Full wwPDB EM Validation Report ⓘ

Nov 29, 2022 – 03:55 PM JST

PDB ID	:	7WKK
EMDB ID	:	EMD-32566
Title	:	Cryo-EM structure of the IR subunit from X. laevis NPC
Authors	:	Huang, G.; Zhan, X.; Shi, Y.
Deposited on	:	2022-01-10
Resolution	:	4.20 Å(reported)

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

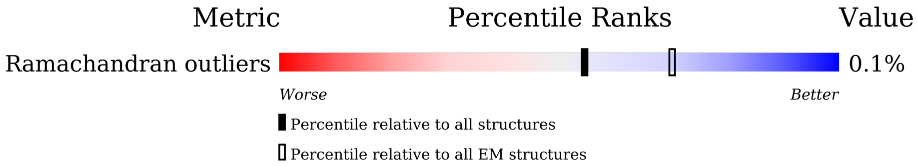
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

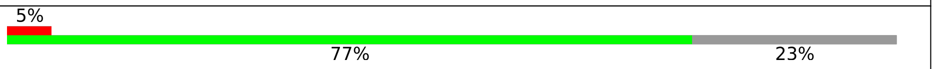
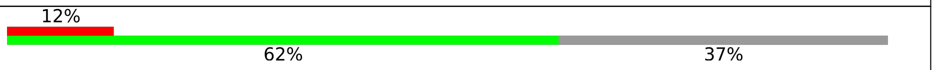
The reported resolution of this entry is 4.20 Å.

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)
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	2011	 • 84% 16%
1	a	2011	 • 83% 17%
2	B	1739	 • 85% 15%
2	b	1739	 • 85% 15%
3	C	820	 5% 77% 23%
3	E	820	 • 76% 24%
3	c	820	 • 77% 23%
3	e	820	 • 76% 24%
4	D	1388	 • 80% 20%
4	F	1388	 • 79% 21%
4	M	1388	 12% 62% 37%

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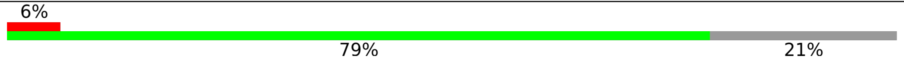
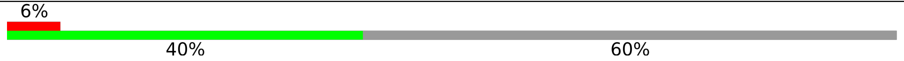
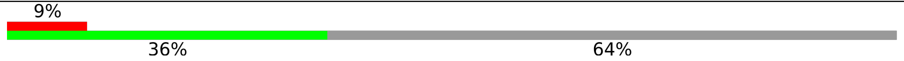
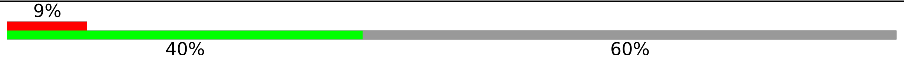
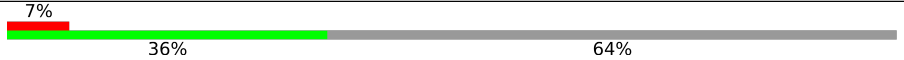
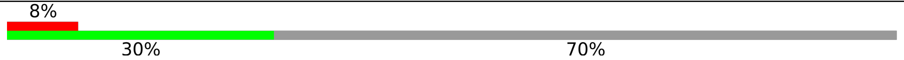
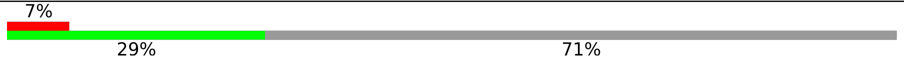
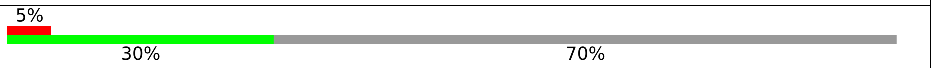
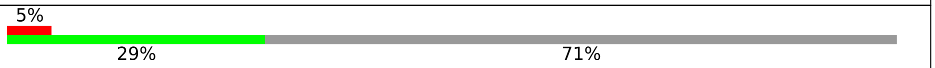
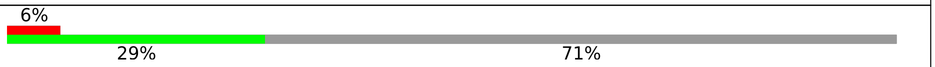
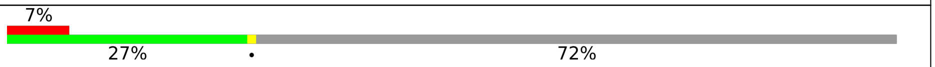
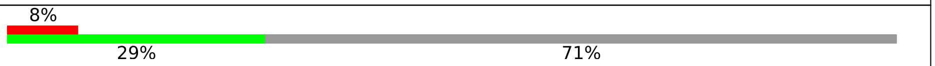
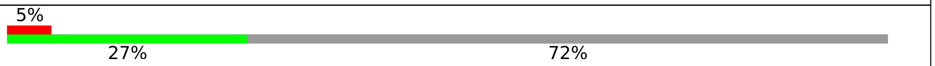
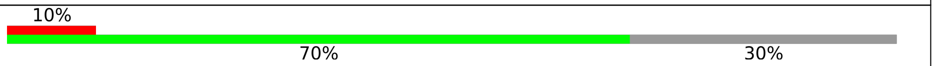
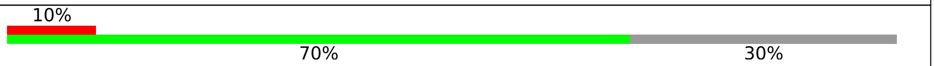
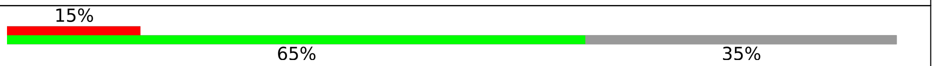
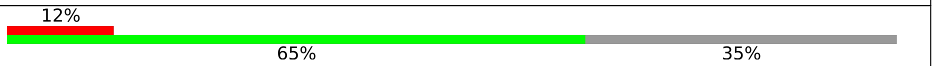
Mol	Chain	Length	Quality of chain
4	d	1388	 81% 19%
4	f	1388	 6% 79% 21%
4	m	1388	 62% 37%
5	G	535	 6% 40% 60%
5	J	535	 9% 36% 64%
5	g	535	 9% 40% 60%
5	j	535	 7% 36% 64%
6	H	547	 8% 30% 70%
6	L	547	 7% 29% 71%
6	h	547	 5% 30% 70%
6	l	547	 5% 29% 71%
7	I	599	 6% 29% 71%
7	K	599	 7% 27% 72%
7	i	599	 8% 29% 71%
7	k	599	 5% 27% 72%
8	O	523	 10% 70% 30%
8	o	523	 10% 70% 30%
9	N	660	 15% 65% 35%
9	n	660	 12% 65% 35%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 92821 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 MGC83295 protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	1684	Total 8339	C 4971	N 1684	O 1684	0	0
1	a	1669	Total 8268	C 4930	N 1669	O 1669	0	0

- Molecule 2 is a protein called Nup188 domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	1482	Total 7347	C 4383	N 1482	O 1482	0	0
2	b	1482	Total 7347	C 4383	N 1482	O 1482	0	0

- Molecule 3 is a protein called Nuclear pore complex protein Nup93.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	633	Total 3144	C 1878	N 633	O 633	0	0
3	E	625	Total 3105	C 1855	N 625	O 625	0	0
3	c	633	Total 3144	C 1878	N 633	O 633	0	0
3	e	625	Total 3105	C 1855	N 625	O 625	0	0

- Molecule 4 is a protein called Nup155-prov protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	1115	Total 5524	C 3294	N 1115	O 1115	0	0
4	F	1094	Total 5417	C 3229	N 1094	O 1094	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	M	869	Total	C	N	O	0	0
			4296	2558	869	869		
4	d	1123	Total	C	N	O	0	0
			5563	3317	1123	1123		
4	f	1097	Total	C	N	O	0	0
			5432	3238	1097	1097		
4	m	869	Total	C	N	O	0	0
			4296	2558	869	869		

- Molecule 5 is a protein called Nup54.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	G	215	Total	C	N	O	0	0
			1063	633	215	215		
5	J	195	Total	C	N	O	0	0
			963	573	195	195		
5	g	215	Total	C	N	O	0	0
			1063	633	215	215		
5	j	195	Total	C	N	O	0	0
			963	573	195	195		

- Molecule 6 is a protein called IL4I1 protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	H	163	Total	C	N	O	0	0
			813	487	163	163		
6	L	156	Total	C	N	O	0	0
			778	466	156	156		
6	h	163	Total	C	N	O	0	0
			813	487	163	163		
6	l	156	Total	C	N	O	0	0
			778	466	156	156		

- Molecule 7 is a protein called MGC84997 protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	I	171	Total	C	N	O	0	0
			853	511	171	171		
7	K	166	Total	C	N	O	0	0
			829	497	166	166		
7	i	171	Total	C	N	O	0	0
			853	511	171	171		

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Mol	Chain	Residues	Atoms				AltConf	Trace
7	k	166	Total 829	C 497	N 166	O 166	0	0

- Molecule 8 is a protein called Aaas-prov protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	O	367	Total 1805	C 1071	N 367	O 367	0	0
8	o	367	Total 1805	C 1071	N 367	O 367	0	0

- Molecule 9 is a protein called Nucleoporin NDC1.

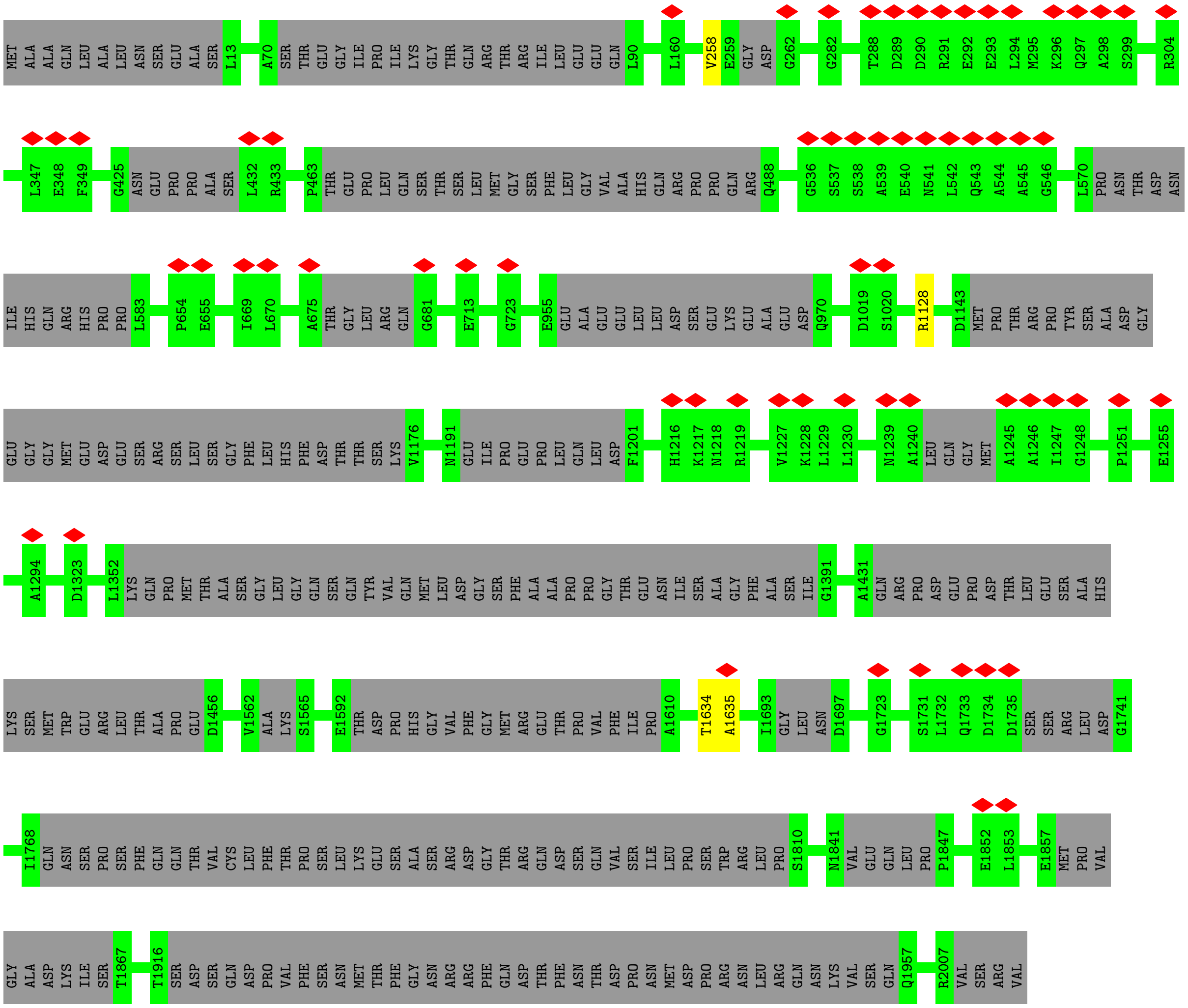
Mol	Chain	Residues	Atoms				AltConf	Trace
9	N	431	Total 2143	C 1281	N 431	O 431	0	0
9	n	431	Total 2143	C 1281	N 431	O 431	0	0

3 Residue-property plots ⓘ

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.

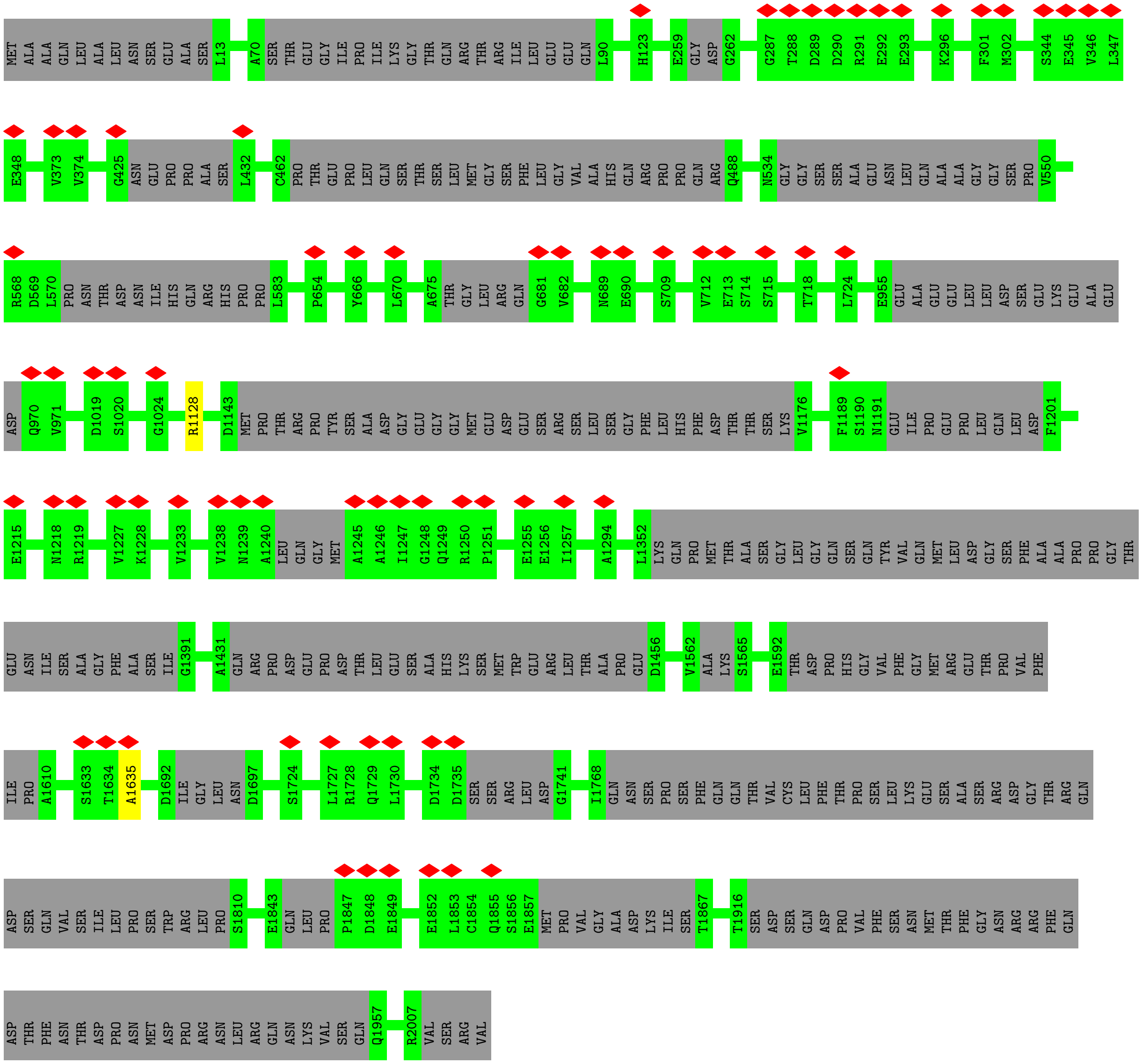
- Molecule 1: MGC83295 protein

Chain A:



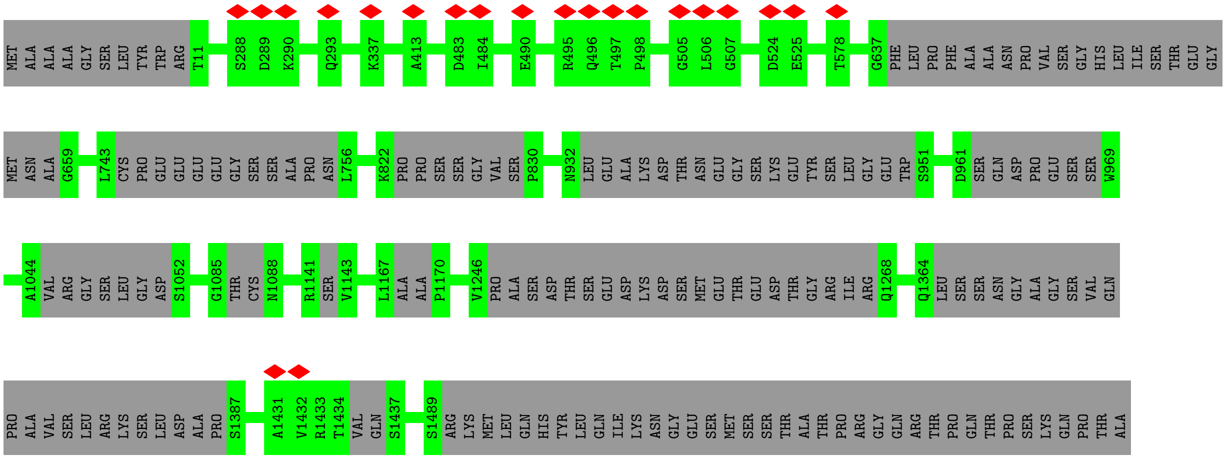
- Molecule 1: MGC83295 protein

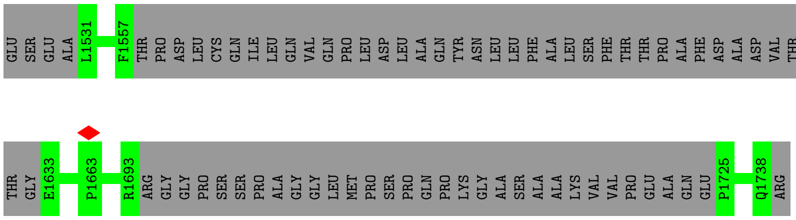
Chain a:



- Molecule 2: Nup188 domain-containing protein

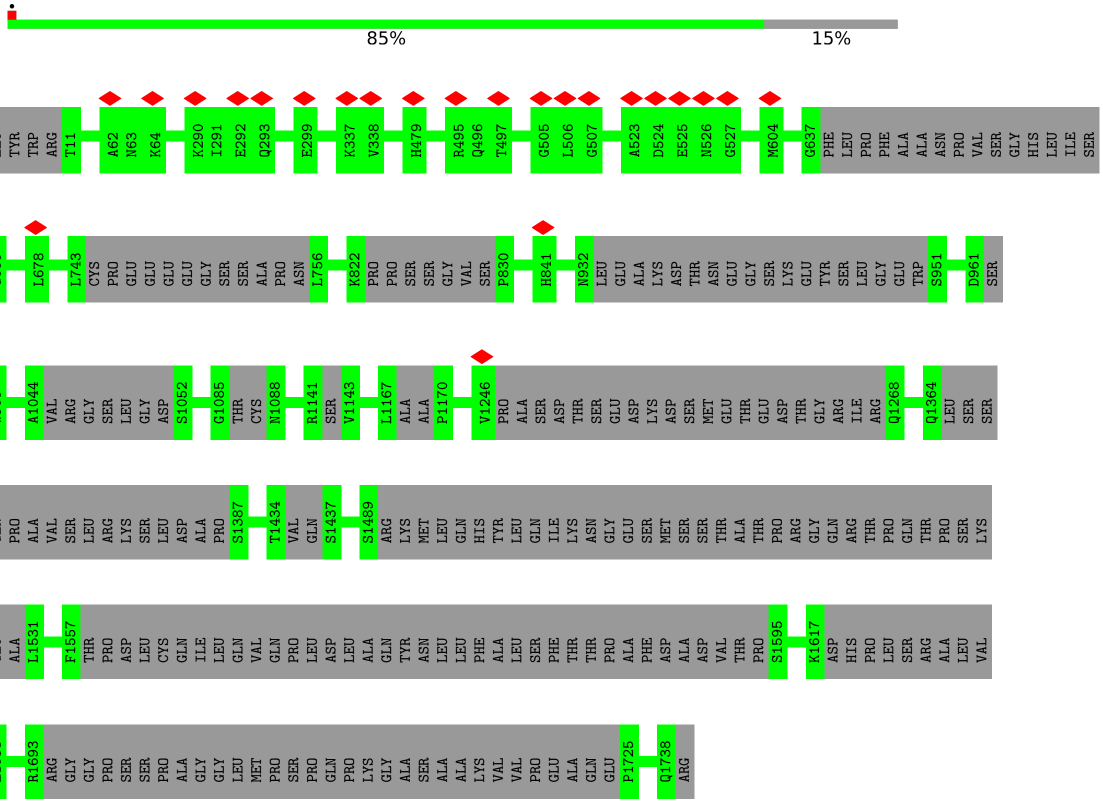
Chain B:





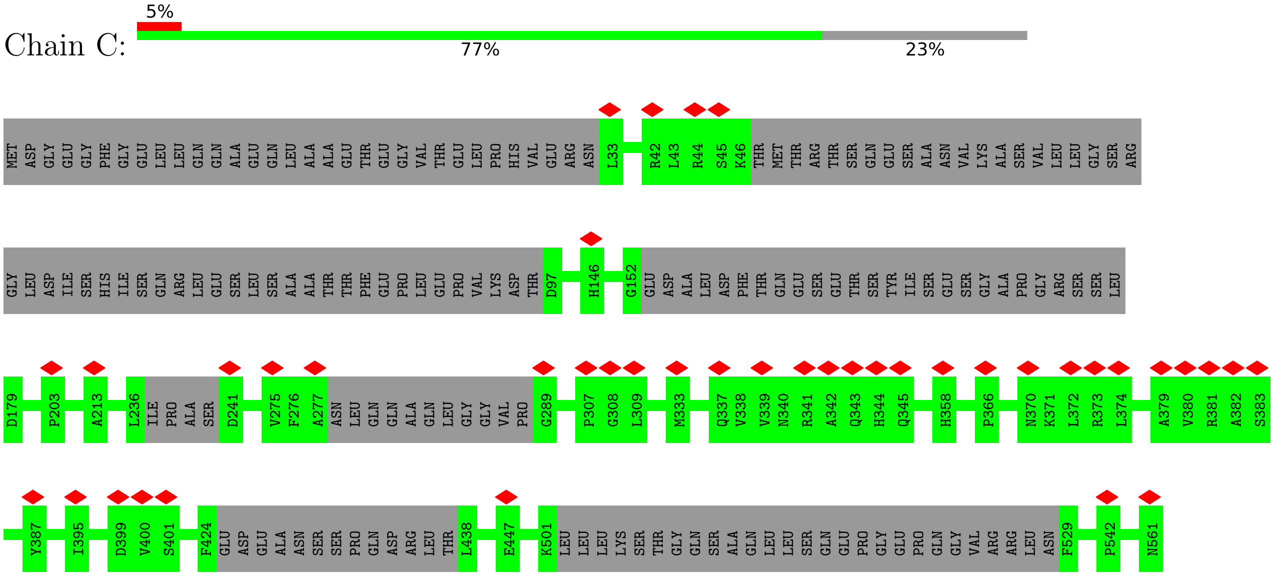
- Molecule 2: Nup188 domain-containing protein

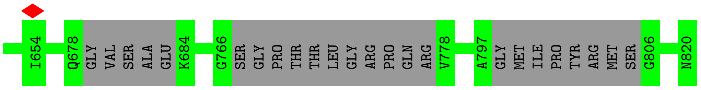
Chain b:



- Molecule 3: Nuclear pore complex protein Nup93

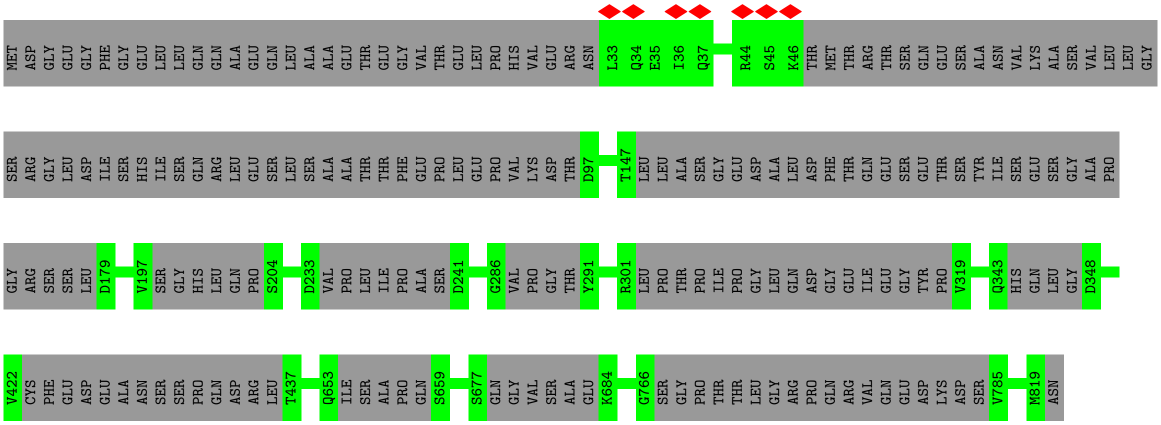
Chain C:





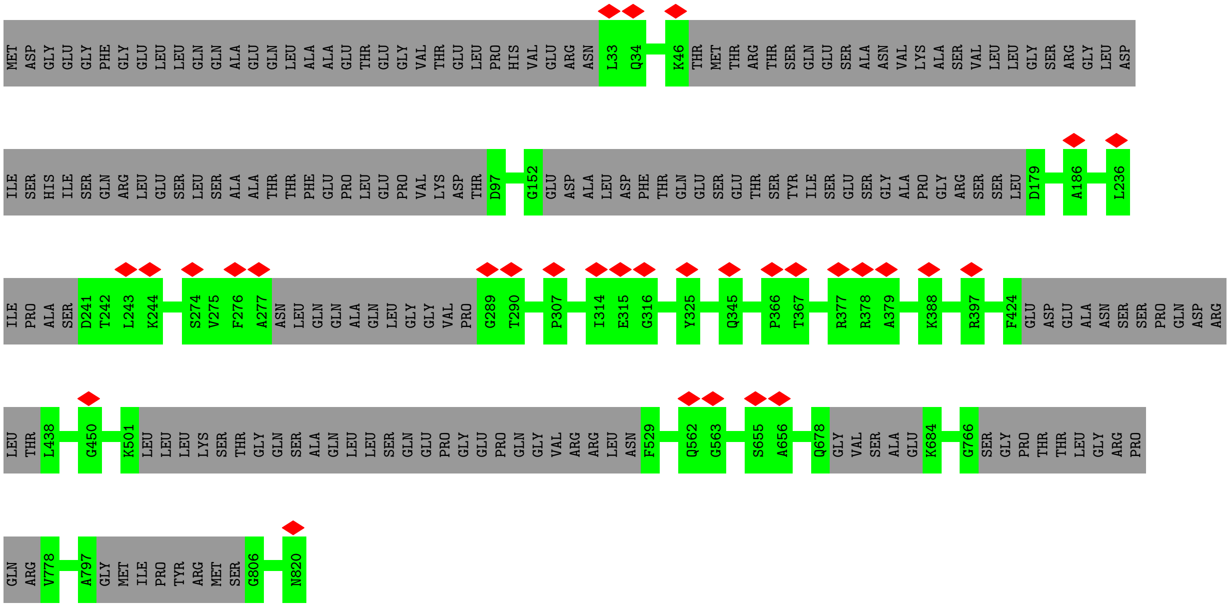
- Molecule 3: Nuclear pore complex protein Nup93

Chain E:



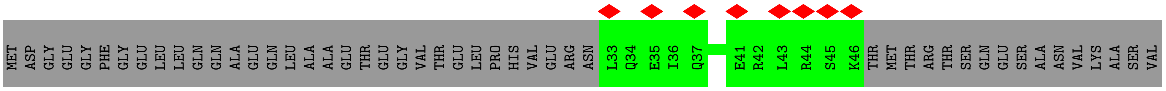
- Molecule 3: Nuclear pore complex protein Nup93

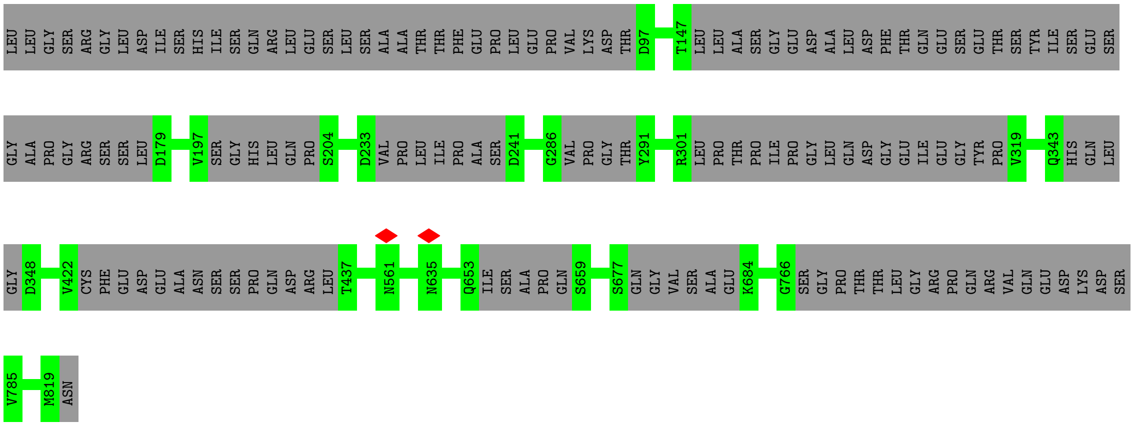
Chain c:



- Molecule 3: Nuclear pore complex protein Nup93

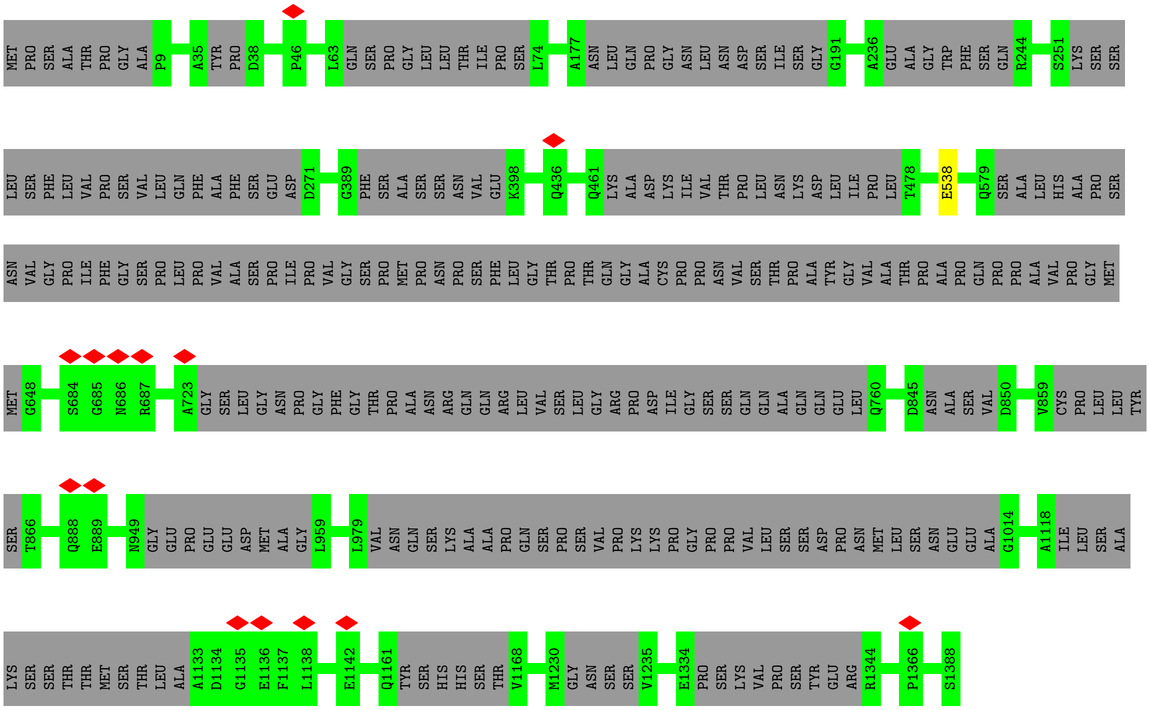
Chain e:





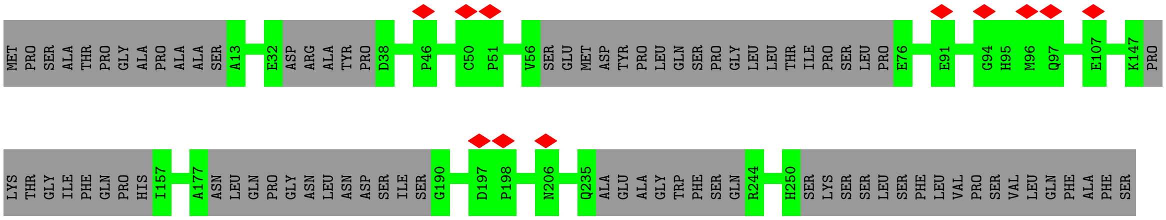
- Molecule 4: Nup155-prov protein

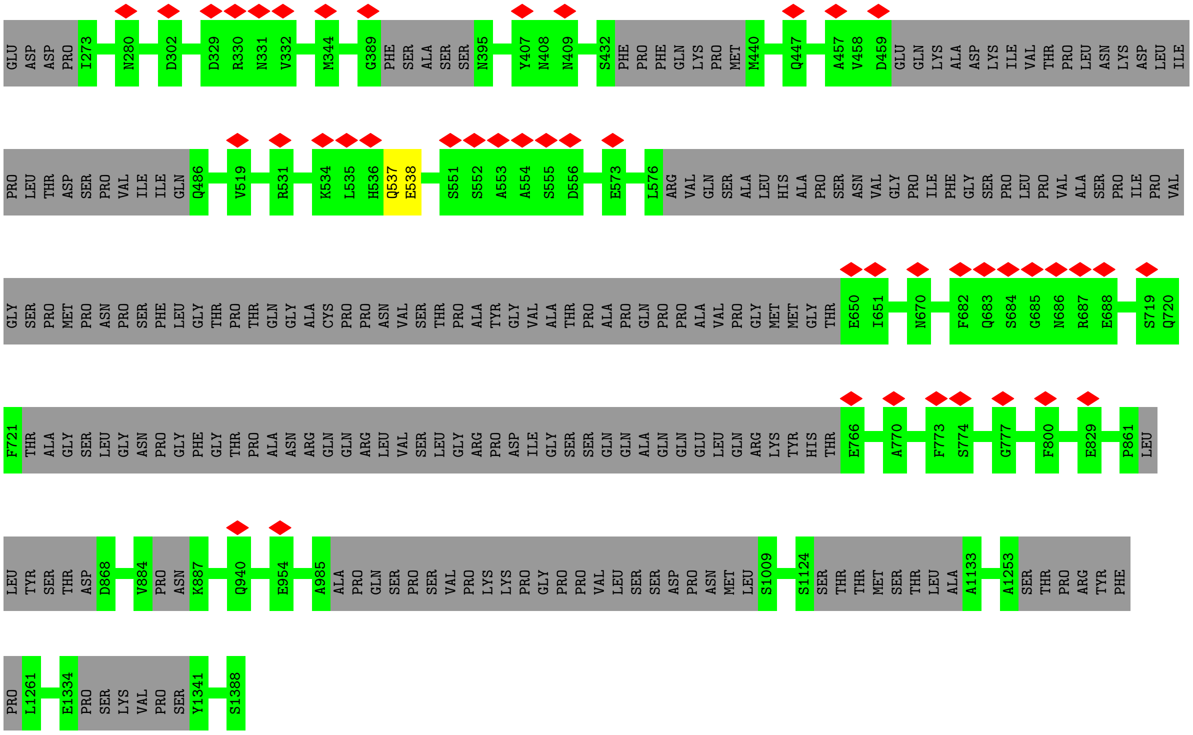
Chain D:



- Molecule 4: Nup155-prov protein

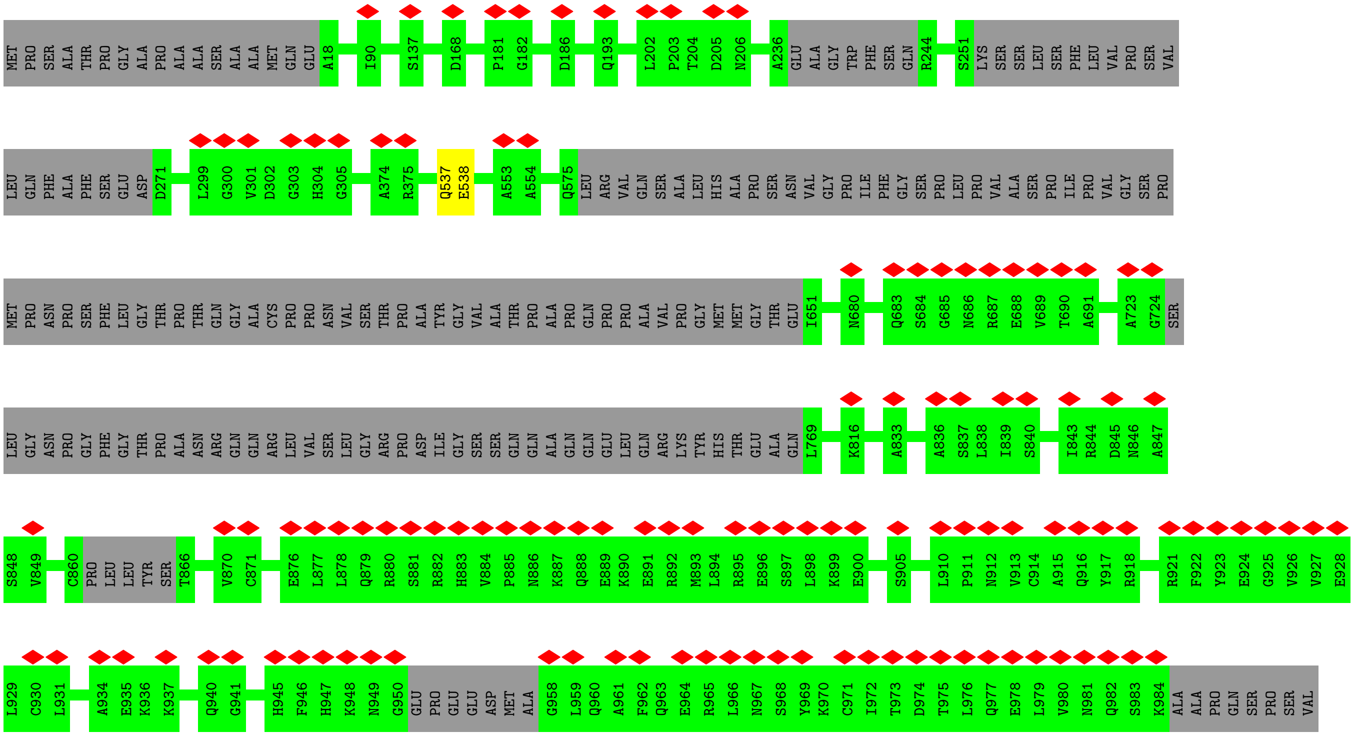
Chain F:

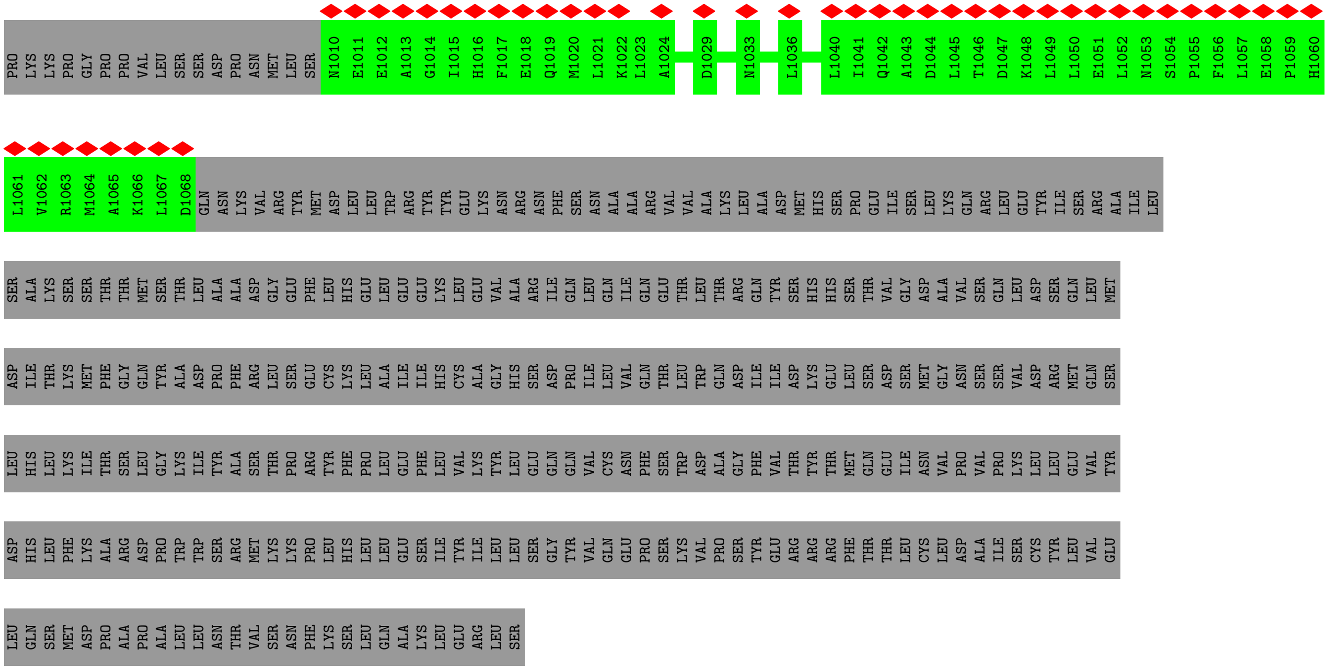




- Molecule 4: Nup155-prov protein

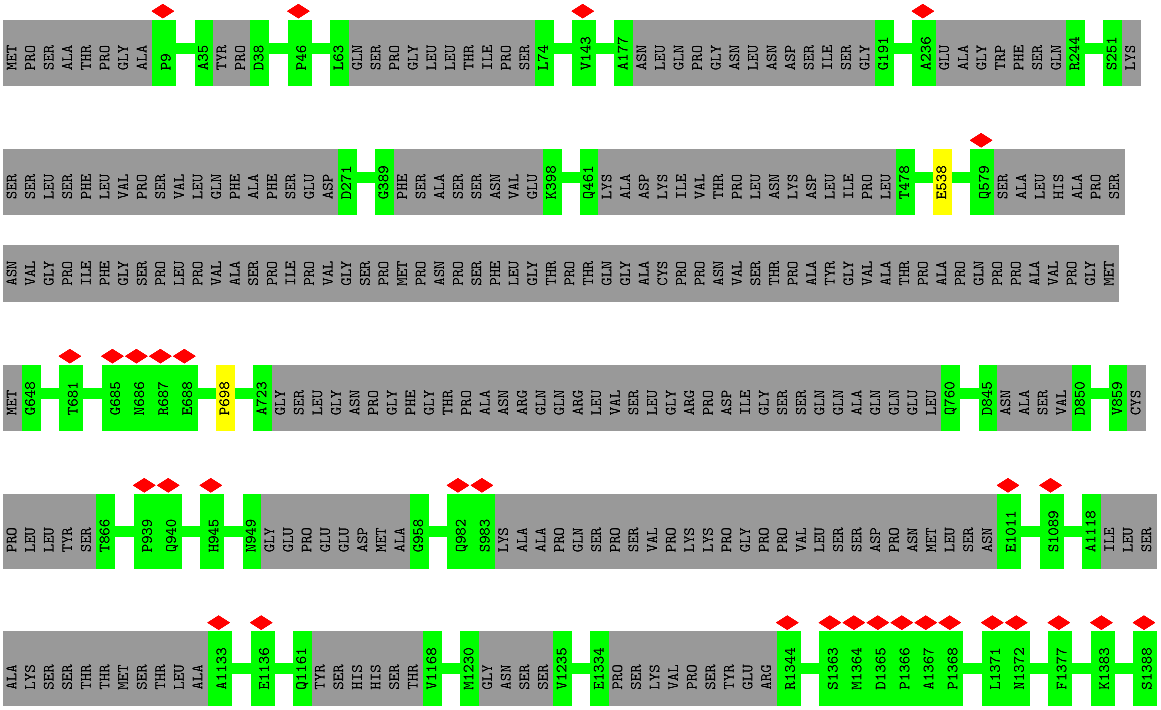
Chain M:





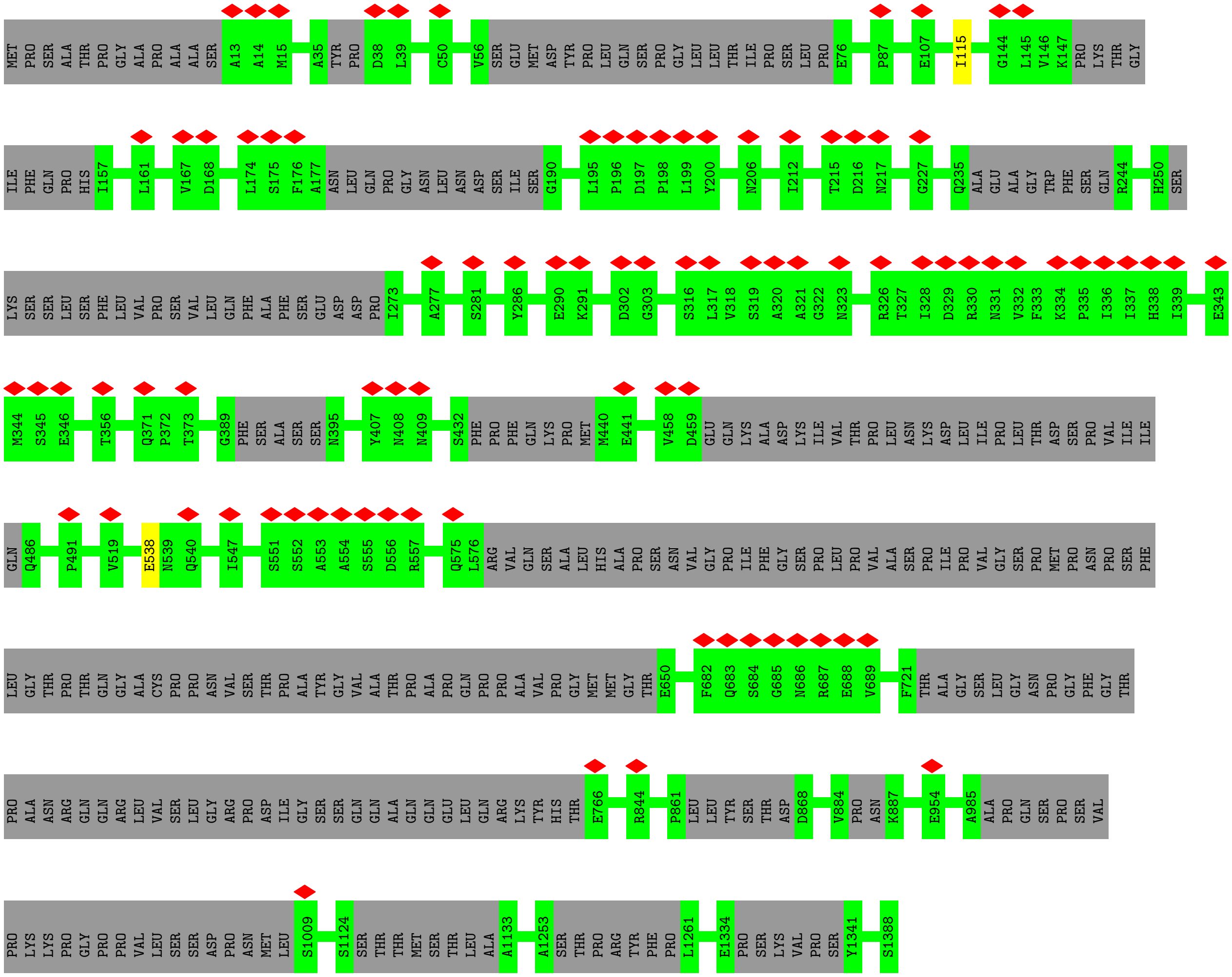
- Molecule 4: Nup155-prov protein

Chain d:



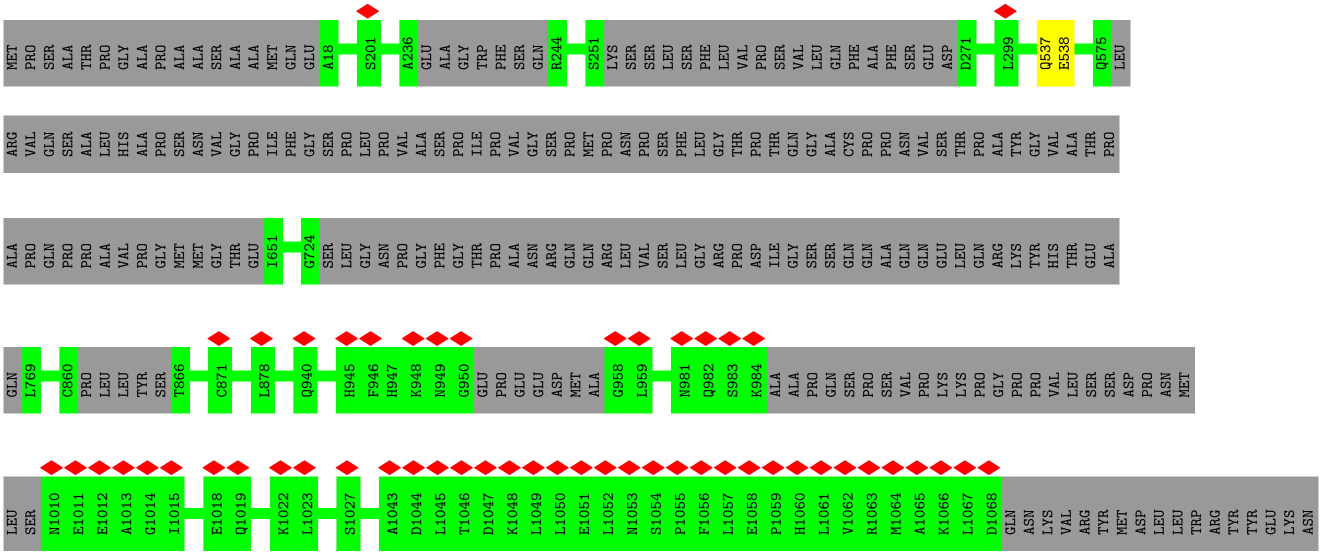
- Molecule 4: Nup155-prov protein

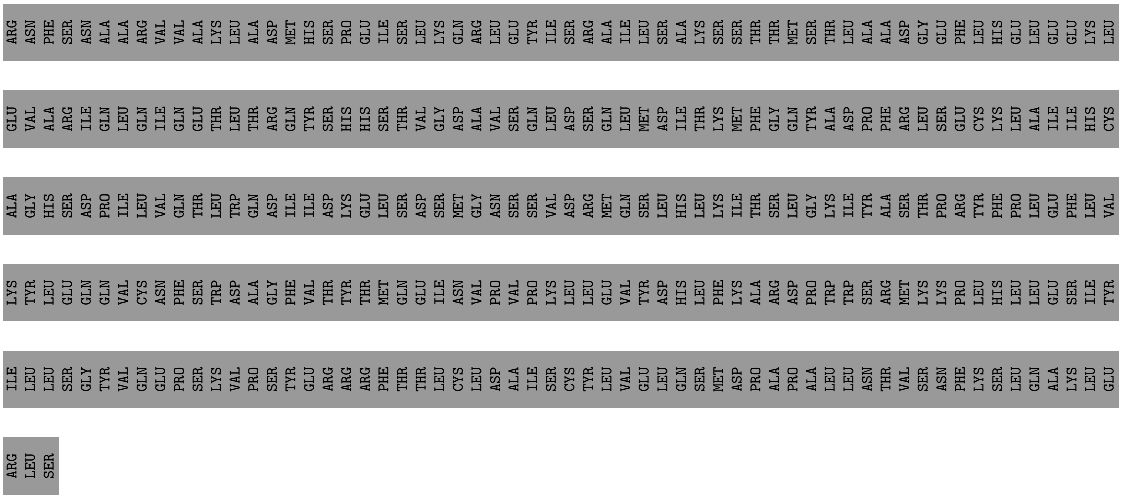
Chain f:



• Molecule 4: Nup155-prov protein

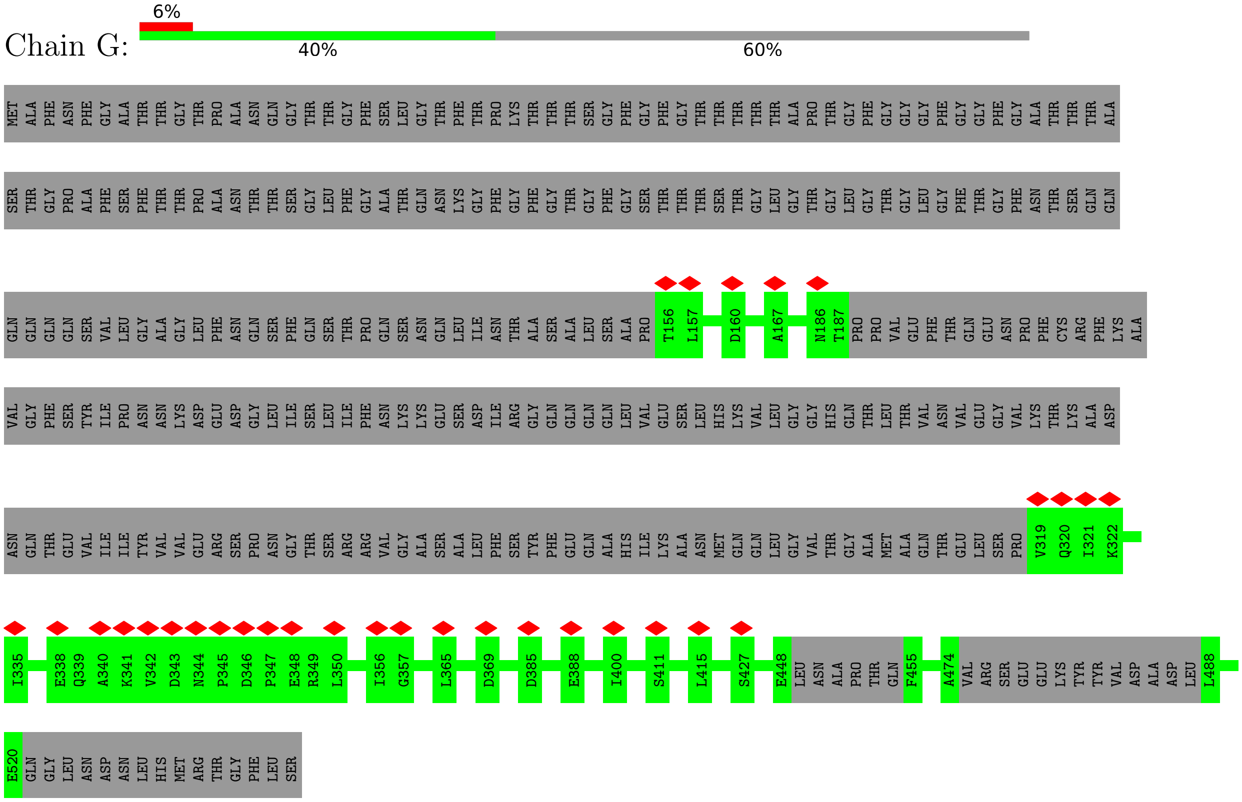
Chain m:





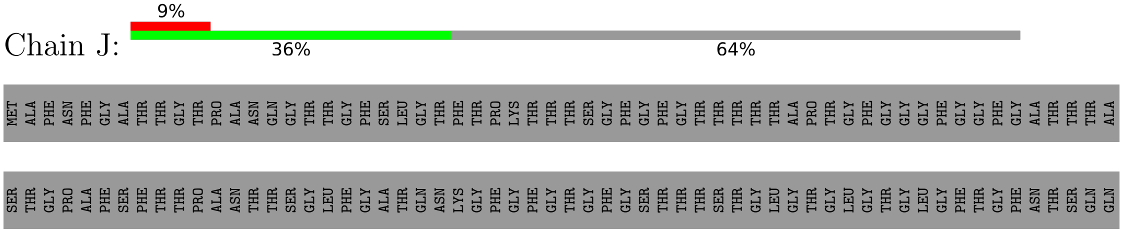
- Molecule 5: Nup54

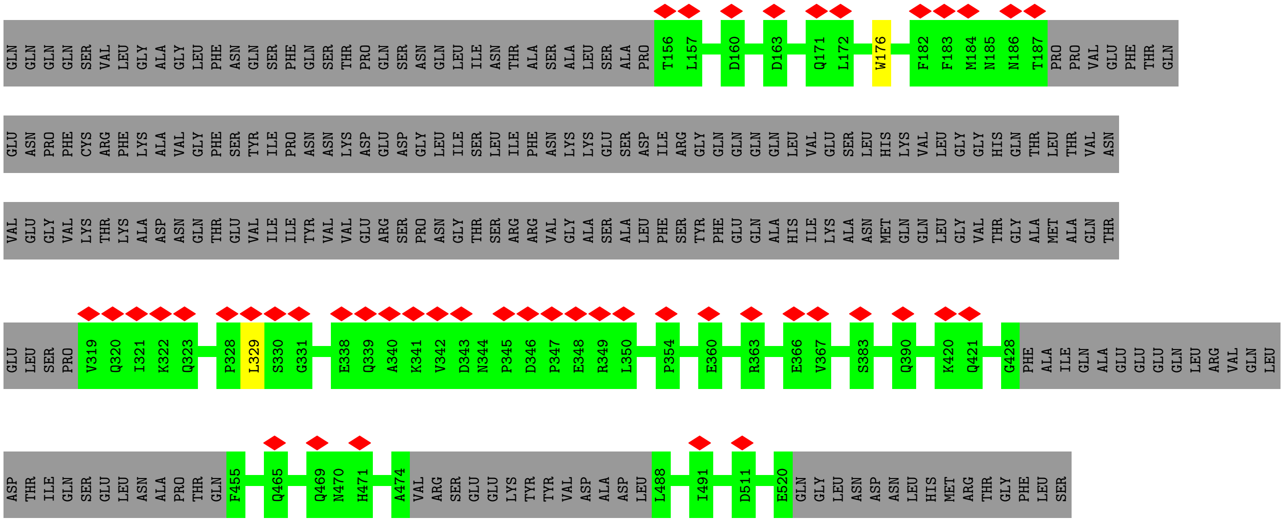
Chain G:



- Molecule 5: Nup54

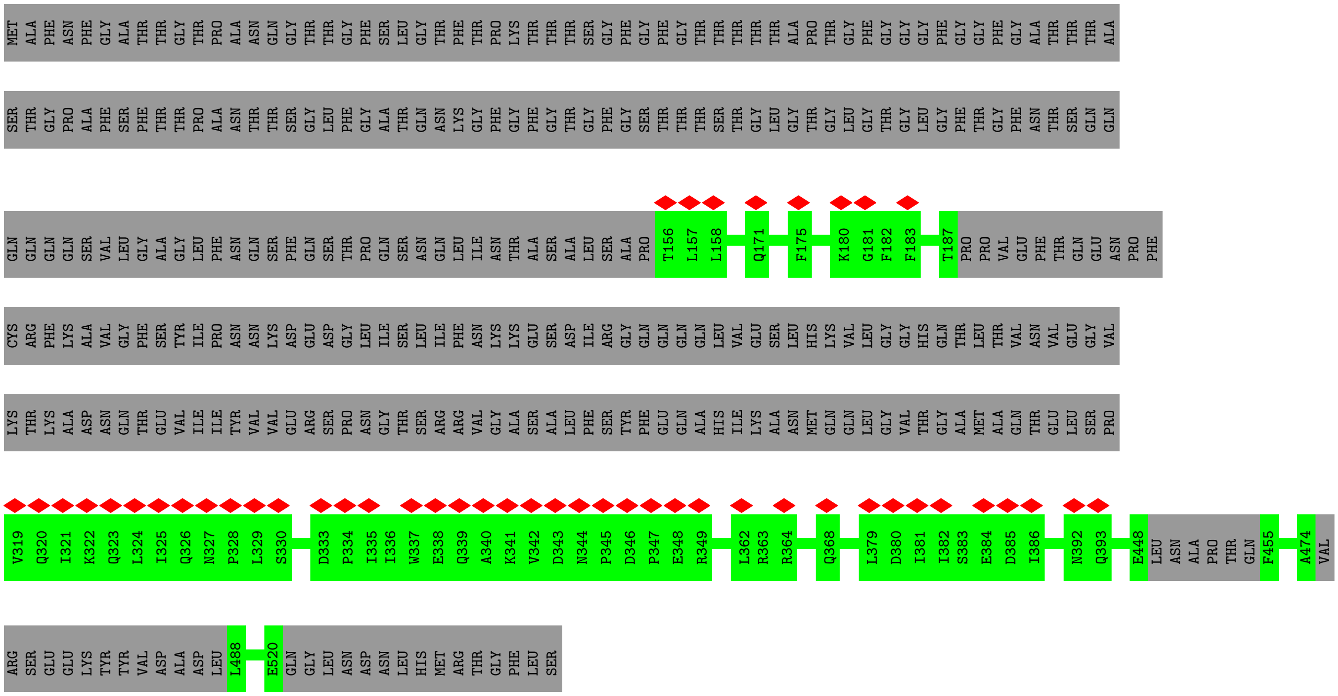
Chain J:





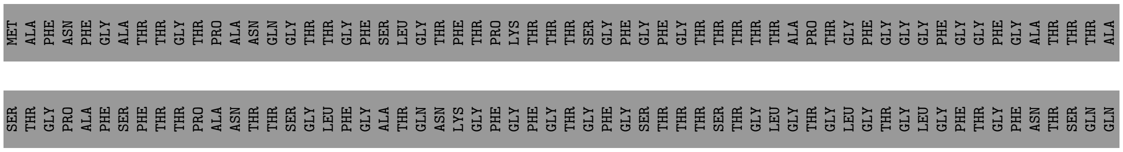
- Molecule 5: Nup54

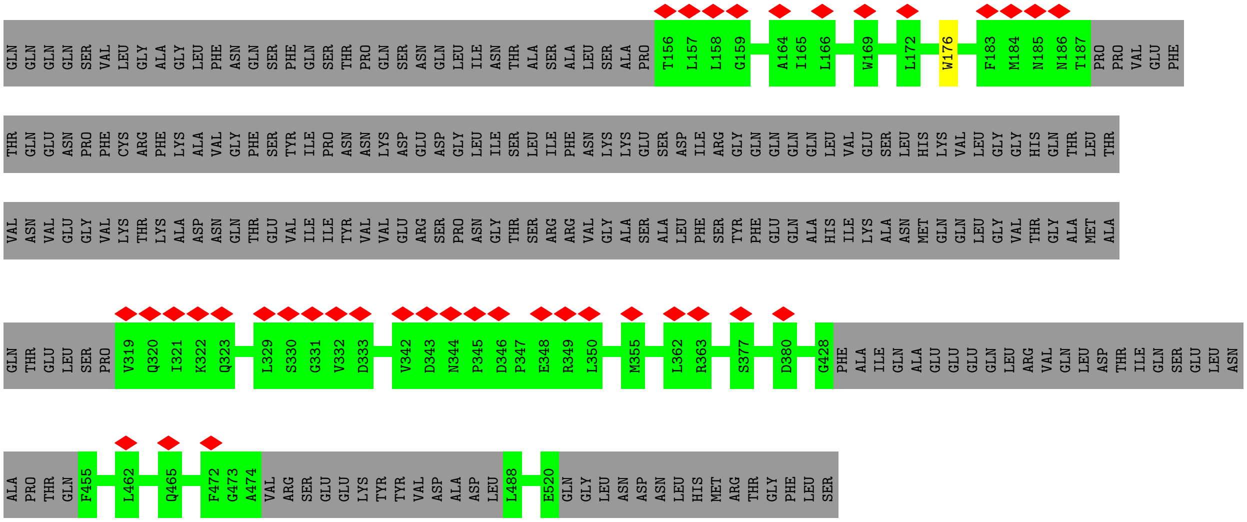
Chain g:



- Molecule 5: Nup54

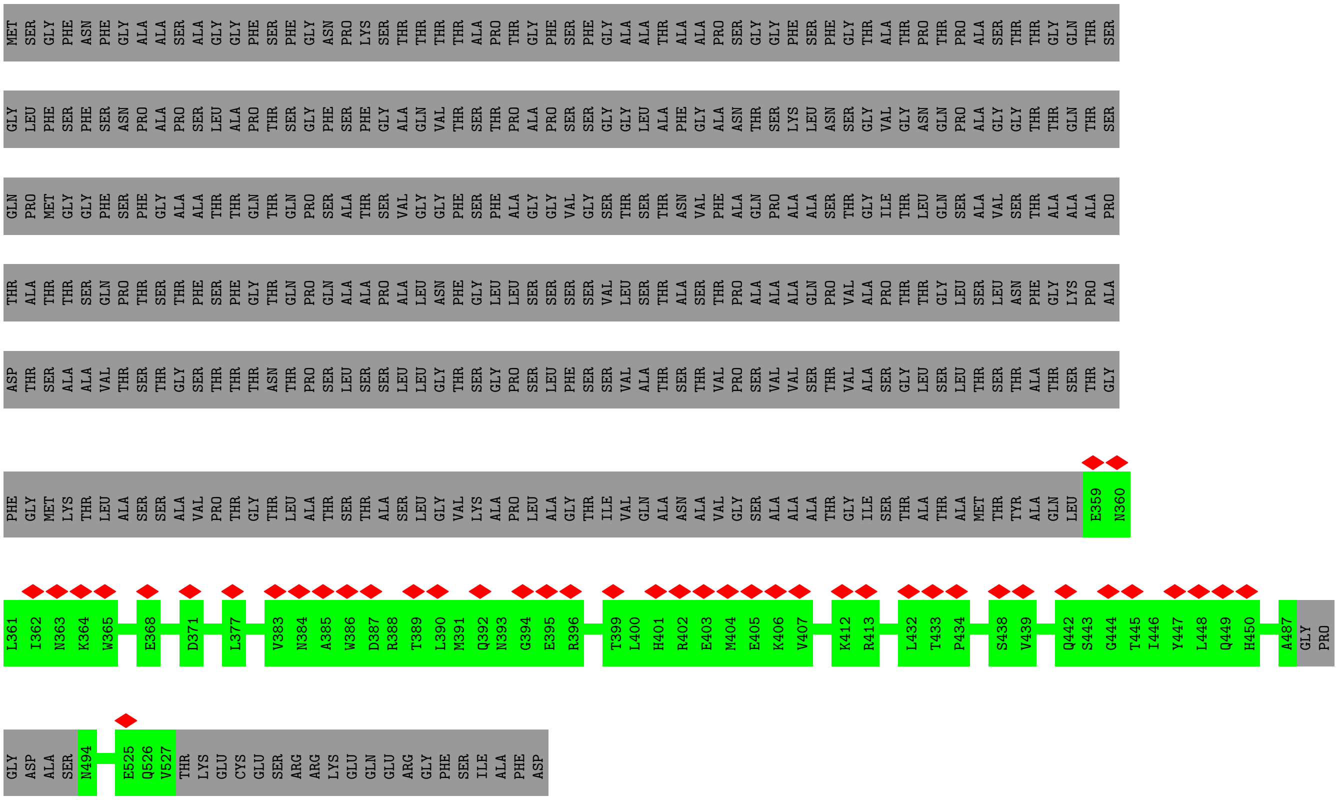
Chain j:





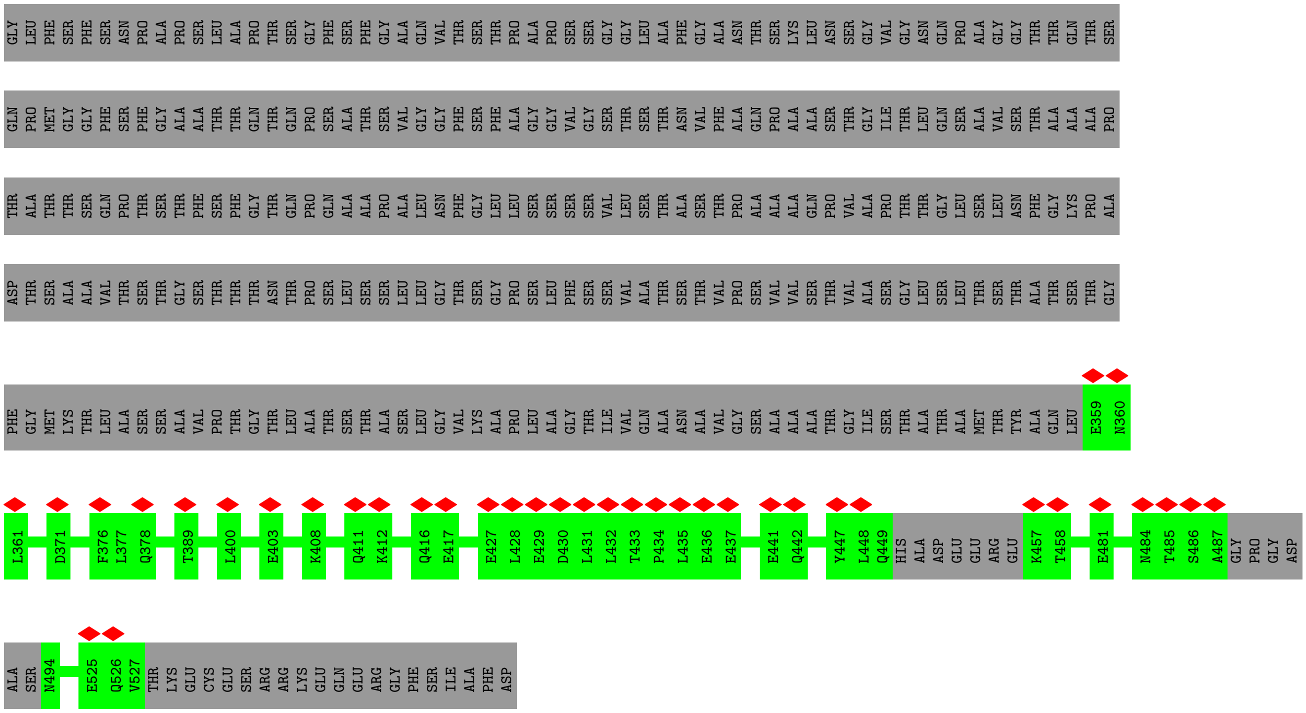
- Molecule 6: IL4I1 protein

Chain H:



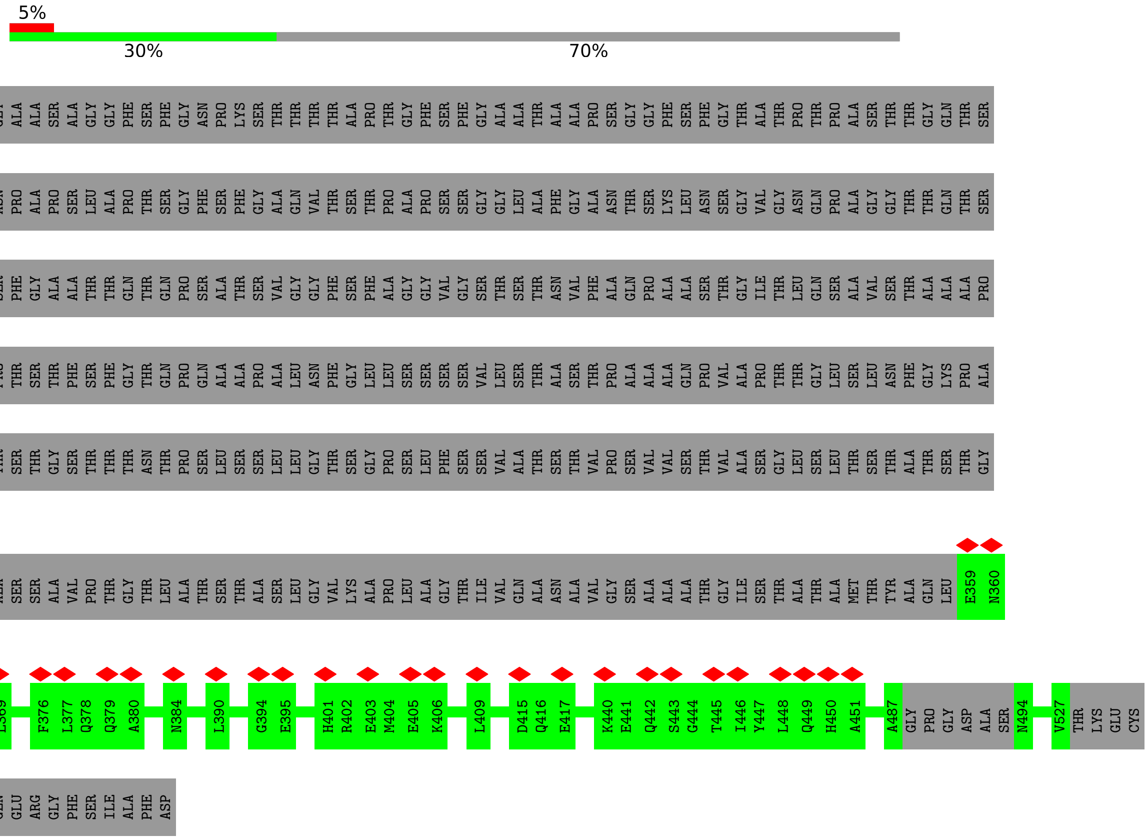
- Molecule 6: IL4I1 protein

Chain L:



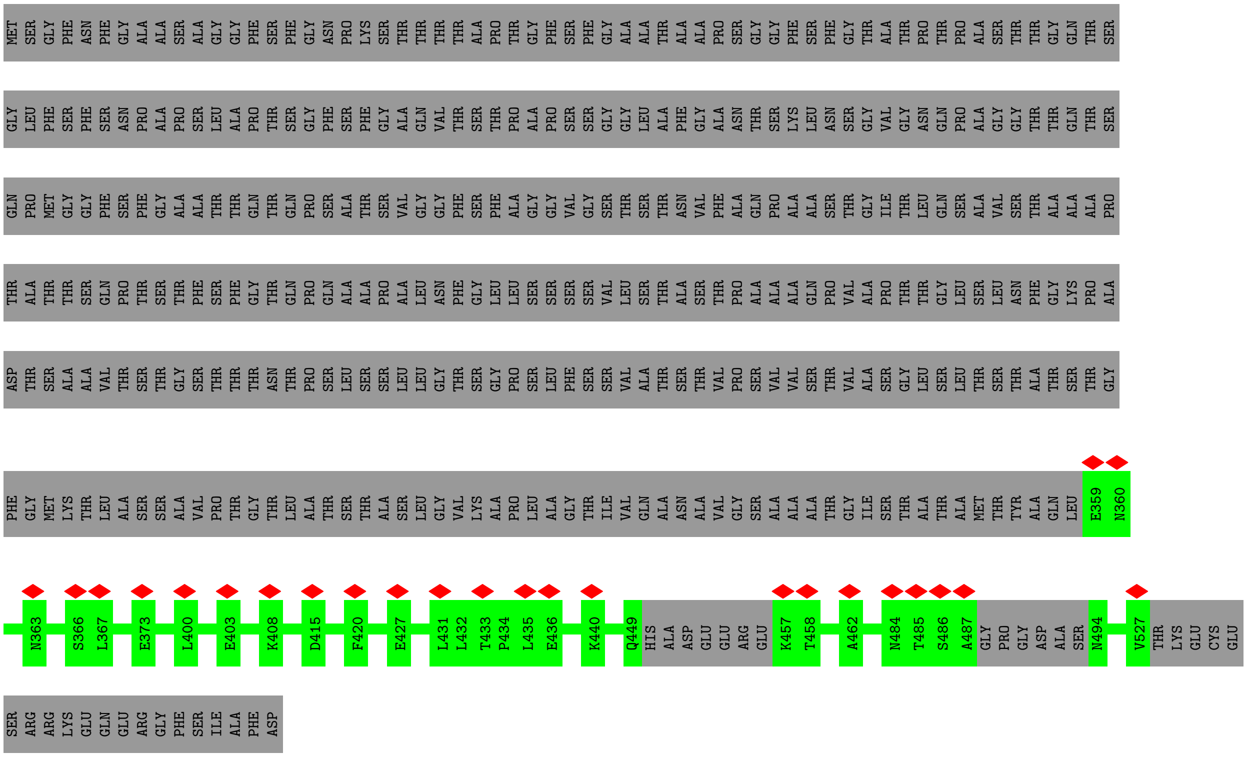
- Molecule 6: IL4I1 protein

Chain h:

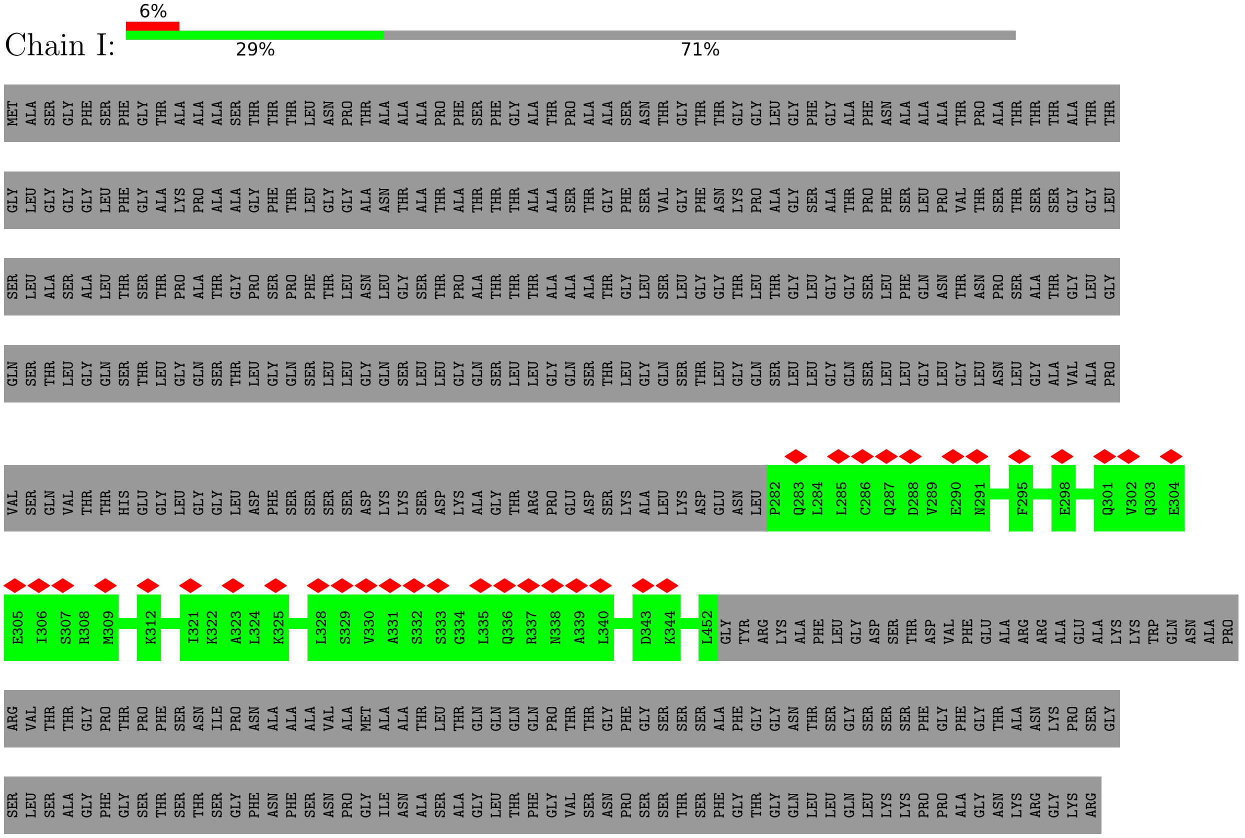


- Molecule 6: IL4I1 protein

Chain l:

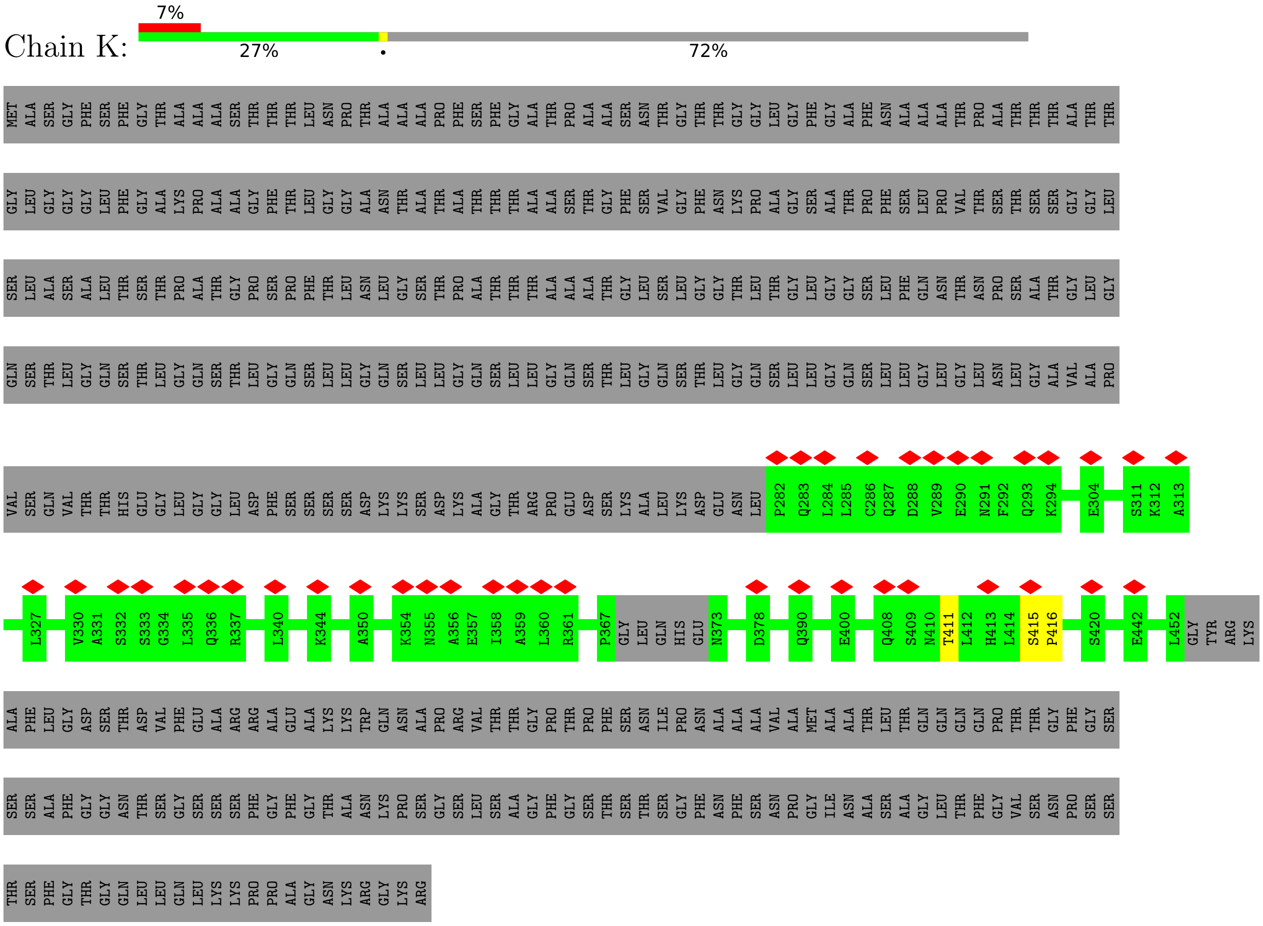


- Molecule 7: MGC84997 protein



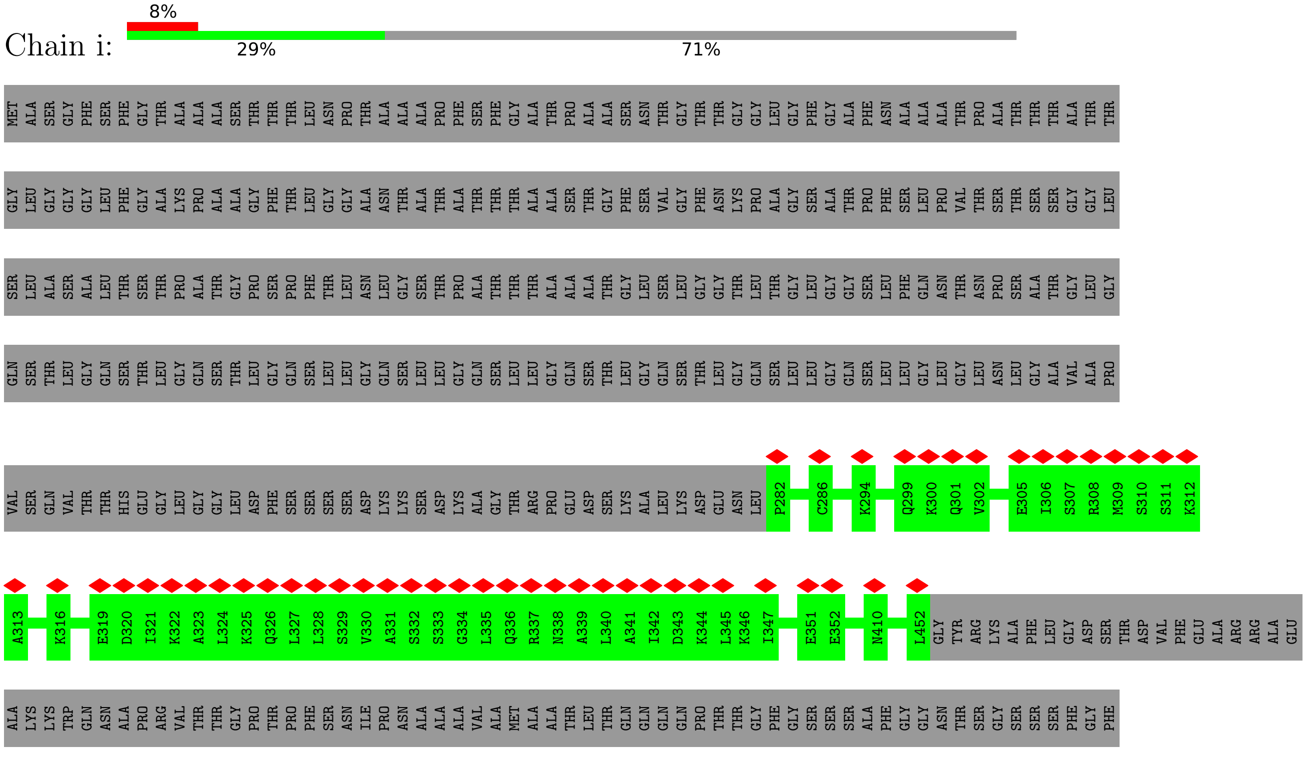
- Molecule 7: MGC84997 protein

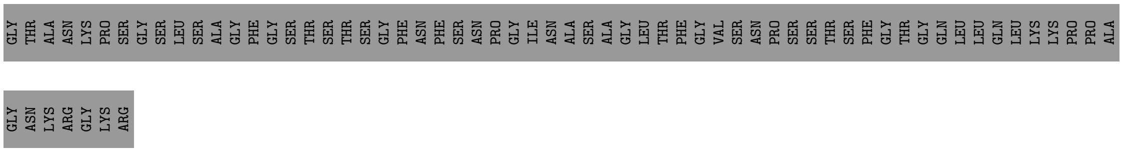
Chain K:



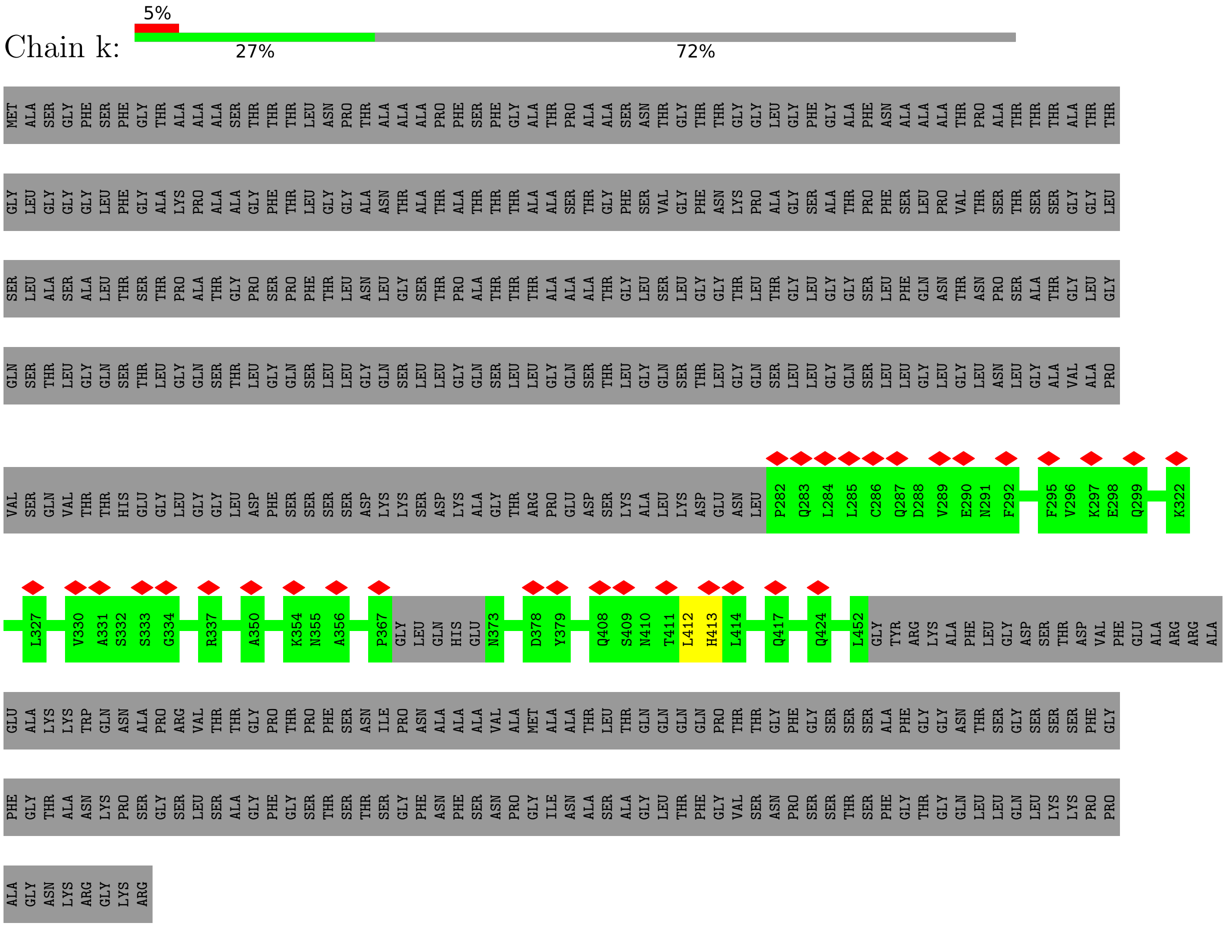
- Molecule 7: MGC84997 protein

Chain i:

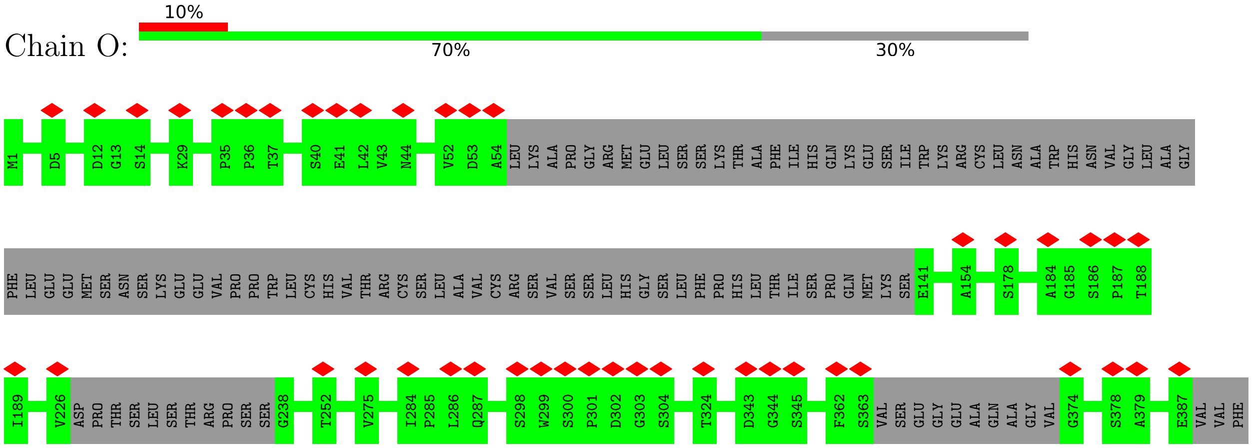


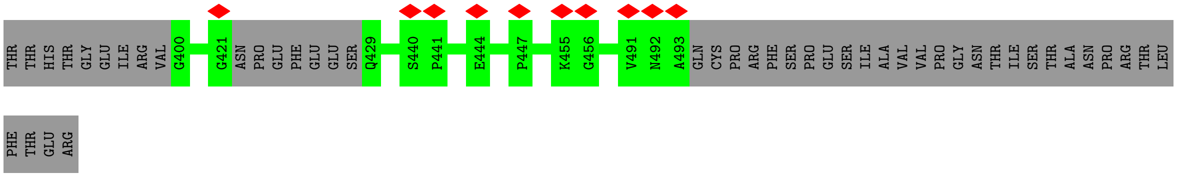


- Molecule 7: MGC84997 protein



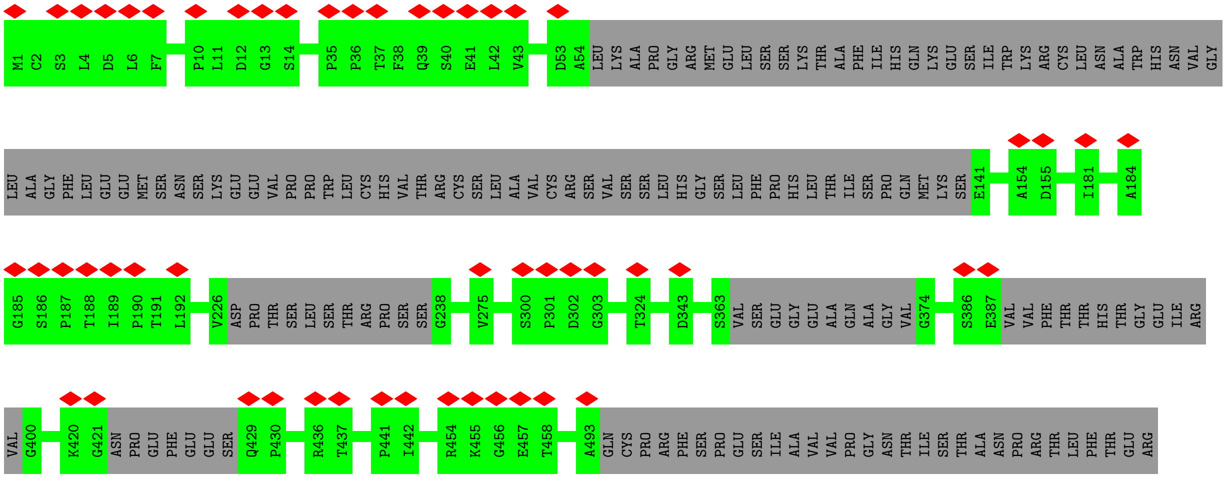
- Molecule 8: Aaas-prov protein





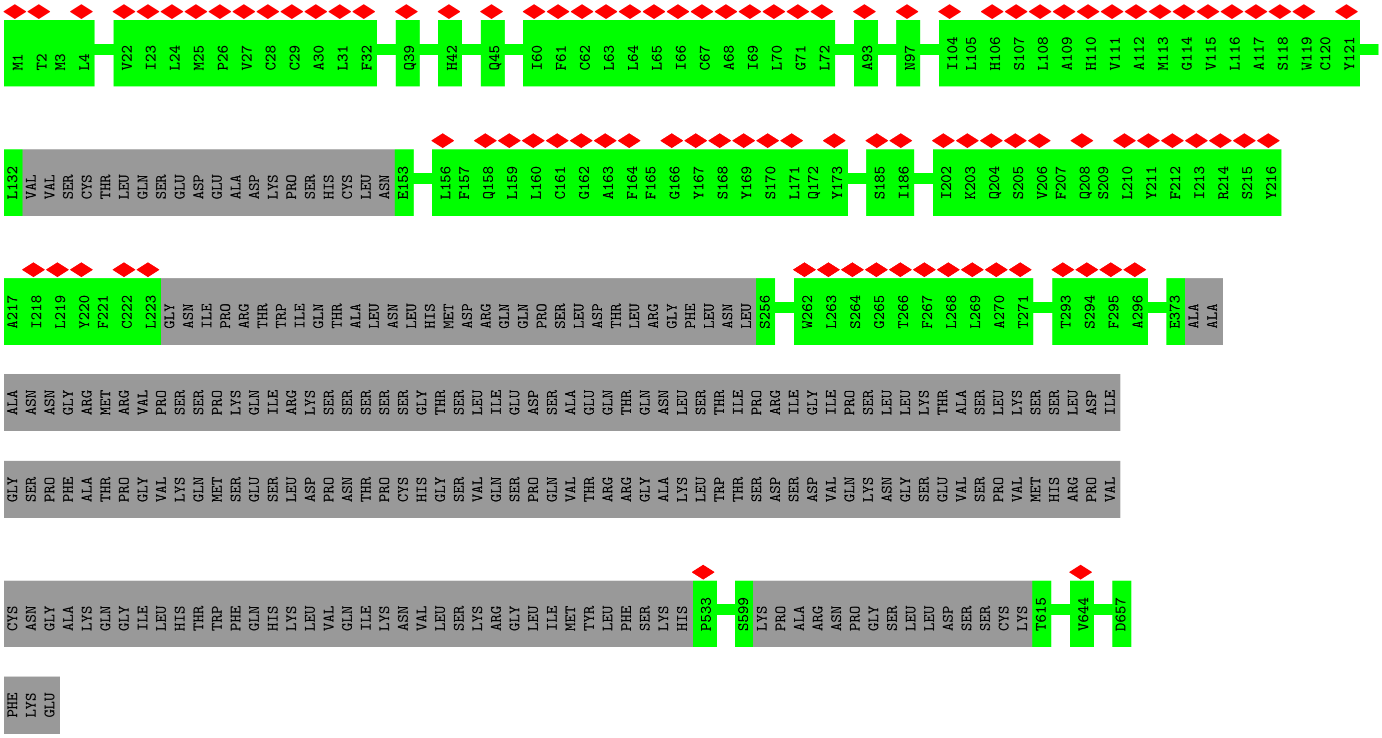
- Molecule 8: Aaas-prov protein

Chain o:

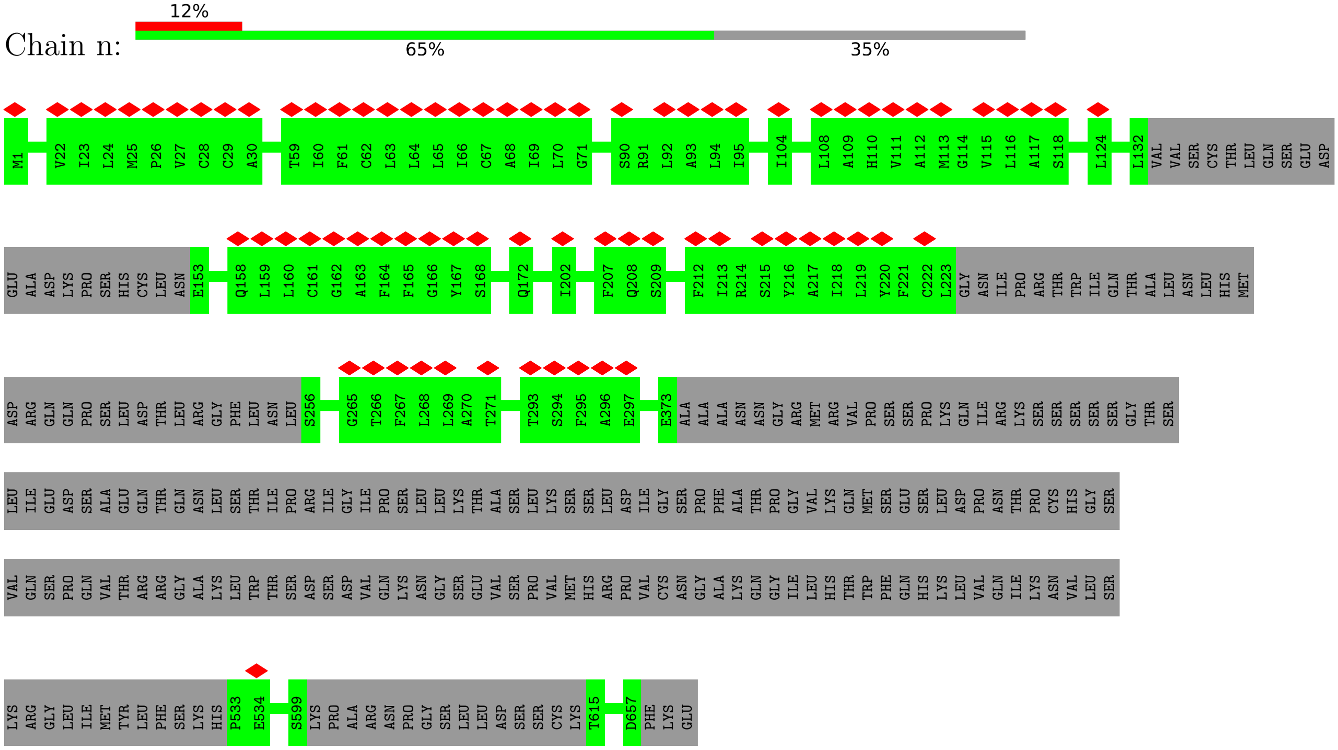


- Molecule 9: Nucleoporin NDC1

Chain N:



- Molecule 9: Nucleoporin NDC1



4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	2093631	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.038	Depositor
Minimum map value	-0.020	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	710.144, 710.144, 710.144	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.387, 1.387, 1.387	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	0.30	0/8318	0.40	0/11563
1	a	0.29	0/8246	0.40	0/11463
2	B	0.25	0/7330	0.38	0/10197
2	b	0.25	0/7330	0.38	0/10197
3	C	0.25	0/3134	0.37	0/4359
3	E	0.33	0/3093	0.41	0/4299
3	c	0.25	0/3134	0.38	0/4359
3	e	0.32	0/3093	0.42	0/4299
4	D	0.29	0/5506	0.43	0/7649
4	F	0.28	0/5399	0.42	0/7498
4	M	0.25	0/4288	0.43	0/5961
4	d	0.29	0/5545	0.44	0/7703
4	f	0.28	0/5414	0.42	0/7519
4	m	0.25	0/4288	0.43	0/5961
5	G	0.26	0/1059	0.41	0/1469
5	J	0.25	0/959	0.39	0/1329
5	g	0.26	0/1059	0.41	0/1469
5	j	0.26	0/959	0.40	0/1329
6	H	0.26	0/811	0.35	0/1131
6	L	0.35	0/775	0.38	0/1079
6	h	0.27	0/811	0.34	0/1131
6	l	0.34	0/775	0.37	0/1079
7	I	0.26	0/852	0.37	0/1190
7	K	0.41	1/827 (0.1%)	0.40	1/1154 (0.1%)
7	i	0.27	0/852	0.36	0/1190
7	k	0.30	0/827	0.37	0/1154
8	O	0.29	0/1799	0.49	0/2491
8	o	0.29	0/1799	0.49	0/2491
9	N	0.26	0/2138	0.36	0/2978
9	n	0.26	0/2138	0.36	0/2978
All	All	0.28	1/92558 (0.0%)	0.41	1/128669 (0.0%)

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
4	F	0	1
4	M	0	1
4	f	0	1
4	m	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	K	415	SER	C-N	7.98	1.49	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	K	415	SER	C-N-CA	5.52	145.19	122.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1634	THR	Peptide
4	F	537	GLN	Peptide
4	M	537	GLN	Peptide
4	f	115	ILE	Peptide
4	m	537	GLN	Peptide

5.2 Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	1642/2011 (82%)	1523 (93%)	116 (7%)	3 (0%)	47	80
1	a	1625/2011 (81%)	1509 (93%)	114 (7%)	2 (0%)	51	85
2	B	1448/1739 (83%)	1406 (97%)	42 (3%)	0	100	100
2	b	1448/1739 (83%)	1407 (97%)	41 (3%)	0	100	100
3	C	613/820 (75%)	593 (97%)	20 (3%)	0	100	100
3	E	601/820 (73%)	542 (90%)	59 (10%)	0	100	100
3	c	613/820 (75%)	592 (97%)	21 (3%)	0	100	100
3	e	601/820 (73%)	547 (91%)	54 (9%)	0	100	100
4	D	1079/1388 (78%)	1020 (94%)	58 (5%)	1 (0%)	51	85
4	F	1058/1388 (76%)	1018 (96%)	39 (4%)	1 (0%)	51	85
4	M	853/1388 (62%)	823 (96%)	29 (3%)	1 (0%)	51	85
4	d	1087/1388 (78%)	1029 (95%)	56 (5%)	2 (0%)	47	80
4	f	1061/1388 (76%)	1014 (96%)	46 (4%)	1 (0%)	51	85
4	m	853/1388 (62%)	823 (96%)	29 (3%)	1 (0%)	51	85
5	G	207/535 (39%)	193 (93%)	14 (7%)	0	100	100
5	J	187/535 (35%)	178 (95%)	7 (4%)	2 (1%)	14	52
5	g	207/535 (39%)	192 (93%)	15 (7%)	0	100	100
5	j	187/535 (35%)	174 (93%)	12 (6%)	1 (0%)	29	68
6	H	159/547 (29%)	154 (97%)	5 (3%)	0	100	100
6	L	150/547 (27%)	150 (100%)	0	0	100	100
6	h	159/547 (29%)	153 (96%)	6 (4%)	0	100	100
6	l	150/547 (27%)	148 (99%)	2 (1%)	0	100	100
7	I	169/599 (28%)	162 (96%)	7 (4%)	0	100	100
7	K	162/599 (27%)	154 (95%)	6 (4%)	2 (1%)	13	50
7	i	169/599 (28%)	159 (94%)	10 (6%)	0	100	100
7	k	162/599 (27%)	156 (96%)	4 (2%)	2 (1%)	13	50
8	O	355/523 (68%)	339 (96%)	16 (4%)	0	100	100
8	o	355/523 (68%)	339 (96%)	16 (4%)	0	100	100
9	N	421/660 (64%)	412 (98%)	9 (2%)	0	100	100
9	n	421/660 (64%)	412 (98%)	9 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	18202/28198 (65%)	17321 (95%)	862 (5%)	19 (0%)	54 85

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1635	ALA
1	a	1635	ALA
1	A	258	VAL
4	F	538	GLU
5	J	176	TRP
4	M	538	GLU
4	m	538	GLU
1	A	1128	ARG
4	D	538	GLU
7	K	411	THR
4	d	538	GLU
4	f	538	GLU
7	k	412	LEU
7	k	413	HIS
7	K	416	PRO
1	a	1128	ARG
5	J	329	LEU
5	j	176	TRP
4	d	698	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 ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

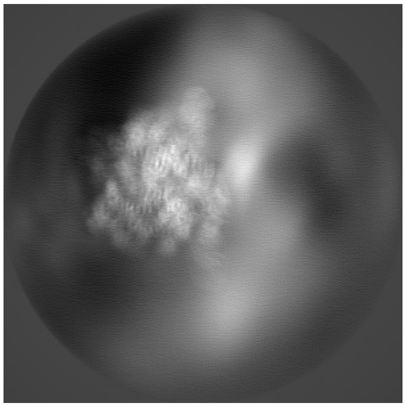
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32566. These allow visual inspection of the internal detail of the map and identification of artifacts.

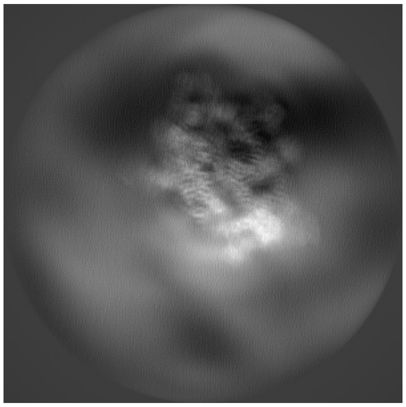
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

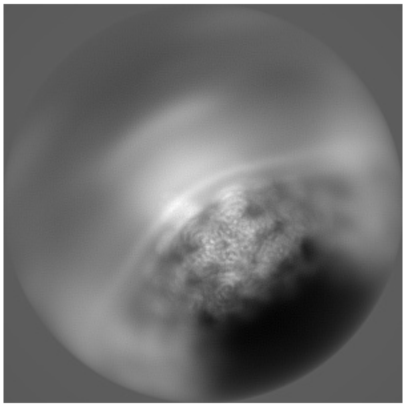
6.1.1 Primary map



X



Y

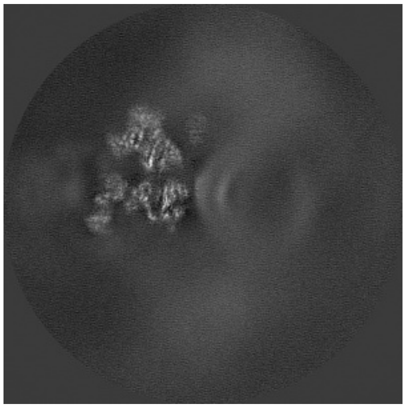


Z

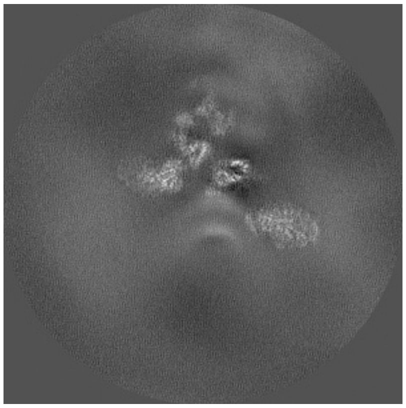
The images above show the map projected in three orthogonal directions.

6.2 Central slices

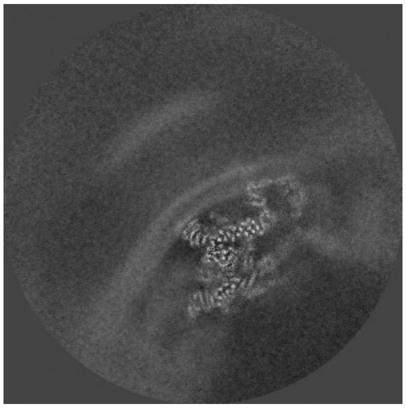
6.2.1 Primary map



X Index: 256



Y Index: 256

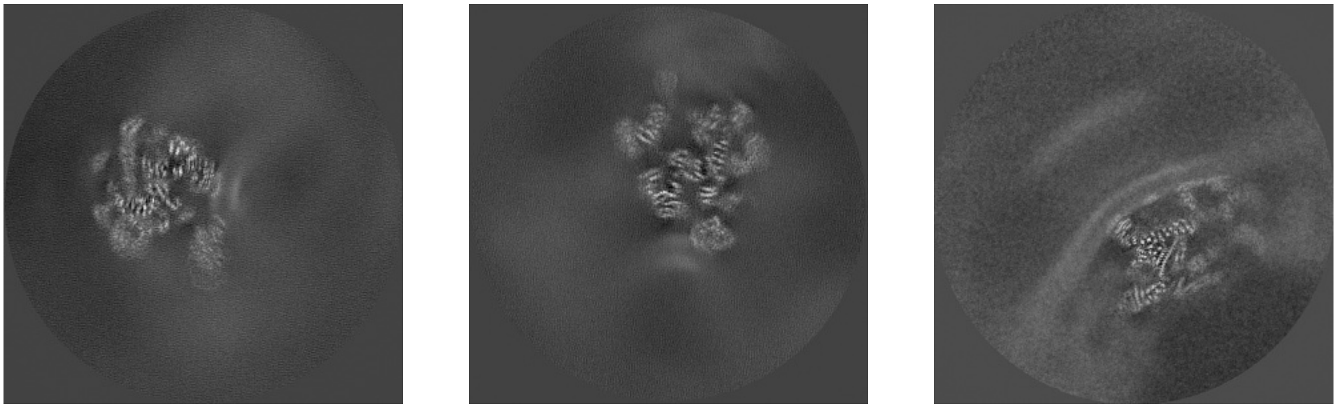


Z Index: 256

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

6.3 Largest variance slices

6.3.1 Primary map



X Index: 293 Y Index: 206 Z Index: 260

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

6.4 Orthogonal surface views

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

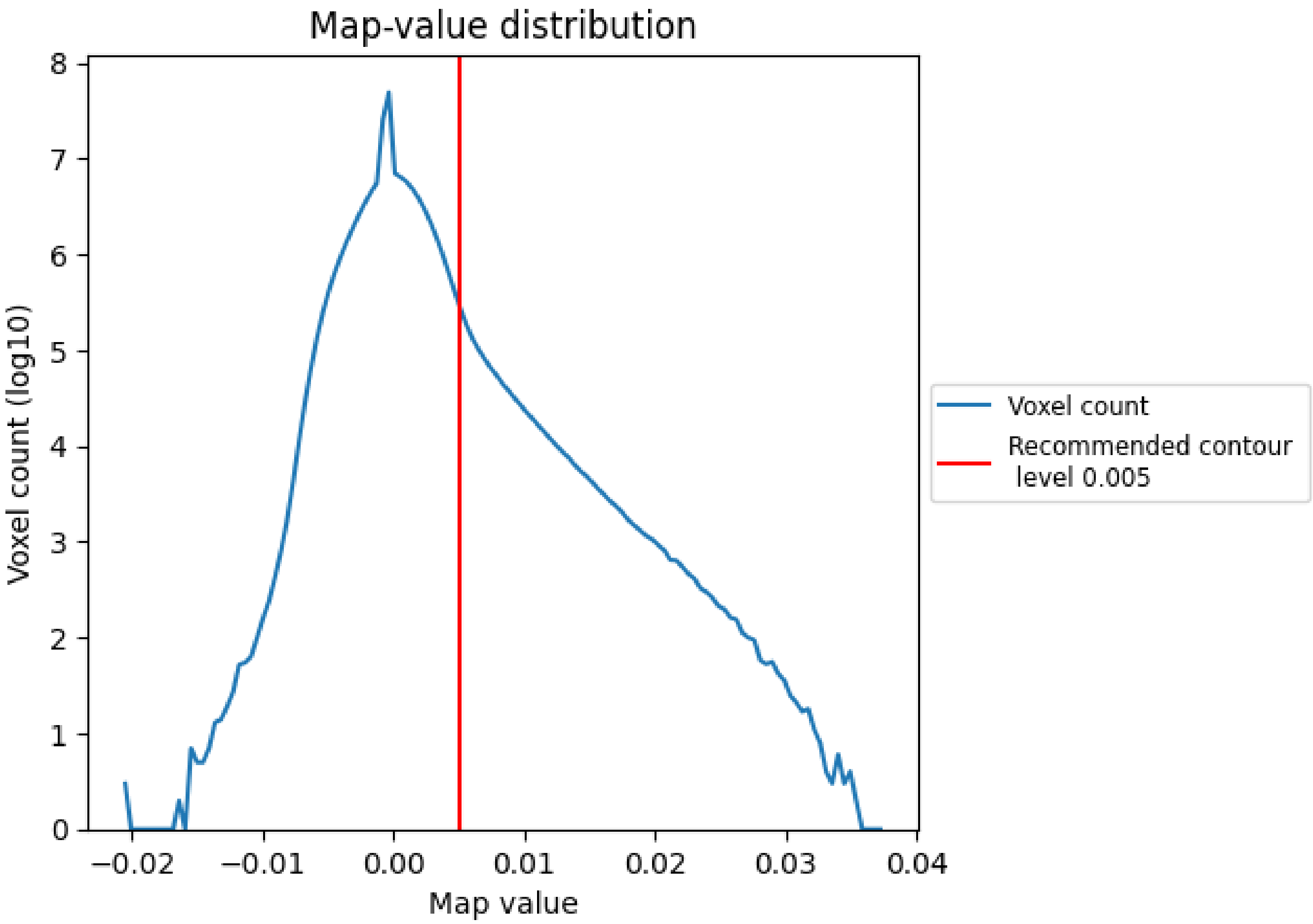
6.5 Mask visualisation ⓘ

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

7 Map analysis ⓘ

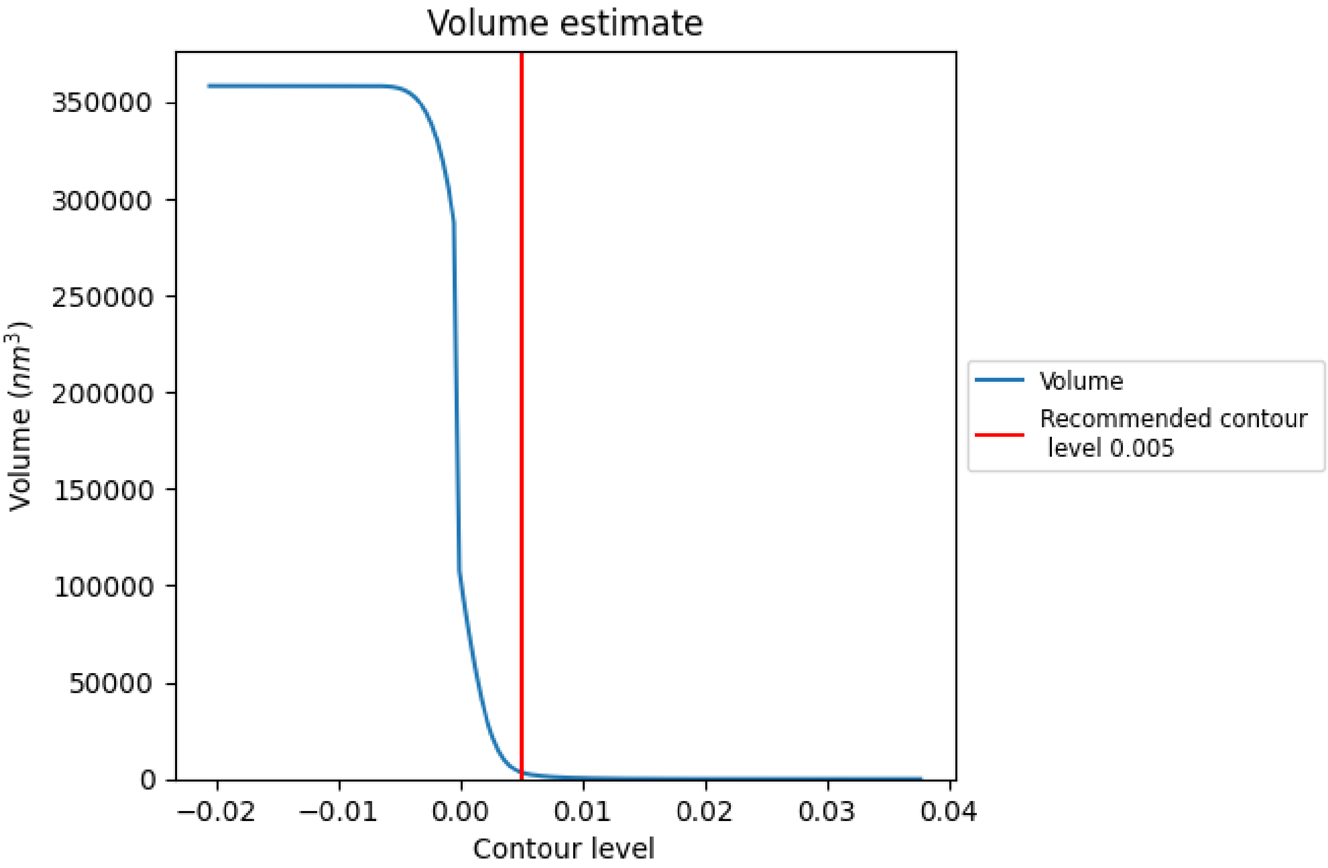
This section contains the results of statistical analysis of the map.

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.

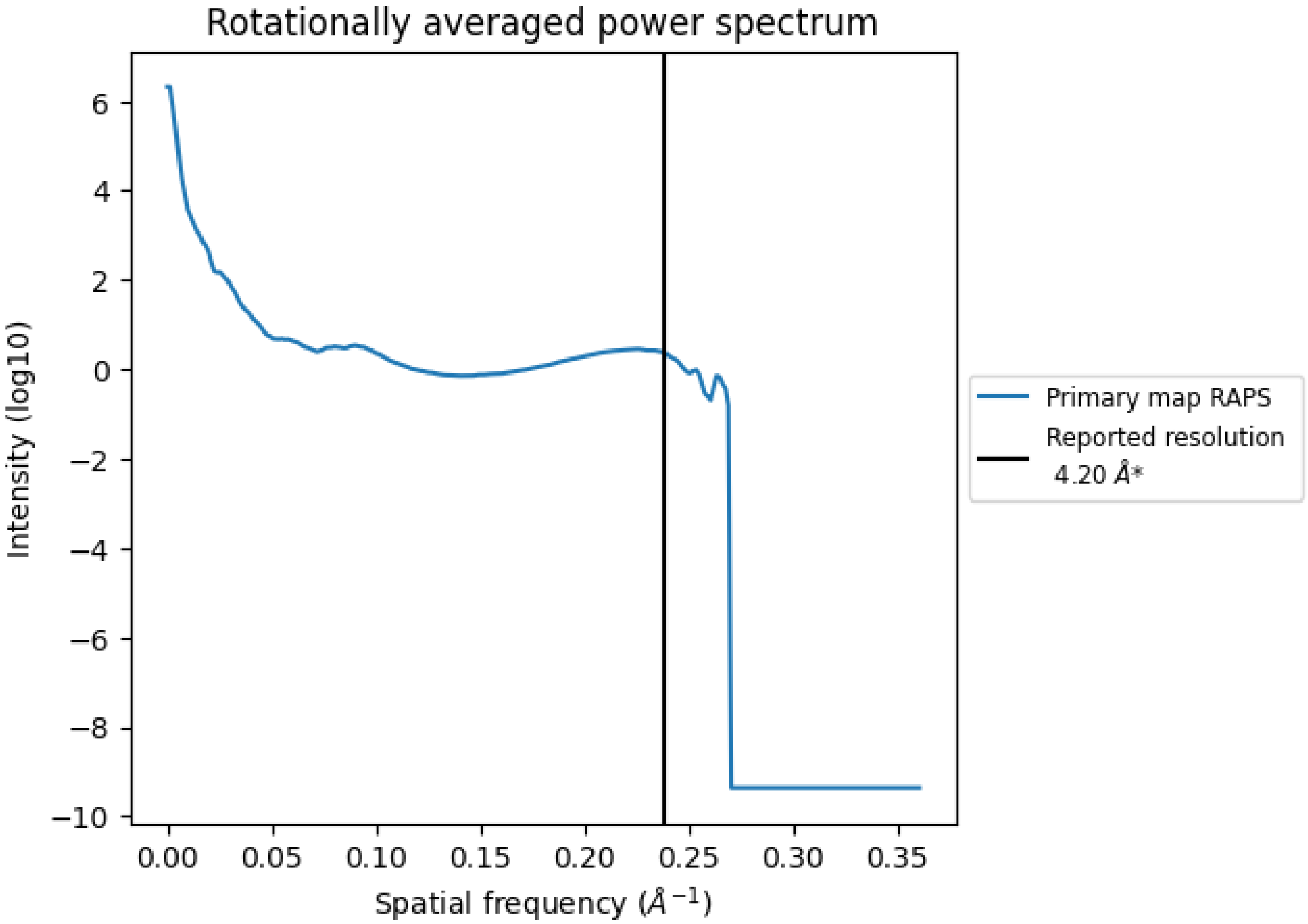
7.2 Volume estimate (i)



The volume at the recommended contour level is 3486 nm^3; this corresponds to an approximate mass of 3149 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

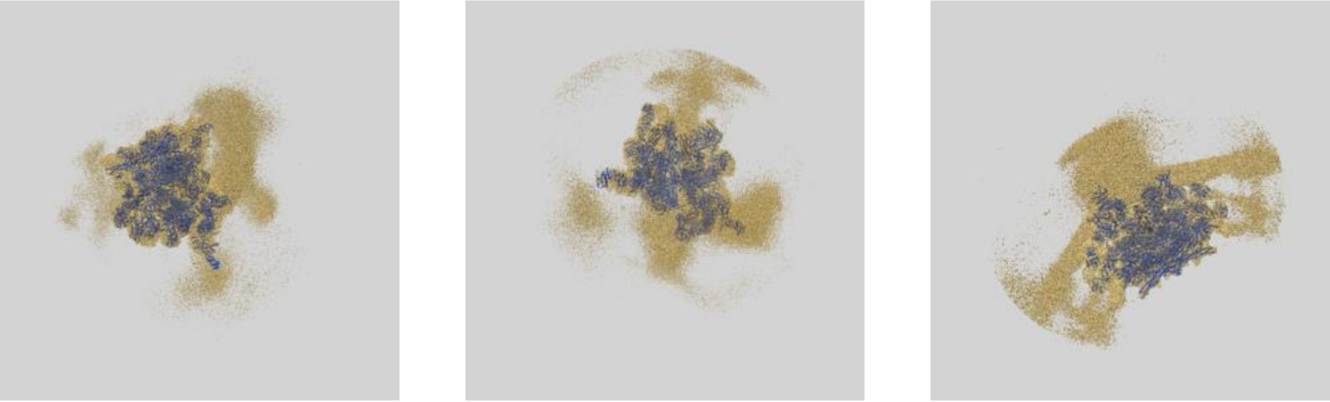
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-32566 and PDB model 7WKK. Per-residue inclusion information can be found in section 3 on page 7.

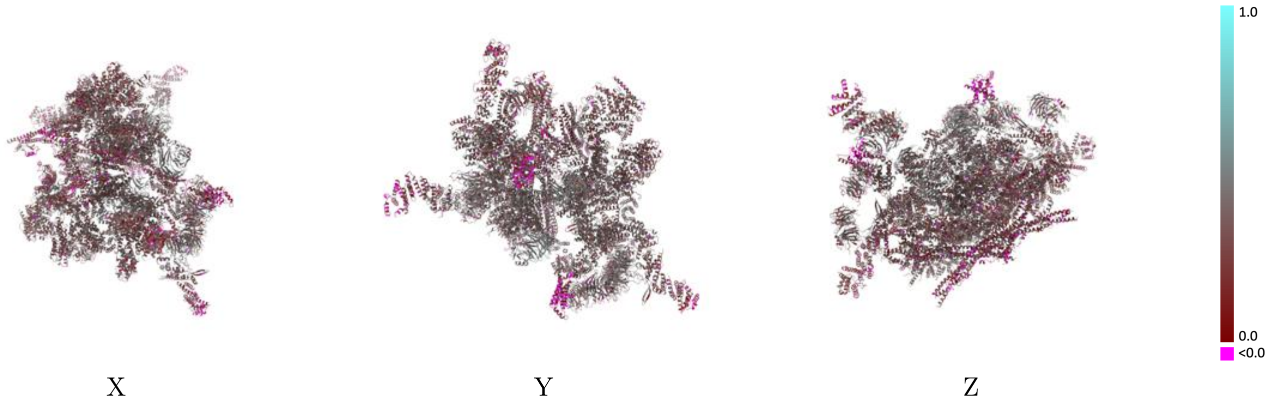
9.1 Map-model overlay ⓘ



X Y Z

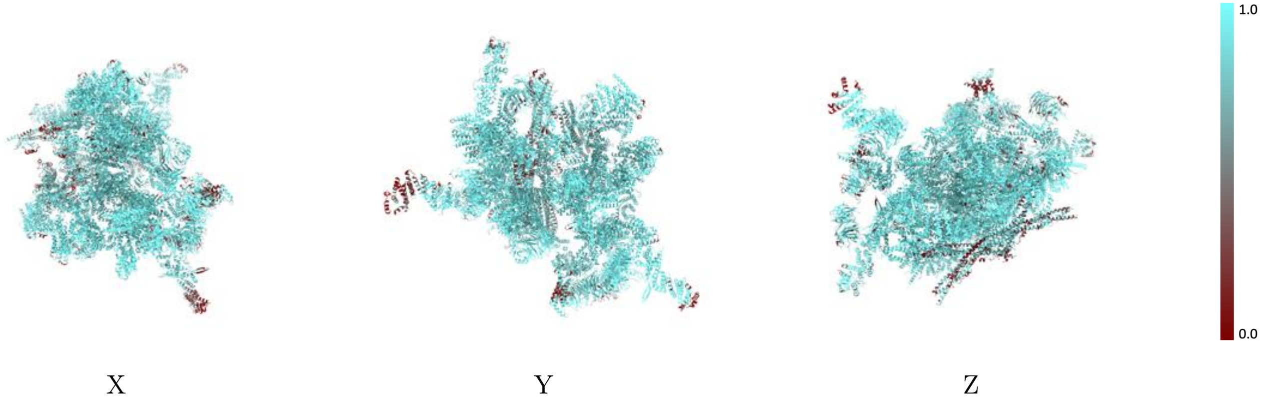
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model



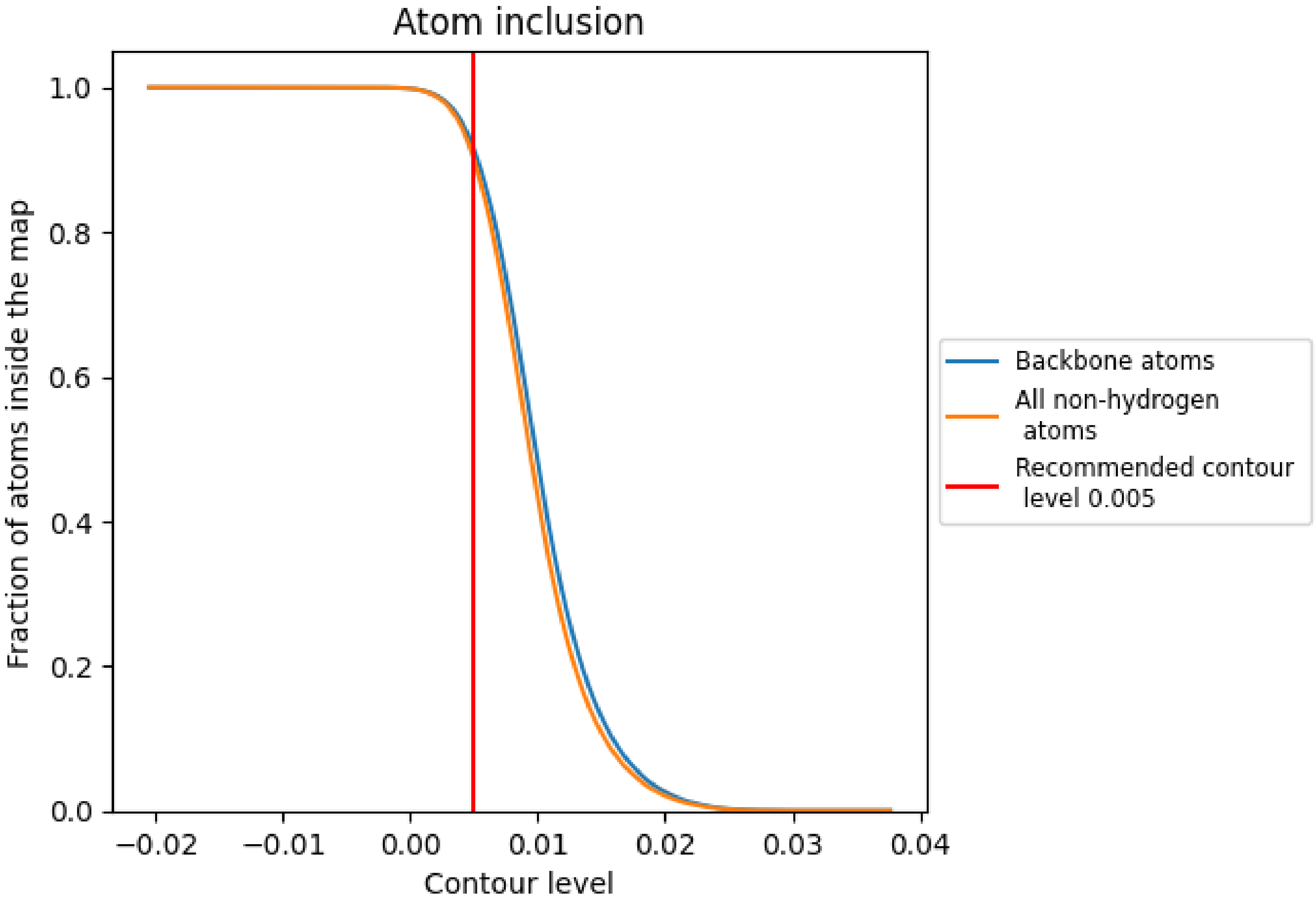
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).

9.4 Atom inclusion ⓘ



At the recommended contour level, 91% of all backbone atoms, 90% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9000	0.3490
A	0.9403	0.3610
B	0.9650	0.3500
C	0.8979	0.3010
D	0.9712	0.4130
E	0.9758	0.4020
F	0.9225	0.3760
G	0.8071	0.3160
H	0.7171	0.2640
I	0.7691	0.2870
J	0.7300	0.2680
K	0.6791	0.2380
L	0.7198	0.2520
M	0.7907	0.3620
N	0.7639	0.2400
O	0.8343	0.3690
a	0.9274	0.3590
b	0.9641	0.3420
c	0.9170	0.3040
d	0.9543	0.4020
e	0.9723	0.3950
f	0.8951	0.3660
g	0.7291	0.2720
h	0.7466	0.2870
i	0.6917	0.2760
j	0.7591	0.2820
k	0.7370	0.2500
l	0.7763	0.2530
m	0.9232	0.3720
n	0.8087	0.2360
o	0.8255	0.3550