



Full wwPDB EM Validation Report ⓘ

Mar 22, 2026 – 12:24 PM UTC

PDB ID : 7APK / pdb_00007apk
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 Full wwPDB EM Validation 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:

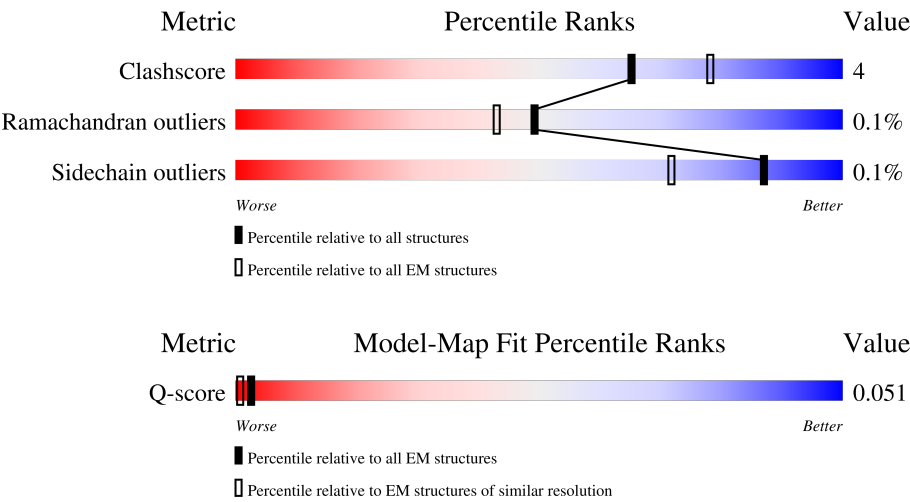
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	
1	I	711	
1	a	711	
1	i	711	

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Mol	Chain	Length	Quality of chain
2	B	1226	
2	J	1226	
2	b	1226	
2	j	1226	
3	C	395	
3	K	395	
3	c	395	
3	k	395	
4	E	683	
4	M	683	
4	e	683	
4	m	683	
5	F	341	
5	N	341	
5	f	341	
5	n	341	
6	G	204	
6	O	204	
6	g	204	
6	o	204	
7	H	451	
7	P	451	
7	h	451	
7	p	451	
8	X	37	

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Mol	Chain	Length	Quality of chain
8	x	37	97% 100%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 72697 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called THO complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	266	Total	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		

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

- Molecule 1: THO complex subunit 1

[illegible][illegible][illegible][illegible]

M247	P248	Q249	Q250	C251	Y252	E253	K254	T255	S256	W257	K258	T259	F260	L261	K262	Y263	S264	E265	E266	Y267	L268	A269	W270	F271	K272	S273	Y274	K275	L276	T277	D278	THR	GLN	ALA	SER	ARG	ARG	LYS	K285	M286	E287	E288	L289	LYS	THR	THR	GLY	GLY	GLU	HIS	Y296	Y297	F298	A299	K300	F301	L302	T303	S304	E305	K306
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PRO	THR	LYS	LYS	ILE	LEU	MET	GLY	ASN	GLU	LEU	THR	ARG	LEU	TRP	ASN	CYS	PRO	ASP	MET	GLU	THR	ARG	GLU	HIS	MET	PRO	THR	LEU	GLU	GLU	PHE	GLU	GLU	ALA	ILE	GLU	GLN	ALA	ASP	PRO	GLU	ASN	MET	VAL	GLU	ASN	GLU	TYR	LYS	ALA
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VAL	ASN	ASN	SER	ASN	TYR	GLY	TRP	ARG	ALA	LEU	ARG	LEU	LEU	LEU	ALA	ARG	SER	PRO	HIS	PHE	PHE	GLN	PRO	THR	ASN	GLN	GLN	PHE	LYS	SER	LEU	PRO	GLU	TYR	LEU	GLU	ASN	MET	VAL	ILE	LYS	LEU	ALA	LYS	GLY	LEU	PRO	PRO	SER	GLU	GLY	ASP	THR
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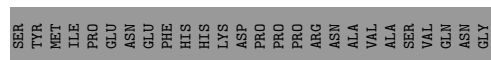
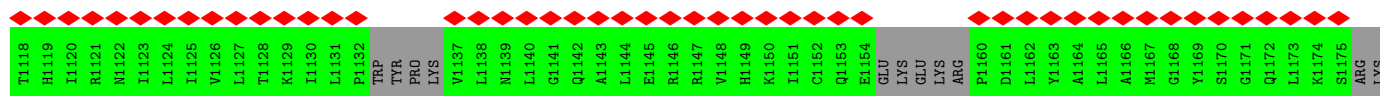
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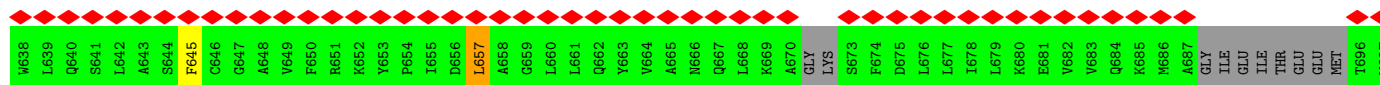
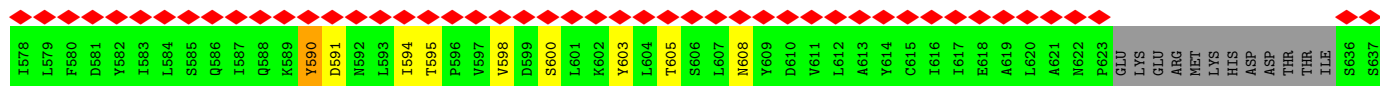
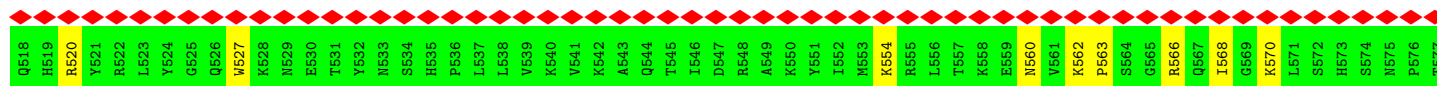
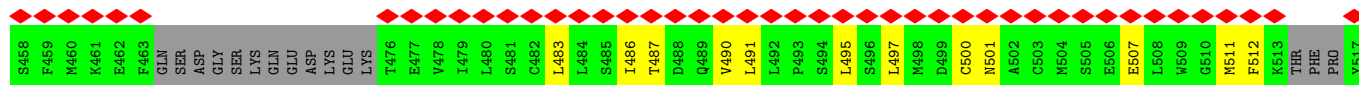
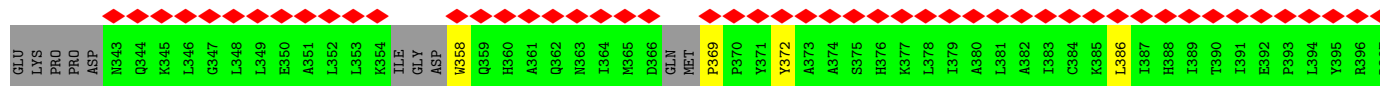
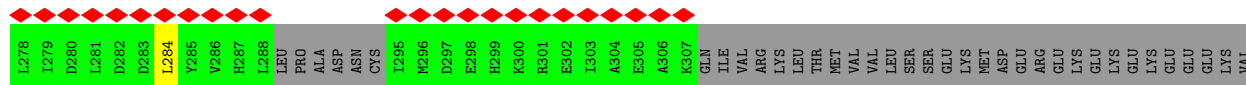
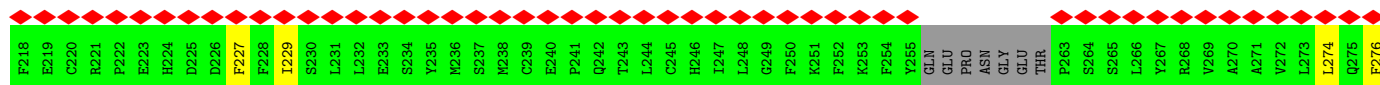
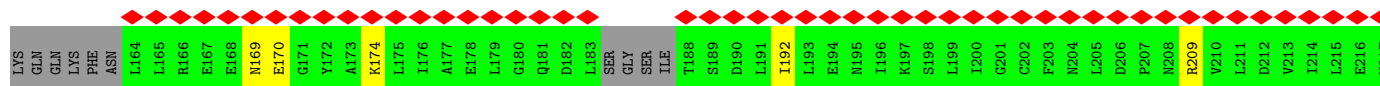
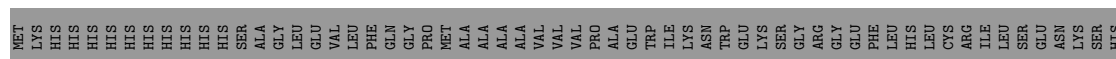
- Molecule 1: THO complex subunit 1



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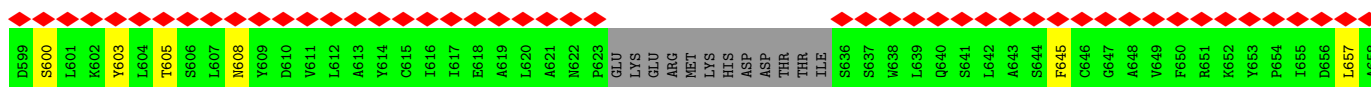
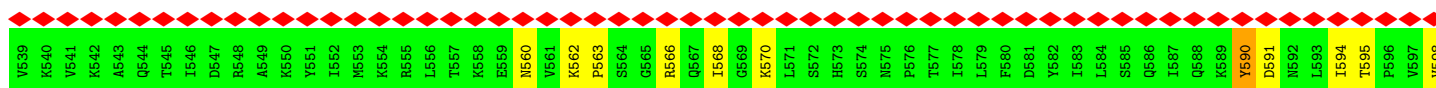
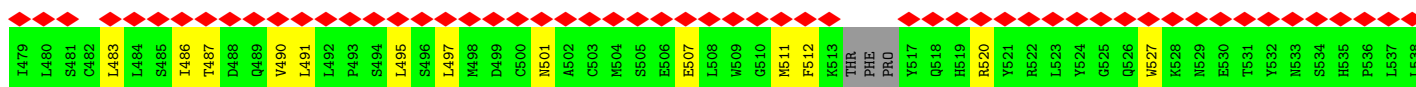
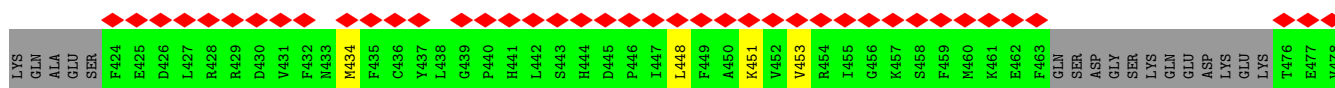
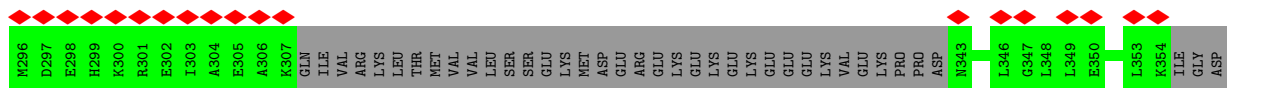
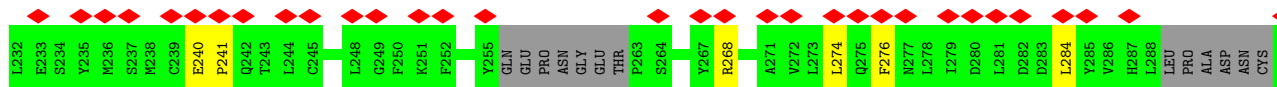
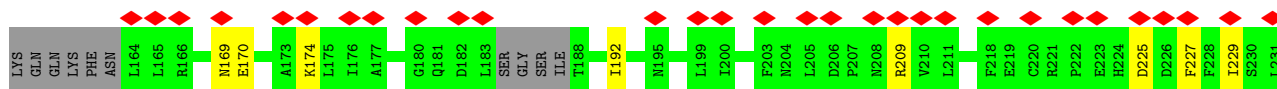
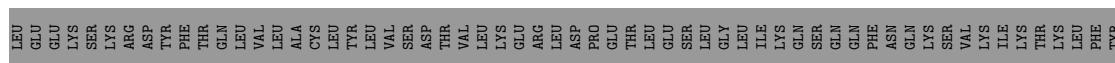
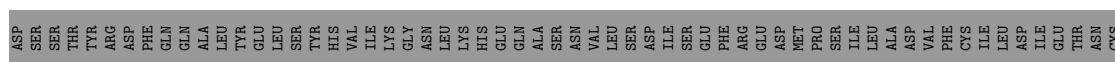
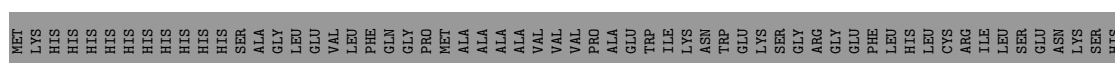
• Molecule 2: THO complex subunit 2

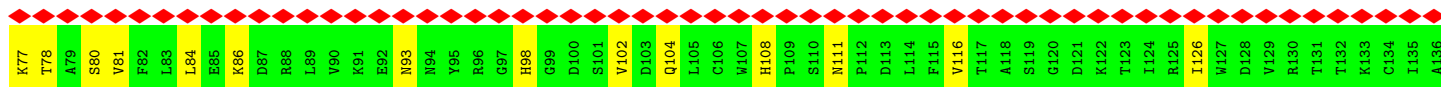


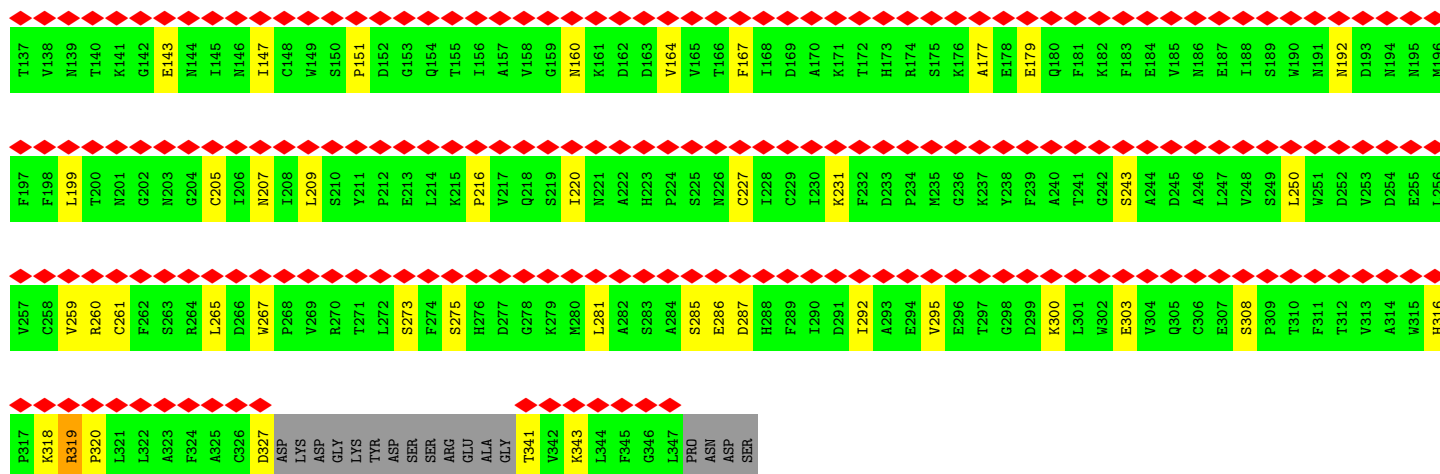
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L938	L939	E940	E941	E942	K943	K944	Q945	M946	E947	H948	V949	Q950	R951	Y952	L953	Q954	R955	L956	K957	L958	E959	LYS	ASP	ASN	TRP	LEU	LEU	LEU	ALA	LYS	THR	THR	N971	E972	T973	I974	T975	K976	F977	L978	Q979	L980	C981	L982	F983	P984	R985	C986	L987	F988	S989	A990	T1051	R1052	W1053	H1054	SER	ASP	ARG					
P878	Q879	F880	Y881	A882	T883	F884	TRP	SER	SER	LEU	THR	M889	Y890	D891	L892	A893	V894	PRO	H896	T897	S898	Y899	E900	R901	E902	Y903	L904	K905	L906	K907	GLN	MET	LYS	ALA	ILE	ASP	ASN	GLN	PRO	MET	LEU	ILE	LYS	VAL	SER	LYS	E927	K928	E929	R930	C931	T932	A933	L934	Q935	D936	K937							
SER	ARG	PRO	MET	ALA	HIS	HIS	ILE	SER	SER	SER	TYR	GLU	LEU	LYS	SER	GLU	LYS	GLY	SER	LYS	GLN	GLN	HIS	LYS	VAL	HIS	LYS	TYR	ILE	THR	CYS	E854	M855	V856	M857	A858	P859	V860	H861	E862	A863	V864	V865	S866	L867	HIS	VAL	SER	LYS	V872	D873	Q874	D875	R876	S877									
GLY	GLY	LYS	HIS	L763	K764	L765	V766	G767	K768	L769	Y770	D771	Q772	C773	H774	D775	T776	L777	V778	Q779	F780	G781	F782	F783	L784	A785	S786	ASN	LEU	THR	GLU	ASP	TYR	ILE	LYS	ARG	VAL	PRO	LEU	ILE	ASP	VAL	ILE	ASP	LEU	ALA	L740	P741	L742	C743	L744	L745	M746	A747	Q748	Q749	ARG	ASN	G752	V753	L754	F755	Q756	E757
E698	Q699	L700	E701	A702	MET	THR	GLY	G706	E707	Q708	L709	K710	A711	E712	G713	G714	TYR	PHE	GLY	GLN	ILE	ARG	ASN	THR	K723	L724	S725	S726	Q727	R728	L729	K730	D731	A732	L733	LEU	ASP	HIS	ASP	LEU	ALA	L740	P741	L742	C743	L744	L745	M746	A747	Q748	Q749	ARG	ASN	G752	V753	L754	F755	Q756	E757					
W638	L639	Q640	S641	L642	A643	S644	F645	C646	G647	A648	V649	F650	R651	K652	Y653	P654	L655	D656	L657	A658	G659	L660	L661	Q662	Y663	V664	A665	M666	Q667	L668	K669	A670	GLY	LYS	S673	F674	D675	L676	L677	L678	L679	K680	E681	V682	V683	Q684	K685	M686	A687	GLY	ILE	GLU	ILE	THR	GLU	MET	T696	M697						
I578	L579	F580	D581	Y582	I583	L584	S585	Q586	Y587	Q588	K589	Y590	D591	N592	L593	I594	T595	P596	V597	V598	D599	S600	L601	K602	Y603	L604	T605	S606	L607	N608	Y609	D610	V611	L612	A613	Y614	C615	I616	I617	E618	A619	L620	A621	N622	P623	GLU	LYS	GLU	ARG	MET	LYS	HIS	ASP	THR	THR	ILE	S636	S637						
Q518	H519	R520	Y521	R522	L523	Y524	G525	Q526	W527	K528	N529	E530	T531	Y532	N533	S534	H535	P536	L537	L538	V539	K540	V541	K542	A543	Q544	T545	I546	D547	R548	A549	K550	Y551	I552	M553	K554	R555	L556	T557	K558	E559	N560	V561	K562	P563	S564	G565	R566	Q567	L568	G569	K570	L571	S572	H573	N575	P576	T577						
S458	F459	M460	K461	E462	F463	GLN	SER	ASP	GLY	SER	LYS	GLN	GLU	ASP	LYS	GLU	LYS	T476	E477	V478	I479	L480	S481	C482	L483	L484	S485	I486	T487	D488	Q489	V490	L491	L492	P493	S494	S496	L497	M498	D499	C500	N501	A502	C503	M504	S505	E506	E507	L508	W509	G510	M511	F512	K513	THR	PHE	PRO	Y517						
V398	GLY	VAL	PRO	LYS	GLY	ALA	LYS	SER	PRO	VAL	ASN	GLN	ASP	LYS	ARG	ALA	PRO	GLY	LYS	GLN	ALA	F424	E425	D426	L427	R428	R429	D430	V431	F432	N433	M434	F435	C436	Y437	L438	G439	P440	H441	L442	S443	H444	A502	D445	C503	M504	S505	L448	F449	A450	K451	V452	R454	I455	G456	K457								
GLU	LYS	PRO	PRO	ASP	N343	Q344	K345	L346	Q347	L348	L349	E350	ASP	ASN	L352	L353	K354	ILE	GLY	ASP	W358	Q359	H360	A361	Q362	N363	I364	M365	D366	GLN	MET	P369	P370	Y371	Y372	A373	A374	S375	H376	K377	L378	I379	A380	A382	I383	C384	K385	L386	I387	H388	I389	T390	I391	E392	P393	L394	Y395	R396	R397					

SER	TYR	MET	ILE	PRO	GLU	ASN	GLU	PHE	HIS	HIS	LYS	ASP	PRO	PRO	PRO	ARG	ASN	ALA	VAL	ALA	SER	SER	VAL	GLN	ASN	GLY
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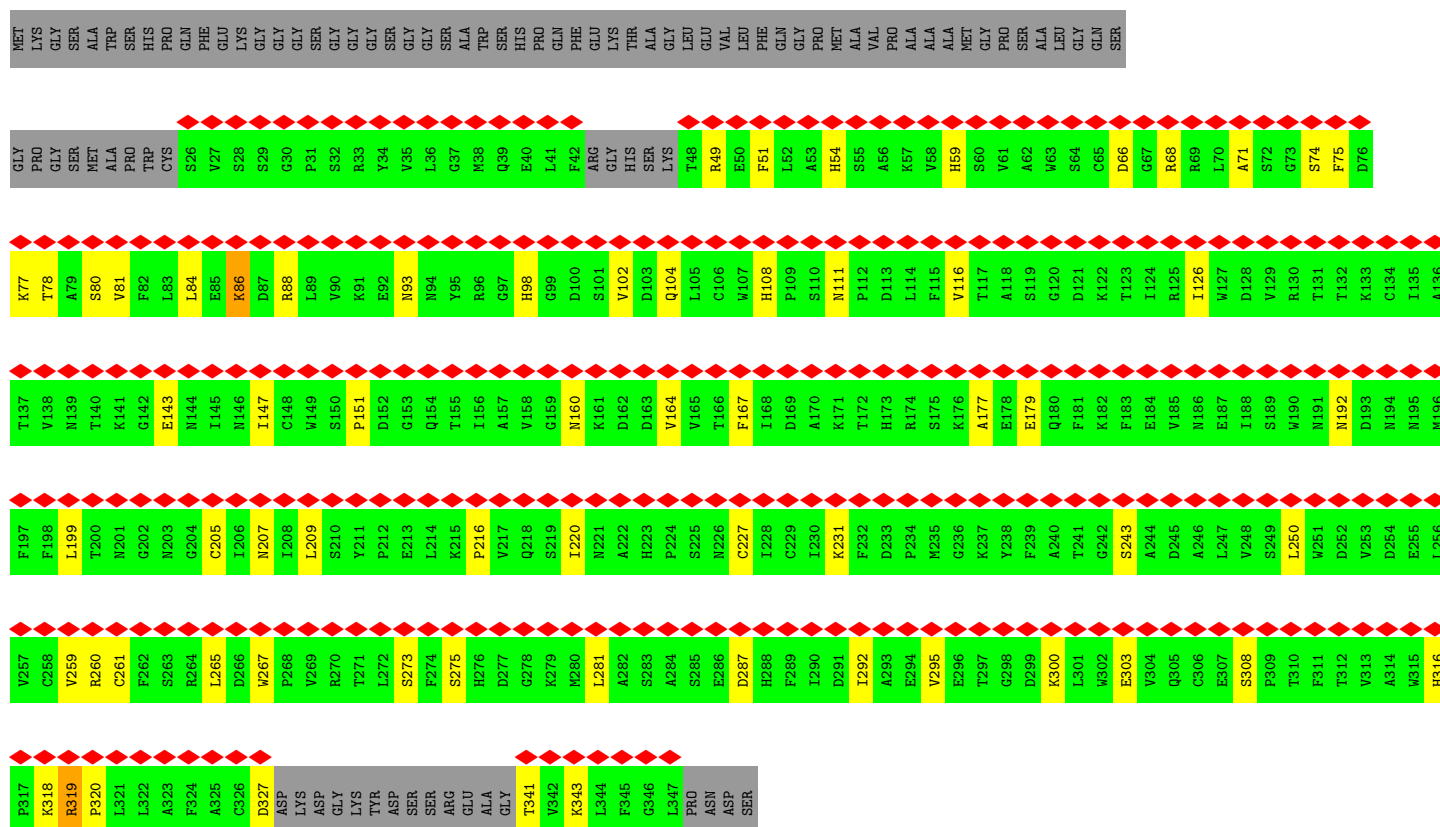
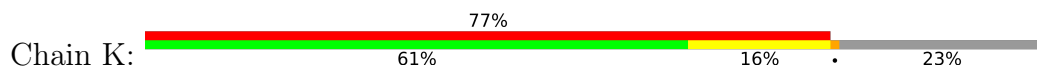
- Molecule 2: THO complex subunit 2



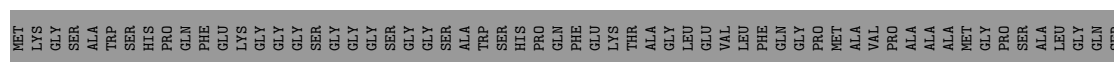
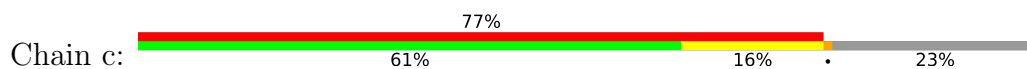


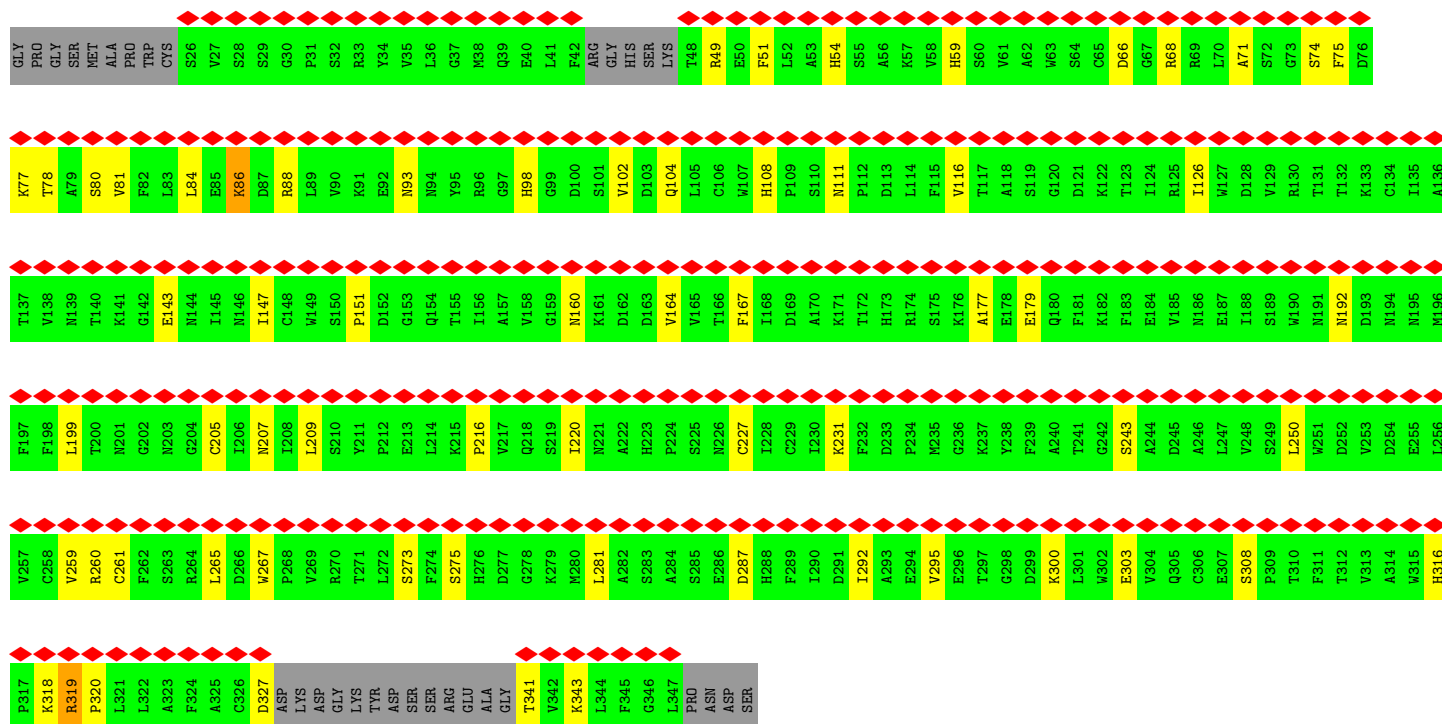


• Molecule 3: THO complex subunit 3

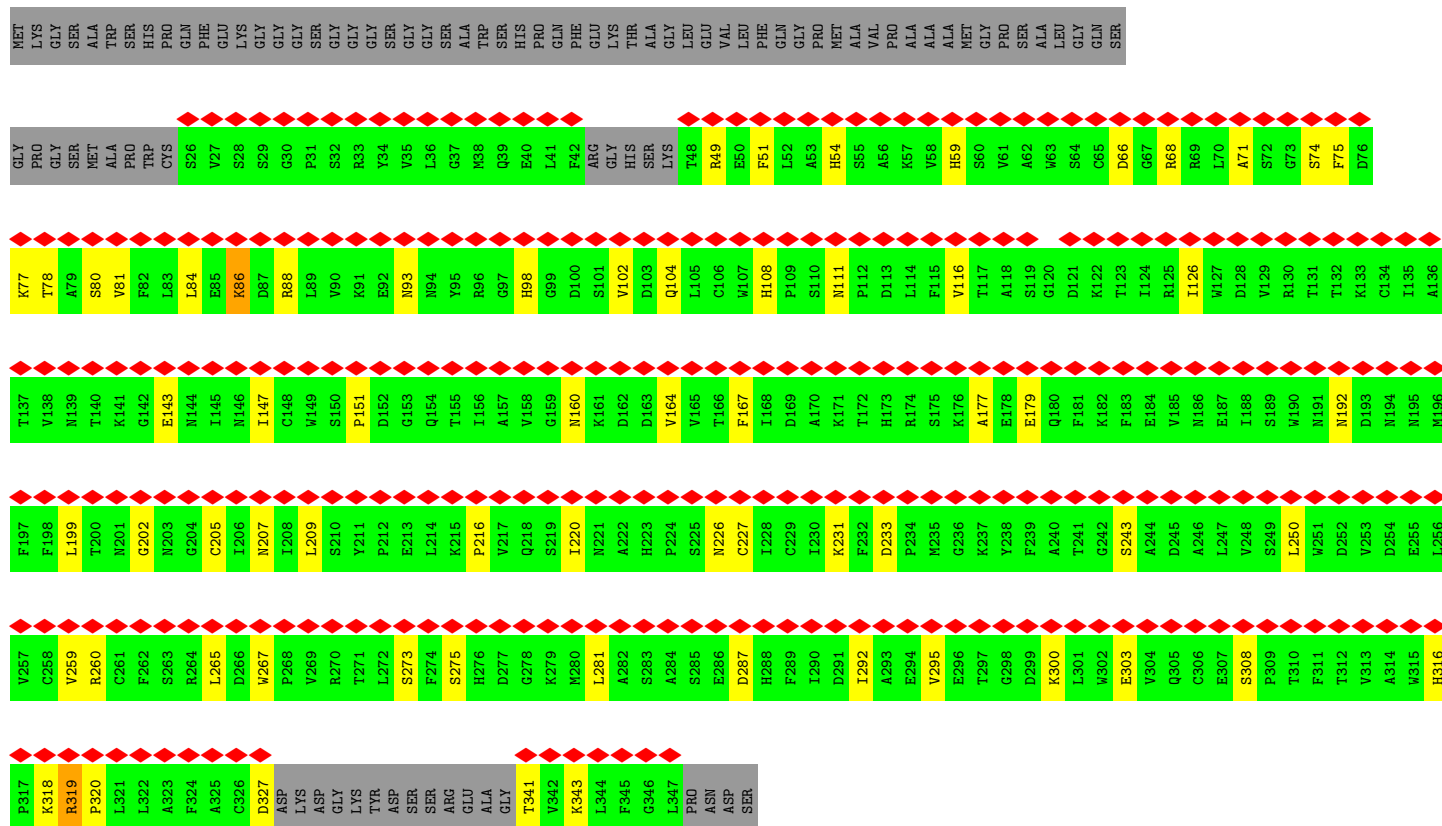
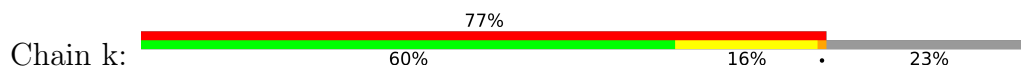


• Molecule 3: THO complex subunit 3



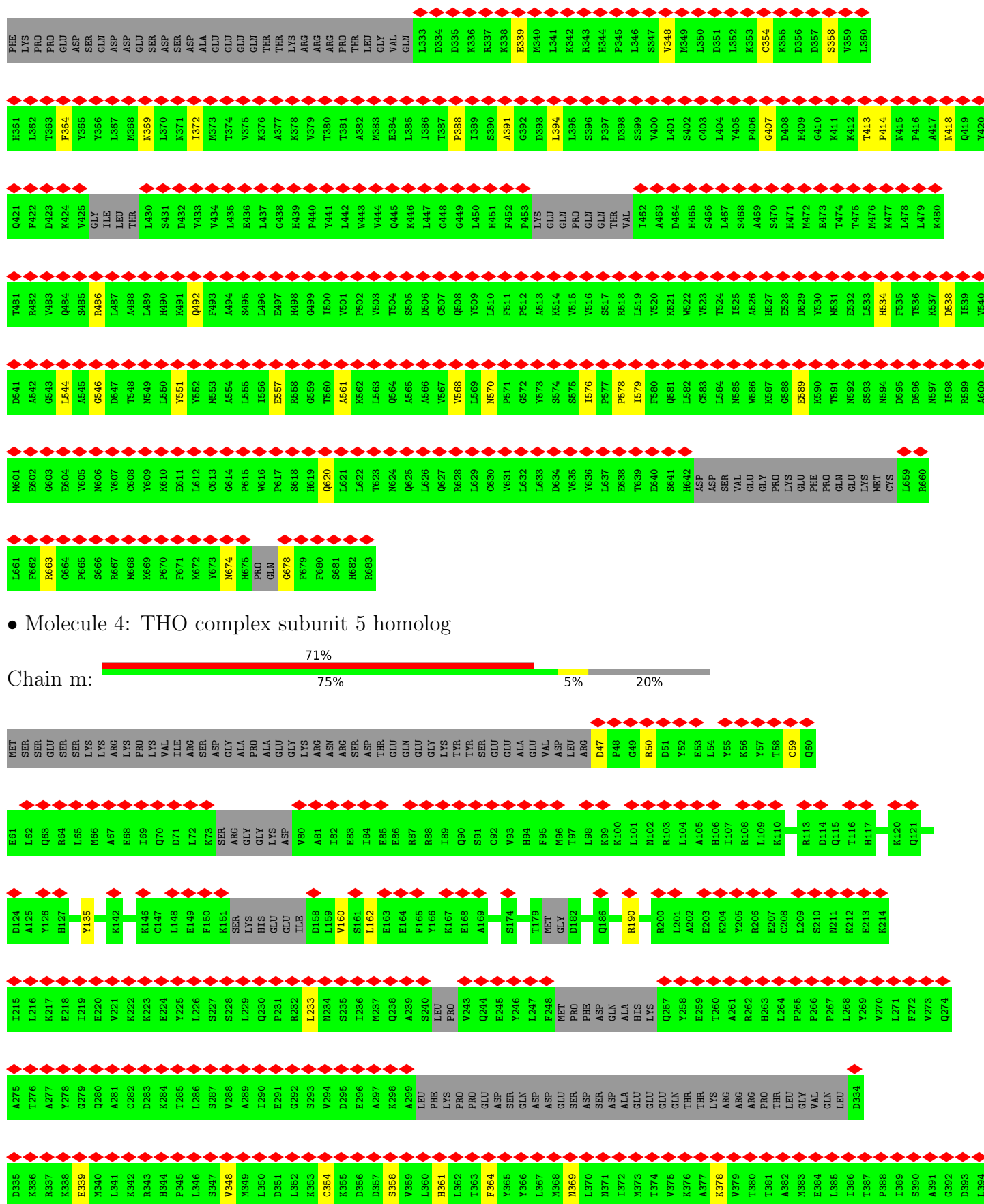


• Molecule 3: THO complex subunit 3

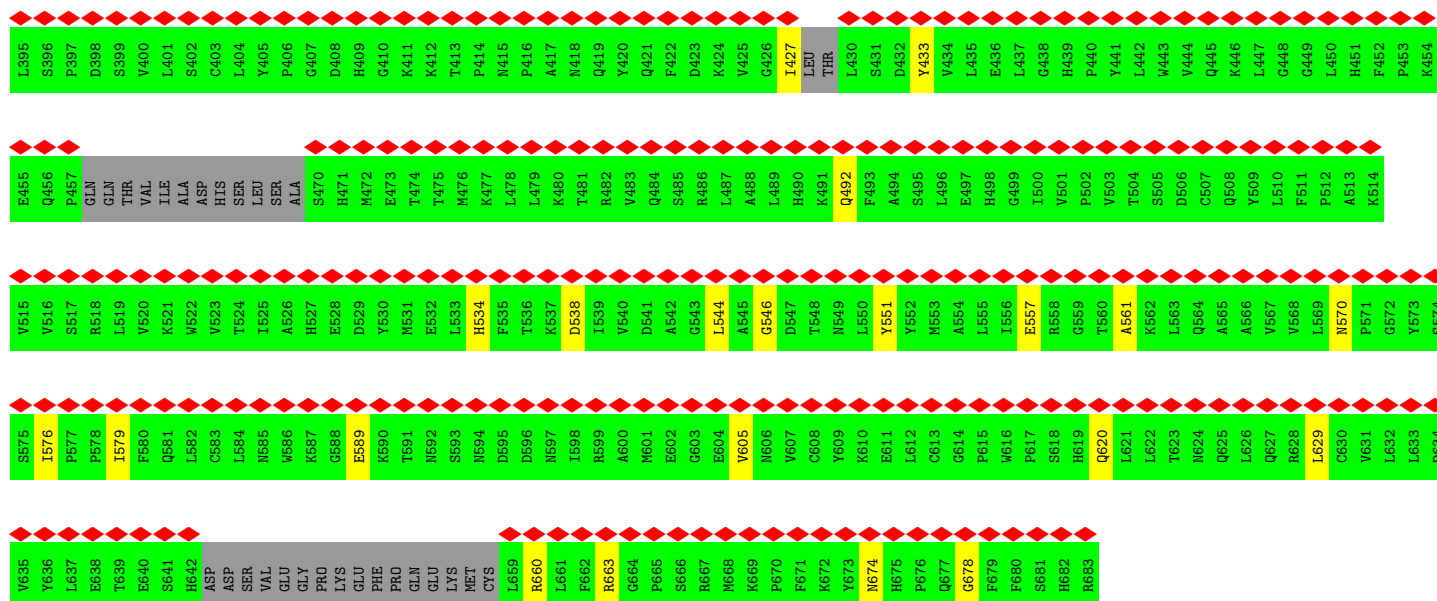


• Molecule 4: THO complex subunit 5 homolog

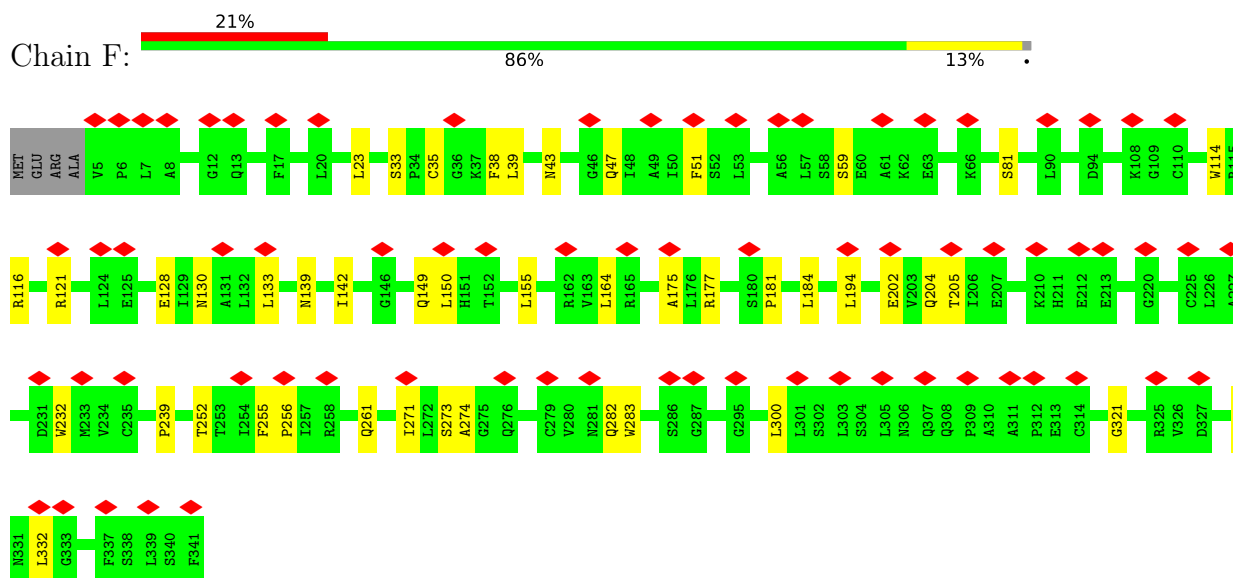




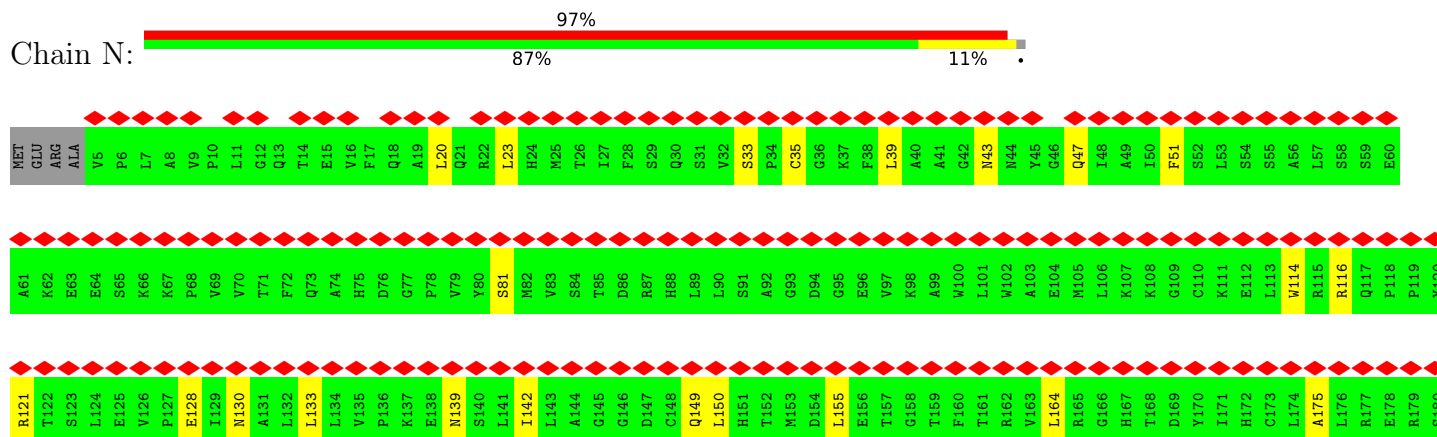
• Molecule 4: THO complex subunit 5 homolog



• Molecule 5: THO complex subunit 6 homolog

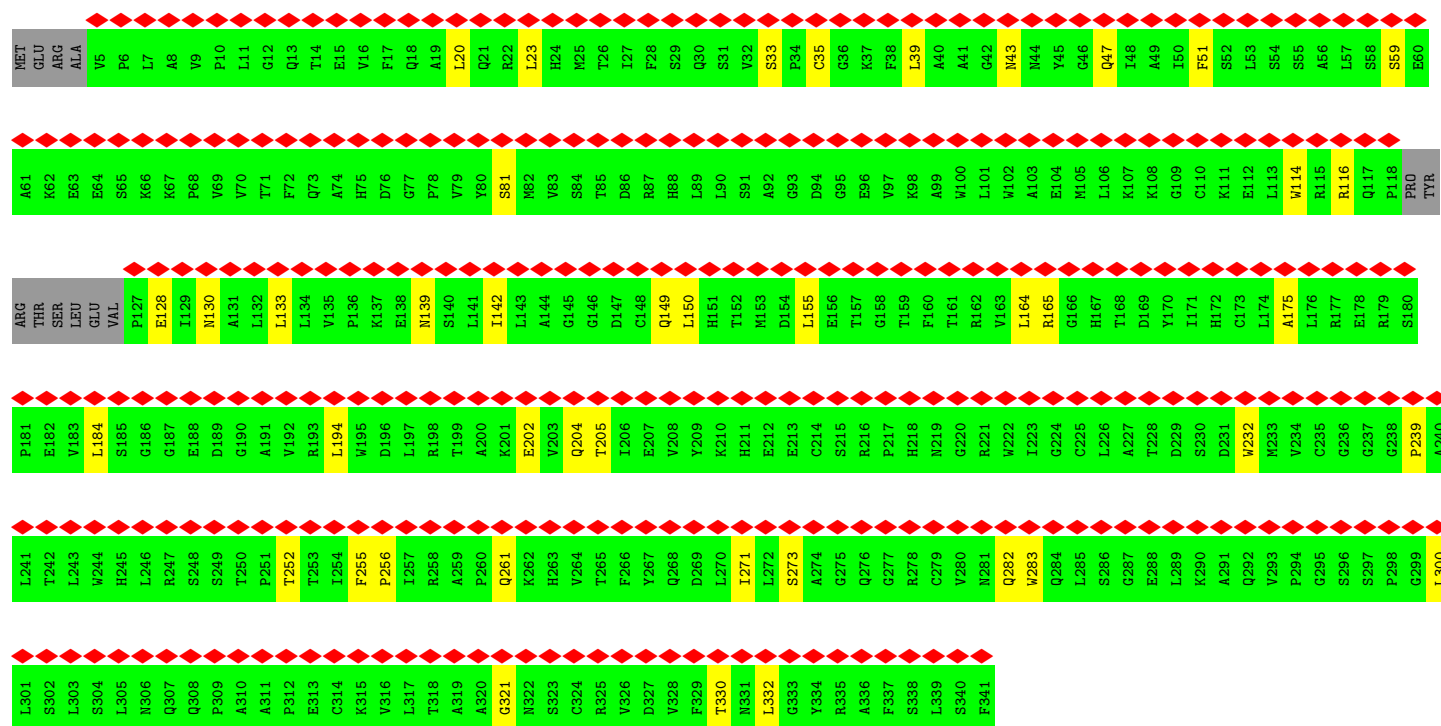
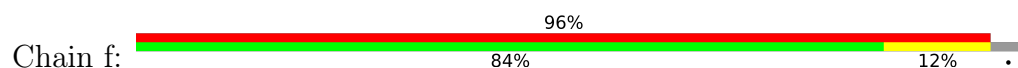


• Molecule 5: THO complex subunit 6 homolog

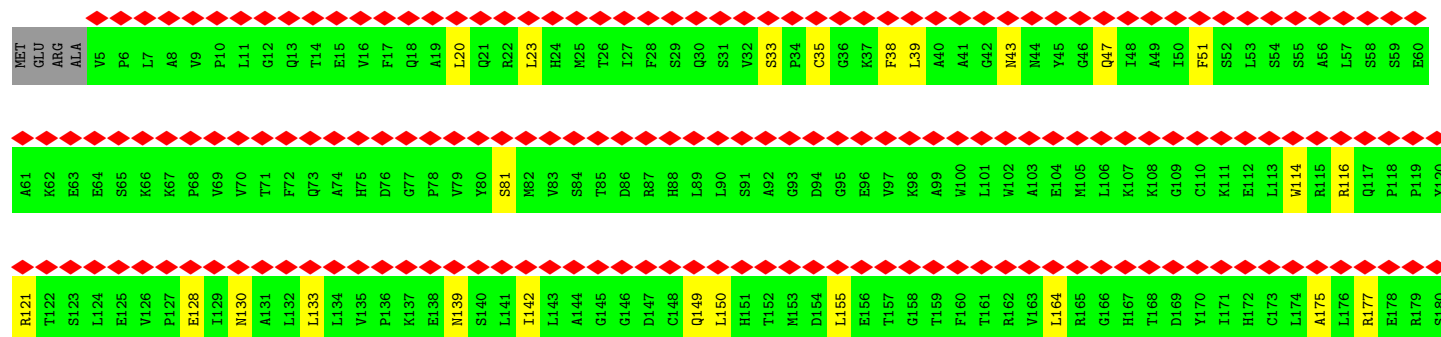
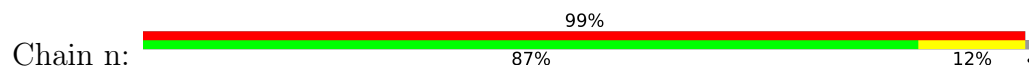




• Molecule 5: THO complex subunit 6 homolog

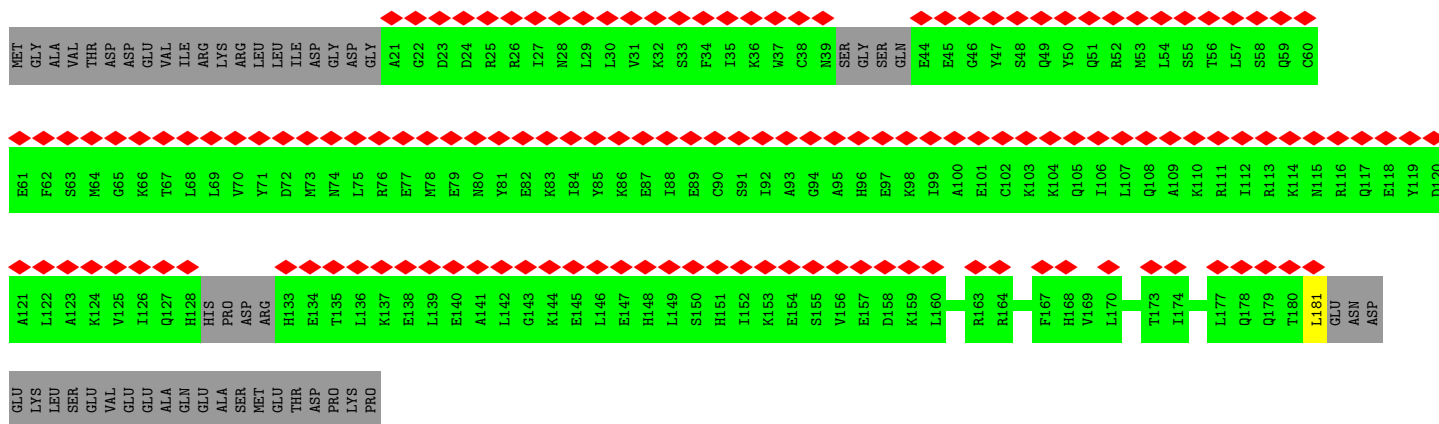
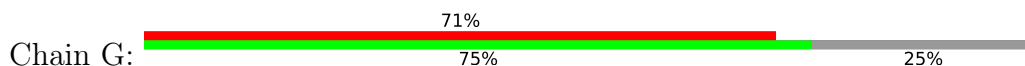


• Molecule 5: THO complex subunit 6 homolog

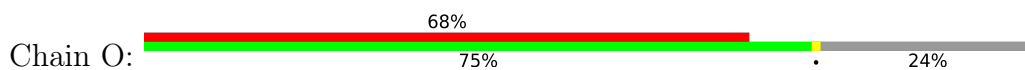




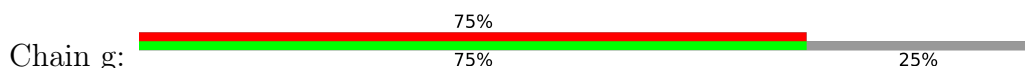
• Molecule 6: THO complex subunit 7 homolog



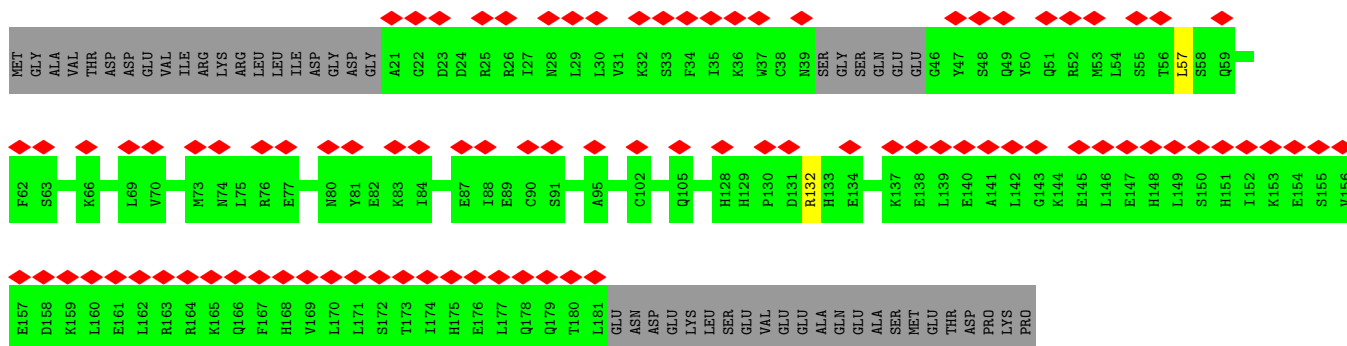
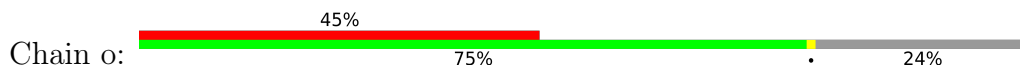
• Molecule 6: THO complex subunit 7 homolog



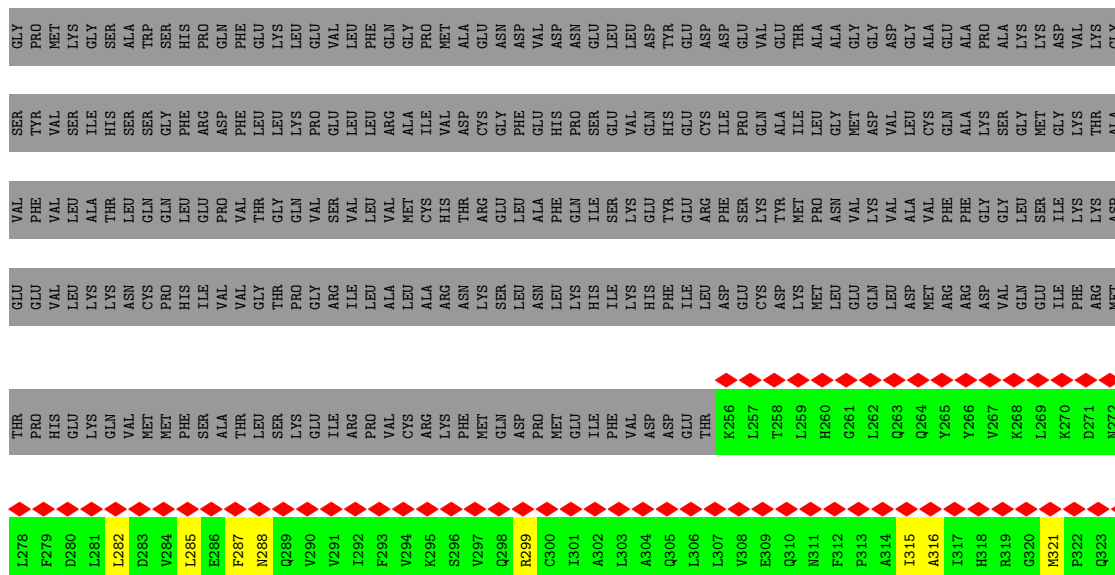
• Molecule 6: THO complex subunit 7 homolog



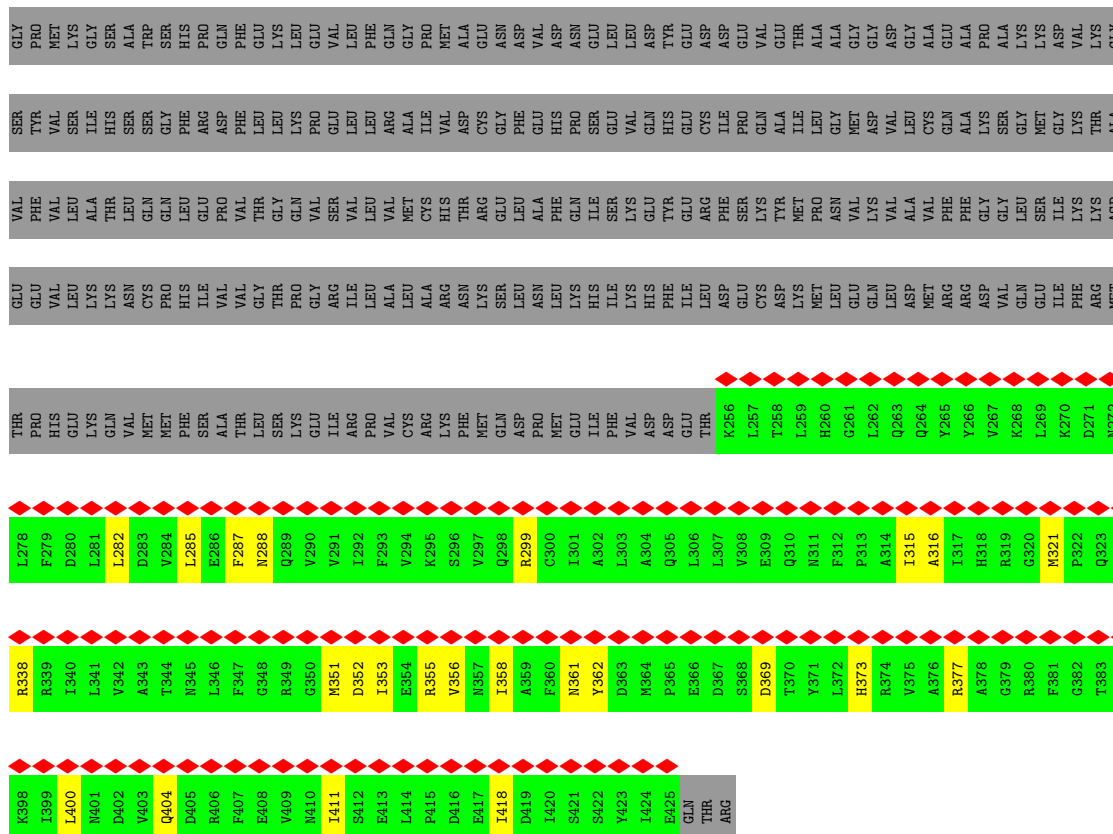
- Molecule 6: THO complex subunit 7 homolog



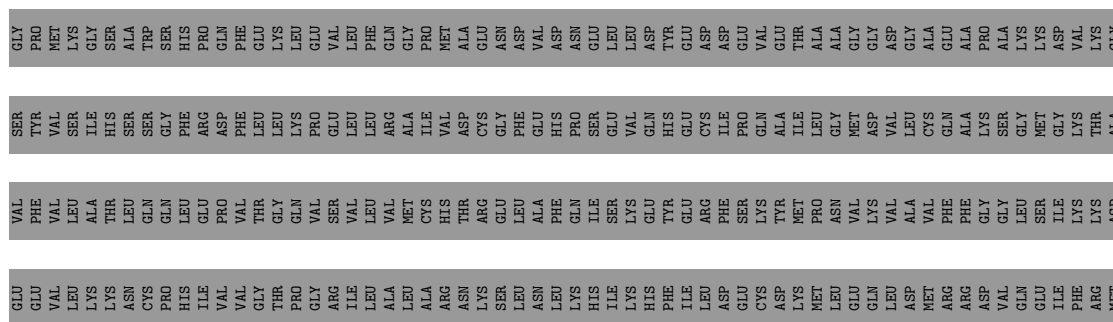
- Molecule 7: Spliceosome RNA helicase DDX39B

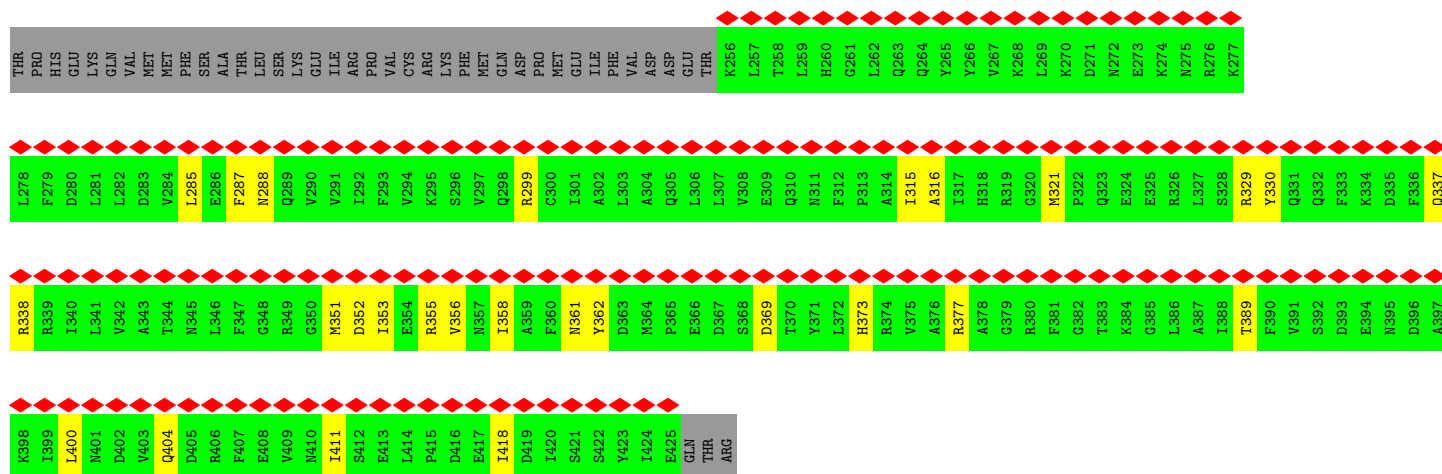


- Molecule 7: Spliceosome RNA helicase DDX39B

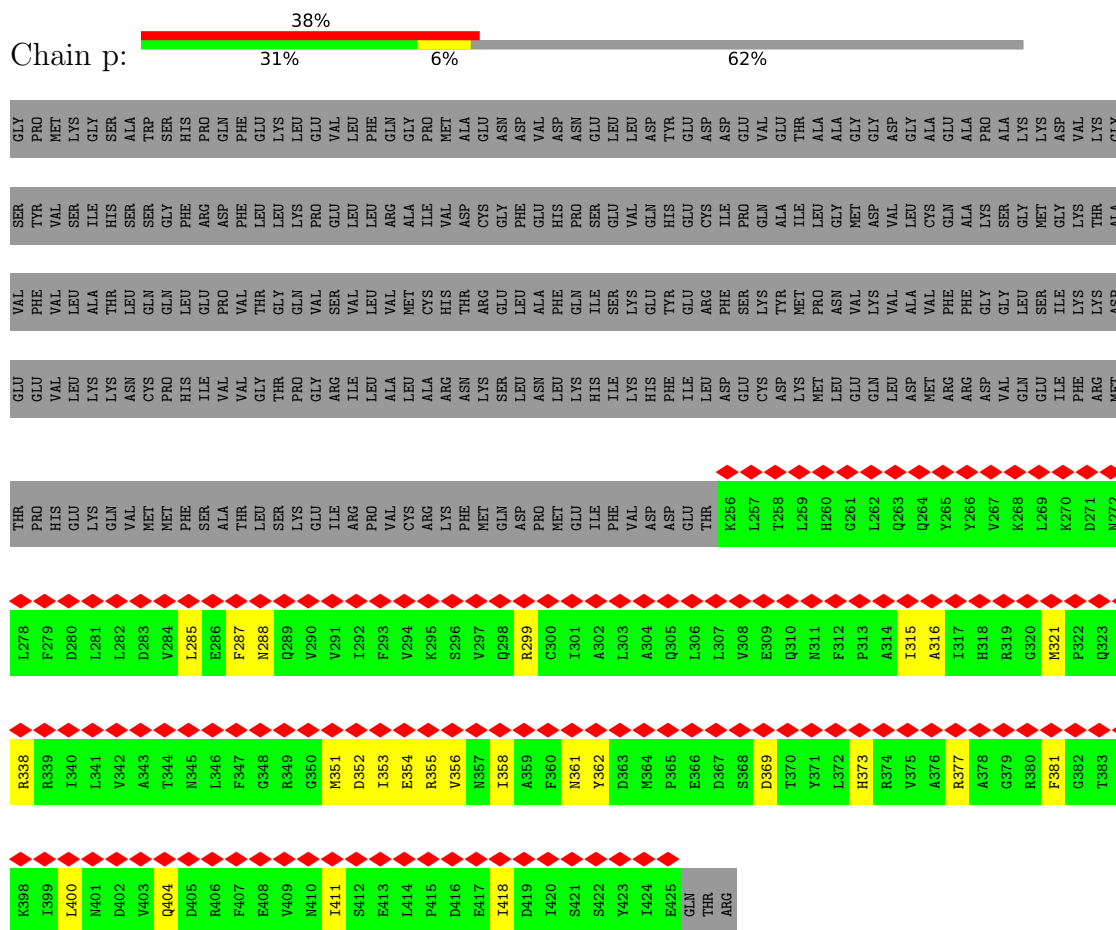


- Molecule 7: Spliceosome RNA helicase DDX39B

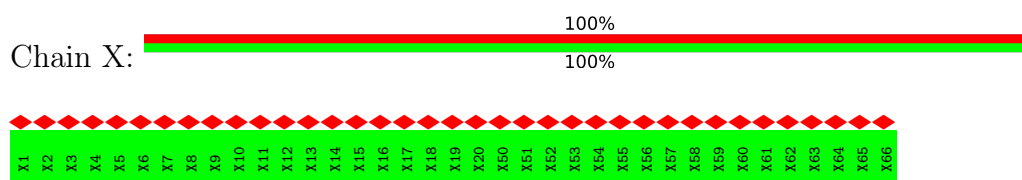




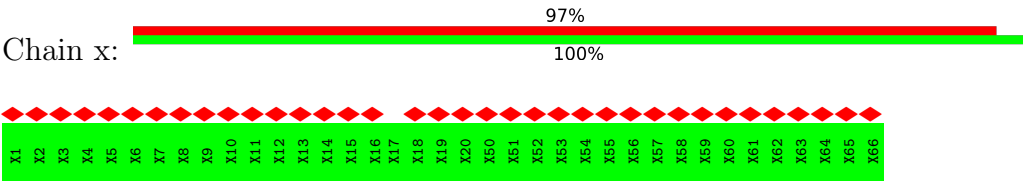
• Molecule 7: Spliceosome RNA helicase DDX39B



• Molecule 8: THOC2 anchor (putative)



● Molecule 8: THOC2 anchor (putative)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	195098	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	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 ($\text{\AA}$)	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 ($\text{\AA}$)	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	0.19	0/2204	0.45	0/2974
1	I	0.24	0/2268	0.51	0/3062
1	a	0.20	0/2204	0.45	0/2974
1	i	0.23	0/2269	0.51	0/3063
2	B	0.23	0/4741	0.45	0/6440
2	J	0.23	0/4743	0.45	0/6444
2	b	0.23	0/4741	0.45	0/6440
2	j	0.23	0/4736	0.45	0/6435
3	C	0.23	0/2404	0.59	0/3265
3	K	0.23	0/2404	0.59	0/3265
3	c	0.24	0/2404	0.59	0/3265
3	k	0.23	0/2404	0.59	0/3265
4	E	0.24	0/3754	0.49	0/5118
4	M	0.24	0/4301	0.51	0/5827
4	e	0.24	0/3661	0.47	2/4991 (0.0%)
4	m	0.24	0/4301	0.51	0/5827
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	0.28	0/2666	0.56	0/3623
6	G	0.17	0/757	0.24	0/1052
6	O	0.21	0/1094	0.36	0/1476
6	g	0.17	0/757	0.24	0/1052
6	o	0.21	0/1094	0.36	0/1476
7	H	0.15	0/1421	0.36	0/1915
7	P	0.16	0/1421	0.36	0/1915
7	h	0.16	0/1421	0.36	0/1915
7	p	0.15	0/1421	0.36	0/1915
All	All	0.23	0/73519	0.49	2/99764 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
2	J	0	2
2	b	0	2
2	j	0	2
3	C	0	2
3	K	0	2
3	c	0	2
3	k	0	2
4	M	0	1
4	m	0	1
All	All	0	18

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	e	407	GLY	CA-C-N	5.04	131.16	121.54
4	e	407	GLY	C-N-CA	5.04	131.16	121.54

There are no chirality outliers.

All (18) planarity outliers are listed below:

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

5.2 Too-close contacts ⓘ

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	2165	0	2114	13	0
1	I	2228	0	2155	18	0
1	a	2165	0	2114	13	0
1	i	2229	0	2158	18	0
2	B	4700	0	3837	37	0
2	J	4702	0	3837	35	0
2	b	4700	0	3837	38	0
2	j	4696	0	3830	32	0
3	C	2349	0	2218	35	0
3	K	2349	0	2218	35	0
3	c	2349	0	2218	35	0
3	k	2349	0	2218	36	0
4	E	3687	0	3239	26	0
4	M	4216	0	4017	27	0
4	e	3598	0	3158	23	0
4	m	4216	0	4017	26	0
5	F	2604	0	2588	26	0
5	N	2604	0	2588	23	0
5	f	2537	0	2521	25	0
5	n	2604	0	2588	25	0
6	G	760	0	332	1	0
6	O	1084	0	916	3	0
6	g	760	0	332	1	0
6	o	1084	0	916	2	0
7	H	1398	0	1394	16	0
7	P	1398	0	1394	16	0
7	h	1398	0	1394	16	0
7	p	1398	0	1394	16	0
8	X	185	0	41	0	0
8	x	185	0	41	0	0
All	All	72697	0	65624	554	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 4.

All (554) 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)
6:G:181:LEU:CB	4:M:233:LEU:CB	2.52	0.87
6:g:181:LEU:CB	4:m:233:LEU:CB	2.58	0.82
4:E:525:ILE:HD13	4:E:553:MET:HG2	1.65	0.76
4:E:524:THR:HA	4:E:552:TYR:HD1	1.56	0.71
2:b:512:PHE:HB3	2:b:520:ARG:HE	1.58	0.69
2:B:512:PHE:HB3	2:B:520:ARG:HE	1.58	0.69
2:J:512:PHE:HB3	2:J:520:ARG:HE	1.58	0.68
4:M:162:LEU:HD13	4:M:190:ARG:HH21	1.58	0.68
4:m:162:LEU:HD13	4:m:190:ARG:HH21	1.58	0.68
2:j:512:PHE:HB3	2:j:520:ARG:HE	1.58	0.67
2:B:221:ARG:HH21	2:B:224:HIS:CD2	2.13	0.67
2:b:221:ARG:HH21	2:b:224:HIS:CD2	2.13	0.66
4:m:579:ILE:HD13	5:n:20:LEU:HD21	1.78	0.66
4:E:524:THR:HB	4:E:552:TYR:CE1	2.31	0.66
4:e:579:ILE:HD13	5:f:20:LEU:HD21	1.78	0.66
1:A:380:HIS:O	1:A:384:THR:HG23	1.97	0.65
4:M:579:ILE:HD13	5:N:20:LEU:HD21	1.78	0.65
1:a:380:HIS:O	1:a:384:THR:HG23	1.97	0.64
7:H:404:GLN:HE21	7:H:411:ILE:HB	1.63	0.64
7:h:404:GLN:HE21	7:h:411:ILE:HB	1.63	0.64
7:P:404:GLN:HE21	7:P:411:ILE:HB	1.63	0.63
7:p:404:GLN:HE21	7:p:411:ILE:HB	1.63	0.63
5:N:150:LEU:HB2	5:N:164:LEU:HB2	1.81	0.62
5:F:150:LEU:HB2	5:F:164:LEU:HB2	1.81	0.62
5:f:43:ASN:HD22	5:f:47:GLN:HB2	1.64	0.61
5:n:43:ASN:HD22	5:n:47:GLN:HB2	1.64	0.61
5:N:43:ASN:HD22	5:N:47:GLN:HB2	1.64	0.61
5:f:150:LEU:HB2	5:f:164:LEU:HB2	1.82	0.61
3:C:68:ARG:HB3	3:C:84:LEU:HB3	1.83	0.61
3:c:68:ARG:HB3	3:c:84:LEU:HB3	1.83	0.61
5:F:175:ALA:HB3	5:F:184:LEU:HB2	1.83	0.61
2:B:221:ARG:NH2	2:B:224:HIS:CD2	2.69	0.61
5:F:43:ASN:HD22	5:F:47:GLN:HB2	1.64	0.61
5:n:175:ALA:HB3	5:n:184:LEU:HB2	1.83	0.61
2:b:221:ARG:NH2	2:b:224:HIS:CD2	2.69	0.60
4:m:579:ILE:CD1	5:n:20:LEU:HD21	2.31	0.60
4:m:348:VAL:HG12	4:m:364:PHE:HB2	1.84	0.60
3:K:68:ARG:HB3	3:K:84:LEU:HB3	1.83	0.60
5:f:175:ALA:HB3	5:f:184:LEU:HB2	1.83	0.60
2:J:487:THR:HA	2:J:490:VAL:HG12	1.84	0.60
5:n:150:LEU:HB2	5:n:164:LEU:HB2	1.82	0.60
4:E:524:THR:HB	4:E:552:TYR:HE1	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:579:ILE:CD1	5:N:20:LEU:HD21	2.31	0.60
3:k:68:ARG:HB3	3:k:84:LEU:HB3	1.83	0.60
4:e:538:ASP:HB3	5:f:23:LEU:HD11	1.84	0.60
4:e:579:ILE:CD1	5:f:20:LEU:HD21	2.31	0.60
4:E:538:ASP:HB3	5:F:23:LEU:HD11	1.84	0.60
5:N:175:ALA:HB3	5:N:184:LEU:HB2	1.83	0.60
4:M:348:VAL:HG12	4:M:364:PHE:HB2	1.83	0.60
4:M:538:ASP:HB3	5:N:23:LEU:HD11	1.83	0.59
4:m:538:ASP:HB3	5:n:23:LEU:HD11	1.84	0.59
2:j:487:THR:HA	2:j:490:VAL:HG12	1.84	0.59
2:b:487:THR:HA	2:b:490:VAL:HG12	1.84	0.59
4:e:348:VAL:HG12	4:e:364:PHE:HB2	1.84	0.59
3:k:160:ASN:HD21	3:k:164:VAL:H	1.50	0.59
2:B:487:THR:HA	2:B:490:VAL:HG12	1.84	0.59
2:B:221:ARG:NH2	2:B:224:HIS:HD2	2.00	0.59
3:c:77:LYS:HB2	3:c:98:HIS:HB2	1.86	0.58
3:C:77:LYS:HB2	3:C:98:HIS:HB2	1.86	0.58
7:h:316:ALA:O	7:h:329:ARG:NH1	2.37	0.58
1:A:377:MET:HG2	2:B:220:CYS:HB3	1.86	0.58
4:E:348:VAL:HG12	4:E:364:PHE:HB2	1.84	0.58
3:K:160:ASN:HD21	3:K:164:VAL:H	1.51	0.58
2:b:219:GLU:O	2:b:268:ARG:NH1	2.36	0.58
3:c:160:ASN:HD21	3:c:164:VAL:H	1.51	0.58
2:J:591:ASP:O	7:P:355:ARG:NH1	2.37	0.58
2:B:221:ARG:HH21	2:B:224:HIS:HD2	1.51	0.57
3:C:160:ASN:HD21	3:C:164:VAL:H	1.51	0.57
4:E:539:ILE:HD12	4:E:579:ILE:HG21	1.85	0.57
2:b:221:ARG:HH21	2:b:224:HIS:HD2	1.52	0.57
2:j:591:ASP:O	7:p:355:ARG:NH1	2.37	0.57
2:B:219:GLU:O	2:B:268:ARG:NH1	2.36	0.57
2:B:591:ASP:O	7:H:355:ARG:NH1	2.37	0.57
1:I:316:ASN:O	1:I:320:HIS:ND1	2.38	0.57
7:p:316:ALA:O	7:p:329:ARG:NH1	2.37	0.57
7:H:316:ALA:O	7:H:329:ARG:NH1	2.37	0.57
7:P:316:ALA:O	7:P:329:ARG:NH1	2.37	0.57
1:a:377:MET:HG2	2:b:220:CYS:HB3	1.86	0.57
2:b:221:ARG:NH2	2:b:224:HIS:HD2	2.01	0.57
3:K:77:LYS:HB2	3:K:98:HIS:HB2	1.86	0.56
3:k:77:LYS:HB2	3:k:98:HIS:HB2	1.86	0.56
5:N:271:ILE:HB	5:N:283:TRP:HB2	1.88	0.56
2:b:591:ASP:O	7:h:355:ARG:NH1	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:590:TYR:HB3	7:h:288:ASN:HD21	1.71	0.56
2:B:566:ARG:HE	2:B:603:TYR:HE2	1.54	0.56
1:i:316:ASN:O	1:i:320:HIS:ND1	2.38	0.56
2:B:358:TRP:NE1	2:B:434:MET:SD	2.75	0.55
2:b:566:ARG:HE	2:b:603:TYR:HE2	1.54	0.55
5:f:271:ILE:HB	5:f:283:TRP:HB2	1.88	0.55
2:j:590:TYR:HB3	7:p:288:ASN:HD21	1.71	0.55
2:B:590:TYR:HB3	7:H:288:ASN:HD21	1.71	0.55
5:f:39:LEU:HB3	5:f:51:PHE:HB2	1.89	0.55
2:j:566:ARG:HE	2:j:603:TYR:HE2	1.54	0.55
5:F:261:GLN:HE21	5:F:273:SER:HB3	1.71	0.55
1:I:114:THR:HG22	1:I:158:ARG:HH22	1.71	0.55
4:e:339:GLU:O	4:e:369:ASN:ND2	2.39	0.55
7:h:299:ARG:NH2	7:h:362:TYR:OH	2.40	0.55
5:n:39:LEU:HB3	5:n:51:PHE:HB2	1.89	0.55
5:F:133:LEU:HD23	5:F:142:ILE:HD12	1.89	0.55
5:F:271:ILE:HB	5:F:283:TRP:HB2	1.88	0.55
5:N:133:LEU:HD23	5:N:142:ILE:HD12	1.89	0.55
5:n:271:ILE:HB	5:n:283:TRP:HB2	1.88	0.55
7:H:299:ARG:NH2	7:H:362:TYR:OH	2.40	0.55
2:J:566:ARG:HE	2:J:603:TYR:HE2	1.54	0.55
2:J:590:TYR:HB3	7:P:288:ASN:HD21	1.71	0.55
4:e:354:CYS:SG	4:e:358:SER:OG	2.65	0.55
2:j:448:LEU:HD23	2:j:451:LYS:HD2	1.89	0.55
7:P:299:ARG:NH2	7:P:362:TYR:OH	2.40	0.55
4:e:394:LEU:O	4:e:486:ARG:NH1	2.40	0.55
2:j:594:ILE:HG23	2:j:645:PHE:HD1	1.72	0.55
4:E:394:LEU:O	4:E:486:ARG:NH1	2.40	0.54
1:I:385:GLU:HG2	2:J:209:ARG:HH22	1.72	0.54
5:n:261:GLN:HE21	5:n:273:SER:HB3	1.72	0.54
1:I:242:GLN:HE22	1:I:324:GLN:HE22	1.54	0.54
2:J:448:LEU:HD23	2:J:451:LYS:HD2	1.89	0.54
5:f:261:GLN:HE21	5:f:273:SER:HB3	1.71	0.54
1:i:114:THR:HG22	1:i:158:ARG:HH22	1.71	0.54
4:E:339:GLU:O	4:E:369:ASN:ND2	2.39	0.54
2:J:594:ILE:HG23	2:J:645:PHE:HD1	1.72	0.54
3:K:227:CYS:HA	3:K:243:SER:HA	1.89	0.54
3:C:227:CYS:HA	3:C:243:SER:HA	1.89	0.54
5:N:39:LEU:HB3	5:N:51:PHE:HB2	1.88	0.54
5:N:261:GLN:HE21	5:N:273:SER:HB3	1.72	0.54
4:E:354:CYS:SG	4:E:358:SER:OG	2.65	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:n:133:LEU:HD23	5:n:142:ILE:HD12	1.89	0.54
7:p:299:ARG:NH2	7:p:362:TYR:OH	2.40	0.54
1:a:142:ASP:OD1	1:a:145:ARG:NH1	2.41	0.54
1:i:63:ILE:HD11	1:i:100:VAL:HG22	1.89	0.54
1:i:242:GLN:HE22	1:i:324:GLN:HE22	1.54	0.54
4:M:339:GLU:O	4:M:369:ASN:ND2	2.41	0.54
2:b:594:ILE:HG23	2:b:645:PHE:HD1	1.72	0.54
4:M:354:CYS:SG	4:M:358:SER:OG	2.65	0.54
2:b:448:LEU:HD23	2:b:451:LYS:HD2	1.89	0.54
2:B:239:CYS:SG	2:B:240:GLU:N	2.81	0.54
2:b:239:CYS:SG	2:b:240:GLU:N	2.81	0.54
2:b:264:SER:HA	2:b:267:TYR:HD2	1.73	0.54
5:f:133:LEU:HD23	5:f:142:ILE:HD12	1.89	0.54
2:B:497:LEU:O	2:B:501:ASN:ND2	2.41	0.53
1:I:319:ARG:NH2	1:I:369:PRO:O	2.41	0.53
2:J:497:LEU:O	2:J:501:ASN:ND2	2.42	0.53
1:i:319:ARG:NH2	1:i:369:PRO:O	2.41	0.53
1:A:142:ASP:OD1	1:A:145:ARG:NH1	2.41	0.53
1:A:272:LYS:HG2	1:A:363:LEU:HD21	1.89	0.53
7:H:353:ILE:O	7:H:377:ARG:NH2	2.42	0.53
1:I:63:ILE:HD11	1:I:100:VAL:HG22	1.89	0.53
2:j:229:ILE:HD13	2:j:276:PHE:CE2	2.43	0.53
3:k:227:CYS:HA	3:k:243:SER:HA	1.89	0.53
4:m:339:GLU:O	4:m:369:ASN:ND2	2.41	0.53
2:J:453:VAL:HG13	2:J:511:MET:HG2	1.91	0.53
2:b:453:VAL:HG13	2:b:511:MET:HG2	1.91	0.53
2:B:448:LEU:HD23	2:B:451:LYS:HD2	1.89	0.53
2:j:453:VAL:HG13	2:j:511:MET:HG2	1.91	0.53
2:B:594:ILE:HG23	2:B:645:PHE:HD1	1.72	0.53
2:B:453:VAL:HG13	2:B:511:MET:HG2	1.91	0.53
4:e:271:LEU:HD12	4:e:348:VAL:HG11	1.91	0.53
1:i:385:GLU:HG2	2:j:209:ARG:HH22	1.72	0.53
1:A:114:THR:HG22	1:A:158:ARG:HH22	1.74	0.53
2:B:512:PHE:O	2:B:520:ARG:NH1	2.39	0.53
2:b:358:TRP:NE1	2:b:434:MET:SD	2.75	0.53
4:E:544:LEU:HD13	4:E:579:ILE:HD13	1.91	0.53
5:F:39:LEU:HB3	5:F:51:PHE:HB2	1.89	0.53
4:m:354:CYS:SG	4:m:358:SER:OG	2.65	0.53
2:J:229:ILE:HD13	2:J:276:PHE:CE2	2.43	0.52
3:c:227:CYS:HA	3:c:243:SER:HA	1.89	0.52
7:h:353:ILE:O	7:h:377:ARG:NH2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:m:47:ASP:HB3	4:m:50:ARG:HB2	1.91	0.52
4:M:47:ASP:HB3	4:M:50:ARG:HB2	1.91	0.52
7:P:353:ILE:O	7:P:377:ARG:NH2	2.42	0.52
1:a:272:LYS:HG2	1:a:363:LEU:HD21	1.89	0.52
2:b:497:LEU:O	2:b:501:ASN:ND2	2.41	0.52
7:p:353:ILE:O	7:p:377:ARG:NH2	2.42	0.52
2:J:274:LEU:HD21	2:J:284:LEU:HD12	1.92	0.52
2:j:497:LEU:O	2:j:501:ASN:ND2	2.42	0.52
2:B:264:SER:HA	2:B:267:TYR:HD2	1.73	0.52
4:E:492:GLN:HE22	4:E:620:GLN:HA	1.75	0.52
4:M:492:GLN:HE22	4:M:620:GLN:HA	1.75	0.52
4:e:492:GLN:HE22	4:e:620:GLN:HA	1.75	0.52
5:F:33:SER:OG	5:F:35:CYS:O	2.26	0.52
7:H:369:ASP:O	7:H:373:HIS:ND1	2.39	0.52
4:M:674:ASN:O	4:M:678:GLY:HA2	2.11	0.51
2:b:453:VAL:HG11	2:b:507:GLU:HB3	1.92	0.51
4:E:271:LEU:HD12	4:E:348:VAL:HG11	1.91	0.51
1:a:242:GLN:NE2	2:b:170:GLU:OE2	2.43	0.51
4:m:492:GLN:HE22	4:m:620:GLN:HA	1.75	0.51
2:B:453:VAL:HG11	2:B:507:GLU:HB3	1.92	0.51
1:I:109:CYS:SG	1:I:146:ARG:NH2	2.83	0.51
1:a:114:THR:HG22	1:a:158:ARG:HH22	1.74	0.51
4:E:674:ASN:O	4:E:678:GLY:HA2	2.11	0.51
5:n:33:SER:OG	5:n:35:CYS:O	2.26	0.51
7:p:369:ASP:O	7:p:373:HIS:ND1	2.39	0.51
3:k:81:VAL:HB	3:k:93:ASN:HB2	1.92	0.51
5:n:282:GLN:HE22	5:n:332:LEU:HB3	1.75	0.51
3:c:81:VAL:HB	3:c:93:ASN:HB2	1.92	0.51
5:f:282:GLN:HE22	5:f:332:LEU:HB3	1.76	0.51
2:j:274:LEU:HD21	2:j:284:LEU:HD12	1.92	0.51
2:j:453:VAL:HG11	2:j:507:GLU:HB3	1.92	0.51
5:F:282:GLN:HE22	5:F:332:LEU:HB3	1.76	0.51
4:M:663:ARG:HH11	5:N:128:GLU:HB3	1.76	0.51
4:e:674:ASN:O	4:e:678:GLY:HA2	2.11	0.51
3:C:81:VAL:HB	3:C:93:ASN:HB2	1.92	0.50
3:K:54:HIS:ND1	3:K:78:THR:OG1	2.45	0.50
3:K:81:VAL:HB	3:K:93:ASN:HB2	1.92	0.50
3:C:300:LYS:NZ	3:C:303:GLU:OE1	2.44	0.50
2:J:453:VAL:HG11	2:J:507:GLU:HB3	1.92	0.50
4:m:674:ASN:O	4:m:678:GLY:HA2	2.11	0.50
7:p:315:ILE:HB	7:p:338:ARG:HD2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:54:HIS:ND1	3:c:78:THR:OG1	2.45	0.50
1:i:242:GLN:NE2	2:j:170:GLU:OE2	2.44	0.50
1:A:242:GLN:NE2	2:B:170:GLU:OE2	2.43	0.50
1:I:242:GLN:NE2	2:J:170:GLU:OE2	2.45	0.50
3:k:54:HIS:ND1	3:k:78:THR:OG1	2.44	0.50
3:C:54:HIS:ND1	3:C:78:THR:OG1	2.44	0.50
3:K:68:ARG:HG2	3:K:84:LEU:HD23	1.94	0.50
2:J:512:PHE:O	2:J:520:ARG:NH1	2.40	0.50
5:N:282:GLN:HE22	5:N:332:LEU:HB3	1.76	0.50
7:P:315:ILE:HB	7:P:338:ARG:HD2	1.94	0.50
1:a:378:VAL:O	1:a:382:LEU:HG	2.12	0.49
7:h:315:ILE:HB	7:h:338:ARG:HD2	1.94	0.49
1:A:378:VAL:O	1:A:382:LEU:HG	2.12	0.49
7:h:369:ASP:O	7:h:373:HIS:ND1	2.39	0.49
1:i:109:CYS:SG	1:i:146:ARG:NH2	2.83	0.49
4:m:663:ARG:HH11	5:n:128:GLU:HB3	1.76	0.49
3:C:68:ARG:HG2	3:C:84:LEU:HD23	1.94	0.49
2:j:512:PHE:O	2:j:520:ARG:NH1	2.40	0.49
3:c:68:ARG:HG2	3:c:84:LEU:HD23	1.94	0.49
3:c:250:LEU:HD21	3:c:295:VAL:HG13	1.95	0.49
3:C:250:LEU:HD21	3:C:295:VAL:HG13	1.95	0.49
2:b:605:THR:OG1	2:b:608:ASN:ND2	2.46	0.49
2:B:605:THR:OG1	2:B:608:ASN:ND2	2.46	0.49
3:K:74:SER:OG	3:K:75:PHE:N	2.46	0.49
1:a:227:SER:OG	1:a:228:ILE:N	2.45	0.49
5:f:33:SER:OG	5:f:35:CYS:O	2.26	0.49
2:j:605:THR:OG1	2:j:608:ASN:ND2	2.46	0.49
3:C:74:SER:OG	3:C:75:PHE:N	2.46	0.49
2:J:495:LEU:HD13	2:J:527:TRP:HZ3	1.78	0.49
3:k:250:LEU:HD21	3:k:295:VAL:HG13	1.95	0.49
2:J:605:THR:OG1	2:J:608:ASN:ND2	2.46	0.48
3:K:300:LYS:NZ	3:K:303:GLU:OE1	2.44	0.48
5:N:33:SER:OG	5:N:35:CYS:O	2.26	0.48
2:b:512:PHE:O	2:b:520:ARG:NH1	2.40	0.48
3:k:68:ARG:HG2	3:k:84:LEU:HD23	1.94	0.48
7:P:369:ASP:O	7:P:373:HIS:ND1	2.39	0.48
1:i:265:GLU:OE2	1:i:352:TRP:NE1	2.46	0.48
7:H:315:ILE:HB	7:H:338:ARG:HD2	1.94	0.48
2:j:495:LEU:HD13	2:j:527:TRP:HZ3	1.78	0.48
2:B:495:LEU:HD13	2:B:527:TRP:HZ3	1.78	0.48
2:b:495:LEU:HD13	2:b:527:TRP:HZ3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:108:HIS:CE1	3:c:111:ASN:H	2.32	0.48
3:K:308:SER:HB2	3:K:327:ASP:HB3	1.96	0.48
4:M:674:ASN:O	4:M:678:GLY:CA	2.62	0.48
3:K:250:LEU:HD21	3:K:295:VAL:HG13	1.95	0.48
3:k:74:SER:OG	3:k:75:PHE:N	2.46	0.48
4:E:674:ASN:O	4:E:678:GLY:CA	2.62	0.47
5:F:81:SER:OG	5:F:130:ASN:O	2.32	0.47
5:f:81:SER:OG	5:f:130:ASN:O	2.32	0.47
5:n:202:GLU:OE2	5:n:205:THR:OG1	2.32	0.47
3:c:74:SER:OG	3:c:75:PHE:N	2.46	0.47
3:C:108:HIS:CE1	3:C:111:ASN:H	2.32	0.47
3:C:267:TRP:HD1	3:C:287:ASP:HB3	1.79	0.47
3:K:108:HIS:CE1	3:K:111:ASN:H	2.32	0.47
4:e:674:ASN:O	4:e:678:GLY:CA	2.62	0.47
5:n:81:SER:OG	5:n:130:ASN:O	2.33	0.47
5:N:202:GLU:OE2	5:N:205:THR:OG1	2.32	0.47
3:K:231:LYS:HD3	3:K:273:SER:HA	1.97	0.47
3:c:267:TRP:HD1	3:c:287:ASP:HB3	1.79	0.47
4:m:674:ASN:O	4:m:678:GLY:CA	2.62	0.47
5:F:202:GLU:OE2	5:F:205:THR:OG1	2.32	0.47
3:K:205:CYS:HA	3:K:220:ILE:O	2.14	0.47
5:N:81:SER:OG	5:N:130:ASN:O	2.32	0.47
3:c:51:PHE:HA	3:c:341:THR:HG23	1.97	0.47
3:c:300:LYS:NZ	3:c:303:GLU:OE1	2.44	0.47
3:k:267:TRP:HD1	3:k:287:ASP:HB3	1.79	0.47
4:m:546:GLY:O	4:m:551:TYR:OH	2.32	0.47
5:n:121:ARG:HH21	5:n:149:GLN:HE21	1.62	0.47
3:C:308:SER:HB2	3:C:327:ASP:HB3	1.96	0.47
5:f:139:ASN:HB3	5:f:155:LEU:HB2	1.97	0.47
3:k:231:LYS:HD3	3:k:273:SER:HA	1.97	0.47
3:k:308:SER:HB2	3:k:327:ASP:HB3	1.96	0.47
5:F:139:ASN:HB3	5:F:155:LEU:HB2	1.97	0.47
1:I:324:GLN:HG3	2:J:169:ASN:HB3	1.97	0.47
3:K:51:PHE:HA	3:K:341:THR:HG23	1.97	0.47
3:K:167:PHE:HB2	3:K:177:ALA:HB3	1.97	0.47
4:m:570:ASN:HD21	4:m:576:ILE:HG21	1.80	0.47
4:E:525:ILE:HG21	4:E:553:MET:CG	2.45	0.47
3:K:267:TRP:HD1	3:K:287:ASP:HB3	1.79	0.47
3:c:167:PHE:HB2	3:c:177:ALA:HB3	1.97	0.47
3:K:316:HIS:CE1	3:K:320:PRO:HD2	2.51	0.46
4:M:546:GLY:O	4:M:551:TYR:OH	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:k:205:CYS:HA	3:k:220:ILE:O	2.15	0.46
5:n:139:ASN:HB3	5:n:155:LEU:HB2	1.98	0.46
4:E:570:ASN:HD21	4:E:576:ILE:HG21	1.81	0.46
1:i:22:ARG:NH2	1:i:61:GLU:OE1	2.48	0.46
1:i:324:GLN:HG3	2:j:169:ASN:HB3	1.97	0.46
4:M:557:GLU:HA	4:M:561:ALA:O	2.15	0.46
5:N:139:ASN:HB3	5:N:155:LEU:HB2	1.98	0.46
3:c:308:SER:HB2	3:c:327:ASP:HB3	1.97	0.46
3:k:108:HIS:CE1	3:k:111:ASN:H	2.32	0.46
3:k:167:PHE:HB2	3:k:177:ALA:HB3	1.97	0.46
4:M:570:ASN:HD21	4:M:576:ILE:HG21	1.81	0.46
5:N:43:ASN:HB3	5:N:47:GLN:H	1.81	0.46
4:e:372:ILE:HD12	4:e:418:ASN:HD22	1.81	0.46
4:e:544:LEU:HD13	4:e:579:ILE:CD1	2.45	0.46
2:j:595:THR:HA	2:j:598:VAL:HG22	1.97	0.46
3:k:316:HIS:CE1	3:k:320:PRO:HD2	2.51	0.46
5:N:121:ARG:HH21	5:N:149:GLN:HE21	1.62	0.46
4:m:544:LEU:HD13	4:m:579:ILE:CD1	2.45	0.46
5:n:43:ASN:HB3	5:n:47:GLN:H	1.81	0.46
3:C:167:PHE:HB2	3:C:177:ALA:HB3	1.97	0.46
3:C:205:CYS:HA	3:C:220:ILE:O	2.15	0.46
3:C:316:HIS:CE1	3:C:320:PRO:HD2	2.51	0.46
2:J:595:THR:HA	2:J:598:VAL:HG22	1.98	0.46
3:c:164:VAL:HA	3:c:179:GLU:O	2.16	0.46
4:E:534:HIS:NE2	4:E:589:GLU:OE2	2.49	0.46
4:M:534:HIS:NE2	4:M:589:GLU:OE2	2.49	0.46
3:c:205:CYS:HA	3:c:220:ILE:O	2.15	0.46
3:c:316:HIS:CE1	3:c:320:PRO:HD2	2.51	0.46
1:I:22:ARG:NH2	1:I:61:GLU:OE1	2.48	0.46
5:f:202:GLU:OE2	5:f:205:THR:OG1	2.32	0.46
3:k:51:PHE:HA	3:k:341:THR:HG23	1.97	0.46
4:E:557:GLU:HA	4:E:561:ALA:O	2.15	0.46
4:M:59:CYS:HB3	6:O:57:LEU:HD11	1.98	0.46
2:b:657:LEU:H	2:b:657:LEU:HG	1.56	0.46
3:c:59:HIS:ND1	3:c:102:VAL:O	2.48	0.46
2:j:192:ILE:HD12	2:j:227:PHE:HZ	1.81	0.46
3:k:300:LYS:NZ	3:k:303:GLU:OE1	2.44	0.46
3:C:231:LYS:HD3	3:C:273:SER:HA	1.97	0.46
3:K:164:VAL:HA	3:K:179:GLU:O	2.16	0.46
3:k:164:VAL:HA	3:k:179:GLU:O	2.16	0.46
4:m:534:HIS:NE2	4:m:589:GLU:OE2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:m:557:GLU:HA	4:m:561:ALA:O	2.15	0.46
5:F:121:ARG:HH21	5:F:149:GLN:HE21	1.62	0.45
4:M:361:HIS:HB2	4:M:378:LYS:HB3	1.97	0.45
4:M:544:LEU:HD13	4:M:579:ILE:CD1	2.45	0.45
4:m:59:CYS:HB3	6:o:57:LEU:HD11	1.98	0.45
5:F:43:ASN:HB3	5:F:47:GLN:H	1.81	0.45
2:J:192:ILE:HD12	2:J:227:PHE:HZ	1.81	0.45
3:c:209:LEU:HG	3:c:216:PRO:HA	1.98	0.45
3:k:209:LEU:HG	3:k:216:PRO:HA	1.98	0.45
1:A:117:GLU:OE1	1:A:158:ARG:NH2	2.48	0.45
1:A:391:TRP:CE2	2:B:250:PHE:HE1	2.35	0.45
4:E:372:ILE:HD12	4:E:418:ASN:HD22	1.81	0.45
2:B:595:THR:HA	2:B:598:VAL:HG22	1.97	0.45
3:C:151:PRO:HG2	3:C:192:ASN:HA	1.98	0.45
3:C:164:VAL:HA	3:C:179:GLU:O	2.16	0.45
3:K:151:PRO:HG2	3:K:192:ASN:HA	1.98	0.45
4:e:534:HIS:NE2	4:e:589:GLU:OE2	2.49	0.45
4:e:557:GLU:HA	4:e:561:ALA:O	2.15	0.45
3:k:59:HIS:ND1	3:k:102:VAL:O	2.48	0.45
4:m:361:HIS:HB2	4:m:378:LYS:HB3	1.97	0.45
4:E:539:ILE:CD1	4:E:579:ILE:HG21	2.46	0.45
5:F:59:SER:O	1:i:236:ARG:NH2	2.48	0.45
1:I:265:GLU:OE2	1:I:352:TRP:NE1	2.46	0.45
3:K:209:LEU:HG	3:K:216:PRO:HA	1.98	0.45
4:e:570:ASN:HD21	4:e:576:ILE:HG21	1.81	0.45
2:j:560:ASN:HD22	2:j:563:PRO:HD2	1.81	0.45
2:B:560:ASN:HD22	2:B:563:PRO:HD2	1.81	0.45
2:B:386:LEU:HD22	2:B:434:MET:HE2	1.99	0.45
3:C:209:LEU:HG	3:C:216:PRO:HA	1.99	0.45
3:K:59:HIS:ND1	3:K:102:VAL:O	2.48	0.45
4:M:160:VAL:HG22	6:O:132:ARG:HH22	1.82	0.45
5:f:43:ASN:HB3	5:f:47:GLN:H	1.81	0.45
4:m:160:VAL:HG22	6:o:132:ARG:HH22	1.81	0.45
2:B:500:CYS:N	3:C:261:CYS:SG	2.87	0.45
3:C:51:PHE:HA	3:C:341:THR:HG23	1.97	0.45
4:e:663:ARG:HH11	5:f:128:GLU:HB3	1.81	0.45
3:C:49:ARG:HG3	3:C:343:LYS:HG2	1.99	0.45
4:E:663:ARG:HH11	5:F:128:GLU:HB3	1.81	0.45
7:H:351:MET:HE2	7:H:356:VAL:HG21	1.99	0.45
2:b:560:ASN:HD22	2:b:563:PRO:HD2	1.81	0.45
7:p:351:MET:HE2	7:p:356:VAL:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:560:ASN:HD22	2:J:563:PRO:HD2	1.82	0.45
3:c:151:PRO:HG2	3:c:192:ASN:HA	1.98	0.45
3:c:231:LYS:HD3	3:c:273:SER:HA	1.97	0.45
2:J:657:LEU:H	2:J:657:LEU:HG	1.57	0.44
7:P:351:MET:HE2	7:P:356:VAL:HG21	1.99	0.44
4:e:546:GLY:O	4:e:551:TYR:OH	2.33	0.44
2:j:570:LYS:NZ	3:k:265:LEU:O	2.50	0.44
3:k:104:GLN:HG2	3:k:147:ILE:H	1.83	0.44
2:j:225:ASP:OD1	2:j:268:ARG:NH1	2.34	0.44
3:C:59:HIS:ND1	3:C:102:VAL:O	2.48	0.44
5:F:232:TRP:HZ3	5:F:252:THR:HG21	1.83	0.44
3:K:104:GLN:HG2	3:K:147:ILE:H	1.82	0.44
1:a:391:TRP:CE2	2:b:250:PHE:HE1	2.35	0.44
2:b:386:LEU:HD22	2:b:434:MET:HE2	1.99	0.44
2:b:595:THR:HA	2:b:598:VAL:HG22	1.97	0.44
3:c:49:ARG:HG3	3:c:343:LYS:HG2	1.99	0.44
5:f:232:TRP:HZ3	5:f:252:THR:HG21	1.83	0.44
3:k:151:PRO:HG2	3:k:192:ASN:HA	1.98	0.44
7:p:330:TYR:OH	7:p:352:ASP:OD1	2.35	0.44
2:B:570:LYS:NZ	3:C:265:LEU:O	2.50	0.44
7:P:321:MET:HE1	7:P:329:ARG:HD2	2.00	0.44
3:c:316:HIS:CE1	3:c:318:LYS:HB2	2.53	0.44
7:h:351:MET:HE2	7:h:356:VAL:HG21	1.99	0.44
2:j:386:LEU:HD22	2:j:434:MET:HE2	1.99	0.44
7:H:321:MET:HE1	7:H:329:ARG:HD2	2.00	0.44
2:J:570:LYS:NZ	3:K:265:LEU:O	2.50	0.44
3:c:275:SER:HB3	3:c:319:ARG:HD2	2.00	0.44
3:C:275:SER:HB3	3:C:319:ARG:HD2	2.00	0.44
3:C:281:LEU:O	3:C:292:ILE:HA	2.18	0.44
4:E:525:ILE:HG21	4:E:553:MET:HG2	1.99	0.44
2:b:352:LEU:HD21	2:b:360:HIS:HB2	2.00	0.44
3:c:281:LEU:O	3:c:292:ILE:HA	2.18	0.44
1:A:163:LEU:HD23	1:A:166:LEU:HD12	2.00	0.44
3:K:316:HIS:CE1	3:K:318:LYS:HB2	2.53	0.44
7:P:330:TYR:OH	7:P:352:ASP:OD1	2.35	0.44
7:H:330:TYR:OH	7:H:352:ASP:OD1	2.35	0.44
2:b:570:LYS:NZ	3:c:265:LEU:O	2.50	0.44
3:k:316:HIS:CE1	3:k:318:LYS:HB2	2.53	0.44
5:F:255:PHE:HA	5:F:256:PRO:HD3	1.86	0.43
3:c:104:GLN:HG2	3:c:147:ILE:H	1.82	0.43
7:h:330:TYR:OH	7:h:352:ASP:OD1	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:i:385:GLU:HG2	2:j:209:ARG:NH2	2.33	0.43
3:k:275:SER:HB3	3:k:319:ARG:HD2	2.00	0.43
3:C:316:HIS:CE1	3:C:318:LYS:HB2	2.53	0.43
3:K:49:ARG:HG3	3:K:343:LYS:HG2	1.99	0.43
3:K:281:LEU:O	3:K:292:ILE:HA	2.18	0.43
5:f:194:LEU:HD13	5:f:204:GLN:HB3	2.00	0.43
7:H:361:ASN:HB2	7:H:389:THR:HA	2.00	0.43
1:I:236:ARG:NH2	5:f:59:SER:O	2.48	0.43
5:N:232:TRP:HZ3	5:N:252:THR:HG21	1.83	0.43
2:b:568:ILE:HG21	2:b:600:SER:HB2	2.00	0.43
5:n:300:LEU:HA	5:n:321:GLY:HA3	2.01	0.43
1:I:299:ALA:O	2:J:174:LYS:NZ	2.41	0.43
2:J:491:LEU:HD13	2:J:527:TRP:HE1	1.84	0.43
7:h:321:MET:HE1	7:h:329:ARG:HD2	2.00	0.43
7:h:361:ASN:HB2	7:h:389:THR:HA	2.00	0.43
7:p:285:LEU:HD21	7:p:418:ILE:HD12	2.01	0.43
3:C:104:GLN:HG2	3:C:147:ILE:H	1.82	0.43
1:I:245:PHE:O	2:J:169:ASN:ND2	2.52	0.43
2:B:369:PRO:HB2	2:B:372:TYR:HB2	2.01	0.43
2:J:386:LEU:HD22	2:J:434:MET:HE2	1.99	0.43
3:K:275:SER:HB3	3:K:319:ARG:HD2	2.00	0.43
1:a:163:LEU:HD23	1:a:166:LEU:HD12	2.00	0.43
3:k:49:ARG:HG3	3:k:343:LYS:HG2	1.99	0.43
2:J:369:PRO:HB2	2:J:372:TYR:HB2	2.01	0.43
3:K:116:VAL:HG22	3:K:126:ILE:HG12	2.00	0.43
1:i:320:HIS:CD2	2:j:174:LYS:HG2	2.54	0.43
2:j:491:LEU:HD13	2:j:527:TRP:HE1	1.84	0.43
3:k:281:LEU:O	3:k:292:ILE:HA	2.18	0.43
7:p:361:ASN:HB2	7:p:389:THR:HA	2.00	0.43
7:P:361:ASN:HB2	7:P:389:THR:HA	2.00	0.43
7:h:400:LEU:HD11	7:h:411:ILE:HG21	2.01	0.43
7:p:400:LEU:HD11	7:p:411:ILE:HG21	2.01	0.43
7:H:400:LEU:HD11	7:H:411:ILE:HG21	2.01	0.43
7:P:400:LEU:HD11	7:P:411:ILE:HG21	2.01	0.43
3:k:71:ALA:HA	3:k:80:SER:O	2.19	0.43
7:p:321:MET:HE1	7:p:329:ARG:HD2	2.00	0.43
3:K:143:GLU:HB3	3:K:160:ASN:HB3	2.01	0.42
5:N:300:LEU:HA	5:N:321:GLY:HA3	2.01	0.42
7:P:285:LEU:HD21	7:P:418:ILE:HD12	2.01	0.42
3:c:71:ALA:HA	3:c:80:SER:O	2.19	0.42
1:i:245:PHE:O	2:j:169:ASN:ND2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:674:ASN:O	4:E:678:GLY:N	2.52	0.42
5:F:194:LEU:HD13	5:F:204:GLN:HB3	2.01	0.42
7:H:285:LEU:HD21	7:H:418:ILE:HD12	2.01	0.42
3:K:71:ALA:HA	3:K:80:SER:O	2.19	0.42
1:a:239:TRP:HH2	1:a:301:PHE:HB3	1.84	0.42
5:n:232:TRP:HZ3	5:n:252:THR:HG21	1.83	0.42
1:A:239:TRP:HH2	1:A:301:PHE:HB3	1.84	0.42
3:C:116:VAL:HG22	3:C:126:ILE:HG12	2.00	0.42
3:C:143:GLU:HB3	3:C:160:ASN:HB3	2.02	0.42
3:C:259:VAL:HG12	3:C:260:ARG:HE	1.85	0.42
5:F:300:LEU:HA	5:F:321:GLY:HA3	2.01	0.42
3:c:116:VAL:HG22	3:c:126:ILE:HG12	2.00	0.42
3:k:116:VAL:HG22	3:k:126:ILE:HG12	2.00	0.42
2:B:352:LEU:HD21	2:B:360:HIS:HB2	2.00	0.42
3:c:259:VAL:HG12	3:c:260:ARG:HE	1.85	0.42
2:B:491:LEU:HD13	2:B:527:TRP:HE1	1.84	0.42
3:C:71:ALA:HA	3:C:80:SER:O	2.19	0.42
5:N:114:TRP:CD1	5:N:116:ARG:HD3	2.55	0.42
7:h:285:LEU:HD21	7:h:418:ILE:HD12	2.01	0.42
5:n:194:LEU:HD13	5:n:204:GLN:HB3	2.01	0.42
7:p:287:PHE:HB3	7:p:358:ILE:HD12	2.02	0.42
1:I:320:HIS:CD2	2:J:174:LYS:HG2	2.54	0.42
4:M:605:VAL:HG21	4:M:629:LEU:HD12	2.02	0.42
1:a:117:GLU:OE1	1:a:158:ARG:NH2	2.48	0.42
2:b:369:PRO:HB2	2:b:372:TYR:HB2	2.01	0.42
1:A:370:ASP:HB3	1:A:373:ARG:HB2	2.02	0.42
5:F:114:TRP:CD1	5:F:116:ARG:HD3	2.55	0.42
3:K:259:VAL:HG12	3:K:260:ARG:HE	1.85	0.42
1:a:370:ASP:HB3	1:a:373:ARG:HB2	2.02	0.42
5:f:114:TRP:CD1	5:f:116:ARG:HD3	2.55	0.42
5:f:255:PHE:HA	5:f:256:PRO:HD3	1.86	0.42
5:f:300:LEU:HA	5:f:321:GLY:HA3	2.01	0.42
2:j:369:PRO:HB2	2:j:372:TYR:HB2	2.01	0.42
2:j:568:ILE:HG21	2:j:600:SER:HB2	2.01	0.42
2:B:568:ILE:HG21	2:B:600:SER:HB2	2.01	0.42
3:c:86:LYS:O	3:c:88:ARG:N	2.52	0.42
4:e:413:THR:HA	4:e:414:PRO:HD3	1.92	0.42
4:e:674:ASN:O	4:e:678:GLY:N	2.52	0.42
7:h:287:PHE:HB3	7:h:358:ILE:HD12	2.02	0.42
3:k:143:GLU:HB3	3:k:160:ASN:HB3	2.01	0.42
3:K:86:LYS:O	3:K:88:ARG:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:330:THR:HG23	1:i:229:PRO:HB2	2.02	0.41
1:I:385:GLU:HG2	2:J:209:ARG:NH2	2.33	0.41
2:j:483:LEU:HA	2:j:486:ILE:HG22	2.02	0.41
1:I:229:PRO:HB2	5:f:330:THR:HG23	2.02	0.41
4:M:674:ASN:O	4:M:678:GLY:N	2.52	0.41
5:N:274:ALA:HB1	5:N:300:LEU:HB2	2.03	0.41
4:m:427:ILE:HD11	4:m:433:TYR:HE2	1.85	0.41
4:E:605:VAL:HG21	4:E:629:LEU:HD12	2.02	0.41
7:H:287:PHE:HB3	7:H:358:ILE:HD12	2.02	0.41
2:b:483:LEU:HA	2:b:486:ILE:HG22	2.01	0.41
3:k:259:VAL:HG12	3:k:260:ARG:HE	1.85	0.41
2:J:483:LEU:HA	2:J:486:ILE:HG22	2.02	0.41
3:c:199:LEU:HG	3:c:207:ASN:HB3	2.02	0.41
7:p:354:GLU:OE2	7:p:381:PHE:N	2.51	0.41
2:J:500:CYS:N	3:K:261:CYS:SG	2.87	0.41
2:j:240:GLU:HA	2:j:241:PRO:HD3	1.92	0.41
3:k:199:LEU:HG	3:k:207:ASN:HB3	2.03	0.41
2:B:483:LEU:HA	2:B:486:ILE:HG22	2.02	0.41
2:B:554:LYS:NZ	7:H:282:LEU:O	2.38	0.41
5:F:274:ALA:HB1	5:F:300:LEU:HB2	2.03	0.41
2:J:554:LYS:NZ	7:P:282:LEU:O	2.38	0.41
5:N:194:LEU:HD13	5:N:204:GLN:HB3	2.01	0.41
2:b:218:PHE:HE1	2:b:225:ASP:HA	1.85	0.41
2:b:491:LEU:HD13	2:b:527:TRP:HE1	1.84	0.41
3:k:86:LYS:O	3:k:88:ARG:N	2.52	0.41
5:n:33:SER:HB3	5:n:38:PHE:HB2	2.03	0.41
5:n:274:ALA:HB1	5:n:300:LEU:HB2	2.03	0.41
1:A:342:ASN:HB3	1:A:343:TYR:H	1.68	0.41
2:J:568:ILE:HG21	2:J:600:SER:HB2	2.01	0.41
3:k:233:ASP:OD1	3:k:233:ASP:N	2.50	0.41
3:C:199:LEU:HG	3:C:207:ASN:HB3	2.03	0.41
4:E:524:THR:HA	4:E:552:TYR:CD1	2.46	0.41
3:K:199:LEU:HG	3:K:207:ASN:HB3	2.02	0.41
2:b:500:CYS:N	3:c:261:CYS:SG	2.88	0.41
4:m:674:ASN:O	4:m:678:GLY:N	2.52	0.41
5:n:114:TRP:CD1	5:n:116:ARG:HD3	2.55	0.41
4:M:427:ILE:HD11	4:M:433:TYR:HE2	1.85	0.41
4:e:544:LEU:HD13	4:e:579:ILE:HD13	2.03	0.41
1:i:70:GLU:OE2	1:i:108:GLN:NE2	2.54	0.41
4:m:544:LEU:HD13	4:m:579:ILE:HD13	2.02	0.41
4:m:605:VAL:HG21	4:m:629:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:285:SER:OG	3:C:286:GLU:N	2.54	0.41
2:J:358:TRP:NE1	2:J:434:MET:SD	2.94	0.41
4:M:116:THR:HG22	6:O:78:MET:HG3	2.03	0.41
4:e:388:PRO:HG2	4:e:391:ALA:HB2	2.03	0.41
5:f:149:GLN:HG2	5:f:165:ARG:HG2	2.03	0.41
5:n:177:ARG:HH21	5:n:181:PRO:HG2	1.86	0.41
2:B:560:ASN:ND2	2:B:563:PRO:HD2	2.36	0.40
1:I:70:GLU:OE2	1:I:108:GLN:NE2	2.54	0.40
4:e:568:VAL:O	4:e:578:PRO:HA	2.21	0.40
1:i:314:ASP:OD2	4:m:135:TYR:OH	2.35	0.40
7:P:287:PHE:HB3	7:P:358:ILE:HD12	2.02	0.40
2:b:560:ASN:ND2	2:b:563:PRO:HD2	2.36	0.40
2:B:218:PHE:HE1	2:B:225:ASP:HA	1.85	0.40
5:F:33:SER:HB3	5:F:38:PHE:HB2	2.03	0.40
3:c:143:GLU:HB3	3:c:160:ASN:HB3	2.02	0.40
3:k:202:GLY:HA2	3:k:226:ASN:HB3	2.03	0.40
5:F:177:ARG:HH21	5:F:181:PRO:HG2	1.86	0.40
4:M:373:MET:HG3	4:M:444:VAL:HG12	2.04	0.40
4:M:544:LEU:HD13	4:M:579:ILE:HD13	2.03	0.40
2:b:559:GLU:HB2	7:h:337:GLN:HG3	2.04	0.40

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	248/711 (35%)	239 (96%)	8 (3%)	1 (0%)	30	60
1	I	255/711 (36%)	241 (94%)	12 (5%)	2 (1%)	16	45
1	a	248/711 (35%)	240 (97%)	7 (3%)	1 (0%)	30	60
1	i	255/711 (36%)	241 (94%)	12 (5%)	2 (1%)	16	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	36	65
3	K	298/395 (75%)	273 (92%)	24 (8%)	1 (0%)	36	65
3	c	298/395 (75%)	273 (92%)	24 (8%)	1 (0%)	36	65
3	k	298/395 (75%)	273 (92%)	24 (8%)	1 (0%)	36	65
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%)	36	65
5	N	335/341 (98%)	307 (92%)	27 (8%)	1 (0%)	36	65
5	f	325/341 (95%)	298 (92%)	26 (8%)	1 (0%)	36	65
5	n	335/341 (98%)	305 (91%)	29 (9%)	1 (0%)	36	65
6	G	147/204 (72%)	147 (100%)	0	0	100	100
6	O	151/204 (74%)	151 (100%)	0	0	100	100
6	g	147/204 (72%)	147 (100%)	0	0	100	100
6	o	151/204 (74%)	151 (100%)	0	0	100	100
7	H	168/451 (37%)	165 (98%)	3 (2%)	0	100	100
7	P	168/451 (37%)	165 (98%)	3 (2%)	0	100	100
7	h	168/451 (37%)	165 (98%)	3 (2%)	0	100	100
7	p	168/451 (37%)	165 (98%)	3 (2%)	0	100	100
All	All	9429/16044 (59%)	8975 (95%)	440 (5%)	14 (0%)	49	75

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	66	ASP
1	I	308	MET
3	K	66	ASP
3	c	66	ASP
1	i	308	MET

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	236/646 (36%)	236 (100%)	0	100	100
1	I	240/646 (37%)	240 (100%)	0	100	100
1	a	236/646 (36%)	236 (100%)	0	100	100
1	i	241/646 (37%)	241 (100%)	0	100	100
2	B	345/1105 (31%)	344 (100%)	1 (0%)	86	86
2	J	345/1105 (31%)	344 (100%)	1 (0%)	86	86
2	b	345/1105 (31%)	344 (100%)	1 (0%)	86	86
2	j	344/1105 (31%)	343 (100%)	1 (0%)	86	86
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%)	318 (99%)	3 (1%)	70	78
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%)	284 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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	153/400 (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%)	6723 (100%)	7 (0%)	87	90

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	657	LEU
4	E	523	VAL
4	E	524	THR
4	E	525	ILE
2	J	657	LEU
2	b	657	LEU
2	j	657	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (128) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	160	GLN
1	A	242	GLN
1	A	320	HIS
1	A	380	HIS
2	B	169	ASN
2	B	204	ASN
2	B	224	HIS
2	B	518	GLN
2	B	560	ASN
2	B	573	HIS
2	B	588	GLN
2	B	592	ASN

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Mol	Chain	Res	Type
2	B	608	ASN
2	B	667	GLN
3	C	104	GLN
3	C	146	ASN
3	C	316	HIS
4	E	274	GLN
4	E	465	HIS
4	E	492	GLN
4	E	508	GLN
4	E	619	HIS
4	E	624	ASN
4	E	674	ASN
4	E	675	HIS
5	F	73	GLN
5	F	130	ASN
5	F	149	GLN
5	F	261	GLN
5	F	282	GLN
5	F	308	GLN
7	H	289	GLN
7	H	357	ASN
7	H	404	GLN
1	I	242	GLN
2	J	169	ASN
2	J	224	HIS
2	J	518	GLN
2	J	560	ASN
2	J	573	HIS
2	J	588	GLN
2	J	608	ASN
2	J	667	GLN
3	K	104	GLN
3	K	139	ASN
3	K	146	ASN
3	K	316	HIS
4	M	492	GLN
4	M	508	GLN
4	M	619	HIS
4	M	624	ASN
4	M	674	ASN
4	M	675	HIS
5	N	73	GLN

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Mol	Chain	Res	Type
5	N	130	ASN
5	N	149	GLN
5	N	151	HIS
5	N	261	GLN
5	N	282	GLN
5	N	308	GLN
6	O	49	GLN
7	P	289	GLN
7	P	357	ASN
7	P	404	GLN
1	a	119	ASN
1	a	242	GLN
1	a	320	HIS
1	a	380	HIS
2	b	169	ASN
2	b	204	ASN
2	b	224	HIS
2	b	518	GLN
2	b	560	ASN
2	b	588	GLN
2	b	592	ASN
2	b	608	ASN
2	b	667	GLN
3	c	104	GLN
3	c	146	ASN
3	c	316	HIS
4	e	274	GLN
4	e	492	GLN
4	e	508	GLN
4	e	619	HIS
4	e	624	ASN
4	e	674	ASN
4	e	675	HIS
5	f	73	GLN
5	f	130	ASN
5	f	151	HIS
5	f	261	GLN
5	f	282	GLN
5	f	308	GLN
7	h	289	GLN
7	h	404	GLN
1	i	242	GLN

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Mol	Chain	Res	Type
2	j	169	ASN
2	j	224	HIS
2	j	518	GLN
2	j	526	GLN
2	j	560	ASN
2	j	573	HIS
2	j	588	GLN
2	j	592	ASN
2	j	608	ASN
2	j	667	GLN
3	k	104	GLN
3	k	146	ASN
3	k	316	HIS
4	m	471	HIS
4	m	492	GLN
4	m	508	GLN
4	m	619	HIS
4	m	624	ASN
4	m	674	ASN
4	m	675	HIS
5	n	73	GLN
5	n	130	ASN
5	n	149	GLN
5	n	151	HIS
5	n	261	GLN
5	n	282	GLN
5	n	308	GLN
6	o	49	GLN
7	p	289	GLN
7	p	357	ASN
7	p	404	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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
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

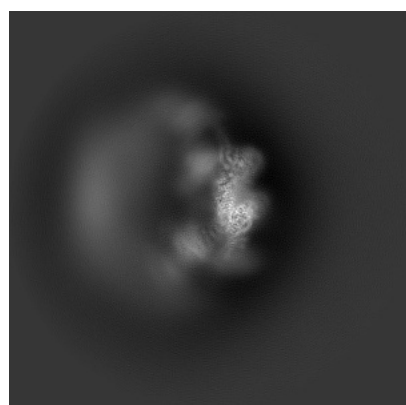
6 Map visualisation [i](#)

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.

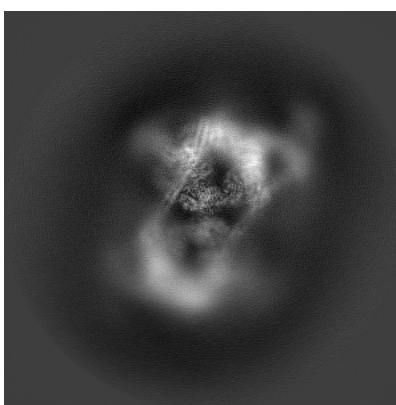
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

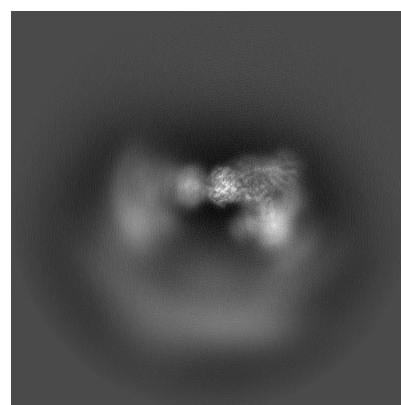
6.1.1 Primary map



X



Y



Z

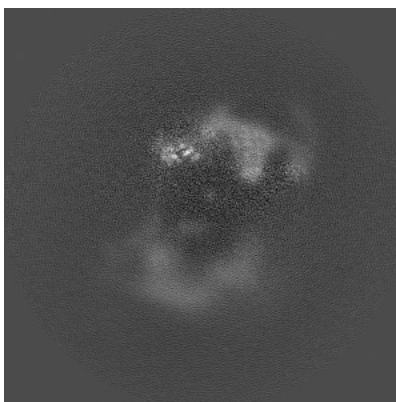
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

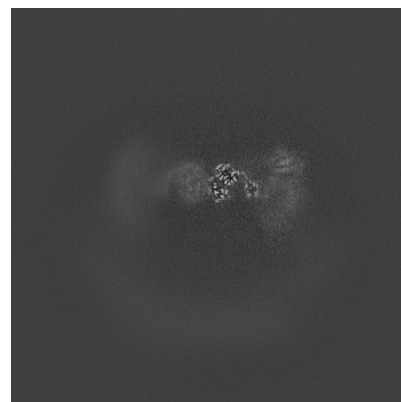
6.2.1 Primary map



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](#)

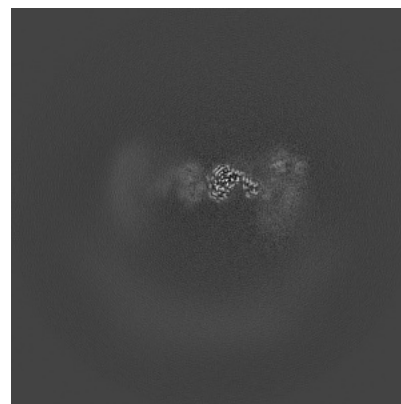
6.3.1 Primary map



X Index: 236



Y Index: 243

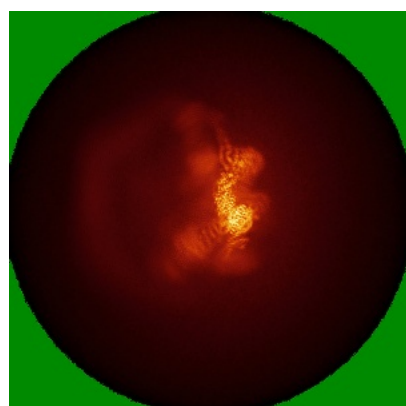


Z Index: 218

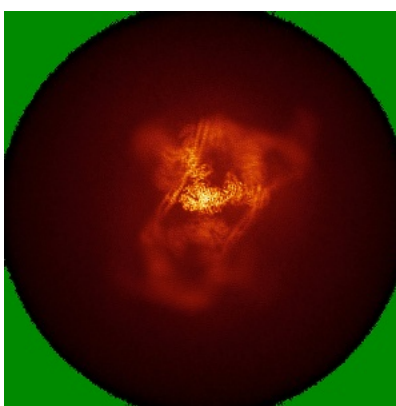
The images above show the largest variance slices of the map in three orthogonal directions.

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

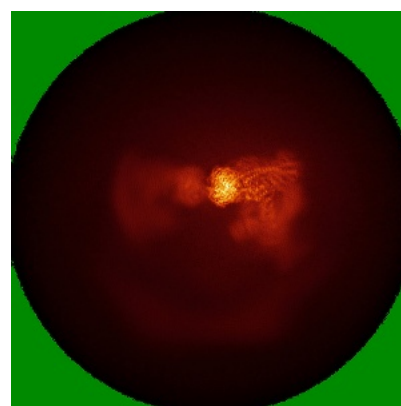
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

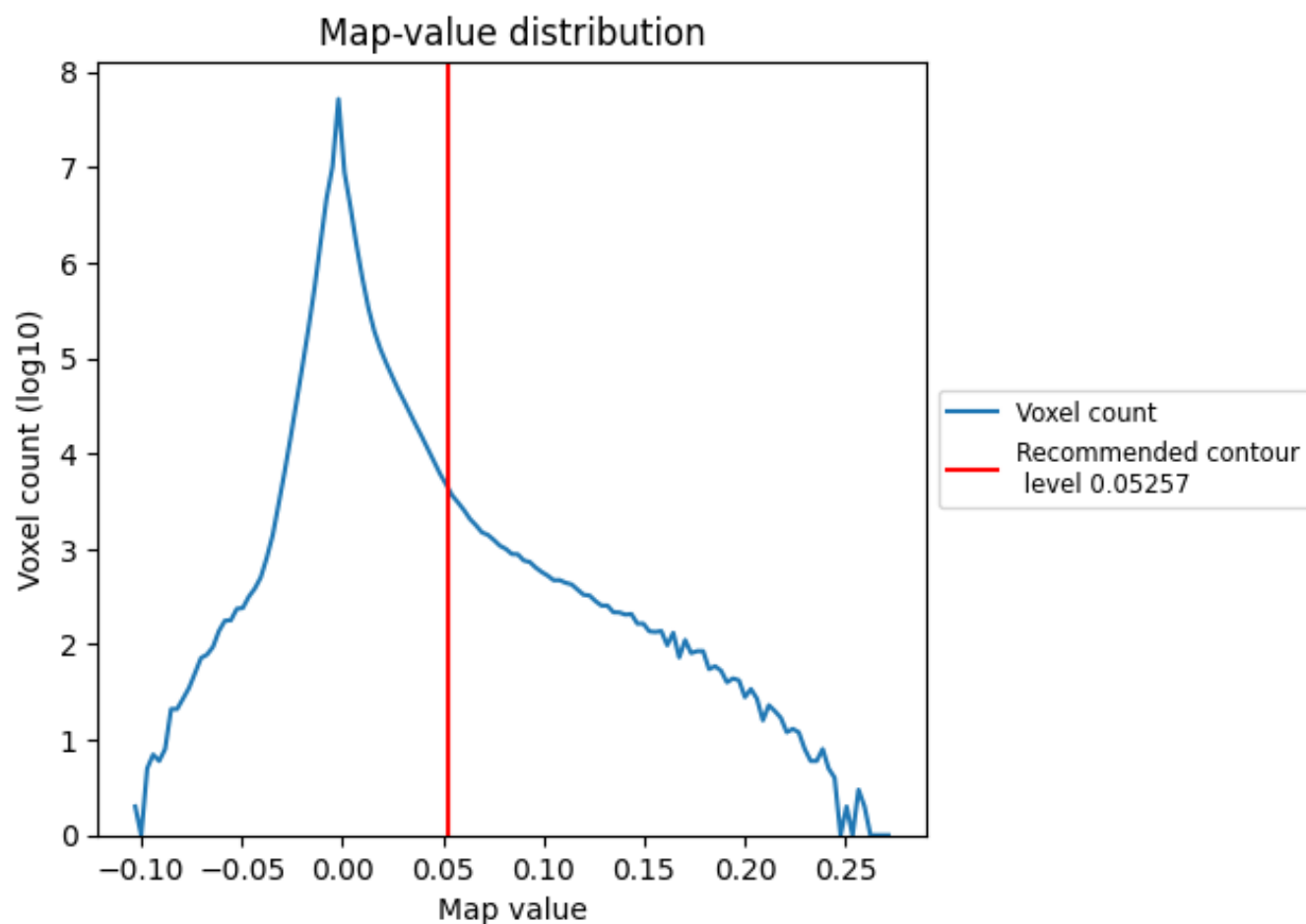
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

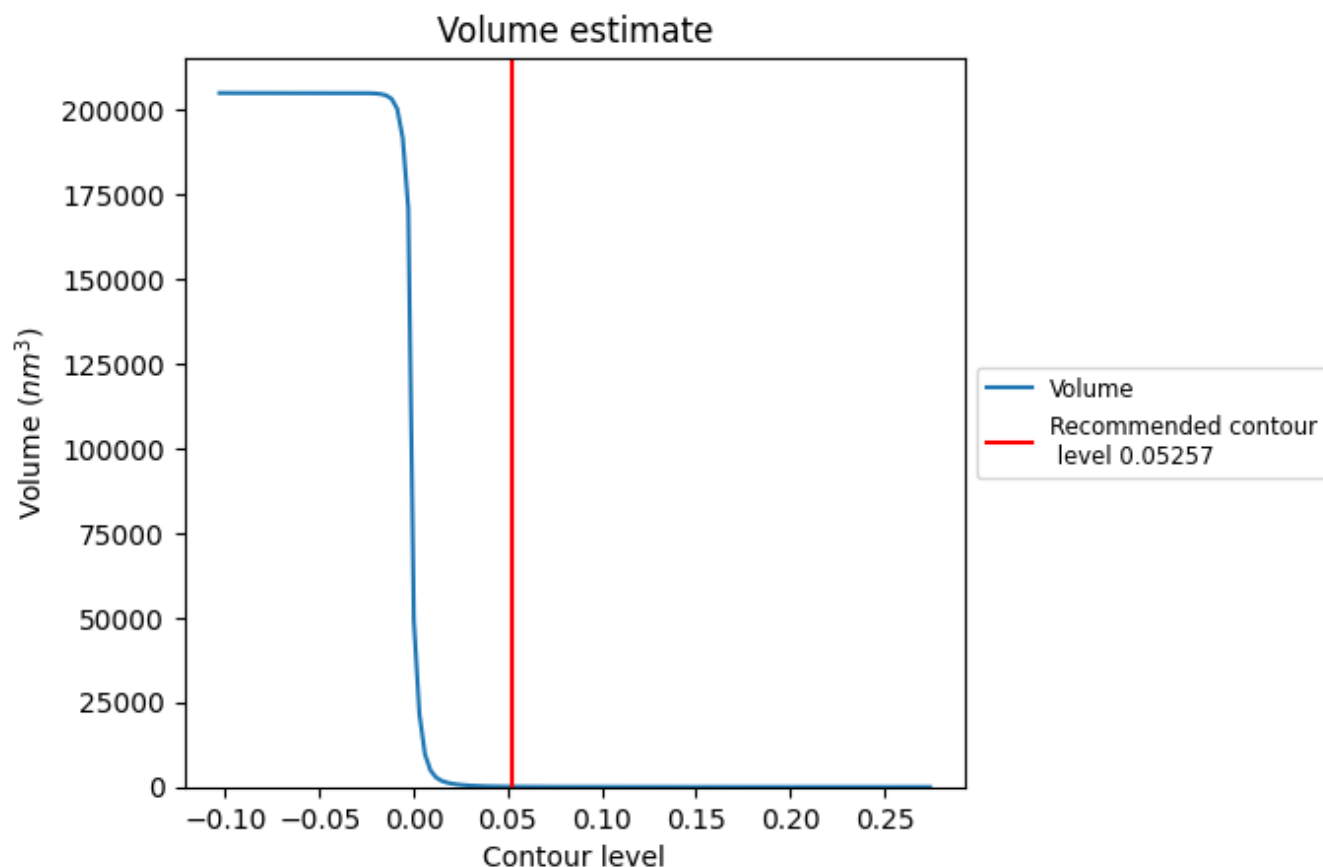
This section contains the results of statistical analysis of the map.

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.

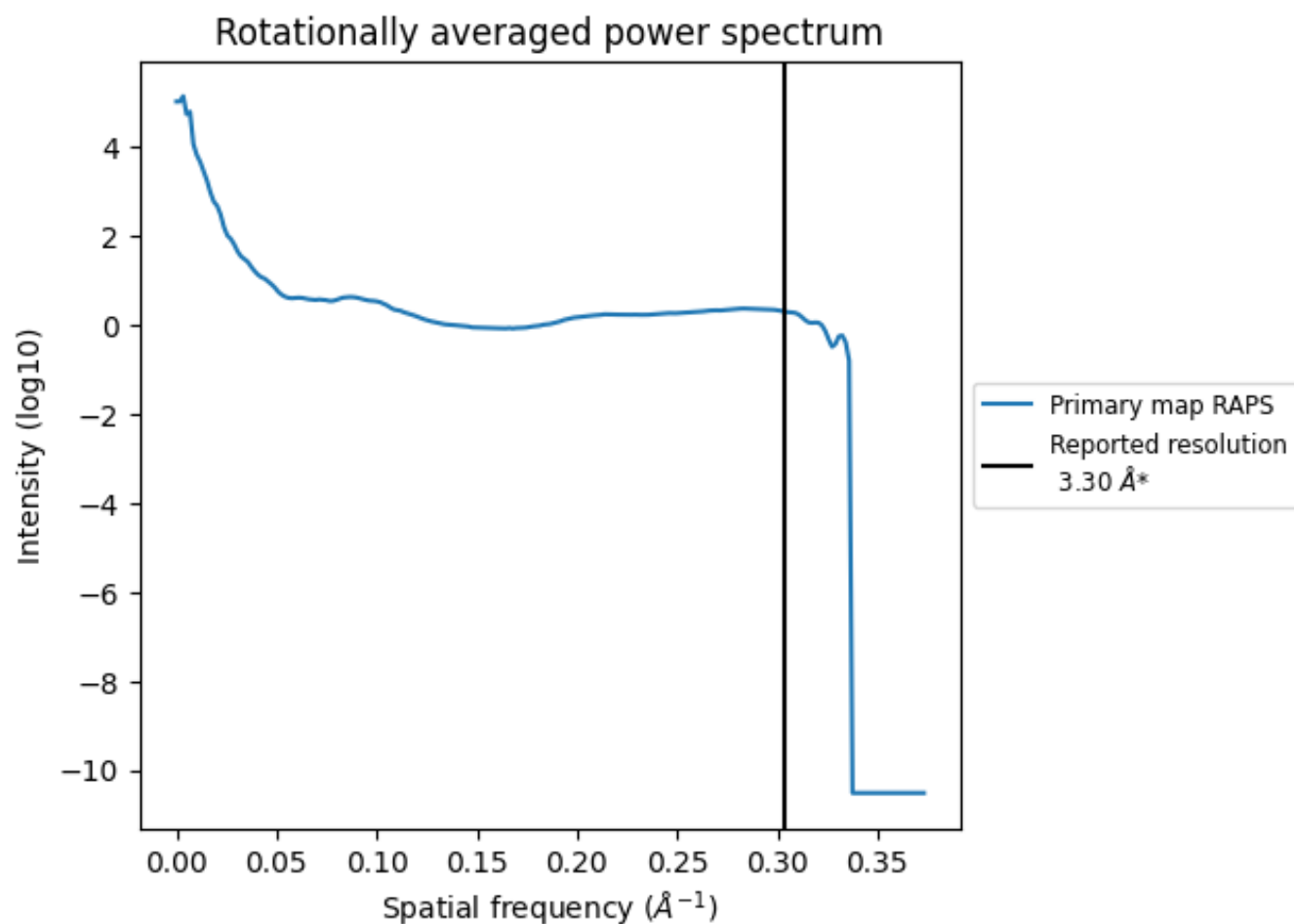
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 81 nm³; 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

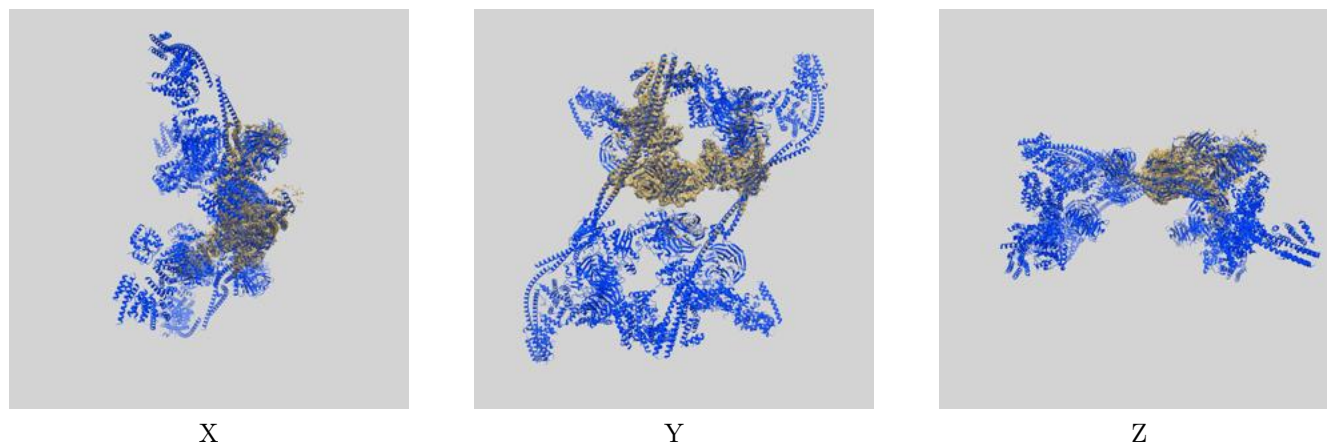
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

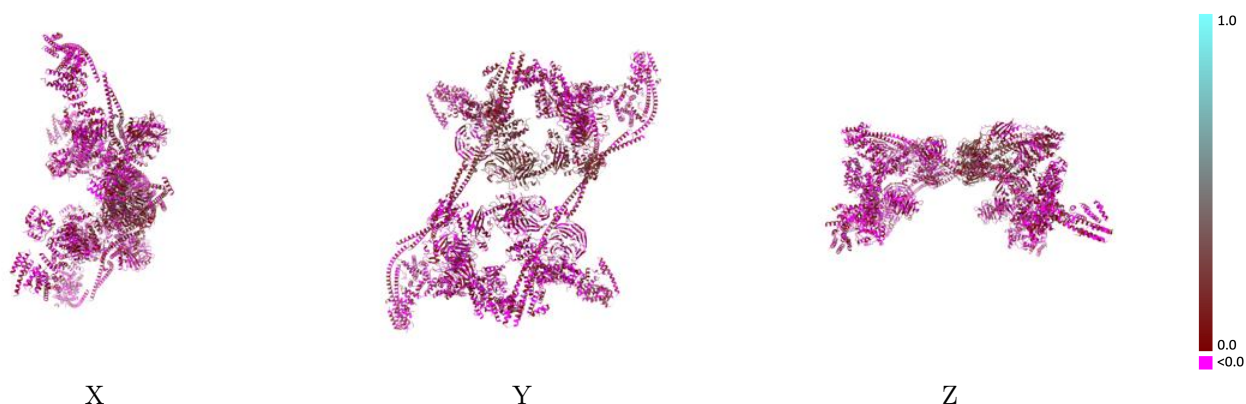
This section contains information regarding the fit between EMDB map EMD-11857 and PDB model 7APK. Per-residue inclusion information can be found in section [3](#) on page [22](#).

9.1 Map-model overlay [i](#)



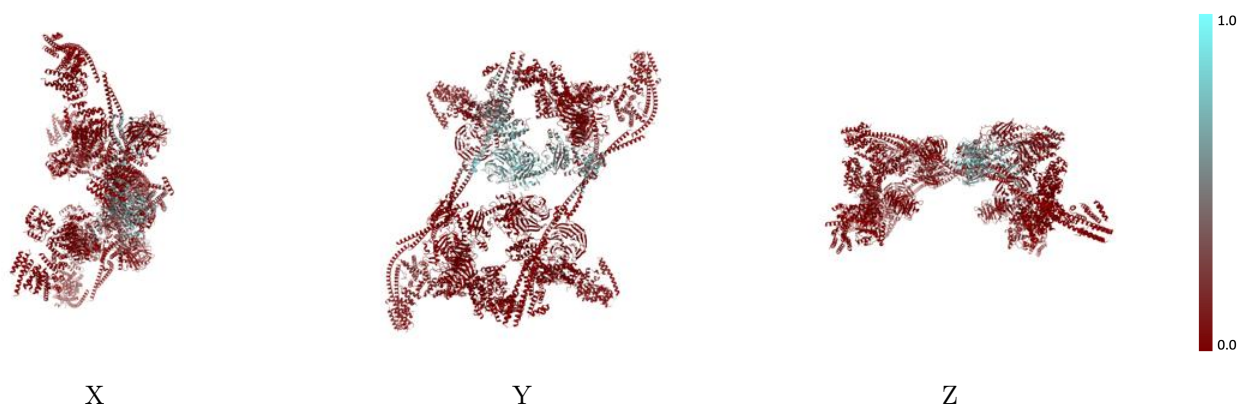
The images above show the 3D surface view of the map at the recommended contour level 0.05257 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



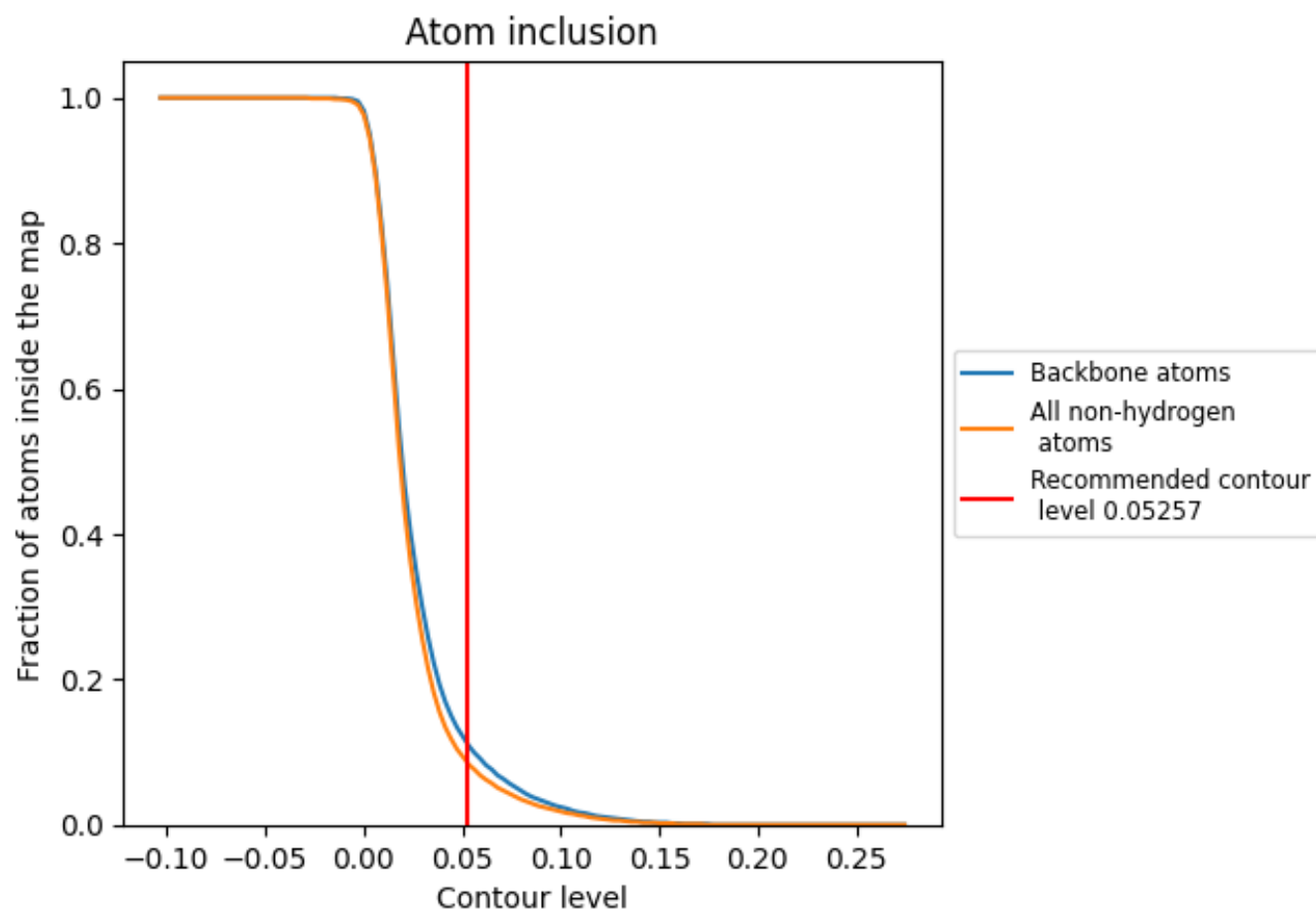
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.0860	 0.0510
A	 0.0000	 0.0080
B	 0.0020	 0.0250
C	 0.0010	 0.0280
E	 0.4380	 0.1750
F	 0.5720	 0.2190
G	 0.0720	 0.0750
H	 0.0000	 0.0090
I	 0.0000	 0.0160
J	 0.0000	 0.0050
K	 0.0000	 0.0090
M	 0.1570	 0.0950
N	 0.0240	 0.0450
O	 0.0900	 0.0620
P	 0.0000	 -0.0090
X	 0.0000	 0.0070
a	 0.0000	 0.0080
b	 0.0000	 0.0090
c	 0.0000	 0.0010
e	 0.0030	 0.0340
f	 0.0140	 0.0160
g	 0.0000	 0.0560
h	 0.0000	 0.0210
i	 0.3650	 0.1810
j	 0.1100	 0.0780
k	 0.0090	 0.0270
m	 0.1060	 0.0600
n	 0.0000	 0.0190
o	 0.3590	 0.1470
p	 0.0000	 -0.0050
x	 0.0540	 0.0840

