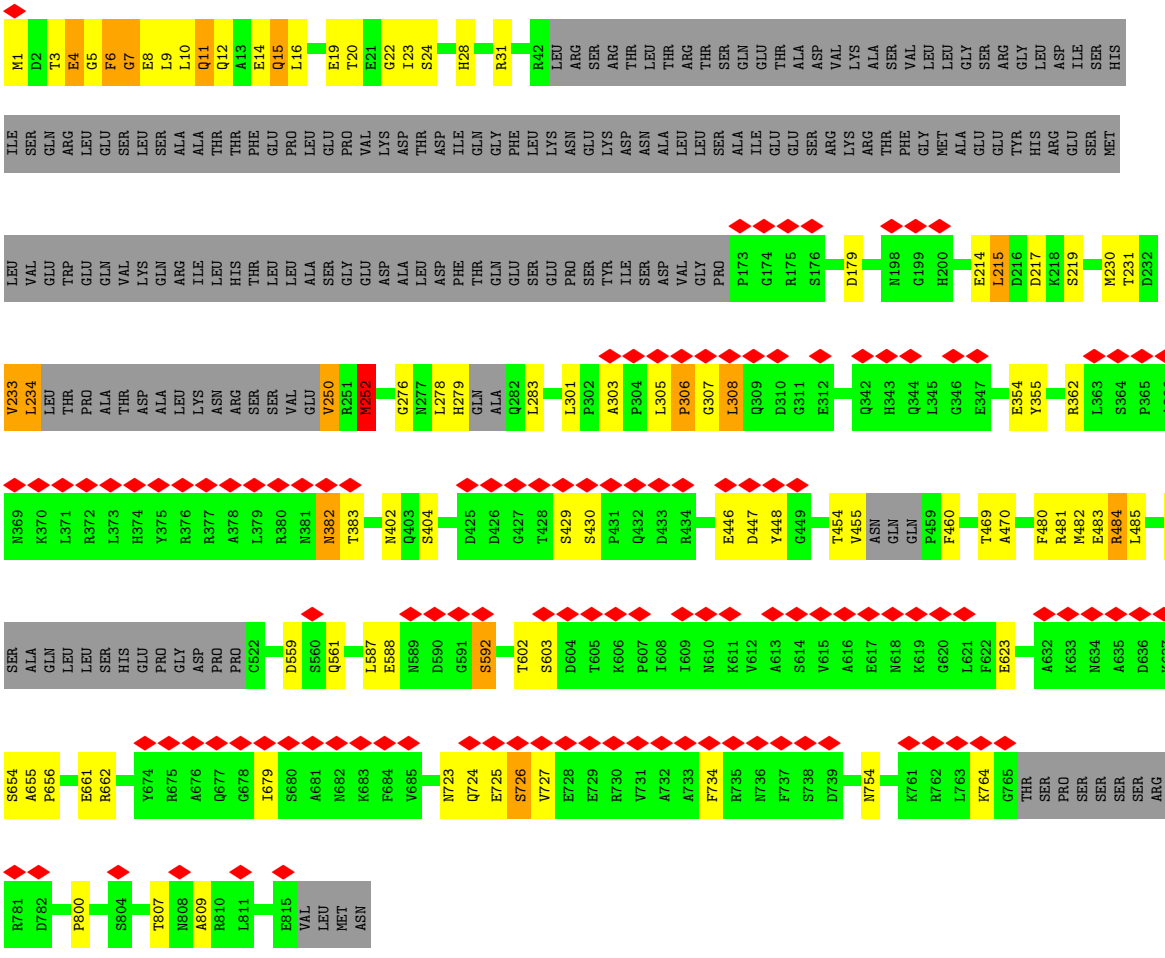
Chain O:





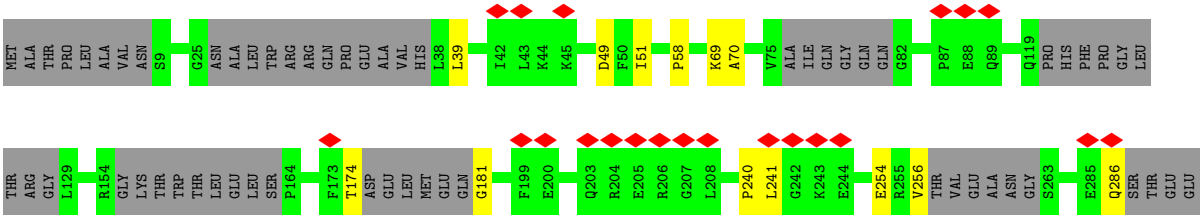
• Molecule 2: Nuclear pore complex protein Nup93

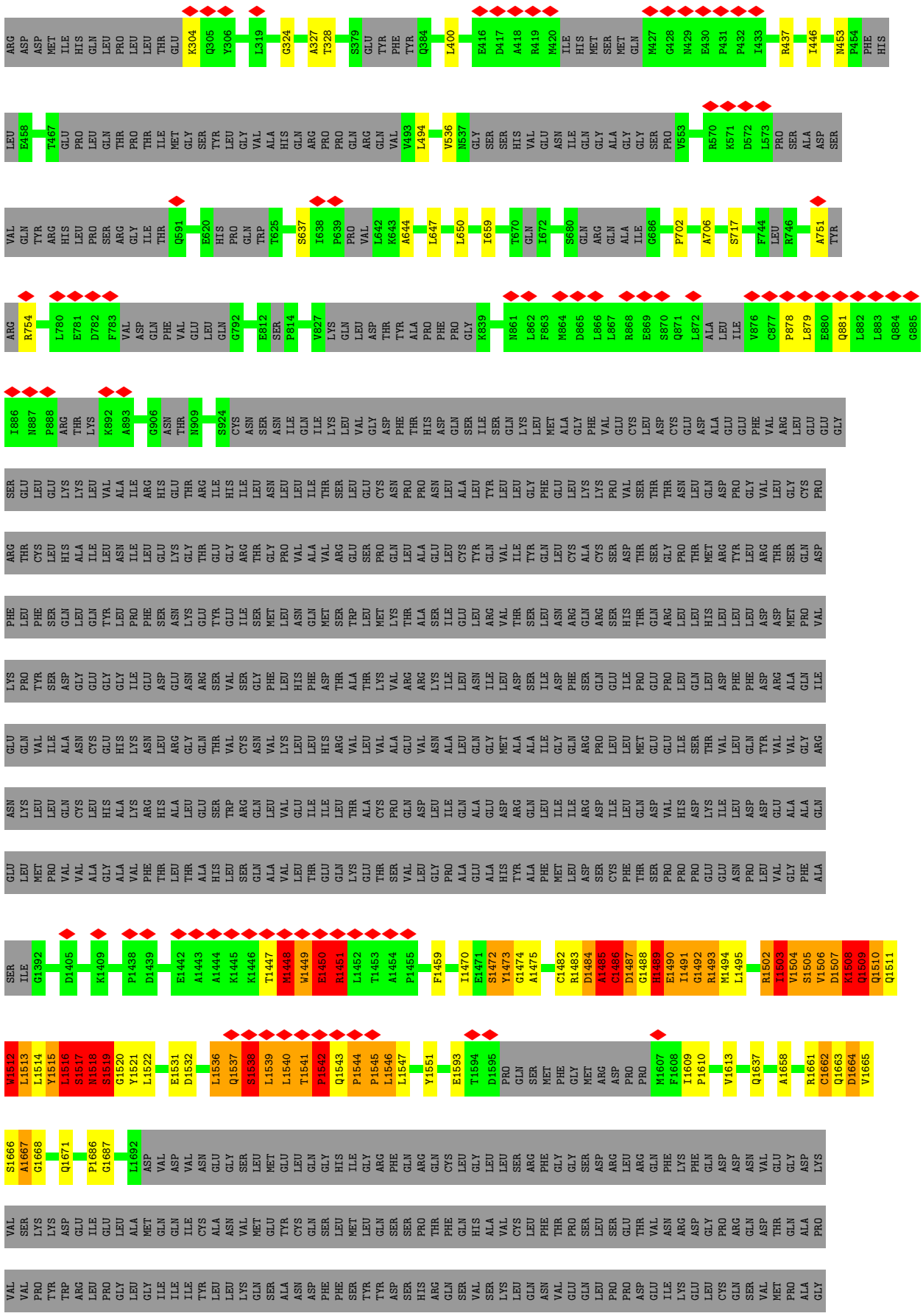
Chain U:



• Molecule 3: Nuclear pore complex protein Nup205

Chain D:

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LEU E458 T467 GLU PRO LEU GLN THR PRO THR ILE MET GLY SER TYR LEU GLY VAL ALA HIS GLN ARG PRO PRO GLN ARG GLN VAL V493 L494 V536 N537 GLY SER SER HIS VAL GLU ASN ILE GLN GLY ALA GLY GLY SER PRO V553 R570 K571 D572 L573 PRO SER ALA ASP SER
VAL GLN TYR ARG HIS LEU PRO SER ARG GLY ILE THR Q591 E620 HIS PRO GLN TRP T625 S637 I638 P639 PRO VAL L642 K643 A644 L647 L650 I659 T670 GLN I672 S680 GLN ARG GLN ALA ILE G686 P702 A706 S717 F744 LEU R746 A751 TYR
ARG R754 L780 E781 D782 F783 VAL ASP GLN PHE VAL GLU LEU GLN G792 E812 SER P814 V827 LYS GLN LEU ASP THR TYR ALA PRO PHE PRO GLY K839 N861 L862 F863 M864 D865 L866 L867 R868 E869 S870 Q871 L872 ALA LEU ILE V876 C877 P878 L879 E880 Q881 L882 L883 Q884 G885
I886 N887 P888 ARG THR LYS K892 A893 G906 ASN THR N909 S924 CYS ASN SER ASN ILE GLN ILE LYS LEU VAL GLY ASP PHE THR HIS ASP GLN SER ILE SER GLN LYS LEU MET ALA GLY PHE VAL GLU CYS LEU ASP CYS GLU ASP ALA GLU GLU PHE VAL ARG LEU GLU GLU GLY
SER GLU LEU GLU LYS LYS LEU VAL ALA ILE ARG HIS GLU THR ARG ILE HIS ILE LEU ASN LEU LEU ILE THR SER LEU GLU CYS ASN PRO PRO ASN LEU ALA LEU TYR LEU LEU GLY PHE GLU LEU LYS LYS PRO VAL SER THR THR ASN LEU GLN ASP PRO GLY VAL LEU GLY CYS PRO
ARG THR CYS LEU HIS ALA ILE LEU ASN ILE LEU GLU LYS GLY THR GLU GLY ARG THR GLY PRO VAL ALA VAL ARG GLU SER PRO GLN LEU ALA GLU LEU CYS TYR GLN VAL ILE TYR GLN LEU CYS ALA CYS SER ASP THR SER GLY PRO THR MET ARG TYR LEU ARG THR SER GLN ASP
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LYS PRO TYR SER ASP GLY GLU GLY GLY ILE GLU ASP GLU ASN ARG SER VAL SER GLY PHE LEU HIS PHE ASP THR ALA THR LYS VAL ARG ARG LYS ILE LEU ASN ILE LEU ASP SER ILE ASP PHE SER GLN GLU ILE PRO GLU PRO LEU GLN ILE PHE ASP ARG ALA GLN ILE
GLU GLN VAL ILE ALA ASN CYS GLU HIS LYS ASN LEU ARG GLY GLN THR VAL CYS ASN VAL LYS LEU LEU LEU HIS ARG VAL LEU VAL ALA GLU VAL ASN ALA LEU GLU GLN GLY MET ALA ALA ILE GLY GLN ARG PRO LEU LEU MET GLU GLU ILE SER THR VAL LEU GLN TYR VAL VAL GLY ARG
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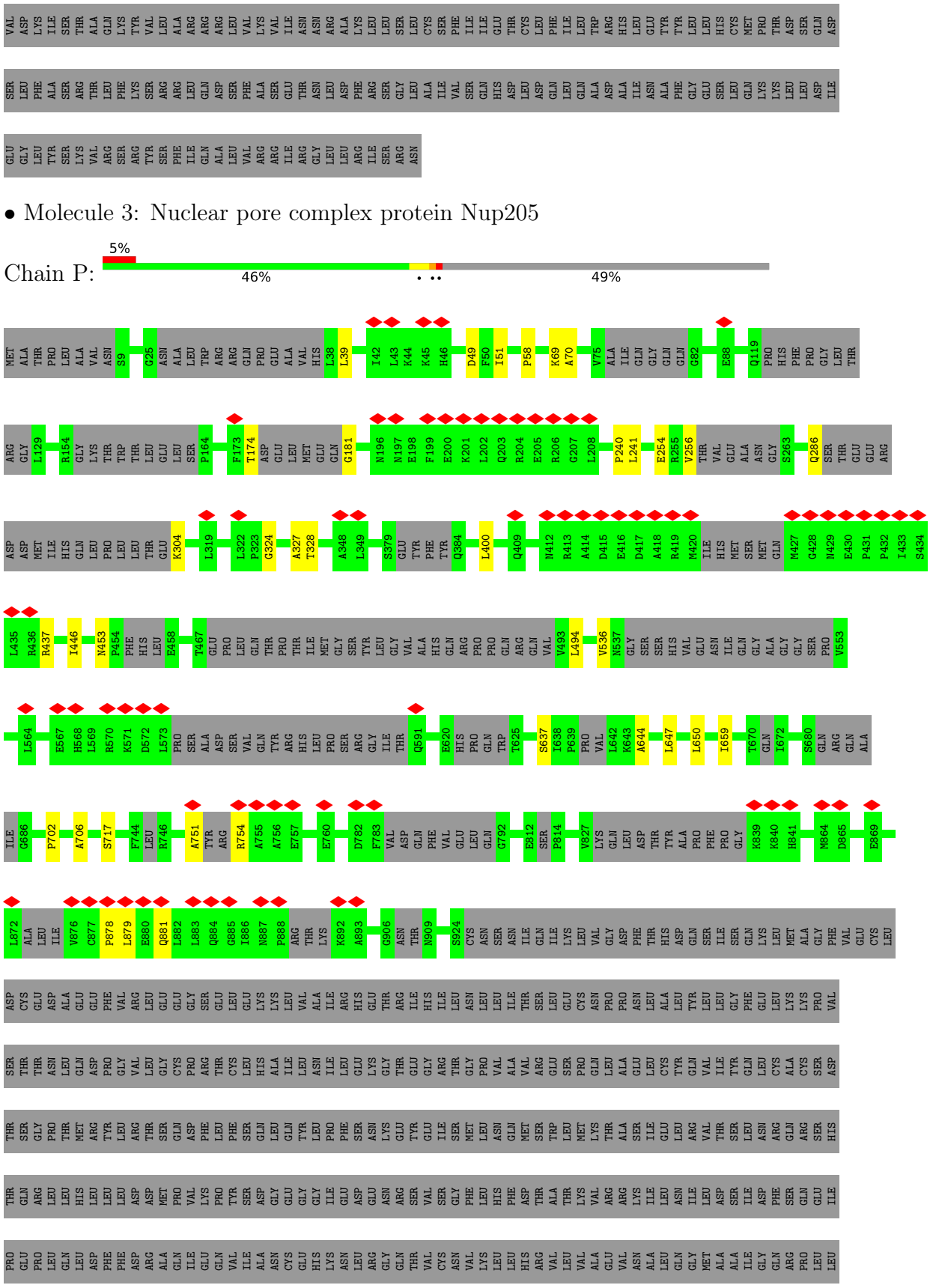
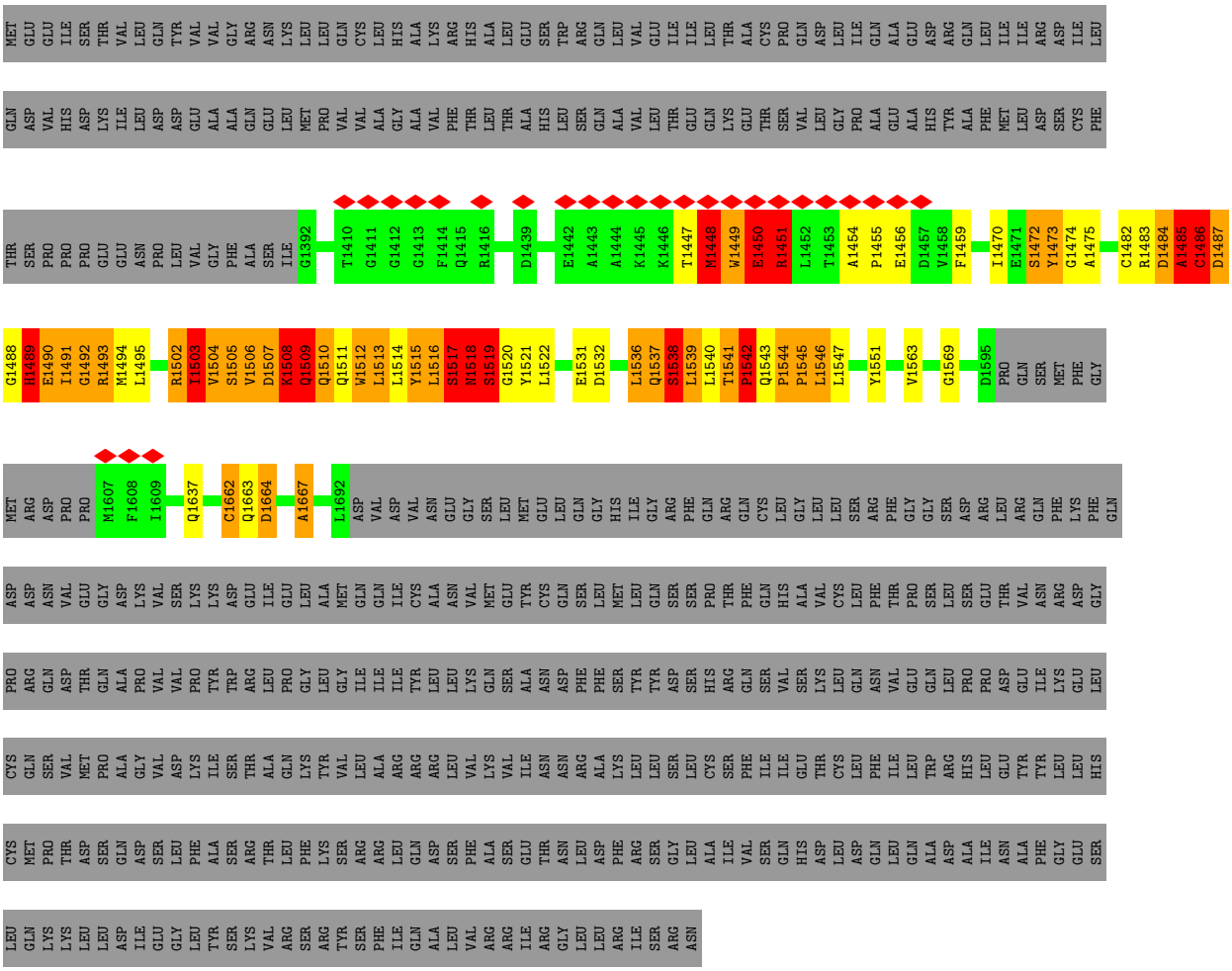
W1512 L1513 L1514 Y1515 L1516 S1517 N1518 S1519 G1520 Y1521 L1522 E1531 D1532 L1536 Q1537 S1538 L1539 L1540 T1541 P1542 Q1543 P1544 P1545 L1546 L1547 Y1551 E1593 T1594 D1595 PRO GLN SER MET PHE GLY MET ARG ASP PRO PRO M1607 F1608 I1609 P1610 V1613 Q1637 A1658 R1661 C1662 Q1663 D1664 V1665
S1666 A1667 G1668 Q1671 P1686 G1687 L1692 ASP VAL ASP VAL ASN GLU GLY SER LEU MET GLU LEU GLN GLY HIS ILE GLY ARG PHE GLN ARG GLN CYS LEU GLY LEU LEU SER ARG PHE GLY GLY SER ASP ARG LEU ARG GLN PHE LYS PHE GLN ASP ASP ASN VAL GLU GLY ASP LYS
VAL SER LYS LYS ASP GLU ILE GLU LEU ALA MET GLN GLN ILE CYS ALA ASN VAL MET GLU TYR CYS GLN SER LEU MET GLU LEU GLN SER SER PRO THR PHE GLN HIS ALA VAL CYS LEU PHE THR PRO PRO GLN ARG GLN ASP GLU THR VAL ASN ARG GLN GLN ASP THR GLN ALA PRO
VAL VAL PRO TYR TRP ARG LEU LEU PRO GLY LEU GLY ILE ILE ILE TYR LEU LEU LYS GLN SER ALA ASN ASP PHE PHE SER TYR TYR ASP SER HIS ARG GLN SER VAL SER LYS LEU GLN ASN VAL GLU GLN LEU PRO PRO ASP GLU ILE LYS GLU LEU CYS GLN SER VAL MET PRO ALA GLY



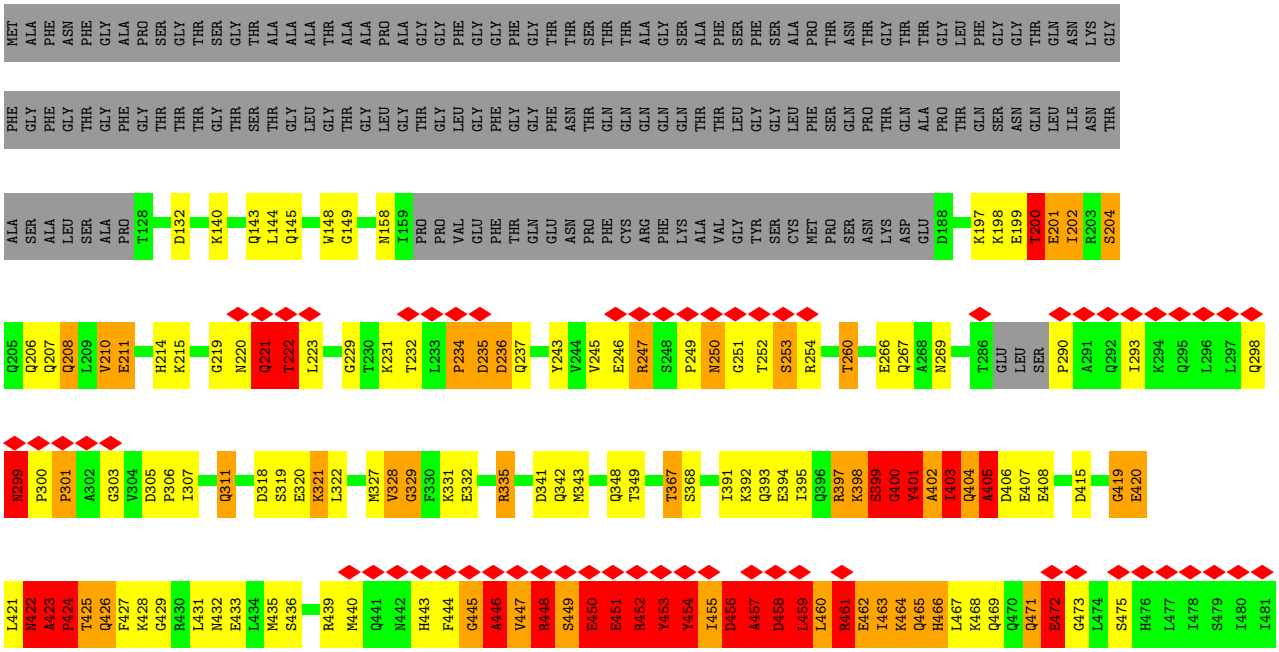
• Molecule 3: Nuclear pore complex protein Nup205

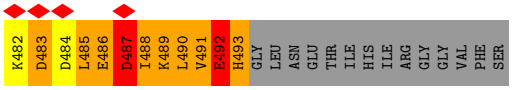
Chain P: 5% 46% 49%



- Molecule 4: Nucleoporin p54

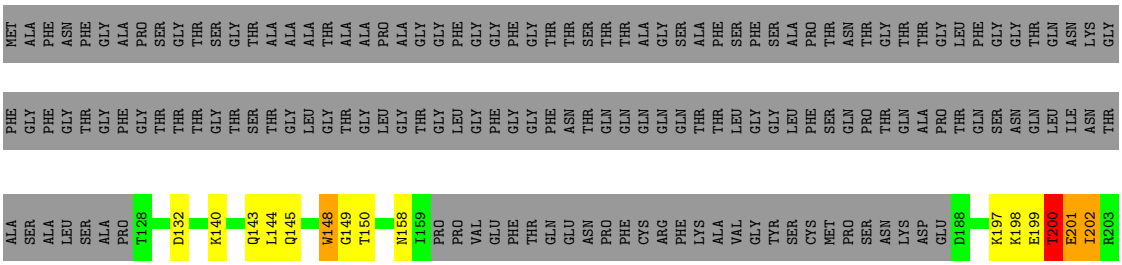
Chain F:





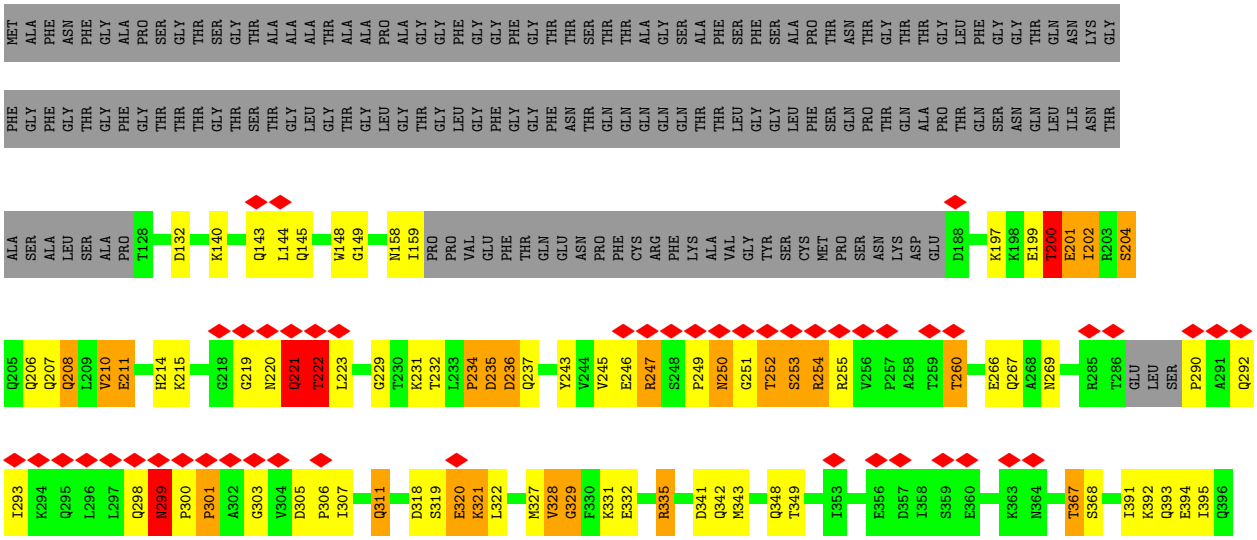
• Molecule 4: Nucleoporin p54

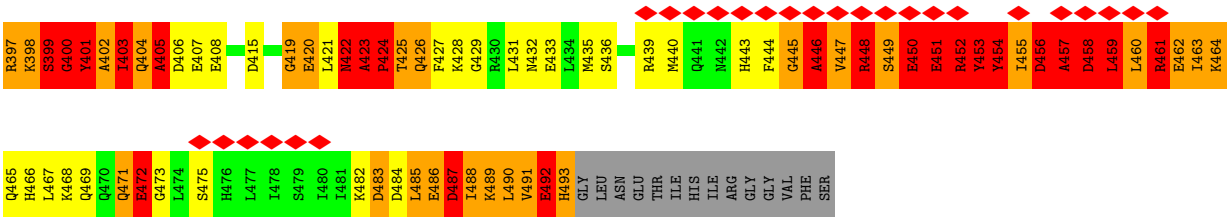
Chain L:



• Molecule 4: Nucleoporin p54

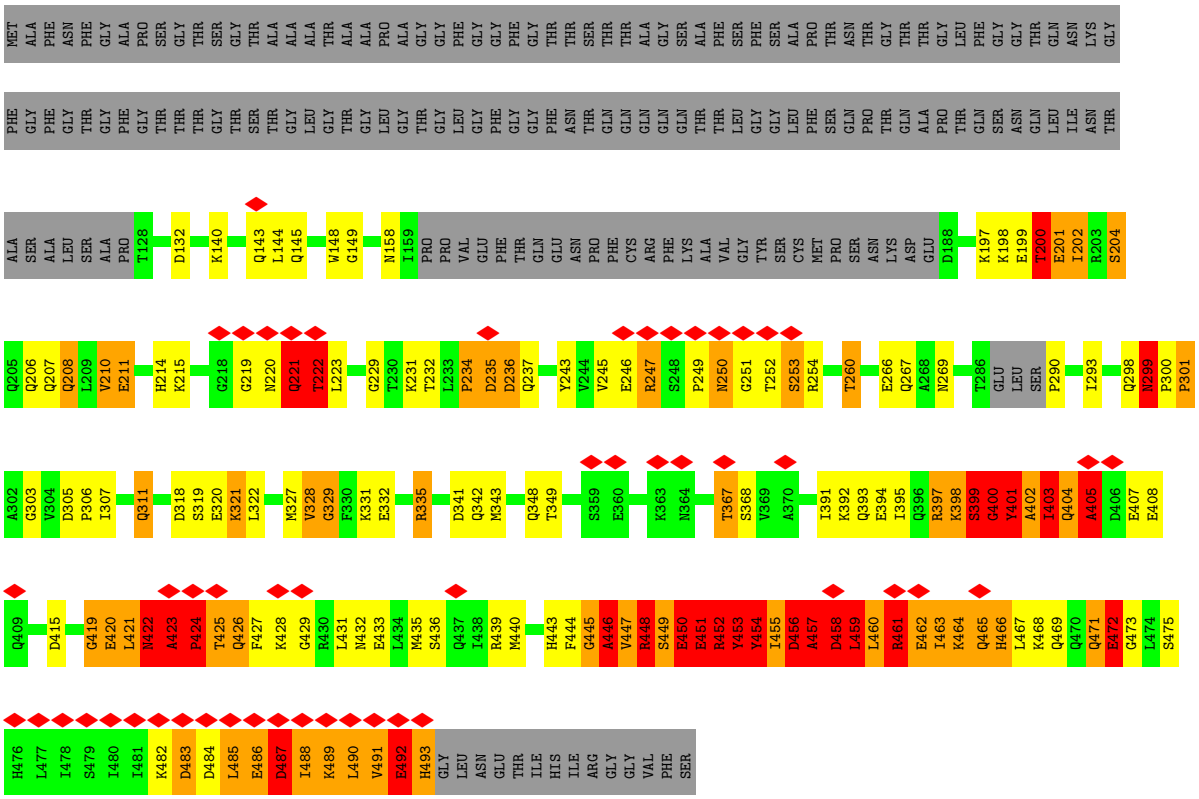
Chain R:





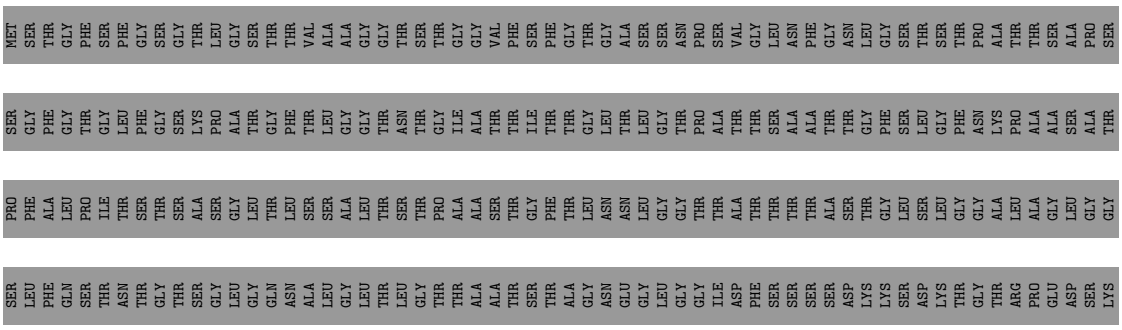
- Molecule 4: Nucleoporin p54

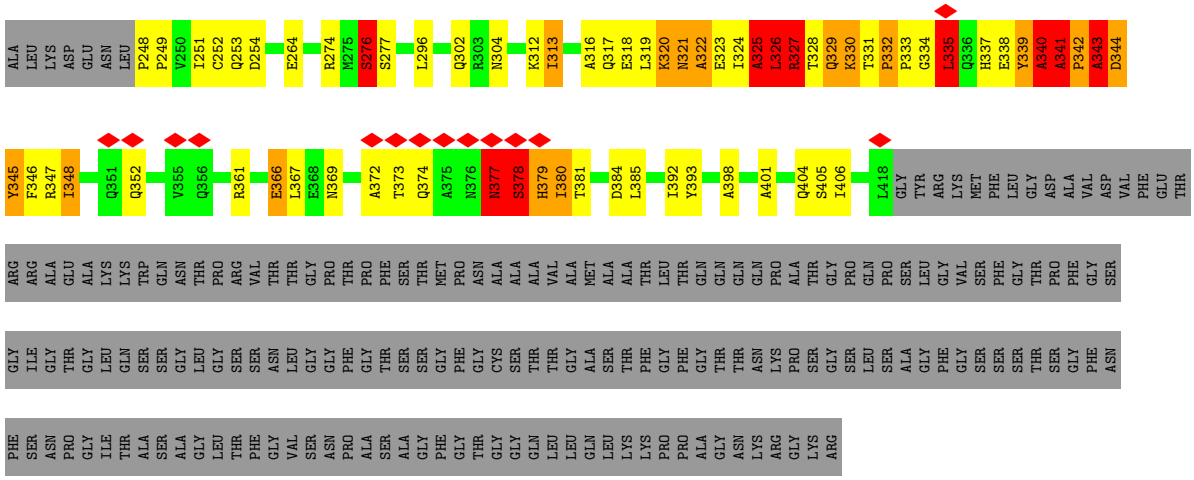
Chain X:



- Molecule 5: Nucleoporin p58/p45

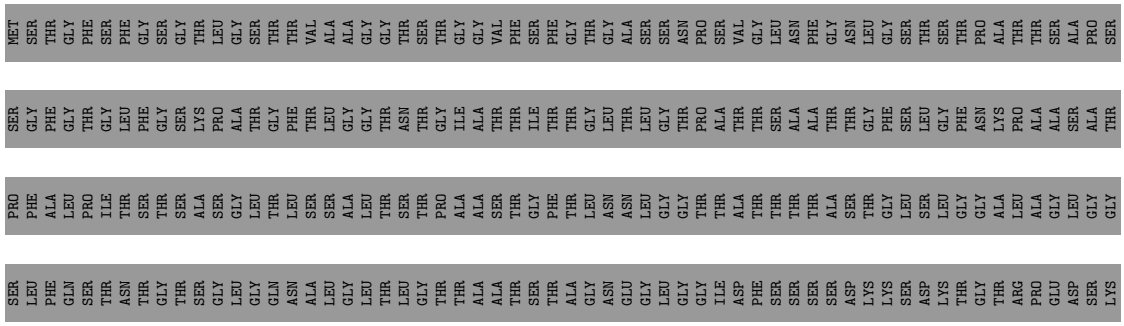
Chain G:

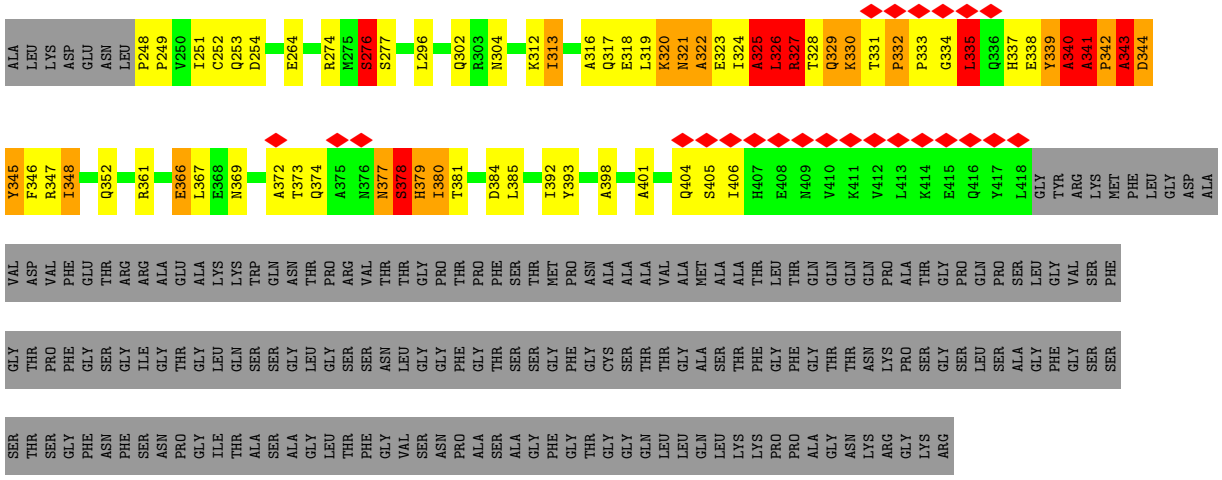




- Molecule 5: Nucleoporin p58/p45

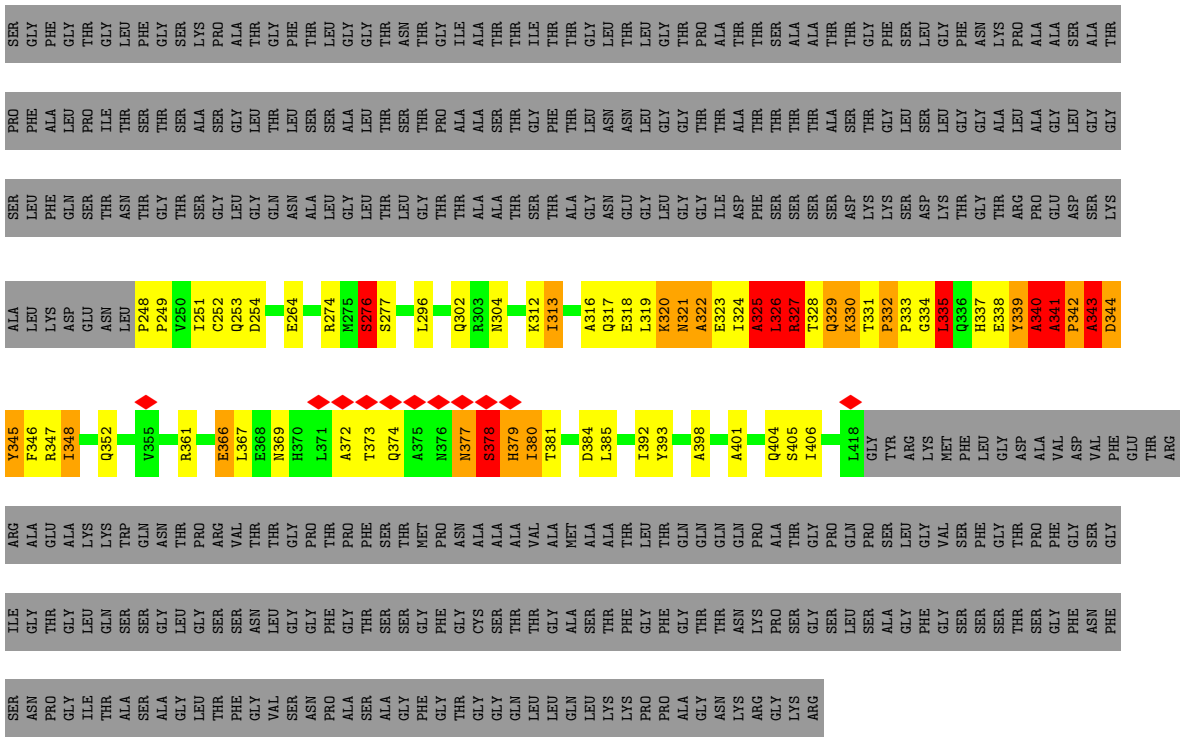
Chain M:





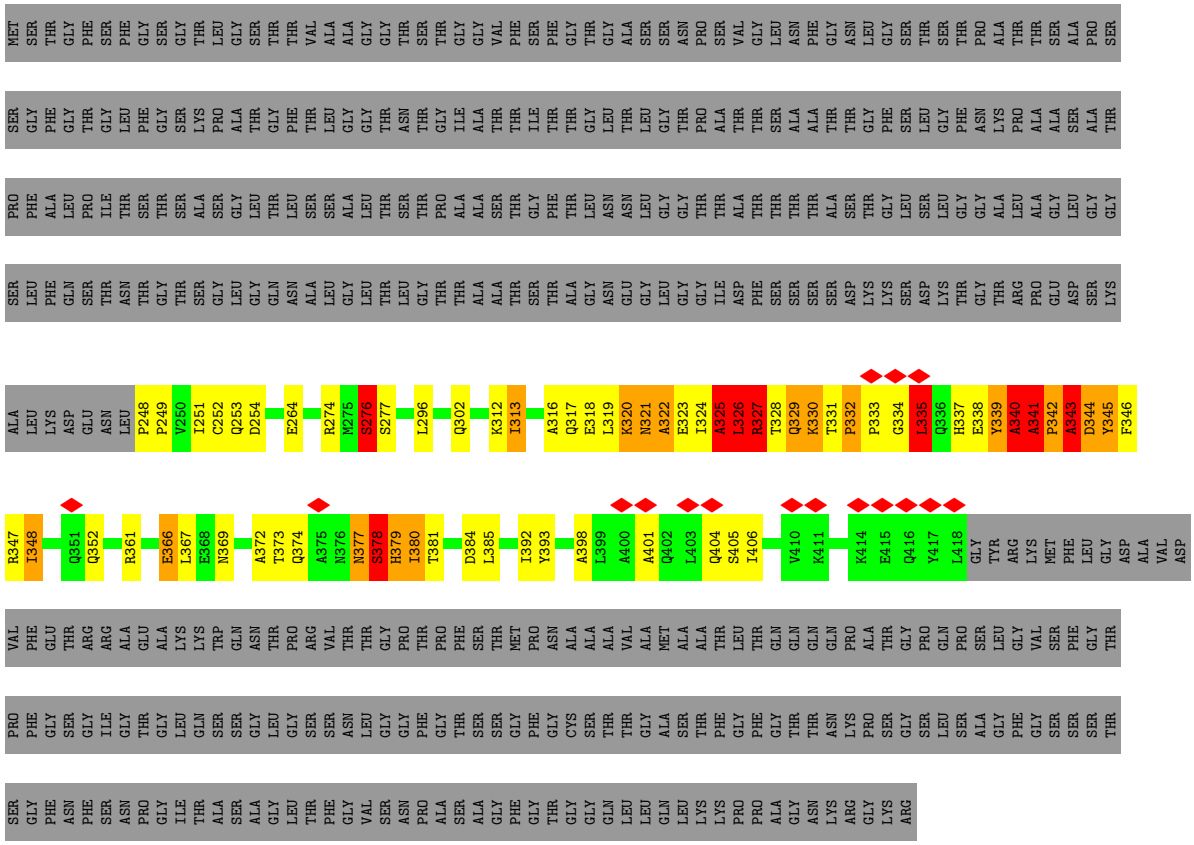
- Molecule 5: Nucleoporin p58/p45

Chain S:



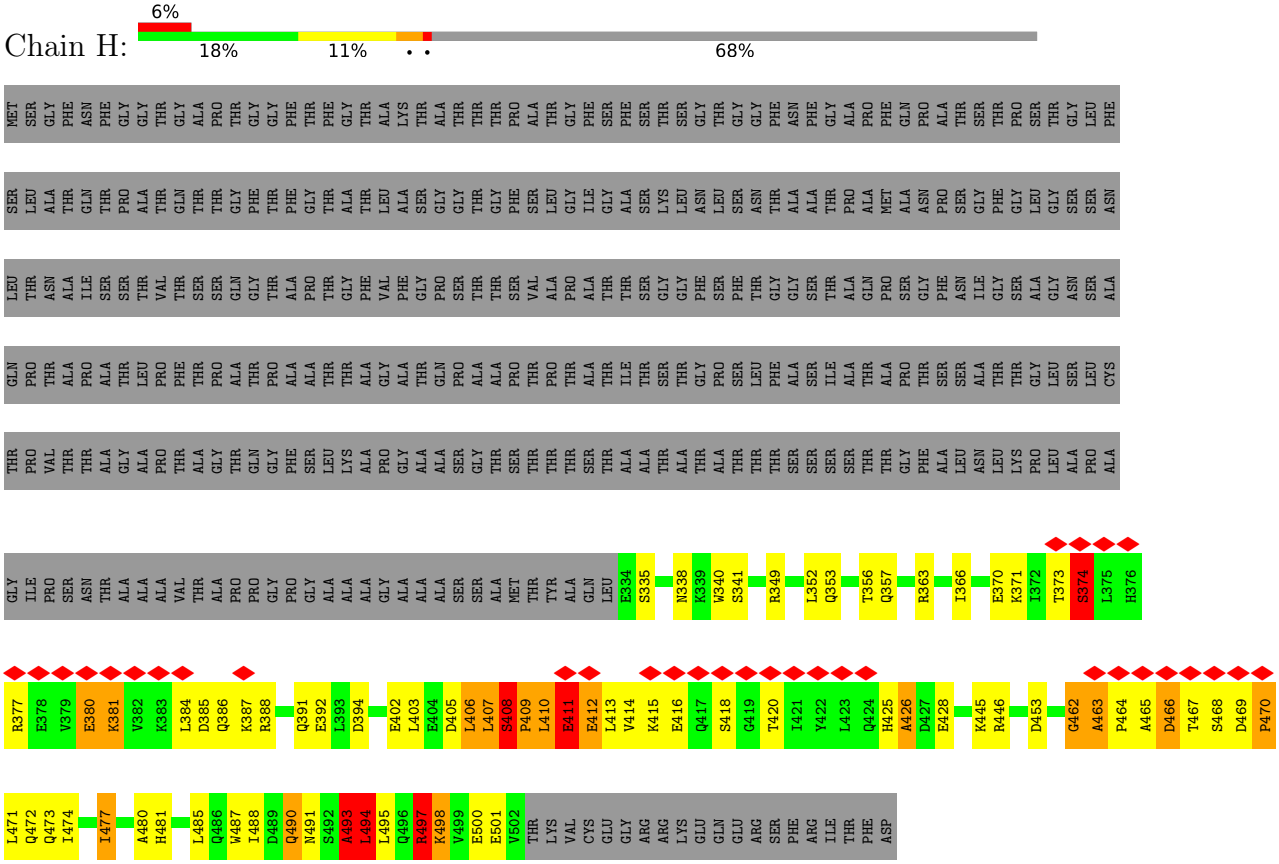
- Molecule 5: Nucleoporin p58/p45

Chain Y:



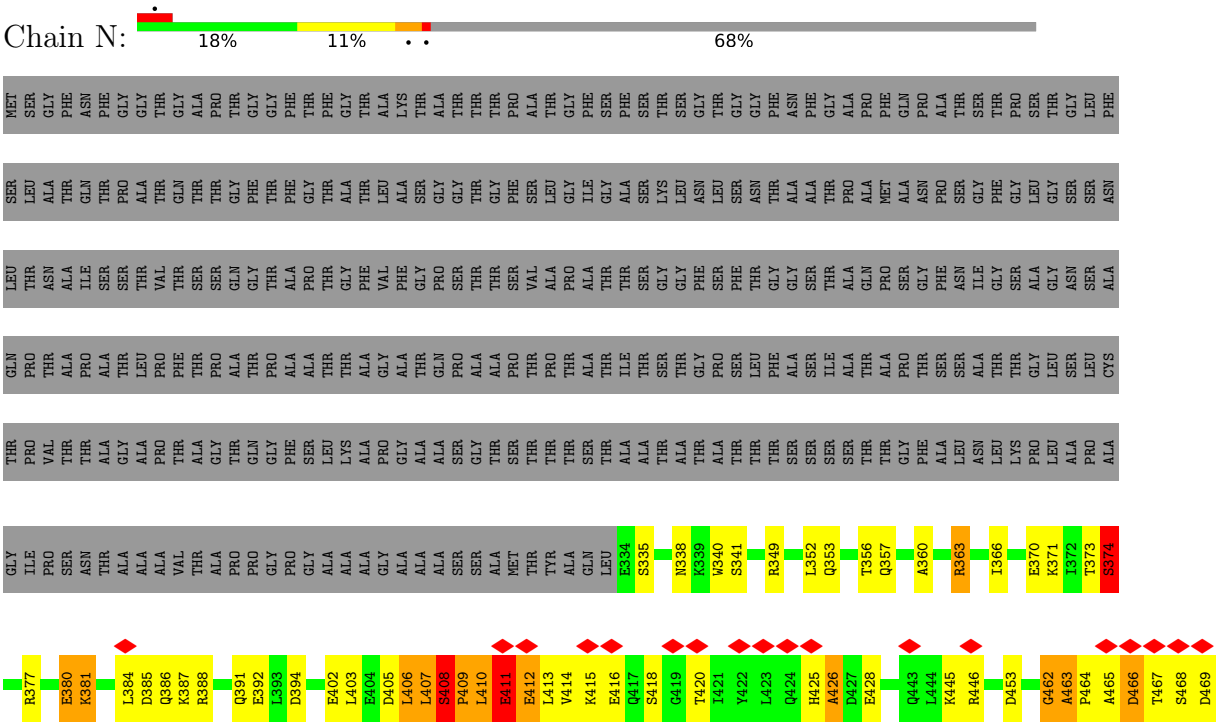
- Molecule 6: Nuclear pore glycoprotein p62

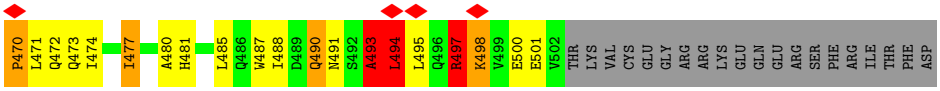
Chain H:



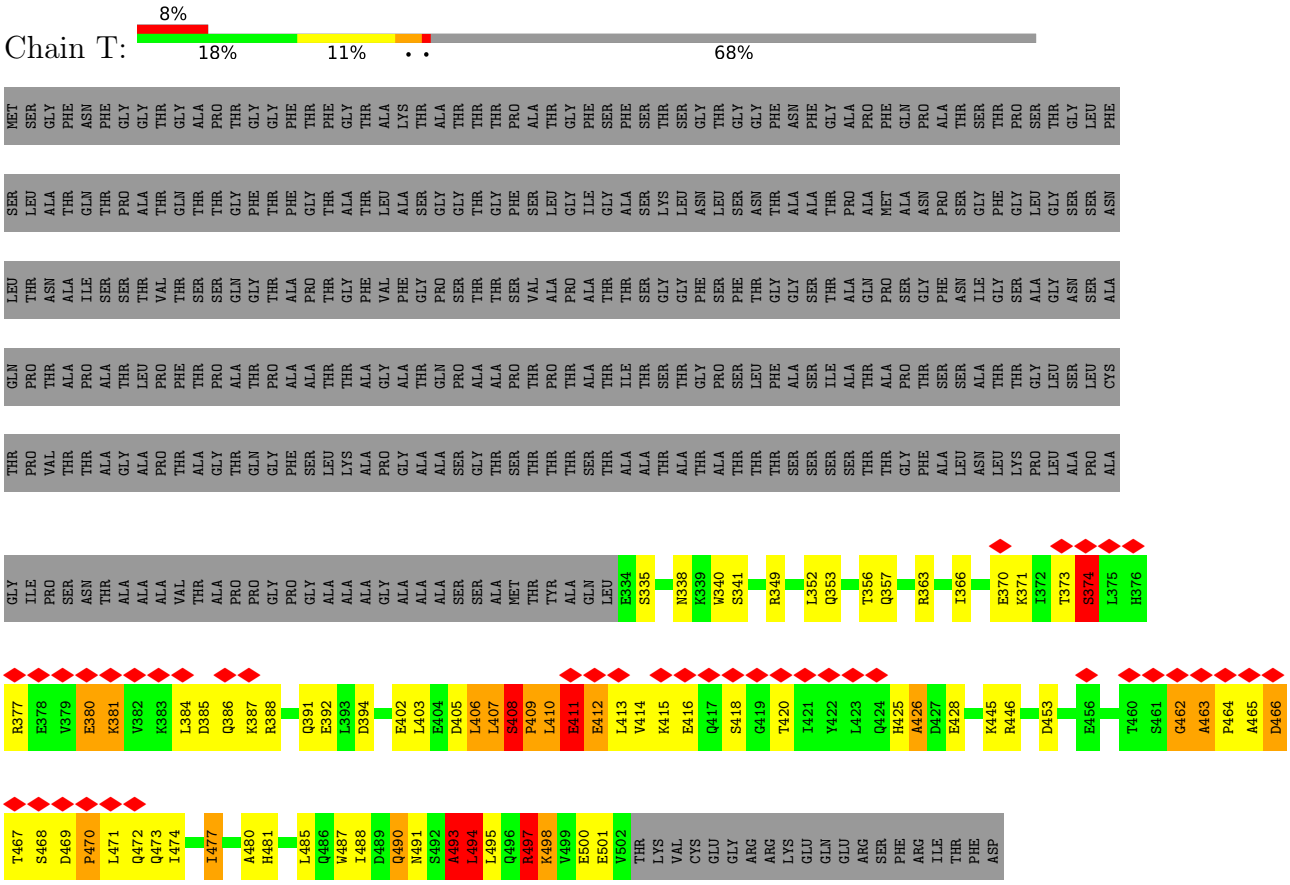
- Molecule 6: Nuclear pore glycoprotein p62

Chain N:

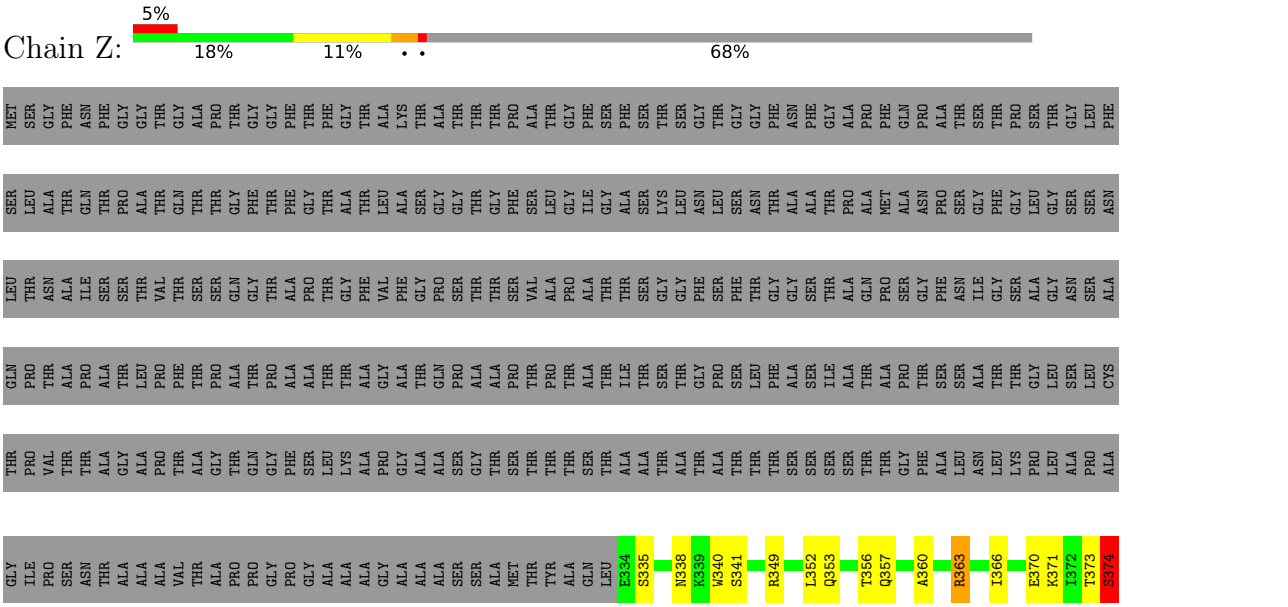


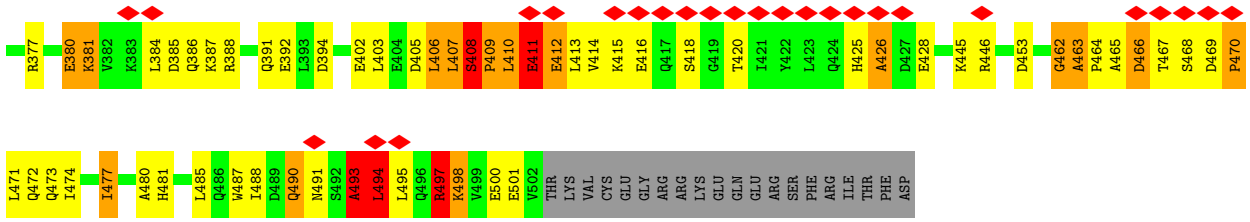


- Molecule 6: Nuclear pore glycoprotein p62



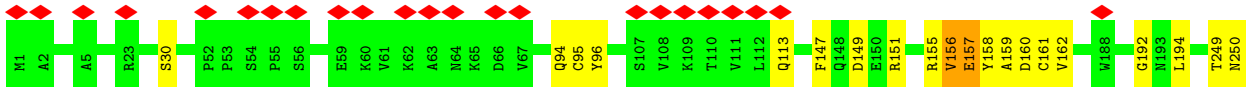
- Molecule 6: Nuclear pore glycoprotein p62

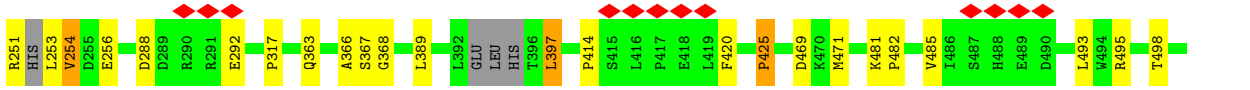


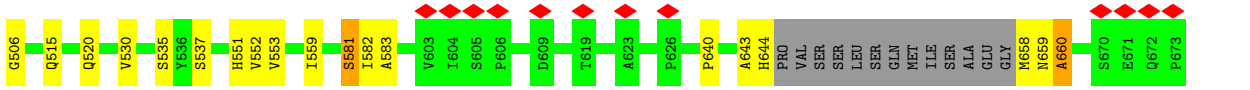


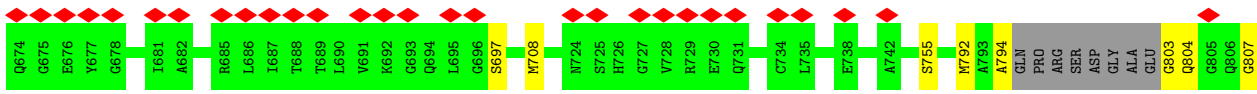
• Molecule 7: Nucleoporin NUP188 homolog

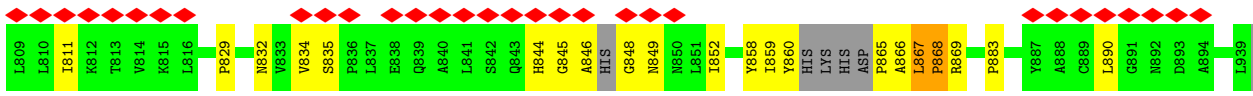
Chain J:

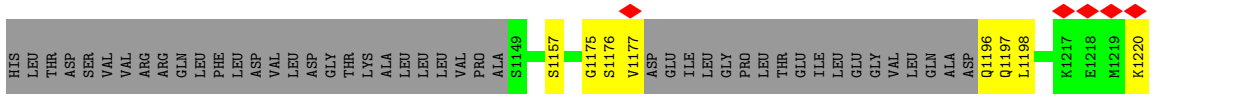


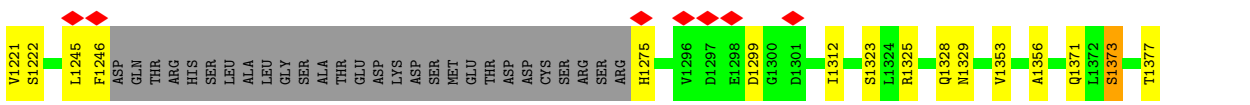


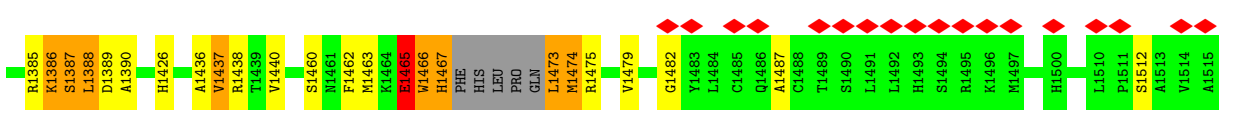


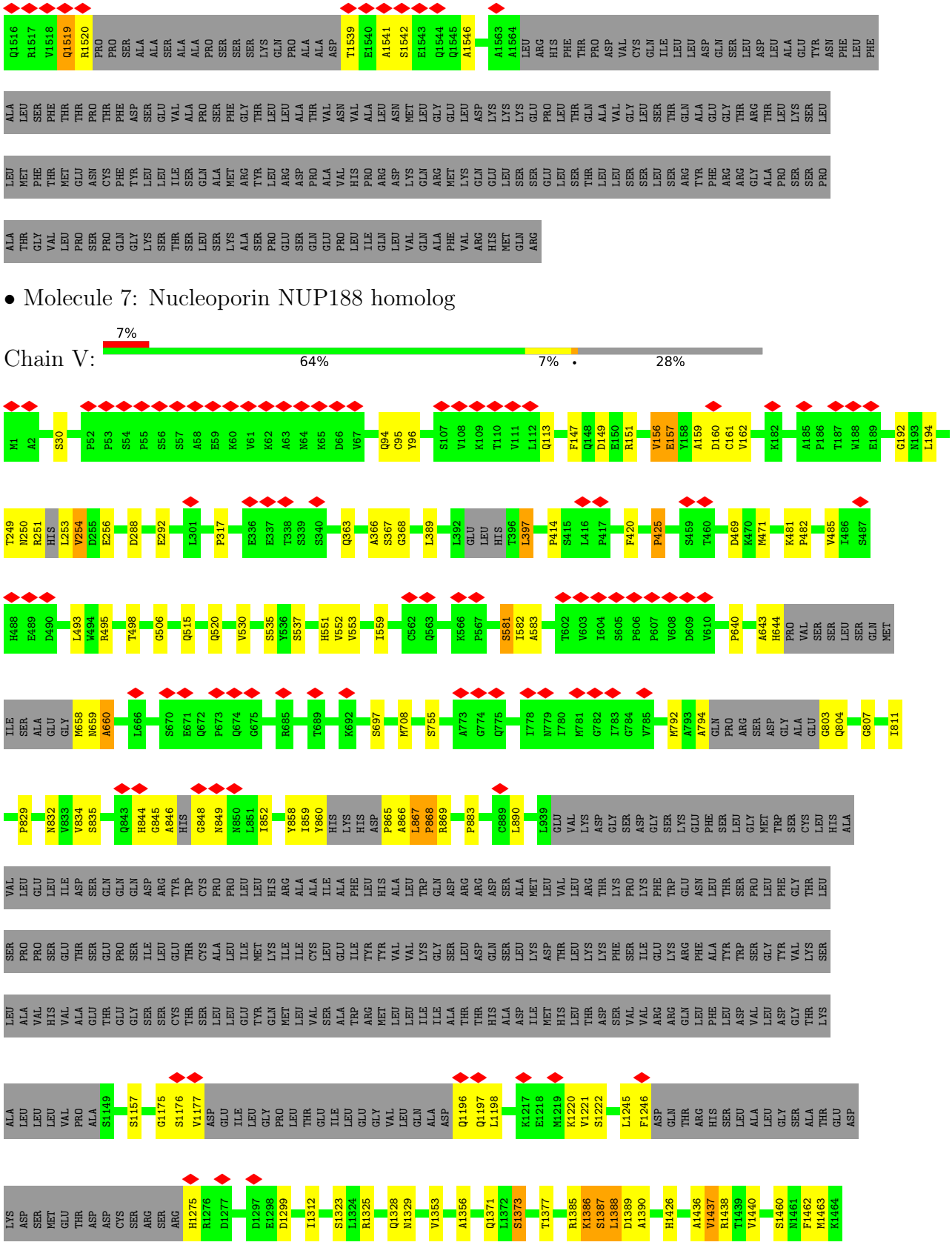




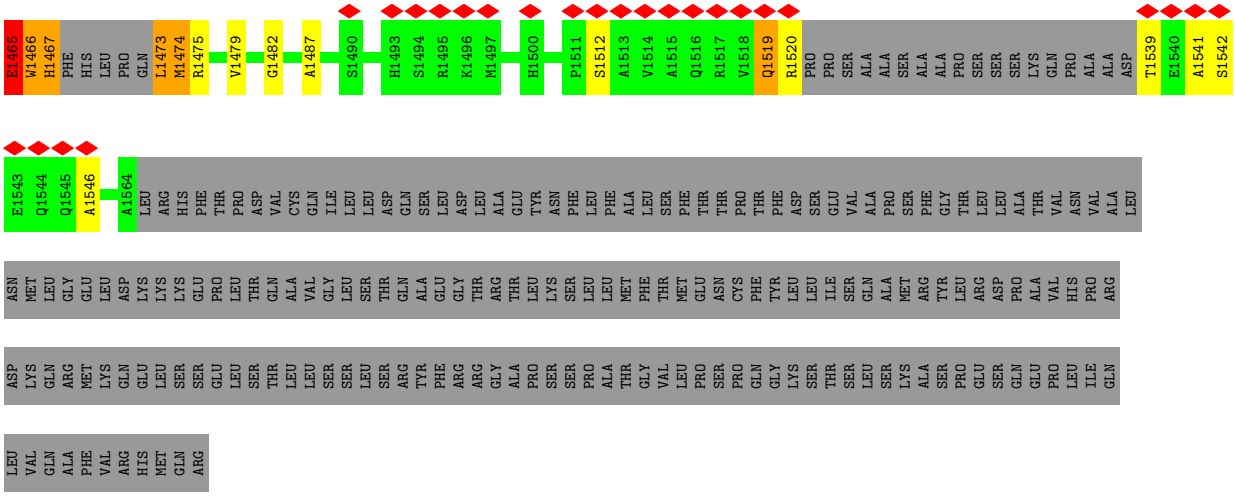








• Molecule 7: Nucleoporin NUP188 homolog


E1465 W1466 H1467 PHE HIS LEU PRO GLN L1473 M1474 R1475 V1479 G1482 A1487 S1490 H1493 S1494 R1495 K1496 M1497 H1500 P1511 S1512 A1513 V1514 A1515 Q1516 R1517 V1518 Q1519 R1520 PRO PRO SER ALA ALA SER ALA ALA PRO SER SER SER LYS GLN PRO ALA ALA ASP T1539 E1540 A1541 S1542
E1543 Q1544 Q1545 A1546 A1564 LEU ARG HIS PHE THR PRO ASP VAL CYS GLN ILE LEU LEU ASP GLN SER LEU ASP LEU ALA GLU TYR ASN PHE LEU PHE ALA LEU SER PHE THR THR PRO THR PHE ASP SER GLU VAL ALA PRO SER PHE GLY THR LEU LEU ALA THR VAL ASN VAL ALA LEU
ASN MET LEU GLY GLU LEU ASP LYS LYS LYS GLU PRO LEU THR GLN ALA VAL GLY LEU SER THR GLN ALA GLU GLY THR ARG THR LEU LYS SER LEU LEU MET PHE THR MET GLU ASN CYS PHE TYR LEU LEU ILE SER GLN ALA MET ARG TYR LEU ARG ASP PRO ALA VAL HIS PRO ARG
ASP LYS GLN ARG MET LYS GLN GLU LEU SER SER GLU LEU SER THR LEU LEU SER SER LEU SER ARG TYR PHE ARG ARG GLY ALA PRO SER SER PRO ALA THR GLY VAL LEU PRO SER PRO GLN GLY LYS SER THR SER LEU SER LYS ALA SER PRO GLU SER GLN GLU PRO LEU ILE GLN
LEU VAL GLN ALA PHE VAL ARG HIS MET GLN ARG

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, Not provided	
Number of subtomograms used	8400	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	3	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	315.784	Depositor
Minimum map value	0.000	Depositor
Average map value	1.328	Depositor
Map value standard deviation	10.659	Depositor
Recommended contour level	36.6	Depositor
Map size (Å)	964.8, 964.8, 964.8	wwPDB
Map dimensions	144, 144, 144	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	6.7, 6.7, 6.7	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	A	0.94	0/3195	1.25	10/4421 (0.2%)
1	B	0.94	0/3195	1.25	10/4421 (0.2%)
1	E	0.93	0/5338	1.17	10/7399 (0.1%)
1	K	0.93	0/5338	1.18	10/7399 (0.1%)
1	Q	0.93	0/5338	1.17	10/7399 (0.1%)
1	W	0.93	0/5338	1.17	10/7399 (0.1%)
2	C	1.13	13/3143 (0.4%)	1.44	45/4369 (1.0%)
2	I	1.13	13/3143 (0.4%)	1.44	45/4369 (1.0%)
2	O	1.13	13/3143 (0.4%)	1.44	45/4369 (1.0%)
2	U	1.13	13/3143 (0.4%)	1.44	45/4369 (1.0%)
3	D	1.22	38/5066 (0.8%)	1.74	122/7020 (1.7%)
3	P	1.22	38/5066 (0.8%)	1.74	121/7020 (1.7%)
4	F	4.14	197/1655 (11.9%)	4.03	272/2302 (11.8%)
4	L	4.14	197/1655 (11.9%)	4.03	272/2302 (11.8%)
4	R	4.14	197/1655 (11.9%)	4.03	272/2302 (11.8%)
4	X	4.14	199/1655 (12.0%)	4.03	273/2302 (11.9%)
5	G	3.95	84/852 (9.9%)	3.81	121/1190 (10.2%)
5	M	3.95	84/852 (9.9%)	3.81	121/1190 (10.2%)
5	S	3.95	84/852 (9.9%)	3.81	121/1190 (10.2%)
5	Y	3.95	85/852 (10.0%)	3.81	120/1190 (10.1%)
6	H	3.44	83/841 (9.9%)	3.10	110/1174 (9.4%)
6	N	3.44	83/841 (9.9%)	3.10	110/1174 (9.4%)
6	T	3.44	83/841 (9.9%)	3.09	109/1174 (9.3%)
6	Z	3.44	83/841 (9.9%)	3.10	110/1174 (9.4%)
7	J	0.92	0/6201	1.20	27/8622 (0.3%)
7	V	0.92	0/6201	1.20	27/8622 (0.3%)
All	All	1.89	1587/76240 (2.1%)	2.00	2548/105862 (2.4%)

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	A	0	1
1	B	0	1
1	E	0	1
1	K	0	1
1	Q	0	1
1	W	0	1
2	C	1	4
2	I	1	4
2	O	1	4
2	U	1	4
3	D	0	21
3	P	0	20
4	F	10	40
4	L	10	40
4	R	10	40
4	X	10	40
5	G	9	10
5	M	9	10
5	S	9	10
5	Y	9	10
6	H	5	5
6	N	5	5
6	T	5	4
6	Z	5	5
7	J	0	3
7	V	0	3
All	All	100	288

The worst 5 of 1587 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	S	380	ILE	N-CA	38.58	2.23	1.46
5	M	380	ILE	N-CA	38.56	2.23	1.46
5	G	380	ILE	N-CA	38.55	2.23	1.46
5	Y	380	ILE	N-CA	38.48	2.23	1.46
5	M	379	HIS	CA-C	37.09	2.49	1.52

The worst 5 of 2548 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	X	452	ARG	CA-C-N	-39.55	30.19	117.20
4	F	452	ARG	CA-C-N	-39.54	30.20	117.20
4	R	452	ARG	CA-C-N	-39.54	30.20	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L	452	ARG	CA-C-N	-39.53	30.24	117.20
5	G	343	ALA	CB-CA-C	-36.23	55.76	110.10

5 of 100 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	11	GLN	CA
4	F	200	THR	CA
4	F	210	VAL	CA
4	F	211	GLU	CA
4	F	305	ASP	CA

5 of 288 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	259	SER	Mainchain
1	B	259	SER	Mainchain
2	C	4	GLU	Mainchain
2	C	6	PHE	Mainchain
2	C	7	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	A	3214	0	1424	23	0
1	B	3214	0	1424	23	0
1	E	5366	0	2364	58	0
1	K	5366	0	2360	73	0
1	Q	5366	0	2364	63	0
1	W	5366	0	2364	56	0
2	C	3152	0	1401	155	0
2	I	3152	0	1406	30	0
2	O	3152	0	1403	88	0
2	U	3152	0	1406	30	0
3	D	5094	0	2272	121	0
3	P	5094	0	2273	77	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	1658	0	715	168	0
4	L	1658	0	715	169	0
4	R	1658	0	714	169	0
4	X	1658	0	715	168	0
5	G	853	0	384	57	0
5	M	853	0	384	55	0
5	S	853	0	384	55	0
5	Y	853	0	384	57	0
6	H	842	0	365	36	0
6	N	842	0	365	39	0
6	T	842	0	365	38	0
6	Z	842	0	365	38	0
7	J	6213	0	2770	79	0
7	V	6213	0	2770	78	0
All	All	76526	0	33856	1791	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 16.

The worst 5 of 1791 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)
5:S:366:GLU:CA	5:S:366:GLU:CB	1.76	1.64
4:F:451:GLU:CA	4:F:451:GLU:CB	1.77	1.63
6:N:490:GLN:CA	6:N:490:GLN:CB	1.75	1.62
4:F:454:TYR:CA	4:F:454:TYR:CB	1.77	1.62
4:X:447:VAL:CA	4:X:447:VAL:CB	1.78	1.62

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	A	612/1391 (44%)	562 (92%)	38 (6%)	12 (2%)	7	38
1	B	612/1391 (44%)	562 (92%)	38 (6%)	12 (2%)	7	38
1	E	1027/1391 (74%)	947 (92%)	58 (6%)	22 (2%)	7	36
1	K	1027/1391 (74%)	947 (92%)	58 (6%)	22 (2%)	7	36
1	Q	1027/1391 (74%)	947 (92%)	58 (6%)	22 (2%)	7	36
1	W	1027/1391 (74%)	947 (92%)	58 (6%)	22 (2%)	7	36
2	C	618/819 (76%)	516 (84%)	59 (10%)	43 (7%)	1	14
2	I	618/819 (76%)	516 (84%)	58 (9%)	44 (7%)	1	14
2	O	618/819 (76%)	516 (84%)	59 (10%)	43 (7%)	1	14
2	U	618/819 (76%)	516 (84%)	59 (10%)	43 (7%)	1	14
3	D	972/2012 (48%)	899 (92%)	59 (6%)	14 (1%)	11	46
3	P	972/2012 (48%)	899 (92%)	59 (6%)	14 (1%)	11	46
4	F	329/507 (65%)	286 (87%)	21 (6%)	22 (7%)	1	15
4	L	329/507 (65%)	286 (87%)	21 (6%)	22 (7%)	1	15
4	R	329/507 (65%)	286 (87%)	21 (6%)	22 (7%)	1	15
4	X	329/507 (65%)	286 (87%)	21 (6%)	22 (7%)	1	15
5	G	169/599 (28%)	153 (90%)	10 (6%)	6 (4%)	3	25
5	M	169/599 (28%)	153 (90%)	11 (6%)	5 (3%)	4	28
5	S	169/599 (28%)	153 (90%)	11 (6%)	5 (3%)	4	28
5	Y	169/599 (28%)	153 (90%)	11 (6%)	5 (3%)	4	28
6	H	167/522 (32%)	152 (91%)	8 (5%)	7 (4%)	3	22
6	N	167/522 (32%)	152 (91%)	8 (5%)	7 (4%)	3	22
6	T	167/522 (32%)	152 (91%)	8 (5%)	7 (4%)	3	22
6	Z	167/522 (32%)	152 (91%)	8 (5%)	7 (4%)	3	22
7	J	1232/1749 (70%)	1111 (90%)	75 (6%)	46 (4%)	3	24
7	V	1232/1749 (70%)	1111 (90%)	75 (6%)	46 (4%)	3	24
All	All	14872/25656 (58%)	13360 (90%)	970 (6%)	542 (4%)	6	25

5 of 542 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	332	ARG
1	A	443	LYS
1	A	543	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	802	GLN
1	B	332	ARG

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
4	F	6
4	L	6
4	R	6
4	X	6
2	C	3

Continued on next page...

Continued from previous page...

Mol	Chain	Number of breaks
2	I	3
2	O	3
2	U	3
5	M	3
5	Y	3
5	G	3
5	S	3
6	H	3
6	N	3
6	T	3
6	Z	3

The worst 5 of 60 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	483:GLU	C	484:ARG	N	4.02
1	I	483:GLU	C	484:ARG	N	4.02
1	O	483:GLU	C	484:ARG	N	4.02
1	U	483:GLU	C	484:ARG	N	4.02
1	C	447:ASP	C	448:TYR	N	3.63

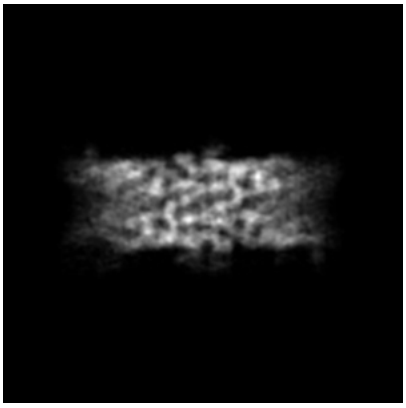
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-8085. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

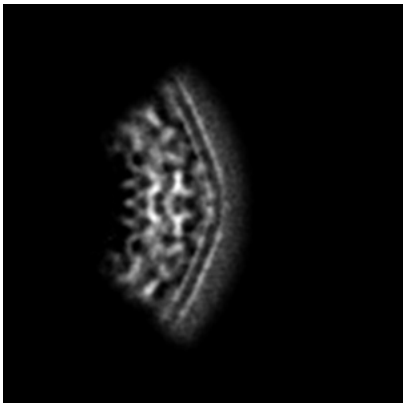
6.1 Orthogonal projections (i)

6.1.1 Primary map



X

Y



Z

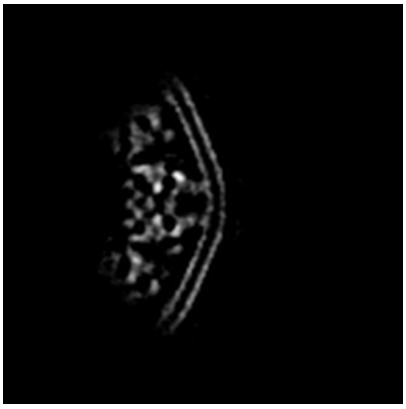
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map

X Index: 72

Y Index: 72

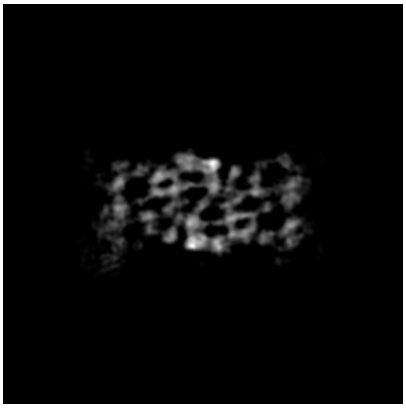


Z Index: 72

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

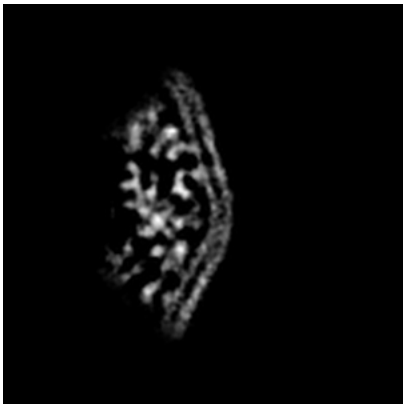
6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 53

Y Index: 76



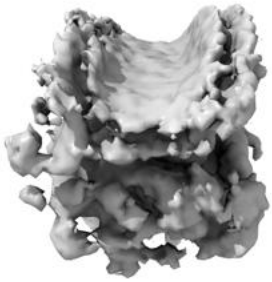
Z Index: 78

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 36.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

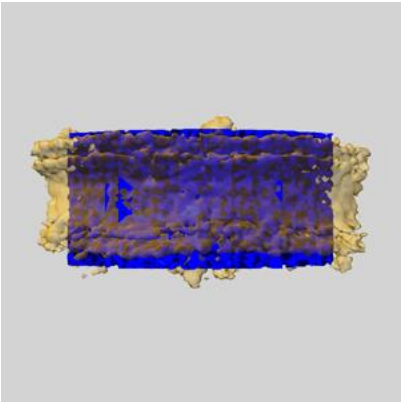
6.5 Mask visualisation (i)

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

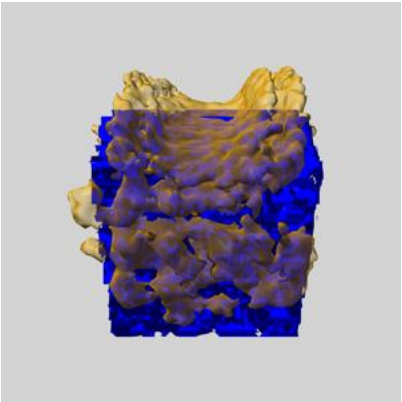
A mask typically either:

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

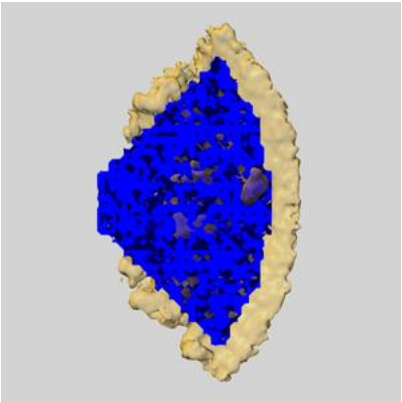
6.5.1 emd_8085_msk_1.map (i)



X



Y

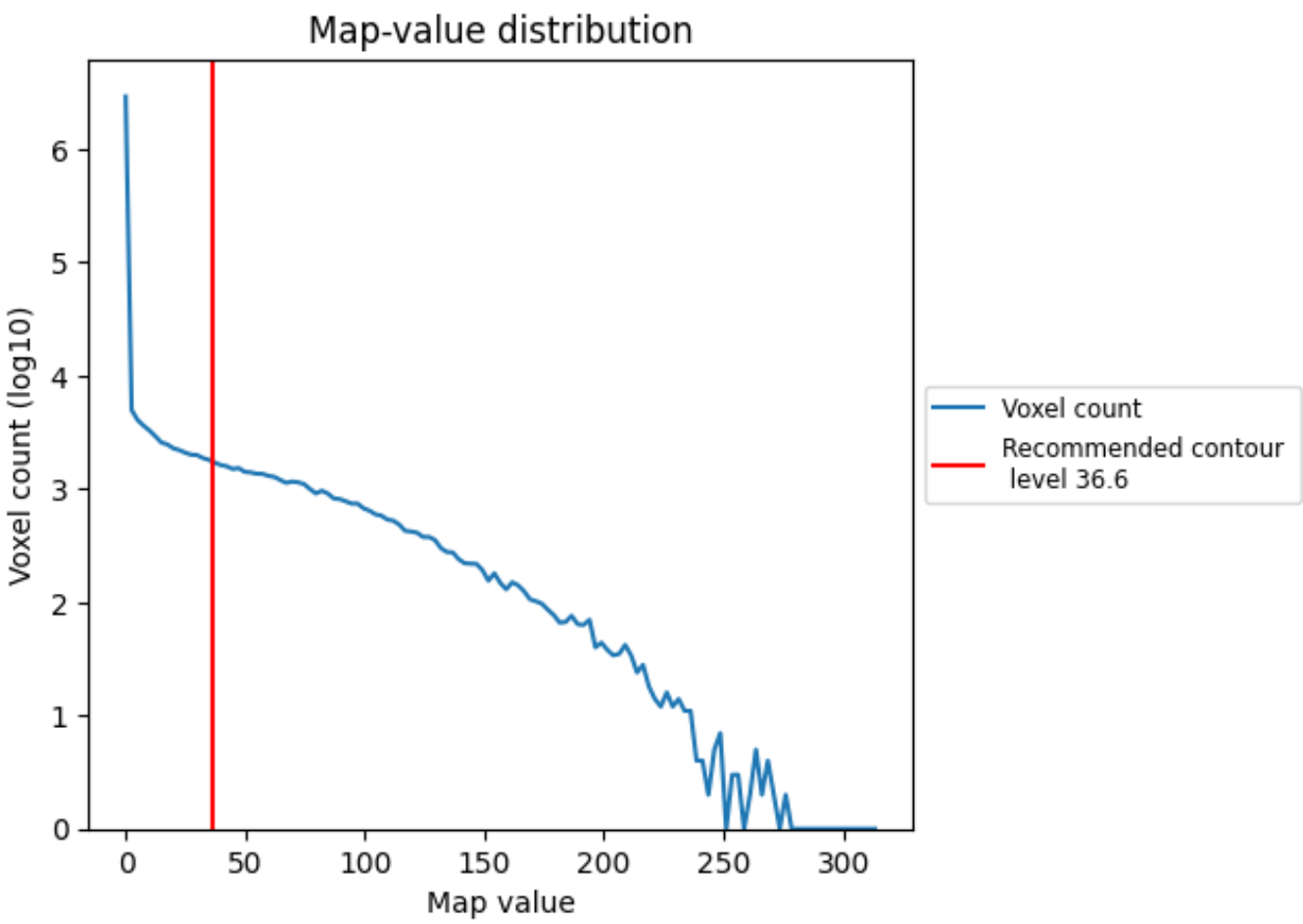


Z

7 Map analysis (i)

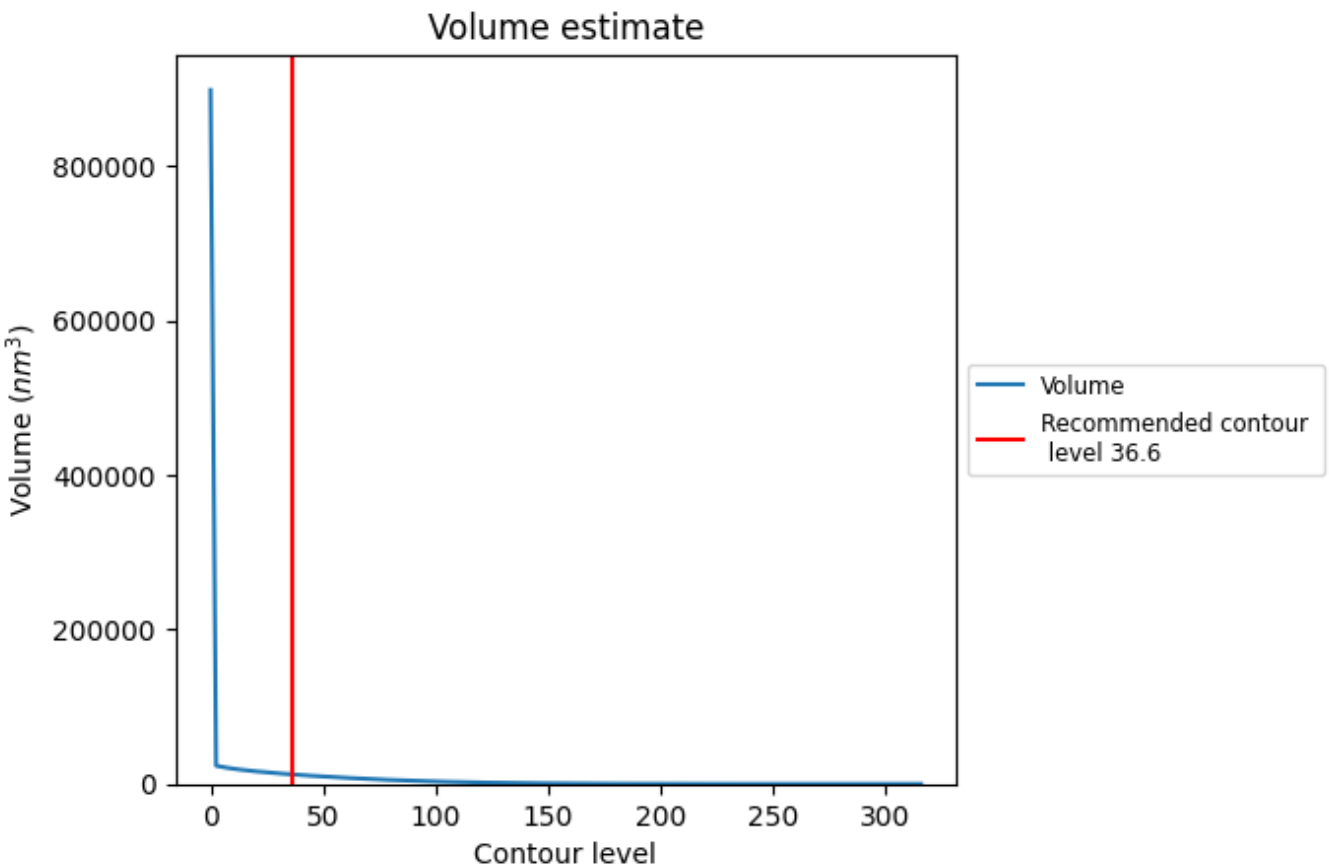
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

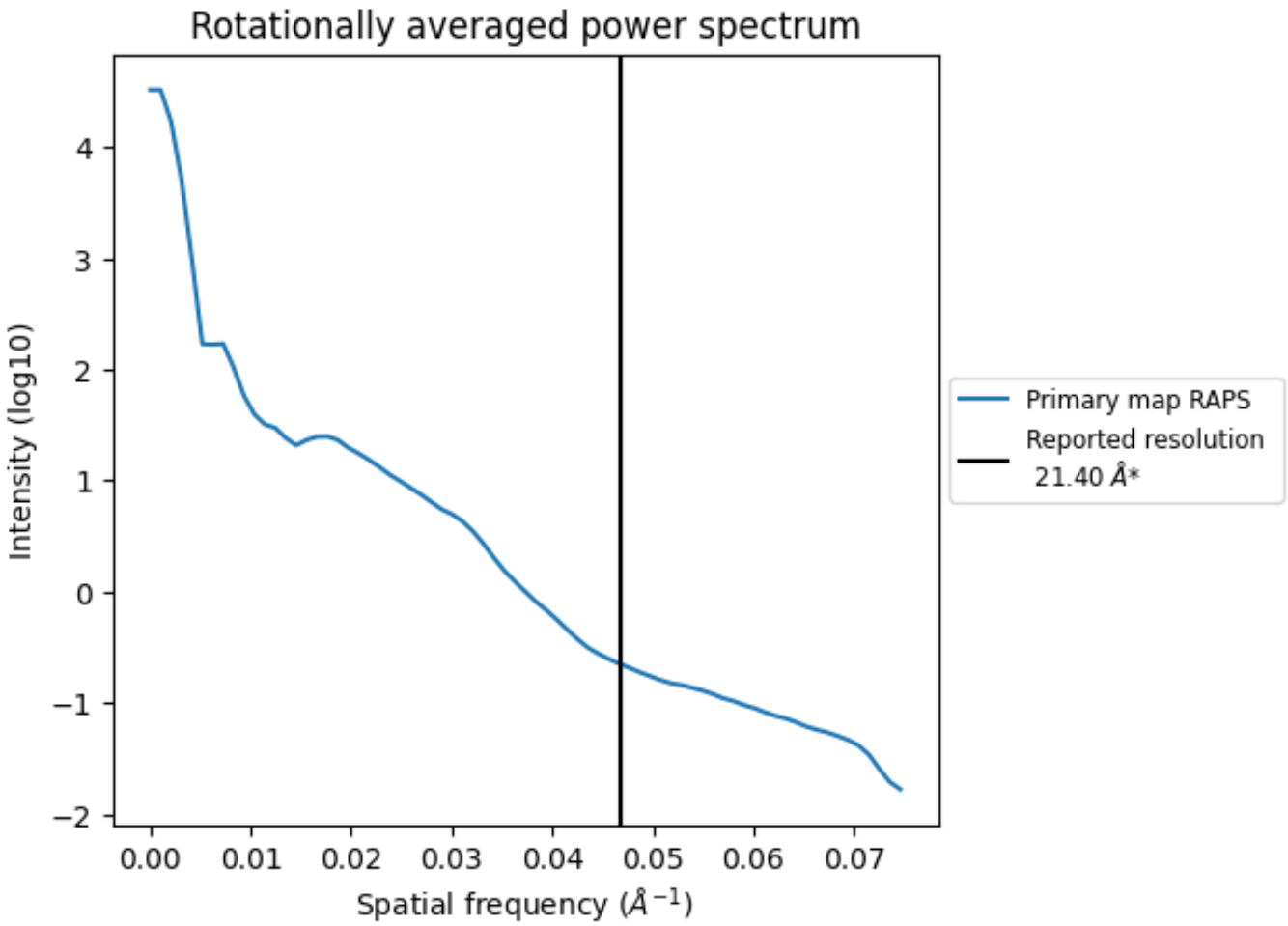
7.2 Volume estimate (i)



The volume at the recommended contour level is 12255 nm^3; this corresponds to an approximate mass of 11070 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 0.047 Å^{-1}

8 Fourier-Shell correlation (i)

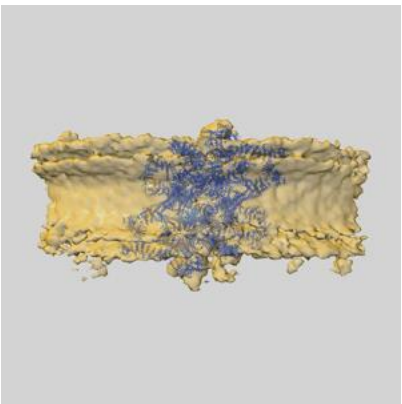
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit (i)

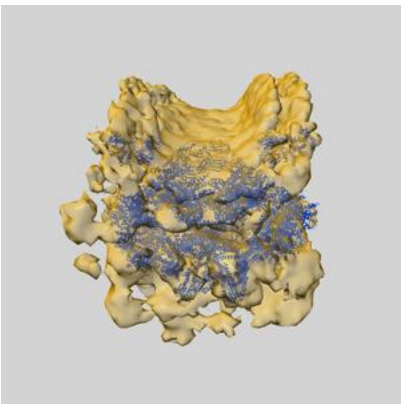
This section contains information regarding the fit between EMDB map EMD-8085 and PDB model 5IJO. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

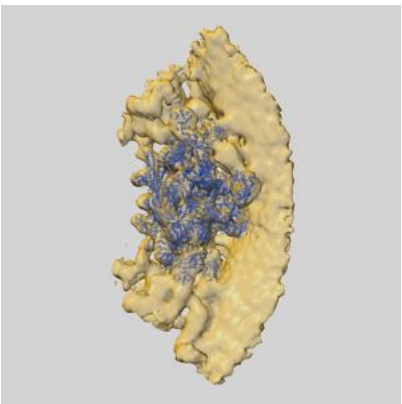
9.1.1 Map-model overlay (i)



X

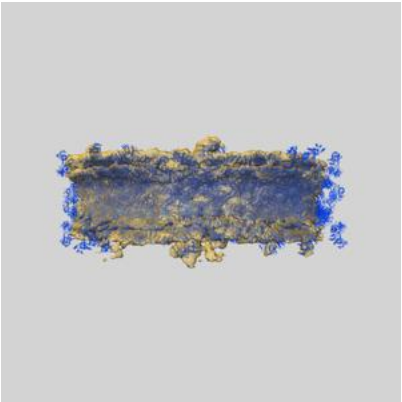


Y

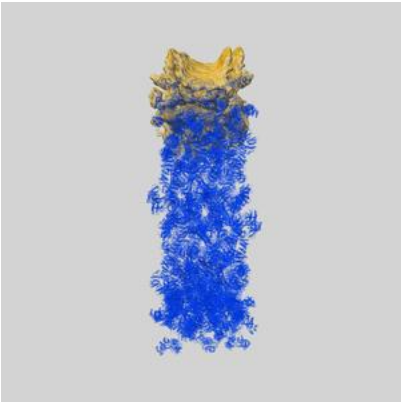


Z

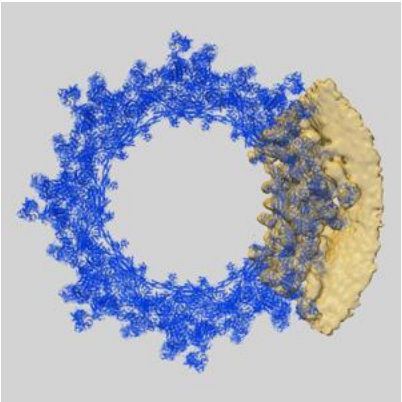
9.1.2 Map-model assembly overlay (i)



X



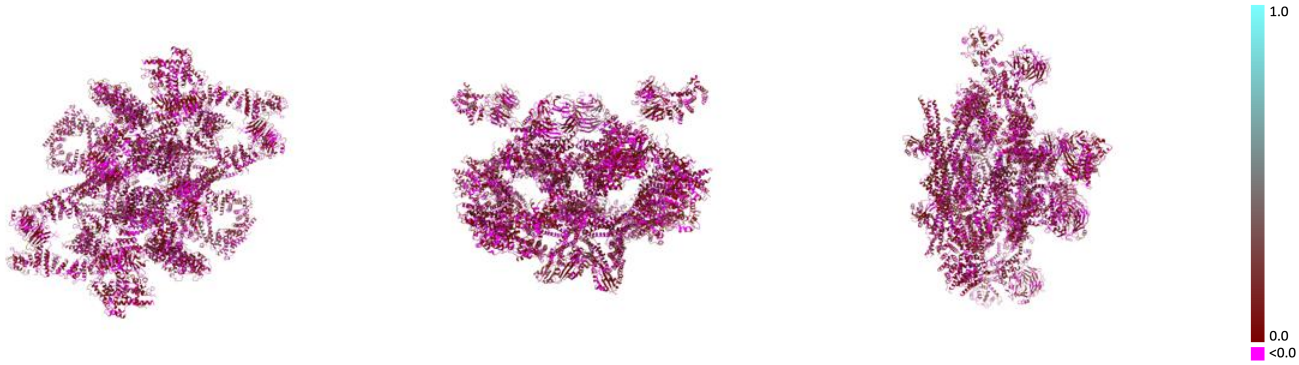
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 36.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

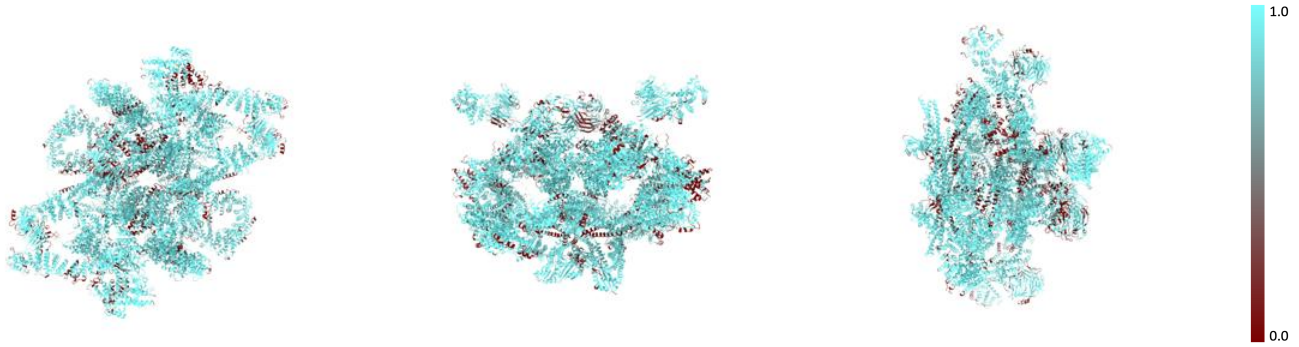
9.2 Q-score mapped to coordinate model (i)



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.

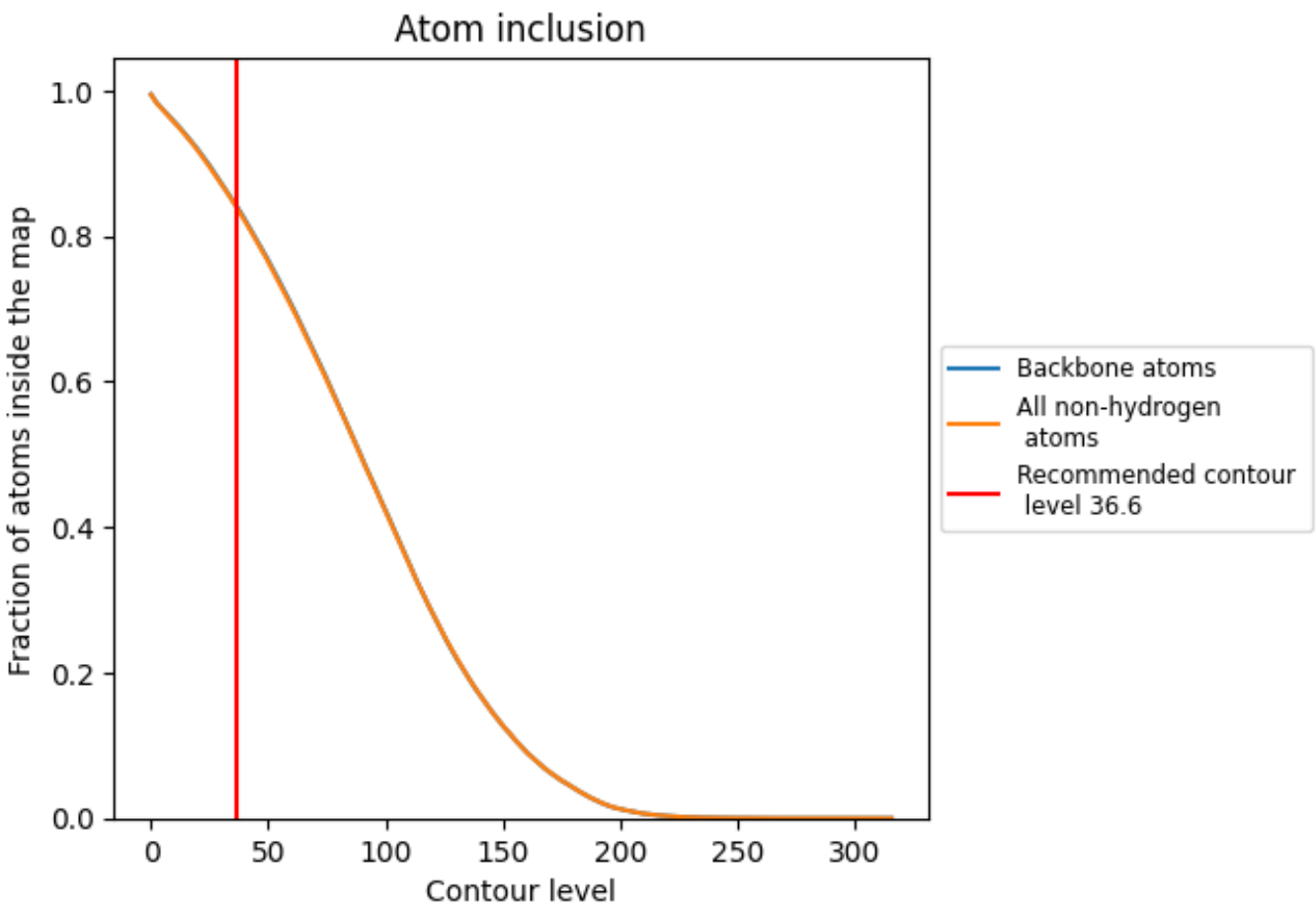
9.3 Atom inclusion mapped to coordinate model (i)



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 (36.6).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (36.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8392	0.0440
A	0.9291	0.0440
B	0.8787	0.0450
C	0.8493	0.0410
D	0.8983	0.0470
E	0.8658	0.0410
F	0.8100	0.0380
G	0.9039	0.0460
H	0.7993	0.0310
I	0.8271	0.0510
J	0.8785	0.0530
K	0.5460	0.0190
L	0.7986	0.0280
M	0.8453	0.0490
N	0.8729	0.0700
O	0.8782	0.0470
P	0.8971	0.0560
Q	0.8813	0.0440
R	0.7762	0.0310
S	0.9332	0.0600
T	0.7482	0.0470
U	0.8004	0.0440
V	0.9036	0.0520
W	0.7753	0.0350
X	0.8372	0.0380
Y	0.9004	0.0550
Z	0.8492	0.0460