



wwPDB EM Validation Summary Report ⓘ

Dec 17, 2022 – 08:30 pm GMT

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)

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:

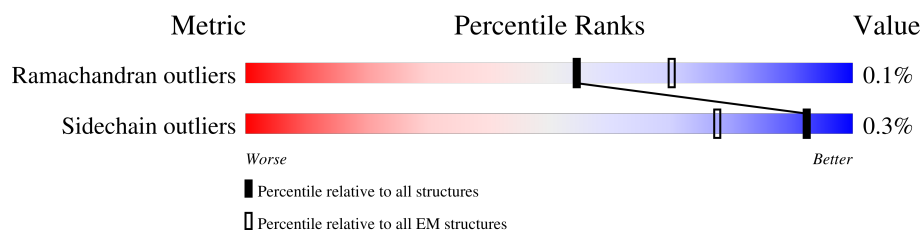
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance

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 $\leq 5\%$. 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	711	<div> <div>37%</div> <div>37%</div> <div>63%</div> </div>
1	I	711	<div> <div>39%</div> <div>38%</div> <div>61%</div> </div>
1	a	711	<div> <div>37%</div> <div>37%</div> <div>63%</div> </div>
1	i	711	<div> <div>23%</div> <div>38%</div> <div>61%</div> </div>
2	B	1226	<div> <div>58%</div> <div>57%</div> <div>42%</div> </div>
2	J	1226	<div> <div>58%</div> <div>57%</div> <div>42%</div> </div>
2	b	1226	<div> <div>58%</div> <div>57%</div> <div>42%</div> </div>
2	j	1226	<div> <div>52%</div> <div>57%</div> <div>42%</div> </div>
3	C	395	<div> <div>77%</div> <div>76%</div> <div>23%</div> </div>

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Mol	Chain	Length	Quality of chain
3	K	395	77% 76% 23%
3	c	395	77% 76% 23%
3	k	395	77% 76% 23%
4	E	683	37% 76% 23%
4	M	683	67% 80% 20%
4	e	683	75% 75% 25%
4	m	683	71% 80% 20%
5	F	341	21% 98% ..
5	N	341	97% 98% ..
5	f	341	96% 96% . .
5	n	341	99% 98% ..
6	G	204	71% 75% 25%
6	O	204	68% 76% 24%
6	g	204	75% 75% 25%
6	o	204	45% 76% 24%
7	H	451	38% 38% 62%
7	P	451	38% 38% 62%
7	h	451	38% 38% 62%
7	p	451	38% 38% 62%
8	X	37	100% 100%
8	x	37	97% 100%

2 Entry composition

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	C	N	O	S	0	0
			2165	1402	357	397	9		
1	I	275	Total	C	N	O	S	0	0
			2228	1441	368	410	9		
1	a	266	Total	C	N	O	S	0	0
			2165	1402	357	397	9		
1	i	275	Total	C	N	O	S	0	0
			2229	1441	368	411	9		

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

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	C	N	O	S	0	0
			2349	1482	407	446	14		
3	K	304	Total	C	N	O	S	0	0
			2349	1482	407	446	14		
3	c	304	Total	C	N	O	S	0	0
			2349	1482	407	446	14		
3	k	304	Total	C	N	O	S	0	0
			2349	1482	407	446	14		

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	C	N	O	S	0	0
			3687	2337	648	681	21		
4	M	549	Total	C	N	O	S	0	0
			4216	2689	734	768	25		
4	e	512	Total	C	N	O	S	0	0
			3598	2281	634	664	19		

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

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	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	153	Total	C	N	O		0	0
			760	454	153	153			
6	O	155	Total	C	N	O	S	0	0
			1084	669	201	207	7		
6	g	153	Total	C	N	O		0	0
			760	454	153	153			
6	o	155	Total	C	N	O	S	0	0
			1084	669	201	207	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		
7	p	170	Total	C	N	O	S	0	0
			1398	888	245	261	4		

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
8	X	37	Total	C	N	O	0	0
			185	111	37	37		
8	x	37	Total	C	N	O	0	0
			185	111	37	37		

[illegible]

- Molecule 1: THO complex subunit 1

[illegible]

- Molecule 1: THO complex subunit 1



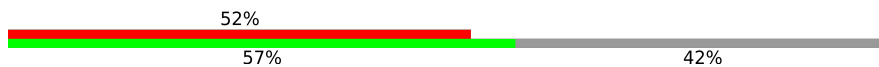


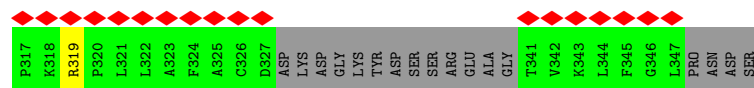




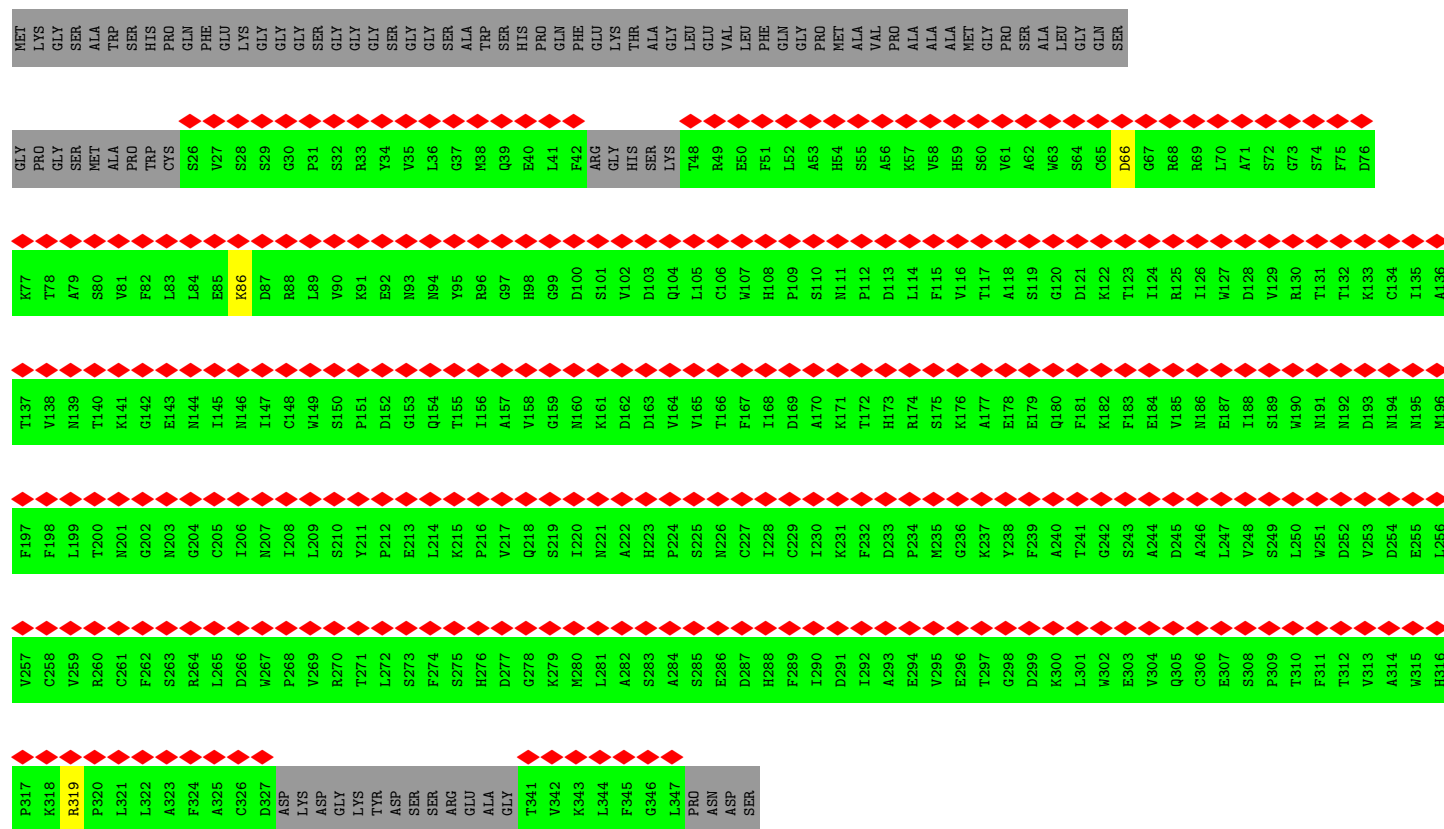
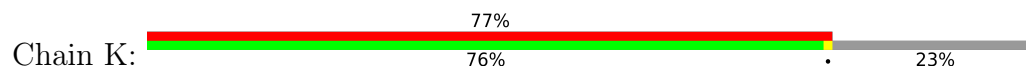


Chain j:

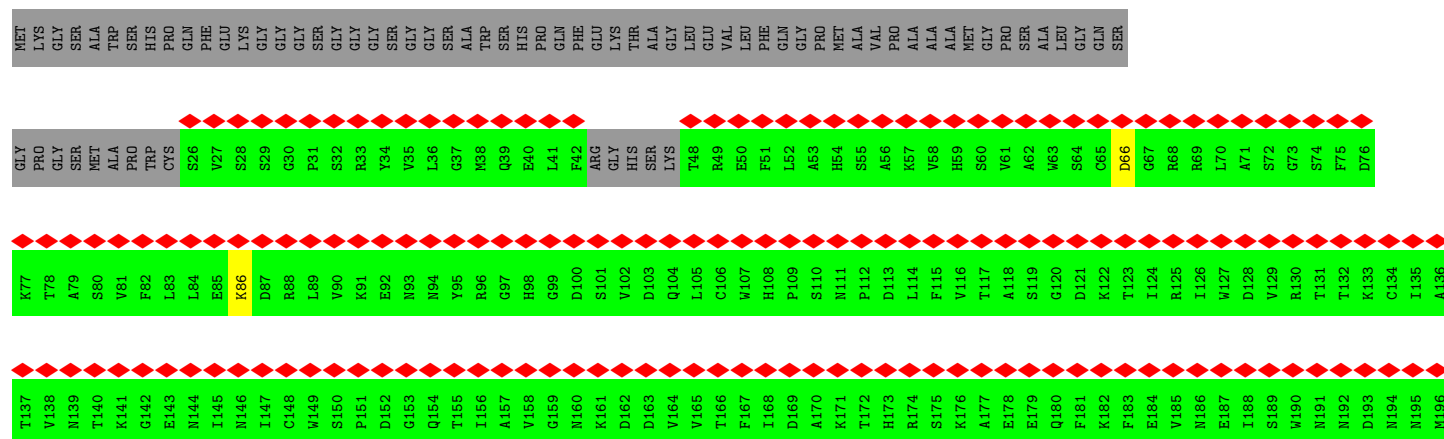
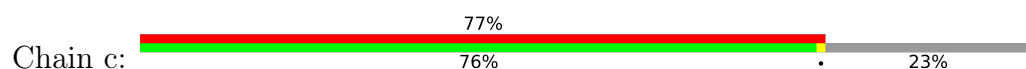




• Molecule 3: THO complex subunit 3

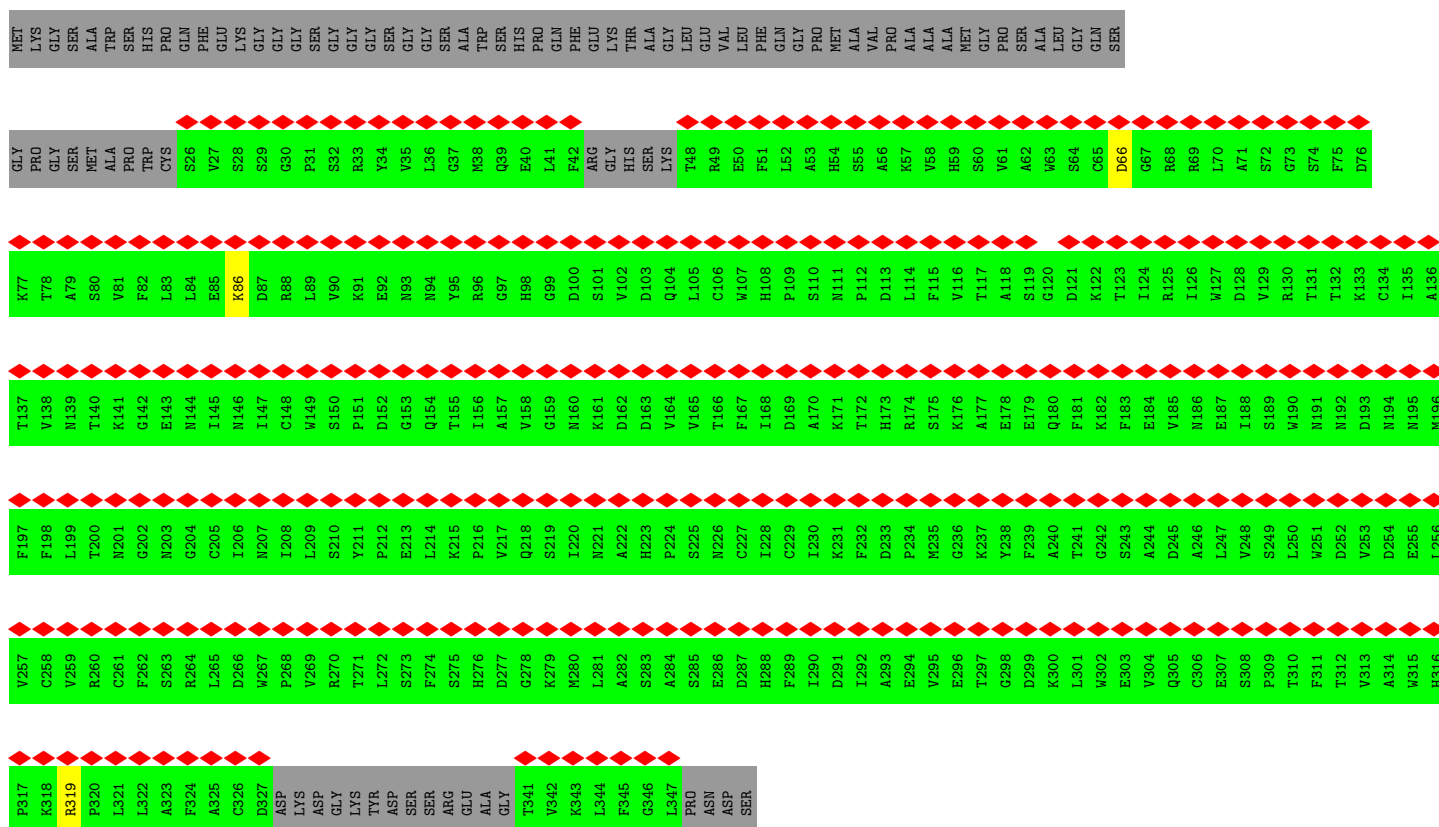
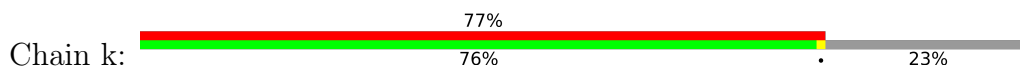


• Molecule 3: THO complex subunit 3

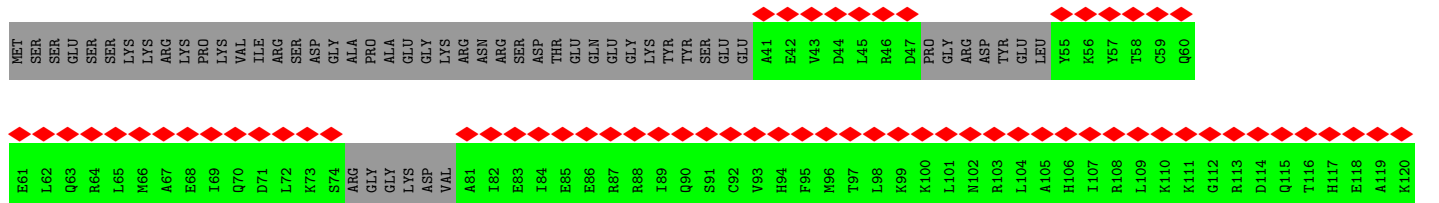
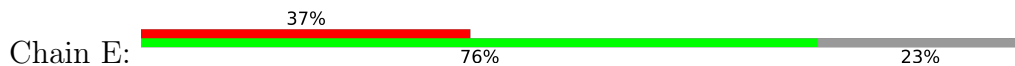


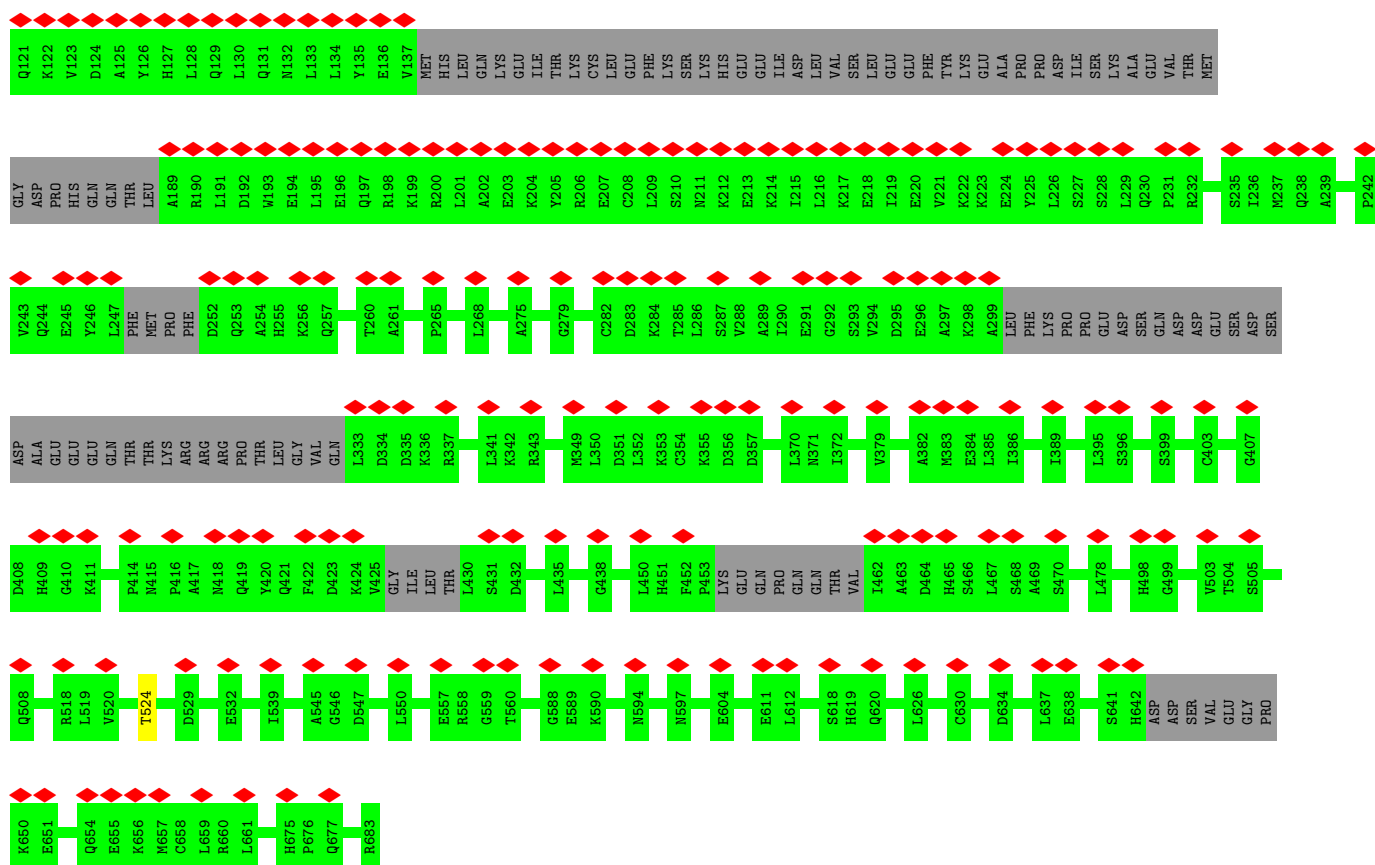


• Molecule 3: THO complex subunit 3

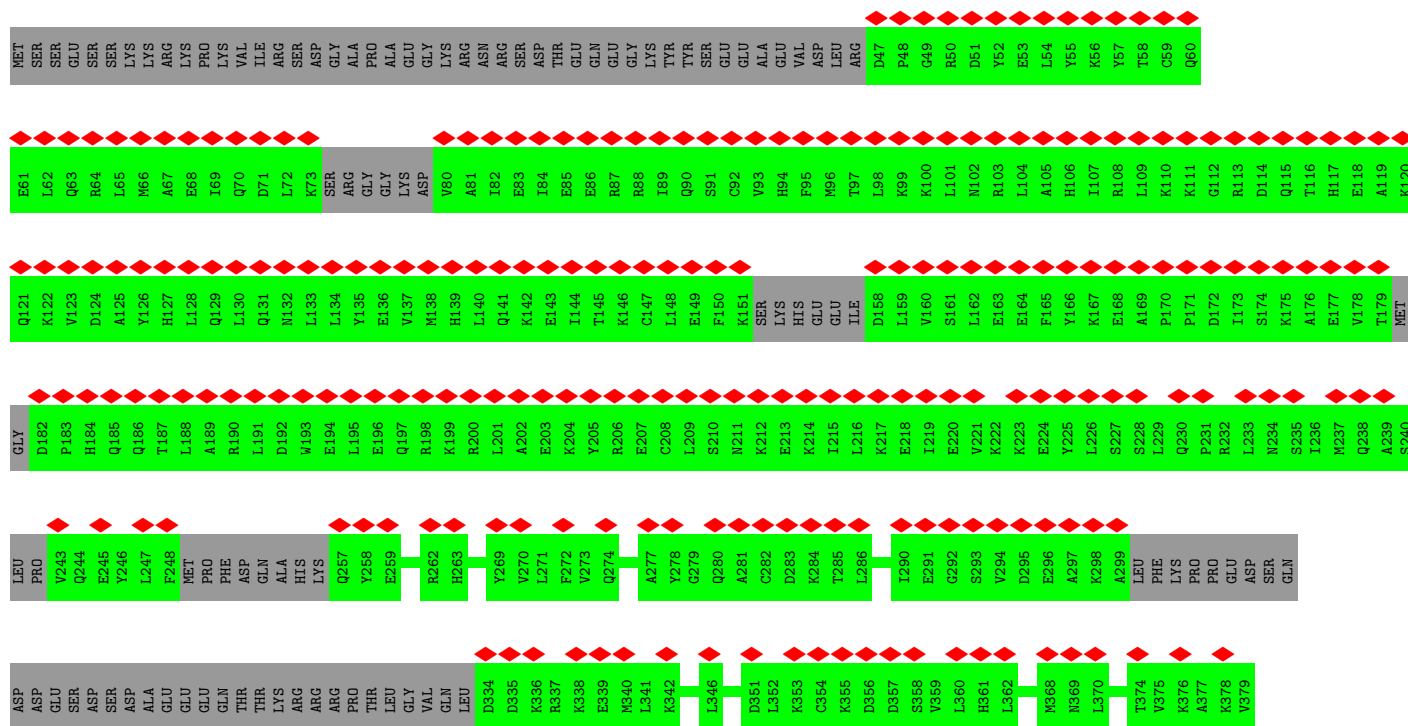
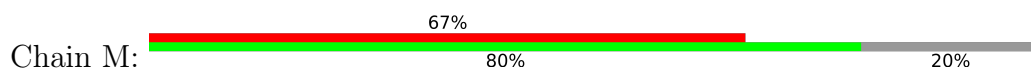


• Molecule 4: THO complex subunit 5 homolog



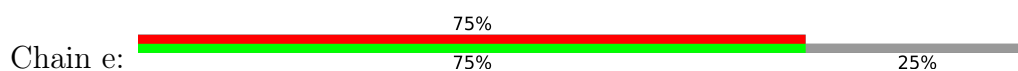


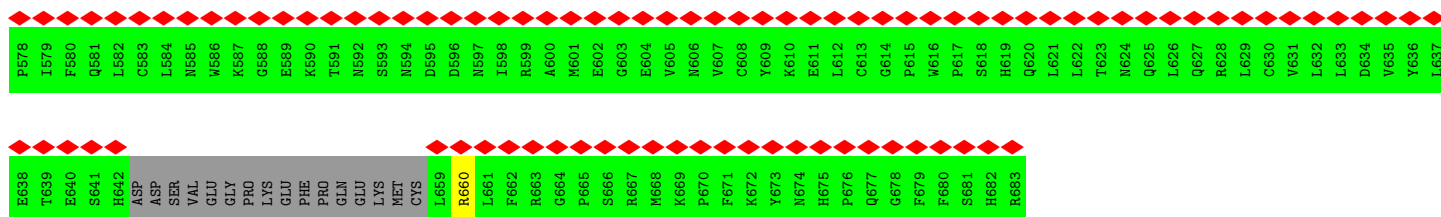
• Molecule 4: THO complex subunit 5 homolog



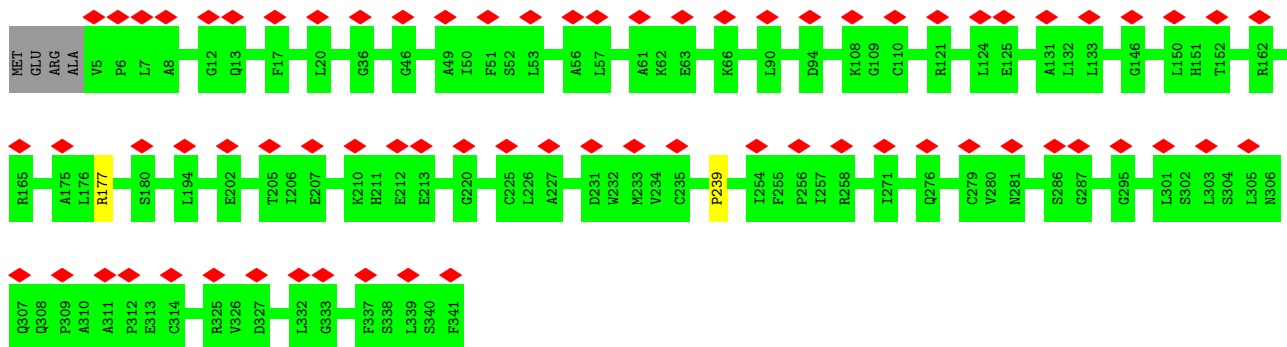


• Molecule 4: THO complex subunit 5 homolog





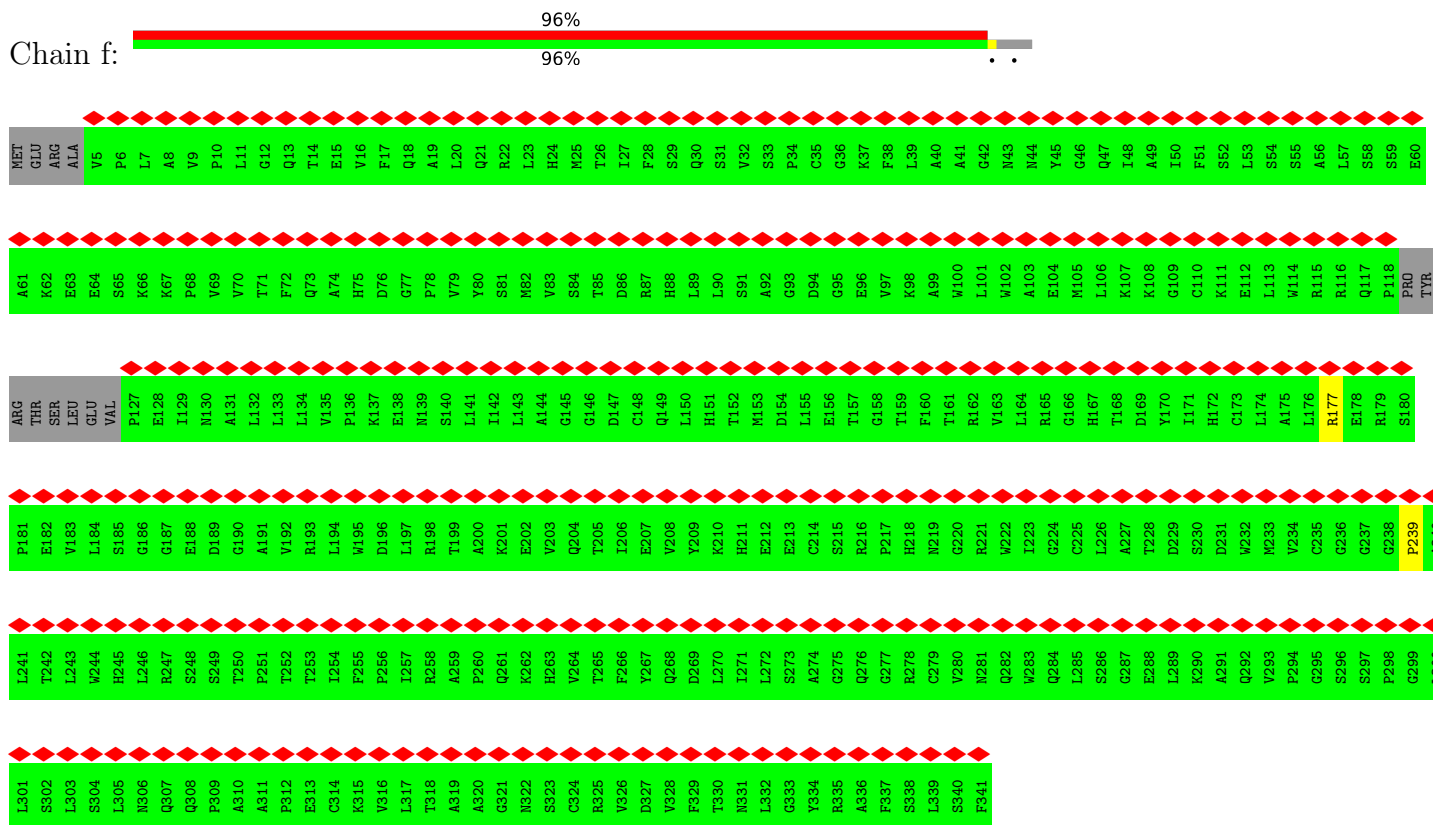
• Molecule 5: THO complex subunit 6 homolog



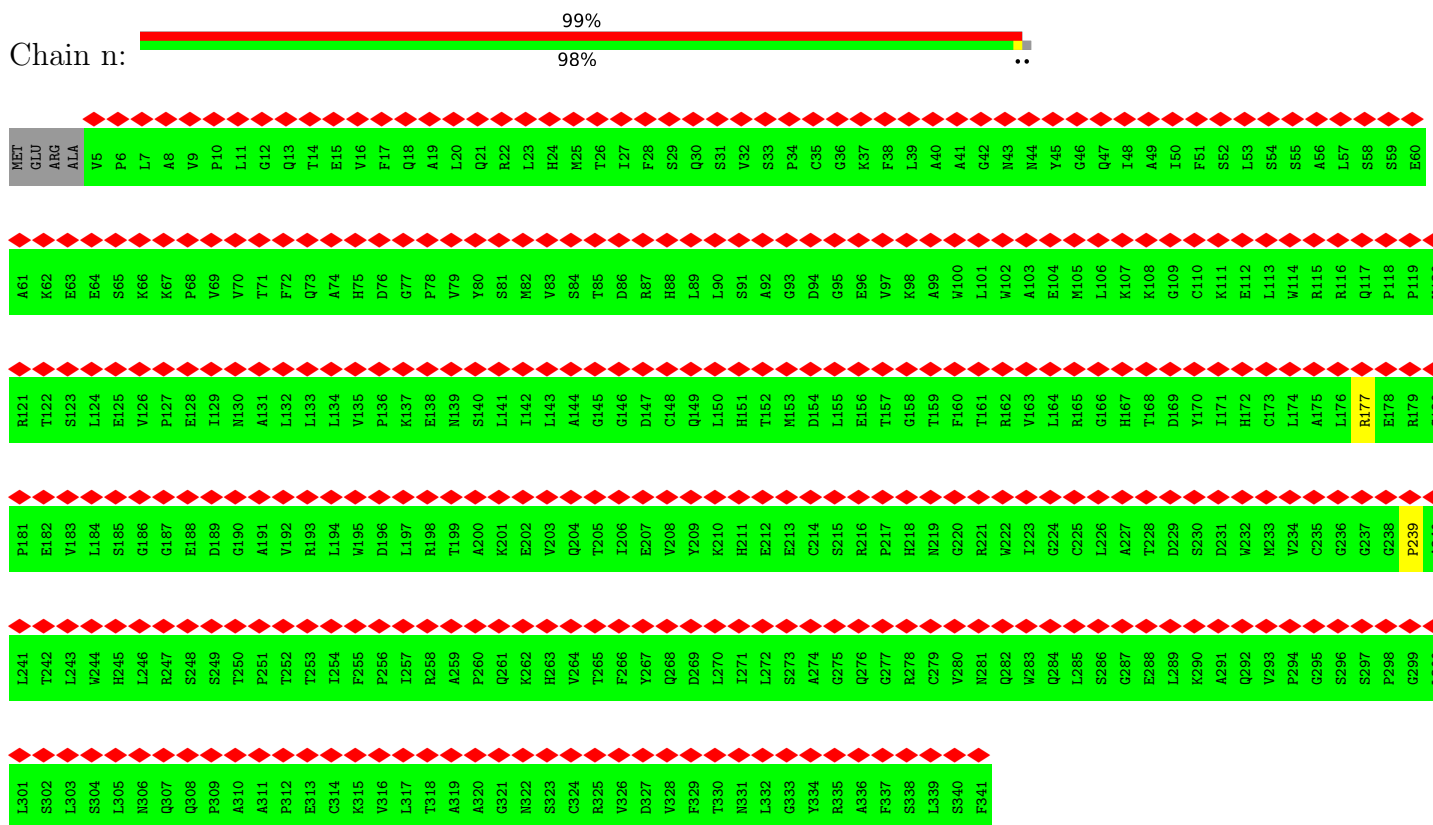
• Molecule 5: THO complex subunit 6 homolog



• Molecule 5: THO complex subunit 6 homolog



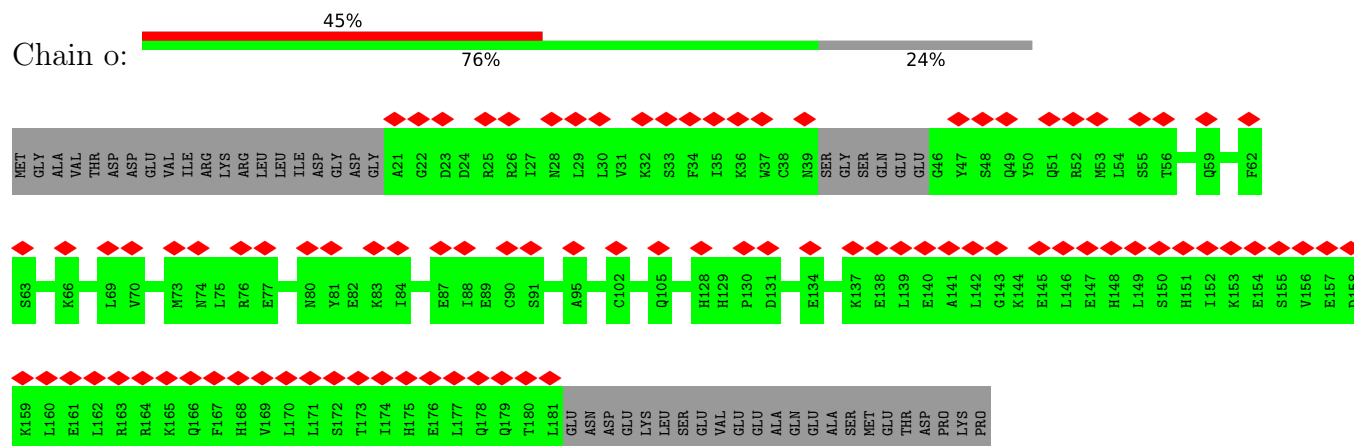
- Molecule 5: THO complex subunit 6 homolog



- Molecule 6: THO complex subunit 7 homolog

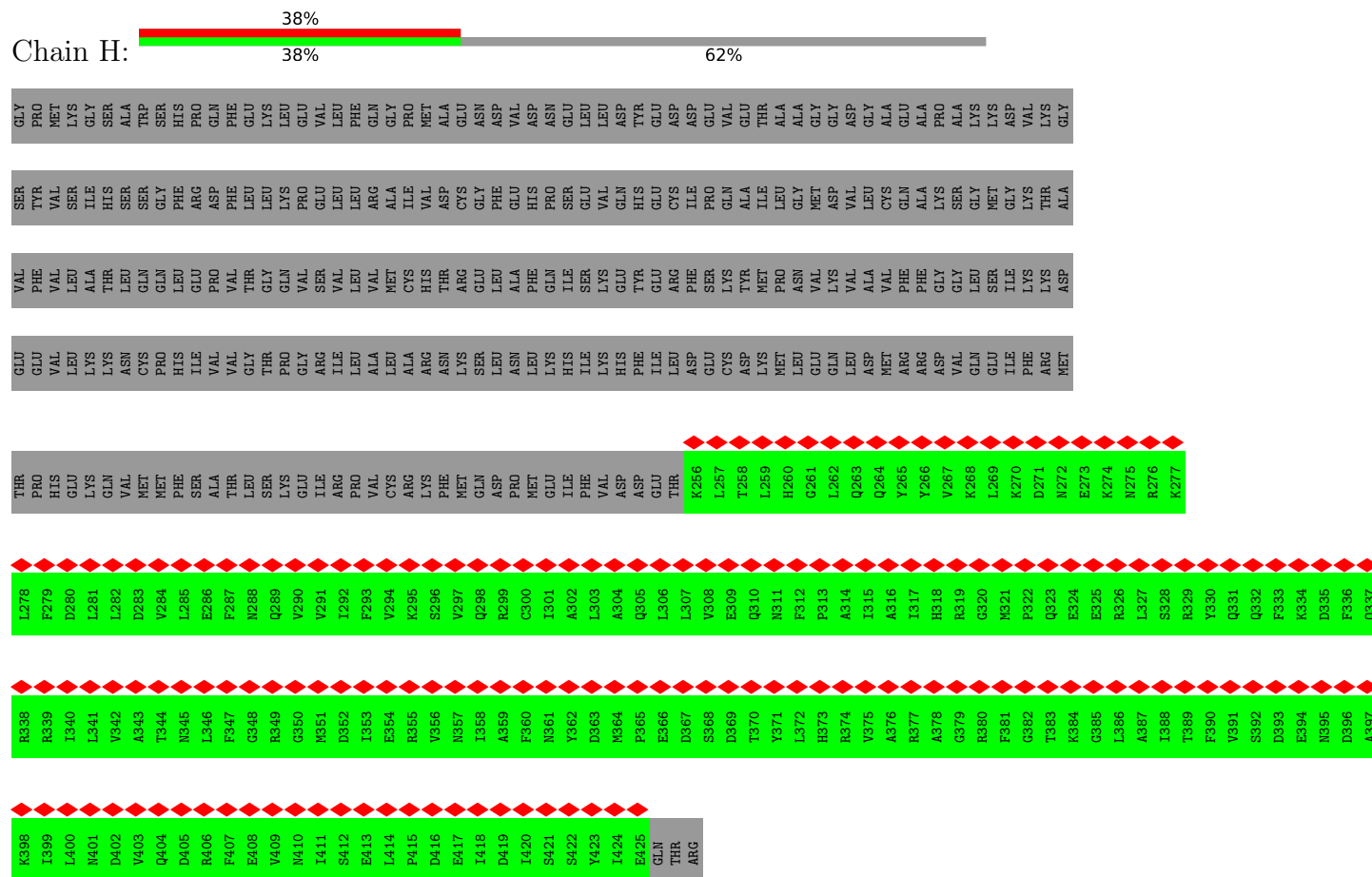
- Molecule 6: THO complex subunit 7 homolog

Chain o:



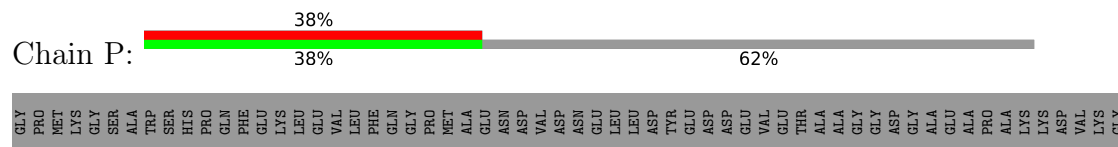
- Molecule 7: Spliceosome RNA helicase DDX39B

Chain H:



- Molecule 7: Spliceosome RNA helicase DDX39B

Chain P:



Chain p:

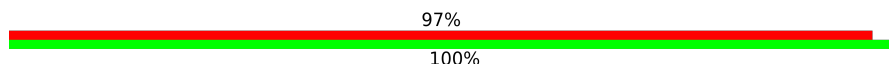
[illegible]

Chain X:



X1	X2	X3	X4	X5	X6	X7	X8	X9	X10	X11	X12	X13	X14	X15	X16	X17	X18	X19	X20	X50	X51	X52	X53	X54	X55	X56	X57	X58	X59	X60	X61	X62	X63	X64	X65	X66
----	----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

Chain x:



X1	X2	X3	X4	X5	X6	X7	X8	X9	X10	X11	X12	X13	X14	X15	X16	X17	X18	X19	X20	X20	X20	X50	X51	X51	X52	X53	X53	X54	X55	X55	X56	X57	X58	X59	X60	X61	X62	X63	X64	X65	X66
----	----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

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 ($e^-/\text{\AA}^2$)	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 (\AA)	589.60004, 589.60004, 589.60004	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	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.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

There are no chirality outliers.

5 of 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

5.2 Too-close contacts [i](#)

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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

5 of 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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	j	560	ASN
5	n	177	ARG
2	J	657	LEU
5	N	177	ARG
2	b	204	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 80 such sidechains are listed below:

Mol	Chain	Res	Type
5	f	172	HIS
4	m	369	ASN
7	h	288	ASN
2	j	518	GLN
5	n	172	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	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

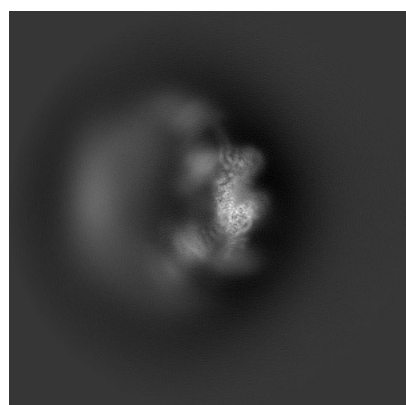
6 Map visualisation [i](#)

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.

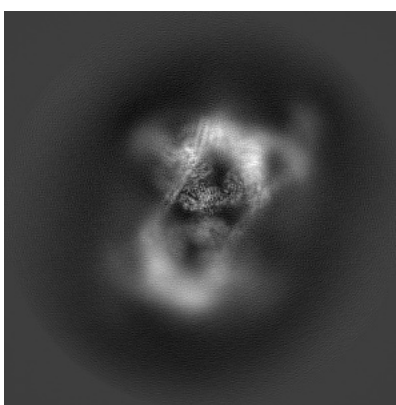
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

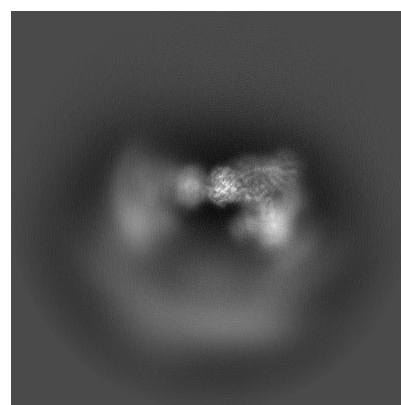
6.1.1 Primary map



X



Y

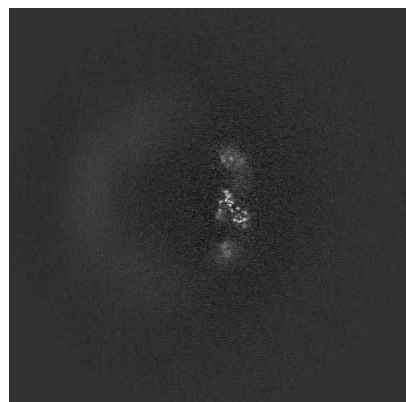


Z

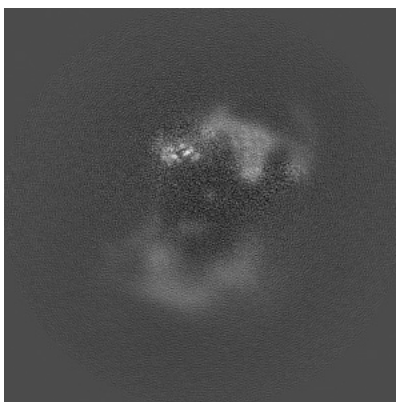
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

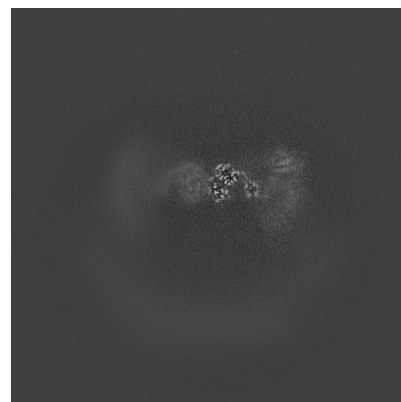
6.2.1 Primary map



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 [i](#)

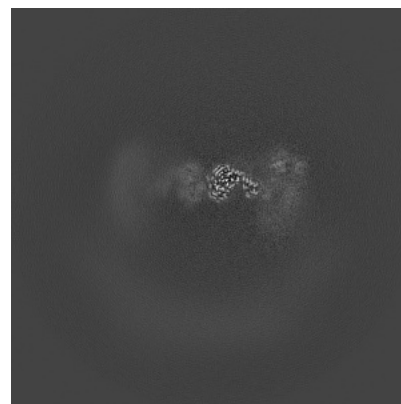
6.3.1 Primary map



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 surface views [i](#)

6.4.1 Primary map



X



Y



Z

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

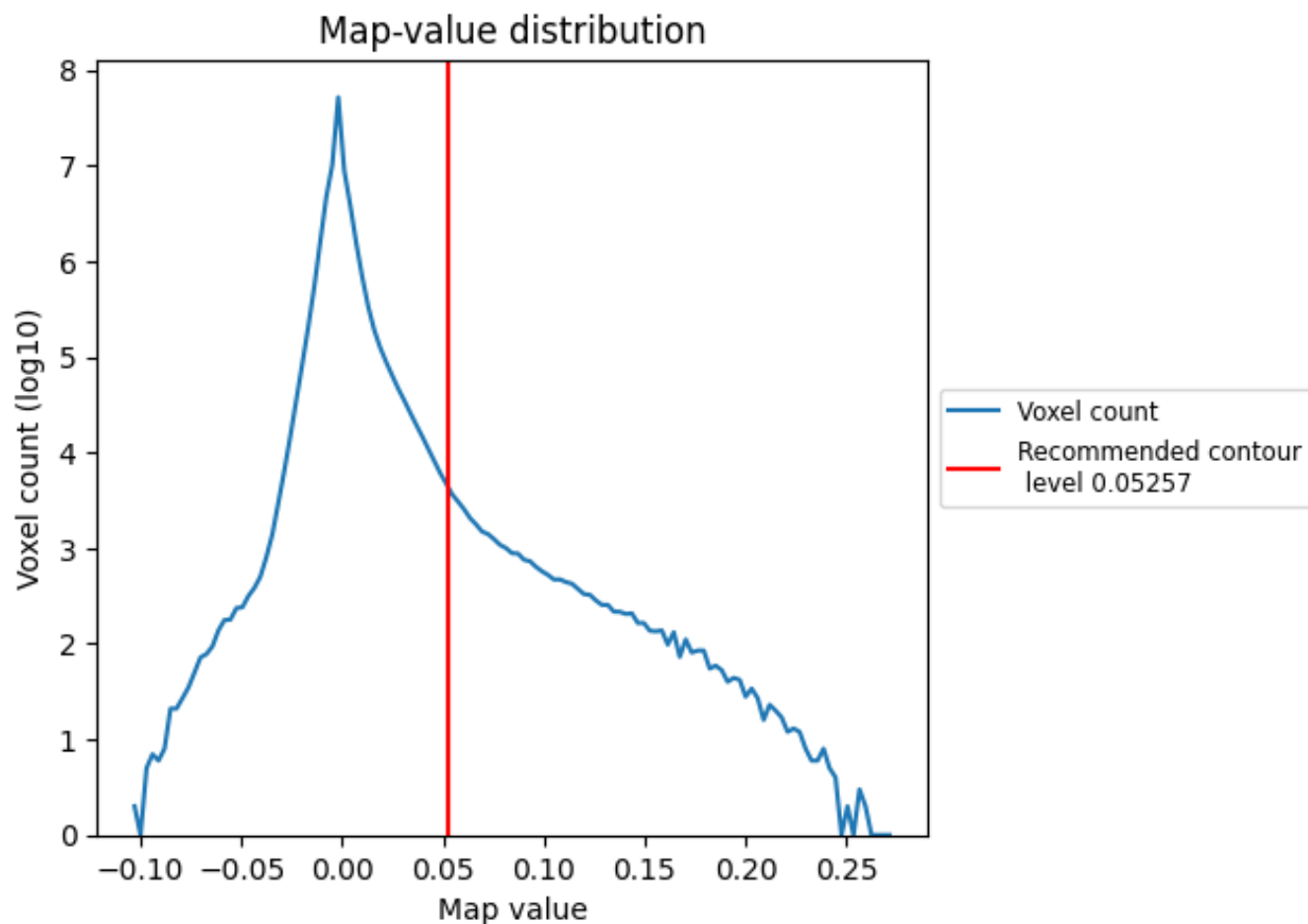
6.5 Mask visualisation

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

7 Map analysis [i](#)

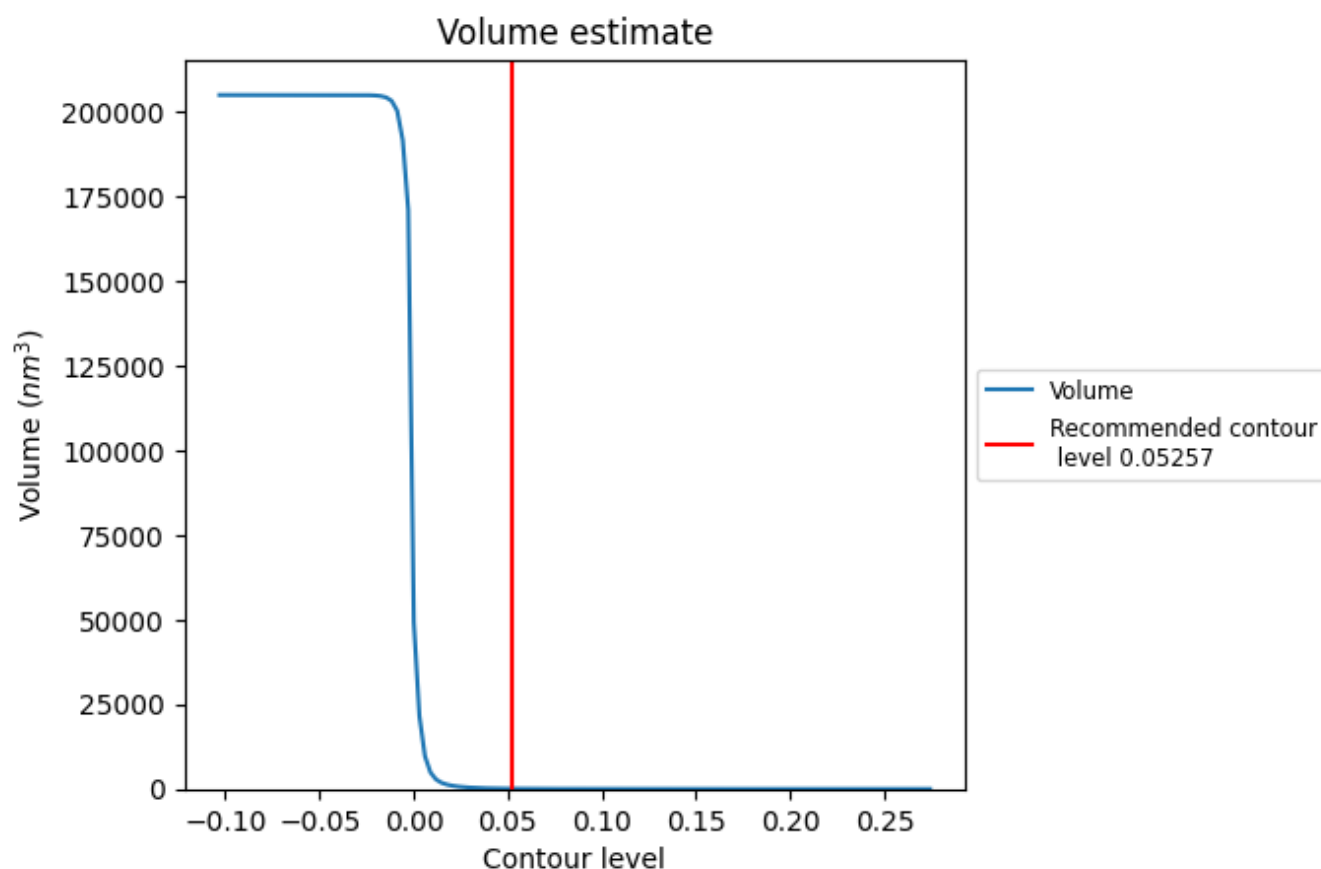
This section contains the results of statistical analysis of the map.

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.

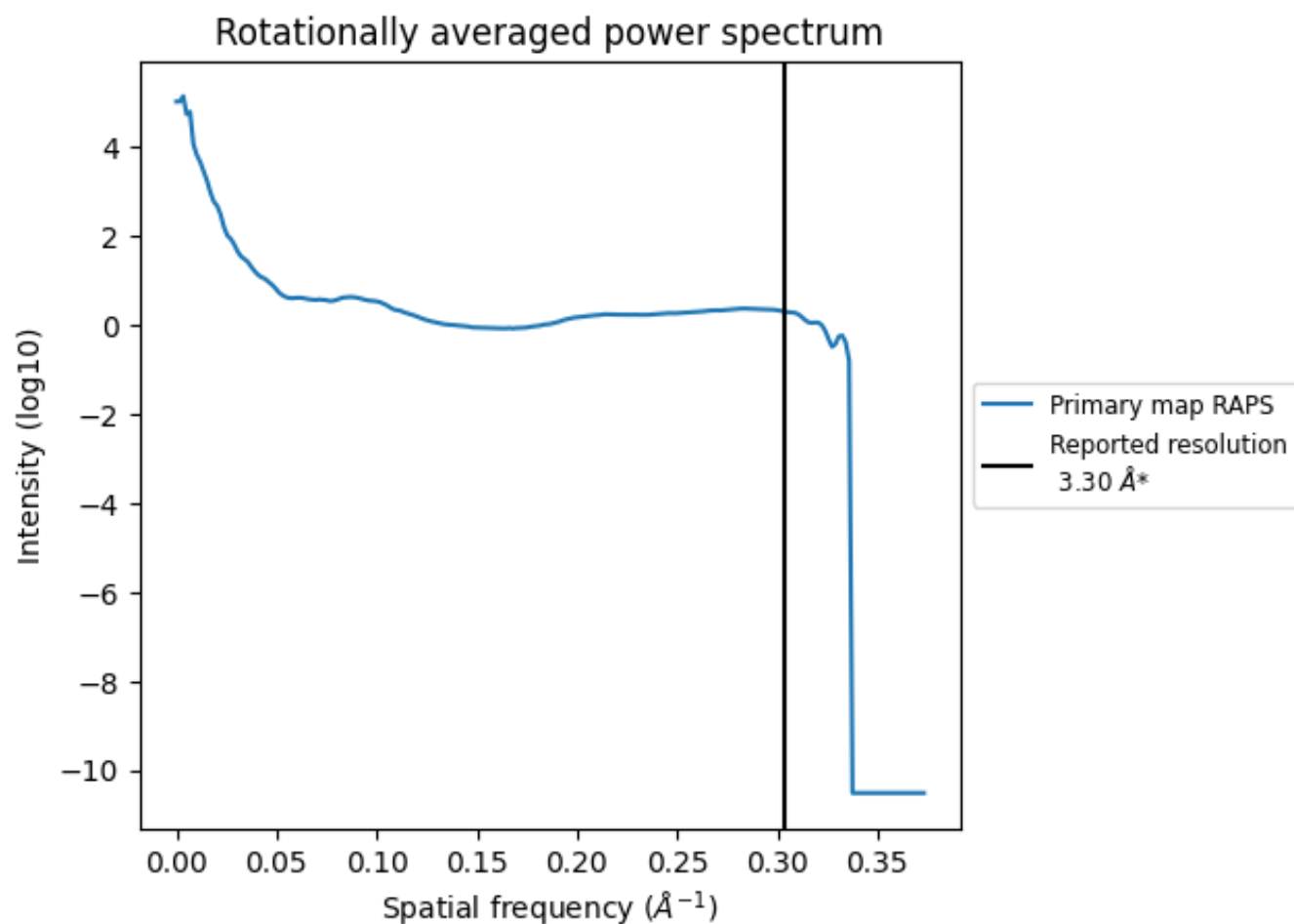
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

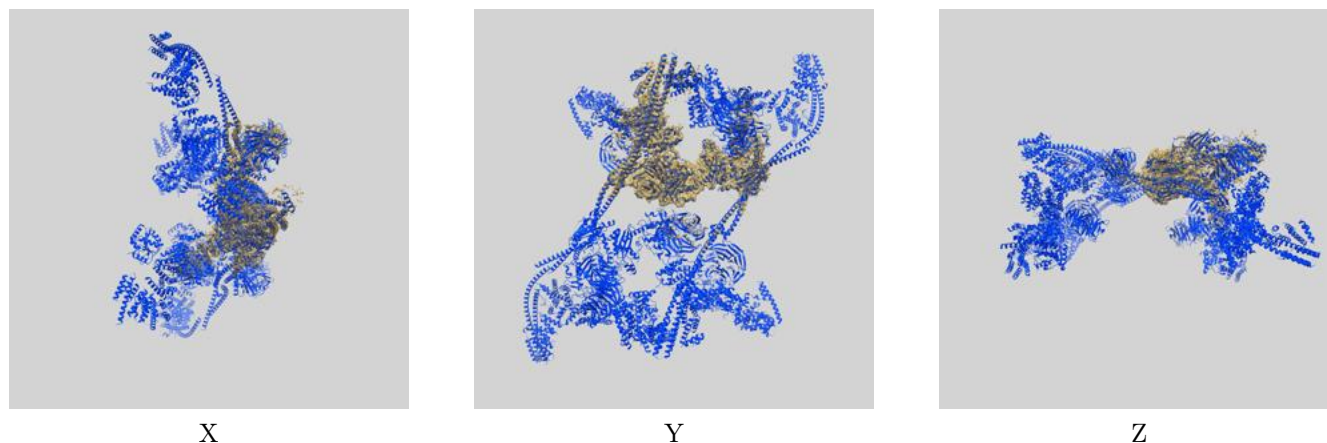
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

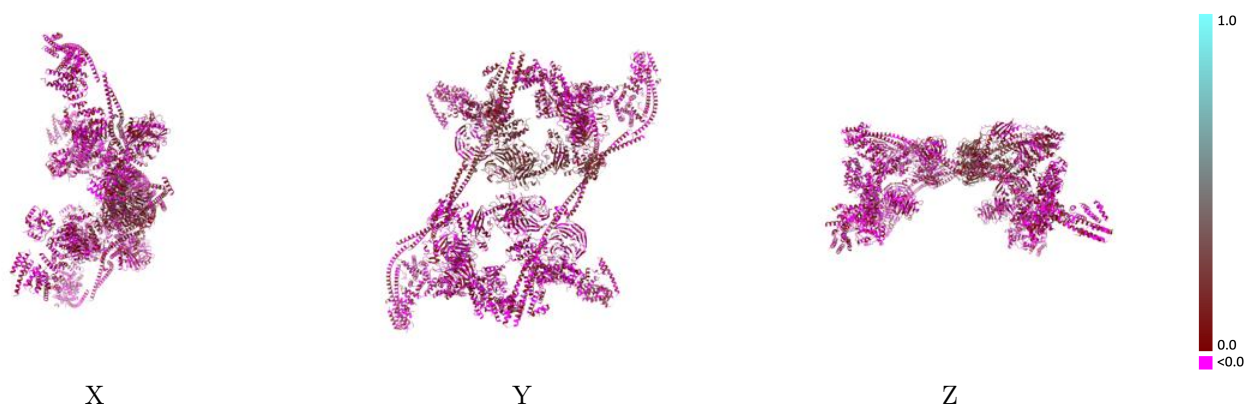
This section contains information regarding the fit between EMDB map EMD-11857 and PDB model 7APK. Per-residue inclusion information can be found in section [3](#) on page [21](#).

9.1 Map-model overlay [i](#)



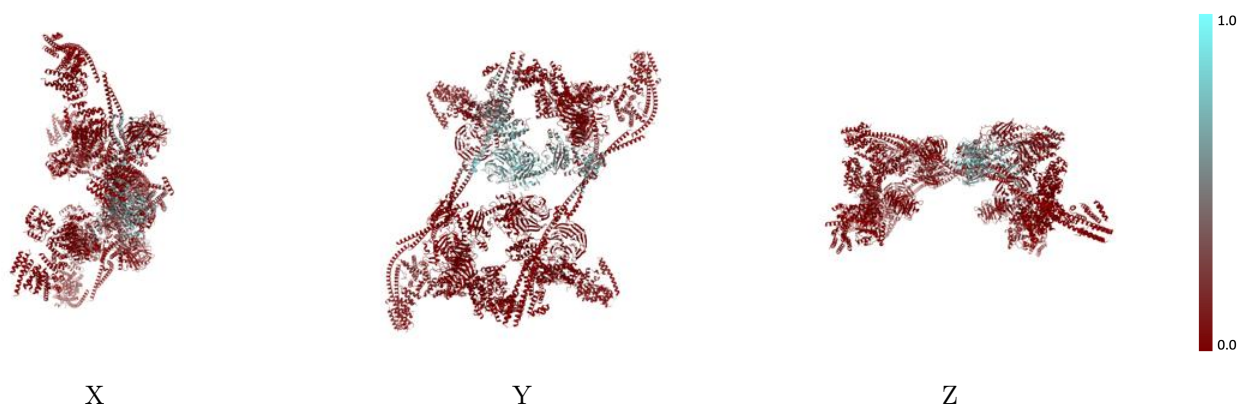
The images above show the 3D surface view of the map at the recommended contour level 0.05257 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



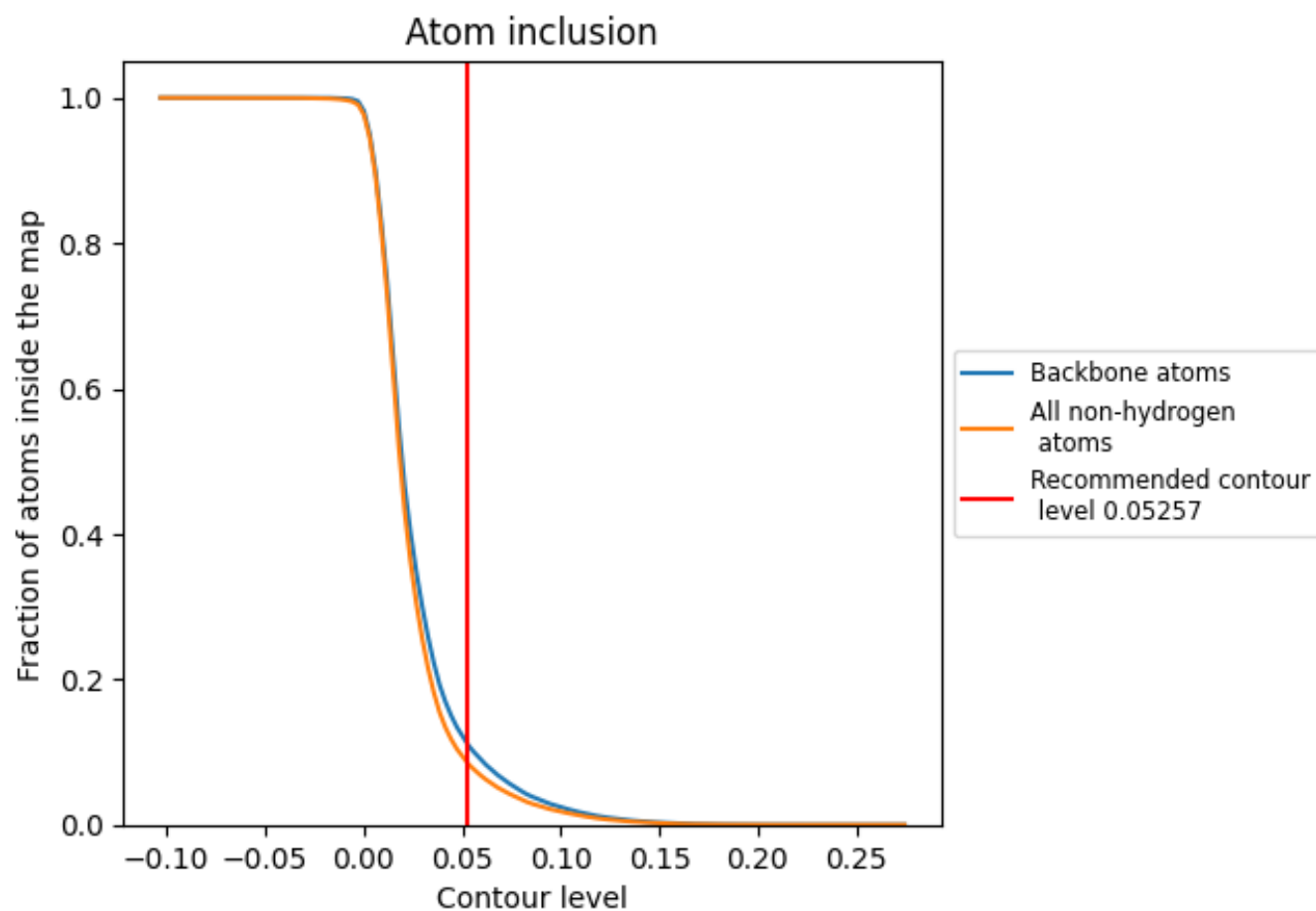
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 [i](#)



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	 0.0856	 0.0510
A	 0.0000	 0.0080
B	 0.0015	 0.0250
C	 0.0009	 0.0280
E	 0.4377	 0.1750
F	 0.5723	 0.2190
G	 0.0724	 0.0750
H	 0.0000	 0.0090
I	 0.0000	 0.0160
J	 0.0000	 0.0050
K	 0.0000	 0.0090
M	 0.1568	 0.0950
N	 0.0235	 0.0450
O	 0.0901	 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	 0.0025	 0.0340
f	 0.0137	 0.0160
g	 0.0000	 0.0560
h	 0.0000	 0.0210
i	 0.3651	 0.1810
j	 0.1096	 0.0780
k	 0.0086	 0.0270
m	 0.1064	 0.0600
n	 0.0000	 0.0190
o	 0.3593	 0.1470
p	 0.0000	 -0.0050
x	 0.0541	 0.0840

