wwPDB EM Validation Summary Report

Nov 20, 2022 – 02:02 PM EST

PDB ID	:	7ML2
EMDB ID	:	EMD-23906
Title	:	RNA polymerase II pre-initiation complex (PIC3)
Authors	:	Yang, C.; Fujiwara, R.; Kim, H.J.; Gorbea Colon, J.J.; Steimle, S.; Garcia, B.A.; Murakami, K.
Deposited on	:	2021-04-27
Resolution	:	3.40 Å(reported)
Based on initial model	:	5OQJ

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 (i) 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 (i)) were used in the production of this report:

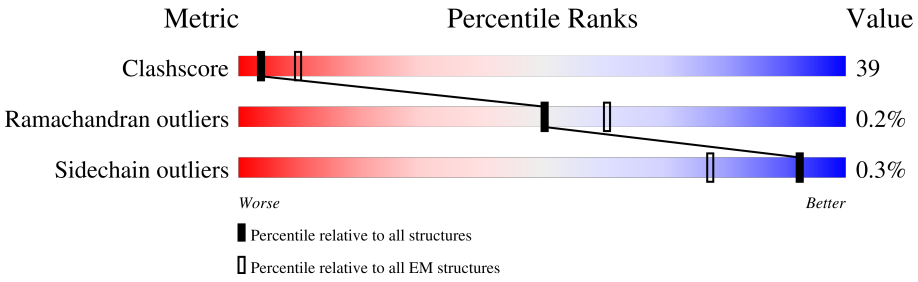
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.40 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1733	35% 45% 19%
2	B	1224	44% 49% 6%
3	C	318	34% 48% 18%
4	D	221	57% 20% 51% 29%
5	E	215	42% 57%
6	F	155	18% 35% 46%
7	G	171	46% 29% 71%
8	H	146	10% 21% 71% 7%

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Mol	Chain	Length	Quality of chain
9	I	122	21% 30% 64% 5%
10	J	70	24% 66% 7%
11	K	120	13% 35% 57% 7%
12	L	70	16% 19% 37% 9% 36%
13	M	345	24% 27% 53% 19%
14	Q	735	8% 12% 80%
15	R	400	13% 26% 22% 52%
16	U	286	16% 8% 8% 84%
17	V	122	36% 14% 26% 60%
18	W	482	23% 20% 20% 60%
19	X	328	20% 33% 14% 52%
20	T	56	14% 41% 54% 5%
21	N	56	18% 23% 68% 9%
22	O	240	10% 34% 41% 25%
23	1	542	23% 42% 26% 32%
24	4	338	11% 42% 41% 16%
25	0	778	27% 38% 58%
26	6	461	13% 35% 41% 24%
27	2	513	24% 50% 39% 10%
28	5	72	33% 36% 56% 8%
29	7	843	28% 31% 43% 25%
30	3	321	26% 21% 22% 57%

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 (i)

There are 33 unique types of molecules in this entry. The entry contains 64550 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1398	10997	6931	1927	2078	61	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1152	9178	5807	1608	1708	55	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	262	2061	1299	343	406	13	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	157	1253	779	220	252	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	213	1744	1107	308	318	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	83	670	428	114	125	3	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1340	861	222	249	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	136	Total	C	N	O	S	0	0
			1089	686	184	215	4		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	116	Total	C	N	O	S	0	0
			944	581	172	181	10		

- Molecule 10 is a protein called DNA-directed RNA polymerases II subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	65	Total	C	N	O	S	0	0
			532	339	93	94	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	112	Total	C	N	O	S	0	0
			904	580	154	168	2		

- Molecule 12 is a protein called DNA-directed RNA polymerases II subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	45	Total	C	N	O	S	0	0
			358	221	71	62	4		

- Molecule 13 is a protein called Transcription initiation factor IIB.

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

- Molecule 14 is a protein called Transcription initiation factor IIF subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Q	148	Total	C	N	O	S	0	0
			1144	733	195	212	4		

- Molecule 15 is a protein called Transcription initiation factor IIF subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	190	Total	C	N	O	S	0	0
			1303	812	238	246	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	U	46	Total	C	N	O	S	0	0
			383	242	67	71	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	V	49	Total	C	N	O	S	0	0
			381	241	63	74	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	191	Total	C	N	O	S	0	0
			1469	932	254	277	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	X	156	Total	C	N	O	S	0	0
			984	608	180	192	4		

- Molecule 20 is a DNA chain called template strand DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	56	Total	C	N	O	P	0	0
			1140	550	188	346	56		

- Molecule 21 is a DNA chain called non-template strand DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	N	56	Total	C	N	O	P	0	0
			1156	552	222	326	56		

- Molecule 22 is a protein called BJ4_G0004860.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	O	180	Total	C	N	O	S	0	0
			1416	921	242	247	6		

- Molecule 23 is a protein called Tfb1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	1	367	Total	C	N	O	S	0	0
			2411	1536	438	430	7		

- Molecule 24 is a protein called Tfb4.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	4	284	Total	C	N	O	S	0	0
			2041	1310	343	376	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	0	754	Total	C	N	O	S	0	0
			6108	3891	1032	1147	38		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	6	351	Total	C	N	O	S	0	0
			2527	1590	454	456	27		

- Molecule 27 is a protein called RNA polymerase II transcription factor B subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	2	460	Total	C	N	O	S	0	0
			3011	1856	562	584	9		

- 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 protein called General transcription and DNA repair factor IIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	7	634	Total	C	N	O	S	0	0
			4447	2722	827	874	24		

- Molecule 30 is a protein called BJ4_G0050160.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	3	138	Total	C	N	O	S	0	0
			860	533	160	160	7		

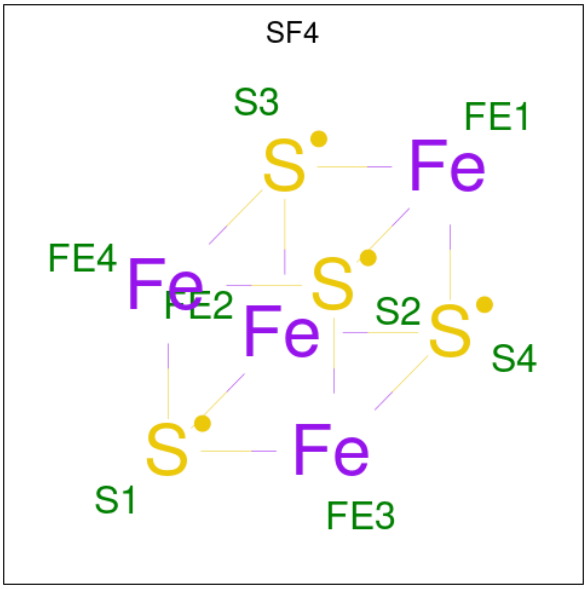
- Molecule 31 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
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	
31	L	1	Total	Zn	0
			1	1	
31	M	1	Total	Zn	0
			1	1	
31	W	1	Total	Zn	0
			1	1	
31	4	1	Total	Zn	0
			1	1	
31	6	4	Total	Zn	0
			4	4	
31	3	2	Total	Zn	0
			2	2	

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 33 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



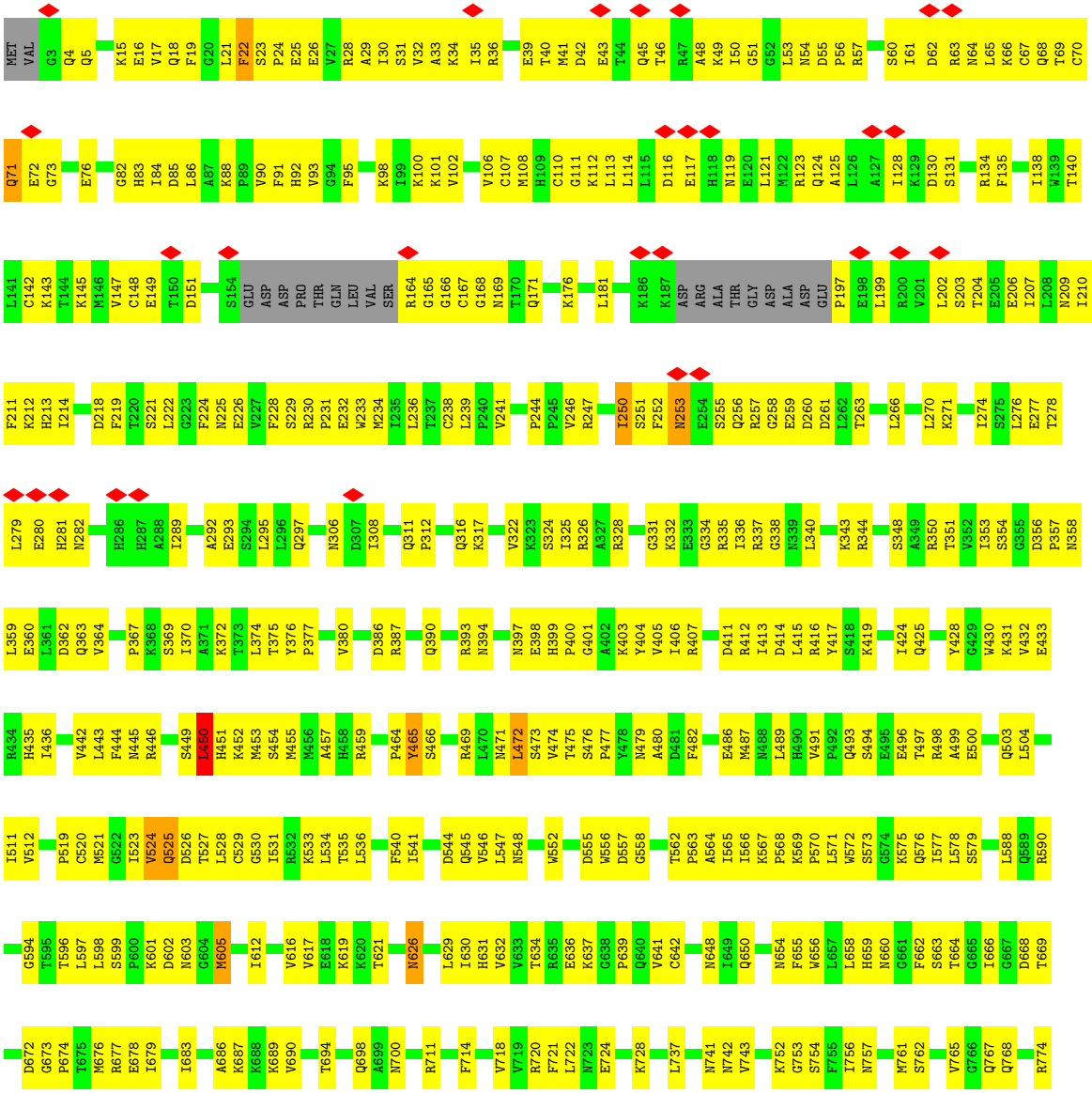
Mol	Chain	Residues	Atoms	AltConf
33	0	1	Total Fe S 8 4 4	0

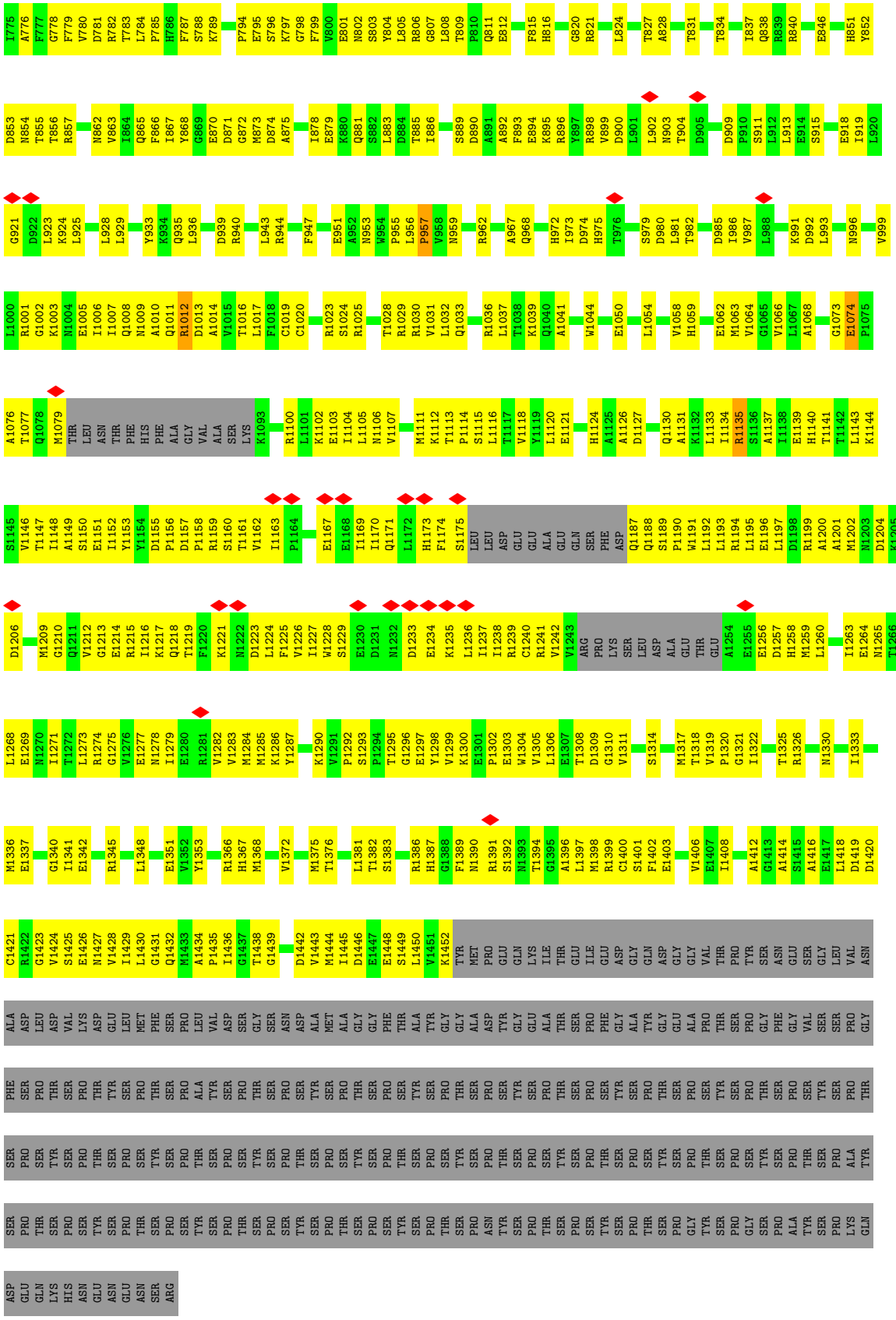
3 Residue-property plots (i)

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: DNA-directed RNA polymerase subunit

Chain A:



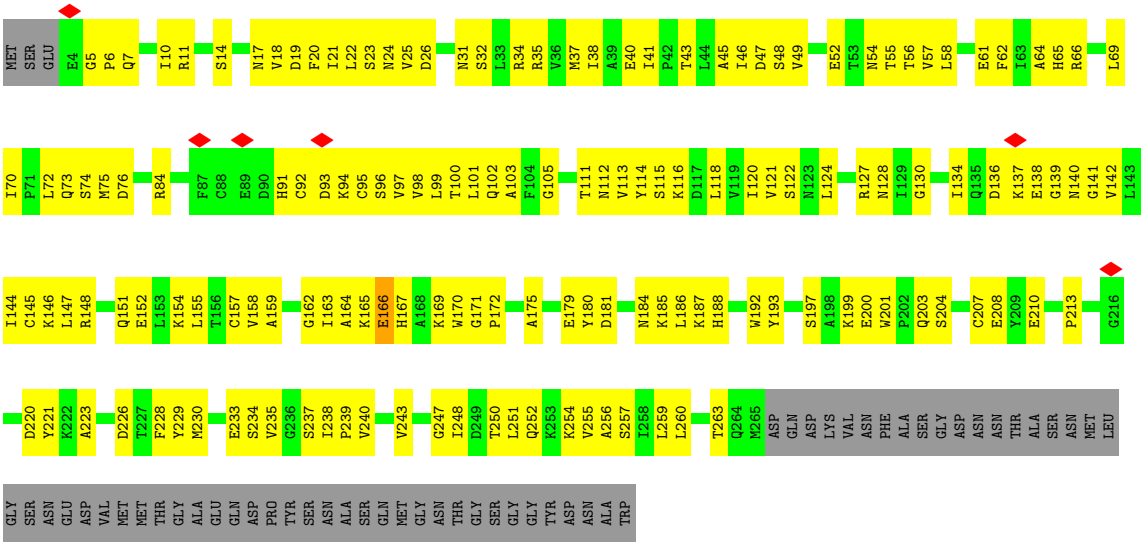


• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain B:

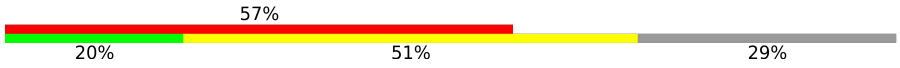
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

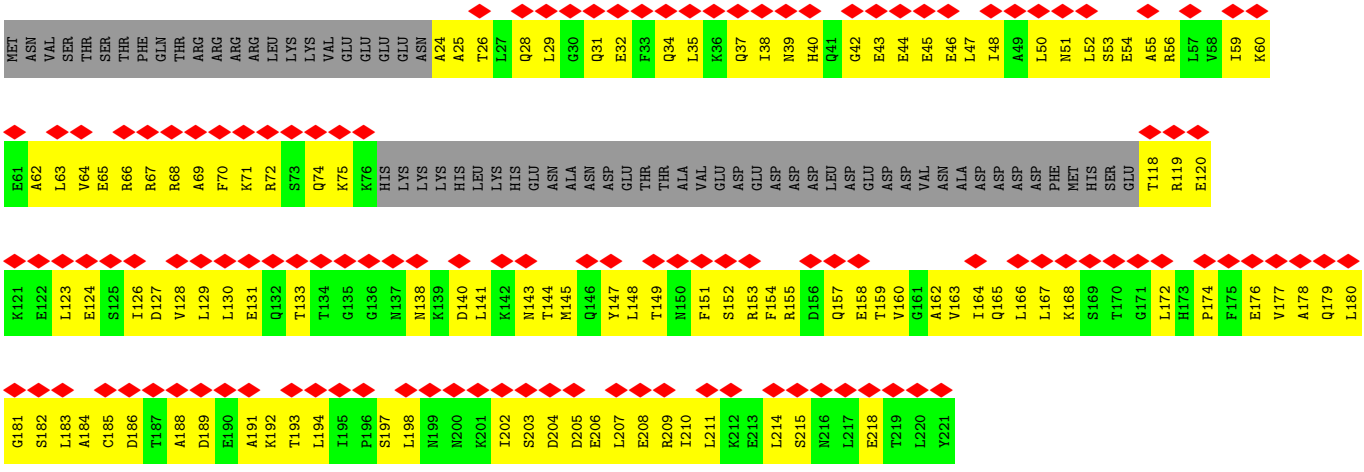
Chain C:



• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

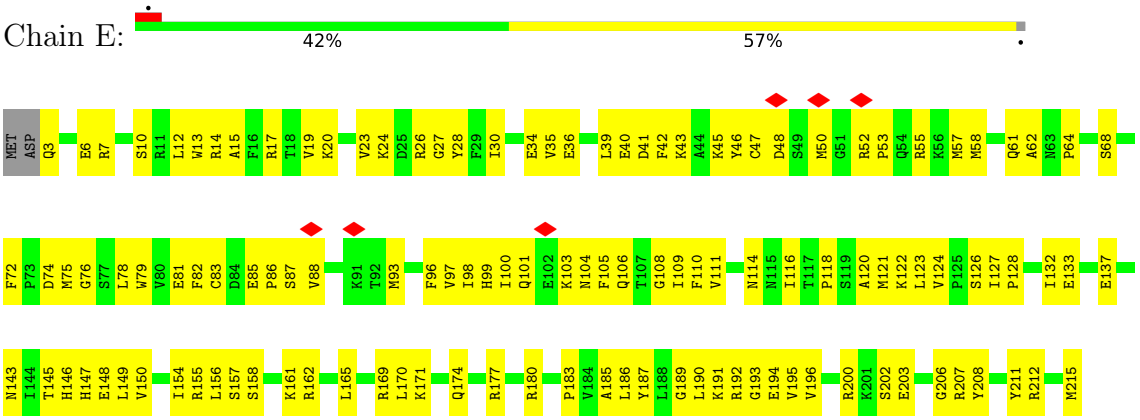
Chain D:





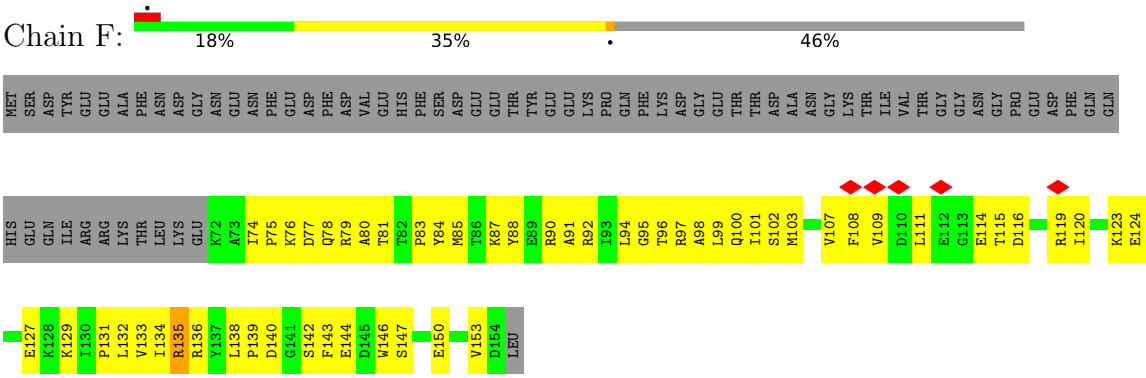
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:



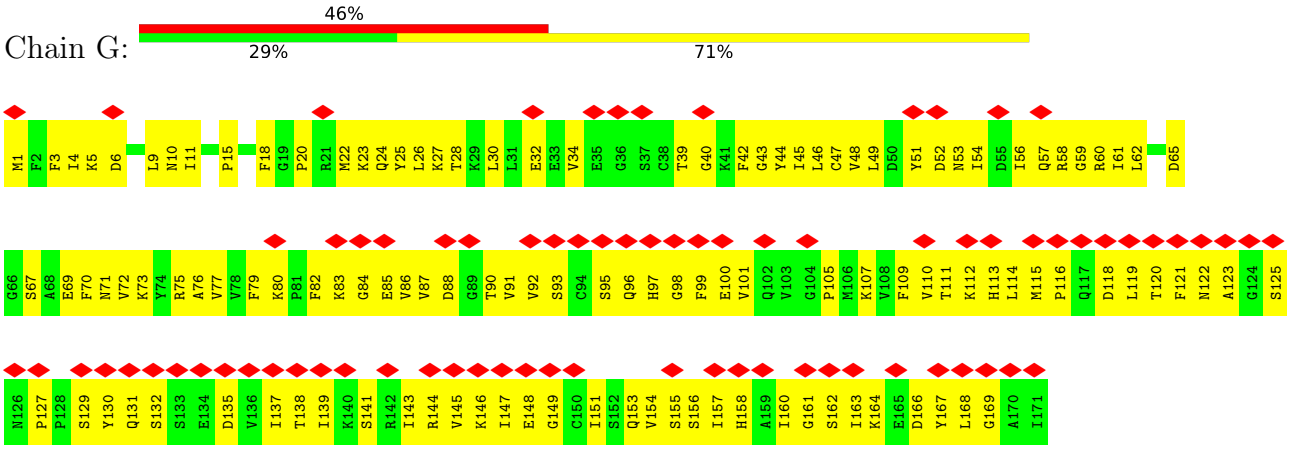
• Molecule 6: DNA-directed RNA polymerases I,II,and III subunit RPABC2

Chain F:



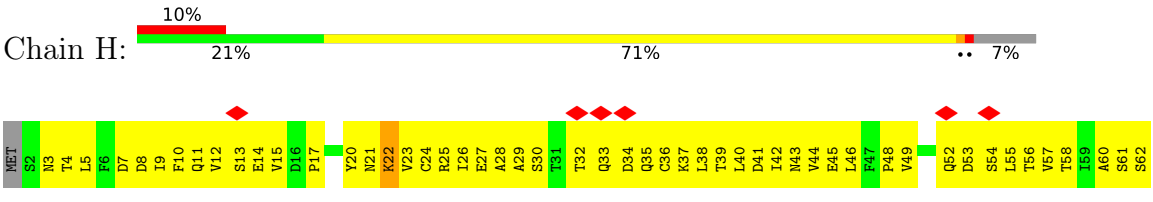
• Molecule 7: DNA-directed RNA polymerase II subunit RPB7

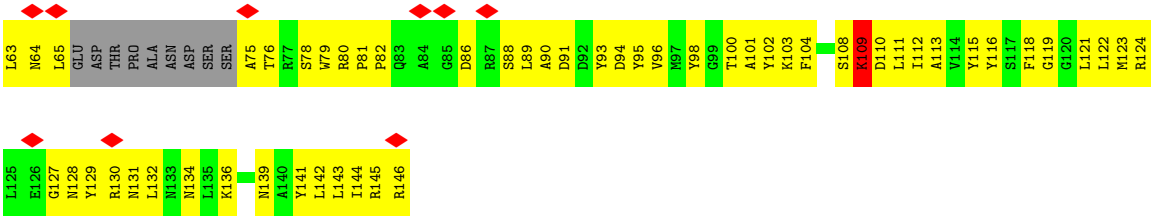
Chain G:



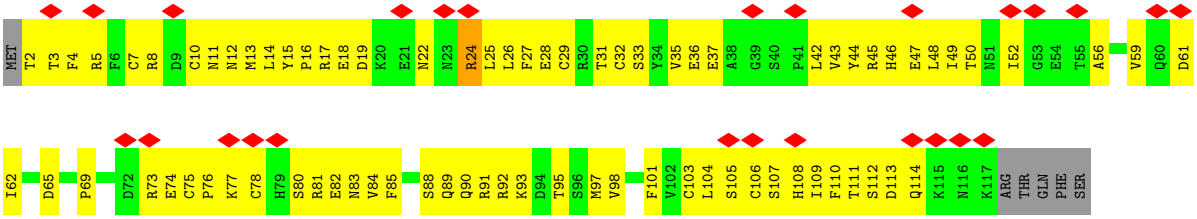
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:

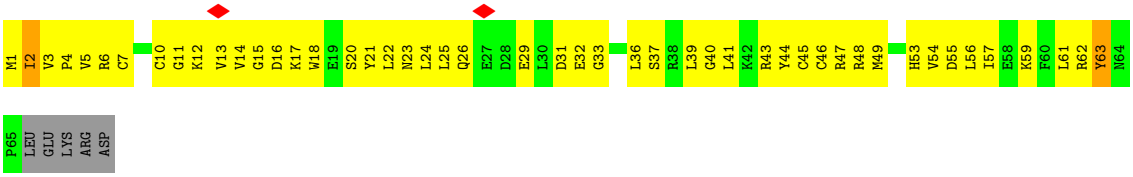




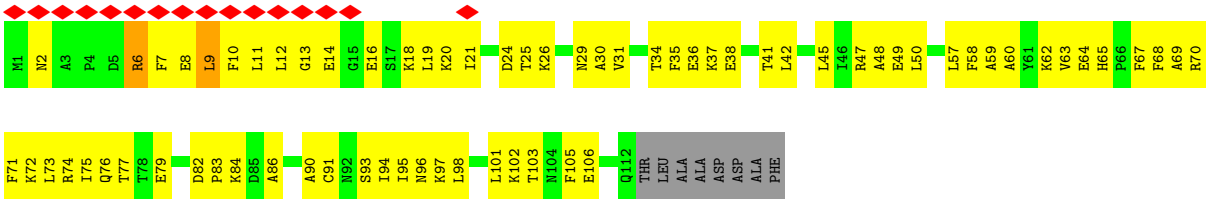
• Molecule 9: DNA-directed RNA polymerase II subunit RPB9



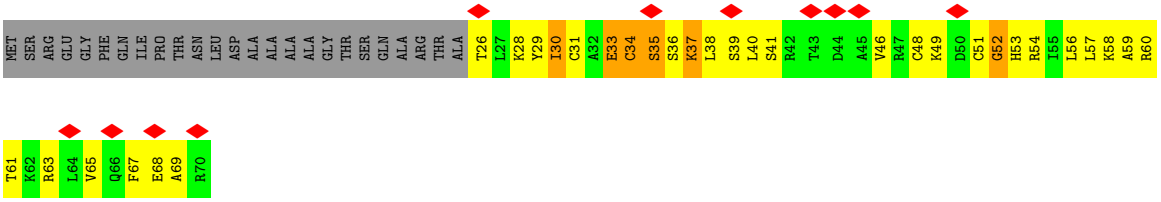
• Molecule 10: DNA-directed RNA polymerases II subunit RPABC5



• Molecule 11: DNA-directed RNA polymerase II subunit RPB11

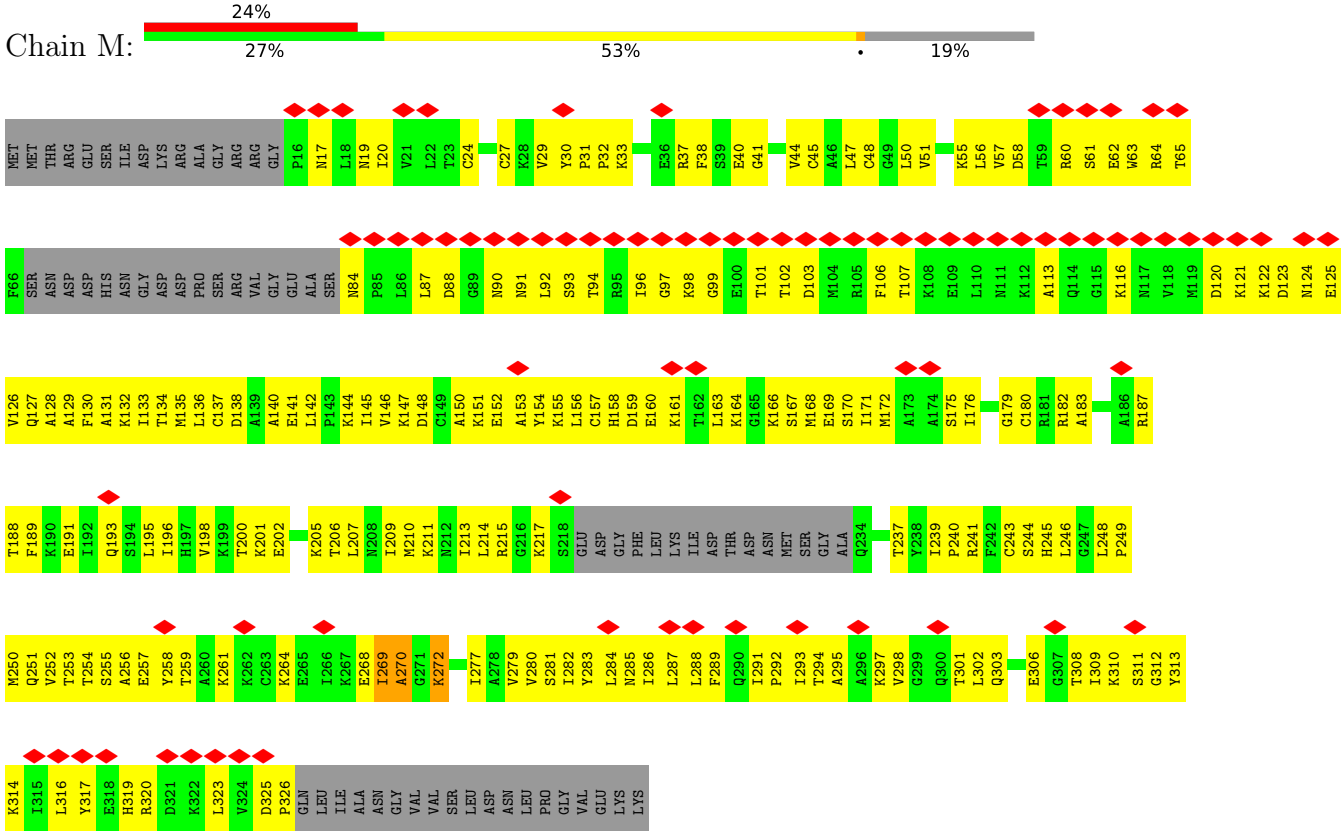


• Molecule 12: DNA-directed RNA polymerases II subunit RPABC4



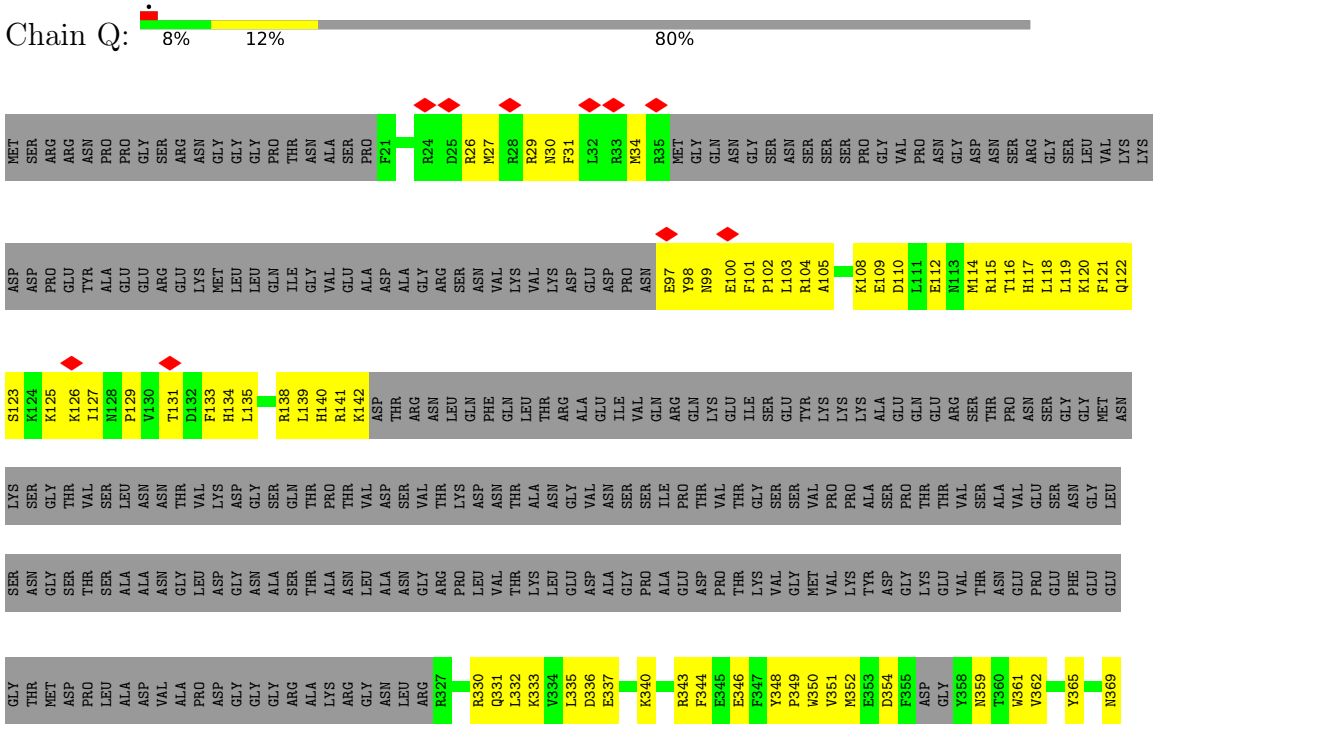
• Molecule 13: Transcription initiation factor IIB

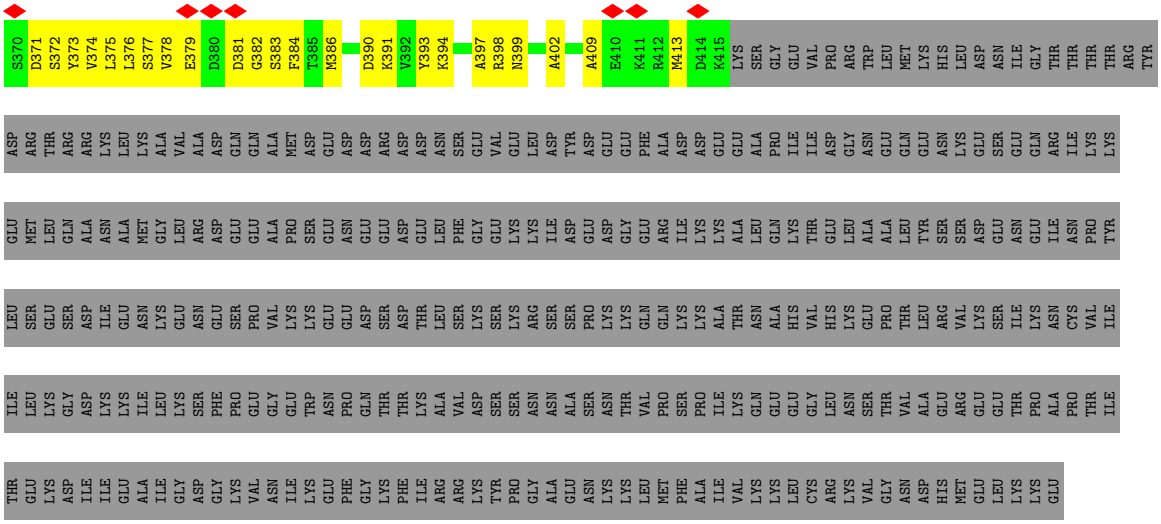
Chain M:



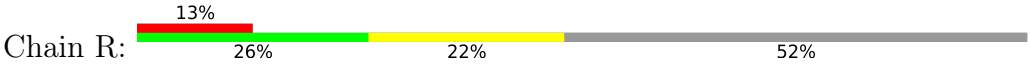
• Molecule 14: Transcription initiation factor IIF subunit alpha

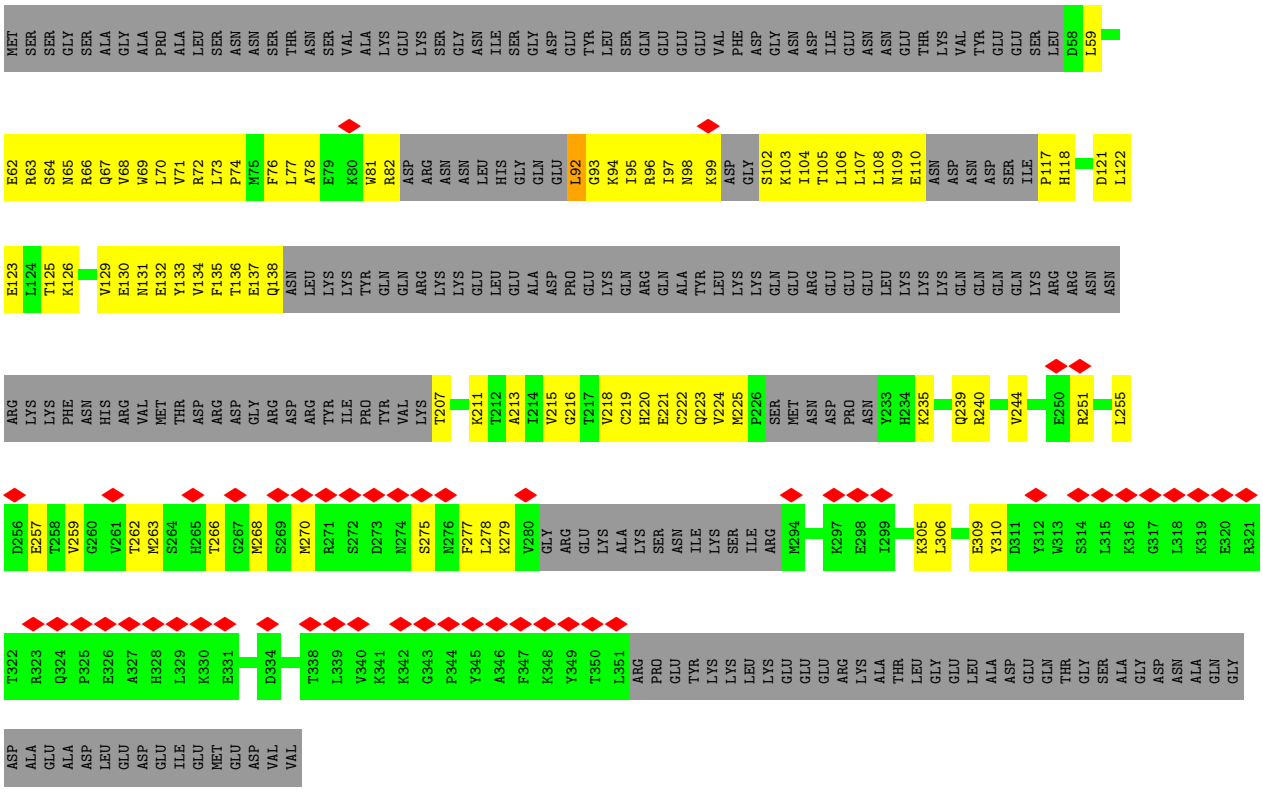
Chain Q:



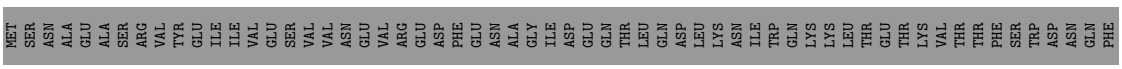


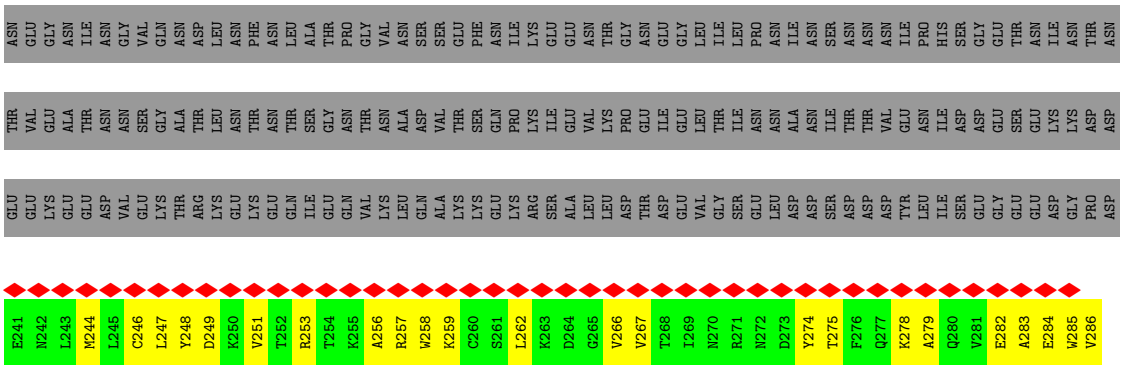
• Molecule 15: Transcription initiation factor IIF subunit beta



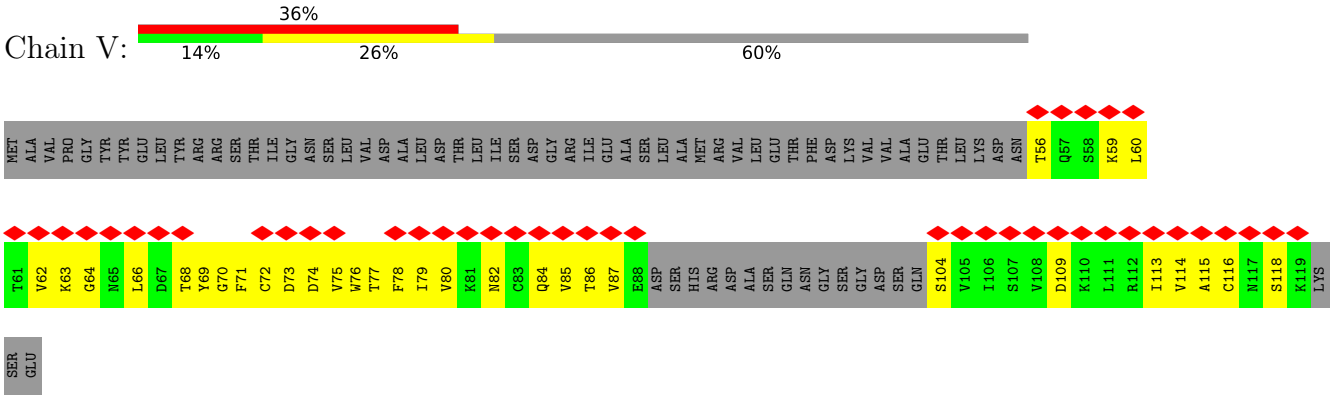


• Molecule 16: Transcription initiation factor IIA large subunit

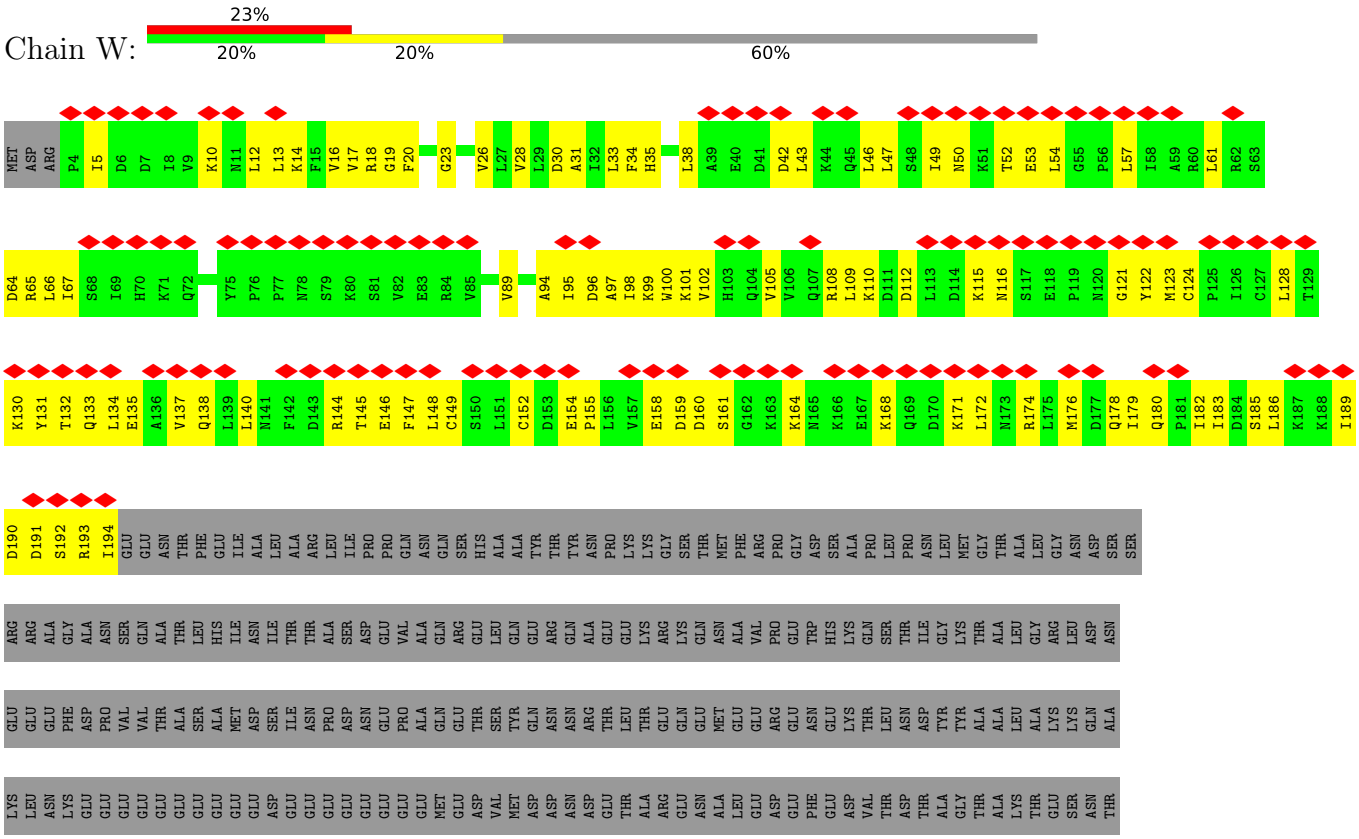




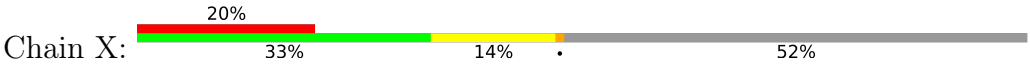
• Molecule 17: Transcription initiation factor IIA subunit 2

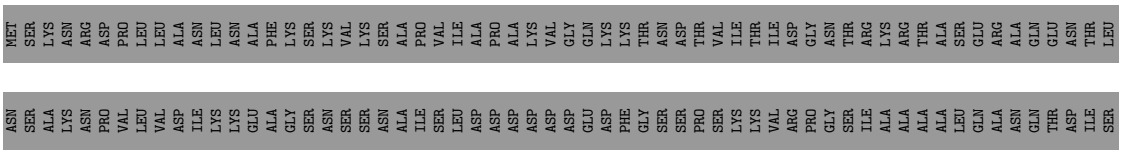


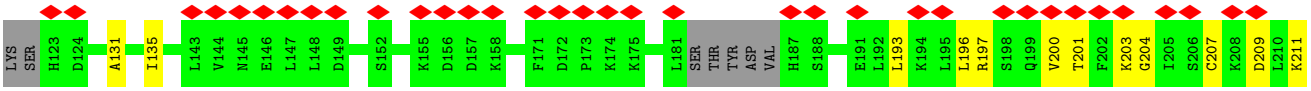
• Molecule 18: Transcription initiation factor IIE subunit alpha

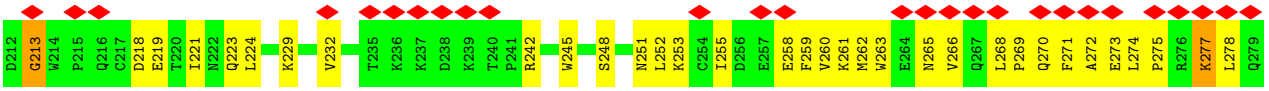


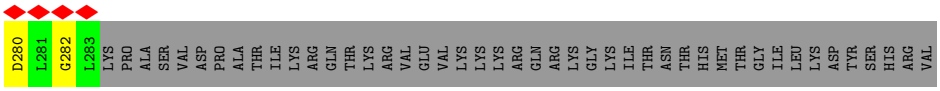
• Molecule 19: Transcription initiation factor IIE subunit beta



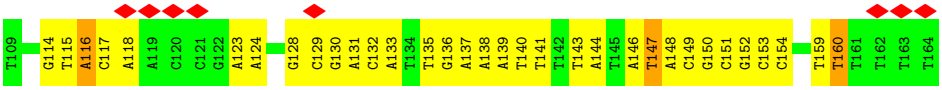




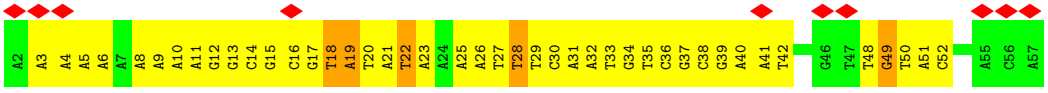




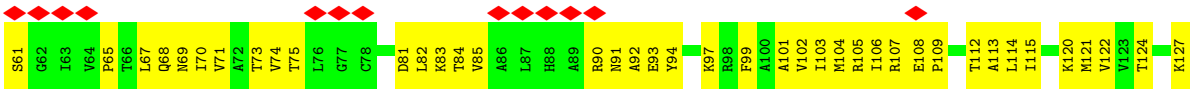
• Molecule 20: template strand DNA

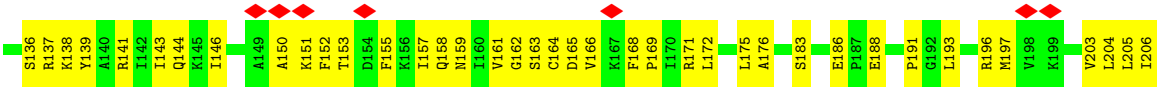


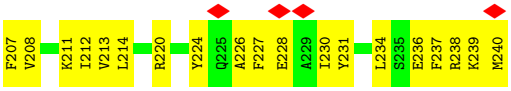
• Molecule 21: non-template strand DNA



• Molecule 22: BJ4_G0004860.mRNA.1.CDS.1

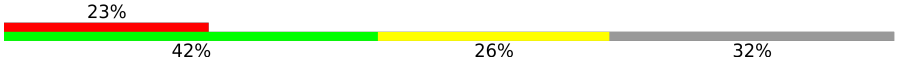


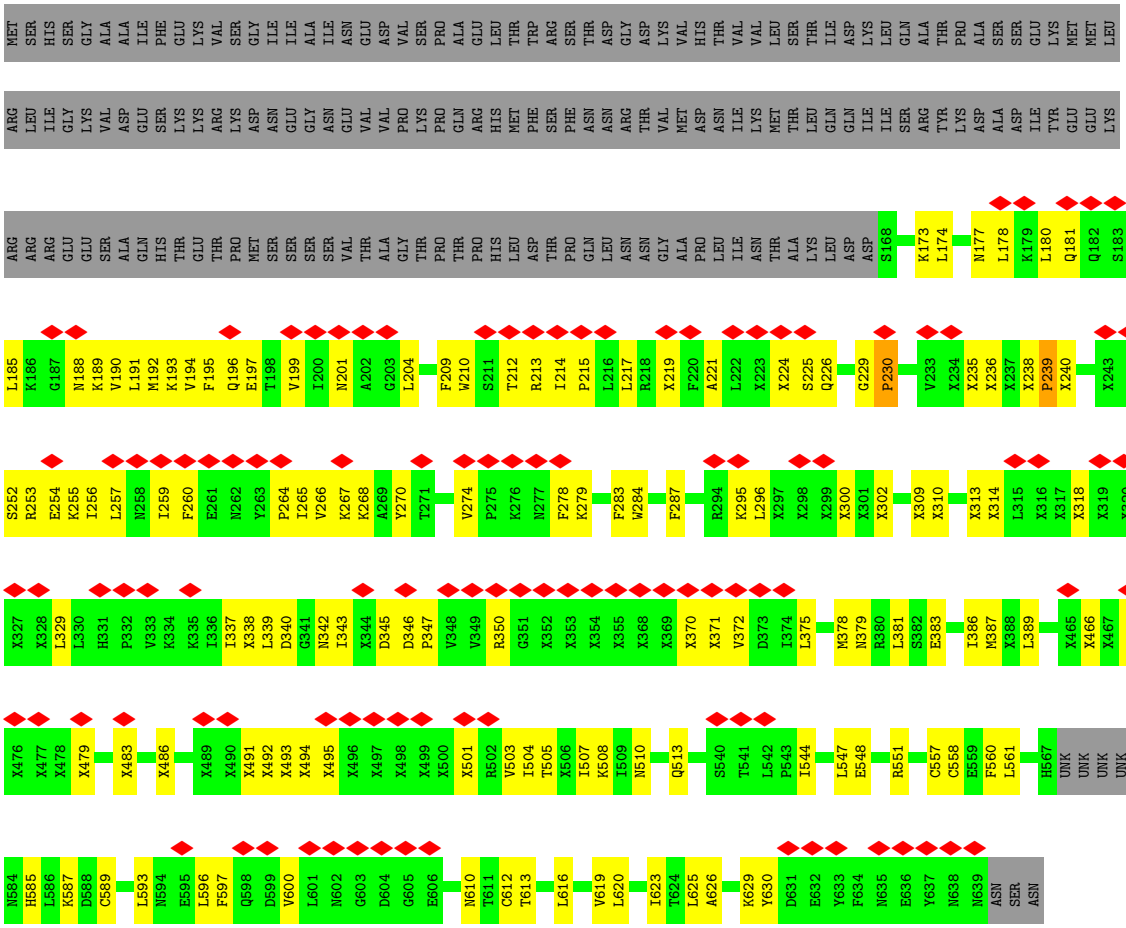




• Molecule 23: Tfb1

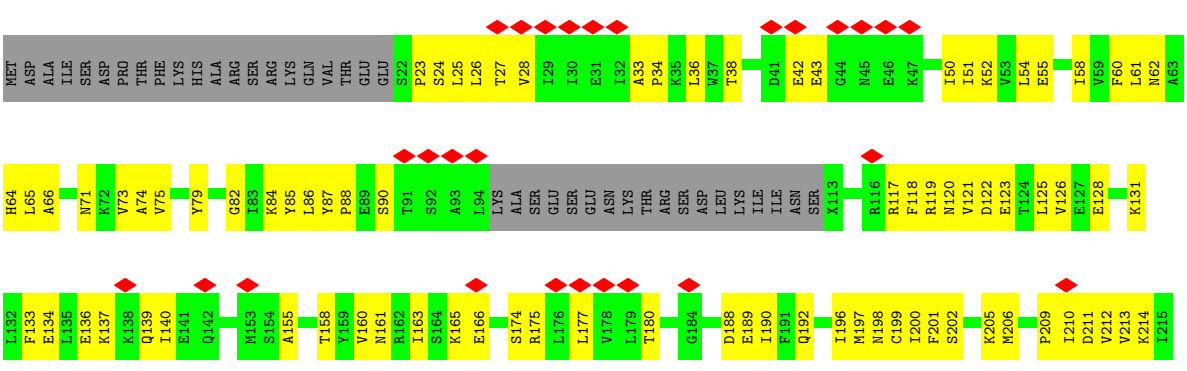
Chain 1:

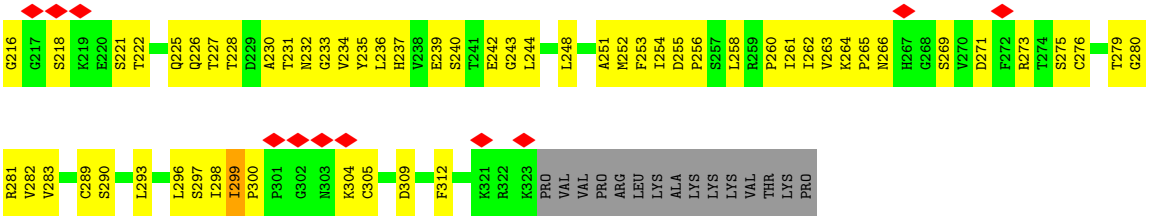




• Molecule 24: Tfb4

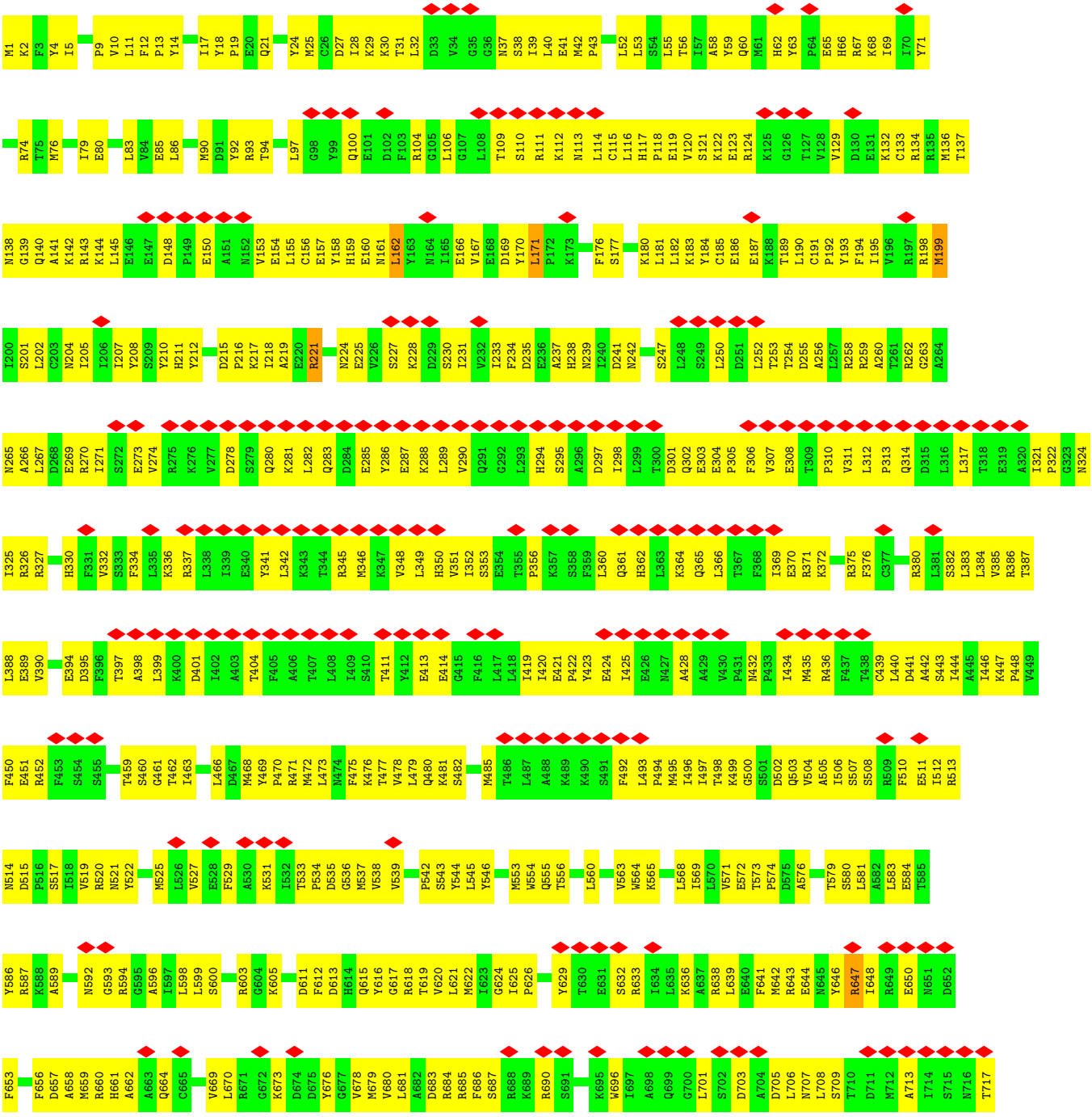
Chain 4:

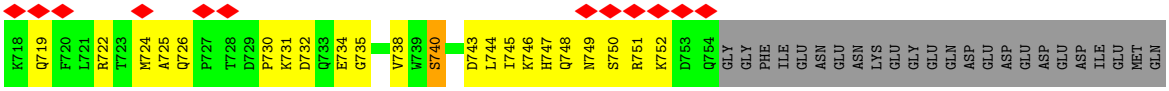




• Molecule 25: General transcription and DNA repair factor IIH helicase subunit XPD

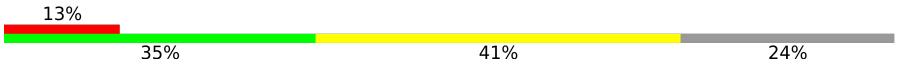
Chain 0:

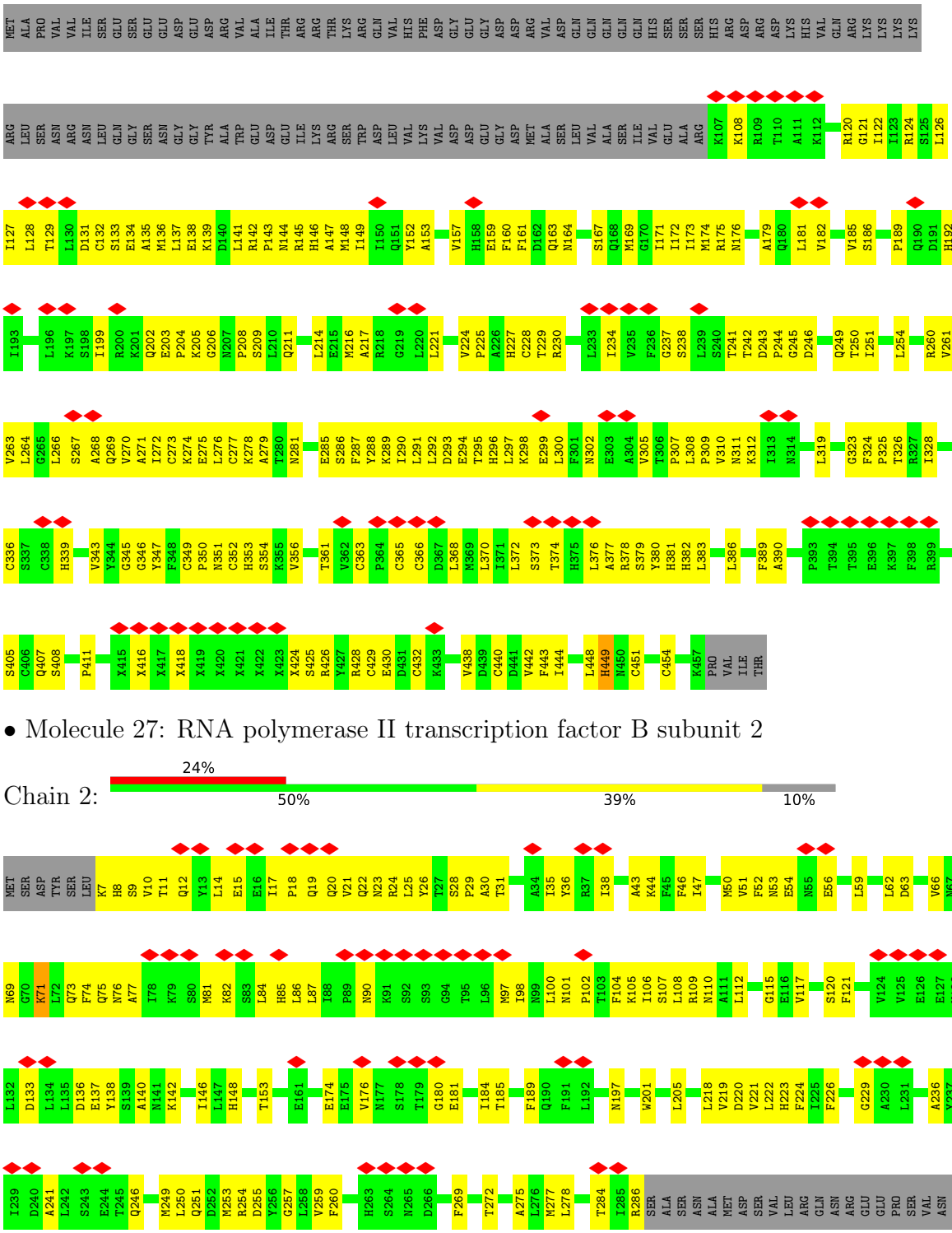




• Molecule 26: General transcription and DNA repair factor IIH

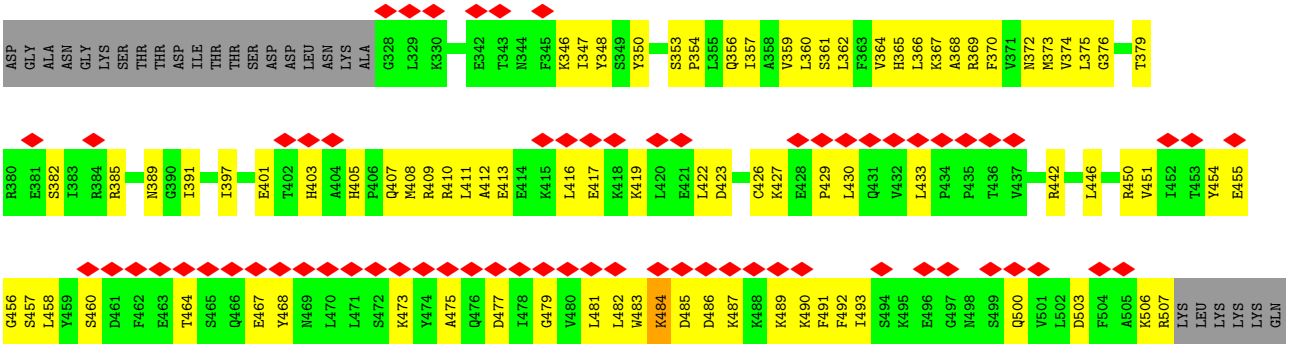
Chain 6:





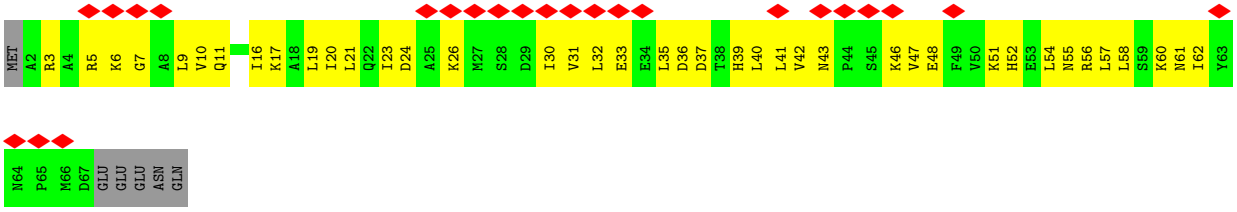
• Molecule 27: RNA polymerase II transcription factor B subunit 2

Chain 2:



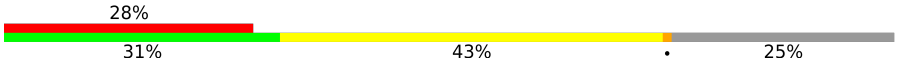
• Molecule 28: General transcription and DNA repair factor IIH subunit TFB5

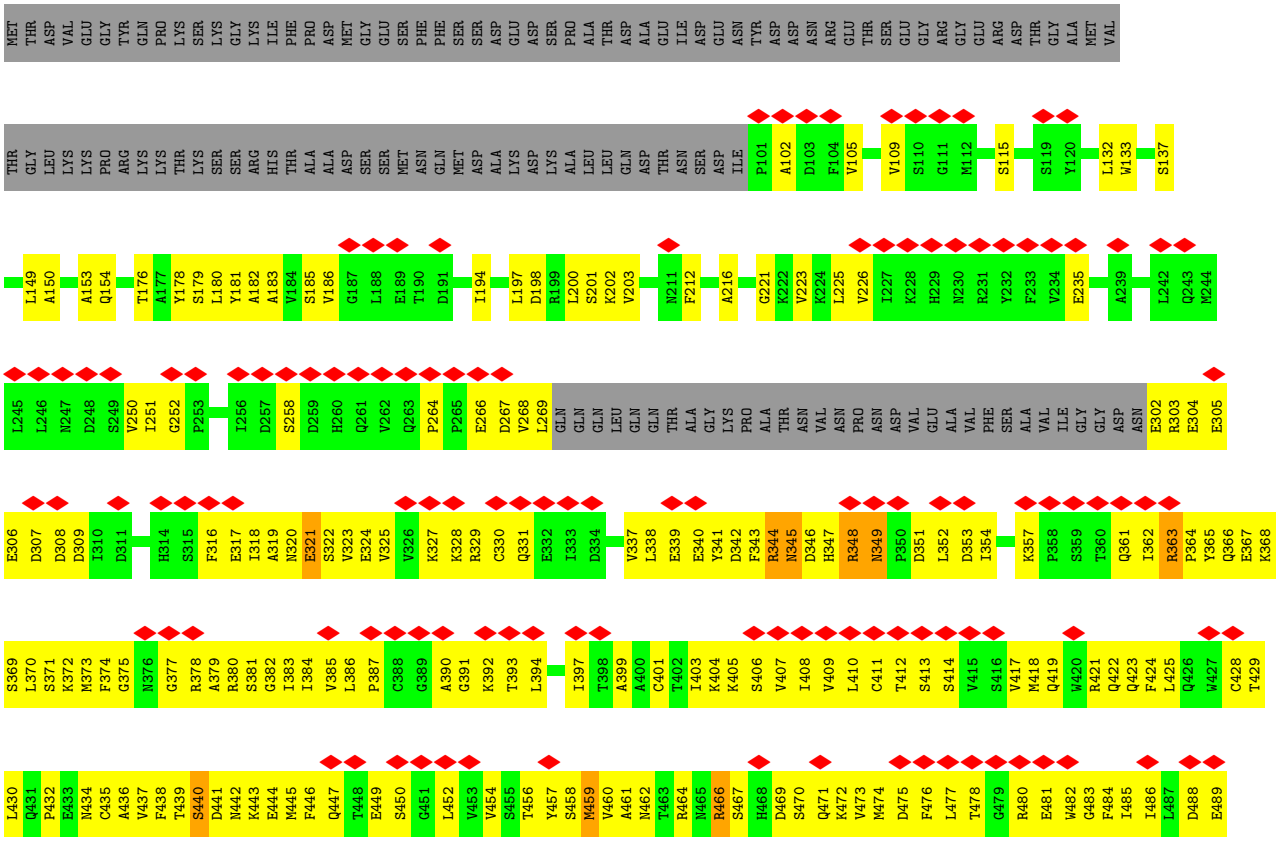
Chain 5:

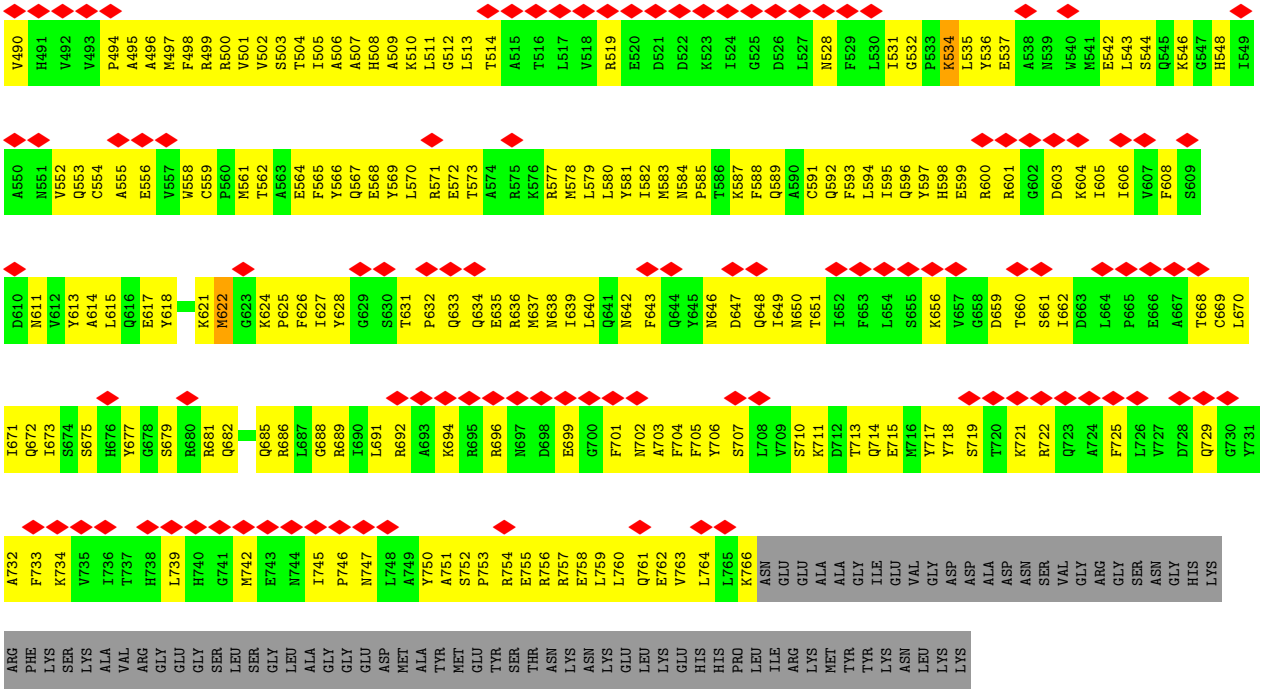


• Molecule 29: General transcription and DNA repair factor IIH helicase subunit XPB

Chain 7:

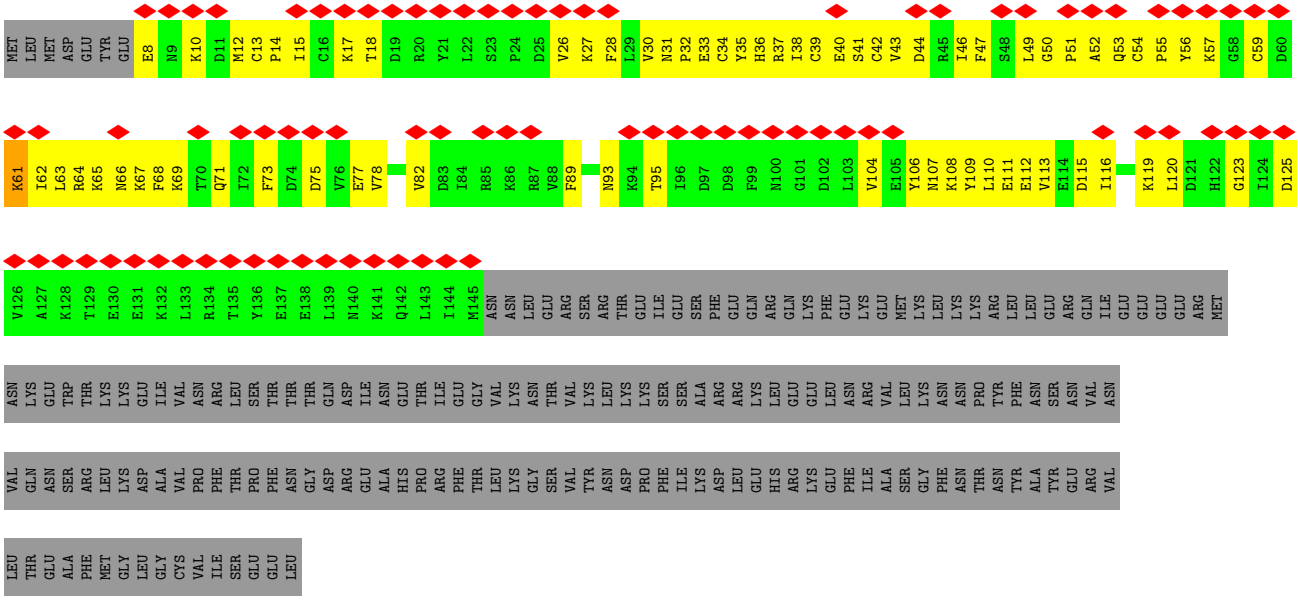






• Molecule 30: BJ4_G0050160.mRNA.1.CDS.1

Chain 3:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	69513	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 ($e^-/Å^2$)	45	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	0.056	Depositor
Minimum map value	0.000	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	474.87997, 501.37997, 473.81998	wwPDB
Map dimensions	448, 473, 447	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.49	3/11192 (0.0%)	0.66	6/15128 (0.0%)
2	B	0.50	0/9357	0.67	4/12618 (0.0%)
3	C	0.55	1/2099 (0.0%)	0.69	0/2845
4	D	0.34	0/1262	0.64	0/1693
5	E	0.45	0/1780	0.62	0/2395
6	F	0.65	1/682 (0.1%)	0.83	1/922 (0.1%)
7	G	0.38	0/1368	0.61	0/1844
8	H	0.55	0/1107	0.76	0/1499
9	I	0.49	0/962	0.77	1/1295 (0.1%)
10	J	0.62	0/541	0.83	1/727 (0.1%)
11	K	0.54	1/922 (0.1%)	0.90	4/1244 (0.3%)
12	L	0.37	0/360	0.71	0/478
13	M	0.37	0/2204	0.62	0/2963
14	Q	0.33	0/1168	0.53	0/1579
15	R	0.32	0/1312	0.57	1/1777 (0.1%)
16	U	0.25	0/389	0.57	0/523
17	V	0.28	0/384	0.48	0/518
18	W	0.29	0/1490	0.49	0/2014
19	X	0.25	0/993	0.50	0/1357
20	T	0.88	2/1273 (0.2%)	1.12	2/1962 (0.1%)
21	N	0.98	1/1301 (0.1%)	1.10	9/2006 (0.4%)
22	O	0.32	0/1443	0.53	0/1942
23	1	0.28	0/1896	0.50	0/2543
24	4	0.33	0/2062	0.57	0/2805
25	0	0.34	0/6226	0.57	2/8407 (0.0%)
26	6	0.33	0/2506	0.58	0/3402
27	2	0.30	0/3057	0.54	0/4071
28	5	0.27	0/502	0.58	0/677
29	7	0.38	0/4521	0.62	2/6036 (0.0%)
30	3	0.52	1/870 (0.1%)	0.62	1/1190 (0.1%)
All	All	0.46	10/65229 (0.0%)	0.66	34/88460 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
2	B	0	4
8	H	0	3
9	I	0	1
10	J	0	1
13	M	0	3
18	W	0	1
19	X	0	1
24	4	0	2
25	0	0	2
26	6	0	1
29	7	0	8
30	3	0	2
All	All	0	36

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1074	GLU	CD-OE2	-10.39	1.14	1.25
30	3	61	LYS	CE-NZ	-7.98	1.29	1.49
3	C	166	GLU	CG-CD	7.34	1.62	1.51
20	T	116	DA	N9-C4	-7.07	1.33	1.37
6	F	135	ARG	CA-CB	-6.59	1.39	1.53

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	K	6	ARG	NE-CZ-NH1	-12.37	114.12	120.30
21	N	22	DT	O4'-C4'-C3'	-8.60	100.84	106.00
20	T	147	DT	O4'-C4'-C3'	-7.76	101.34	106.00
2	B	935	ARG	NE-CZ-NH1	-6.57	117.02	120.30
21	N	51	DA	O4'-C4'-C3'	-6.39	101.94	104.50

There are no chirality outliers.

5 of 36 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	22	PHE	Peptide

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Mol	Chain	Res	Type	Group
1	A	250	ILE	Peptide
1	A	450	LEU	Peptide
1	A	465	TYR	Peptide
1	A	71	GLN	Peptide

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	A	10997	0	11081	800	0
2	B	9178	0	9195	614	0
3	C	2061	0	2029	154	0
4	D	1253	0	1275	127	0
5	E	1744	0	1772	120	0
6	F	670	0	690	66	0
7	G	1340	0	1357	132	0
8	H	1089	0	1062	124	0
9	I	944	0	899	106	0
10	J	532	0	542	62	0
11	K	904	0	911	87	0
12	L	358	0	383	39	0
13	M	2175	0	2283	217	0
14	Q	1144	0	1034	113	0
15	R	1303	0	1110	122	0
16	U	383	0	384	24	0
17	V	381	0	388	35	0
18	W	1469	0	1432	110	0
19	X	984	0	722	58	0
20	T	1140	0	641	71	0
21	N	1156	0	631	87	0
22	O	1416	0	1493	99	0
23	1	2411	0	1881	121	0
24	4	2041	0	1954	140	0
25	0	6108	0	6168	537	0
26	6	2527	0	2321	221	0
27	2	3011	0	2600	225	0
28	5	498	0	506	58	0
29	7	4447	0	3905	483	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	3	860	0	623	103	0
31	3	2	0	0	0	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	W	1	0	0	0	0
32	A	1	0	0	0	0
33	0	8	0	0	3	0
All	All	64550	0	61272	4827	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 39.

The worst 5 of 4827 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)
12:L:48:CYS:SG	12:L:53:HIS:HB3	1.70	1.32
12:L:34:CYS:SG	12:L:36:SER:OG	1.98	1.18
2:B:649:LYS:NZ	2:B:736:THR:O	1.83	1.11
25:0:162:LEU:HD22	25:0:194:PHE:HB3	1.27	1.09
1:A:253:ASN:HA	2:B:935:ARG:HH12	1.17	1.07

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1386/1733 (80%)	1192 (86%)	189 (14%)	5 (0%)	34	67
2	B	1136/1224 (93%)	987 (87%)	146 (13%)	3 (0%)	41	72
3	C	260/318 (82%)	214 (82%)	46 (18%)	0	100	100
4	D	153/221 (69%)	135 (88%)	18 (12%)	0	100	100
5	E	211/215 (98%)	193 (92%)	18 (8%)	0	100	100
6	F	81/155 (52%)	69 (85%)	12 (15%)	0	100	100
7	G	169/171 (99%)	152 (90%)	17 (10%)	0	100	100
8	H	132/146 (90%)	106 (80%)	24 (18%)	2 (2%)	10	36
9	I	114/122 (93%)	94 (82%)	20 (18%)	0	100	100
10	J	63/70 (90%)	44 (70%)	19 (30%)	0	100	100
11	K	110/120 (92%)	95 (86%)	15 (14%)	0	100	100
12	L	43/70 (61%)	33 (77%)	7 (16%)	3 (7%)	1	7
13	M	273/345 (79%)	221 (81%)	52 (19%)	0	100	100
14	Q	140/735 (19%)	120 (86%)	20 (14%)	0	100	100
15	R	176/400 (44%)	163 (93%)	13 (7%)	0	100	100
16	U	44/286 (15%)	38 (86%)	6 (14%)	0	100	100
17	V	45/122 (37%)	44 (98%)	1 (2%)	0	100	100
18	W	189/482 (39%)	182 (96%)	7 (4%)	0	100	100
19	X	152/328 (46%)	136 (90%)	16 (10%)	0	100	100
22	O	178/240 (74%)	167 (94%)	11 (6%)	0	100	100
23	1	256/542 (47%)	234 (91%)	19 (7%)	3 (1%)	13	41
24	4	279/338 (82%)	222 (80%)	57 (20%)	0	100	100
25	0	752/778 (97%)	670 (89%)	82 (11%)	0	100	100
26	6	336/461 (73%)	298 (89%)	36 (11%)	2 (1%)	25	57
27	2	456/513 (89%)	390 (86%)	66 (14%)	0	100	100
28	5	64/72 (89%)	58 (91%)	6 (9%)	0	100	100
29	7	630/843 (75%)	539 (86%)	90 (14%)	1 (0%)	47	78
30	3	136/321 (42%)	105 (77%)	31 (23%)	0	100	100
All	All	7964/11371 (70%)	6901 (87%)	1044 (13%)	19 (0%)	50	78

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	465	TYR
2	B	364	ILE
8	H	110	ASP
26	6	411	PRO
29	7	349	ASN

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	A	1221/1520 (80%)	1218 (100%)	3 (0%)	93 98
2	B	1000/1061 (94%)	1000 (100%)	0	100 100
3	C	230/274 (84%)	230 (100%)	0	100 100
4	D	139/200 (70%)	139 (100%)	0	100 100
5	E	195/197 (99%)	195 (100%)	0	100 100
6	F	73/137 (53%)	73 (100%)	0	100 100
7	G	152/152 (100%)	152 (100%)	0	100 100
8	H	119/128 (93%)	118 (99%)	1 (1%)	81 91
9	I	110/116 (95%)	110 (100%)	0	100 100
10	J	60/65 (92%)	60 (100%)	0	100 100
11	K	97/102 (95%)	97 (100%)	0	100 100
12	L	40/57 (70%)	34 (85%)	6 (15%)	3 12
13	M	245/299 (82%)	245 (100%)	0	100 100
14	Q	109/641 (17%)	109 (100%)	0	100 100
15	R	107/363 (30%)	107 (100%)	0	100 100
16	U	42/260 (16%)	42 (100%)	0	100 100
17	V	46/108 (43%)	46 (100%)	0	100 100
18	W	155/429 (36%)	155 (100%)	0	100 100
19	X	62/295 (21%)	61 (98%)	1 (2%)	62 81
22	O	152/205 (74%)	151 (99%)	1 (1%)	84 92

Continued on next page...

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
23	1	169/395 (43%)	169 (100%)	0	100 100
24	4	198/298 (66%)	198 (100%)	0	100 100
25	0	686/707 (97%)	684 (100%)	2 (0%)	92 97
26	6	247/406 (61%)	246 (100%)	1 (0%)	91 95
27	2	258/468 (55%)	255 (99%)	3 (1%)	71 85
28	5	53/66 (80%)	53 (100%)	0	100 100
29	7	414/737 (56%)	413 (100%)	1 (0%)	93 98
30	3	53/303 (18%)	53 (100%)	0	100 100
All	All	6432/9989 (64%)	6413 (100%)	19 (0%)	92 97

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
26	6	108	LYS
27	2	484	LYS
29	7	534	LYS
27	2	410	ARG
12	L	38	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
23	1	196	GLN
26	6	163	GLN
25	0	60	GLN
25	0	294	HIS
26	6	302	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 monosaccharides 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	801	25	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	25	-	-	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 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	0	801	SF4	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
23	1	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	393:UNK	C	465:UNK	N	84.96
1	1	519:UNK	C	537:GLU	N	11.53
1	1	355:UNK	C	368:UNK	N	10.44

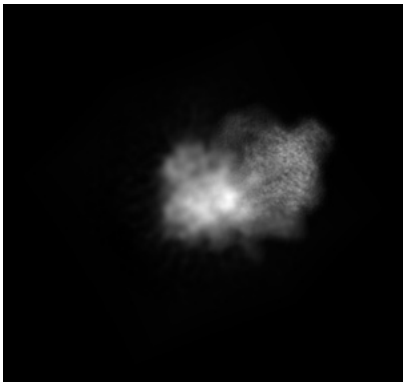
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23906. These allow visual inspection of the internal detail of the map and identification of artifacts.

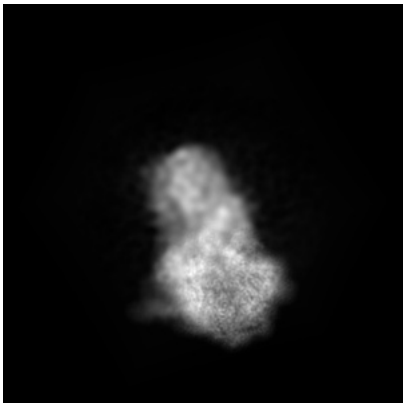
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

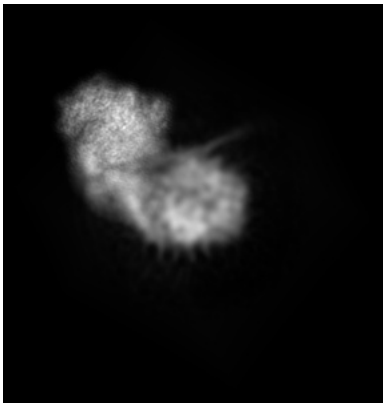
6.1.1 Primary map



X



Y

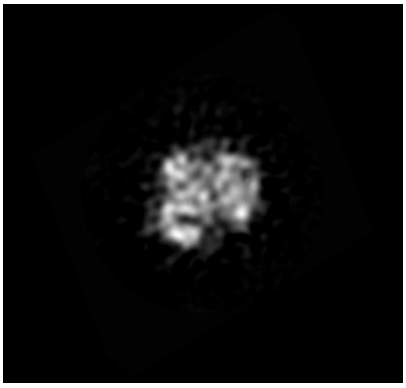


Z

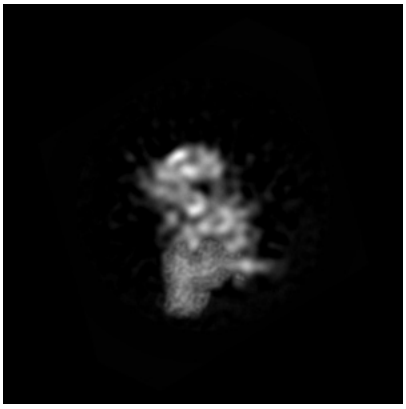
The images above show the map projected in three orthogonal directions.

6.2 Central slices

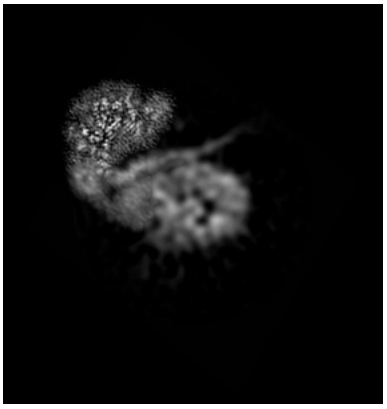
6.2.1 Primary map



X Index: 224



Y Index: 236

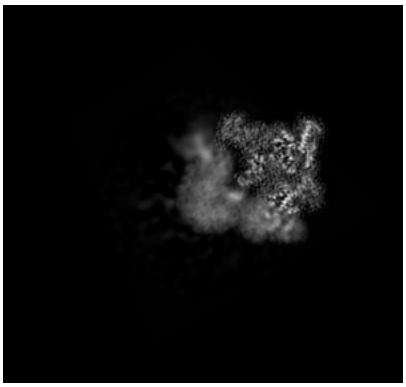


Z Index: 223

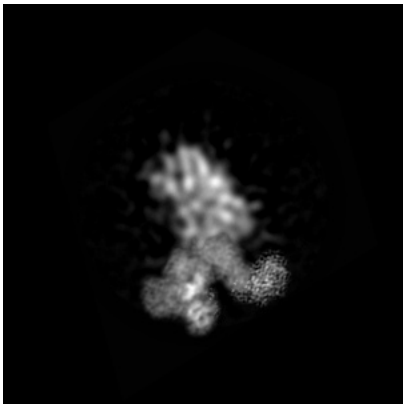
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

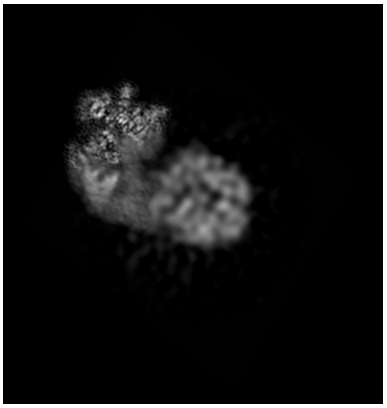
6.3.1 Primary map



X Index: 152



Y Index: 263

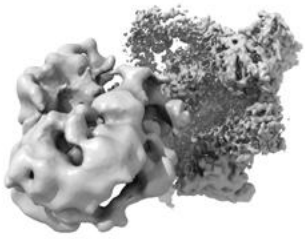


Z Index: 210

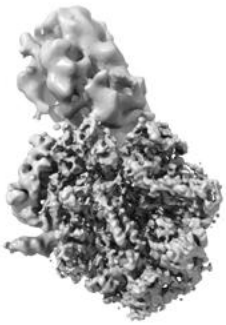
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

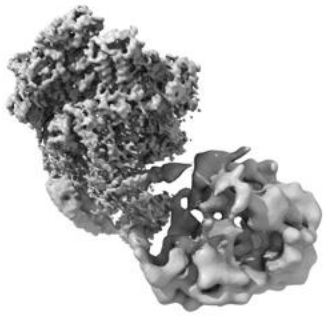
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.018. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

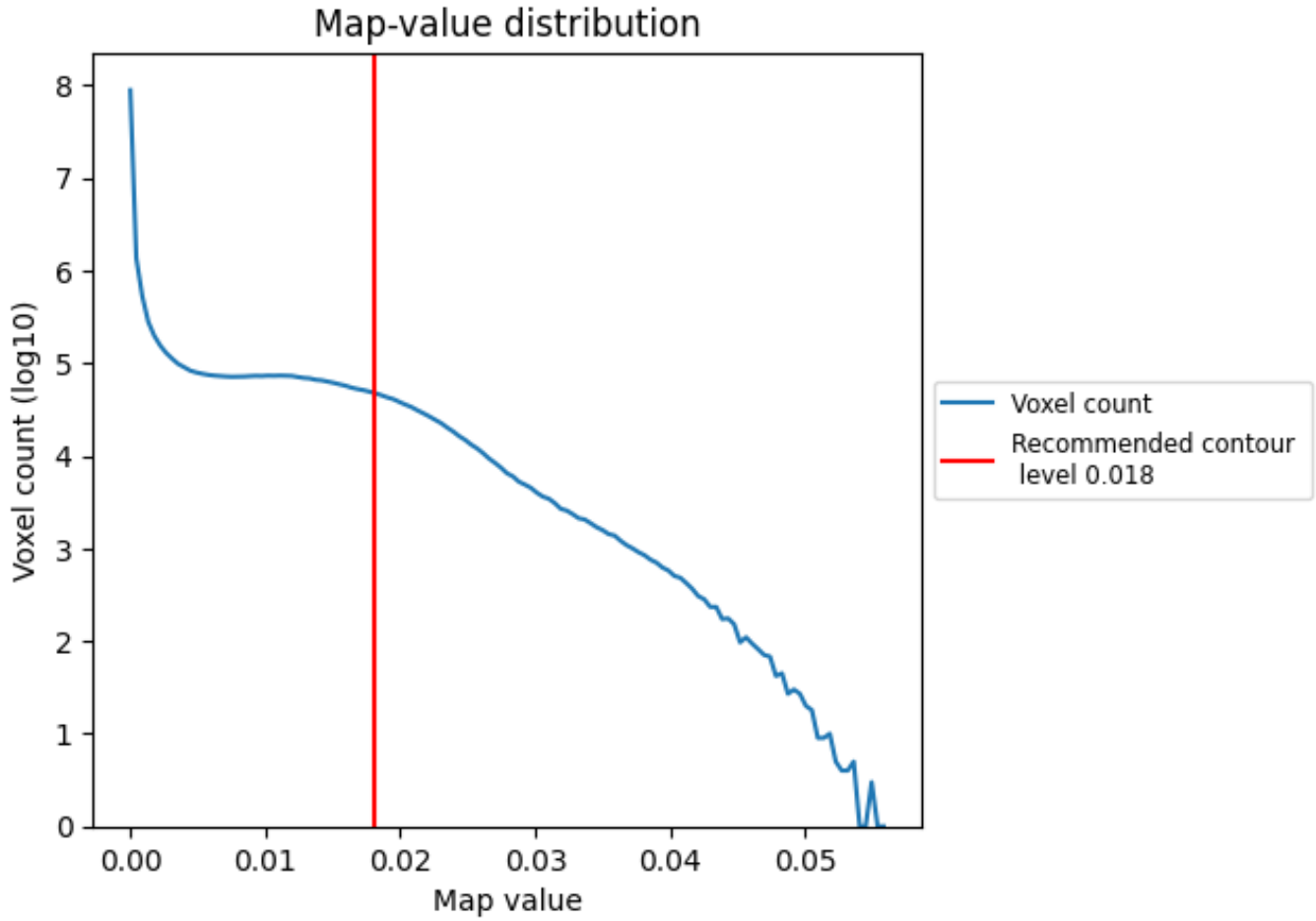
6.5 Mask visualisation (i)

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

7 Map analysis

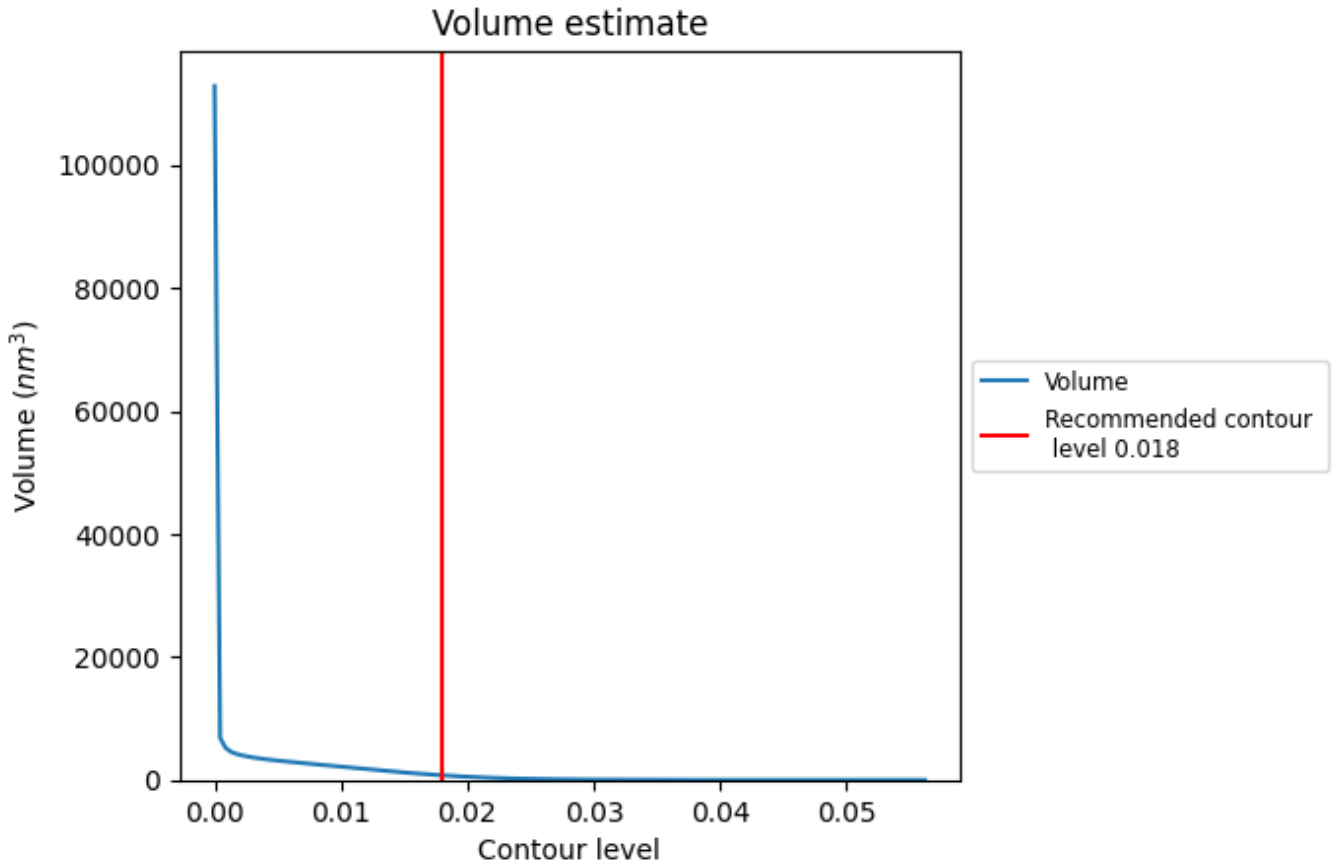
This section contains the results of statistical analysis of the map.

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 762 nm^3; this corresponds to an approximate mass of 688 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.

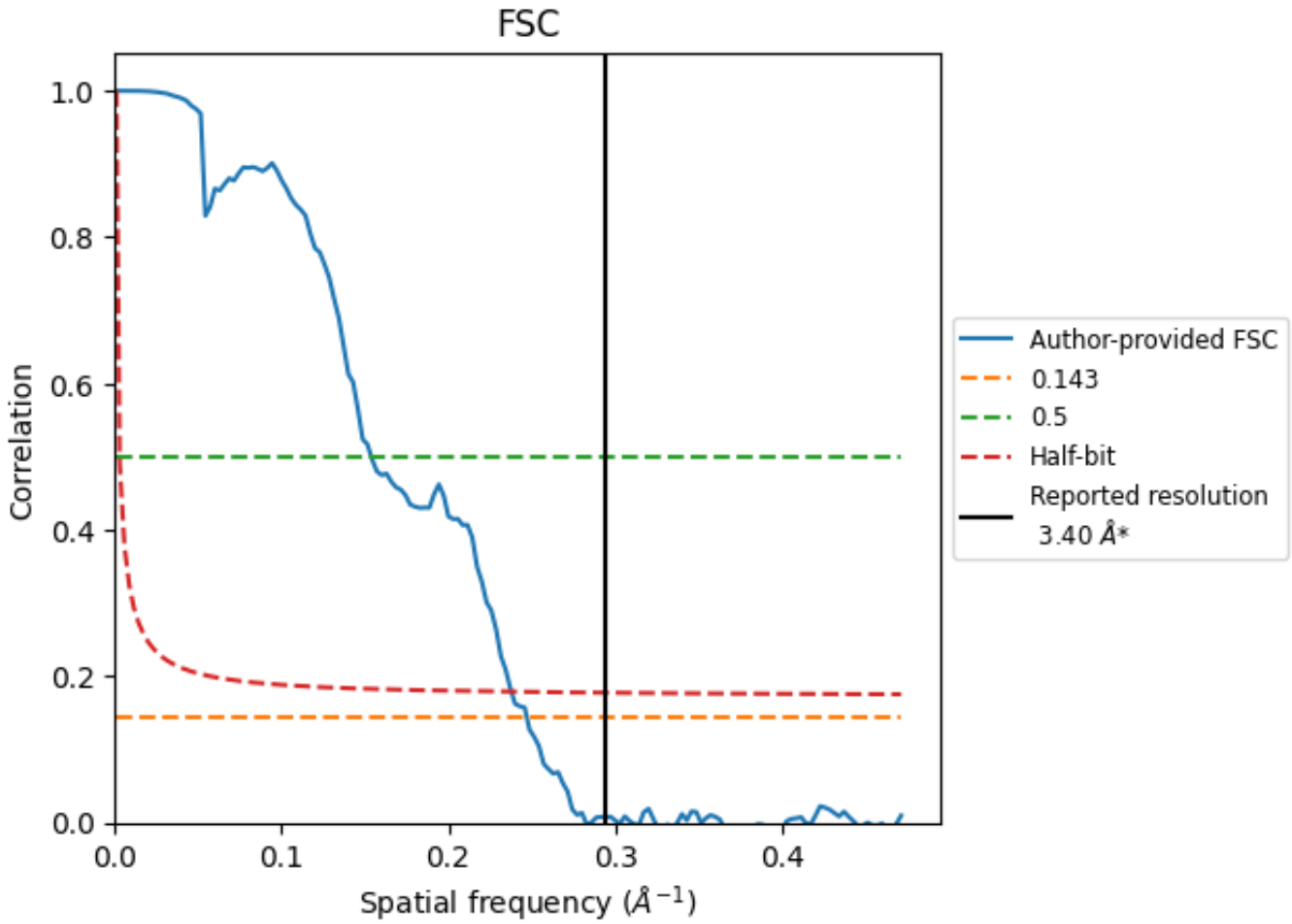
7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

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 0.294 Å^{-1}

8.2 Resolution estimates (i)

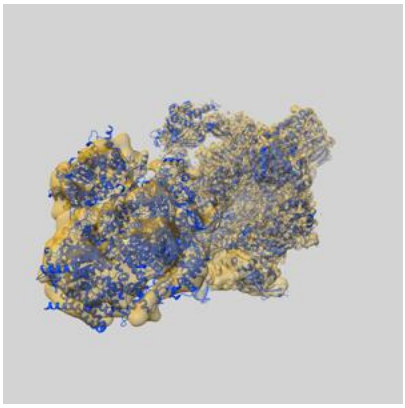
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	4.05	6.50	4.20
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.05 differs from the reported value 3.4 by more than 10 %

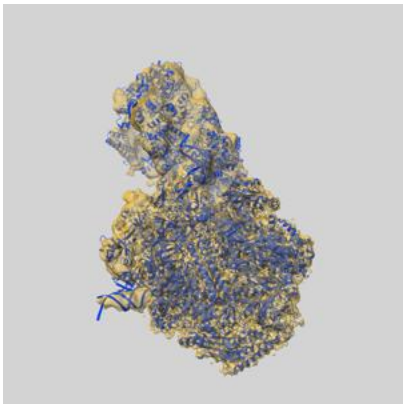
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23906 and PDB model 7ML2. Per-residue inclusion information can be found in section 3 on page 11.

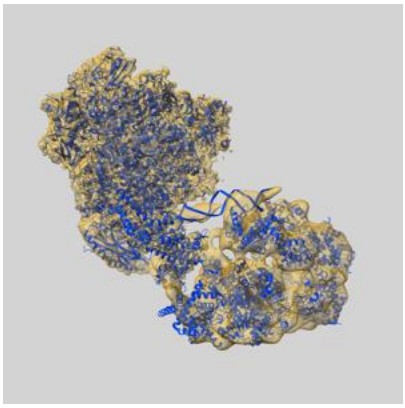
9.1 Map-model overlay



X



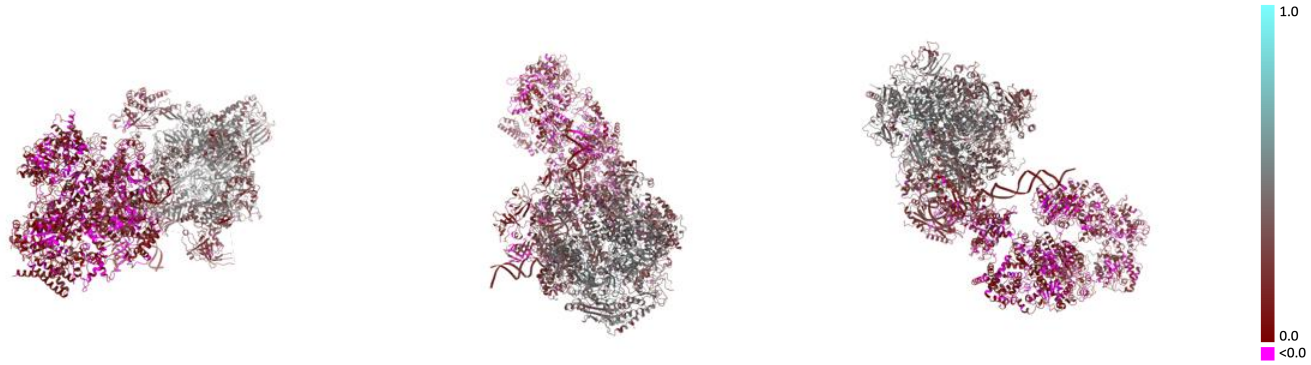
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.018 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.

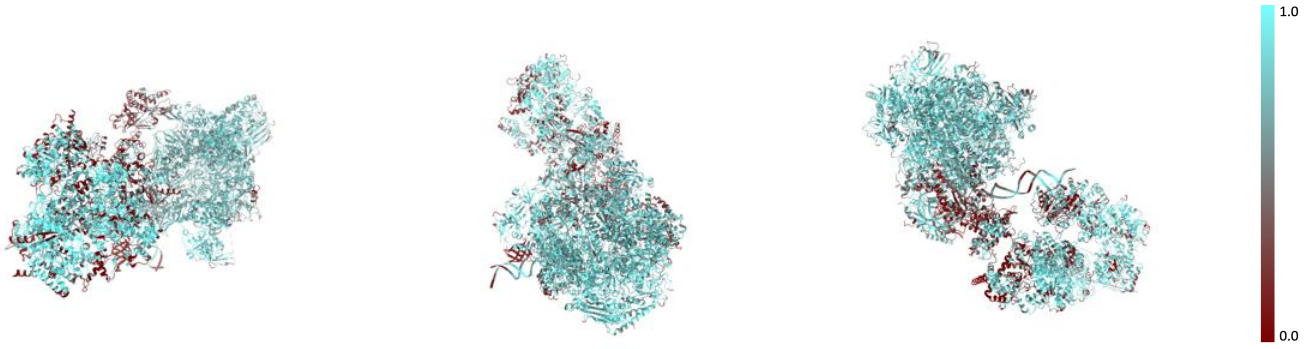
9.2 Q-score mapped to coordinate model



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.

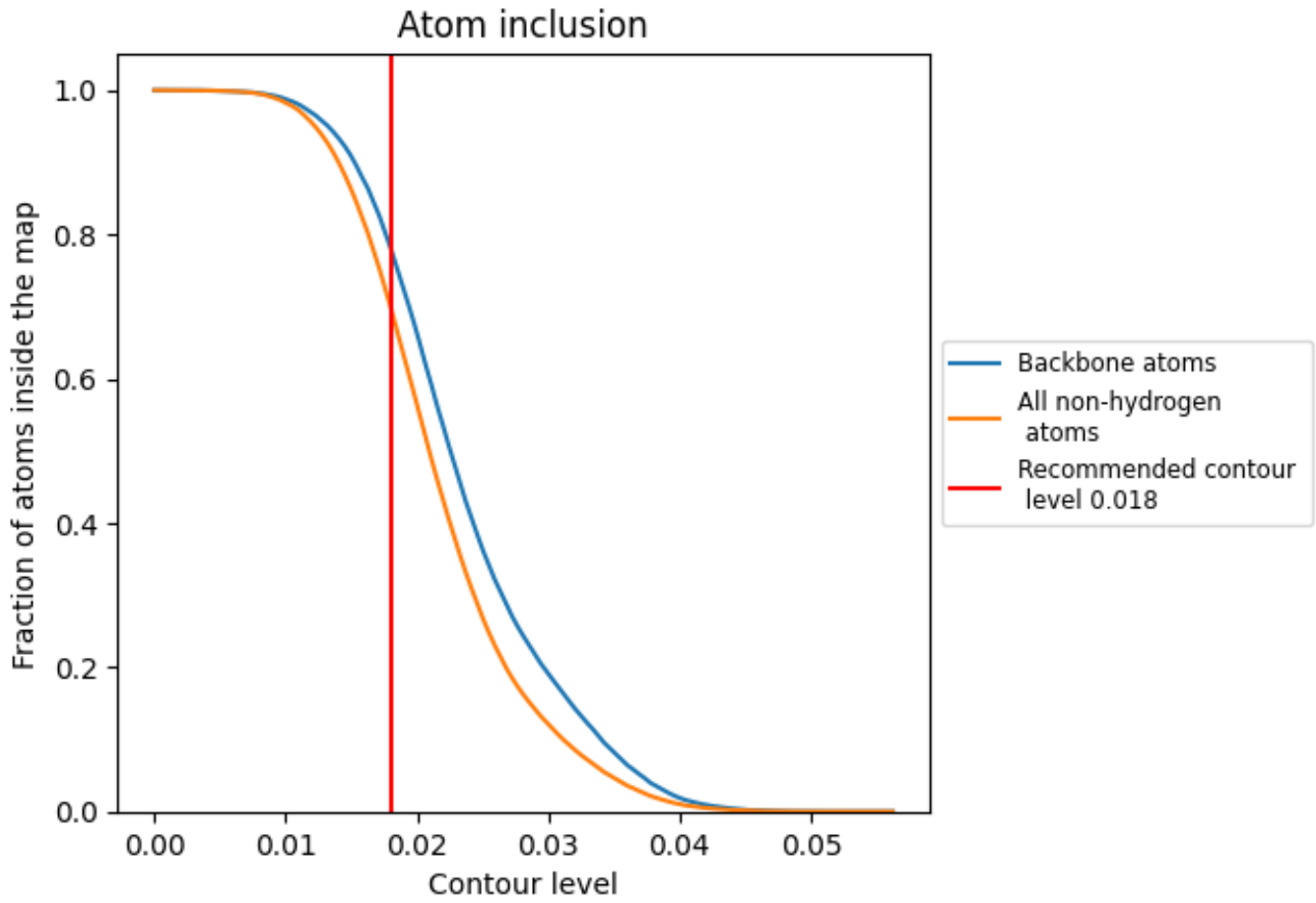
9.3 Atom inclusion mapped to coordinate model



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 (0.018).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 70% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6983	0.2410
0	0.6761	0.0760
1	0.6296	0.0700
2	0.6611	0.0730
3	0.3782	0.0870
4	0.8349	0.0840
5	0.6362	0.0880
6	0.8017	0.0860
7	0.5854	0.0670
A	0.7976	0.4070
B	0.8270	0.4220
C	0.8412	0.4250
D	0.2474	0.2040
E	0.7772	0.3820
F	0.7929	0.3810
G	0.4357	0.2550
H	0.7370	0.3440
I	0.6102	0.2690
J	0.8375	0.4100
K	0.7149	0.3710
L	0.6965	0.2880
M	0.5480	0.2340
N	0.6981	0.1450
O	0.7608	0.1580
Q	0.8077	0.2110
R	0.6770	0.1820
T	0.7070	0.1650
U	0.0295	0.0510
V	0.1141	0.0470
W	0.4044	0.0900
X	0.5358	0.0920