wwPDB EM Validation Summary Report (i)

Nov 6, 2022 – 01:51 PM EST

PDB ID	:	6MZL
EMDB ID	:	EMD-9305
Title	:	Human TFIID canonical state
Authors	:	Patel, A.B.; Louder, R.K.; Greber, B.J.; Grunberg, S.; Luo, J.; Fang, J.; Liu, Y.; Ranish, J.; Hahn, S.; Nogales, E.
Deposited on	:	2018-11-05
Resolution	:	23.00 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 (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:

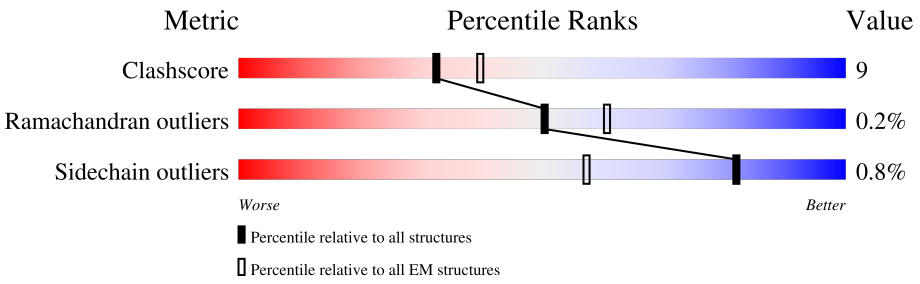
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 23.00 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	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	1872	14% 22% • 75%
2	B	1199	16% 52% 27% • 19%
3	C	929	• 9% • 90%
4	D	1085	• 9% • 91%
4	E	1085	• 8% • 91%
5	F	800	16% 48% 10% 41%
5	G	800	9% 42% 17% • 41%
6	H	677	7% 35% 13% 51%

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Mol	Chain	Length	Quality of chain
7	I	677	10% 36% 13% 50%
8	J	349	27% 30% 5% 65%
9	K	310	52% 14% 35%
10	L	264	36% 61%
10	M	264	11% 32% 7% 61%
11	N	218	5% 32% 6% 62%
11	O	218	28% 10% 62%
12	P	211	12% 32% 9% 58%
13	Q	161	6% 37% 9% 54%
13	R	161	34% 12% 54%
14	S	124	29% 6% 64%
15	T	339	12% 45% 7% 47%
16	Y	96	54% 98%
17	Z	238	15% 90% 10%

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 36618 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	472	3772	2397	659	693	23	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	968	7832	5031	1322	1421	58	0	0

- Molecule 3 is a protein called Transcription initiation factor TFIID subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	93	742	467	128	141	6	0	0

- Molecule 4 is a protein called Transcription initiation factor TFIID subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	102	686	423	130	133	0	0
4	E	102	686	423	130	133	0	0

- Molecule 5 is a protein called Transcription initiation factor TFIID subunit 5,TAF5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	473	3646	2314	638	679	15	0	0
5	G	473	3646	2314	638	679	15	0	0

- Molecule 6 is a protein called Transcription initiation factor TFIID subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	H	329	2494	1575	439	464	16	0	0

- Molecule 7 is a protein called Transcription initiation factor TFIID subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	I	339	2520	1585	445	474	16	0	0

- Molecule 8 is a protein called Transcription initiation factor TFIID subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	J	123	998	638	184	172	4	0	0

- Molecule 9 is a protein called Transcription initiation factor TFIID subunit 8,TAF8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	K	202	1449	906	260	278	5	0	0

- Molecule 10 is a protein called Transcription initiation factor TFIID subunit 9, TAF9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	L	104	732	456	129	142	5	0	0
10	M	104	732	456	129	142	5	0	0

- Molecule 11 is a protein called Transcription initiation factor TFIID subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	N	82	645	413	102	126	4	0	0
11	O	82	645	413	102	126	4	0	0

- Molecule 12 is a protein called Transcription initiation factor TFIID subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	P	89	707	447	127	128	5	0	0

- Molecule 13 is a protein called Transcription initiation factor TFIID subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	Q	74	611	381	107	120	3	0	0
13	R	74	611	381	107	120	3	0	0

- Molecule 14 is a protein called Transcription initiation factor TFIID subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	S	45	365	233	54	73	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	T	180	1429	927	252	243	7	0	0

- Molecule 16 is a protein called poly(UNK).

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	Y	96	480	288	96	96	0	0

- Molecule 17 is a protein called poly(UNK).

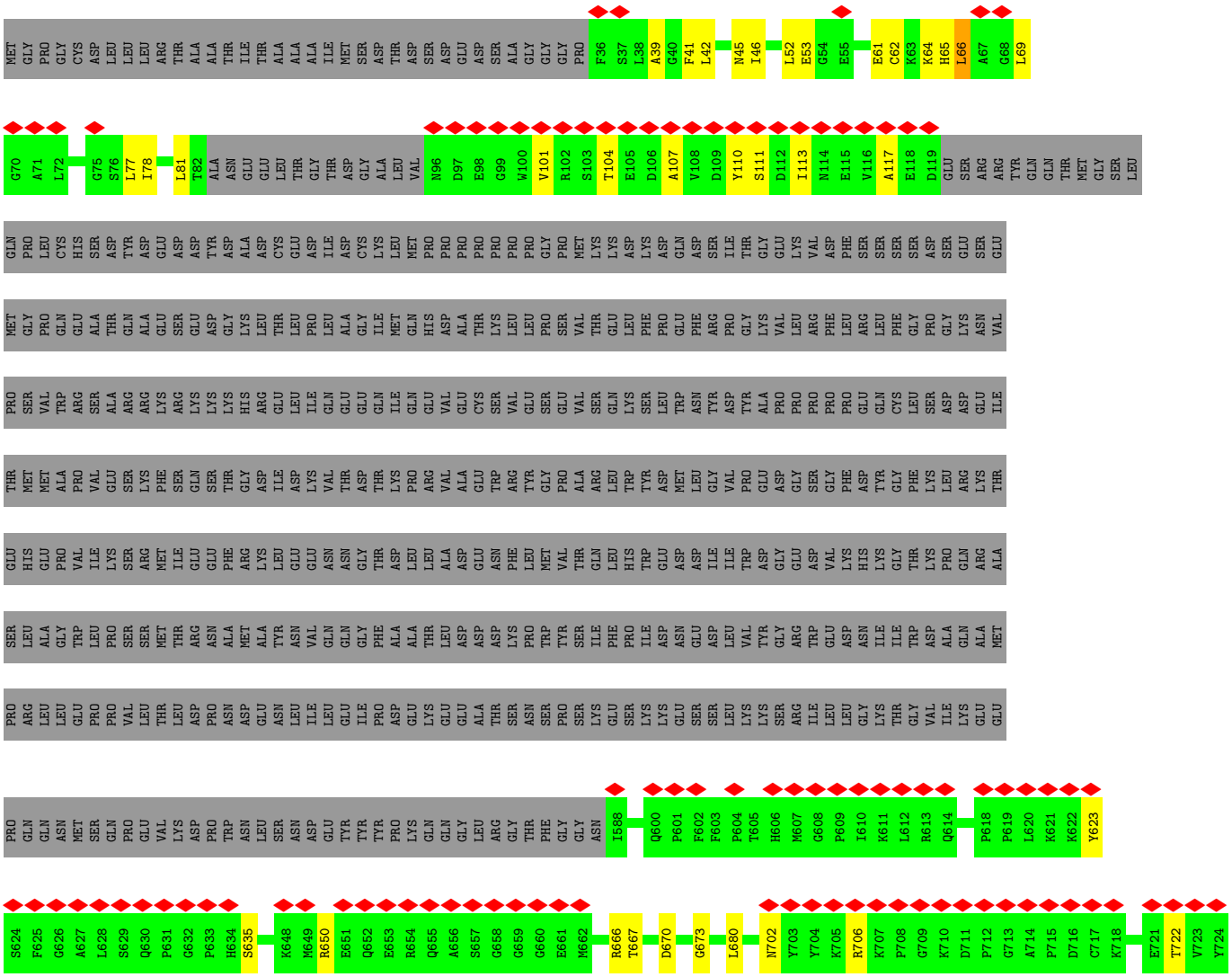
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	Z	238	1190	714	238	238	0	0

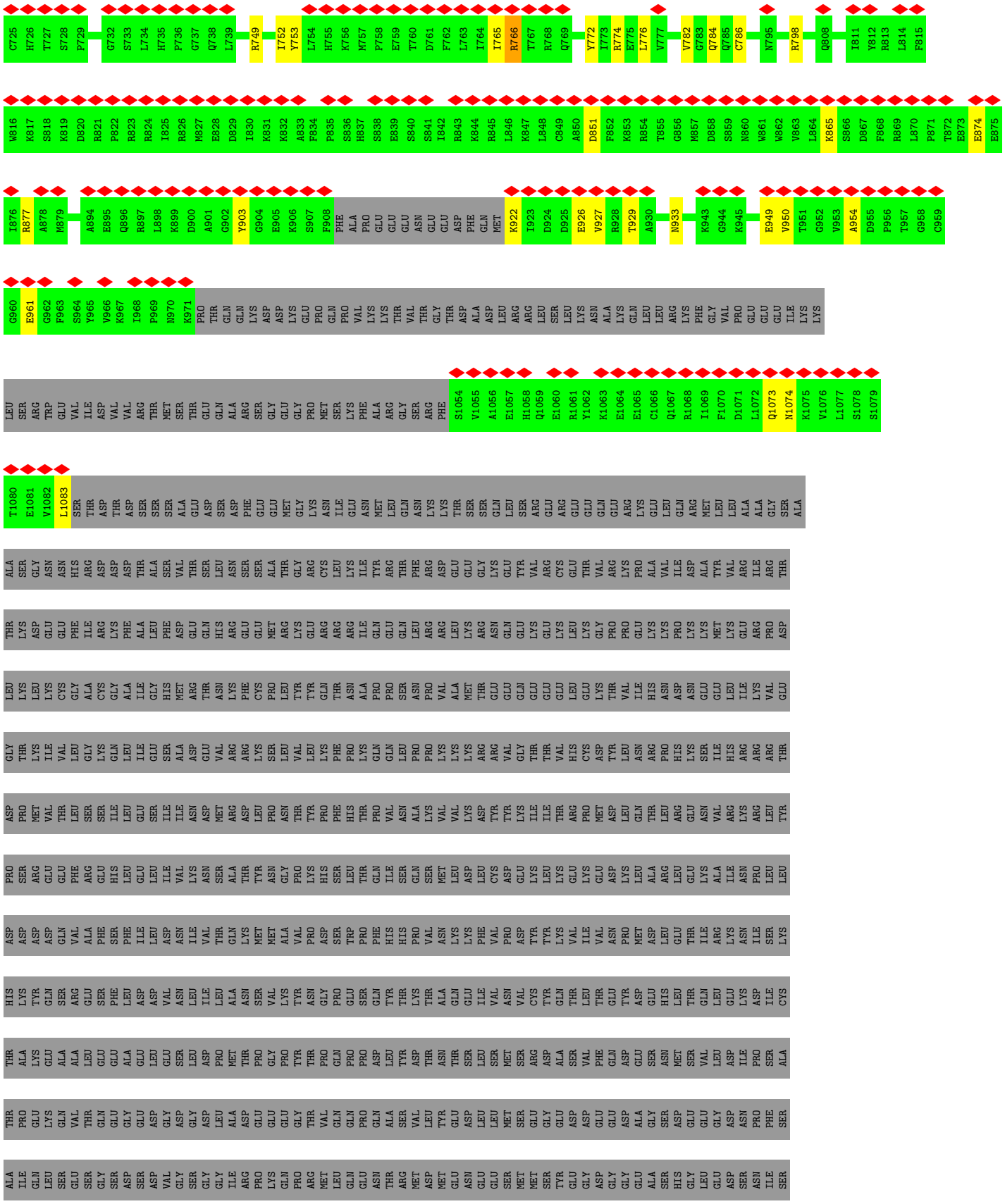
3 Residue-property plots (i)

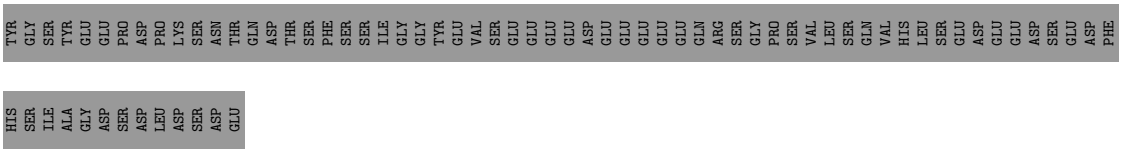
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Transcription initiation factor TFIID subunit 1

Chain A:

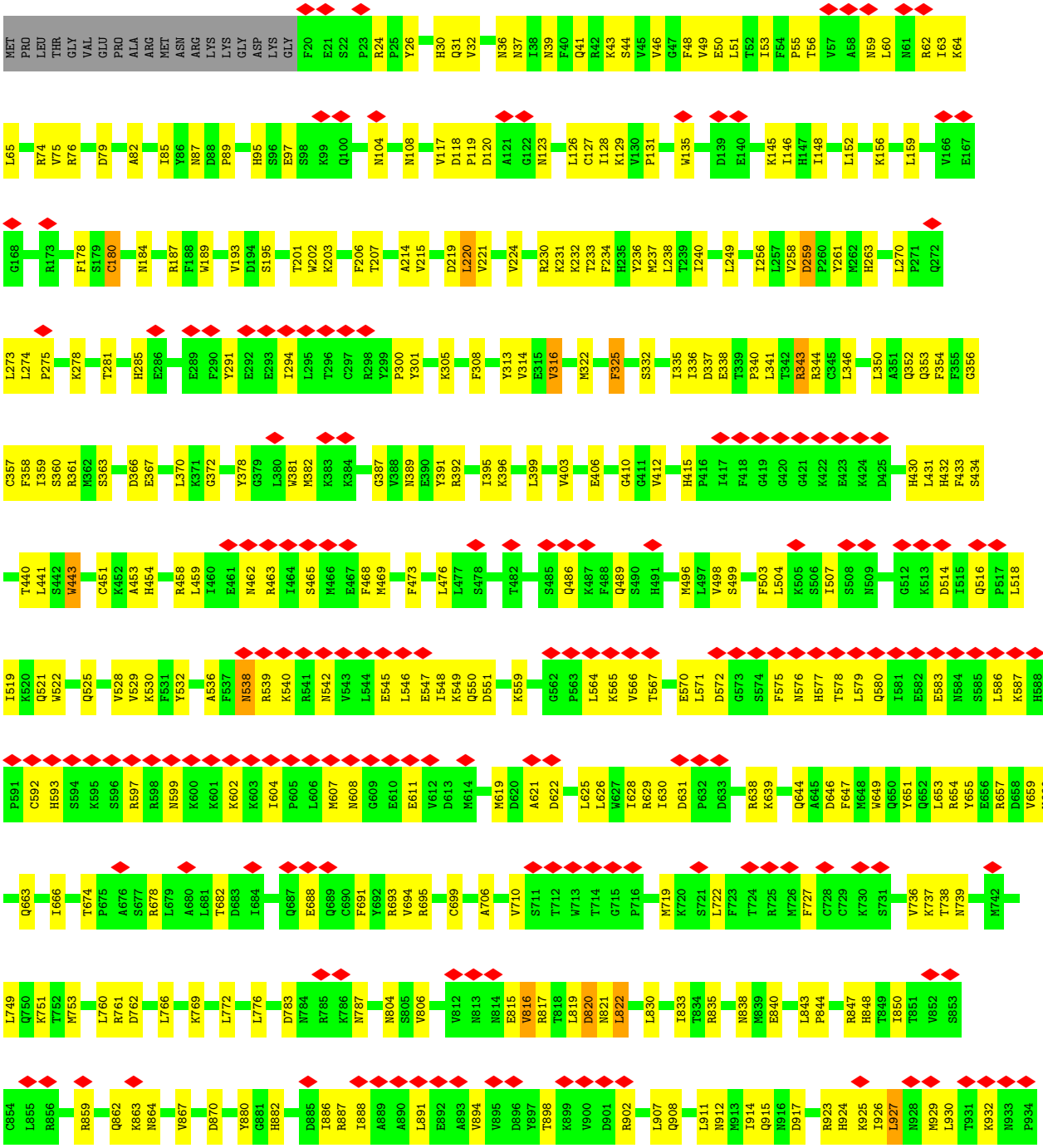


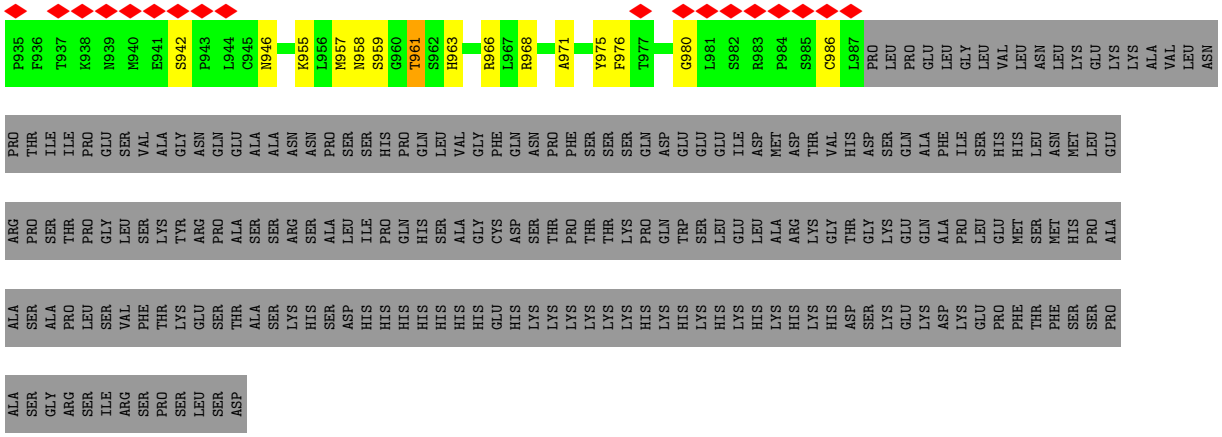

C725 H726 T727 S728 P729 G732 S733 L734 H735 P736 G737 Q738 L739 R749 I752 V753 L754 H755 K756 M757 P758 E759 T760 D761 F762 L763 I764 I765 R766 T767 R768 Q769 Y772 I773 R774 E775 L776 V777 V782 G783 Q784 Q785 C786 N795 R798 Q808 I811 Y812 R813 L814 F815
W816 K817 S818 K819 D820 R821 P822 R823 R824 I825 R826 M827 E828 D829 I830 K831 K832 A833 F834 P835 S836 H837 S838 E839 S840 S841 I842 R843 K844 R845 L846 K847 L848 C849 A850 D851 F852 K853 R854 T855 G856 M857 D858 S859 N860 W861 W862 V863 L864 K865 S866 D867 F868 R869 L870 P871 T872 E873 E874 E875
I876 R877 A878 M879 A894 E895 Q896 R897 L898 K899 D900 A901 G902 Y903 G904 E905 K906 S907 F908 PHE ALA PRO GLU GLU GLU ASN GLU GLU ASP PHE GLN MET K922 I923 D924 D925 E926 V927 R928 T929 A930 N933 K943 G944 K945 E949 V950 T951 G952 V953 A954 D955 P956 T957 G958 C959
G960 E961 G962 F963 S964 Y965 V966 K967 I968 P969 N970 K971 PRO THR GLN GLN LYS ASP ASP LYS GLU PRO GLN PRO VAL LYS LYS THR VAL THR GLY THR ASP ALA ASP LEU ARG ARG LEU SER LEU LYS ASN ALA LYS GLN LEU LEU ARG LYS PHE GLY VAL PRO GLU GLU GLU ILE LYS LYS
LEU SER ARG TRP GLU VAL ILE ASP VAL VAL ARG THR MET SER THR GLU GLN ALA ARG SER GLY GLU GLY PRO MET SER LYS PHE ALA ARG GLY SER ARG PHE S1054 V1055 A1056 E1057 H1058 Q1059 E1060 R1061 Y1062 K1063 E1064 E1065 C1066 Q1067 R1068 I1069 F1070 D1071 L1072 Q1073 N1074 K1075 V1076 L1077 S1078 S1079
T1080 E1081 V1082 L1083 SER THR ASP THR ASP SER SER SER ALA GLU ASP SER ASP PHE GLU GLU MET GLY LYS ASN ILE GLU ASN MET LEU GLN ASN LYS LYS THR SER SER GLN LEU SER ARG GLU ARG GLU GLU GLU GLN GLU ARG LYS GLU LEU GLN ARG MET LEU LEU ALA ALA GLY SER ALA
ALA SER GLY ASN ASN HIS ARG ASP ASP ASP THR ALA SER VAL THR SER LEU ASN SER SER ALA THR GLY ARG CYS LEU LYS ILE TYR ARG THR PHE ARG ASP GLU GLU GLY LYS GLU TYR VAL ARG CYS GLU THR VAL ARG LYS PRO ALA VAL ILE ASP ALA TYR VAL ARG ILE ARG THR
THR LYS ASP GLU GLU PHE ILE ARG LYS PHE ALA LEU PHE ASP GLU GLN HIS ARG GLU GLU MET ARG LYS GLU ARG ARG ARG ILE GLN GLU GLN GLN LEU ARG ARG LEU LYS ARG ASN GLN GLU LYS GLU LYS LEU LYS GLY PRO PRO GLU LYS LYS LYS PRO LYS LYS MET LYS GLU ARG
LEU LYS LEU LYS CYS GLY ALA CYS GLY ALA ILE GLY HIS MET ARG THR ASN LYS PHE CYS PRO LEU TYR TYR GLN THR ASN ALA PRO PRO PRO SER ASN PRO VAL ALA MET THR GLU GLU GLN GLU GLU LEU LEU LEU LYS THR VAL ILE HIS ASN ASP ASN GLU GLU LEU ILE LYS VAL GLU
GLY THR LYS ILE VAL LEU GLY LYS GLN LEU ILE GLU SER ALA ASP GLU VAL ARG ARG LYS SER LEU VAL VAL LEU LYS PHE PRO LYS GLN GLN LEU PRO PRO LYS LYS LYS ARG ARG VAL GLY THR THR THR VAL HIS CYS ASP TYR THR LEU ASN ARG PRO HIS LYS SER ILE HIS ARG ARG ARG THR
ASP PRO MET VAL THR LEU SER SER ILE LEU GLU SER ILE ILE ASN ASP MET ARG ASP LEU PRO ASN THR TYR PRO PHE HIS THR PRO VAL ASN ALA LYS VAL VAL LYS ASP TYR TYR LYS ILE ILE THR ARG PRO MET ASP LEU GLN THR LEU ARG LYS VAL ILE ARG ILE LYS ARG LEU TYR
PRO SER ARG GLU GLU PHE ARG GLU HIS SER LEU GLU GLU LEU ILE LYS ASN SER ALA THR TYR ASN GLY PRO LYS HIS SER LEU THR GLN ILE SER GLN SER MET LEU ASP LEU CYS ASP GLU LYS LEU LYS GLU LYS GLU ASP LYS LEU ALA ARG LEU GLU LYS ALA ILE ASN PRO LEU LEU
ASP ASP ASP ASP GLN VAL ALA PHE SER PHE PHE LEU ILE LEU ASP ASN ILE VAL THR GLN LYS MET MET ALA VAL PRO ASP SER TRP PRO PHE HIS HIS PRO VAL ASN LYS LYS PHE VAL PRO ASP TYR TYR LYS VAL ILE VAL ASN PRO MET ASP LEU GLN THR ARG LEU GLU THR ILE ARG LYS ASN ILE SER LYS
HIS LYS TYR GLN SER ARG GLU SER PHE LEU ASP ASP VAL ASN LEU ILE LEU ALA ASN SER VAL LYS TYR ASN GLY PRO GLU SER GLN TYR THR LYS THR ALA GLN GLU ILE VAL ASN VAL CYS TYR GLN THR LEU THR GLU TYR ASP GLU LYS GLU LYS ASP ILE CYS
THR ALA LYS GLU ALA ALA LEU GLU GLU ALA GLU LEU GLU GLU SER LEU ASP PRO MET THR PRO GLN PRO PRO ASP LEU TYR ASP THR ASN THR SER LEU SER MET SER ARG ASP ALA SER VAL PHE GLN GLU ASP GLU SER ASN MET SER VAL LEU ASP ILE PRO SER ALA
THR PRO GLU LYS GLN VAL THR GLN GLU GLY GLY ASP GLY GLY LEU ALA ASP PRO GLU GLU GLN GLN PRO GLN ALA SER VAL LEU TYR GLU GLY THR VAL GLN GLU GLY GLU ASP ASP GLU GLU GLU ASP ALA GLY SER ASP GLU LEU GLY ASP ASN PRO SER PHE
ALA ILE GLN LEU SER GLU SER GLY SER ASP SER ASP VAL GLY SER GLY LEU ILE ARG PRO LYS GLN PRO ARG MET LEU GLN GLU ASN THR ARG MET ASP MET GLU ASN GLU GLU SER MET MET MET SER TYR GLU GLY ASP GLY GLY GLU ALA SER HIS GLY LEU GLU ASP GLY GLU ASP ILE SER



• Molecule 2: Transcription initiation factor TFIID subunit 2

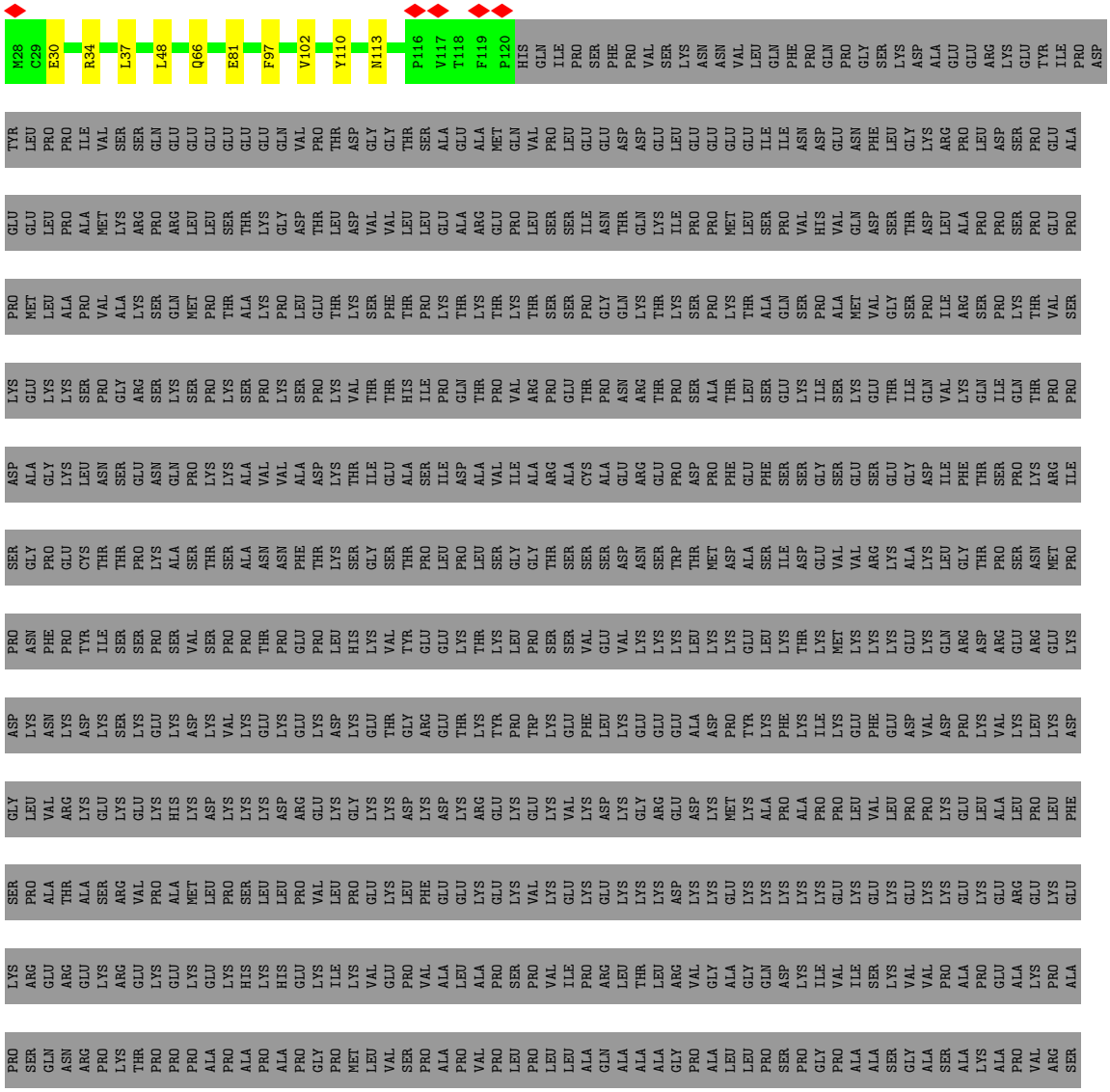
Chain B:

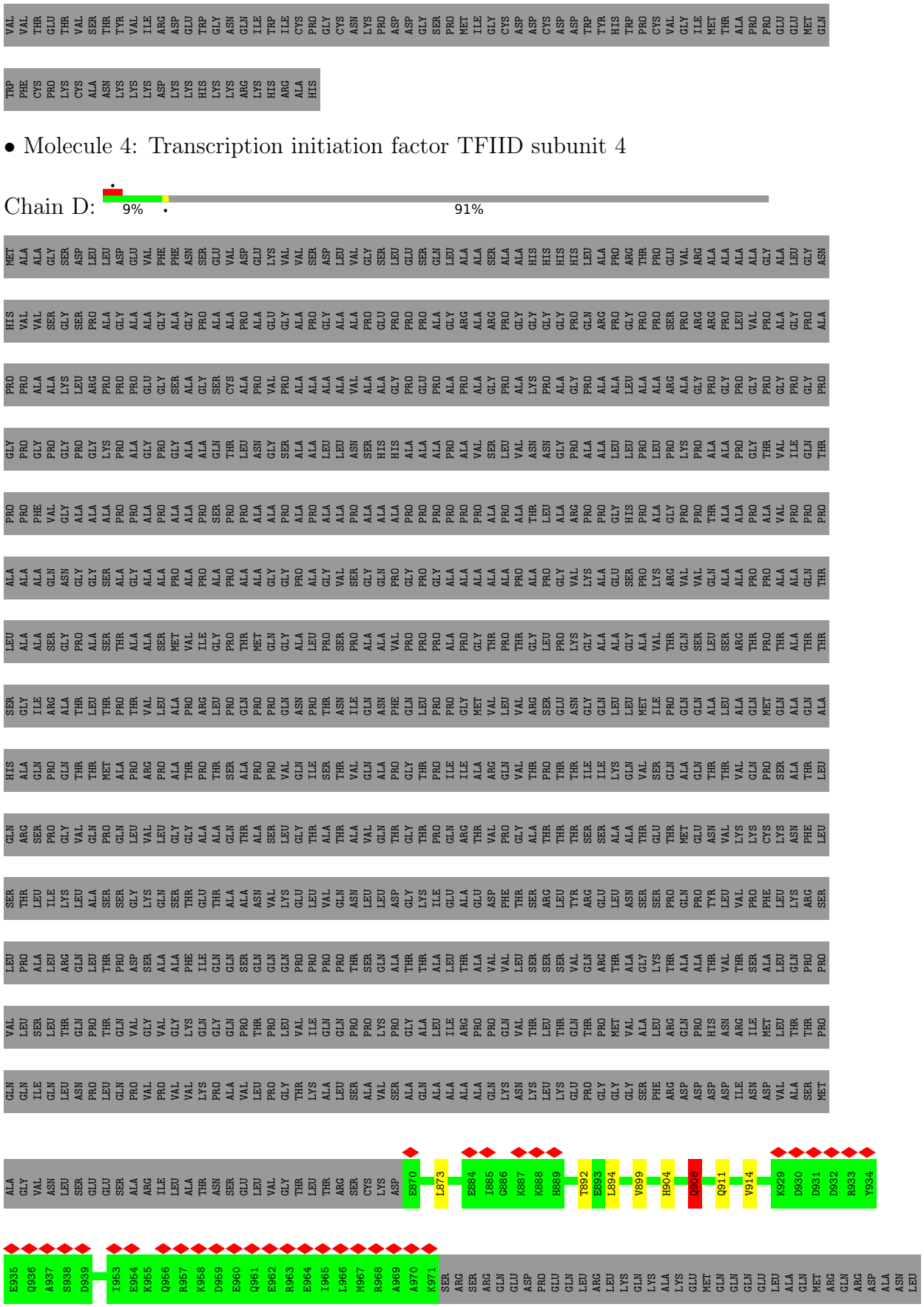




• Molecule 3: Transcription initiation factor TFIID subunit 3

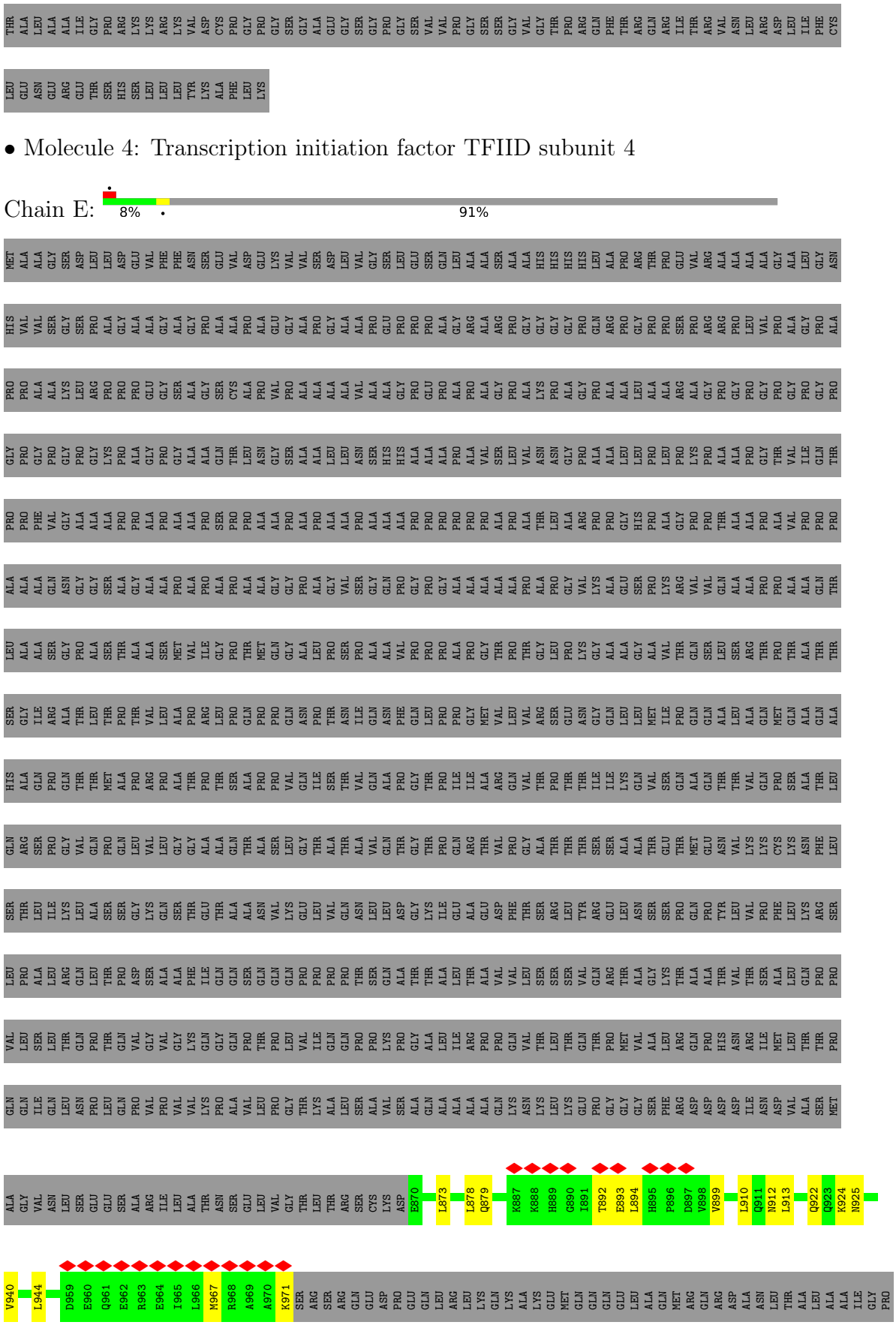
Chain C: 9% 90%





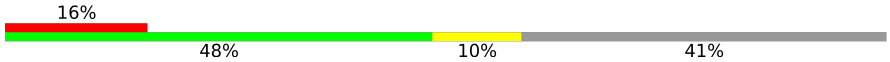
• Molecule 4: Transcription initiation factor TFIID subunit 4

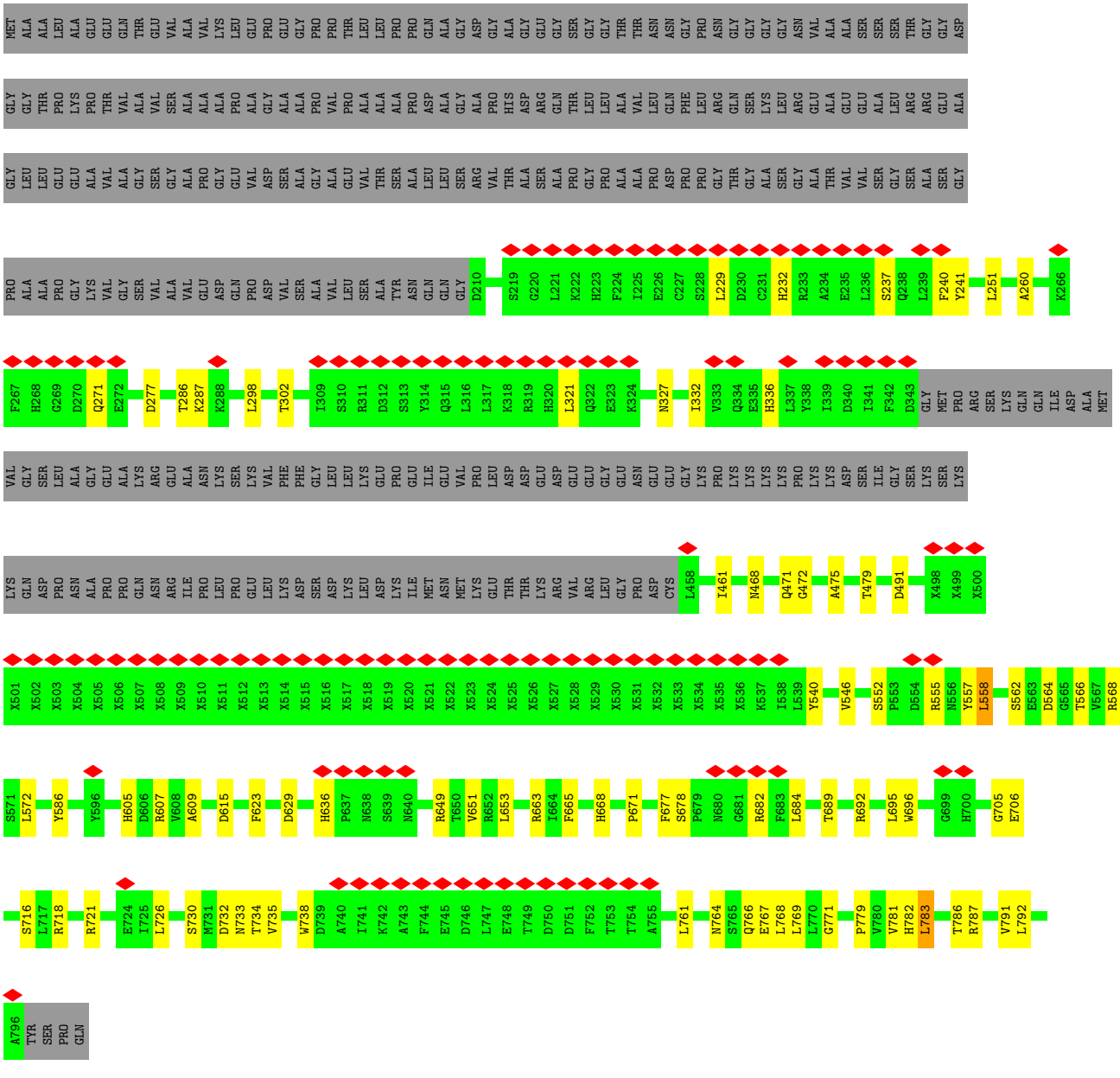
Chain D:


THR ALA LEU ALA ALA ILE GLY PRO ARG LYS LYS ARG LYS VAL ASP CYS PRO GLY PRO GLY SER GLY ALA GLU GLY SER GLY PRO GLY SER VAL VAL PRO GLY SER SER GLY VAL GLY THR PRO ARG GLN PHE THR ARG GLN ARG ILE THR ARG VAL ASN LEU ARG ASP LEU ILE PHE CYS
LEU GLU ASN GLU ARG GLU THR SER HIS SER LEU LEU LEU LEU TYR LYS ALA PHE LEU LYS
• Molecule 4: Transcription initiation factor TFIID subunit 4
Chain E:
8%
91%
MET ALA ALA GLY SER ASP LEU LEU ASP GLU VAL PHE PHE ASN SER GLU VAL ASP GLU LYS VAL VAL SER ASP LEU VAL GLY SER LEU GLU SER GLN LEU ALA ALA SER ALA ALA HIS HIS HIS HIS LEU ALA PRO ARG THR PRO GLU VAL ARG ALA ALA ALA ALA GLY
HIS VAL VAL SER GLY SER PRO ALA GLY ALA ALA GLY ALA GLY PRO ALA PRO ALA GLU GLU GLY ALA PRO GLY ALA ALA PRO GLU PRO PRO PRO ALA GLY ARG ALA ARG PRO GLY GLY GLY PRO GLN ARG PRO GLY PRO PRO SER PRO ARG ARG PRO LEU VAL PRO ALA GLY ALA
PRO PRO ALA ALA LYS LEU ARG PRO PRO GLU GLY SER ALA GLY SER CYS ALA PRO VAL PRO ALA ALA ALA ALA VAL ALA ALA GLY PRO GLU PRO ALA PRO ALA GLY PRO ALA LYS PRO ALA GLY PRO ALA ALA LEU ALA ALA ARG GLY PRO GLY PRO GLY PRO
GLY PRO GLY PRO GLY PRO GLY LYS PRO ALA GLY PRO GLY ALA ALA GLN THR LEU ASN GLY SER ALA ALA LEU LEU ASN SER HIS HIS ALA ALA ALA PRO ALA VAL SER LEU VAL ASN ASN GLY PRO ALA ALA LEU LEU PRO LEU PRO LYS PRO ALA ALA GLY THR VAL ILE GLN THR
PRO PRO PHE VAL GLY ALA ALA ALA PRO PRO ALA PRO ALA PRO ALA PRO SER PRO PRO ALA ALA PRO ALA ALA ALA PRO PRO PRO PRO PRO ALA PRO ALA ALA ARG PRO PRO GLY HIS PRO ALA GLY PRO PRO THR ALA ALA PRO ALA VAL PRO PRO PRO
ALA ALA ALA GLN ASN GLY GLY SER ALA GLY ALA ALA PRO ALA PRO ALA ALA ALA GLY VAL SER GLY GLN PRO GLY PRO GLY ALA ALA ALA ALA ALA PRO ALA PRO GLY VAL LYS ALA GLU SER PRO LYS ARG VAL VAL GLN ALA ALA PRO PRO ALA ALA GLN THR
LEU ALA ALA SER GLY PRO ALA SER THR ALA ALA SER MET VAL ILE GLY PRO THR MET GLN GLY ALA LEU PRO SER PRO ALA ALA VAL PRO PRO PRO ALA PRO GLY THR PRO THR GLY LEU PRO LYS GLY ALA ALA GLY VAL THR GLN SER LEU SER ARG THR PRO THR ALA ALA THR THR
SER GLY ILE ARG ALA THR LEU THR PRO THR VAL LEU ALA PRO ARG LEU PRO GLN PRO PRO GLN ASN PRO THR ASN ILE GLN ASN PHE GLN LEU PRO PRO GLY MET VAL LEU VAL ARG SER GLU ASN GLY GLN LEU LEU MET ILE PRO GLN GLN GLN ALA LEU ALA GLN MET GLN ALA GLN ALA
HIS ALA GLN PRO GLN THR THR MET ALA PRO ARG PRO ALA ARG PRO ALA PRO PRO VAL GLN ILE SER THR VAL GLN ALA PRO GLY THR PRO ILE ILE ALA ARG GLN VAL THR PRO THR THR ILE ILE LYS GLN VAL SER GLN ALA GLN THR LEU VAL GLN PRO SER ALA THR LEU
GLN ARG SER PRO GLY VAL GLN PRO GLN LEU LEU VAL LEU GLY GLY VAL ALA ALA GLN THR ALA SER GLY GLY THR ALA THR ALA VAL GLN THR GLY THR PRO GLN ARG THR VAL PRO GLY ALA THR THR THR SER SER ALA ALA THR GLU THR MET GLU ASN VAL LYS LYS CYS LYS ASN PHE LEU
SER THR LEU ILE LYS LEU ALA SER SER GLY LYS GLN SER THR GLU THR ALA ALA ASN VAL LYS GLU LEU VAL GLN ASN LEU LEU ASP GLY LYS ILE GLU ALA GLU ASP PHE THR SER ARG LEU TYR ARG GLU LEU ASN SER PRO GLN PRO TYR LEU VAL PRO LEU LEU ARG SER
LEU PRO ALA LEU ARG GLN LEU THR PRO ASP SER ALA ALA PHE ILE GLN GLN SER GLN GLN GLN PRO PRO PRO PRO THR SER GLN ALA THR ALA LEU THR ALA VAL PRO GLN GLN ARG THR ALA ALA THR VAL THR VAL GLN ARG ILE LEU LEU SER THR ALA GLY LYS THR ALA ALA THR THR ILE ILE ASP ASP ILE ASN ARG PRO PRO
VAL LEU SER LEU THR GLN PRO THR GLN VAL GLY VAL LYS GLN GLN PRO THR VAL GLN GLN GLN PRO LYS PRO GLY ALA LEU ILE ARG PRO PRO GLN VAL THR LEU THR GLN THR PRO MET VAL ALA LEU ARG GLN PRO HIS ASN ARG ILE MET LEU THR THR PRO
GLN GLN ILE GLN LEU ASN PRO LEU GLN PRO VAL LYS GLN ALA VAL LEU PRO GLY THR LYS ALA LEU SER ALA VAL SER ALA GLN LYS ALA ALA ALA GLN LYS ASN LYS LEU LYS GLU PRO GLY GLY GLY SER PHE ARG ASP ASP ASP ILE ASN ASP VAL ALA SER MET
ALA GLY VAL ASN LEU SER GLU GLU SER ALA ARG ILE LEU ALA THR ASN SER GLU LEU VAL GLY THR LEU THR ARG SER CYS LYS ASP E870 L873 L878 Q879 K887 K888 H889 G890 I891 T892 E893 L894 H895 P896 D897 V898 V899 L910 Q911 N912 L913 Q922 Q923 K924 N925
V940 L944 D959 E960 Q961 E962 R963 E964 I965 L966 M967 R968 A969 A970 K971 SER ARG SER ARG GLN GLU ASP PRO GLU GLN LEU ARG LEU LYS GLN LYS ALA LYS GLU MET GLN GLN GLN GLU LEU ALA GLN MET MET ARG GLN ARG ASP ALA ASN LEU THR ALA LEU ALA ALA ILE GLY PRO

• Molecule 5: Transcription initiation factor TFIID subunit 5,TAF5

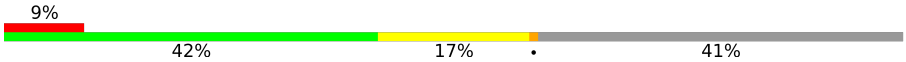
Chain F:

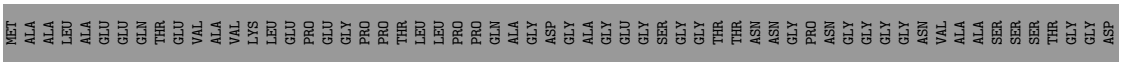


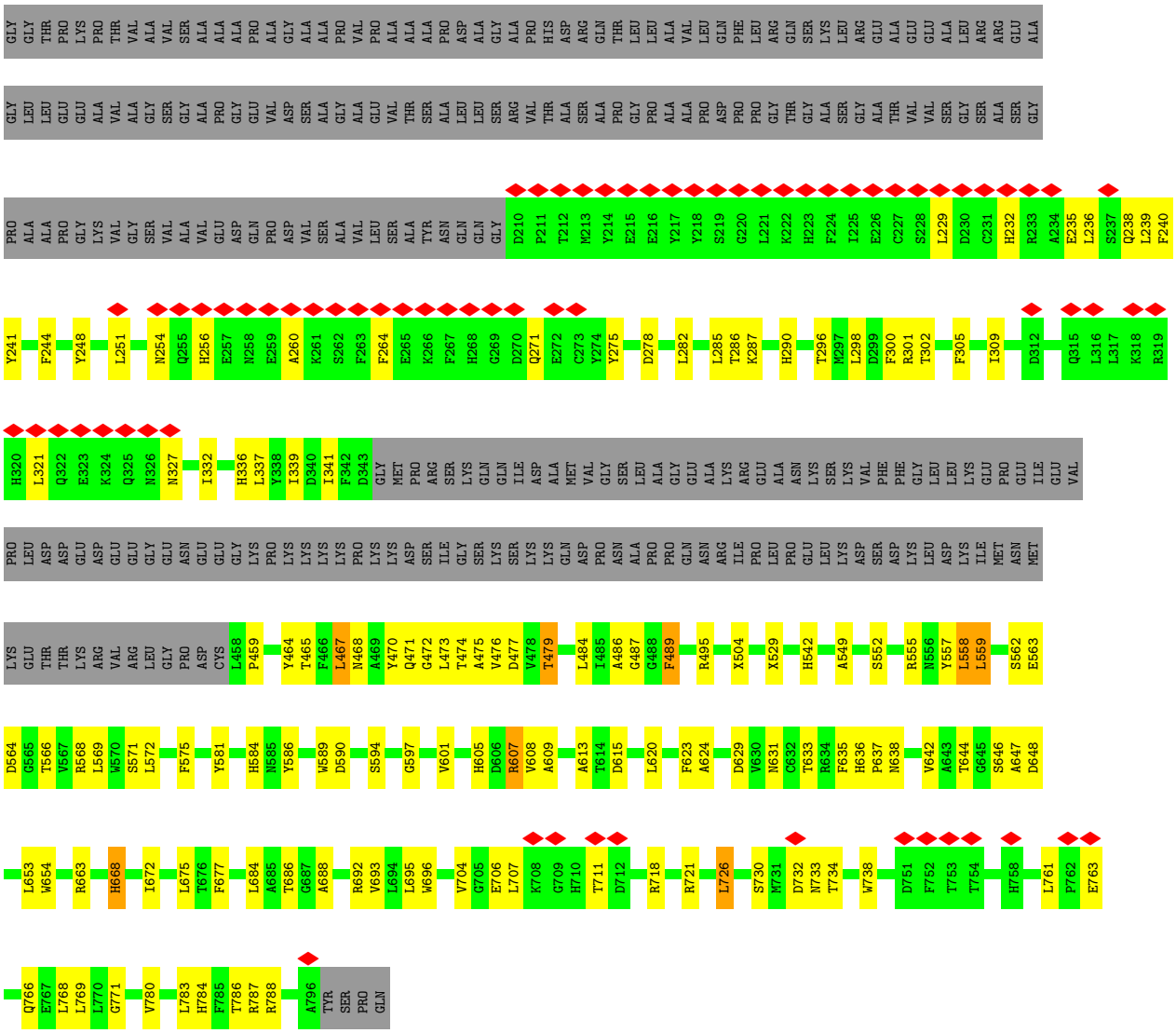


• Molecule 5: Transcription initiation factor TFIID subunit 5,TAF5

Chain G:

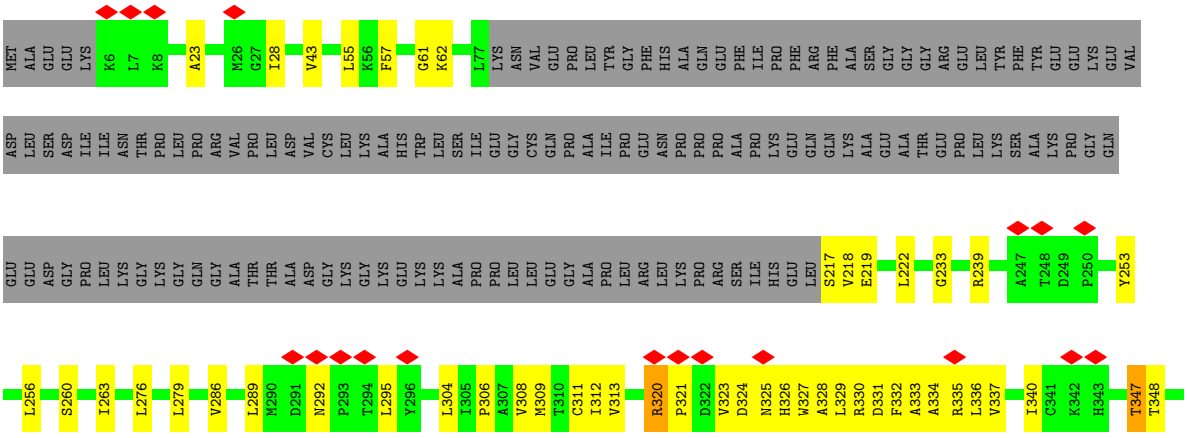


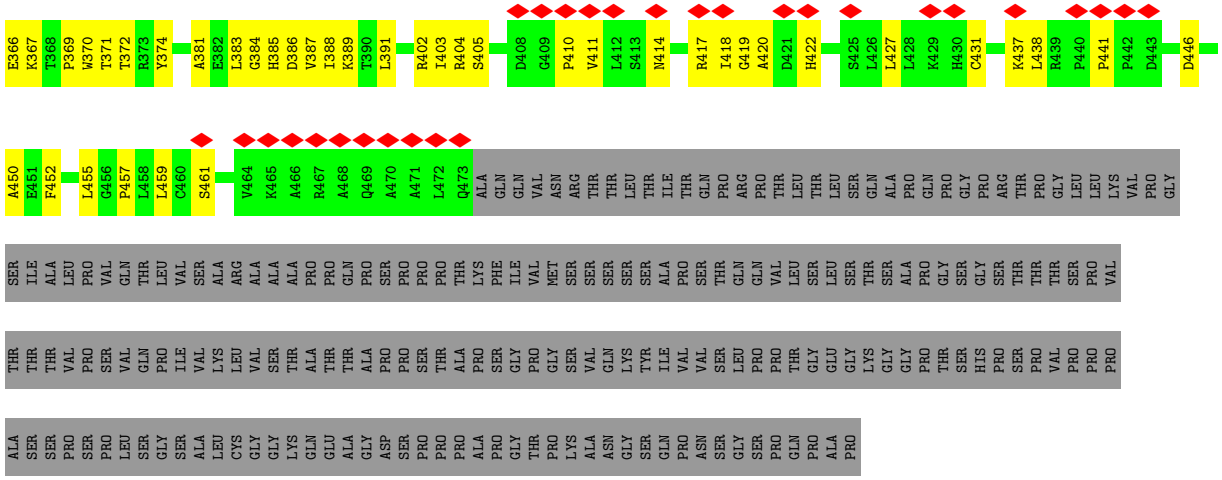




• Molecule 6: Transcription initiation factor TFIID subunit 6

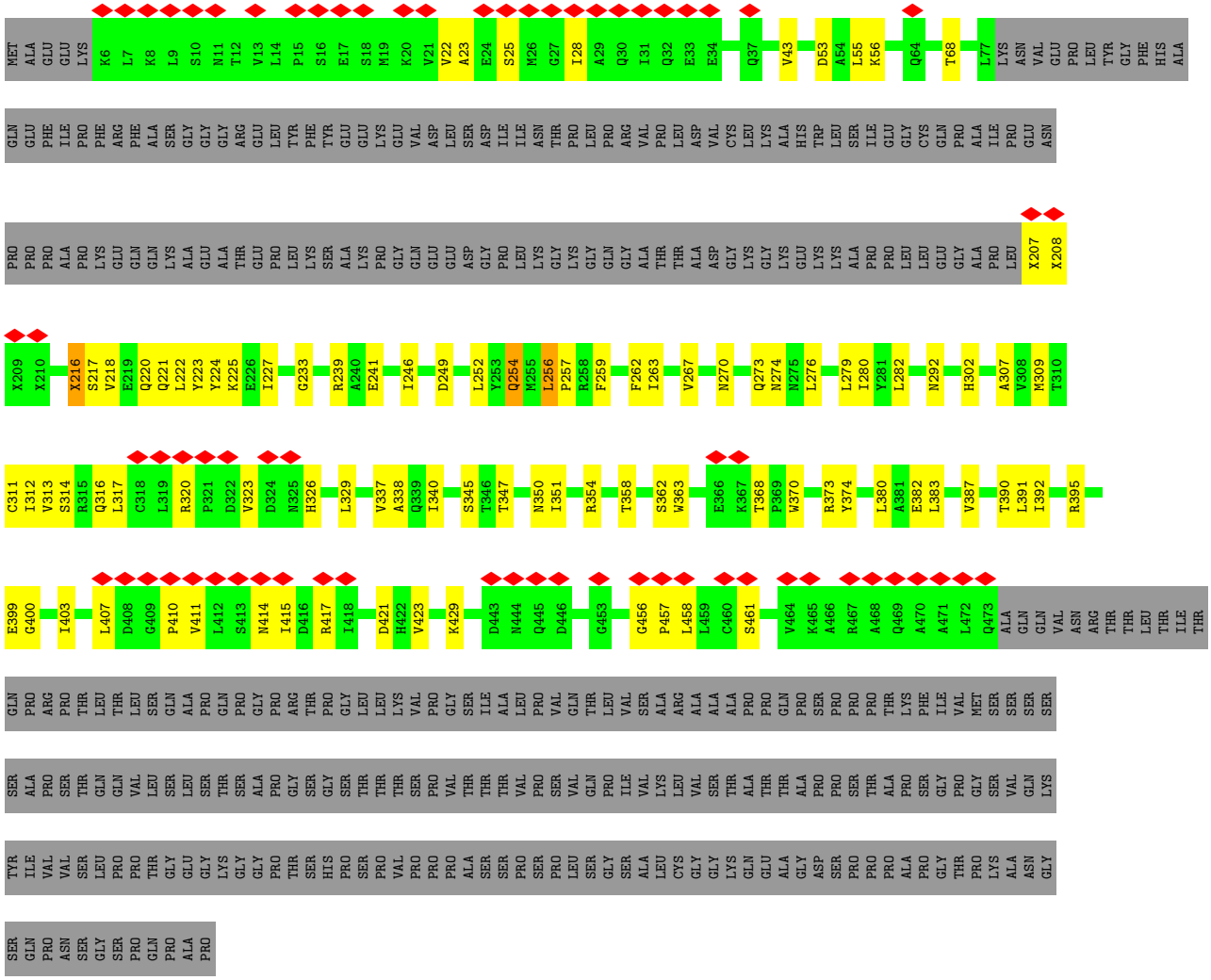
Chain H:





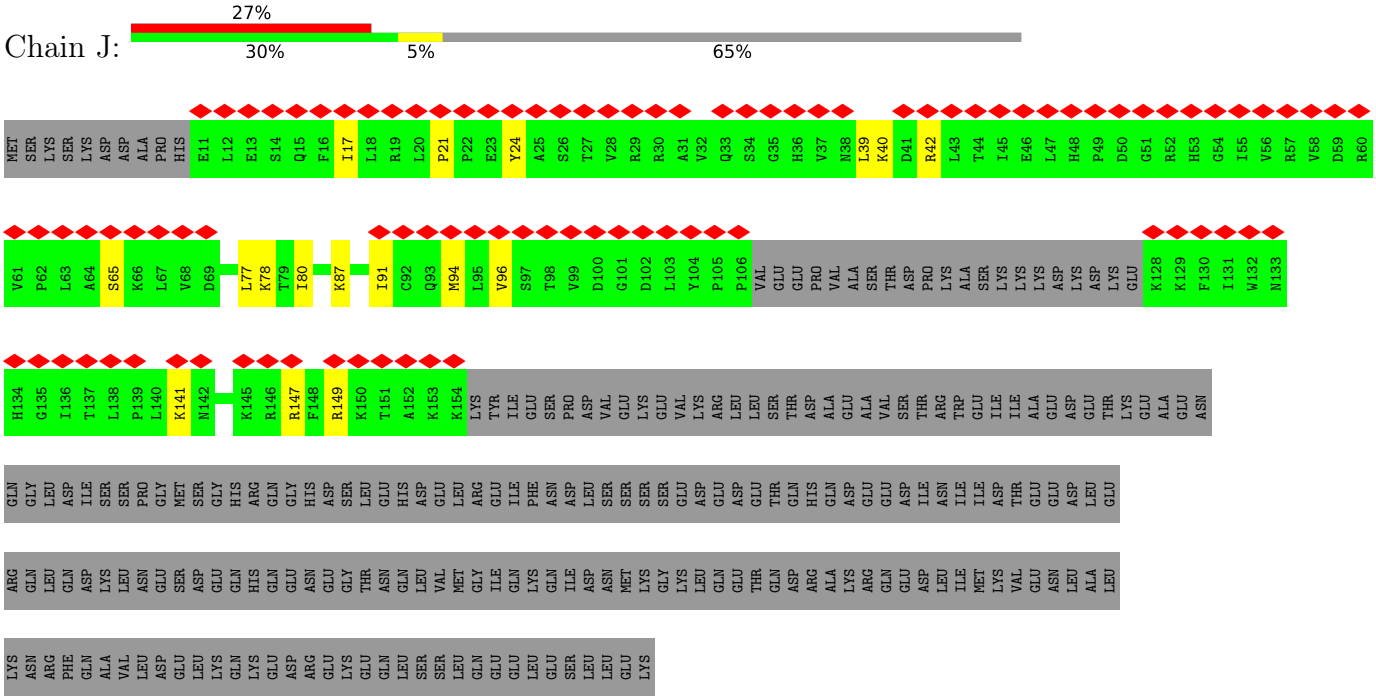
- Molecule 7: Transcription initiation factor TFIID subunit 6

Chain I:



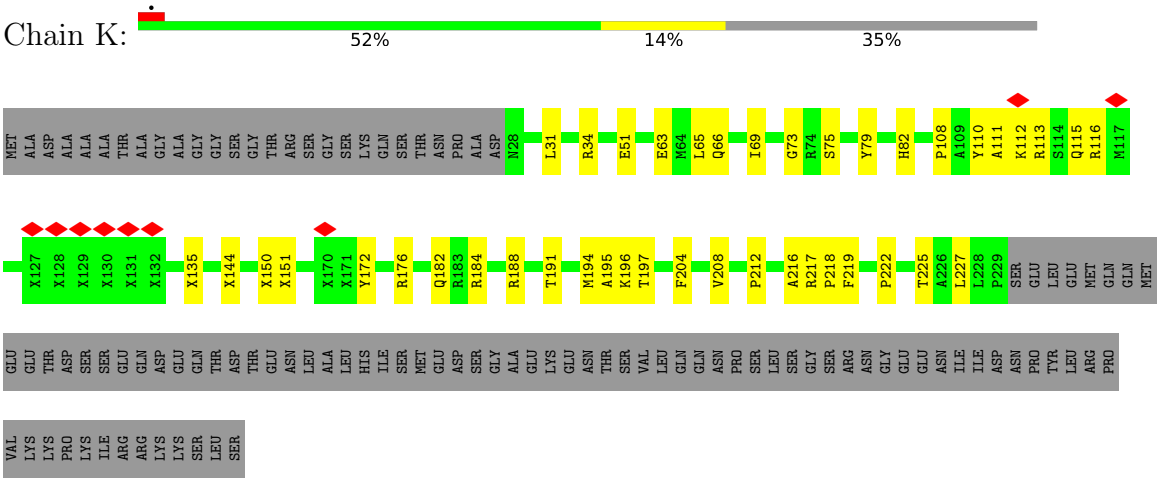
- Molecule 8: Transcription initiation factor TFIID subunit 7

Chain J:



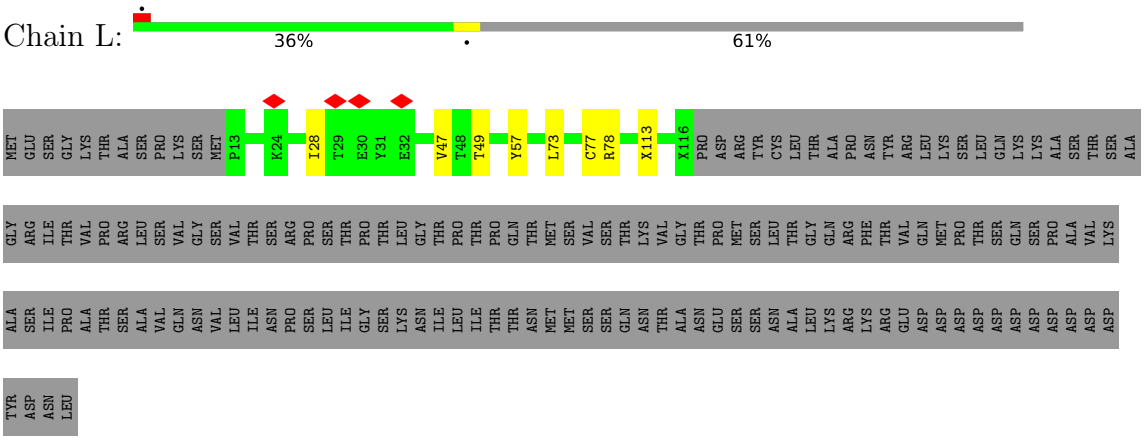
- Molecule 9: Transcription initiation factor TFIID subunit 8,TAF8

Chain K:



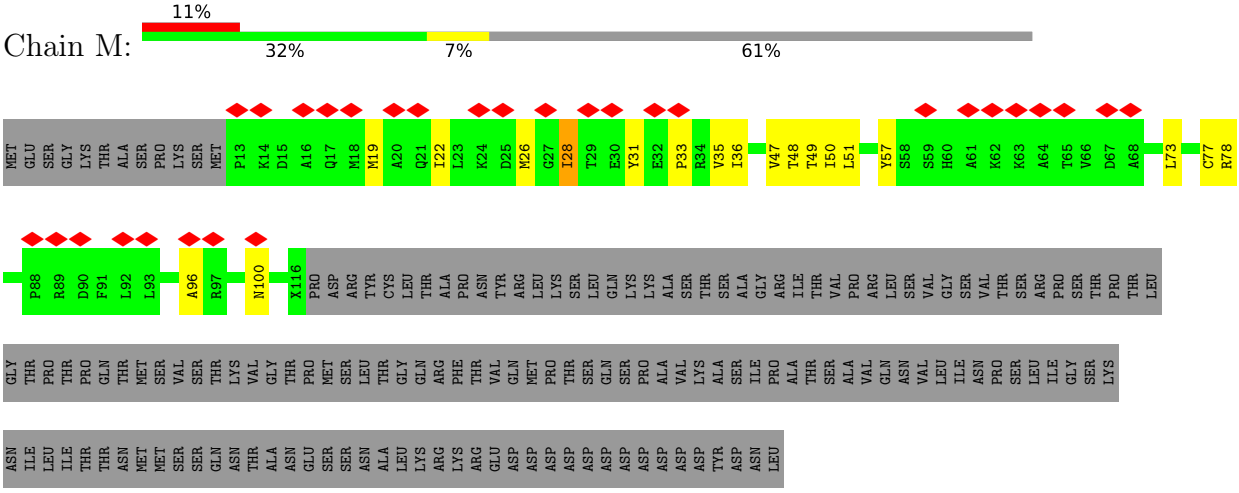
- Molecule 10: Transcription initiation factor TFIID subunit 9, TAF9

Chain L:



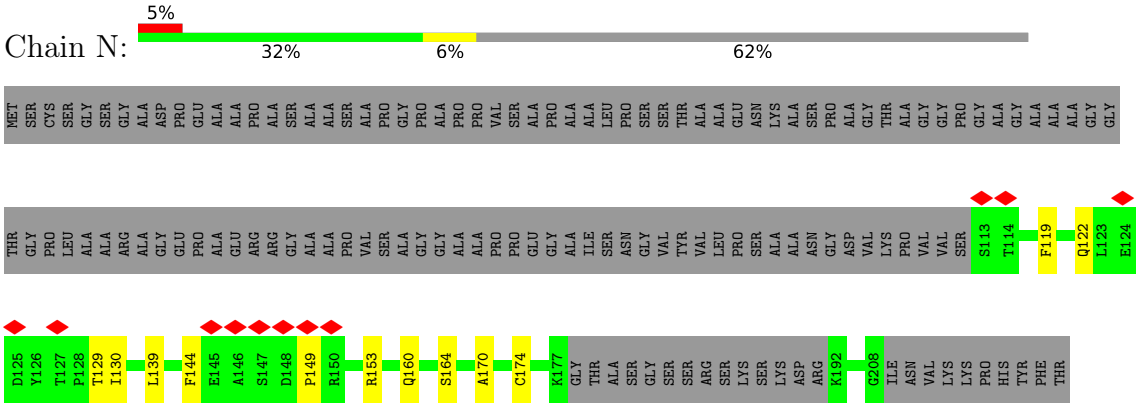
- Molecule 10: Transcription initiation factor TFIID subunit 9, TAF9

Chain M:



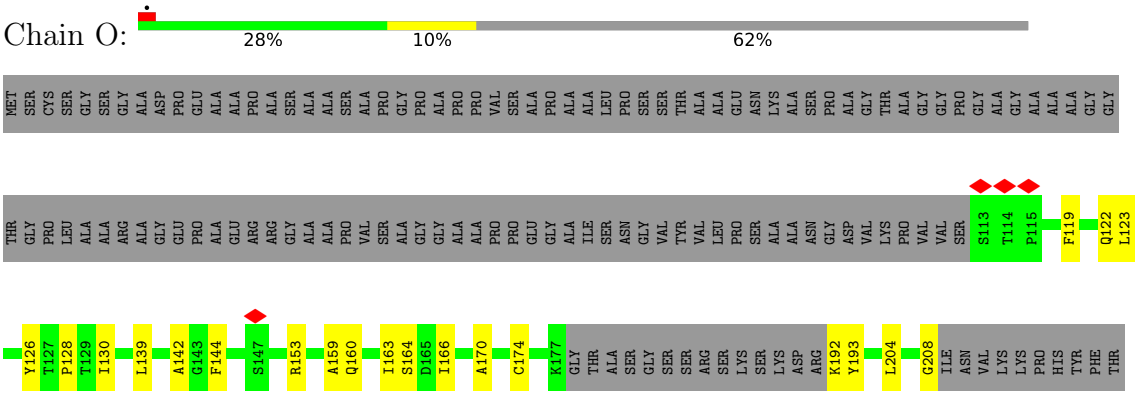
- Molecule 11: Transcription initiation factor TFIID subunit 10

Chain N:



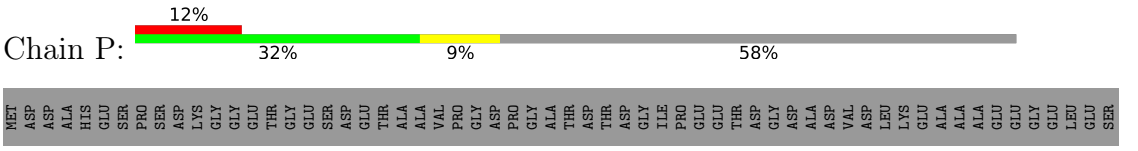
- Molecule 11: Transcription initiation factor TFIID subunit 10

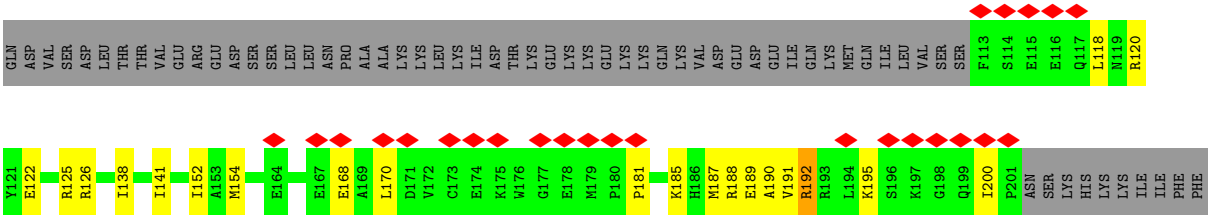
Chain O:



- Molecule 12: Transcription initiation factor TFIID subunit 11

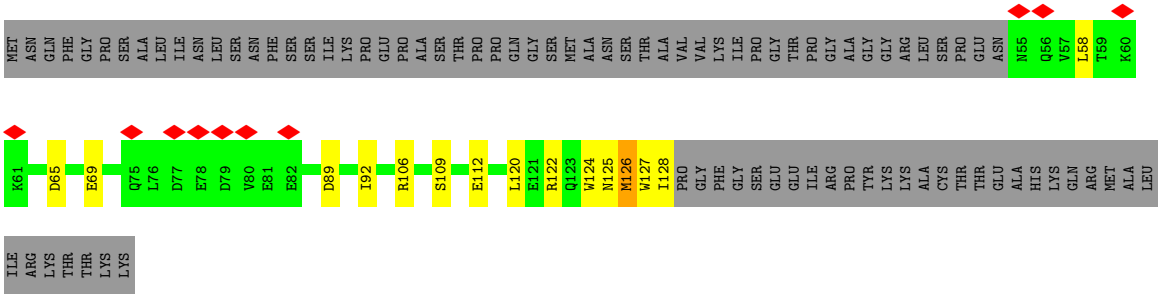
Chain P:





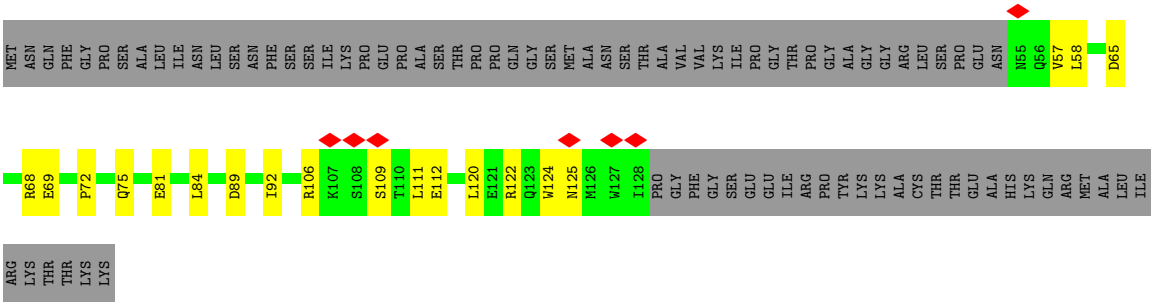
- Molecule 13: Transcription initiation factor TFIID subunit 12

Chain Q:



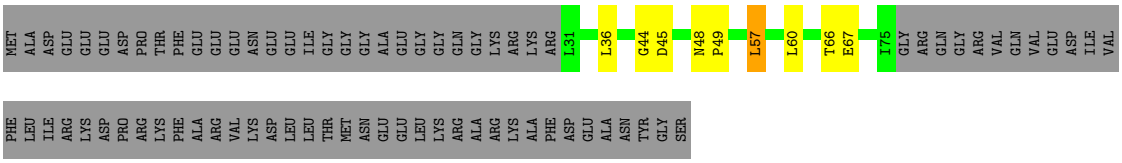
- Molecule 13: Transcription initiation factor TFIID subunit 12

Chain R:



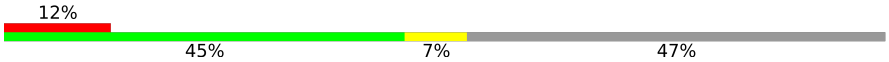
- Molecule 14: Transcription initiation factor TFIID subunit 13

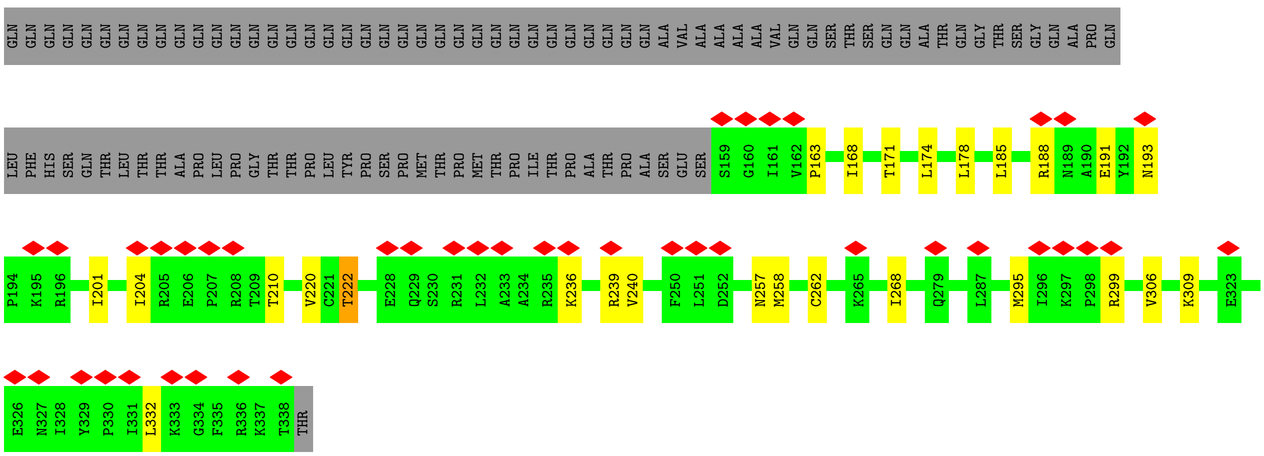
Chain S:



- Molecule 15: TATA-box-binding protein

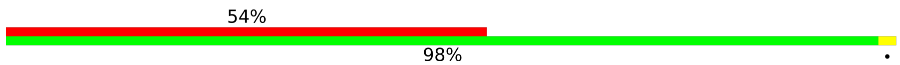
Chain T:

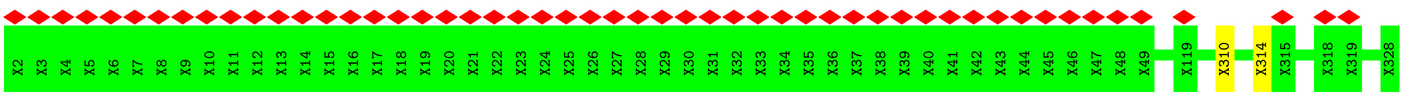




• Molecule 16: poly(UNK)

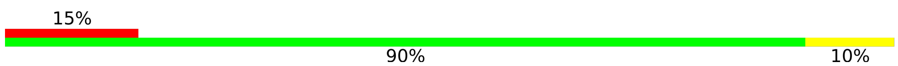
Chain Y:

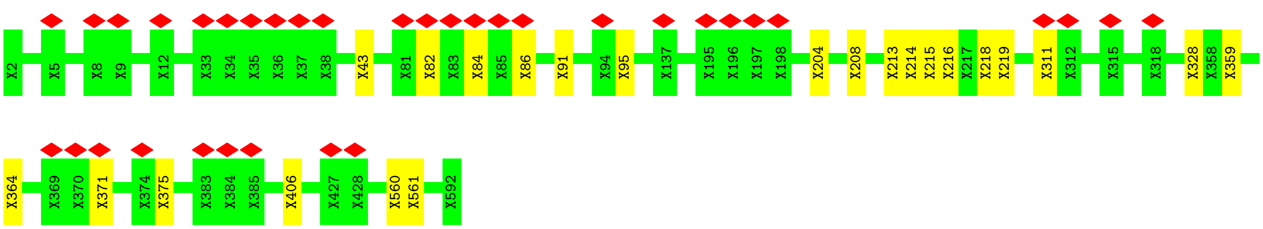




• Molecule 17: poly(UNK)

Chain Z:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	107900	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.065	Depositor
Minimum map value	-0.017	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.026	Depositor
Map size (Å)	380.16, 380.16, 380.16	wwPDB
Map dimensions	144, 144, 144	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.64, 2.64, 2.64	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.27	0/3858	0.53	2/5193 (0.0%)
2	B	0.57	2/8029 (0.0%)	0.74	3/10882 (0.0%)
3	C	0.28	0/757	0.52	0/1027
4	D	0.34	0/692	0.61	1/945 (0.1%)
4	E	0.31	0/692	0.50	0/945
5	F	0.27	0/3537	0.58	0/4802
5	G	0.52	0/3537	0.72	2/4802 (0.0%)
6	H	0.46	0/2533	0.66	0/3439
7	I	0.44	0/2506	0.64	0/3402
8	J	0.26	0/1017	0.53	0/1370
9	K	0.43	0/1212	0.59	0/1640
10	L	0.25	0/705	0.48	0/955
10	M	0.37	0/705	0.59	0/955
11	N	0.27	0/657	0.47	0/891
11	O	0.38	0/657	0.51	0/891
12	P	0.37	0/719	0.72	4/965 (0.4%)
13	Q	0.31	0/618	0.62	1/835 (0.1%)
13	R	0.33	0/618	0.55	0/835
14	S	0.28	0/371	0.52	0/498
15	T	0.31	0/1455	0.55	0/1958
All	All	0.42	2/34875 (0.0%)	0.64	13/47230 (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	1
2	B	0	17
5	F	0	3
5	G	0	8
6	H	0	6

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	I	0	4
9	K	0	2
10	M	0	1
17	Z	0	1
All	All	0	43

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	443	TRP	CB-CG	-7.44	1.36	1.50
2	B	381	TRP	CB-CG	-5.07	1.41	1.50

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	220	LEU	CA-CB-CG	7.67	132.93	115.30
12	P	192	ARG	CG-CD-NE	6.62	125.71	111.80
2	B	927	LEU	CA-CB-CG	-6.32	100.76	115.30
1	A	69	LEU	CA-CB-CG	6.27	129.72	115.30
5	G	726	LEU	CB-CG-CD2	-6.05	100.72	111.00

There are no chirality outliers.

5 of 43 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	949	GLU	Peptide
2	B	193	VAL	Peptide
2	B	259	ASP	Peptide
2	B	316	VAL	Peptide
2	B	325	PHE	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	3772	0	3742	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	7832	0	7789	217	0
3	C	742	0	719	8	0
4	D	686	0	572	8	0
4	E	686	0	572	13	0
5	F	3646	0	3312	48	0
5	G	3646	0	3312	95	0
6	H	2494	0	2474	58	0
7	I	2520	0	2422	61	0
8	J	998	0	1055	12	0
9	K	1449	0	1281	33	0
10	L	732	0	624	6	0
10	M	732	0	623	13	0
11	N	645	0	640	7	0
11	O	645	0	640	15	0
12	P	707	0	730	24	0
13	Q	611	0	610	16	0
13	R	611	0	610	16	0
14	S	365	0	351	10	0
15	T	1429	0	1521	18	0
16	Y	480	0	112	1	0
17	Z	1190	0	280	16	0
All	All	36618	0	33991	655	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 9.

The worst 5 of 655 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)
1:A:874:GLU:HG2	2:B:468:PHE:HZ	1.27	0.99
2:B:566:VAL:O	2:B:577:HIS:HA	1.64	0.97
2:B:532:TYR:O	2:B:551:ASP:HB2	1.67	0.94
2:B:50:GLU:HA	2:B:146:ILE:O	1.70	0.92
1:A:874:GLU:HG2	2:B:468:PHE:CZ	2.04	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	A	462/1872 (25%)	454 (98%)	7 (2%)	1 (0%)	47	81
2	B	966/1199 (81%)	781 (81%)	183 (19%)	2 (0%)	47	81
3	C	91/929 (10%)	89 (98%)	2 (2%)	0	100	100
4	D	100/1085 (9%)	93 (93%)	7 (7%)	0	100	100
4	E	100/1085 (9%)	94 (94%)	6 (6%)	0	100	100
5	F	429/800 (54%)	382 (89%)	47 (11%)	0	100	100
5	G	429/800 (54%)	352 (82%)	77 (18%)	0	100	100
6	H	325/677 (48%)	293 (90%)	31 (10%)	1 (0%)	41	77
7	I	326/677 (48%)	292 (90%)	32 (10%)	2 (1%)	25	66
8	J	119/349 (34%)	117 (98%)	2 (2%)	0	100	100
9	K	149/310 (48%)	133 (89%)	15 (10%)	1 (1%)	22	63
10	L	96/264 (36%)	93 (97%)	3 (3%)	0	100	100
10	M	96/264 (36%)	89 (93%)	7 (7%)	0	100	100
11	N	78/218 (36%)	75 (96%)	3 (4%)	0	100	100
11	O	78/218 (36%)	74 (95%)	4 (5%)	0	100	100
12	P	87/211 (41%)	86 (99%)	1 (1%)	0	100	100
13	Q	72/161 (45%)	71 (99%)	1 (1%)	0	100	100
13	R	72/161 (45%)	68 (94%)	4 (6%)	0	100	100
14	S	43/124 (35%)	43 (100%)	0	0	100	100
15	T	178/339 (52%)	177 (99%)	1 (1%)	0	100	100
All	All	4296/11743 (37%)	3856 (90%)	433 (10%)	7 (0%)	50	81

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	950	VAL

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Mol	Chain	Res	Type
7	I	256	LEU
6	H	321	PRO
7	I	257	PRO
9	K	218	PRO

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	407/1665 (24%)	403 (99%)	4 (1%)	76	86
2	B	879/1083 (81%)	872 (99%)	7 (1%)	81	89
3	C	83/833 (10%)	83 (100%)	0	100	100
4	D	52/815 (6%)	51 (98%)	1 (2%)	57	75
4	E	52/815 (6%)	52 (100%)	0	100	100
5	F	367/619 (59%)	365 (100%)	2 (0%)	88	93
5	G	367/619 (59%)	362 (99%)	5 (1%)	67	80
6	H	260/574 (45%)	259 (100%)	1 (0%)	91	94
7	I	252/564 (45%)	251 (100%)	1 (0%)	91	94
8	J	113/322 (35%)	113 (100%)	0	100	100
9	K	132/223 (59%)	132 (100%)	0	100	100
10	L	61/229 (27%)	60 (98%)	1 (2%)	62	79
10	M	61/229 (27%)	60 (98%)	1 (2%)	62	79
11	N	71/154 (46%)	71 (100%)	0	100	100
11	O	71/154 (46%)	71 (100%)	0	100	100
12	P	78/182 (43%)	78 (100%)	0	100	100
13	Q	70/141 (50%)	69 (99%)	1 (1%)	67	80
13	R	70/141 (50%)	69 (99%)	1 (1%)	67	80
14	S	42/106 (40%)	40 (95%)	2 (5%)	25	51
15	T	155/293 (53%)	153 (99%)	2 (1%)	69	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3643/9761 (37%)	3614 (99%)	29 (1%)	82 89

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	G	558	LEU
15	T	193	ASN
5	G	607	ARG
13	R	125	ASN
5	G	589	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 67 such sidechains are listed below:

Mol	Chain	Res	Type
11	N	122	GLN
11	O	122	GLN
15	T	193	ASN
2	B	924	HIS
2	B	912	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)

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
17	Z	8
16	Y	2

The worst 5 of 10 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Z	95:UNK	C	119:UNK	N	129.81
1	Z	52:UNK	C	81:UNK	N	116.40
1	Z	143:UNK	C	195:UNK	N	95.92
1	Z	223:UNK	C	309:UNK	N	54.56
1	Y	143:UNK	C	309:UNK	N	54.12

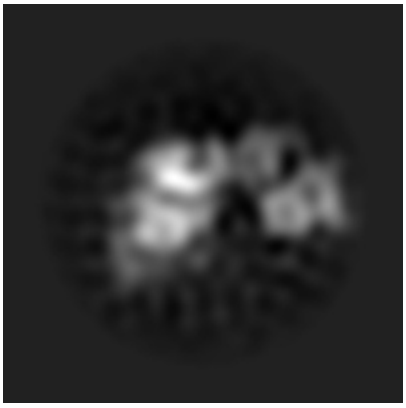
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-9305. These allow visual inspection of the internal detail of the map and identification of artifacts.

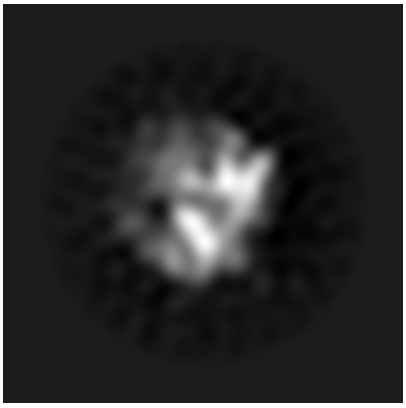
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

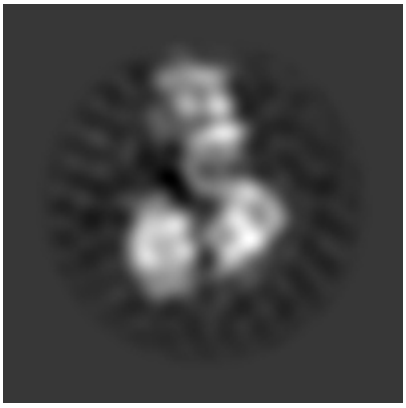
6.1.1 Primary map



X



Y



Z

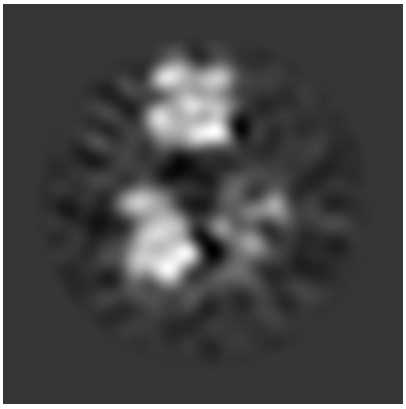
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map

X Index: 72

Y Index: 72

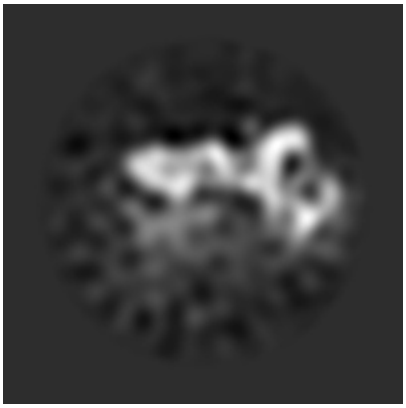


Z Index: 72

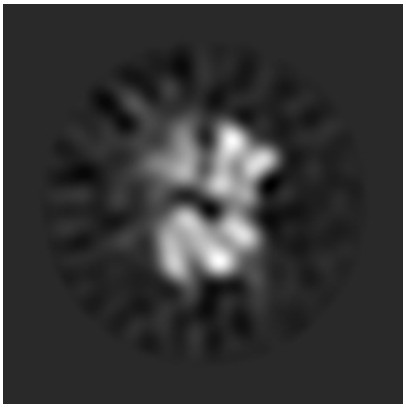
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 79



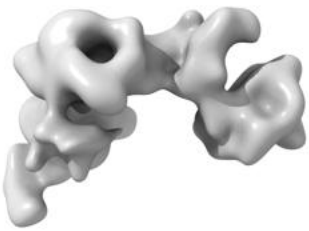
Y Index: 62

Z Index: 80

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

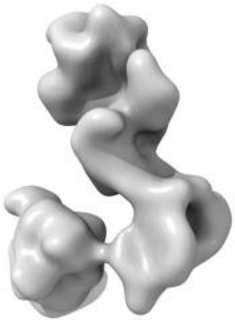
6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.026. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

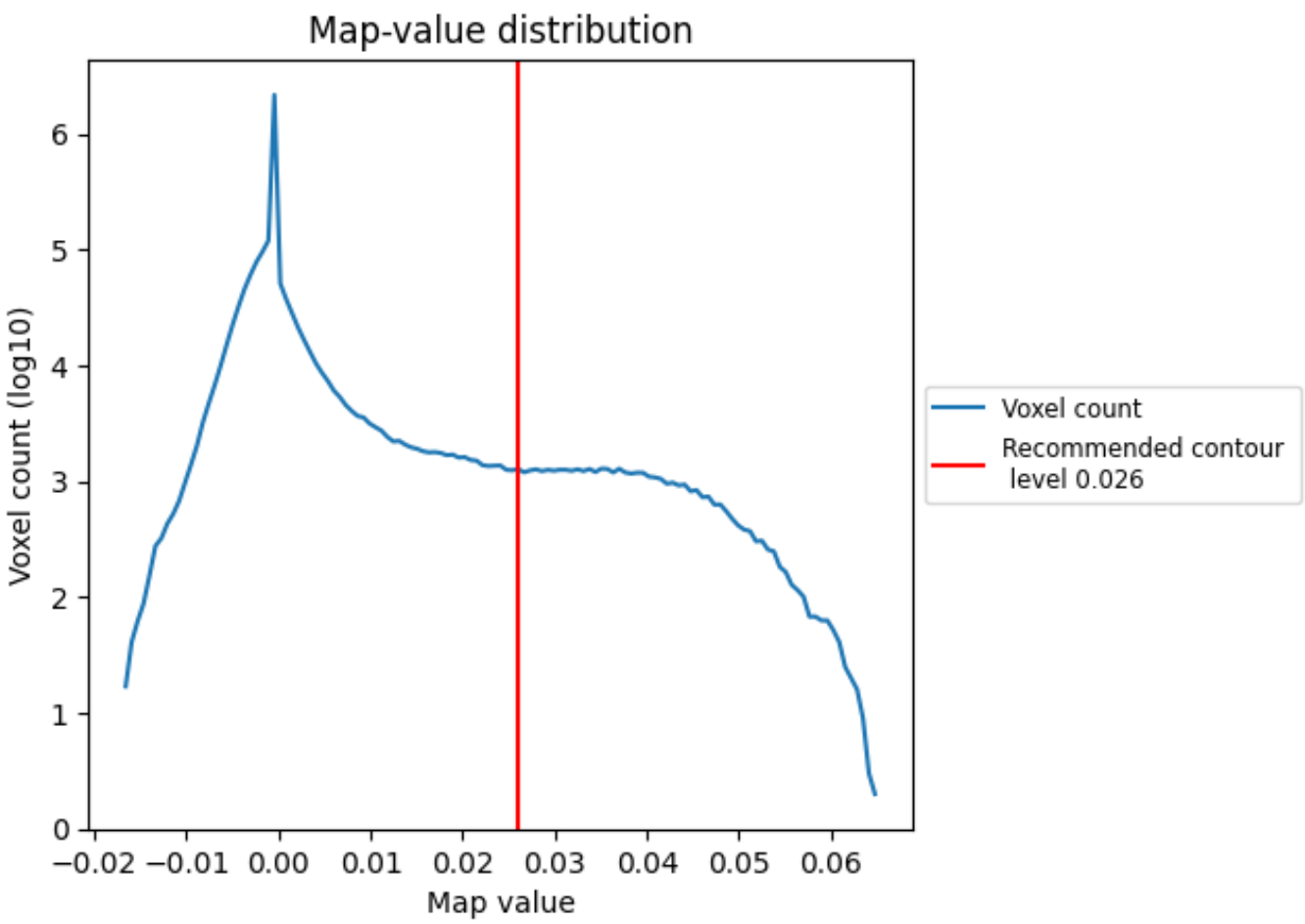
6.5 Mask visualisation (i)

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

7 Map analysis (i)

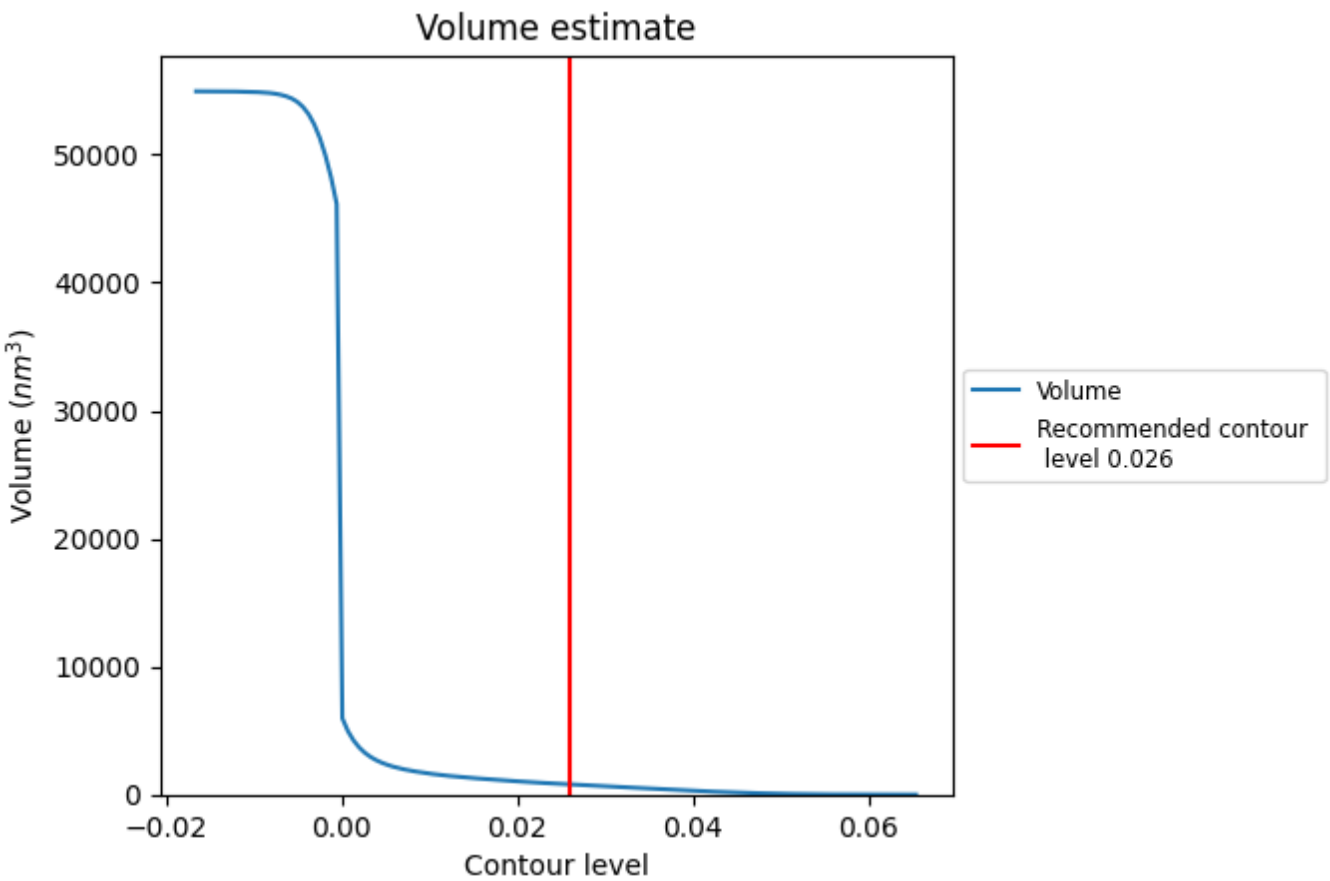
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

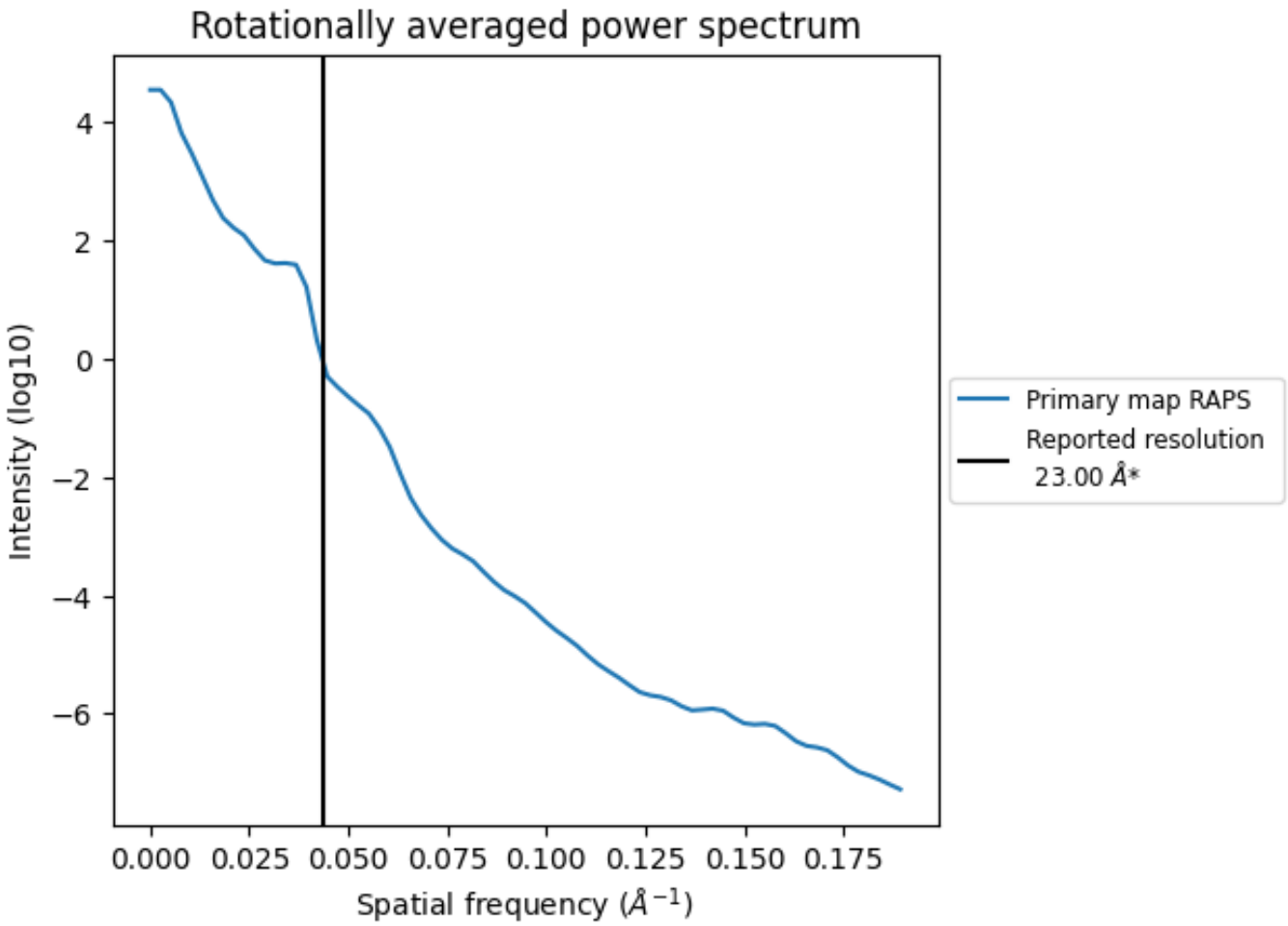
7.2 Volume estimate (i)



The volume at the recommended contour level is 794 nm^3; this corresponds to an approximate mass of 717 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 0.043 Å^{-1}

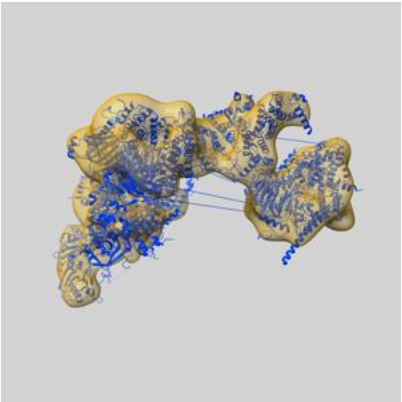
8 Fourier-Shell correlation (i)

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

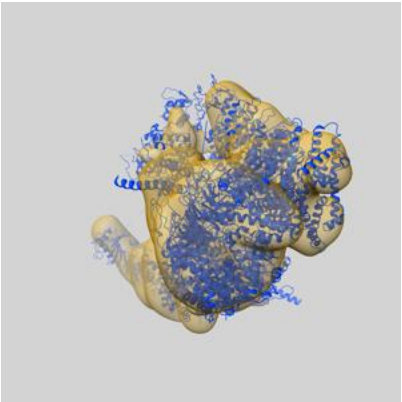
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-9305 and PDB model 6MZL. Per-residue inclusion information can be found in section 3 on page 7.

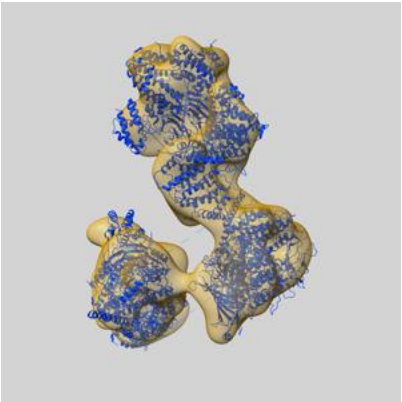
9.1 Map-model overlay (i)



X



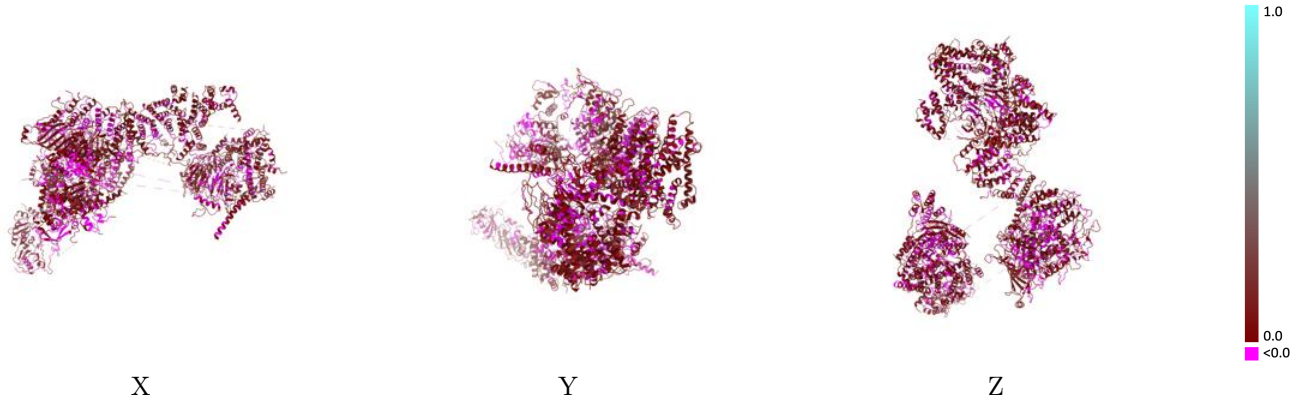
Y



Z

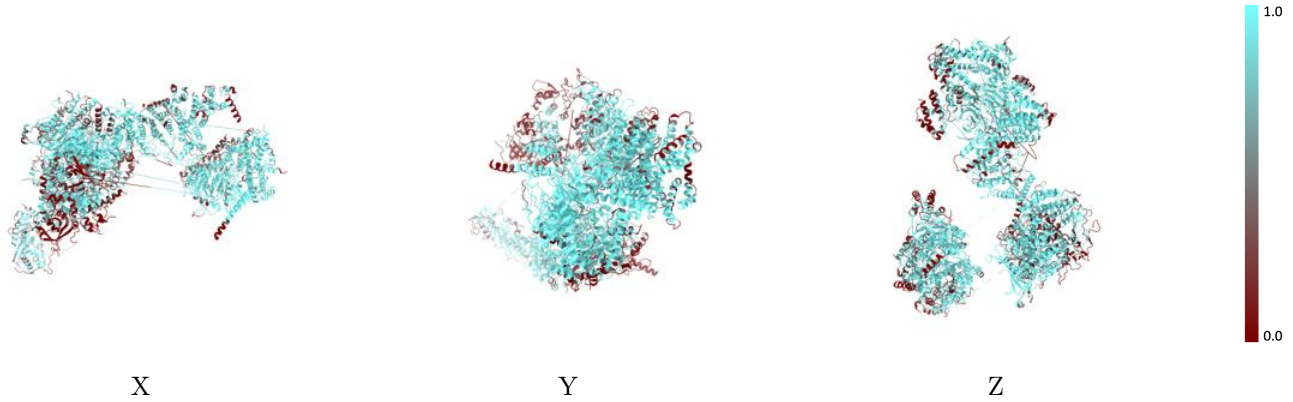
The images above show the 3D surface view of the map at the recommended contour level 0.026 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



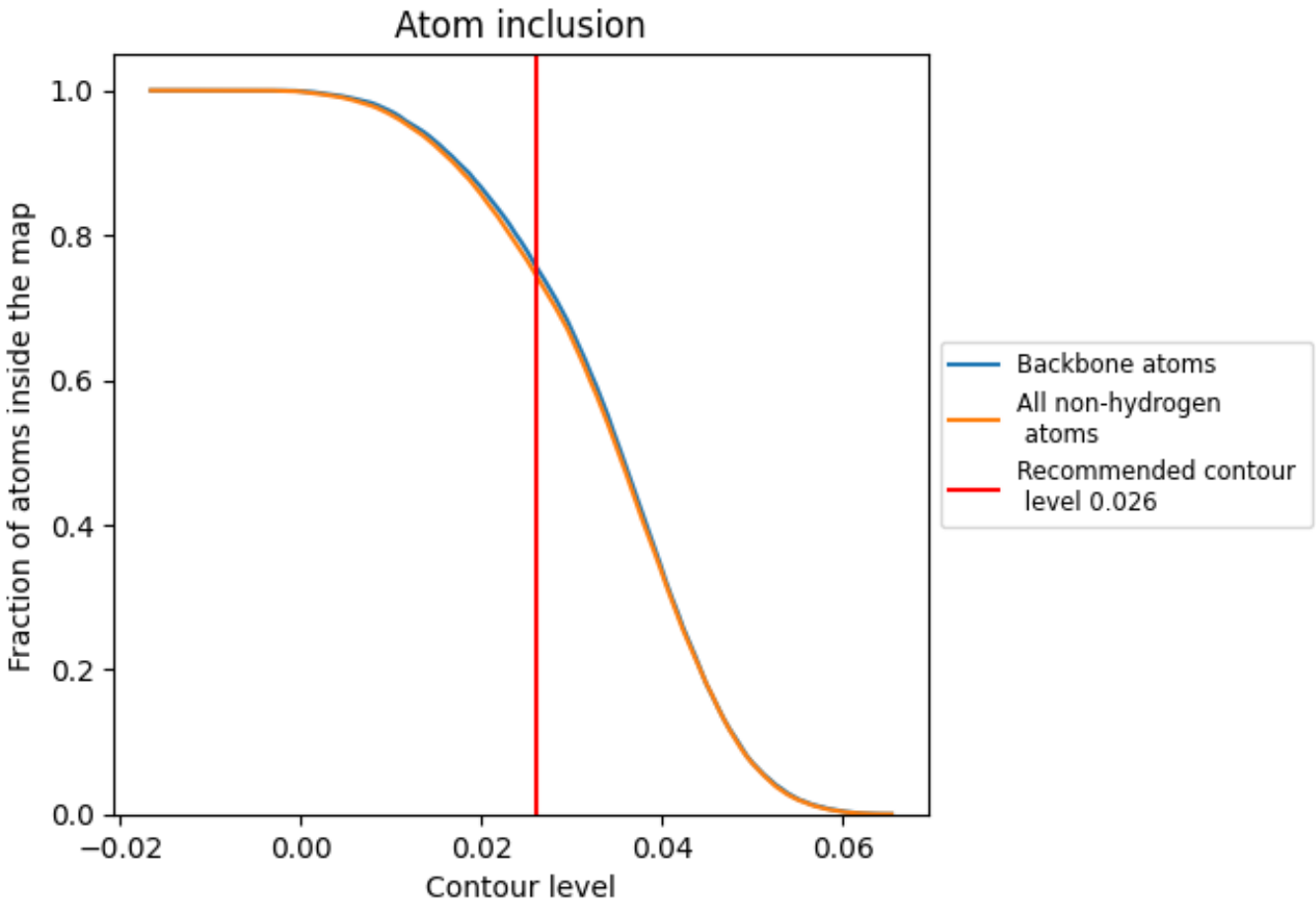
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.026).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.026) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7460	0.0510
A	0.4127	0.0390
B	0.7835	0.0480
C	0.9420	0.0820
D	0.6922	0.0730
E	0.7923	0.0700
F	0.7465	0.0340
G	0.8162	0.0530
H	0.8452	0.0500
I	0.8021	0.0650
J	0.2058	0.0100
K	0.9386	0.0760
L	0.9362	0.0420
M	0.7171	0.0580
N	0.8628	0.0590
O	0.9432	0.0750
P	0.6942	0.0320
Q	0.8170	0.0450
R	0.8403	0.0710
S	0.9668	0.0990
T	0.7176	0.0690
Y	0.4792	0.0320
Z	0.8571	0.0550