wwPDB EM Validation Summary Report

Sep 17, 2024 – 02:25 pm BST

PDB ID	:	6TBM
EMDB ID	:	EMD-10446
Title	:	Structure of SAGA bound to TBP, including Spt8 and DUB
Authors	:	Papai, G.; Frechard, A.; Kolesnikova, O.; Crucifix, C.; Schultz, P.; Ben-Shem, A.
Deposited on	:	2019-11-01
Resolution	:	20.00 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

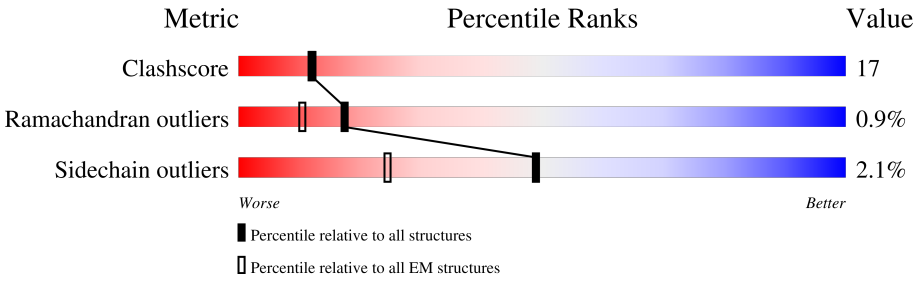
EMDB validation analysis	:	0.0.1.dev112
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

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 20.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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	M	240	10% 37% 32% 6% 25%
2	A	448	9% 31% 7% 61%
3	C	698	5% 9% · 86%
4	F	517	· 33% 7% 59%
5	D	341	7% 37% 21% · 39%
6	E	1191	10% · · 87%
7	J	217	· 36% 7% 56%
8	K	609	· 17% 7% · 75%

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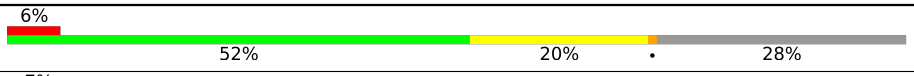
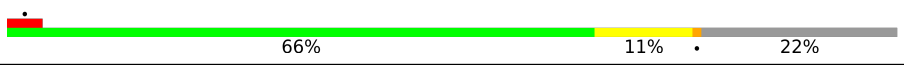
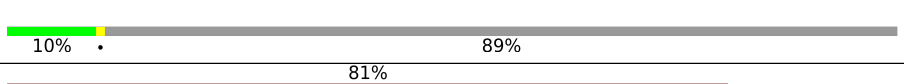
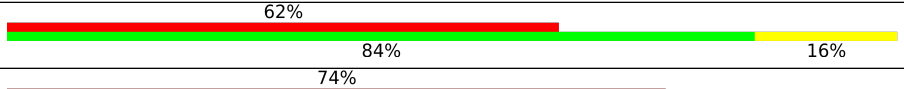
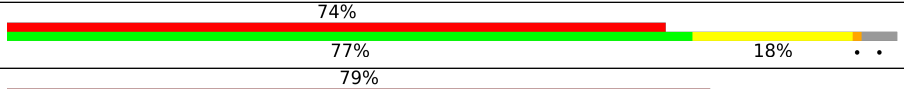
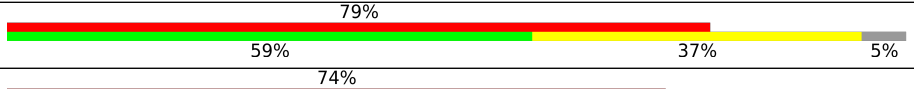
Mol	Chain	Length	Quality of chain
9	G	722	
10	H	485	
11	I	153	
12	L	3825	
13	B	722	
14	N	400	
15	R	76	
16	Q	502	
17	O	123	
18	P	96	

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 48800 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 TATA-box Binding Protein (TBP).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	M	180	1415	921	242	246	6	0	0

- Molecule 2 is a protein called Transcriptional coactivator HFI1/ADA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	173	1300	816	228	250	6	0	0

- Molecule 3 is a protein called Subunit of SAGA histone acetyltransferase complex.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	95	761	480	142	133	6	0	0

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	645	LEU	-	expression tag	UNP C4QZ39
C	646	GLU	-	expression tag	UNP C4QZ39
C	647	GLY	-	expression tag	UNP C4QZ39
C	648	GLY	-	expression tag	UNP C4QZ39
C	649	GLY	-	expression tag	UNP C4QZ39
C	650	GLY	-	expression tag	UNP C4QZ39
C	651	SER	-	expression tag	UNP C4QZ39
C	652	MET	-	expression tag	UNP C4QZ39
C	653	ASP	-	expression tag	UNP C4QZ39
C	654	GLU	-	expression tag	UNP C4QZ39
C	655	LYS	-	expression tag	UNP C4QZ39
C	656	THR	-	expression tag	UNP C4QZ39
C	657	THR	-	expression tag	UNP C4QZ39
C	658	GLY	-	expression tag	UNP C4QZ39
C	659	TRP	-	expression tag	UNP C4QZ39

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Chain	Residue	Modelled	Actual	Comment	Reference
C	660	ARG	-	expression tag	UNP C4QZ39
C	661	GLY	-	expression tag	UNP C4QZ39
C	662	GLY	-	expression tag	UNP C4QZ39
C	663	HIS	-	expression tag	UNP C4QZ39
C	664	VAL	-	expression tag	UNP C4QZ39
C	665	VAL	-	expression tag	UNP C4QZ39
C	666	GLU	-	expression tag	UNP C4QZ39
C	667	GLY	-	expression tag	UNP C4QZ39
C	668	LEU	-	expression tag	UNP C4QZ39
C	669	ALA	-	expression tag	UNP C4QZ39
C	670	GLY	-	expression tag	UNP C4QZ39
C	671	GLU	-	expression tag	UNP C4QZ39
C	672	LEU	-	expression tag	UNP C4QZ39
C	673	GLU	-	expression tag	UNP C4QZ39
C	674	GLN	-	expression tag	UNP C4QZ39
C	675	LEU	-	expression tag	UNP C4QZ39
C	676	ARG	-	expression tag	UNP C4QZ39
C	677	ALA	-	expression tag	UNP C4QZ39
C	678	ARG	-	expression tag	UNP C4QZ39
C	679	LEU	-	expression tag	UNP C4QZ39
C	680	GLU	-	expression tag	UNP C4QZ39
C	681	HIS	-	expression tag	UNP C4QZ39
C	682	HIS	-	expression tag	UNP C4QZ39
C	683	PRO	-	expression tag	UNP C4QZ39
C	684	GLN	-	expression tag	UNP C4QZ39
C	685	GLY	-	expression tag	UNP C4QZ39
C	686	GLN	-	expression tag	UNP C4QZ39
C	687	ARG	-	expression tag	UNP C4QZ39
C	688	GLU	-	expression tag	UNP C4QZ39
C	689	PRO	-	expression tag	UNP C4QZ39
C	690	GLY	-	expression tag	UNP C4QZ39
C	691	GLY	-	expression tag	UNP C4QZ39
C	692	SER	-	expression tag	UNP C4QZ39
C	693	HIS	-	expression tag	UNP C4QZ39
C	694	HIS	-	expression tag	UNP C4QZ39
C	695	HIS	-	expression tag	UNP C4QZ39
C	696	HIS	-	expression tag	UNP C4QZ39
C	697	HIS	-	expression tag	UNP C4QZ39
C	698	HIS	-	expression tag	UNP C4QZ39

- Molecule 4 is a protein called Spt20.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	210	Total	C	N	O	S	0	0
			1682	1071	292	315	4		

- Molecule 5 is a protein called Subunit of the SAGA and SAGA-like transcriptional regulatory complexes, interacts with Spt15p to act.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	209	Total	C	N	O	S	0	0
			1616	1016	298	295	7		

- Molecule 6 is a protein called Subunit of the SAGA transcriptional regulatory complex, involved in proper assembly of the complex.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	154	Total	C	N	O	S	0	0
			1232	784	208	233	7		

- Molecule 7 is a protein called Transcription initiation factor TFIID subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	96	Total	C	N	O	S	0	0
			768	489	120	156	3		

- Molecule 8 is a protein called Subunit (61/68 kDa) of TFIID and SAGA complexes.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	154	Total	C	N	O	S	0	0
			1192	747	216	226	3		

- Molecule 9 is a protein called Subunit (90 kDa) of TFIID and SAGA complexes.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	522	Total	C	N	O	S	0	0
			4075	2581	719	756	19		

- Molecule 10 is a protein called Subunit (60 kDa) of TFIID and SAGA complexes.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	421	Total	C	N	O	S	0	0
			3263	2084	556	617	6		

- Molecule 11 is a protein called Subunit (17 kDa) of TFIID and SAGA complexes, involved

in RNA polymerase II transcription initiation.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	123	Total	C	N	O	S	0	0
			981	632	169	178	2		

- Molecule 12 is a protein called Transcription-associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	2968	Total	C	N	O	S	0	0
			22318	14296	3864	4071	87		

- Molecule 13 is a protein called Transcriptional regulator involved in glucose repression of Gal4p-regulated genes.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	B	76	Total	C	N	O	0	0
			373	221	76	76		

- Molecule 14 is a protein called Spt8.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	N	335	Total	C	N	O	0	0
			1648	978	335	335		

- Molecule 15 is a protein called Polyubiquitin-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	76	Total	C	N	O	S	2	0
			611	384	105	121	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	76	GLZ	-	expression tag	UNP J3QS39

- Molecule 16 is a protein called Ubiquitin carboxyl-terminal hydrolase.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	482	Total	C	N	O	S	0	0
			3817	2410	657	719	31		

- Molecule 17 is a protein called SAGA-associated factor 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	117	Total	C	N	O	S	0	0
			922	563	169	184	6		

- Molecule 18 is a protein called Transcription and mRNA export factor SUS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	P	90	Total	C	N	O	S	0	0
			735	470	122	142	1		

- Molecule 19 is water.

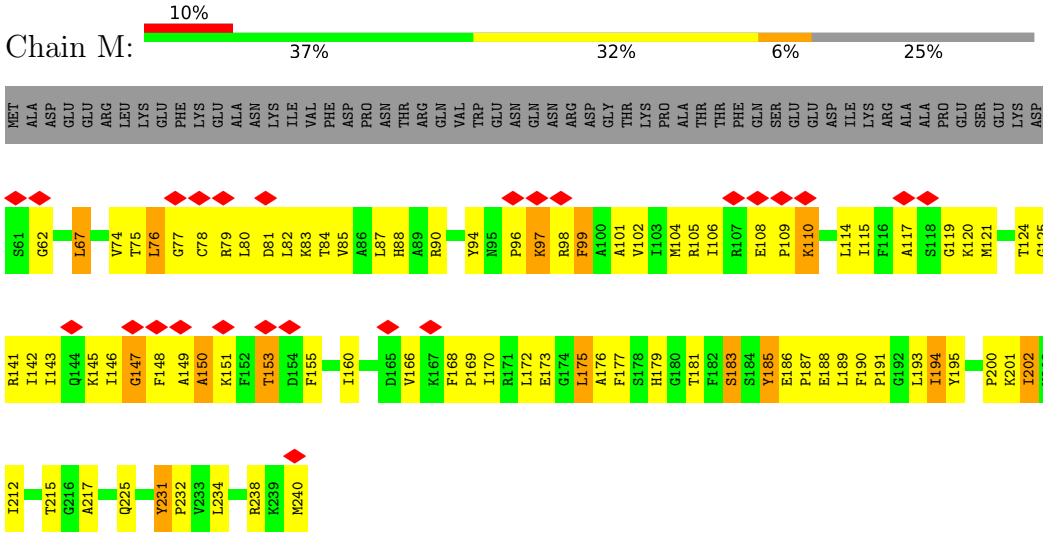
Mol	Chain	Residues	Atoms		AltConf
19	R	83	Total	O	0
			83	83	
19	Q	8	Total	O	0
			8	8	

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.

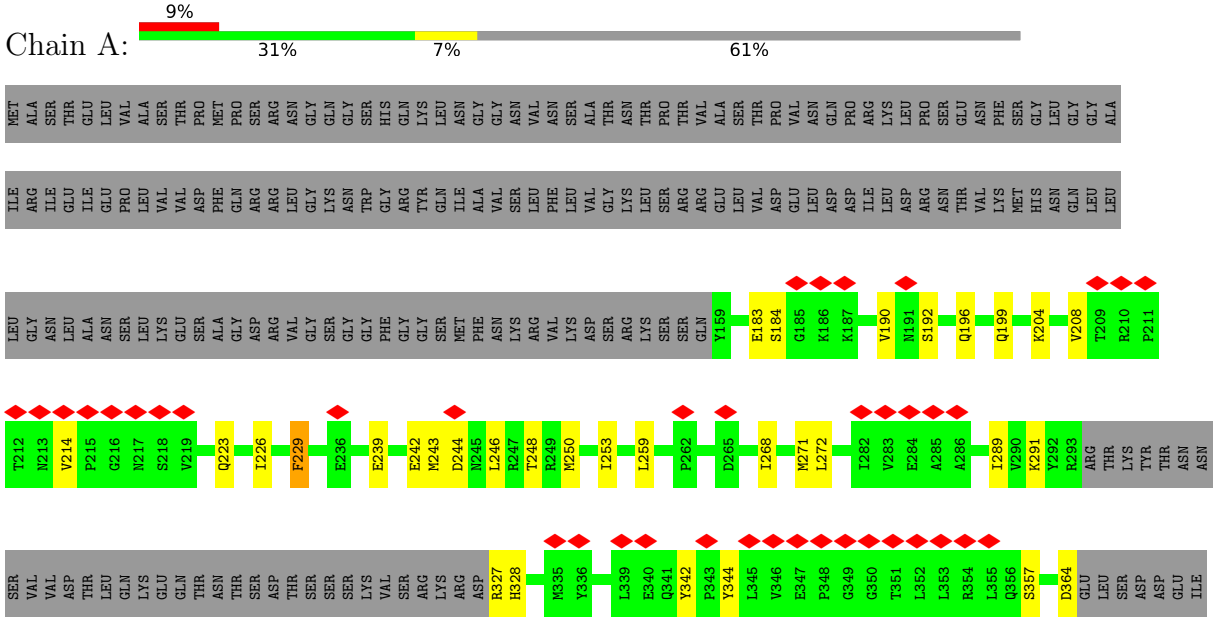
• Molecule 1: TATA-box Binding Protein (TBP)

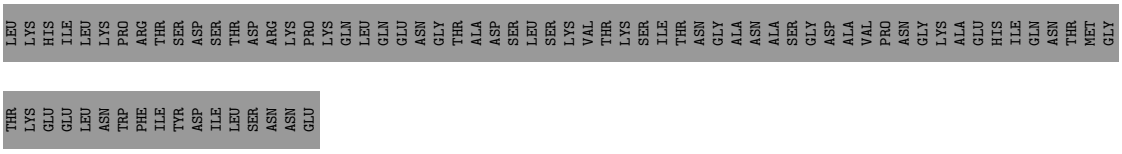
Chain M:



• Molecule 2: Transcriptional coactivator HFI1/ADA1

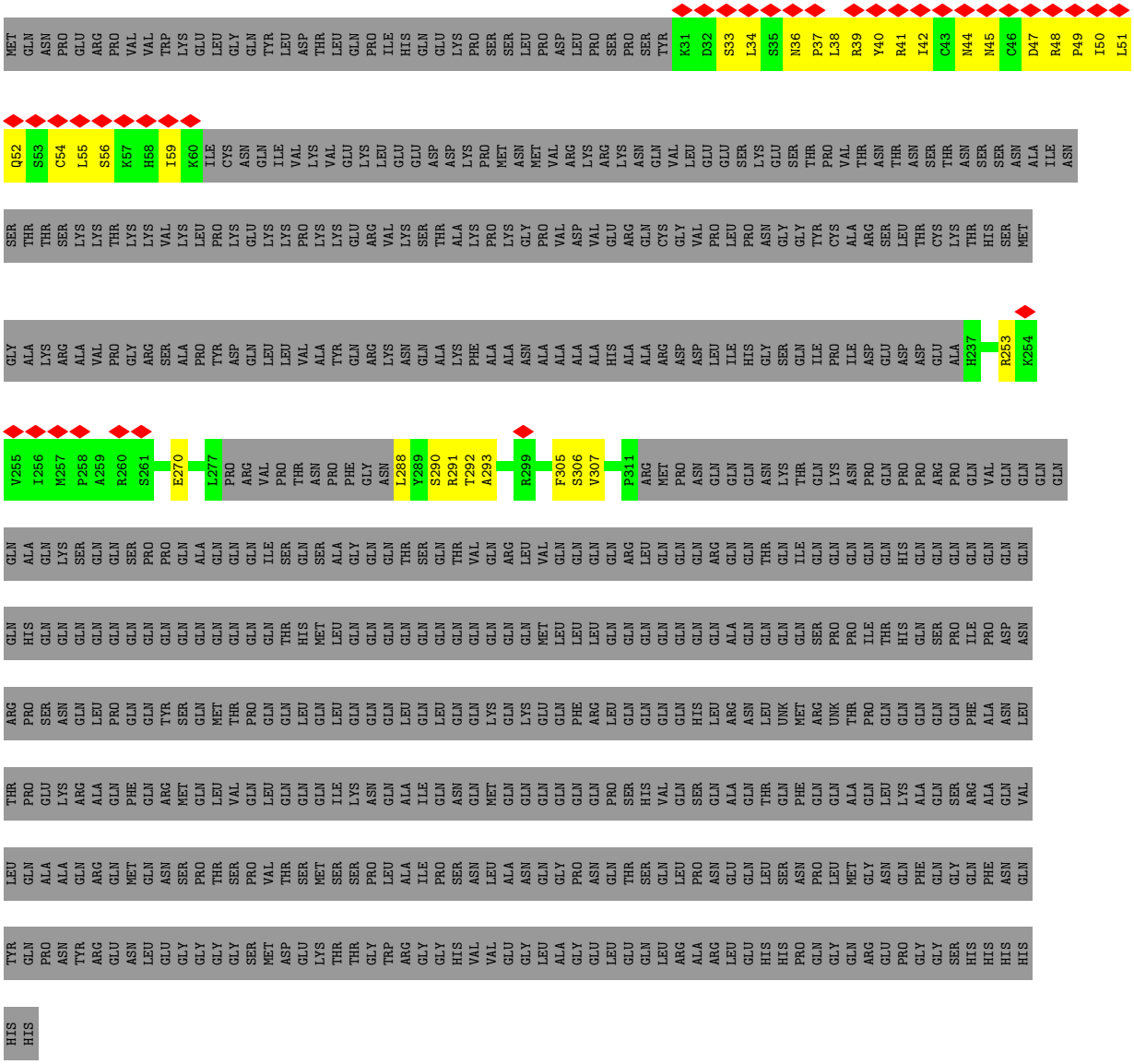
Chain A:





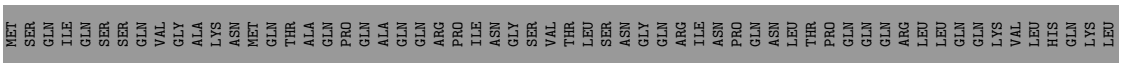
• Molecule 3: Subunit of SAGA histone acetyltransferase complex

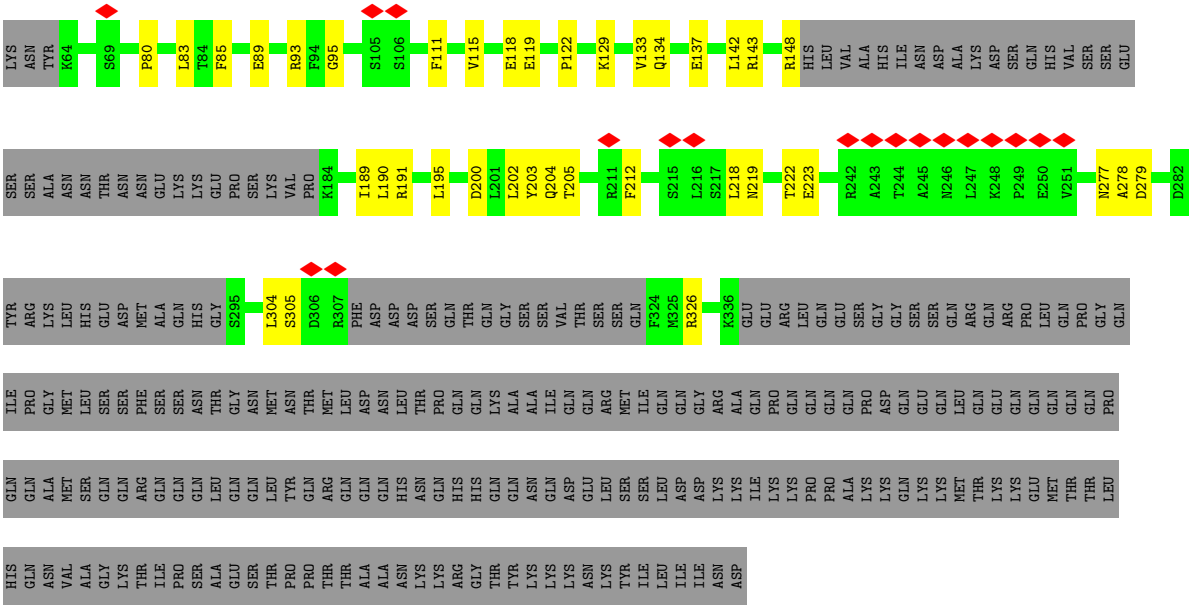
Chain C:



• Molecule 4: Spt20

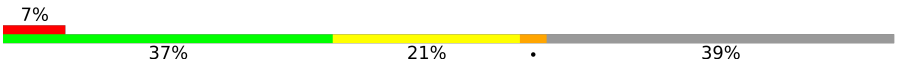
Chain F:

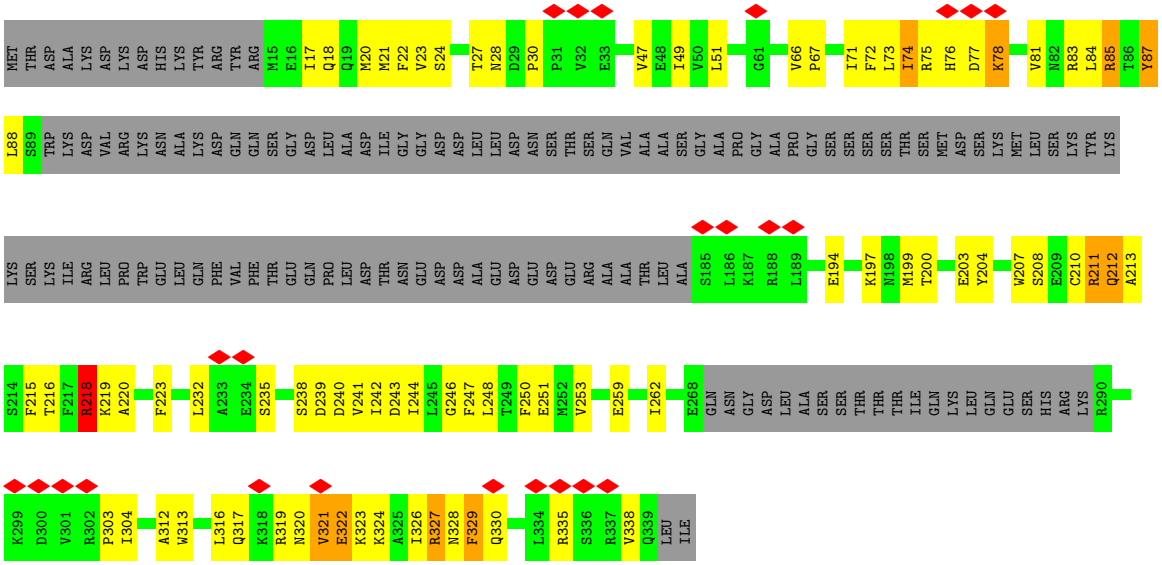




• Molecule 5: Subunit of the SAGA and SAGA-like transcriptional regulatory complexes, interacts with Spt15p to act

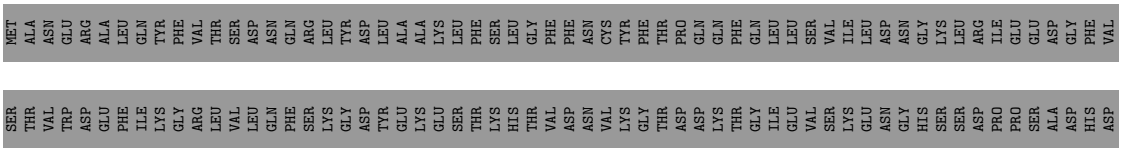
Chain D:

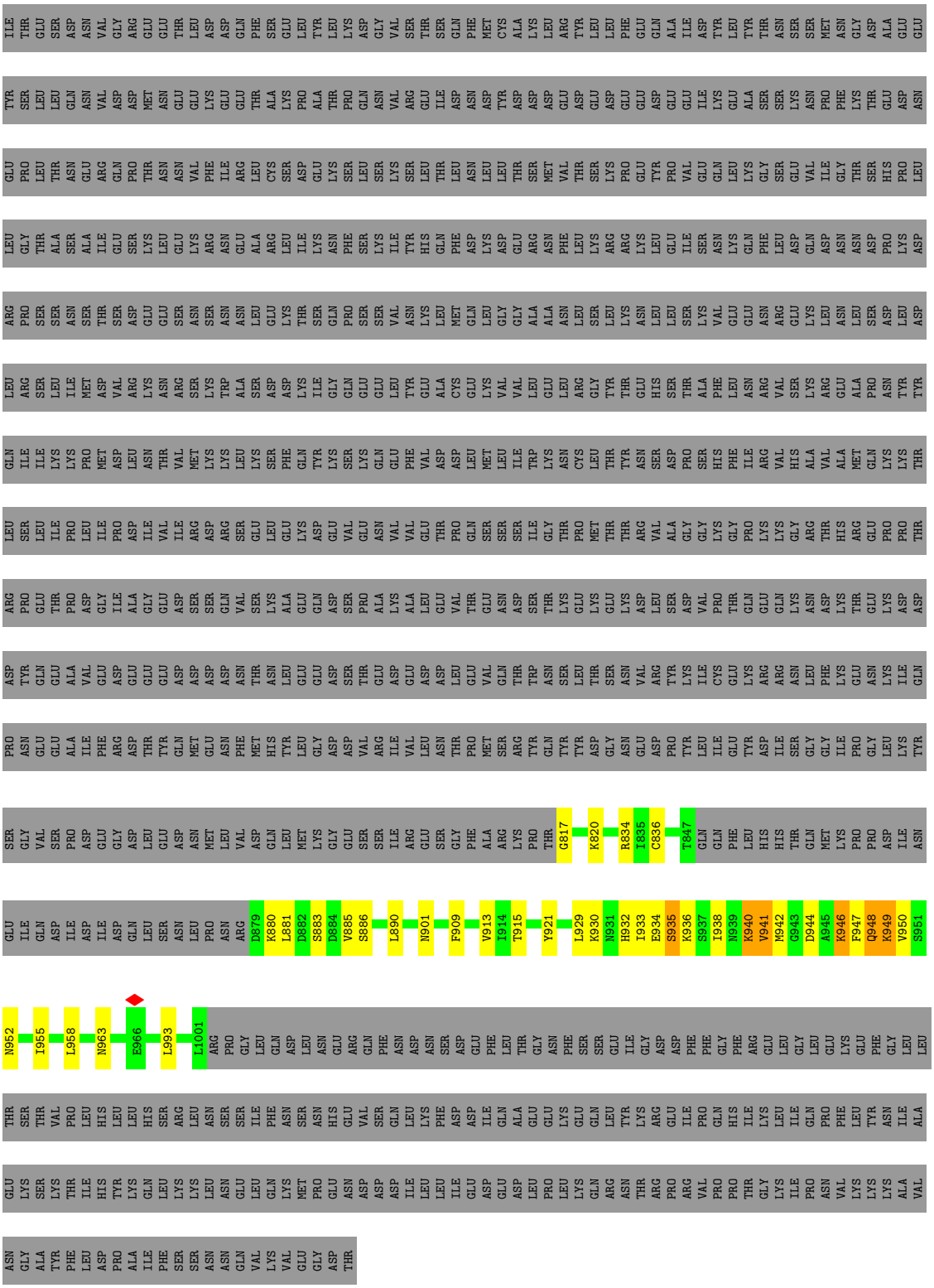




• Molecule 6: Subunit of the SAGA transcriptional regulatory complex, involved in proper assembly of the complex

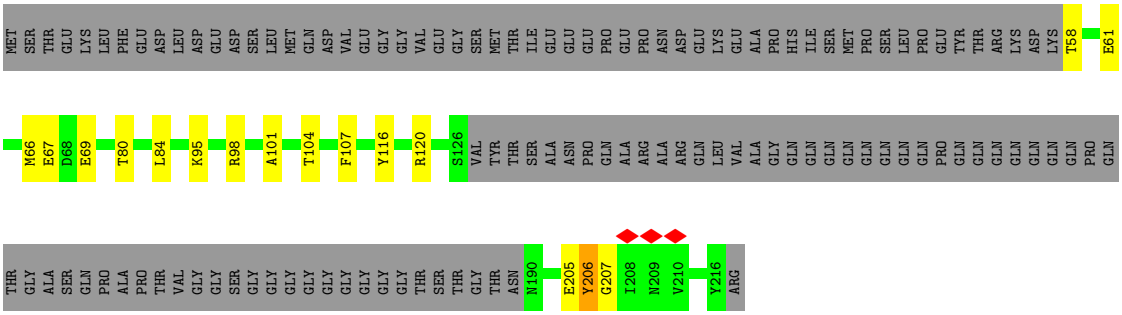
Chain E:





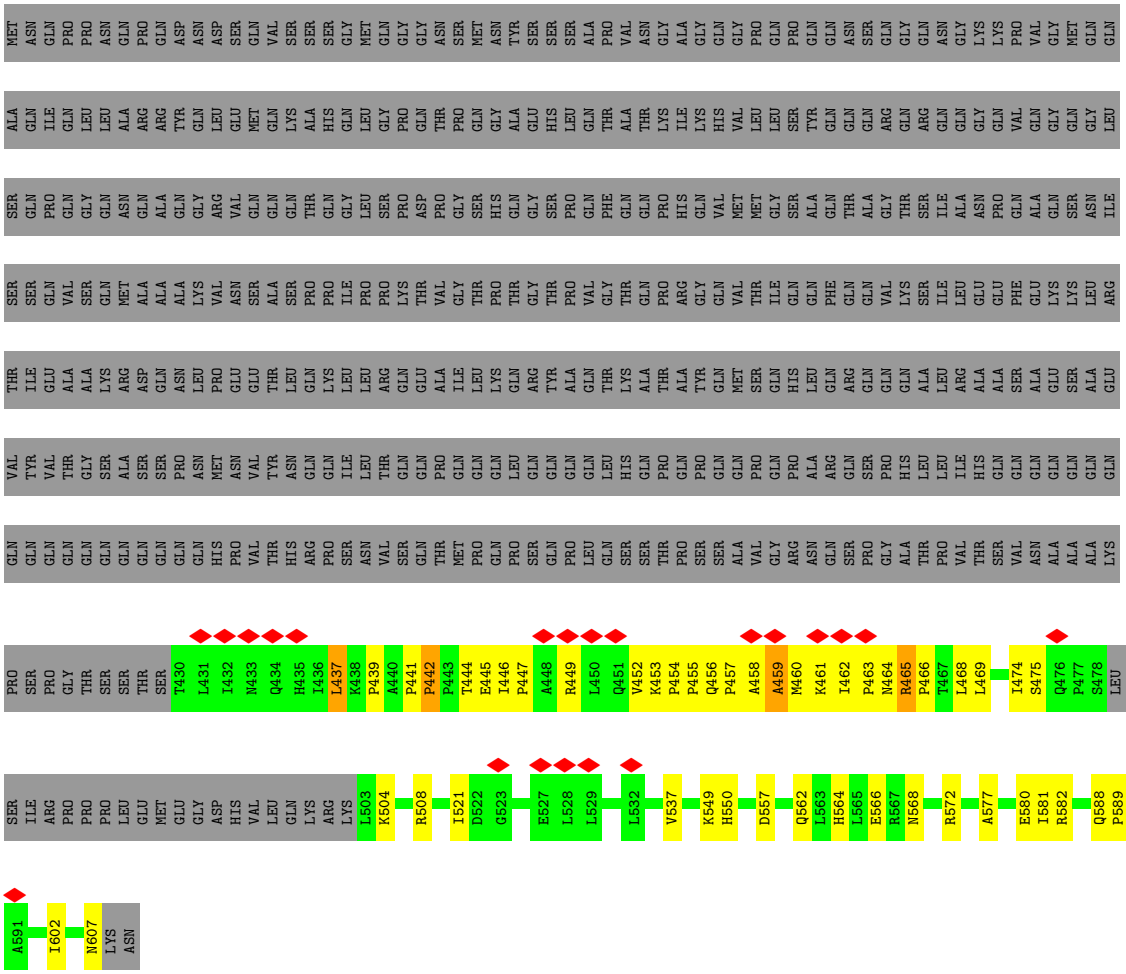
• Molecule 7: Transcription initiation factor TFIID subunit 10

Chain J:



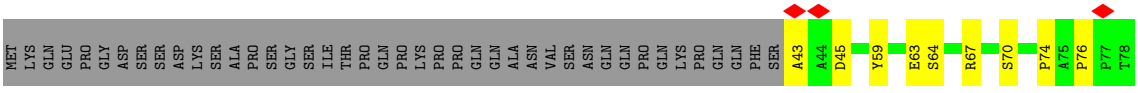
• Molecule 8: Subunit (61/68 kDa) of TFIID and SAGA complexes

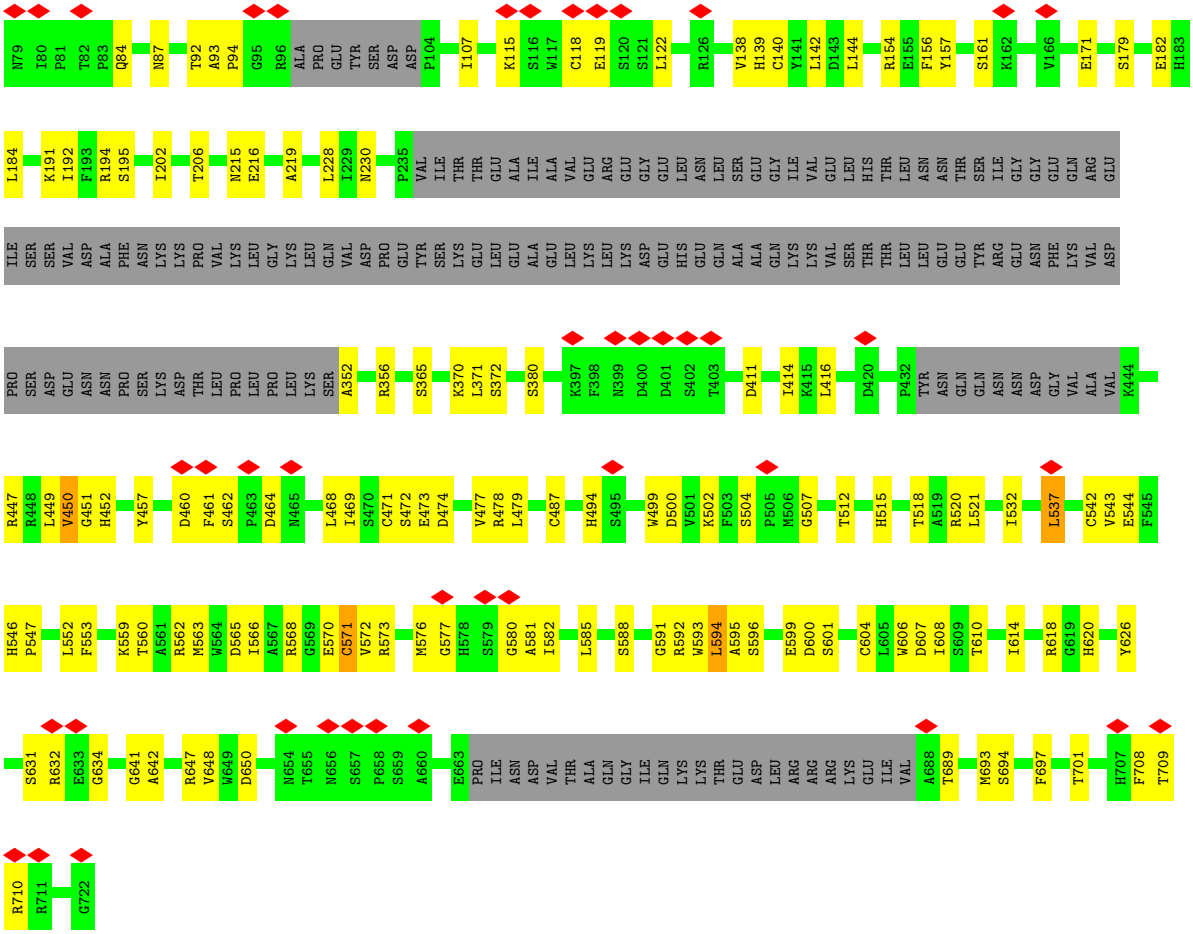
Chain K:



• Molecule 9: Subunit (90 kDa) of TFIID and SAGA complexes

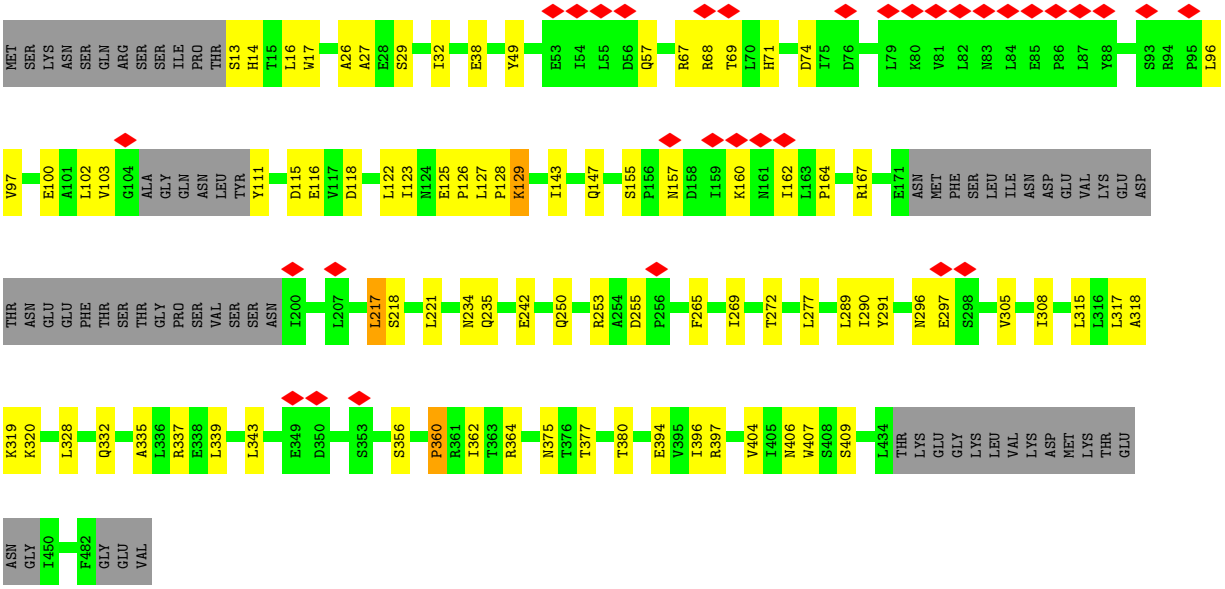
Chain G:





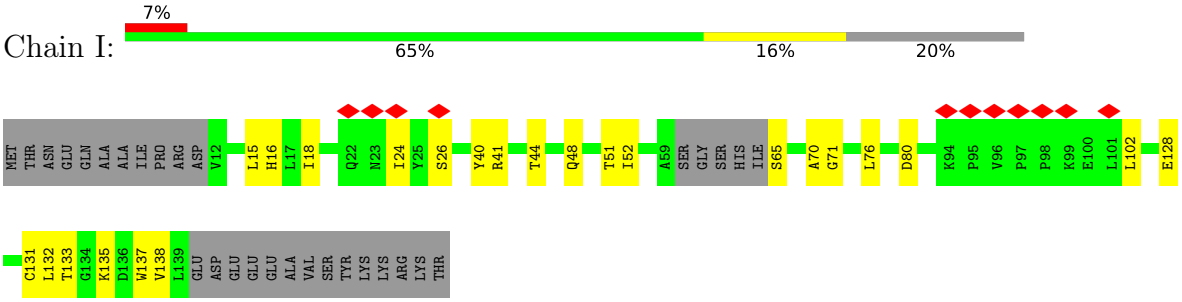
• Molecule 10: Subunit (60 kDa) of TFIID and SAGA complexes

Chain H:



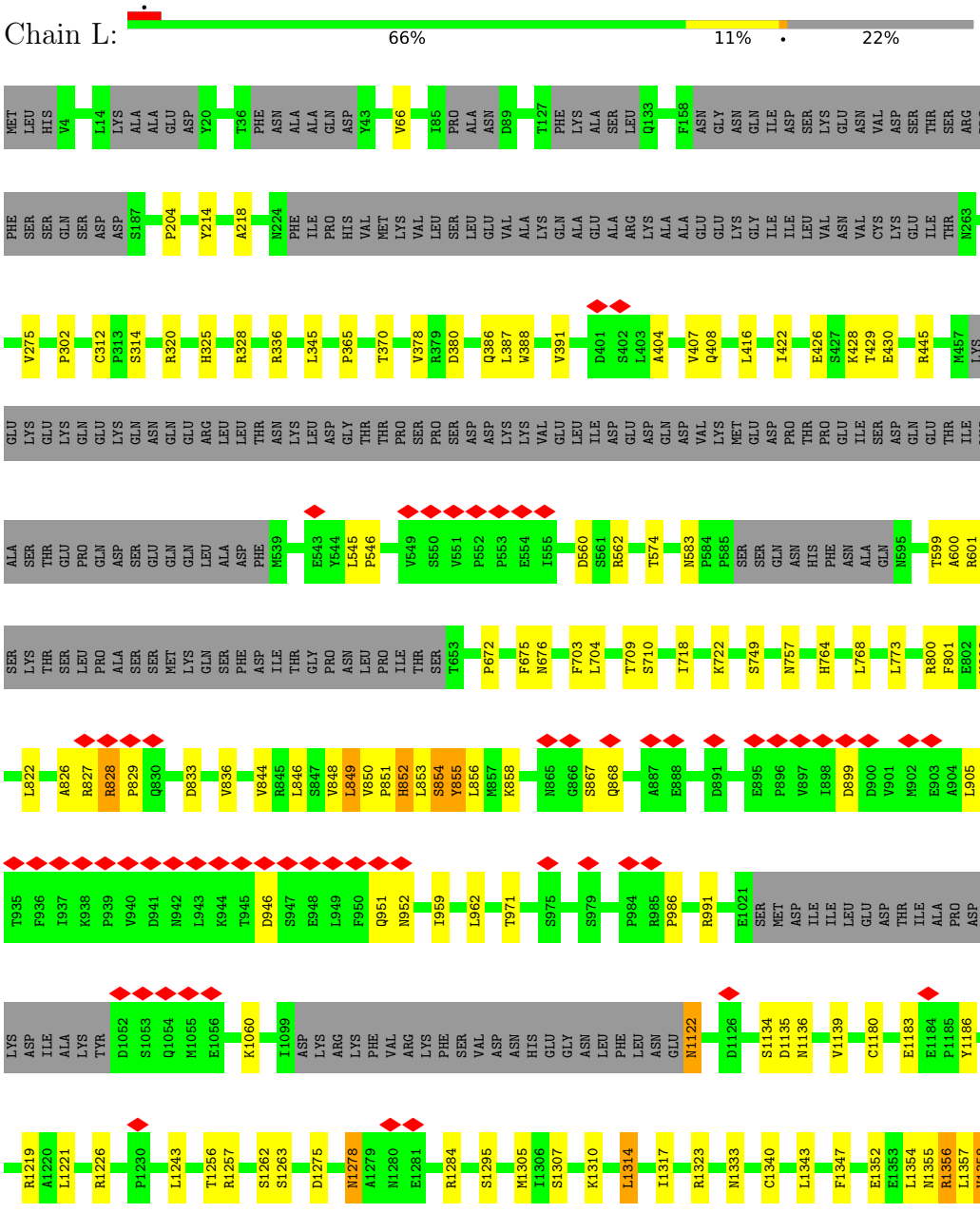
• Molecule 11: Subunit (17 kDa) of TFIID and SAGA complexes, involved in RNA polymerase II transcription initiation

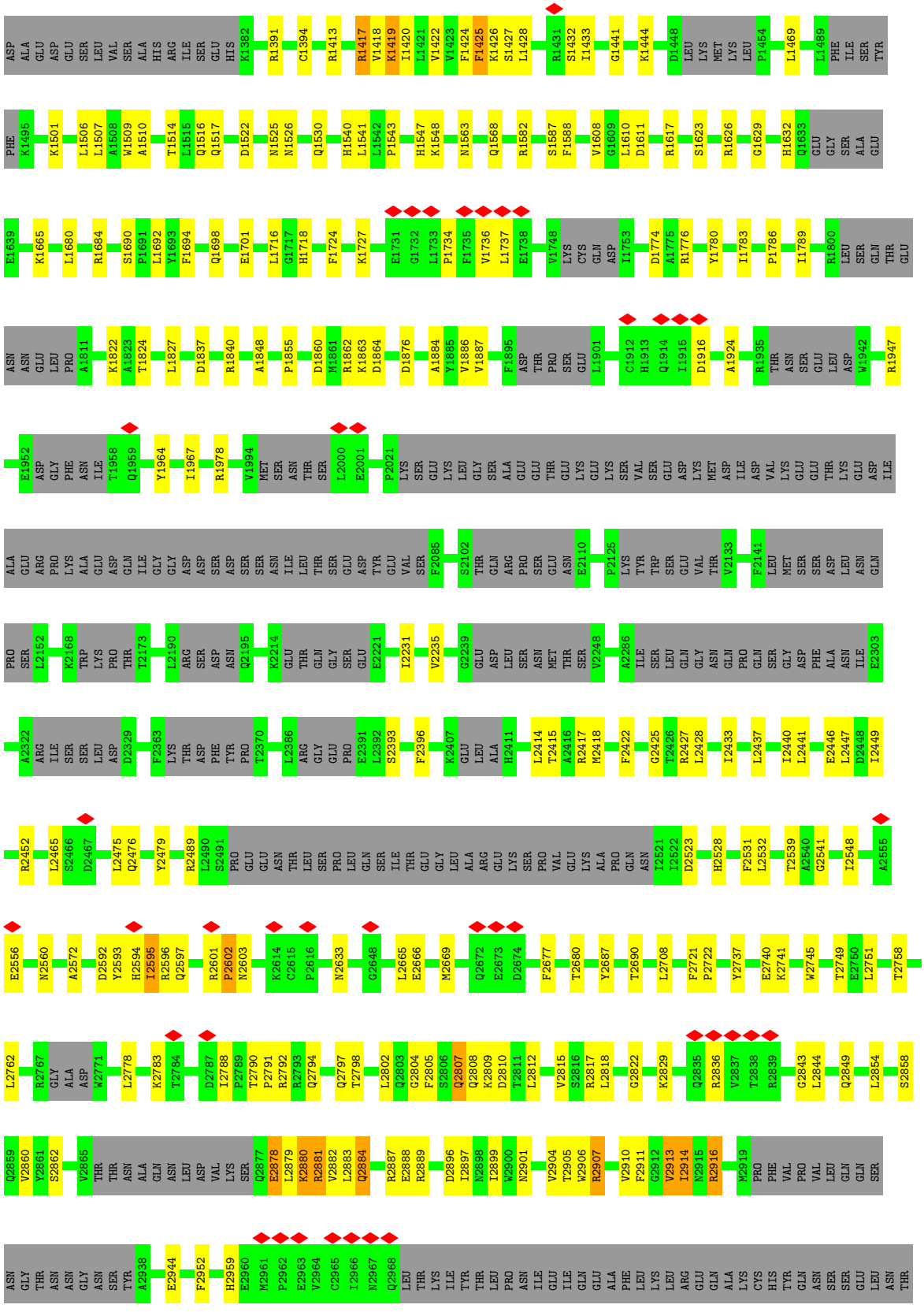
Chain I:

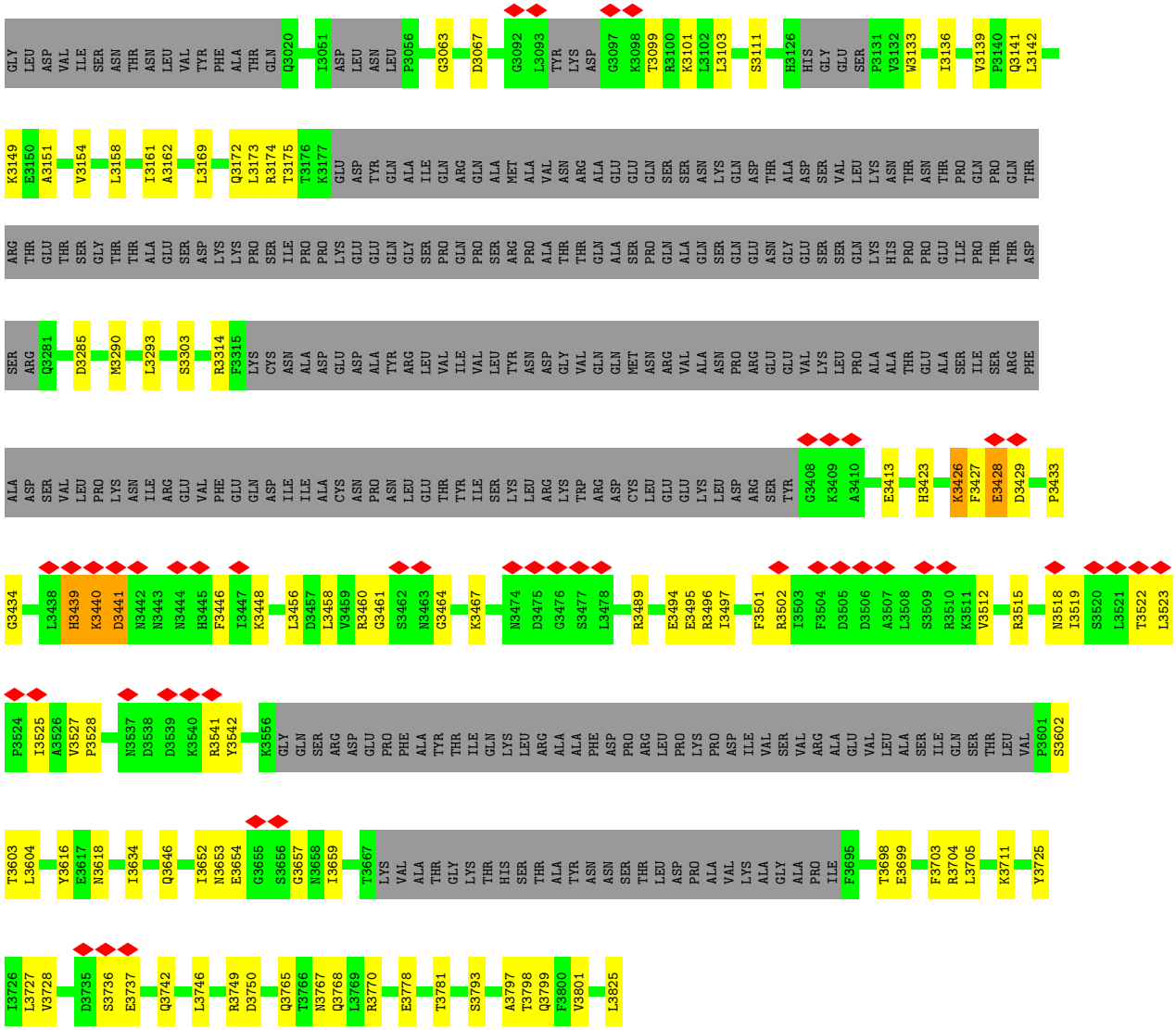


• Molecule 12: Transcription-associated protein

Chain L:







• Molecule 13: Transcriptional regulator involved in glucose repression of Gal4p-regulated genes

Chain B: 10% • 89%

GLU ASP ILE LYS PHE LEU LYS LYS GLN TYR ASN LEU PRO GLN ASN LEU PRO LYS ASN TYR ASP PRO ASN VAL THR PRO PHE VAL ILE PRO LYS PHE GLY ALA HIS TYR ARG ASP THR TRP TYR GLU GLU ASP ILE ASN THR GLY MET ILE LYS LYS LYS PRO ASN ASP VAL ASP PRO ARG

LEU ALA ASP GLN LYS MET ARG GLN ASP ALA LEU ILE PRO LYS GLY SER GLY ALA SER LEU THR ASP ASP VAL LEU GLU THR GLU LYS VAL SER CYS GLY PRO LEU ALA SER ARG LEU LEU SER ALA LEU LEU LYS ASN GLY ASP ASP THR GLU ASP GLY GLU PRO VAL ASP ASN ASP ASP

ASN ASN ASN VAL SER SER ALA ILE GLY ASN GLU GLY TRP THR PRO SER VAL GLU THR SER ASP TYR GLU THR LEU ASP GLN ARG LEU ARG ARG GLU LEU LYS TYR ILE GLY VAL PHE MET ASN VAL GLU GLN THR LEU LYS ARG GLU GLY HIS ALA ASP GLU LEU VAL ASN SER VAL GLY

VAL THR SER GLY ASN GLY GLU PHE GLU GLU ASP TRP LEU ASN SER ARG GLU ASP ASP GLU ILE SER ALA GLU MET ARG SER LEU GLN ARG GLU LEU ARG ARG LEU THR ARG LYS ASN VAL ARG ARG LYS GLU LYS LEU ILE PRO ILE VAL GLU GLU GLN LEU ALA TRP GLN GLU TYR GLN

SER ILE LEU GLU ASP LEU ASP LYS GLN VAL ASP GLN ALA TYR LEU ARG ARG ILE ARG VAL PRO ARG LYS ASN LYS ARG LYS ASN GLU SER GLN SER SER GLY GLN GLN THR GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN ASP GLN GLN GLN THR GLY PHE LYS ALA LEU

LEU ASP LYS ARG THR ARG TRP ILE GLU LYS ILE GLY PRO LEU PHE LYS PRO PRO HIS LEU MET ARG ARG PRO PRO SER GLU SER VAL PHE LYS ASP VAL ASP LEU GLU ASN ASP ASP GLU GLU LEU GLU GLU ASP ASP GLU MET LYS VAL ASP ILE ASP LEU ARG

- Molecule 14: Spt8

Chain N:

81%

72% 12% 16%

X83 X84 X85 X86 X87 X88 X89 X90 X91 X92 X93 X94 X95 X96 X97 X98 X99 X100 X101 X102 X103 X104 X105 X106 X107 X108 X109 X110 X111 X112 X113 X114 X115 X116 X117 X172 X173 X174 X175 X176 X177 X178 X179 X180 X181 X182 X183 X184 X185 X186 X187 X188 X189 X190 X191 X192 X193 X194 X195 X196

X197 X198 X199 X200 X201 X202 X203 X204 X205 X206 X207 X208 X209 X210 X211 X212 X213 X214 X215 X216 X217 X218 X219 X220 X221 X222 X223 X224 X225 X226 X227 X228 X229 X230 X231 X232 X233 X234 X235 X236 X237 X238 X239 X240 X241 X242 X243 X244 X245 X246 X247 X248 X249 X250 X251 X252 X253 X254 X255 X256

X257 X258 X259 X260 X261 X262 X263 X264 X265 X266 X267 X268 X269 X270 X271 X272 X273 X274 X275 X276 X277 X278 X279 X280 X281 X282 X283 X284 X285 X286 X287 X332 X333 X334 X335 X336 X337 X338 X339 X340 X341 X342 X343 X344 X345 X346 X347 X348 X349 X350 X351 X352 X353 X354 X355 X356 X357 X358 X359 X360

X361 X362 X363 X364 X365 X366 X367 X368 X369 X370 X371 X372 X373 X374 X375 X376 X377 X378 X379 X380 X381 X382 X383 X384 X385 X386 X387 X388 X389 X390 X391 X392 X393 X394 X395 X396 X397 X398 X399 X400 X401 X402 X403 X404 X405 X406 X407 X408 X409 X410 X411 X412 X413 X414 X415 X416 X417 X418 X419 X420

X421 X422 X423 X424 X425 X426 X427 X428 X429 X430 X431 X432 X433 X434 X435 X436 X437 X438 X439 X440 X441 X442 X443 X444 X445 X446 X447 X448 X449 X450 X451 X452 X453 X454 X455 X456 X457 X458 X459 X460 X461 X462 X463 X464 X465 X466 X467 X468 X469 X470 X471 X472 X473 X474 X475 X476 X477 X478 X479 X480

X481 X482 X483 X484 X485 X486 X487 X488 X489 X490 X493 X494 X495 X496 X497 X498 X499 X500 X501 X502 X503 X504 X505 X506 X507 X508 X509 X510 X511 X512 X513 X514 X515 UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK

UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK

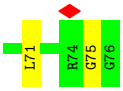
- Molecule 15: Polyubiquitin-B

Chain R:

62%

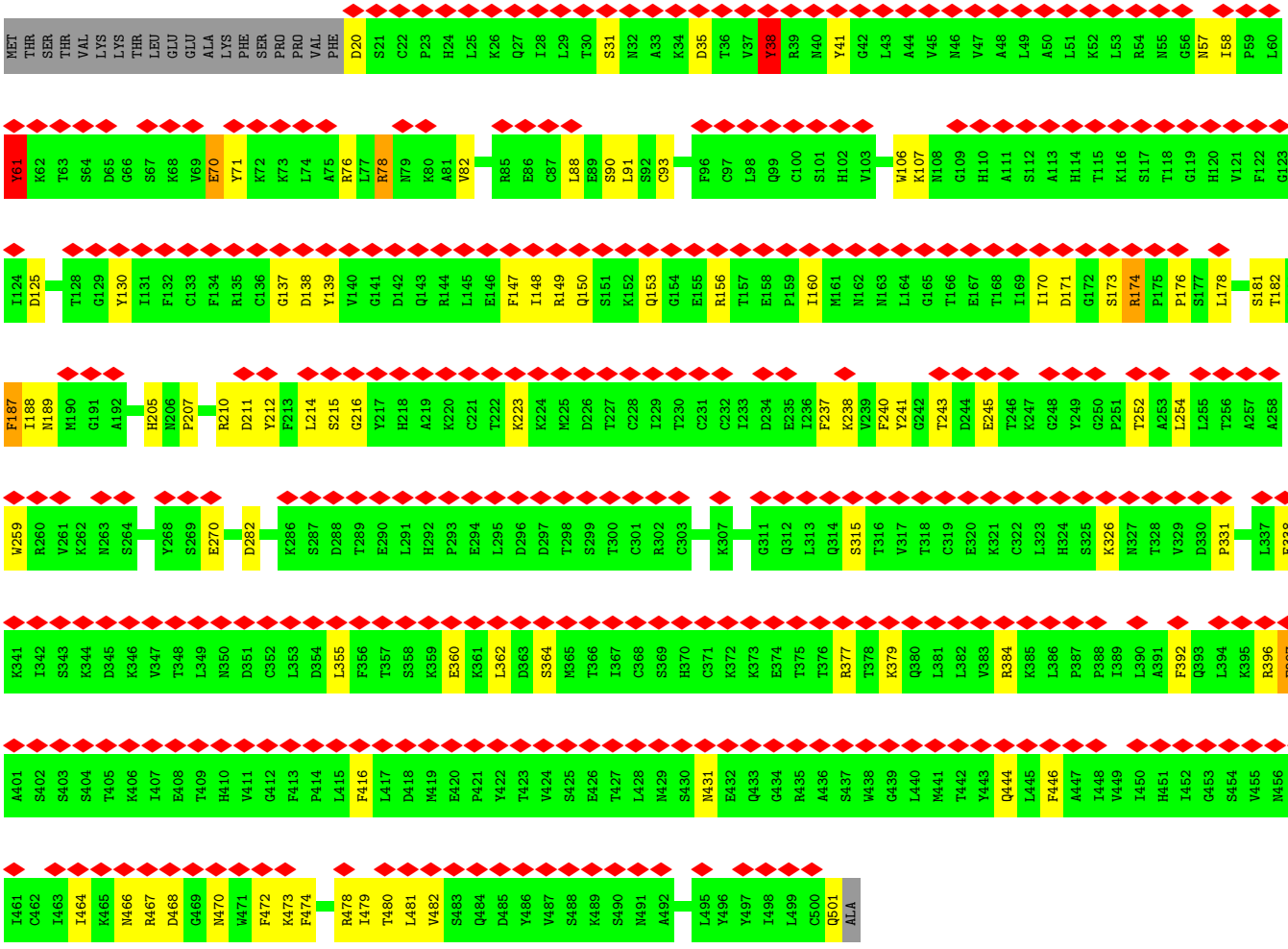
84% 16%

M1 Q2 I3 F4 L8 T9 G10 K11 T12 I13 T14 L15 E16 V17 E18 P19 S20 D21 T22 I23 E24 N25 A28 Q31 D32 K33 E34 G35 I36 P37 P38 D39 Q40 Q41 R42 A46 Q49 D52 G53 R54 T55 L56 S57 D58 Y59 N60 I61 Q62 K63 E64 S65 T66 L67 H68



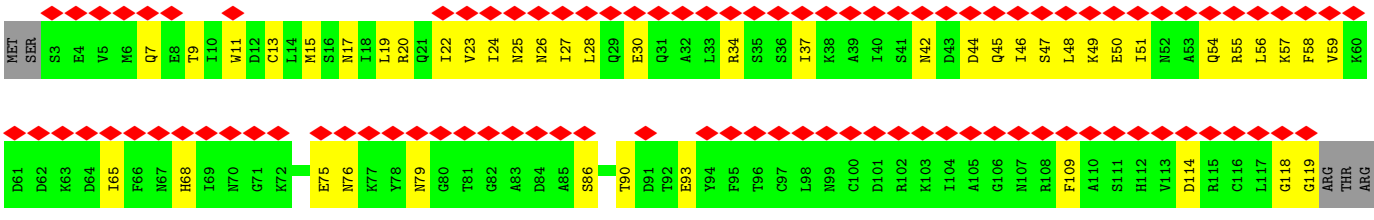
• Molecule 16: Ubiquitin carboxyl-terminal hydrolase

Chain Q:



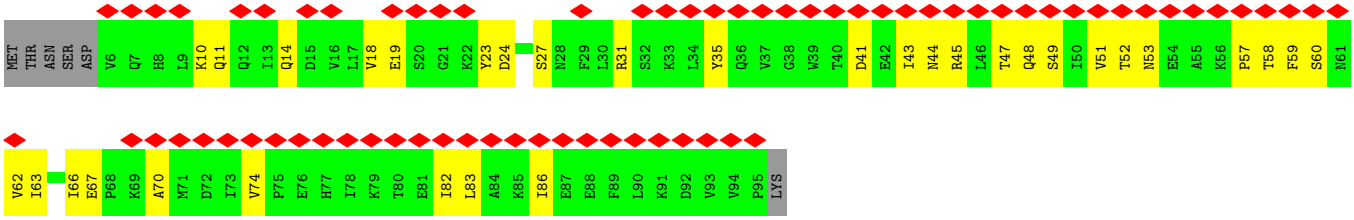
• Molecule 17: SAGA-associated factor 11

Chain O:



• Molecule 18: Transcription and mRNA export factor SUS1

Chain P:


MET THR ASN SER ASP V6 Q7 H8 L9 K10 Q11 Q12 I13 Q14 D15 V16 L17 V18 E19 S20 G21 K22 Y23 D24 S27 N28 F29 L30 R31 S32 K33 L34 Y35 Q36 V37 G38 W39 T40 D41 E42 I43 N44 R45 L46 T47 Q48 S49 I50 V51 T52 N53 E54 A55 K56 P57 T58 F59 S60 N61
V62 I63 I66 E67 P68 K69 A70 M71 D72 I73 V74 P75 E76 H77 I78 K79 T80 E81 I82 L83 A84 K85 I86 E87 E88 F89 L90 K91 D92 V93 V94 P95 LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	354104	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 ($e^-/Å^2$)	52.8	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.032	Depositor
Minimum map value	-0.024	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.004	Depositor
Map size (Å)	558.08, 558.08, 558.08	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.18, 2.18, 2.18	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GLZ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	M	0.88	2/1442 (0.1%)	0.78	2/1942 (0.1%)
2	A	0.44	0/1319	0.60	0/1794
3	C	0.53	0/774	0.75	0/1039
4	F	0.34	0/1718	0.58	0/2335
5	D	0.51	0/1641	0.65	0/2213
6	E	0.45	0/1246	0.62	0/1667
7	J	0.47	0/779	0.60	0/1051
8	K	0.42	0/1213	0.66	0/1647
9	G	0.52	0/4177	0.60	0/5661
10	H	0.38	0/3315	0.60	0/4500
11	I	0.44	0/1006	0.63	0/1374
12	L	0.33	0/22712	0.54	0/30825
13	B	0.64	0/370	0.70	1/509 (0.2%)
15	R	0.83	1/619 (0.2%)	0.75	0/833
16	Q	0.71	0/3897	1.09	15/5265 (0.3%)
17	O	0.79	0/931	1.13	2/1250 (0.2%)
18	P	0.75	0/747	1.01	0/1011
All	All	0.47	3/47906 (0.0%)	0.67	20/64916 (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	M	0	1
16	Q	2	5
All	All	2	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	194	ILE	C-N	27.38	1.97	1.34
1	M	183	SER	C-N	6.38	1.48	1.34
15	R	24	GLU	CB-CG	-5.25	1.42	1.52

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	Q	61	TYR	CB-CG-CD1	9.83	126.90	121.00
16	Q	61	TYR	CB-CG-CD2	-9.38	115.37	121.00
1	M	62	GLY	N-CA-C	6.94	130.46	113.10
16	Q	78	ARG	NE-CZ-NH1	-6.80	116.90	120.30
13	B	527	PRO	N-CA-CB	6.57	111.18	103.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
16	Q	31	SER	CA
16	Q	222	THR	CA

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	183	SER	Mainchain
16	Q	149	ARG	Sidechain
16	Q	212	TYR	Sidechain
16	Q	38	TYR	Sidechain
16	Q	61	TYR	Sidechain

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	M	1415	0	1491	102	0
2	A	1300	0	1254	30	0
3	C	761	0	779	194	0
4	F	1682	0	1622	30	0
5	D	1616	0	1558	122	0
6	E	1232	0	1276	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	J	768	0	754	11	0
8	K	1192	0	1214	89	0
9	G	4075	0	3934	102	0
10	H	3263	0	3258	69	0
11	I	981	0	982	18	0
12	L	22318	0	20960	376	0
13	B	373	0	190	2	0
14	N	1648	0	382	61	0
15	R	611	0	636	20	0
16	Q	3817	0	3772	521	0
17	O	922	0	897	411	0
18	P	735	0	743	191	0
19	Q	8	0	0	10	0
19	R	83	0	0	7	0
All	All	48800	0	45702	1602	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 17.

The worst 5 of 1602 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)
16:Q:472:PHE:CZ	17:O:45:GLN:HB3	1.29	1.65
17:O:11:TRP:CD1	18:P:83:LEU:HD23	1.14	1.61
16:Q:479:ILE:HG23	17:O:47:SER:CA	1.19	1.61
16:Q:479:ILE:CG2	17:O:47:SER:HA	1.14	1.60
17:O:34:ARG:HH11	18:P:57:PRO:CB	1.11	1.58

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	M	178/240 (74%)	147 (83%)	24 (14%)	7 (4%)	2 19
2	A	169/448 (38%)	151 (89%)	18 (11%)	0	100 100
3	C	89/698 (13%)	83 (93%)	6 (7%)	0	100 100
4	F	202/517 (39%)	177 (88%)	24 (12%)	1 (0%)	25 64
5	D	203/341 (60%)	177 (87%)	19 (9%)	7 (3%)	3 21
6	E	150/1191 (13%)	135 (90%)	13 (9%)	2 (1%)	10 43
7	J	92/217 (42%)	82 (89%)	9 (10%)	1 (1%)	12 47
8	K	150/609 (25%)	125 (83%)	23 (15%)	2 (1%)	10 43
9	G	512/722 (71%)	448 (88%)	63 (12%)	1 (0%)	44 78
10	H	413/485 (85%)	365 (88%)	48 (12%)	0	100 100
11	I	119/153 (78%)	98 (82%)	21 (18%)	0	100 100
12	L	2874/3825 (75%)	2623 (91%)	233 (8%)	18 (1%)	22 60
13	B	70/722 (10%)	63 (90%)	7 (10%)	0	100 100
15	R	76/76 (100%)	75 (99%)	1 (1%)	0	100 100
16	Q	480/502 (96%)	444 (92%)	30 (6%)	6 (1%)	10 43
17	O	115/123 (94%)	103 (90%)	6 (5%)	6 (5%)	1 15
18	P	88/96 (92%)	85 (97%)	3 (3%)	0	100 100
All	All	5980/10965 (54%)	5381 (90%)	548 (9%)	51 (1%)	17 52

5 of 51 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	77	GLY
1	M	99	PHE
1	M	110	LYS
5	D	200	THR
5	D	327	ARG

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	M	152/205 (74%)	138 (91%)	14 (9%)	7 23
2	A	134/394 (34%)	132 (98%)	2 (2%)	60 75
3	C	85/627 (14%)	85 (100%)	0	100 100
4	F	179/471 (38%)	179 (100%)	0	100 100
5	D	166/306 (54%)	154 (93%)	12 (7%)	12 32
6	E	142/1101 (13%)	136 (96%)	6 (4%)	25 46
7	J	85/183 (46%)	84 (99%)	1 (1%)	67 78
8	K	133/524 (25%)	130 (98%)	3 (2%)	45 64
9	G	439/635 (69%)	430 (98%)	9 (2%)	48 66
10	H	352/438 (80%)	348 (99%)	4 (1%)	70 80
11	I	104/130 (80%)	103 (99%)	1 (1%)	73 82
12	L	2156/3450 (62%)	2114 (98%)	42 (2%)	52 69
15	R	70/68 (103%)	69 (99%)	1 (1%)	62 75
16	Q	431/449 (96%)	425 (99%)	6 (1%)	62 75
17	O	103/109 (94%)	102 (99%)	1 (1%)	73 82
18	P	85/91 (93%)	85 (100%)	0	100 100
All	All	4816/9181 (52%)	4714 (98%)	102 (2%)	49 66

5 of 102 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	L	1122	ASN
12	L	2489	ARG
16	Q	254	LEU
12	L	1314	LEU
12	L	1419	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
12	L	2884	GLN
17	O	76	ASN
15	R	60	ASN
18	P	36	GLN
17	O	26	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)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	$\#\|Z\| > 2$
15	GLZ	R	76	15,16	3,3,3	0.70	0	0,2,2	-	-

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
15	GLZ	R	76	15,16	-	0/0/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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
14	N	6
13	B	2
1	M	1

The worst 5 of 9 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	414:ASP	C	462:ALA	N	28.86
1	B	471:ASP	C	509:ASP	N	23.98
1	N	117:UNK	C	172:UNK	N	15.59
1	N	287:UNK	C	332:UNK	N	5.97
1	N	213:UNK	C	214:UNK	N	4.21

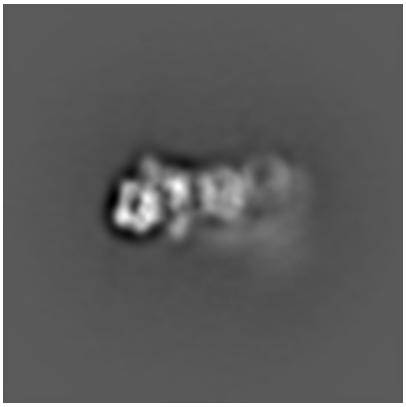
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10446. These allow visual inspection of the internal detail of the map and identification of artifacts.

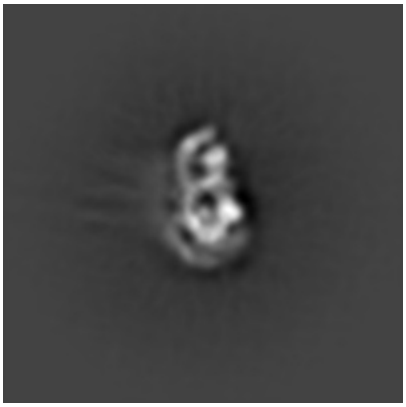
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

6.1.1 Primary map



X



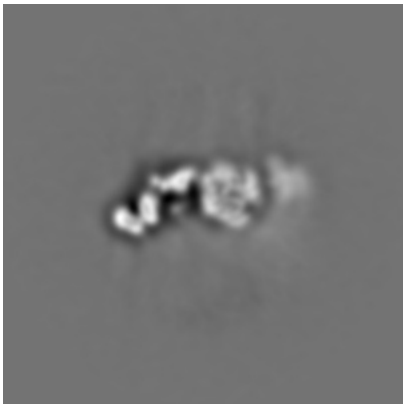
Y

Z

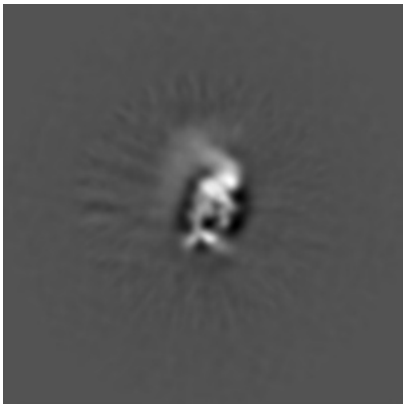
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map



X Index: 128



Y Index: 128

Z Index: 128

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: 121

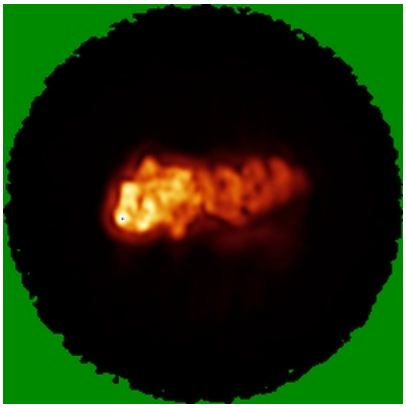
Y Index: 93

Z Index: 133

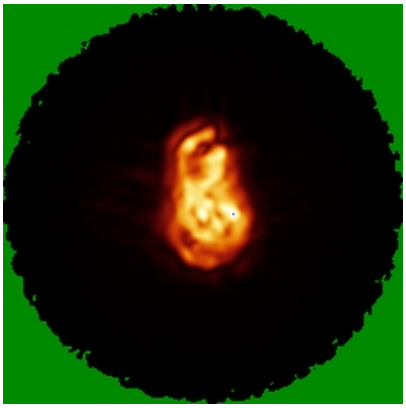
The images above show the largest variance slices of the map in three orthogonal directions.

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

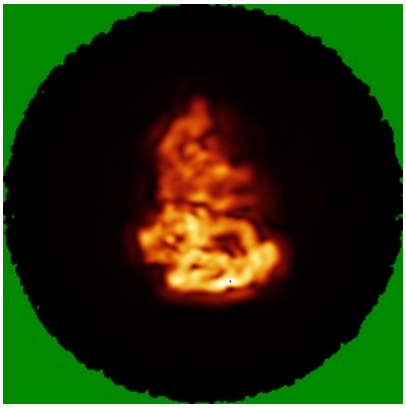
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.004. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

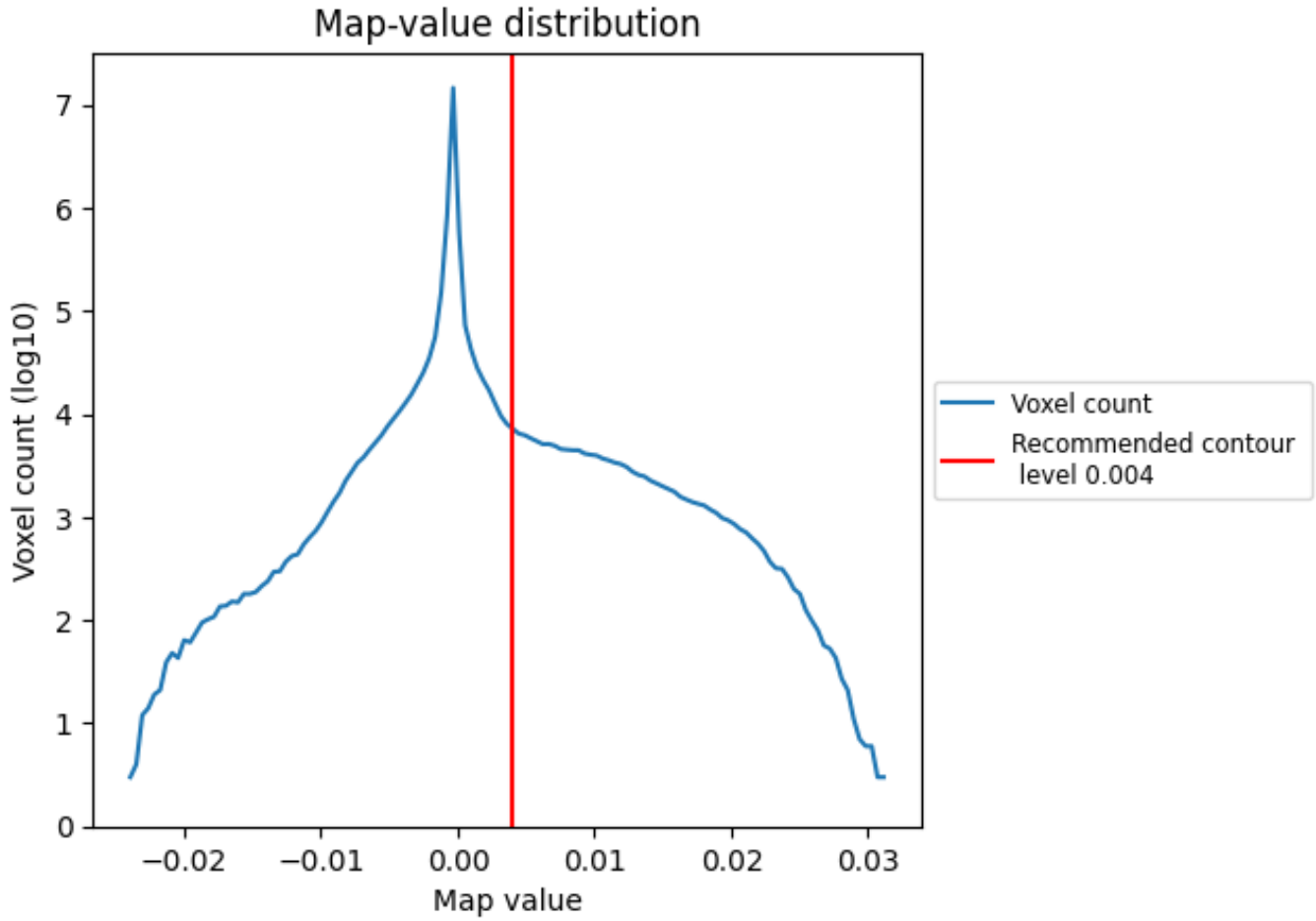
6.6 Mask visualisation (i)

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

7 Map analysis

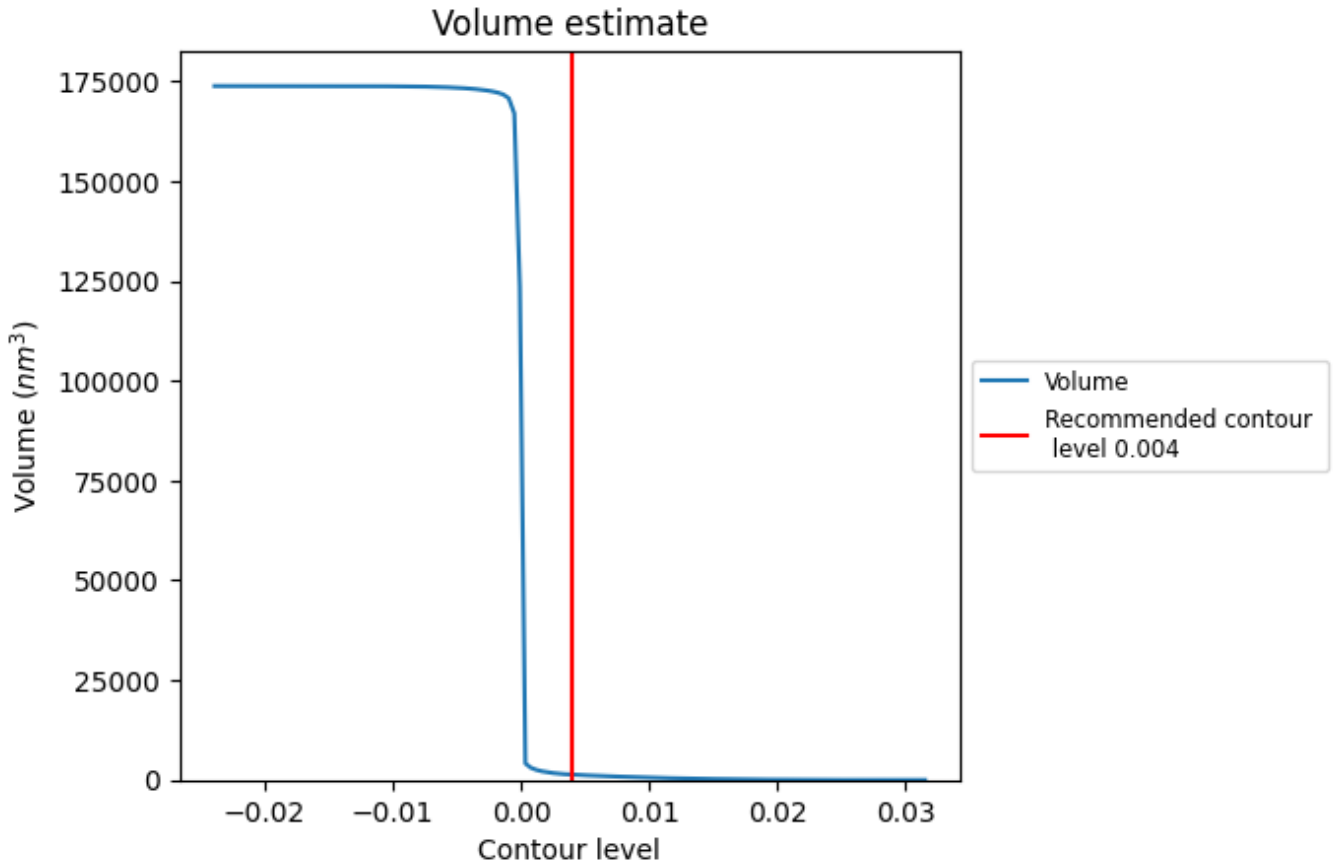
This section contains the results of statistical analysis of the map.

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.

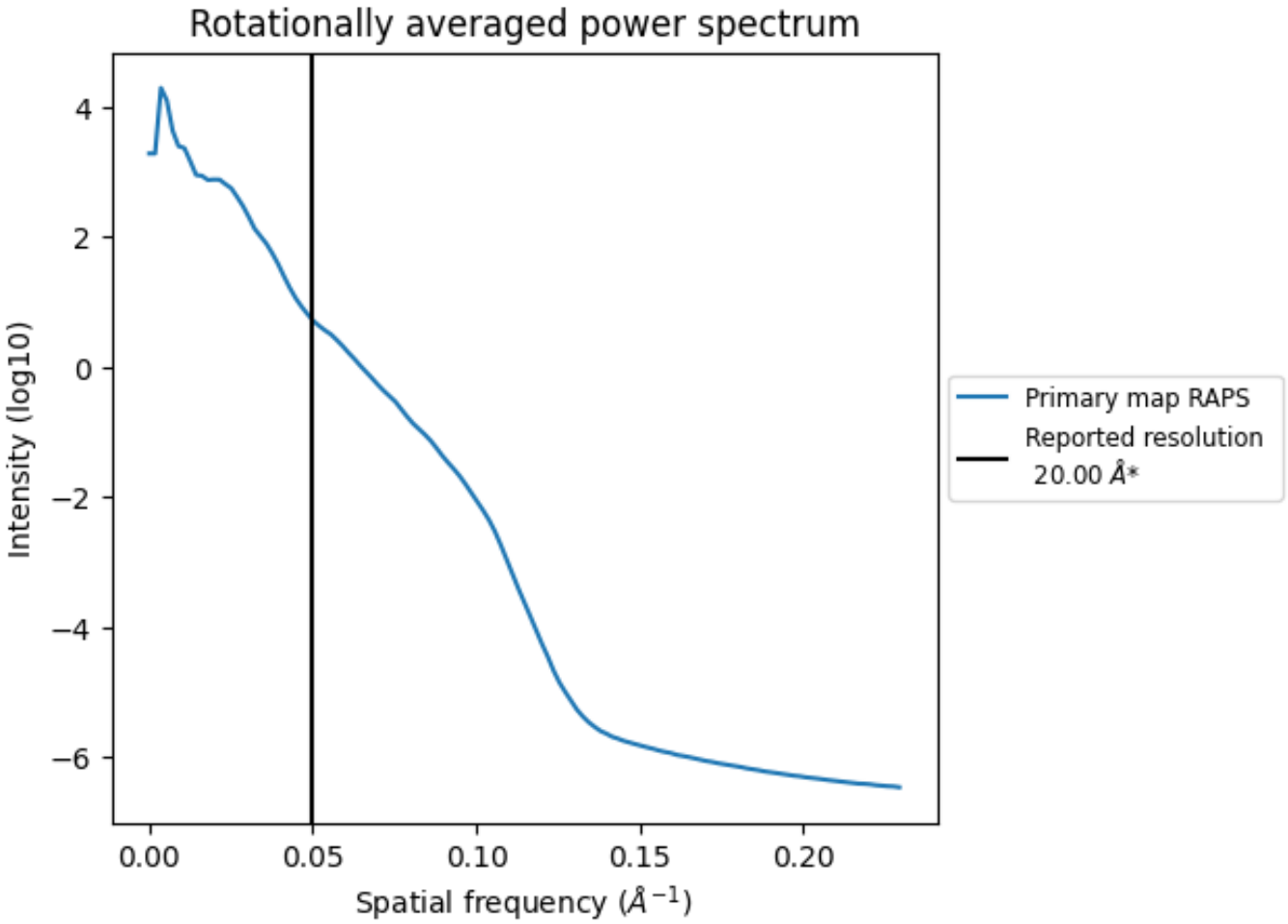
7.2 Volume estimate (i)



The volume at the recommended contour level is 1341 nm^3; this corresponds to an approximate mass of 1211 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 0.050 Å^{-1}

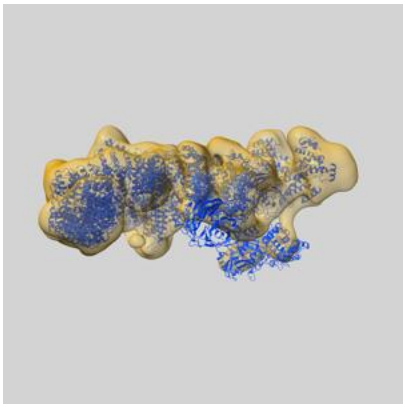
8 Fourier-Shell correlation

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

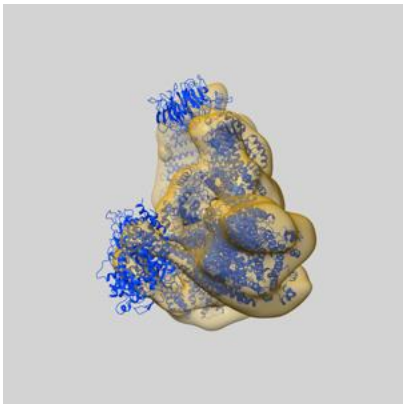
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10446 and PDB model 6TBM. Per-residue inclusion information can be found in section 3 on page 9.

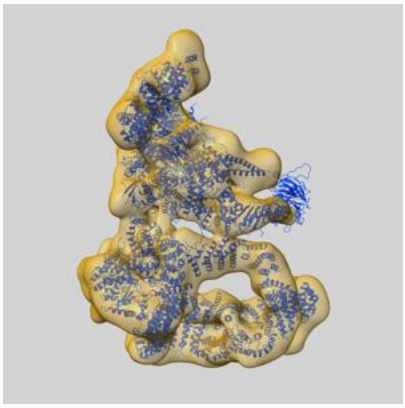
9.1 Map-model overlay



X



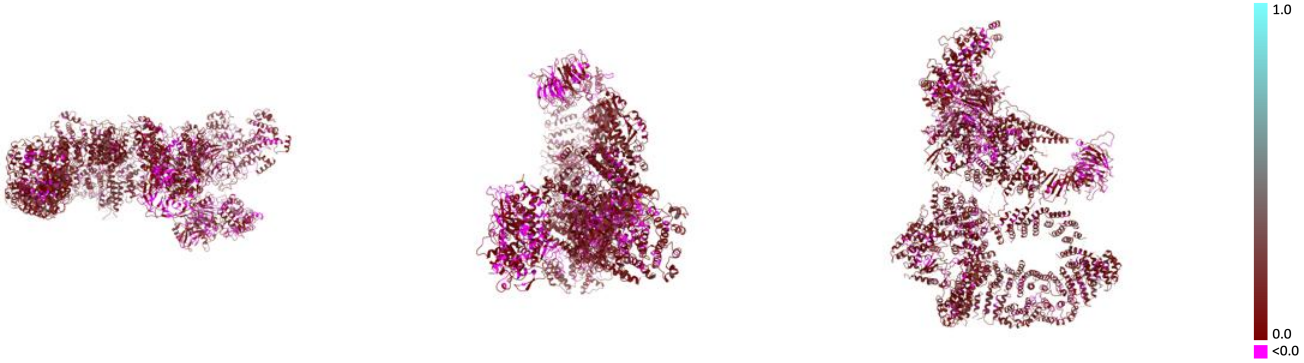
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.004 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.

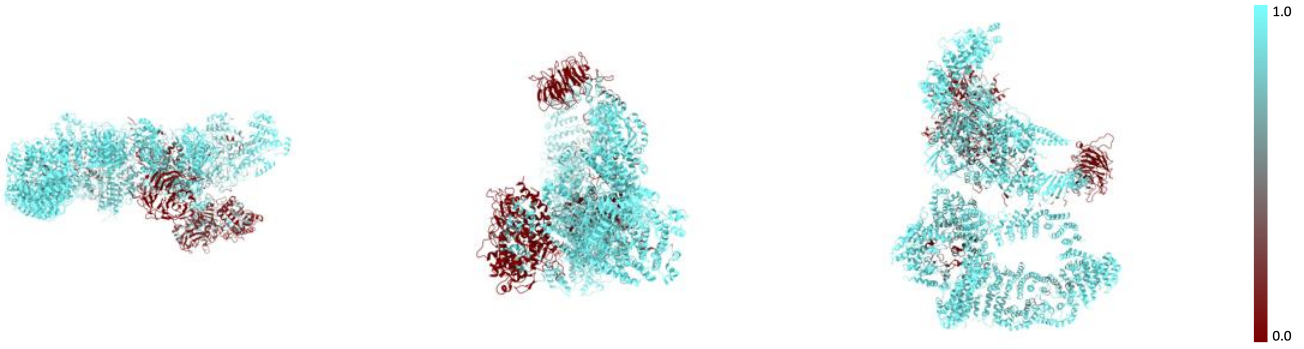
9.2 Q-score mapped to coordinate model



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.

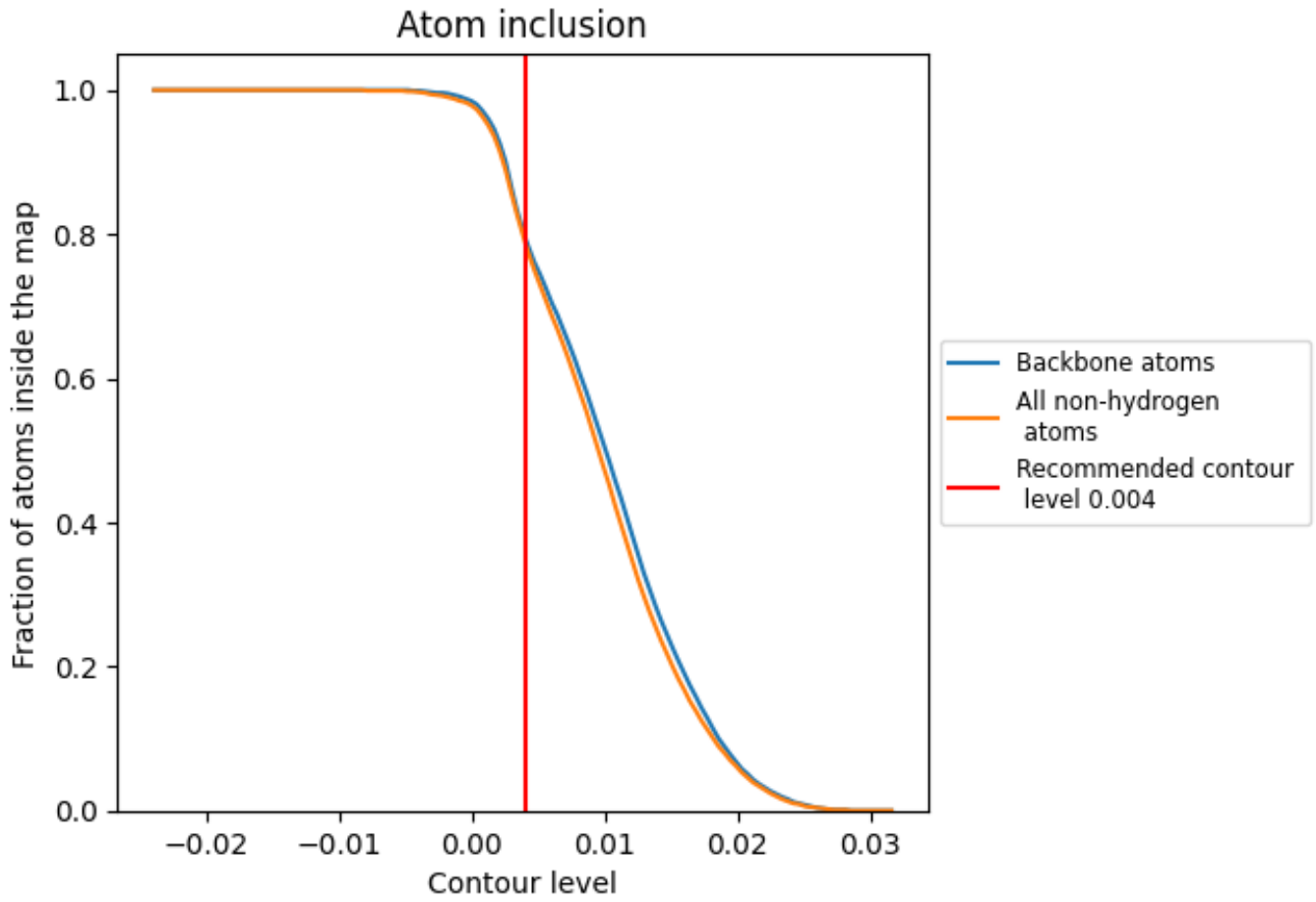
9.3 Atom inclusion mapped to coordinate model



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 (0.004).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 79% 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 (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7880	0.0800
A	0.7340	0.0550
B	1.0000	0.1030
C	0.5900	0.0520
D	0.8780	0.0850
E	0.9840	0.1110
F	0.8990	0.0920
G	0.8960	0.0740
H	0.9010	0.0800
I	0.8680	0.0710
J	0.9480	0.0730
K	0.8180	0.0500
L	0.9280	0.1010
M	0.8060	0.0760
N	0.0380	0.0210
O	0.1700	0.0130
P	0.2190	0.0410
Q	0.2220	0.0270
R	0.3800	0.0620