



wwPDB EM Validation Summary Report ⓘ

Aug 6, 2026 – 06:39 PM JST

PDB ID : 8IUE / pdb_00008iue
EMDB ID : EMD-35719
Title : RNA polymerase III pre-initiation complex melting complex 1
Authors : Hou, H.; Jin, Q.; Ren, Y.; Wang, Q.; Xu, Y.
Deposited on : 2023-03-24
Resolution : 4.10 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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
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) : 2.50

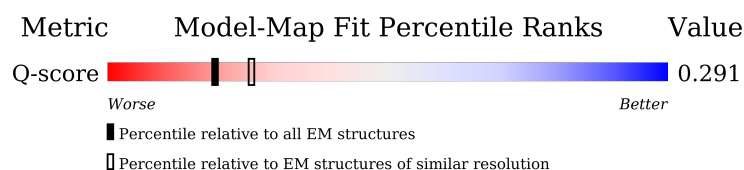
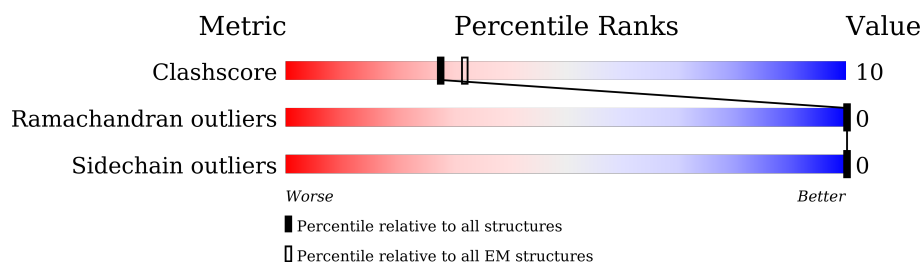
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 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	6458 (3.60 - 4.60)

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	1390	
2	B	1133	
3	C	346	
4	D	148	

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Mol	Chain	Length	Quality of chain
5	E	210	
6	F	127	
7	G	204	
8	H	150	
9	I	108	
10	J	67	
11	K	133	
12	L	58	
13	M	708	
14	N	317	
15	O	534	
16	P	316	
17	Q	223	
18	X	464	
19	Y	464	
20	1	368	
21	3	411	
22	4	1469	
23	U	339	
24	V	419	
25	W	2624	

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 57927 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 DNA-directed RNA polymerase III subunit RPC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1378	Total	C	N	O	S	0	0
			10814	6850	1886	2005	73		

- Molecule 2 is a protein called DNA-directed RNA polymerase III subunit RPC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1105	Total	C	N	O	S	0	0
			8741	5538	1529	1605	69		

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	343	Total	C	N	O	S	0	0
			2736	1723	488	514	11		

- Molecule 4 is a protein called DNA-directed RNA polymerase III subunit RPC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	122	Total	C	N	O	S	0	0
			985	614	172	196	3		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	209	Total	C	N	O	S	0	0
			1715	1083	300	324	8		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	76	Total	C	N	O	S	0	0
			610	392	103	110	5		

- Molecule 7 is a protein called DNA-directed RNA polymerase III subunit RPC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	166	Total	C	N	O	S	0	0
			1337	876	211	245	5		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase III subunit RPC10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	107	Total	C	N	O	S	0	0
			848	525	157	153	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	24	ALA	SER	variant	UNP Q9Y2Y1

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	65	Total	C	N	O	S	0	0
			512	331	87	88	6		

- Molecule 11 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	103	Total	C	N	O	S	0	0
			822	513	145	157	7		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	46	Total	C	N	O	S	0	0
			388	241	75	66	6		

- Molecule 13 is a protein called DNA-directed RNA polymerase III subunit RPC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	422	Total	C	N	O	S	0	0
			3382	2138	588	636	20		

- Molecule 14 is a protein called DNA-directed RNA polymerase III subunit RPC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	146	Total	C	N	O	S	0	0
			1128	710	191	221	6		

There are 81 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	?	-	LYS	deletion	UNP P05423
N	?	-	ASP	deletion	UNP P05423
N	?	-	ASP	deletion	UNP P05423
N	?	-	PHE	deletion	UNP P05423
N	?	-	LEU	deletion	UNP P05423
N	?	-	ASP	deletion	UNP P05423
N	?	-	ASP	deletion	UNP P05423
N	?	-	PRO	deletion	UNP P05423
N	?	-	GLY	deletion	UNP P05423
N	?	-	LEU	deletion	UNP P05423
N	?	-	ARG	deletion	UNP P05423
N	?	-	ASN	deletion	UNP P05423
N	?	-	ASP	deletion	UNP P05423
N	?	-	THR	deletion	UNP P05423
N	?	-	ARG	deletion	UNP P05423
N	?	-	ASN	deletion	UNP P05423
N	?	-	MET	deletion	UNP P05423
N	?	-	PRO	deletion	UNP P05423
N	?	-	VAL	deletion	UNP P05423
N	?	-	GLN	deletion	UNP P05423
N	?	-	LEU	deletion	UNP P05423
N	?	-	PRO	deletion	UNP P05423
N	?	-	LEU	deletion	UNP P05423
N	?	-	ALA	deletion	UNP P05423
N	?	-	HIS	deletion	UNP P05423
N	?	-	SER	deletion	UNP P05423
N	?	-	GLY	deletion	UNP P05423
N	?	-	TRP	deletion	UNP P05423
N	?	-	LEU	deletion	UNP P05423
N	?	-	PHE	deletion	UNP P05423
N	?	-	LYS	deletion	UNP P05423

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Chain	Residue	Modelled	Actual	Comment	Reference
N	?	-	GLU	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	ASN	deletion	UNP P05423
N	?	-	ASP	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	PRO	deletion	UNP P05423
N	?	-	ASP	deletion	UNP P05423
N	?	-	VAL	deletion	UNP P05423
N	?	-	LYS	deletion	UNP P05423
N	?	-	PRO	deletion	UNP P05423
N	?	-	TRP	deletion	UNP P05423
N	?	-	LEU	deletion	UNP P05423
N	?	-	ALA	deletion	UNP P05423
N	?	-	GLY	deletion	UNP P05423
N	?	-	PRO	deletion	UNP P05423
N	?	-	LYS	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	ASP	deletion	UNP P05423
N	?	-	MET	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	VAL	deletion	UNP P05423
N	?	-	ASP	deletion	UNP P05423
N	?	-	ILE	deletion	UNP P05423
N	?	-	PRO	deletion	UNP P05423
N	?	-	ALA	deletion	UNP P05423
N	?	-	VAL	deletion	UNP P05423
N	?	-	LYS	deletion	UNP P05423
N	?	-	VAL	deletion	UNP P05423
N	?	-	LYS	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	PRO	deletion	UNP P05423
N	?	-	ARG	deletion	UNP P05423
N	?	-	ASP	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	ALA	deletion	UNP P05423
N	?	-	LYS	deletion	UNP P05423
N	?	-	MET	deletion	UNP P05423

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Chain	Residue	Modelled	Actual	Comment	Reference
N	?	-	LYS	deletion	UNP P05423
N	?	-	ALA	deletion	UNP P05423
N	?	-	PRO	deletion	UNP P05423
N	?	-	PRO	deletion	UNP P05423
N	?	-	LYS	deletion	UNP P05423
N	?	-	ALA	deletion	UNP P05423
N	?	-	ALA	deletion	UNP P05423
N	?	-	ARG	deletion	UNP P05423

- Molecule 15 is a protein called DNA-directed RNA polymerase III subunit RPC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	512	Total	C	N	O	S	0	0
			4075	2565	712	774	24		

- Molecule 16 is a protein called DNA-directed RNA polymerase III subunit RPC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	303	Total	C	N	O	S	0	0
			2403	1516	411	460	16		

- Molecule 17 is a protein called DNA-directed RNA polymerase III subunit RPC7.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	87	Total	C	N	O	S	0	0
			754	488	126	134	6		

- Molecule 18 is a DNA chain called Human gene for U 6 RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	X	74	Total	C	N	O	P	0	0
			1517	727	263	453	74		

- Molecule 19 is a DNA chain called DNA (74-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Y	70	Total	C	N	O	P	0	0
			1437	686	271	410	70		

- Molecule 20 is a protein called snRNA-activating protein complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	1	146	Total	C	N	O	S	0	0
			1233	804	212	209	8		

- Molecule 21 is a protein called snRNA-activating protein complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	3	374	Total	C	N	O	S	0	0
			3037	1925	521	570	21		

- Molecule 22 is a protein called snRNA-activating protein complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	4	365	Total	C	N	O	S	0	0
			3058	1921	573	555	9		

- Molecule 23 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	176	Total	C	N	O	S	1	0
			1396	907	244	238	7		

- Molecule 24 is a protein called Transcription factor IIIB 50 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	V	361	Total	C	N	O	S	1	0
			2853	1792	507	531	23		

- Molecule 25 is a protein called Transcription factor TFIIB component B'' homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	W	111	Total	C	N	O	S	0	0
			943	606	163	170	4		

- Molecule 26 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
26	A	2	Total	Zn	0
			2	2	
26	B	1	Total	Zn	0
			1	1	
26	I	2	Total	Zn	0
			2	2	

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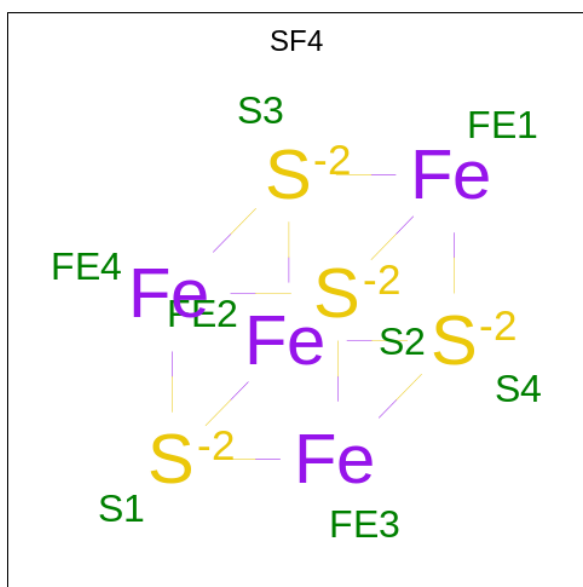
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Mol	Chain	Residues	Atoms		AltConf
26	J	1	Total	Zn	0
			1	1	
26	L	1	Total	Zn	0
			1	1	
26	V	1	Total	Zn	0
			1	1	

- Molecule 27 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
27	A	1	Total	Mg	0
			1	1	

- Molecule 28 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).

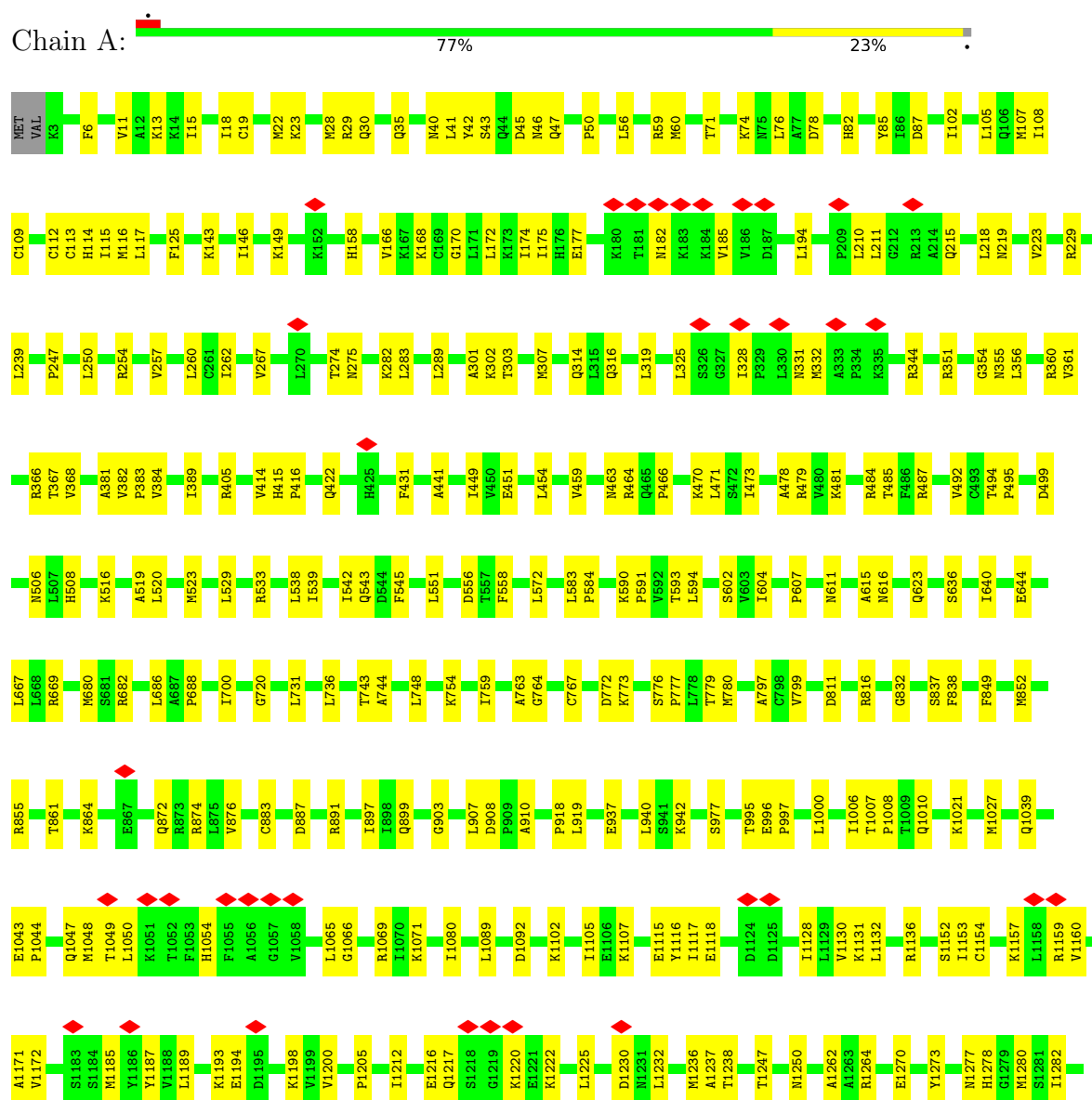


Mol	Chain	Residues	Atoms			AltConf
28	P	1	Total	Fe	S	0
			8	4	4	

3 Residue-property plots

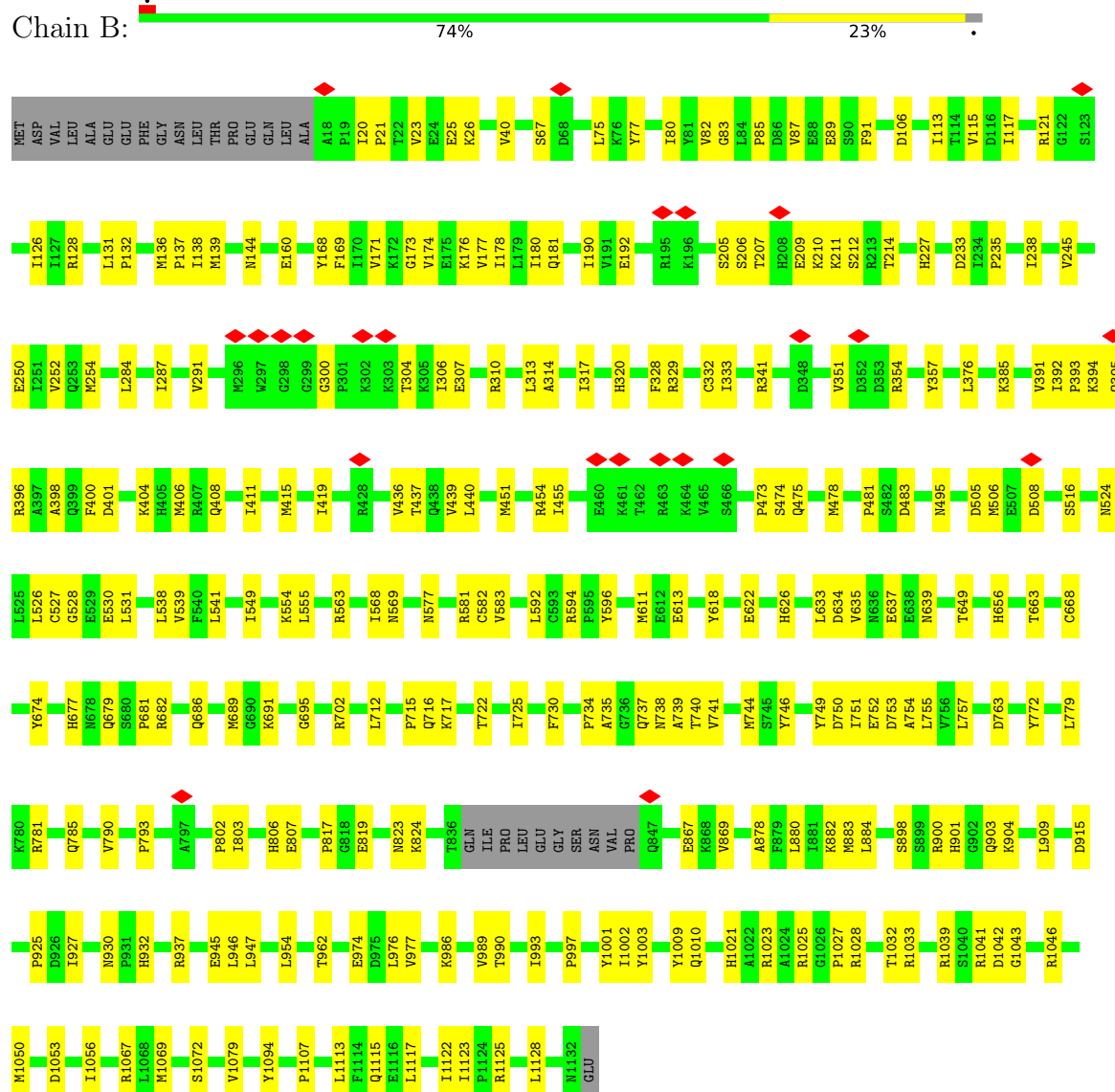
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA-directed RNA polymerase III subunit RPC1

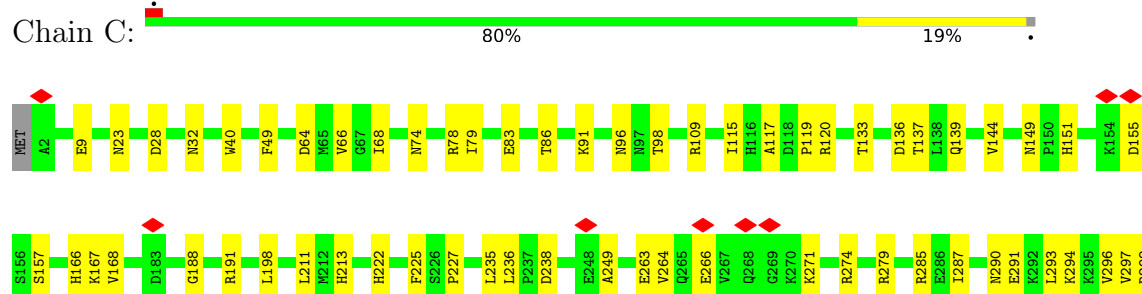


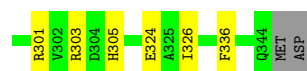


• Molecule 2: DNA-directed RNA polymerase III subunit RPC2

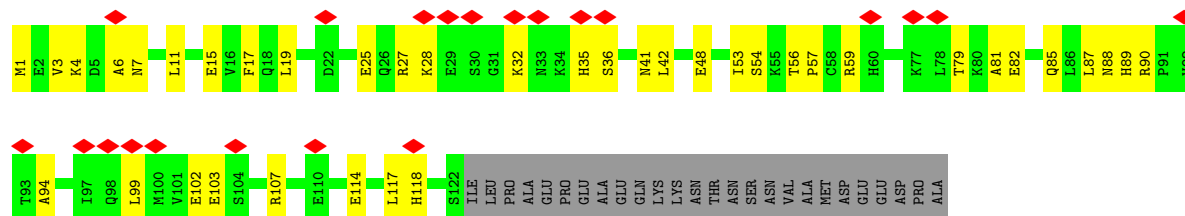


• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

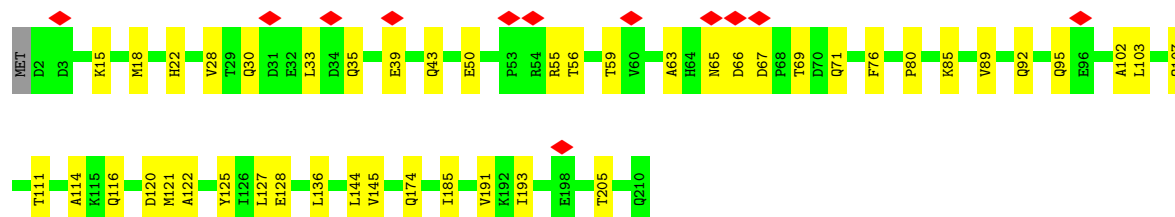
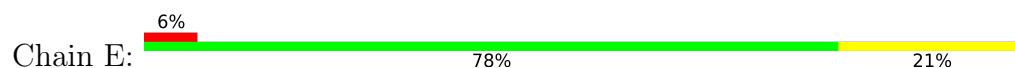




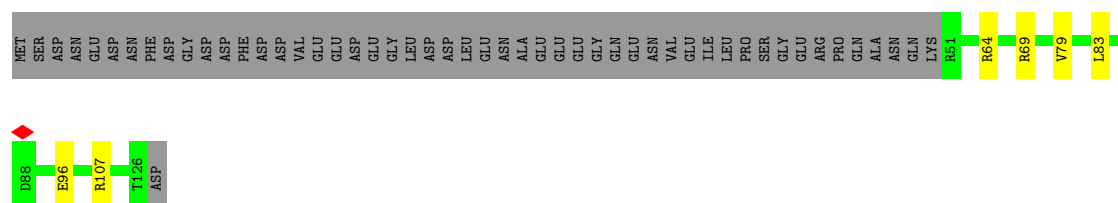
• Molecule 4: DNA-directed RNA polymerase III subunit RPC9



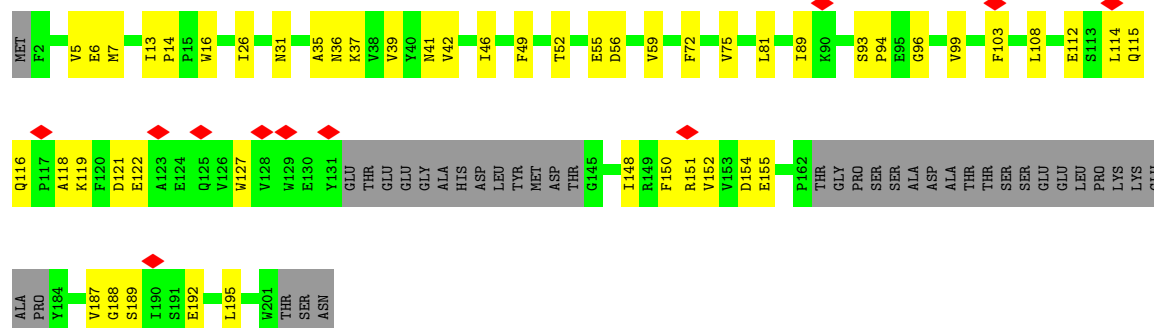
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



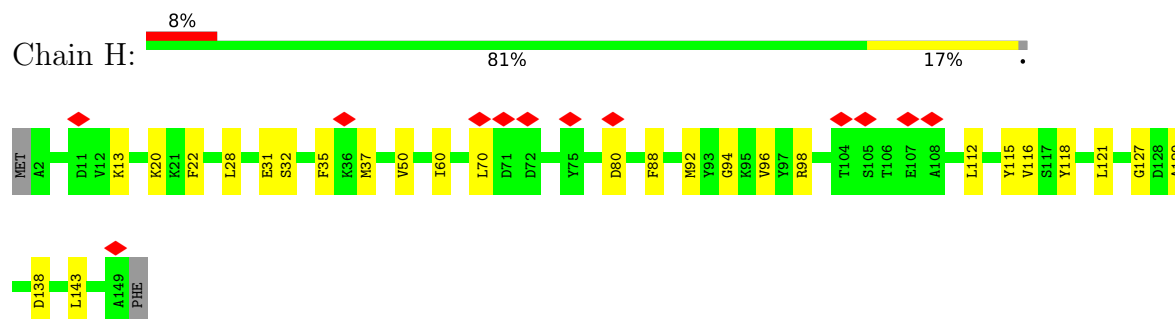
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



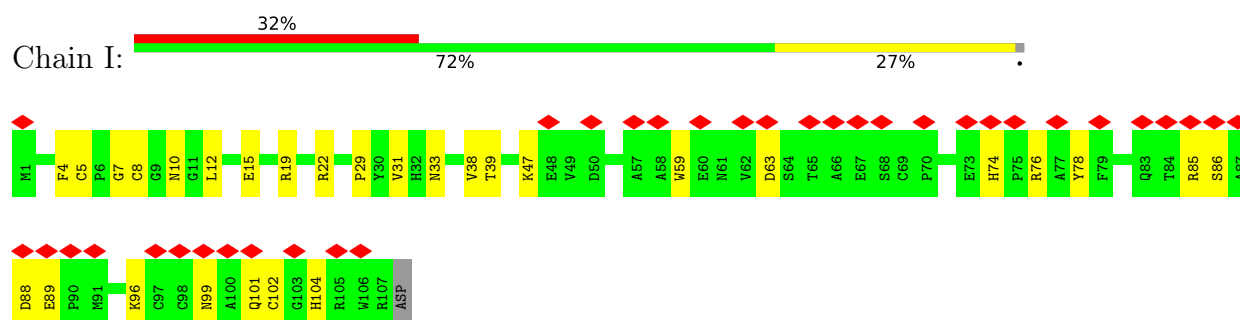
• Molecule 7: DNA-directed RNA polymerase III subunit RPC8



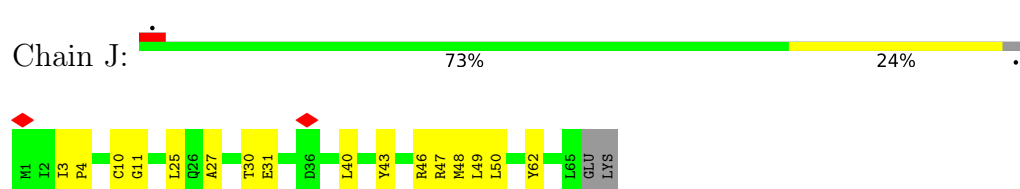
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



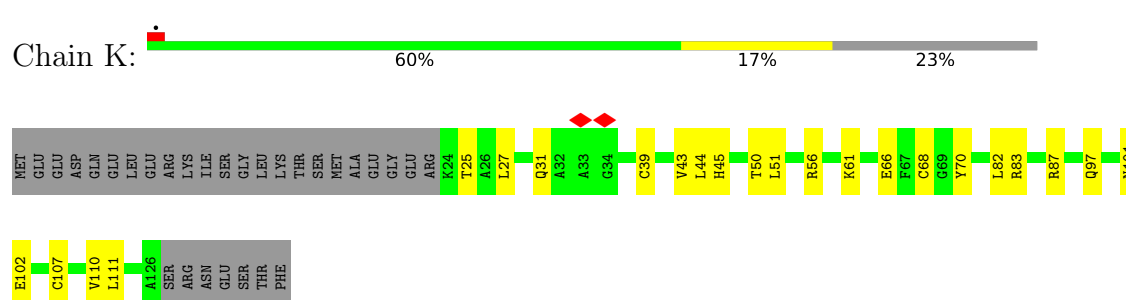
- Molecule 9: DNA-directed RNA polymerase III subunit RPC10



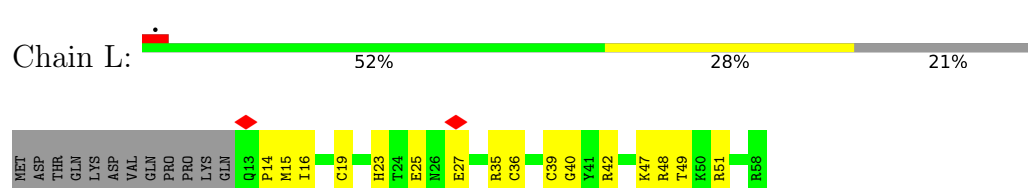
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



- Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2



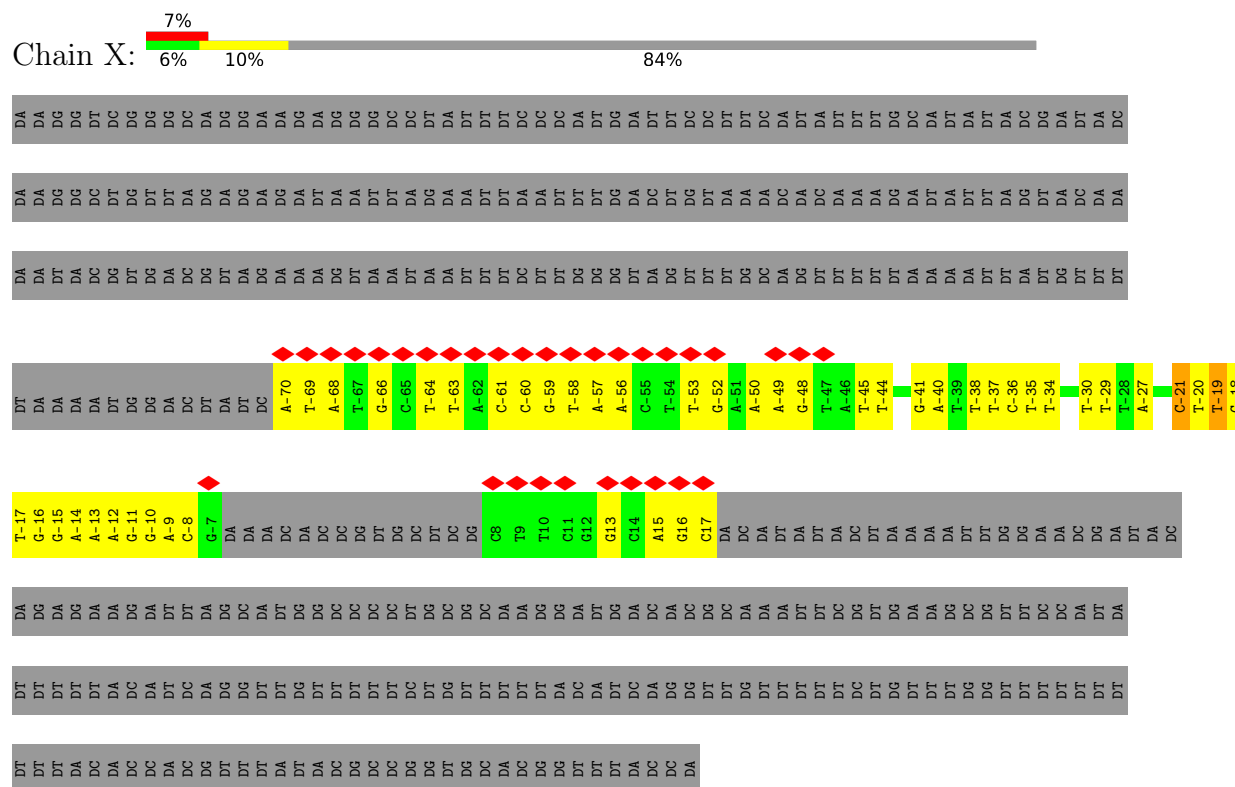
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



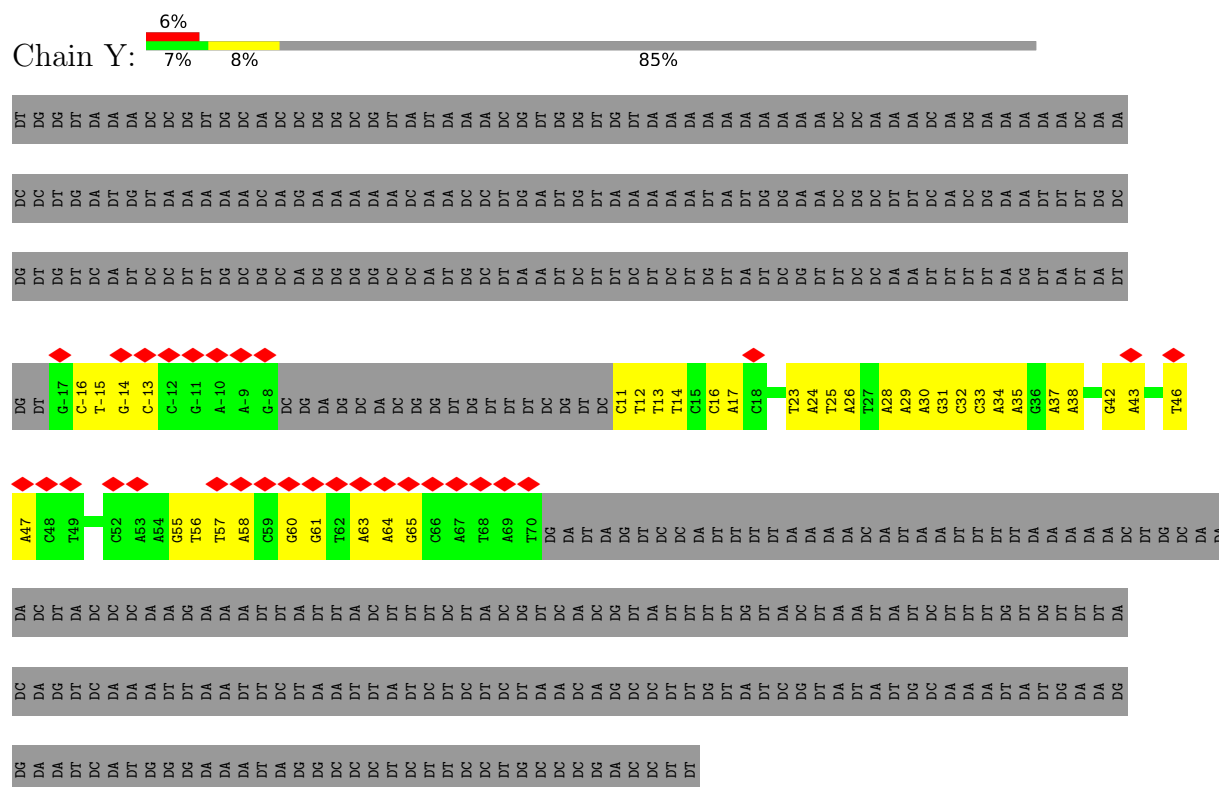
- Molecule 13: DNA-directed RNA polymerase III subunit RPC5



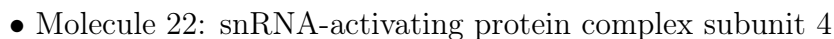
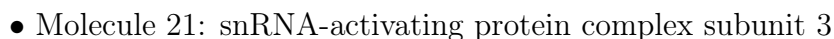
- Molecule 18: Human gene for U 6 RNA



- Molecule 19: DNA (74-MER)



- Molecule 20: snRNA-activating protein complex subunit 1





[illegible]

- Molecule 23: TATA-box-binding protein

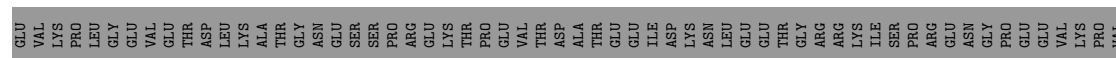


K383	T204	LEU	GLN	MET
G394	R205	PHE	GLN	ASP
PHE	E206	HIS	GLN	ASN
ARG	P207	SER	GLN	ASN
LYS	R208	GLN	GLN	SER
THR		THR	GLN	LEU
THR	L212	LEU	GLN	PRO
	I213	THR	GLN	PRO
	F214	ALA	GLN	TYR
		PRO	GLN	ALA
	R218	LEU	GLN	GLN
		PRO	GLN	GLY
	T222	GLY	GLN	LEU
	G223	THR	GLN	ALA
	A224	THR	GLN	PRO
	R225	PRO	GLN	SER
	E226	LEU	GLN	GLN
	S227	TYR	GLN	GLY
	E228	PRO	GLN	ALA
		SER	GLN	MET
		PRO	GLN	THR
	R235	PRO	GLN	PRO
		MET	GLN	GLY
		THR	GLN	ILE
	R239	PRO	GLN	PRO
	V240	MET	GLN	ILE
	V241	THR	GLN	PHE
	Q242	PRO	GLN	SER
	R243	ILE	GLN	SER
	L244	THR	GLN	PRO
	G245	PRO	GLN	MET
	F246	ALA	GLN	MET
	P247	THR	GLN	TYR
	A248	ALA	GLN	GLY
	R249	SER	ALA	THR
	F250	GLU	VAL	GLY
	L251	SER	ALA	LEU
	D252	SER	ALA	PRO
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		G160	ALA	GLN
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		I168	VAL	ILE
		V169	GLN	GLN
			GLN	GLN
		N173	SER	THR
		L174	THR	ASN
		G175	SER	ASN
		C176	GLN	SER
		K177	GLN	LEU
			ALA	SER
			THR	ILE
			GLN	LEU
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		A187	THR	GLU
		R188	SER	GLN
		N189	GLY	GLN
		A190	GLN	ARG
			ALA	GLN
			PRO	GLN
		K195	GLN	GLN

- Molecule 24: Transcription factor IIIB 50 kDa subunit



R284	L133	PRO	R285	T134	GLY	R286	M135	ARG	R287	G136	GLY	R288	A137	R6	R289	L141	R290	K158	R291	L159	L15	R292	V173	S19	R293	K174	H20	R294	T175	Y21	R295	Q184	L26	R296	P187	G32	R297	S188	R298	V189	F44	R299	L207	E47	R300	N212	G48	R301	F213	N49	R302	T214	L50	R303	V217	R51	R304	P222	E52	R305	L223	T54	R306	L224	V53	R307	G225	Y55	R308	L226	R309	Q238	S58	R310	R242	R67	R311	L243	S69	R312	G244	V76	R313	L253	H82	R314	D257	P86	R315	P261	F89	R316	A262	R317	G263	R318	S264	R319	R265	R320	L266	R321	Q267	R322	L276	R323	L280	R324	A281	R325	L282	R326	L283	R327	PRO	R328	GLN	R329	GLY	R330	LEU	R331	PRO	R332	GLN	R333	GLY	R334	GLY	R335	GLY	R336	GLY	R337	GLY	R338	GLY	R339	GLY	R340	GLY	R341	GLY	R342	GLY	R343	GLY	R344	GLY	R345	GLY	R346	GLY	R347	GLY	R348	GLY	R349	GLY	R350	GLY	R351	GLY	R352	GLY	R353	GLY	R354	GLY	R355	GLY	R356	GLY	R357	GLY	R358	GLY	R359	GLY	R360	GLY	R361	GLY	R362	GLY	R363	GLY	R364	GLY	R365	GLY	R366	GLY	R367	GLY	R368	GLY	R369	GLY	R370	GLY	R371	GLY	R372	GLY	R373	GLY	R374	GLY	R375	GLY	R376	GLY	R377	GLY	R378	GLY	R379	GLY	R380	GLY	R381	GLY	R382	GLY	R383	PRO	R384	PRO	R385	PRO	R386	PRO	R387	PRO	R388	PRO	R389	PRO	R390	PRO	R391	PRO	R392	PRO	R393	PRO	R394	PRO	R395	PRO	R396	PRO	R397	PRO	R398	PRO	R399	PRO	R400	PRO	R401	PRO	R402	PRO	R403	PRO	R404	PRO	R405	PRO	R406	PRO	R407	PRO	R408	PRO	R409	PRO	R410	PRO	R411	PRO	R412	PRO	R413	PRO	R414	PRO	R415	PRO	R416	PRO	R417	PRO	R418	PRO	R419	PRO	R420	PRO	R421	PRO	R422	PRO	R423	PRO	R424	PRO	R425	PRO	R426	PRO	R427	PRO	R428	PRO	R429	PRO	R430	PRO	R431	PRO	R432	PRO	R433	PRO	R434	PRO	R435	PRO	R436	PRO	R437	PRO	R438	PRO	R439	PRO	R440	PRO	R441	PRO	R442	PRO	R443	PRO	R444	PRO	R445	PRO	R446	PRO	R447	PRO	R448	PRO	R449	PRO	R450	PRO	R451	PRO	R452	PRO	R453	PRO	R454	PRO	R455	PRO	R456	PRO	R457	PRO	R458	PRO	R459	PRO	R460	PRO	R461	PRO	R462	PRO	R463	PRO	R464	PRO	R465	PRO	R466	PRO	R467	PRO	R468	PRO	R469	PRO	R470	PRO	R471	PRO	R472	PRO	R473	PRO	R474	PRO	R475	PRO	R476	PRO	R477	PRO	R478	PRO	R479	PRO	R480	PRO	R481	PRO	R482	PRO	R483	PRO	R484	PRO	R485	PRO	R486	PRO	R487	PRO	R488	PRO	R489	PRO	R490	PRO	R491	PRO	R492	PRO	R493	PRO	R494	PRO	R495	PRO	R496	PRO	R497	PRO	R498	PRO	R499	PRO	R500	PRO	R501	PRO	R502	PRO	R503	PRO	R504	PRO	R505	PRO	R506	PRO	R507	PRO	R508	PRO	R509	PRO	R510	PRO	R511	PRO	R512	PRO	R513	PRO	R514	PRO	R515	PRO	R516	PRO	R517	PRO	R518	PRO	R519	PRO	R520	PRO	R521	PRO	R522	PRO	R523	PRO	R524	PRO	R525	PRO	R526	PRO	R527	PRO	R528	PRO	R529	PRO	R530	PRO	R531	PRO	R532	PRO	R533	PRO	R534	PRO	R535	PRO	R536	PRO	R537	PRO	R538	PRO	R539	PRO	R540	PRO	R541	PRO	R542	PRO	R543	PRO	R544	PRO	R545	PRO	R546	PRO	R547	PRO	R548	PRO	R549	PRO	R550	PRO	R551	PRO	R552	PRO	R553	PRO	R554	PRO	R555	PRO	R556	PRO	R557	PRO	R558	PRO	R559	PRO	R560	PRO	R561	PRO	R562	PRO	R563	PRO	R564	PRO	R565	PRO	R566	PRO	R567	PRO	R568	PRO	R569	PRO	R570	PRO	R571	PRO	R572	PRO	R573	PRO	R574	PRO	R575	PRO	R576	PRO	R577	PRO	R578	PRO	R579	PRO	R580	PRO	R581	PRO	R582	PRO	R583	PRO	R584	PRO	R585	PRO	R586	PRO	R587	PRO	R588	PRO	R589	PRO	R590	PRO	R591	PRO	R592	PRO	R593	PRO	R594	PRO	R595	PRO	R596	PRO	R597	PRO	R598	PRO	R599	PRO	R600	PRO	R601	PRO	R602	PRO	R603	PRO	R604	PRO	R605	PRO	R606	PRO	R607	PRO	R608	PRO	R609	PRO	R610	PRO	R611	PRO	R612	PRO	R613	PRO	R614	PRO	R615	PRO	R616	PRO	R617	PRO	R618	PRO	R619	PRO	R620	PRO	R621	PRO	R622	PRO	R623	PRO	R624	PRO	R625	PRO	R626	PRO	R627	PRO	R628	PRO	R629	PRO	R630	PRO	R631	PRO	R632	PRO	R633	PRO	R634	PRO	R635	PRO	R636	PRO	R637	PRO	R638	PRO	R639	PRO	R640	PRO	R641	PRO	R642	PRO	R643	PRO	R644	PRO	R645	PRO	R646	PRO	R647	PRO	R648	PRO	R649	PRO	R650	PRO	R651	PRO	R652	PRO	R653	PRO	R654	PRO	R655	PRO	R656	PRO	R657	PRO	R658	PRO	R659	PRO	R660	PRO	R661	PRO	R662	PRO	R663	PRO	R664	PRO	R665	PRO	R666	PRO	R667	PRO	R668	PRO	R669	PRO	R670	PRO	R671	PRO	R672	PRO	R673	PRO	R674	PRO	R675	PRO	R676	PRO	R677	PRO	R678	PRO	R679	PRO	R680	PRO	R681	PRO	R682	PRO	R683	PRO	R684	PRO	R685	PRO	R686	PRO	R687	PRO	R688	PRO	R689	PRO	R690	PRO	R691	PRO	R692	PRO	R693	PRO	R694	PRO	R695	PRO	R696	PRO	R697	PRO	R698	PRO	R699	PRO	R700	PRO	R701	PRO	R702	PRO	R703	PRO	R704	PRO	R705	PRO	R706	PRO	R707	PRO	R708	PRO	R709	PRO	R710	PRO	R711	PRO	R712	PRO	R713	PRO	R714	PRO	R715	PRO	R716	PRO	R717	PRO	R718	PRO	R719	PRO	R720	PRO	R721	PRO	R722	PRO	R723	PRO	R724	PRO	R725	PRO	R726	PRO	R727	PRO	R728	PRO	R729	PRO	R730	PRO	R731	PRO	R732	PRO	R733	PRO	R734	PRO	R735	PRO	R736	PRO	R737	PRO	R738	PRO	R739	PRO	R740	PRO	R741	PRO	R742	PRO	R743	PRO	R744	PRO	R745	PRO	R746	PRO	R747	PRO	R748	PRO	R749	PRO	R750	PRO	R751	PRO	R752	PRO	R753	PRO	R754	PRO	R755	PRO	R756	PRO	R757	PRO	R758	PRO	R759	PRO	R760	PRO	R761	PRO	R762	PRO	R763	PRO	R764	PRO	R765	PRO	R766	PRO	R767	PRO	R768	PRO	R769	PRO	R770	PRO	R771	PRO	R772	PRO	R773	PRO	R774	PRO	R775	PRO	R776	PRO	R777	PRO	R778	PRO	R779	PRO	R780	PRO	R781	PRO	R782	PRO	R783	PRO	R784	PRO	R785	PRO	R786	PRO	R787	PRO	R788	PRO	R789	PRO	R790	PRO	R791	PRO	R792	PRO	R793	PRO	R794	PRO	R795	PRO	R796	PRO	R797	PRO	R798	PRO	R799	PRO	R800	PRO	R801	PRO	R802	PRO	R803	PRO	R804	PRO	R805	PRO	R806	PRO	R807	PRO	R808	PRO	R809	PRO	R810	PRO	R811	PRO	R812	PRO	R813	PRO	R814	PRO	R815	PRO	R816	PRO	R817	PRO	R818	PRO	R819	PRO	R820	PRO	R821	PRO	R822	PRO	R823	PRO	R824	PRO	R825	PRO	R826	PRO	R827	PRO	R828	PRO	R829	PRO	R830	PRO	R831	PRO	R832	PRO	R833	PRO	R834	PRO	R835	PRO	R836	PRO	R837	PRO	R838	PRO	R839	PRO	R840	PRO	R841	PRO	R842	PRO	R843	PRO	R844	PRO	R845	PRO	R846	PRO	R847	PRO	R848	PRO	R849	PRO	R850	PRO	R851	PRO	R852	PRO	R853	PRO	R854	PRO	R855	PRO	R856	PRO	R857	PRO	R858	PRO	R859	PRO	R860	PRO	R861	PRO	R862	PRO	R863	PRO	R864	PRO	R865	PRO	R866	PRO	R867	PRO	R868	PRO	R869	PRO	R870	PRO	R871	PRO	R872	PRO	R873	PRO	R874	PRO	R875	PRO	R876	PRO	R877	PRO	R878	PRO	R879	PRO	R880	PRO	R881	PRO	R882	PRO	R883	PRO	R884	PRO	R885	PRO	R886	PRO	R887	PRO	R888	PRO	R889	PRO	R890	PRO	R891	PRO	R892	PRO	R893	PRO	R894	PRO	R895	PRO	R896	PRO	R897	PRO	R898	PRO	R899	PRO	R900	PRO	R901	PRO	R902	PRO	R903	PRO	R904	PRO	R905	PRO	R906	PRO	R907	PRO	R908	PRO	R909	PRO	R910	PRO	R911	PRO	R912	PRO	R913	PRO	R914	PRO	R915	PRO	R916	PRO	R917	PRO	R918	PRO	R919	PRO	R920	PRO	R921	PRO	R922	PRO	R923	PRO	R924	PRO	R925	PRO	R926	PRO	R927	PRO	R928	PRO	R929	PRO	R930	PRO	R931	PRO	R932	PRO	R933	PRO	R934	PRO	R935	PRO	R936	PRO	R937	PRO	R938	PRO	R939	PRO	R940	PRO	R941	PRO	R942	PRO	R943	PRO	R944	PRO	R945	PRO	R946	PRO	R947	PRO	R948	PRO	R949	PRO	R950	PRO	R951	PRO	R952	PRO	R953	PRO	R954	PRO	R955	PRO	R956	PRO	R957	PRO	R958	PRO	R959	PRO	R960	PRO	R961	PRO	R962	PRO	R963	PRO	R964	PRO	R965	PRO	R966	PRO	R967	PRO	R968	PRO	R969	PRO	R970	PRO	R971	PRO	R972	PRO	R973	PRO	R974	PRO	R975	PRO	R976	PRO	R977	PRO	R978	PRO	R979	PRO	R980	PRO	R981	PRO	R982	PRO	R983	PRO	R984	PRO	R985	PRO	R986	PRO	R987	PRO	R988	PRO	R989	PRO	R990	PRO	R991	PRO	R992	PRO	R993	PRO	R994	PRO	R995	PRO	R996	PRO	R997	PRO	R998	PRO	R999	PRO	R1000	PRO
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PRO	GLN	GLU	ARG	SER	GLY	SER	GLY	VAL	PRO
ALA	ASP	GLU	SER	ARG	PHE	ARG	LEU	ILE	VAL
VAL	LEU	GLY	THR	GLY	LEU	SER	THR	THR	ILE
SER	VAL	GLY	THR	SER	THR	SER	THR	THR	THR
GLU	ASN	MET	ARG	SER	ILE	SER	ILE	GLN	GLU
THR	LEU	SER	ASP	ASP	ASP	PRO	CYS	SER	GLY
GLY	VAL	ILE	ASP	ASP	GLY	ASP	ALA	THR	LEU
THR	ALA	PRO	THR	THR	THR	THR	THR	THR	GLY
PRO	GLN	THR	THR	THR	THR	THR	THR	THR	GLY
CYS	ASN	GLN	CYS	CYS	GLN	GLN	GLN	GLN	GLN
THR	VAL	PRO	GLU	MET	ASP	ASP	ASP	ASP	THR
LEU	PRO	ASP	TYR	THR	THR	SER	GLU	GLU	GLY
GLY	GLN	ASP	SER	SER	LEU	PRO	GLN	GLN	GLY
LEU	GLN	ALA	LYS	THR	GLY	THR	GLN	GLN	GLY
GLY	GLN	THR	THR	THR	GLY	THR	GLY	GLY	GLY
LEU	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP	LYS	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ALA	THR	THR	GLY	THR	GLY	GLY	GLY
GLY	GLN	ASP							

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	37656	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.184	Depositor
Minimum map value	-0.056	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.024	Depositor
Map size (Å)	426.88, 426.88, 426.88	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.334, 1.334, 1.334	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SF4, MG

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	0.10	0/11008	0.29	0/14842
2	B	0.10	0/8910	0.30	0/12018
3	C	0.10	0/2790	0.30	0/3782
4	D	0.10	0/997	0.29	0/1343
5	E	0.10	0/1745	0.30	0/2358
6	F	0.11	0/620	0.27	0/839
7	G	0.12	0/1374	0.33	0/1868
8	H	0.11	0/1207	0.31	0/1628
9	I	0.14	0/869	0.34	0/1174
10	J	0.10	0/521	0.28	0/703
11	K	0.10	0/837	0.31	0/1129
12	L	0.12	0/394	0.34	0/524
13	M	0.10	0/3455	0.28	0/4673
14	N	0.10	0/1137	0.29	0/1530
15	O	0.10	0/4141	0.28	0/5592
16	P	0.10	0/2446	0.30	0/3301
17	Q	0.11	0/777	0.31	0/1050
18	X	0.80	1/1697 (0.1%)	0.52	4/2616 (0.2%)
19	Y	0.14	0/1614	0.30	0/2485
20	1	0.13	0/1266	0.28	0/1708
21	3	0.12	0/3112	0.33	0/4206
22	4	0.11	0/3121	0.31	0/4181
23	U	0.11	0/1424	0.29	0/1918
24	V	0.11	0/2904	0.31	0/3941
25	W	0.10	0/967	0.29	0/1293
All	All	0.17	1/59333 (0.0%)	0.31	4/80702 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	X	-21	DC	O3'-P	-31.92	1.13	1.61

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	X	-21	DC	O3'-P-O5'	-10.98	87.53	104.00
18	X	-18	DG	C4'-C3'-O3'	7.94	121.91	110.00
18	X	-21	DC	P-O3'-C3'	-6.65	110.22	120.20
18	X	-19	DT	C2'-C3'-O3'	-5.90	102.65	111.50

There are no chirality outliers.

There are no planarity outliers.

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	10814	0	11057	234	0
2	B	8741	0	8867	217	0
3	C	2736	0	2712	54	0
4	D	985	0	1006	34	0
5	E	1715	0	1733	38	0
6	F	610	0	642	6	0
7	G	1337	0	1306	45	0
8	H	1186	0	1147	17	0
9	I	848	0	811	47	0
10	J	512	0	525	14	0
11	K	822	0	810	18	0
12	L	388	0	395	19	0
13	M	3382	0	3376	60	0
14	N	1128	0	1181	35	0
15	O	4075	0	4149	54	0
16	P	2403	0	2409	48	0
17	Q	754	0	759	25	0
18	X	1517	0	844	61	0
19	Y	1437	0	789	32	0
20	1	1233	0	1231	35	0
21	3	3037	0	2911	84	0
22	4	3058	0	3064	70	0
23	U	1396	0	1490	15	0
24	V	2853	0	2892	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	W	943	0	924	8	0
26	A	2	0	0	0	0
26	B	1	0	0	0	0
26	I	2	0	0	0	0
26	J	1	0	0	0	0
26	L	1	0	0	0	0
26	V	1	0	0	0	0
27	A	1	0	0	0	0
28	P	8	0	0	1	0
All	All	57927	0	57030	1104	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 10.

The worst 5 of 1104 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)
9:I:76:ARG:CD	9:I:99:ASN:HB2	1.23	1.60
2:B:741:VAL:CG2	2:B:1009:TYR:CE2	1.87	1.55
18:X:-21:DC:O3'	18:X:-20:DT:P	1.13	1.52
2:B:741:VAL:HG21	2:B:1009:TYR:CZ	1.36	1.52
9:I:76:ARG:CD	9:I:99:ASN:CB	1.99	1.38

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	1376/1390 (99%)	1342 (98%)	34 (2%)	0	100	100
2	B	1101/1133 (97%)	1072 (97%)	29 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	341/346 (99%)	336 (98%)	5 (2%)	0	100	100
4	D	120/148 (81%)	115 (96%)	5 (4%)	0	100	100
5	E	207/210 (99%)	205 (99%)	2 (1%)	0	100	100
6	F	74/127 (58%)	73 (99%)	1 (1%)	0	100	100
7	G	160/204 (78%)	151 (94%)	9 (6%)	0	100	100
8	H	146/150 (97%)	146 (100%)	0	0	100	100
9	I	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
10	J	63/67 (94%)	61 (97%)	2 (3%)	0	100	100
11	K	101/133 (76%)	100 (99%)	1 (1%)	0	100	100
12	L	44/58 (76%)	42 (96%)	2 (4%)	0	100	100
13	M	418/708 (59%)	403 (96%)	15 (4%)	0	100	100
14	N	140/317 (44%)	140 (100%)	0	0	100	100
15	O	508/534 (95%)	497 (98%)	11 (2%)	0	100	100
16	P	301/316 (95%)	295 (98%)	6 (2%)	0	100	100
17	Q	85/223 (38%)	82 (96%)	3 (4%)	0	100	100
20	1	144/368 (39%)	142 (99%)	2 (1%)	0	100	100
21	3	368/411 (90%)	356 (97%)	12 (3%)	0	100	100
22	4	363/1469 (25%)	350 (96%)	13 (4%)	0	100	100
23	U	175/339 (52%)	173 (99%)	2 (1%)	0	100	100
24	V	358/419 (85%)	349 (98%)	9 (2%)	0	100	100
25	W	109/2624 (4%)	105 (96%)	4 (4%)	0	100	100
All	All	6807/11802 (58%)	6636 (98%)	171 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	1200/1212 (99%)	1200 (100%)	0	100	100
2	B	964/988 (98%)	964 (100%)	0	100	100
3	C	299/302 (99%)	299 (100%)	0	100	100
4	D	114/136 (84%)	114 (100%)	0	100	100
5	E	191/192 (100%)	191 (100%)	0	100	100
6	F	66/111 (60%)	66 (100%)	0	100	100
7	G	149/181 (82%)	149 (100%)	0	100	100
8	H	129/131 (98%)	129 (100%)	0	100	100
9	I	92/93 (99%)	92 (100%)	0	100	100
10	J	53/56 (95%)	53 (100%)	0	100	100
11	K	92/119 (77%)	92 (100%)	0	100	100
12	L	43/55 (78%)	43 (100%)	0	100	100
13	M	377/622 (61%)	377 (100%)	0	100	100
14	N	131/276 (48%)	131 (100%)	0	100	100
15	O	458/476 (96%)	458 (100%)	0	100	100
16	P	269/280 (96%)	269 (100%)	0	100	100
17	Q	84/195 (43%)	84 (100%)	0	100	100
20	1	130/334 (39%)	130 (100%)	0	100	100
21	3	330/356 (93%)	330 (100%)	0	100	100
22	4	321/1213 (26%)	321 (100%)	0	100	100
23	U	152/293 (52%)	152 (100%)	0	100	100
24	V	325/365 (89%)	325 (100%)	0	100	100
25	W	102/2381 (4%)	102 (100%)	0	100	100
All	All	6071/10367 (59%)	6071 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 94 such sidechains are listed below:

Mol	Chain	Res	Type
14	N	395	HIS
20	1	95	GLN
15	O	60	HIS
15	O	498	GLN
21	3	314	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 9 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
28	SF4	P	401	-	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	SF4	P	401	-	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	P	401	SF4	1	0

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
18	X	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	X	-21:DC	O3'	-20:DT	P	1.13

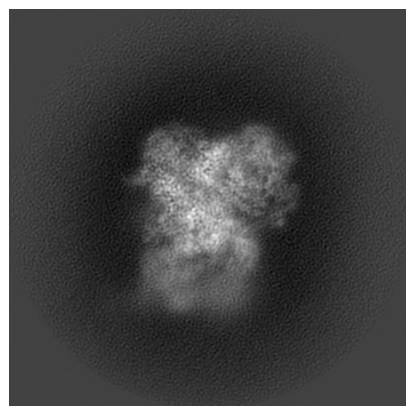
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35719. These allow visual inspection of the internal detail of the map and identification of artifacts.

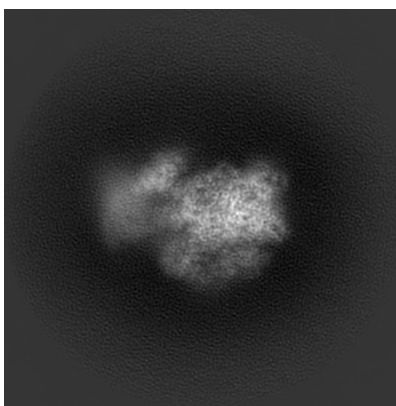
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

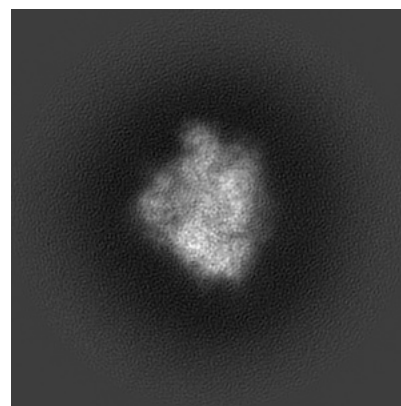
6.1.1 Primary map



X

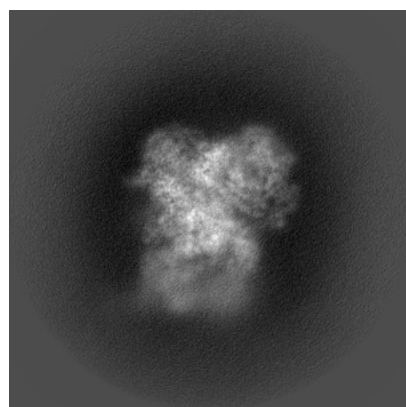


Y

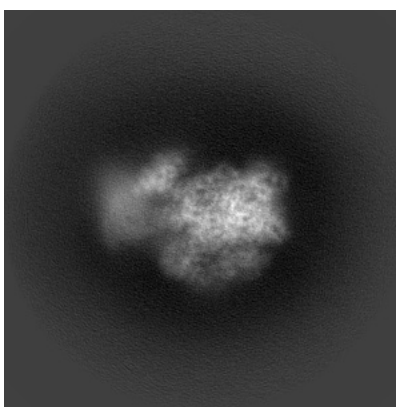


Z

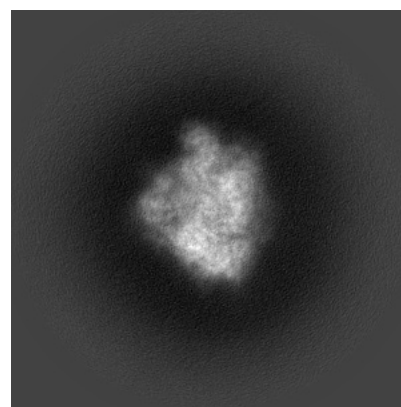
6.1.2 Raw map



X



Y

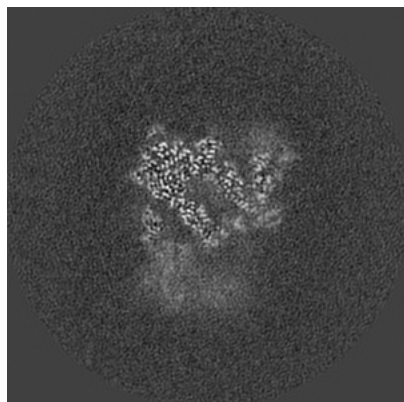


Z

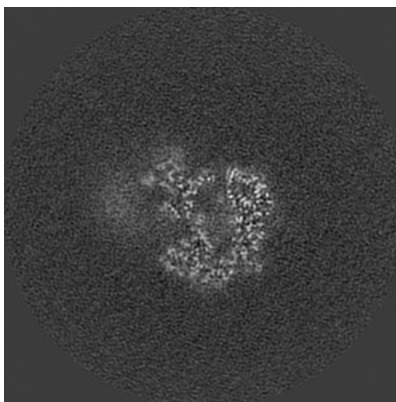
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

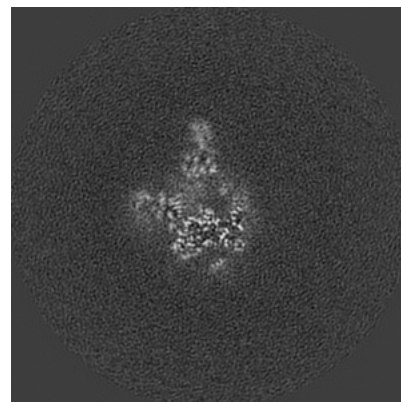
6.2.1 Primary map



X Index: 160

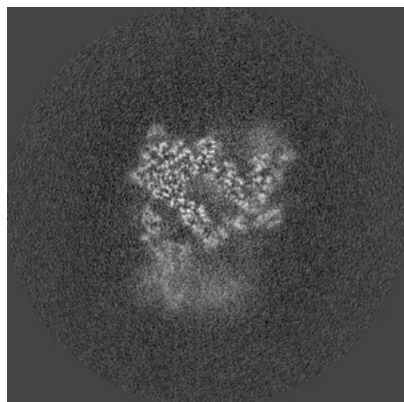


Y Index: 160

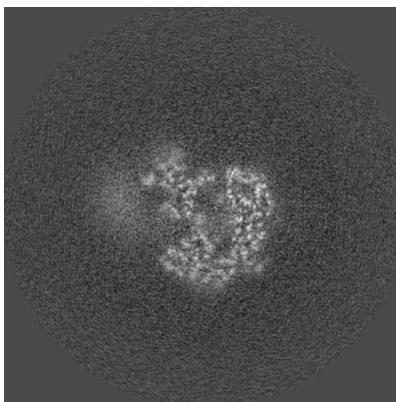


Z Index: 160

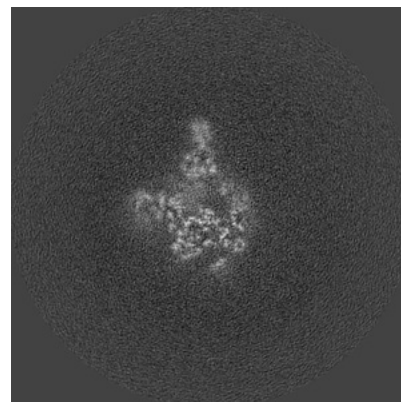
6.2.2 Raw map



X Index: 160



Y Index: 160

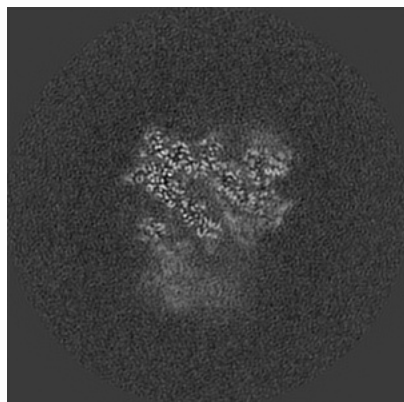


Z Index: 160

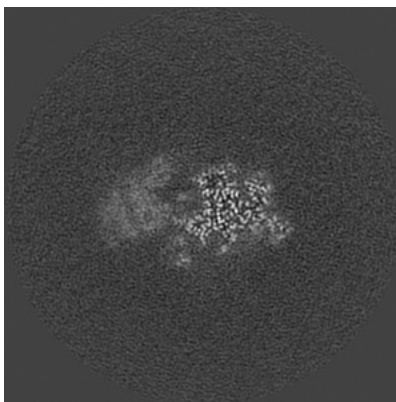
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

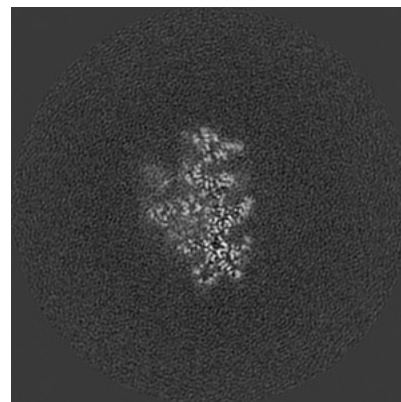
6.3.1 Primary map



X Index: 156

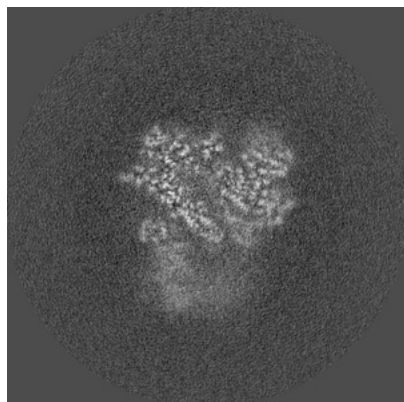


Y Index: 130

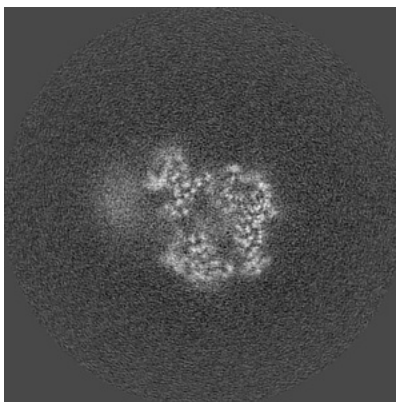


Z Index: 186

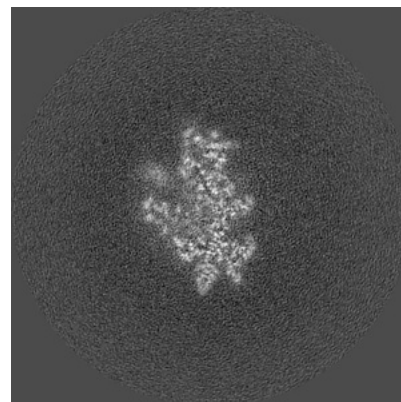
6.3.2 Raw map



X Index: 154



Y Index: 164

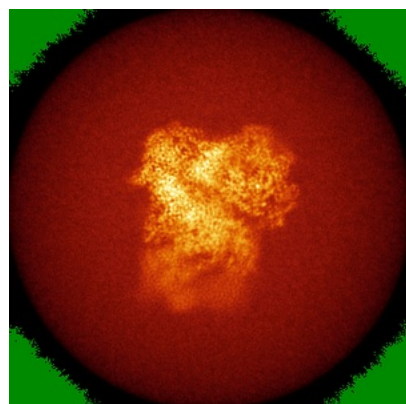


Z Index: 182

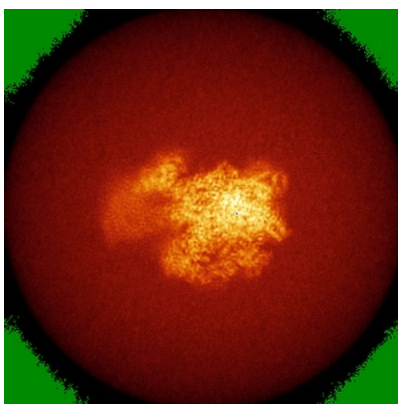
The images above show the largest variance slices of the map in three orthogonal directions.

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

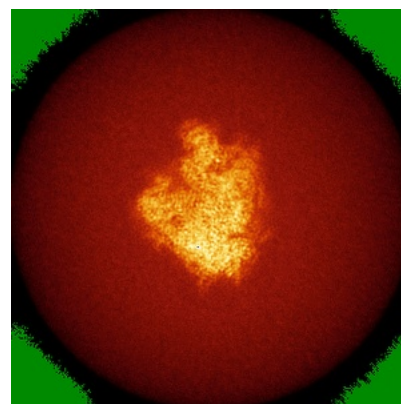
6.4.1 Primary map



X

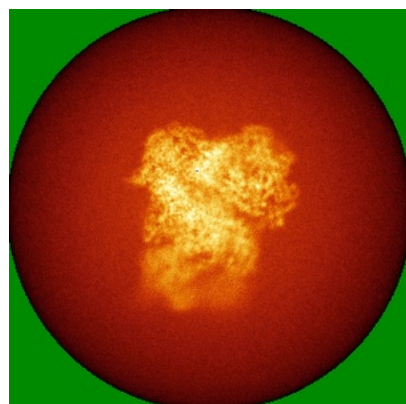


Y

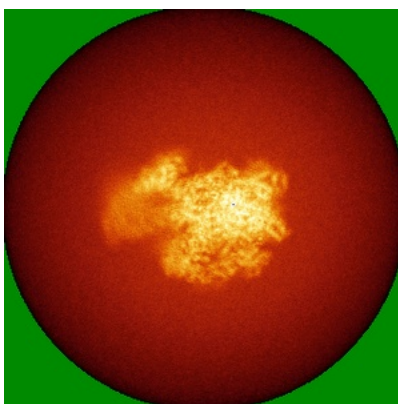


Z

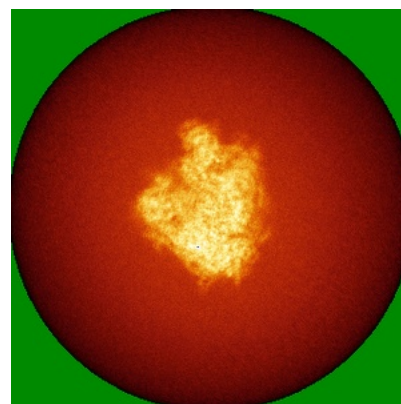
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.024. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

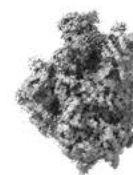
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

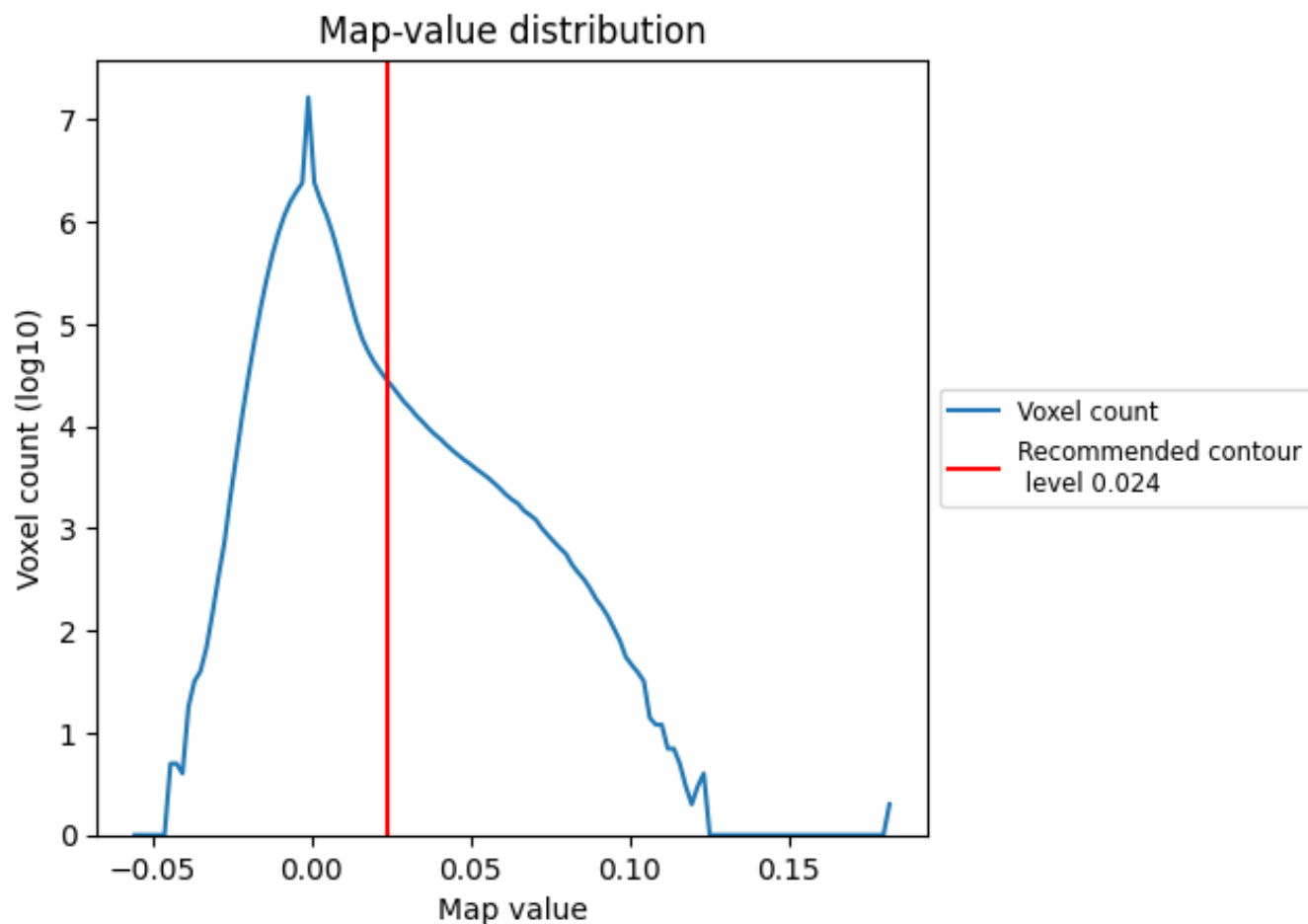
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

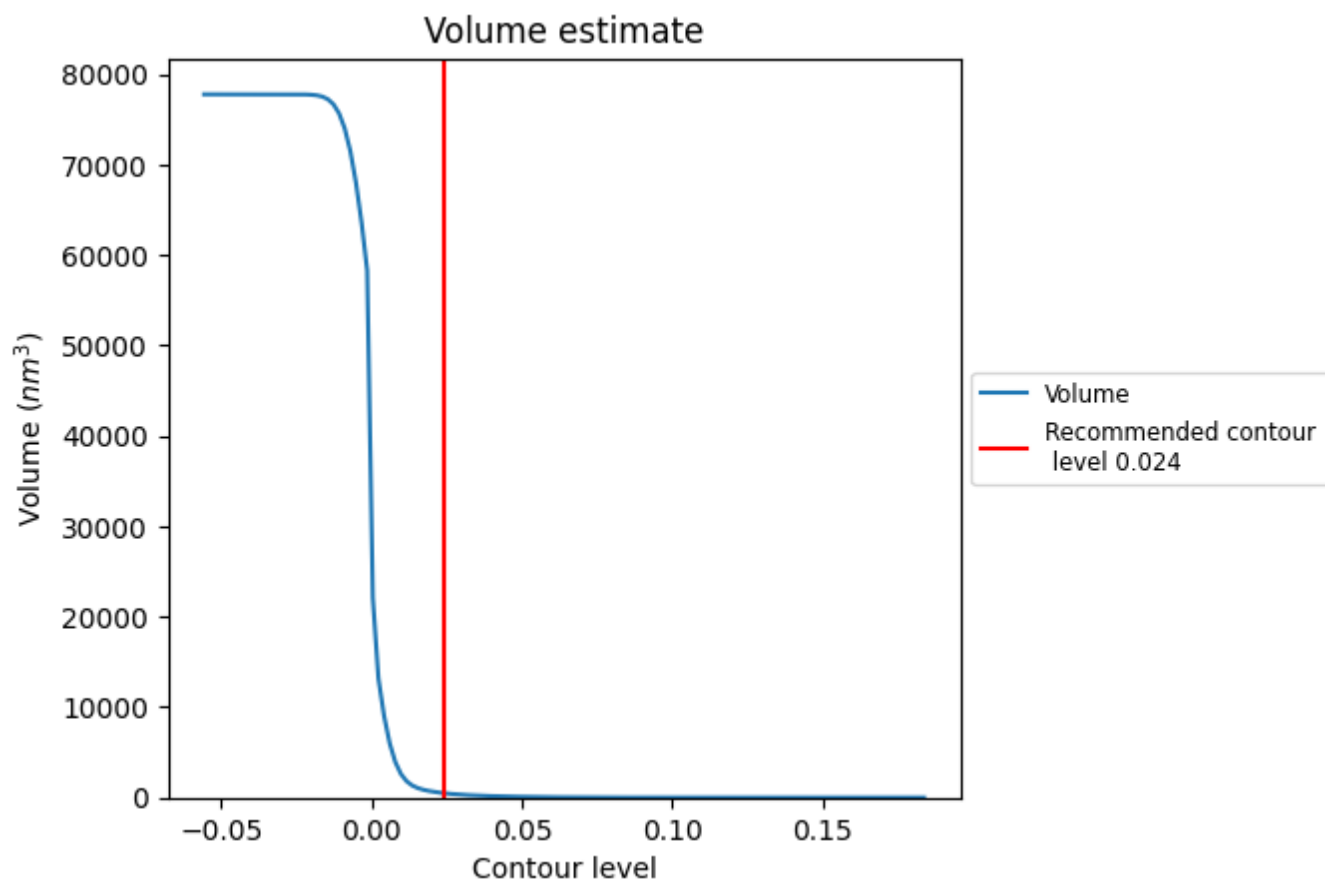
This section contains the results of statistical analysis of the map.

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.

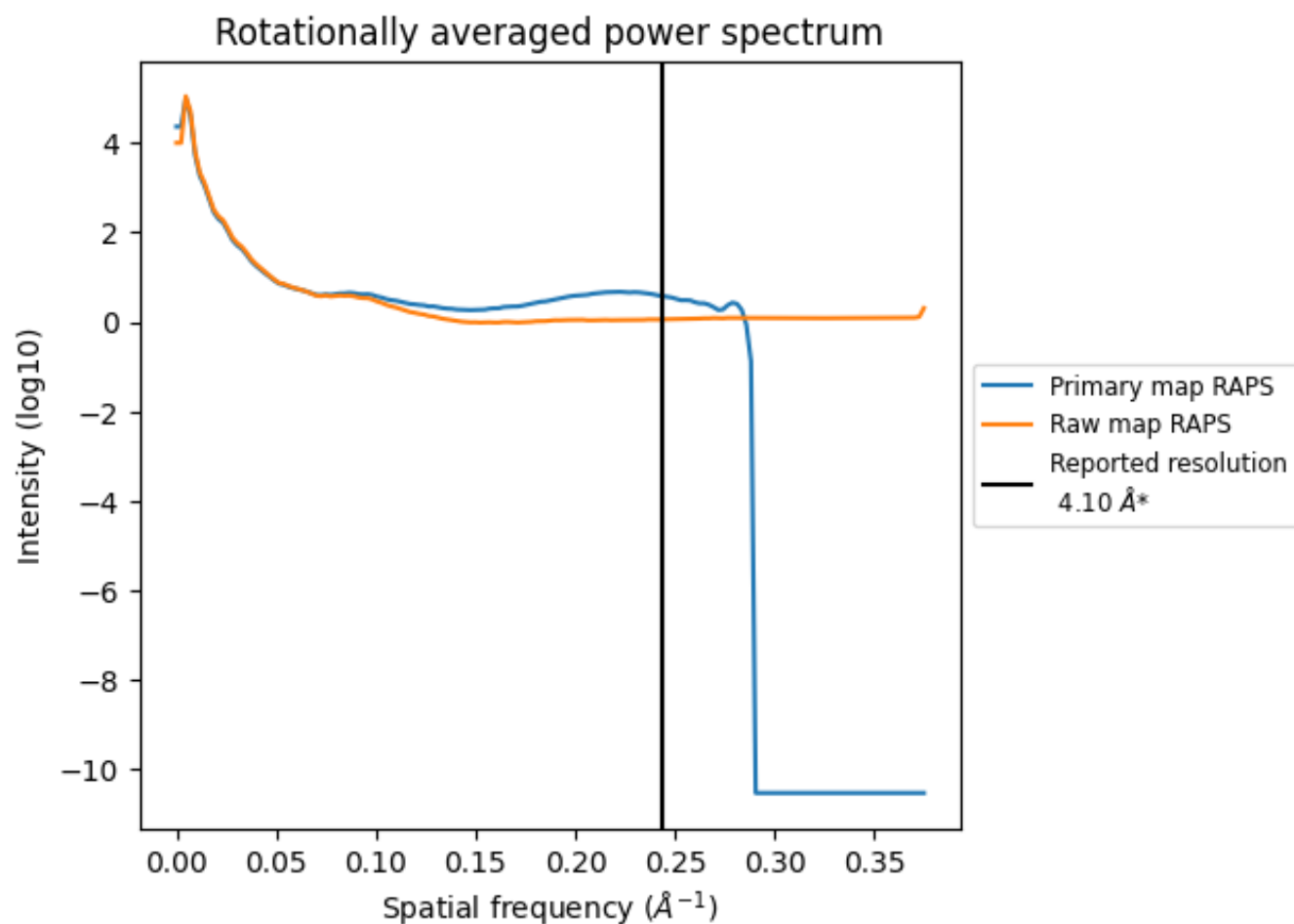
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 491 nm³; this corresponds to an approximate mass of 443 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 ⓘ

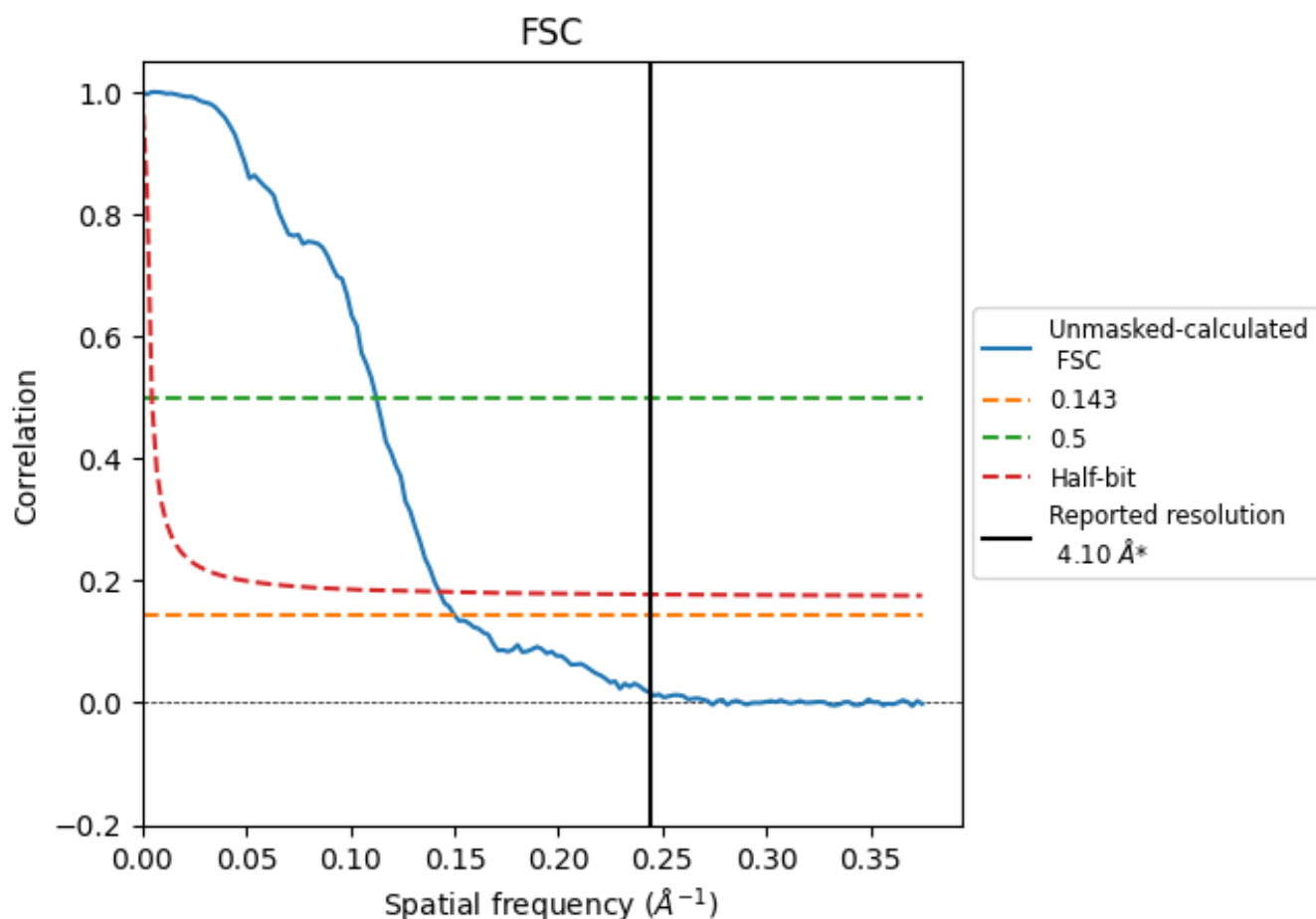


*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

8.2 Resolution estimates [i](#)

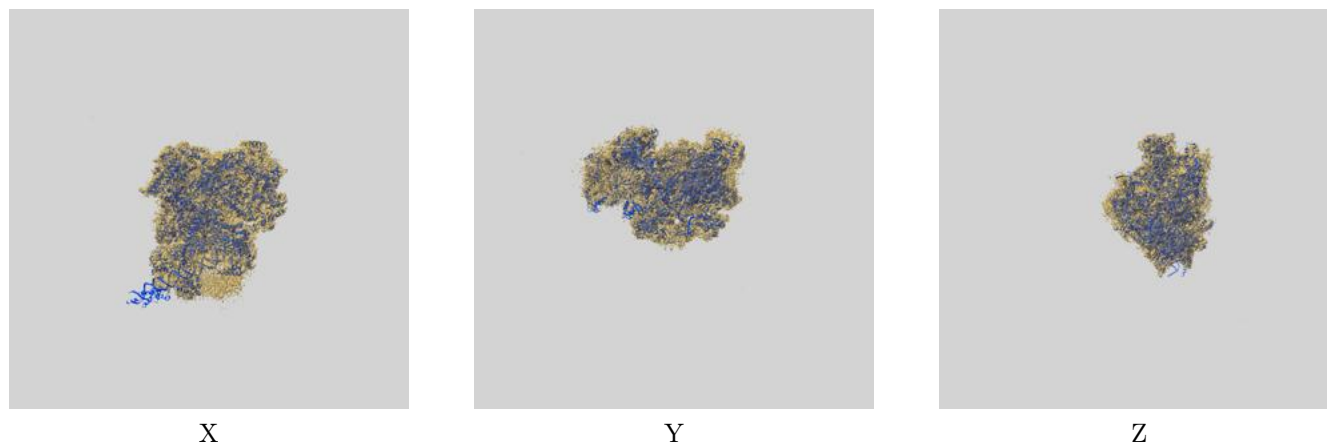
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.66	8.89	7.00

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.66 differs from the reported value 4.1 by more than 10 %

9 Map-model fit [i](#)

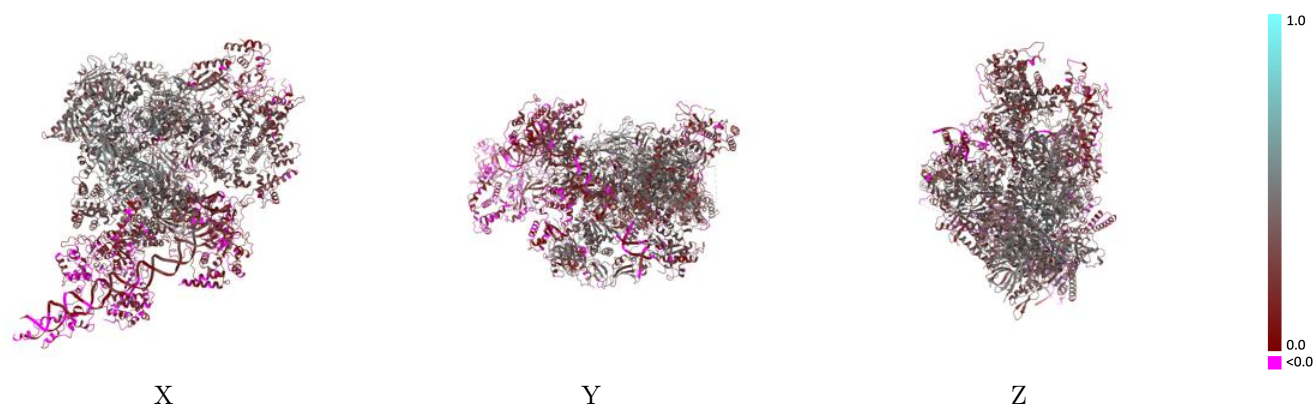
This section contains information regarding the fit between EMDB map EMD-35719 and PDB model 8IUE. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



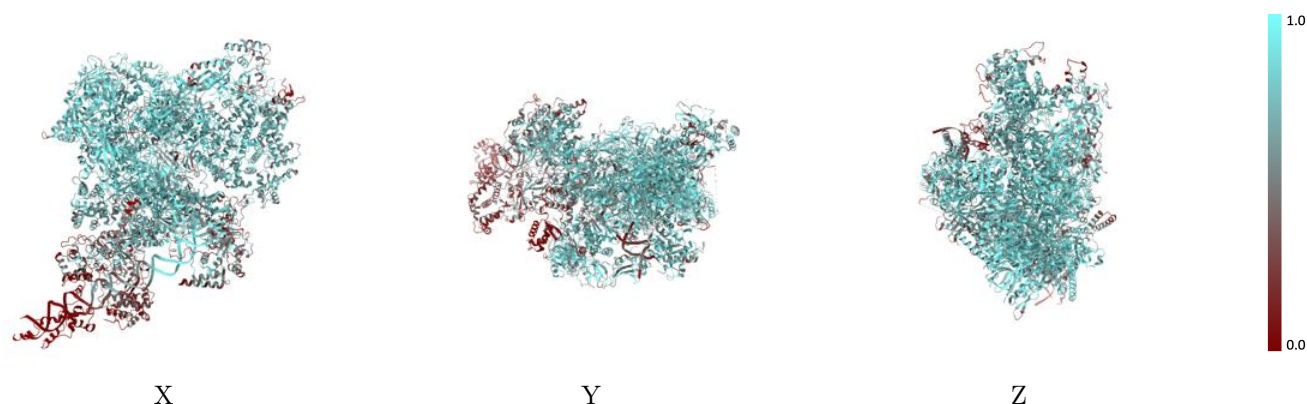
The images above show the 3D surface view of the map at the recommended contour level 0.024 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



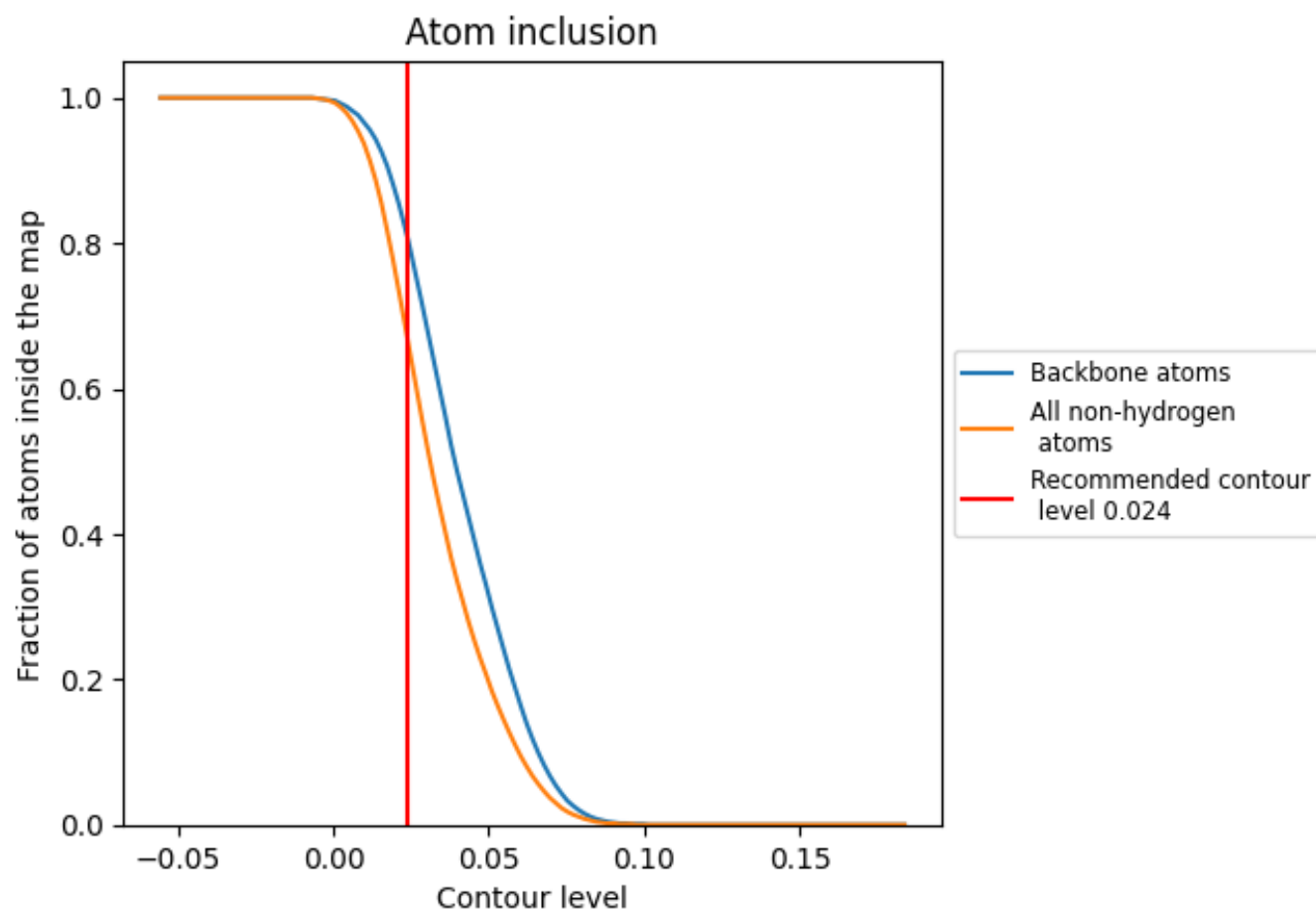
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.024).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 66% 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 (0.024) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6640	 0.2910
1	 0.2820	 0.0650
3	 0.3490	 0.0760
4	 0.2470	 0.0710
A	 0.8020	 0.3840
B	 0.8210	 0.4140
C	 0.8060	 0.4180
D	 0.6290	 0.2170
E	 0.7260	 0.3030
F	 0.8490	 0.4300
G	 0.7610	 0.2970
H	 0.7430	 0.3900
I	 0.5820	 0.2510
J	 0.8360	 0.4250
K	 0.8050	 0.4080
L	 0.8120	 0.3960
M	 0.6600	 0.2980
N	 0.6300	 0.2830
O	 0.6900	 0.3000
P	 0.4530	 0.1740
Q	 0.6580	 0.2710
U	 0.6290	 0.2020
V	 0.6670	 0.2600
W	 0.5160	 0.1200
X	 0.4920	 0.1070
Y	 0.5000	 0.1160

