



## wwPDB EM Validation Summary Report ⓘ

May 4, 2025 – 03:16 PM EDT

PDB ID : 8UOQ / pdb\_00008uoq  
EMDB ID : EMD-42437  
Title : Composite map of PIC\_delta\_TFIIF form2  
Authors : Yang, C.; Murakami, K.  
Deposited on : 2023-10-20  
Resolution : 3.80 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev118  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

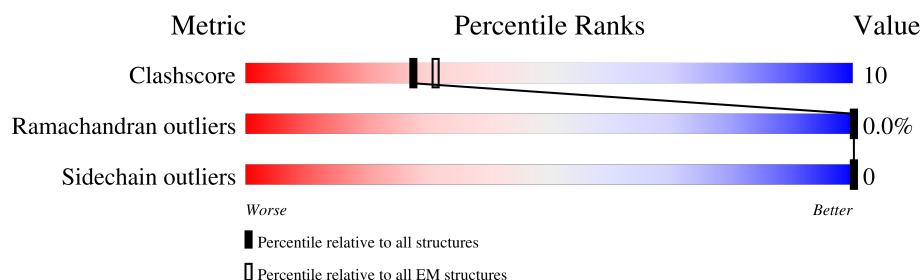
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 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.





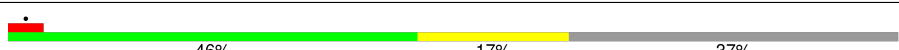


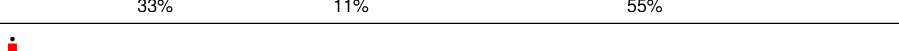
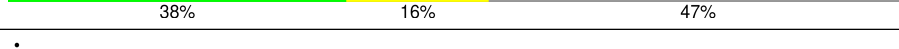



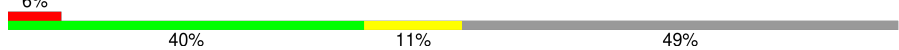

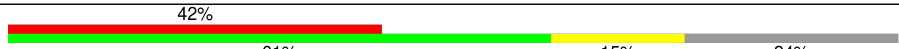


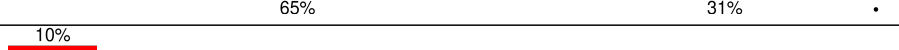






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	M	345	
2	A	1733	
3	B	1224	
4	C	318	
5	E	215	
6	F	155	
7	H	146	
8	I	122	

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Mol	Chain	Length	Quality of chain
9	J	70	
10	K	120	
11	L	70	
12	Q	735	
13	P	400	
14	S	309	
15	O	240	
16	U	286	
17	V	122	
18	W	482	
19	X	328	
20	D	221	
21	G	171	
22	0	778	
23	1	642	
24	4	338	
25	6	461	
26	7	843	
27	2	513	
28	5	72	
29	N	64	
30	T	64	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	SF4	0	801	-	-	X	-

## 2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 70481 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 Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	M	279	Total	C	N	O	S	0	0
			2175	1382	373	403	17		

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	1425	Total	C	N	O	S	0	0
			11167	7036	1948	2121	62		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	1166	Total	C	N	O	S	0	0
			9227	5823	1619	1729	56		

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	265	Total	C	N	O	S	0	0
			2086	1312	347	414	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	214	Total	C	N	O	S	0	0
			1752	1111	309	321	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	87	Total	C	N	O	S	0	0
			705	451	119	132	3		

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	135	Total	C	N	O	S	0	0
			1080	679	182	214	5		

- Molecule 8 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	114	Total	C	N	O	S	0	0
			927	571	168	178	10		

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	66	Total	C	N	O	S	0	0
			540	345	94	95	6		

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	115	Total	C	N	O	S	0	0
			924	593	157	172	2		

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	44	Total	C	N	O	S	0	0
			352	217	70	61	4		

- Molecule 12 is a protein called Transcription initiation factor IIF subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Q	214	Total	C	N	O	S	0	0
			1619	1017	297	299	6		

- Molecule 13 is a protein called Transcription initiation factor IIF subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	P	179	Total	C	N	O	S	0	0
			1484	941	258	279	6		

- Molecule 14 is a protein called Transcription elongation factor S-II.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	S	164	Total	C	N	O	S	0	0
			1294	809	230	247	8		

- Molecule 15 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	181	Total	C	N	O	S	0	0
			1422	925	243	248	6		

- Molecule 16 is a protein called Transcription initiation factor IIA large subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	U	107	Total	C	N	O	S	0	0
			885	559	147	176	3		

- Molecule 17 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	V	104	Total	C	N	O	S	0	0
			815	511	136	164	4		

- Molecule 18 is a protein called Transcription initiation factor IIE subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	247	Total	C	N	O	S	0	0
			2010	1275	347	381	7		

- Molecule 19 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	X	160	Total	C	N	O	S	0	0
			1288	826	212	245	5		

- Molecule 20 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	D	168	Total	C	N	O	S	0	0
			1331	822	237	270	2		

- Molecule 21 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	G	171	Total	C	N	O	S	0	0
			1335	858	221	248	8		

- Molecule 22 is a protein called General transcription and DNA repair factor IIH helicase subunit XPD/RAD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	0	752	Total	C	N	O	S	0	0
			6091	3882	1029	1142	38		

- Molecule 23 is a protein called General transcription and DNA repair factor IIH subunit TFB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	1	417	Total	C	N	O	S	0	0
			3382	2139	587	640	16		

- Molecule 24 is a protein called General transcription and DNA repair factor IIH subunit TFB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	4	292	Total	C	N	O	S	0	0
			2267	1449	376	428	14		

- Molecule 25 is a protein called General transcription and DNA repair factor IIH subunit SSL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	6	355	Total	C	N	O	S	0	0
			2786	1765	481	512	28		

- Molecule 26 is a protein called General transcription and DNA repair factor IIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	7	608	Total	C	N	O	S	0	0
			4889	3110	847	906	26		

- Molecule 27 is a protein called General transcription and DNA repair factor IIH subunit TFB2.



Mol	Chain	Residues	Atoms					AltConf	Trace
27	2	445	Total	C	N	O	S	0	0
			3546	2291	585	654	16		

- Molecule 28 is a protein called General transcription and DNA repair factor IIH subunit TFB5.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	5	66	Total	C	N	O	S	0	0
			498	314	89	93	2		

- Molecule 29 is a DNA chain called non-template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	N	63	Total	C	N	O	P	0	0
			1288	621	225	380	62		

- Molecule 30 is a DNA chain called template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	T	63	Total	C	N	O	P	0	0
			1291	619	236	373	63		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	-10	DC	DT	conflict	GB 2567904391

- Molecule 31 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
31	M	1	Total	Zn	0
			1	1	
31	A	2	Total	Zn	0
			2	2	
31	B	1	Total	Zn	0
			1	1	
31	C	1	Total	Zn	0
			1	1	
31	I	2	Total	Zn	0
			2	2	
31	J	1	Total	Zn	0
			1	1	

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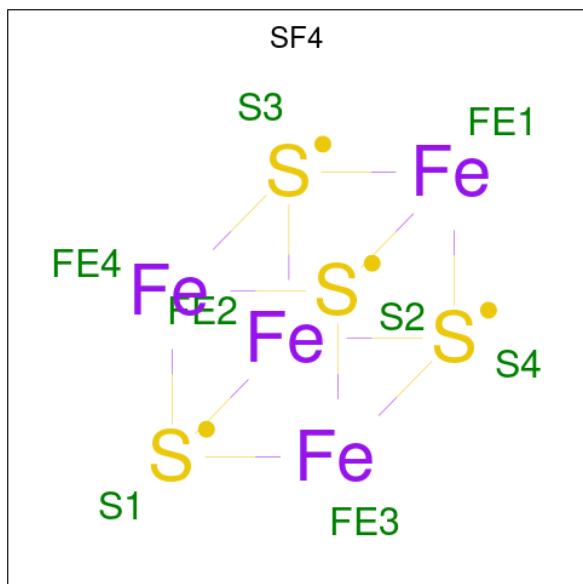
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Mol	Chain	Residues	Atoms		AltConf
31	L	1	Total	Zn	0
			1	1	
31	S	1	Total	Zn	0
			1	1	
31	4	1	Total	Zn	0
			1	1	
31	6	4	Total	Zn	0
			4	4	

- Molecule 32 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
32	A	1	Total	Mg	0
			1	1	
32	7	1	Total	Mg	0
			1	1	

- Molecule 33 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).

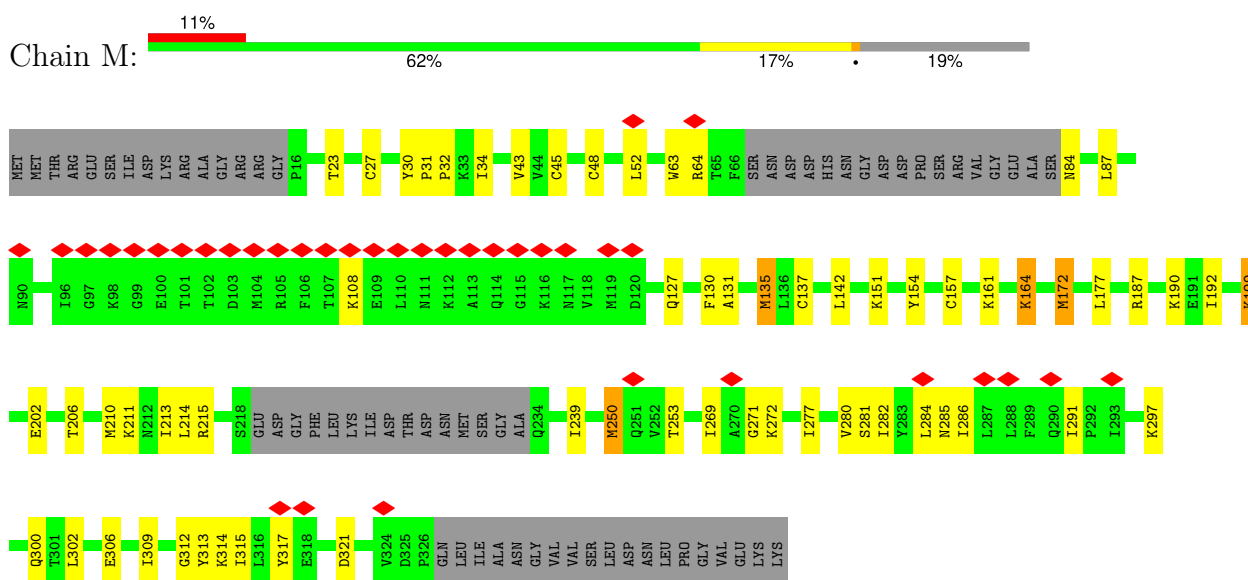


Mol	Chain	Residues	Atoms			AltConf
33	0	1	Total	Fe	S	0
			8	4	4	

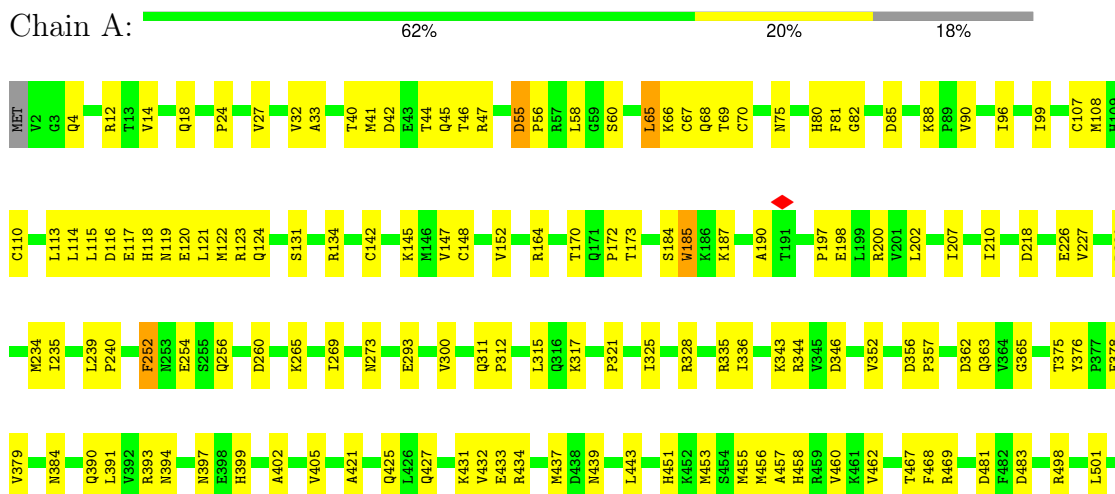
### 3 Residue-property plots

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: Transcription initiation factor IIB



#### • Molecule 2: DNA-directed RNA polymerase II subunit RPB1



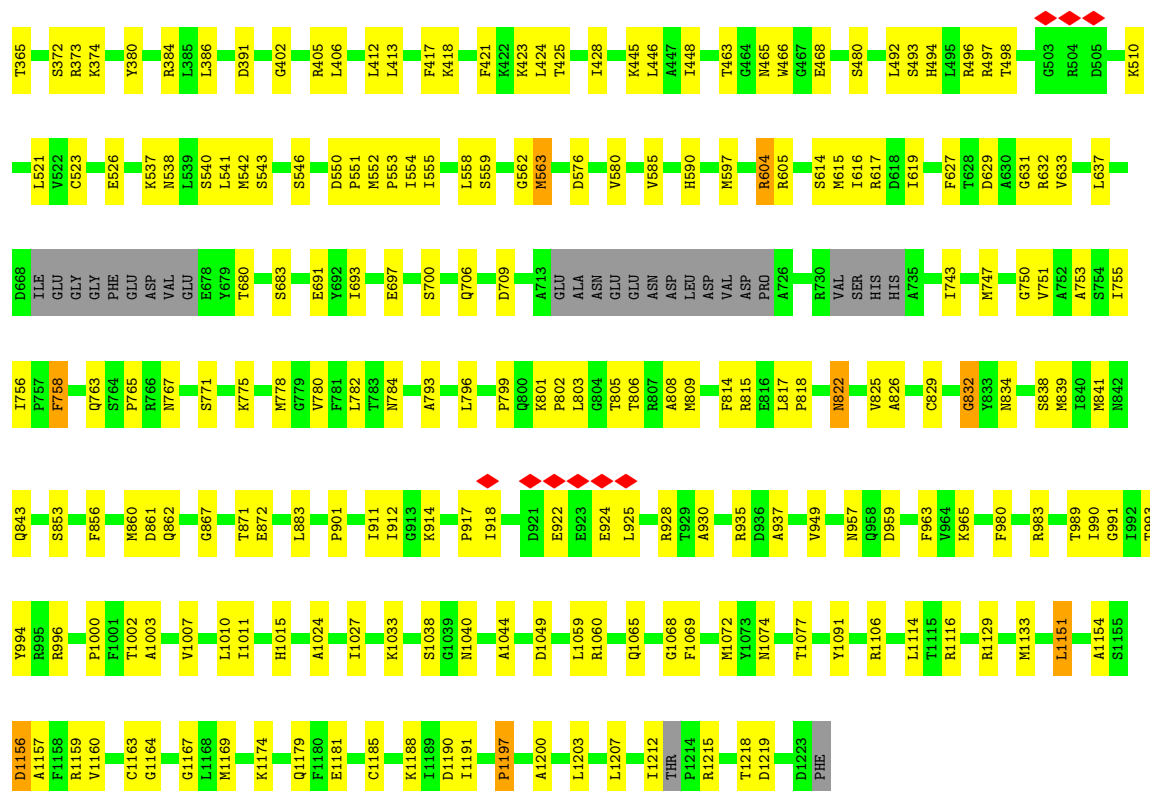
C506	T675	E846	I1007	S1180	P1245	T1376	VAL	PRO	PRO	ALA	LYS
Q510	M676	M849	Q1008	T1161	LYS	T1377	ASN	THR	THR	TYR	GLN
I511	L691	M856	N1009	V1162	SER	T1384	ALA	GLY	THR	PRO	ASP
V512	L698	N851	D1013	I1170	ASP	T1385	LEU	PRO	THR	THR	GLN
P519	Q698	H852	D1023	I1170	ALA	G1388	ASP	SER	TYR	PRO	LYS
Q525	R711	T855	R1024	H1173	GLU	T1394	VAL	PRO	PRO	THR	ASN
L528	N742	T856	S1024	F1174	THR	T1394	LYS	PRO	THR	TYR	ASN
R532	N743	R857	R1025	S1175	GLU	G1395	ASP	THR	THR	THR	GLN
R537	K744	N858	W1044	LEU	E1256	G1397	MET	PRO	PRO	PRO	ASN
R537	Q745	G861	V1045	LEU	E1256	M1398	PHE	THR	THR	THR	SER
D544	M746	T864	N1048	GLU	M1259	R1399	SER	SER	PRO	PRO	ARG
L547	V747	Q865	M1063	GLU	R1274	C1400	PRO	PRO	PRO	THR	ASN
N548	A749	Q865	M1063	ALA	R1274	G1401	LEU	THR	THR	TYR	GLY
W552	G750	D871	Q1070	GLN	I1279	E1402	VAL	THR	THR	THR	LYS
T562	K752	N873	Q1070	SER	V1282	E1403	ASP	PRO	PRO	THR	ASN
I566	G753	D874	L1081	F1185	V1283	D1419	GLY	THR	THR	THR	SER
K567	S754	Q881	ASN	D1186	V1283	L1430	ASN	PRO	PRO	PRO	PRO
W572	S754	Q881	THR	Q1187	M1284	L1430	ASP	PRO	THR	THR	TYR
R590	N757	D884	HIS	Q1188	M1285	G1431	ALA	THR	THR	THR	TYR
D592	M761	T885	ALA	R1194	S1293	Q1432	MET	PRO	PRO	PRO	SER
S599	C764	I886	GLY	L1195	E1297	V1443	ALA	THR	THR	THR	THR
N603	V765	E894	VAL	E1196	K1300	D1446	GLY	PRO	PRO	PRO	PRO
G604	G769	R898	ALA	D1198	T1308	S1449	THR	THR	THR	THR	THR
M605	K773	N903	LYS	R1199	T1309	K1452	ALA	PRO	PRO	PRO	PRO
K619	R782	T907	K1093	A1201	G1310	M1454	TYR	PRO	PRO	PRO	PRO
K620	T783	S907	V1094	K1205	M1317	PRO	GLY	PRO	PRO	PRO	PRO
T621	L784	T907	R1100	D1206	T1318	GLY	ALA	THR	THR	THR	THR
H631	N802	D939	V1107	T1207	T1318	GLY	THR	THR	THR	THR	THR
R635	S803	R944	S1115	G1210	T1319	GLY	ALA	THR	THR	THR	THR
E636	L805	D949	L1116	Q1211	V1319	GLY	ALA	THR	THR	THR	THR
Y804	R806	D949	E1121	R1215	M1330	GLY	ALA	THR	THR	THR	THR
F646	G807	T963	P1122	K1216	S1331	GLY	ALA	THR	THR	THR	THR
Q650	T834	R962	G1123	K1217	F1332	ASP	ALA	THR	THR	THR	THR
K651	I837	N953	K1132	Q1218	T1335	ASP	GLY	THR	THR	THR	THR
D668	R840	N954	R1135	K1221	M1336	GLY	GLY	THR	THR	THR	THR
T669	L841	P955	I1138	I1227	L1339	GLY	ALA	PRO	PRO	PRO	PRO
I670	R840	L964	T1142	V1228	E1351	VAL	PRO	THR	THR	THR	THR
A671	L841	R964	T1142	S1229	S1361	THR	THR	THR	THR	THR	THR
D672	K843	K977	S1145	D1231	R1366	TYR	THR	THR	THR	THR	THR
		G1002	V1146	D1233	L1371	ASN	PHE	THR	THR	THR	THR
		K1003	A1149	R1239	V1372	GLY	GLY	PRO	PRO	PRO	PRO
		R1004	V1146	C1240	D1373	GLY	VAL	THR	THR	THR	THR
		E1005	P1158	R1241		LEU	SER	THR	THR	THR	THR
		I1006	R1159				SER	THR	THR	THR	THR

• Molecule 3: DNA-directed RNA polymerase II subunit RPB2

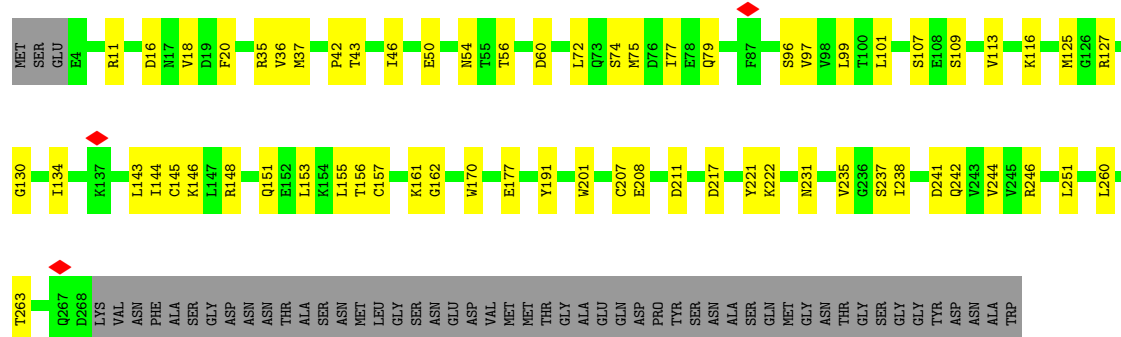
Chain B:



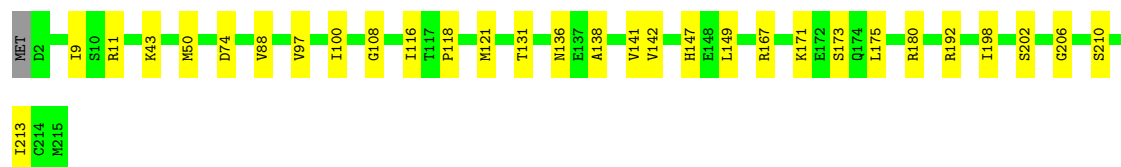
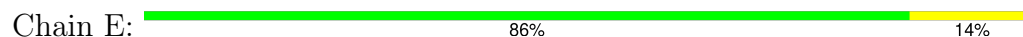
GLY	LYS	MET	D90	D159	H300	GLY	GLY	GLY	GLY	GLY	GLY
S264	ARG	SER	E28	K164	I301	ASP	ASP	ASP	ASP	ASP	ASP
S265	Y137	LEU	L43	M173	C302	ALA	ALA	ALA	ALA	ALA	ALA
A266	A139	ALA	V44	K177	D303	GLY	GLY	GLY	GLY	GLY	GLY
R267	E146	SER	S45	N178	Y304	GLY	GLY	GLY	GLY	GLY	GLY
A271	L147	GLY	Q46	C179	D306	GLY	GLY	GLY	GLY	GLY	GLY
I280	E150	THR	N52	Y180	I297	GLY	GLY	GLY	GLY	GLY	GLY
I284	LEU	THR	I62	E194	H300	GLY	GLY	GLY	GLY	GLY	GLY
R287	ILE	THR	T68	C195	I301	GLY	GLY	GLY	GLY	GLY	GLY
D294	ALA	PRO	L69	D198	C302	GLY	GLY	GLY	GLY	GLY	GLY
G295	GLY	THR	Q73	Y202	D303	GLY	GLY	GLY	GLY	GLY	GLY
E296	GLY	THR	L74	I205	Y304	GLY	GLY	GLY	GLY	GLY	GLY
I297	ASP	THR	A75	S208	D306	GLY	GLY	GLY	GLY	GLY	GLY
		THR	Q76	I213	M310	GLY	GLY	GLY	GLY	GLY	GLY
		THR	T79	G335	M313	GLY	GLY	GLY	GLY	GLY	GLY
		THR	E80	Q215	L314	GLY	GLY	GLY	GLY	GLY	GLY
		THR	S81	E216	V323	GLY	GLY	GLY	GLY	GLY	GLY
		THR	D82	S232	I324	GLY	GLY	GLY	GLY	GLY	GLY
		THR	N83	P233	G326	GLY	GLY	GLY	GLY	GLY	GLY
		THR	S85	I234	D326	GLY	GLY	GLY	GLY	GLY	GLY
		THR	I90	L244	F333	GLY	GLY	GLY	GLY	GLY	GLY
		THR	V102	E245	I334	GLY	GLY	GLY	GLY	GLY	GLY
		THR	L112	S248	R336	GLY	GLY	GLY	GLY	GLY	GLY
		THR	R120	K257	T339	GLY	GLY	GLY	GLY	GLY	GLY
		THR	F129	L258	A340	GLY	GLY	GLY	GLY	GLY	GLY
		THR	K133	Y259	L341	GLY	GLY	GLY	GLY	GLY	GLY
		THR		G260	K344	GLY	GLY	GLY	GLY	GLY	GLY
		THR		H363	K347	GLY	GLY	GLY	GLY	GLY	GLY
		THR		I364	R348	GLY	GLY	GLY	GLY	GLY	GLY



• Molecule 4: DNA-directed RNA polymerase II subunit RPB3

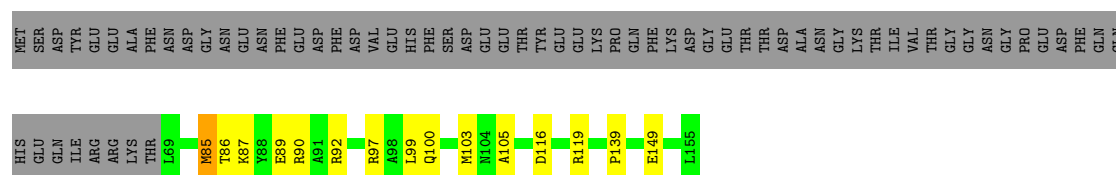


• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



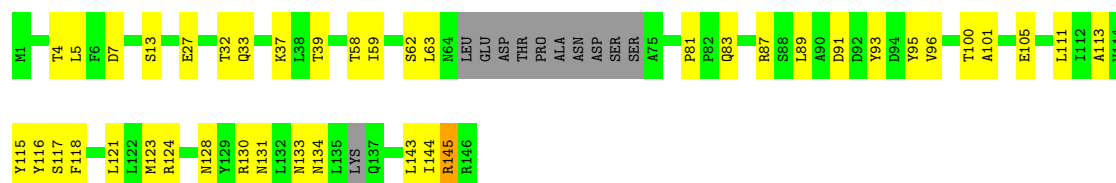
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 



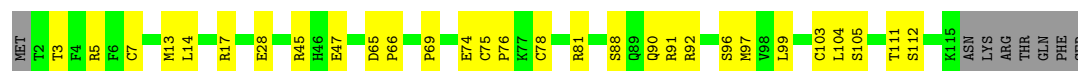
- Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 



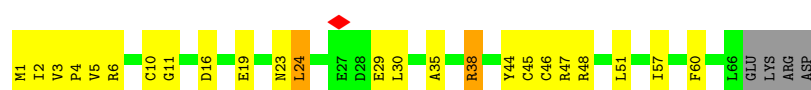
- Molecule 8: DNA-directed RNA polymerase II subunit RPB9

Chain I: 




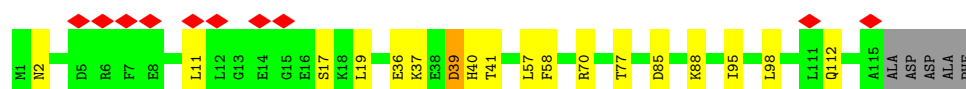
- Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 



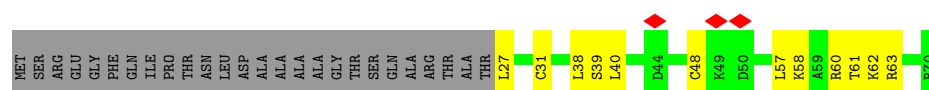
- Molecule 10: DNA-directed RNA polymerase II subunit RPB11

Chain K: 

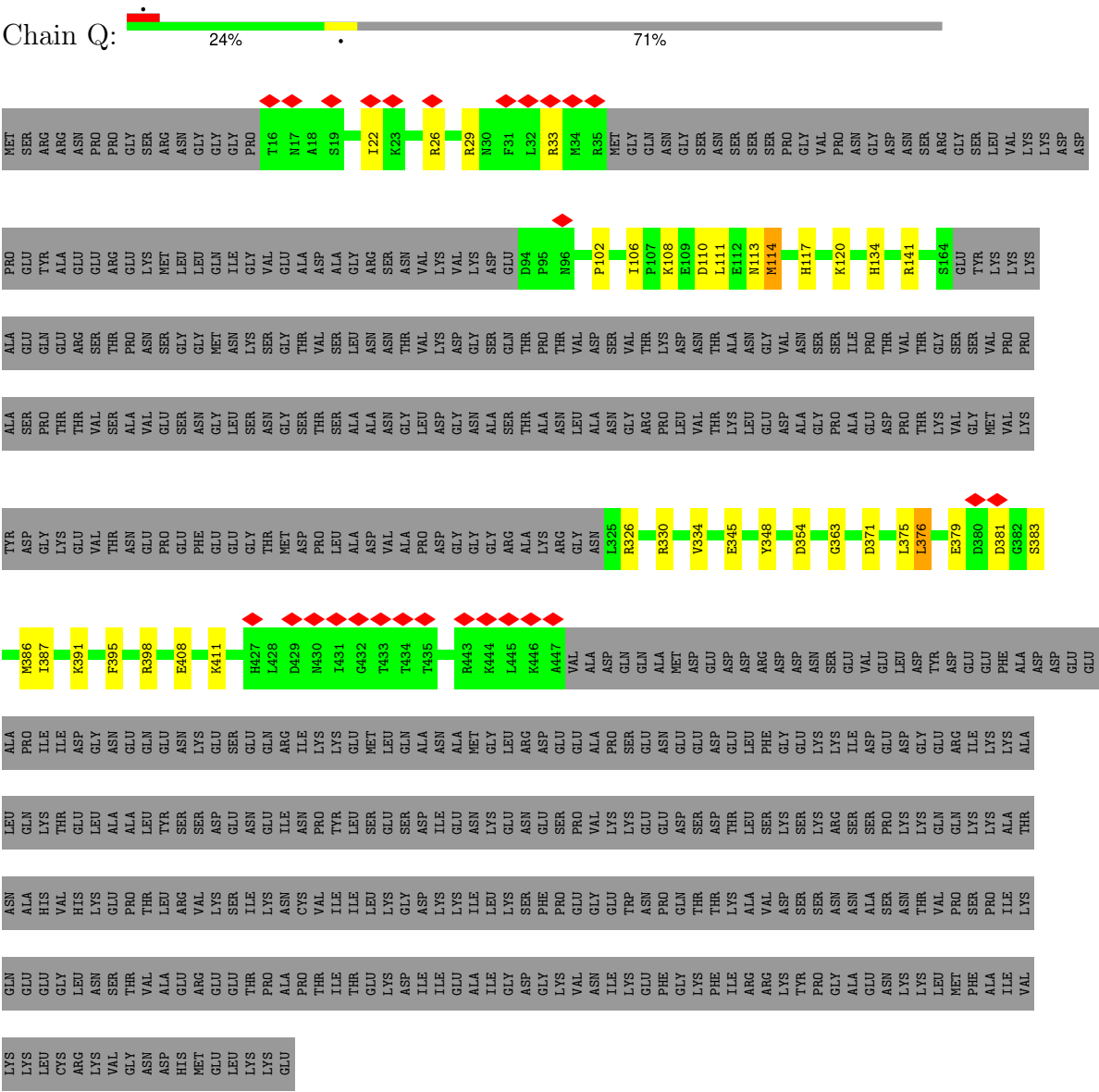


- Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC4

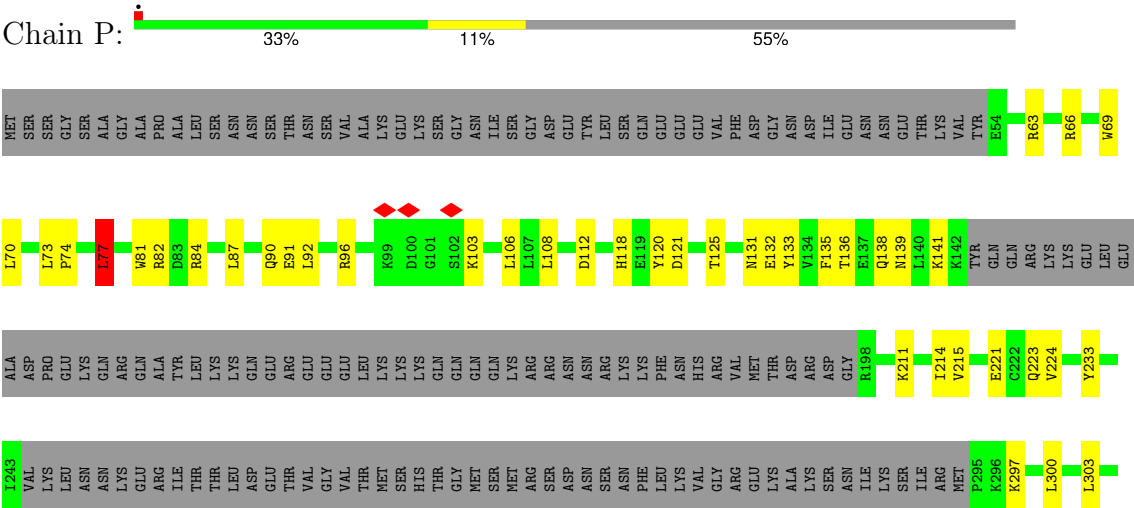
Chain L: 



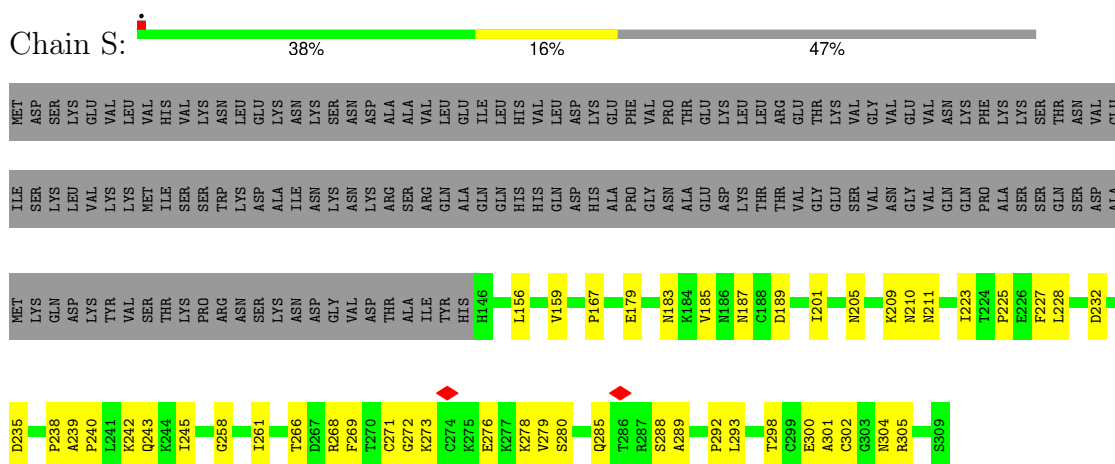
- Molecule 12: Transcription initiation factor IIF subunit alpha



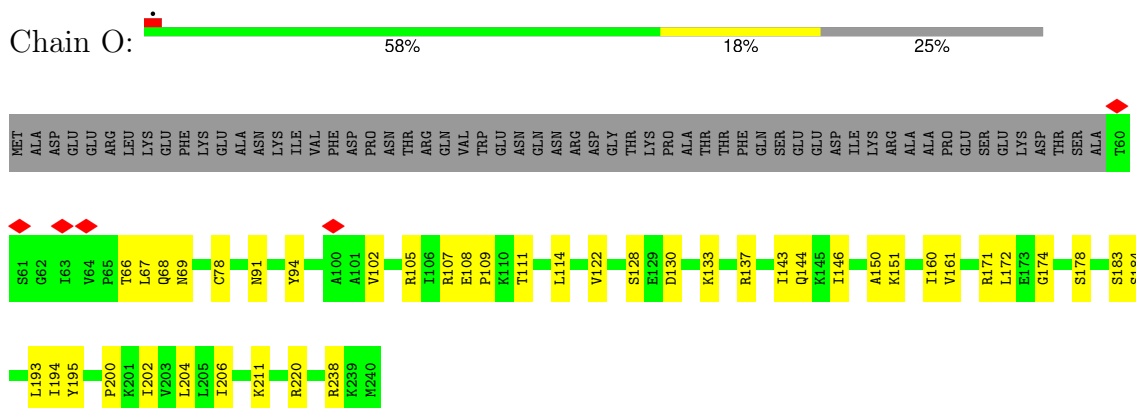
● Molecule 13: Transcription initiation factor IIF subunit beta



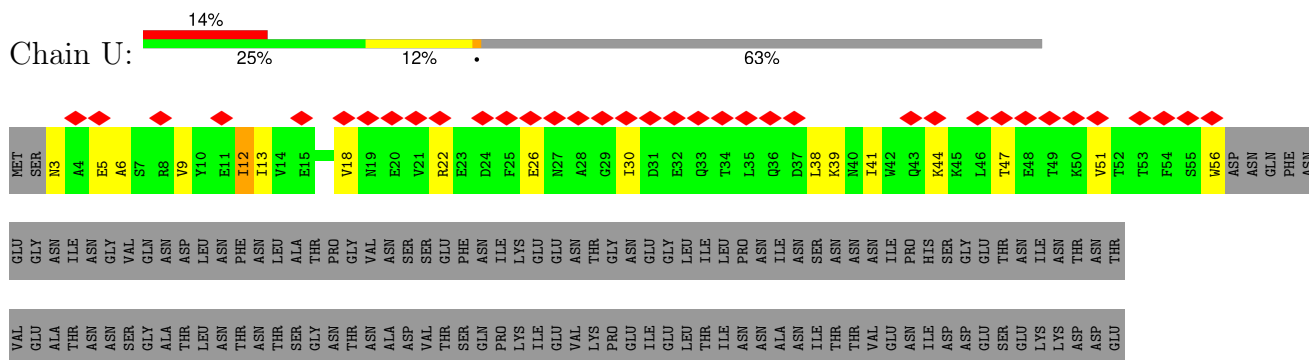
- Molecule 14: Transcription elongation factor S-II



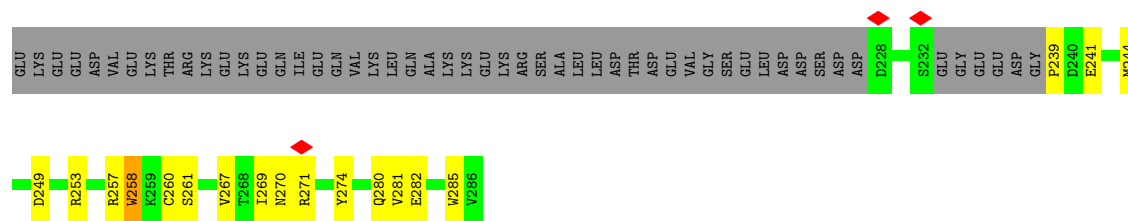
- Molecule 15: TATA-box-binding protein



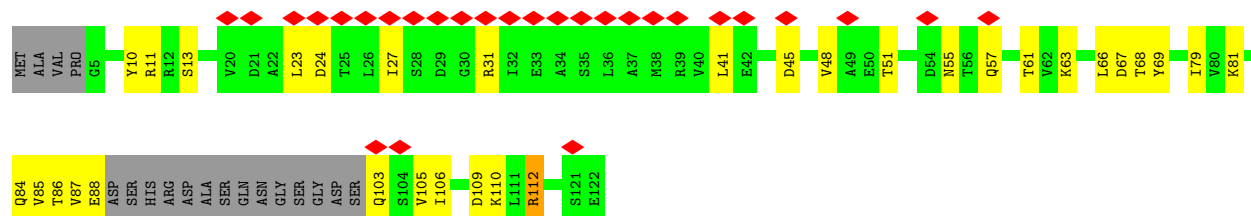
- Molecule 16: Transcription initiation factor IIA large subunit



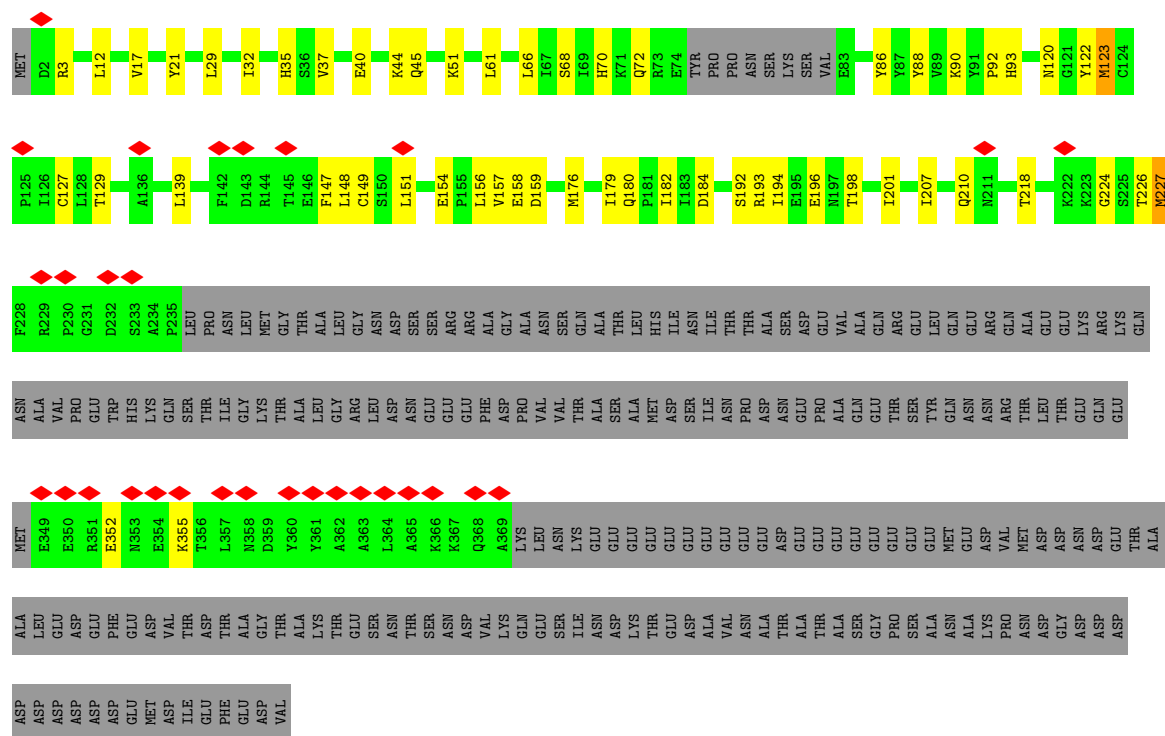
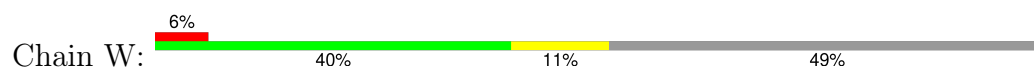




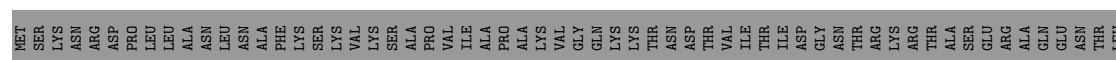
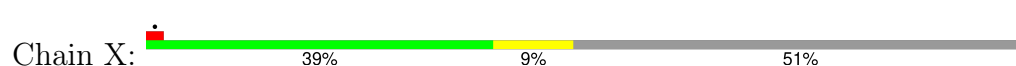
• Molecule 17: Transcription initiation factor IIA subunit 2

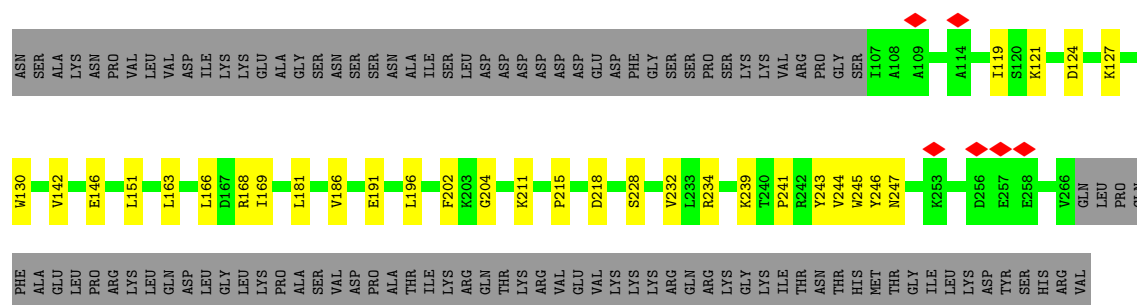


• Molecule 18: Transcription initiation factor IIE subunit alpha

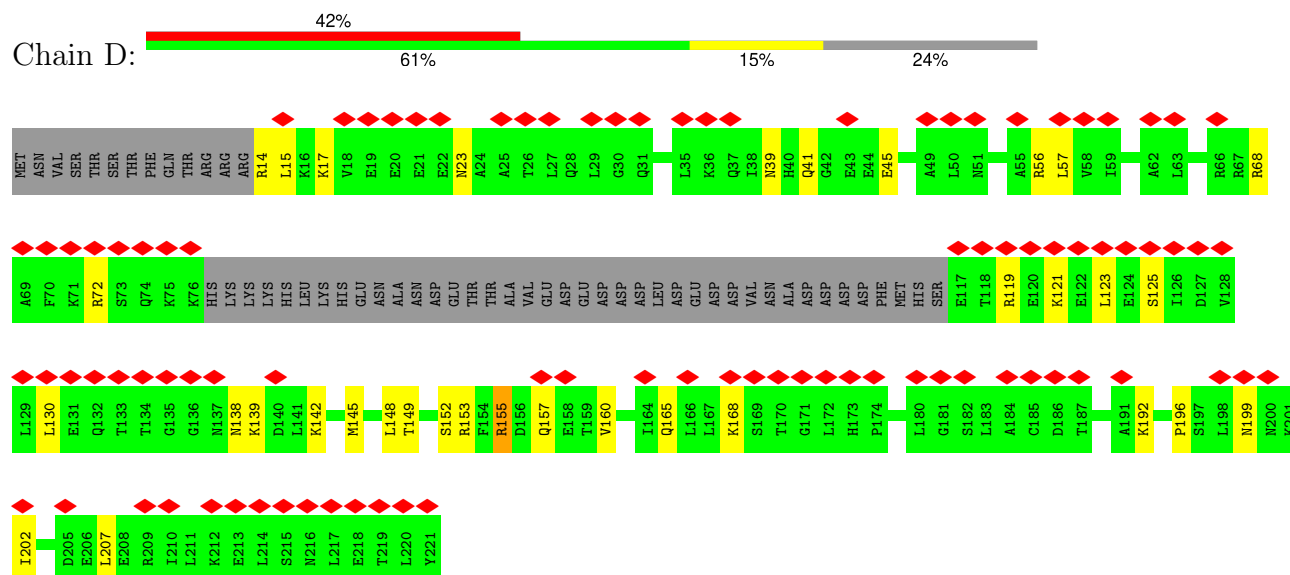


• Molecule 19: Transcription initiation factor IIE subunit beta

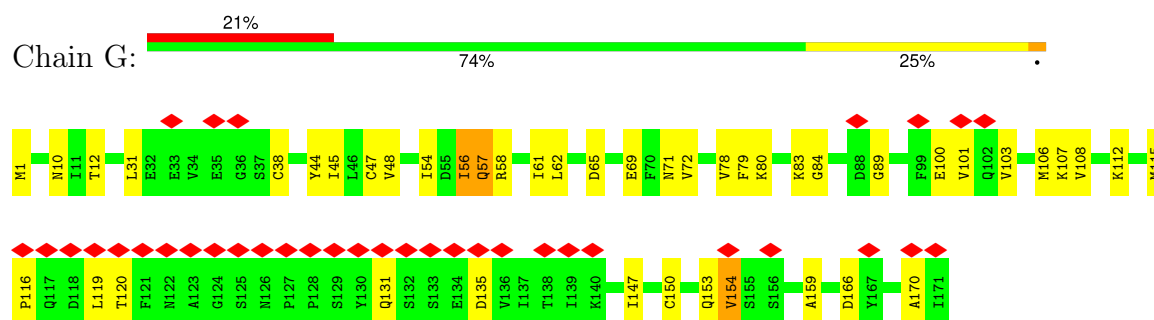




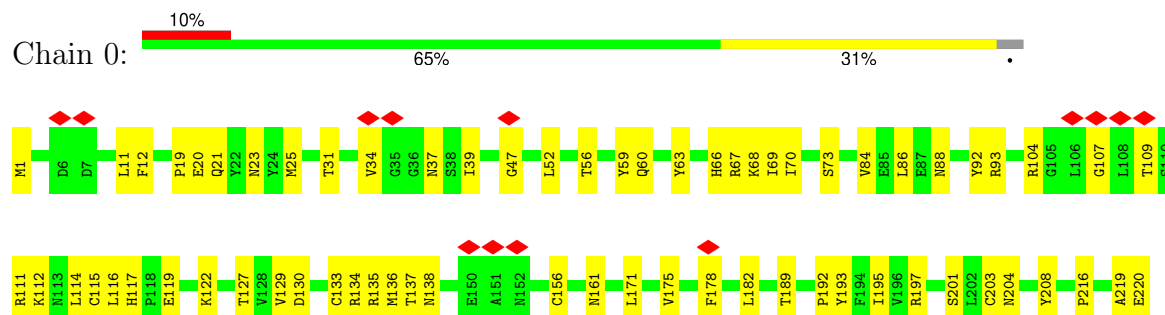
- Molecule 20: DNA-directed RNA polymerase II subunit RPB4

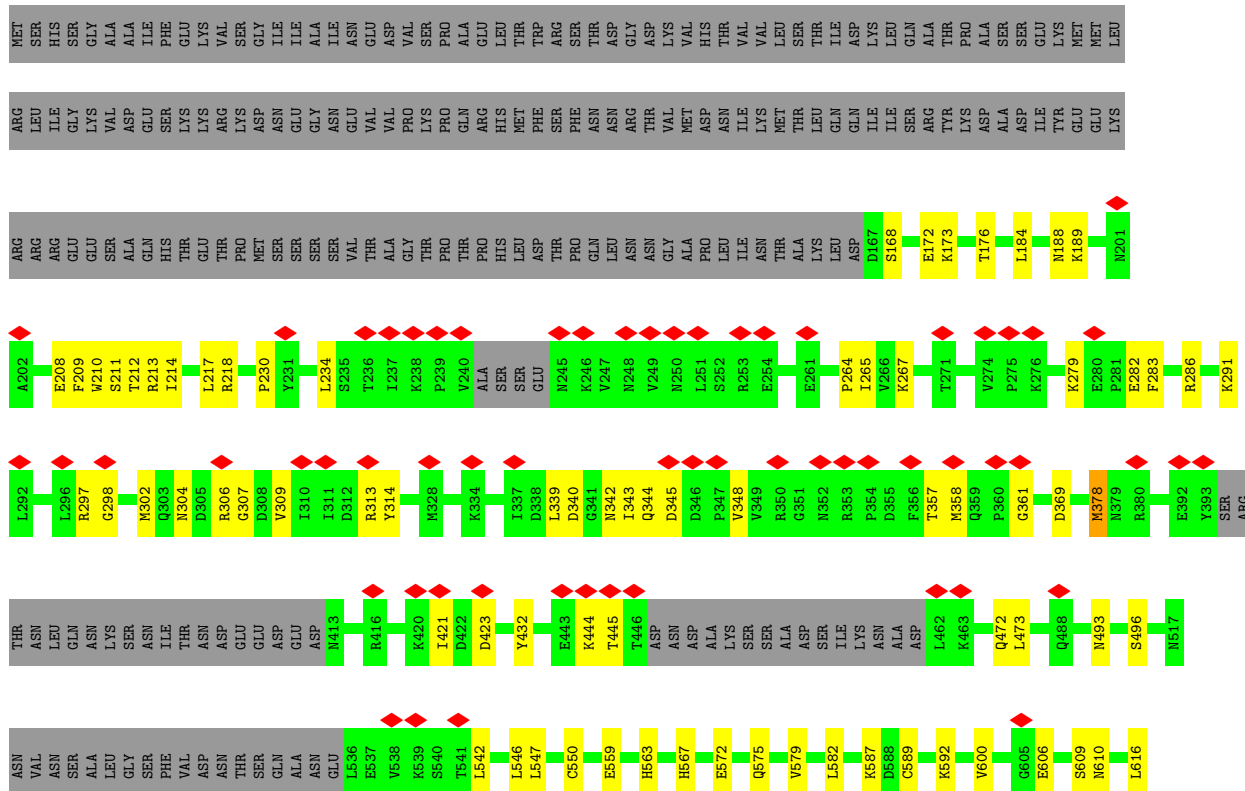


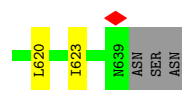
- Molecule 21: DNA-directed RNA polymerase II subunit RPB7



- Molecule 22: General transcription and DNA repair factor IIH helicase subunit XPD/RAD3

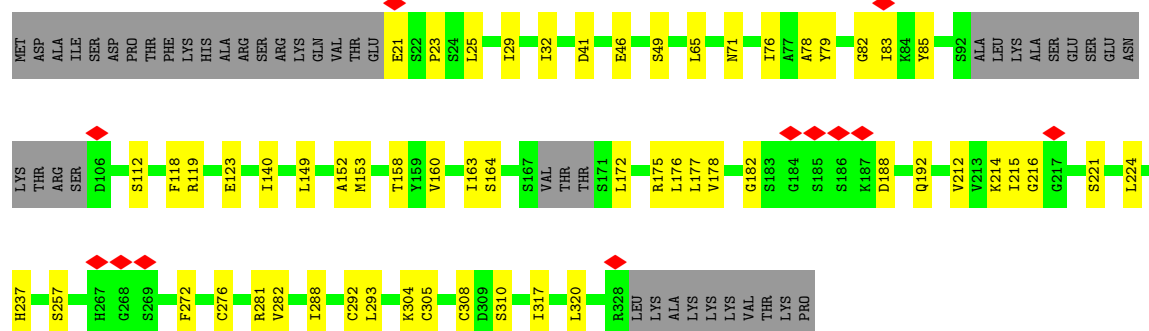






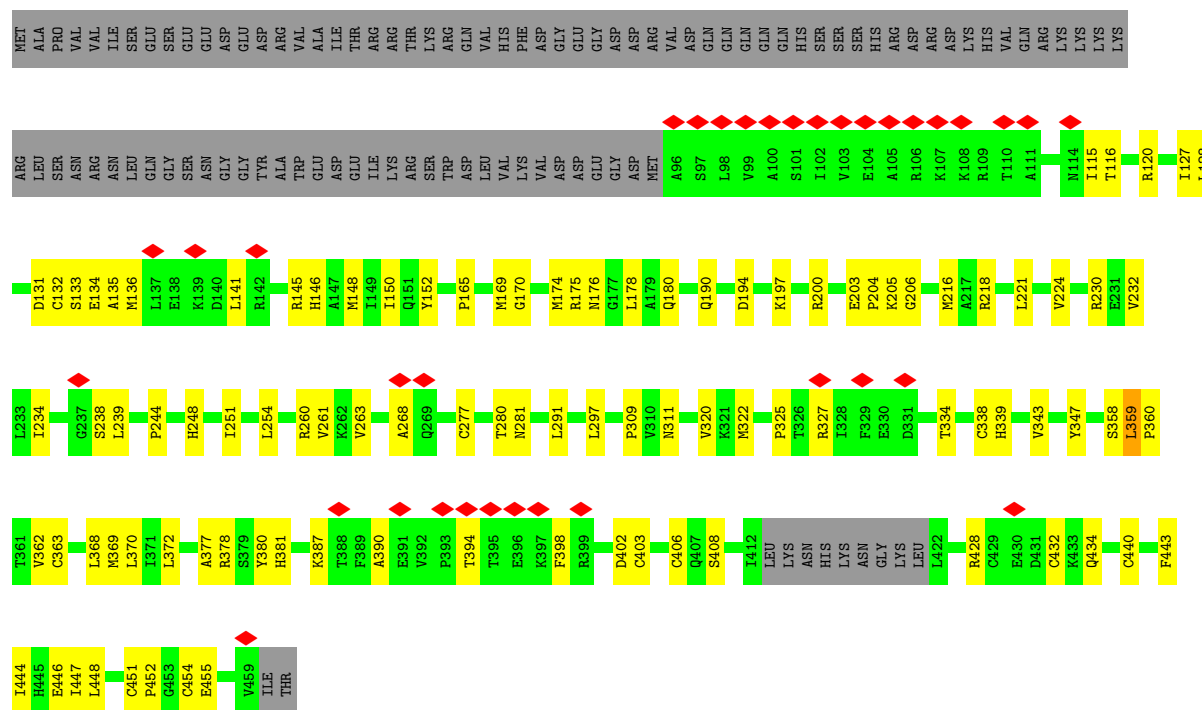
- Molecule 24: General transcription and DNA repair factor IIH subunit TFB4

Chain 4: 70% 17% 14%



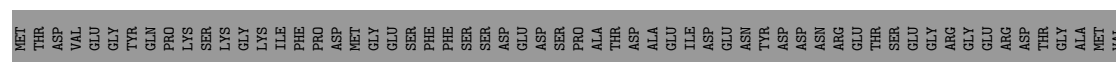
- Molecule 25: General transcription and DNA repair factor IIH subunit SSL1

Chain 6: 8% 55% 21% 23%

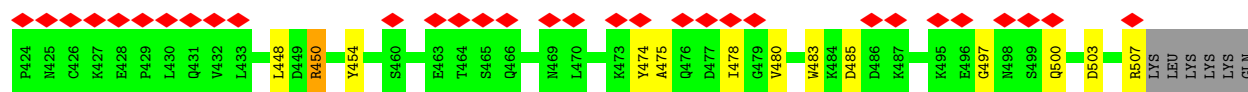


- Molecule 26: General transcription and DNA repair factor IIH helicase subunit XPB

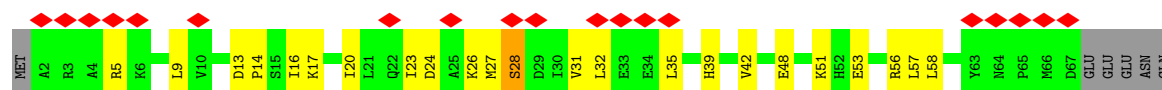
Chain 7: 6% 52% 19% 28%







- Molecule 28: General transcription and DNA repair factor IIH subunit TFB5



- Molecule 29: non-template strand



- Molecule 30: template strand



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	90136	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.25	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	1750	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.054	Depositor
Minimum map value	0.000	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size ( $\text{\AA}$ )	414.72003, 414.72003, 414.72003	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.08, 1.08, 1.08	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	M	0.46	2/2204 (0.1%)	0.85	8/2963 (0.3%)
2	A	0.44	1/11368 (0.0%)	0.85	15/15383 (0.1%)
3	B	0.49	5/9402 (0.1%)	0.89	26/12680 (0.2%)
4	C	0.43	0/2124	0.80	1/2879 (0.0%)
5	E	0.39	0/1788	0.72	0/2406
6	F	0.43	0/717	0.86	1/967 (0.1%)
7	H	0.56	1/1097 (0.1%)	0.86	0/1484
8	I	0.38	0/945	0.65	1/1273 (0.1%)
9	J	0.89	5/549 (0.9%)	1.41	9/738 (1.2%)
10	K	0.41	0/942	0.76	2/1272 (0.2%)
11	L	0.48	0/354	1.00	0/468
12	Q	0.45	0/1648	0.80	4/2226 (0.2%)
13	P	0.44	1/1511 (0.1%)	0.79	6/2035 (0.3%)
14	S	0.42	0/1317	0.85	2/1778 (0.1%)
15	O	0.36	0/1449	0.66	0/1952
16	U	0.63	2/898 (0.2%)	0.83	0/1212
17	V	0.51	0/822	0.84	0/1109
18	W	0.36	0/2045	0.65	2/2757 (0.1%)
19	X	0.32	0/1312	0.58	0/1767
20	D	0.36	0/1339	0.67	0/1793
21	G	0.42	0/1363	0.80	3/1840 (0.2%)
22	0	0.38	2/6209 (0.0%)	0.67	2/8384 (0.0%)
23	1	0.42	2/3434 (0.1%)	0.72	1/4624 (0.0%)
24	4	0.33	0/2305	0.64	0/3117
25	6	0.41	1/2843 (0.0%)	0.66	3/3845 (0.1%)
26	7	0.39	1/4992 (0.0%)	0.69	4/6754 (0.1%)
27	2	0.42	0/3611	0.72	3/4881 (0.1%)
28	5	0.48	1/502 (0.2%)	0.93	3/677 (0.4%)
29	N	0.39	0/1443	0.63	0/2226
30	T	0.39	0/1449	0.63	0/2233
All	All	0.43	24/71982 (0.0%)	0.78	96/97723 (0.1%)



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
1	M	0	5
2	A	0	8
3	B	0	6
7	H	0	1
9	J	0	1
10	K	0	1
11	L	0	1
12	Q	0	1
13	P	0	1
14	S	0	2
15	O	0	1
17	V	0	1
20	D	0	1
21	G	0	1
22	0	0	2
27	2	0	1
All	All	0	34

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	758	PHE	C-O	14.17	1.30	1.23
3	B	1156	ASP	CG-OD2	-13.41	0.99	1.25
26	7	575	ARG	CG-CD	-8.96	1.25	1.52
9	J	24	LEU	CB-CG	-8.12	1.37	1.53
16	U	12	ILE	CG1-CD1	-8.01	1.20	1.51

The worst 5 of 96 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	J	24	LEU	CB-CG-CD2	-15.31	64.77	110.70
3	B	79	THR	CA-C-N	13.48	145.96	121.70
3	B	79	THR	C-N-CA	13.48	145.96	121.70
2	A	1107	VAL	CA-C-N	12.48	144.17	121.70
2	A	1107	VAL	C-N-CA	12.48	144.17	121.70

There are no chirality outliers.

5 of 34 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	269	ILE	Peptide
1	M	271	GLY	Peptide
1	M	272	LYS	Peptide
1	M	30	TYR	Peptide
1	M	31	PRO	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	M	2175	0	2283	37	0
2	A	11167	0	11189	235	0
3	B	9227	0	9200	196	0
4	C	2086	0	2045	37	0
5	E	1752	0	1776	21	0
6	F	705	0	731	10	0
7	H	1080	0	1049	30	0
8	I	927	0	881	19	0
9	J	540	0	553	16	0
10	K	924	0	934	11	0
11	L	352	0	375	9	0
12	Q	1619	0	1452	36	0
13	P	1484	0	1480	31	0
14	S	1294	0	1289	28	0
15	O	1422	0	1500	28	0
16	U	885	0	866	27	0
17	V	815	0	822	27	0
18	W	2010	0	2026	38	0
19	X	1288	0	1307	19	0
20	D	1331	0	1345	21	0
21	G	1335	0	1346	28	0
22	0	6091	0	6155	159	0
23	1	3382	0	3436	55	0
24	4	2267	0	2323	38	0
25	6	2786	0	2804	60	0
26	7	4889	0	4876	104	0
27	2	3546	0	3593	63	0
28	5	498	0	506	13	0
29	N	1288	0	719	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	T	1291	0	713	12	0
31	4	1	0	0	0	0
31	6	4	0	0	0	0
31	A	2	0	0	0	0
31	B	1	0	0	0	0
31	C	1	0	0	0	0
31	I	2	0	0	0	0
31	J	1	0	0	0	0
31	L	1	0	0	0	0
31	M	1	0	0	0	0
31	S	1	0	0	0	0
32	7	1	0	0	0	0
32	A	1	0	0	0	0
33	0	8	0	0	2	0
All	All	70481	0	69574	1323	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 1323 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:J:24:LEU:CG	9:J:24:LEU:CD1	1.74	1.56
2:A:107:CYS:HB3	2:A:110:CYS:SG	2.01	1.00
25:6:406:CYS:HB3	25:6:440:CYS:SG	2.04	0.96
22:0:134:ARG:O	22:0:138:ASN:HB2	1.68	0.91
2:A:1170:ILE:O	2:A:1174:PHE:HB2	1.76	0.85

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	M	273/345 (79%)	238 (87%)	35 (13%)	0	100	100
2	A	1417/1733 (82%)	1249 (88%)	168 (12%)	0	100	100
3	B	1150/1224 (94%)	1000 (87%)	148 (13%)	2 (0%)	44	74
4	C	263/318 (83%)	231 (88%)	32 (12%)	0	100	100
5	E	212/215 (99%)	193 (91%)	19 (9%)	0	100	100
6	F	85/155 (55%)	78 (92%)	7 (8%)	0	100	100
7	H	129/146 (88%)	109 (84%)	20 (16%)	0	100	100
8	I	112/122 (92%)	98 (88%)	14 (12%)	0	100	100
9	J	64/70 (91%)	55 (86%)	9 (14%)	0	100	100
10	K	113/120 (94%)	107 (95%)	6 (5%)	0	100	100
11	L	42/70 (60%)	30 (71%)	12 (29%)	0	100	100
12	Q	208/735 (28%)	198 (95%)	10 (5%)	0	100	100
13	P	173/400 (43%)	161 (93%)	12 (7%)	0	100	100
14	S	162/309 (52%)	143 (88%)	18 (11%)	1 (1%)	22	55
15	O	179/240 (75%)	168 (94%)	11 (6%)	0	100	100
16	U	101/286 (35%)	96 (95%)	5 (5%)	0	100	100
17	V	100/122 (82%)	97 (97%)	3 (3%)	0	100	100
18	W	241/482 (50%)	230 (95%)	11 (5%)	0	100	100
19	X	158/328 (48%)	145 (92%)	13 (8%)	0	100	100
20	D	164/221 (74%)	159 (97%)	5 (3%)	0	100	100
21	G	169/171 (99%)	154 (91%)	14 (8%)	1 (1%)	22	55
22	0	750/778 (96%)	715 (95%)	35 (5%)	0	100	100
23	1	407/642 (63%)	394 (97%)	13 (3%)	0	100	100
24	4	286/338 (85%)	276 (96%)	10 (4%)	0	100	100
25	6	351/461 (76%)	334 (95%)	17 (5%)	0	100	100
26	7	604/843 (72%)	564 (93%)	40 (7%)	0	100	100
27	2	435/513 (85%)	417 (96%)	18 (4%)	0	100	100
28	5	64/72 (89%)	55 (86%)	9 (14%)	0	100	100
All	All	8412/11459 (73%)	7694 (92%)	714 (8%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	364	ILE
3	B	363	HIS
21	G	57	GLN
14	S	167	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	M	245/299 (82%)	245 (100%)	0	100	100
2	A	1235/1520 (81%)	1235 (100%)	0	100	100
3	B	1000/1061 (94%)	1000 (100%)	0	100	100
4	C	233/274 (85%)	233 (100%)	0	100	100
5	E	196/197 (100%)	196 (100%)	0	100	100
6	F	77/137 (56%)	77 (100%)	0	100	100
7	H	118/128 (92%)	118 (100%)	0	100	100
8	I	108/116 (93%)	108 (100%)	0	100	100
9	J	61/65 (94%)	61 (100%)	0	100	100
10	K	99/102 (97%)	99 (100%)	0	100	100
11	L	39/57 (68%)	39 (100%)	0	100	100
12	Q	147/641 (23%)	147 (100%)	0	100	100
13	P	166/363 (46%)	166 (100%)	0	100	100
14	S	141/274 (52%)	141 (100%)	0	100	100
15	O	153/205 (75%)	153 (100%)	0	100	100
16	U	99/260 (38%)	99 (100%)	0	100	100
17	V	94/108 (87%)	94 (100%)	0	100	100
18	W	224/429 (52%)	224 (100%)	0	100	100
19	X	144/295 (49%)	144 (100%)	0	100	100
20	D	146/200 (73%)	146 (100%)	0	100	100
21	G	151/152 (99%)	151 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	0	684/707 (97%)	684 (100%)	0	100	100
23	1	389/589 (66%)	389 (100%)	0	100	100
24	4	259/300 (86%)	259 (100%)	0	100	100
25	6	322/418 (77%)	322 (100%)	0	100	100
26	7	540/737 (73%)	540 (100%)	0	100	100
27	2	394/468 (84%)	394 (100%)	0	100	100
28	5	53/66 (80%)	53 (100%)	0	100	100
All	All	7517/10168 (74%)	7517 (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 101 such sidechains are listed below:

Mol	Chain	Res	Type
19	X	136	GLN
23	1	610	ASN
27	2	352	ASN
20	D	28	GLN
22	0	645	ASN

### 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 18 ligands modelled in this entry, 17 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	$\# Z  > 2$
33	SF4	0	801	-	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
33	SF4	0	801	-	-	-	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 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	0	801	SF4	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

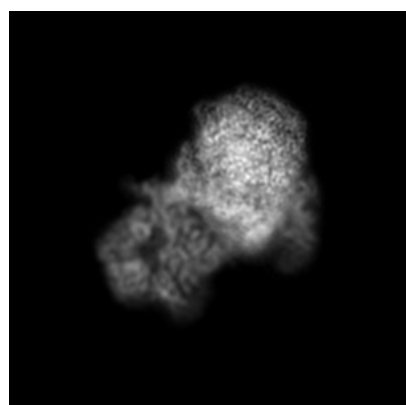
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42437. These allow visual inspection of the internal detail of the map and identification of artifacts.

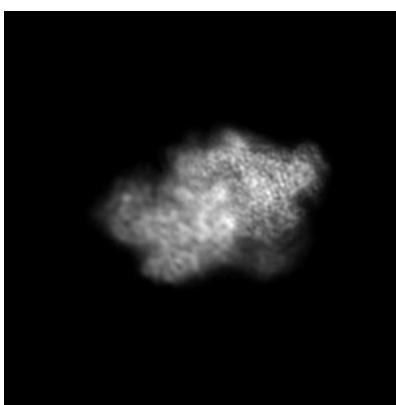
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

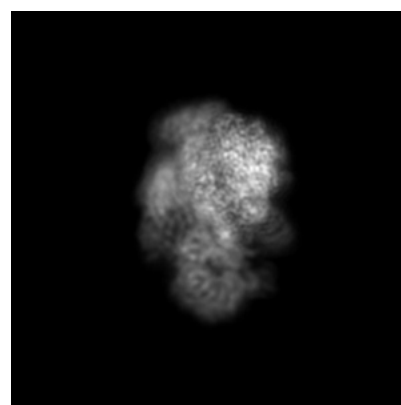
#### 6.1.1 Primary map



X



Y



Z

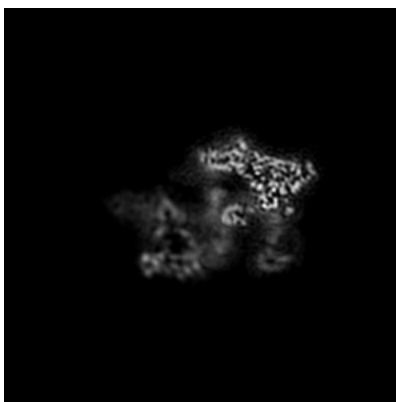
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

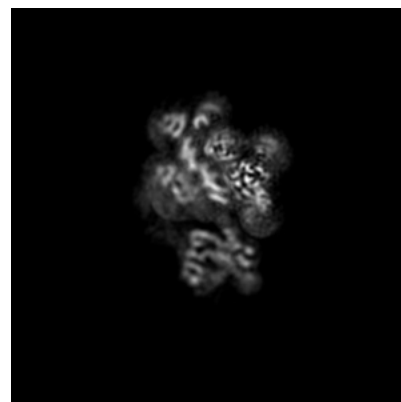
#### 6.2.1 Primary map



X Index: 192



Y Index: 192



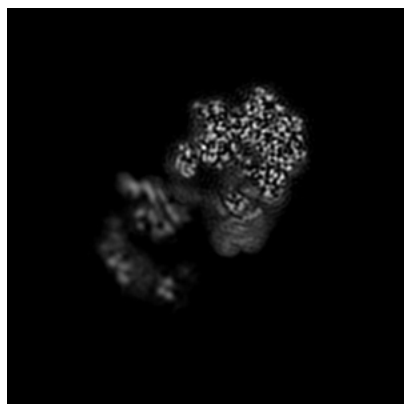
Z Index: 192



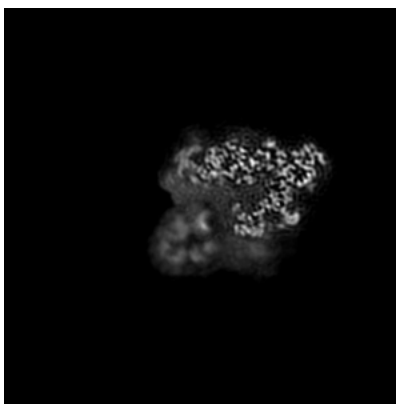
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

### 6.3.1 Primary map



X Index: 216



Y Index: 232

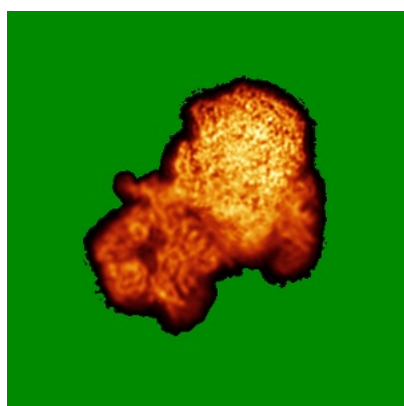


Z Index: 210

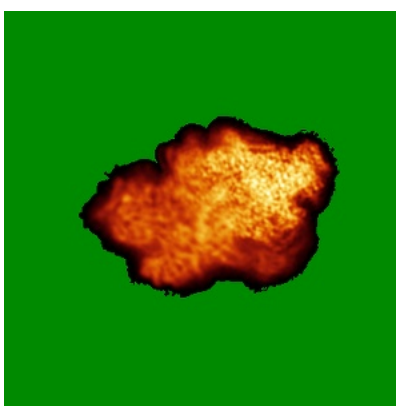
The images above show the largest variance slices of the map in three orthogonal directions.

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

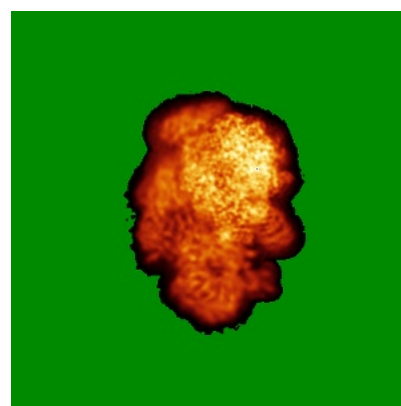
### 6.4.1 Primary map



X



Y

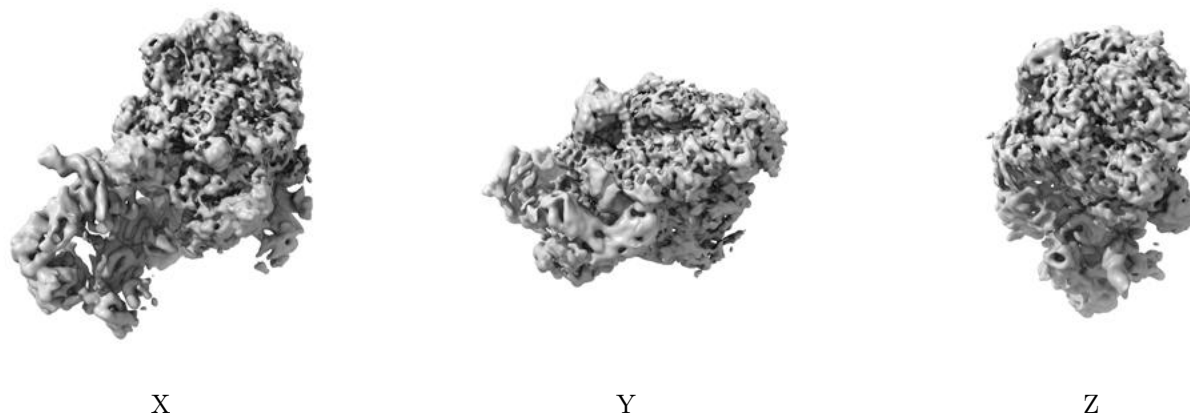


Z

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 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

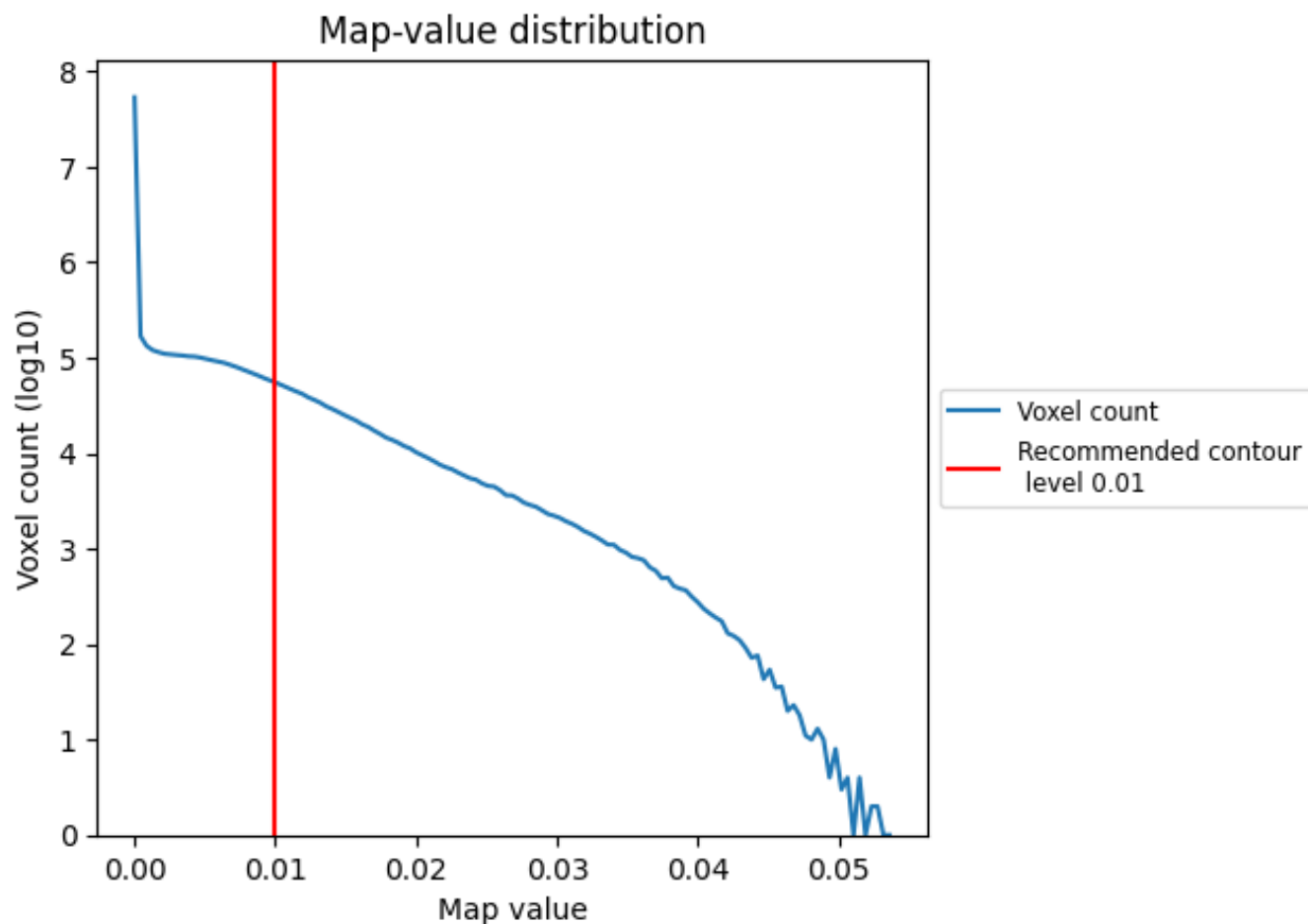
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

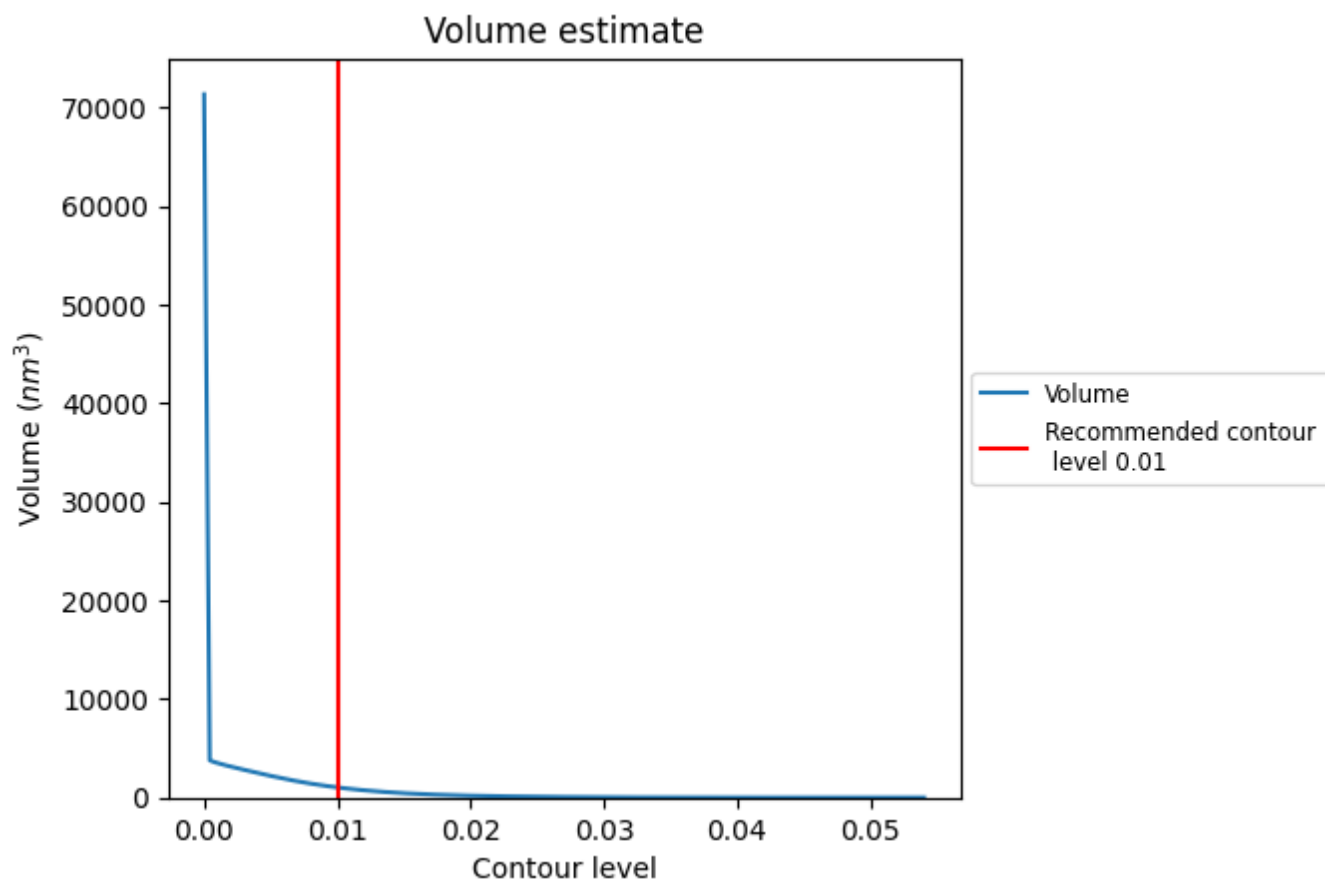
This section contains the results of statistical analysis of the map.

### 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.

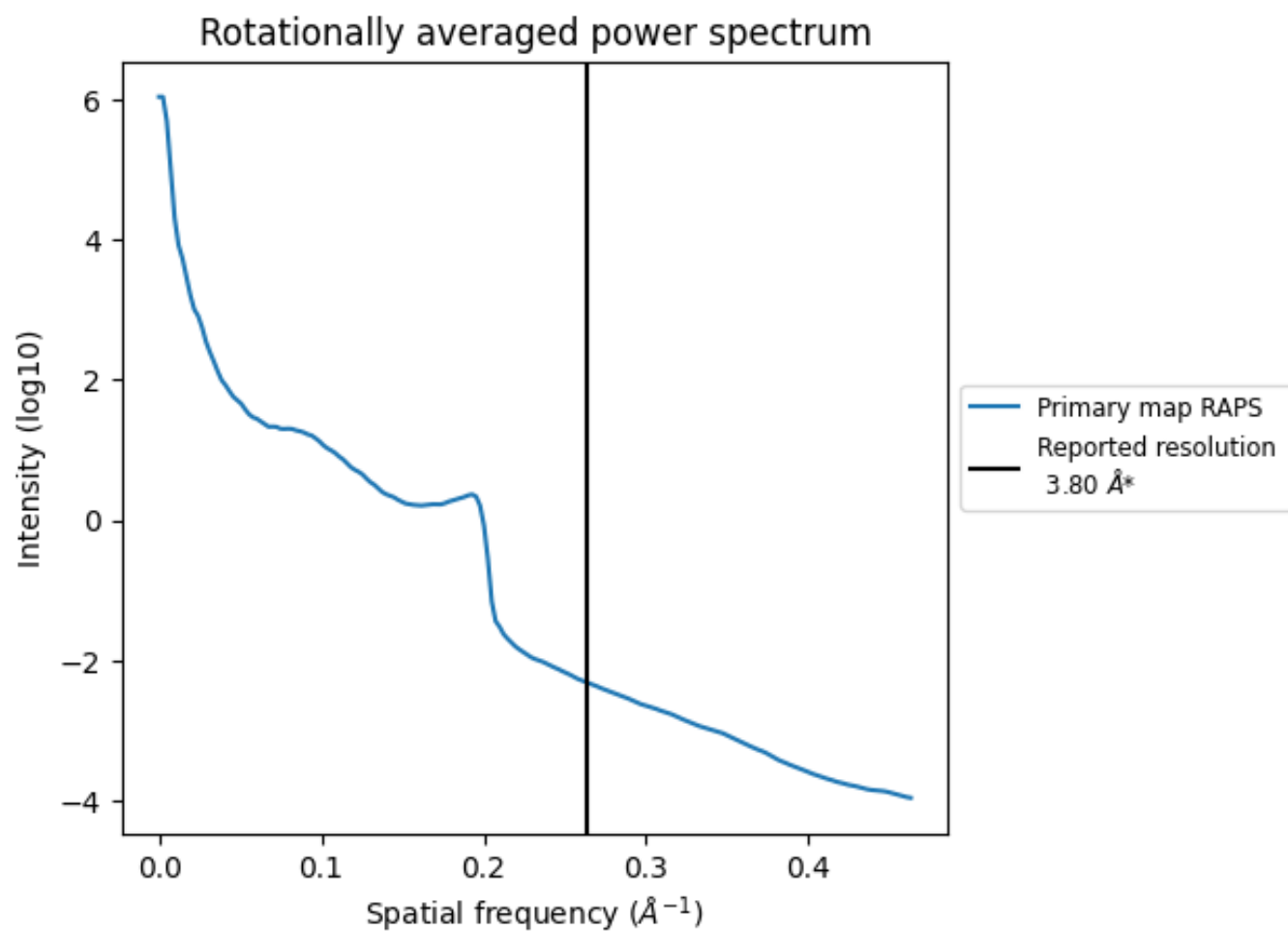
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1031  $\text{nm}^3$ ; this corresponds to an approximate mass of 932 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 0.263 Å<sup>-1</sup>

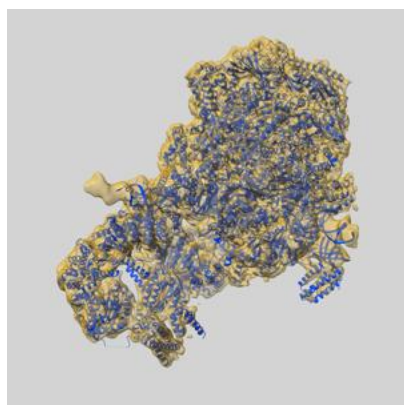
## 8 Fourier-Shell correlation

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

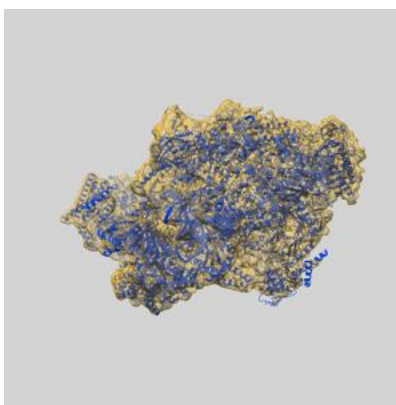
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42437 and PDB model 8UOQ. Per-residue inclusion information can be found in section [3](#) on page [11](#).

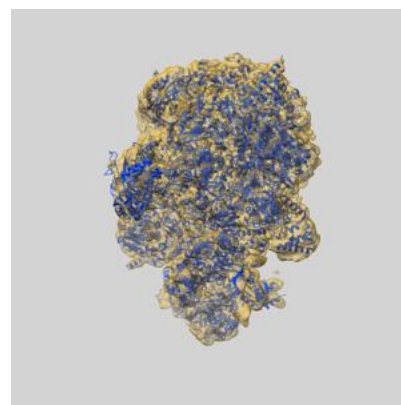
### 9.1 Map-model overlay [i](#)



X



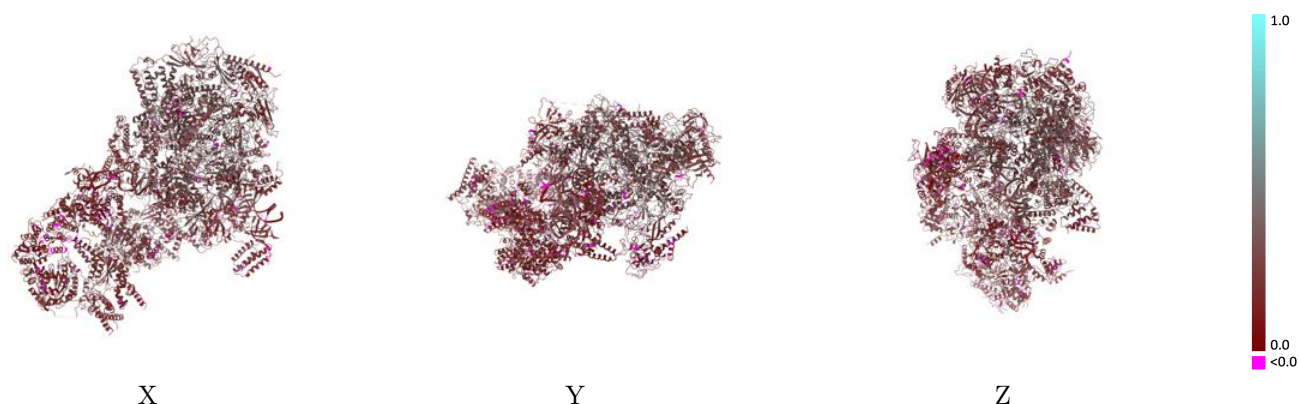
Y



Z

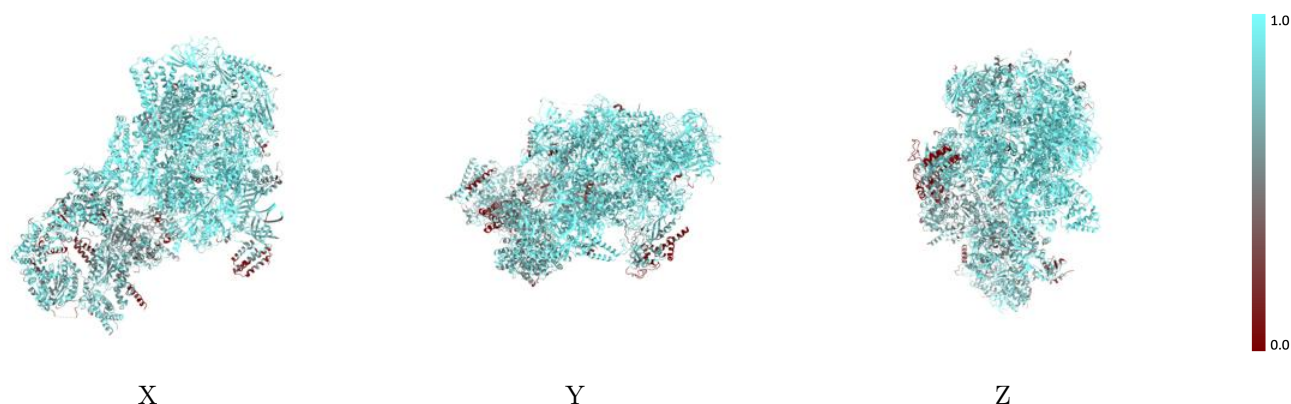
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

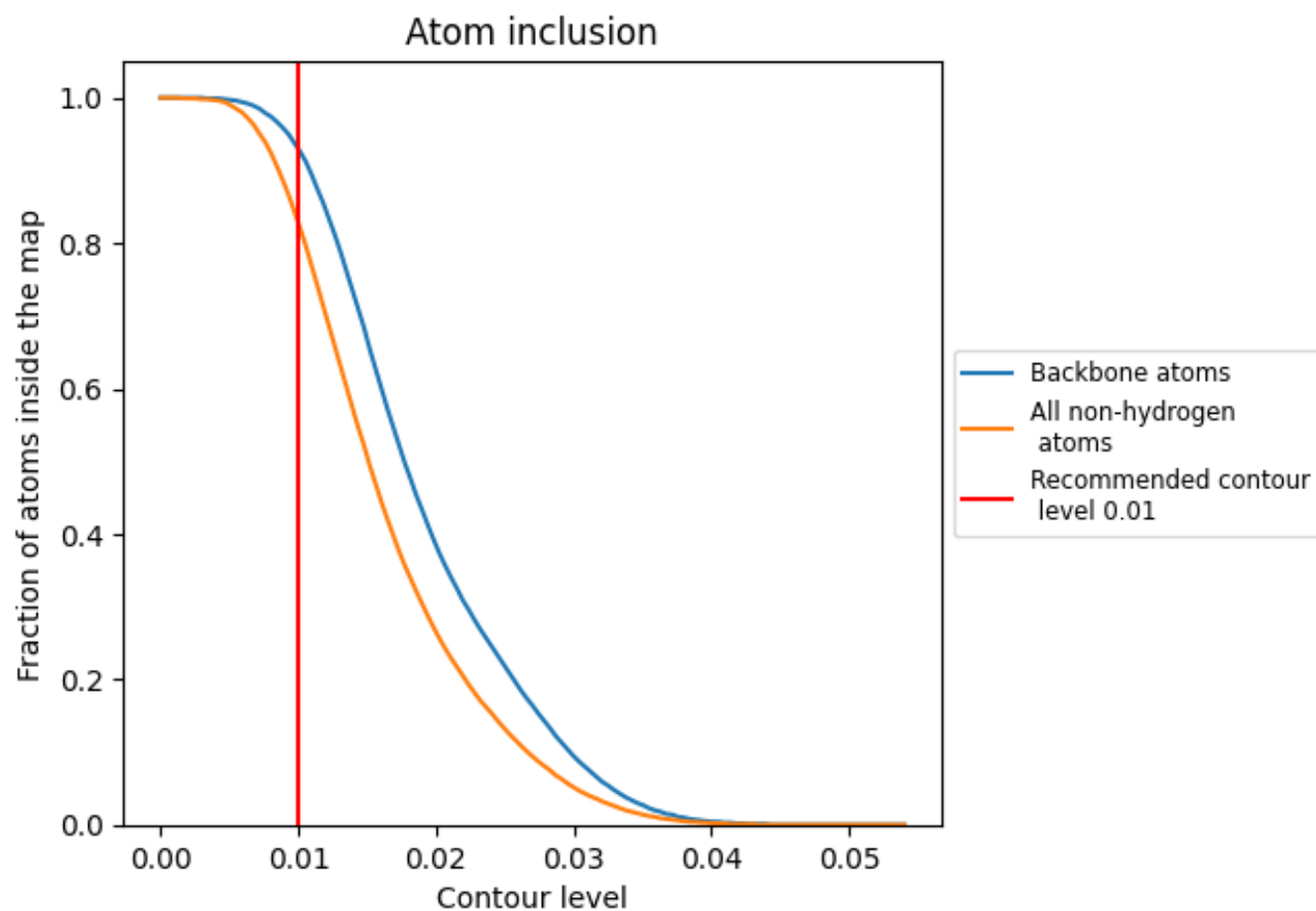
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.01).

































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 83% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8280	 0.2390
0	 0.6950	 0.1780
1	 0.6570	 0.1870
2	 0.7450	 0.1480
4	 0.7750	 0.1900
5	 0.6180	 0.1540
6	 0.7370	 0.1850
7	 0.7490	 0.1710
A	 0.9580	 0.3280
B	 0.9520	 0.3380
C	 0.9020	 0.2690
D	 0.3700	 0.1540
E	 0.9640	 0.3190
F	 0.9300	 0.3100
G	 0.6530	 0.1970
H	 0.9270	 0.3000
I	 0.9470	 0.3070
J	 0.9010	 0.2700
K	 0.8330	 0.2730
L	 0.7940	 0.1800
M	 0.7590	 0.2010
N	 0.9490	 0.2210
O	 0.9000	 0.1860
P	 0.9170	 0.2080
Q	 0.8310	 0.2520
S	 0.9020	 0.1940
T	 0.9480	 0.2290
U	 0.5180	 0.1400
V	 0.6040	 0.1810
W	 0.8160	 0.1690
X	 0.8750	 0.1570

