wwPDB EM Validation Summary Report

Aug 6, 2026 – 08:40 PM JST

PDB ID	:	8WAP / pdb_00008wap
EMDB ID	:	EMD-37400
Title	:	Structure of transcribing complex 6 (TC6), the initially transcribing complex with Pol II positioned 6nt downstream of TSS.
Authors	:	Chen, X.; Liu, W.; Wang, Q.; Wang, X.; Ren, Y.; Qu, X.; Li, W.; Xu, Y.
Deposited on	:	2023-09-08
Resolution	:	5.85 Å(reported)

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

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

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

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

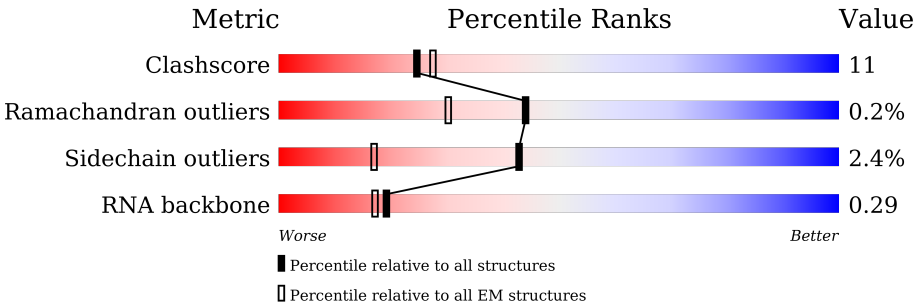
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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

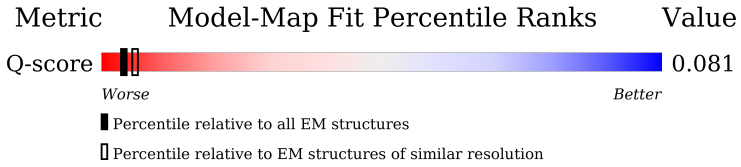
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 5.85 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	480 (5.35 - 6.35)

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	309	50% 38% 16% • 45%
2	1	548	15% 40% 8% 52%
3	2	395	7% 66% 17% 17%

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Mol	Chain	Length	Quality of chain
4	3	308	10% 65% 19% 15%
5	4	462	20% 66% 18% 15%
6	5	71	37% 54% 18% 24%
7	6	782	28% 65% 13% 23%
8	7	760	24% 72% 22% 6%
9	N	8	25% 25% 50%
10	Z	6	33% 50% 17%
11	A	1872	22% 24% 5% 70%
12	B	1199	5% 69% 11% 20%
13	D	1085	10% 12% 85%
13	d	1085	15% 13% 85%
14	E	800	22% 55% 12% 32%
14	e	800	60% 56% 10% 33%
15	F	677	35% 44% 15% 39%
15	f	677	31% 48% 10% 40%
16	G	349	41% 36% 59%
17	H	310	10% 51% 14% 33%
18	I	264	24% 39% 6% 55%
18	i	264	41% 42% 54%
19	J	218	15% 32% 8% 59%
19	j	218	39% 36% 7% 56%
20	L	161	40% 32% 12% 53%
20	l	161	66% 59% 7% 34%
21	O	109	75% 16% 9%
22	P	339	47% 6% 47%

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Mol	Chain	Length	Quality of chain
23	Q	376	27% 70%
24	R	316	75% 14% 11%
25	S	517	24% 9% 66%
26	T	249	73% 16% 11%
27	U	439	23% 19% 58%
28	V	291	23% 33% 43%
29	X	99	27% 36% 36%
30	Y	99	35% 38% 26%
31	c	929	10% 12% 86%
32	k	211	46% 42% 54%
33	m	124	70% 48% 17% 5% 30%
34	o	1970	57% 17% 26%
35	p	1174	77% 21%
36	q	275	76% 17% 7%
37	r	142	64% 26% 10%
38	s	210	82% 17%
39	t	127	60% 5% 35%
40	u	172	68% 31%
41	v	150	87% 12%
42	w	125	70% 20% 9%
43	x	67	76% 22%
44	y	117	80% 17%
45	z	58	57% 19% 24%

2 Entry composition (i)

There are 49 unique types of molecules in this entry. The entry contains 108642 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 CDK-activating kinase assembly factor MAT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	171	1420	882	249	279	10	0	0

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

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

- Molecule 3 is a protein called General transcription factor IIH subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	329	2567	1621	440	479	27	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	263	2066	1323	344	380	19	0	0

- Molecule 5 is a protein called General transcription factor IIH subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	394	3189	2068	552	557	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	5	54	428	277	67	82	2	0	0

- Molecule 7 is a protein called General transcription and DNA repair factor IIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	605	Total	C	N	O	S	0	0
			4890	3127	848	885	30		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	714	Total	C	N	O	S	0	0
			5751	3683	999	1040	29		

- Molecule 9 is a protein called Alpha-amanitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	N	8	Total	C	N	O	S	0	0
			64	39	10	14	1		

- Molecule 10 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Z	6	Total	C	N	O	P	0	0
			139	59	25	47	8		

- Molecule 11 is a protein called Transcription initiation factor TFIID subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	559	Total	C	N	O	S	0	0
			4580	2924	795	834	27		

- Molecule 12 is a protein called Transcription initiation factor TFIID subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	B	963	Total	C	N	O	S	0	0
			7796	5011	1315	1412	58		

- Molecule 13 is a protein called Transcription initiation factor TFIID subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	164	Total	C	N	O	S	0	0
			1366	851	256	255	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	d	158	Total 1307	C 814	N 238	O 252	S 3	0	0

- Molecule 14 is a protein called Transcription initiation factor TFIID subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	E	547	Total 4376	C 2774	N 759	O 822	S 21	0	0
14	e	539	Total 4327	C 2746	N 748	O 814	S 19	0	0

- Molecule 15 is a protein called Transcription initiation factor TFIID subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	F	412	Total 3143	C 1994	N 548	O 583	S 18	0	0
15	f	403	Total 3081	C 1954	N 533	O 576	S 18	0	0

- Molecule 16 is a protein called Transcription initiation factor TFIID subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	G	144	Total 1171	C 742	N 215	O 210	S 4	0	0

- Molecule 17 is a protein called Transcription initiation factor TFIID subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	H	209	Total 1633	C 1034	N 283	O 311	S 5	0	0

- Molecule 18 is a protein called Transcription initiation factor TFIID subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	I	120	Total 959	C 610	N 166	O 177	S 6	0	0
18	i	121	Total 967	C 615	N 167	O 178	S 7	0	0

- Molecule 19 is a protein called Transcription initiation factor TFIID subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	J	90	Total 720	C 466	N 115	O 135	S 4	0	0
19	j	95	Total 759	C 488	N 124	O 143	S 4	0	0

- Molecule 20 is a protein called Transcription initiation factor TFIID subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	76	Total 622	C 388	N 109	O 122	S 3	0	0
20	l	107	Total 876	C 547	N 158	O 166	S 5	0	0

- Molecule 21 is a protein called Transcription initiation factor IIA subunit 2.

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

- Molecule 22 is a protein called TATA-box-binding protein.

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

- Molecule 23 is a protein called Transcription initiation factor IIA beta chain.

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

- Molecule 24 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R	282	Total 2167	C 1353	N 384	O 412	S 18	0	0

- Molecule 25 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	S	176	Total 1461	C 921	N 268	O 268	S 4	0	0

- Molecule 26 is a protein called General transcription factor IIF subunit 2.

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

- Molecule 27 is a protein called General transcription factor IIE subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U	184	Total	C	N	O	S	0	0
			1520	957	272	280	11		

- Molecule 28 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	V	165	Total	C	N	O	S	0	0
			1357	865	235	253	4		

- Molecule 29 is a DNA chain called non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	X	63	Total	C	N	O	P	0	0
			1304	616	248	377	63		

- Molecule 30 is a DNA chain called template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Y	73	Total	C	N	O	P	0	0
			1484	706	266	439	73		

- Molecule 31 is a protein called Transcription initiation factor TFIID subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	c	127	Total	C	N	O	S	0	0
			1011	638	174	193	6		

- Molecule 32 is a protein called Transcription initiation factor TFIID subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	k	98	Total	C	N	O	S	0	0
			785	499	142	139	5		

- Molecule 33 is a protein called Transcription initiation factor TFIID subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	m	87	Total	C	N	O	S	0	0
			724	456	131	131	6		

- Molecule 34 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	o	1452	Total	C	N	O	S	0	0
			11510	7235	2056	2146	73		

- Molecule 35 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	p	1149	Total	C	N	O	S	0	0
			9175	5796	1614	1701	64		

- Molecule 36 is a protein called DNA-directed RNA polymerase II subunit RPB3.

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

- Molecule 37 is a protein called DNA-directed RNA polymerase II subunit RPB4.

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

- Molecule 38 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	s	209	Total	C	N	O	S	0	0
			1720	1089	300	323	8		

- Molecule 39 is a protein called DNA-directed RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	t	82	Total	C	N	O	S	0	0
			657	418	113	121	5		

- Molecule 40 is a protein called DNA-directed RNA polymerase II subunit RPB7.

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

- Molecule 41 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 42 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	w	114	Total	C	N	O	S	0	0
			927	571	166	179	11		

- Molecule 43 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	x	67	Total	C	N	O	S	0	0
			533	345	90	92	6		

- Molecule 44 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

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

- Molecule 45 is a protein called RPB12.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	z	44	Total	C	N	O	S	0	0
			372	231	72	63	6		

- Molecule 46 is ZINC ION (CCD ID: ZN) (formula: Zn).

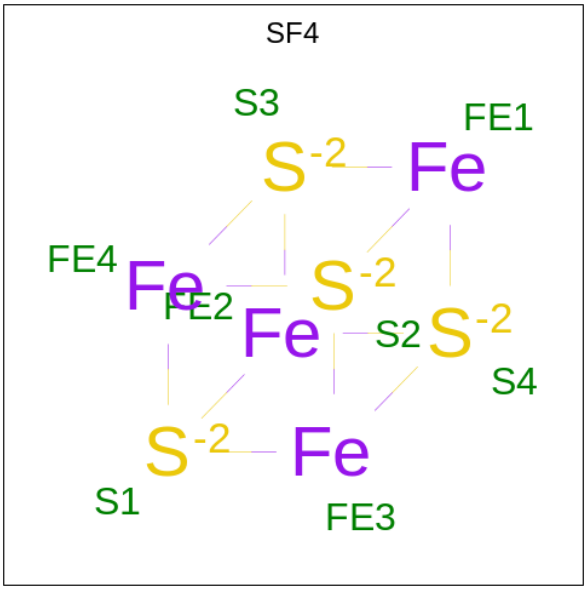
Mol	Chain	Residues	Atoms		AltConf
46	0	2	Total	Zn	0
			2	2	
46	2	3	Total	Zn	0
			3	3	
46	3	2	Total	Zn	0
			2	2	

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Mol	Chain	Residues	Atoms	AltConf
46	R	1	Total Zn 1 1	0
46	U	1	Total Zn 1 1	0
46	o	2	Total Zn 2 2	0
46	p	1	Total Zn 1 1	0
46	q	1	Total Zn 1 1	0
46	w	2	Total Zn 2 2	0
46	x	1	Total Zn 1 1	0
46	z	1	Total Zn 1 1	0

- Molecule 47 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).

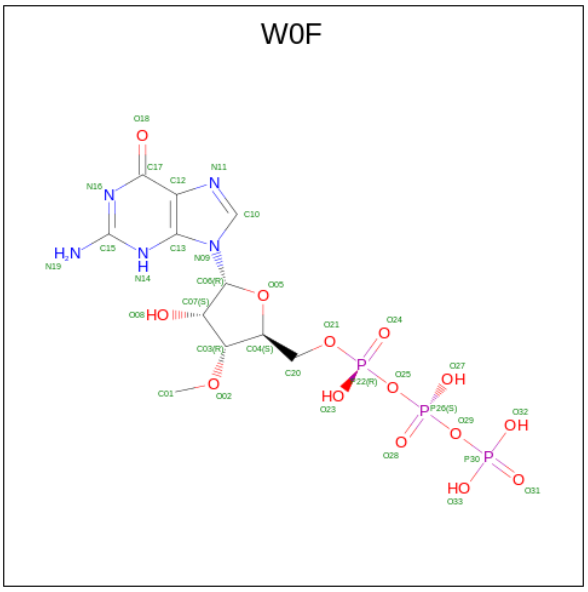


Mol	Chain	Residues	Atoms	AltConf
47	7	1	Total Fe S 8 4 4	0

- Molecule 48 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
48	o	1	Total	Mg	0
			1	1	

- Molecule 49 is [[(2 {S},3 {R},4 {S},5 {R})-5-(2-azanyl-6-oxidanylidene-3 {H}-purin-9-yl)-3-methoxy-4-oxidanyl-oxolan-2-yl]methoxy-oxidanyl-phosphoryl] phosphono hydrogen phosphate (CCD ID: W0F) (formula: $C_{11}H_{18}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).

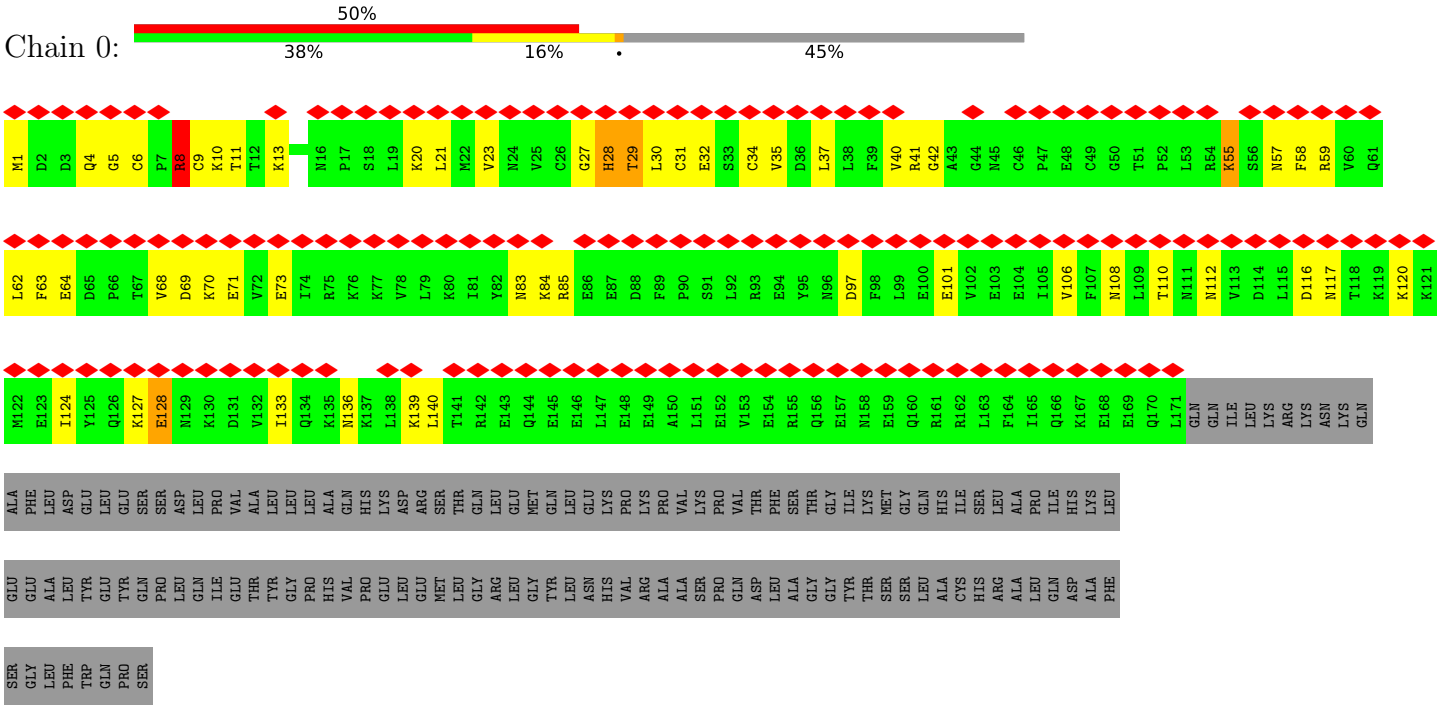


Mol	Chain	Residues	Atoms					AltConf
49	p	1	Total	C	N	O	P	0
			33	11	5	14	3	

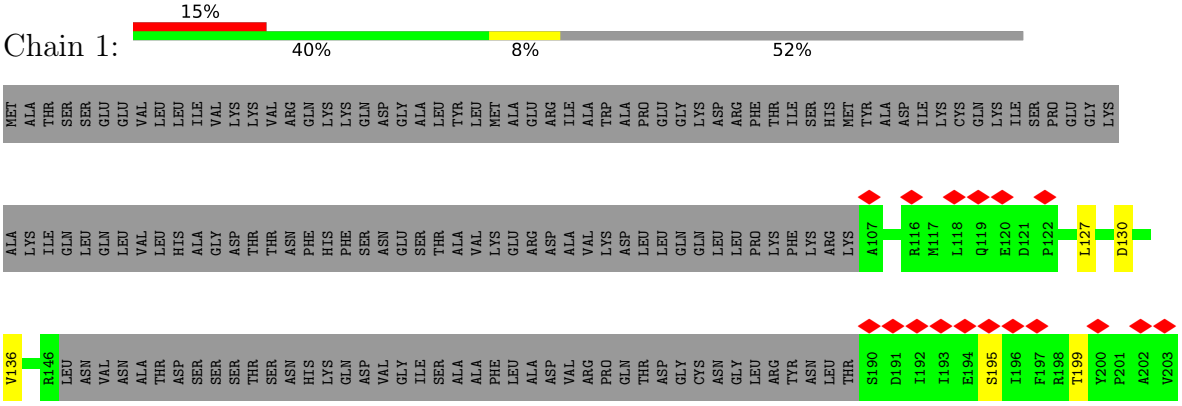
3 Residue-property plots (i)

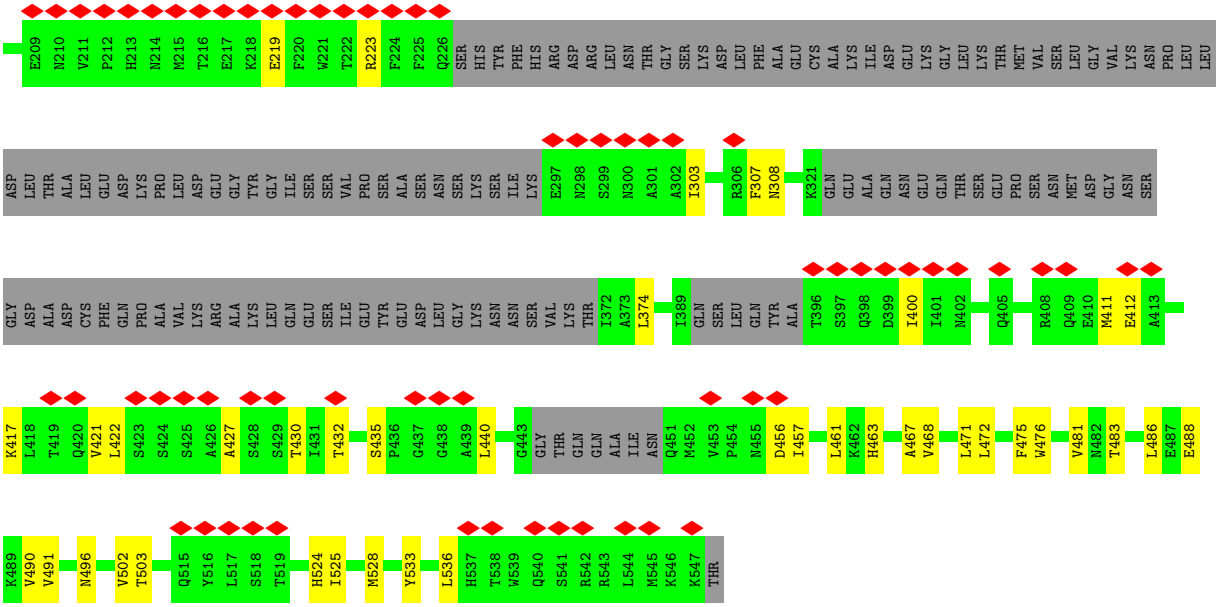
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: CDK-activating kinase assembly factor MAT1



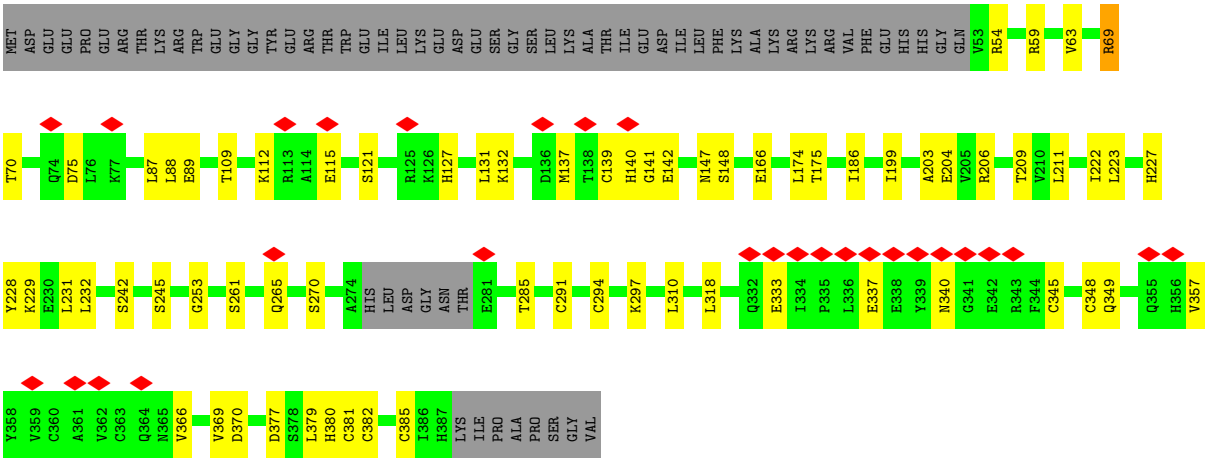
• Molecule 2: General transcription factor IIH subunit 1





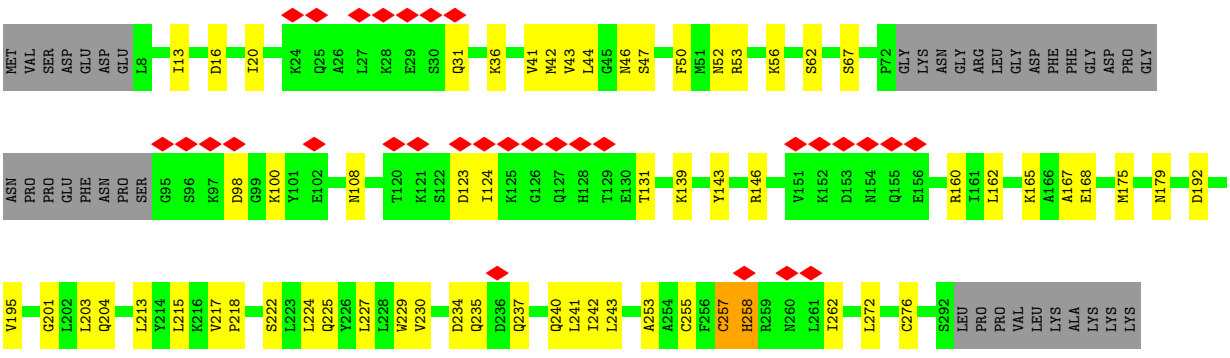
• Molecule 3: General transcription factor IIH subunit 2





• Molecule 4: General transcription factor IIH subunit 3



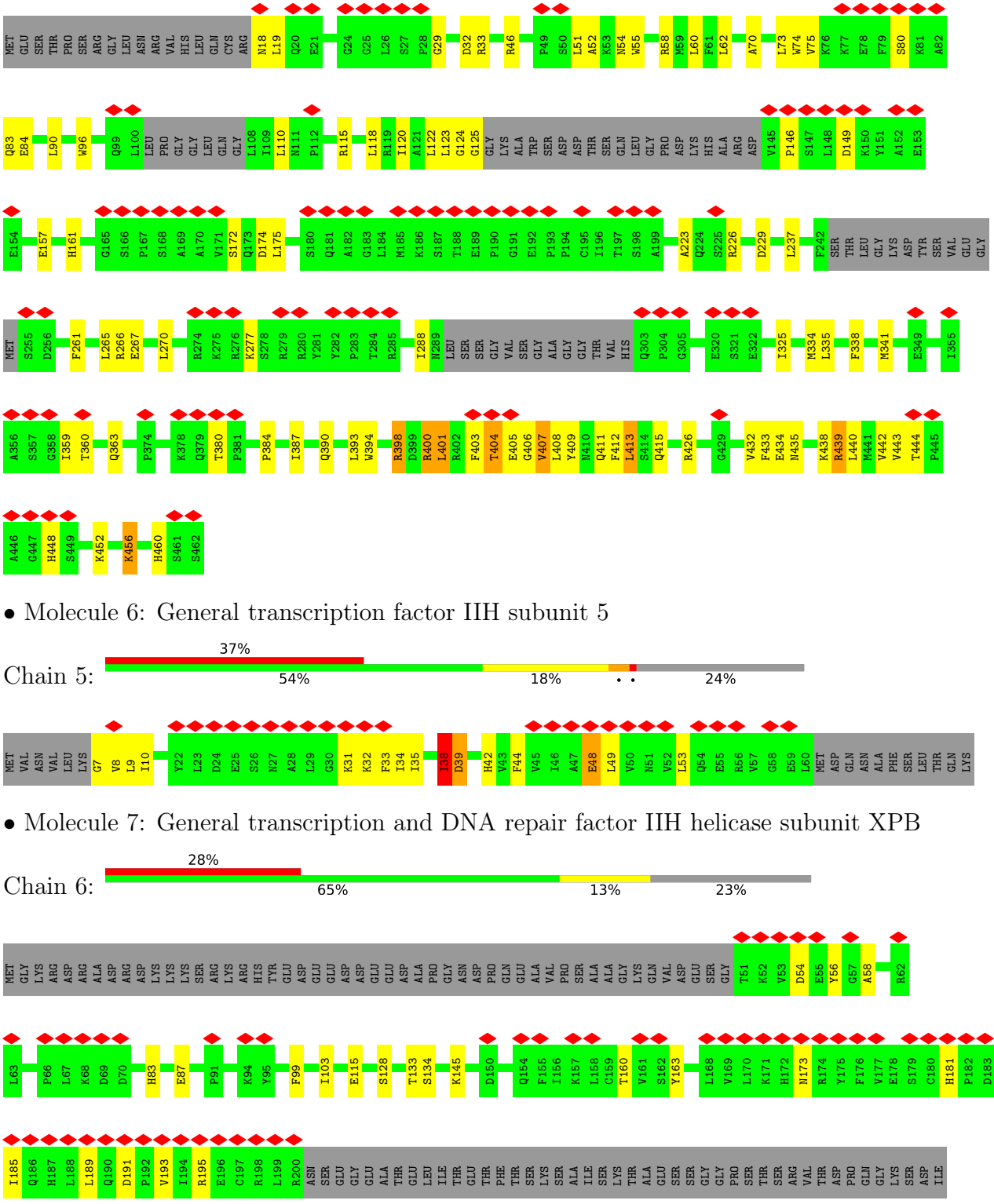




• Molecule 5: General transcription factor IIH subunit 4

Chain 4:



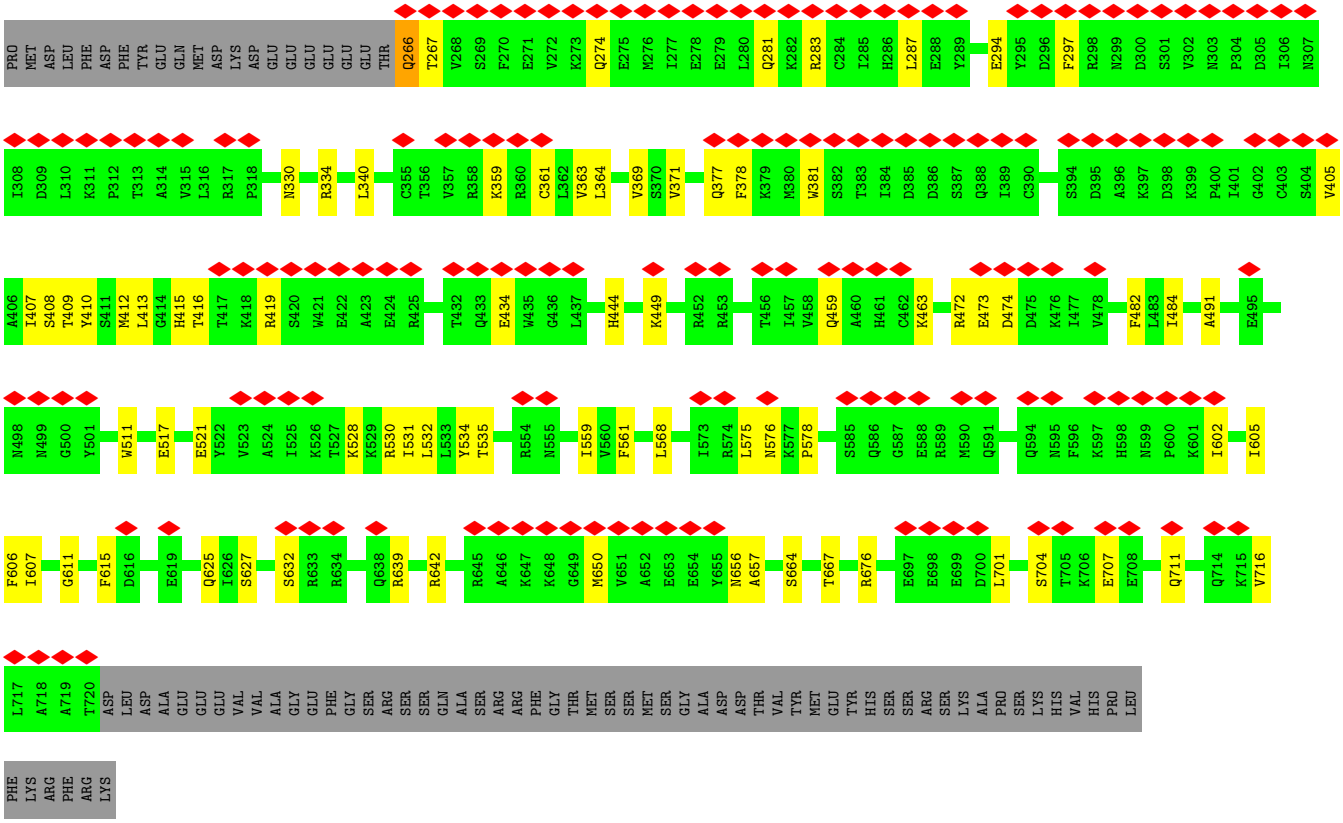


• Molecule 6: General transcription factor IIH subunit 5

Chain 5:

• Molecule 7: General transcription and DNA repair factor IIH helicase subunit XPB

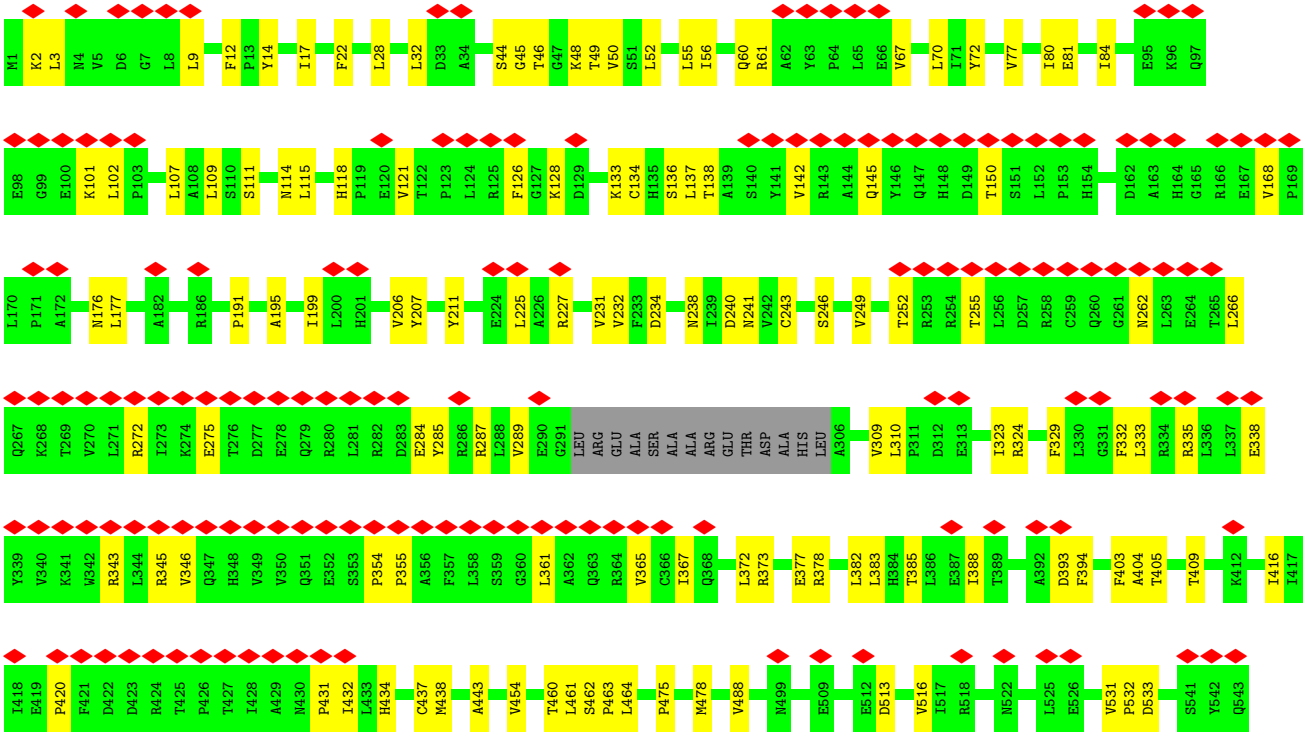
Chain 6:

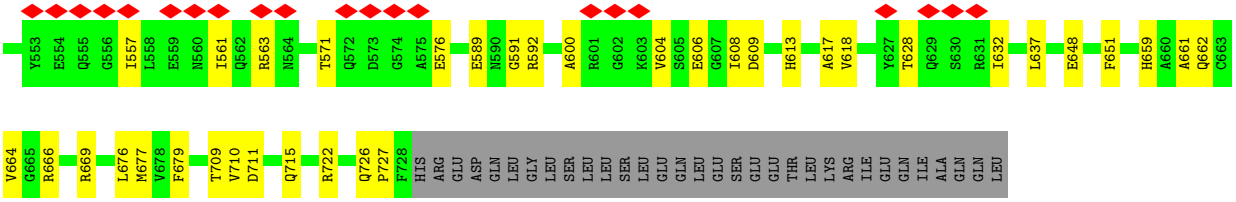


• Molecule 8: General transcription and DNA repair factor IIH helicase subunit XPD

Chain 7:







• Molecule 9: Alpha-amanitin

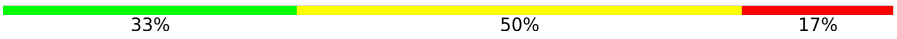
Chain N:

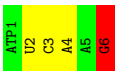




• Molecule 10: RNA

Chain Z:

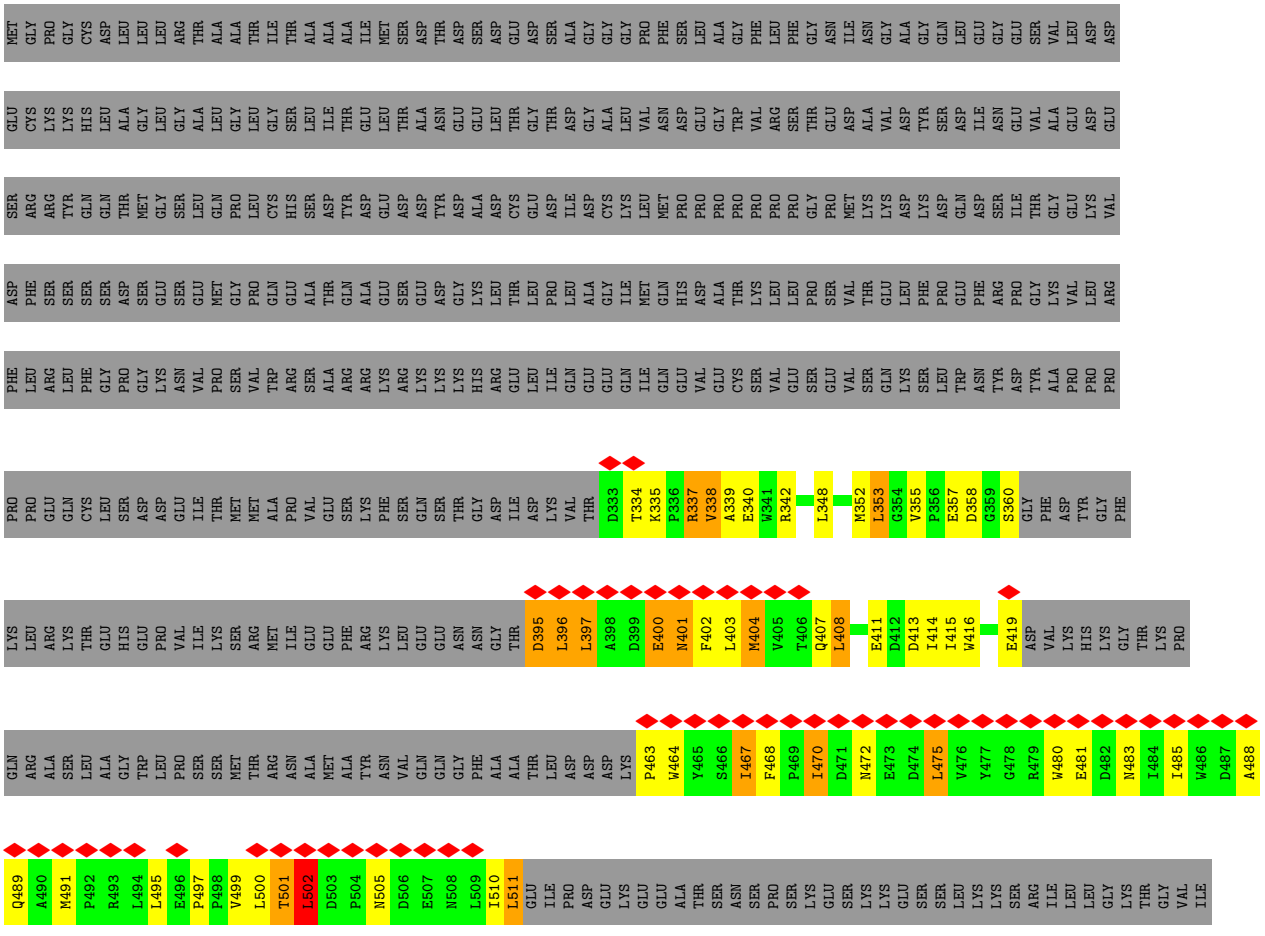


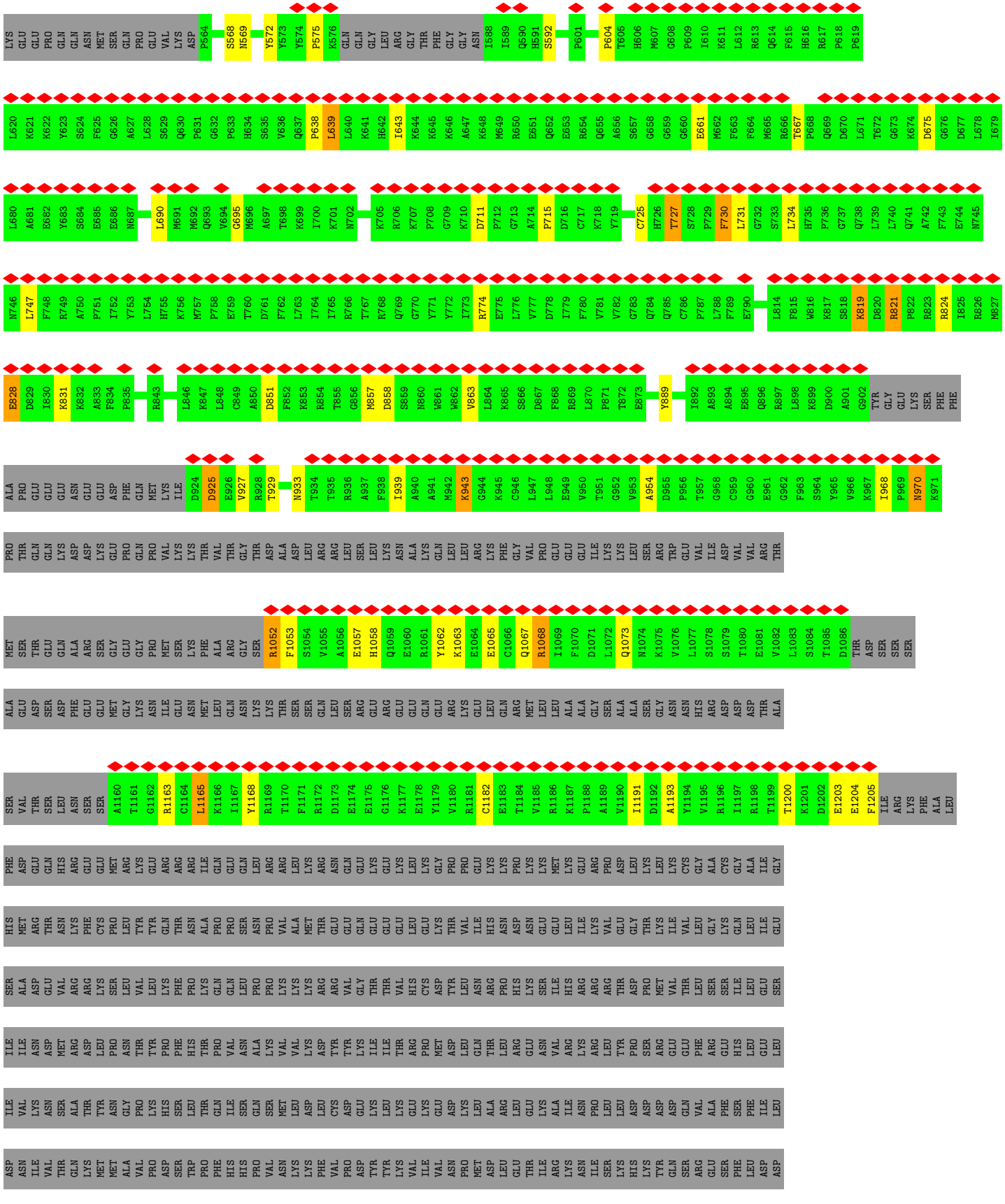


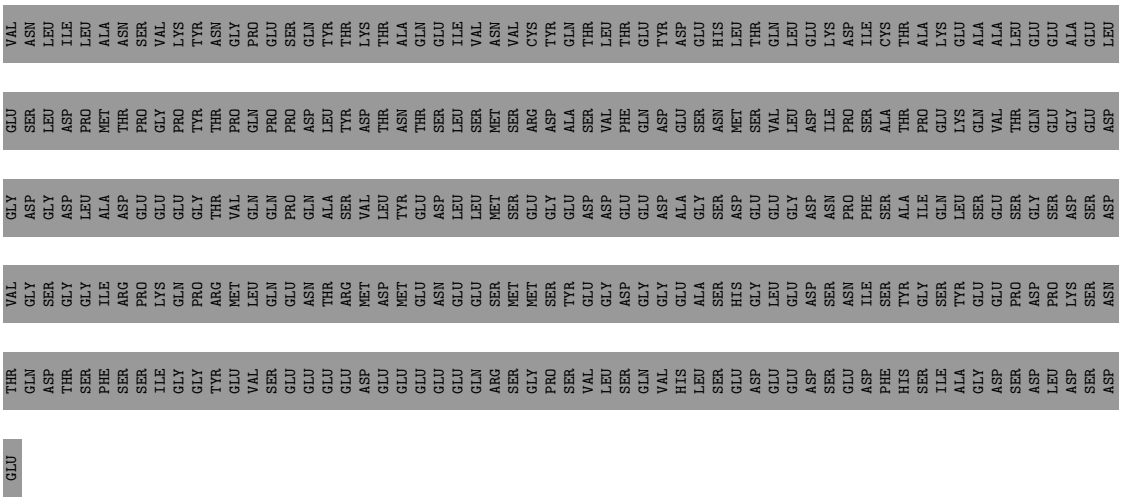
• Molecule 11: Transcription initiation factor TFIID subunit 1

Chain A:





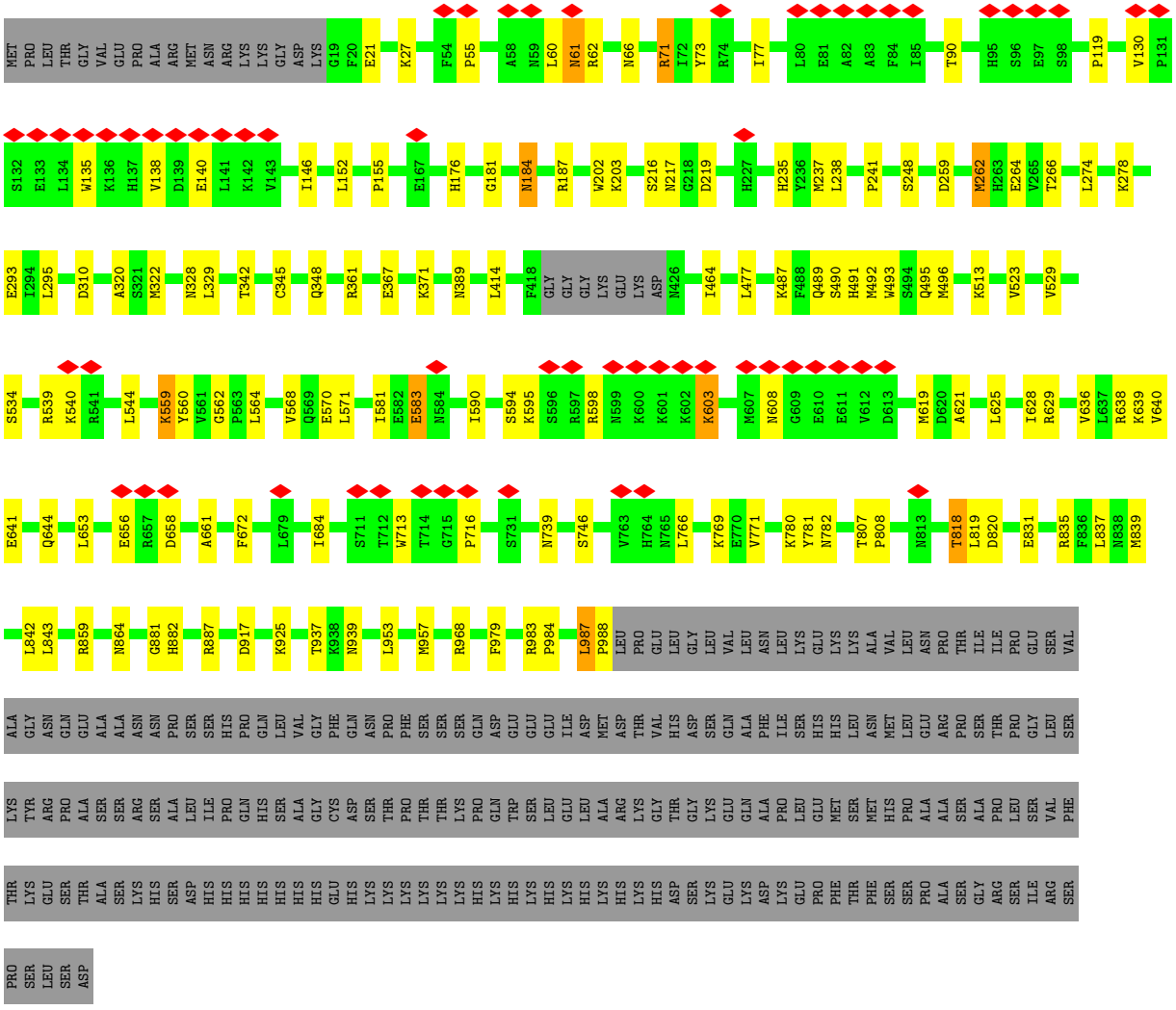

LYS GLU GLU PRO GLN GLN ASN MET SER GLN PRO GLU VAL LYS ASP P564 S568 N569 Y572 Y573 Y574 P575 K576 GLN GLN GLY LEU ARG GLY THR PHE GLY GLY ASN I588 I589 Q590 H591 S592 P601 P604 T605 H606 M607 G608 P609 I610 K611 L612 R613 Q614 F615 H616 R617 P618 P619
L620 K621 K622 Y623 S624 F625 G626 A627 L628 S629 Q630 P631 G632 P633 H634 S635 V636 Q637 P638 L639 L640 K641 H642 I643 K644 K645 K646 A647 K648 M649 R650 E651 Q652 E653 R654 Q655 A656 S657 G658 G659 G660 E661 M662 F663 F664 M665 R666 T667 F668 Q669 D670 L671 T672 G673 K674 D675 G676 D677 L678 I679
L680 A681 E682 Y683 S684 E685 E686 N687 L690 M691 M692 Q693 V694 G695 M696 A697 T698 K699 I700 K701 N702 K705 R706 K707 P708 G709 K710 D711 P712 G713 A714 P715 D716 C717 K718 Y719 G725 H726 T727 S728 P729 F730 L731 G732 S733 L734 H735 P736 G737 Q738 L739 L740 Q741 A742 F743 E744 N745
N746 L747 F748 R749 A750 P751 I752 Y753 L754 H755 K756 M757 P758 E759 T760 D761 F762 L763 I764 I765 R766 T767 R768 Q769 G770 Y771 Y772 I773 R774 E775 L776 V777 D778 I779 F780 V781 V782 G783 Q784 Q785 C786 P787 L788 F789 E790 L814 F815 W816 K817 S818 K819 D820 R821 P822 R823 R824 I825 R826 M827
E828 D829 I830 K831 K832 A833 F834 P835 R843 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 Y889 I892 A893 A894 E895 Q896 R897 L898 K899 D900 A901 G902 TYR GLY GLU LYS SER PHE PHE
ALA PRO GLU GLU GLU ASN GLU GLU ASP PHE GLN MET LYS ILE D924 D925 E926 V927 R928 T929 N933 T934 T935 R936 A937 F938 I939 A940 A941 N942 K943 G944 K945 C946 L947 L948 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 R1052 F1053 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 S1084 T1085 D1086 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 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 THR ALA
SER VAL THR SER LEU ASN SER SER A1160 T1161 G1162 R1163 C1164 L1165 K1166 I1167 Y1168 R1169 T1170 F1171 R1172 D1173 E1174 E1175 G1176 K1177 E1178 Y1179 V1180 R1181 C1182 E1183 T1184 V1185 R1186 K1187 P1188 A1189 V1190 I1191 D1192 A1193 Y1194 V1195 R1196 I1197 R1198 T1199 T1200 K1201 D1202 E1203 E1204 F1205 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 LEU ARG ARG LEU LYS ARG ASN GLN GLU LYS GLU LYS LEU LYS GLY PRO PRO GLU LYS LYS PRO LYS LYS MET LYS GLU ASP 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 SER ASN PRO VAL ALA MET THR GLU GLN GLU GLU LEU GLU 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 LEU LYS PHE PRO LYS GLN GLN LEU PRO PRO PRO LYS LYS LYS ARG ARG VAL GLY THR THR VAL HIS CYS ASP TYR 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 GLU GLU ASN VAL ARG LYS ARG LEU TYR PRO SER ARG GLU GLU PHE ARG GLU HIS LEU GLU LEU
ILE VAL 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 GLU LYS ALA ILE ASN PRO LEU LEU ASP ASP ASP GLN VAL ALA PHE SER PHE ILE LEU
ASP ASN ILE VAL THR GLN LYS MET MET ALA VAL PRO HIS HIS PRO VAL ASN LYS LYS PHE VAL PRO ASP TYR TYR LYS VAL ILE VAL ASN PRO MET ASP LEU GLU THR ILE ARG LYS ASN ILE SER LYS HIS LYS TYR GLN SER ARG GLU SER PHE LEU ASP



• Molecule 12: Transcription initiation factor TFIID subunit 2

Chain B:

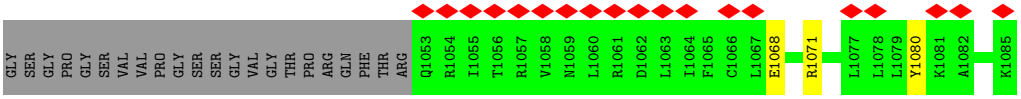




• Molecule 13: Transcription initiation factor TFIID subunit 4

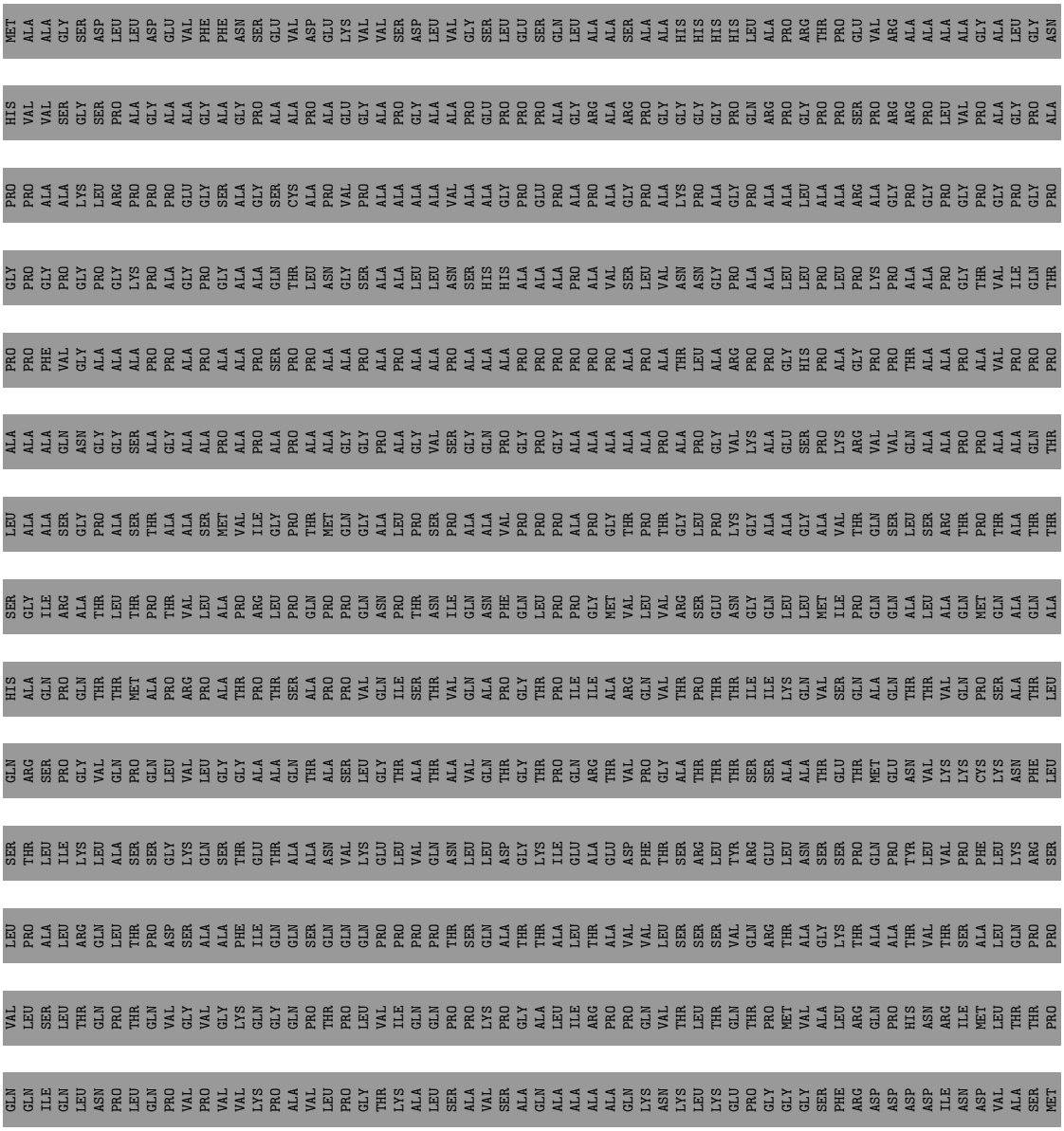
Chain D:

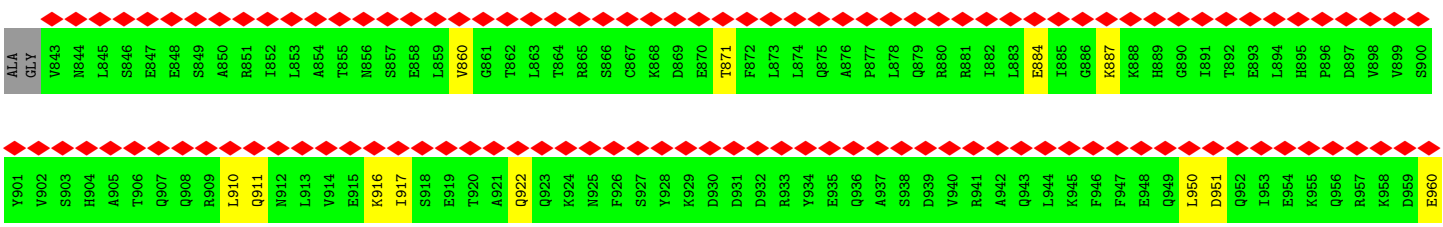


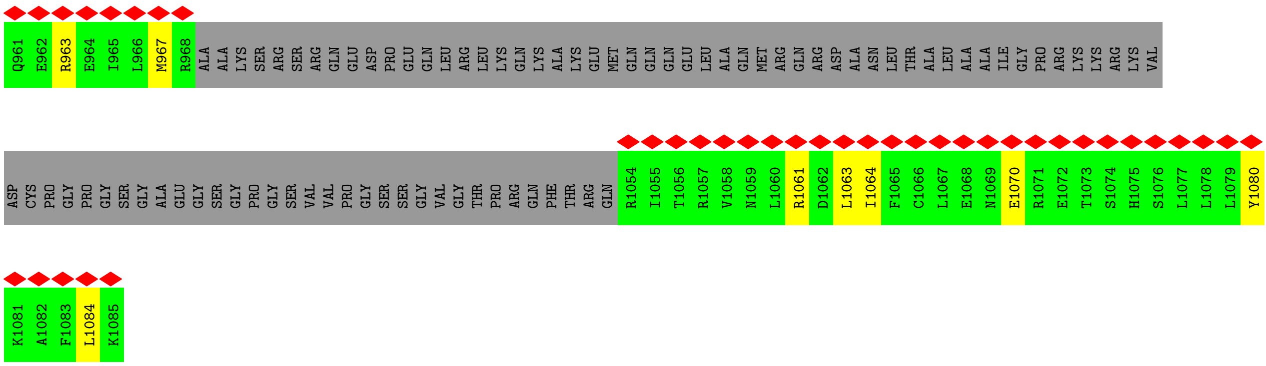


• Molecule 13: Transcription initiation factor TFIID subunit 4





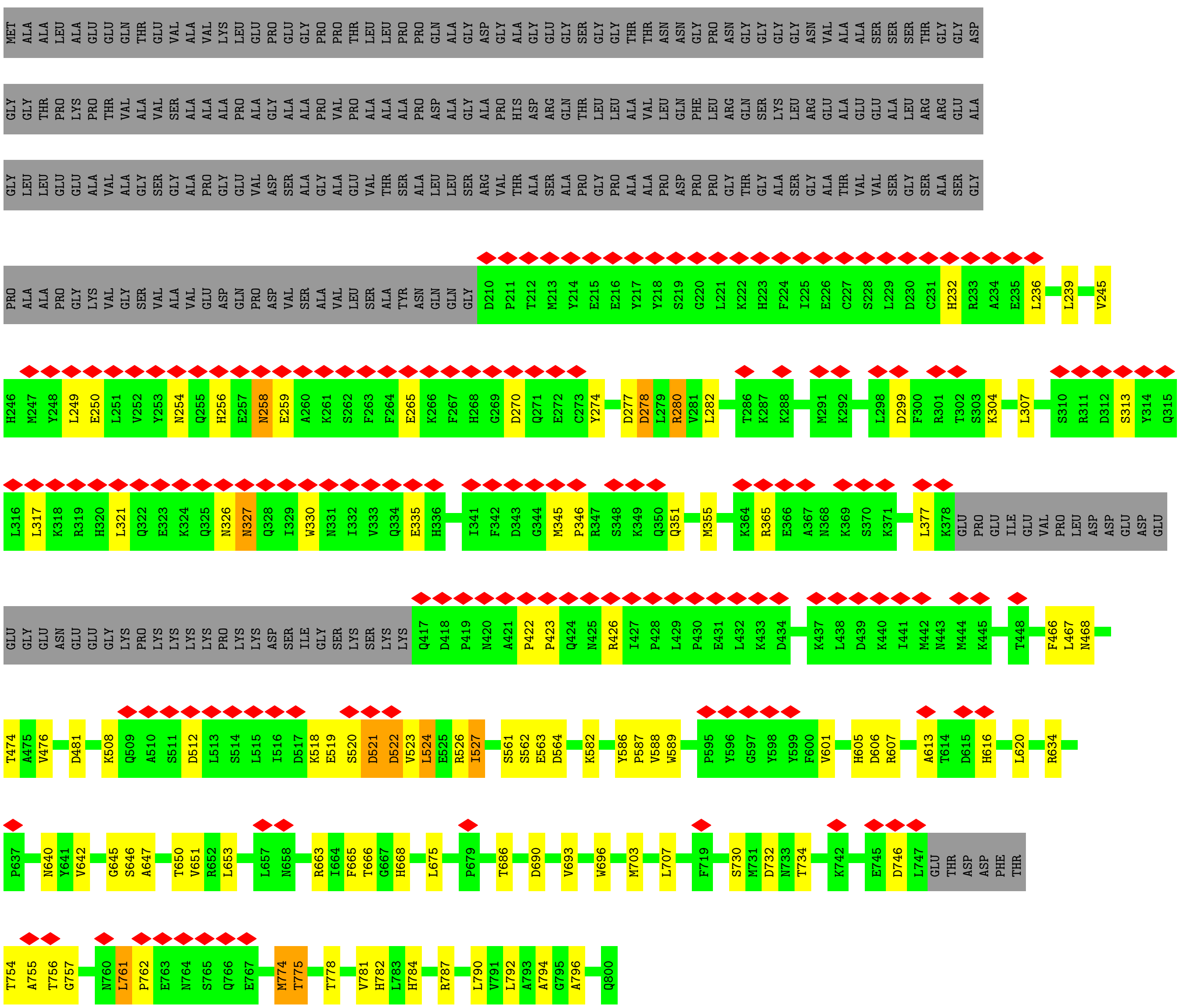




• Molecule 14: Transcription initiation factor TFIID subunit 5

Chain E:

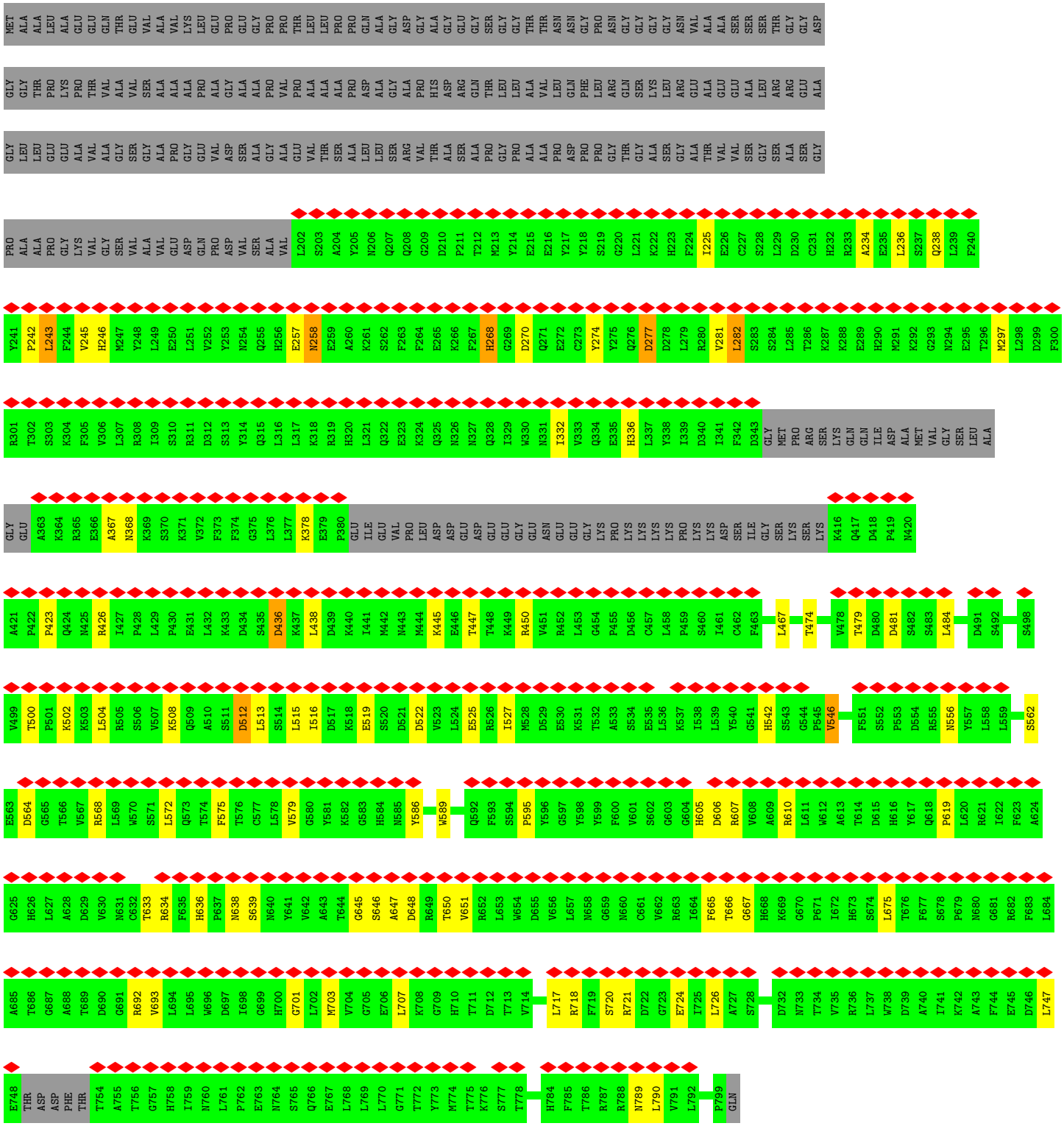




• Molecule 14: Transcription initiation factor TFIID subunit 5

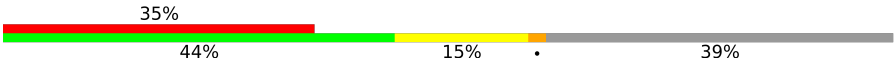
Chain e:

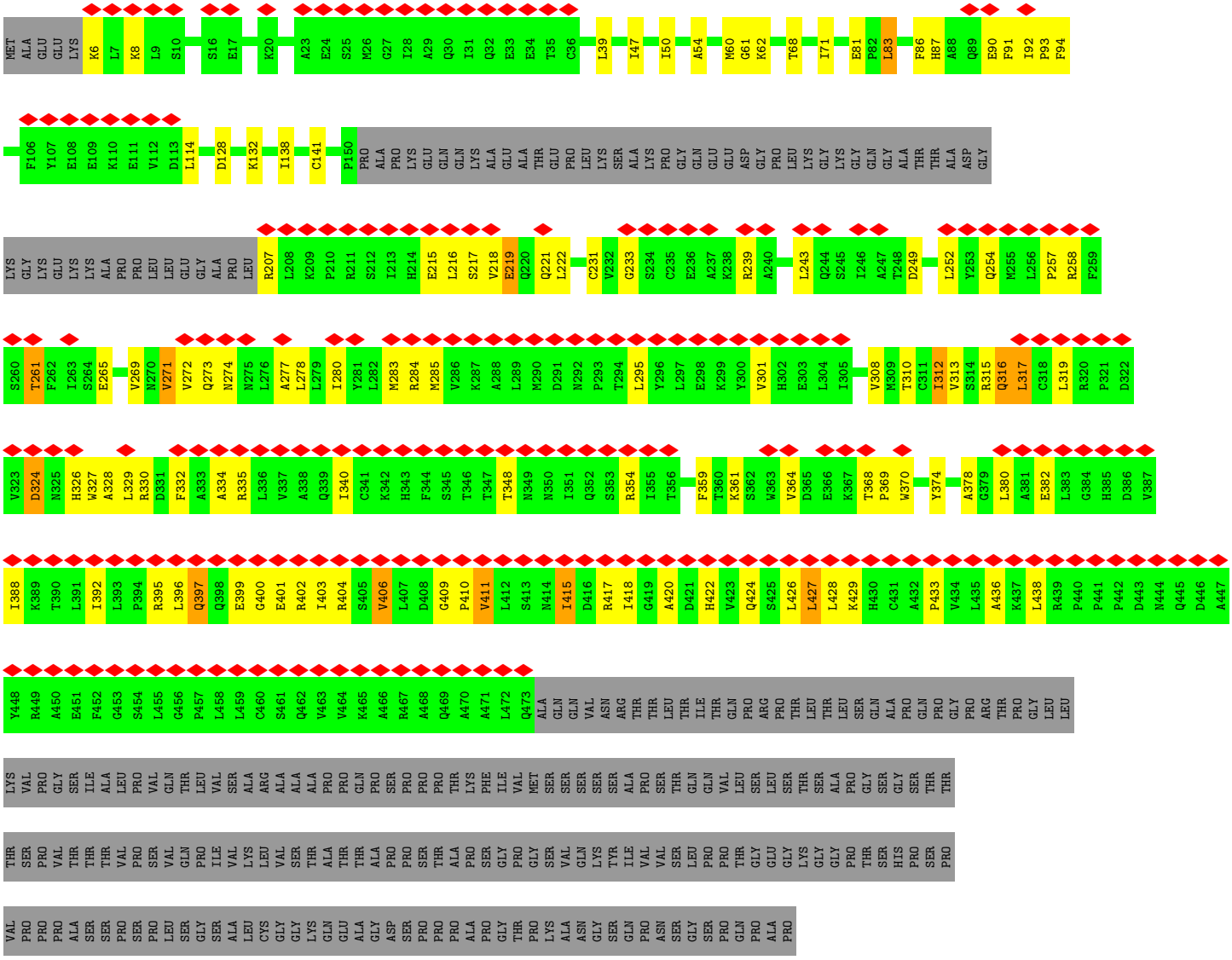




• Molecule 15: Transcription initiation factor TFIID subunit 6

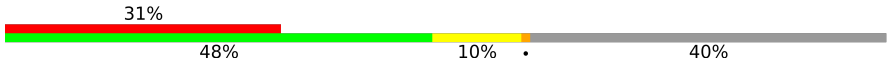
Chain F:

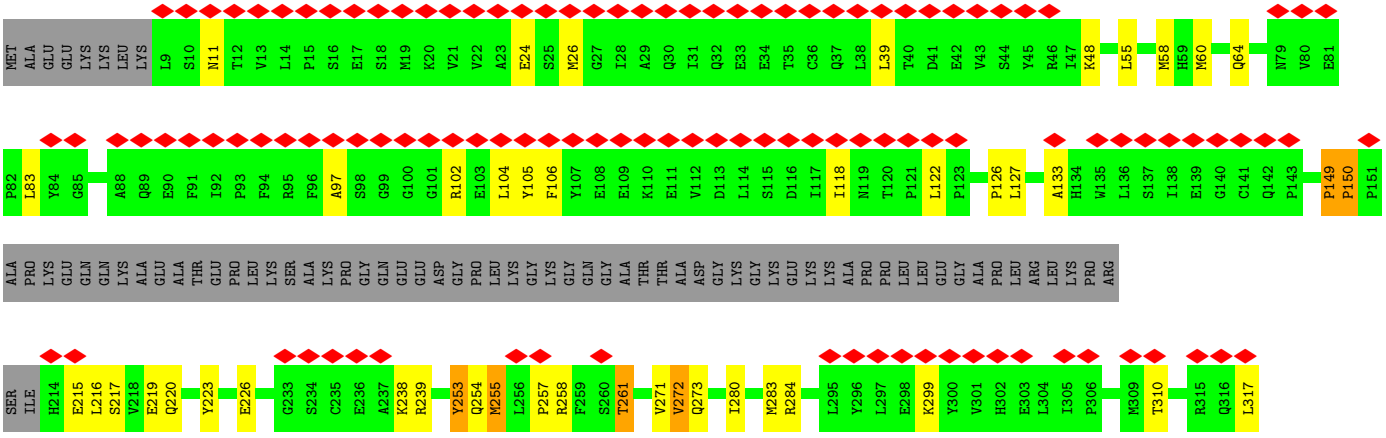


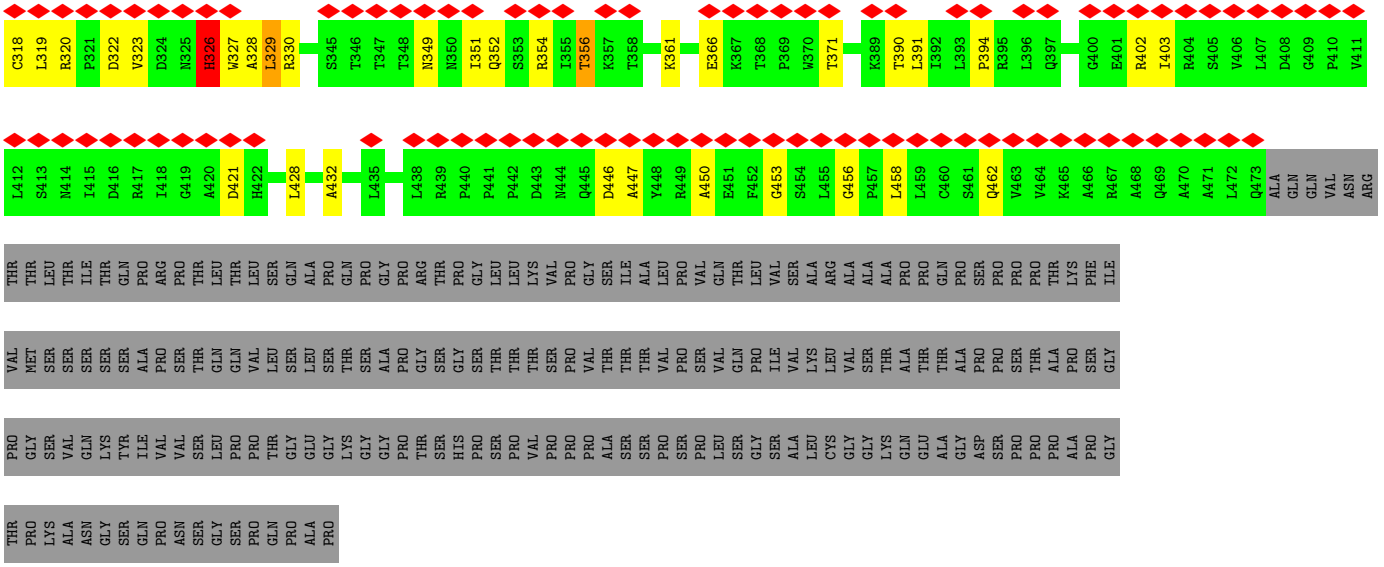


• Molecule 15: Transcription initiation factor TFIID subunit 6

Chain f:



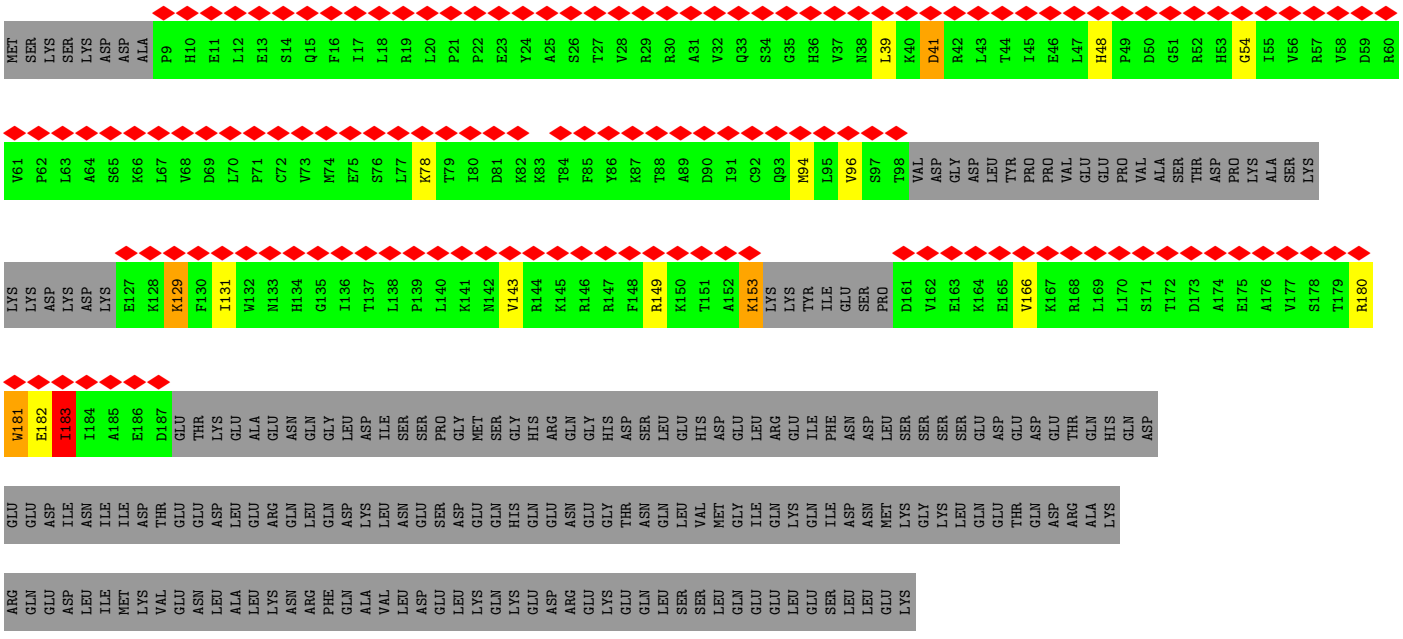




• Molecule 16: Transcription initiation factor TFIID subunit 7

Chain G:

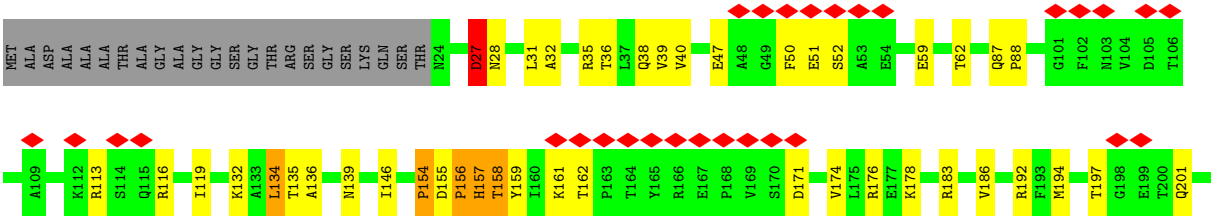


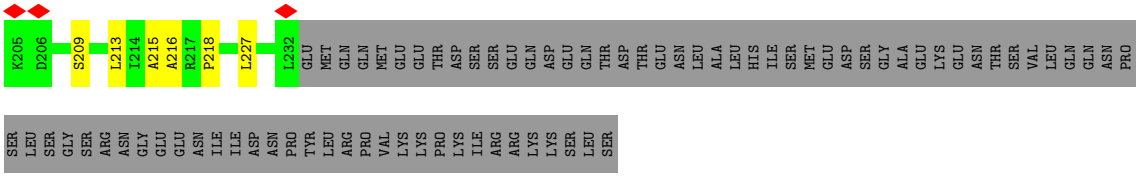


• Molecule 17: Transcription initiation factor TFIID subunit 8

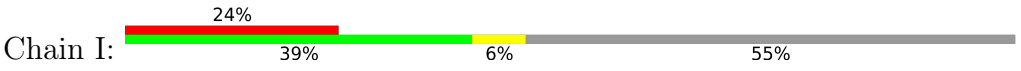
Chain H:

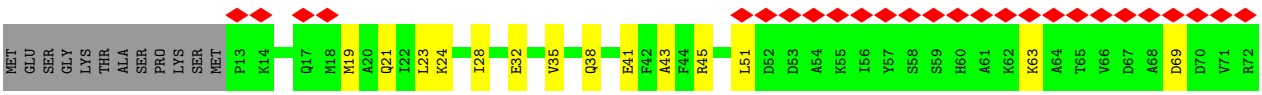


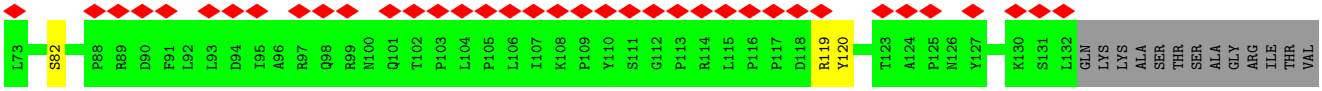




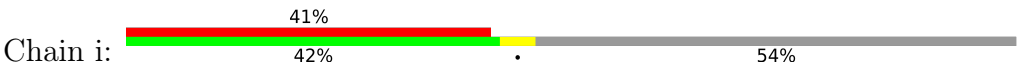
• Molecule 18: Transcription initiation factor TFIID subunit 9

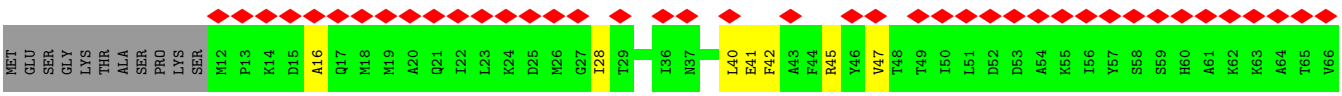


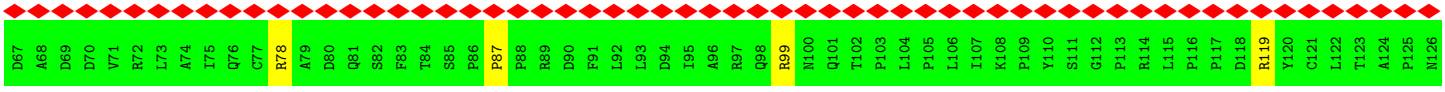




• Molecule 18: Transcription initiation factor TFIID subunit 9



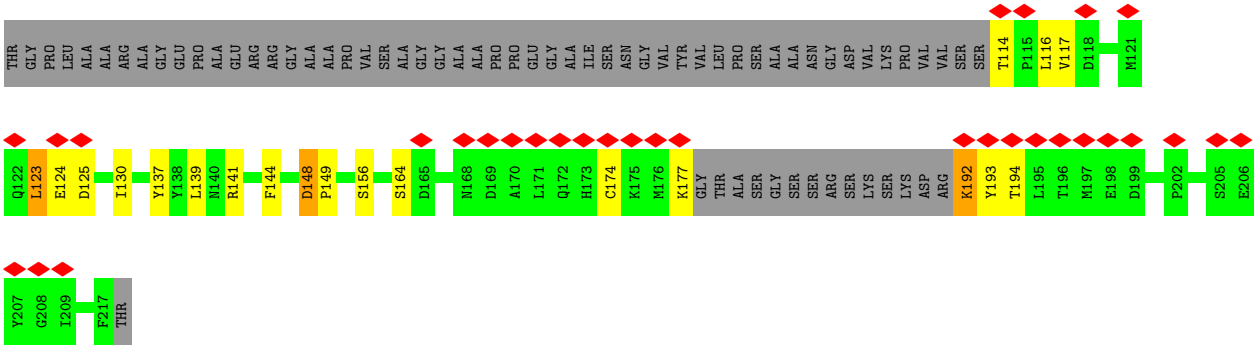




• Molecule 19: Transcription initiation factor TFIID subunit 10



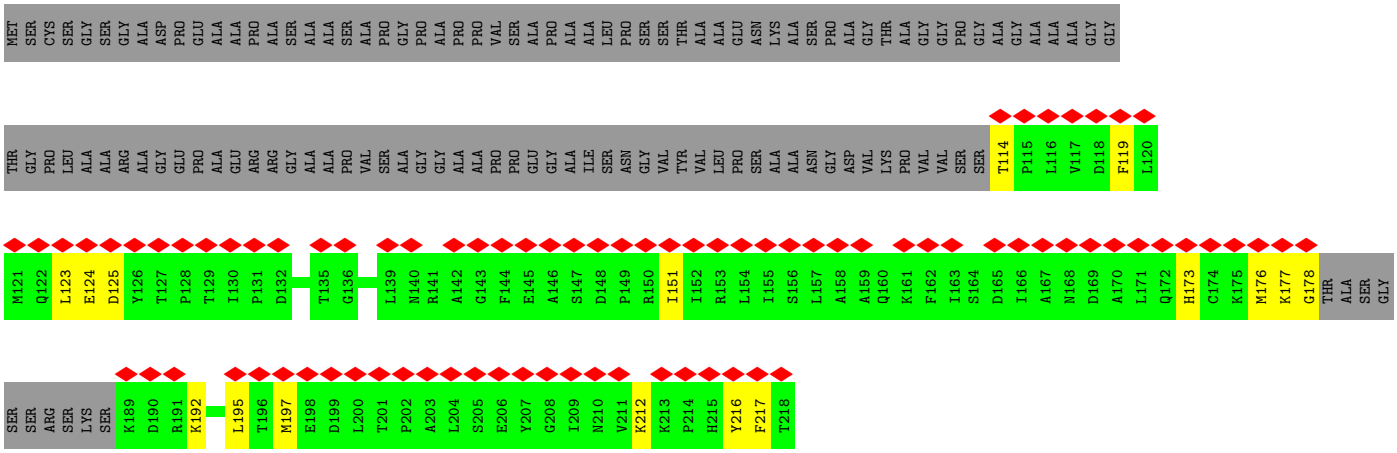




• Molecule 19: Transcription initiation factor TFIID subunit 10

Chain j:

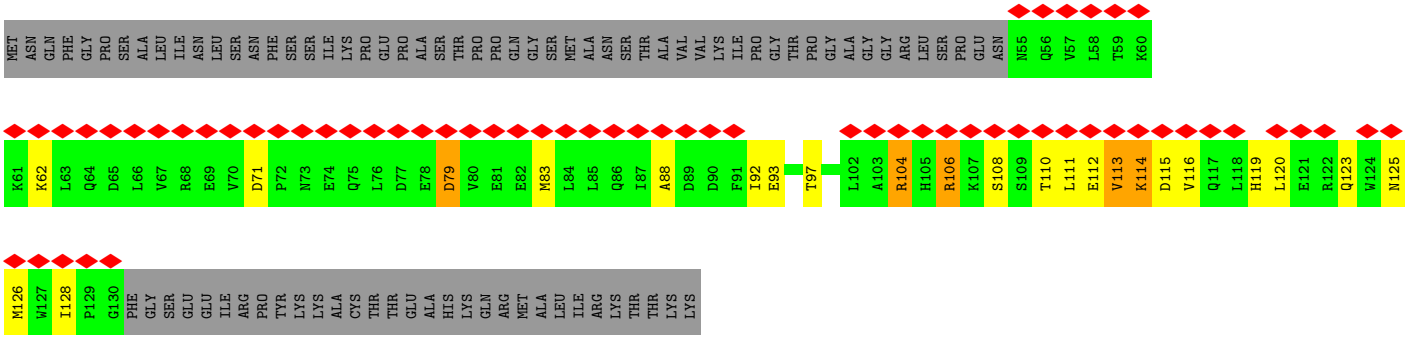




• Molecule 20: Transcription initiation factor TFIID subunit 12

Chain L:





• Molecule 20: Transcription initiation factor TFIID subunit 12

Chain l:





K61 K62 L63 Q64 D65 L66 V67 R68 E69 V70 D71 P72 N73 E74 Q75 L76 D77 E78 D79 V80 E81 E82 M83 L84 L85 Q86 I87 A88 D89 D90 F91 I92 E93 S94 V95 V96 T97 A98 A99 C100 Q101 L102 A103 R104 H105 R106 K107 S108 S109 T110 L111 E112 V113 K114 D115 V116 Q117 L118 H119 L120

E121 R122 Q123 W124 N125 M126 W127 I128 P129 G130 F131 G132 S133 E134 E135 I136 R137 P138 Y139 K140 K141 A142 C143 T144 T145 E146 A147 H148 K149 Q150 R151 M152 A153 L154 I155 R156 K157 T158 T159 K160 K161

- Molecule 21: Transcription initiation factor IIA subunit 2

Chain O: 75% 16% 9%

M1 L11 Q16 D20 Q24 T29 L32 I44 L48 R51 N57 F58 L62 N63 T64 Y65 D69 T73 L76 D99 GLY LYS ASN THR GLY SER ASN THR THR GLU

- Molecule 22: TATA-box-binding protein

Chain P: 47% 6% 47%

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

GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN ALA VAL ALA ALA ALA ALA VAL GLN GLN SER THR SER GLN GLN ALA THR GLN GLY THR SER GLY GLN ALA PRO GLN

LEU PHE HIS SER GLN THR LEU THR THR ALA PRO LEU PRO GLY THR THR PRO LEU TYR PRO SER PRO MET THR PRO MET THR PRO ILE THR PRO ALA THR PRO ALA SER GLU SER S159 V169 L174 L178 R186 A187 R188 R203 E206 P207 R208 T222 E227

K236 L244 M295 I296 K297 P298 R299 I300 R318 E323 K337 THR THR

- Molecule 23: Transcription initiation factor IIA beta chain

Chain Q: 27% 70%

MET ALA ASN SER ALA ASN THR ASN T9 R15 I18 E19 D20 V21 I22 D31 L39 W46 M51 GLN SER ARG ALA VAL ASP GLY PHE HIS SER GLU GLU GLN GLN LEU LEU LEU GLN VAL GLN GLN GLN HIS GLN PRO GLN GLN GLN GLN HIS HIS HIS HIS HIS HIS

HIS GLN GLN ALA GLN PRO GLN GLN THR VAL PRO GLN GLN ALA GLN THR GLN GLN VAL LEU ILE PRO ALA SER GLN GLN ALA THR ALA PRO GLN VAL ILE VAL PRO ASP SER LYS LEU ILE GLN HIS MET ASN ALA SER ASN MET SER ALA ALA ALA THR ALA ALA THR LEU ALA LEU PRO

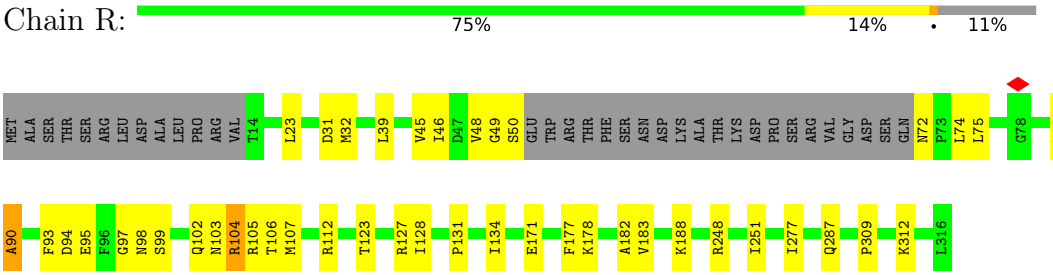
ALA GLY VAL THR PRO VAL GLN GLN ILE LEU THR ASN SER GLY GLN LEU LEU GLN VAL VAL ARG ALA ALA ASN GLY ALA GLN TYR ILE PHE GLN PRO GLN GLN SER VAL VAL LEU GLN GLN GLN VAL ILE PRO GLN MET GLN PRO GLY GLY VAL GLN ALA PRO VAL ILE GLN GLN VAL LEU

ALA PRO LEU PRO GLY GLY ILE SER PRO GLN THR GLY VAL ILE ILE GLN PRO GLN GLN ILE LEU PHE THR GLY ASN LYS THR GLN VAL ILE PRO THR THR VAL ALA ALA PRO THR PRO ALA GLN ALA GLN ILE THR ALA THR GLY GLN GLN GLN PRO GLN ALA GLN PRO ALA GLN THR GLN

ALA PRO LEU VAL LEU GLN VAL ASP GLY THR GLY ASP THR SER SER GLU GLU ASP GLU ASP GLU GLU GLU ASP TYR ASP ASP ASP GLU GLU GLU ASP LYS GLU LYS ASP GLY ALA GLU ASP G307 Q308 V309 S321 D322 E332 K346 I366 W376

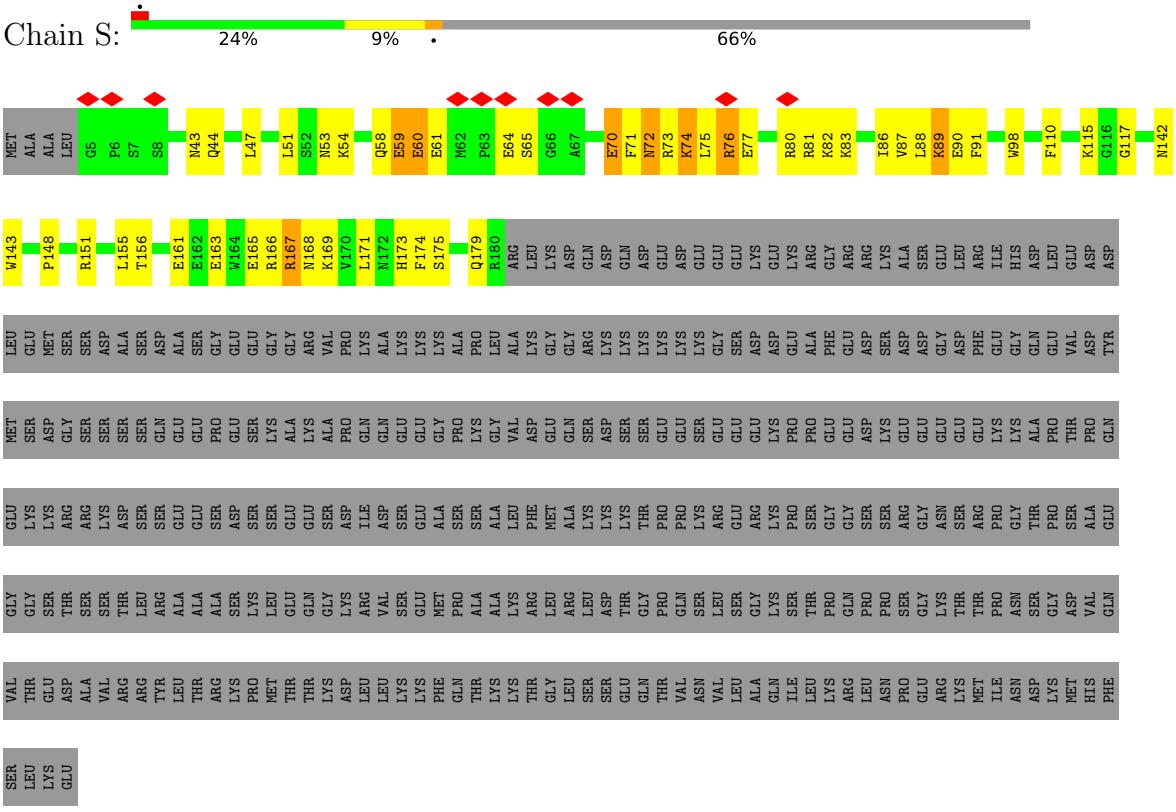
- Molecule 24: Transcription initiation factor IIB

Chain R:



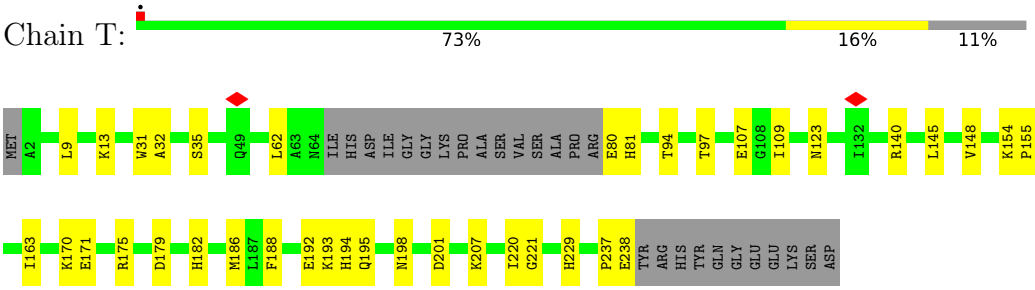
• Molecule 25: General transcription factor IIF subunit 1

Chain S:



• Molecule 26: General transcription factor IIF subunit 2

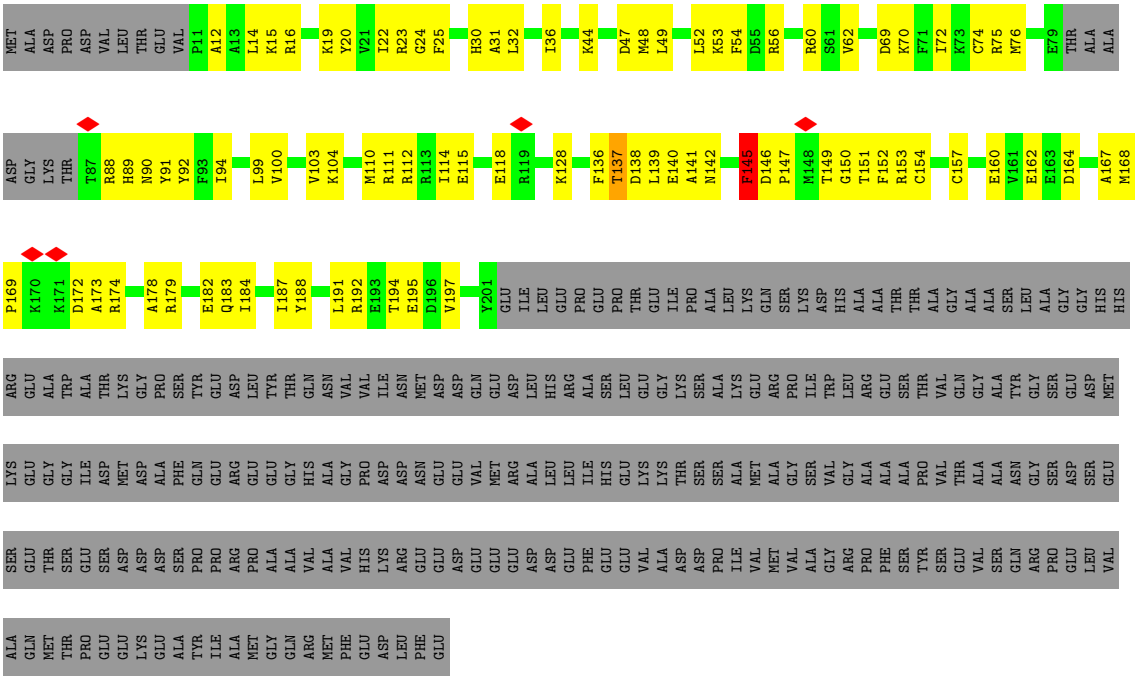
Chain T:



• Molecule 27: General transcription factor IIE subunit 1

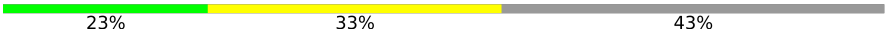
Chain U:

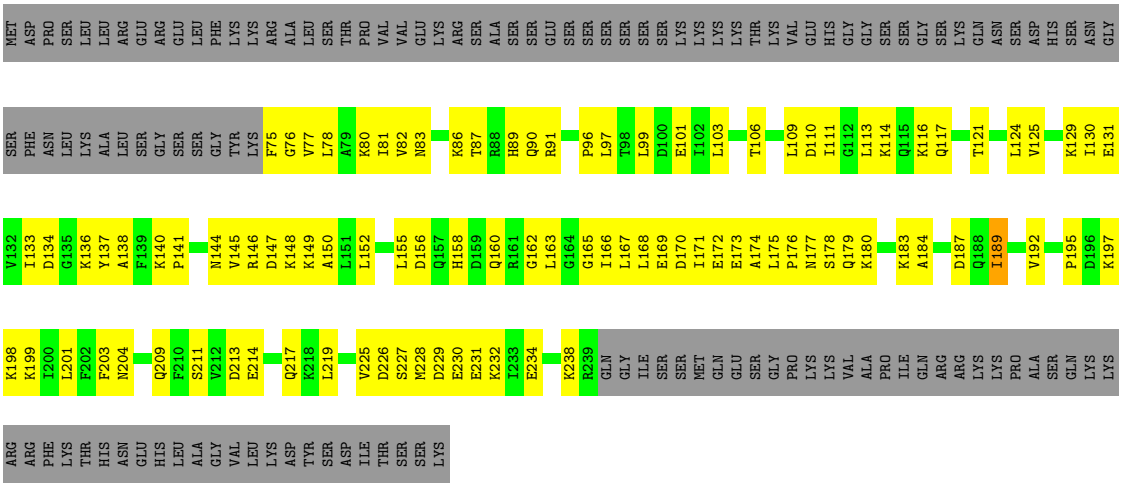




• Molecule 28: Transcription initiation factor IIE subunit beta

Chain V:

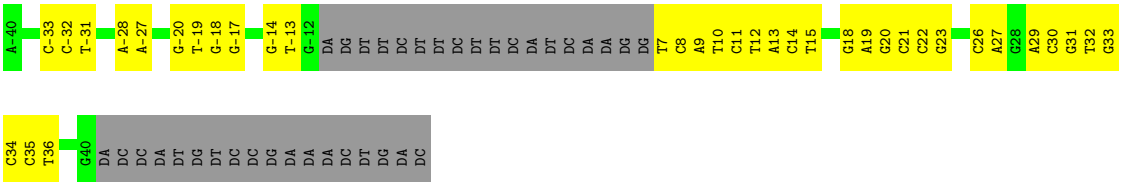




• Molecule 29: non-template DNA

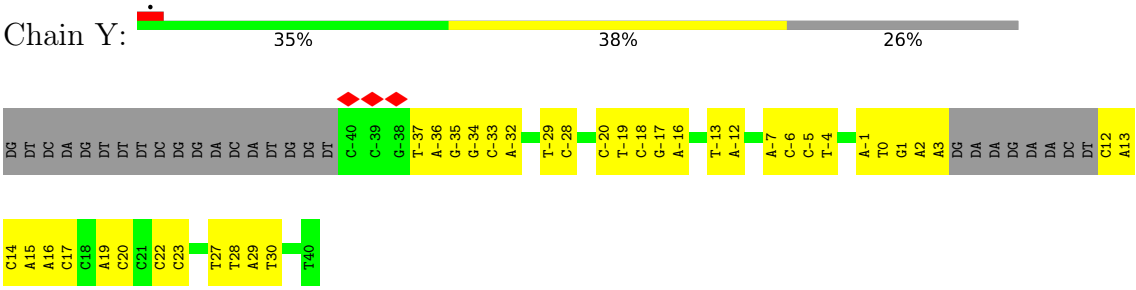
Chain X:





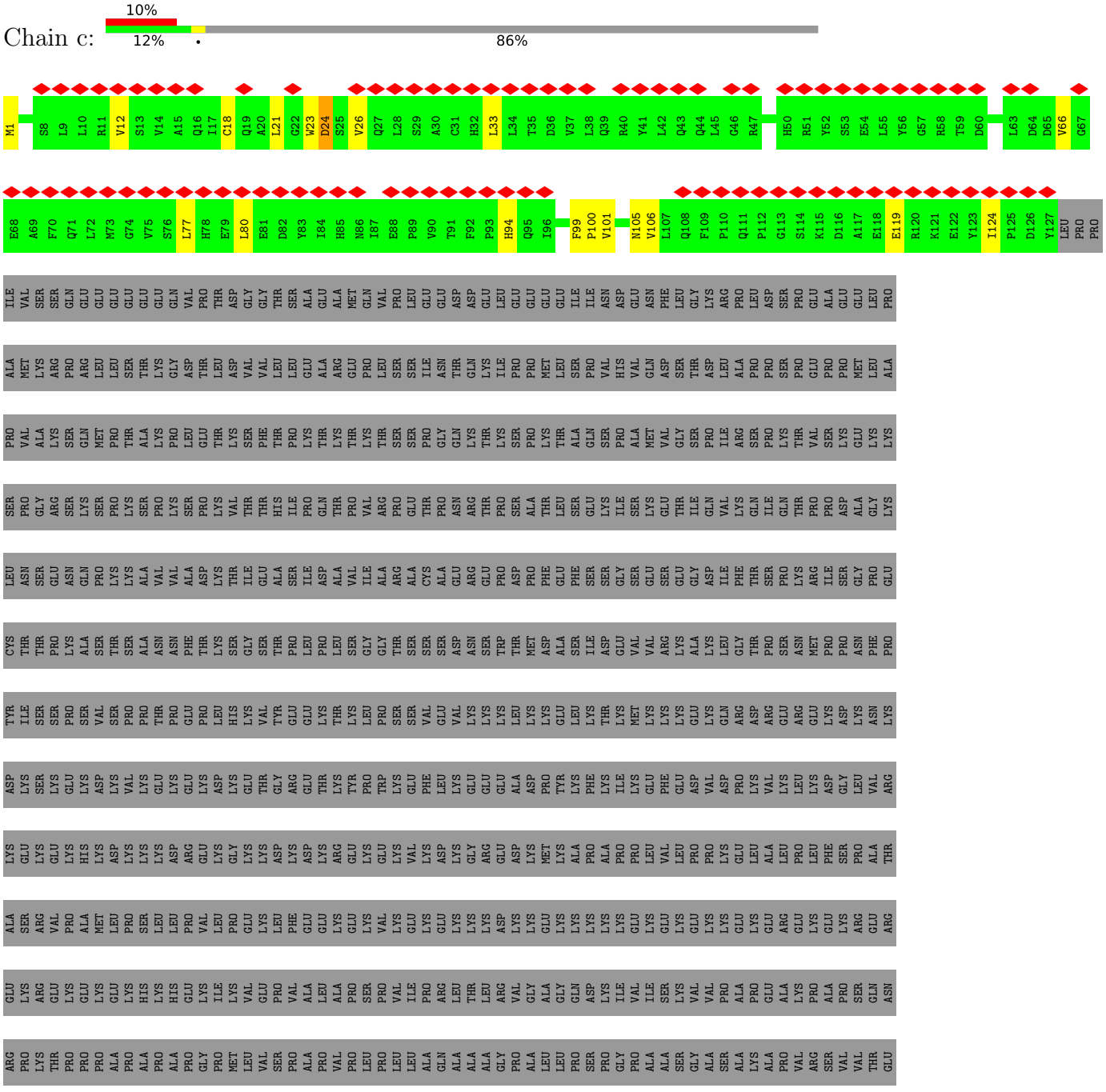
• Molecule 30: template DNA

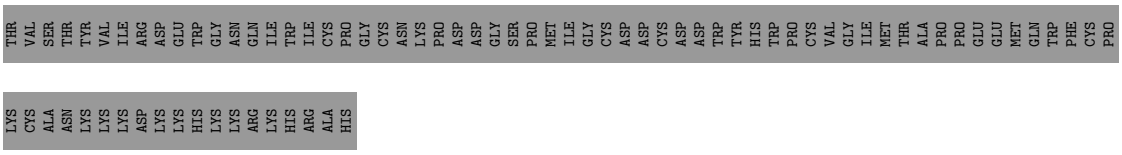
Chain Y:



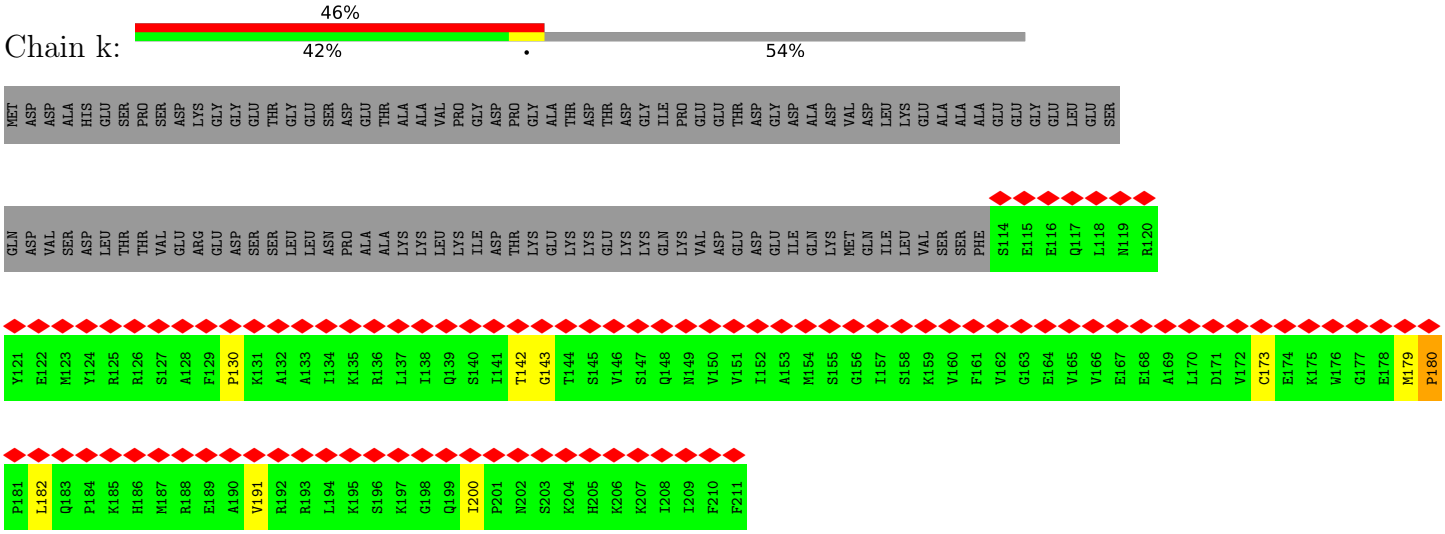
• Molecule 31: Transcription initiation factor TFIID subunit 3

Chain c:

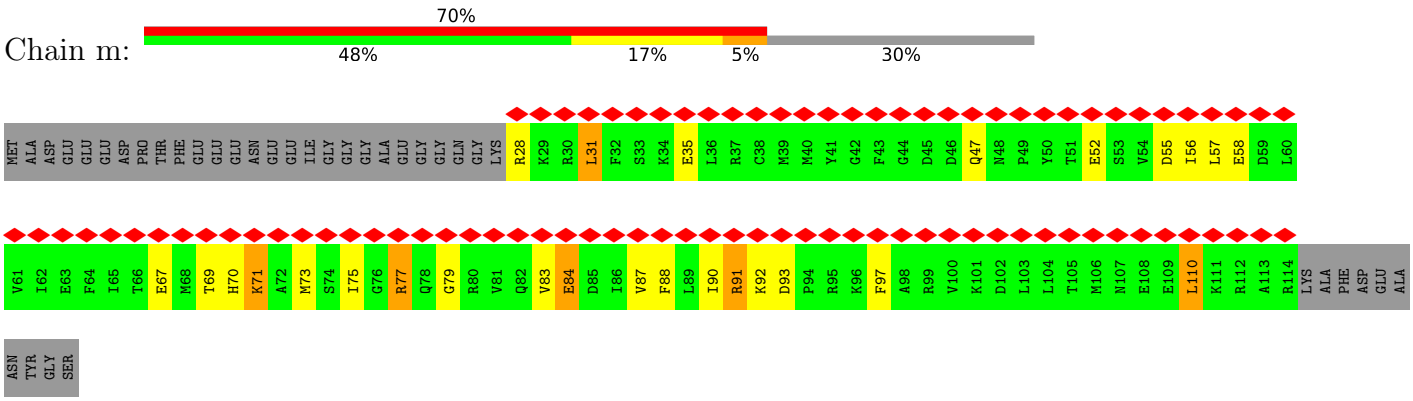




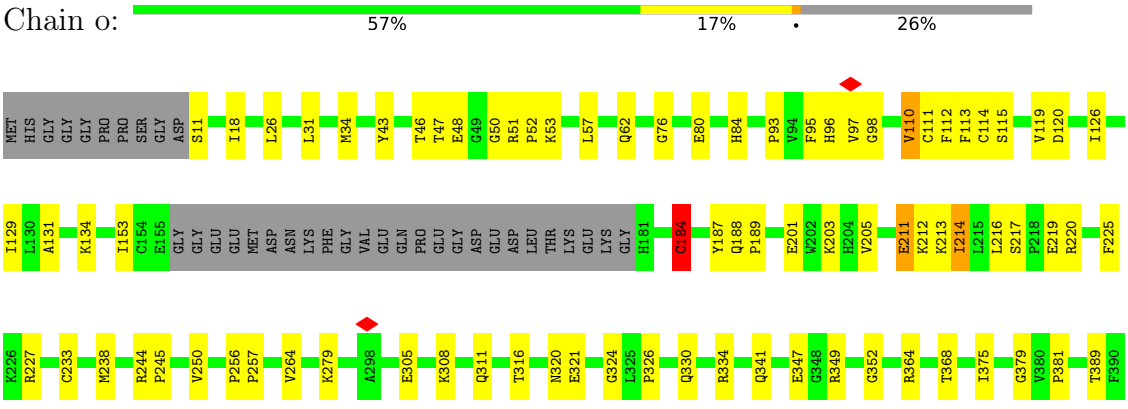
• Molecule 32: Transcription initiation factor TFIID subunit 11

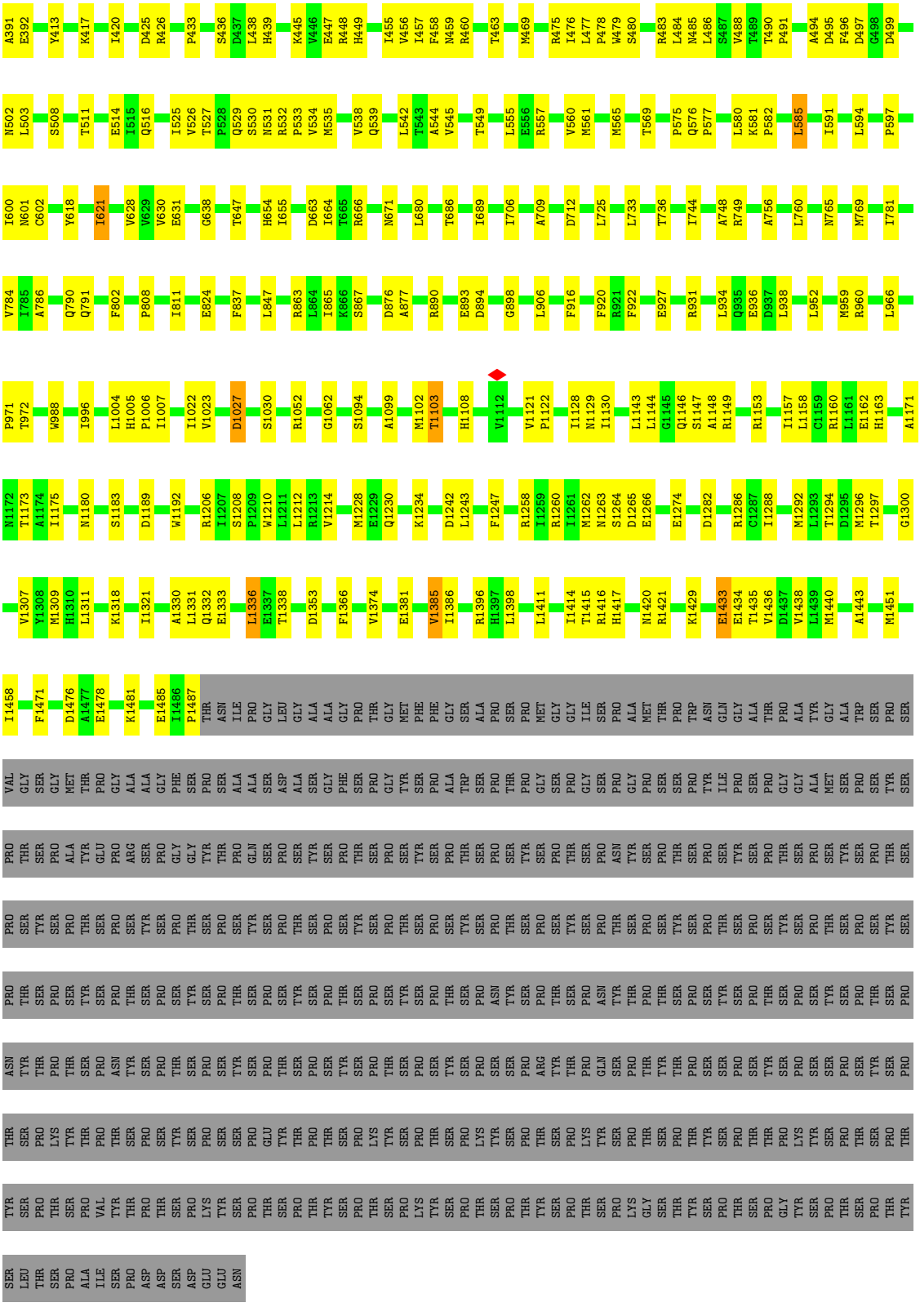


• Molecule 33: Transcription initiation factor TFIID subunit 13



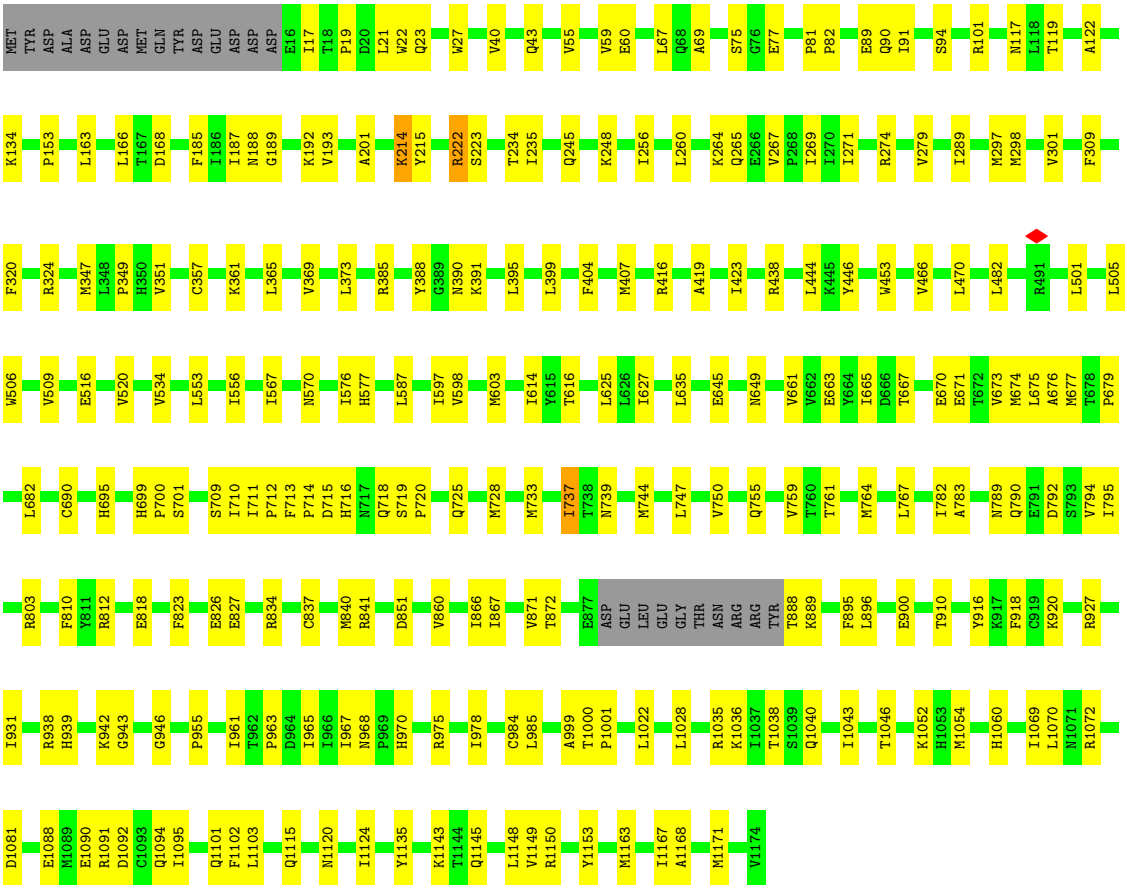
• Molecule 34: DNA-directed RNA polymerase subunit





• Molecule 35: DNA-directed RNA polymerase subunit beta

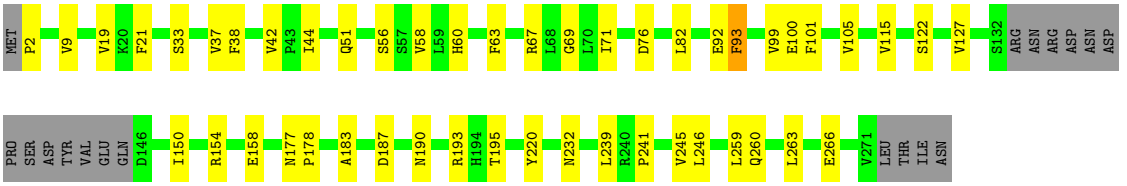
Chain p: 77% 21%



• Molecule 36: DNA-directed RNA polymerase II subunit RPB3

Chain q:

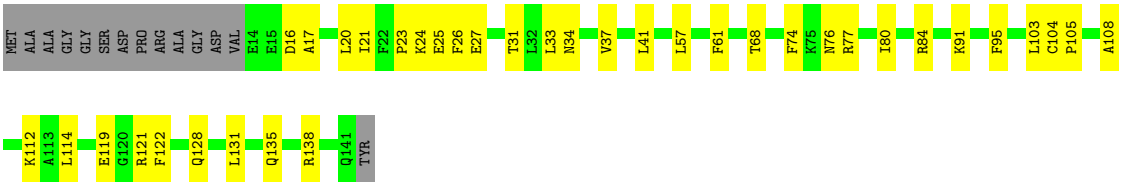




• Molecule 37: DNA-directed RNA polymerase II subunit RPB4

Chain r:

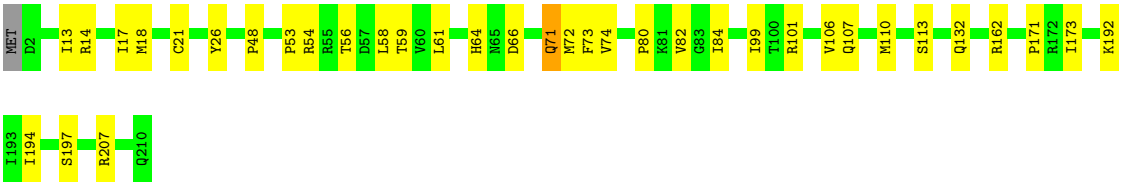




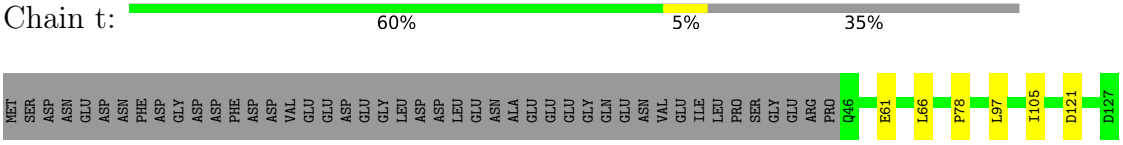
• Molecule 38: DNA-directed RNA polymerase II subunit E

Chain s:

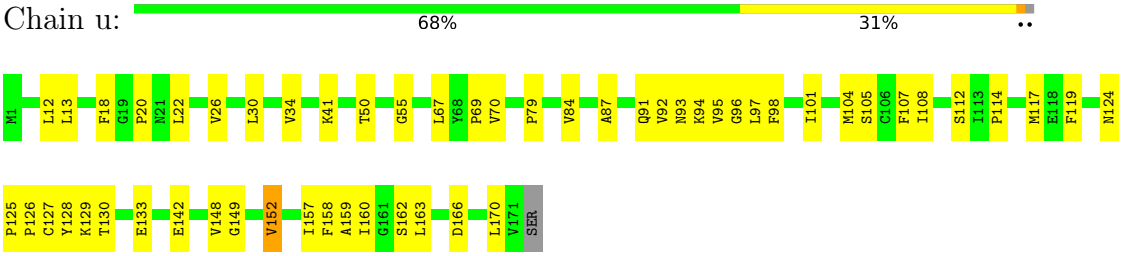




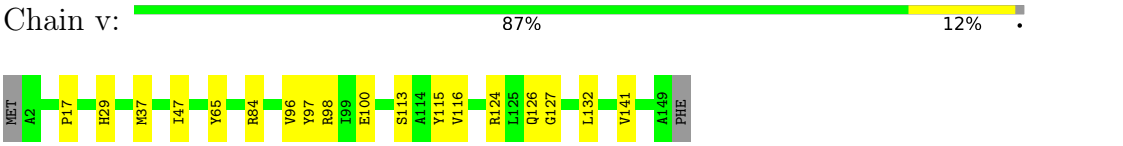
• Molecule 39: DNA-directed RNA polymerase II subunit F



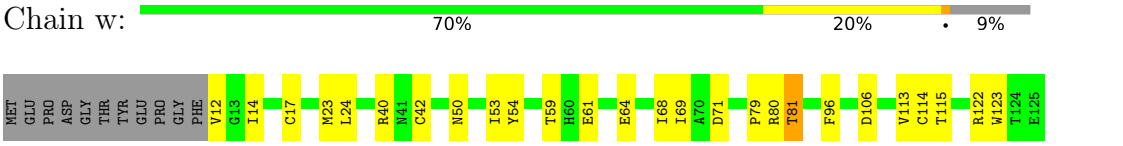
• Molecule 40: DNA-directed RNA polymerase II subunit RPB7



• Molecule 41: DNA-directed RNA polymerases I, II, and III subunit RPABC3



• Molecule 42: DNA-directed RNA polymerase II subunit RPB9



• Molecule 43: DNA-directed RNA polymerases I, II, and III subunit RPABC5



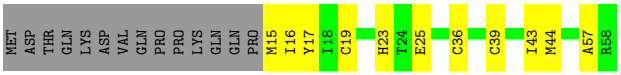
• Molecule 44: DNA-directed RNA polymerase II subunit RPB11-a





• Molecule 45: RPB12





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	4867	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.331	Depositor
Minimum map value	-1.901	Depositor
Average map value	0.035	Depositor
Map value standard deviation	0.176	Depositor
Recommended contour level	0.48	Depositor
Map size (Å)	426.88, 426.88, 426.88	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.334, 1.334, 1.334	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, CSX, HYP, MG, SF4, W0F, ILX, TRX, G2L, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	0	0.41	0/1437	0.71	3/1926 (0.2%)
2	1	0.20	0/2210	0.34	0/2975
3	2	0.19	0/2624	0.33	1/3555 (0.0%)
4	3	0.24	0/2103	0.36	0/2846
5	4	0.31	0/3262	0.45	1/4418 (0.0%)
6	5	0.40	0/433	0.79	1/585 (0.2%)
7	6	0.19	0/4994	0.33	0/6745
8	7	0.17	0/5875	0.30	0/7955
9	N	0.41	0/22	0.98	0/26
10	Z	0.36	0/93	0.59	0/142
11	A	0.63	0/4698	0.95	5/6345 (0.1%)
12	B	0.46	1/7993 (0.0%)	0.69	6/10836 (0.1%)
13	D	0.56	0/1379	0.88	3/1843 (0.2%)
13	d	0.47	0/1321	0.71	0/1772
14	E	0.45	1/4482 (0.0%)	0.72	3/6069 (0.0%)
14	e	0.55	1/4433 (0.0%)	0.77	0/6004
15	F	0.63	1/3201 (0.0%)	1.00	7/4347 (0.2%)
15	f	0.47	0/3140	0.80	6/4268 (0.1%)
16	G	0.68	0/1190	0.94	1/1601 (0.1%)
17	H	0.63	3/1673 (0.2%)	0.86	5/2285 (0.2%)
18	I	0.20	0/981	0.41	0/1332
18	i	0.22	0/989	0.40	0/1343
19	J	0.83	0/736	1.15	2/998 (0.2%)
19	j	0.74	0/775	0.97	0/1049
20	L	0.69	0/630	1.14	1/852 (0.1%)
20	l	0.59	0/888	0.88	0/1194
21	O	0.27	0/816	0.36	0/1105
22	P	0.12	0/1448	0.24	0/1948
23	Q	0.19	0/945	0.36	0/1274
24	R	0.18	0/2199	0.38	0/2967
25	S	0.19	0/1496	0.38	0/2013
26	T	0.15	0/1817	0.29	0/2445

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
27	U	0.35	0/1545	0.69	1/2075 (0.0%)
28	V	0.24	0/1380	0.58	0/1854
29	X	0.34	0/1464	0.61	0/2258
30	Y	0.38	0/1660	0.59	0/2554
31	c	0.48	0/1035	0.67	0/1406
32	k	0.28	0/799	0.53	1/1070 (0.1%)
33	m	0.84	0/733	1.18	1/977 (0.1%)
34	o	0.25	0/11723	0.38	0/15830
35	p	0.27	0/9358	0.37	0/12633
36	q	0.31	1/2102 (0.0%)	0.38	0/2857
37	r	0.11	0/1064	0.23	0/1428
38	s	0.24	0/1751	0.34	0/2366
39	t	0.22	0/667	0.31	0/901
40	u	0.19	0/1382	0.31	0/1874
41	v	0.22	0/1207	0.31	0/1628
42	w	0.20	0/948	0.31	0/1284
43	x	0.26	0/542	0.37	0/730
44	y	0.26	0/939	0.34	0/1271
45	z	0.22	0/377	0.34	0/500
All	All	0.38	8/110959 (0.0%)	0.59	48/150559 (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
24	R	0	1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	H	28	ASN	C-O	-7.45	1.15	1.24
17	H	27	ASP	C-O	-7.05	1.15	1.24
17	H	31	LEU	C-O	-6.31	1.16	1.24
12	B	61	ASN	C-O	-6.12	1.18	1.24
14	E	524	LEU	C-O	5.72	1.30	1.24

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	55	LYS	CB-CA-C	-11.48	94.97	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	B	491	HIS	N-CA-C	-9.46	100.97	111.28
15	f	149	PRO	O-C-N	9.13	125.51	121.31
14	E	756	THR	N-CA-C	-8.40	103.16	113.50
17	H	32	ALA	N-CA-C	-8.21	102.29	111.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
24	R	106	THR	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	1420	0	1420	125	0
2	1	2167	0	2175	39	0
3	2	2567	0	2539	95	0
4	3	2066	0	2097	102	0
5	4	3189	0	3243	141	0
6	5	428	0	434	43	0
7	6	4890	0	4949	93	0
8	7	5751	0	5794	146	0
9	N	64	0	51	8	0
10	Z	139	0	64	4	0
11	A	4580	0	4502	99	0
12	B	7796	0	7751	117	0
13	D	1366	0	1390	73	0
13	d	1307	0	1318	14	0
14	E	4376	0	4256	74	0
14	e	4327	0	4197	60	0
15	F	3143	0	3093	99	0
15	f	3081	0	3012	71	0
16	G	1171	0	1222	15	0
17	H	1633	0	1621	36	0
18	I	959	0	969	13	0
18	i	967	0	977	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	J	720	0	719	12	0
19	j	759	0	759	14	0
20	L	622	0	620	19	0
20	l	876	0	893	10	0
21	O	806	0	818	18	0
22	P	1422	0	1514	17	0
23	Q	930	0	888	12	0
24	R	2167	0	2193	32	0
25	S	1461	0	1429	39	0
26	T	1788	0	1819	54	0
27	U	1520	0	1520	215	0
28	V	1357	0	1381	90	0
29	X	1304	0	708	44	0
30	Y	1484	0	822	45	0
31	c	1011	0	975	18	0
32	k	785	0	818	8	0
33	m	724	0	744	23	0
34	o	11510	0	11615	239	0
35	p	9175	0	9196	178	0
36	q	2059	0	2007	30	0
37	r	1050	0	1033	23	0
38	s	1720	0	1737	22	0
39	t	657	0	684	6	0
40	u	1351	0	1358	133	0
41	v	1186	0	1147	12	0
42	w	927	0	860	23	0
43	x	533	0	553	12	0
44	y	920	0	942	16	0
45	z	372	0	378	9	0
46	0	2	0	0	0	0
46	2	3	0	0	0	0
46	3	2	0	0	0	0
46	R	1	0	0	0	0
46	U	1	0	0	0	0
46	o	2	0	0	0	0
46	p	1	0	0	0	0
46	q	1	0	0	0	0
46	w	2	0	0	0	0
46	x	1	0	0	0	0
46	z	1	0	0	0	0
47	7	8	0	0	0	0
48	o	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	p	33	0	0	8	0
All	All	108642	0	107204	2279	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 11.

The worst 5 of 2279 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)
27:U:152:PHE:CE1	40:u:95:VAL:HB	1.23	1.65
27:U:139:LEU:HB2	40:u:160:ILE:CG1	1.22	1.58
1:0:41:ARG:CG	27:U:169:PRO:HG2	1.34	1.54
27:U:139:LEU:CB	40:u:160:ILE:HG12	1.41	1.49
6:5:33:PHE:CE1	6:5:49:LEU:HD12	1.44	1.49

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	169/309 (55%)	156 (92%)	13 (8%)	0	100 100
2	1	253/548 (46%)	243 (96%)	10 (4%)	0	100 100
3	2	325/395 (82%)	313 (96%)	12 (4%)	0	100 100
4	3	259/308 (84%)	253 (98%)	6 (2%)	0	100 100
5	4	384/462 (83%)	365 (95%)	19 (5%)	0	100 100
6	5	52/71 (73%)	48 (92%)	2 (4%)	2 (4%)	2 19
7	6	601/782 (77%)	573 (95%)	27 (4%)	1 (0%)	43 77
8	7	710/760 (93%)	683 (96%)	27 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
9	N	4/8 (50%)	3 (75%)	1 (25%)	0	100 100
11	A	543/1872 (29%)	519 (96%)	23 (4%)	1 (0%)	43 77
12	B	959/1199 (80%)	911 (95%)	48 (5%)	0	100 100
13	D	158/1085 (15%)	153 (97%)	5 (3%)	0	100 100
13	d	154/1085 (14%)	150 (97%)	4 (3%)	0	100 100
14	E	541/800 (68%)	518 (96%)	22 (4%)	1 (0%)	43 77
14	e	531/800 (66%)	482 (91%)	48 (9%)	1 (0%)	43 77
15	F	408/677 (60%)	392 (96%)	15 (4%)	1 (0%)	43 77
15	f	399/677 (59%)	379 (95%)	20 (5%)	0	100 100
16	G	138/349 (40%)	135 (98%)	3 (2%)	0	100 100
17	H	207/310 (67%)	189 (91%)	13 (6%)	5 (2%)	4 26
18	I	118/264 (45%)	115 (98%)	3 (2%)	0	100 100
18	i	119/264 (45%)	115 (97%)	4 (3%)	0	100 100
19	J	86/218 (39%)	82 (95%)	4 (5%)	0	100 100
19	j	91/218 (42%)	85 (93%)	4 (4%)	2 (2%)	5 28
20	L	74/161 (46%)	72 (97%)	2 (3%)	0	100 100
20	l	105/161 (65%)	100 (95%)	5 (5%)	0	100 100
21	O	97/109 (89%)	95 (98%)	2 (2%)	0	100 100
22	P	177/339 (52%)	175 (99%)	2 (1%)	0	100 100
23	Q	109/376 (29%)	102 (94%)	7 (6%)	0	100 100
24	R	278/316 (88%)	263 (95%)	13 (5%)	2 (1%)	18 55
25	S	174/517 (34%)	163 (94%)	10 (6%)	1 (1%)	21 59
26	T	218/249 (88%)	211 (97%)	7 (3%)	0	100 100
27	U	180/439 (41%)	153 (85%)	26 (14%)	1 (1%)	21 59
28	V	163/291 (56%)	139 (85%)	24 (15%)	0	100 100
31	c	125/929 (14%)	116 (93%)	9 (7%)	0	100 100
32	k	96/211 (46%)	91 (95%)	5 (5%)	0	100 100
33	m	85/124 (68%)	82 (96%)	3 (4%)	0	100 100
34	o	1448/1970 (74%)	1398 (96%)	46 (3%)	4 (0%)	36 72
35	p	1145/1174 (98%)	1106 (97%)	39 (3%)	0	100 100
36	q	253/275 (92%)	245 (97%)	8 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	r	126/142 (89%)	126 (100%)	0	0	100	100
38	s	207/210 (99%)	203 (98%)	4 (2%)	0	100	100
39	t	80/127 (63%)	79 (99%)	1 (1%)	0	100	100
40	u	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
41	v	146/150 (97%)	141 (97%)	5 (3%)	0	100	100
42	w	112/125 (90%)	109 (97%)	3 (3%)	0	100	100
43	x	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
44	y	113/117 (97%)	110 (97%)	3 (3%)	0	100	100
45	z	42/58 (72%)	40 (95%)	2 (5%)	0	100	100
All	All	12996/22270 (58%)	12409 (96%)	565 (4%)	22 (0%)	44	77

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	5	48	GLU
14	E	523	VAL
17	H	156	PRO
25	S	87	VAL
34	o	1103	THR

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	164/283 (58%)	158 (96%)	6 (4%)	30	51
2	1	241/484 (50%)	241 (100%)	0	100	100
3	2	295/352 (84%)	294 (100%)	1 (0%)	86	85
4	3	234/272 (86%)	232 (99%)	2 (1%)	70	78
5	4	346/399 (87%)	339 (98%)	7 (2%)	48	66
6	5	48/64 (75%)	47 (98%)	1 (2%)	47	65
7	6	536/688 (78%)	535 (100%)	1 (0%)	87	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	7	624/664 (94%)	624 (100%)	0	100 100
9	N	2/2 (100%)	2 (100%)	0	100 100
11	A	496/1665 (30%)	452 (91%)	44 (9%)	9 27
12	B	876/1083 (81%)	862 (98%)	14 (2%)	55 69
13	D	147/815 (18%)	136 (92%)	11 (8%)	12 32
13	d	146/815 (18%)	144 (99%)	2 (1%)	59 72
14	E	480/657 (73%)	467 (97%)	13 (3%)	39 60
14	e	475/657 (72%)	462 (97%)	13 (3%)	39 60
15	F	328/574 (57%)	307 (94%)	21 (6%)	16 37
15	f	322/574 (56%)	312 (97%)	10 (3%)	35 56
16	G	132/322 (41%)	124 (94%)	8 (6%)	17 38
17	H	181/270 (67%)	175 (97%)	6 (3%)	33 54
18	I	106/235 (45%)	106 (100%)	0	100 100
18	i	107/235 (46%)	107 (100%)	0	100 100
19	J	79/154 (51%)	72 (91%)	7 (9%)	9 27
19	j	83/154 (54%)	82 (99%)	1 (1%)	63 74
20	L	71/141 (50%)	66 (93%)	5 (7%)	14 35
20	l	98/141 (70%)	97 (99%)	1 (1%)	68 77
21	O	90/98 (92%)	90 (100%)	0	100 100
22	P	154/293 (53%)	154 (100%)	0	100 100
23	Q	105/324 (32%)	105 (100%)	0	100 100
24	R	238/268 (89%)	233 (98%)	5 (2%)	47 65
25	S	154/448 (34%)	134 (87%)	20 (13%)	4 15
26	T	196/218 (90%)	193 (98%)	3 (2%)	57 71
27	U	167/373 (45%)	166 (99%)	1 (1%)	78 82
28	V	150/261 (58%)	149 (99%)	1 (1%)	76 81
31	c	113/833 (14%)	111 (98%)	2 (2%)	51 67
32	k	87/182 (48%)	87 (100%)	0	100 100
33	m	80/106 (76%)	71 (89%)	9 (11%)	5 19
34	o	1280/1749 (73%)	1259 (98%)	21 (2%)	55 69
35	p	1004/1027 (98%)	987 (98%)	17 (2%)	53 68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
36	q	234/252 (93%)	227 (97%)	7 (3%)	36 56
37	r	118/126 (94%)	118 (100%)	0	100 100
38	s	191/192 (100%)	188 (98%)	3 (2%)	55 69
39	t	71/111 (64%)	71 (100%)	0	100 100
40	u	152/153 (99%)	150 (99%)	2 (1%)	61 73
41	v	129/131 (98%)	128 (99%)	1 (1%)	73 79
42	w	103/112 (92%)	99 (96%)	4 (4%)	28 49
43	x	56/56 (100%)	53 (95%)	3 (5%)	20 40
44	y	104/106 (98%)	101 (97%)	3 (3%)	37 57
45	z	41/55 (74%)	40 (98%)	1 (2%)	43 63
All	All	11634/19174 (61%)	11357 (98%)	277 (2%)	43 63

5 of 277 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
36	q	100	GLU
41	v	141	VAL
14	e	512	ASP
14	E	761	LEU
14	E	521	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 207 such sidechains are listed below:

Mol	Chain	Res	Type
27	U	183	GLN
34	o	783	GLN
15	f	273	GLN
28	V	157	GLN
34	o	273	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	Z	4/6 (66%)	2 (50%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
10	Z	4	A
10	Z	6	G2L

There are no RNA pucker outliers to report.

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

5 non-standard protein/DNA/RNA residues are 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	$\#\|Z\| > 2$
10	G2L	Z	6	30,10,48	23,26,30	1.20	3 (13%)	32,38,44	2.06	7 (21%)
9	HYP	N	8	9	6,8,9	0.77	0	5,10,12	2.19	2 (40%)
9	TRX	N	2	9	15,16,17	1.00	1 (6%)	19,22,24	1.54	2 (10%)
9	CSX	N	6	9	3,6,7	1.06	0	1,6,8	2.25	1 (100%)
9	ILX	N	1	9	8,9,10	0.61	0	9,11,13	1.32	2 (22%)

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
10	G2L	Z	6	30,10,48	-	2/9/27/31	0/3/3/3
9	HYP	N	8	9	-	0/0/11/13	0/1/1/1
9	TRX	N	2	9	-	2/5/6/8	0/2/2/2
9	CSX	N	6	9	-	1/1/5/7	-
9	ILX	N	1	9	-	7/11/12/14	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	Z	6	G2L	C5-C4	3.13	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	Z	6	G2L	C6-N1	-2.37	1.34	1.38
10	Z	6	G2L	C5-N7	-2.14	1.34	1.39
9	N	2	TRX	CD2-CE2	2.08	1.44	1.41

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	Z	6	G2L	C5-C4-N3	-6.14	118.50	128.46
9	N	2	TRX	CA-CB-CG	5.20	123.45	113.51
10	Z	6	G2L	C2-N3-C4	4.89	121.02	112.30
10	Z	6	G2L	N9-C4-N3	4.57	135.11	125.94
9	N	8	HYP	O-C-CA	-3.28	116.19	124.78

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	N	1	ILX	C-CA-CB-CG2
9	N	1	ILX	OD1-CD1-CG1-CB
9	N	1	ILX	OD1-CD1-CG1-OG1
9	N	6	CSX	N-CA-CB-SG
10	Z	6	G2L	C3'-C4'-C5'-O5'

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	Z	6	G2L	3	0
9	N	8	HYP	1	0
9	N	2	TRX	2	0
9	N	6	CSX	1	0
9	N	1	ILX	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 18 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
47	SF4	7	1000	8	0,12,12	-	-	-		
49	W0F	p	1201	-	31,35,35	2.89	10 (32%)	38,55,55	3.53	16 (42%)

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
47	SF4	7	1000	8	-	-	0/6/5/5
49	W0F	p	1201	-	-	3/24/40/40	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	p	1201	W0F	C03-C04	-9.40	1.27	1.52
49	p	1201	W0F	O05-C04	6.83	1.60	1.45
49	p	1201	W0F	O05-C06	-5.84	1.28	1.42
49	p	1201	W0F	C12-C13	5.70	1.47	1.38
49	p	1201	W0F	C13-N09	-3.12	1.34	1.37

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	p	1201	W0F	O05-C06-N09	-14.44	75.37	108.36
49	p	1201	W0F	C07-C06-N09	8.15	136.31	113.22
49	p	1201	W0F	O05-C04-C03	-5.66	92.74	104.87
49	p	1201	W0F	O05-C04-C20	4.79	125.13	109.37
49	p	1201	W0F	O05-C06-C07	-4.10	97.70	106.64

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
49	p	1201	W0F	C20-O21-P22-O24
49	p	1201	W0F	C20-O21-P22-O25
49	p	1201	W0F	C03-C04-C20-O21

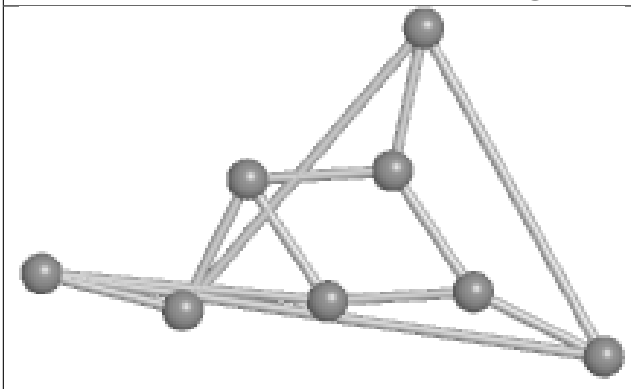
There are no ring outliers.

1 monomer is involved in 8 short contacts:

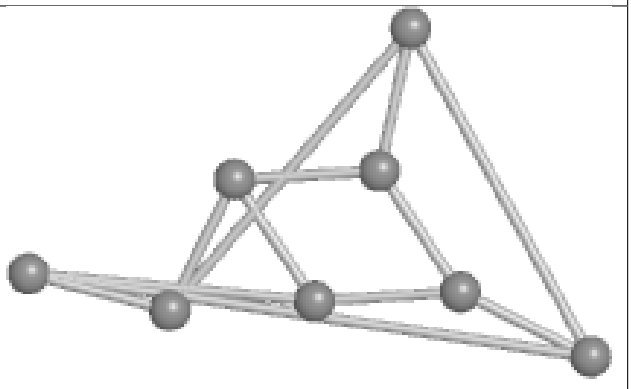
Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	p	1201	W0F	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

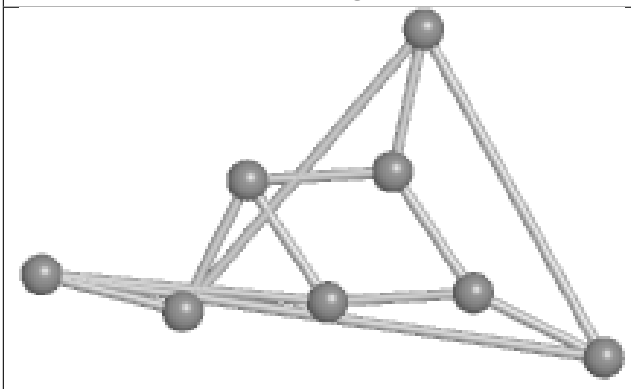
Ligand SF4 7 1000



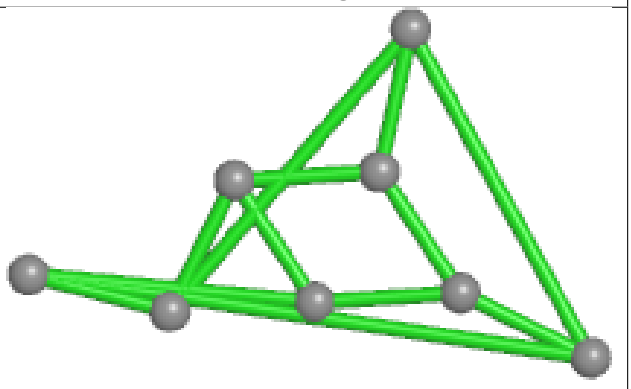
Bond lengths



Bond angles

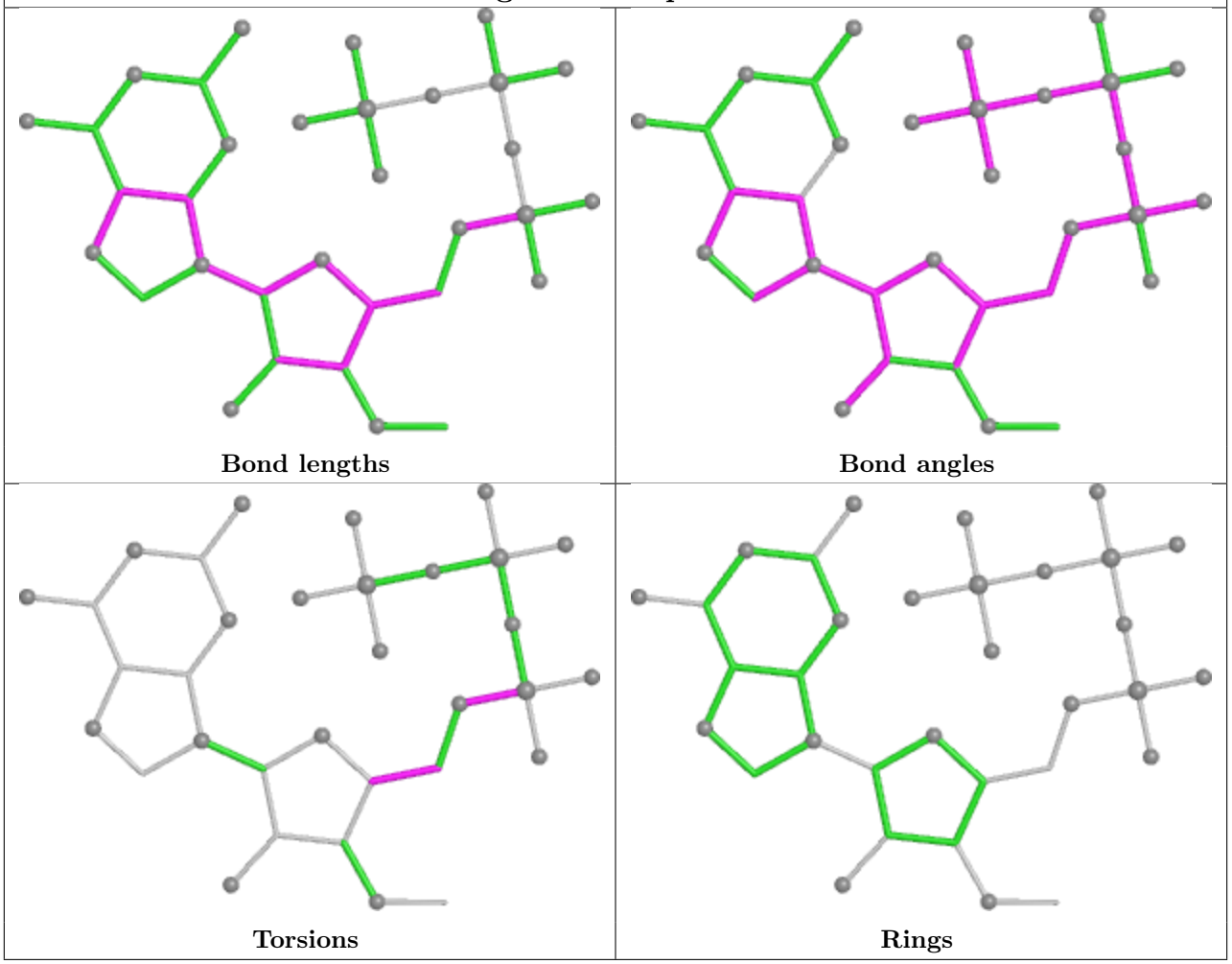


Torsions



Rings

Ligand W0F p 1201



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.

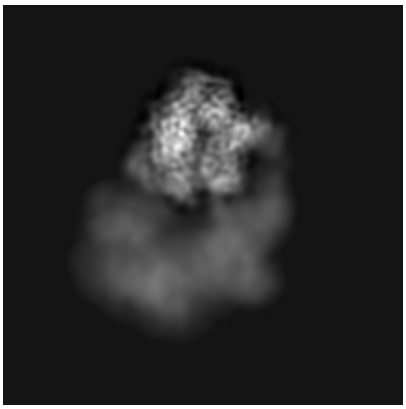
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-37400. These allow visual inspection of the internal detail of the map and identification of artifacts.

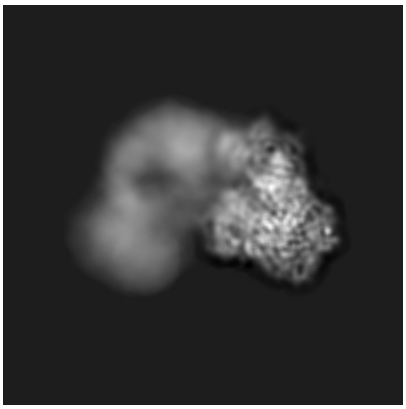
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

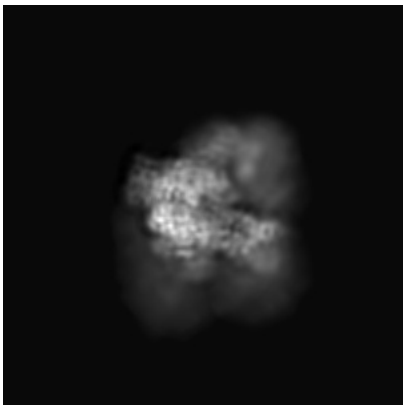
6.1.1 Primary map



X

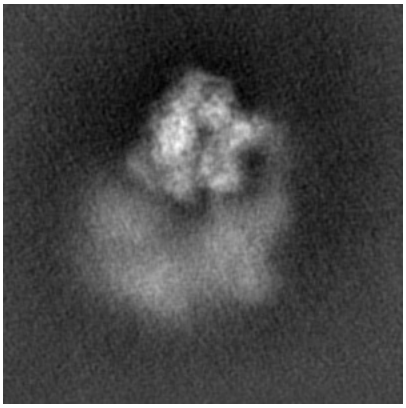


Y

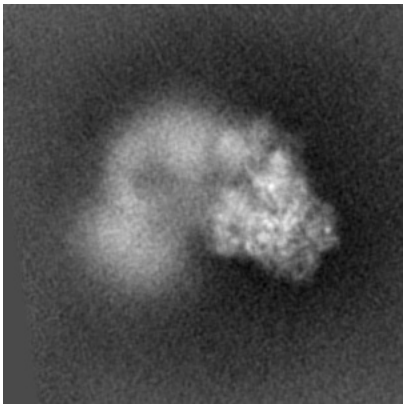


Z

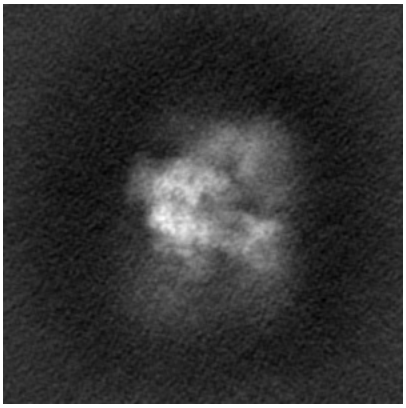
6.1.2 Raw map



X



Y

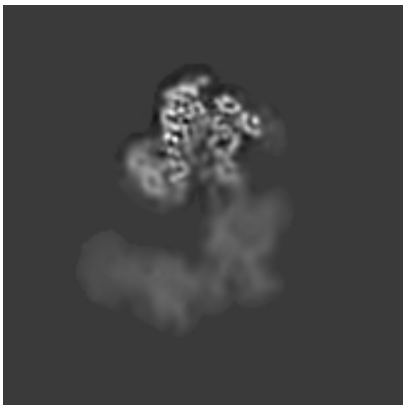


Z

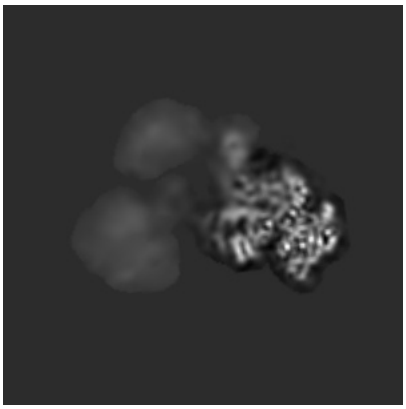
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

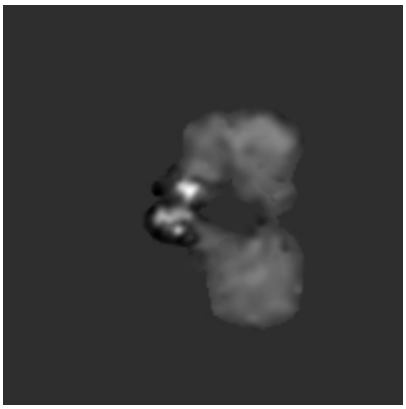
6.2.1 Primary map



X Index: 160

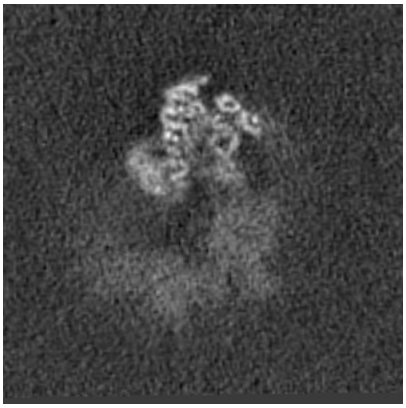


Y Index: 160

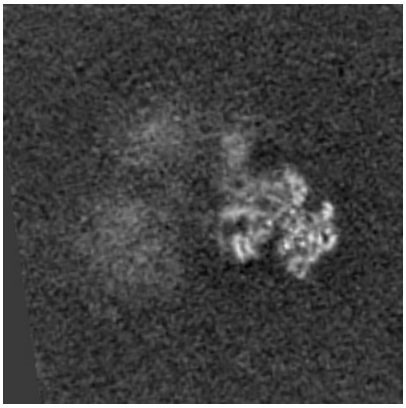


Z Index: 160

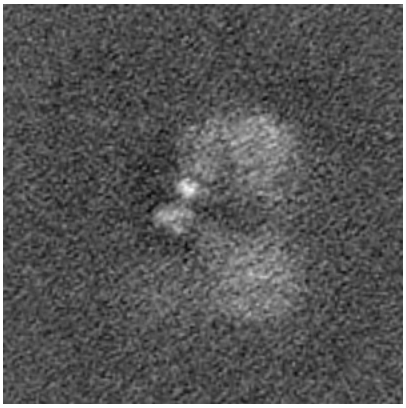
6.2.2 Raw map



X Index: 160



Y Index: 160

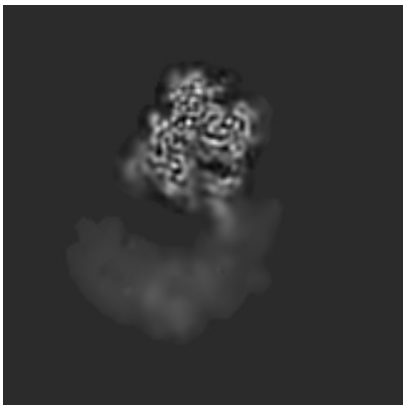


Z Index: 160

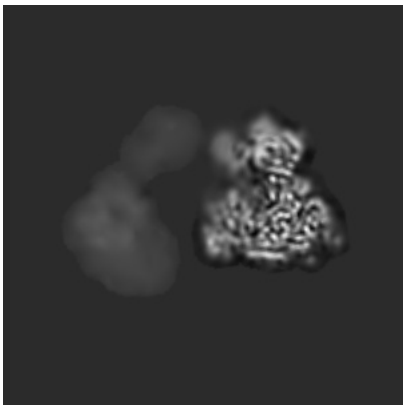
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 146

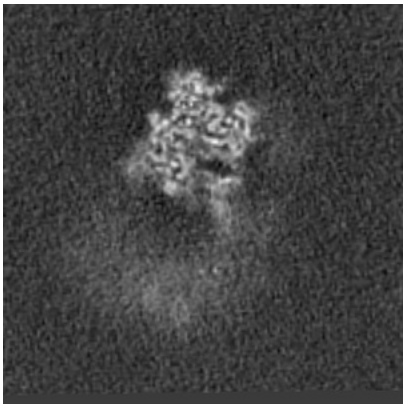


Y Index: 142

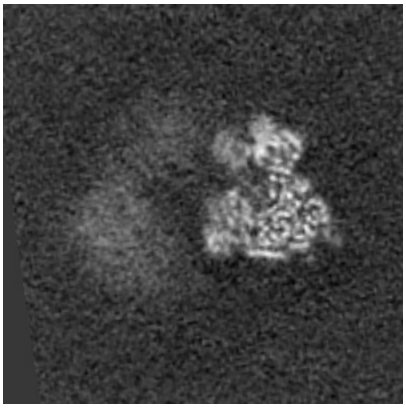


Z Index: 221

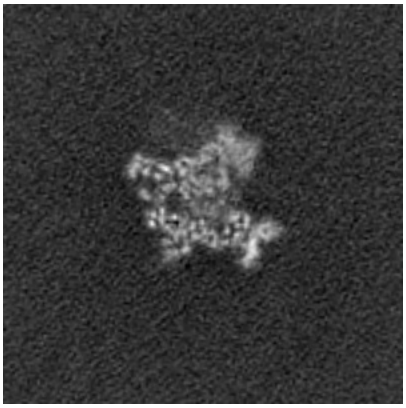
6.3.2 Raw map



X Index: 146



Y Index: 142

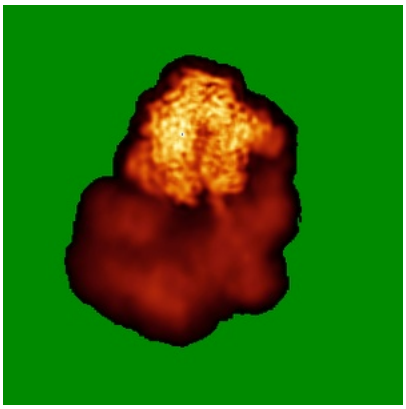


Z Index: 220

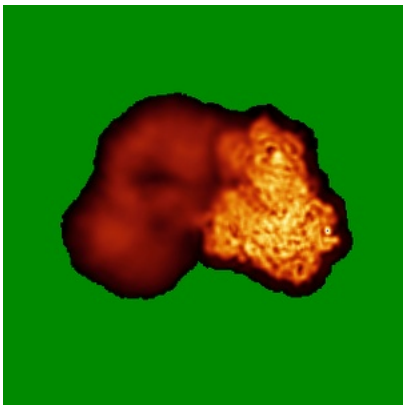
The images above show the largest variance slices of the map in three orthogonal directions.

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

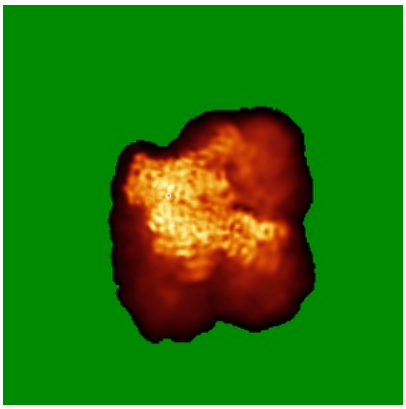
6.4.1 Primary map



X

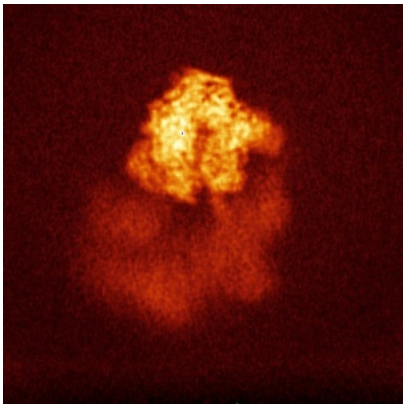


Y

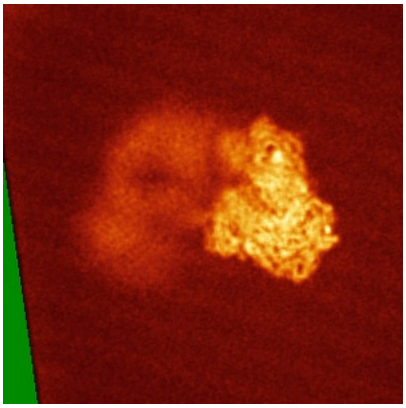


Z

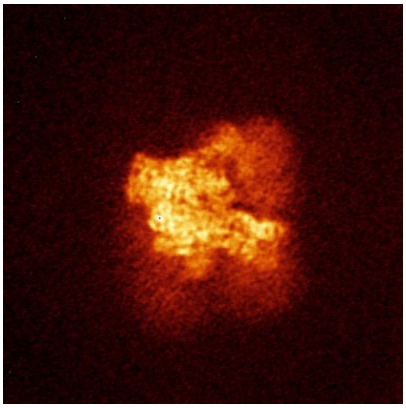
6.4.2 Raw map



X



Y

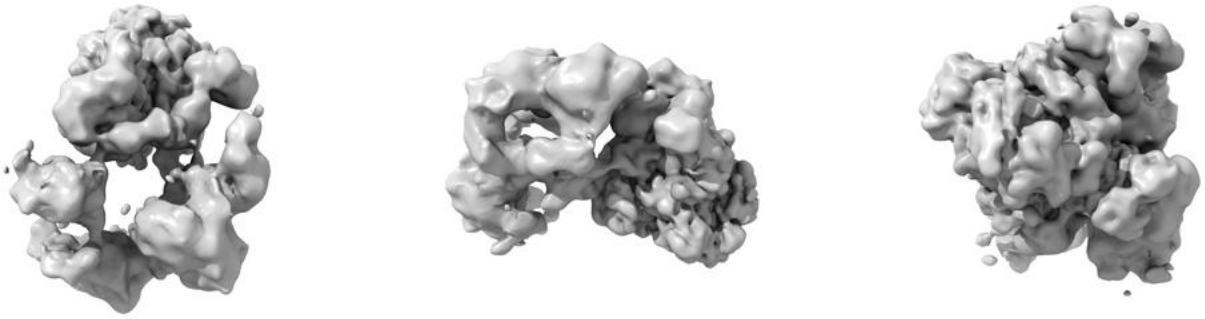


Z

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)

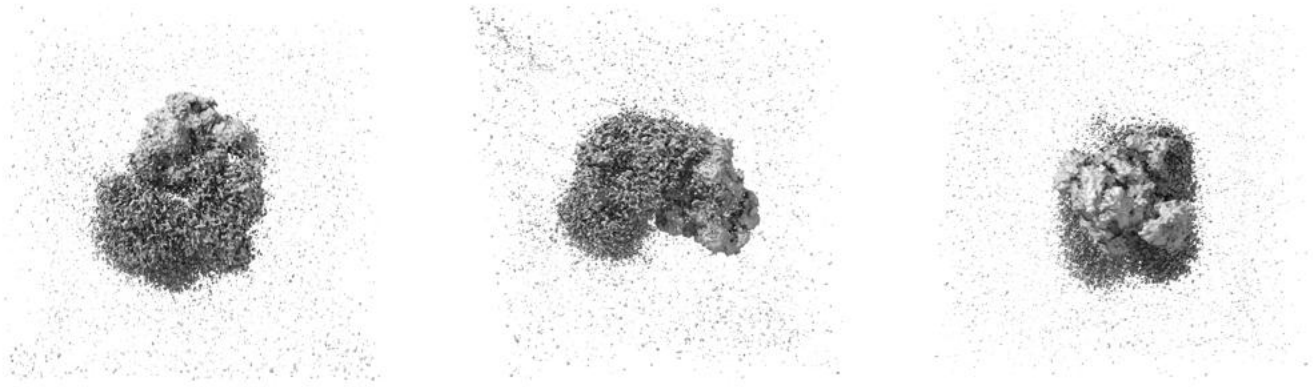
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.48. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

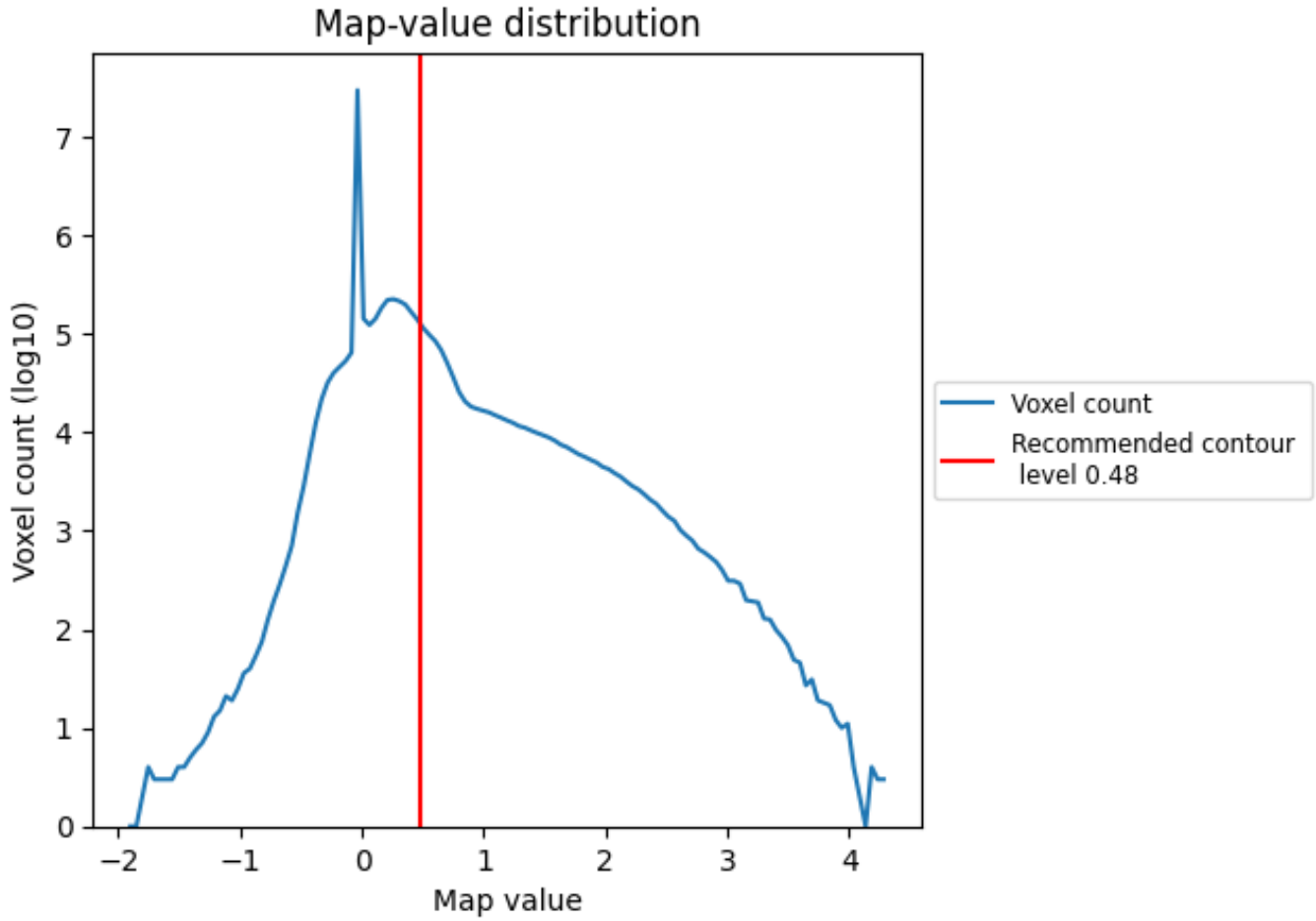
6.6 Mask visualisation (i)

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

7 Map analysis

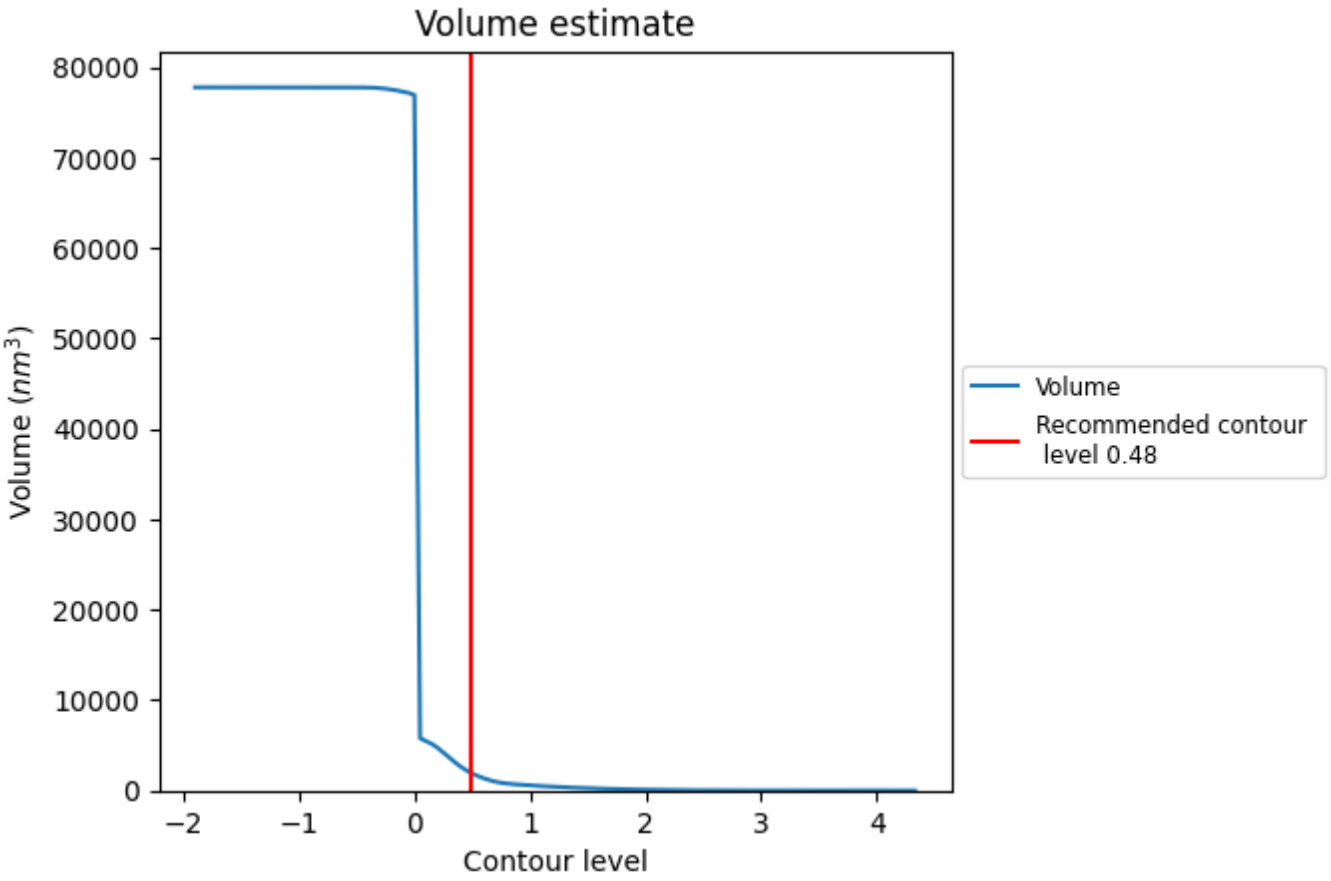
This section contains the results of statistical analysis of the map.

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.

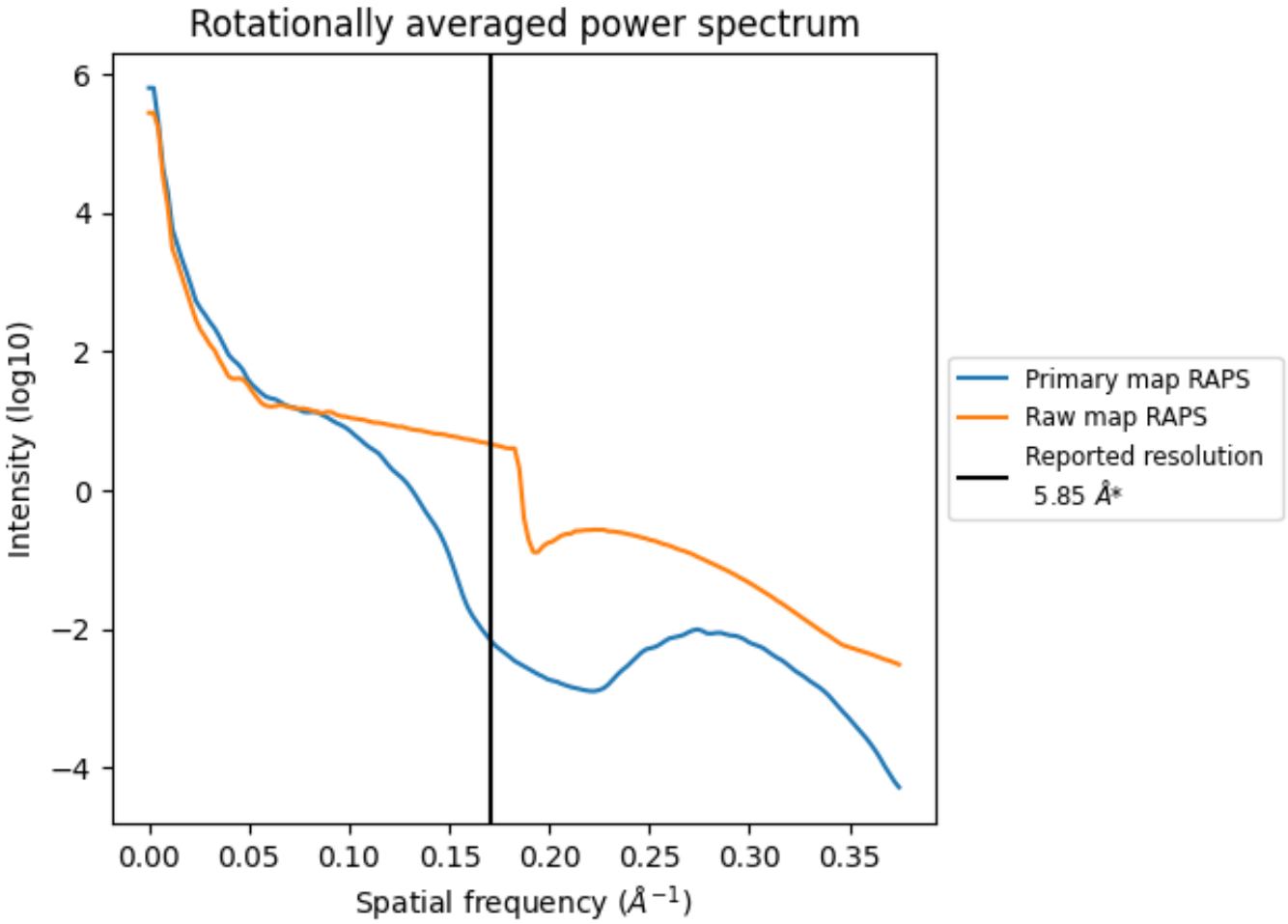
7.2 Volume estimate (i)



The volume at the recommended contour level is 2009 nm^3; this corresponds to an approximate mass of 1814 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)

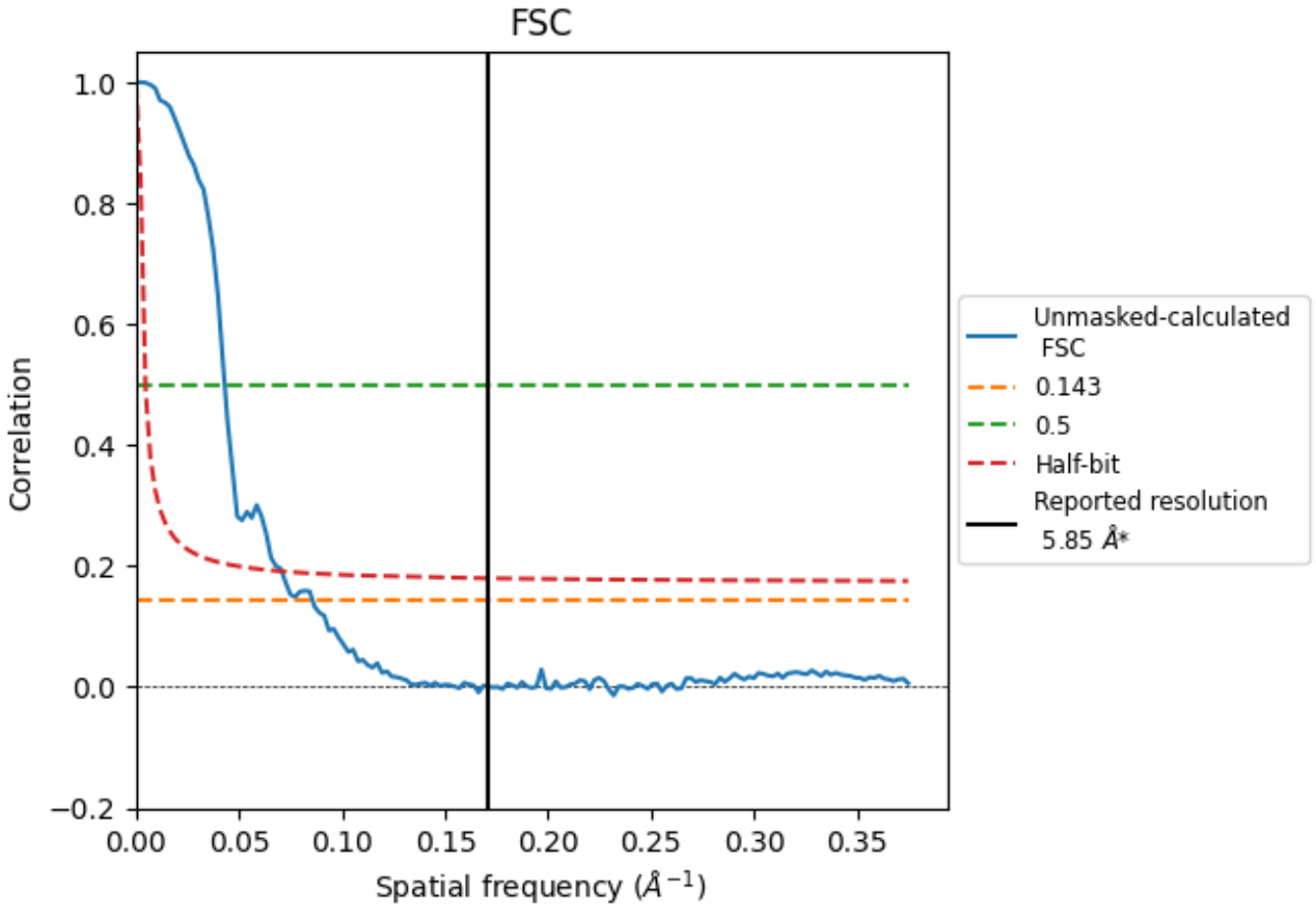


*Reported resolution corresponds to spatial frequency of 0.171 Å^{-1}

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 0.171 Å^{-1}

8.2 Resolution estimates (i)

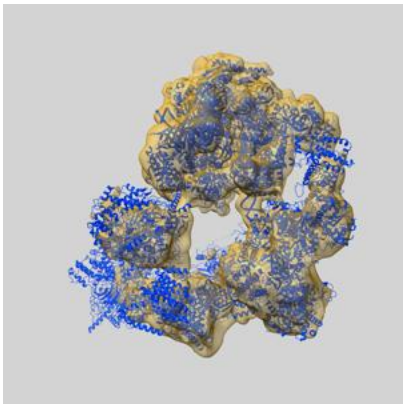
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.85	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	11.67	23.20	14.14

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 11.67 differs from the reported value 5.85 by more than 10 %

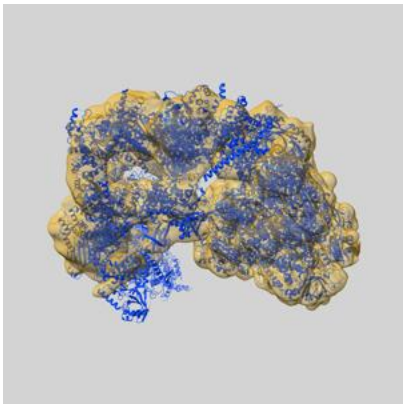
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-37400 and PDB model 8WAP. Per-residue inclusion information can be found in section 3 on page 14.

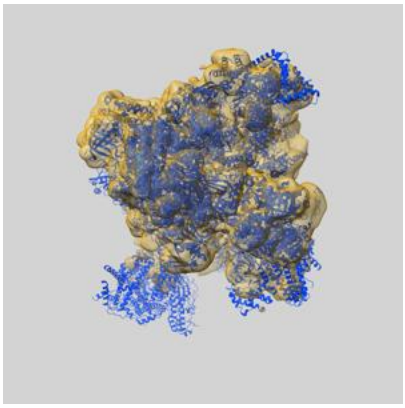
9.1 Map-model overlay



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.48 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.

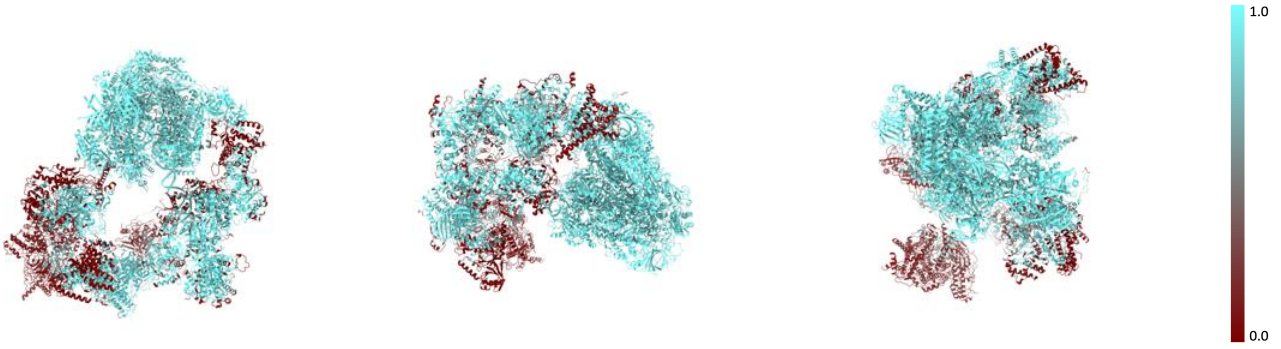
9.2 Q-score mapped to coordinate model (i)



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.

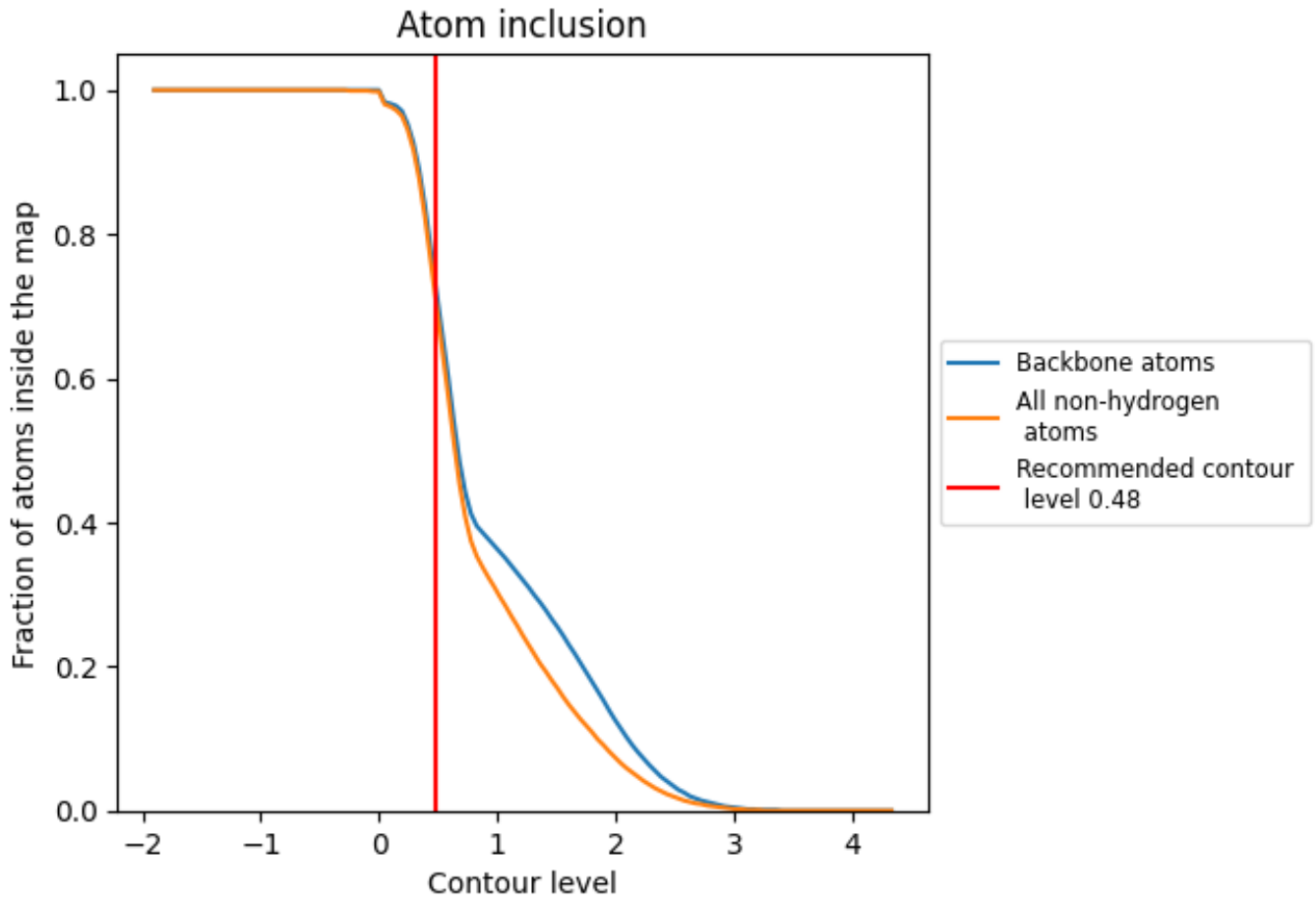
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.48).

9.4 Atom inclusion (i)



At the recommended contour level, 73% of all backbone atoms, 71% 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 (0.48) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7070	0.0810
0	0.0850	0.0580
1	0.6720	0.0530
2	0.9000	0.0640
3	0.8560	0.0400
4	0.7540	0.0630
5	0.5150	0.0160
6	0.6080	0.0420
7	0.7250	0.0570
A	0.2400	0.0310
B	0.9210	0.0510
D	0.3090	0.0290
E	0.6590	0.0430
F	0.4410	0.0270
G	0.0060	0.0170
H	0.8210	0.0420
I	0.4600	0.0240
J	0.6430	0.0680
L	0.1310	0.0450
N	0.9680	0.1310
O	0.9630	0.0830
P	0.9880	0.1260
Q	0.9510	0.1080
R	0.9600	0.1440
S	0.9270	0.0970
T	0.9660	0.1290
U	0.9530	0.0850
V	0.9700	0.1040
X	0.9870	0.1710
Y	0.9310	0.1480
Z	0.8990	0.1510
c	0.2340	0.0380
d	0.0000	0.0040
e	0.0980	0.0150
f	0.4770	0.0540



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Chain	Atom inclusion	Q-score
i	0.1270	0.0230
j	0.1030	0.0390
k	0.0000	-0.0130
l	0.0020	0.0420
m	0.0000	-0.0040
o	0.9420	0.1420
p	0.9310	0.1390
q	0.9610	0.1560
r	0.9860	0.1340
s	0.9670	0.1590
t	0.9670	0.1550
u	0.9830	0.1100
v	0.9680	0.1590
w	0.9630	0.1380
x	0.9420	0.1270
y	0.9580	0.1560
z	0.9780	0.1610