



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 05:41 AM UTC

PDB ID : 7ZNL / pdb_00007znl
EMDB ID : EMD-14808
Title : Structure of the human TREX core THO-UAP56 complex
Authors : Pacheco-Fiallos, F.B.; Vorlaender, M.K.; Plaschka, C.
Deposited on : 2022-04-21
Resolution : 3.45 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

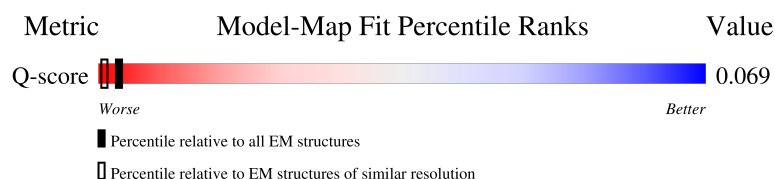
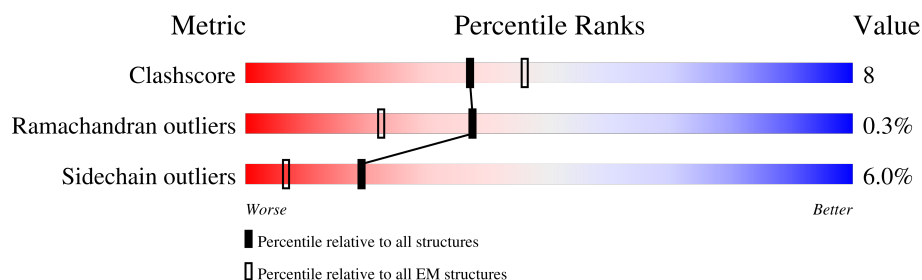
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.45 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13836 (2.95 - 3.95)

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 $\leq 5\%$. 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	657	
1	I	657	
1	a	657	
1	i	657	

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Mol	Chain	Length	Quality of chain
2	B	1593	
2	J	1593	
2	b	1593	
2	j	1593	
3	C	351	
3	K	351	
3	c	351	
3	k	351	
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	428	
7	P	428	
7	h	428	
7	p	428	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 84821 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	356	Total	C	N	O	S	0	0
			2889	1864	481	531	13		
1	I	363	Total	C	N	O	S	0	0
			2935	1894	489	539	13		
1	a	356	Total	C	N	O	S	0	0
			2889	1864	481	531	13		
1	i	363	Total	C	N	O	S	0	0
			2936	1894	489	540	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	919	Total	C	N	O	S	0	0
			7012	4486	1206	1278	42		
2	J	914	Total	C	N	O	S	0	0
			6956	4452	1194	1268	42		
2	b	919	Total	C	N	O	S	0	0
			7012	4486	1206	1278	42		
2	j	914	Total	C	N	O	S	0	0
			6956	4452	1194	1268	42		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	309	Total	C	N	O	S	0	0
			2433	1538	423	457	15		
3	K	309	Total	C	N	O	S	0	0
			2433	1538	423	457	15		
3	c	309	Total	C	N	O	S	0	0
			2433	1538	423	457	15		
3	k	309	Total	C	N	O	S	0	0
			2433	1538	423	457	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	538	Total	C	N	O	S	0	0
			3763	2383	663	696	21		
4	M	549	Total	C	N	O	S	0	0
			4134	2634	725	752	23		
4	e	527	Total	C	N	O	S	0	0
			3674	2327	649	679	19		
4	m	549	Total	C	N	O	S	0	0
			4134	2634	725	752	23		

- 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	0	0
			2604	1647	459	483	15		
5	N	337	Total	C	N	O	S	0	0
			2604	1647	459	483	15		
5	f	329	Total	C	N	O	S	0	0
			2537	1604	448	470	15		
5	n	337	Total	C	N	O	S	0	0
			2604	1647	459	483	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	161	Total	C	N	O		0	0
			800	478	161	161			
6	O	164	Total	C	N	O	S	0	0
			1129	696	210	216	7		
6	g	161	Total	C	N	O		0	0
			800	478	161	161			
6	o	164	Total	C	N	O	S	0	0
			1129	696	210	216	7		

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

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

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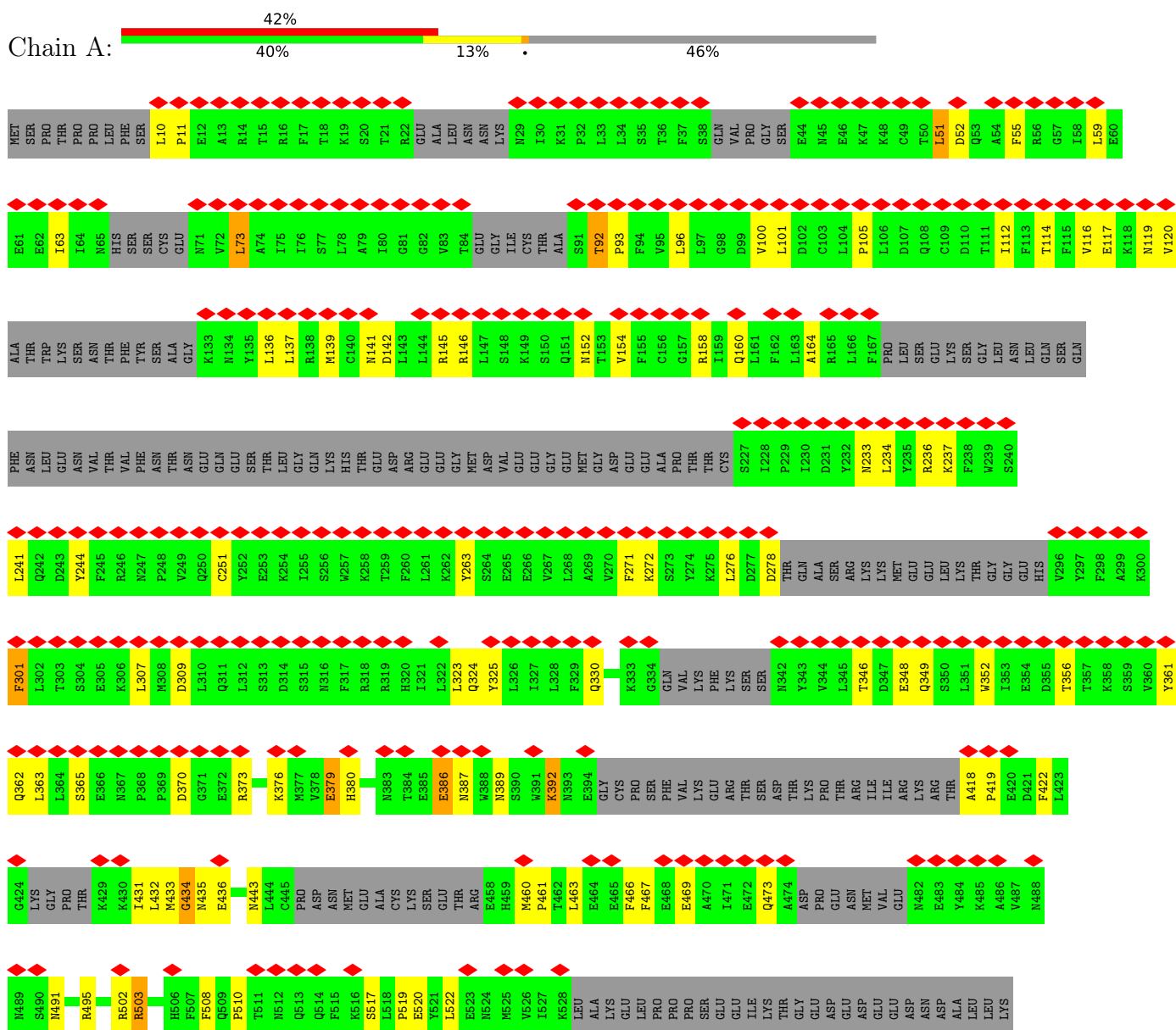
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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	p	170	1398	888	245	261	4	0	0

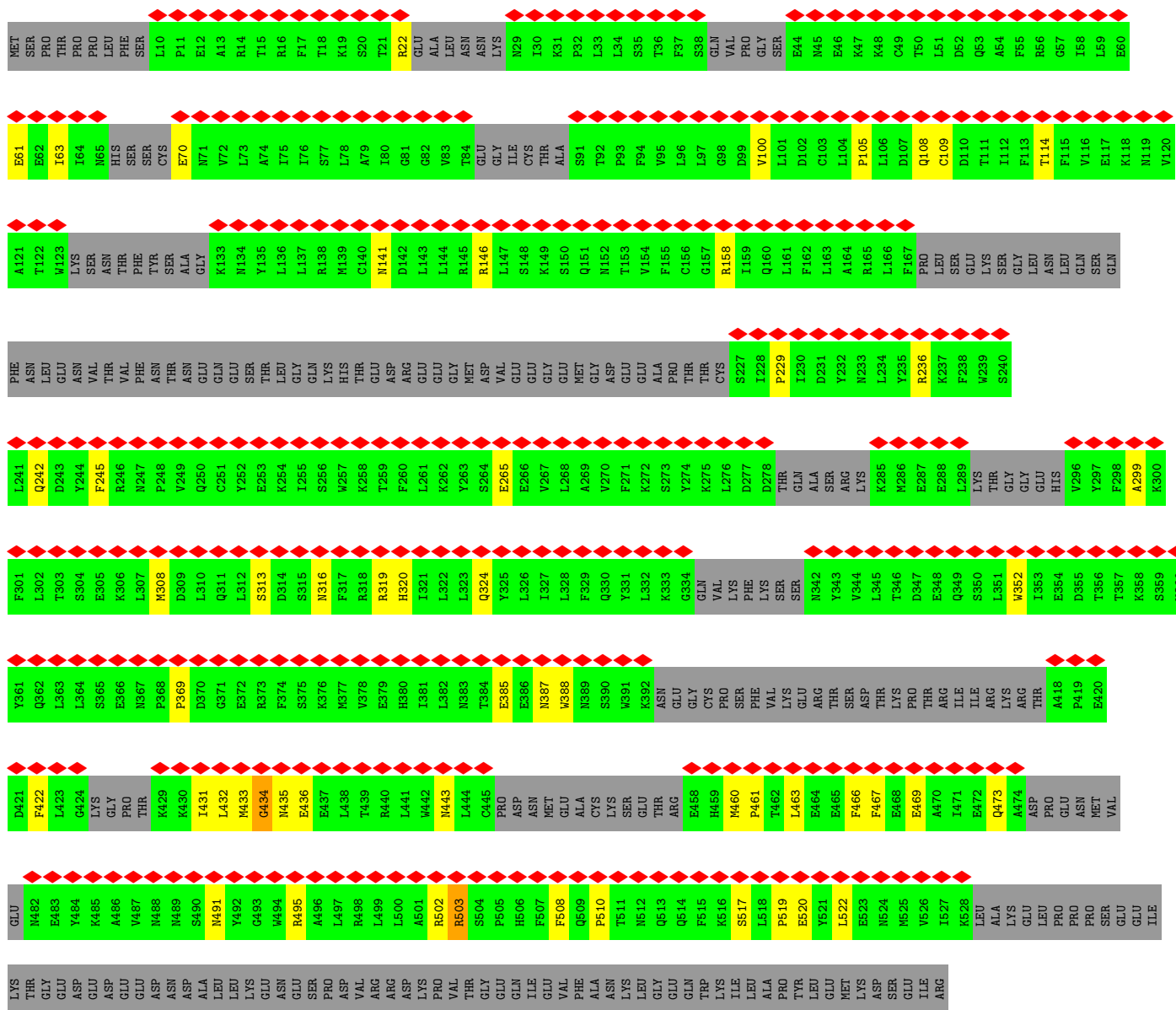
3 Residue-property plots

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: THO complex subunit 1



- Molecule 1: THO complex subunit 1



- Molecule 1: THO complex subunit 1





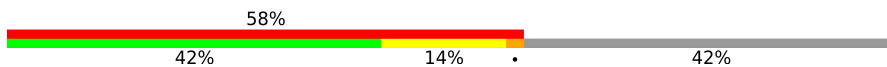






• Molecule 2: THO complex subunit 2

Chain b:



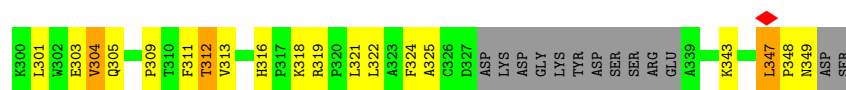
THR	Q181	P241	R301	A361	A421	S481	V541	L601	L661	M721
VAL	D182	Q242	E302	Q362	E422	C482	K542	K602	Q662	T722
LEU	L183	T243	I303	N363	S423	L483	A543	K603	Y663	K723
ALA	GLY	L244	A304	I364	F424	L484	Q544	L604	V664	K724
ARG	ASP	C245	E305	M365	E425	S485	T545	K605	A665	S725
VAL	LEU	H246	A306	D366	D426	L486	T546	S606	N666	S726
PRO	ASP	I247	K307	Q367	L427	T487	D547	L607	Q667	Q727
GLU	LEU	L248	Q308	M368	R428	D488	R548	N608	L668	R728
TRP	GLU	G249	VAL	P369	D429	A489	A549	Y609	K669	L729
ILE	LEU	F250	ARG	P370	R430	V490	K550	D610	A670	K730
K14	I73	K251	LYS	Y371	V431	L491	Y551	V611	G671	D731
N15	S74	F252	THR	Y372	F432	L492	T552	L612	K672	A732
W16	E75	K253	MET	A373	N433	P493	M553	A613	S673	L733
E17	F76	F254	VAL	A374	M434	S494	K554	V614	P674	L734
K18	R77	Y255	VAL	S375	F435	L495	R555	C615	D675	D735
S19	E78	Q256	LEU	H376	C436	S496	L556	T616	L676	H736
G20	M80	E257	SER	K377	Y437	L497	T557	L617	L677	D737
R21	PRU	S198	SER	L378	L438	M498	K558	E618	L678	L738
G22	SER	I200	LYS	L379	G439	D499	E559	A619	L679	A739
E23	I83	G201	ASP	A380	P440	C500	N560	L620	K680	L740
PHE	L84	C202	GLU	L381	H441	N501	V561	A621	E681	F741
LEU	A85	F203	ARG	A382	L442	A502	K562	K622	V682	L742
HIS	D86	N204	GLU	I383	S443	C503	P563	F623	V683	C743
LEU	V87	L205	GLU	C384	H444	M504	S564	GLY	D684	L744
CYS	D206	L206	LYS	K385	D445	S505	G565	LYS	K685	L745
ARG	F88	K150	GLU	L386	P446	E506	R566	ARG	M686	M746
ILE	C89	I151	GLU	L387	I447	E507	Q567	MET	A687	A747
LEU	N208	R268	GLU	H388	L448	L508	I568	K629	G688	Q748
SER	I90	V269	GLU	T389	F449	W509	G569	H630	L689	Q749
GLU	L91	A270	GLU	L390	A450	G510	K570	D631	E690	R750
ASN	D92	A271	LYS	I391	K451	M511	L571	D632	T691	M751
LYS	I93	V272	VAL	S392	V452	F512	S572	T633	THR	G752
HIS	E94	L155	GLU	P393	R453	K513	H573	T634	GLU	V753
ASP	T95	Y157	PRO	L394	R454	T514	S574	T635	E694	V754
S39	N96	K158	ASP	Y395	I455	F515	N575	T636	M695	F755
S40	C97	Q159	PRO	R396	G456	P516	P576	T637	T696	G756
T41	L98	Q160	ASP	R397	K457	Y517	T577	M638	M697	E757
Y42	E99	K161	ASP	V398	S458	Q518	F578	L639	E698	E758
R43	E100	F162	ASP	G399	F459	H519	L579	Q640	Q699	G759
D44	LYS	M163	ASP	V400	M460	R520	F580	S641	L700	L760
F45	LYS	L164	ASP	P401	K461	Y521	D581	L642	E701	K761
Q46	ARG	L165	ASP	K402	E462	R522	R582	A643	A702	H762
Q47	ASP	R166	ASP	G403	F463	L523	L583	S644	H703	L763
A48	TYR	E167	ASP	A404	Q464	Y524	L584	F645	T704	K764
L49	F107	E168	ASP	K405	S465	G525	S585	C646	GLY	L765
Y50	T108	N169	ASP	G406	ASP	Q526	Q586	Q647	GLY	V766
E51	Q109	E170	ASP	S407	GLY	W527	L587	A648	E707	G767
L52	L110	G171	ASP	P408	LYS	K528	Q588	V649	Q708	K768
S63	V111	L112	ASP	V409	GLN	N529	K589	F650	L709	L769
Y54	A113	C114	ASP	N410	ASP	E530	Y590	K652	K710	Y770
H55	L115	L116	ASP	A411	K473	T531	D591	V653	A711	D771
V56	I57	Y117	ASP	L412	E474	Y532	N592	P654	E712	G772
I57	L117	A177	ASP	Q413	K475	N533	L593	T654	GLY	C773
LYS	V118	E178	ASP	N414	T476	S534	T594	I655	TVR	H774
GLY	S119	L179	ASP	K415	E477	H535	T595	D656	PHE	D775
ASN	ASP	G180	ASP	R416	V478	P536	P596	L657	GLY	T776
				E298	I479	L537	V597	A658	ILE	L777
				C239	K419	V539	D599	L660		V778
				E240	Q420	K540	S600			R779
										F780

LYS	GLN	GLN	HIS	GLU	GLY	ALA	ARG	SER	ASN	VAL	LEU	SER	D72	I73	S74	E75	F76	R77	E78	D79	M80	PRO	SER	I83	L84	A85	D86	V87	F88	C89	I90	L91	D92	I93	E94	T95	N96	C97	L98	E99	E100	LYS	SER	LYS	ARG	ASP	TYR	F107	T108	Q109	L110	V111	L112	A113	C114	L115	Y116	L117	V118	S119	ASP
THR	VAL	LEU	LYS	GLU	GLY	ARG	LEU	ASP	PRO	GLU	THR	LEU	Q142	Q143	F144	N145	Q146	K147	S148	V149	K150	I151	K152	T153	K154	L155	F156	Y157	K158	GLN	GLN	PHE	ASN	L164	L165	R166	E167	E168	N169	E170	G171	Y172	A173	K174	L175	L176	A177	E178	L179	G180											
Q181	D182	L183	SER	GLY	SER	ILE	T188	S189	D190	L191	I192	L193	E194	N195	I196	K197	S198	L199	I200	G201	C202	F203	N204	L205	D206	P207	N208	R209	L210	L211	D212	V213	I214	L215	E216	V217	F218	E219	C220	R221	P222	E223	H224	D225	D226	F227	F228	L229	P230	L231	L232	E233	S234	Y235	M236	S237	M238	C239	E240		
P241	Q242	T243	L244	H245	H246	I247	L248	G249	K251	F252	K253	L254	Y255	Q256	E257	PRO	ASN	GLY	GLU	T262	P263	S264	S265	L266	Y267	R268	V269	A270	A271	V272	L273	L274	Q275	F276	N277	L278	I279	D280	L281	D282	D283	L284	Y285	V286	H287	L288	L289	A291	D292	N293	C294	I295	M296	D297	E298	H299	K300				
R301	E302	I303	A304	E305	A306	K307	Q308	ILE	VAL	ARG	LYS	THR	LEU	MET	VAL	LEU	SER	SER	GLU	LYS	MET	ASP	GLU	ARG	GLU	LYS	GLU	GLY	PRO	PRD	N343	Q344	G345	L346	G347	L348	L349	E350	A351	L352	L353	K354	I355	G356	D357	V358	L359	H360													
A361	Q362	N363	L364	M365	D366	Q367	M368	P369	P370	Y371	Y372	A373	A374	S375	H376	K377	L378	I379	A380	L381	A382	I383	C384	K385	L386	I387	H388	T389	G390	I391	E392	L393	Y395	R396	R397	V398	G399	V400	F401	G402	G403	A404	K405	G406	S407	P408	V409	N410	A411	L412	Q413	N414	K415	R416	A417	P418	K419	Q420			
A421	E422	S423	F424	E425	D426	L427	R428	R429	D430	V431	F432	M433	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	F462	F463	Q464	S465	ASP	GLY	SER	GLN	ASP	K473	E474	K475	L476	E477	V478	L479	L480				
S481	C482	L483	L484	S485	L486	T487	D488	Q489	V490	L491	L492	P493	S494	L495	S496	L497	M498	D499	C500	N501	A502	C503	M504	S505	E506	E507	L508	N509	M510	N511	F512	K513	T514	F515	P516	V517	Q518	H519	R520	Y521	R522	L523	Y524	G525	Q526	N527	K528	N529	E530	T531	Y532	N533	S534	H535	P536	L537	L538	V539	K540		
V541	K542	A543	Q544	T545	L546	D547	R548	A549	K550	Y551	L552	M553	K554	R555	L556	T557	K558	E559	N560	V561	K562	P563	S564	G565	R566	Q567	I568	G569	L570	L571	S572	H573	S574	N575	P576	T577	L578	L579	F580	D581	Y582	L583	L584	S585	Q586	L587	Q588	K589	Y590	D591	N592	L593	T594	T595	P596	V597	V598	D599	S600		
L601	K602	Y603	L604	T605	S606	L607	N608	Y609	D610	V611	L612	A613	Y614	S615	I616	L617	E618	A619	L620	A621	N622	P623	GLU	LYS	GLU	ARG	MET	K629	H630	D631	D632	T633	T634	L635	S636	S637	V638	L639	Q640	S641	L642	A643	S644	F645	C646	A648	V649	F650	R651	K652	P653	P654	L655	D656	L657	A658	G659	L660			
L661	Q662	Y663	V664	A665	N666	Q667	L668	K669	A670	G671	K672	S673	F674	D675	L676	L677	L678	L679	K680	E681	V682	V683	Q684	K685	M686	A687	G688	L689	E690	T691	THR	GLU	E694	M695	T696	M697	E698	Q699	L700	E701	A702	M703	T704	GLY	GLY	E707	Q708	L709	K710	A711	E712	G713	GLY	TYR	PHE	GLY	ILE	R720			
M721	T722	K723	K724	S725	S726	Q727	R728	Y729	K730	D731	A732	L733	L734	D735	H736	D737	L738	A739	L740	F741	L742	G743	L744	L745	M746	A747	Q748	Q749	R750	M751	G752	V753	L754	F755	Q756	E757	G758	GLY	GLU	K761	H762	L763	K764	L765	V766	G767	K768	L769	Y770	D771	Q772	H774	D775	T776	V778	Q779	F780				
G781	G782	F783	L784	A785	S786	M787	L788	S789	T790	E791	D792	Y793	L794	K795	R796	Y797	P798	S799	I800	D801	S802	L803	C804	N805	E806	F807	H808	T809	P810	H811	D812	A813	A814	F815	F816	L817	S818	R819	P820	M821	H822	A823	HIS	HIS	ILE	SER	LYS	TYR	ASP	GLU	LEU	LYS	LYS	SER	GLU	LYS	GLY	SER			
V860	H861	E862	A863	V864	V865	S866	L867	H868	SER	LYS	VAL	TRP	ASP	ASP	ILE	S877	P878	Q879	F880	Y881	A882	T883	F884	W885	S886	L887	T888	M889	Y890	D891	L892	A893	V894	P895	HIS	T899	S900	Y901	E902																						

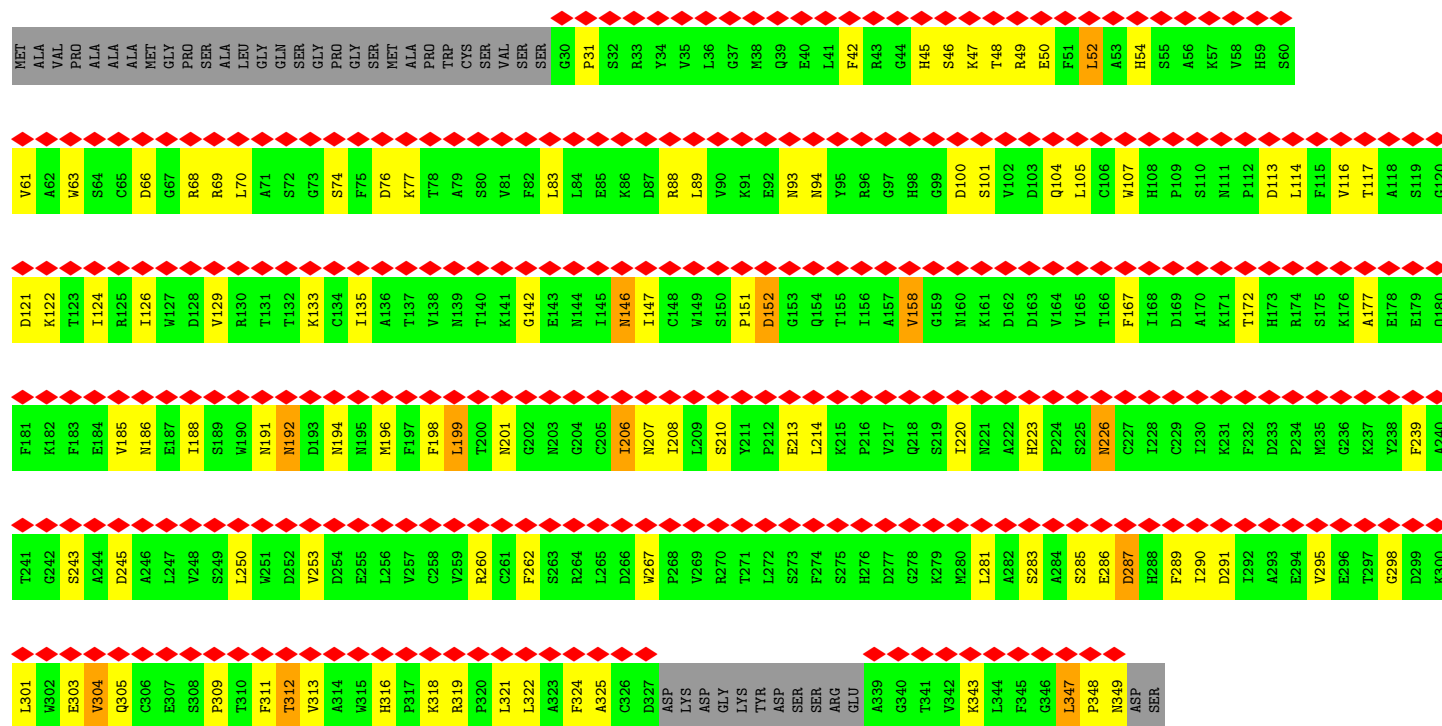
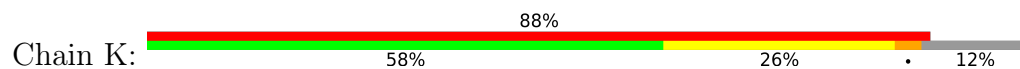


Frequency	Percentage
Daily	58%
Weekly	27%
Monthly	12%
Other	3%

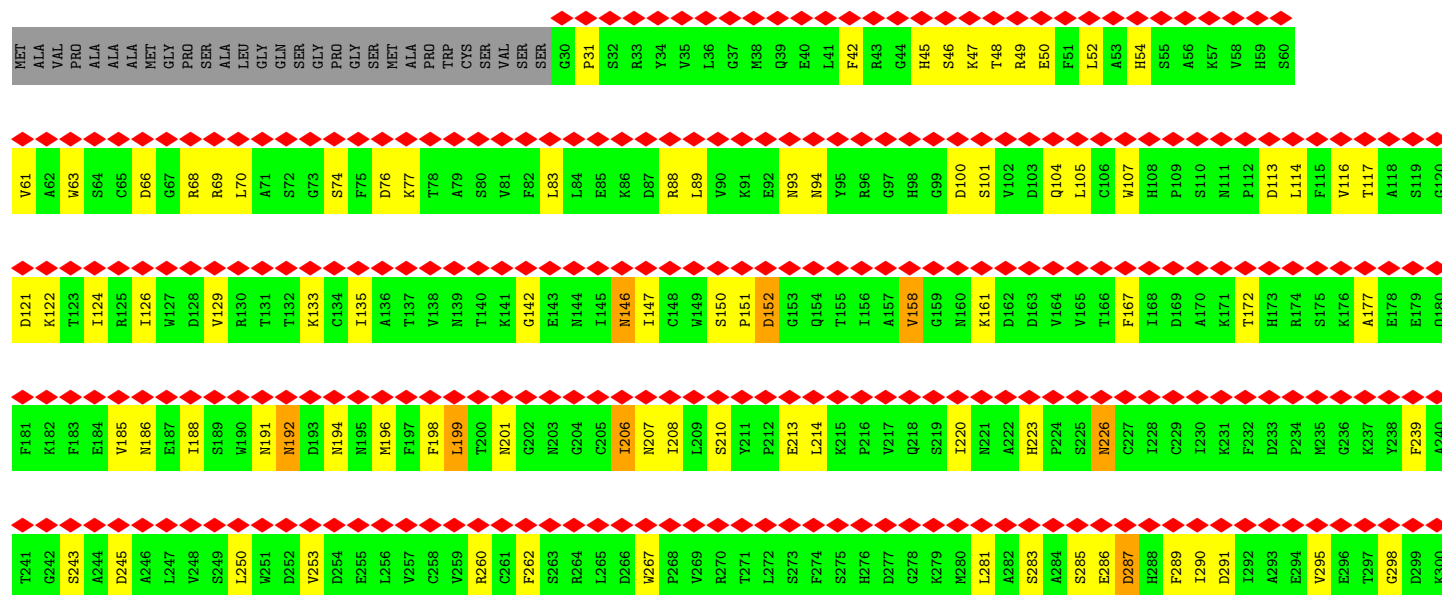
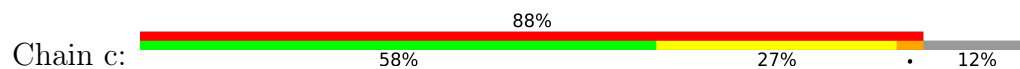


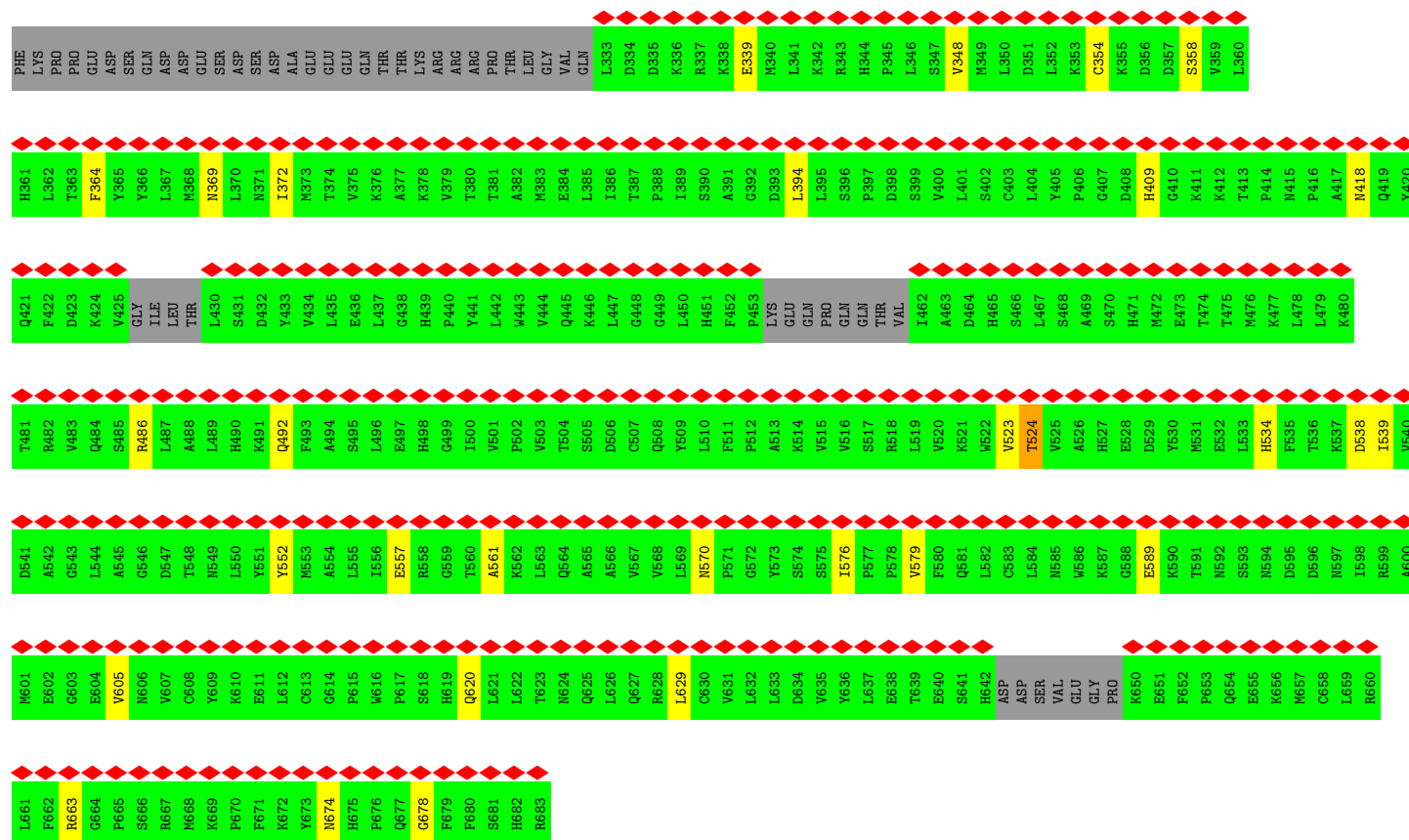


• Molecule 3: THO complex subunit 3

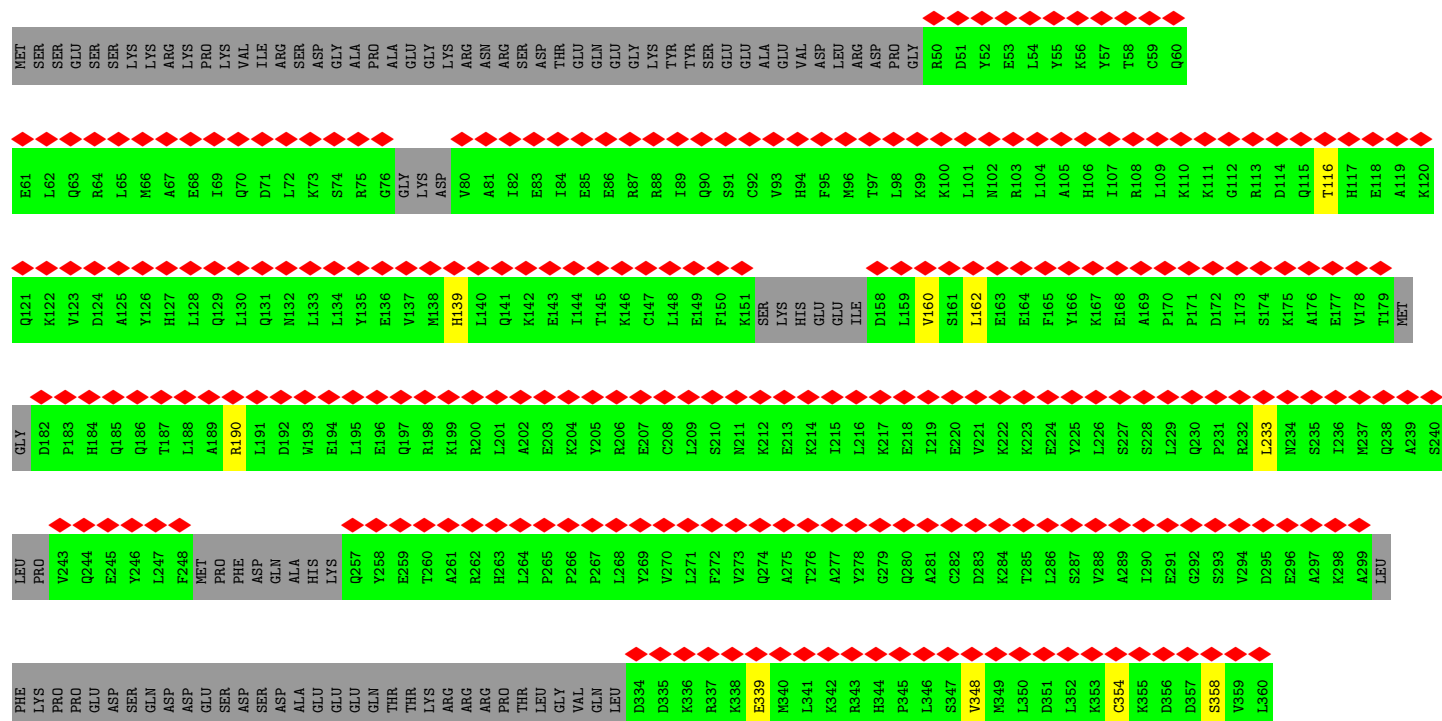
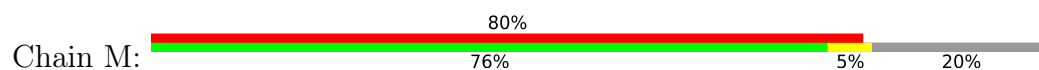


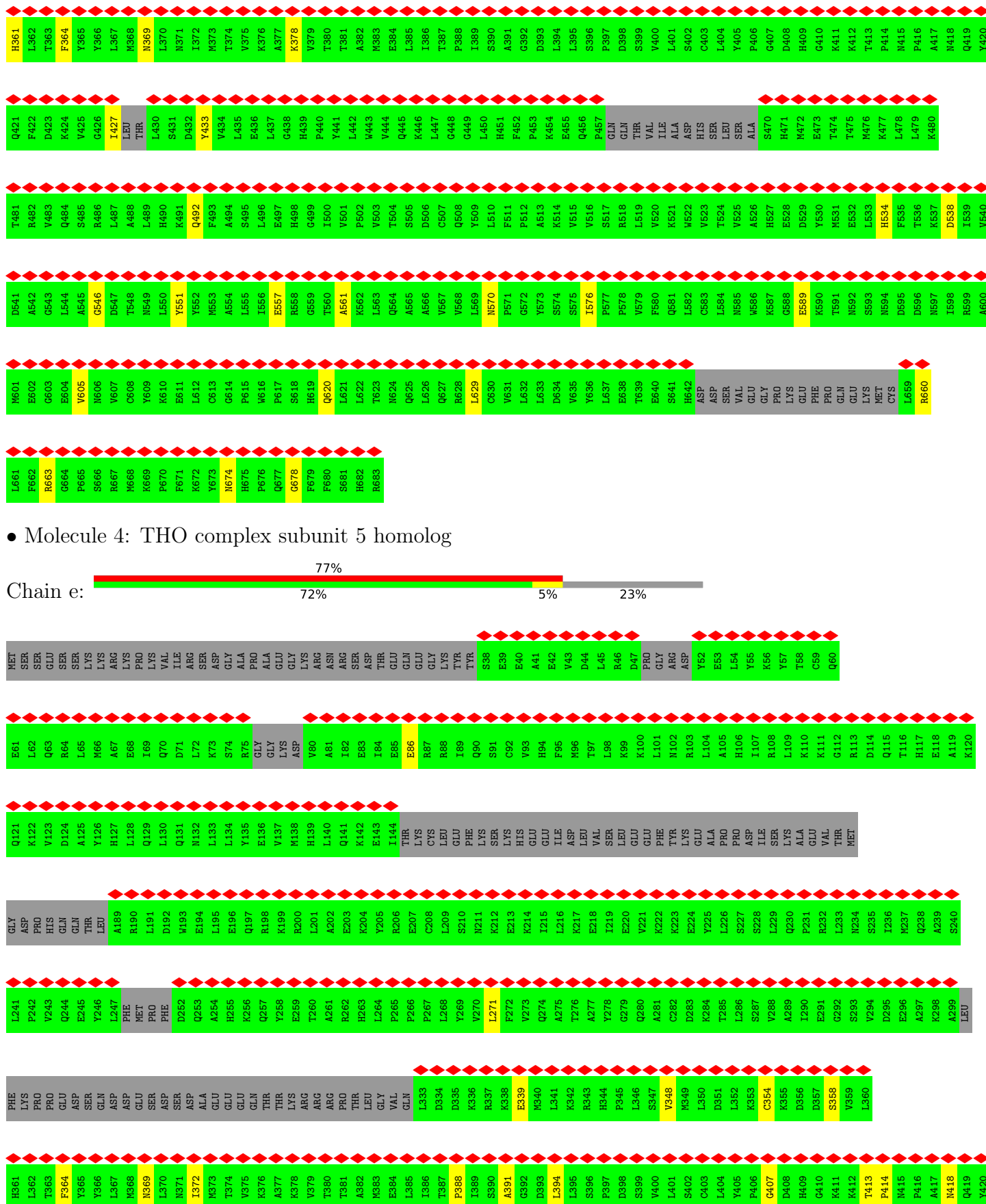
• Molecule 3: THO complex subunit 3



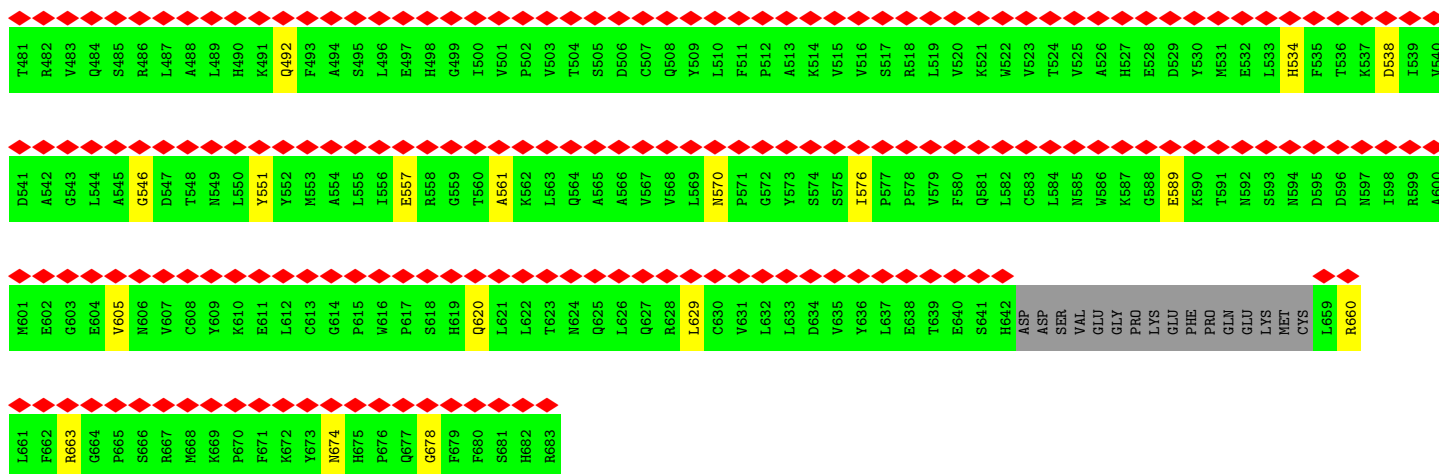


• Molecule 4: THO complex subunit 5 homolog

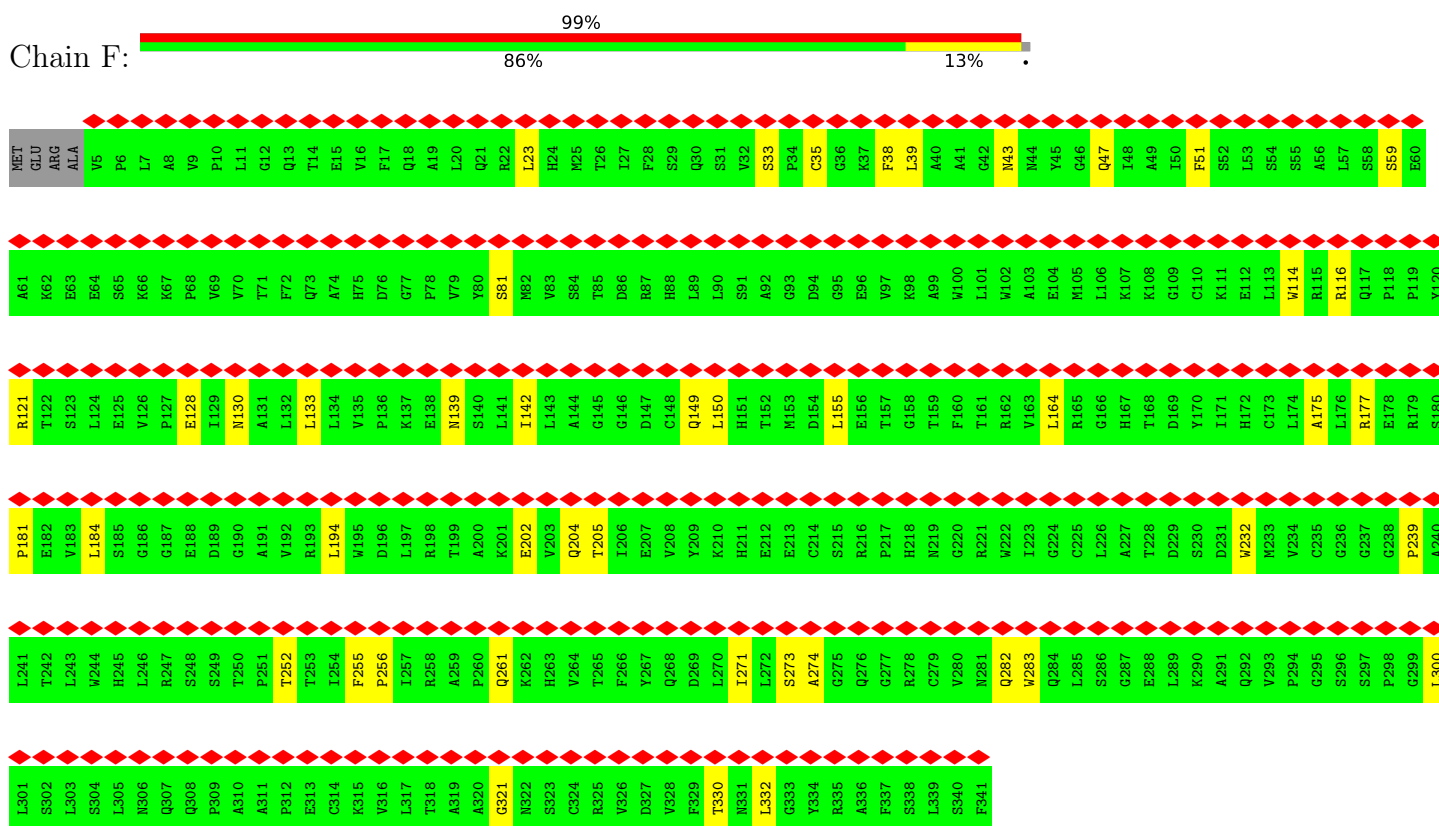




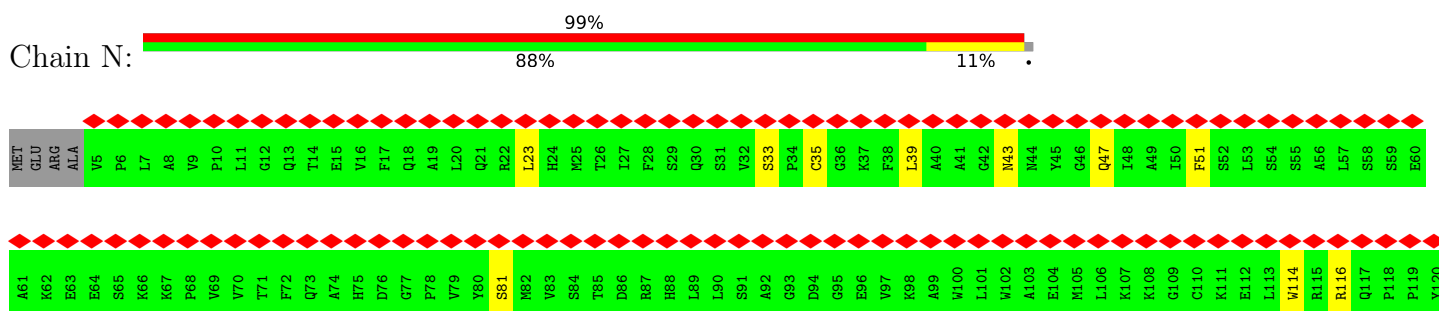


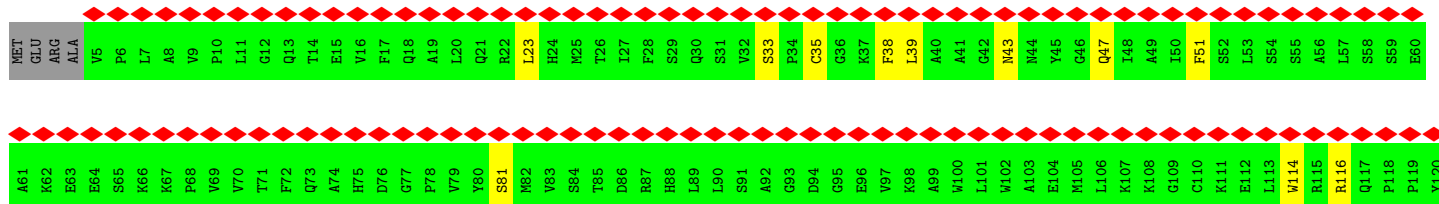


• Molecule 5: THO complex subunit 6 homolog

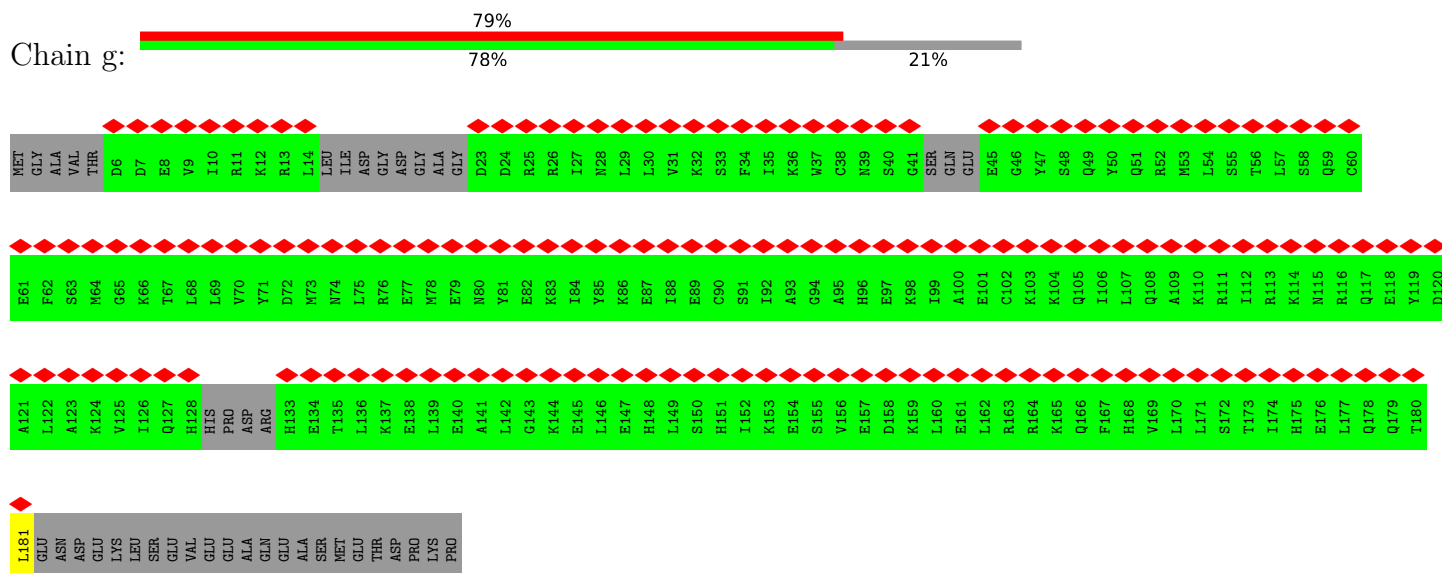


• Molecule 5: THO complex subunit 6 homolog

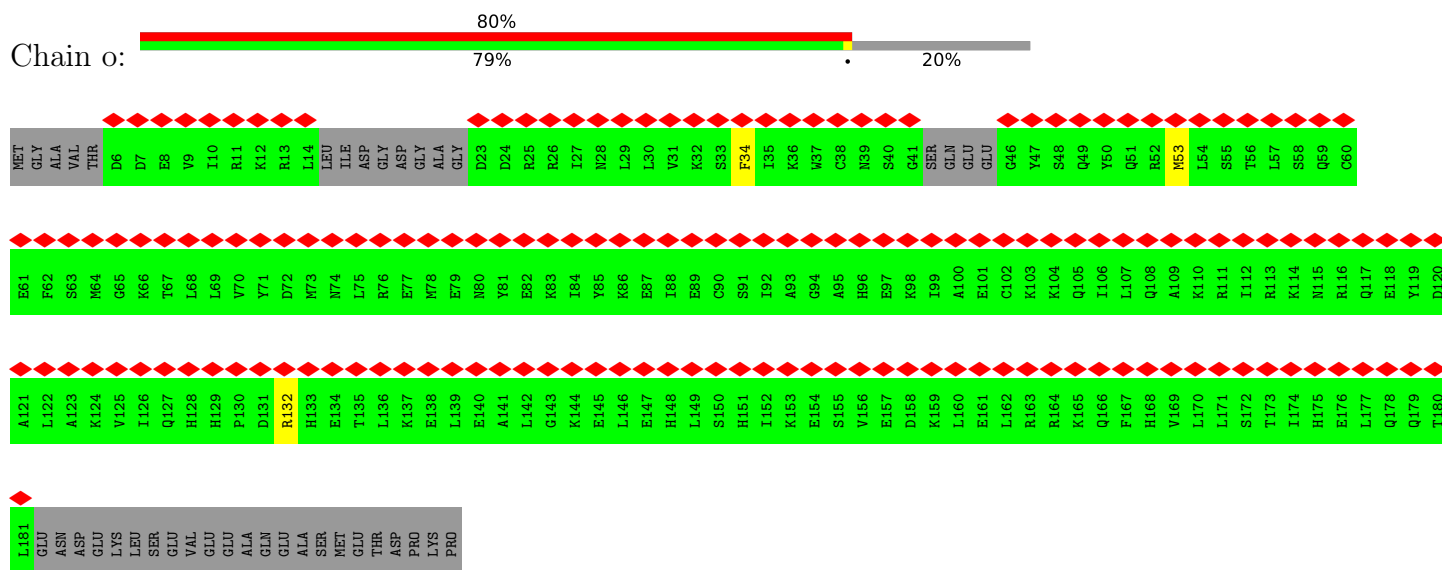




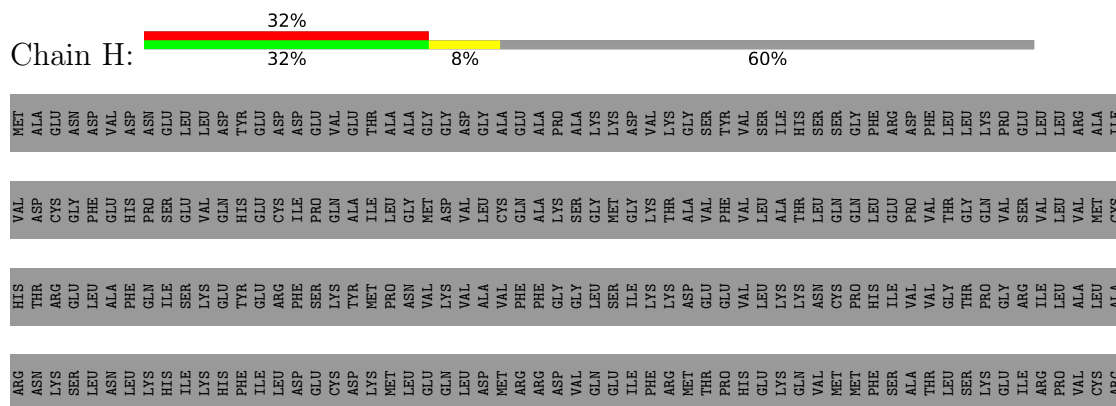
- Molecule 6: THO complex subunit 7 homolog



- Molecule 6: THO complex subunit 7 homolog

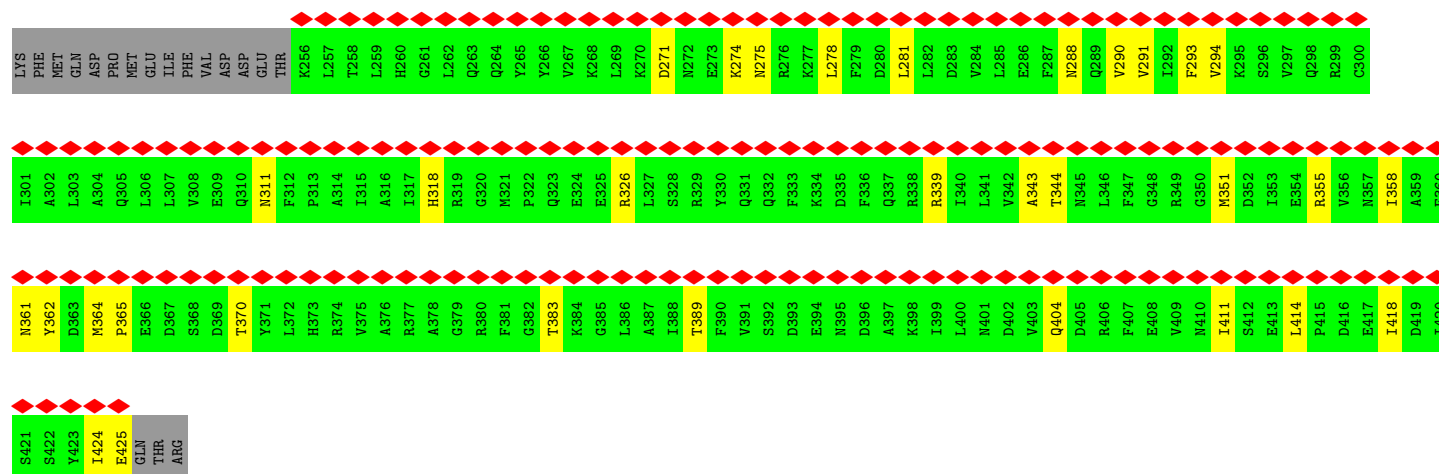
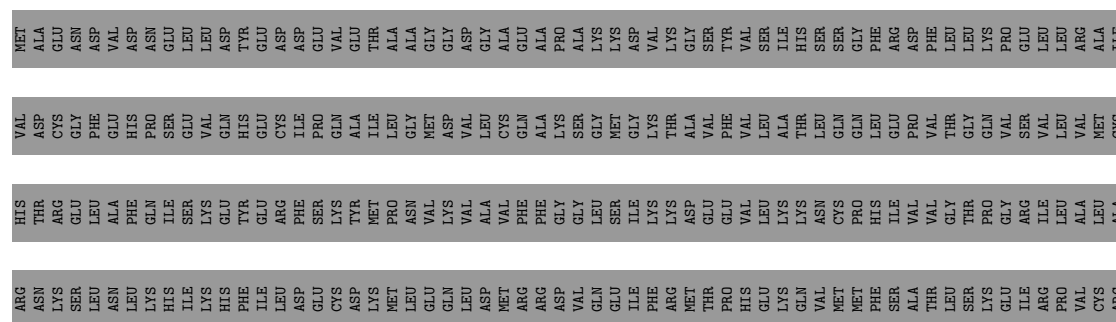


- Molecule 7: Spliceosome RNA helicase DDX39B

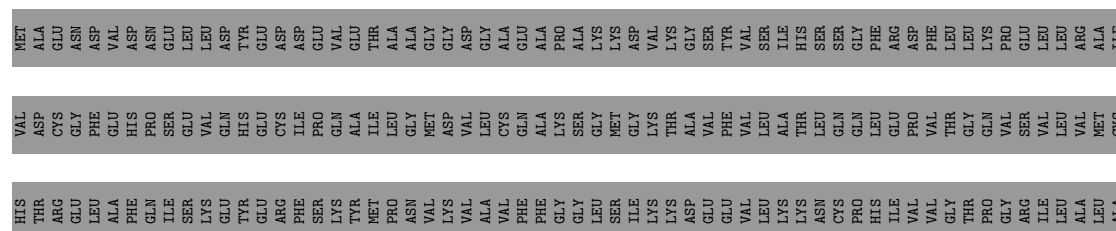




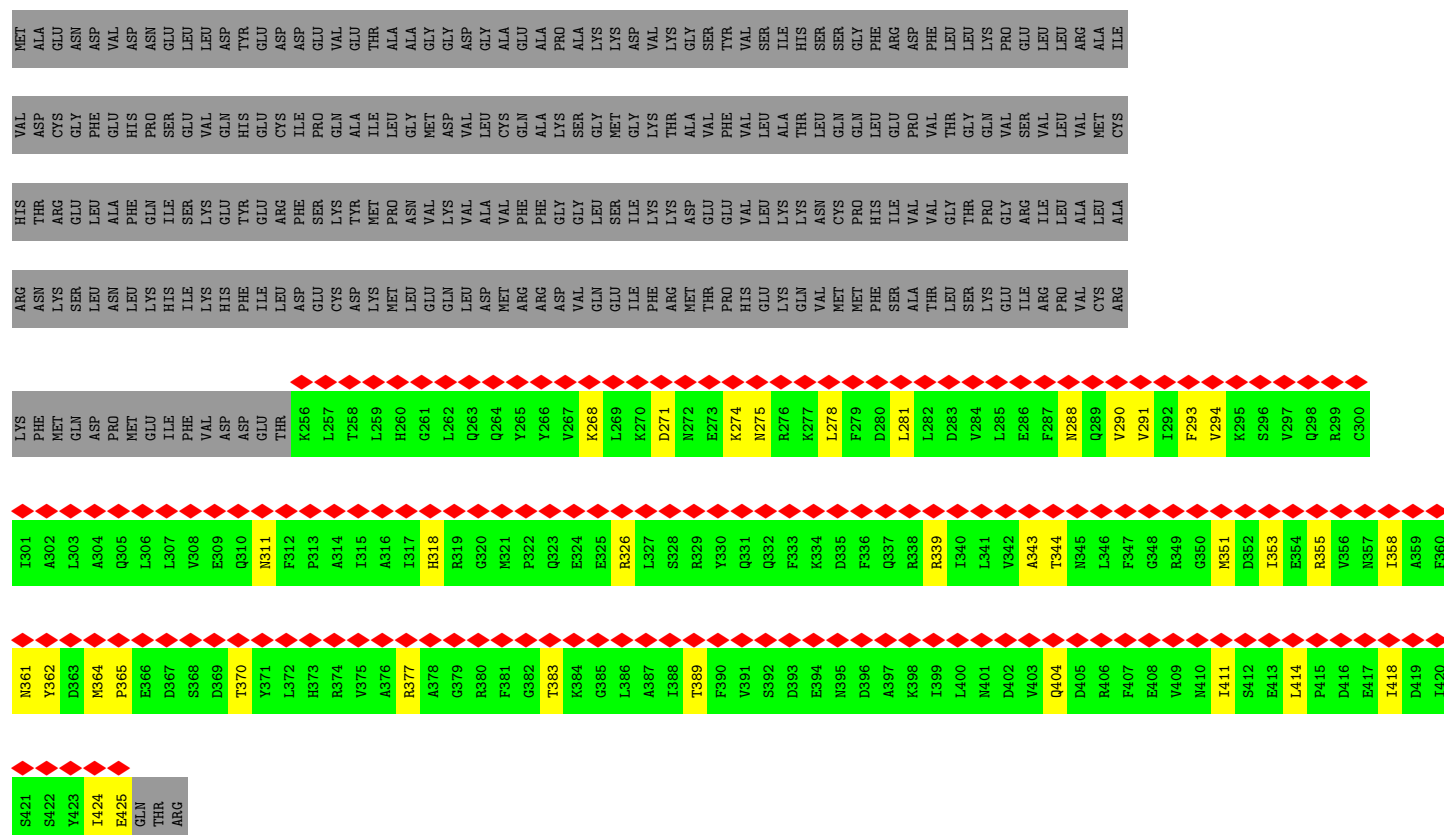
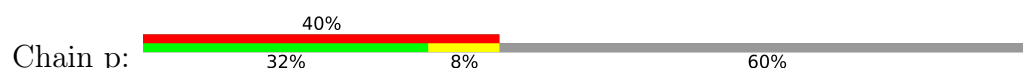
• Molecule 7: Spliceosome RNA helicase DDX39B



• Molecule 7: Spliceosome RNA helicase DDX39B



- Molecule 7: Spliceosome RNA helicase DDX39B



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	246457	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	3700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	6.605	Depositor
Minimum map value	-4.523	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.048	Depositor
Recommended contour level	0.9	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 [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	0.16	0/2942	0.37	0/3969
1	I	0.22	0/2989	0.49	0/4034
1	a	0.16	0/2942	0.37	0/3969
1	i	0.22	0/2990	0.49	0/4035
2	B	0.20	0/7129	0.46	0/9633
2	J	0.22	1/7071 (0.0%)	0.47	1/9556 (0.0%)
2	b	0.20	0/7129	0.47	0/9633
2	j	0.22	1/7071 (0.0%)	0.47	1/9556 (0.0%)
3	C	0.26	0/2494	0.57	0/3384
3	K	0.26	0/2494	0.56	0/3384
3	c	0.26	0/2494	0.56	0/3384
3	k	0.26	0/2494	0.57	0/3384
4	E	0.38	1/3830 (0.0%)	0.50	0/5225
4	M	0.25	0/4215	0.52	0/5717
4	e	0.39	1/3737 (0.0%)	0.48	2/5098 (0.0%)
4	m	0.25	0/4215	0.52	0/5717
5	F	0.28	0/2666	0.56	0/3623
5	N	0.28	0/2666	0.56	0/3623
5	f	0.28	0/2596	0.56	0/3524
5	n	0.29	0/2666	0.56	0/3623
6	G	0.16	0/796	0.24	0/1105
6	O	0.22	0/1138	0.36	0/1536
6	g	0.16	0/796	0.23	0/1105
6	o	0.21	0/1138	0.36	0/1536
7	H	0.13	0/1421	0.32	0/1915
7	P	0.13	0/1421	0.32	0/1915
7	h	0.13	0/1421	0.32	0/1915
7	p	0.13	0/1421	0.32	0/1915
All	All	0.24	4/86382 (0.0%)	0.48	4/117013 (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	5
2	J	0	4
2	b	0	5
2	j	0	4
3	C	0	1
3	K	0	1
3	c	0	1
3	k	0	1
4	M	0	1
4	m	0	1
All	All	0	24

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	e	86	GLU	C-N	-18.01	1.11	1.33
4	E	86	GLU	C-N	-17.98	1.11	1.33
2	j	234	SER	C-N	-9.37	1.20	1.33
2	J	234	SER	C-N	-9.30	1.20	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	234	SER	O-C-N	-5.66	114.84	122.43
2	j	234	SER	O-C-N	-5.56	114.97	122.43
4	e	407	GLY	CA-C-N	5.03	131.14	121.54
4	e	407	GLY	C-N-CA	5.03	131.14	121.54

There are no chirality outliers.

5 of 24 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1116	GLU	Peptide
2	B	163	ASN	Peptide
2	B	557	THR	Peptide
2	B	562	LYS	Peptide
2	B	788	LEU	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2889	0	2791	71	0
1	I	2935	0	2820	60	0
1	a	2889	0	2791	71	0
1	i	2936	0	2823	63	0
2	B	7012	0	6687	160	0
2	J	6956	0	6627	170	0
2	b	7012	0	6687	168	0
2	j	6956	0	6627	169	0
3	C	2433	0	2346	52	0
3	K	2433	0	2346	52	0
3	c	2433	0	2346	51	0
3	k	2433	0	2346	52	0
4	E	3763	0	3273	22	0
4	M	4134	0	3884	21	0
4	e	3674	0	3192	20	0
4	m	4134	0	3884	21	0
5	F	2604	0	2588	26	0
5	N	2604	0	2588	21	0
5	f	2537	0	2521	23	0
5	n	2604	0	2588	23	0
6	G	800	0	344	1	0
6	O	1129	0	930	3	0
6	g	800	0	344	1	0
6	o	1129	0	930	2	0
7	H	1398	0	1394	24	0
7	P	1398	0	1394	22	0
7	h	1398	0	1394	23	0
7	p	1398	0	1394	25	0
All	All	84821	0	79879	1253	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 1253 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:219:GLU:HG2	2:B:269:VAL:HG21	1.26	1.16
1:i:387:ASN:CG	2:j:254:PHE:CZ	2.25	1.15
1:I:387:ASN:CG	2:J:254:PHE:CZ	2.25	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:219:GLU:HG2	2:b:269:VAL:HG21	1.26	1.13
1:A:392:LYS:HG2	2:B:250:PHE:CE1	1.85	1.12

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	330/657 (50%)	309 (94%)	19 (6%)	2 (1%)	21	53
1	I	335/657 (51%)	309 (92%)	23 (7%)	3 (1%)	14	46
1	a	330/657 (50%)	309 (94%)	19 (6%)	2 (1%)	21	53
1	i	335/657 (51%)	309 (92%)	23 (7%)	3 (1%)	14	46
2	B	871/1593 (55%)	805 (92%)	62 (7%)	4 (0%)	24	57
2	J	864/1593 (54%)	802 (93%)	59 (7%)	3 (0%)	36	67
2	b	871/1593 (55%)	805 (92%)	62 (7%)	4 (0%)	24	57
2	j	864/1593 (54%)	802 (93%)	59 (7%)	3 (0%)	36	67
3	C	305/351 (87%)	267 (88%)	37 (12%)	1 (0%)	36	67
3	K	305/351 (87%)	268 (88%)	36 (12%)	1 (0%)	36	67
3	c	305/351 (87%)	267 (88%)	37 (12%)	1 (0%)	36	67
3	k	305/351 (87%)	267 (88%)	37 (12%)	1 (0%)	36	67
4	E	520/683 (76%)	494 (95%)	25 (5%)	1 (0%)	43	74
4	M	529/683 (78%)	504 (95%)	25 (5%)	0	100	100
4	e	507/683 (74%)	485 (96%)	22 (4%)	0	100	100
4	m	529/683 (78%)	503 (95%)	26 (5%)	0	100	100
5	F	335/341 (98%)	305 (91%)	29 (9%)	1 (0%)	36	67
5	N	335/341 (98%)	306 (91%)	28 (8%)	1 (0%)	36	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	f	325/341 (95%)	298 (92%)	26 (8%)	1 (0%)	36	67
5	n	335/341 (98%)	305 (91%)	29 (9%)	1 (0%)	36	67
6	G	153/204 (75%)	153 (100%)	0	0	100	100
6	O	158/204 (78%)	158 (100%)	0	0	100	100
6	g	153/204 (75%)	153 (100%)	0	0	100	100
6	o	158/204 (78%)	158 (100%)	0	0	100	100
7	H	168/428 (39%)	162 (96%)	6 (4%)	0	100	100
7	P	168/428 (39%)	162 (96%)	6 (4%)	0	100	100
7	h	168/428 (39%)	162 (96%)	6 (4%)	0	100	100
7	p	168/428 (39%)	162 (96%)	6 (4%)	0	100	100
All	All	10729/17028 (63%)	9989 (93%)	707 (7%)	33 (0%)	37	67

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	789	SER
2	J	789	SER
2	b	789	SER
2	j	789	SER
2	B	557	THR

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	310/601 (52%)	288 (93%)	22 (7%)	13	40
1	I	312/601 (52%)	307 (98%)	5 (2%)	55	71
1	a	310/601 (52%)	288 (93%)	22 (7%)	13	40
1	i	313/601 (52%)	308 (98%)	5 (2%)	55	71
2	B	704/1442 (49%)	622 (88%)	82 (12%)	5	25
2	J	697/1442 (48%)	623 (89%)	74 (11%)	6	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	704/1442 (49%)	622 (88%)	82 (12%)	5	25
2	j	697/1442 (48%)	623 (89%)	74 (11%)	6	27
3	C	268/300 (89%)	232 (87%)	36 (13%)	4	20
3	K	268/300 (89%)	232 (87%)	36 (13%)	4	20
3	c	268/300 (89%)	232 (87%)	36 (13%)	4	20
3	k	268/300 (89%)	232 (87%)	36 (13%)	4	20
4	E	322/615 (52%)	320 (99%)	2 (1%)	78	80
4	M	404/615 (66%)	404 (100%)	0	100	100
4	e	312/615 (51%)	312 (100%)	0	100	100
4	m	404/615 (66%)	404 (100%)	0	100	100
5	F	284/287 (99%)	284 (100%)	0	100	100
5	N	284/287 (99%)	284 (100%)	0	100	100
5	f	276/287 (96%)	276 (100%)	0	100	100
5	n	284/287 (99%)	284 (100%)	0	100	100
6	O	85/184 (46%)	85 (100%)	0	100	100
6	o	85/184 (46%)	85 (100%)	0	100	100
7	H	153/381 (40%)	153 (100%)	0	100	100
7	P	153/381 (40%)	153 (100%)	0	100	100
7	h	153/381 (40%)	153 (100%)	0	100	100
7	p	153/381 (40%)	153 (100%)	0	100	100
All	All	8471/14872 (57%)	7959 (94%)	512 (6%)	19	45

5 of 512 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	j	996	CYS
3	k	48	THR
2	j	987	ILE
2	J	748	GLN
2	J	679	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 192 such sidechains are listed below:

Mol	Chain	Res	Type
2	b	640	GLN
7	h	404	GLN
2	b	779	GLN
4	e	274	GLN
2	j	256	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	E	1
4	e	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	86:GLU	C	87:ARG	N	1.11
1	e	86:GLU	C	87:ARG	N	1.11

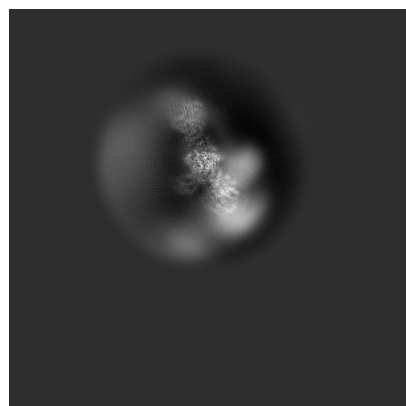
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14808. These allow visual inspection of the internal detail of the map and identification of artifacts.

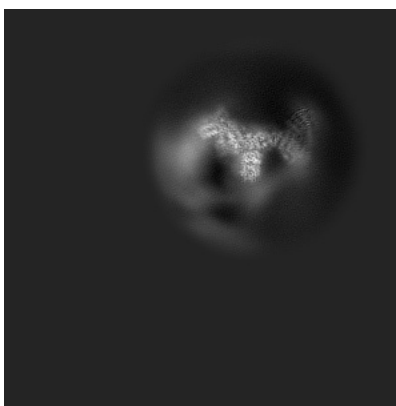
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

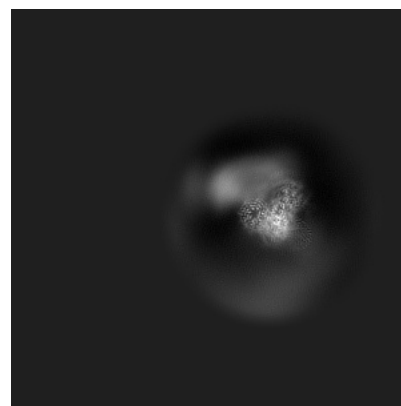
6.1.1 Primary map



X

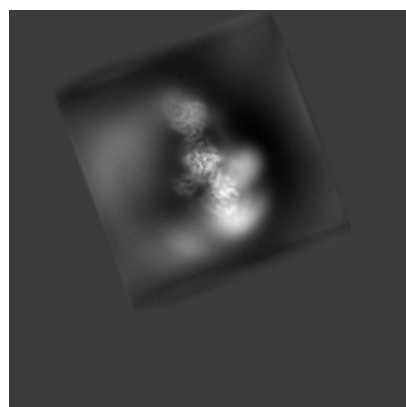


Y

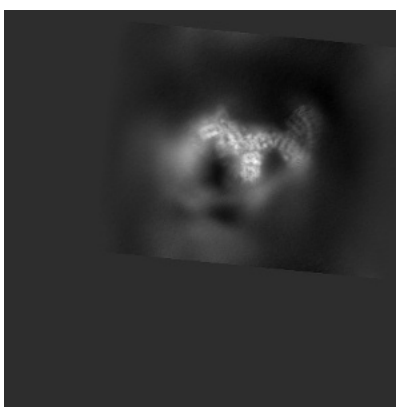


Z

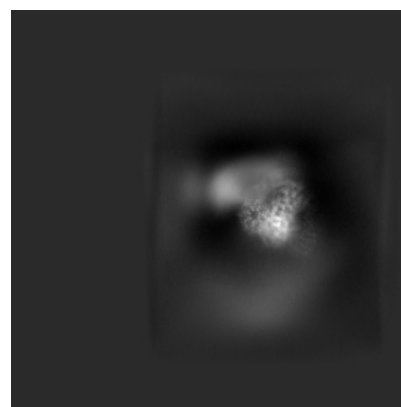
6.1.2 Raw map



X



Y

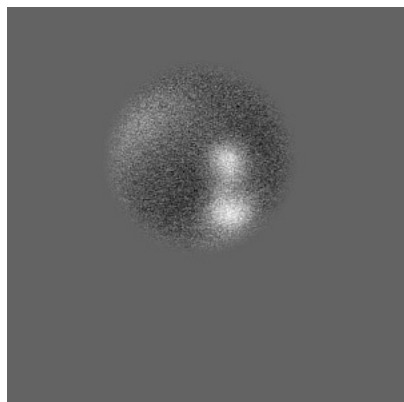


Z

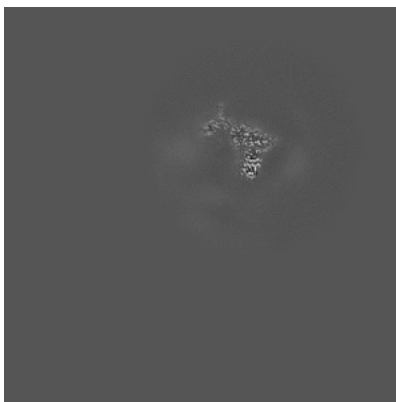
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

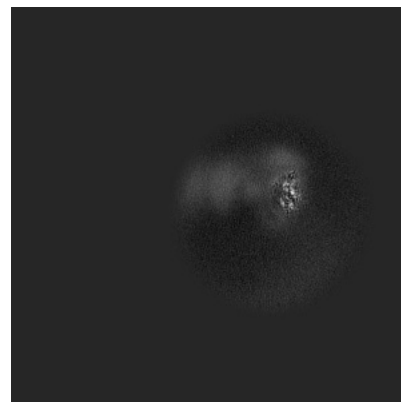
6.2.1 Primary map



X Index: 220

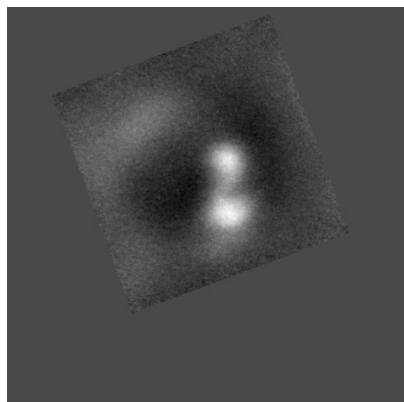


Y Index: 220

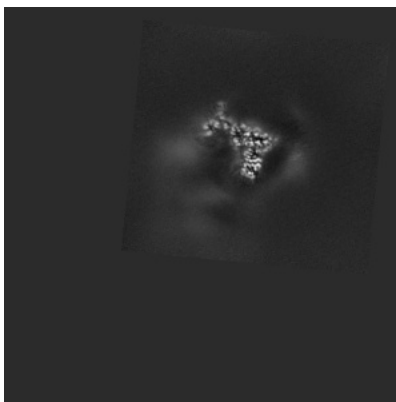


Z Index: 220

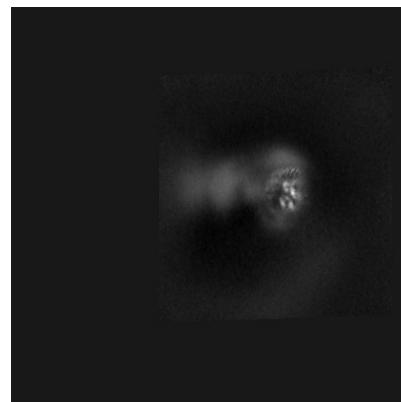
6.2.2 Raw map



X Index: 220



Y Index: 220

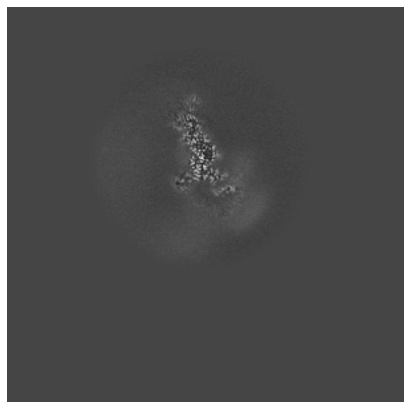


Z Index: 220

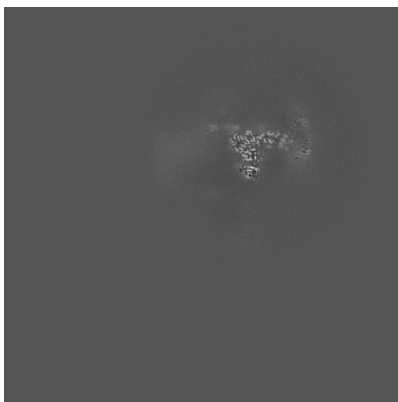
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

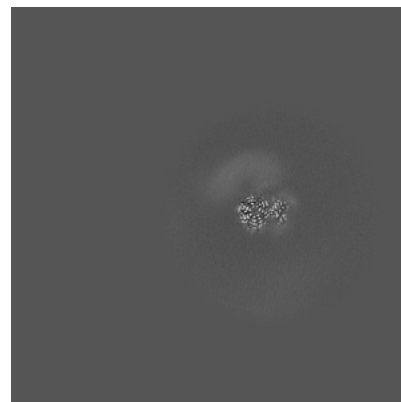
6.3.1 Primary map



X Index: 295

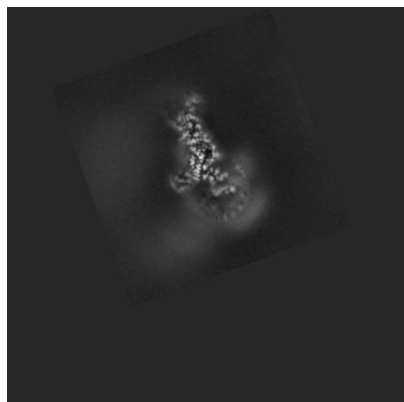


Y Index: 211

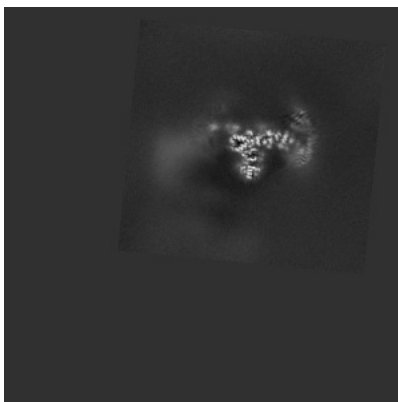


Z Index: 272

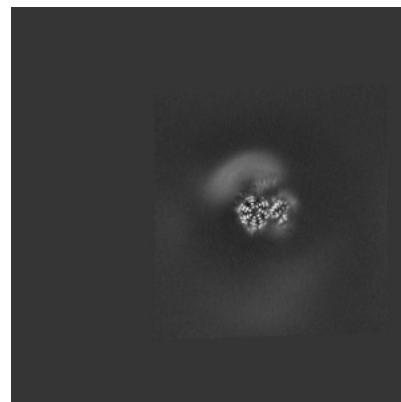
6.3.2 Raw map



X Index: 295



Y Index: 210

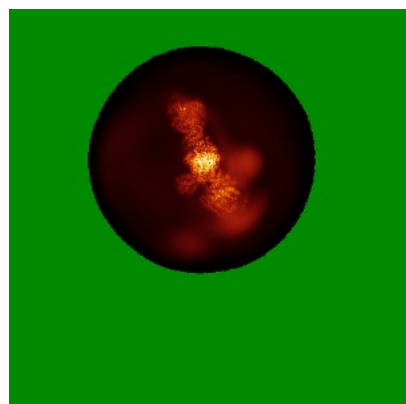


Z Index: 272

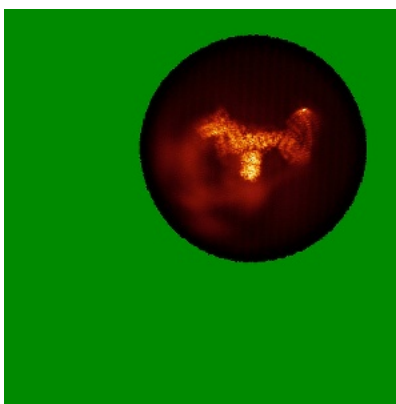
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

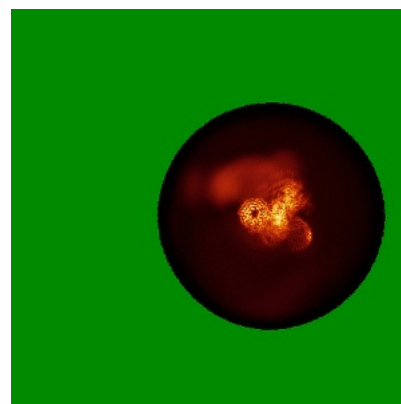
6.4.1 Primary map



X

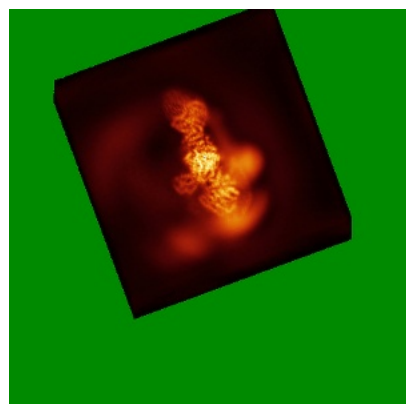


Y

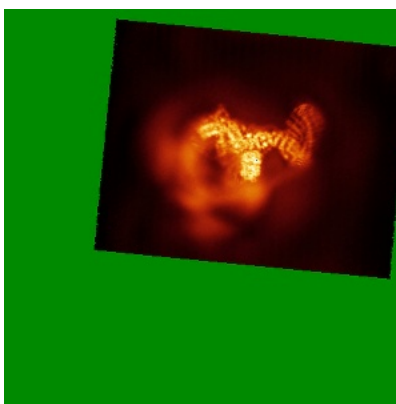


Z

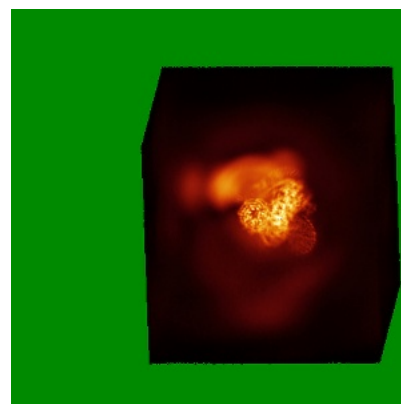
6.4.2 Raw map



X



Y

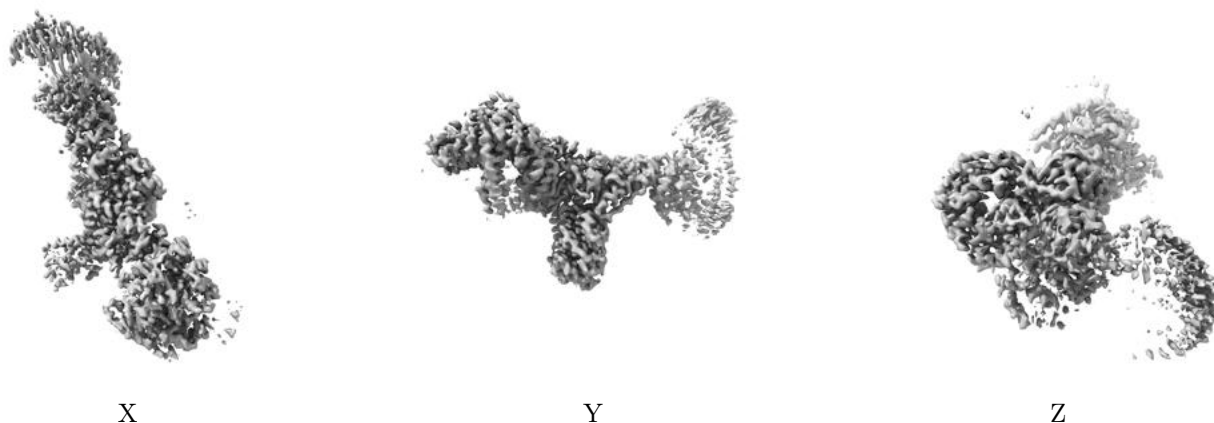


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.9. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

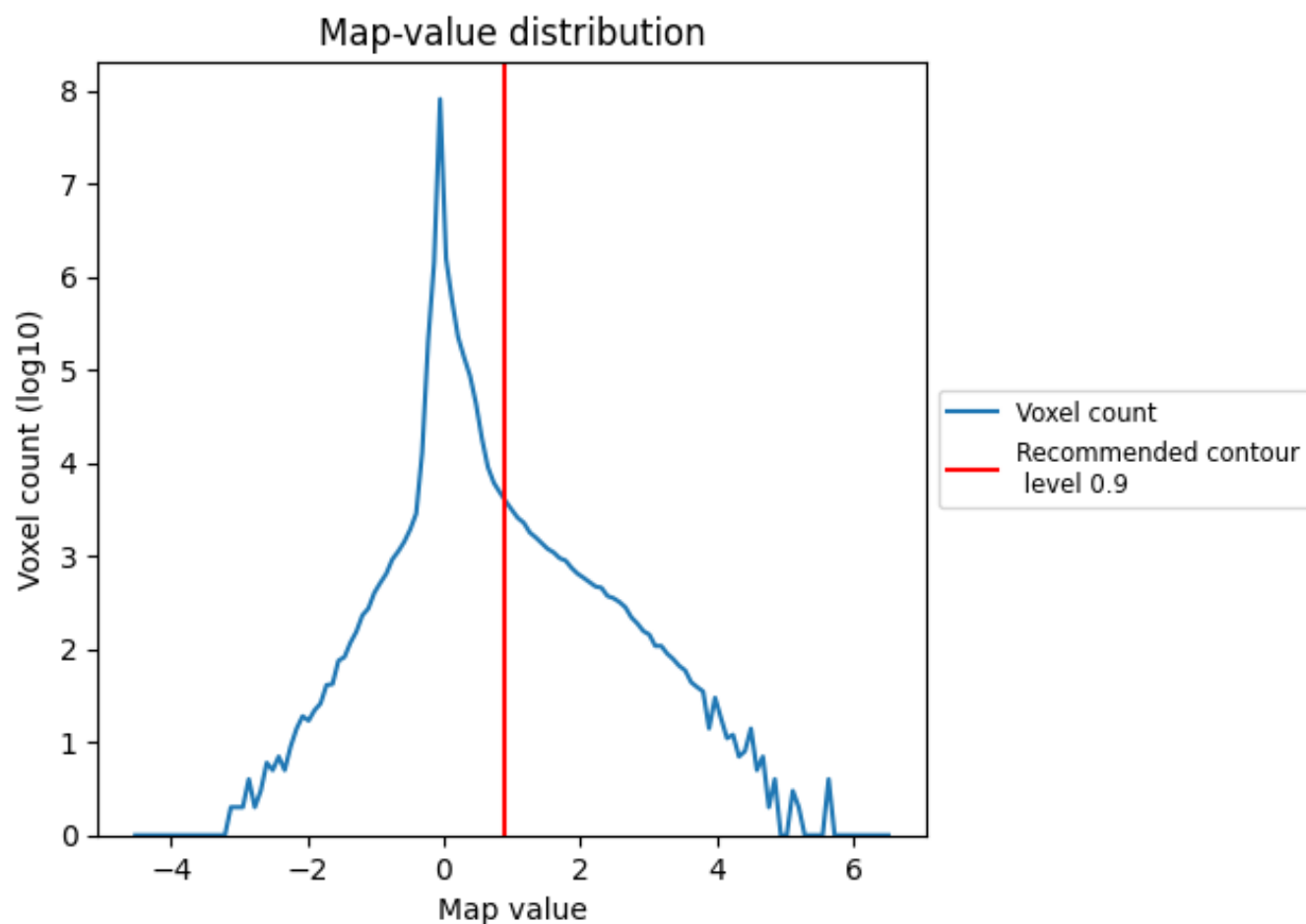
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

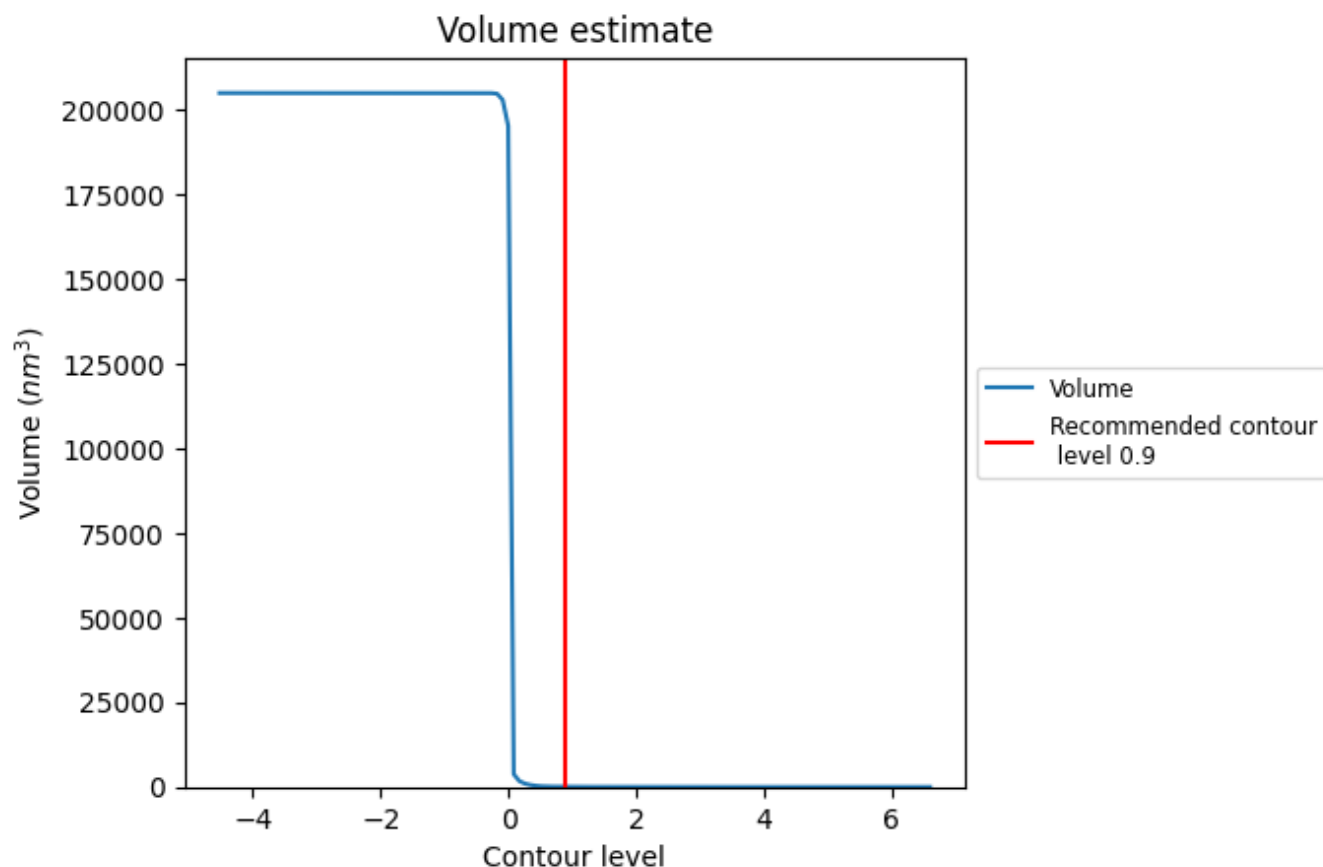
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

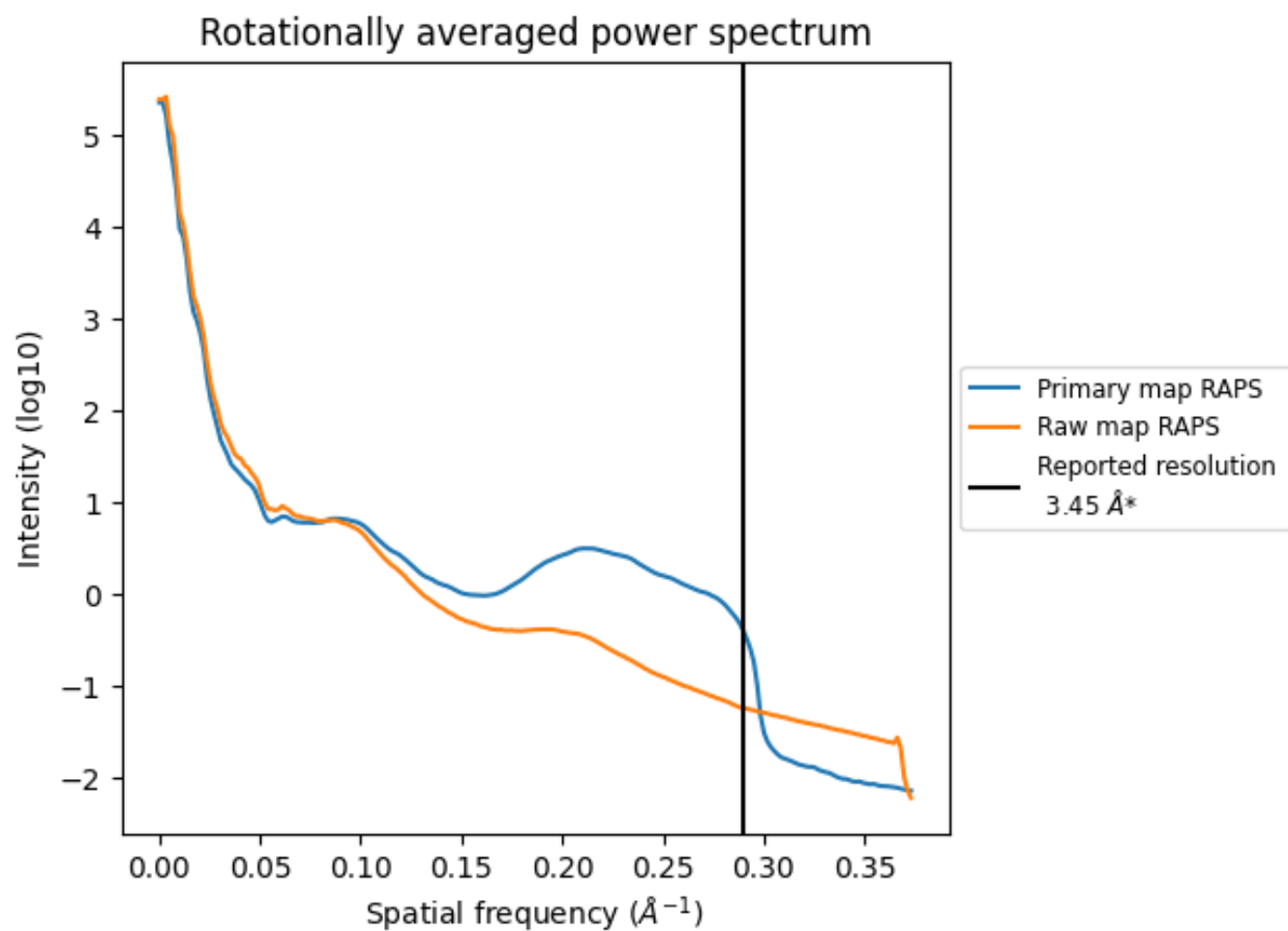
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 66 nm^3 ; this corresponds to an approximate mass of 60 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 ⓘ

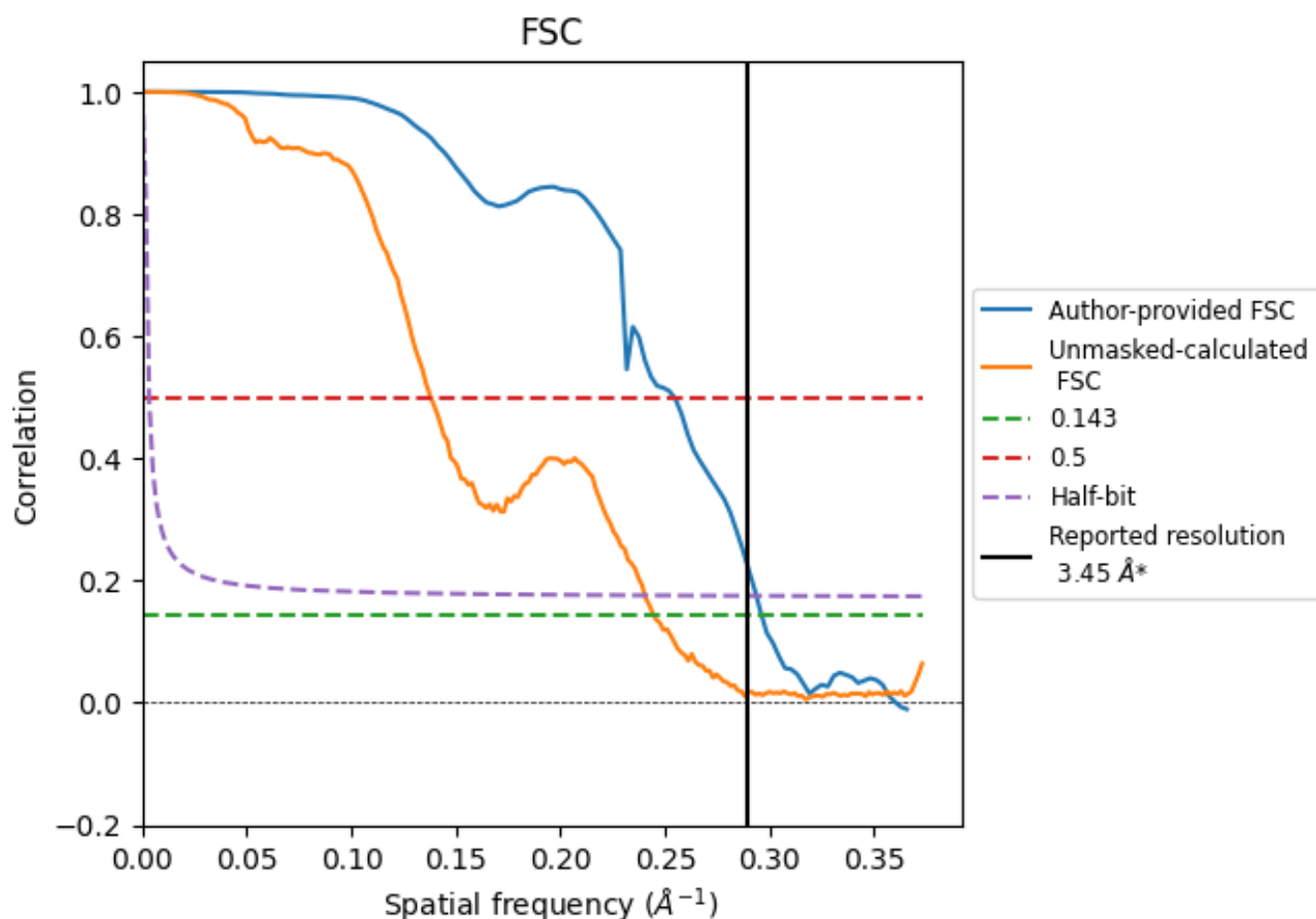


*Reported resolution corresponds to spatial frequency of 0.290 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.290 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.45	-	-
Author-provided FSC curve	3.37	3.93	3.41
Unmasked-calculated*	4.08	7.25	4.16

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.08 differs from the reported value 3.45 by more than 10 %

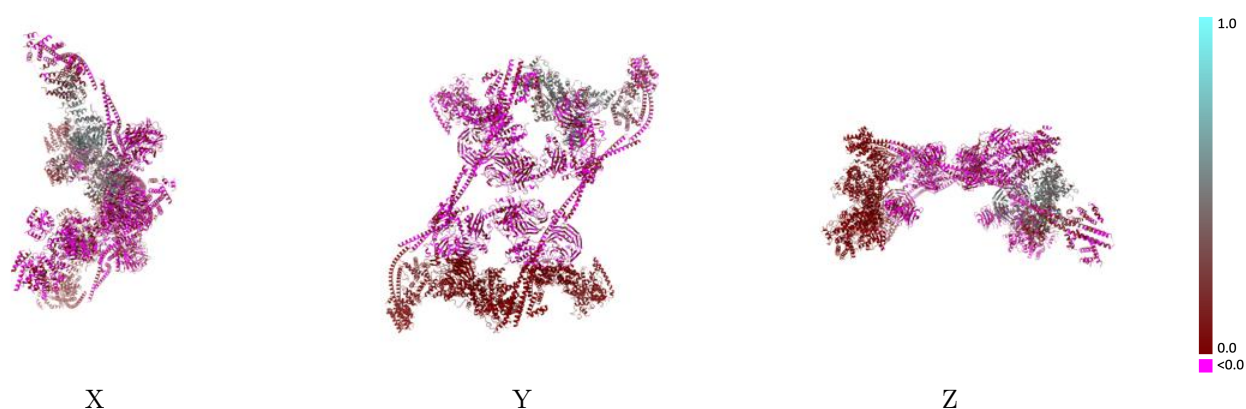
9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-14808 and PDB model 7ZNL. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay ⓘ

This section was not generated.

9.2 Q-score mapped to coordinate model ⓘ

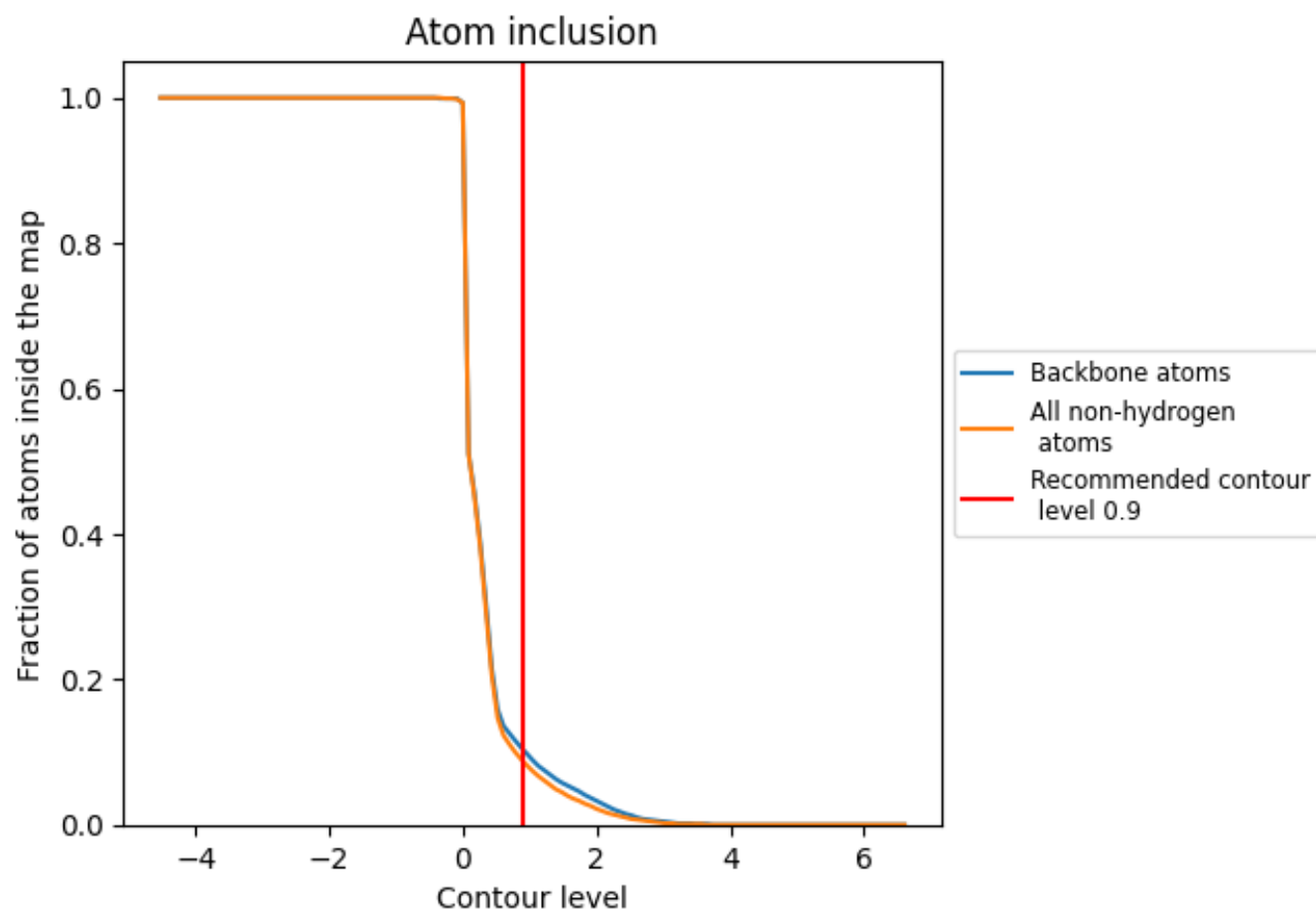


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 10% 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 (0.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.0870	 0.0690
A	 0.2270	 0.2380
B	 0.6300	 0.4210
C	 0.7970	 0.5090
E	 0.0090	 0.0360
F	 0.0000	 0.0190
G	 0.0750	 0.0590
H	 0.1960	 0.3320
I	 0.0000	 -0.0080
J	 0.0000	 0.0010
K	 0.0000	 -0.0060
M	 0.0000	 0.0170
N	 0.0000	 0.0240
O	 0.0000	 -0.0040
P	 0.0000	 -0.0000
a	 0.0000	 0.0000
b	 0.0000	 0.0000
c	 0.0000	 0.0080
e	 0.0000	 0.0040
f	 0.0000	 0.0200
g	 0.0000	 -0.0010
h	 0.0000	 0.0000
i	 0.0000	 0.0180
j	 0.0000	 0.0040
k	 0.0000	 0.0140
m	 0.0000	 -0.0070
n	 0.0000	 -0.0030
o	 0.0000	 0.0020
p	 0.0000	 -0.0130

