wwPDB EM Validation Summary Report ⓘ

Aug 25, 2026 – 11:53 pm BST

PDB ID	:	7NVZ / pdb_00007nvz
EMDB ID	:	EMD-12618
Title	:	RNA polymerase II pre-initiation complex with closed promoter DNA in distal position
Authors	:	Aibara, S.; Schilbach, S.; Cramer, P.
Deposited on	:	2021-03-16
Resolution	:	7.20 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:

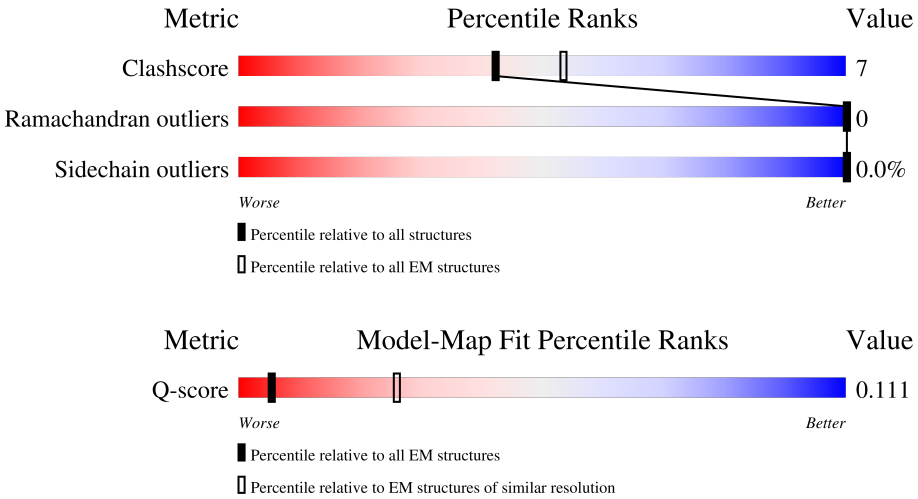
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal 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 (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 7.20 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	444 (6.70 - 7.70)

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 <=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	0	760	12% 74% 20% 6%
2	1	548	19% 42% 6% 52%
3	2	462	20% 71% 13% 16%
4	3	309	20% 37% 11% 52%

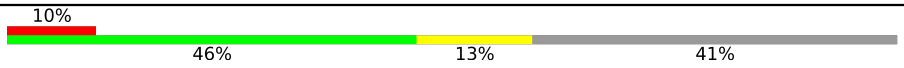
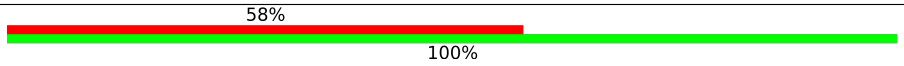
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Mol	Chain	Length	Quality of chain
5	4	308	19% 65% 20% 15%
6	5	71	32% 80% 13% 7%
7	6	395	13% 73% 15% 12%
8	7	782	15% 65% 13% 23%
9	A	1970	6% 61% 11% 28%
10	B	1174	7% 83% 13%
11	C	275	81% 13% 7%
12	D	142	26% 79% 11% 10%
13	E	210	80% 19%
14	F	127	54% 9% 38%
15	G	172	12% 91% 8%
16	H	150	5% 89% 9%
17	I	125	6% 80% 11% 9%
18	J	67	13% 76% 19%
19	K	117	7% 81% 17%
20	L	58	67% 9% 24%
21	M	316	5% 72% 8% 20%
22	N	106	5% 39% 22% 40%
23	O	339	6% 46% 7% 47%
24	Q	517	5% 24% 73%
25	R	249	14% 79% 10% 11%
26	T	106	49% 11% 40%
27	U	376	27% 26% 5% 70%
28	V	109	74% 76% 15% 9%
29	W	439	10% 33% 13% 54%

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Mol	Chain	Length	Quality of chain
30	X	291	
31	Y	19	
32	Z	8	

2 Entry composition (i)

There are 35 unique types of molecules in this entry. The entry contains 67474 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 TFIIH basal transcription factor complex helicase XPD subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	714	5751	3683	999	1040	29	0	0

- Molecule 2 is a protein called General transcription factor IIH subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	265	2167	1382	378	395	12	0	0

- Molecule 3 is a protein called General transcription factor IIH subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	390	3158	2050	545	551	12	0	0

- Molecule 4 is a protein called CDK-activating kinase assembly factor MAT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	149	1225	763	212	240	10	0	0

- Molecule 5 is a protein called General transcription factor IIH subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	263	2066	1323	344	380	19	0	0

- Molecule 6 is a protein called General transcription factor IIH subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	5	66	523	337	83	100	3	0	0

- Molecule 7 is a protein called General transcription factor IIH subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	347	Total	C	N	O	S	0	0
			2732	1726	471	508	27		

- Molecule 8 is a protein called General transcription and DNA repair factor IIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	605	Total	C	N	O	S	0	0
			4890	3127	848	885	30		

- Molecule 9 is a protein called RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	1423	Total	C	N	O	S	0	0
			11274	7092	2016	2094	72		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	1136	Total	C	N	O	S	0	0
			9076	5739	1597	1676	64		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	257	Total	C	N	O	S	0	0
			2059	1294	351	408	6		

- Molecule 12 is a protein called RPOL4c domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	128	Total	C	N	O	S	0	0
			1050	656	178	212	4		

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	209	Total	C	N	O	S	0	0
			1721	1089	300	324	8		

- Molecule 14 is a protein called DNA-directed RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	79	Total	C	N	O	S	0	0
			636	406	108	117	5		

- Molecule 15 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	G	171	Total	C	N	O	S	0	0
			1351	875	219	249	8		

- Molecule 16 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 17 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I	114	Total	C	N	O	S	0	0
			928	571	166	180	11		

- Molecule 18 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	J	64	Total	C	N	O	S	0	0
			507	328	86	87	6		

- Molecule 19 is a protein called RNA_pol_L_2 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	115	Total	C	N	O	S	0	0
			920	593	152	173	2		

- Molecule 20 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	44	Total	C	N	O	S	0	0
			373	231	72	64	6		

- Molecule 21 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	M	252	Total	C	N	O	S	0	0
			1953	1224	346	366	17		

- Molecule 22 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	N	64	Total	C	N	O	P	0	0
			1318	624	243	388	63		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	O	179	Total	C	N	O	S	0	0
			1422	923	251	241	7		

- Molecule 24 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Q	138	Total	C	N	O	S	0	0
			1138	719	208	208	3		

- Molecule 25 is a protein called General transcription factor IIF subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	R	222	Total	C	N	O	S	0	0
			1788	1127	320	338	3		

- Molecule 26 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T	64	Total	C	N	O	P	0	0
			1303	616	245	378	64		

- Molecule 27 is a protein called Transcription initiation factor IIA subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U	113	Total	C	N	O	S	0	0
			930	585	152	189	4		

- Molecule 28 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	V	99	Total	C	N	O	S	0	0
			806	510	142	151	3		

- Molecule 29 is a protein called General transcription factor IIE subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	W	202	Total	C	N	O	S	0	0
			1659	1042	299	307	11		

- Molecule 30 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	X	171	Total	C	N	O	S	0	0
			1403	895	243	261	4		

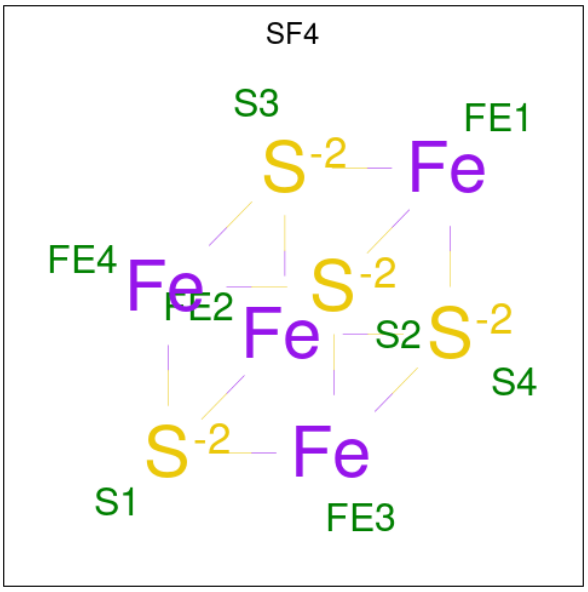
- Molecule 31 is a protein called Unassigned peptide, likely TFIIE-beta.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	Y	19	Total	C	N	O	0	0
			95	57	19	19		

- Molecule 32 is a protein called Unassigned peptide, likely XPB.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	Z	8	Total	C	N	O	0	0
			40	24	8	8		

- Molecule 33 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 34 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
34	3	2	Total	Zn	0
			2	2	
34	4	2	Total	Zn	0
			2	2	
34	6	3	Total	Zn	0
			3	3	
34	A	2	Total	Zn	0
			2	2	
34	B	1	Total	Zn	0
			1	1	
34	C	1	Total	Zn	0
			1	1	
34	I	2	Total	Zn	0
			2	2	
34	J	1	Total	Zn	0
			1	1	
34	L	1	Total	Zn	0
			1	1	
34	M	1	Total	Zn	0
			1	1	
34	W	1	Total	Zn	0
			1	1	

- Molecule 35 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

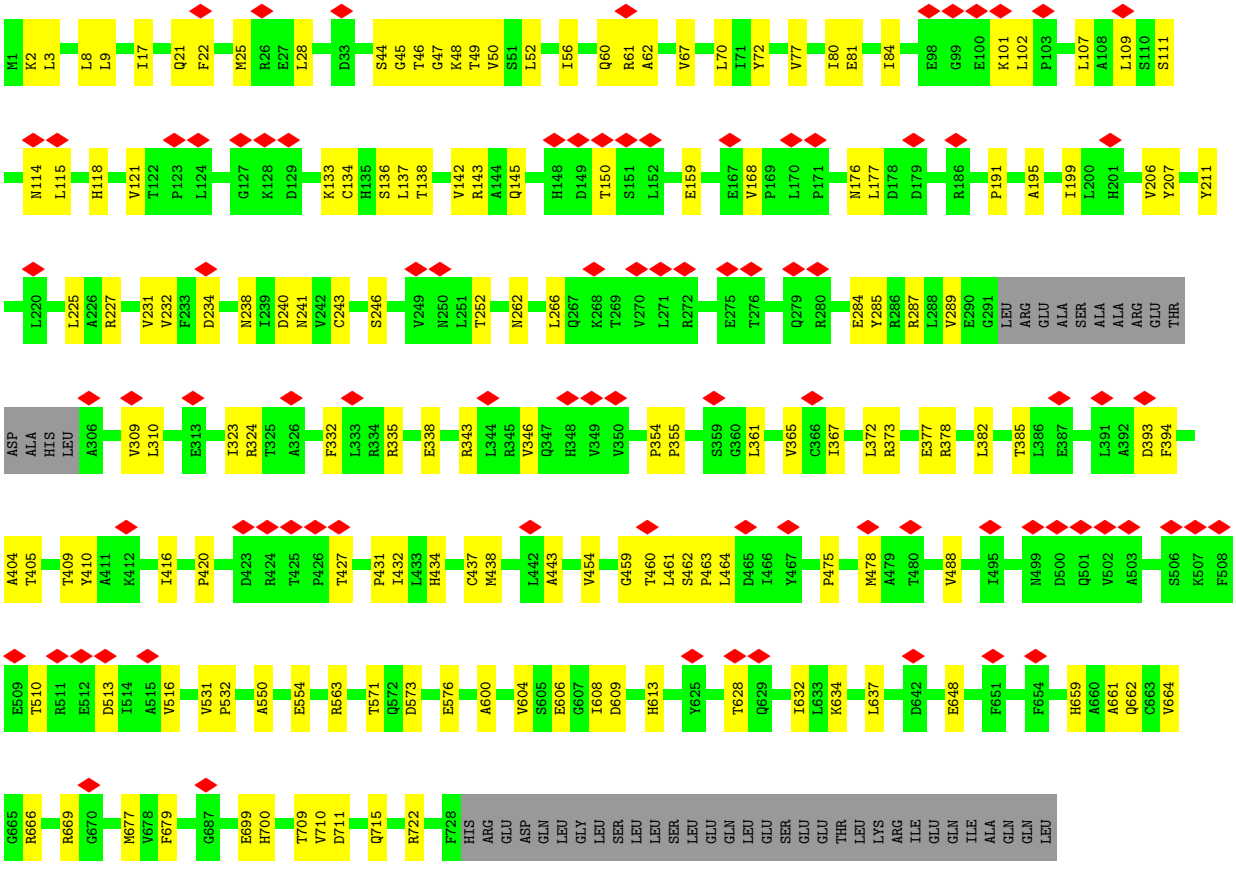
3 Residue-property plots (i)

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: TFIIH basal transcription factor complex helicase XPD subunit

Chain 0:



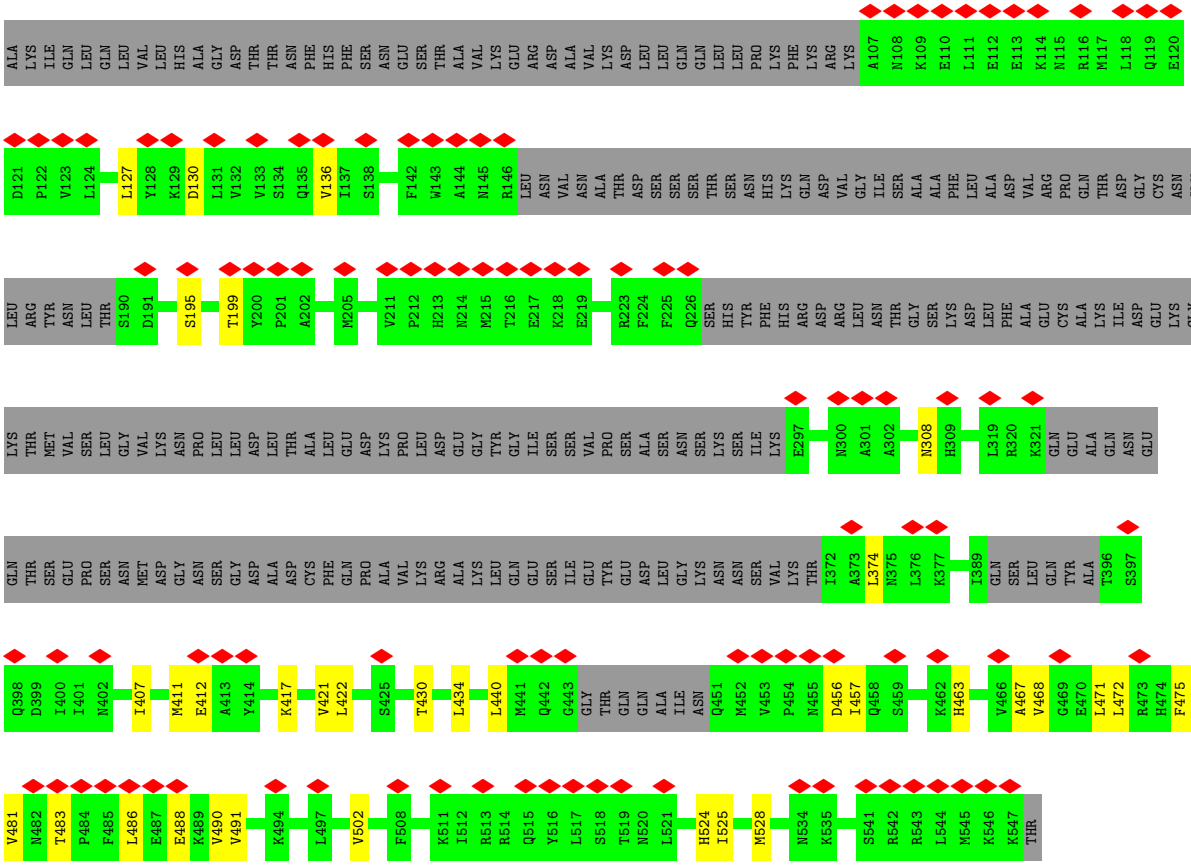


• Molecule 2: General transcription factor IIH subunit 1

Chain 1:



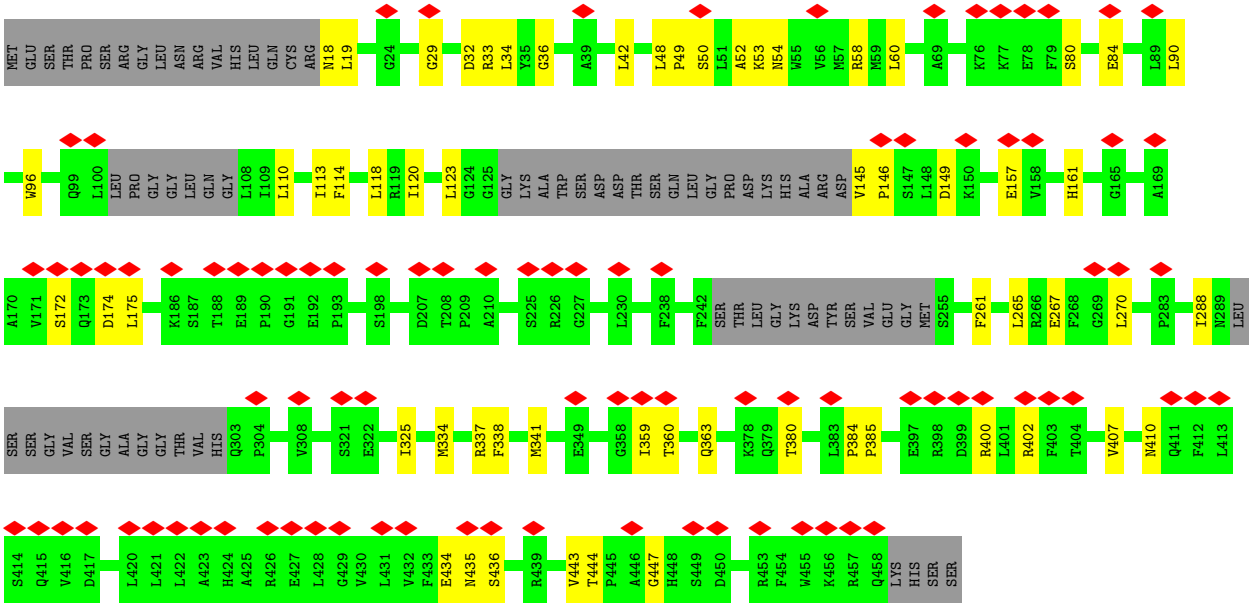




• Molecule 3: General transcription factor IIH subunit 4

Chain 2:

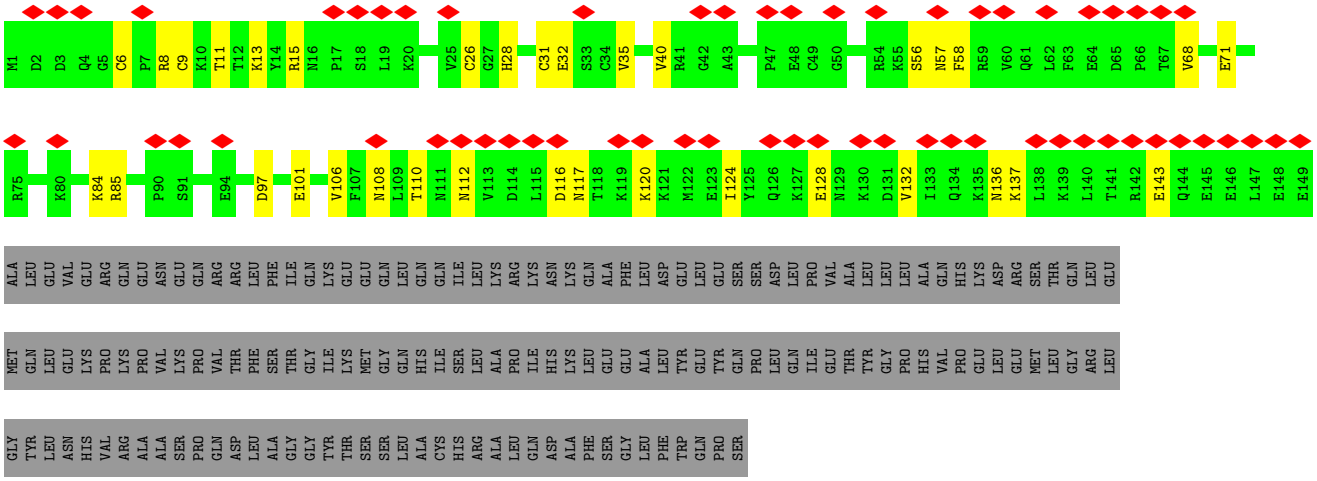




• Molecule 4: CDK-activating kinase assembly factor MAT1

Chain 3:

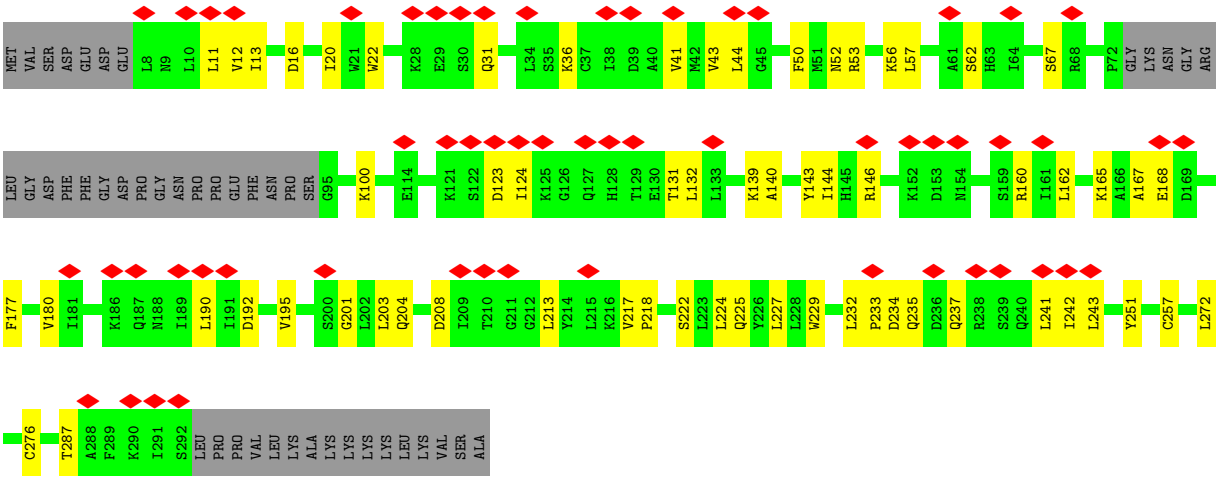




• Molecule 5: General transcription factor IIH subunit 3

Chain 4:

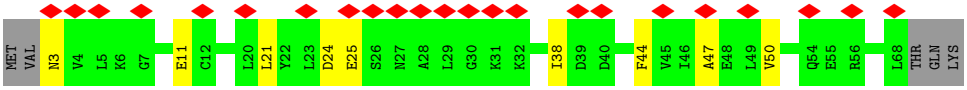




• Molecule 6: General transcription factor IIH subunit 5

Chain 5:

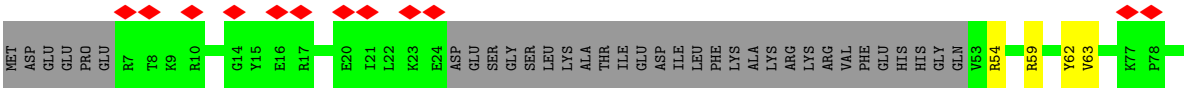


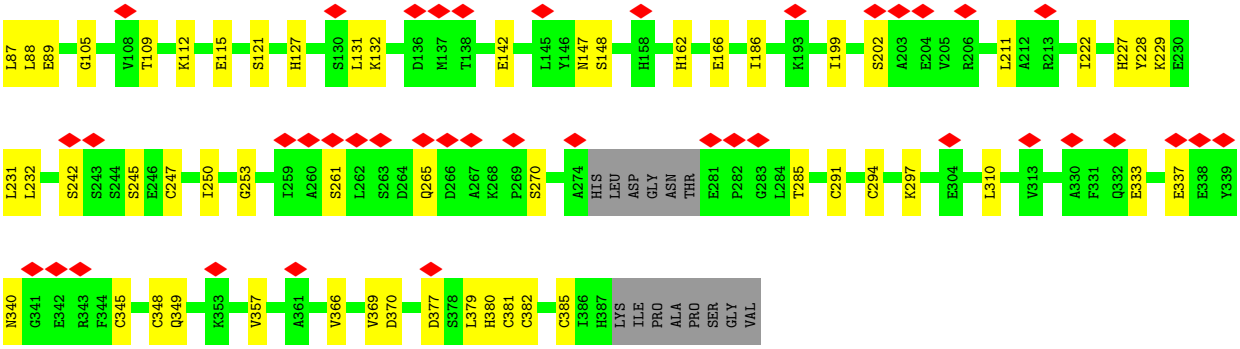


• Molecule 7: General transcription factor IIH subunit 2

Chain 6:



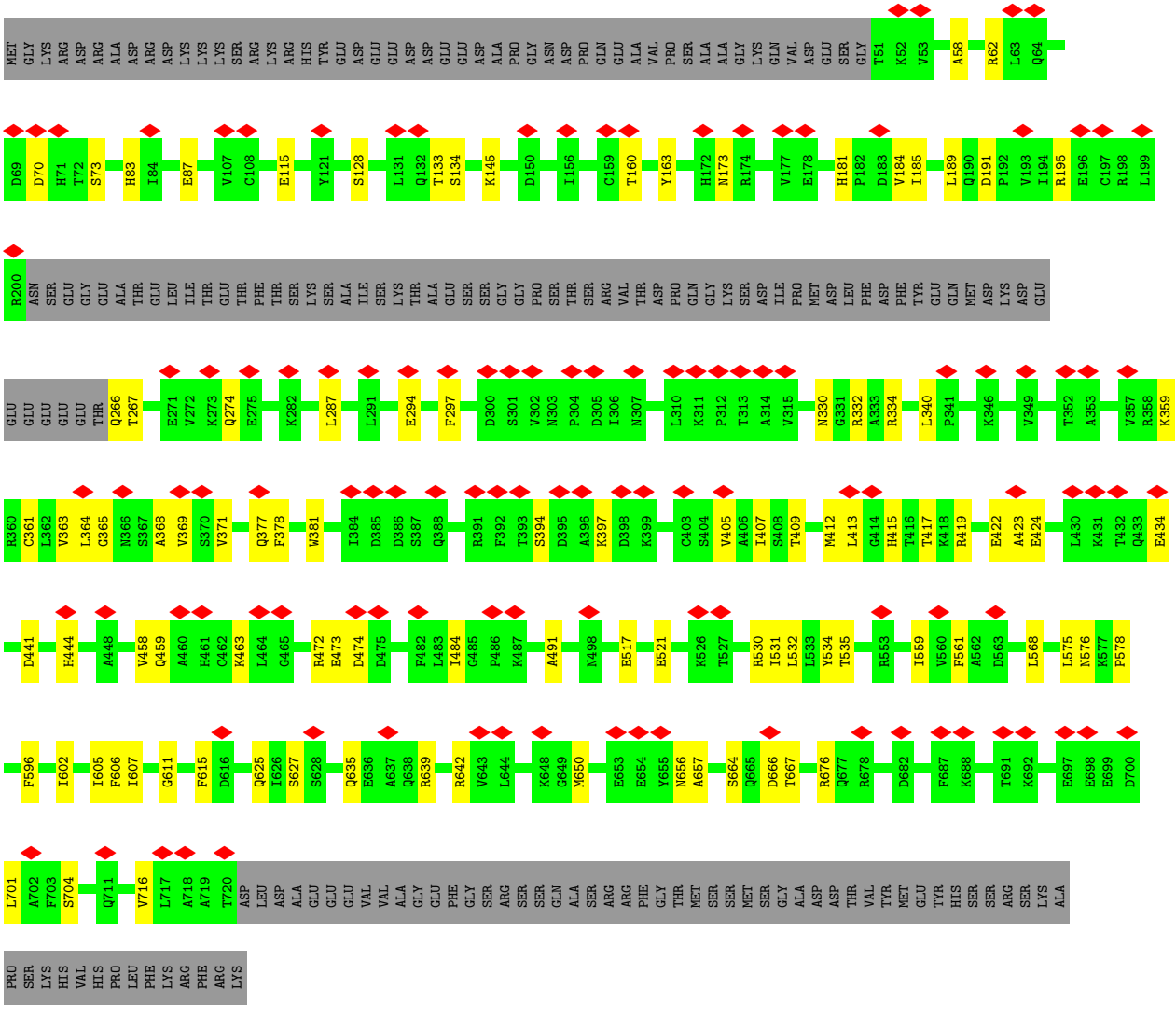




• Molecule 8: General transcription and DNA repair factor IIH helicase subunit XPB

Chain 7:

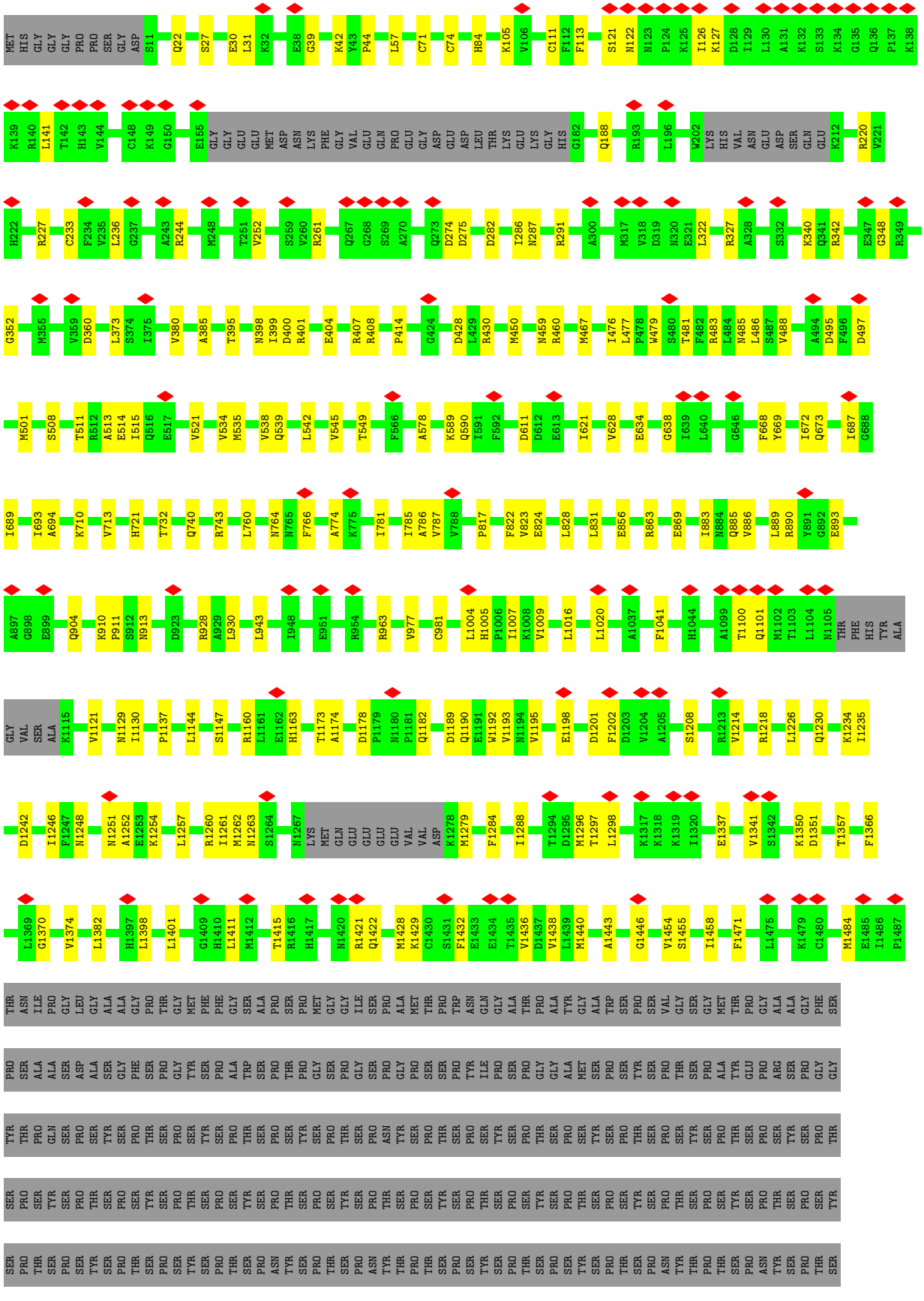


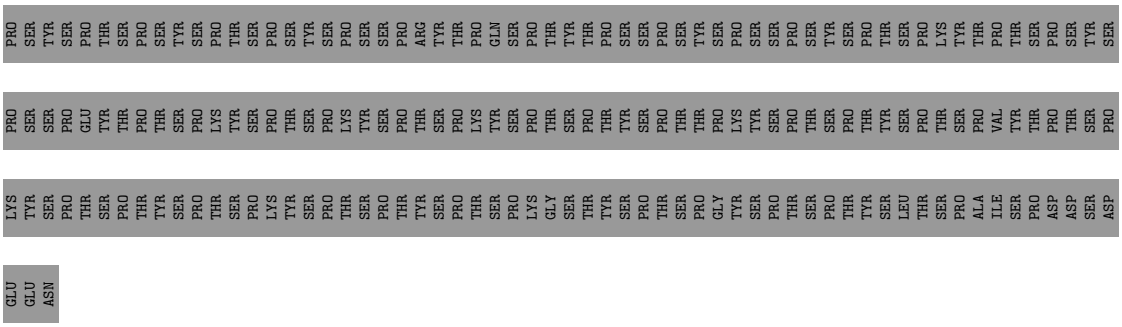


• Molecule 9: RPB1

Chain A:



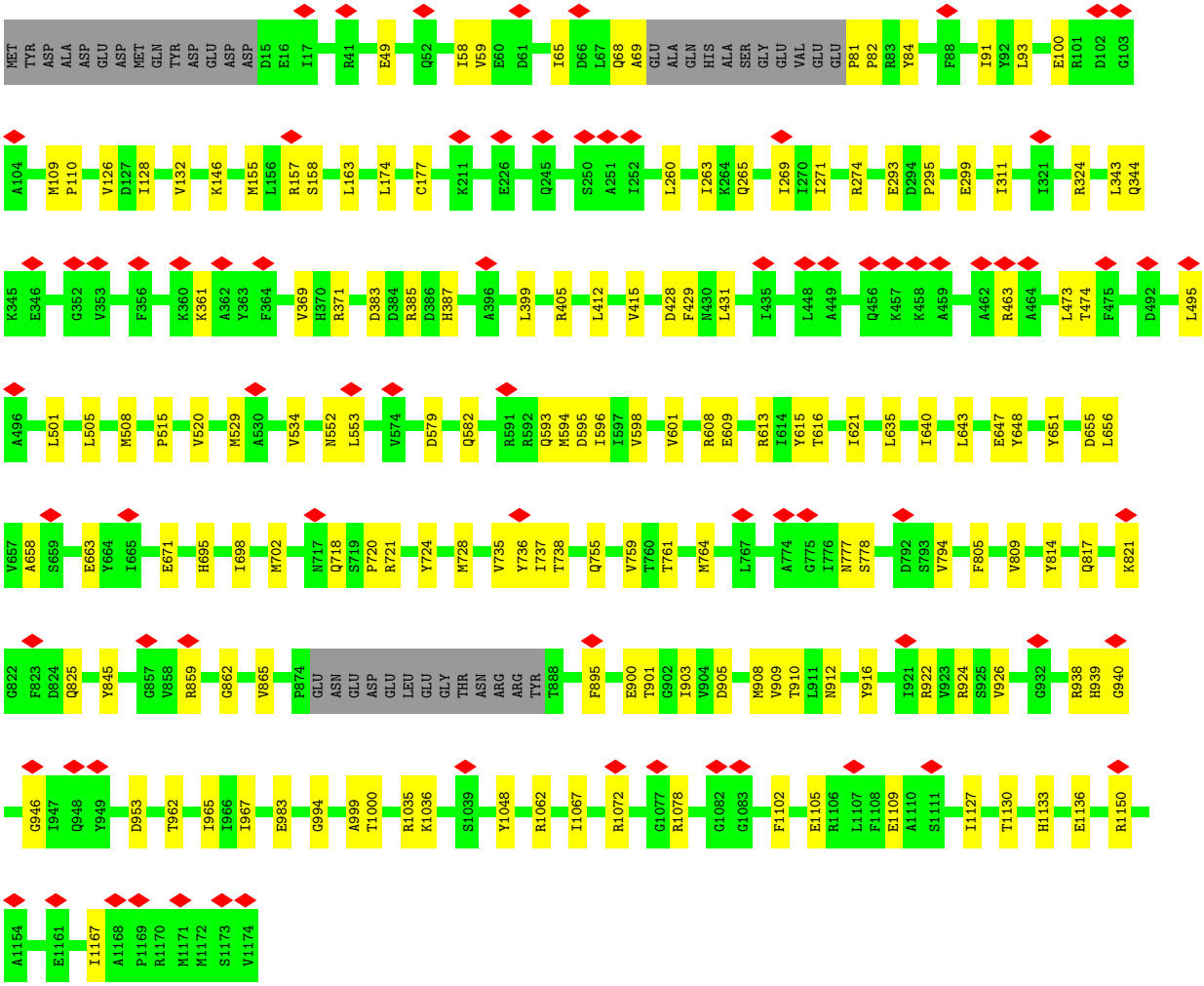

MET HIS GLY GLY GLY PRO PRO SER GLY ASP S11 Q22 S27 E30 L31 K32 E38 G39 K42 Y43 P44 L57 C71 C74 H84 K105 V106 C111 F112 F113 S121 N122 N123 P124 K125 I126 K127 D128 I129 L130 A131 K132 S133 K134 G135 Q136 P137 K138
K139 R140 L141 T142 H143 V144 C148 K149 G150 E155 GLY GLY GLU GLU MET ASP ASN LYS PHE GLY VAL GLU GLN PRO GLU GLY ASP GLU ASP LEU THR LYS GLU LYS GLY HIS G182 Q188 R193 L196 W202 LYS HIS VAL ASN GLU ASP SER GLN GLU K212 R220 Y221
H222 R227 C233 F234 V235 L236 G237 A243 R244 M248 T251 V252 S259 V260 R261 Q267 G268 S269 A270 Q273 D274 D275 D282 I286 N287 R291 A300 M317 V318 D319 N320 E321 L322 R327 A328 S332 K340 Q341 R342 E347 G348 R349
G352 M355 V359 D360 L373 S374 I375 V380 A385 T395 N398 I399 D400 R401 E404 R407 R408 P414 G424 D428 L429 R430 M450 N459 R460 M467 I476 L477 P478 W479 S480 T481 F482 R483 L484 N485 L486 S487 V488 A494 D495 F496 D497
M501 S508 T511 R512 A513 E514 I515 Q516 E517 V521 V534 M535 V538 Q539 L542 V545 T549 F566 A578 K689 Q590 I591 F592 D611 D612 E613 I621 V628 E634 G638 I639 L640 G646 F668 Y669 I672 Q673 I687 G688
I689 I693 A694 K710 V713 H721 T732 Q740 R743 L760 N764 N765 F766 A774 K775 I781 I785 A786 V787 V788 P817 F822 V823 E824 L828 L831 E856 R863 E869 I883 N884 Q885 V886 L889 R890 Y891 G892 E893
A897 G898 E899 Q904 K910 P911 S912 N913 D923 R928 A929 L930 L943 I948 E951 R954 R963 V977 C981 L1004 H1005 P1006 I1007 K1008 V1009 L1016 L1020 A1037 F1041 H1044 A1099 T1100 Q1101 M1102 T1103 L1104 N1105 THR PHE HIS TYR ALA
GLY VAL SER ALA K1115 V1121 N1129 I1130 P1137 L1144 S1147 R1160 L1161 E1162 H1163 T1173 A1174 D1178 P1179 N1180 P1181 Q1182 D1189 Q1190 E1191 W1192 V1193 N1194 V1195 E1198 D1201 F1202 D1203 V1204 A1205 S1208 R1213 V1214 R1218 L1226 Q1230 K1234 I1235
D1242 I1246 F1247 N1248 N1251 A1252 E1253 K1254 L1257 R1260 I1261 M1262 N1263 S1264 N1267 LYS MET GLN GLU GLU GLU GLU VAL VAL ASP K1278 M1279 F1284 I1288 T1294 D1295 M1296 T1297 L1298 K1317 K1318 K1319 I1320 E1337 V1341 S1342 K1350 D1351 T1357 F1366
L1369 G1370 V1374 L1382 H1397 L1398 L1401 G1409 H1410 L1411 M1412 T1415 R1416 H1417 N1420 R1421 Q1422 M1428 K1429 C1430 S1431 F1432 E1433 E1434 T1435 V1436 D1437 V1438 L1439 M1440 A1443 G1446 V1454 S1455 I1458 F1471 L1475 K1479 C1480 M1484 E1485 I1486 P1487
THR ASN ILE PRO GLY LEU GLY ALA ALA GLY PRO THR GLY MET PHE PHE GLY SER ALA PRO SER PRO MET MET GLY GLY ILE GLY GLU GLU GLU GLU VAL VAL ASP ALA MET THR PRO TRP ASN GLN GLY ALA THR PRO ALA ALA TYR GLY ALA TRP SER PRO SER VAL GLY SER GLY MET THR PRO THR GLY GLY PHE SER
PRO SER ALA ALA SER ASP ALA SER GLY PHE SER PRO GLY TYR SER PRO ALA TRP SER PRO THR PRO GLY SER PRO GLY PRO SER PRO TYR ILE PRO SER PRO GLY GLY ALA MET SER PRO SER TYR SER PRO THR SER PRO ALA THR GLU PRO ARG SER PRO GLY GLY
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• Molecule 10: DNA-directed RNA polymerase subunit beta

Chain B:

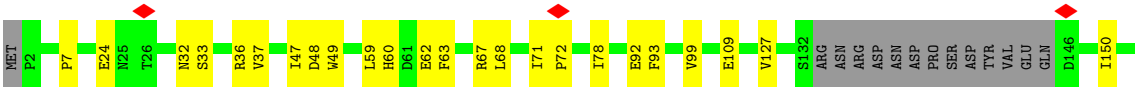


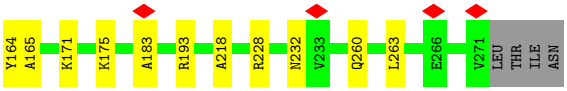


• Molecule 11: DNA-directed RNA polymerase II subunit RPB3

Chain C:



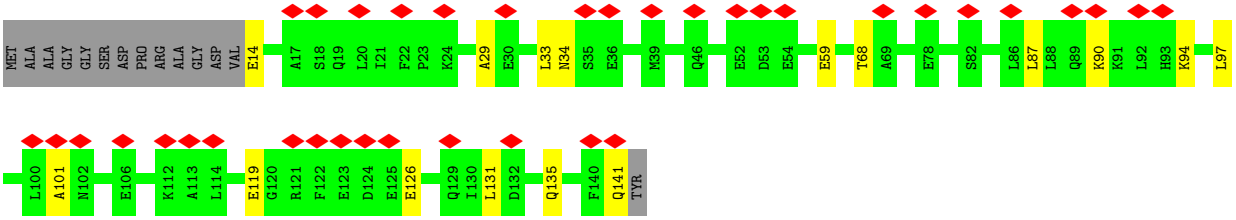




• Molecule 12: RPOL4c domain-containing protein

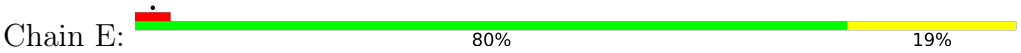
Chain D:

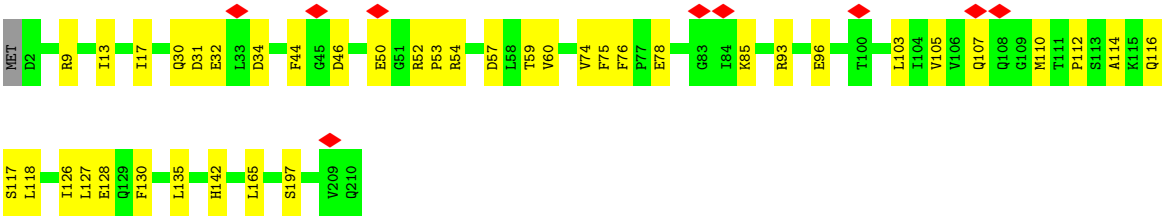




• Molecule 13: DNA-directed RNA polymerase II subunit E

Chain E:

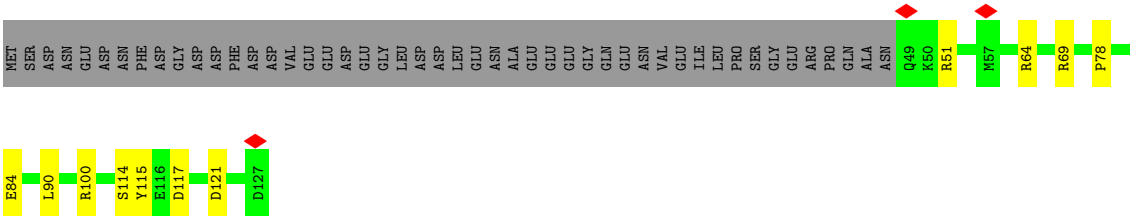




• Molecule 14: DNA-directed RNA polymerase II subunit F

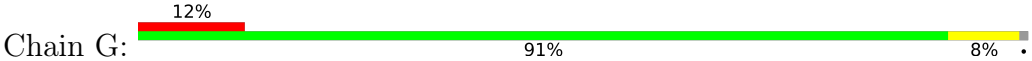
Chain F:

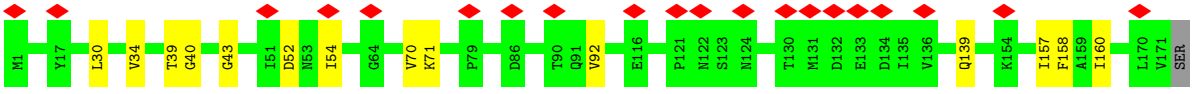




• Molecule 15: DNA-directed RNA polymerase II subunit RPB7

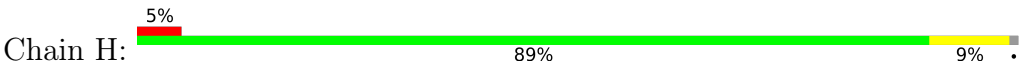
Chain G:

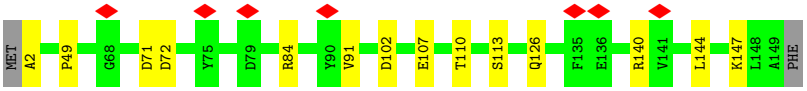




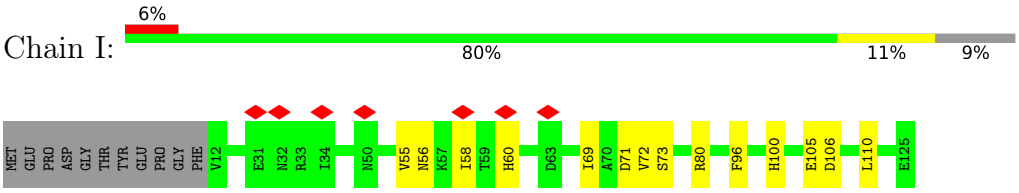
• Molecule 16: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:

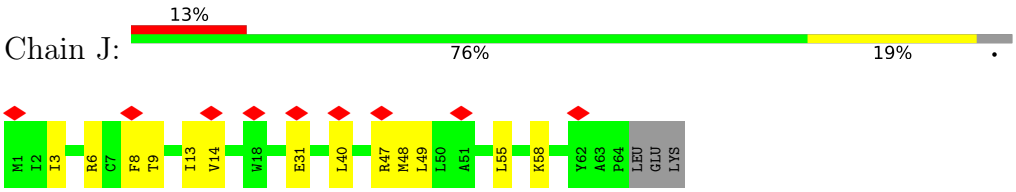




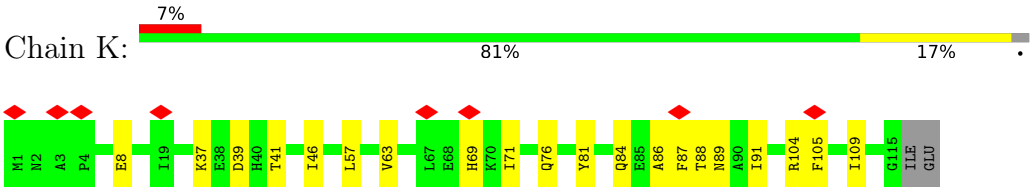
• Molecule 17: DNA-directed RNA polymerase II subunit RPB9



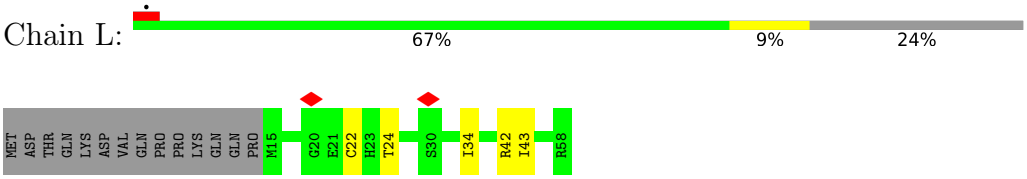
• Molecule 18: DNA-directed RNA polymerases I, II, and III subunit RPABC5



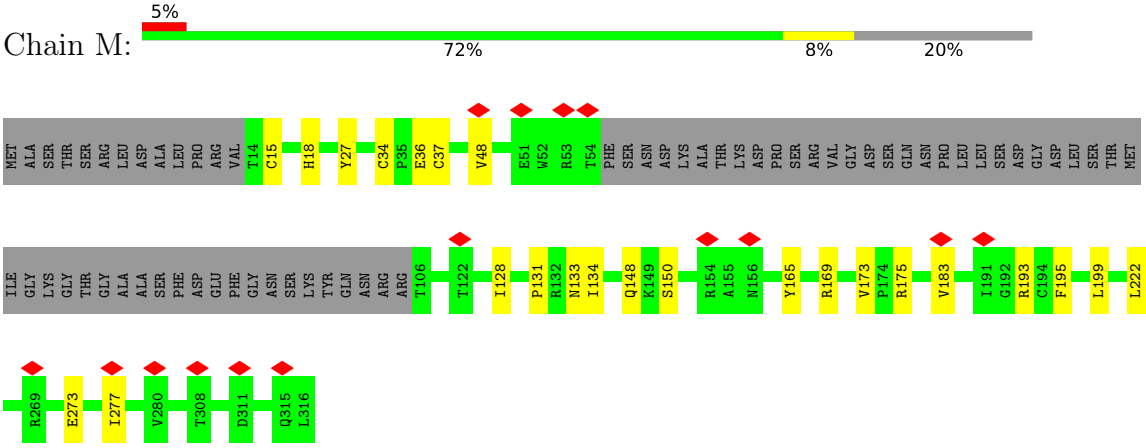
• Molecule 19: RNA_pol_L_2 domain-containing protein



• Molecule 20: RNA polymerase II subunit K

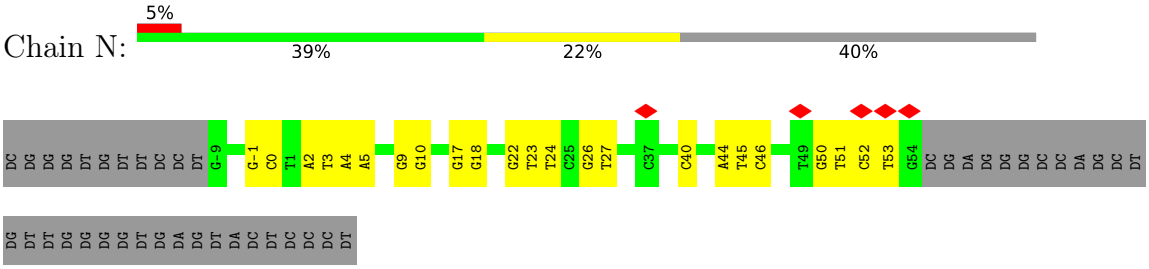


• Molecule 21: Transcription initiation factor IIB



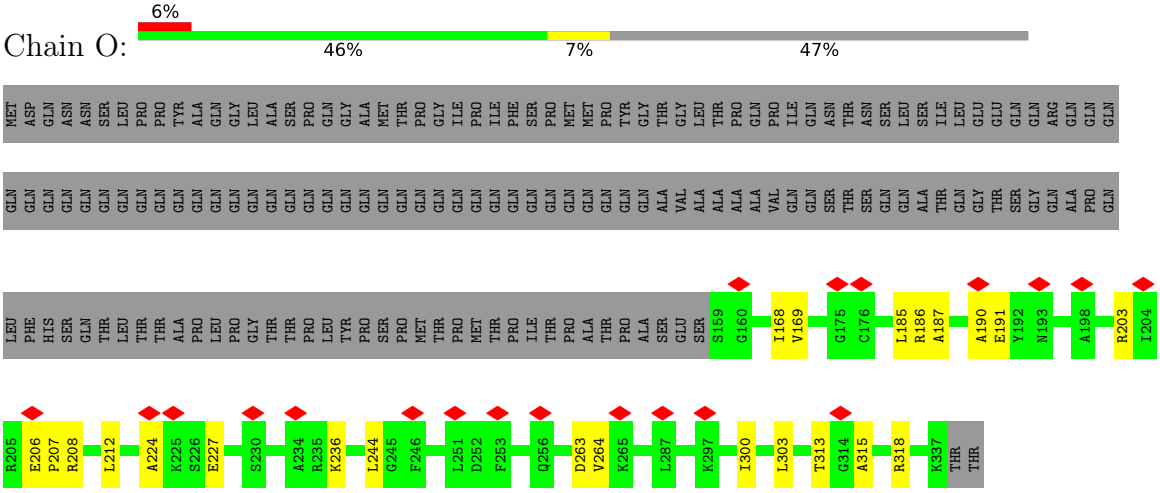
• Molecule 22: Non-template DNA

Chain N:



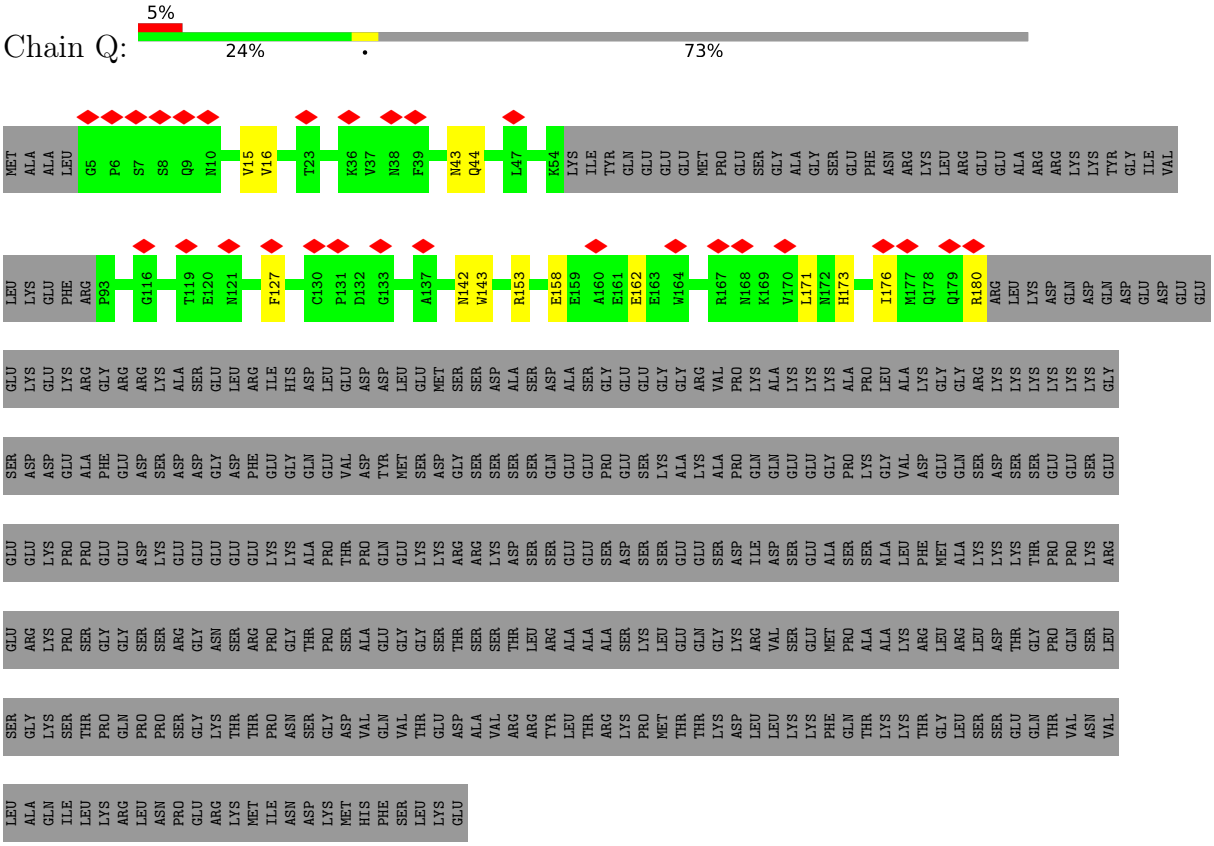
• Molecule 23: TATA-box-binding protein

Chain O:



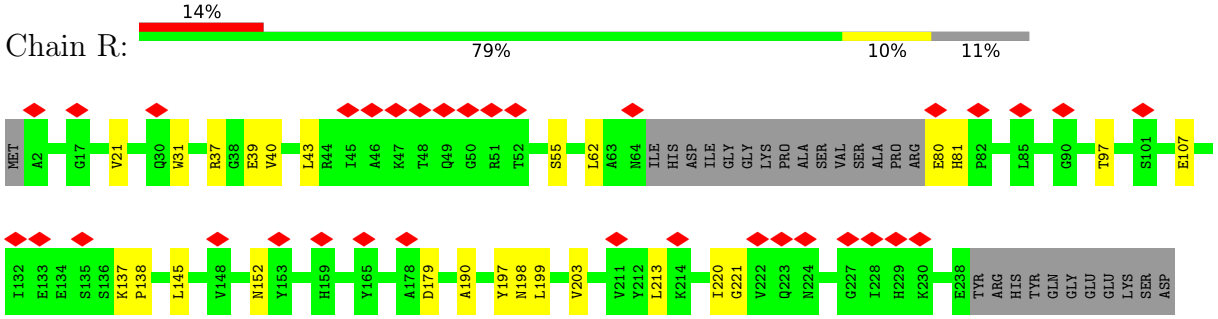
• Molecule 24: General transcription factor IIF subunit 1

Chain Q:



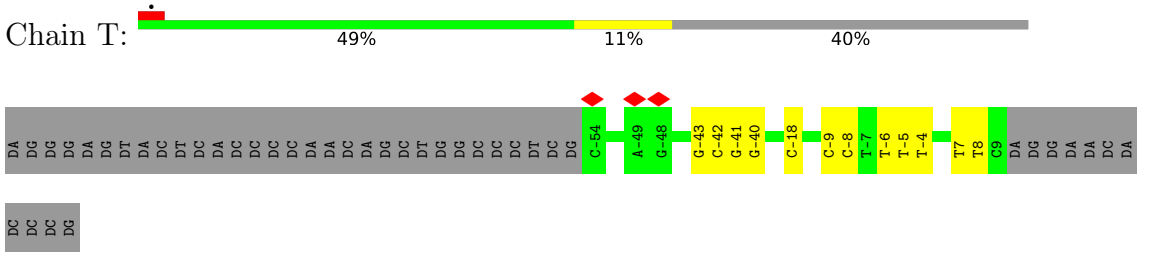
• Molecule 25: General transcription factor IIF subunit 2

Chain R:



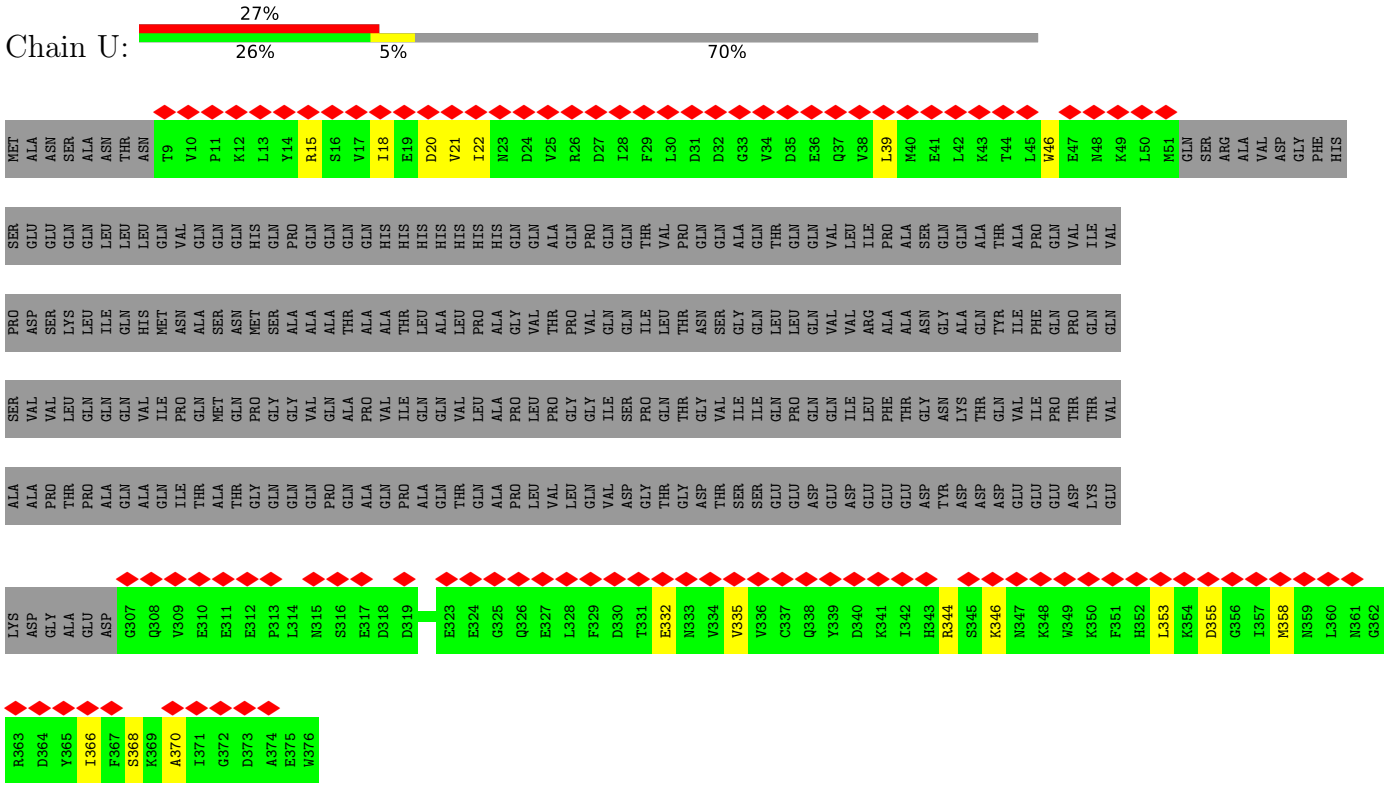
• Molecule 26: Template DNA

Chain T:



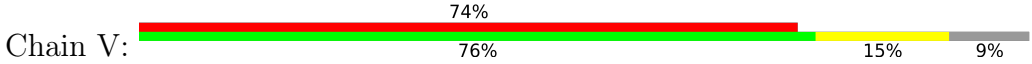
• Molecule 27: Transcription initiation factor IIA subunit 1

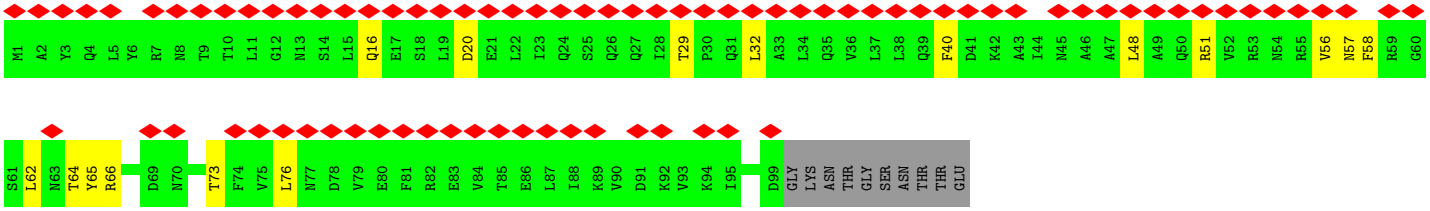
Chain U:



• Molecule 28: Transcription initiation factor IIA subunit 2

Chain V:

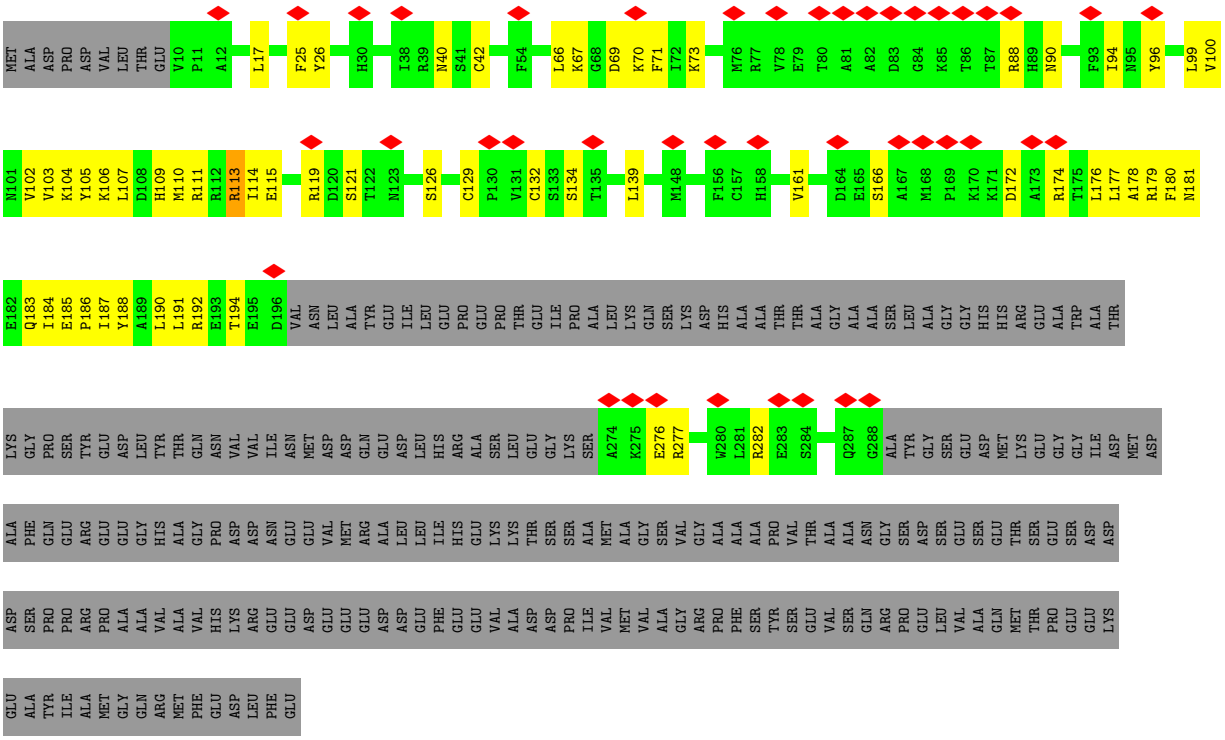




• Molecule 29: General transcription factor IIE subunit 1

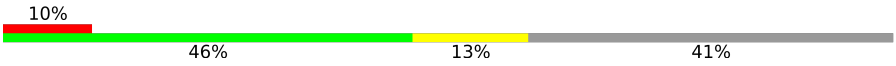
Chain W:

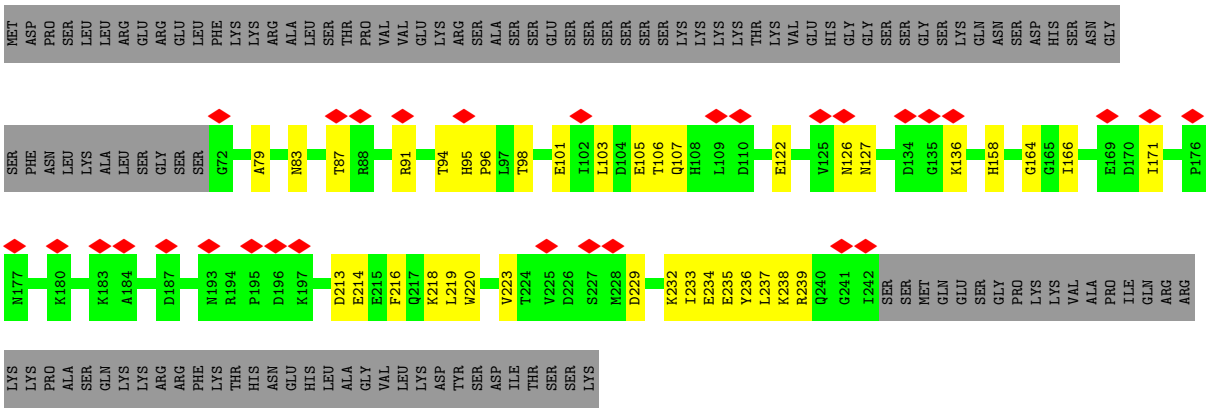




• Molecule 30: Transcription initiation factor IIE subunit beta

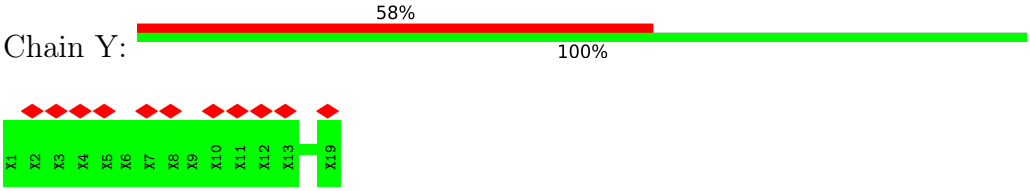
Chain X:





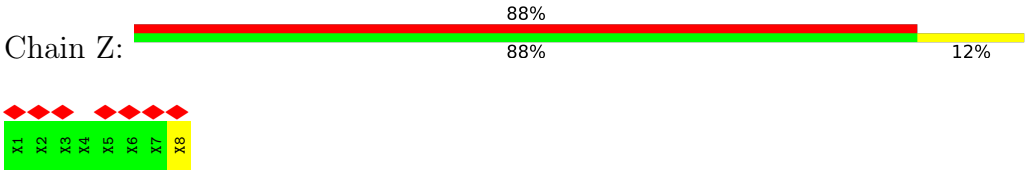
• Molecule 31: Unassigned peptide, likely TFIIE-beta

Chain Y:



• Molecule 32: Unassigned peptide, likely XPB

Chain Z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	11412	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 ($e^-/Å^2$)	41.1	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	27.888	Depositor
Minimum map value	-14.326	Depositor
Average map value	-0.005	Depositor
Map value standard deviation	0.967	Depositor
Recommended contour level	4	Depositor
Map size (Å)	472.49997, 472.49997, 472.49997	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

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

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	0	0.13	0/5875	0.32	0/7955
2	1	0.14	0/2210	0.31	0/2975
3	2	0.13	0/3230	0.29	0/4376
4	3	0.23	0/1241	0.41	0/1665
5	4	0.13	0/2103	0.32	0/2846
6	5	0.11	0/529	0.27	0/714
7	6	0.12	0/2793	0.29	0/3780
8	7	0.13	0/4994	0.32	0/6745
9	A	0.12	0/11479	0.30	0/15496
10	B	0.12	0/9257	0.29	0/12493
11	C	0.12	0/2102	0.28	0/2857
12	D	0.12	0/1064	0.26	0/1428
13	E	0.14	0/1752	0.33	0/2366
14	F	0.12	0/646	0.28	0/871
15	G	0.10	0/1382	0.24	0/1874
16	H	0.11	0/1207	0.30	0/1628
17	I	0.10	0/949	0.26	0/1284
18	J	0.13	0/516	0.28	0/696
19	K	0.13	0/939	0.28	0/1271
20	L	0.12	0/378	0.26	0/500
21	M	0.13	0/1983	0.28	0/2679
22	N	0.18	0/1478	0.42	0/2283
23	O	0.11	0/1448	0.27	0/1948
24	Q	0.10	0/1167	0.26	0/1576
25	R	0.11	0/1817	0.27	0/2445
26	T	0.18	0/1461	0.42	0/2249
27	U	0.12	0/945	0.34	0/1274
28	V	0.13	0/816	0.28	0/1105
29	W	0.25	0/1686	0.49	0/2266
30	X	0.15	0/1427	0.34	0/1916
All	All	0.13	0/68874	0.31	0/93561

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	5751	0	5794	104	0
2	1	2167	0	2175	34	0
3	2	3158	0	3213	45	0
4	3	1225	0	1224	39	0
5	4	2066	0	2097	51	0
6	5	523	0	530	8	0
7	6	2732	0	2698	46	0
8	7	4890	0	4949	76	0
9	A	11274	0	11406	152	0
10	B	9076	0	9116	109	0
11	C	2059	0	2007	27	0
12	D	1050	0	1033	10	0
13	E	1721	0	1737	30	0
14	F	636	0	665	7	0
15	G	1351	0	1358	12	0
16	H	1186	0	1147	9	0
17	I	928	0	859	12	0
18	J	507	0	523	14	0
19	K	920	0	942	17	0
20	L	373	0	378	4	0
21	M	1953	0	1987	16	0
22	N	1318	0	721	19	0
23	O	1422	0	1514	16	0
24	Q	1138	0	1103	8	0
25	R	1788	0	1819	16	0
26	T	1303	0	714	15	0
27	U	930	0	888	14	0
28	V	806	0	818	12	0
29	W	1659	0	1666	69	0
30	X	1403	0	1428	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	Y	95	0	24	0	0
32	Z	40	0	10	1	0
33	0	8	0	0	0	0
34	3	2	0	0	0	0
34	4	2	0	0	0	0
34	6	3	0	0	0	0
34	A	2	0	0	0	0
34	B	1	0	0	0	0
34	C	1	0	0	0	0
34	I	2	0	0	0	0
34	J	1	0	0	0	0
34	L	1	0	0	0	0
34	M	1	0	0	0	0
34	W	1	0	0	0	0
35	A	1	0	0	0	0
All	All	67474	0	66543	896	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 7.

The worst 5 of 896 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)
4:3:8:ARG:NH2	29:W:177:LEU:O	1.88	1.06
1:0:571:THR:OG1	1:0:573:ASP:OD1	1.91	0.88
1:0:722:ARG:NH2	7:6:202:SER:OG	2.09	0.86
3:2:120:ILE:O	5:4:100:LYS:NZ	2.09	0.86
11:C:36:ARG:NH1	19:K:41:THR:OG1	2.09	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	0	710/760 (93%)	680 (96%)	30 (4%)	0	100	100
2	1	253/548 (46%)	241 (95%)	12 (5%)	0	100	100
3	2	380/462 (82%)	366 (96%)	14 (4%)	0	100	100
4	3	147/309 (48%)	138 (94%)	9 (6%)	0	100	100
5	4	259/308 (84%)	253 (98%)	6 (2%)	0	100	100
6	5	64/71 (90%)	63 (98%)	1 (2%)	0	100	100
7	6	341/395 (86%)	328 (96%)	13 (4%)	0	100	100
8	7	601/782 (77%)	570 (95%)	31 (5%)	0	100	100
9	A	1413/1970 (72%)	1377 (98%)	36 (2%)	0	100	100
10	B	1130/1174 (96%)	1094 (97%)	36 (3%)	0	100	100
11	C	253/275 (92%)	249 (98%)	4 (2%)	0	100	100
12	D	126/142 (89%)	125 (99%)	1 (1%)	0	100	100
13	E	207/210 (99%)	201 (97%)	6 (3%)	0	100	100
14	F	77/127 (61%)	76 (99%)	1 (1%)	0	100	100
15	G	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
16	H	146/150 (97%)	140 (96%)	6 (4%)	0	100	100
17	I	112/125 (90%)	105 (94%)	7 (6%)	0	100	100
18	J	62/67 (92%)	60 (97%)	2 (3%)	0	100	100
19	K	113/117 (97%)	112 (99%)	1 (1%)	0	100	100
20	L	42/58 (72%)	39 (93%)	3 (7%)	0	100	100
21	M	248/316 (78%)	242 (98%)	6 (2%)	0	100	100
23	O	177/339 (52%)	175 (99%)	2 (1%)	0	100	100
24	Q	134/517 (26%)	128 (96%)	6 (4%)	0	100	100
25	R	218/249 (88%)	213 (98%)	5 (2%)	0	100	100
27	U	109/376 (29%)	102 (94%)	7 (6%)	0	100	100
28	V	97/109 (89%)	94 (97%)	3 (3%)	0	100	100
29	W	198/439 (45%)	196 (99%)	2 (1%)	0	100	100
30	X	169/291 (58%)	164 (97%)	5 (3%)	0	100	100
All	All	7955/10858 (73%)	7697 (97%)	258 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	0	624/664 (94%)	624 (100%)	0	100	100
2	1	241/484 (50%)	241 (100%)	0	100	100
3	2	342/399 (86%)	342 (100%)	0	100	100
4	3	143/283 (50%)	143 (100%)	0	100	100
5	4	234/272 (86%)	234 (100%)	0	100	100
6	5	59/64 (92%)	59 (100%)	0	100	100
7	6	311/352 (88%)	311 (100%)	0	100	100
8	7	536/688 (78%)	536 (100%)	0	100	100
9	A	1254/1749 (72%)	1254 (100%)	0	100	100
10	B	994/1027 (97%)	994 (100%)	0	100	100
11	C	234/252 (93%)	234 (100%)	0	100	100
12	D	118/126 (94%)	118 (100%)	0	100	100
13	E	191/192 (100%)	191 (100%)	0	100	100
14	F	69/111 (62%)	69 (100%)	0	100	100
15	G	152/153 (99%)	152 (100%)	0	100	100
16	H	129/131 (98%)	129 (100%)	0	100	100
17	I	103/112 (92%)	103 (100%)	0	100	100
18	J	53/56 (95%)	53 (100%)	0	100	100
19	K	104/106 (98%)	104 (100%)	0	100	100
20	L	41/55 (74%)	41 (100%)	0	100	100
21	M	215/268 (80%)	215 (100%)	0	100	100
23	O	154/293 (53%)	154 (100%)	0	100	100
24	Q	121/448 (27%)	121 (100%)	0	100	100
25	R	196/218 (90%)	196 (100%)	0	100	100
27	U	105/324 (32%)	105 (100%)	0	100	100
28	V	90/98 (92%)	90 (100%)	0	100	100

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Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
29	W	182/373 (49%)	181 (100%)	1 (0%)	81 83
30	X	154/261 (59%)	154 (100%)	0	100 100
All	All	7149/9559 (75%)	7148 (100%)	1 (0%)	100 100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
29	W	113	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
16	H	76	ASN
21	M	140	ASN
16	H	133	HIS
19	K	49	GLN
25	R	64	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 19 ligands modelled in this entry, 18 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	1000	1	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	1000	1	-	-	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.

No monomer is involved in short contacts.

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.

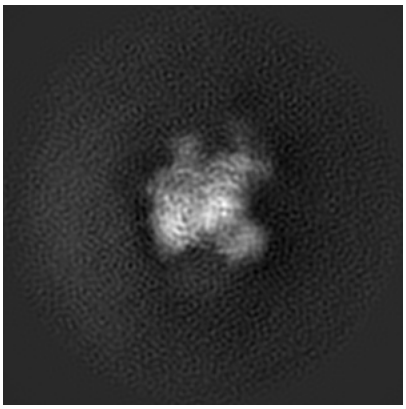
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12618. These allow visual inspection of the internal detail of the map and identification of artifacts.

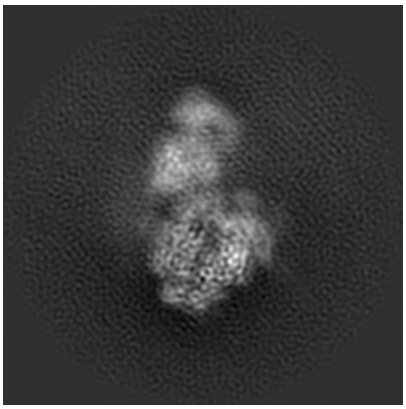
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

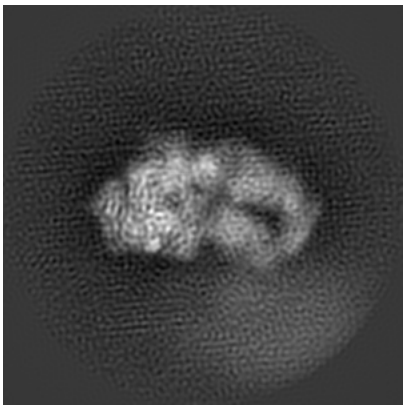
6.1.1 Primary map



X

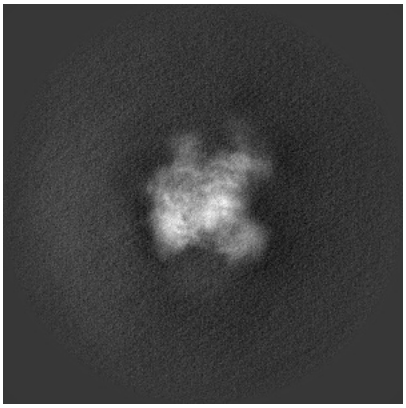


Y

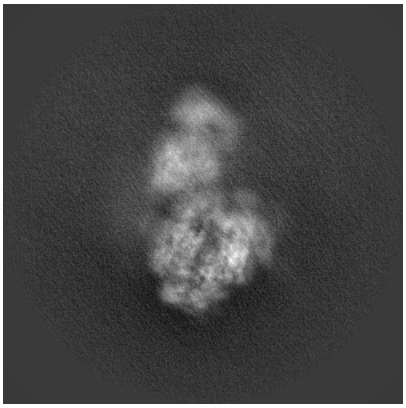


Z

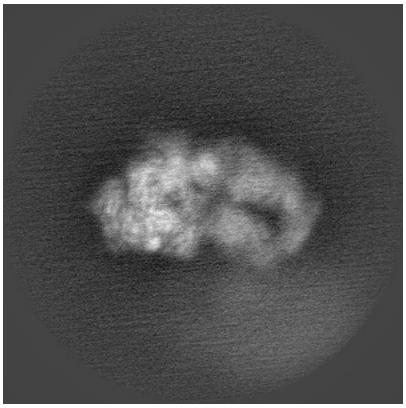
6.1.2 Raw map



X



Y

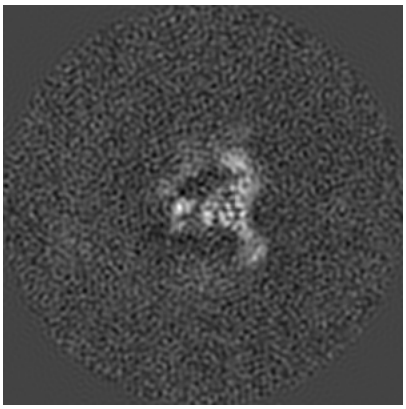


Z

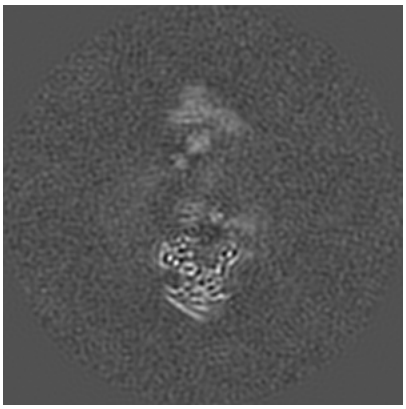
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

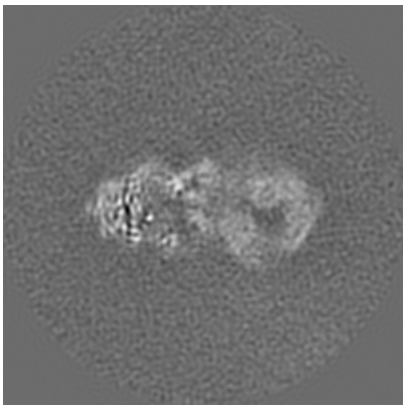
6.2.1 Primary map



X Index: 225

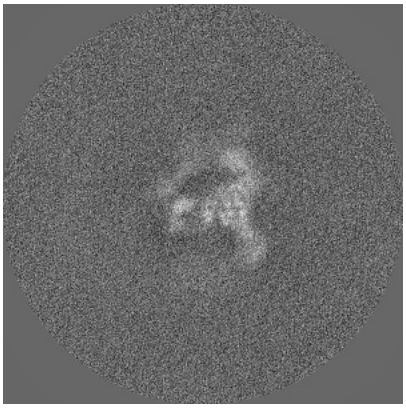


Y Index: 225

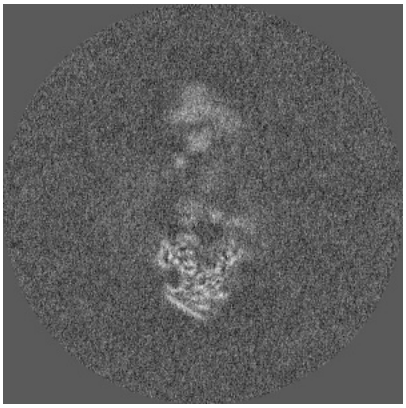


Z Index: 225

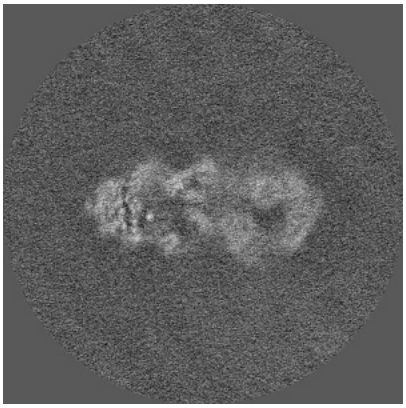
6.2.2 Raw map



X Index: 225



Y Index: 225

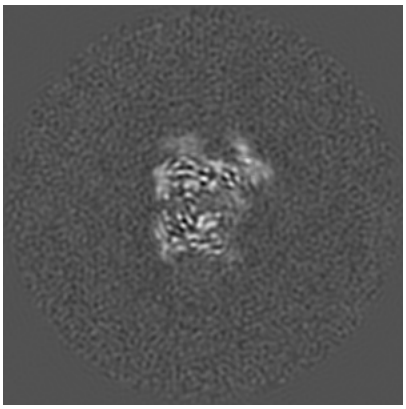


Z Index: 225

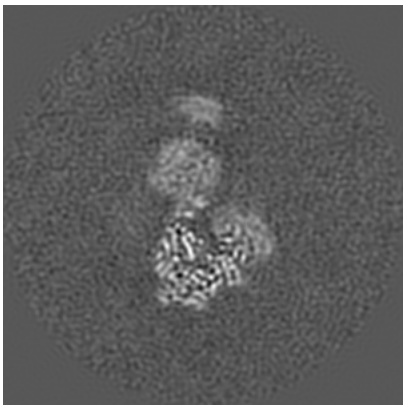
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

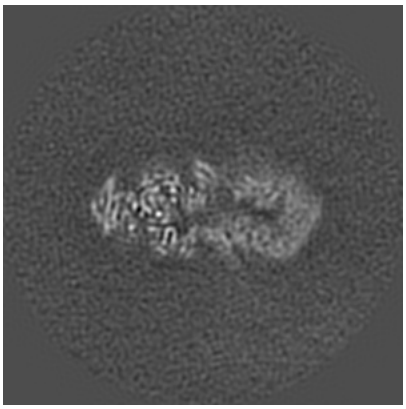
6.3.1 Primary map



X Index: 169

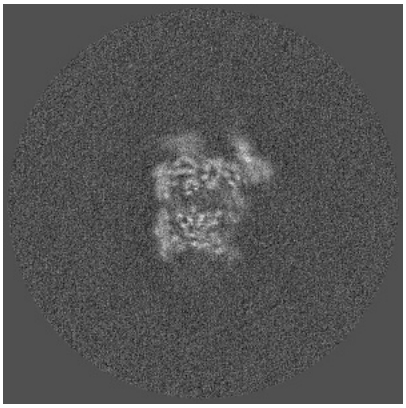


Y Index: 198

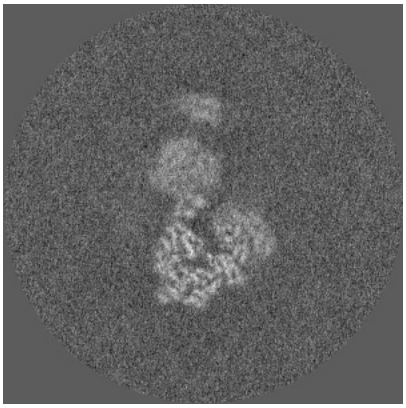


Z Index: 213

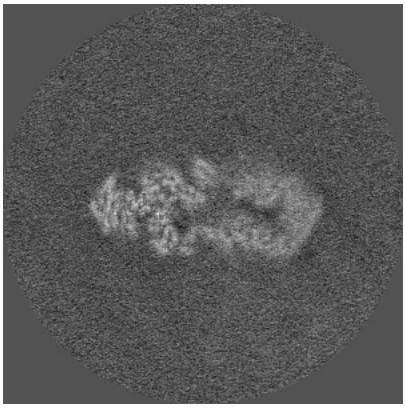
6.3.2 Raw map



X Index: 170



Y Index: 198

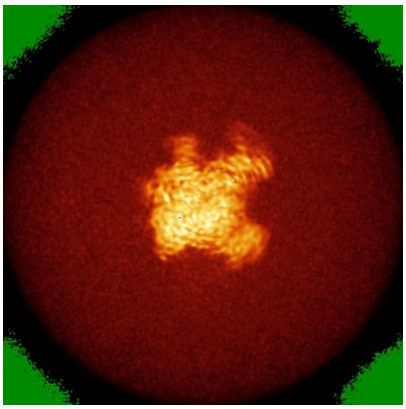


Z Index: 214

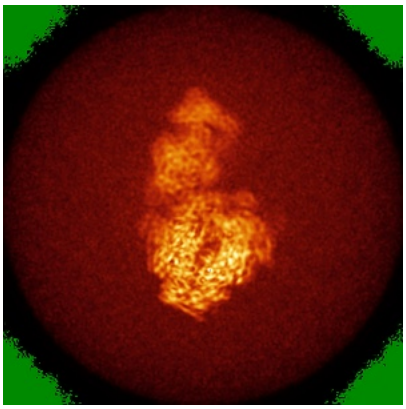
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

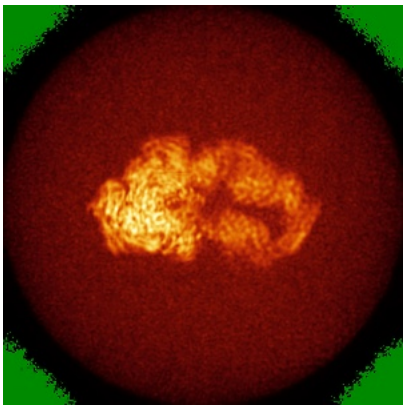
6.4.1 Primary map



X

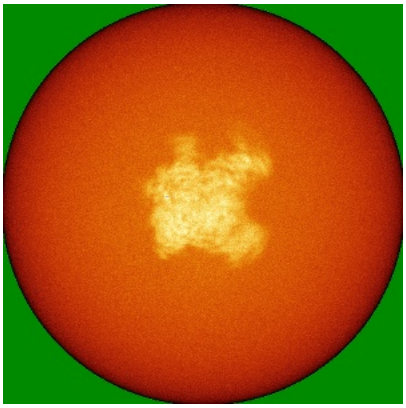


Y

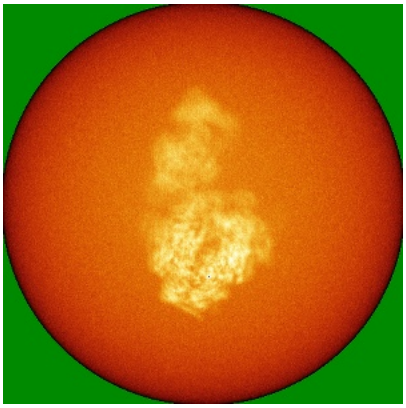


Z

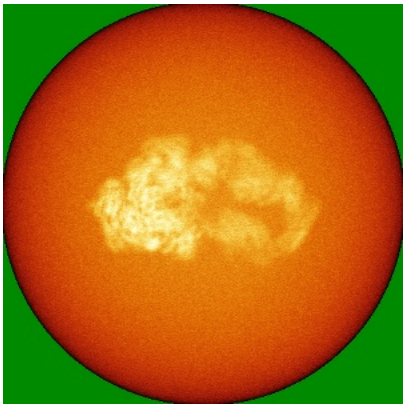
6.4.2 Raw map



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)

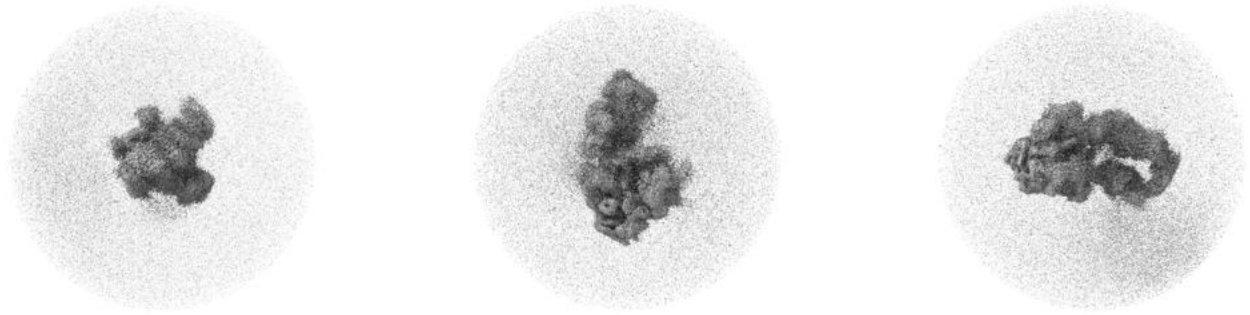
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 4.0. 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.

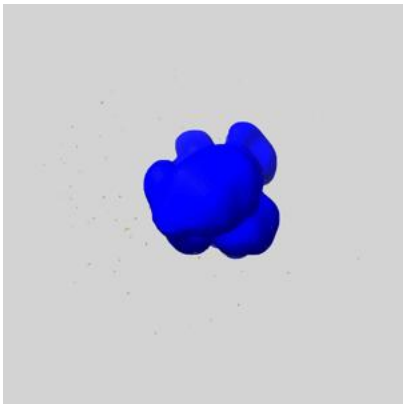
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

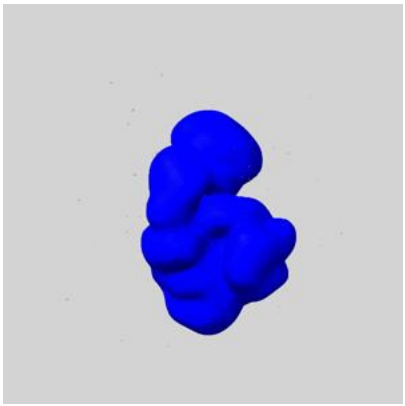
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

6.6.1 emd_12618_msk_1.map (i)



X



Y

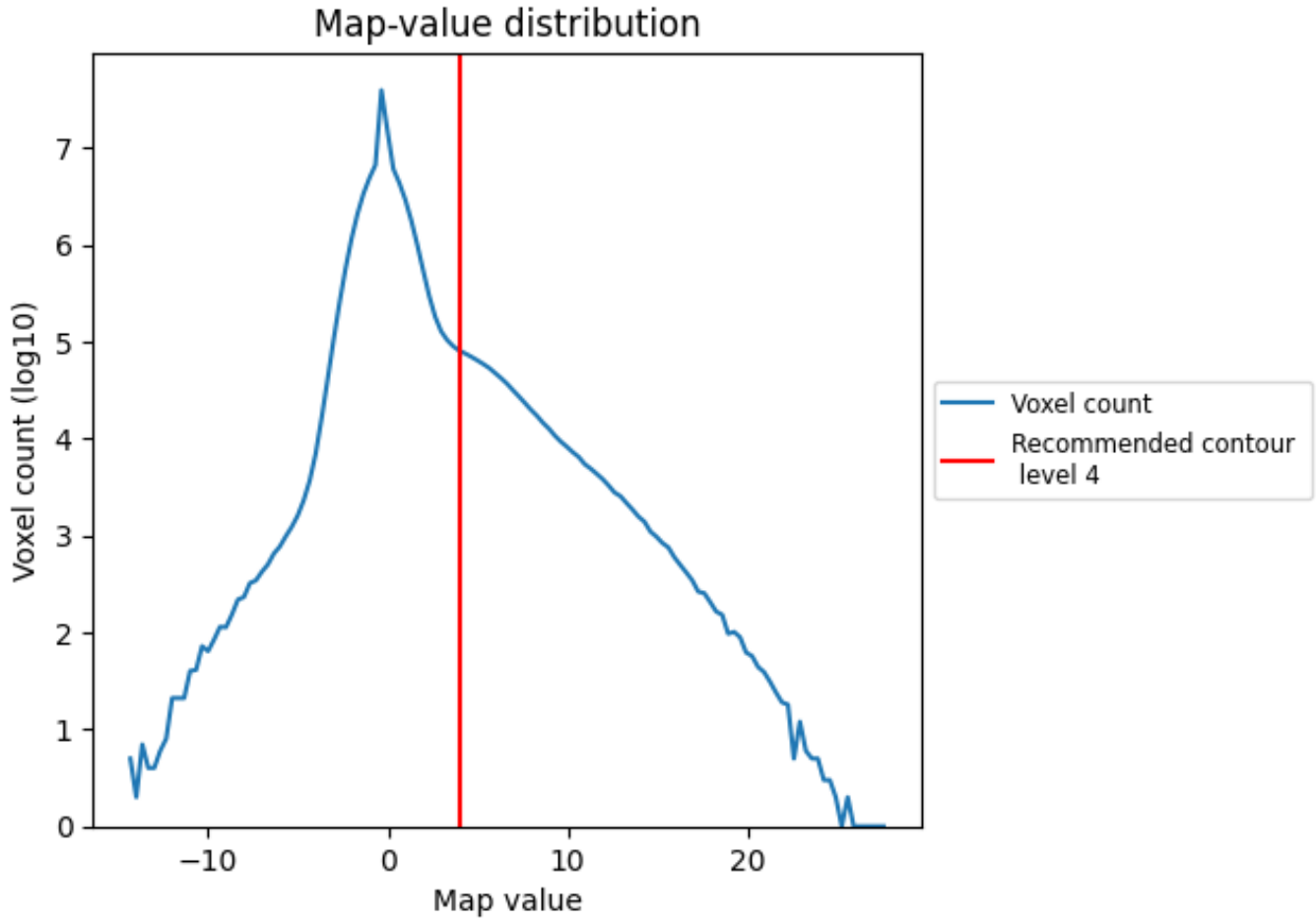


Z

7 Map analysis

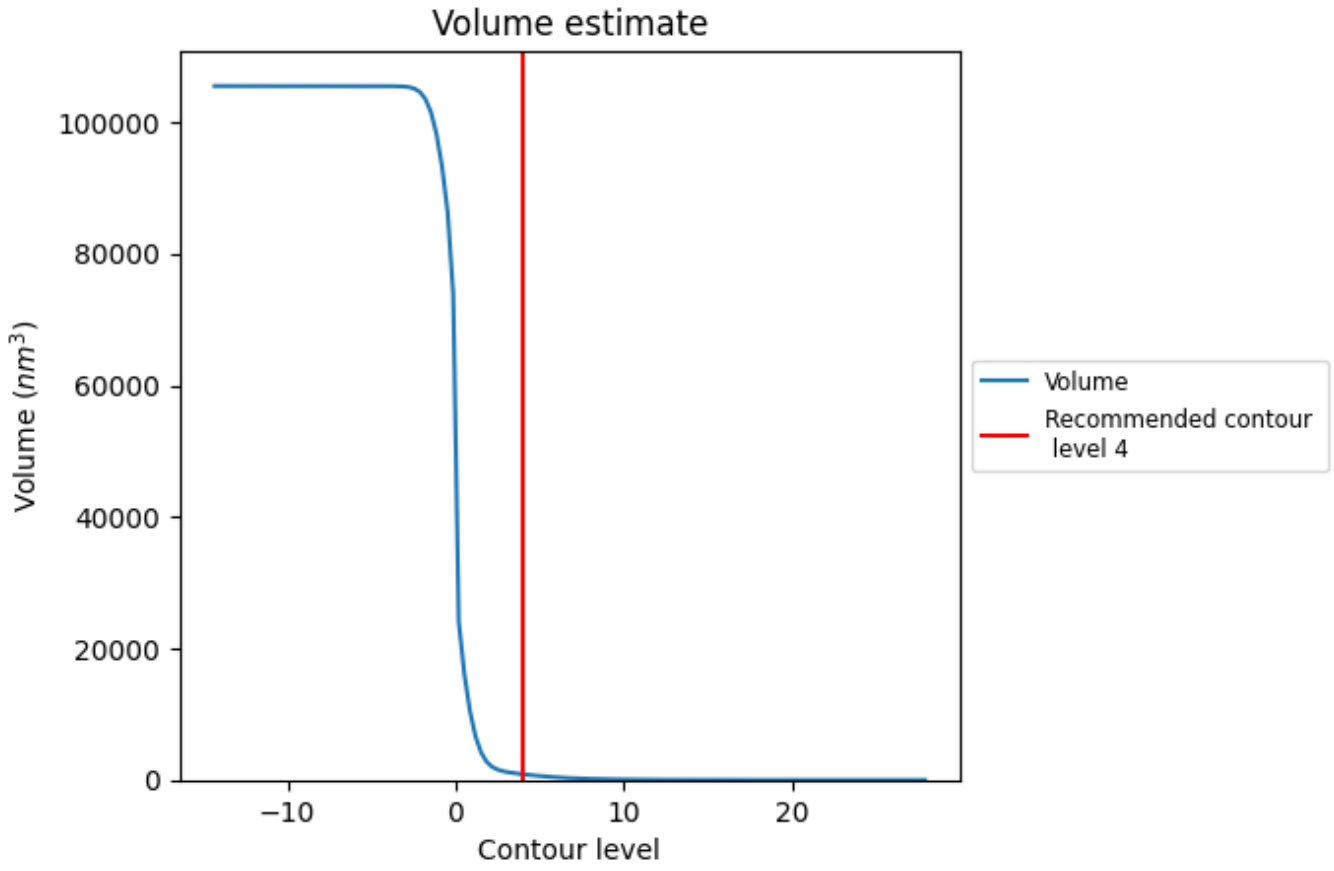
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

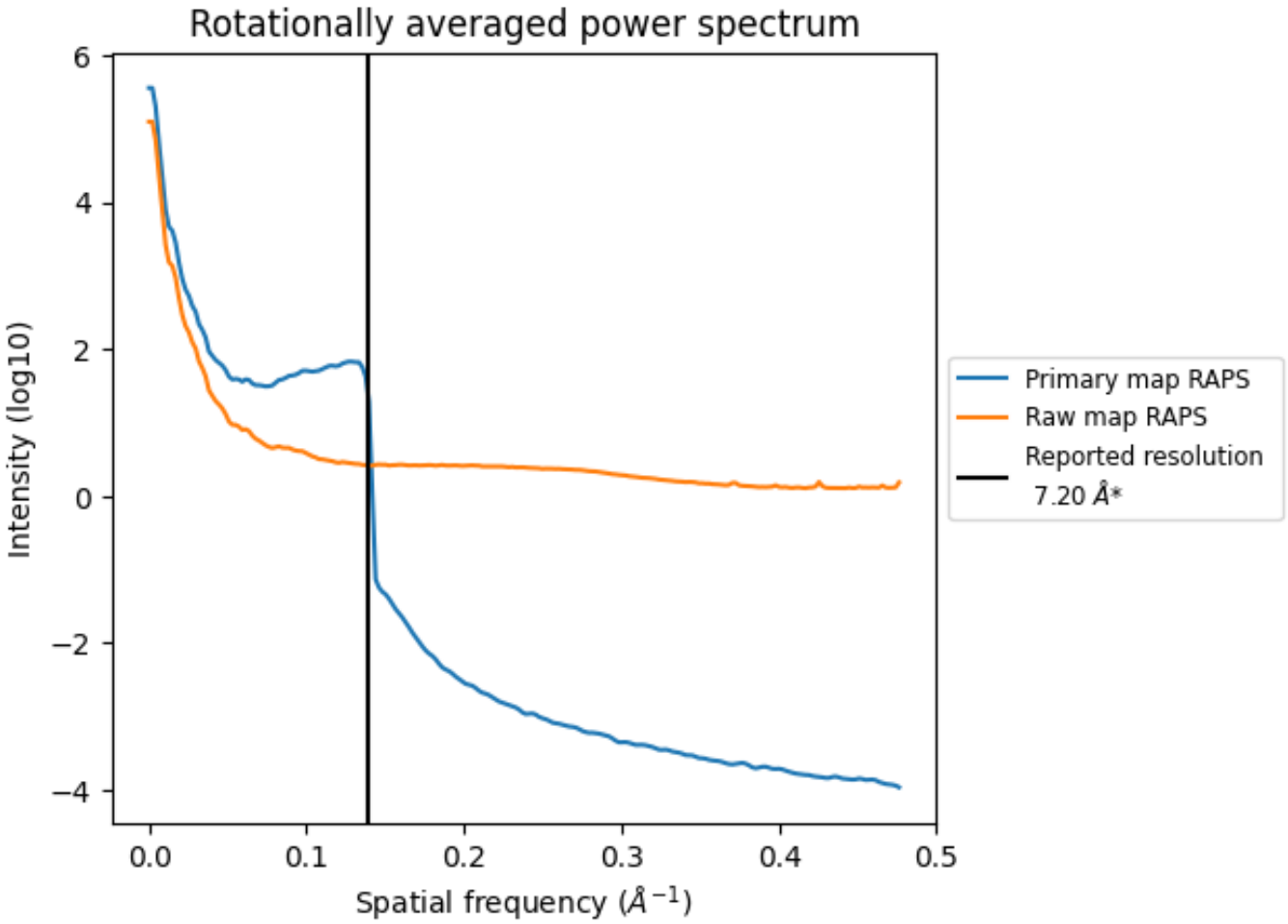
7.2 Volume estimate (i)



The volume at the recommended contour level is 864 nm^3; this corresponds to an approximate mass of 781 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 (i)

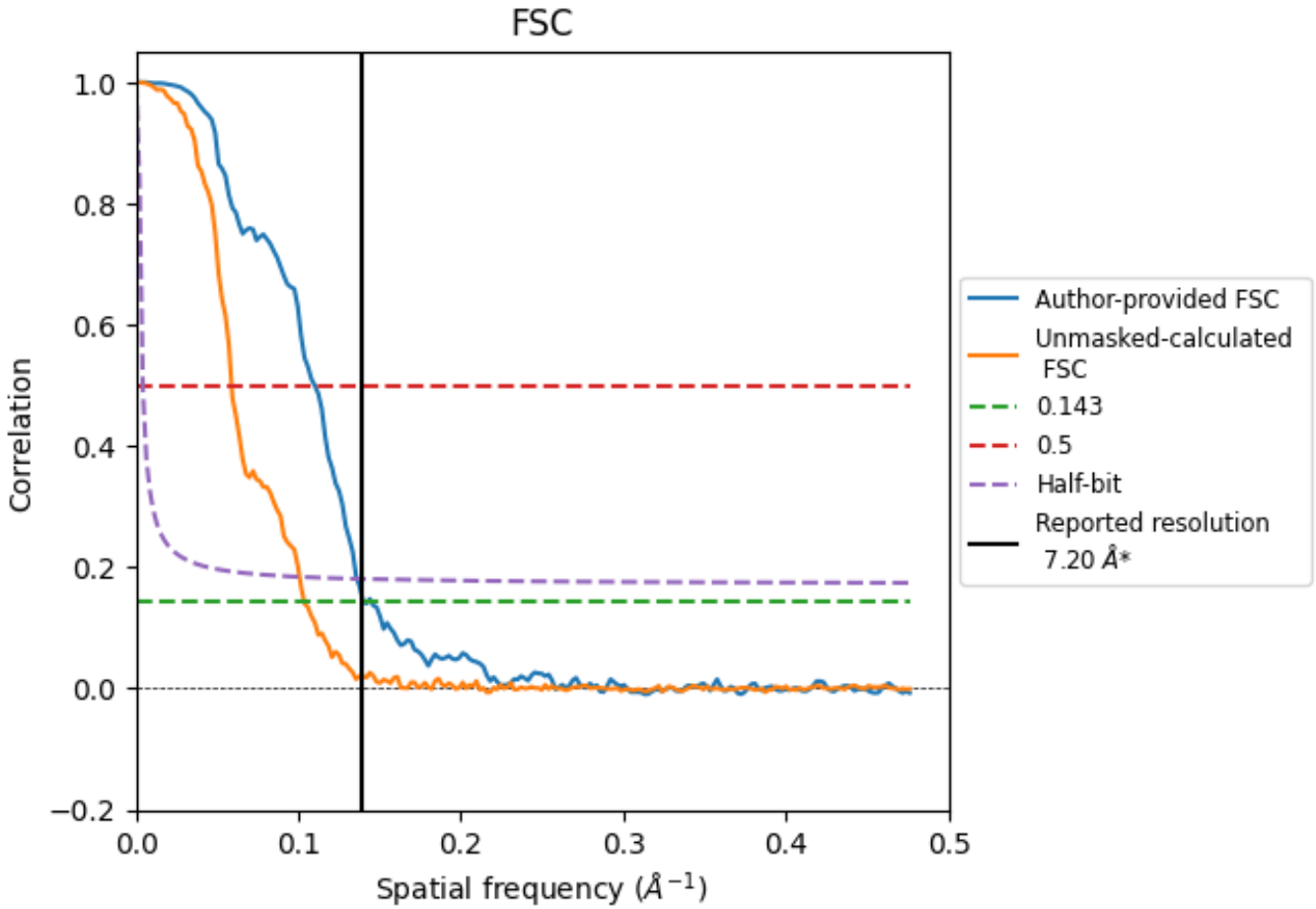


*Reported resolution corresponds to spatial frequency of 0.139 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.139 Å^{-1}

8.2 Resolution estimates (i)

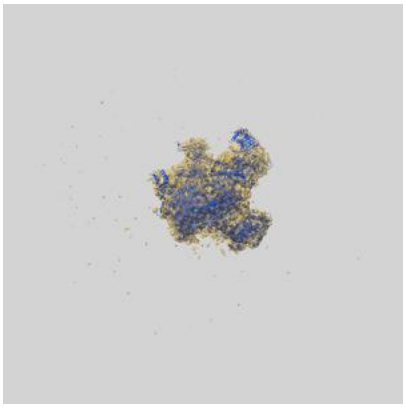
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.20	-	-
Author-provided FSC curve	7.13	9.10	7.35
Unmasked-calculated*	9.66	17.01	9.94

*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 9.66 differs from the reported value 7.2 by more than 10 %

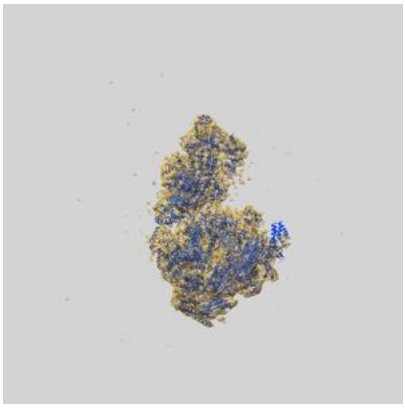
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12618 and PDB model 7NVZ. Per-residue inclusion information can be found in section 3 on page 12.

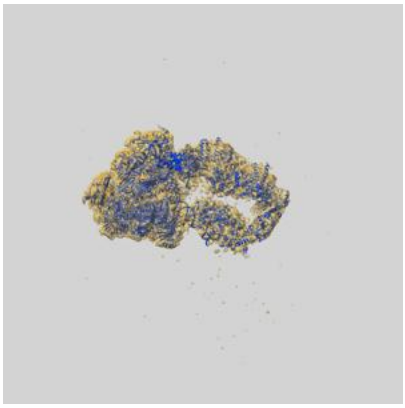
9.1 Map-model overlay



X



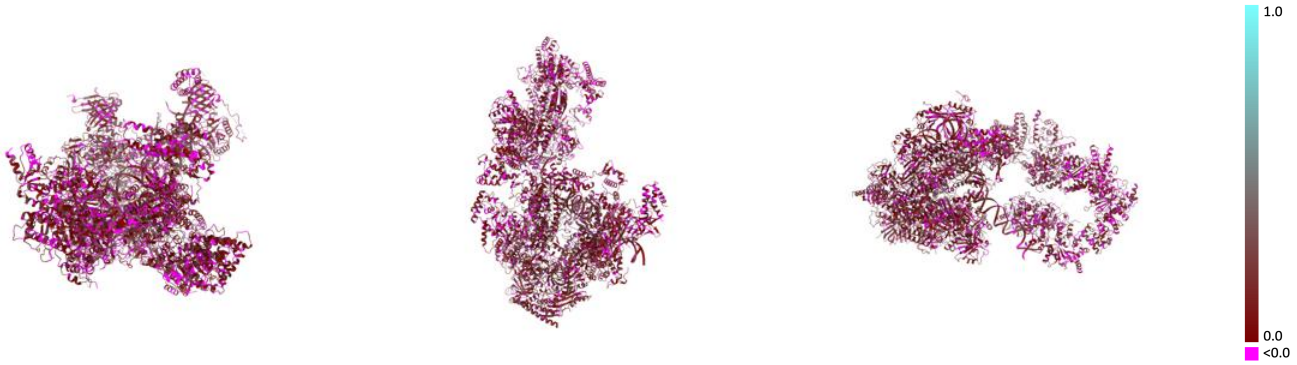
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.0 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.

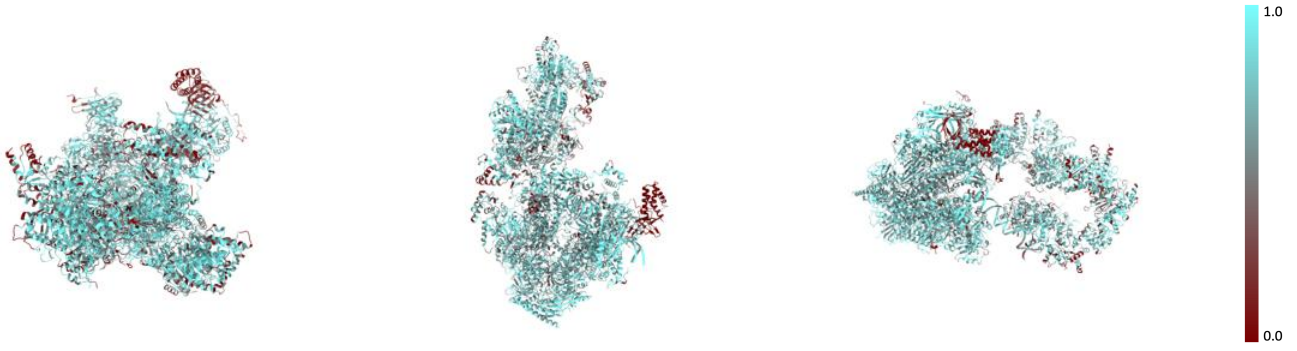
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according 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.

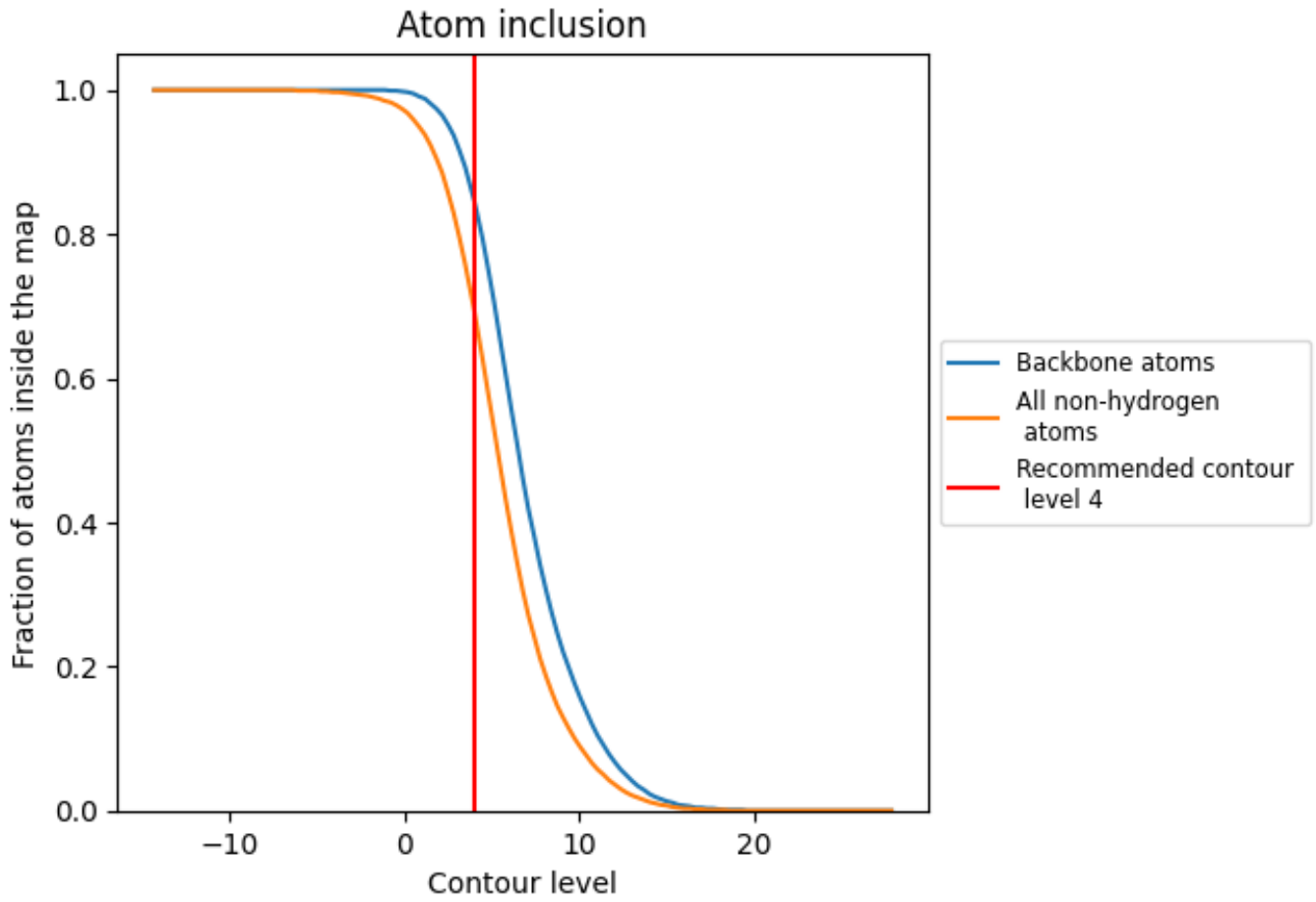
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (4).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 69% 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 (4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6940	0.1110
0	0.7350	0.0990
1	0.5210	0.0610
2	0.6720	0.0790
3	0.5530	0.0920
4	0.7020	0.0680
5	0.5690	0.1000
6	0.7290	0.0770
7	0.6750	0.0790
A	0.7090	0.1350
B	0.7140	0.1320
C	0.8080	0.1380
D	0.5930	0.0890
E	0.7240	0.1480
F	0.7490	0.1340
G	0.7370	0.0990
H	0.7870	0.1240
I	0.8150	0.1320
J	0.7370	0.1240
K	0.7460	0.1420
L	0.8120	0.1560
M	0.7310	0.1420
N	0.7970	0.1650
O	0.7660	0.0970
Q	0.7100	0.1100
R	0.6950	0.1060
T	0.8150	0.1550
U	0.1460	0.0370
V	0.1420	0.0420
W	0.6650	0.0970
X	0.7240	0.1160
Y	0.3370	0.0640
Z	0.2000	0.1200

