Full wwPDB EM Validation Report ⓘ

Apr 23, 2024 – 08:43 am BST

PDB ID	:	7APK
EMDB ID	:	EMD-11857
Title	:	Structure of the human THO - UAP56 complex
Authors	:	Hohmann, U.; Puehringer, T.; Plaschka, C.
Deposited on	:	2020-10-17
Resolution	:	3.30 Å(reported)

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

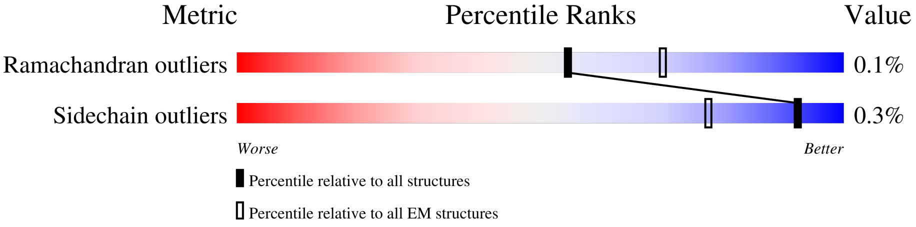
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.30 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
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	711	37% 37% 63%
1	I	711	39% 38% 61%
1	a	711	37% 37% 63%
1	i	711	23% 38% 61%
2	B	1226	58% 57% • 42%
2	J	1226	58% 57% 42%
2	b	1226	58% 57% • 42%
2	j	1226	52% 57% 42%
3	C	395	77% 76% • 23%

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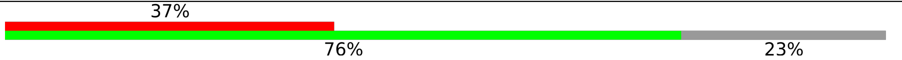
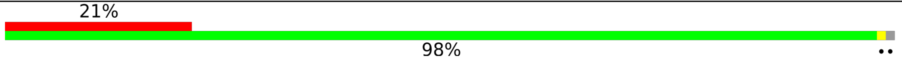
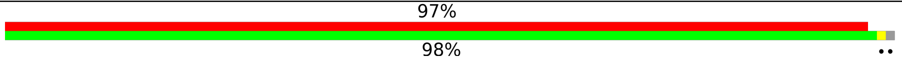
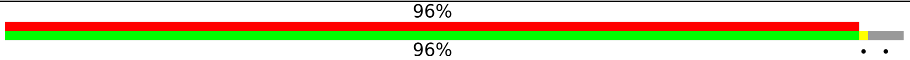
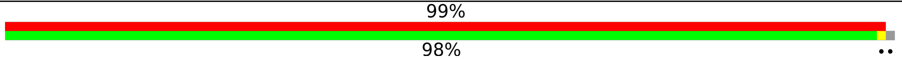
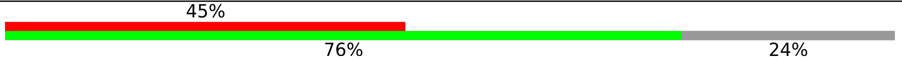
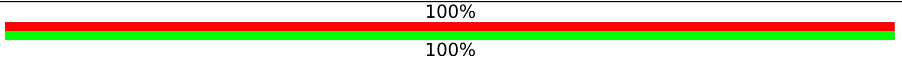
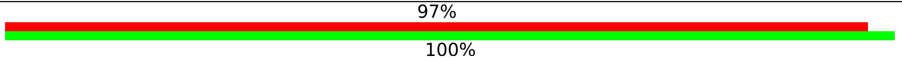
Mol	Chain	Length	Quality of chain
3	K	395	
3	c	395	
3	k	395	
4	E	683	
4	M	683	
4	e	683	
4	m	683	
5	F	341	
5	N	341	
5	f	341	
5	n	341	
6	G	204	
6	O	204	
6	g	204	
6	o	204	
7	H	451	
7	P	451	
7	h	451	
7	p	451	
8	X	37	
8	x	37	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 72697 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 THO complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	266	Total 2165	C 1402	N 357	O 397	S 9	0	0
1	I	275	Total 2228	C 1441	N 368	O 410	S 9	0	0
1	a	266	Total 2165	C 1402	N 357	O 397	S 9	0	0
1	i	275	Total 2229	C 1441	N 368	O 411	S 9	0	0

There are 220 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-53	MET	-	initiating methionine	UNP Q96FV9
A	-52	GLY	-	expression tag	UNP Q96FV9
A	-51	LYS	-	expression tag	UNP Q96FV9
A	-50	PRO	-	expression tag	UNP Q96FV9
A	-49	ILE	-	expression tag	UNP Q96FV9
A	-48	PRO	-	expression tag	UNP Q96FV9
A	-47	ASN	-	expression tag	UNP Q96FV9
A	-46	PRO	-	expression tag	UNP Q96FV9
A	-45	LEU	-	expression tag	UNP Q96FV9
A	-44	LEU	-	expression tag	UNP Q96FV9
A	-43	GLY	-	expression tag	UNP Q96FV9
A	-42	LEU	-	expression tag	UNP Q96FV9
A	-41	ASP	-	expression tag	UNP Q96FV9
A	-40	SER	-	expression tag	UNP Q96FV9
A	-39	THR	-	expression tag	UNP Q96FV9
A	-38	GLY	-	expression tag	UNP Q96FV9
A	-37	SER	-	expression tag	UNP Q96FV9
A	-36	GLY	-	expression tag	UNP Q96FV9
A	-35	LYS	-	expression tag	UNP Q96FV9
A	-34	PRO	-	expression tag	UNP Q96FV9
A	-33	ILE	-	expression tag	UNP Q96FV9
A	-32	PRO	-	expression tag	UNP Q96FV9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-31	ASN	-	expression tag	UNP Q96FV9
A	-30	PRO	-	expression tag	UNP Q96FV9
A	-29	LEU	-	expression tag	UNP Q96FV9
A	-28	LEU	-	expression tag	UNP Q96FV9
A	-27	GLY	-	expression tag	UNP Q96FV9
A	-26	LEU	-	expression tag	UNP Q96FV9
A	-25	ASP	-	expression tag	UNP Q96FV9
A	-24	SER	-	expression tag	UNP Q96FV9
A	-23	THR	-	expression tag	UNP Q96FV9
A	-22	GLY	-	expression tag	UNP Q96FV9
A	-21	SER	-	expression tag	UNP Q96FV9
A	-20	GLY	-	expression tag	UNP Q96FV9
A	-19	LYS	-	expression tag	UNP Q96FV9
A	-18	PRO	-	expression tag	UNP Q96FV9
A	-17	ILE	-	expression tag	UNP Q96FV9
A	-16	PRO	-	expression tag	UNP Q96FV9
A	-15	ASN	-	expression tag	UNP Q96FV9
A	-14	PRO	-	expression tag	UNP Q96FV9
A	-13	LEU	-	expression tag	UNP Q96FV9
A	-12	LEU	-	expression tag	UNP Q96FV9
A	-11	GLY	-	expression tag	UNP Q96FV9
A	-10	LEU	-	expression tag	UNP Q96FV9
A	-9	ASP	-	expression tag	UNP Q96FV9
A	-8	SER	-	expression tag	UNP Q96FV9
A	-7	THR	-	expression tag	UNP Q96FV9
A	-6	LEU	-	expression tag	UNP Q96FV9
A	-5	GLU	-	expression tag	UNP Q96FV9
A	-4	VAL	-	expression tag	UNP Q96FV9
A	-3	LEU	-	expression tag	UNP Q96FV9
A	-2	PHE	-	expression tag	UNP Q96FV9
A	-1	GLN	-	expression tag	UNP Q96FV9
A	0	GLY	-	expression tag	UNP Q96FV9
A	1	PRO	-	expression tag	UNP Q96FV9
I	-53	MET	-	initiating methionine	UNP Q96FV9
I	-52	GLY	-	expression tag	UNP Q96FV9
I	-51	LYS	-	expression tag	UNP Q96FV9
I	-50	PRO	-	expression tag	UNP Q96FV9
I	-49	ILE	-	expression tag	UNP Q96FV9
I	-48	PRO	-	expression tag	UNP Q96FV9
I	-47	ASN	-	expression tag	UNP Q96FV9
I	-46	PRO	-	expression tag	UNP Q96FV9
I	-45	LEU	-	expression tag	UNP Q96FV9

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-44	LEU	-	expression tag	UNP Q96FV9
I	-43	GLY	-	expression tag	UNP Q96FV9
I	-42	LEU	-	expression tag	UNP Q96FV9
I	-41	ASP	-	expression tag	UNP Q96FV9
I	-40	SER	-	expression tag	UNP Q96FV9
I	-39	THR	-	expression tag	UNP Q96FV9
I	-38	GLY	-	expression tag	UNP Q96FV9
I	-37	SER	-	expression tag	UNP Q96FV9
I	-36	GLY	-	expression tag	UNP Q96FV9
I	-35	LYS	-	expression tag	UNP Q96FV9
I	-34	PRO	-	expression tag	UNP Q96FV9
I	-33	ILE	-	expression tag	UNP Q96FV9
I	-32	PRO	-	expression tag	UNP Q96FV9
I	-31	ASN	-	expression tag	UNP Q96FV9
I	-30	PRO	-	expression tag	UNP Q96FV9
I	-29	LEU	-	expression tag	UNP Q96FV9
I	-28	LEU	-	expression tag	UNP Q96FV9
I	-27	GLY	-	expression tag	UNP Q96FV9
I	-26	LEU	-	expression tag	UNP Q96FV9
I	-25	ASP	-	expression tag	UNP Q96FV9
I	-24	SER	-	expression tag	UNP Q96FV9
I	-23	THR	-	expression tag	UNP Q96FV9
I	-22	GLY	-	expression tag	UNP Q96FV9
I	-21	SER	-	expression tag	UNP Q96FV9
I	-20	GLY	-	expression tag	UNP Q96FV9
I	-19	LYS	-	expression tag	UNP Q96FV9
I	-18	PRO	-	expression tag	UNP Q96FV9
I	-17	ILE	-	expression tag	UNP Q96FV9
I	-16	PRO	-	expression tag	UNP Q96FV9
I	-15	ASN	-	expression tag	UNP Q96FV9
I	-14	PRO	-	expression tag	UNP Q96FV9
I	-13	LEU	-	expression tag	UNP Q96FV9
I	-12	LEU	-	expression tag	UNP Q96FV9
I	-11	GLY	-	expression tag	UNP Q96FV9
I	-10	LEU	-	expression tag	UNP Q96FV9
I	-9	ASP	-	expression tag	UNP Q96FV9
I	-8	SER	-	expression tag	UNP Q96FV9
I	-7	THR	-	expression tag	UNP Q96FV9
I	-6	LEU	-	expression tag	UNP Q96FV9
I	-5	GLU	-	expression tag	UNP Q96FV9
I	-4	VAL	-	expression tag	UNP Q96FV9
I	-3	LEU	-	expression tag	UNP Q96FV9

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-2	PHE	-	expression tag	UNP Q96FV9
I	-1	GLN	-	expression tag	UNP Q96FV9
I	0	GLY	-	expression tag	UNP Q96FV9
I	1	PRO	-	expression tag	UNP Q96FV9
a	-53	MET	-	initiating methionine	UNP Q96FV9
a	-52	GLY	-	expression tag	UNP Q96FV9
a	-51	LYS	-	expression tag	UNP Q96FV9
a	-50	PRO	-	expression tag	UNP Q96FV9
a	-49	ILE	-	expression tag	UNP Q96FV9
a	-48	PRO	-	expression tag	UNP Q96FV9
a	-47	ASN	-	expression tag	UNP Q96FV9
a	-46	PRO	-	expression tag	UNP Q96FV9
a	-45	LEU	-	expression tag	UNP Q96FV9
a	-44	LEU	-	expression tag	UNP Q96FV9
a	-43	GLY	-	expression tag	UNP Q96FV9
a	-42	LEU	-	expression tag	UNP Q96FV9
a	-41	ASP	-	expression tag	UNP Q96FV9
a	-40	SER	-	expression tag	UNP Q96FV9
a	-39	THR	-	expression tag	UNP Q96FV9
a	-38	GLY	-	expression tag	UNP Q96FV9
a	-37	SER	-	expression tag	UNP Q96FV9
a	-36	GLY	-	expression tag	UNP Q96FV9
a	-35	LYS	-	expression tag	UNP Q96FV9
a	-34	PRO	-	expression tag	UNP Q96FV9
a	-33	ILE	-	expression tag	UNP Q96FV9
a	-32	PRO	-	expression tag	UNP Q96FV9
a	-31	ASN	-	expression tag	UNP Q96FV9
a	-30	PRO	-	expression tag	UNP Q96FV9
a	-29	LEU	-	expression tag	UNP Q96FV9
a	-28	LEU	-	expression tag	UNP Q96FV9
a	-27	GLY	-	expression tag	UNP Q96FV9
a	-26	LEU	-	expression tag	UNP Q96FV9
a	-25	ASP	-	expression tag	UNP Q96FV9
a	-24	SER	-	expression tag	UNP Q96FV9
a	-23	THR	-	expression tag	UNP Q96FV9
a	-22	GLY	-	expression tag	UNP Q96FV9
a	-21	SER	-	expression tag	UNP Q96FV9
a	-20	GLY	-	expression tag	UNP Q96FV9
a	-19	LYS	-	expression tag	UNP Q96FV9
a	-18	PRO	-	expression tag	UNP Q96FV9
a	-17	ILE	-	expression tag	UNP Q96FV9
a	-16	PRO	-	expression tag	UNP Q96FV9

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Chain	Residue	Modelled	Actual	Comment	Reference
a	-15	ASN	-	expression tag	UNP Q96FV9
a	-14	PRO	-	expression tag	UNP Q96FV9
a	-13	LEU	-	expression tag	UNP Q96FV9
a	-12	LEU	-	expression tag	UNP Q96FV9
a	-11	GLY	-	expression tag	UNP Q96FV9
a	-10	LEU	-	expression tag	UNP Q96FV9
a	-9	ASP	-	expression tag	UNP Q96FV9
a	-8	SER	-	expression tag	UNP Q96FV9
a	-7	THR	-	expression tag	UNP Q96FV9
a	-6	LEU	-	expression tag	UNP Q96FV9
a	-5	GLU	-	expression tag	UNP Q96FV9
a	-4	VAL	-	expression tag	UNP Q96FV9
a	-3	LEU	-	expression tag	UNP Q96FV9
a	-2	PHE	-	expression tag	UNP Q96FV9
a	-1	GLN	-	expression tag	UNP Q96FV9
a	0	GLY	-	expression tag	UNP Q96FV9
a	1	PRO	-	expression tag	UNP Q96FV9
i	-53	MET	-	initiating methionine	UNP Q96FV9
i	-52	GLY	-	expression tag	UNP Q96FV9
i	-51	LYS	-	expression tag	UNP Q96FV9
i	-50	PRO	-	expression tag	UNP Q96FV9
i	-49	ILE	-	expression tag	UNP Q96FV9
i	-48	PRO	-	expression tag	UNP Q96FV9
i	-47	ASN	-	expression tag	UNP Q96FV9
i	-46	PRO	-	expression tag	UNP Q96FV9
i	-45	LEU	-	expression tag	UNP Q96FV9
i	-44	LEU	-	expression tag	UNP Q96FV9
i	-43	GLY	-	expression tag	UNP Q96FV9
i	-42	LEU	-	expression tag	UNP Q96FV9
i	-41	ASP	-	expression tag	UNP Q96FV9
i	-40	SER	-	expression tag	UNP Q96FV9
i	-39	THR	-	expression tag	UNP Q96FV9
i	-38	GLY	-	expression tag	UNP Q96FV9
i	-37	SER	-	expression tag	UNP Q96FV9
i	-36	GLY	-	expression tag	UNP Q96FV9
i	-35	LYS	-	expression tag	UNP Q96FV9
i	-34	PRO	-	expression tag	UNP Q96FV9
i	-33	ILE	-	expression tag	UNP Q96FV9
i	-32	PRO	-	expression tag	UNP Q96FV9
i	-31	ASN	-	expression tag	UNP Q96FV9
i	-30	PRO	-	expression tag	UNP Q96FV9
i	-29	LEU	-	expression tag	UNP Q96FV9

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Chain	Residue	Modelled	Actual	Comment	Reference
i	-28	LEU	-	expression tag	UNP Q96FV9
i	-27	GLY	-	expression tag	UNP Q96FV9
i	-26	LEU	-	expression tag	UNP Q96FV9
i	-25	ASP	-	expression tag	UNP Q96FV9
i	-24	SER	-	expression tag	UNP Q96FV9
i	-23	THR	-	expression tag	UNP Q96FV9
i	-22	GLY	-	expression tag	UNP Q96FV9
i	-21	SER	-	expression tag	UNP Q96FV9
i	-20	GLY	-	expression tag	UNP Q96FV9
i	-19	LYS	-	expression tag	UNP Q96FV9
i	-18	PRO	-	expression tag	UNP Q96FV9
i	-17	ILE	-	expression tag	UNP Q96FV9
i	-16	PRO	-	expression tag	UNP Q96FV9
i	-15	ASN	-	expression tag	UNP Q96FV9
i	-14	PRO	-	expression tag	UNP Q96FV9
i	-13	LEU	-	expression tag	UNP Q96FV9
i	-12	LEU	-	expression tag	UNP Q96FV9
i	-11	GLY	-	expression tag	UNP Q96FV9
i	-10	LEU	-	expression tag	UNP Q96FV9
i	-9	ASP	-	expression tag	UNP Q96FV9
i	-8	SER	-	expression tag	UNP Q96FV9
i	-7	THR	-	expression tag	UNP Q96FV9
i	-6	LEU	-	expression tag	UNP Q96FV9
i	-5	GLU	-	expression tag	UNP Q96FV9
i	-4	VAL	-	expression tag	UNP Q96FV9
i	-3	LEU	-	expression tag	UNP Q96FV9
i	-2	PHE	-	expression tag	UNP Q96FV9
i	-1	GLN	-	expression tag	UNP Q96FV9
i	0	GLY	-	expression tag	UNP Q96FV9
i	1	PRO	-	expression tag	UNP Q96FV9

- Molecule 2 is a protein called THO complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	706	4700	2972	834	874	20	0	0
2	J	707	4702	2975	832	875	20	0	0
2	b	706	4700	2972	834	874	20	0	0
2	j	707	4696	2969	832	875	20	0	0

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-22	MET	-	initiating methionine	UNP Q8NI27
B	-21	LYS	-	expression tag	UNP Q8NI27
B	-20	HIS	-	expression tag	UNP Q8NI27
B	-19	HIS	-	expression tag	UNP Q8NI27
B	-18	HIS	-	expression tag	UNP Q8NI27
B	-17	HIS	-	expression tag	UNP Q8NI27
B	-16	HIS	-	expression tag	UNP Q8NI27
B	-15	HIS	-	expression tag	UNP Q8NI27
B	-14	HIS	-	expression tag	UNP Q8NI27
B	-13	HIS	-	expression tag	UNP Q8NI27
B	-12	HIS	-	expression tag	UNP Q8NI27
B	-11	HIS	-	expression tag	UNP Q8NI27
B	-10	SER	-	expression tag	UNP Q8NI27
B	-9	ALA	-	expression tag	UNP Q8NI27
B	-8	GLY	-	expression tag	UNP Q8NI27
B	-7	LEU	-	expression tag	UNP Q8NI27
B	-6	GLU	-	expression tag	UNP Q8NI27
B	-5	VAL	-	expression tag	UNP Q8NI27
B	-4	LEU	-	expression tag	UNP Q8NI27
B	-3	PHE	-	expression tag	UNP Q8NI27
B	-2	GLN	-	expression tag	UNP Q8NI27
B	-1	GLY	-	expression tag	UNP Q8NI27
B	0	PRO	-	expression tag	UNP Q8NI27
J	-22	MET	-	initiating methionine	UNP Q8NI27
J	-21	LYS	-	expression tag	UNP Q8NI27
J	-20	HIS	-	expression tag	UNP Q8NI27
J	-19	HIS	-	expression tag	UNP Q8NI27
J	-18	HIS	-	expression tag	UNP Q8NI27
J	-17	HIS	-	expression tag	UNP Q8NI27
J	-16	HIS	-	expression tag	UNP Q8NI27
J	-15	HIS	-	expression tag	UNP Q8NI27
J	-14	HIS	-	expression tag	UNP Q8NI27
J	-13	HIS	-	expression tag	UNP Q8NI27
J	-12	HIS	-	expression tag	UNP Q8NI27
J	-11	HIS	-	expression tag	UNP Q8NI27
J	-10	SER	-	expression tag	UNP Q8NI27
J	-9	ALA	-	expression tag	UNP Q8NI27
J	-8	GLY	-	expression tag	UNP Q8NI27
J	-7	LEU	-	expression tag	UNP Q8NI27
J	-6	GLU	-	expression tag	UNP Q8NI27
J	-5	VAL	-	expression tag	UNP Q8NI27
J	-4	LEU	-	expression tag	UNP Q8NI27

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-3	PHE	-	expression tag	UNP Q8NI27
J	-2	GLN	-	expression tag	UNP Q8NI27
J	-1	GLY	-	expression tag	UNP Q8NI27
J	0	PRO	-	expression tag	UNP Q8NI27
b	-22	MET	-	initiating methionine	UNP Q8NI27
b	-21	LYS	-	expression tag	UNP Q8NI27
b	-20	HIS	-	expression tag	UNP Q8NI27
b	-19	HIS	-	expression tag	UNP Q8NI27
b	-18	HIS	-	expression tag	UNP Q8NI27
b	-17	HIS	-	expression tag	UNP Q8NI27
b	-16	HIS	-	expression tag	UNP Q8NI27
b	-15	HIS	-	expression tag	UNP Q8NI27
b	-14	HIS	-	expression tag	UNP Q8NI27
b	-13	HIS	-	expression tag	UNP Q8NI27
b	-12	HIS	-	expression tag	UNP Q8NI27
b	-11	HIS	-	expression tag	UNP Q8NI27
b	-10	SER	-	expression tag	UNP Q8NI27
b	-9	ALA	-	expression tag	UNP Q8NI27
b	-8	GLY	-	expression tag	UNP Q8NI27
b	-7	LEU	-	expression tag	UNP Q8NI27
b	-6	GLU	-	expression tag	UNP Q8NI27
b	-5	VAL	-	expression tag	UNP Q8NI27
b	-4	LEU	-	expression tag	UNP Q8NI27
b	-3	PHE	-	expression tag	UNP Q8NI27
b	-2	GLN	-	expression tag	UNP Q8NI27
b	-1	GLY	-	expression tag	UNP Q8NI27
b	0	PRO	-	expression tag	UNP Q8NI27
j	-22	MET	-	initiating methionine	UNP Q8NI27
j	-21	LYS	-	expression tag	UNP Q8NI27
j	-20	HIS	-	expression tag	UNP Q8NI27
j	-19	HIS	-	expression tag	UNP Q8NI27
j	-18	HIS	-	expression tag	UNP Q8NI27
j	-17	HIS	-	expression tag	UNP Q8NI27
j	-16	HIS	-	expression tag	UNP Q8NI27
j	-15	HIS	-	expression tag	UNP Q8NI27
j	-14	HIS	-	expression tag	UNP Q8NI27
j	-13	HIS	-	expression tag	UNP Q8NI27
j	-12	HIS	-	expression tag	UNP Q8NI27
j	-11	HIS	-	expression tag	UNP Q8NI27
j	-10	SER	-	expression tag	UNP Q8NI27
j	-9	ALA	-	expression tag	UNP Q8NI27
j	-8	GLY	-	expression tag	UNP Q8NI27

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Chain	Residue	Modelled	Actual	Comment	Reference
j	-7	LEU	-	expression tag	UNP Q8NI27
j	-6	GLU	-	expression tag	UNP Q8NI27
j	-5	VAL	-	expression tag	UNP Q8NI27
j	-4	LEU	-	expression tag	UNP Q8NI27
j	-3	PHE	-	expression tag	UNP Q8NI27
j	-2	GLN	-	expression tag	UNP Q8NI27
j	-1	GLY	-	expression tag	UNP Q8NI27
j	0	PRO	-	expression tag	UNP Q8NI27

- Molecule 3 is a protein called THO complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	304	Total 2349	C 1482	N 407	O 446	S 14	0	0
3	K	304	Total 2349	C 1482	N 407	O 446	S 14	0	0
3	c	304	Total 2349	C 1482	N 407	O 446	S 14	0	0
3	k	304	Total 2349	C 1482	N 407	O 446	S 14	0	0

There are 176 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-43	MET	-	initiating methionine	UNP Q96J01
C	-42	LYS	-	expression tag	UNP Q96J01
C	-41	GLY	-	expression tag	UNP Q96J01
C	-40	SER	-	expression tag	UNP Q96J01
C	-39	ALA	-	expression tag	UNP Q96J01
C	-38	TRP	-	expression tag	UNP Q96J01
C	-37	SER	-	expression tag	UNP Q96J01
C	-36	HIS	-	expression tag	UNP Q96J01
C	-35	PRO	-	expression tag	UNP Q96J01
C	-34	GLN	-	expression tag	UNP Q96J01
C	-33	PHE	-	expression tag	UNP Q96J01
C	-32	GLU	-	expression tag	UNP Q96J01
C	-31	LYS	-	expression tag	UNP Q96J01
C	-30	GLY	-	expression tag	UNP Q96J01
C	-29	GLY	-	expression tag	UNP Q96J01
C	-28	GLY	-	expression tag	UNP Q96J01
C	-27	SER	-	expression tag	UNP Q96J01
C	-26	GLY	-	expression tag	UNP Q96J01

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-25	GLY	-	expression tag	UNP Q96J01
C	-24	GLY	-	expression tag	UNP Q96J01
C	-23	SER	-	expression tag	UNP Q96J01
C	-22	GLY	-	expression tag	UNP Q96J01
C	-21	GLY	-	expression tag	UNP Q96J01
C	-20	SER	-	expression tag	UNP Q96J01
C	-19	ALA	-	expression tag	UNP Q96J01
C	-18	TRP	-	expression tag	UNP Q96J01
C	-17	SER	-	expression tag	UNP Q96J01
C	-16	HIS	-	expression tag	UNP Q96J01
C	-15	PRO	-	expression tag	UNP Q96J01
C	-14	GLN	-	expression tag	UNP Q96J01
C	-13	PHE	-	expression tag	UNP Q96J01
C	-12	GLU	-	expression tag	UNP Q96J01
C	-11	LYS	-	expression tag	UNP Q96J01
C	-10	THR	-	expression tag	UNP Q96J01
C	-9	ALA	-	expression tag	UNP Q96J01
C	-8	GLY	-	expression tag	UNP Q96J01
C	-7	LEU	-	expression tag	UNP Q96J01
C	-6	GLU	-	expression tag	UNP Q96J01
C	-5	VAL	-	expression tag	UNP Q96J01
C	-4	LEU	-	expression tag	UNP Q96J01
C	-3	PHE	-	expression tag	UNP Q96J01
C	-2	GLN	-	expression tag	UNP Q96J01
C	-1	GLY	-	expression tag	UNP Q96J01
C	0	PRO	-	expression tag	UNP Q96J01
K	-43	MET	-	initiating methionine	UNP Q96J01
K	-42	LYS	-	expression tag	UNP Q96J01
K	-41	GLY	-	expression tag	UNP Q96J01
K	-40	SER	-	expression tag	UNP Q96J01
K	-39	ALA	-	expression tag	UNP Q96J01
K	-38	TRP	-	expression tag	UNP Q96J01
K	-37	SER	-	expression tag	UNP Q96J01
K	-36	HIS	-	expression tag	UNP Q96J01
K	-35	PRO	-	expression tag	UNP Q96J01
K	-34	GLN	-	expression tag	UNP Q96J01
K	-33	PHE	-	expression tag	UNP Q96J01
K	-32	GLU	-	expression tag	UNP Q96J01
K	-31	LYS	-	expression tag	UNP Q96J01
K	-30	GLY	-	expression tag	UNP Q96J01
K	-29	GLY	-	expression tag	UNP Q96J01
K	-28	GLY	-	expression tag	UNP Q96J01

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-27	SER	-	expression tag	UNP Q96J01
K	-26	GLY	-	expression tag	UNP Q96J01
K	-25	GLY	-	expression tag	UNP Q96J01
K	-24	GLY	-	expression tag	UNP Q96J01
K	-23	SER	-	expression tag	UNP Q96J01
K	-22	GLY	-	expression tag	UNP Q96J01
K	-21	GLY	-	expression tag	UNP Q96J01
K	-20	SER	-	expression tag	UNP Q96J01
K	-19	ALA	-	expression tag	UNP Q96J01
K	-18	TRP	-	expression tag	UNP Q96J01
K	-17	SER	-	expression tag	UNP Q96J01
K	-16	HIS	-	expression tag	UNP Q96J01
K	-15	PRO	-	expression tag	UNP Q96J01
K	-14	GLN	-	expression tag	UNP Q96J01
K	-13	PHE	-	expression tag	UNP Q96J01
K	-12	GLU	-	expression tag	UNP Q96J01
K	-11	LYS	-	expression tag	UNP Q96J01
K	-10	THR	-	expression tag	UNP Q96J01
K	-9	ALA	-	expression tag	UNP Q96J01
K	-8	GLY	-	expression tag	UNP Q96J01
K	-7	LEU	-	expression tag	UNP Q96J01
K	-6	GLU	-	expression tag	UNP Q96J01
K	-5	VAL	-	expression tag	UNP Q96J01
K	-4	LEU	-	expression tag	UNP Q96J01
K	-3	PHE	-	expression tag	UNP Q96J01
K	-2	GLN	-	expression tag	UNP Q96J01
K	-1	GLY	-	expression tag	UNP Q96J01
K	0	PRO	-	expression tag	UNP Q96J01
c	-43	MET	-	initiating methionine	UNP Q96J01
c	-42	LYS	-	expression tag	UNP Q96J01
c	-41	GLY	-	expression tag	UNP Q96J01
c	-40	SER	-	expression tag	UNP Q96J01
c	-39	ALA	-	expression tag	UNP Q96J01
c	-38	TRP	-	expression tag	UNP Q96J01
c	-37	SER	-	expression tag	UNP Q96J01
c	-36	HIS	-	expression tag	UNP Q96J01
c	-35	PRO	-	expression tag	UNP Q96J01
c	-34	GLN	-	expression tag	UNP Q96J01
c	-33	PHE	-	expression tag	UNP Q96J01
c	-32	GLU	-	expression tag	UNP Q96J01
c	-31	LYS	-	expression tag	UNP Q96J01
c	-30	GLY	-	expression tag	UNP Q96J01

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Chain	Residue	Modelled	Actual	Comment	Reference
c	-29	GLY	-	expression tag	UNP Q96J01
c	-28	GLY	-	expression tag	UNP Q96J01
c	-27	SER	-	expression tag	UNP Q96J01
c	-26	GLY	-	expression tag	UNP Q96J01
c	-25	GLY	-	expression tag	UNP Q96J01
c	-24	GLY	-	expression tag	UNP Q96J01
c	-23	SER	-	expression tag	UNP Q96J01
c	-22	GLY	-	expression tag	UNP Q96J01
c	-21	GLY	-	expression tag	UNP Q96J01
c	-20	SER	-	expression tag	UNP Q96J01
c	-19	ALA	-	expression tag	UNP Q96J01
c	-18	TRP	-	expression tag	UNP Q96J01
c	-17	SER	-	expression tag	UNP Q96J01
c	-16	HIS	-	expression tag	UNP Q96J01
c	-15	PRO	-	expression tag	UNP Q96J01
c	-14	GLN	-	expression tag	UNP Q96J01
c	-13	PHE	-	expression tag	UNP Q96J01
c	-12	GLU	-	expression tag	UNP Q96J01
c	-11	LYS	-	expression tag	UNP Q96J01
c	-10	THR	-	expression tag	UNP Q96J01
c	-9	ALA	-	expression tag	UNP Q96J01
c	-8	GLY	-	expression tag	UNP Q96J01
c	-7	LEU	-	expression tag	UNP Q96J01
c	-6	GLU	-	expression tag	UNP Q96J01
c	-5	VAL	-	expression tag	UNP Q96J01
c	-4	LEU	-	expression tag	UNP Q96J01
c	-3	PHE	-	expression tag	UNP Q96J01
c	-2	GLN	-	expression tag	UNP Q96J01
c	-1	GLY	-	expression tag	UNP Q96J01
c	0	PRO	-	expression tag	UNP Q96J01
k	-43	MET	-	initiating methionine	UNP Q96J01
k	-42	LYS	-	expression tag	UNP Q96J01
k	-41	GLY	-	expression tag	UNP Q96J01
k	-40	SER	-	expression tag	UNP Q96J01
k	-39	ALA	-	expression tag	UNP Q96J01
k	-38	TRP	-	expression tag	UNP Q96J01
k	-37	SER	-	expression tag	UNP Q96J01
k	-36	HIS	-	expression tag	UNP Q96J01
k	-35	PRO	-	expression tag	UNP Q96J01
k	-34	GLN	-	expression tag	UNP Q96J01
k	-33	PHE	-	expression tag	UNP Q96J01
k	-32	GLU	-	expression tag	UNP Q96J01

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Chain	Residue	Modelled	Actual	Comment	Reference
k	-31	LYS	-	expression tag	UNP Q96J01
k	-30	GLY	-	expression tag	UNP Q96J01
k	-29	GLY	-	expression tag	UNP Q96J01
k	-28	GLY	-	expression tag	UNP Q96J01
k	-27	SER	-	expression tag	UNP Q96J01
k	-26	GLY	-	expression tag	UNP Q96J01
k	-25	GLY	-	expression tag	UNP Q96J01
k	-24	GLY	-	expression tag	UNP Q96J01
k	-23	SER	-	expression tag	UNP Q96J01
k	-22	GLY	-	expression tag	UNP Q96J01
k	-21	GLY	-	expression tag	UNP Q96J01
k	-20	SER	-	expression tag	UNP Q96J01
k	-19	ALA	-	expression tag	UNP Q96J01
k	-18	TRP	-	expression tag	UNP Q96J01
k	-17	SER	-	expression tag	UNP Q96J01
k	-16	HIS	-	expression tag	UNP Q96J01
k	-15	PRO	-	expression tag	UNP Q96J01
k	-14	GLN	-	expression tag	UNP Q96J01
k	-13	PHE	-	expression tag	UNP Q96J01
k	-12	GLU	-	expression tag	UNP Q96J01
k	-11	LYS	-	expression tag	UNP Q96J01
k	-10	THR	-	expression tag	UNP Q96J01
k	-9	ALA	-	expression tag	UNP Q96J01
k	-8	GLY	-	expression tag	UNP Q96J01
k	-7	LEU	-	expression tag	UNP Q96J01
k	-6	GLU	-	expression tag	UNP Q96J01
k	-5	VAL	-	expression tag	UNP Q96J01
k	-4	LEU	-	expression tag	UNP Q96J01
k	-3	PHE	-	expression tag	UNP Q96J01
k	-2	GLN	-	expression tag	UNP Q96J01
k	-1	GLY	-	expression tag	UNP Q96J01
k	0	PRO	-	expression tag	UNP Q96J01

- Molecule 4 is a protein called THO complex subunit 5 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	523	Total 3687	C 2337	N 648	O 681	S 21	0	0
4	M	549	Total 4216	C 2689	N 734	O 768	S 25	0	0
4	e	512	Total 3598	C 2281	N 634	O 664	S 19	0	0

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Mol	Chain	Residues	Atoms	AltConf	Trace
4	m	549	Total C N O S 4216 2689 734 768 25	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	525	ILE	VAL	conflict	UNP Q13769
E	579	ILE	VAL	conflict	UNP Q13769
M	525	ILE	VAL	conflict	UNP Q13769
M	579	ILE	VAL	conflict	UNP Q13769
e	525	ILE	VAL	conflict	UNP Q13769
e	579	ILE	VAL	conflict	UNP Q13769
m	525	ILE	VAL	conflict	UNP Q13769
m	579	ILE	VAL	conflict	UNP Q13769

- Molecule 5 is a protein called THO complex subunit 6 homolog.

Mol	Chain	Residues	Atoms	AltConf	Trace
5	F	337	Total C N O S 2604 1647 459 483 15	0	0
5	N	337	Total C N O S 2604 1647 459 483 15	0	0
5	f	329	Total C N O S 2537 1604 448 470 15	0	0
5	n	337	Total C N O S 2604 1647 459 483 15	0	0

- Molecule 6 is a protein called THO complex subunit 7 homolog.

Mol	Chain	Residues	Atoms	AltConf	Trace
6	G	153	Total C N O 760 454 153 153	0	0
6	O	155	Total C N O S 1084 669 201 207 7	0	0
6	g	153	Total C N O 760 454 153 153	0	0
6	o	155	Total C N O S 1084 669 201 207 7	0	0

- Molecule 7 is a protein called Spliceosome RNA helicase DDX39B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	H	170	1398	888	245	261	4	0	0
7	P	170	1398	888	245	261	4	0	0
7	h	170	1398	888	245	261	4	0	0
7	p	170	1398	888	245	261	4	0	0

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-22	GLY	-	expression tag	UNP Q13838
H	-21	PRO	-	expression tag	UNP Q13838
H	-20	MET	-	expression tag	UNP Q13838
H	-19	LYS	-	expression tag	UNP Q13838
H	-18	GLY	-	expression tag	UNP Q13838
H	-17	SER	-	expression tag	UNP Q13838
H	-16	ALA	-	expression tag	UNP Q13838
H	-15	TRP	-	expression tag	UNP Q13838
H	-14	SER	-	expression tag	UNP Q13838
H	-13	HIS	-	expression tag	UNP Q13838
H	-12	PRO	-	expression tag	UNP Q13838
H	-11	GLN	-	expression tag	UNP Q13838
H	-10	PHE	-	expression tag	UNP Q13838
H	-9	GLU	-	expression tag	UNP Q13838
H	-8	LYS	-	expression tag	UNP Q13838
H	-7	LEU	-	expression tag	UNP Q13838
H	-6	GLU	-	expression tag	UNP Q13838
H	-5	VAL	-	expression tag	UNP Q13838
H	-4	LEU	-	expression tag	UNP Q13838
H	-3	PHE	-	expression tag	UNP Q13838
H	-2	GLN	-	expression tag	UNP Q13838
H	-1	GLY	-	expression tag	UNP Q13838
H	0	PRO	-	expression tag	UNP Q13838
P	-22	GLY	-	expression tag	UNP Q13838
P	-21	PRO	-	expression tag	UNP Q13838
P	-20	MET	-	expression tag	UNP Q13838
P	-19	LYS	-	expression tag	UNP Q13838
P	-18	GLY	-	expression tag	UNP Q13838
P	-17	SER	-	expression tag	UNP Q13838
P	-16	ALA	-	expression tag	UNP Q13838
P	-15	TRP	-	expression tag	UNP Q13838

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Chain	Residue	Modelled	Actual	Comment	Reference
P	-14	SER	-	expression tag	UNP Q13838
P	-13	HIS	-	expression tag	UNP Q13838
P	-12	PRO	-	expression tag	UNP Q13838
P	-11	GLN	-	expression tag	UNP Q13838
P	-10	PHE	-	expression tag	UNP Q13838
P	-9	GLU	-	expression tag	UNP Q13838
P	-8	LYS	-	expression tag	UNP Q13838
P	-7	LEU	-	expression tag	UNP Q13838
P	-6	GLU	-	expression tag	UNP Q13838
P	-5	VAL	-	expression tag	UNP Q13838
P	-4	LEU	-	expression tag	UNP Q13838
P	-3	PHE	-	expression tag	UNP Q13838
P	-2	GLN	-	expression tag	UNP Q13838
P	-1	GLY	-	expression tag	UNP Q13838
P	0	PRO	-	expression tag	UNP Q13838
h	-22	GLY	-	expression tag	UNP Q13838
h	-21	PRO	-	expression tag	UNP Q13838
h	-20	MET	-	expression tag	UNP Q13838
h	-19	LYS	-	expression tag	UNP Q13838
h	-18	GLY	-	expression tag	UNP Q13838
h	-17	SER	-	expression tag	UNP Q13838
h	-16	ALA	-	expression tag	UNP Q13838
h	-15	TRP	-	expression tag	UNP Q13838
h	-14	SER	-	expression tag	UNP Q13838
h	-13	HIS	-	expression tag	UNP Q13838
h	-12	PRO	-	expression tag	UNP Q13838
h	-11	GLN	-	expression tag	UNP Q13838
h	-10	PHE	-	expression tag	UNP Q13838
h	-9	GLU	-	expression tag	UNP Q13838
h	-8	LYS	-	expression tag	UNP Q13838
h	-7	LEU	-	expression tag	UNP Q13838
h	-6	GLU	-	expression tag	UNP Q13838
h	-5	VAL	-	expression tag	UNP Q13838
h	-4	LEU	-	expression tag	UNP Q13838
h	-3	PHE	-	expression tag	UNP Q13838
h	-2	GLN	-	expression tag	UNP Q13838
h	-1	GLY	-	expression tag	UNP Q13838
h	0	PRO	-	expression tag	UNP Q13838
p	-22	GLY	-	expression tag	UNP Q13838
p	-21	PRO	-	expression tag	UNP Q13838
p	-20	MET	-	expression tag	UNP Q13838
p	-19	LYS	-	expression tag	UNP Q13838

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Chain	Residue	Modelled	Actual	Comment	Reference
p	-18	GLY	-	expression tag	UNP Q13838
p	-17	SER	-	expression tag	UNP Q13838
p	-16	ALA	-	expression tag	UNP Q13838
p	-15	TRP	-	expression tag	UNP Q13838
p	-14	SER	-	expression tag	UNP Q13838
p	-13	HIS	-	expression tag	UNP Q13838
p	-12	PRO	-	expression tag	UNP Q13838
p	-11	GLN	-	expression tag	UNP Q13838
p	-10	PHE	-	expression tag	UNP Q13838
p	-9	GLU	-	expression tag	UNP Q13838
p	-8	LYS	-	expression tag	UNP Q13838
p	-7	LEU	-	expression tag	UNP Q13838
p	-6	GLU	-	expression tag	UNP Q13838
p	-5	VAL	-	expression tag	UNP Q13838
p	-4	LEU	-	expression tag	UNP Q13838
p	-3	PHE	-	expression tag	UNP Q13838
p	-2	GLN	-	expression tag	UNP Q13838
p	-1	GLY	-	expression tag	UNP Q13838
p	0	PRO	-	expression tag	UNP Q13838

- Molecule 8 is a protein called THOC2 anchor (putative).

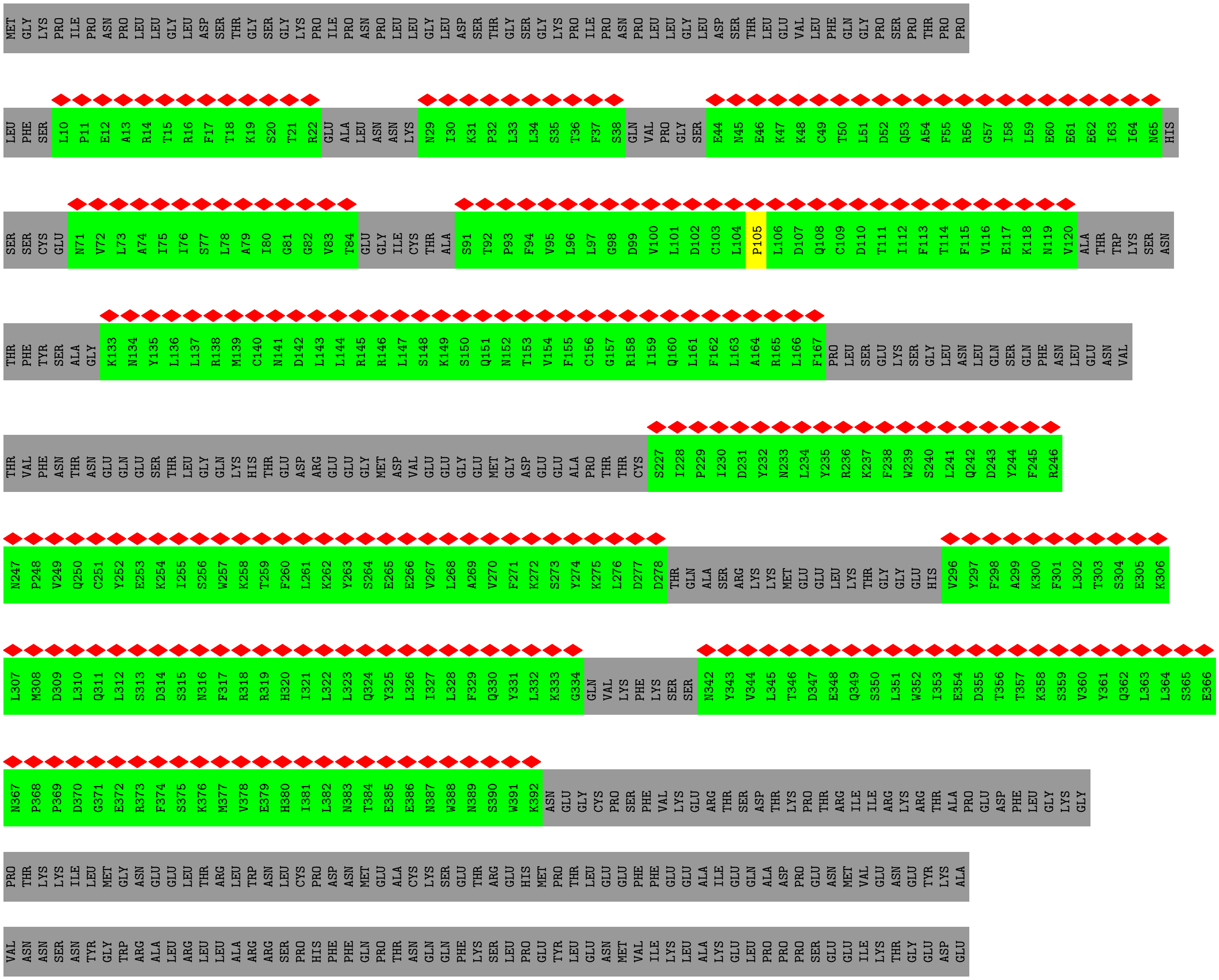
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	X	37	185	111	37	37	0	0
			Total	C	N	O		
8	x	37	185	111	37	37	0	0

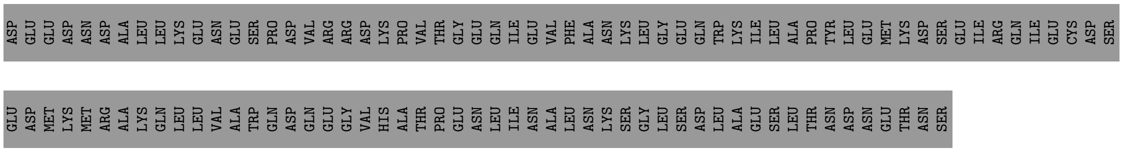
3 Residue-property plots (i)

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: THO complex subunit 1

Chain A:



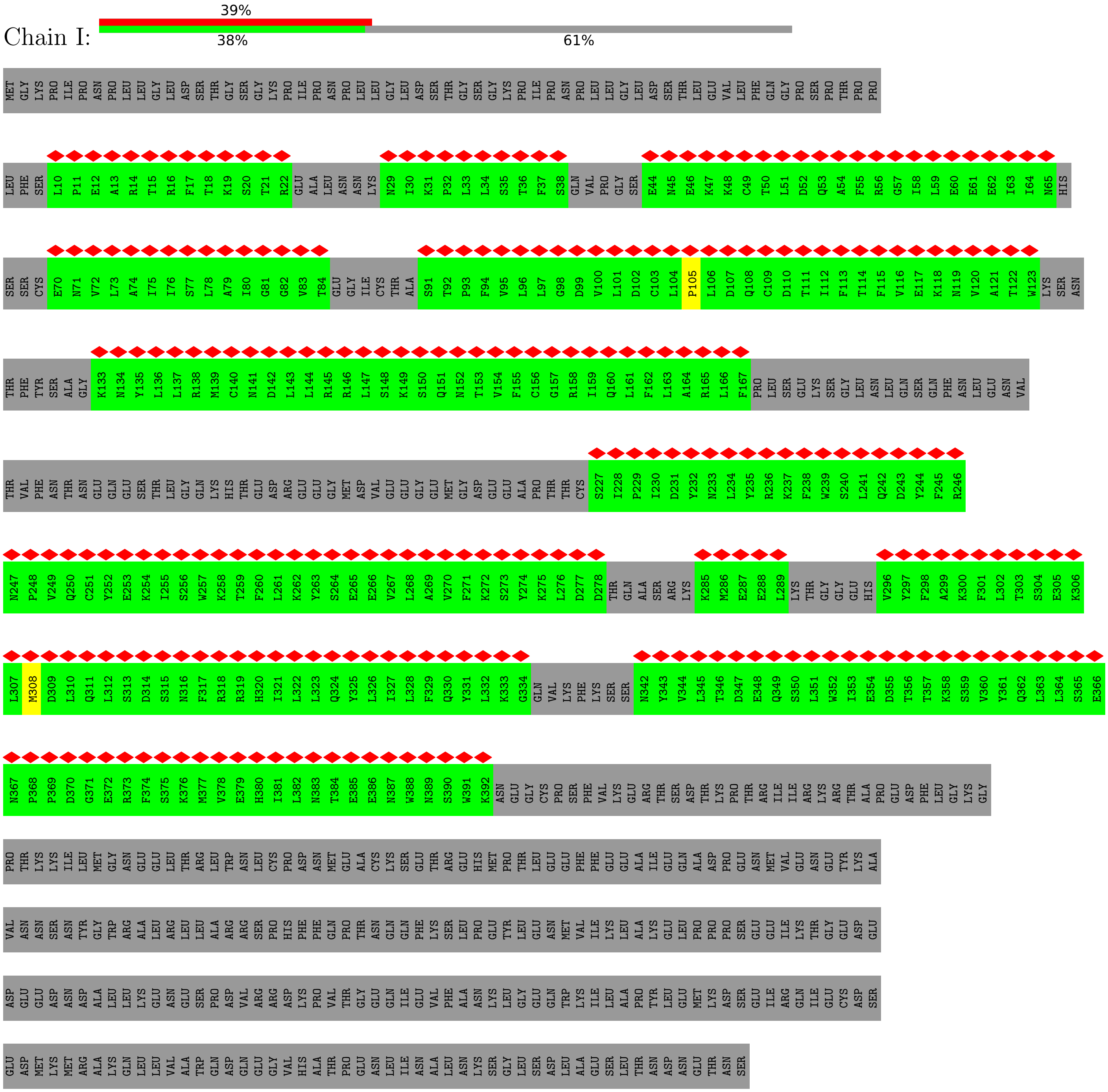


ASP GLU GLU ASP ASN ASP ALA LEU LEU LYS GLU ASN GLU SER PRO ASP VAL ARG ARG ASP LYS PRO VAL THR GLY GLU GLN ILE GLU VAL PHE ALA ASN LYS LEU GLY GLU GLN TRP LYS ILE LEU ALA PRO TYR LEU GLU MET LYS ASP SER GLU ILE ARG GLN ILE GLU CYS ASP SER

GLU ASP MET LYS MET ARG ALA LYS GLN LEU LEU VAL ALA TRP GLN ASP GLN GLU GLY VAL HIS ALA THR PRO GLU ASN LEU ILE ASN ALA LEU ASN LYS SER GLY LEU SER ASP LEU ALA GLU SER LEU THR ASN ASP ASN GLU THR ASN SER

- Molecule 1: THO complex subunit 1

Chain I:



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LEU PHE SER L10 P11 E12 A13 R14 T15 R16 F17 T18 K19 S20 T21 R22 GLU ALA LEU ASN ASN LYS N29 I30 K31 P32 L33 L34 S35 T36 F37 S38 GLN VAL PRO GLY SER E44 N45 E46 K47 K48 C49 T50 L51 D52 Q53 A54 F55 R56 G57 I58 L59 E60 E61 E62 I63 I64 N65 HIS

SER SER CYS E70 N71 V72 L73 A74 I75 I76 S77 L78 A79 I80 G81 G82 V83 T84 GLU GLY ILE CYS THR ALA S91 T92 P93 F94 V95 L96 L97 G98 D99 V100 L101 D102 C103 L104 P105 L106 D107 Q108 C109 D110 T111 I112 F113 T114 F115 V116 E117 K118 N119 V120 A121 T122 W123 LYS SER ASN

THR PHE TYR SER ALA GLY K133 N134 Y135 L136 L137 R138 M139 C140 N141 D142 L143 L144 R145 R146 L147 S148 K149 S150 Q151 N152 T153 V154 F155 C156 G157 R158 I159 Q160 L161 F162 L163 A164 R165 L166 F167 PRO LEU SER GLU LYS SER GLY LEU ASN LEU GLN SER GLN PHE ASN LEU GLU ASN VAL

THR VAL PHE ASN THR ASN GLU GLN GLU SER THR LEU GLY GLN LYS HIS THR GLU ASP ARG GLU GLU GLY MET ASP VAL GLU GLU GLY GLU MET GLY ASP GLU GLU ALA PRO THR THR CYS S227 I228 P229 I230 D231 Y232 N233 L234 Y235 R236 K237 F238 W239 S240 L241 Q242 D243 Y244 F245 R246

N247 P248 V249 Q250 C251 Y252 E253 K254 I255 S256 W257 K258 T259 F260 L261 K262 Y263 S264 E265 E266 V267 L268 A269 V270 F271 K272 S273 Y274 K275 L276 D277 D278 THR GLN ALA SER ARG LYS K285 M286 E287 E288 L289 LYS THR GLY GLY GLU HIS V296 Y297 F298 A299 K300 F301 L302 T303 S304 E305 K306

L307 M308 D309 L310 Q311 L312 S313 D314 S315 N316 F317 R318 R319 H320 I321 L322 L323 Q324 Y325 L326 I327 L328 F329 Q330 Y331 L332 K333 G334 GLN VAL LYS PHE LYS SER SER N342 Y343 V344 L345 T346 D347 E348 Q349 S350 L351 W352 I353 E354 D355 T356 T357 K358 S359 V360 Y361 Q362 L363 L364 S365 E366

N367 P368 P369 D370 G371 E372 R373 F374 S375 K376 M377 V378 E379 H380 I381 L382 N383 T384 E385 E386 N387 W388 N389 S390 W391 K392 ASN GLU GLY CYS PRO SER PHE VAL LYS GLU ARG THR SER ASP THR LYS PRO THR ARG ILE ILE ARG LYS ARG THR ALA PRO GLU ASP PHE LEU GLY LYS GLY

PRO THR LYS LYS ILE LEU MET GLY ASN GLU GLU LEU THR ARG LEU TRP ASN LEU CYS PRO ASP ASN MET GLU ALA CYS LYS SER GLU THR ARG GLU HIS MET PRO THR LEU GLU GLU PHE PHE GLU GLU ALA ILE GLU GLN ALA ASP PRO GLU ASN MET VAL GLU ASN GLU TYR LYS ALA

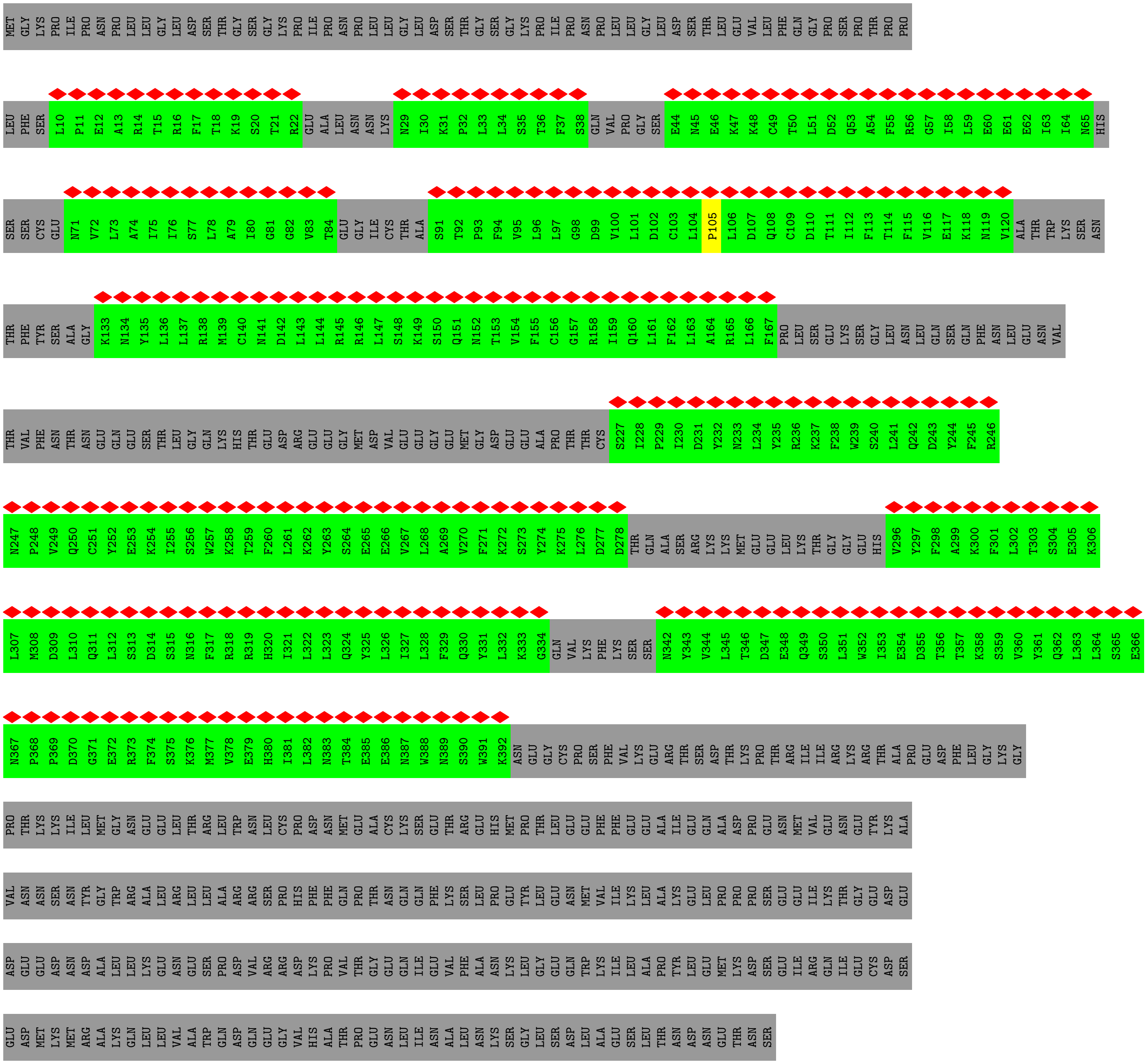
VAL ASN ASN SER ASN TYR GLY TRP ARG ALA LEU ARG LEU LEU ALA ARG ARG SER PRO HIS PHE PHE GLN PRO THR ASN GLN GLN PHE LYS SER LEU PRO GLU TYR LEU GLU ASN MET VAL ILE LYS LEU ALA LYS GLU LEU PRO PRO PRO SER GLU GLU ILE LYS THR GLY GLU ASP GLU

ASP GLU GLU ASP ASN ASP ALA LEU LEU LYS GLU ASN GLU SER PRO ASP VAL ARG ARG ASP LYS PRO VAL THR GLY GLU GLN ILE GLU VAL PHE ALA ASN LYS LEU GLY GLU GLN TRP LYS ILE LEU ALA PRO TYR LEU GLU MET LYS ASP SER GLU ILE ARG GLN ILE GLU CYS ASP SER

GLU ASP MET LYS MET ARG ALA LYS GLN LEU LEU VAL ALA TRP GLN ASP GLN GLU GLY VAL HIS ALA THR PRO GLU ASN LEU ILE ASN ALA LEU ASN LYS SER GLY LEU SER ASP LEU ALA GLU SER LEU THR ASN ASP ASN GLU THR ASN SER

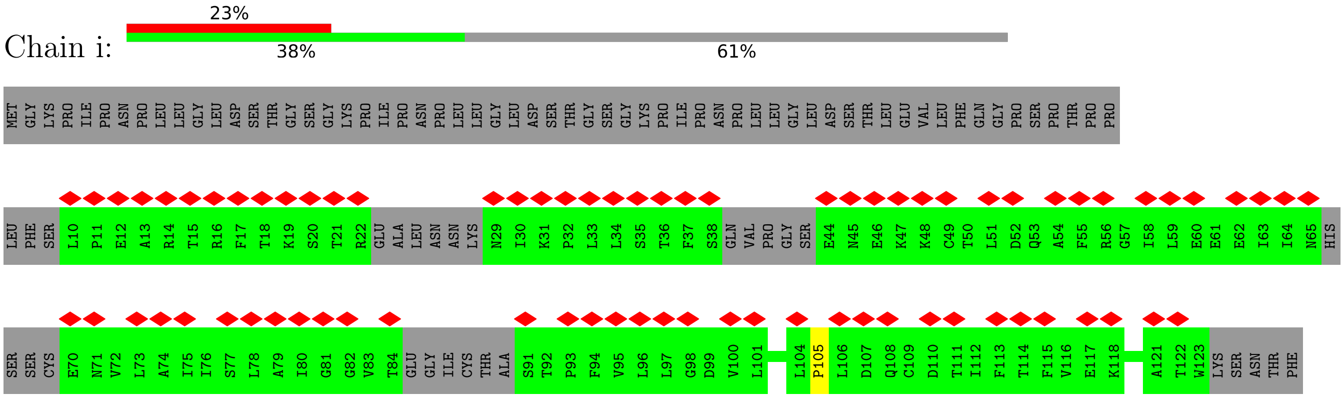
- Molecule 1: THO complex subunit 1

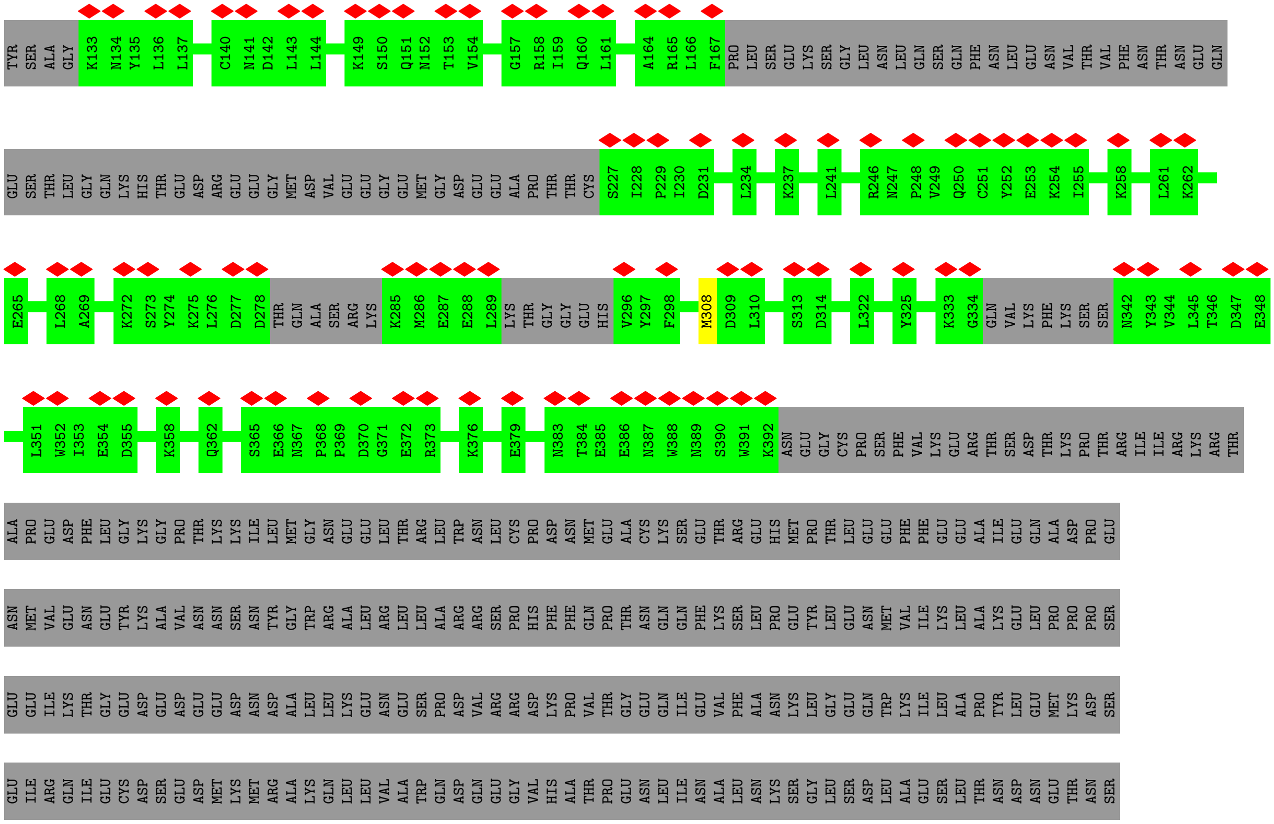
Chain a:



- Molecule 1: THO complex subunit 1

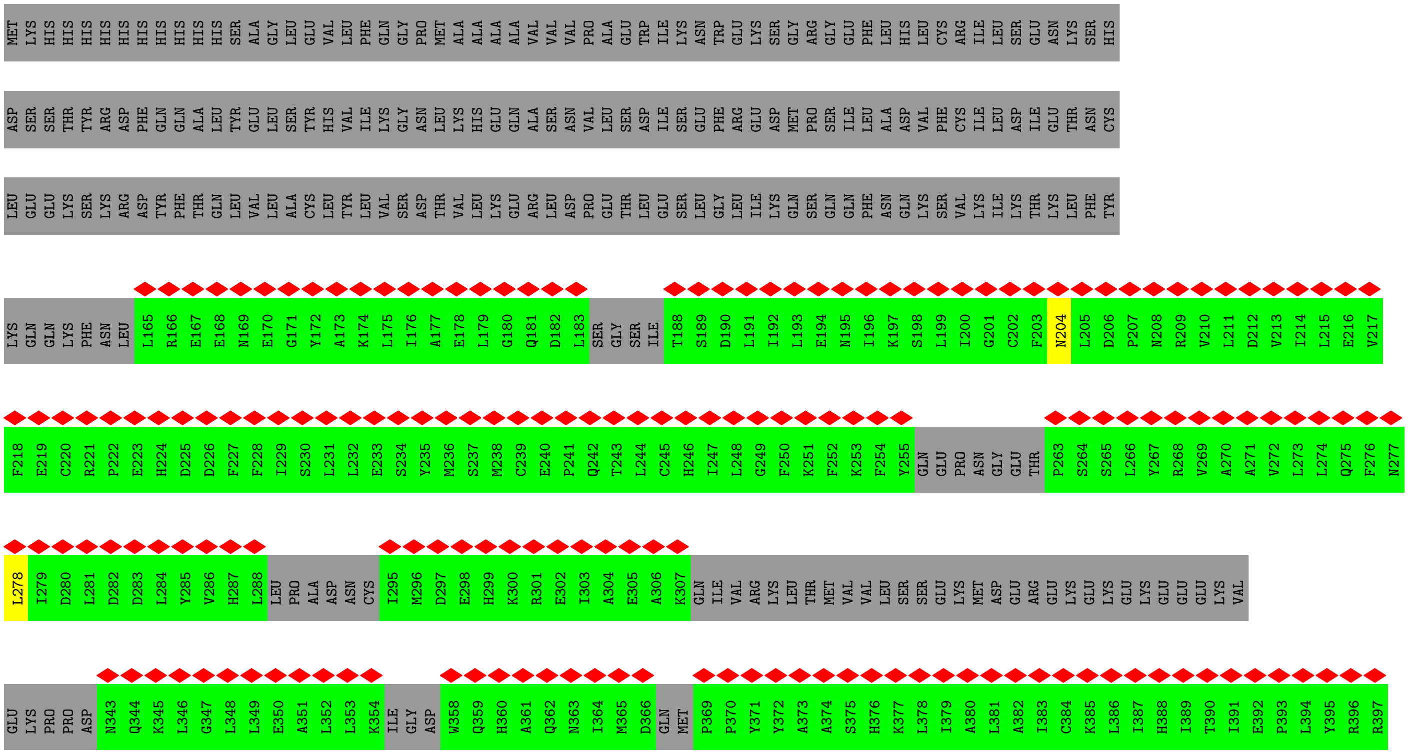
Chain i:

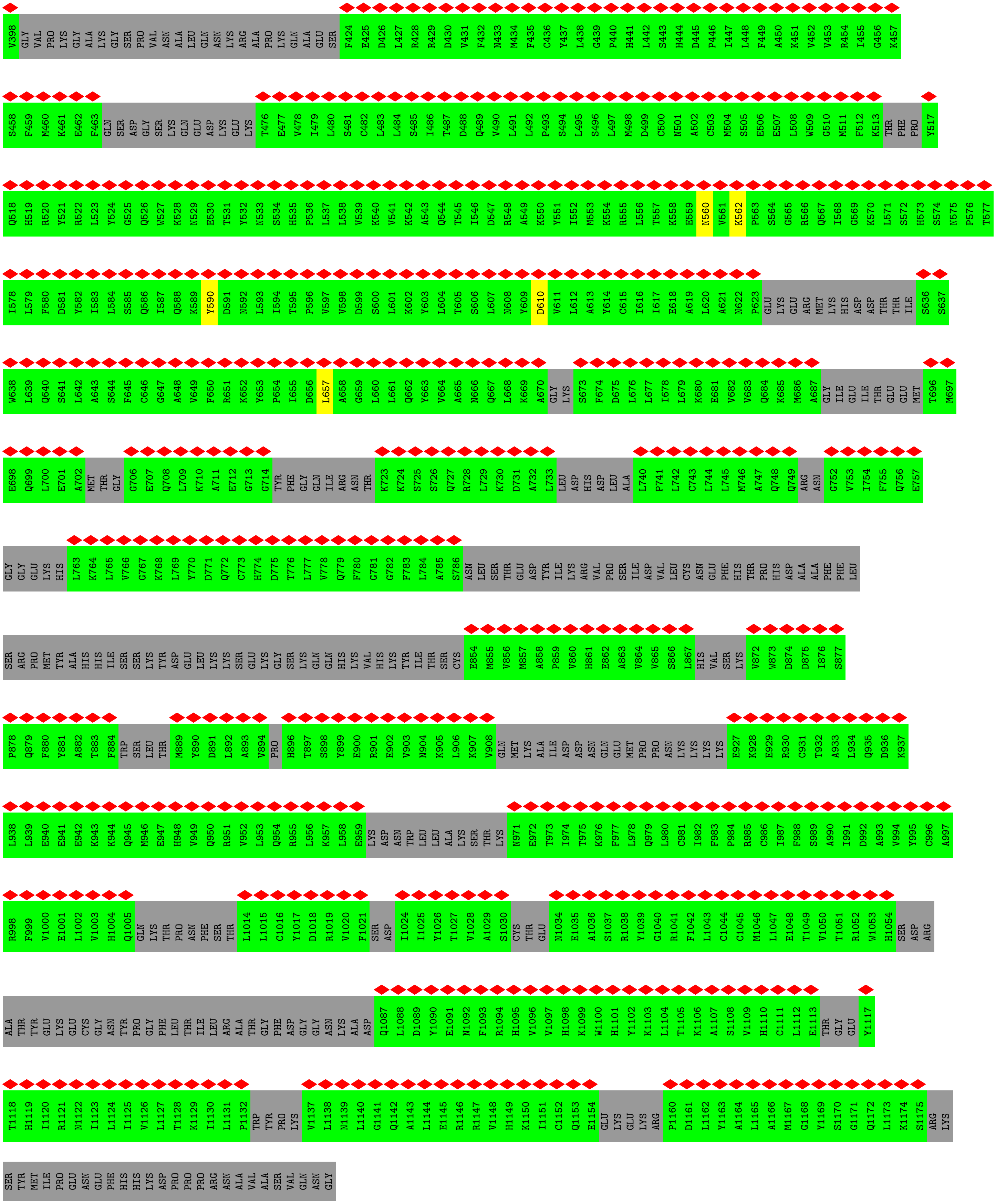




- Molecule 2: THO complex subunit 2

Chain B:

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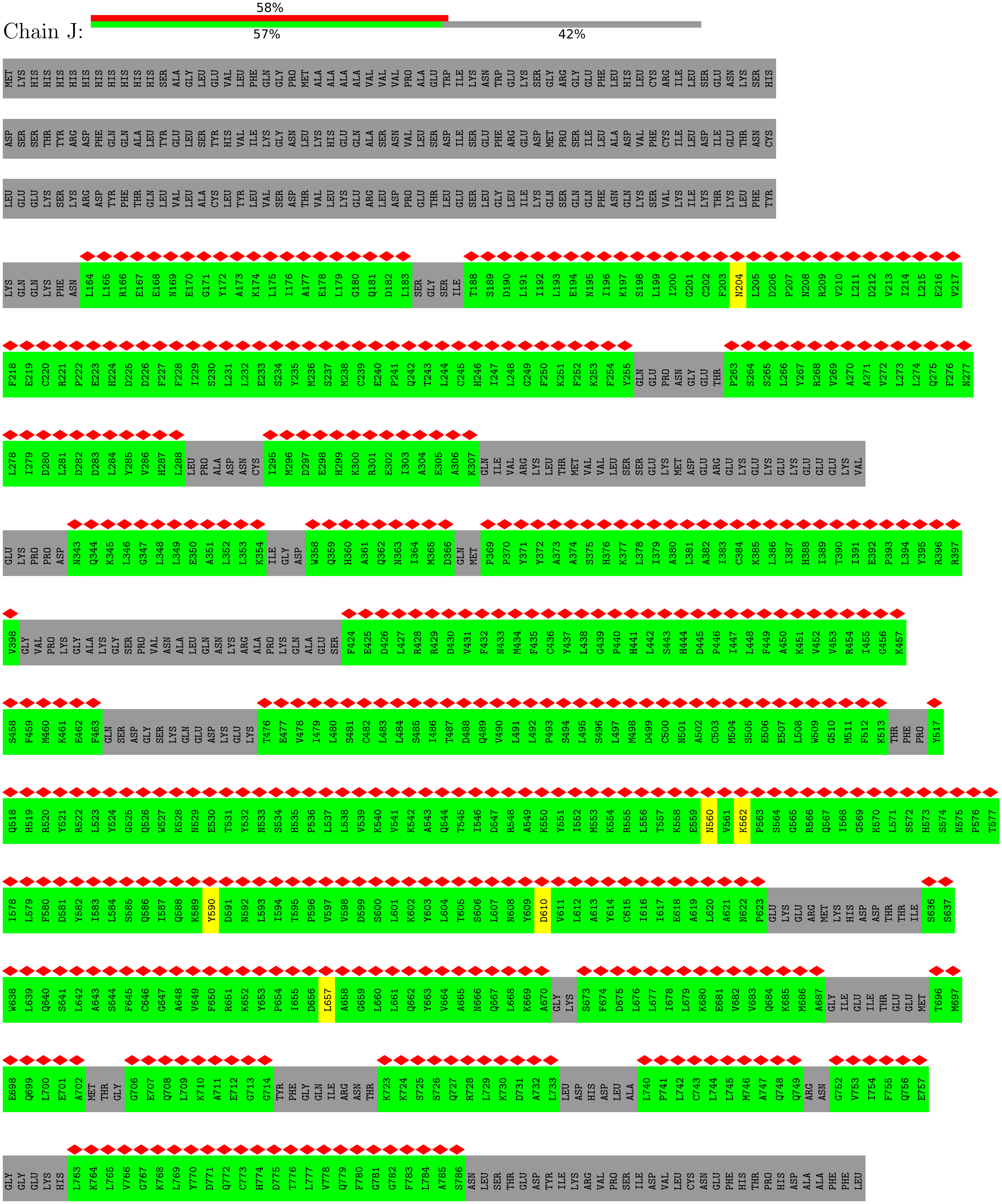
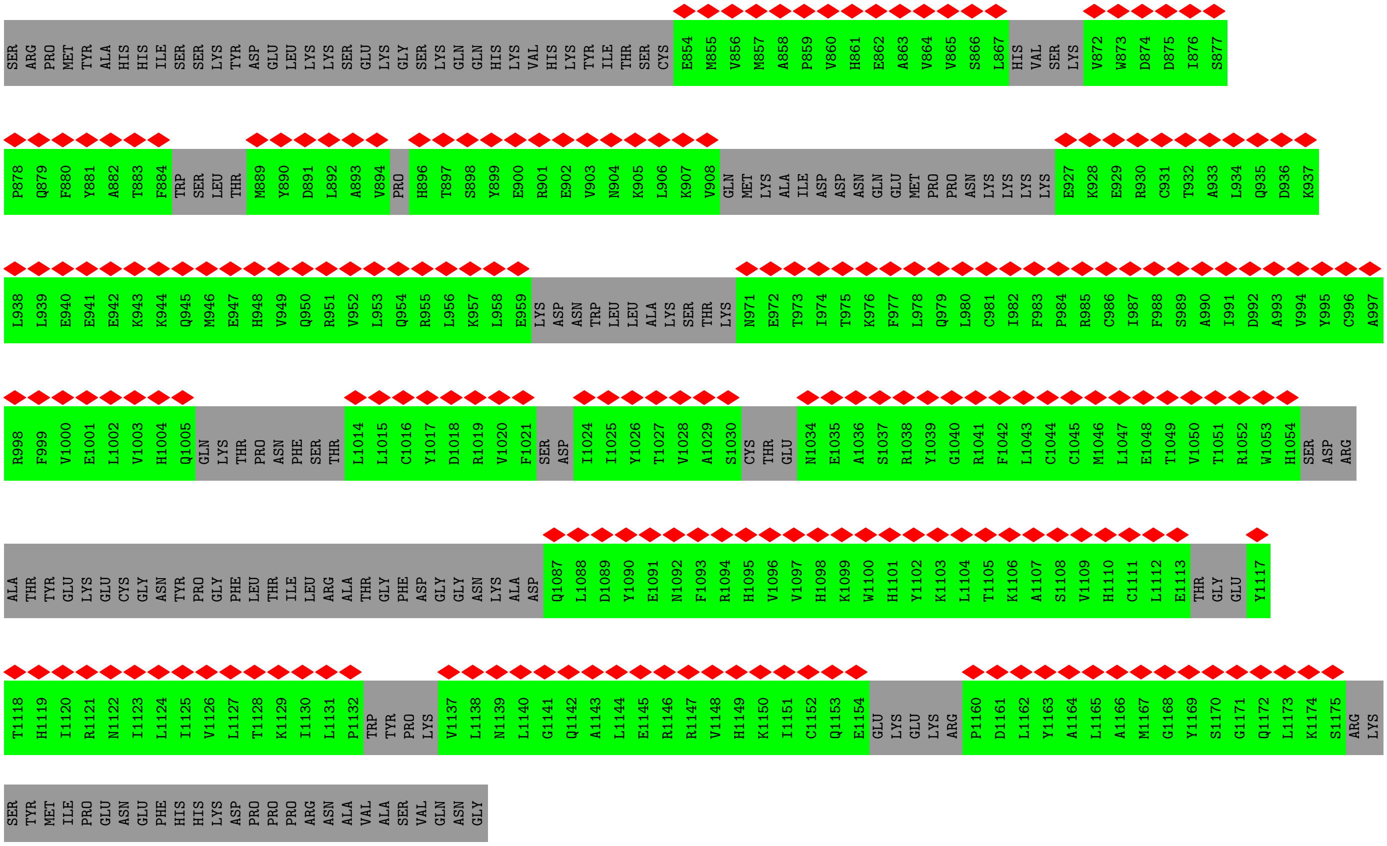
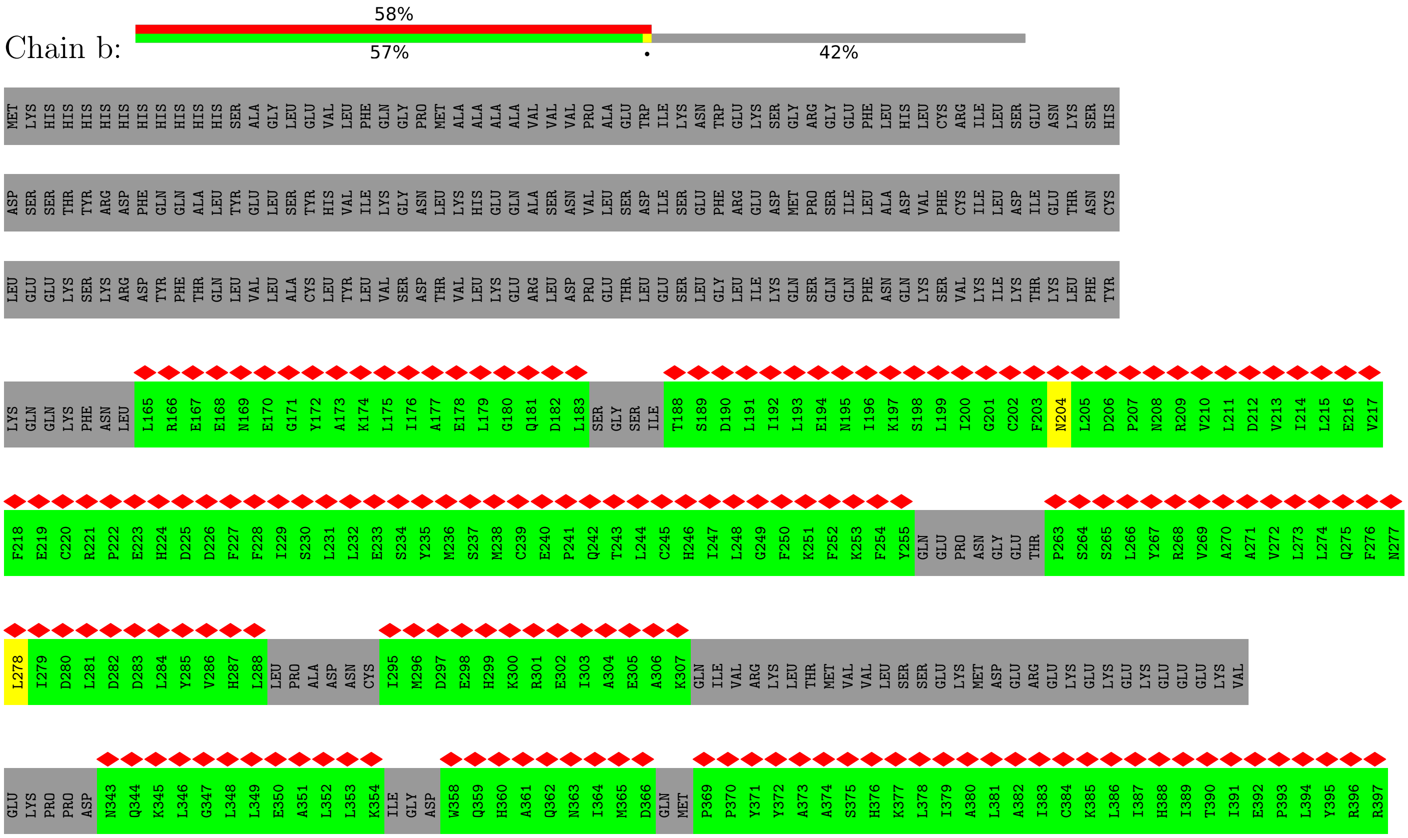
S458 F459 M460 K461 E462 F463 GLN SER ASP GLY SER LYS GLN GLU ASP LYS GLU LYS T476 E477 V478 I479 L480 S481 C482 L483 L484 S485 I486 T487 D488 Q489 V490 L491 L492 P493 S494 L495 S496 L497 M498 D499 C500 N501 A502 C503 M504 S505 E506 E507 L508 W509 G510 M511 F512 K513 THR PHE PRO Y517
Q518 H519 R520 Y521 R522 L523 Y524 G525 Q526 W527 K528 N529 E530 T531 Y532 N533 S534 H535 P536 L537 L538 V539 K540 V541 K542 A543 Q544 T545 I546 D547 R548 A549 K550 Y551 I552 M553 K554 R555 L556 T557 K558 E559 N560 V561 K562 P563 S564 G565 R566 Q567 I568 G569 K570 L571 S572 H573 S574 N575 P576 T577
I578 L579 F580 D581 Y582 I583 L584 S585 Q586 I587 Q588 K589 Y590 D591 N592 L593 I594 T595 P596 V597 V598 D599 S600 L601 K602 Y603 L604 T605 S606 L607 N608 Y609 D610 V611 L612 A613 Y614 C615 I616 I617 E618 A619 L620 A621 N622 P623 GLU LYS GLU ARG MET LYS HIS ASP ASP THR THR ILE S636 S637
W638 L639 Q640 S641 L642 A643 S644 F645 C646 G647 A648 V649 F650 R651 K652 Y653 P654 I655 D656 L657 A658 G659 L660 L661 Q662 Y663 V664 A665 N666 Q667 L668 K669 A670 GLY LYS S673 F674 D675 L676 L677 I678 L679 K680 E681 V682 V683 Q684 K685 M686 A687 GLY ILE GLU ILE THR GLU MET T696 M697
E698 Q699 L700 E701 A702 MET THR GLY G706 E707 Q708 L709 K710 A711 E712 G713 G714 TYR PHE GLY GLN ILE ARG ASN THR K723 K724 S725 S726 Q727 R728 L729 K730 D731 A732 L733 LEU ASP HIS ASP LEU ALA L740 P741 L742 C743 L744 L745 M746 A747 Q748 Q749 ARG ASN G752 V753 I754 F755 Q756 E757
GLY GLY GLU LYS HIS L763 K764 L765 V766 G767 K768 L769 Y770 D771 Q772 C773 H774 D775 T776 L777 V778 Q779 F780 G781 G782 F783 L784 A785 S786 ASN LEU SER THR GLU ASP TYR ILE LYS ARG VAL PRO SER ILE ASP VAL LEU CYS ASN GLU PHE HIS THR PRO HIS ASP ALA ALA PHE PHE LEU
SER ARG PRO MET TYR ALA HIS HIS ILE SER SER LYS TYR ASP GLU LEU LYS LYS SER GLU LYS GLY SER LYS GLN GLN HIS LYS VAL HIS LYS TYR ILE THR SER CYS E854 M855 V856 M857 A858 P859 V860 H861 E862 A863 V864 V865 S866 L867 HIS VAL SER LYS V872 W873 D874 D875 I876 S877
P878 Q879 F880 Y881 A882 T883 F884 TRP SER LEU THR M889 Y890 D891 L892 A893 V894 PRO H896 T897 S898 Y899 E900 R901 E902 V903 N904 K905 L906 K907 V908 GLN MET LYS ALA ILE ASP ASP ASN GLN GLU MET PRO PRO ASN LYS LYS LYS LYS E927 K928 E929 R930 C931 T932 A933 L934 Q935 D936 K937
L938 L939 E940 E941 E942 K943 K944 Q945 M946 E947 H948 V949 Q950 R951 V952 L953 Q954 R955 L956 K957 L958 E959 LYS ASP ASN TRP LEU LEU ALA LYS SER THR LYS N971 E972 T973 I974 T975 K976 F977 L978 Q979 L980 C981 I982 F983 P984 R985 C986 I987 F988 S989 A990 I991 D992 A993 V994 Y995 C996 A997
R998 F999 V1000 E1001 L1002 V1003 H1004 Q1005 GLN LYS THR PRO ASN PHE SER THR L1014 L1015 C1016 Y1017 D1018 R1019 V1020 F1021 SER ASP I1024 I1025 Y1026 T1027 V1028 A1029 S1030 CYS THR GLU N1034 E1035 A1036 S1037 R1038 Y1039 G1040 R1041 F1042 L1043 C1044 C1045 M1046 L1047 E1048 T1049 V1050 T1051 R1052 W1053 H1054 SER ASP ARG
ALA THR TYR GLU LYS GLU CYS GLY ASN TYR PRO GLY PHE LEU THR ILE LEU ARG ALA THR GLY PHE ASP GLY GLY ASN LYS ALA ASP Q1087 L1088 D1089 Y1090 E1091 N1092 F1093 R1094 H1095 V1096 V1097 H1098 K1099 W1100 H1101 Y1102 K1103 L1104 T1105 K1106 A1107 S1108 V1109 H1110 C1111 L1112 E1113 THR GLY GLU Y1117
T1118 H1119 I1120 R1121 N1122 I1123 L1124 I1125 V1126 L1127 T1128 K1129 I1130 L1131 P1132 TRP TYR PRO LYS V1137 L1138 N1139 L1140 G1141 Q1142 A1143 L1144 E1145 R1146 P1147 V1148 H1149 K1150 I1151 C1152 Q1153 E1154 GLU LYS GLU LYS ARG P1160 D1161 L1162 Y1163 A1164 L1165 A1166 M1167 G1168 Y1169 S1170 G1171 Q1172 L1173 K1174 S1175 ARG LYS
SER TYR MET ILE PRO GLU ASN GLU PHE HIS LYS ASP PRO PRO ARG ASN ALA VAL ALA SER VAL GLN ASN GLY

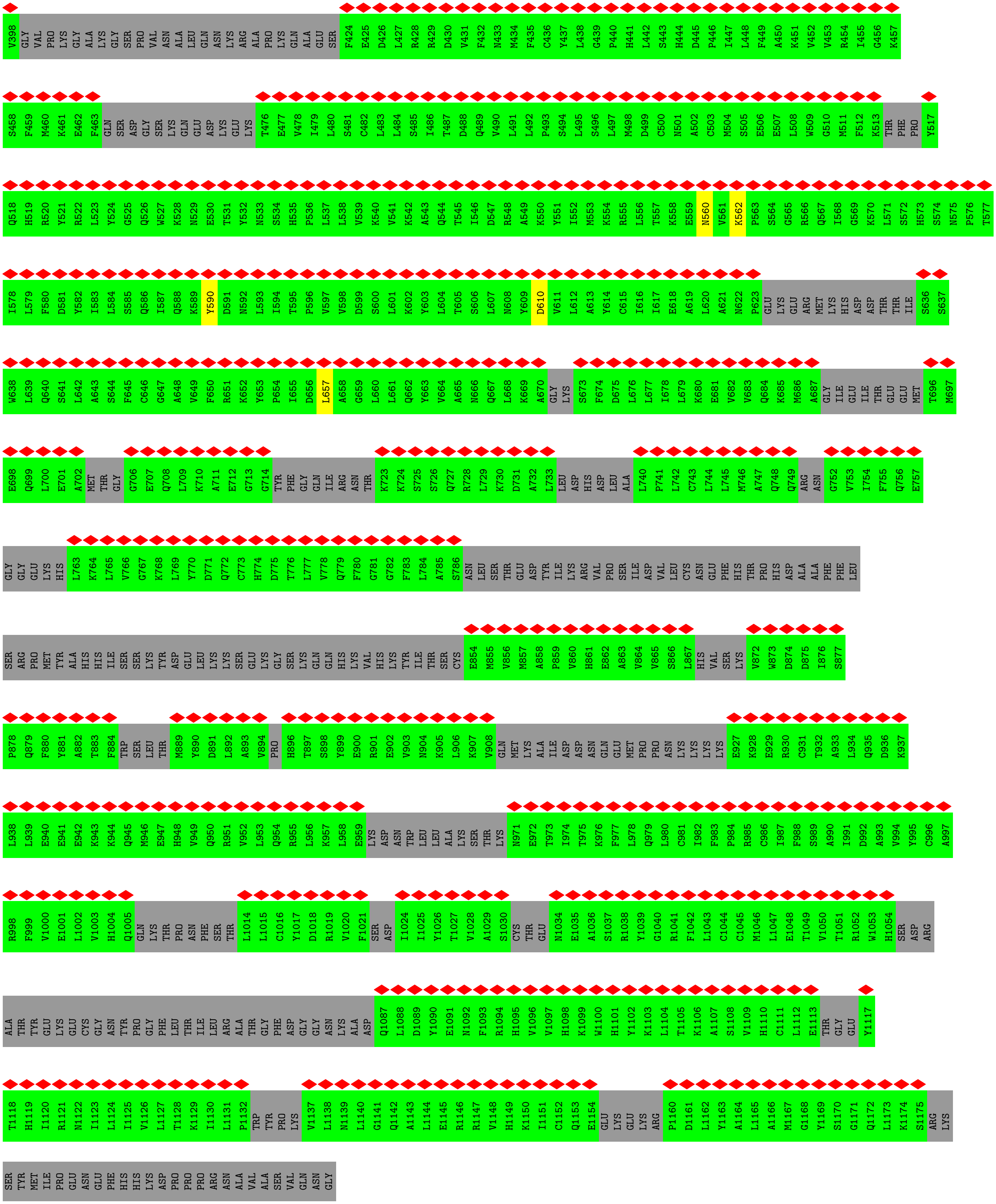
- Molecule 2: THO complex subunit 2





- Molecule 2: THO complex subunit 2





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S458 F459 M460 K461 E462 F463 GLN SER ASP GLY SER LYS GLN GLU ASP LYS GLU LYS T476 E477 V478 I479 L480 S481 C482 L483 L484 S485 I486 T487 D488 Q489 V490 L491 L492 P493 S494 L495 S496 L497 M498 D499 C500 N501 A502 C503 M504 S505 E506 E507 L508 W509 G510 M511 F512 K513 THR PHE PRO Y517

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I578 L579 F580 D581 Y582 I583 L584 S585 Q586 I587 Q588 K589 Y590 D591 N592 L593 I594 T595 P596 V597 V598 D599 S600 L601 K602 Y603 L604 T605 S606 L607 N608 Y609 D610 V611 L612 A613 Y614 C615 I616 I617 E618 A619 L620 A621 N622 P623 GLU LYS GLU ARG MET LYS HIS ASP ASP THR THR ILE S636 S637

W638 L639 Q640 S641 L642 A643 S644 F645 C646 G647 A648 V649 F650 R651 K652 Y653 P654 I655 D656 L657 A658 G659 L660 L661 Q662 Y663 V664 A665 N666 Q667 L668 K669 A670 GLY LYS S673 F674 D675 L676 L677 I678 L679 K680 E681 V682 V683 Q684 K685 M686 A687 GLY ILE GLU ILE THR GLU MET T696 M697

E698 Q699 L700 E701 A702 MET THR GLY G706 E707 Q708 L709 K710 A711 E712 G713 G714 TYR PHE GLY GLN ILE ARG ASN THR K723 K724 S725 S726 Q727 R728 L729 K730 D731 A732 L733 LEU ASP HIS ASP LEU ALA L740 P741 L742 C743 L744 L745 M746 A747 Q748 Q749 ARG ASN G752 V753 I754 F755 Q756 E757

GLY GLY GLU LYS HIS L763 K764 L765 V766 G767 K768 L769 Y770 D771 Q772 C773 H774 D775 T776 L777 V778 Q779 F780 G781 G782 F783 L784 A785 S786 ASN LEU SER THR GLU ASP TYR ILE LYS ARG VAL PRO SER ILE ASP VAL LEU CYS ASN GLU PHE HIS THR PRO HIS ASP ALA ALA PHE PHE LEU

SER ARG PRO MET TYR ALA HIS HIS ILE SER SER LYS TYR ASP GLU LEU LYS LYS SER GLU LYS GLY SER LYS GLN GLN HIS LYS VAL HIS LYS TYR ILE THR SER CYS E854 M855 V856 M857 A858 P859 V860 H861 E862 A863 V864 V865 S866 L867 HIS VAL SER LYS V872 W873 D874 D875 I876 S877

P878 Q879 F880 Y881 A882 T883 F884 TRP SER LEU THR M889 Y890 D891 L892 A893 V894 PRO H896 T897 S898 Y899 E900 R901 E902 V903 N904 K905 L906 K907 V908 GLN MET LYS ALA ILE ASP ASP ASN GLN GLU MET PRO PRO ASN LYS LYS LYS LYS E927 K928 E929 R930 C931 T932 A933 L934 Q935 D936 K937

L938 L939 E940 E941 E942 K943 K944 Q945 M946 E947 H948 V949 Q950 R951 V952 L953 Q954 R955 L956 K957 L958 E959 LYS ASP ASN TRP LEU LEU ALA LYS SER THR LYS N971 E972 T973 I974 T975 K976 F977 L978 Q979 L980 C981 I982 F983 P984 R985 C986 I987 F988 S989 A990 I991 D992 A993 V994 Y995 C996 A997

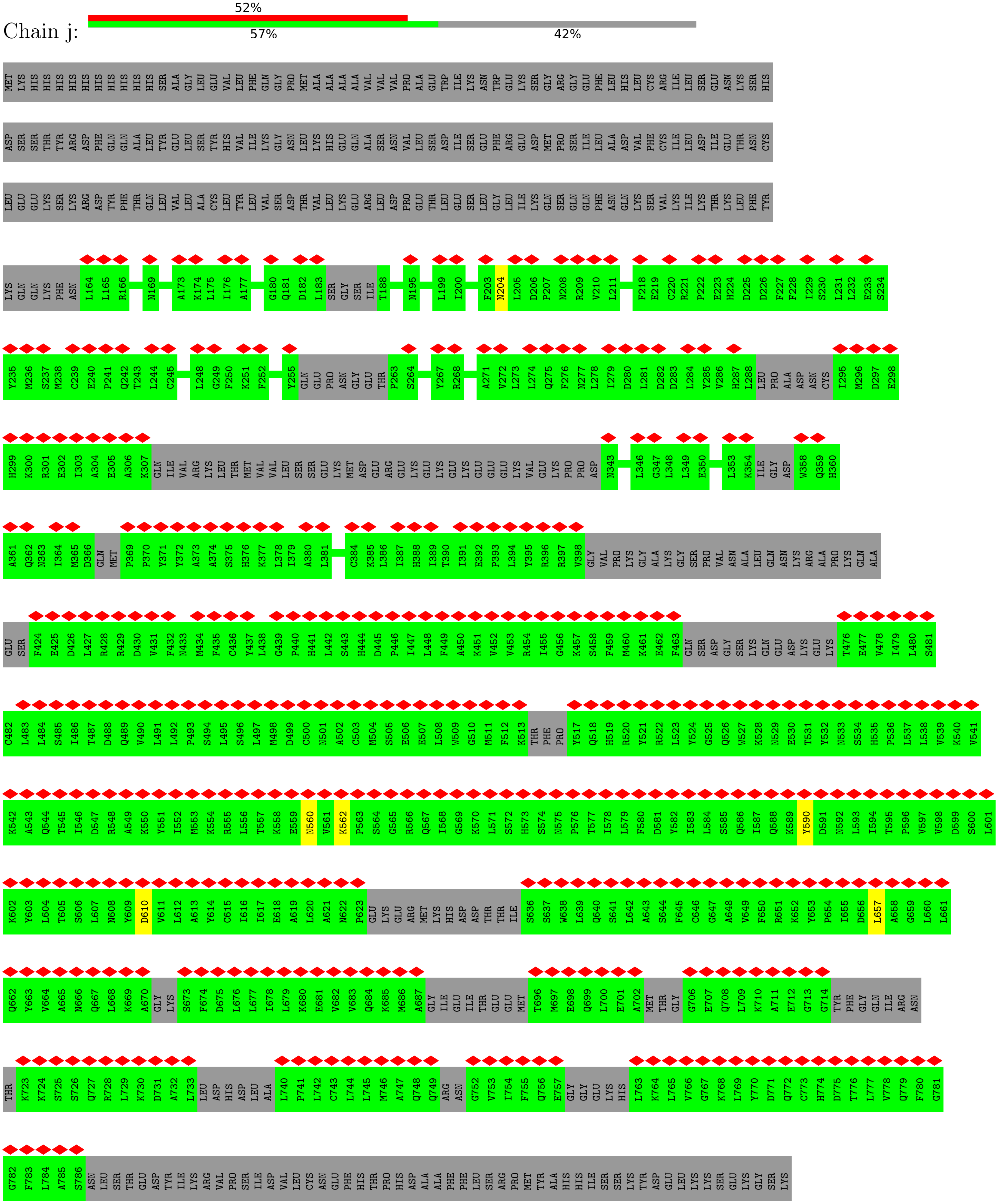
R998 F999 V1000 E1001 L1002 V1003 H1004 Q1005 GLN LYS THR PRO ASN PHE SER THR L1014 L1015 C1016 Y1017 D1018 R1019 V1020 F1021 SER ASP I1024 L1025 Y1026 T1027 V1028 A1029 S1030 CYS THR GLU N1034 E1035 A1036 S1037 R1038 Y1039 G1040 R1041 F1042 L1043 C1044 C1045 M1046 L1047 E1048 T1049 V1050 T1051 R1052 W1053 H1054 SER ASP ARG

ALA THR TYR GLU LYS GLU CYS GLY ASN TYR PRO GLY PHE LEU THR ILE LEU ARG ALA THR GLY PHE ASP GLY GLY ASN LYS ALA ASP Q1087 L1088 D1089 Y1090 E1091 N1092 F1093 R1094 H1095 V1096 V1097 H1098 K1099 W1100 H1101 Y1102 K1103 L1104 T1105 K1106 A1107 S1108 V1109 H1110 C1111 L1112 E1113 THR GLY GLU Y1117

T1118 H1119 I1120 R1121 N1122 I1123 L1124 I1125 V1126 L1127 T1128 K1129 I1130 L1131 P1132 TRP TYR PRO LYS V1137 L1138 N1139 L1140 G1141 Q1142 A1143 L1144 E1145 R1146 P1147 V1148 H1149 K1150 I1151 C1152 Q1153 E1154 GLU LYS GLU LYS ARG P1160 D1161 L1162 Y1163 A1164 L1165 A1166 M1167 G1168 Y1169 S1170 G1171 Q1172 L1173 K1174 S1175 ARG LYS

SER TYR MET ILE PRO GLU ASN GLU PHE HIS HIS LYS ASP PRO PRO ARG ASN ALA VAL ALA SER VAL GLN ASN GLY

- Molecule 2: THO complex subunit 2



MET LYS HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS SER ALA GLY LEU GLU VAL LEU PHE GLN GLY PRO MET ALA ALA ALA ALA VAL VAL VAL PRO ALA GLU TRP ILE LYS ASN TRP GLU LYS SER GLY ARG GLY GLU PHE LEU HIS LEU CYS ARG ILE LEU SER GLU ASN LYS SER HIS

ASP SER SER THR TYR ARG ASP PHE GLN GLN ALA LEU TYR GLU LEU SER TYR HIS VAL ILE LYS GLY ASN LEU LYS HIS GLU GLN ALA SER ASN VAL LEU SER ASP ILE SER GLU PHE ARG GLU ASP MET PRO SER ILE LEU ALA ASP VAL PHE CYS ILE LEU ASP ILE GLU THR ASN CYS

LEU GLU GLU LYS SER LYS ARG ASP TYR PHE THR GLN LEU VAL LEU ALA CYS LEU TYR LEU VAL SER ASP THR VAL LEU LYS GLU ARG LEU ASP PRO GLU THR LEU GLU SER LEU GLY LEU ILE LYS GLN SER GLN GLN PHE ASN GLN LYS SER VAL LYS ILE LYS THR LYS LEU PHE TYR

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GLU SER F424 E425 D426 L427 R428 R429 D430 V431 F432 N433 M434 F435 C436 Y437 L438 G439 P440 H441 L442 S443 H444 D445 P446 I447 L448 F449 A450 K451 V452 V453 R454 I455 G456 K457 S458 F459 M460 K461 E462 F463 GLN SER ASP GLY SER LYS GLN GLU ASP LYS GLU LYS T476 E477 V478 I479 L480 S481

C482 L483 L484 S485 I486 T487 D488 Q489 V490 L491 L492 P493 S494 L495 S496 L497 M498 D499 C500 N501 A502 C503 M504 S505 E506 E507 L508 W509 G510 M511 F512 K513 THR PHE PRO Y517 Q518 H519 R520 Y521 R522 L523 Y524 G525 Q526 W527 K528 N529 E530 T531 Y532 N533 S534 H535 P536 L537 L538 V539 K540 V541

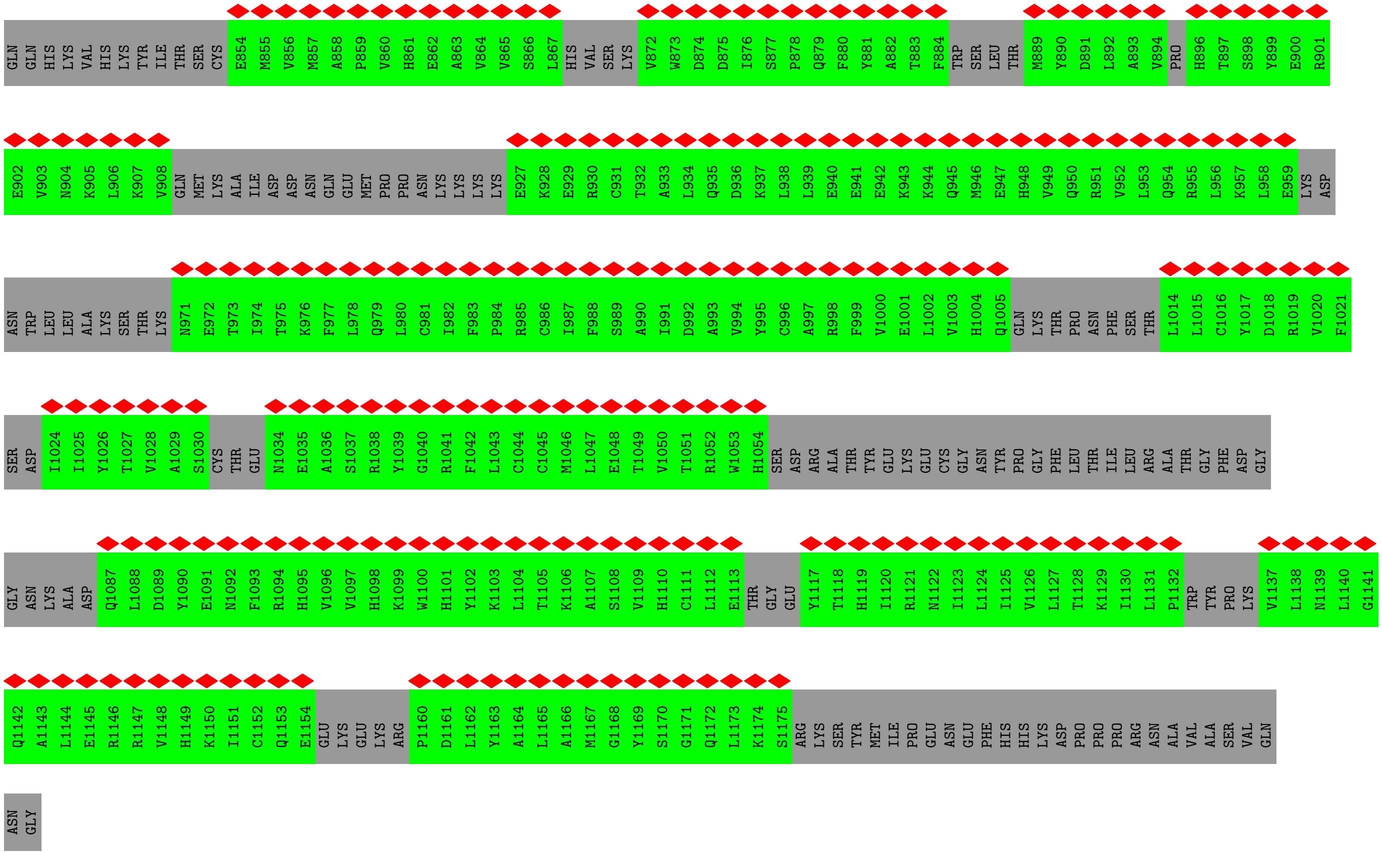
K542 A543 Q544 T545 I546 D547 R548 A549 K550 Y551 I552 M553 K554 R555 L556 T557 K558 E559 N560 V561 K562 P563 S564 G565 R566 Q567 I568 G569 K570 L571 S572 H573 S574 N575 P576 T577 I578 L579 F580 D581 Y582 I583 L584 S585 Q586 I587 Q588 K589 Y590 D591 N592 L593 I594 T595 P596 V597 V598 D599 S600 L601

K602 Y603 L604 T605 S606 L607 N608 Y609 D610 V611 L612 A613 Y614 C615 I616 I617 E618 A619 L620 A621 N622 P623 GLU LYS GLU ARG MET LYS HIS ASP ASP THR THR ILE S636 S637 W638 L639 Q640 S641 L642 A643 S644 F645 C646 G647 A648 V649 F650 R651 K652 Y653 P654 I655 D656 L657 A658 G659 L660 L661

Q662 Y663 V664 A665 N666 Q667 L668 K669 A670 GLY LYS S673 F674 D675 L676 L677 I678 L679 K680 E681 V682 V683 Q684 K685 M686 A687 GLY ILE GLU ILE THR GLU GLU MET T696 M697 E698 Q699 L700 E701 A702 MET THR GLY G706 E707 Q708 L709 K710 A711 E712 G713 G714 TYR PHE GLY GLN ILE ARG ASN

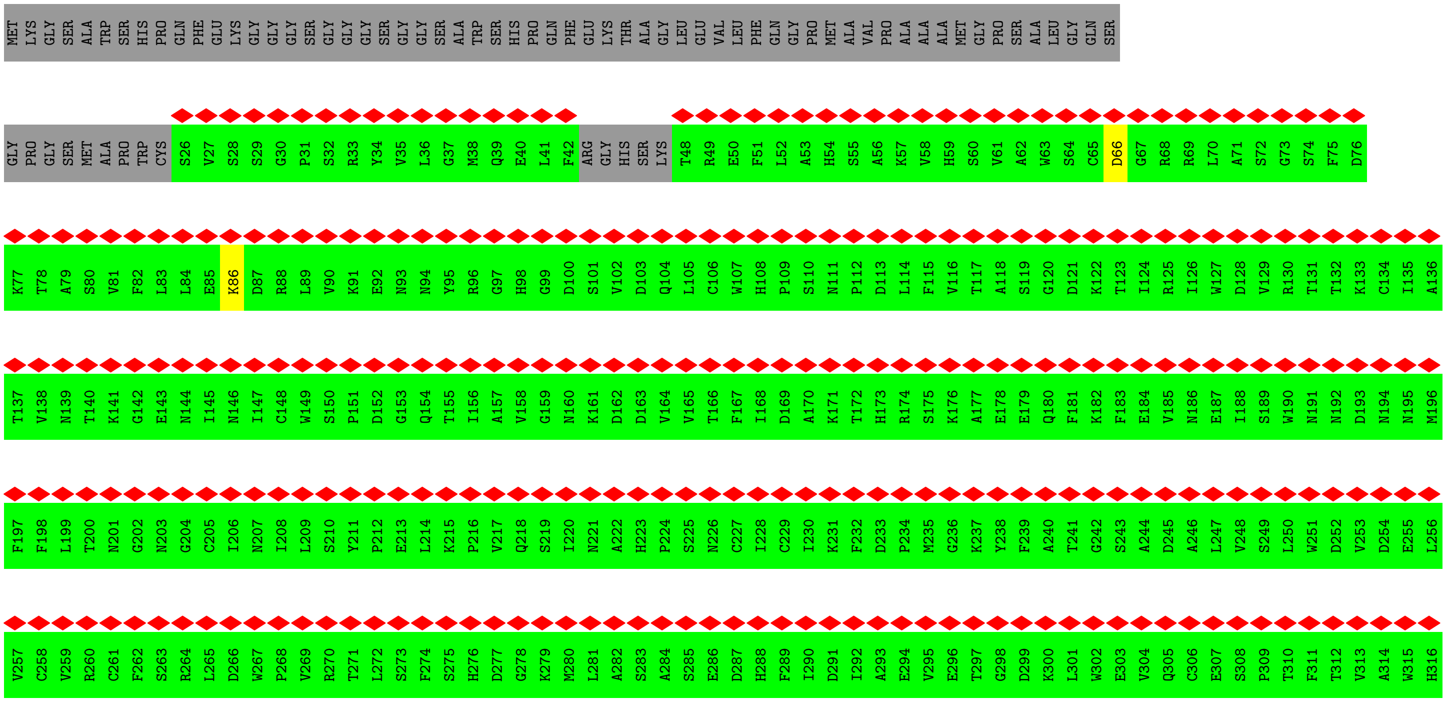
THR K723 K724 S725 S726 Q727 R728 L729 K730 D731 A732 L733 LEU ASP HIS ASP LEU ALA L740 P741 L742 C743 L744 L745 M746 A747 Q748 Q749 ARG ASN G752 V753 I754 F755 Q756 E757 GLY GLY GLU LYS HIS L763 K764 L765 V766 G767 K768 L769 Y770 D771 Q772 C773 H774 D775 T776 L777 V778 Q779 F780 G781

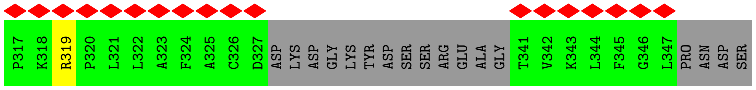
G782 F783 L784 A785 S786 ASN LEU SER THR GLU ASP TYR ILE LYS ARG VAL PRO SER ILE ASP VAL LEU CYS ASN GLU PHE HIS THR PRO HIS ASP ALA ALA PHE PHE LEU SER ARG PRO MET TYR ALA HIS HIS ILE SER SER LYS TYR ASP GLU LEU LYS LYS SER GLU LYS GLY SER LYS



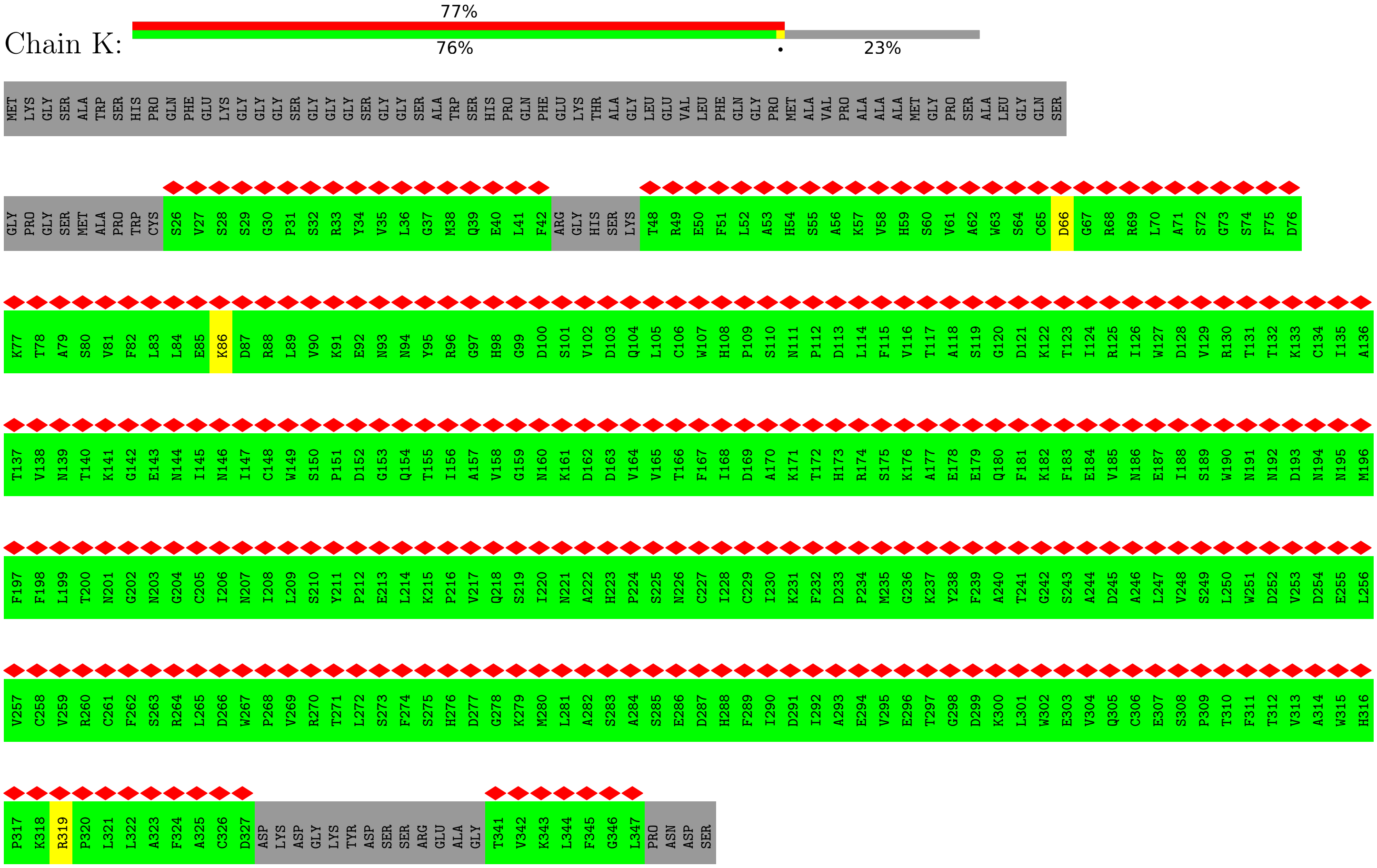
- Molecule 3: THO complex subunit 3

Chain C:

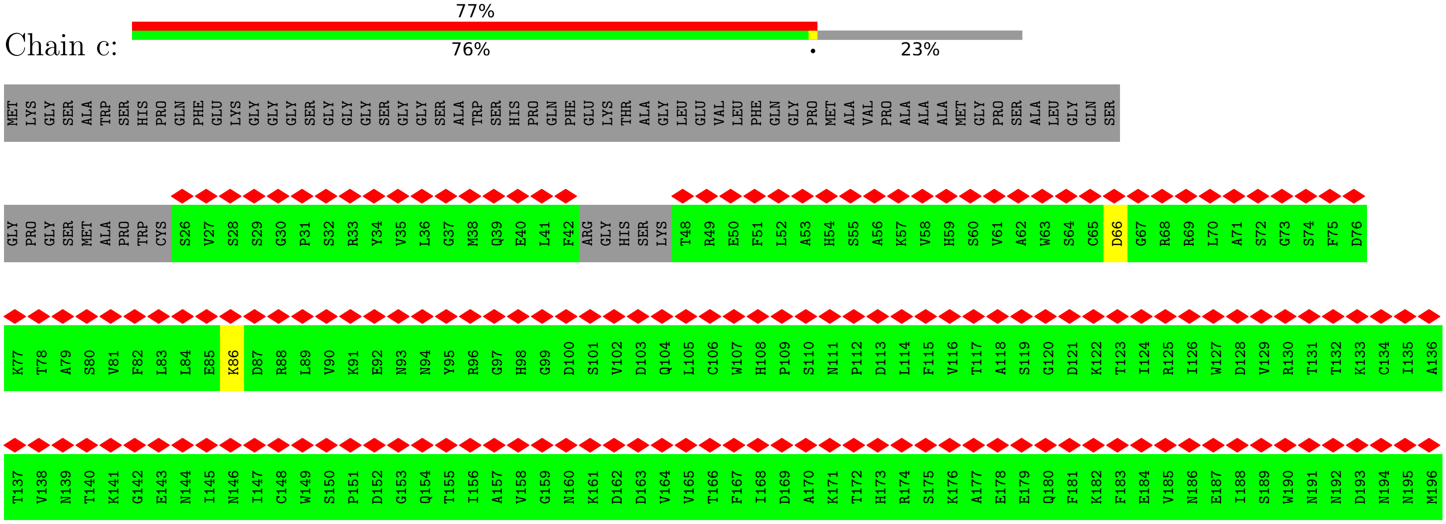


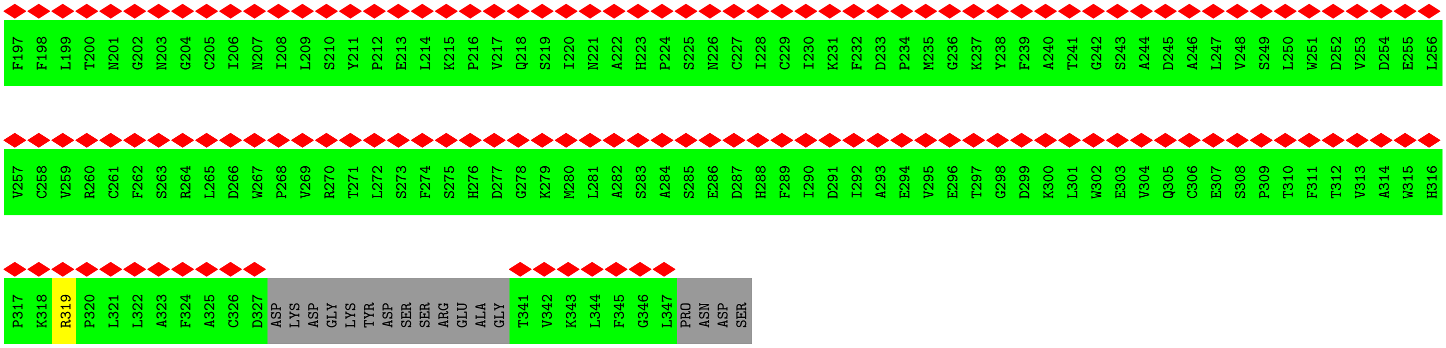


- Molecule 3: THO complex subunit 3

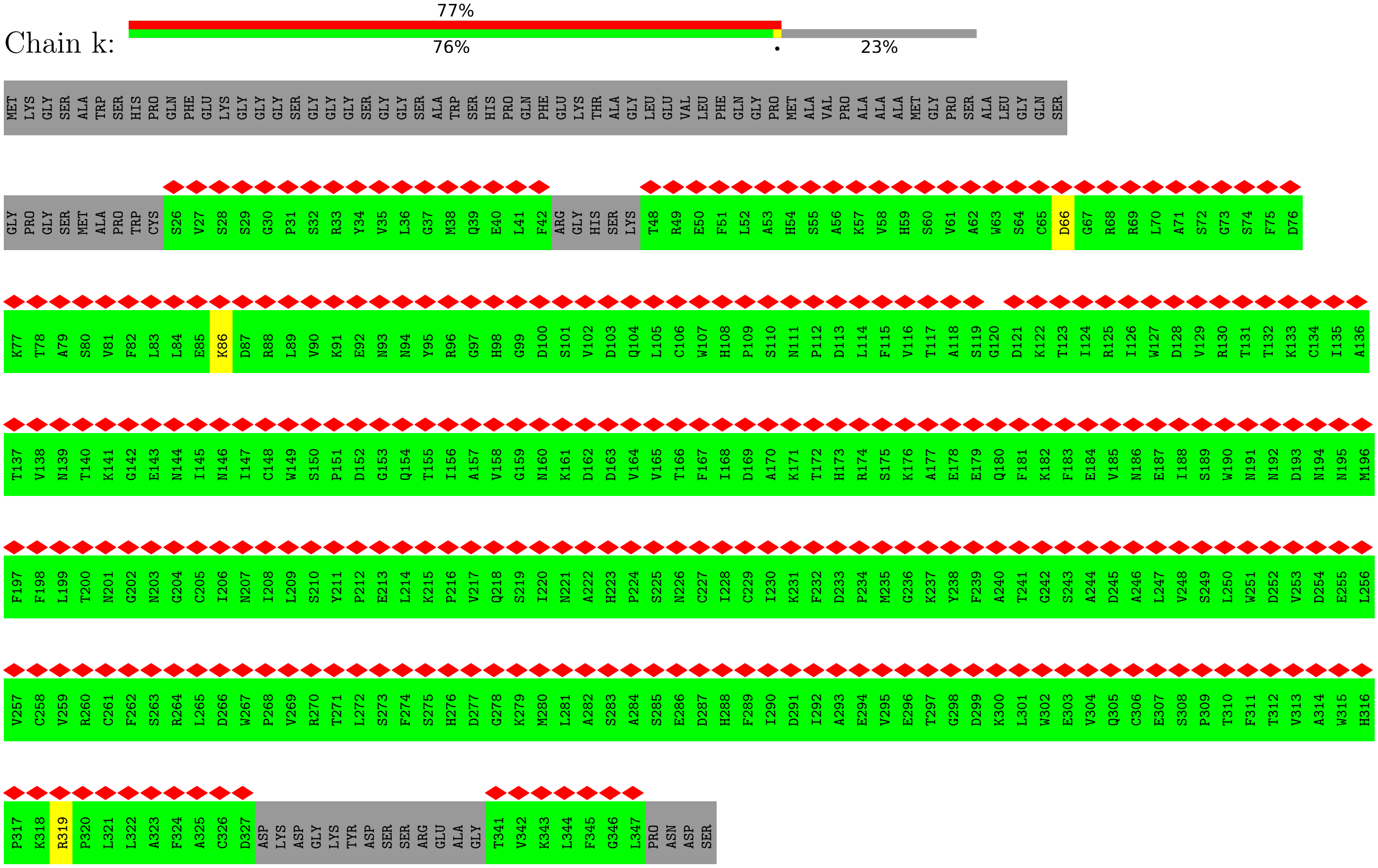


- Molecule 3: THO complex subunit 3

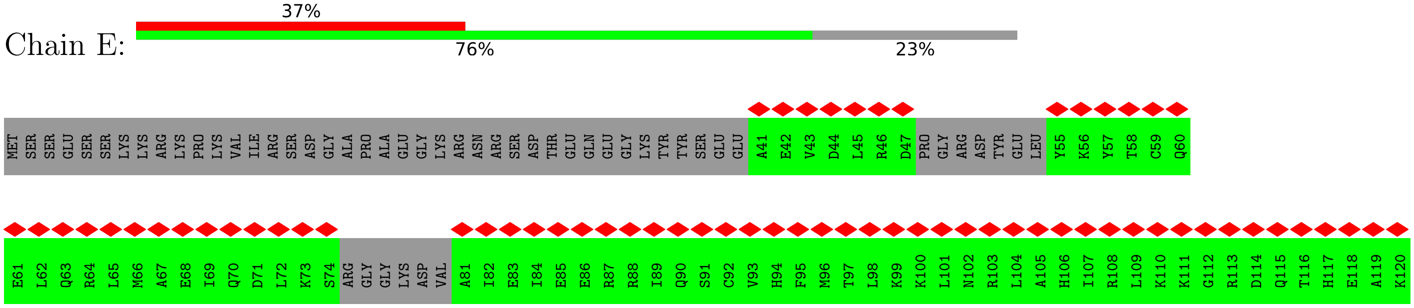


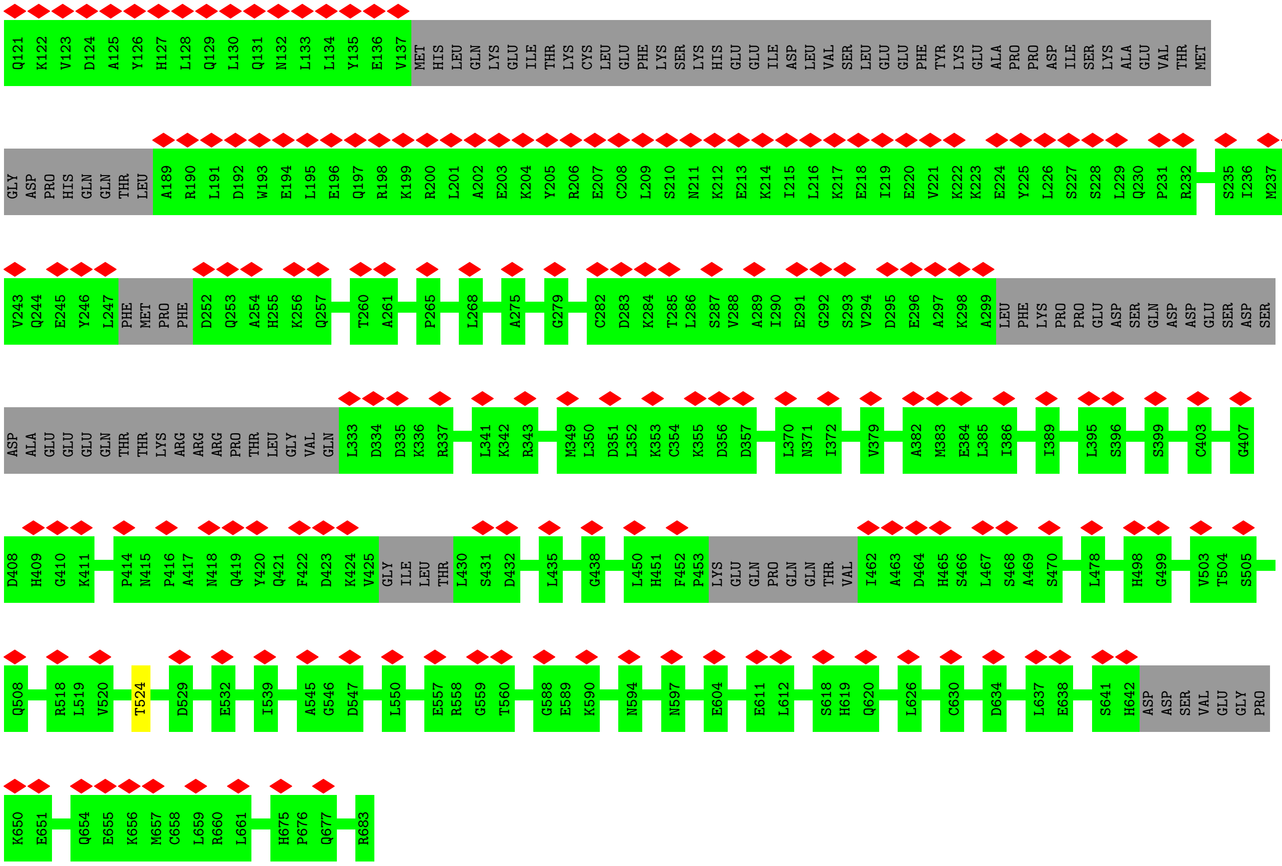


- Molecule 3: THO complex subunit 3



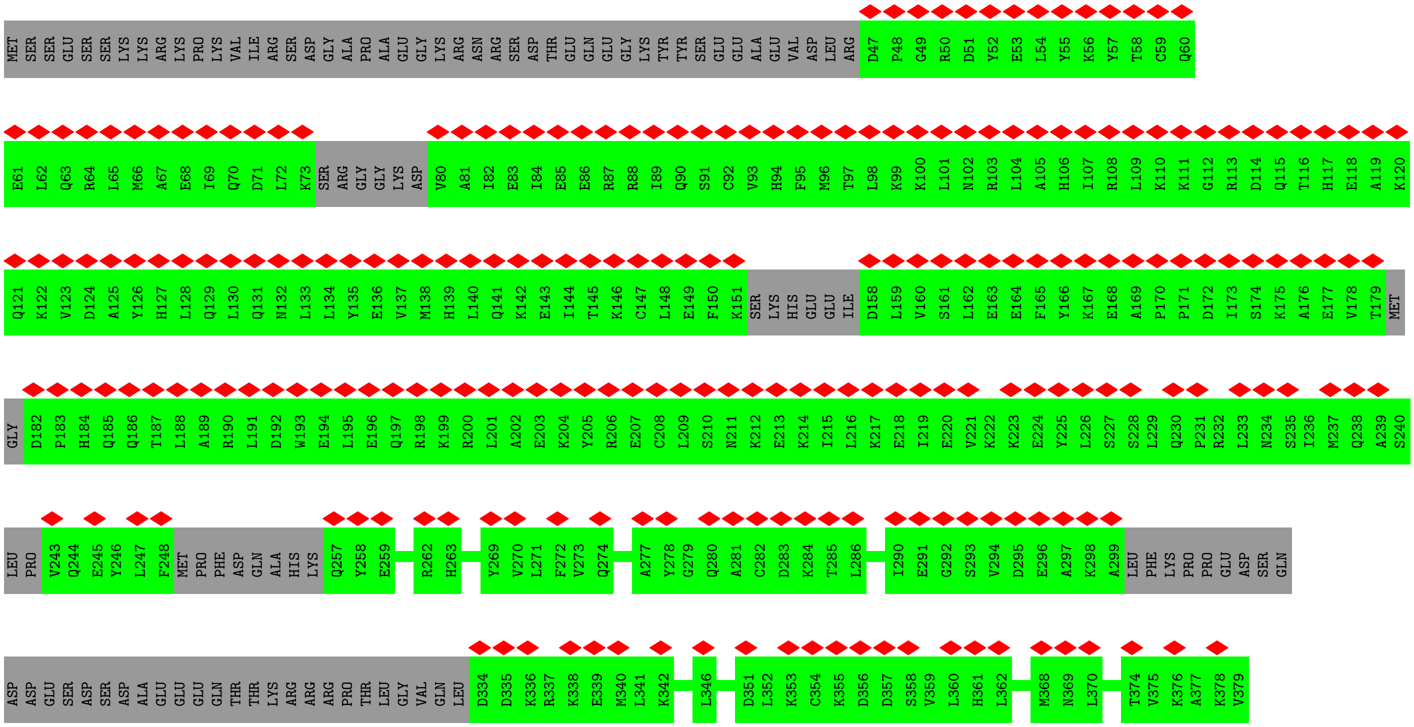
- Molecule 4: THO complex subunit 5 homolog

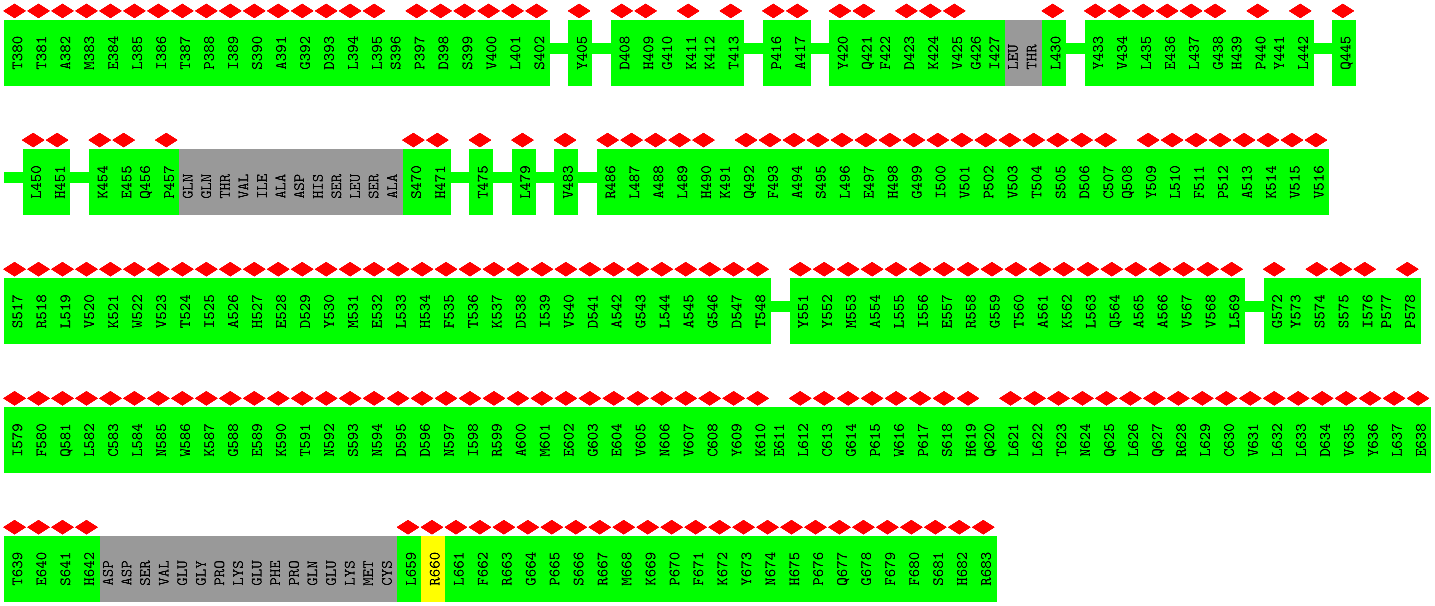




- Molecule 4: THO complex subunit 5 homolog

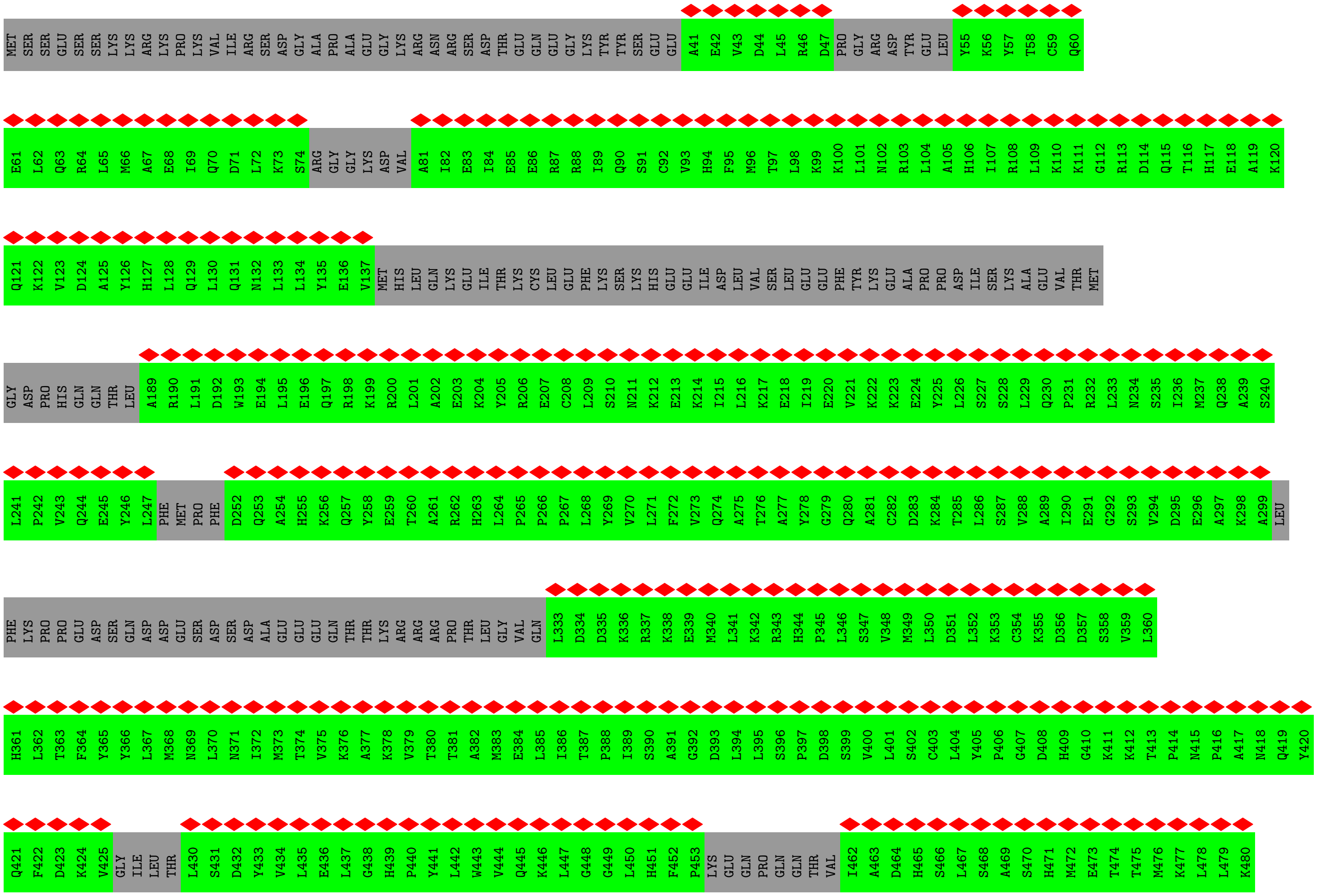
Chain M:

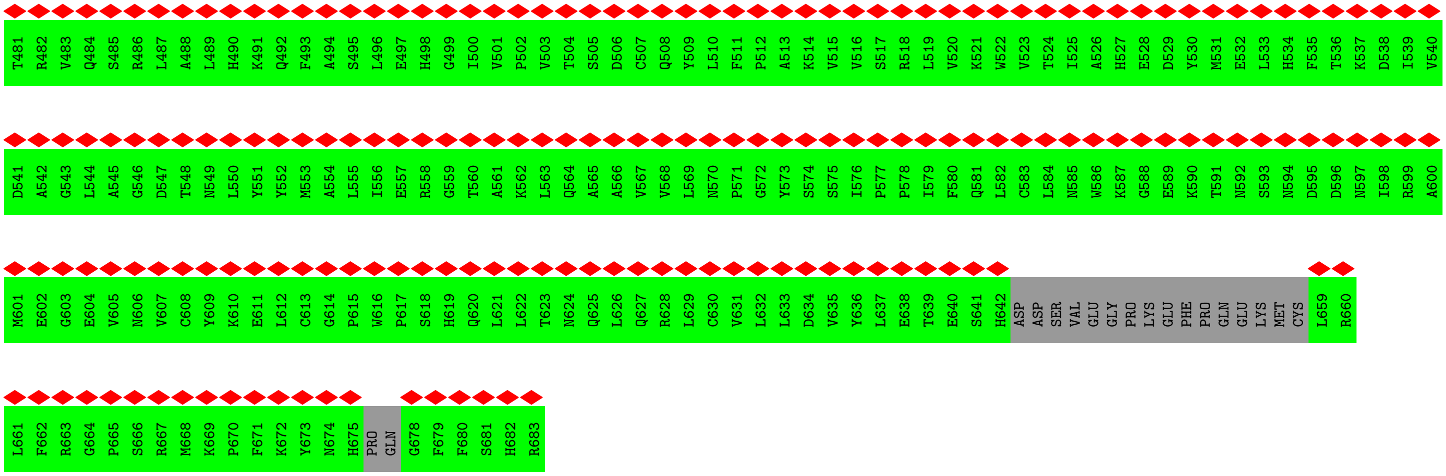





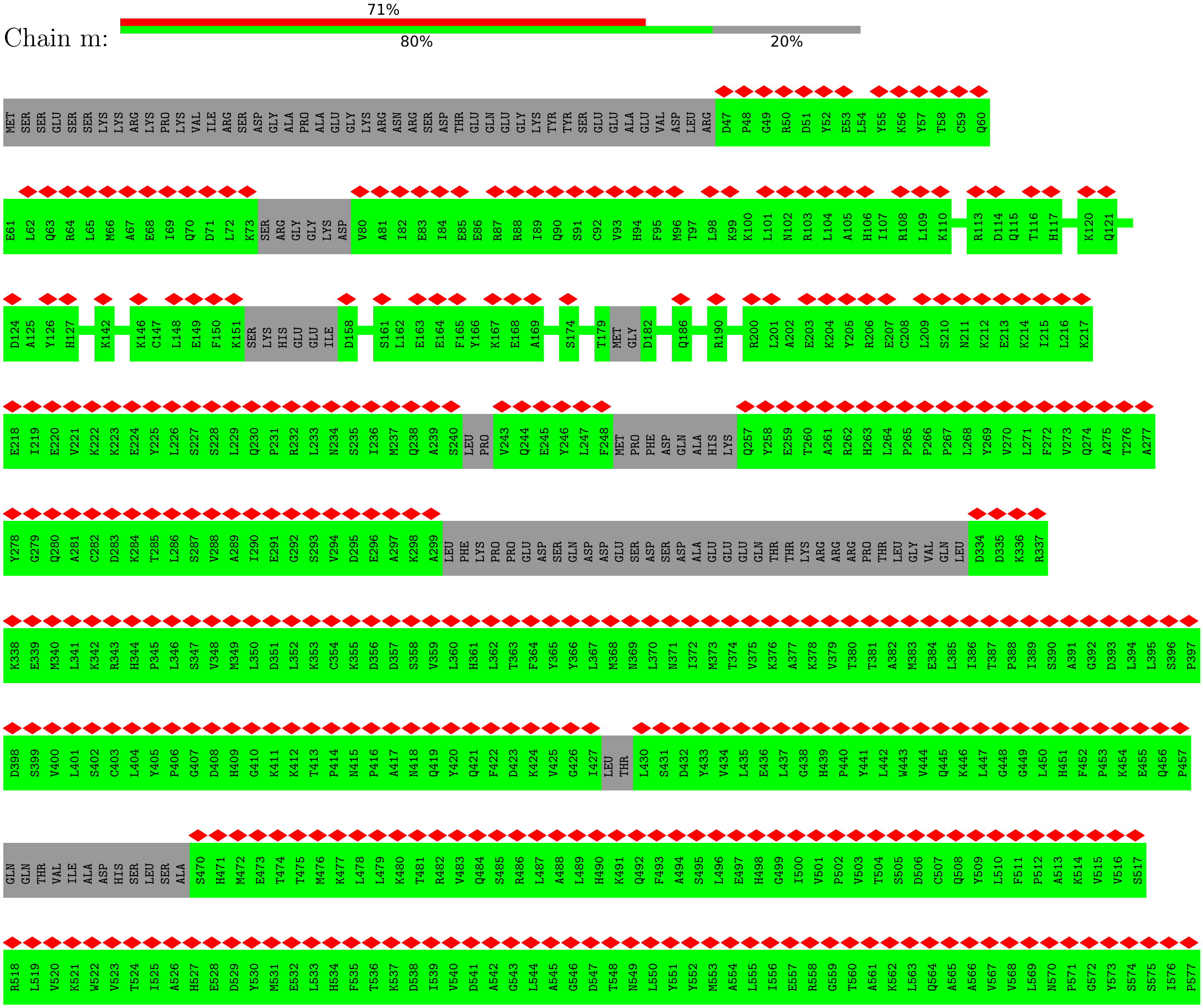
- Molecule 4: THO complex subunit 5 homolog

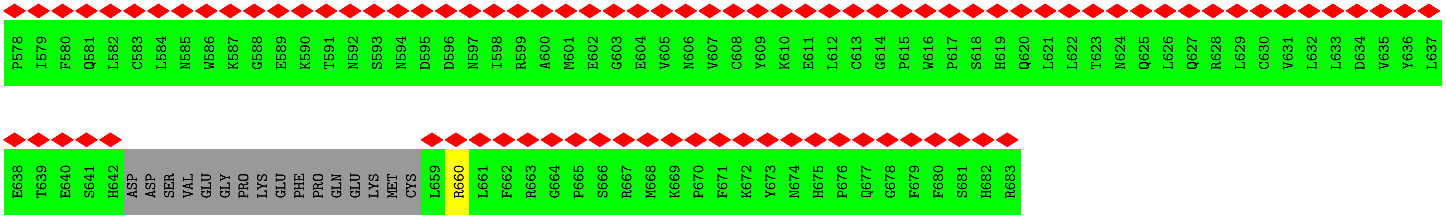
Chain e:





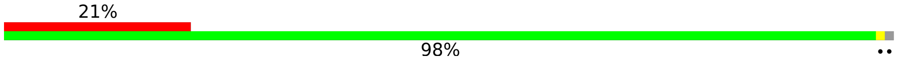
• Molecule 4: THO complex subunit 5 homolog

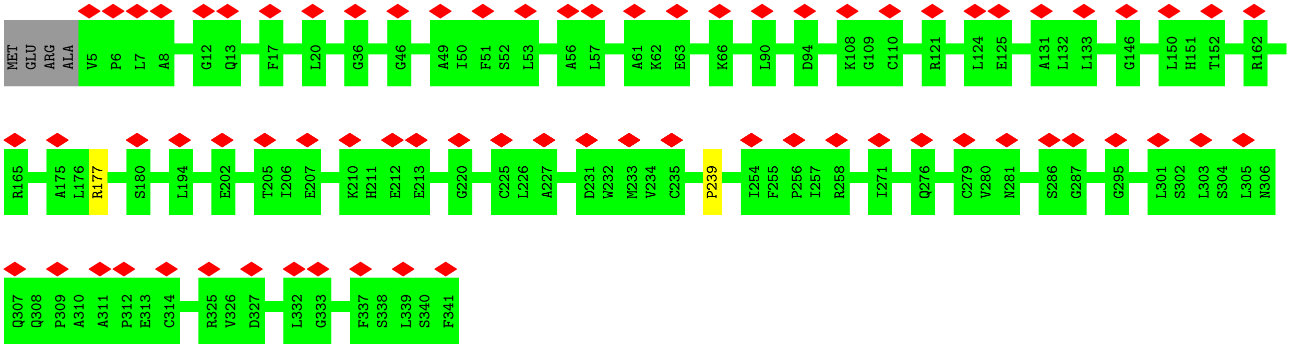




- Molecule 5: THO complex subunit 6 homolog

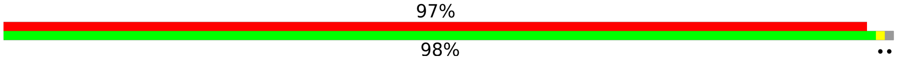
Chain F:

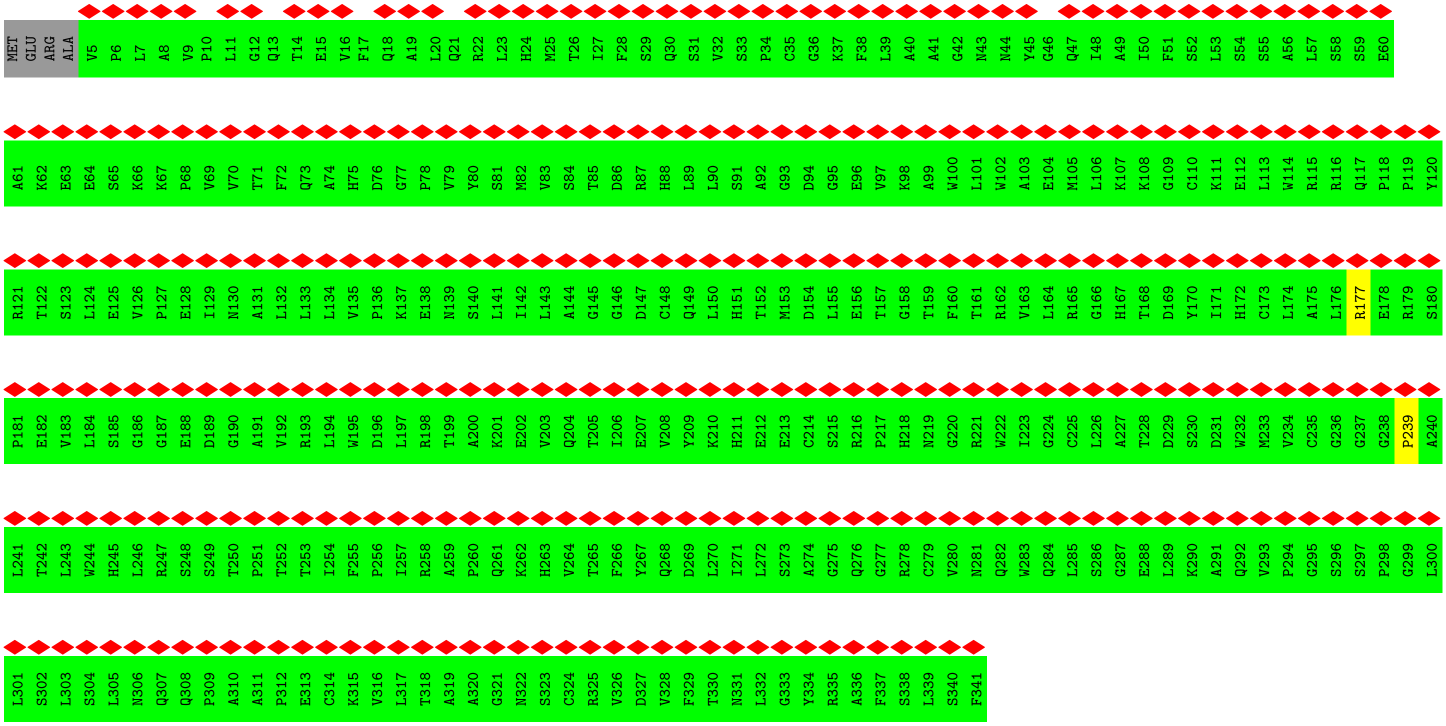




- Molecule 5: THO complex subunit 6 homolog

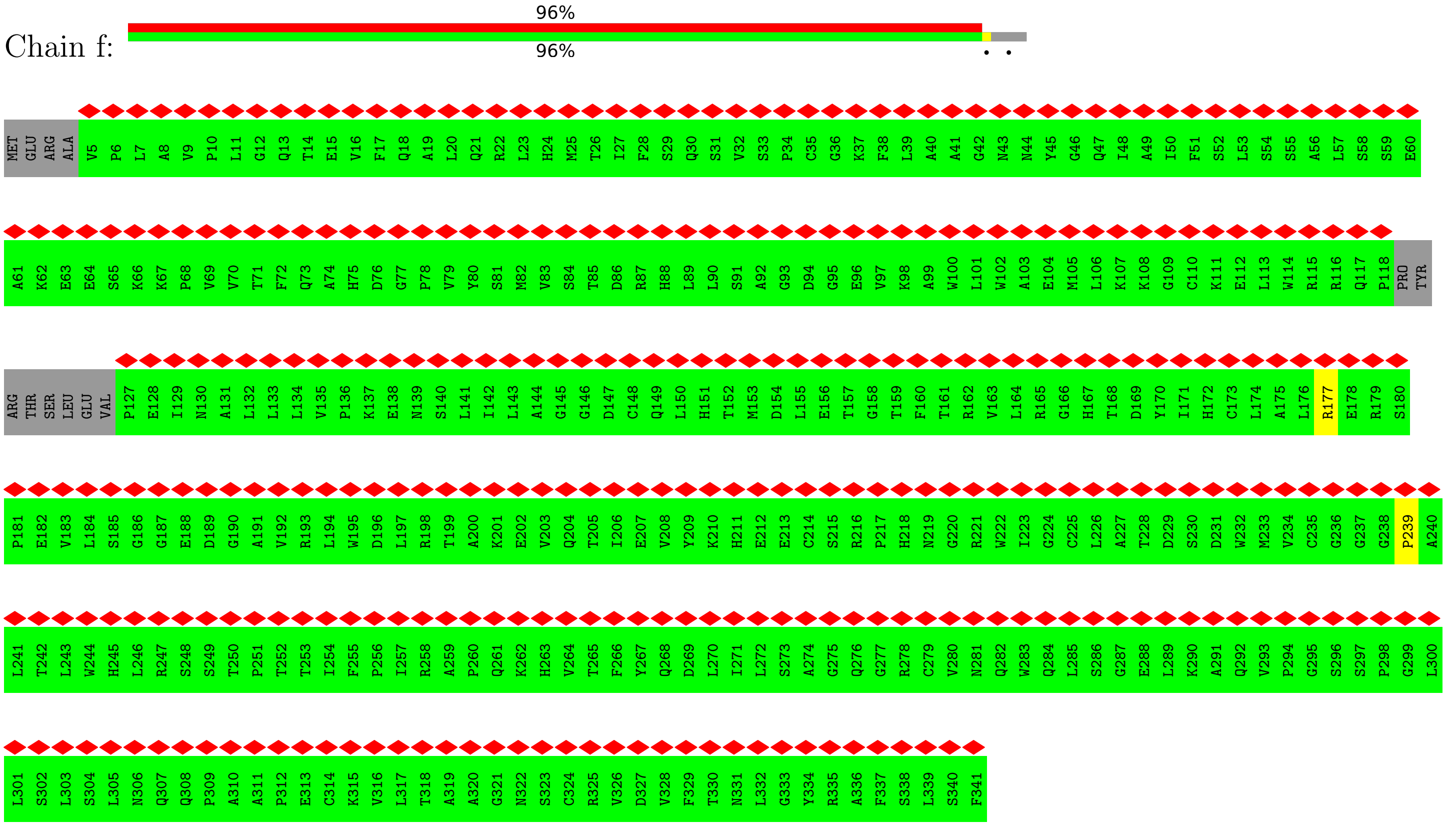
Chain N:





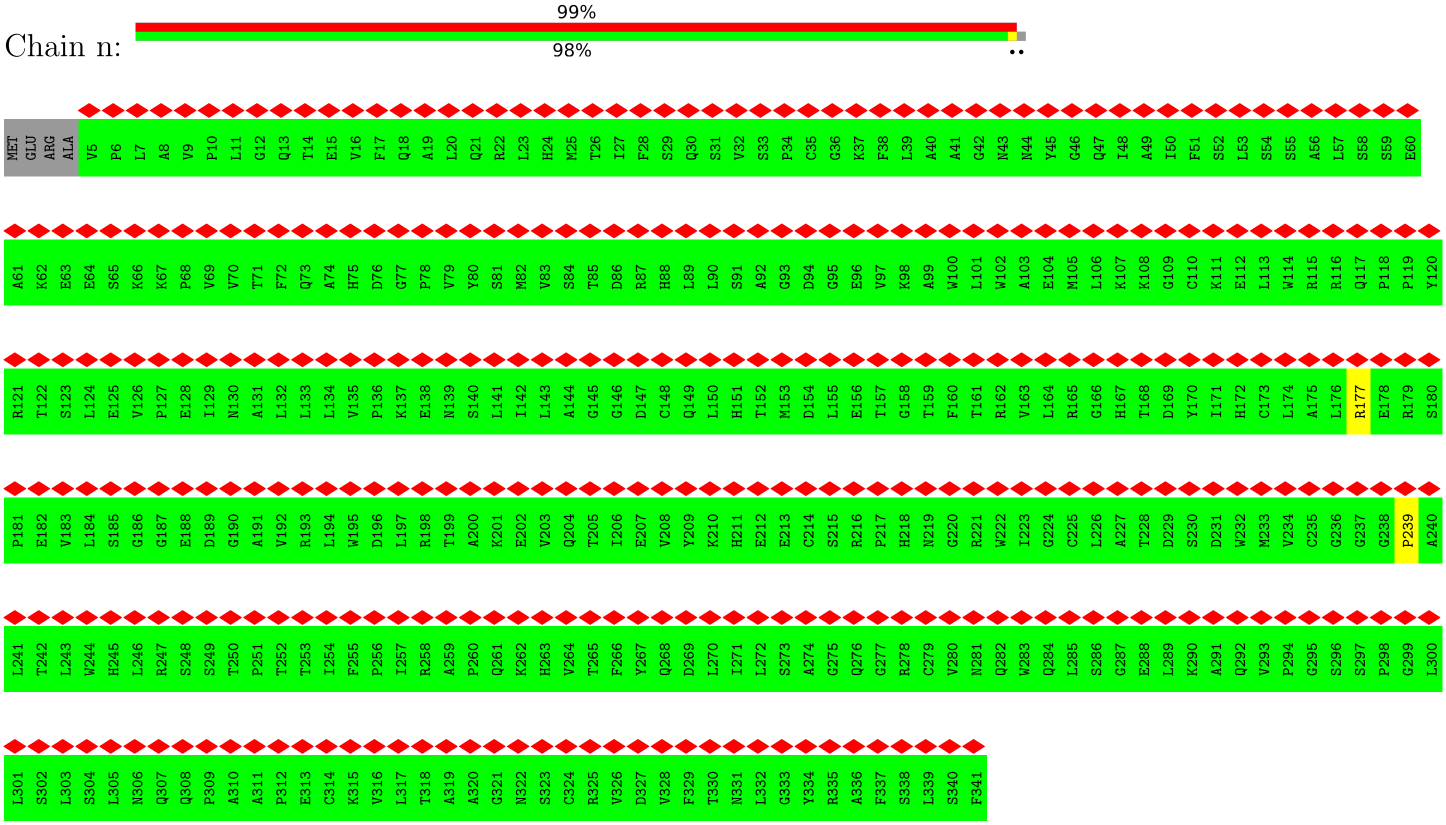
- Molecule 5: THO complex subunit 6 homolog

Chain f:

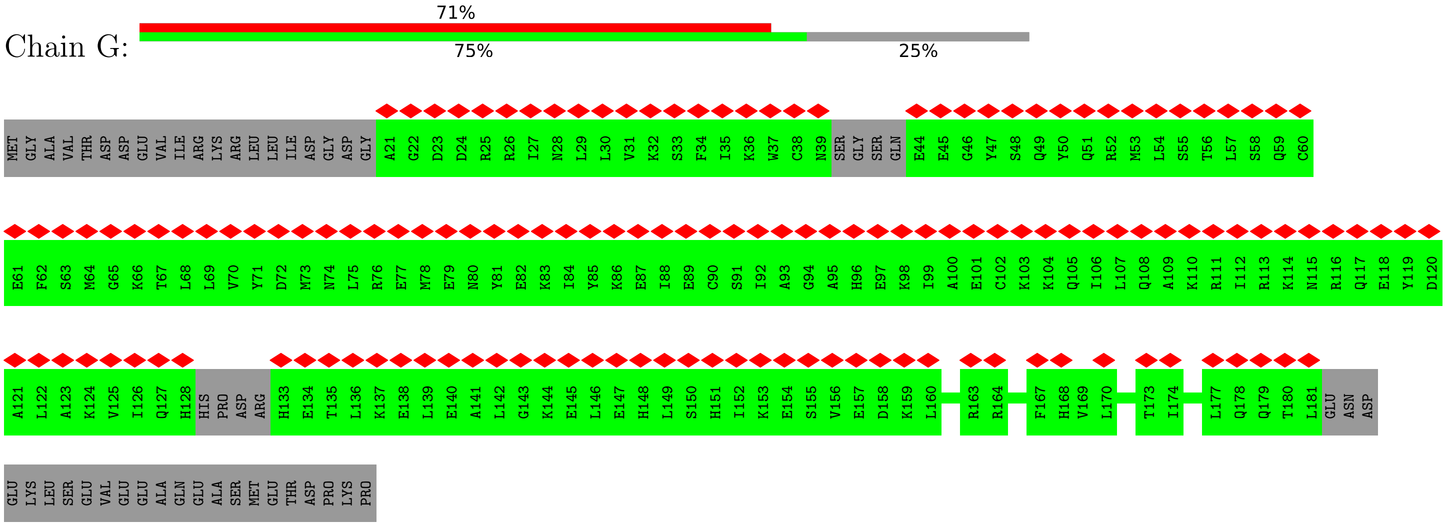


- Molecule 5: THO complex subunit 6 homolog

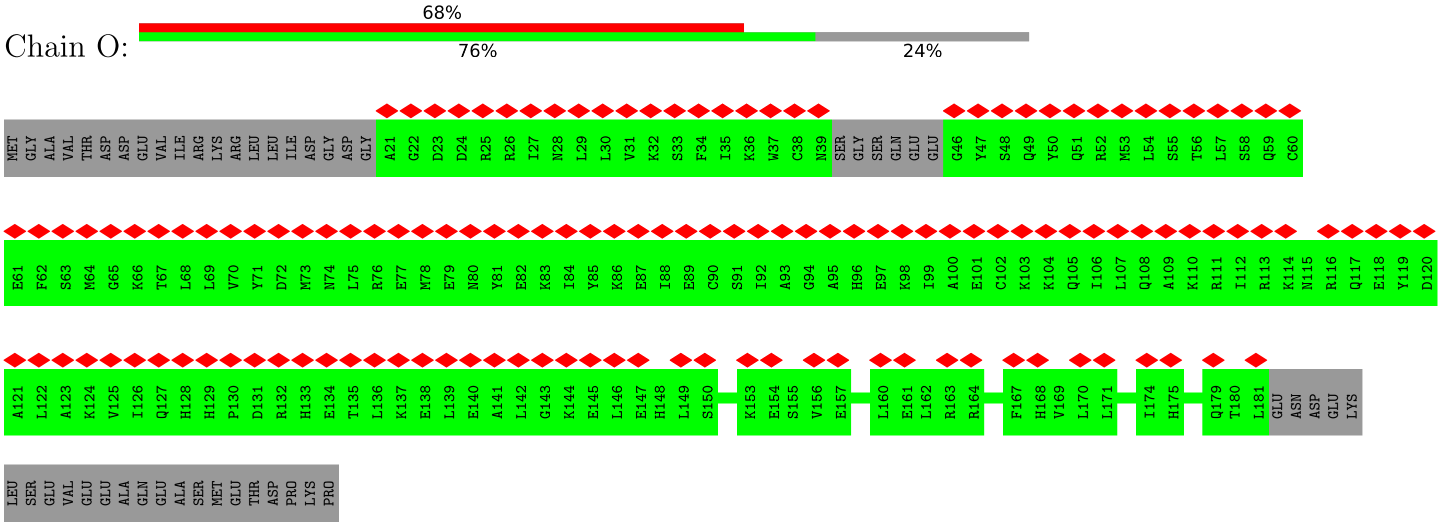
Chain n:



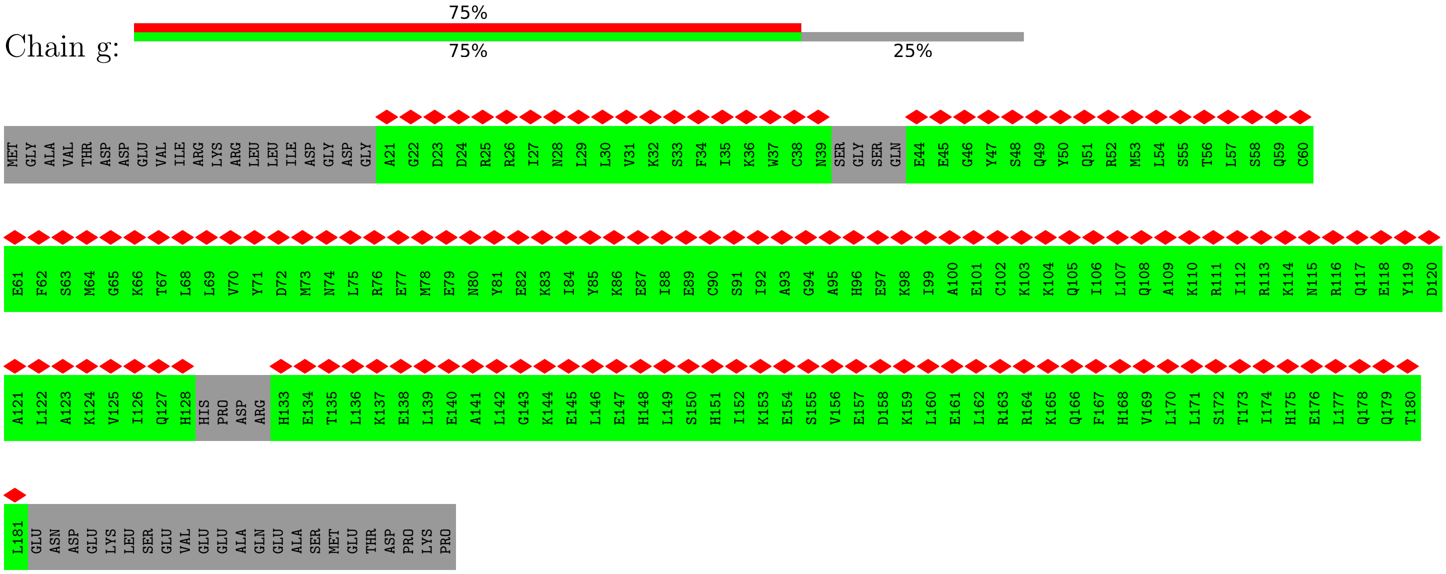
- Molecule 6: THO complex subunit 7 homolog



- Molecule 6: THO complex subunit 7 homolog

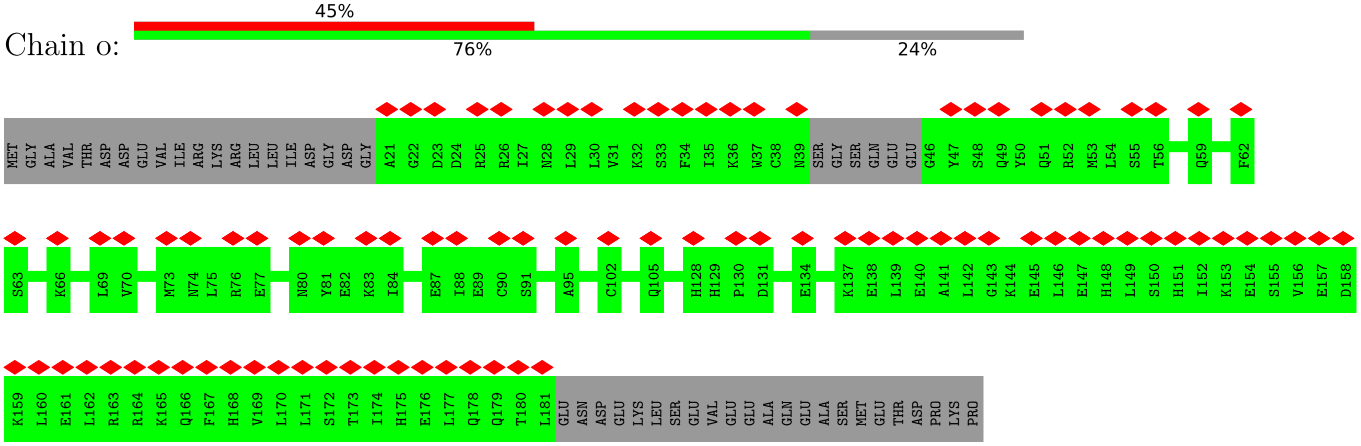


- Molecule 6: THO complex subunit 7 homolog



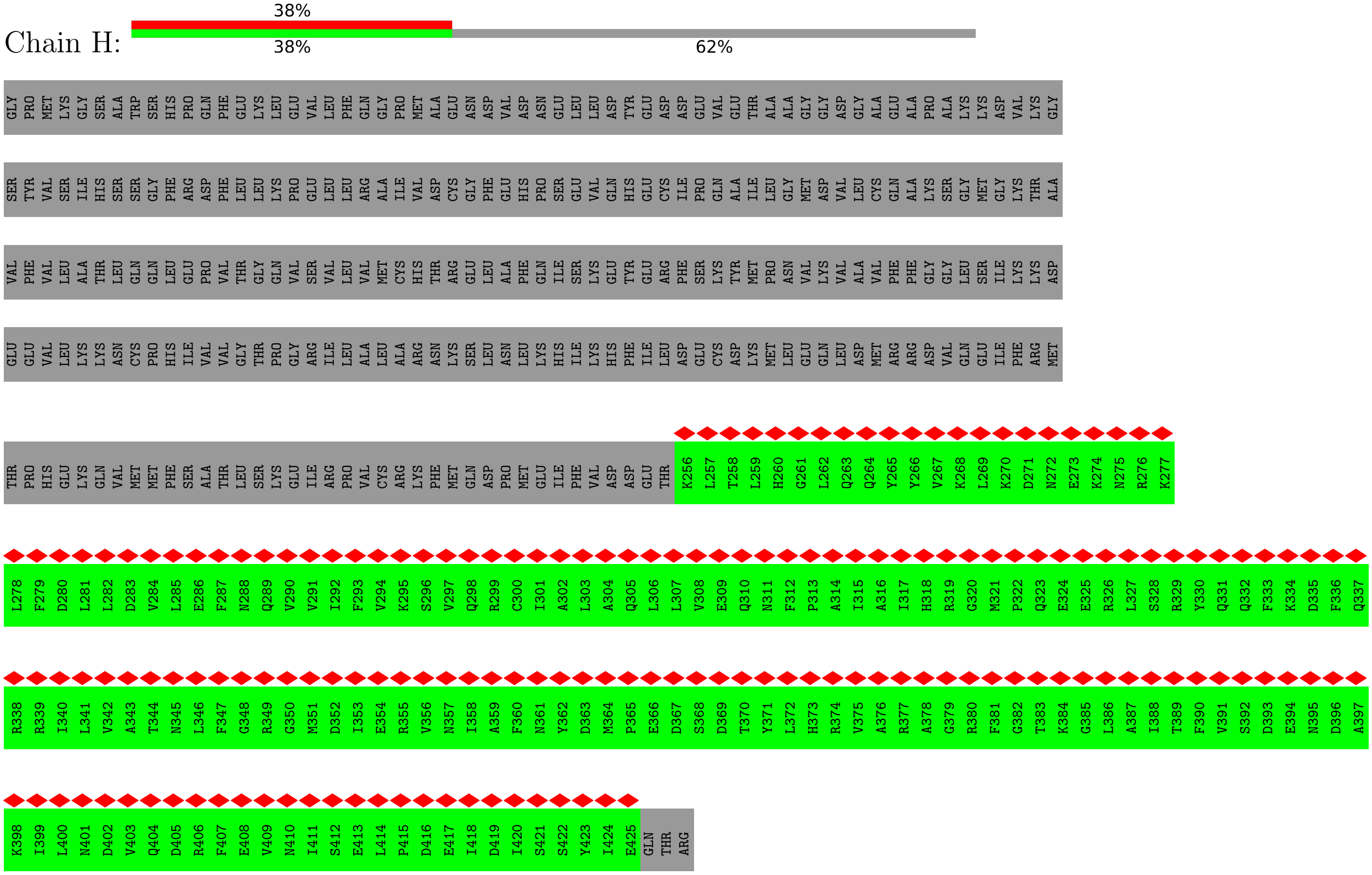
- Molecule 6: THO complex subunit 7 homolog

Chain o:



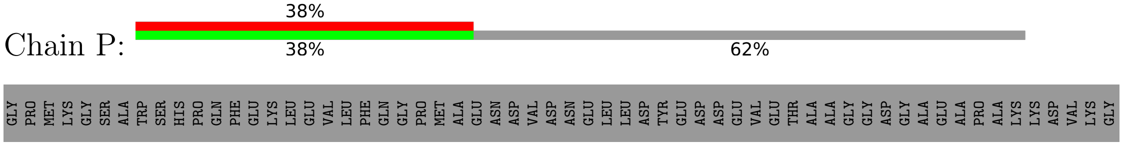
- Molecule 7: Spliceosome RNA helicase DDX39B

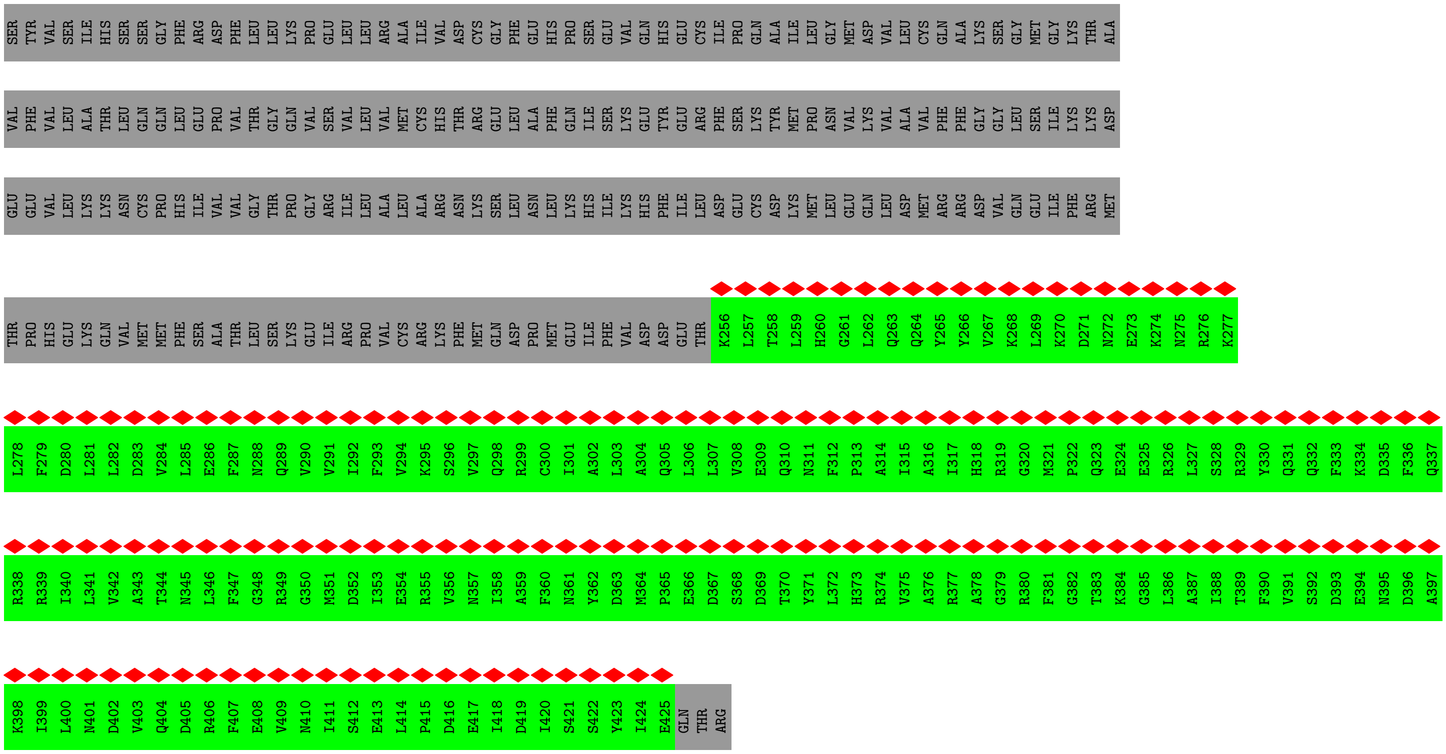
Chain H:



- Molecule 7: Spliceosome RNA helicase DDX39B

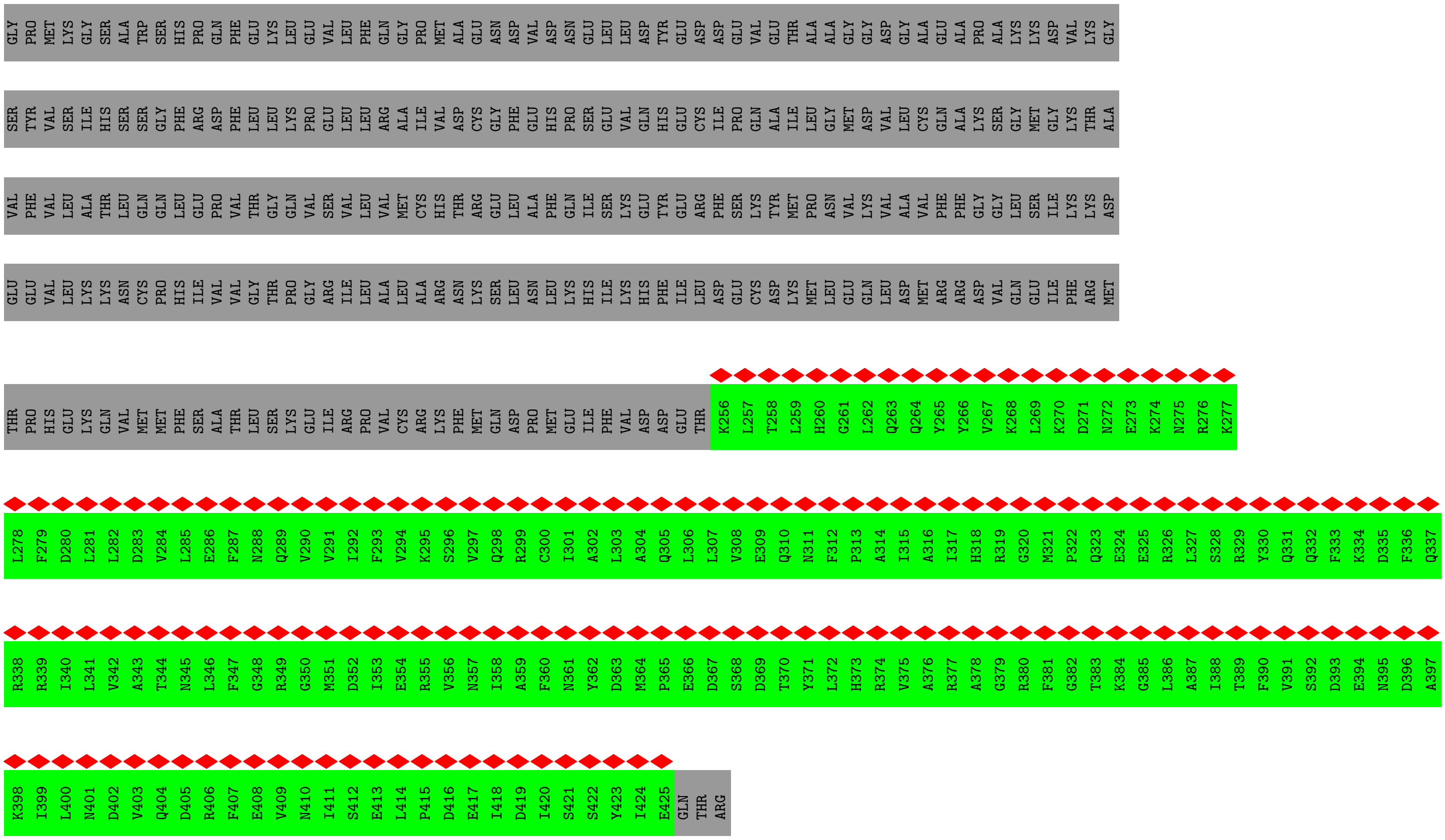
Chain P:



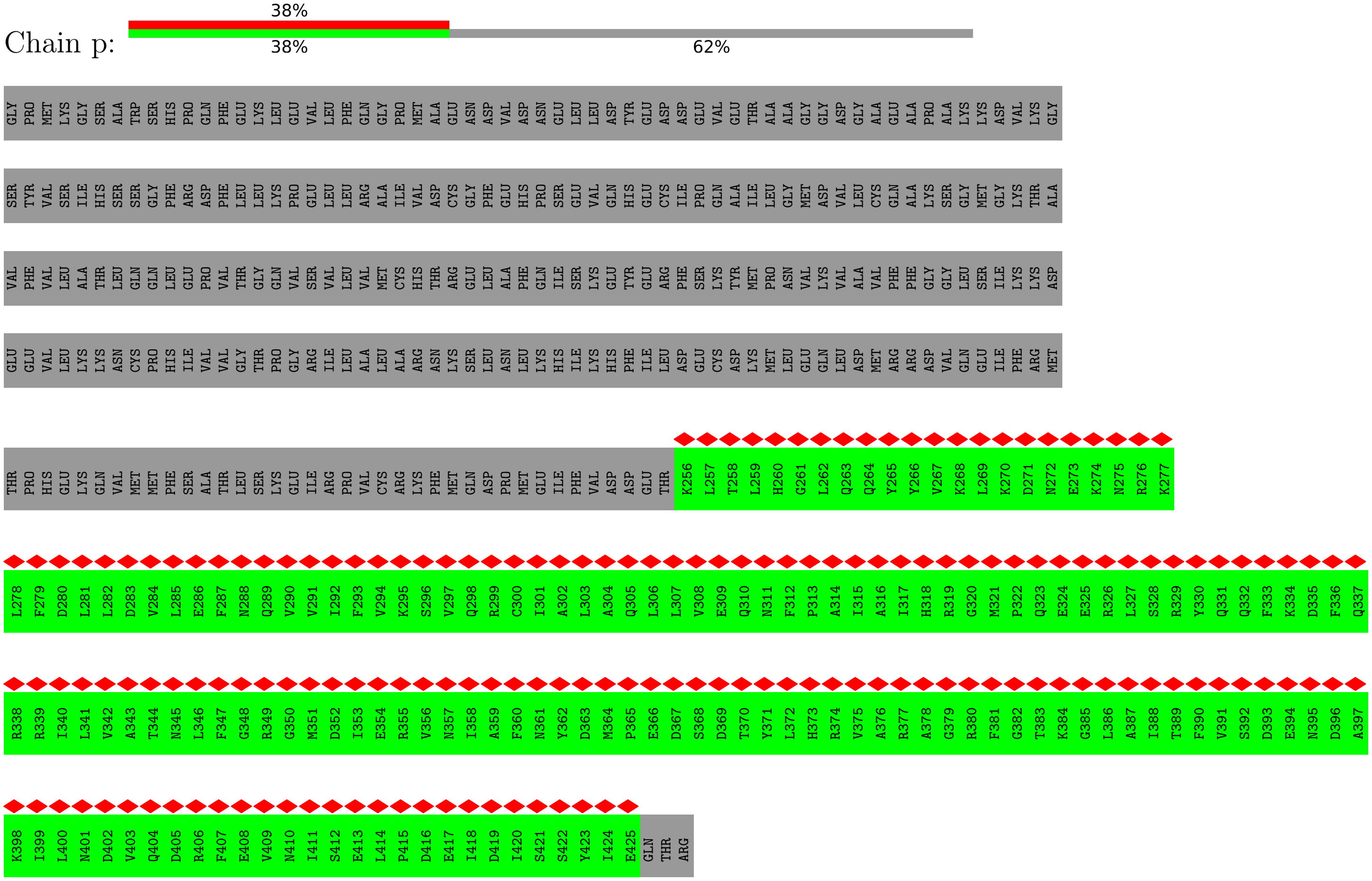


• Molecule 7: Spliceosome RNA helicase DDX39B

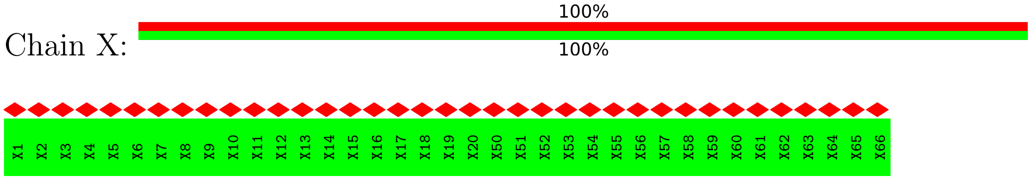
Chain h:



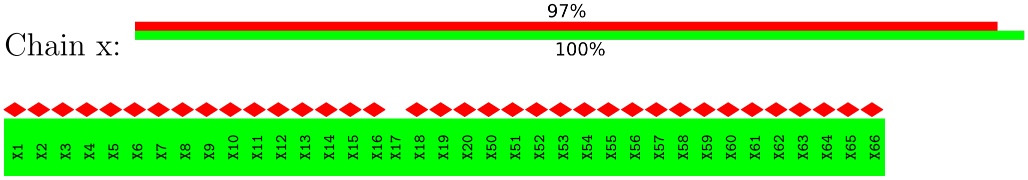
- Molecule 7: Spliceosome RNA helicase DDX39B



- Molecule 8: THOC2 anchor (putative)



- Molecule 8: THOC2 anchor (putative)



4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	195098	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)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.274	Depositor
Minimum map value	-0.103	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.05257	Depositor
Map size (Å)	589.60004, 589.60004, 589.60004	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	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	A	0.27	0/2204	0.45	0/2974
1	I	0.29	0/2268	0.48	0/3062
1	a	0.27	0/2204	0.45	0/2974
1	i	0.29	0/2269	0.48	0/3063
2	B	0.27	0/4741	0.45	2/6440 (0.0%)
2	J	0.28	0/4743	0.44	1/6444 (0.0%)
2	b	0.28	0/4741	0.45	2/6440 (0.0%)
2	j	0.27	0/4736	0.44	1/6435 (0.0%)
3	C	0.29	0/2404	0.56	0/3265
3	K	0.29	0/2404	0.56	0/3265
3	c	0.29	0/2404	0.56	0/3265
3	k	0.29	0/2404	0.56	0/3265
4	E	0.30	0/3754	0.49	0/5118
4	M	0.29	0/4301	0.49	0/5827
4	e	0.30	0/3661	0.48	0/4991
4	m	0.29	0/4301	0.49	0/5827
5	F	0.32	0/2666	0.57	0/3623
5	N	0.32	0/2666	0.56	0/3623
5	f	0.32	0/2596	0.57	0/3524
5	n	0.32	0/2666	0.57	0/3623
6	G	0.24	0/757	0.27	0/1052
6	O	0.27	0/1094	0.39	0/1476
6	g	0.24	0/757	0.27	0/1052
6	o	0.27	0/1094	0.39	0/1476
7	H	0.26	0/1421	0.44	0/1915
7	P	0.26	0/1421	0.44	0/1915
7	h	0.26	0/1421	0.44	0/1915
7	p	0.26	0/1421	0.44	0/1915
All	All	0.29	0/73519	0.49	6/99764 (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
2	B	0	2
2	J	0	2
2	b	0	2
2	j	0	2
3	C	0	2
3	K	0	2
3	c	0	2
3	k	0	2
4	M	0	1
4	m	0	1
All	All	0	18

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	b	278	LEU	CA-CB-CG	6.95	131.29	115.30
2	B	278	LEU	CA-CB-CG	6.92	131.21	115.30
2	J	610	ASP	CB-CG-OD2	5.33	123.09	118.30
2	B	610	ASP	CB-CG-OD2	5.17	122.96	118.30
2	b	610	ASP	CB-CG-OD2	5.17	122.96	118.30
2	j	610	ASP	CB-CG-OD2	5.16	122.95	118.30

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	562	LYS	Peptide
2	B	590	TYR	Peptide
3	C	319	ARG	Peptide
3	C	86	LYS	Peptide
2	J	562	LYS	Peptide
2	J	590	TYR	Peptide
3	K	319	ARG	Peptide
3	K	86	LYS	Peptide
4	M	660	ARG	Peptide
2	b	562	LYS	Peptide
2	b	590	TYR	Peptide
3	c	319	ARG	Peptide
3	c	86	LYS	Peptide
2	j	562	LYS	Peptide
2	j	590	TYR	Peptide

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Mol	Chain	Res	Type	Group
3	k	319	ARG	Peptide
3	k	86	LYS	Peptide
4	m	660	ARG	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	248/711 (35%)	239 (96%)	8 (3%)	1 (0%)	34	66
1	I	255/711 (36%)	241 (94%)	12 (5%)	2 (1%)	19	51
1	a	248/711 (35%)	240 (97%)	7 (3%)	1 (0%)	34	66
1	i	255/711 (36%)	241 (94%)	12 (5%)	2 (1%)	19	51
2	B	644/1226 (52%)	625 (97%)	19 (3%)	0	100	100
2	J	645/1226 (53%)	623 (97%)	22 (3%)	0	100	100
2	b	644/1226 (52%)	625 (97%)	19 (3%)	0	100	100
2	j	645/1226 (53%)	623 (97%)	22 (3%)	0	100	100
3	C	298/395 (75%)	273 (92%)	24 (8%)	1 (0%)	41	71
3	K	298/395 (75%)	273 (92%)	24 (8%)	1 (0%)	41	71
3	c	298/395 (75%)	273 (92%)	24 (8%)	1 (0%)	41	71
3	k	298/395 (75%)	273 (92%)	24 (8%)	1 (0%)	41	71
4	E	505/683 (74%)	479 (95%)	26 (5%)	0	100	100
4	M	529/683 (78%)	503 (95%)	26 (5%)	0	100	100
4	e	492/683 (72%)	470 (96%)	22 (4%)	0	100	100
4	m	529/683 (78%)	503 (95%)	26 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	F	335/341 (98%)	305 (91%)	29 (9%)	1 (0%)	41	71
5	N	335/341 (98%)	307 (92%)	27 (8%)	1 (0%)	41	71
5	f	325/341 (95%)	298 (92%)	26 (8%)	1 (0%)	41	71
5	n	335/341 (98%)	305 (91%)	29 (9%)	1 (0%)	41	71
6	G	147/204 (72%)	147 (100%)	0	0	100	100
6	O	151/204 (74%)	151 (100%)	0	0	100	100
6	g	147/204 (72%)	147 (100%)	0	0	100	100
6	o	151/204 (74%)	151 (100%)	0	0	100	100
7	H	168/451 (37%)	165 (98%)	3 (2%)	0	100	100
7	P	168/451 (37%)	165 (98%)	3 (2%)	0	100	100
7	h	168/451 (37%)	165 (98%)	3 (2%)	0	100	100
7	p	168/451 (37%)	165 (98%)	3 (2%)	0	100	100
All	All	9429/16044 (59%)	8975 (95%)	440 (5%)	14 (0%)	54	81

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	66	ASP
1	I	308	MET
3	K	66	ASP
3	c	66	ASP
1	i	308	MET
3	k	66	ASP
1	I	105	PRO
1	i	105	PRO
1	A	105	PRO
1	a	105	PRO
5	F	239	PRO
5	N	239	PRO
5	f	239	PRO
5	n	239	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	236/646 (36%)	236 (100%)	0	100	100
1	I	240/646 (37%)	240 (100%)	0	100	100
1	a	236/646 (36%)	236 (100%)	0	100	100
1	i	241/646 (37%)	241 (100%)	0	100	100
2	B	345/1105 (31%)	342 (99%)	3 (1%)	78	87
2	J	345/1105 (31%)	342 (99%)	3 (1%)	78	87
2	b	345/1105 (31%)	342 (99%)	3 (1%)	78	87
2	j	344/1105 (31%)	341 (99%)	3 (1%)	78	87
3	C	252/330 (76%)	252 (100%)	0	100	100
3	K	252/330 (76%)	252 (100%)	0	100	100
3	c	252/330 (76%)	252 (100%)	0	100	100
3	k	252/330 (76%)	252 (100%)	0	100	100
4	E	321/615 (52%)	320 (100%)	1 (0%)	92	96
4	M	424/615 (69%)	424 (100%)	0	100	100
4	e	311/615 (51%)	311 (100%)	0	100	100
4	m	424/615 (69%)	424 (100%)	0	100	100
5	F	284/287 (99%)	283 (100%)	1 (0%)	91	95
5	N	284/287 (99%)	283 (100%)	1 (0%)	91	95
5	f	276/287 (96%)	275 (100%)	1 (0%)	91	95
5	n	284/287 (99%)	283 (100%)	1 (0%)	91	95
6	O	85/184 (46%)	85 (100%)	0	100	100
6	o	85/184 (46%)	85 (100%)	0	100	100
7	H	153/400 (38%)	153 (100%)	0	100	100
7	P	153/400 (38%)	153 (100%)	0	100	100
7	h	153/400 (38%)	153 (100%)	0	100	100
7	p	153/400 (38%)	153 (100%)	0	100	100
All	All	6730/13900 (48%)	6713 (100%)	17 (0%)	92	96

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	204	ASN
2	B	560	ASN
2	B	657	LEU
4	E	524	THR
5	F	177	ARG
2	J	204	ASN
2	J	560	ASN
2	J	657	LEU
5	N	177	ARG
2	b	204	ASN
2	b	560	ASN
2	b	657	LEU
5	f	177	ARG
2	j	204	ASN
2	j	560	ASN
2	j	657	LEU
5	n	177	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	242	GLN
1	A	320	HIS
1	A	380	HIS
2	B	204	ASN
2	B	224	HIS
2	B	518	GLN
2	B	560	ASN
2	B	588	GLN
2	B	608	ASN
2	B	667	GLN
3	C	316	HIS
4	E	274	GLN
4	E	369	ASN
4	E	465	HIS
4	E	492	GLN
4	E	675	HIS
5	F	130	ASN
5	F	149	GLN
5	F	172	HIS
5	F	261	GLN
7	H	288	ASN
7	H	357	ASN

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Mol	Chain	Res	Type
7	H	404	GLN
1	I	242	GLN
2	J	204	ASN
2	J	224	HIS
2	J	518	GLN
2	J	560	ASN
2	J	588	GLN
2	J	608	ASN
2	J	667	GLN
3	K	316	HIS
4	M	369	ASN
4	M	492	GLN
4	M	675	HIS
5	N	149	GLN
5	N	172	HIS
5	N	261	GLN
7	P	288	ASN
7	P	357	ASN
7	P	404	GLN
1	a	242	GLN
1	a	320	HIS
1	a	380	HIS
2	b	204	ASN
2	b	224	HIS
2	b	518	GLN
2	b	560	ASN
2	b	588	GLN
2	b	608	ASN
2	b	667	GLN
3	c	316	HIS
4	e	274	GLN
4	e	369	ASN
4	e	492	GLN
4	e	675	HIS
5	f	130	ASN
5	f	172	HIS
5	f	261	GLN
7	h	288	ASN
7	h	357	ASN
7	h	404	GLN
1	i	242	GLN
2	j	204	ASN

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Mol	Chain	Res	Type
2	j	224	HIS
2	j	518	GLN
2	j	560	ASN
2	j	588	GLN
2	j	608	ASN
2	j	667	GLN
3	k	316	HIS
4	m	369	ASN
4	m	492	GLN
4	m	675	HIS
5	n	149	GLN
5	n	172	HIS
5	n	261	GLN
7	p	288	ASN
7	p	357	ASN
7	p	404	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

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 ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	X	1
8	x	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	X	20:UNK	C	50:UNK	N	23.23
1	x	20:UNK	C	50:UNK	N	23.23

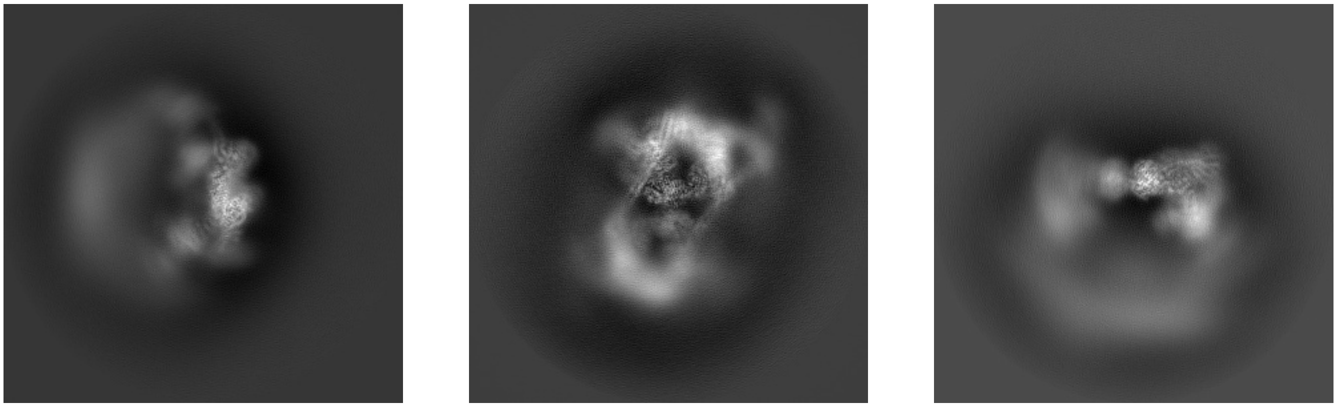
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-11857. 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

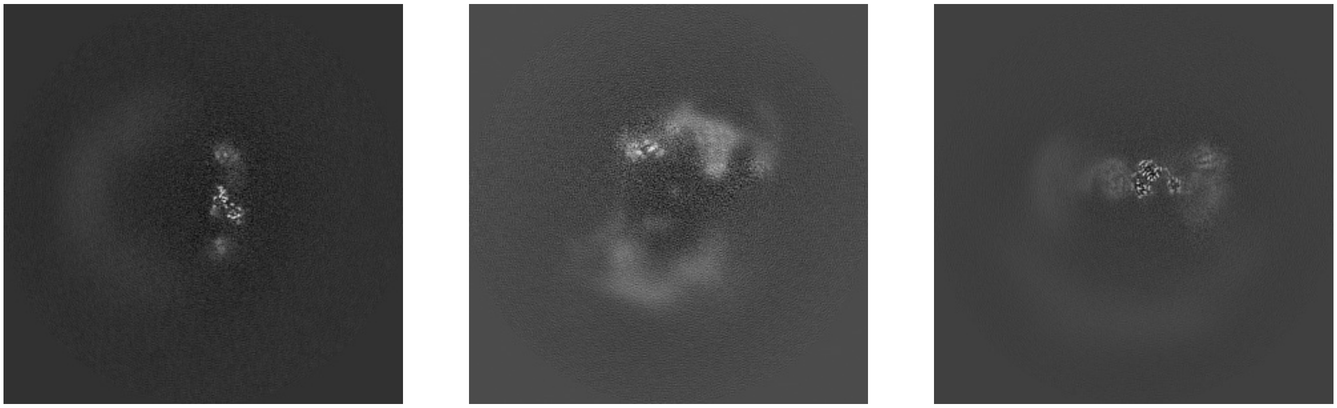


X Y Z

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

6.2 Central slices (i)

6.2.1 Primary map



X Index: 220 Y Index: 220 Z Index: 220

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

6.3 Largest variance slices

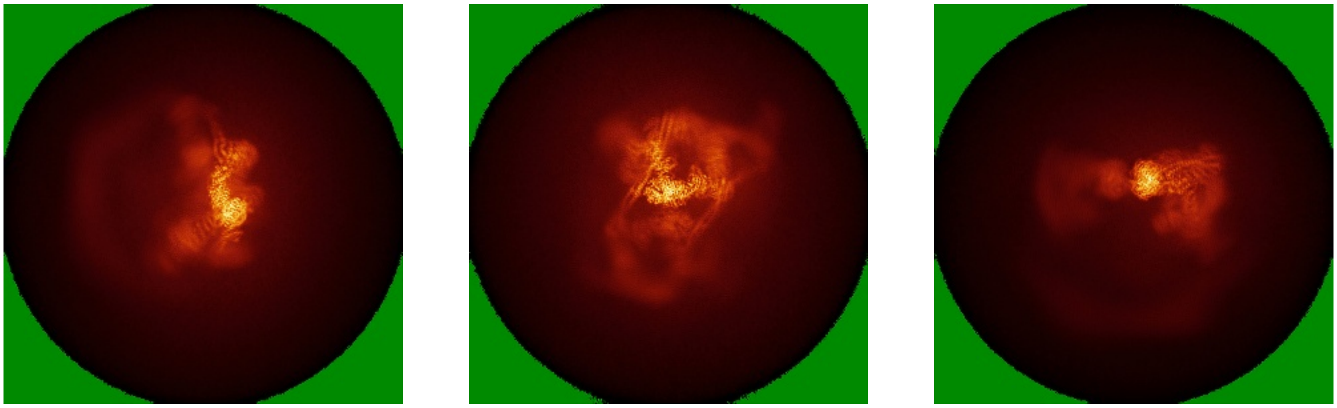
6.3.1 Primary map

X Index: 236 Y Index: 243 Z Index: 218

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

6.4 Orthogonal standard-deviation projections (False-color)

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 ⓘ

6.5.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.05257. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

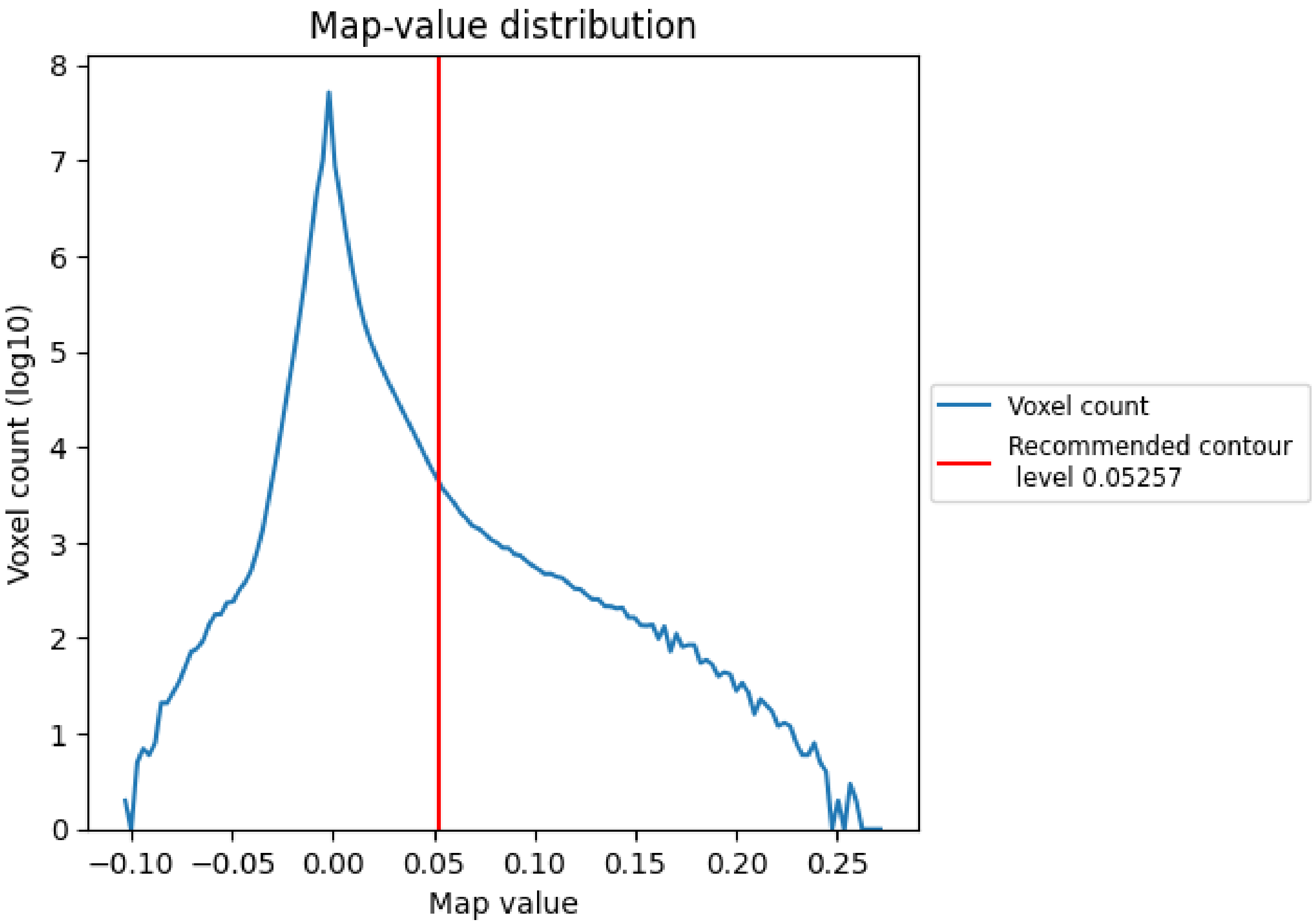
6.6 Mask visualisation ⓘ

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

7 Map analysis ⓘ

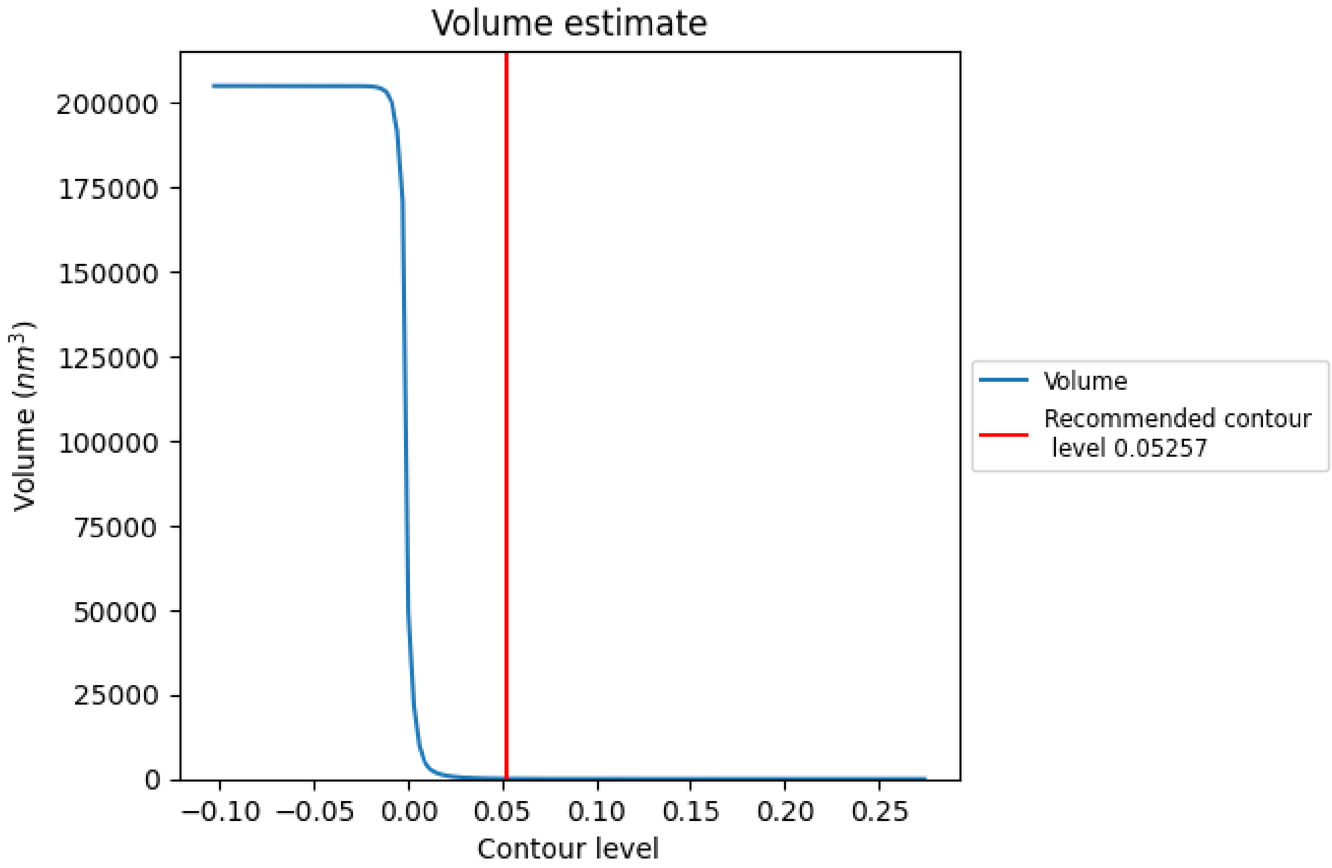
This section contains the results of statistical analysis of the map.

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.

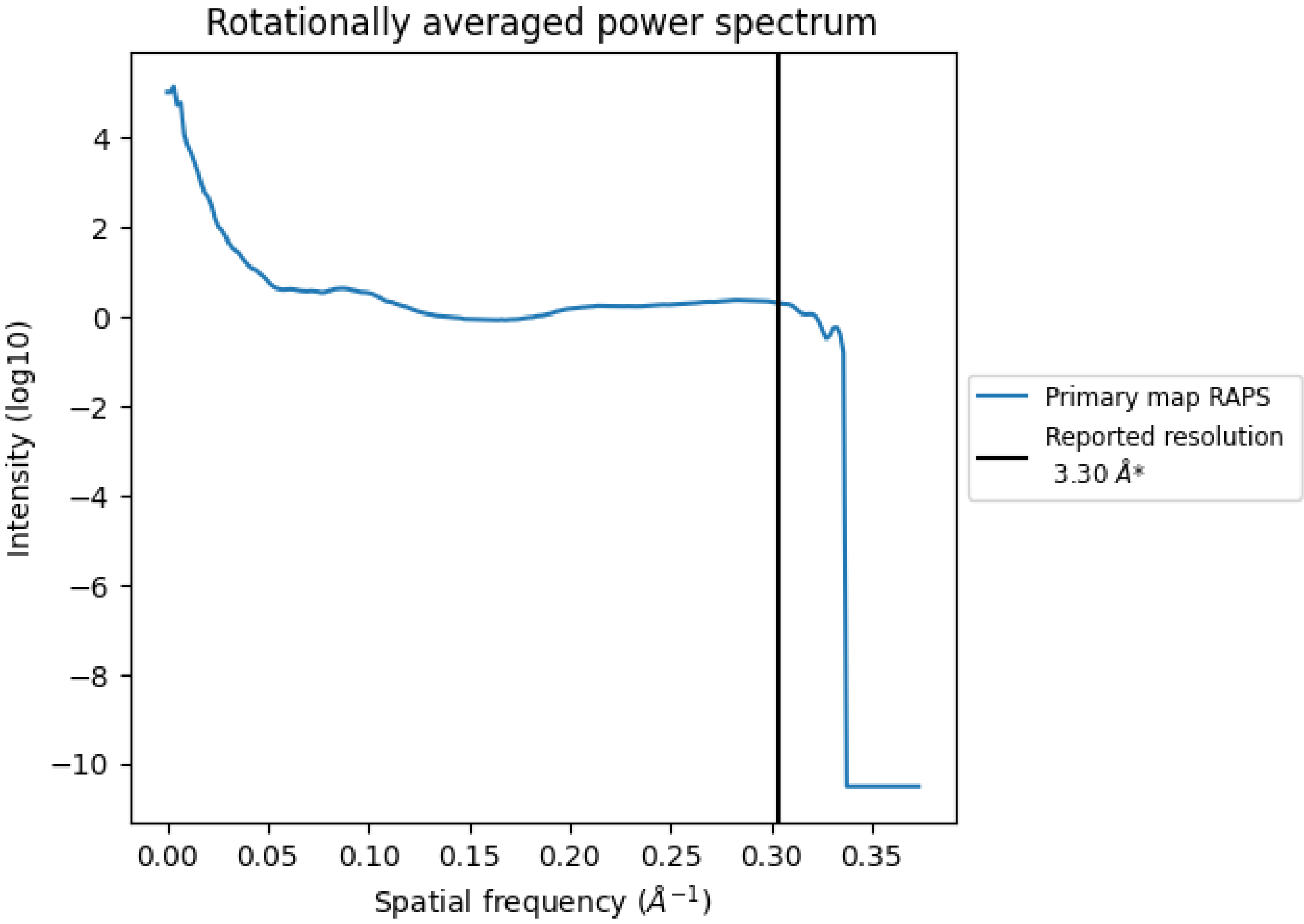
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 81 nm^3; this corresponds to an approximate mass of 73 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 0.303 Å^{-1}

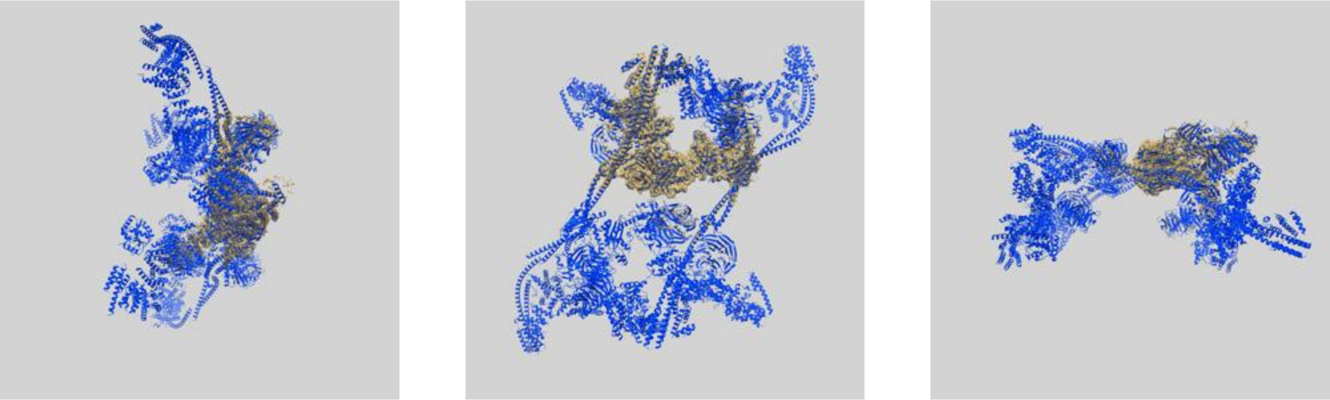
8 Fourier-Shell correlation ⓘ

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-11857 and PDB model 7APK. Per-residue inclusion information can be found in section 3 on page 21.

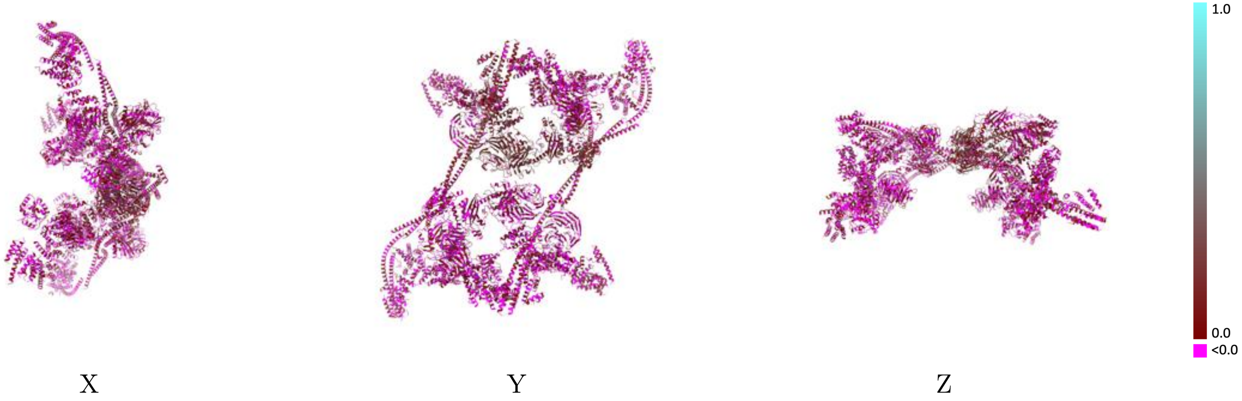
9.1 Map-model overlay ⓘ



X Y Z

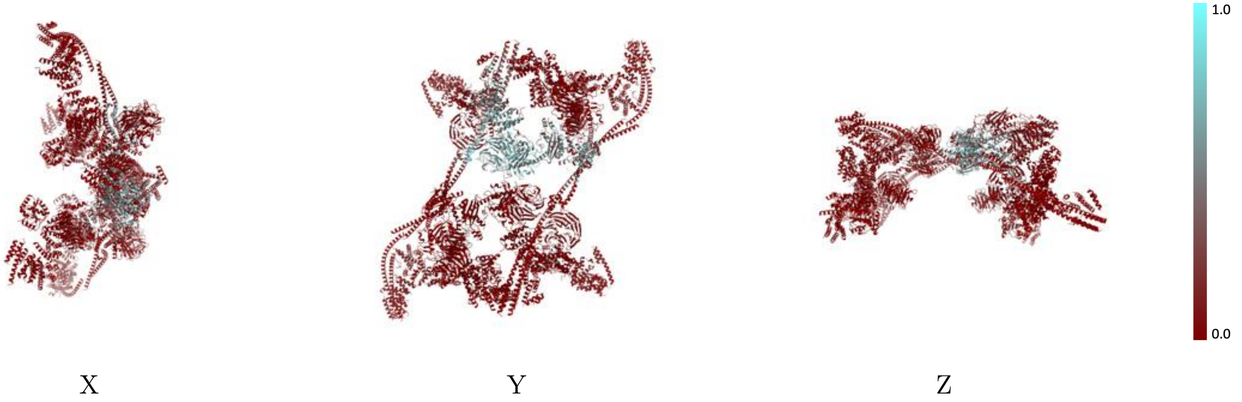
The images above show the 3D surface view of the map at the recommended contour level 0.05257 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model



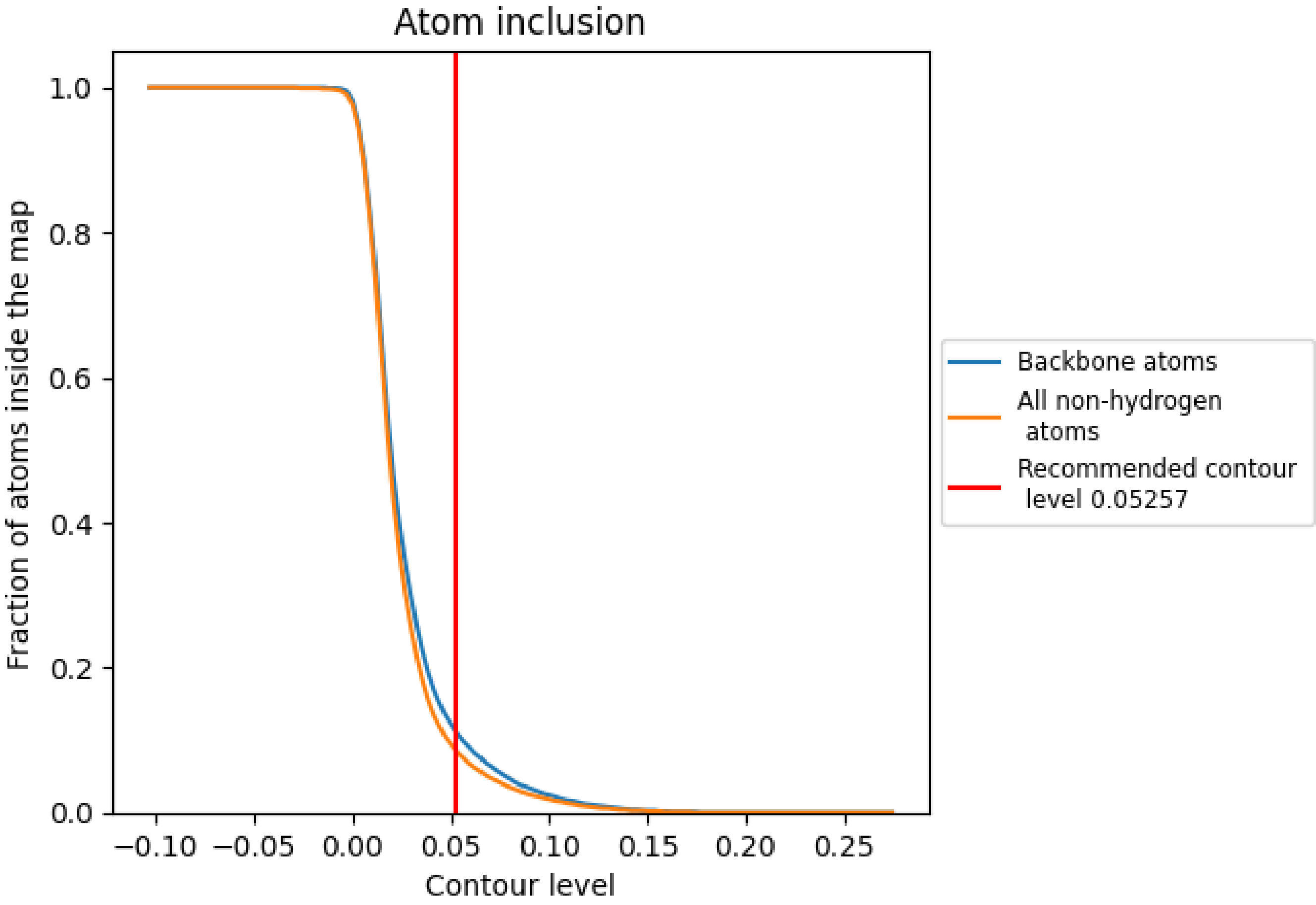
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05257).

9.4 Atom inclusion ⓘ



At the recommended contour level, 11% of all backbone atoms, 9% 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 (0.05257) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.0860	0.0510
A	0.0000	0.0080
B	0.0020	0.0250
C	0.0010	0.0280
E	0.4380	0.1750
F	0.5720	0.2190
G	0.0720	0.0750
H	0.0000	0.0090
I	0.0000	0.0160
J	0.0000	0.0050
K	0.0000	0.0090
M	0.1570	0.0950
N	0.0240	0.0450
O	0.0900	0.0620
P	0.0000	-0.0090
X	0.0000	0.0070
a	0.0000	0.0080
b	0.0000	0.0090
c	0.0000	0.0010
e	0.0030	0.0340
f	0.0140	0.0160
g	0.0000	0.0560
h	0.0000	0.0210
i	0.3650	0.1810
j	0.1100	0.0780
k	0.0090	0.0270
m	0.1060	0.0600
n	0.0000	0.0190
o	0.3590	0.1470
p	0.0000	-0.0050
x	0.0540	0.0840