wwPDB EM Validation Summary Report (i)

Aug 5, 2026 – 09:14 AM EDT

PDB ID	:	8UMI / pdb_00008umi
EMDB ID	:	EMD-42380
Title	:	consensus map of PICdeltaTFIIK form1
Authors	:	Yang, C.; Murakami, K.
Deposited on	:	2023-10-17
Resolution	:	3.70 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 (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:

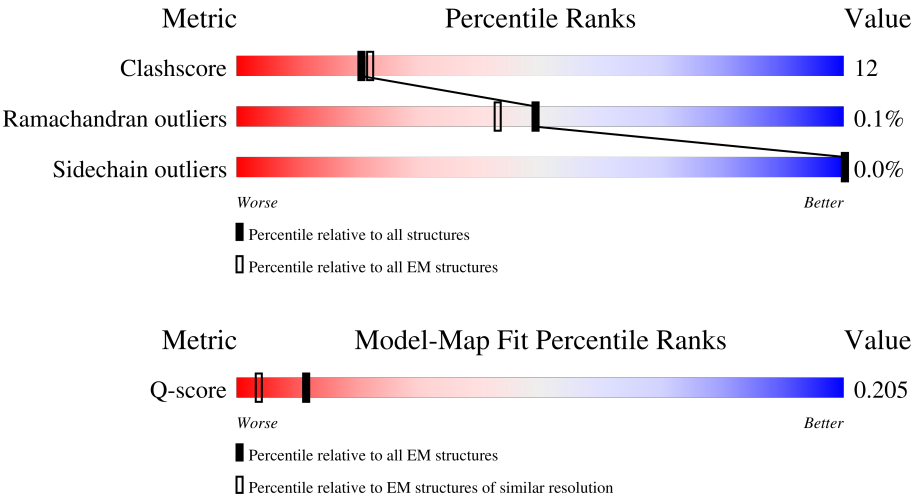
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
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 3.70 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	11569 (3.20 - 4.20)

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	778	7% 63% 33% .
2	1	642	10% 51% 14% 35%
3	2	513	17% 59% 28% 13%
4	4	338	5% 64% 22% 14%

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Mol	Chain	Length	Quality of chain
5	6	461	7% 52% 25% 23%
6	7	843	11% 48% 24% 28%
7	M	345	9% 58% 23% 19%
8	A	1733	61% 21% 18%
9	B	1224	70% 25% 5%
10	C	318	62% 21% 17%
11	D	221	13% 56% 20% 24%
12	E	215	72% 27%
13	F	155	40% 16% 44%
14	G	171	61% 38%
15	H	146	63% 29% 8%
16	I	122	61% 33% 7%
17	J	70	59% 36% 6%
18	K	120	76% 20%
19	L	70	39% 23% 37%
20	Q	735	23% 6% 71%
21	P	400	31% 14% 55%
22	S	309	36% 17% 47%
23	O	240	55% 21% 25%
24	U	286	14% 24% 14% 63%
25	V	122	32% 63% 22% 15%
26	W	482	38% 13% 49%
27	X	328	34% 15% 51%
28	5	72	56% 61% 31% 8%
29	N	64	17% 53% 47%

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Mol	Chain	Length	Quality of chain
30	T	64	11% 62% 38%

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
31	SF4	0	801	-	-	X	-

2 Entry composition (i)

There are 33 unique types of molecules in this entry. The entry contains 70523 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 General transcription and DNA repair factor IIH helicase subunit XPD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	752	6091	3882	1029	1142	38	0	0

- Molecule 2 is a protein called TFB1 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	417	3382	2139	587	640	16	0	0

- Molecule 3 is a protein called RNA polymerase II transcription factor B subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	445	3546	2291	585	654	16	0	0

- Molecule 4 is a protein called General transcription and DNA repair factor IIH subunit TFB4.

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

- Molecule 5 is a protein called General transcription and DNA repair factor IIH.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	6	355	2786	1765	481	512	28	0	0

- Molecule 6 is a protein called General transcription and DNA repair factor IIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	608	Total	C	N	O	S	0	0
			4889	3110	847	906	26		

- Molecule 7 is a protein called Transcription initiation factor IIB.

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

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

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

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

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

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB3.

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

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB4.

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

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

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

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

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

- Molecule 14 is a protein called DNA-directed RNA polymerase II subunit RPB7.

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

- Molecule 15 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 16 is a protein called DNA-directed RNA polymerase II subunit RPB9.

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

- Molecule 17 is a protein called DNA-directed RNA polymerases II subunit RPABC5.

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

- Molecule 18 is a protein called DNA-directed RNA polymerase II subunit RPB11.

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

- Molecule 19 is a protein called DNA-directed RNA polymerases II subunit RPABC4.

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

- Molecule 20 is a protein called Transcription initiation factor IIF subunit alpha.

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

- Molecule 21 is a protein called Transcription initiation factor IIF subunit beta.

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

- Molecule 22 is a protein called Transcription elongation factor.

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

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

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

- Molecule 24 is a protein called Transcription initiation factor IIA large subunit.

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

- Molecule 25 is a protein called Transcription initiation factor IIA subunit 2.

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

- Molecule 26 is a protein called Transcription initiation factor IIE subunit alpha.

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

- Molecule 27 is a protein called Transcription initiation factor IIE subunit beta.

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

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

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

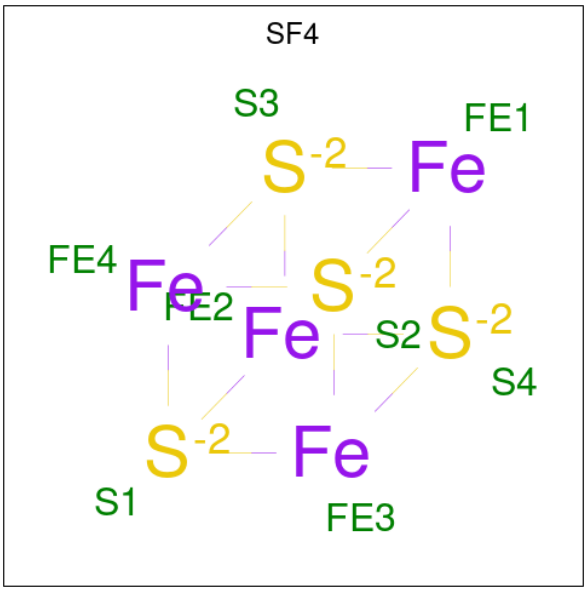
- Molecule 29 is a DNA chain called DNA (64-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
29	N	64	Total	C	N	O	P	0	0
			1307	630	228	386	63		

- Molecule 30 is a DNA chain called DNA (64-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
30	T	64	Total	C	N	O	P	0	0
			1314	630	240	380	64		

- Molecule 31 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
31	0	1	Total	Fe	S	0
			8	4	4	

- Molecule 32 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
32	4	1	Total Zn 1 1	0
32	6	4	Total Zn 4 4	0
32	M	1	Total Zn 1 1	0
32	A	2	Total Zn 2 2	0
32	B	1	Total Zn 1 1	0
32	C	1	Total Zn 1 1	0
32	I	2	Total Zn 2 2	0
32	J	1	Total Zn 1 1	0
32	L	1	Total Zn 1 1	0
32	S	1	Total Zn 1 1	0

- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

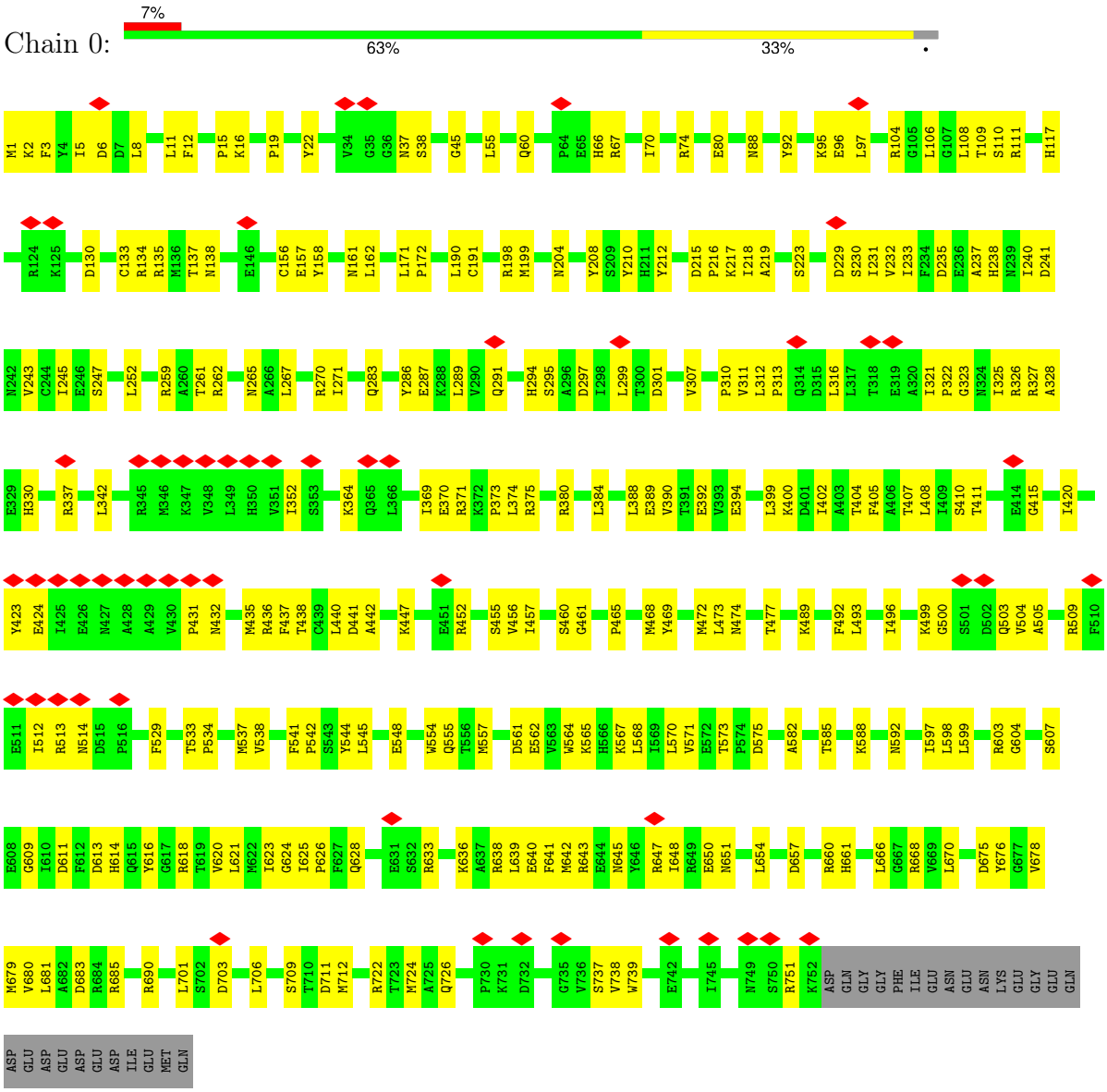
Mol	Chain	Residues	Atoms	AltConf
33	7	1	Total Mg 1 1	0
33	A	1	Total Mg 1 1	0

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.

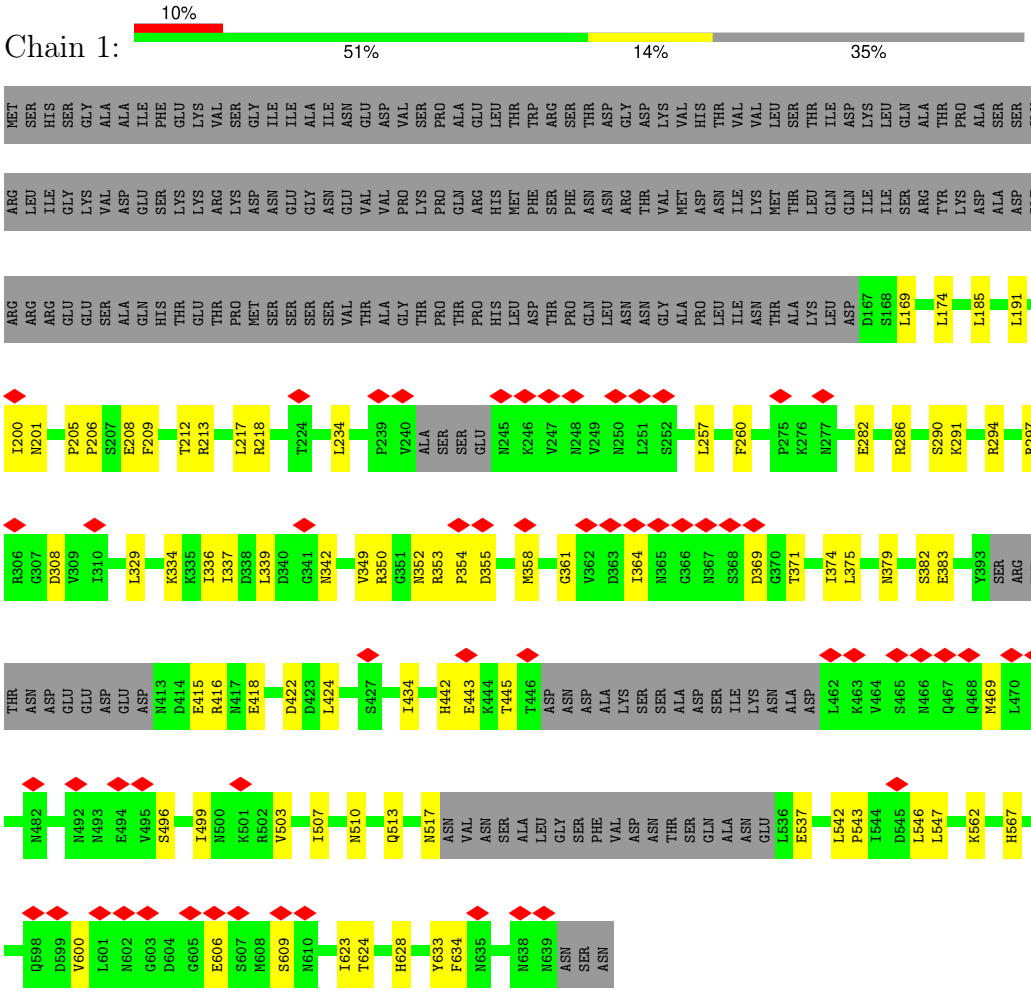
• Molecule 1: General transcription and DNA repair factor IIH helicase subunit XPD

Chain 0:



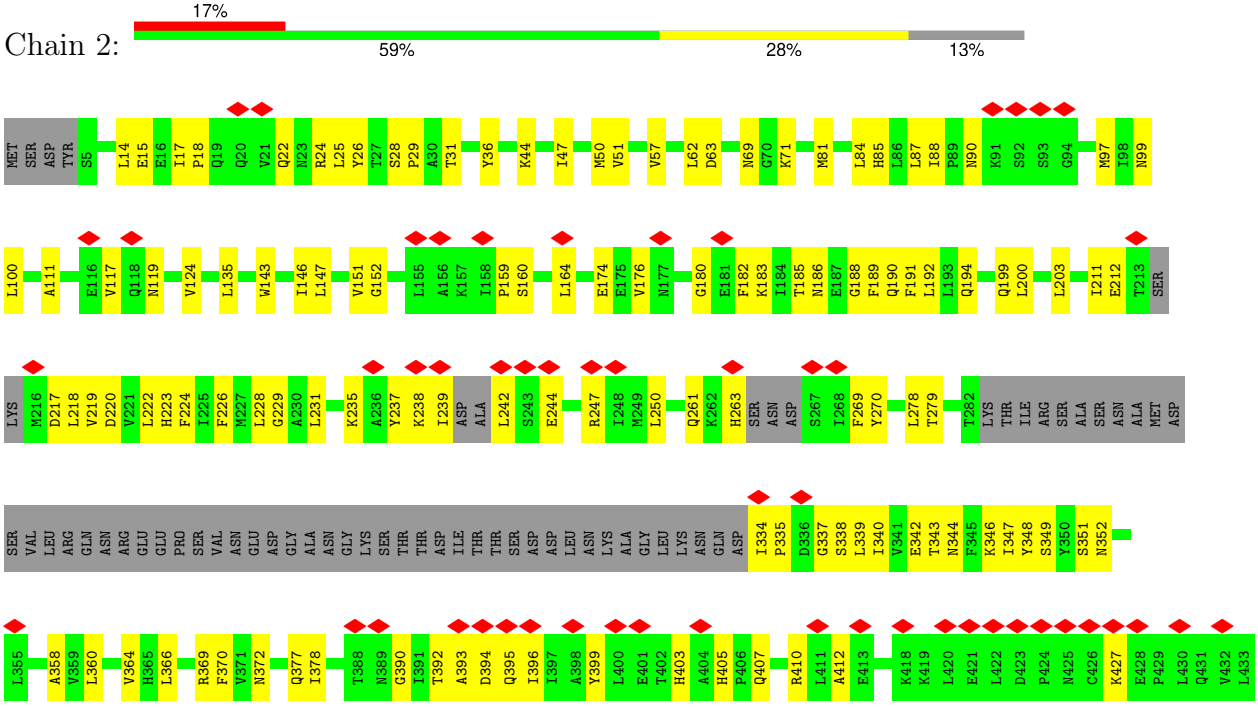
• Molecule 2: TFB1 isoform 1

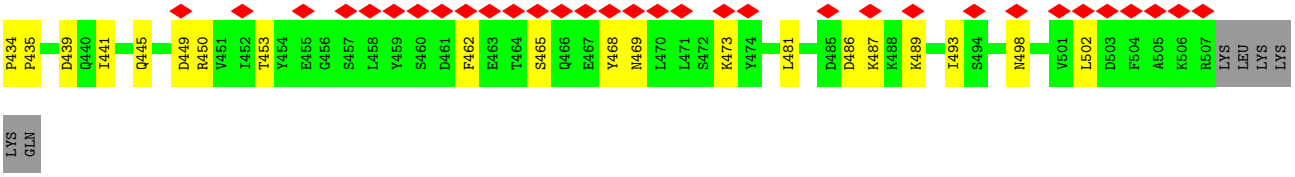
Chain 1:



• Molecule 3: RNA polymerase II transcription factor B subunit 2

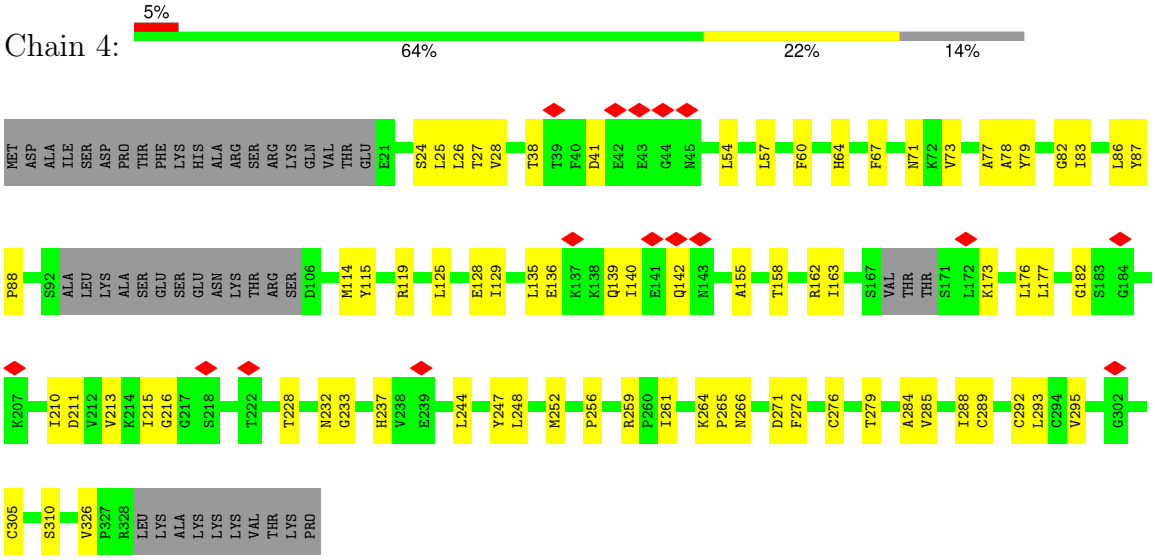
Chain 2:





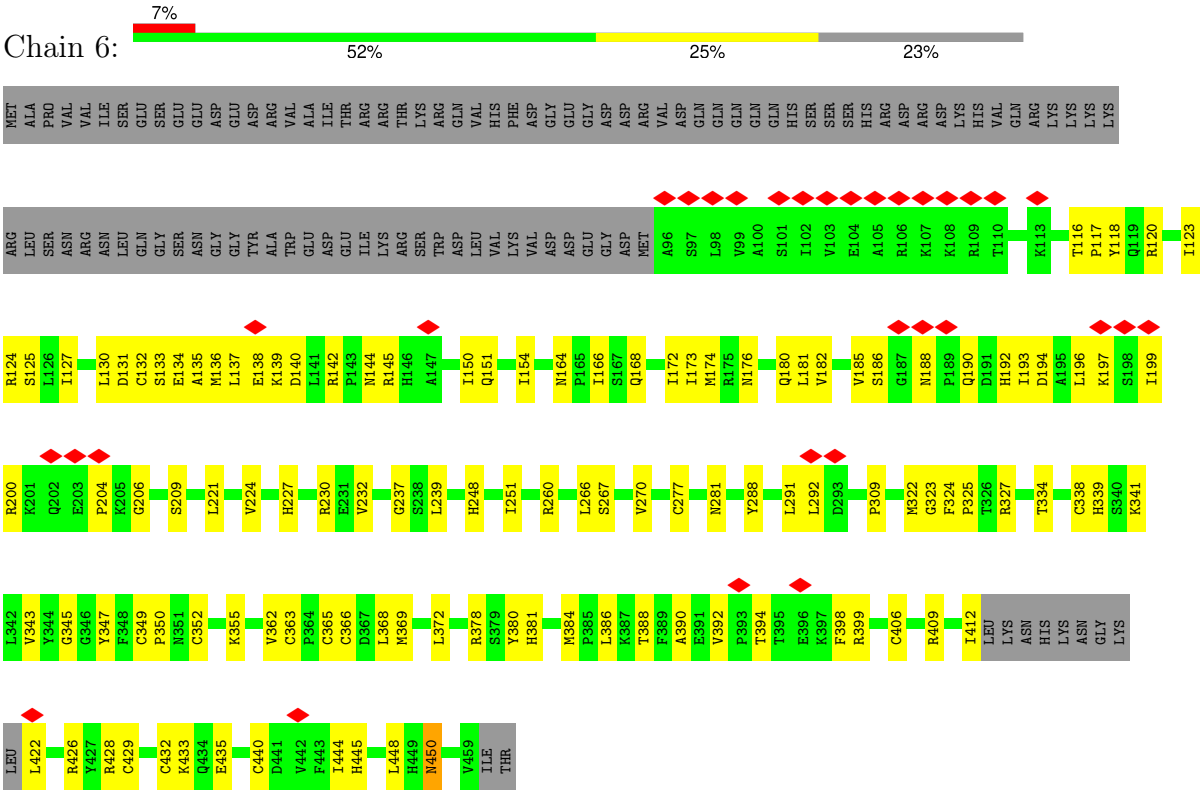
• Molecule 4: General transcription and DNA repair factor IIH subunit TFB4

Chain 4:



• Molecule 5: General transcription and DNA repair factor IIH

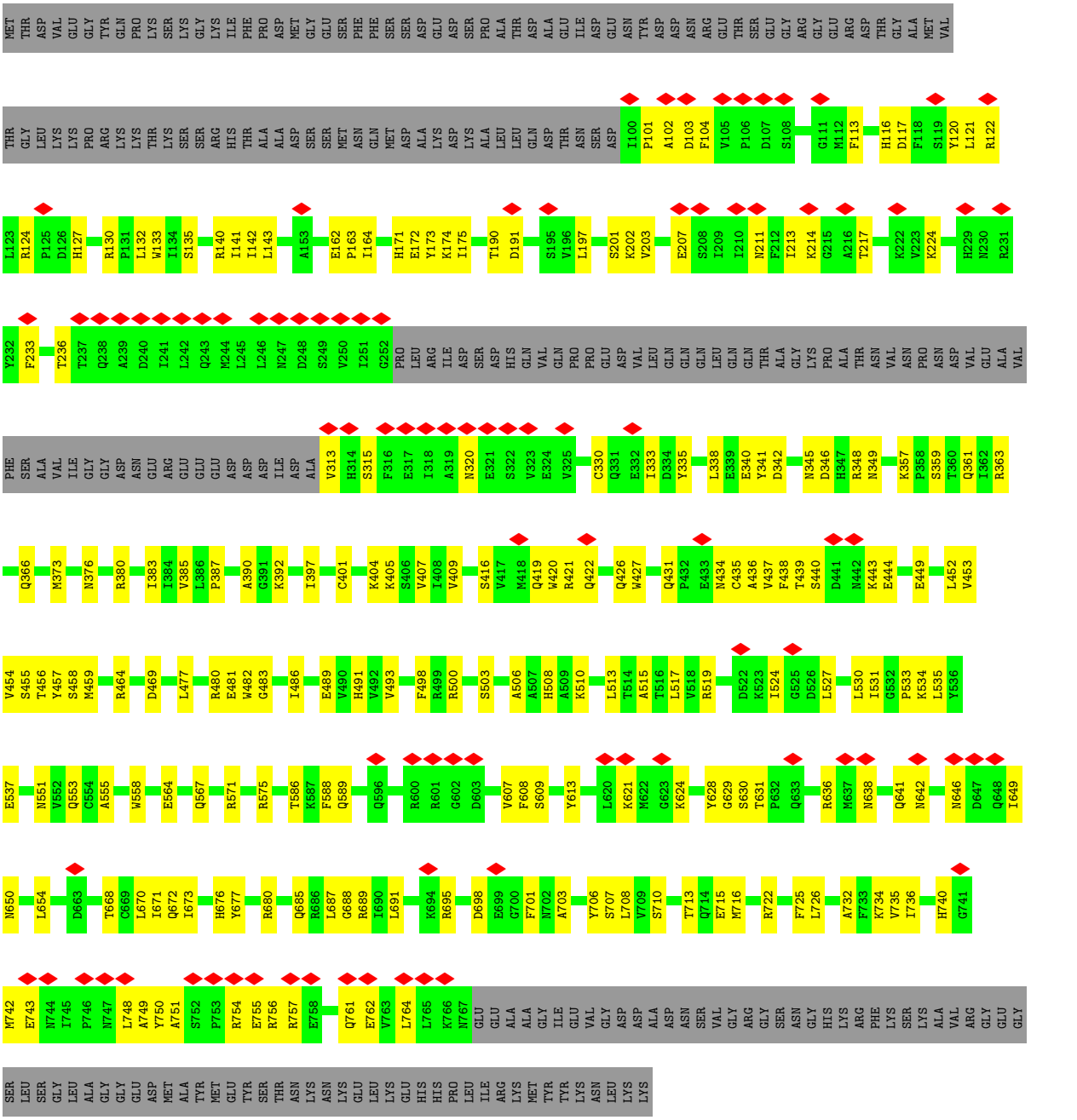
Chain 6:



• Molecule 6: General transcription and DNA repair factor IIH helicase subunit XPB

Chain 7:

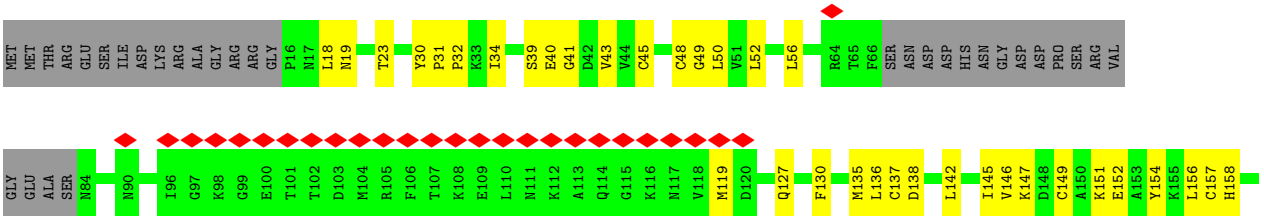


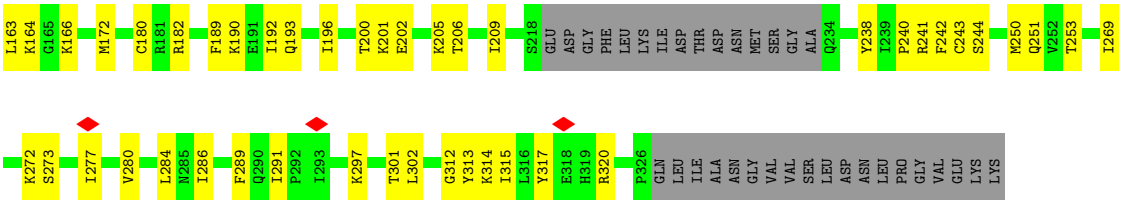


• Molecule 7: Transcription initiation factor IIB

Chain M:



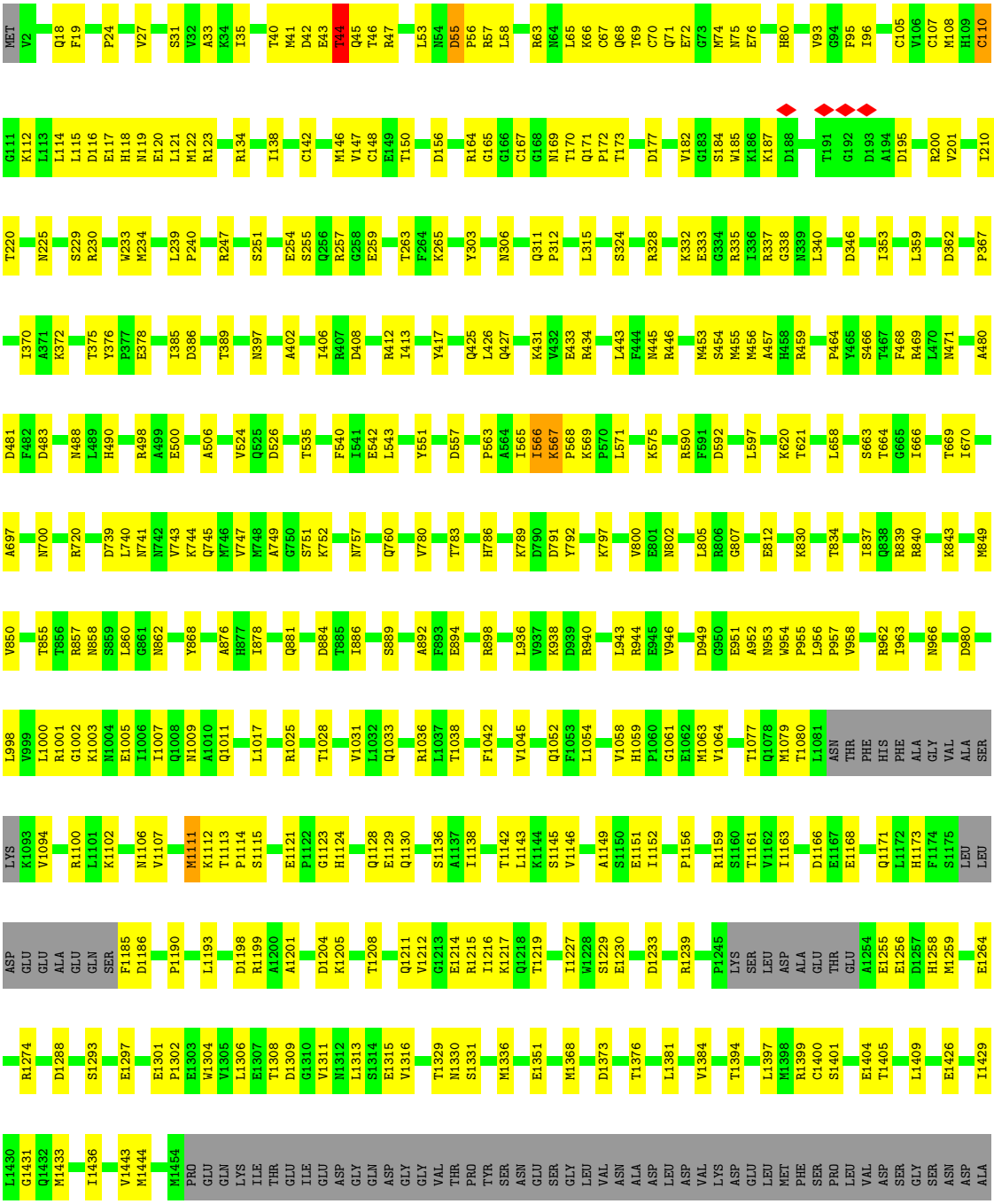


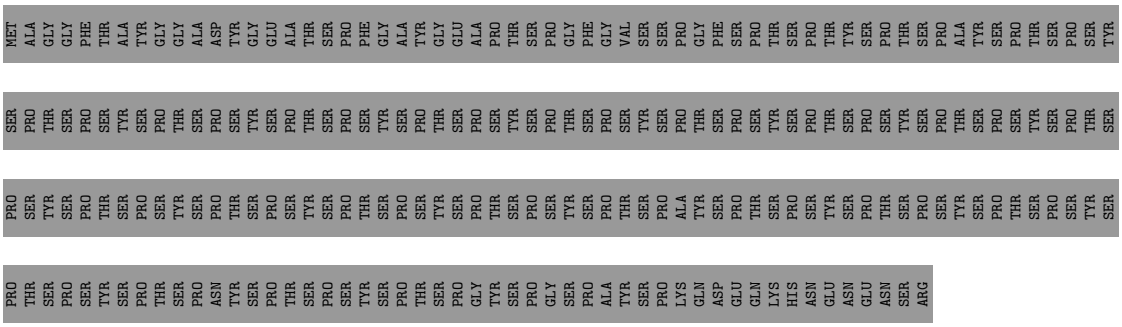


• Molecule 8: DNA-directed RNA polymerase subunit

Chain A:



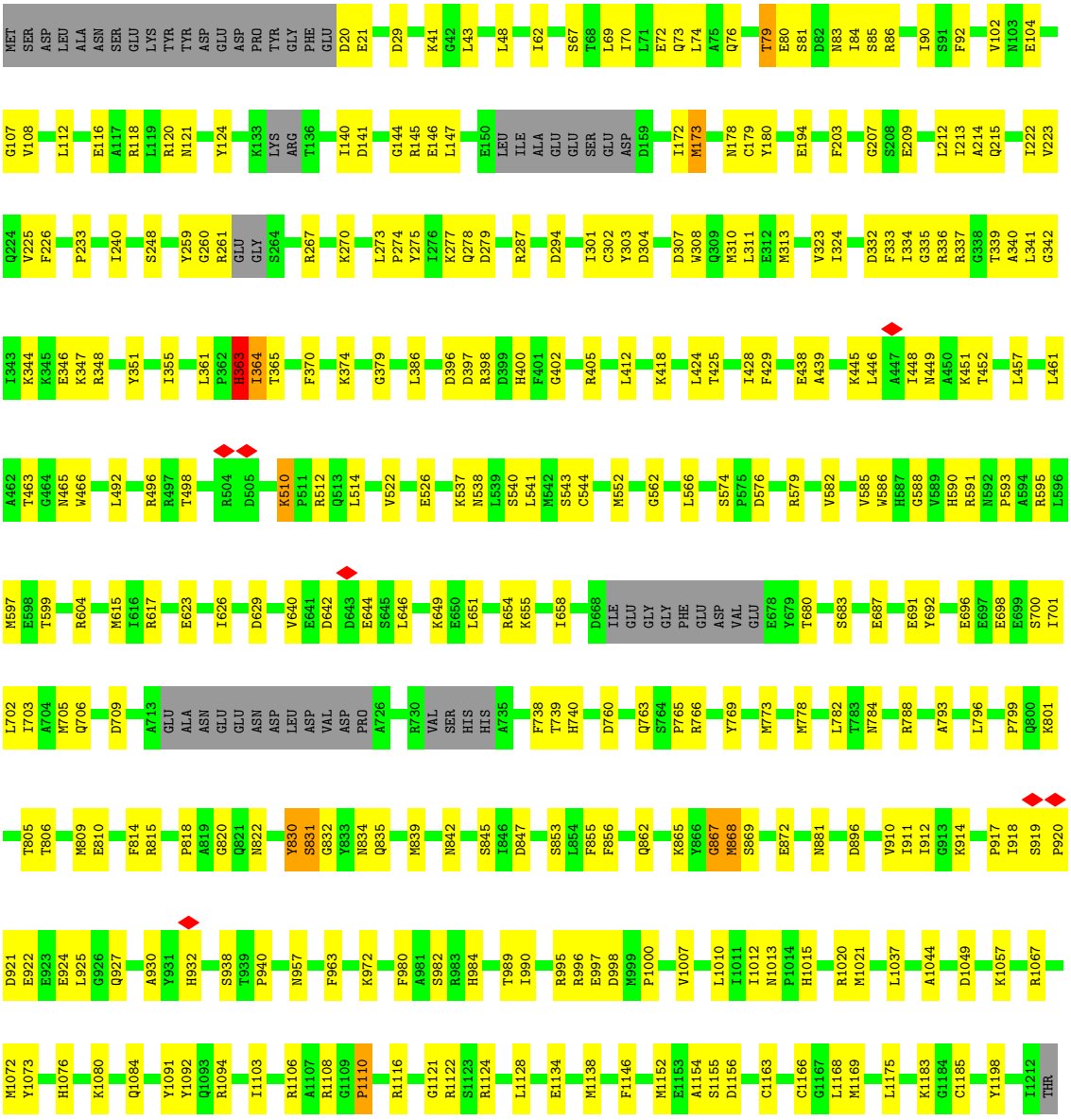




• Molecule 9: DNA-directed RNA polymerase subunit beta

Chain B:

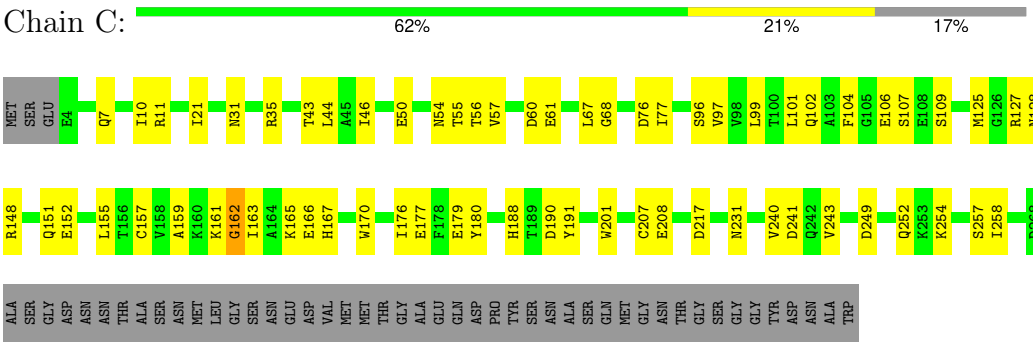






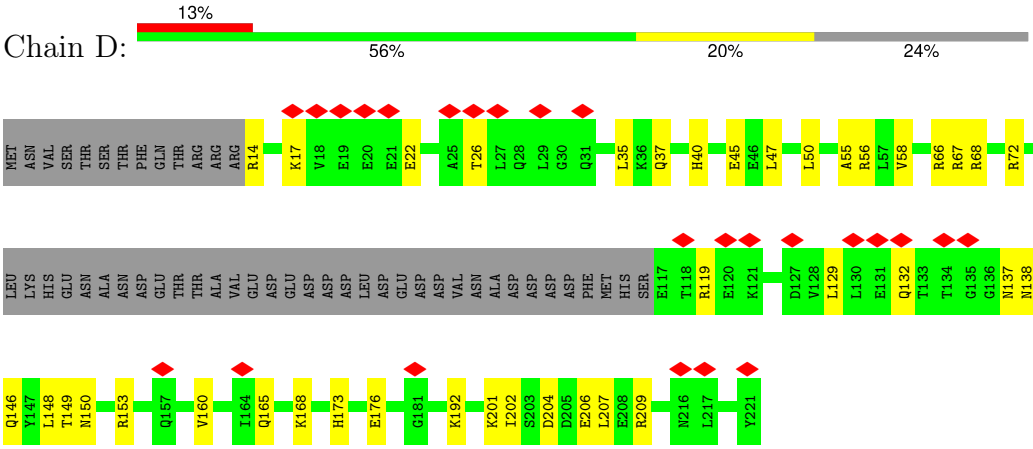
• Molecule 10: DNA-directed RNA polymerase II subunit RPB3

Chain C:



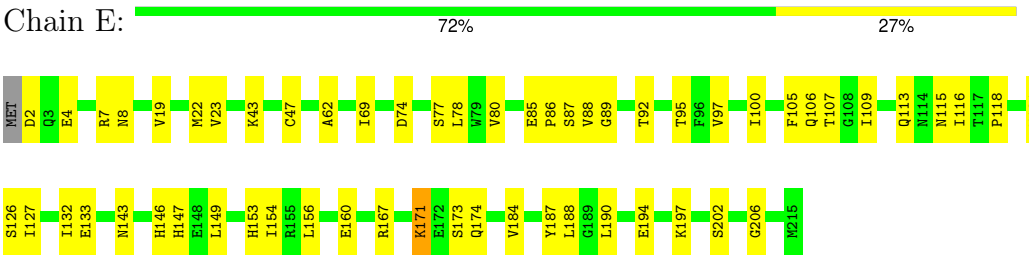
• Molecule 11: DNA-directed RNA polymerase II subunit RPB4

Chain D:



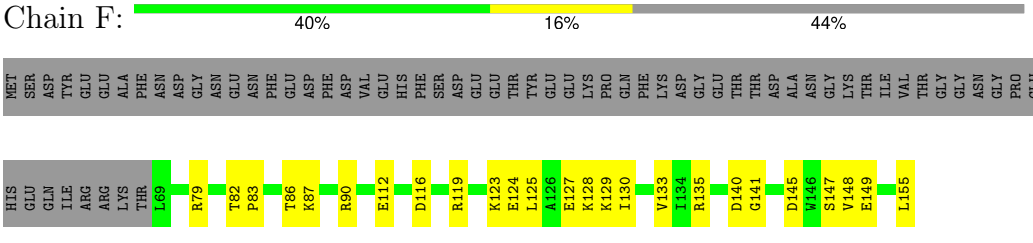
• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:



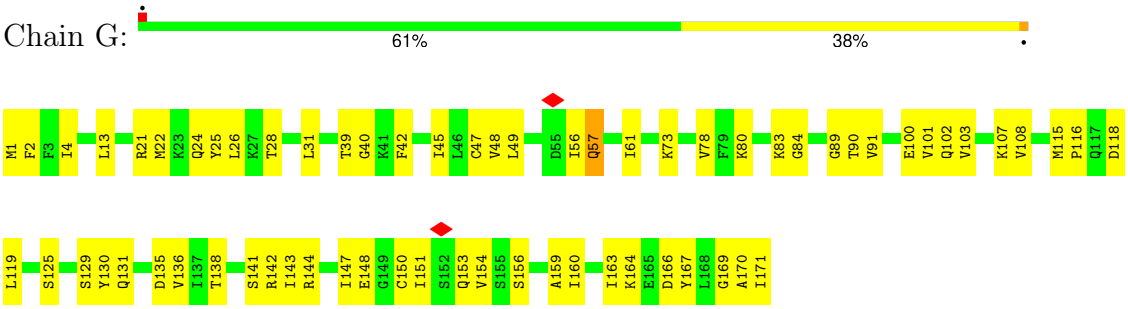
• Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:



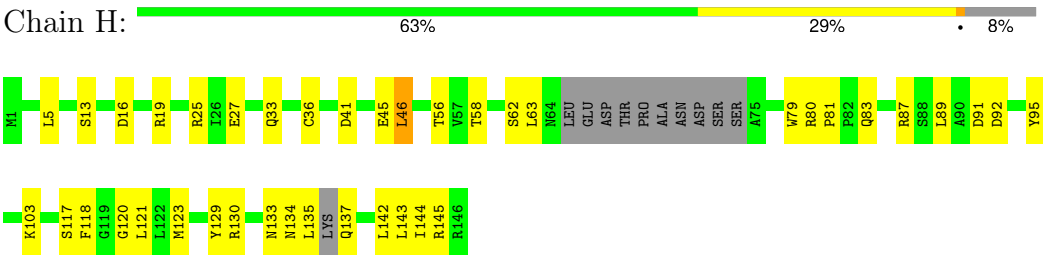
• Molecule 14: DNA-directed RNA polymerase II subunit RPB7

Chain G:



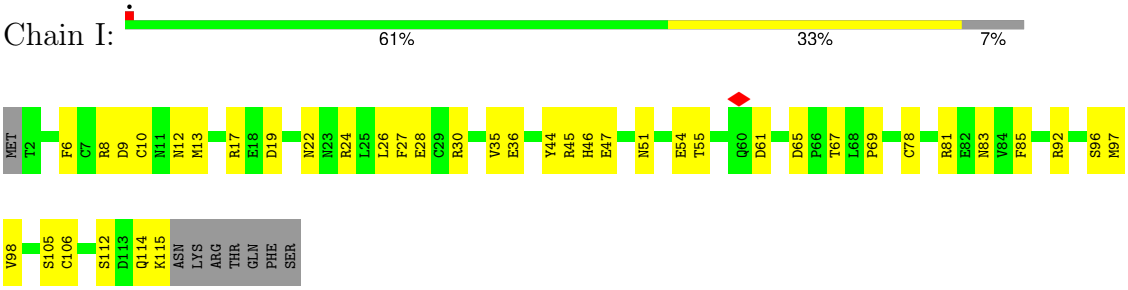
• Molecule 15: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



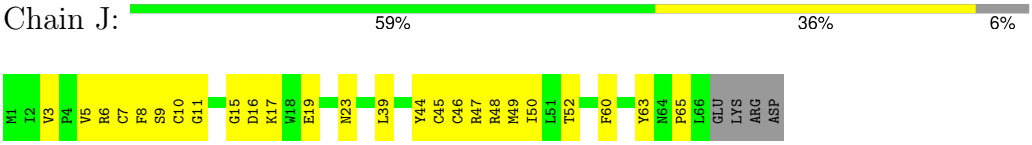
• Molecule 16: DNA-directed RNA polymerase II subunit RPB9

Chain I:



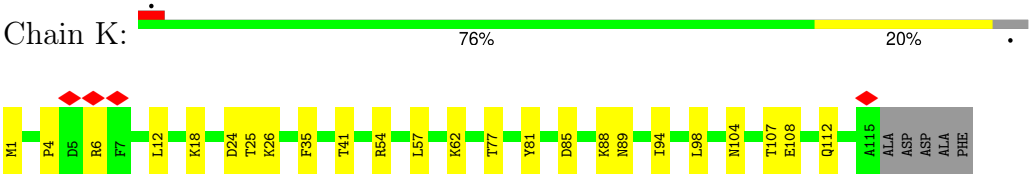
• Molecule 17: DNA-directed RNA polymerases II subunit RPABC5

Chain J:



• Molecule 18: DNA-directed RNA polymerase II subunit RPB11

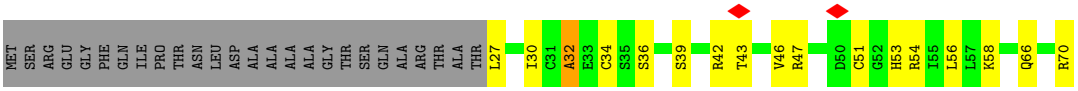
Chain K:



• Molecule 19: DNA-directed RNA polymerases II subunit RPABC4

Chain L:

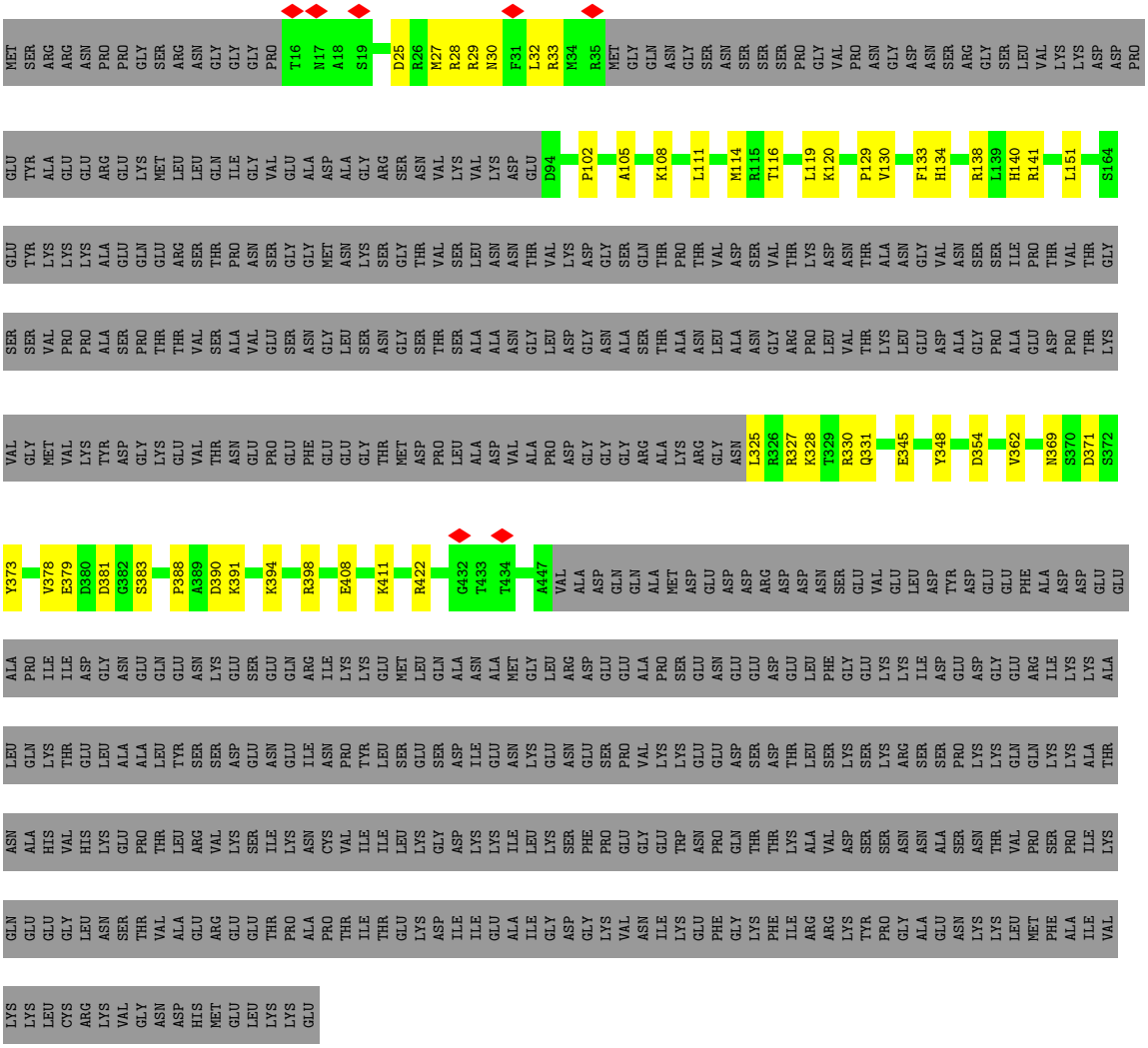




• Molecule 20: Transcription initiation factor IIF subunit alpha

Chain Q:

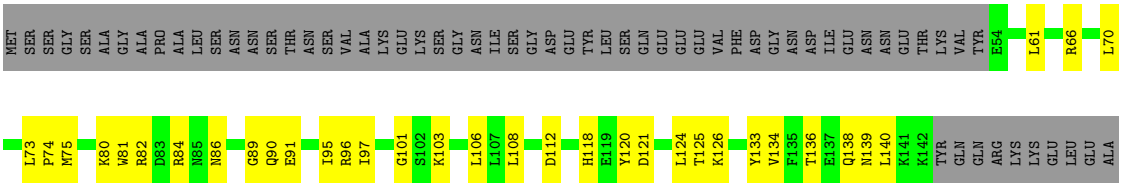


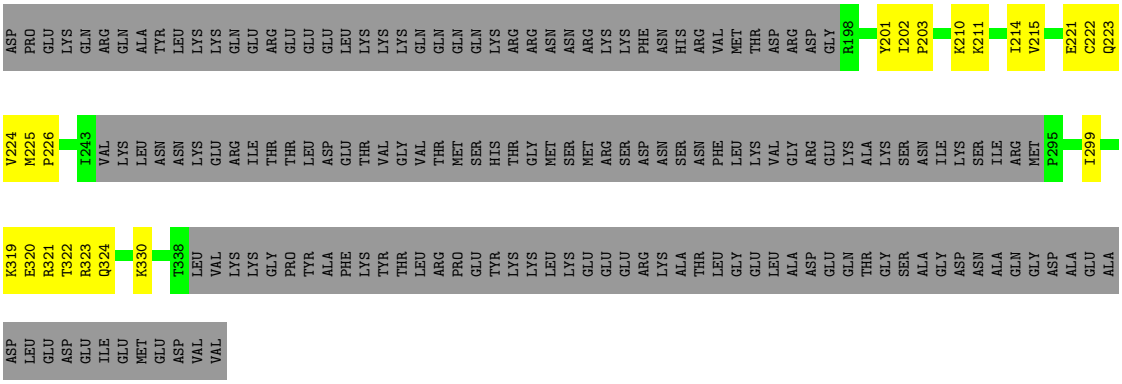


• Molecule 21: Transcription initiation factor IIF subunit beta

Chain P:



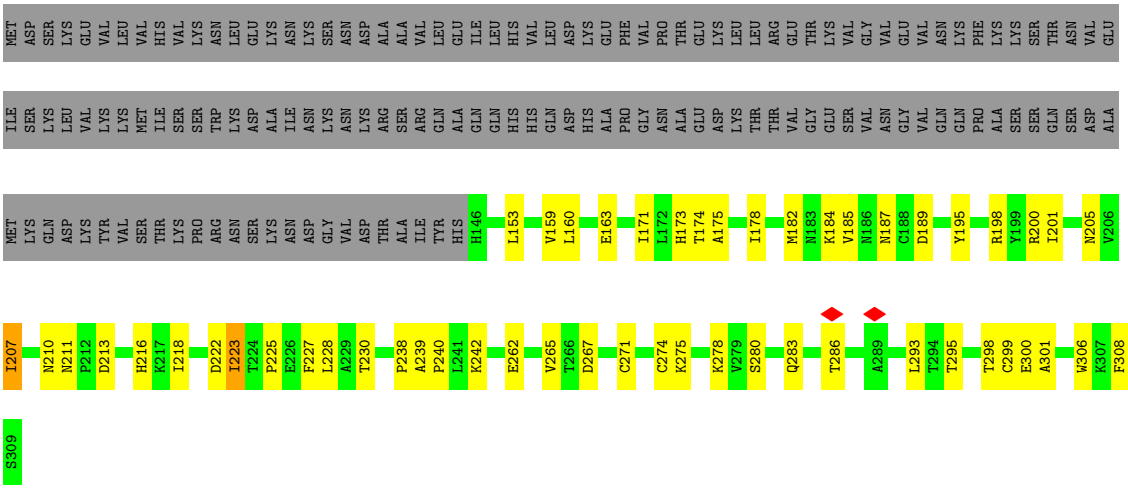




• Molecule 22: Transcription elongation factor

Chain S:

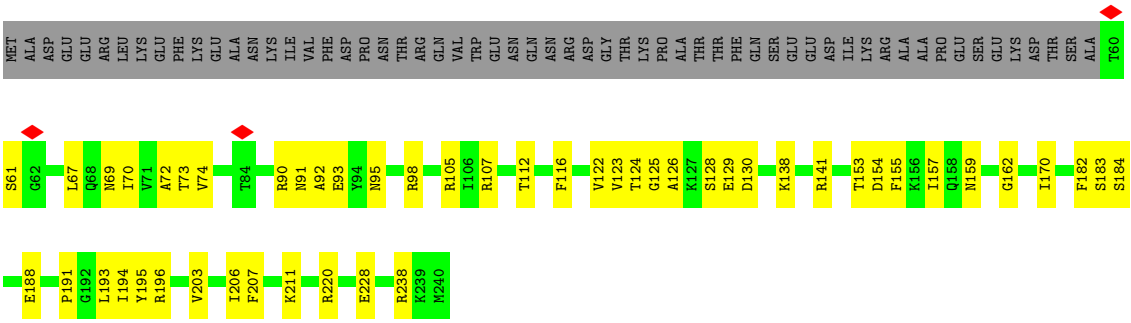




• Molecule 23: TATA-box-binding protein

Chain O:

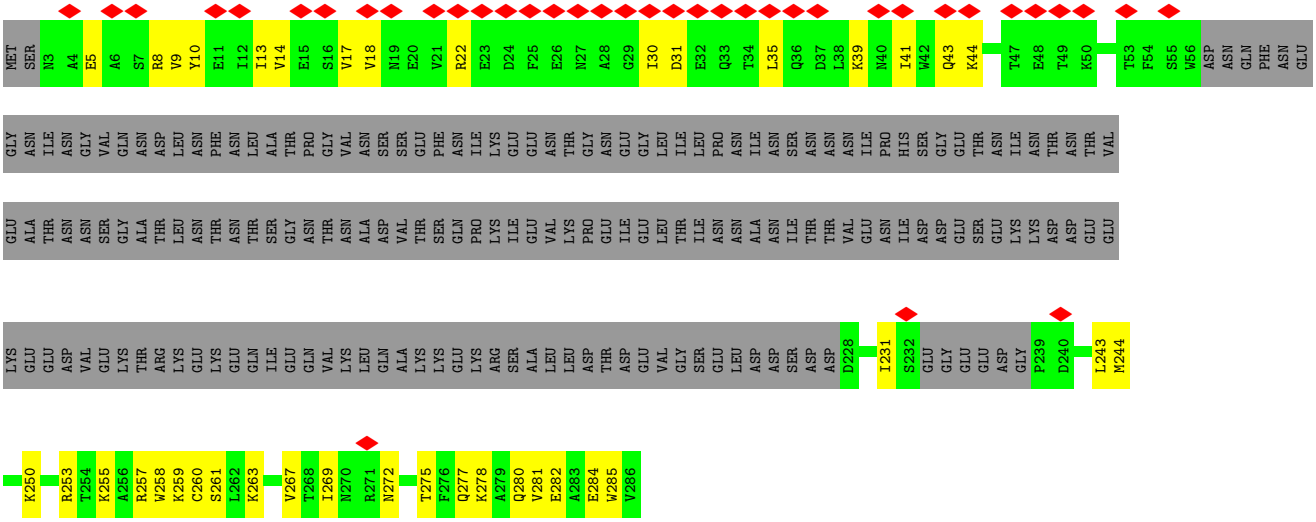




• Molecule 24: Transcription initiation factor IIA large subunit

Chain U:

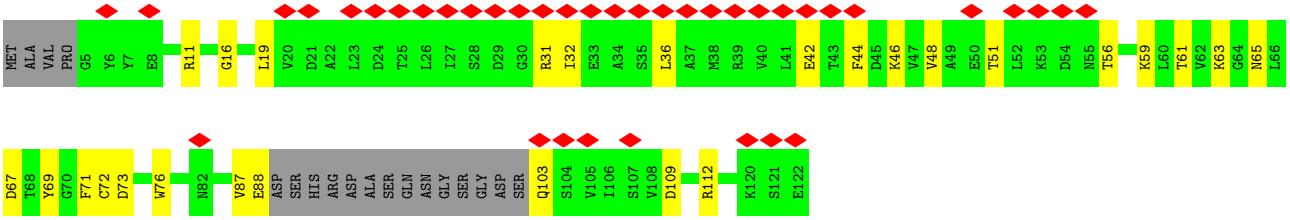




• Molecule 25: Transcription initiation factor IIA subunit 2

Chain V:

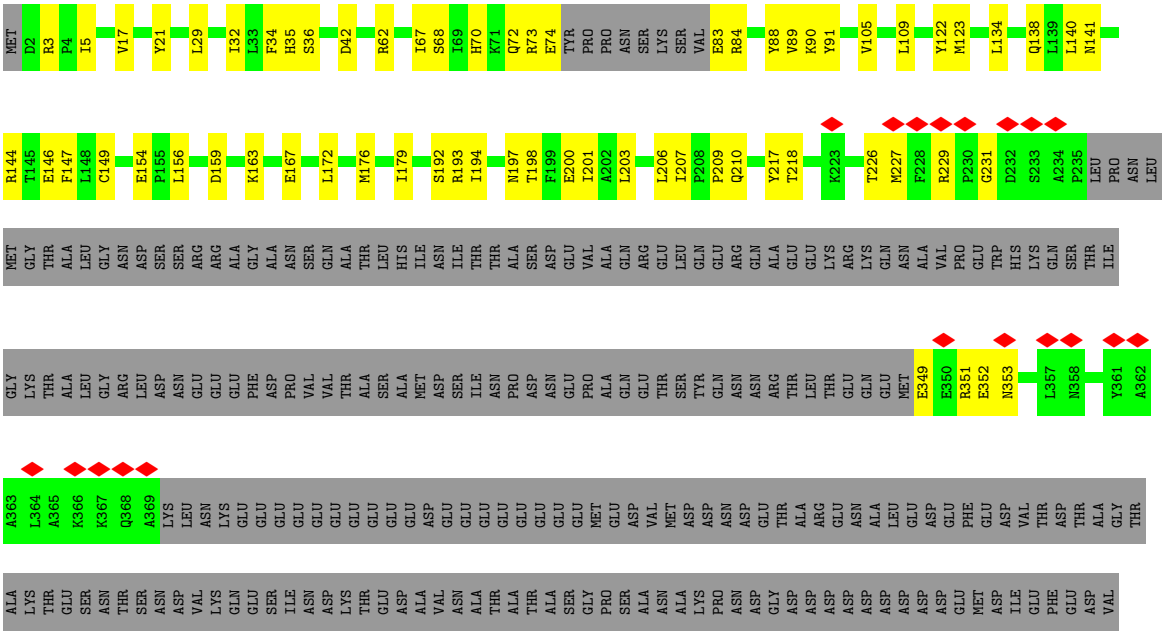




• Molecule 26: Transcription initiation factor IIE subunit alpha

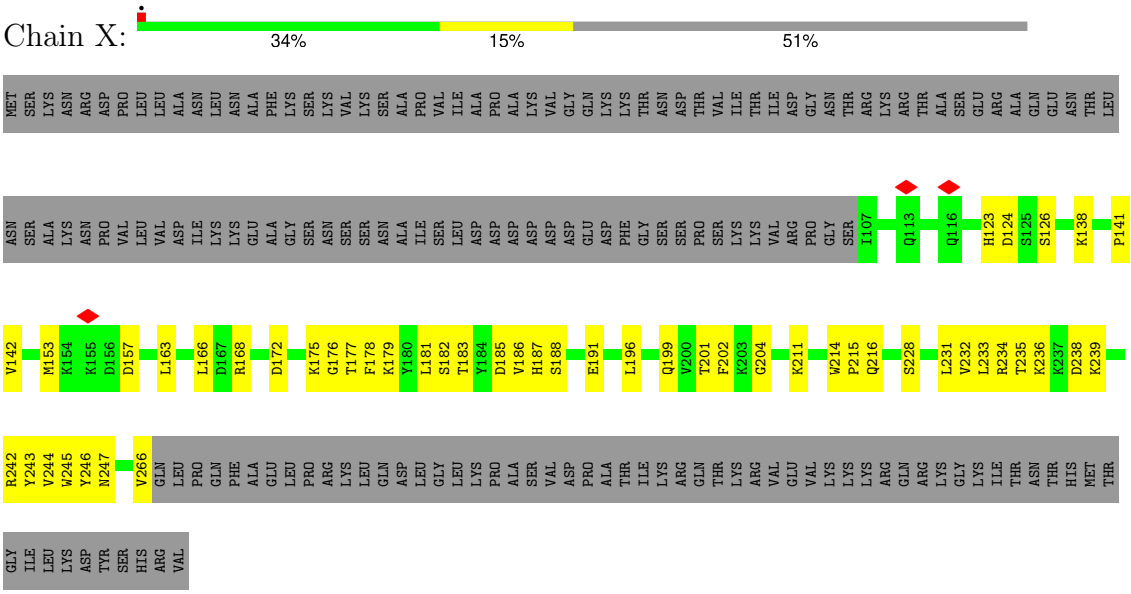
Chain W:





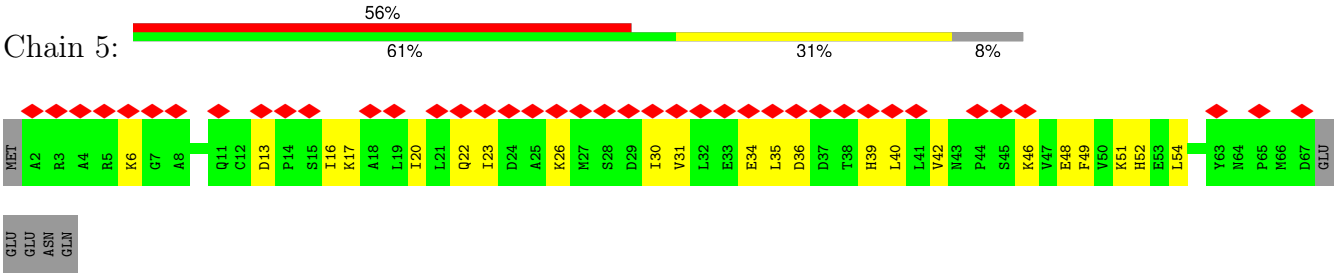
• Molecule 27: Transcription initiation factor IIE subunit beta

Chain X:



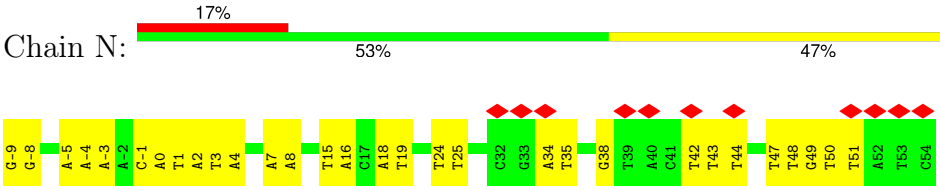
• Molecule 28: General transcription and DNA repair factor IIH subunit TFB5

Chain 5:



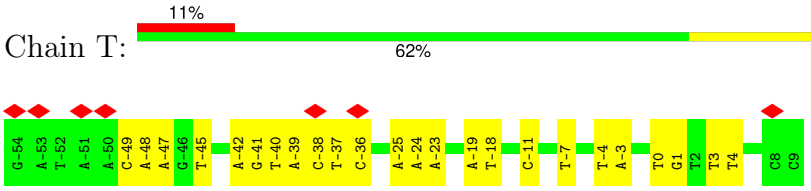
• Molecule 29: DNA (64-MER)

Chain N:



• Molecule 30: DNA (64-MER)

Chain T:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	138691	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.25	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	1750	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.083	Depositor
Minimum map value	-0.029	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0054	Depositor
Map size (Å)	414.72003, 414.72003, 414.72003	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, 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	0	0.29	0/6209	0.51	0/8384
2	1	0.25	0/3434	0.49	0/4624
3	2	0.23	0/3611	0.54	1/4881 (0.0%)
4	4	0.24	0/2305	0.46	0/3117
5	6	0.28	0/2843	0.49	0/3845
6	7	0.20	0/4992	0.48	0/6754
7	M	0.27	0/2204	0.63	0/2963
8	A	0.59	0/11368	0.74	6/15383 (0.0%)
9	B	0.64	0/9402	0.77	13/12680 (0.1%)
10	C	0.68	0/2124	0.72	0/2879
11	D	0.22	0/1339	0.59	2/1793 (0.1%)
12	E	0.53	0/1788	0.66	1/2406 (0.0%)
13	F	0.61	0/717	0.76	0/967
14	G	0.28	0/1363	0.66	2/1840 (0.1%)
15	H	0.57	0/1097	0.78	2/1484 (0.1%)
16	I	0.41	0/945	0.61	0/1273
17	J	0.85	0/549	0.84	0/738
18	K	0.62	0/942	0.68	0/1272
19	L	0.48	0/354	0.98	3/468 (0.6%)
20	Q	0.28	0/1648	0.57	0/2226
21	P	0.26	0/1511	0.52	0/2035
22	S	0.29	0/1317	0.70	2/1778 (0.1%)
23	O	0.25	0/1449	0.55	0/1952
24	U	0.25	0/898	0.60	0/1212
25	V	0.25	0/822	0.60	0/1109
26	W	0.23	0/2045	0.45	0/2757
27	X	0.21	0/1312	0.43	0/1767
28	5	0.29	0/502	0.79	1/677 (0.1%)
29	N	0.49	0/1464	0.69	0/2258
30	T	0.46	0/1475	0.58	0/2274
All	All	0.44	0/72029	0.63	33/97796 (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
7	M	0	3
8	A	0	11
9	B	0	7
12	E	0	1
13	F	0	1
15	H	0	1
19	L	0	1
22	S	0	1
All	All	0	26

There are no bond length outliers.

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	79	THR	CA-C-N	7.98	136.07	121.70
9	B	79	THR	C-N-CA	7.98	136.07	121.70
9	B	918	ILE	CA-C-N	6.89	134.10	121.70
9	B	918	ILE	C-N-CA	6.89	134.10	121.70
8	A	1107	VAL	CA-C-N	6.83	133.99	121.70

There are no chirality outliers.

5 of 26 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	A	44	THR	Peptide
8	A	55	ASP	Peptide
7	M	269	ILE	Peptide
7	M	30	TYR	Peptide
7	M	31	PRO	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	0	6091	0	6155	186	0
2	1	3382	0	3436	70	0
3	2	3546	0	3593	88	0
4	4	2267	0	2323	57	0
5	6	2786	0	2804	88	0
6	7	4889	0	4877	139	0
7	M	2175	0	2283	52	0
8	A	11167	0	11189	282	0
9	B	9227	0	9201	242	0
10	C	2086	0	2045	52	0
11	D	1331	0	1345	36	0
12	E	1752	0	1776	37	0
13	F	705	0	731	17	0
14	G	1335	0	1346	40	0
15	H	1080	0	1049	39	0
16	I	927	0	881	33	0
17	J	540	0	553	20	0
18	K	924	0	934	20	0
19	L	352	0	374	12	0
20	Q	1619	0	1452	42	0
21	P	1484	0	1480	41	0
22	S	1294	0	1289	38	0
23	O	1422	0	1500	44	0
24	U	885	0	866	32	0
25	V	815	0	822	28	0
26	W	2010	0	2026	46	0
27	X	1288	0	1307	34	0
28	5	498	0	506	18	0
29	N	1307	0	730	31	0
30	T	1314	0	725	25	0
31	0	8	0	0	3	0
32	4	1	0	0	0	0
32	6	4	0	0	0	0
32	A	2	0	0	0	0
32	B	1	0	0	0	0
32	C	1	0	0	0	0
32	I	2	0	0	0	0
32	J	1	0	0	0	0
32	L	1	0	0	0	0
32	M	1	0	0	0	0
32	S	1	0	0	0	0
33	7	1	0	0	0	0
33	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	70523	0	69598	1693	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 12.

The worst 5 of 1693 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)
7:M:45:CYS:HB3	7:M:48:CYS:SG	1.97	1.05
5:6:406:CYS:HB3	5:6:440:CYS:SG	1.99	1.02
19:L:27:LEU:N	19:L:39:SER:HG	1.62	0.95
29:N:38:DG:N1	30:T:-38:DC:O2	2.01	0.92
1:0:134:ARG:O	1:0:138:ASN:HB2	1.70	0.91

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	750/778 (96%)	709 (94%)	41 (6%)	0	100	100
2	1	407/642 (63%)	390 (96%)	17 (4%)	0	100	100
3	2	435/513 (85%)	413 (95%)	22 (5%)	0	100	100
4	4	286/338 (85%)	274 (96%)	12 (4%)	0	100	100
5	6	351/461 (76%)	335 (95%)	16 (5%)	0	100	100
6	7	604/843 (72%)	578 (96%)	26 (4%)	0	100	100
7	M	273/345 (79%)	240 (88%)	33 (12%)	0	100	100
8	A	1417/1733 (82%)	1252 (88%)	164 (12%)	1 (0%)	48	78
9	B	1150/1224 (94%)	981 (85%)	166 (14%)	3 (0%)	36	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
10	C	263/318 (83%)	227 (86%)	35 (13%)	1 (0%)	30 60
11	D	164/221 (74%)	151 (92%)	13 (8%)	0	100 100
12	E	212/215 (99%)	194 (92%)	18 (8%)	0	100 100
13	F	85/155 (55%)	78 (92%)	7 (8%)	0	100 100
14	G	169/171 (99%)	147 (87%)	21 (12%)	1 (1%)	21 52
15	H	129/146 (88%)	105 (81%)	24 (19%)	0	100 100
16	I	112/122 (92%)	97 (87%)	15 (13%)	0	100 100
17	J	64/70 (91%)	57 (89%)	7 (11%)	0	100 100
18	K	113/120 (94%)	105 (93%)	8 (7%)	0	100 100
19	L	42/70 (60%)	25 (60%)	17 (40%)	0	100 100
20	Q	208/735 (28%)	190 (91%)	18 (9%)	0	100 100
21	P	173/400 (43%)	161 (93%)	12 (7%)	0	100 100
22	S	162/309 (52%)	142 (88%)	20 (12%)	0	100 100
23	O	179/240 (75%)	166 (93%)	13 (7%)	0	100 100
24	U	101/286 (35%)	97 (96%)	4 (4%)	0	100 100
25	V	100/122 (82%)	98 (98%)	2 (2%)	0	100 100
26	W	241/482 (50%)	234 (97%)	7 (3%)	0	100 100
27	X	158/328 (48%)	149 (94%)	9 (6%)	0	100 100
28	5	64/72 (89%)	58 (91%)	6 (9%)	0	100 100
All	All	8412/11459 (73%)	7653 (91%)	753 (9%)	6 (0%)	49 78

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	B	364	ILE
14	G	57	GLN
9	B	363	HIS
8	A	1112	LYS
9	B	705	MET

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	684/707 (97%)	684 (100%)	0	100	100
2	1	389/589 (66%)	389 (100%)	0	100	100
3	2	394/468 (84%)	394 (100%)	0	100	100
4	4	259/300 (86%)	259 (100%)	0	100	100
5	6	322/418 (77%)	321 (100%)	1 (0%)	86	83
6	7	540/737 (73%)	540 (100%)	0	100	100
7	M	245/299 (82%)	245 (100%)	0	100	100
8	A	1235/1520 (81%)	1235 (100%)	0	100	100
9	B	1000/1061 (94%)	1000 (100%)	0	100	100
10	C	233/274 (85%)	233 (100%)	0	100	100
11	D	146/200 (73%)	146 (100%)	0	100	100
12	E	196/197 (100%)	196 (100%)	0	100	100
13	F	77/137 (56%)	77 (100%)	0	100	100
14	G	151/152 (99%)	151 (100%)	0	100	100
15	H	118/128 (92%)	118 (100%)	0	100	100
16	I	108/116 (93%)	108 (100%)	0	100	100
17	J	61/65 (94%)	61 (100%)	0	100	100
18	K	99/102 (97%)	99 (100%)	0	100	100
19	L	39/57 (68%)	39 (100%)	0	100	100
20	Q	147/641 (23%)	147 (100%)	0	100	100
21	P	166/363 (46%)	166 (100%)	0	100	100
22	S	141/274 (52%)	141 (100%)	0	100	100
23	O	153/205 (75%)	153 (100%)	0	100	100
24	U	99/260 (38%)	99 (100%)	0	100	100
25	V	94/108 (87%)	94 (100%)	0	100	100
26	W	224/429 (52%)	224 (100%)	0	100	100
27	X	144/295 (49%)	143 (99%)	1 (1%)	76	77
28	5	53/66 (80%)	53 (100%)	0	100	100
All	All	7517/10168 (74%)	7515 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	6	450	ASN
27	X	216	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 82 such sidechains are listed below:

Mol	Chain	Res	Type
12	E	113	GLN
22	S	205	ASN
12	E	146	HIS
18	K	110	ASN
24	U	43	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 17 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
31	SF4	0	801	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
31	SF4	0	801	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.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	0	801	SF4	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

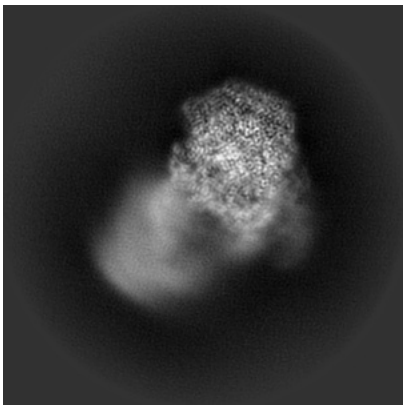
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-42380. These allow visual inspection of the internal detail of the map and identification of artifacts.

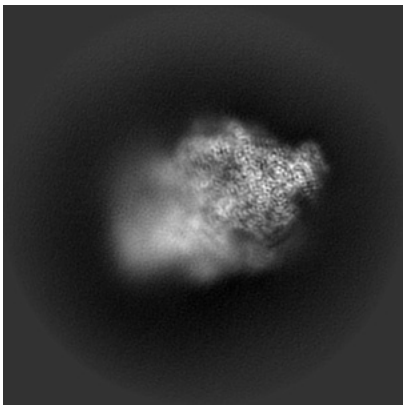
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

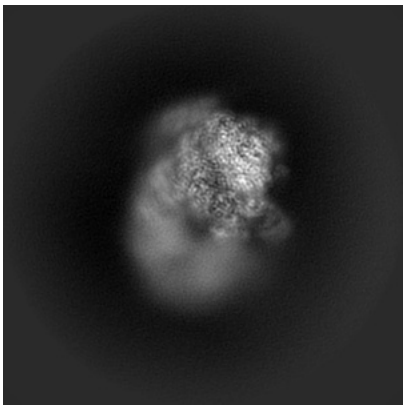
6.1.1 Primary map



X

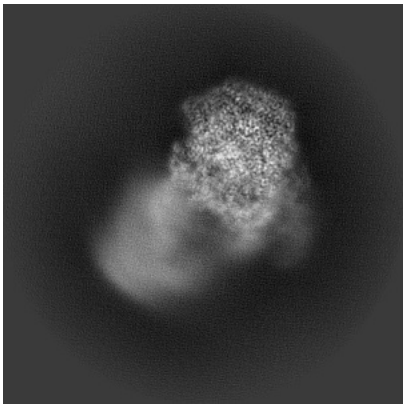


Y

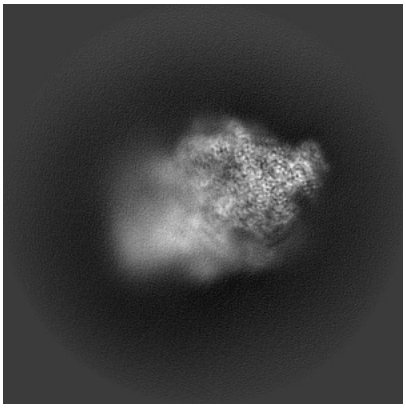


Z

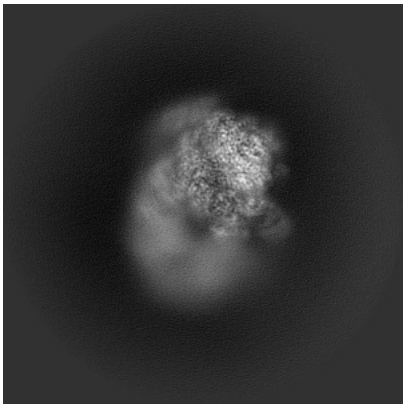
6.1.2 Raw map



X



Y

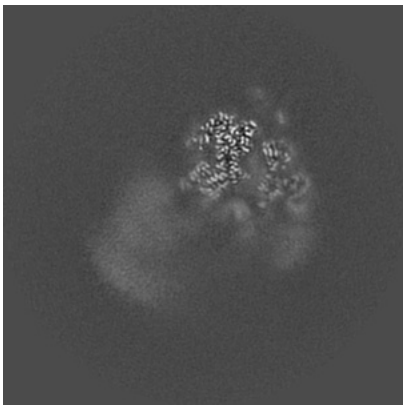


Z

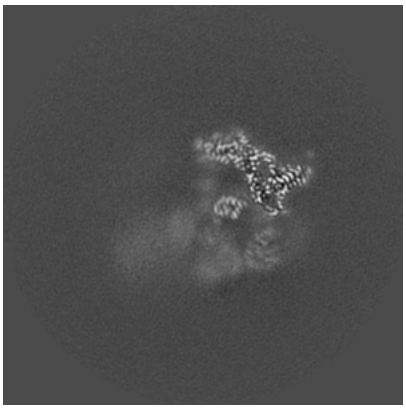
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

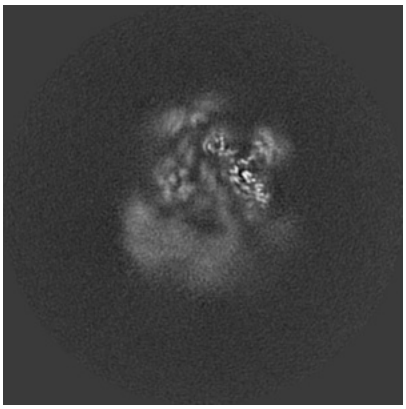
6.2.1 Primary map



X Index: 192

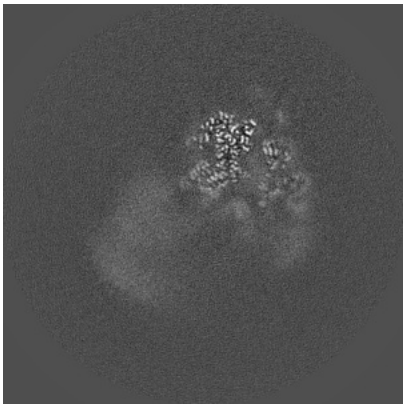


Y Index: 192

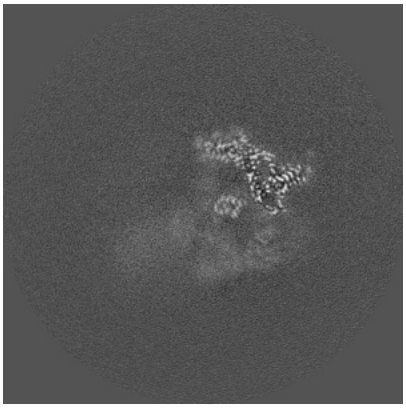


Z Index: 192

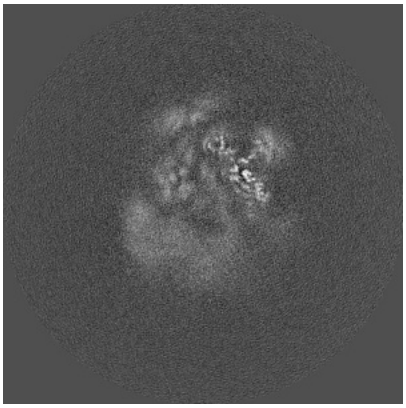
6.2.2 Raw map



X Index: 192



Y Index: 192

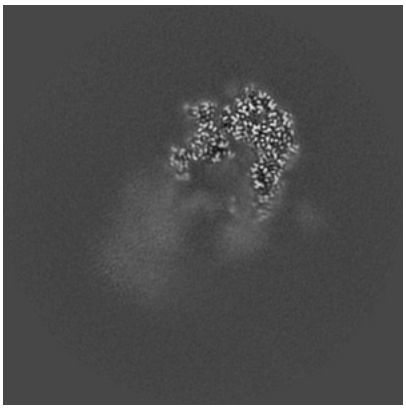


Z Index: 192

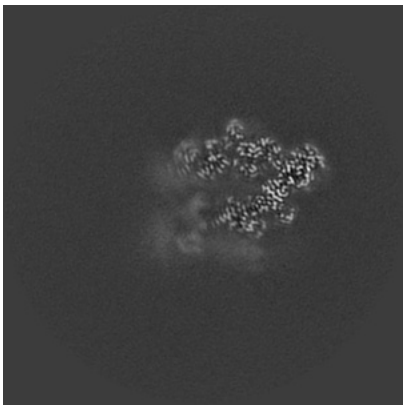
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

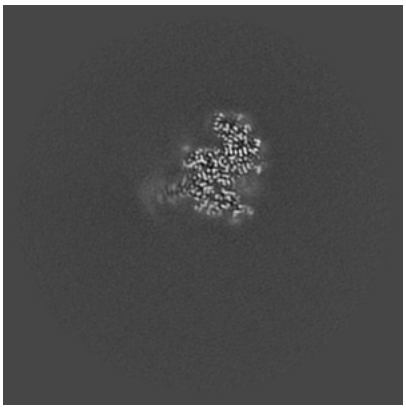
6.3.1 Primary map



X Index: 214

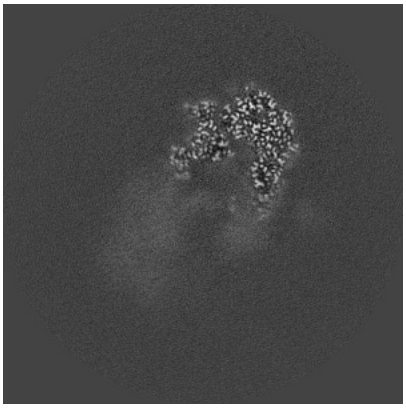


Y Index: 225

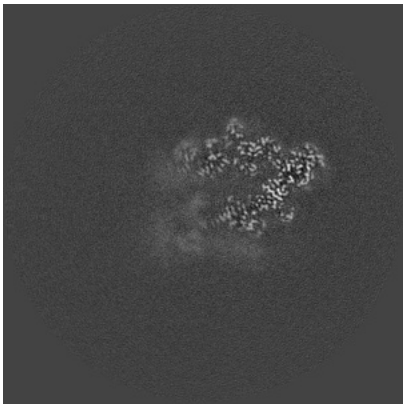


Z Index: 265

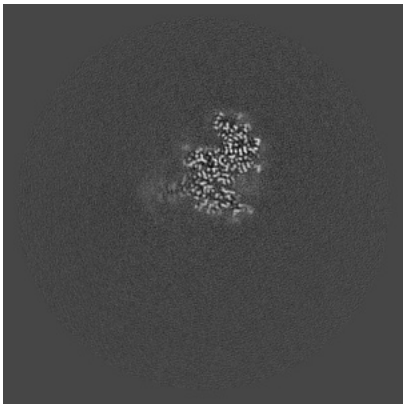
6.3.2 Raw map



X Index: 214



Y Index: 225

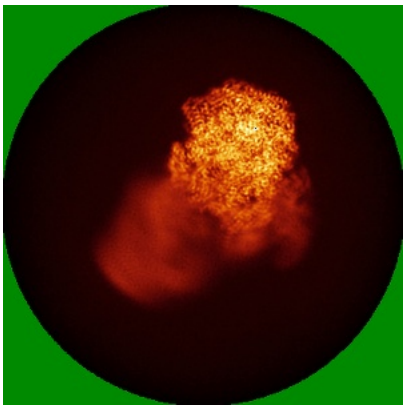


Z Index: 265

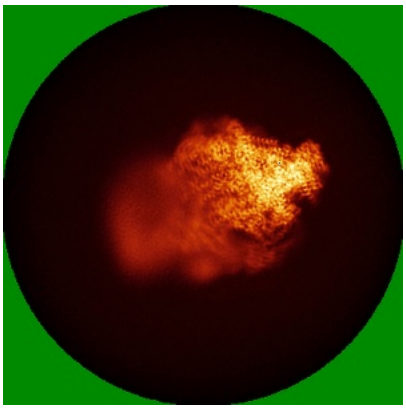
The images above show the largest variance slices of the map in three orthogonal directions.

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

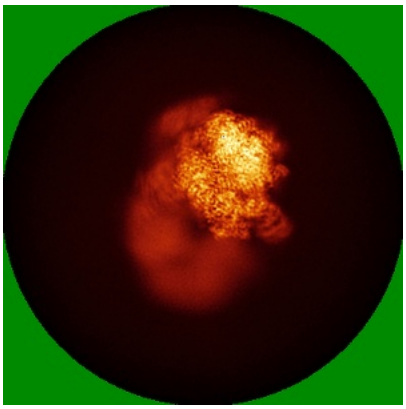
6.4.1 Primary map



X

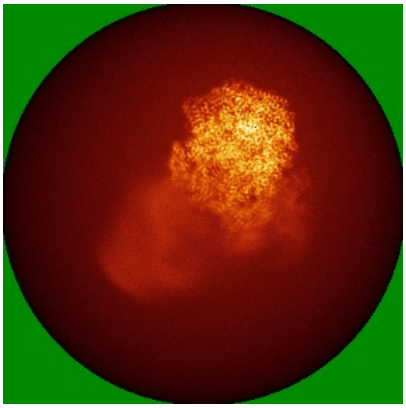


Y

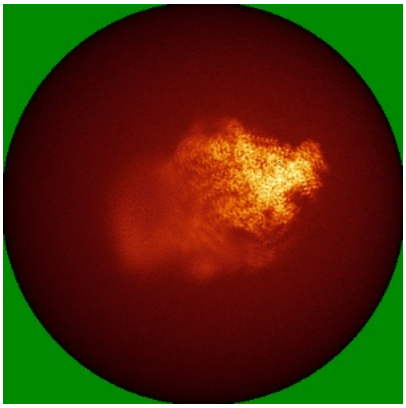


Z

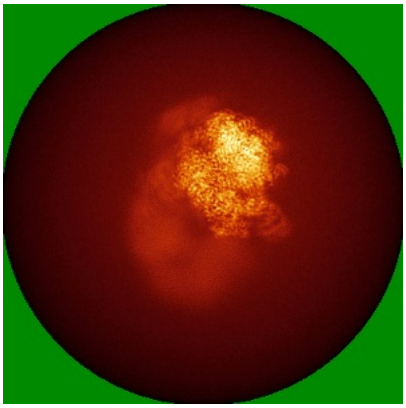
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

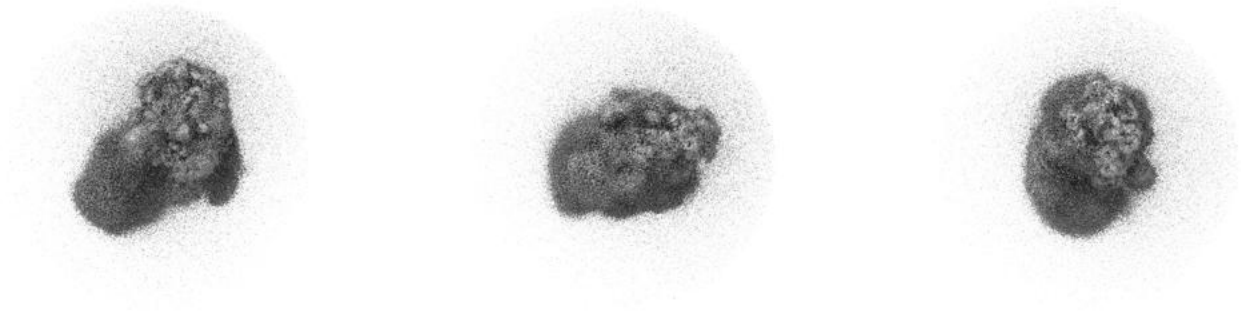
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0054. 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.

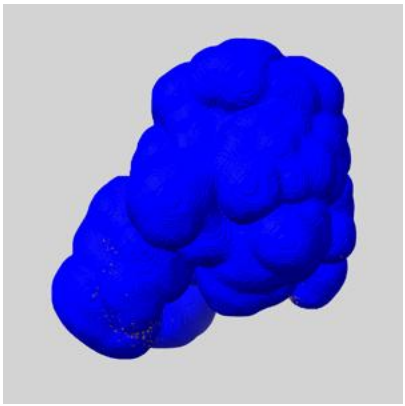
6.6 Mask visualisation

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

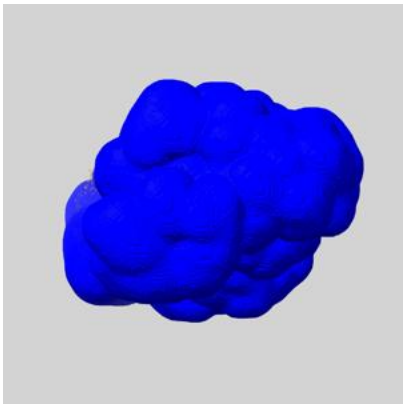
A mask typically either:

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

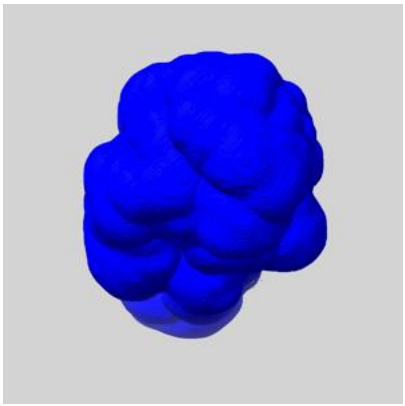
6.6.1 emd_42380_msk_1.map



X



Y

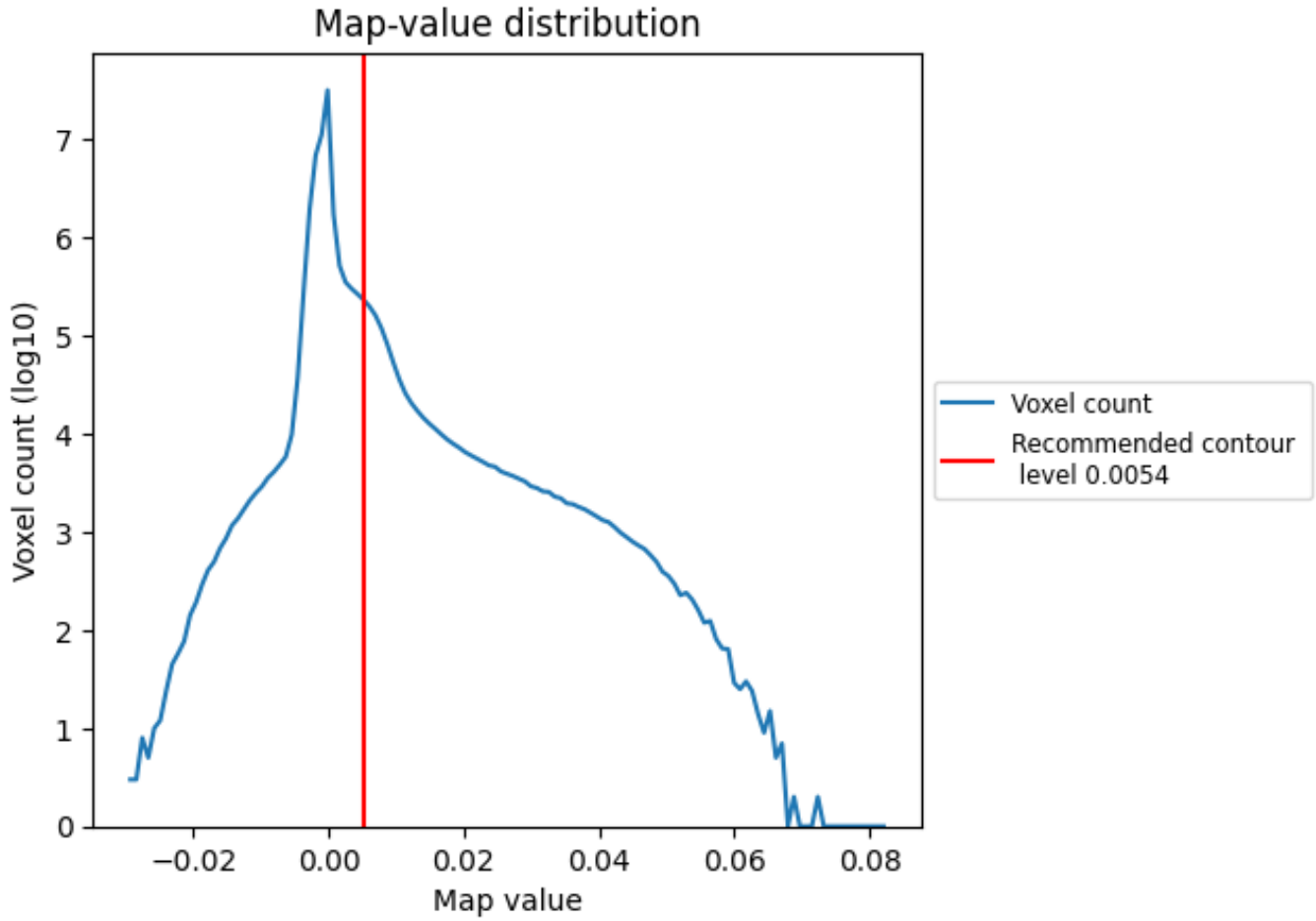


Z

7 Map analysis

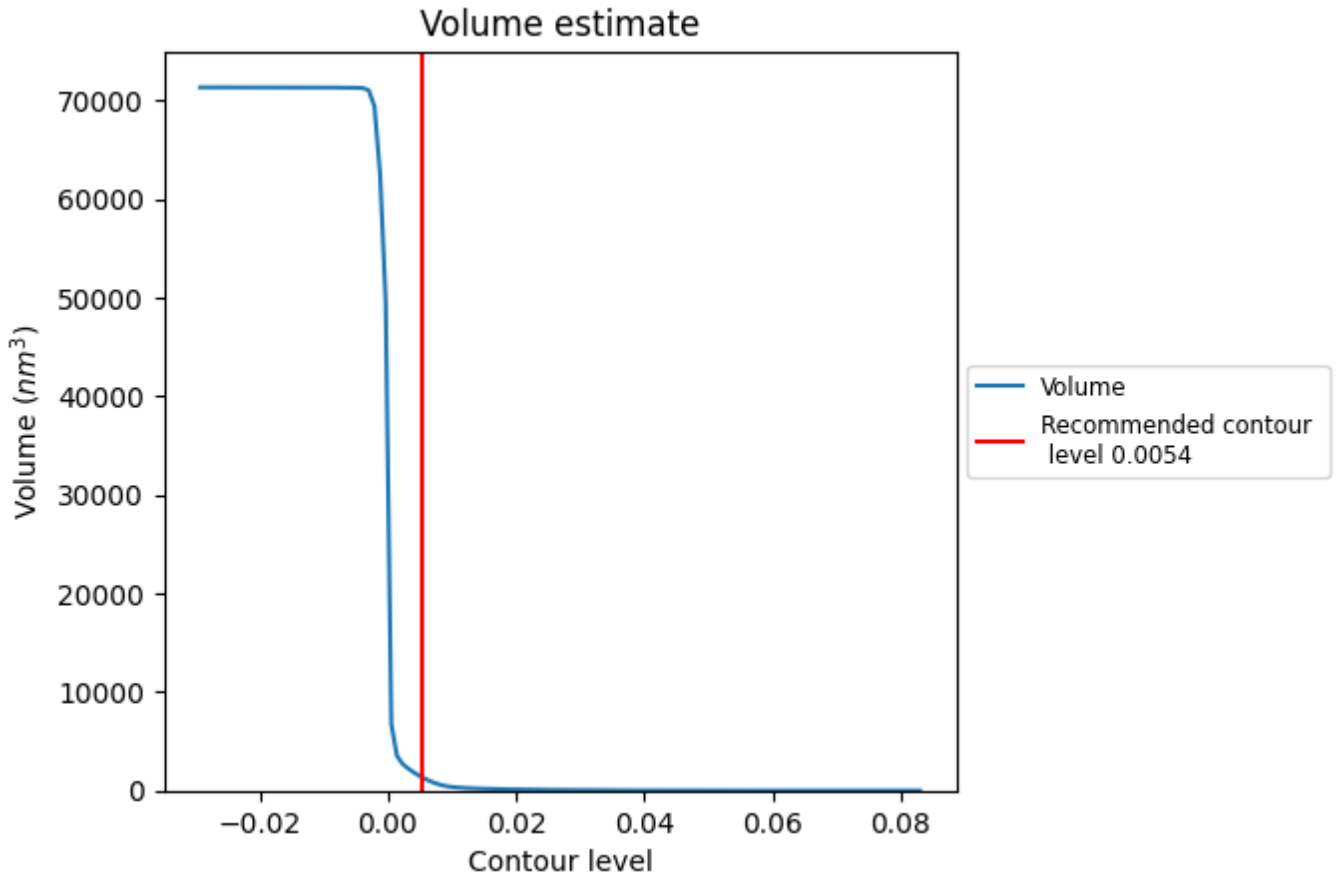
This section contains the results of statistical analysis of the map.

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.

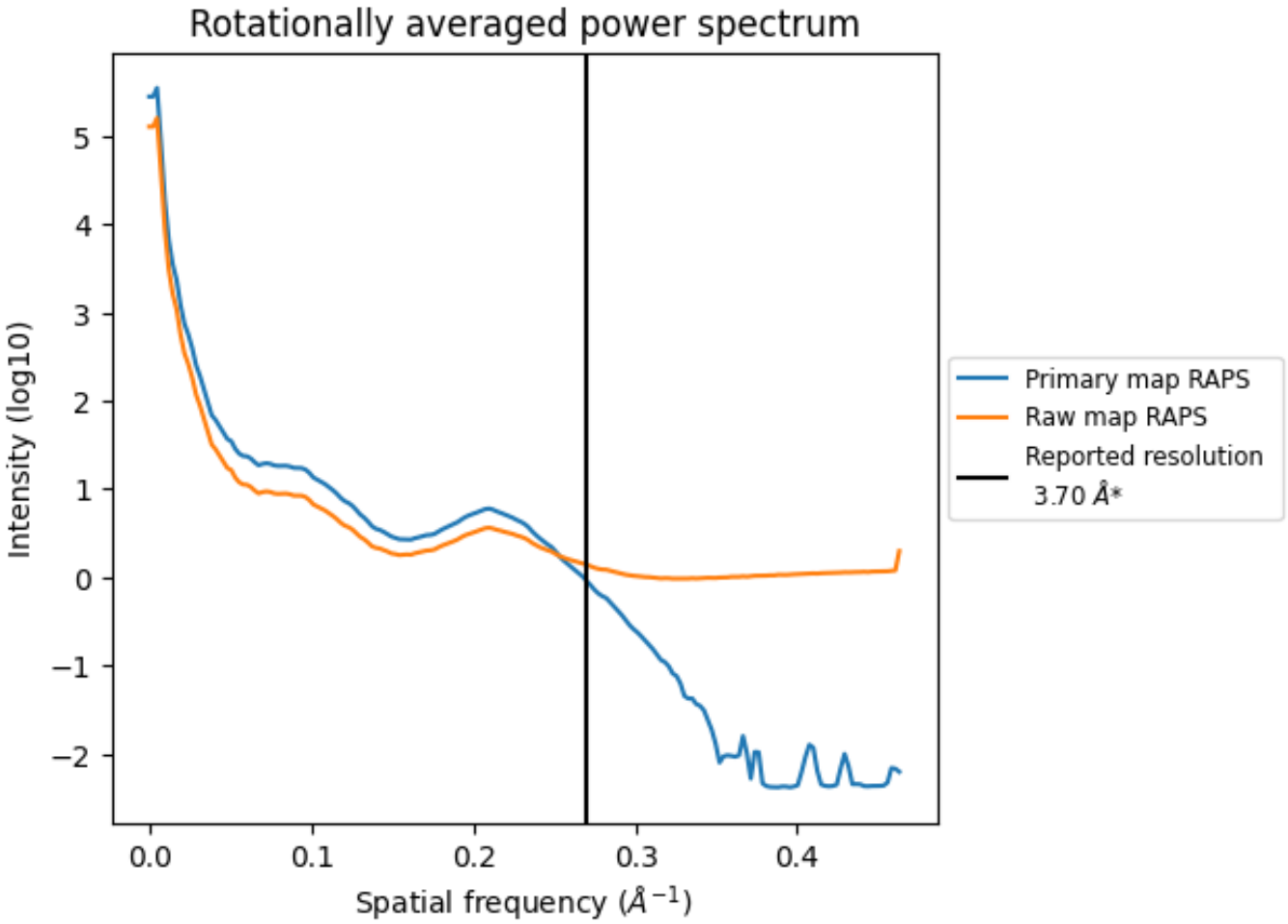
7.2 Volume estimate (i)



The volume at the recommended contour level is 1335 nm^3; this corresponds to an approximate mass of 1206 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)

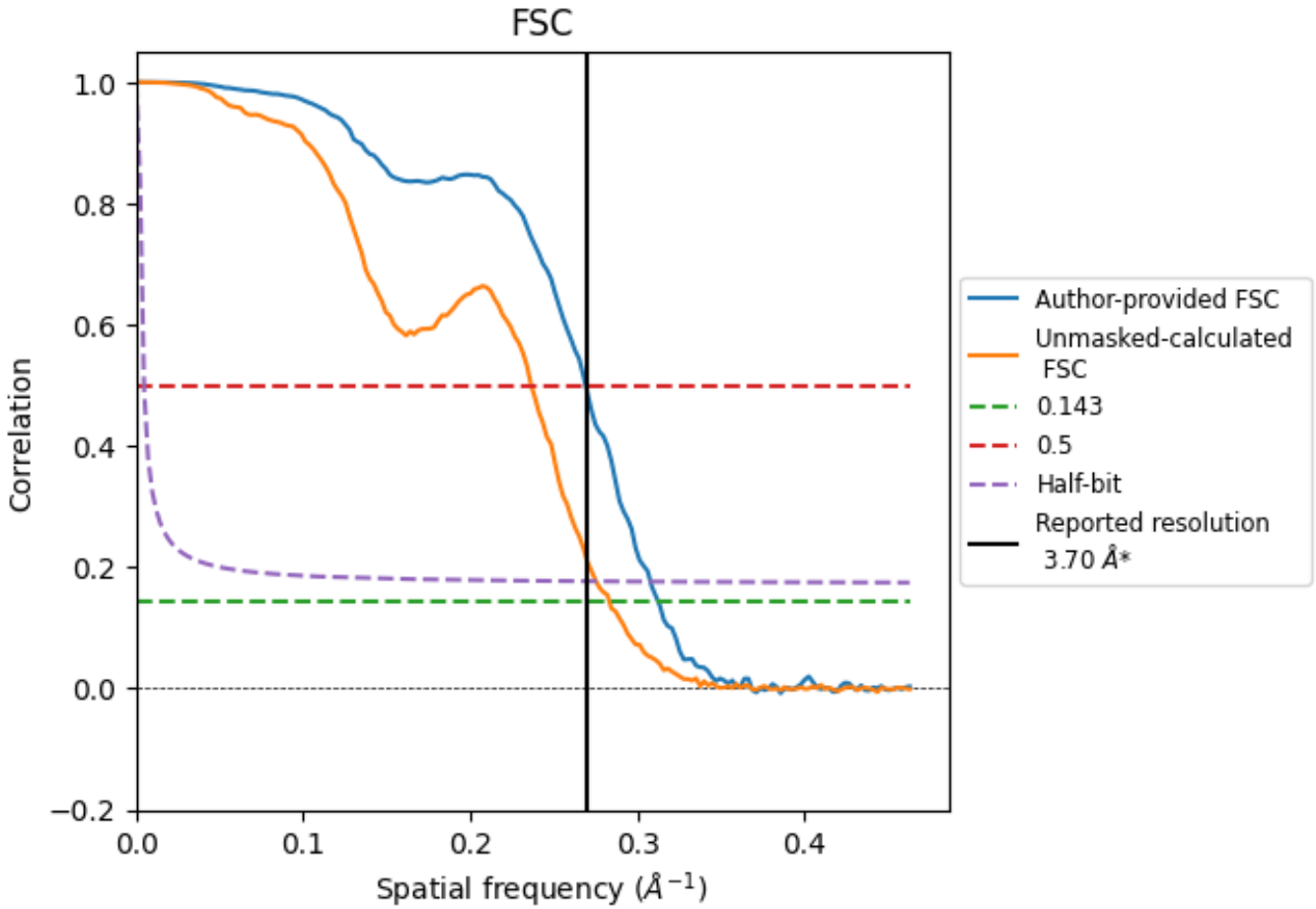


*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

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 0.270 Å^{-1}

8.2 Resolution estimates (i)

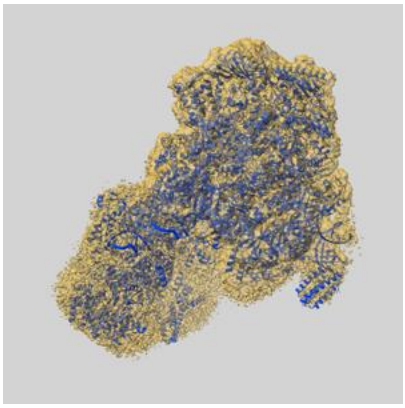
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.20	3.72	3.25
Unmasked-calculated*	3.53	4.23	3.63

*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 3.20 differs from the reported value 3.7 by more than 10 %

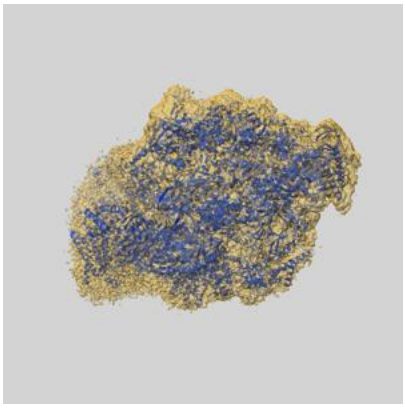
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-42380 and PDB model 8UMI. Per-residue inclusion information can be found in section 3 on page 11.

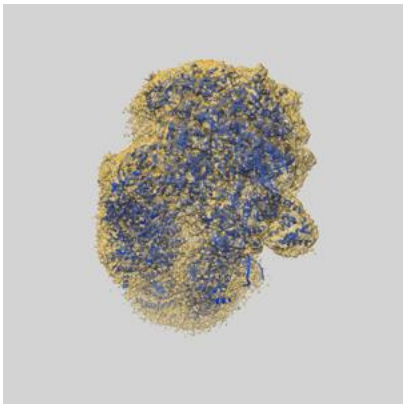
9.1 Map-model overlay



X



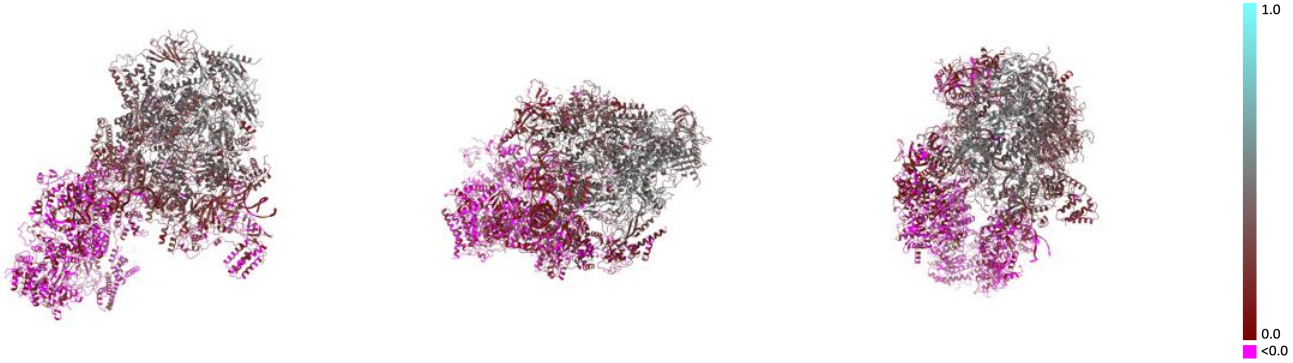
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0054 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

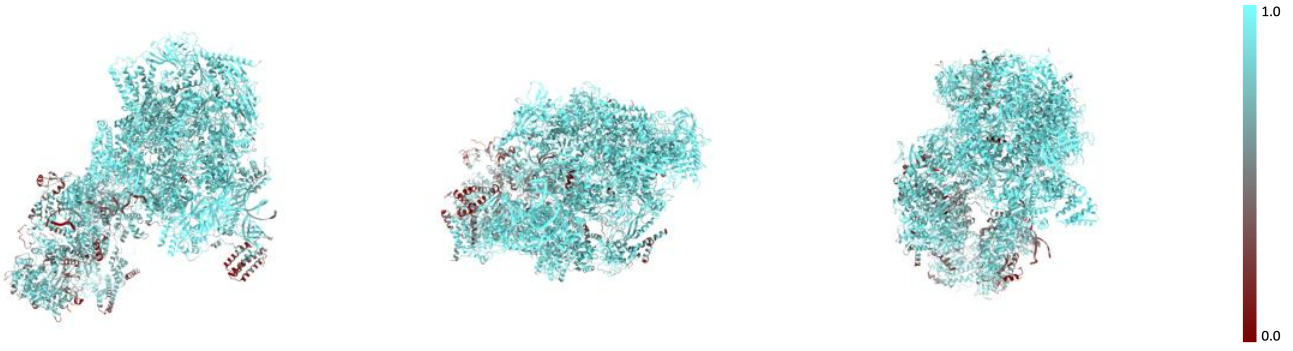
9.2 Q-score mapped to coordinate model (i)



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.

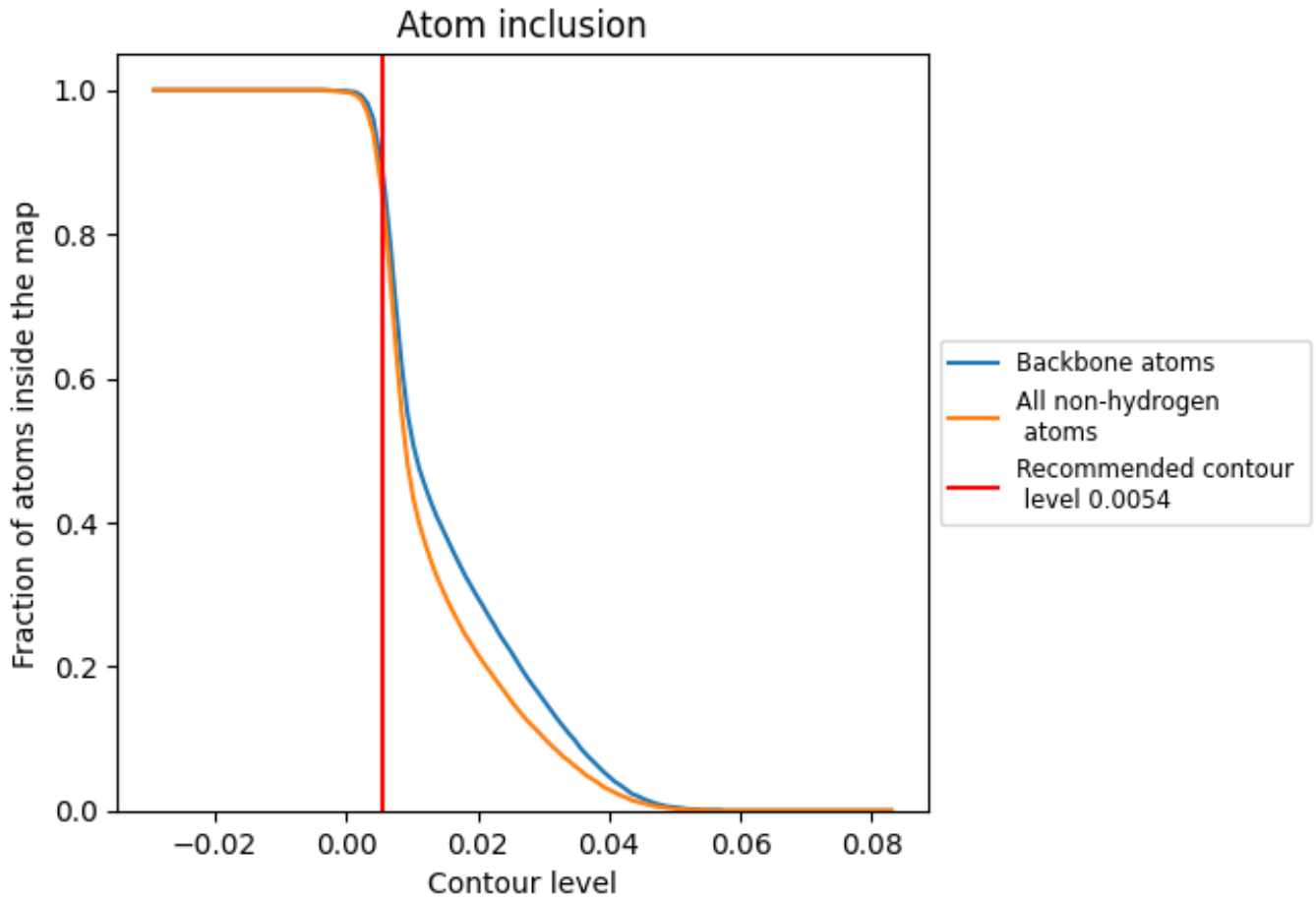
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0054).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 86% 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 (0.0054) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8600	0.2050
0	0.8550	0.0420
1	0.7390	0.0160
2	0.6880	0.0100
4	0.8760	0.0130
5	0.4550	-0.0180
6	0.8410	0.0250
7	0.7520	0.0160
A	0.9410	0.3910
B	0.9350	0.3890
C	0.9660	0.4230
D	0.7230	0.1410
E	0.9640	0.3520
F	0.9460	0.4080
G	0.8860	0.2390
H	0.9450	0.3120
I	0.9390	0.2900
J	0.9450	0.4060
K	0.9250	0.4120
L	0.9230	0.2780
M	0.7790	0.2550
N	0.7440	0.1110
O	0.9360	0.1010
P	0.9720	0.1490
Q	0.9080	0.2310
S	0.9230	0.2020
T	0.7540	0.1120
U	0.5920	0.0610
V	0.5680	0.0410
W	0.8770	0.1670
X	0.9570	0.1000

