Full wwPDB EM Validation Report (i)

Nov 22, 2022 – 01:06 PM JST

PDB ID	:	7EGA
EMDB ID	:	EMD-31110
Title	:	TFIID-based intermediate PIC on PUMA promoter
Authors	:	Chen, X.; Wu, Z.; Hou, H.; Qi, Y.; Wang, X.; Li, J.; Xu, Y.
Deposited on	:	2021-03-24
Resolution	:	4.10 Å(reported)

This is a Full wwPDB EM Validation 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:

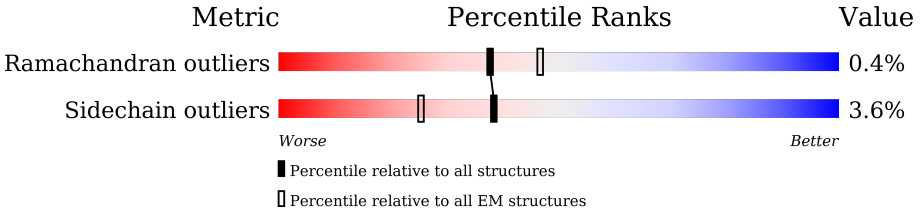
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 4.10 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)
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	12% 29% • 68%
2	B	1199	14% 78% • 20%
3	D	1085	• 12% • 85%
3	d	1085	15% 15% 85%
4	E	800	16% 67% • 32%
4	e	800	58% 67% 33%
5	F	677	19% 56% • 40%
5	f	677	24% 58% • 40%
6	G	349	14% 40% • 58%

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Mol	Chain	Length	Quality of chain
7	H	310	16% 63% 5% 33%
8	I	264	6% 44% 55%
8	i	264	44% 45% 54%
9	J	218	40% 59%
9	j	218	44% 44% 56%
10	L	161	15% 45% 53%
10	l	161	66% 64% 34%
11	O	109	82% 6% 11%
12	P	339	46% 6% 48%
13	Q	376	31% 68%
14	R	316	75% 21%
15	S	517	20% 79%
16	T	249	8% 80% 9% 11%
17	U	439	7% 33% 7% 59%
18	V	291	9% 45% 14% 41%
19	c	929	14% 13% 86%
20	k	211	46% 46% 54%
21	m	124	70% 69% 30%
22	o	1487	95%
23	p	1174	96%
24	q	273	94% 6%
25	r	142	13% 89% 10%
26	s	210	99%
27	t	127	62% 38%
28	v	150	99%

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Mol	Chain	Length	Quality of chain
29	w	125	91% 9%
30	x	64	100%
31	y	117	100%
32	z	58	76% 24%
33	X	85	19% 98%
34	Y	85	21% 100%
35	u	172	8% 98%

2 Entry composition (i)

There are 37 unique types of molecules in this entry. The entry contains 85697 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	602	4927	3142	858	899	28	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	963	7796	5011	1315	1412	58	0	0

- Molecule 3 is a protein called Transcription initiation factor TFIID subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	164	1366	851	256	255	4	0	0
3	d	158	1307	814	238	252	3	0	0

- Molecule 4 is a protein called Transcription initiation factor TFIID subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	546	4364	2766	757	820	21	0	0
4	e	539	4327	2746	748	814	19	0	0

- Molecule 5 is a protein called Transcription initiation factor TFIID subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	404	3081	1954	537	572	18	0	0
5	f	403	3081	1954	533	576	18	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	145	1180	748	217	211	4	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	J	89	709	457	114	134	4	0	0
9	j	95	759	488	124	143	4	0	0

- Molecule 10 is a protein called Transcription initiation factor TFIID subunit 12.

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

- Molecule 11 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	O	97	771	491	133	145	2	0	0

- Molecule 12 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	P	177	1412	918	249	238	7	0	0

- Molecule 13 is a protein called Transcription initiation factor IIA subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	Q	122	996	623	162	207	4	0	0

- Molecule 14 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	R	251	1939	1214	344	364	17	0	0

- Molecule 15 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	S	108	872	558	153	159	2	0	0

- Molecule 16 is a protein called General transcription factor IIF subunit 2.

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

- Molecule 17 is a protein called General transcription factor IIE subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	U	179	1476	932	261	272	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	V	172	1404	893	243	264	4	0	0

- Molecule 19 is a protein called Transcription initiation factor TFIID subunit 3.

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

- Molecule 20 is a protein called Transcription initiation factor TFIID subunit 11.

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

- Molecule 21 is a protein called Transcription initiation factor TFIID subunit 13.

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

- Molecule 22 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	o	1427	11308	7114	2023	2099	72	0	0

- Molecule 23 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	p	1134	9062	5732	1595	1671	64	0	0

- Molecule 24 is a protein called DNA-directed RNA polymerase II subunit RPB3.

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

- Molecule 25 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	r	128	1005	632	172	197	4	0	0

- Molecule 26 is a protein called DNA-directed RNA polymerase II subunit E.

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

- Molecule 27 is a protein called DNA-directed RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	t	79	635	406	108	116	5	0	0

- Molecule 28 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 29 is a protein called DNA-directed RNA polymerase II subunit RPB9.

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

- Molecule 30 is a protein called RPB10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	x	64	507	328	86	87	6	0	0

- Molecule 31 is a protein called RNA_pol_L_2 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	y	117	937	604	154	177	2	0	0

- Molecule 32 is a protein called RPB12.

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

- Molecule 33 is a DNA chain called DNA (85-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
33	X	85	1751	829	329	508	85	0	0

- Molecule 34 is a DNA chain called DNA (85-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
34	Y	85	1734	824	313	512	85	0	0

- Molecule 35 is a protein called DNA-directed RNA polymerase II subunit RPB7.

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

- Molecule 36 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 37 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

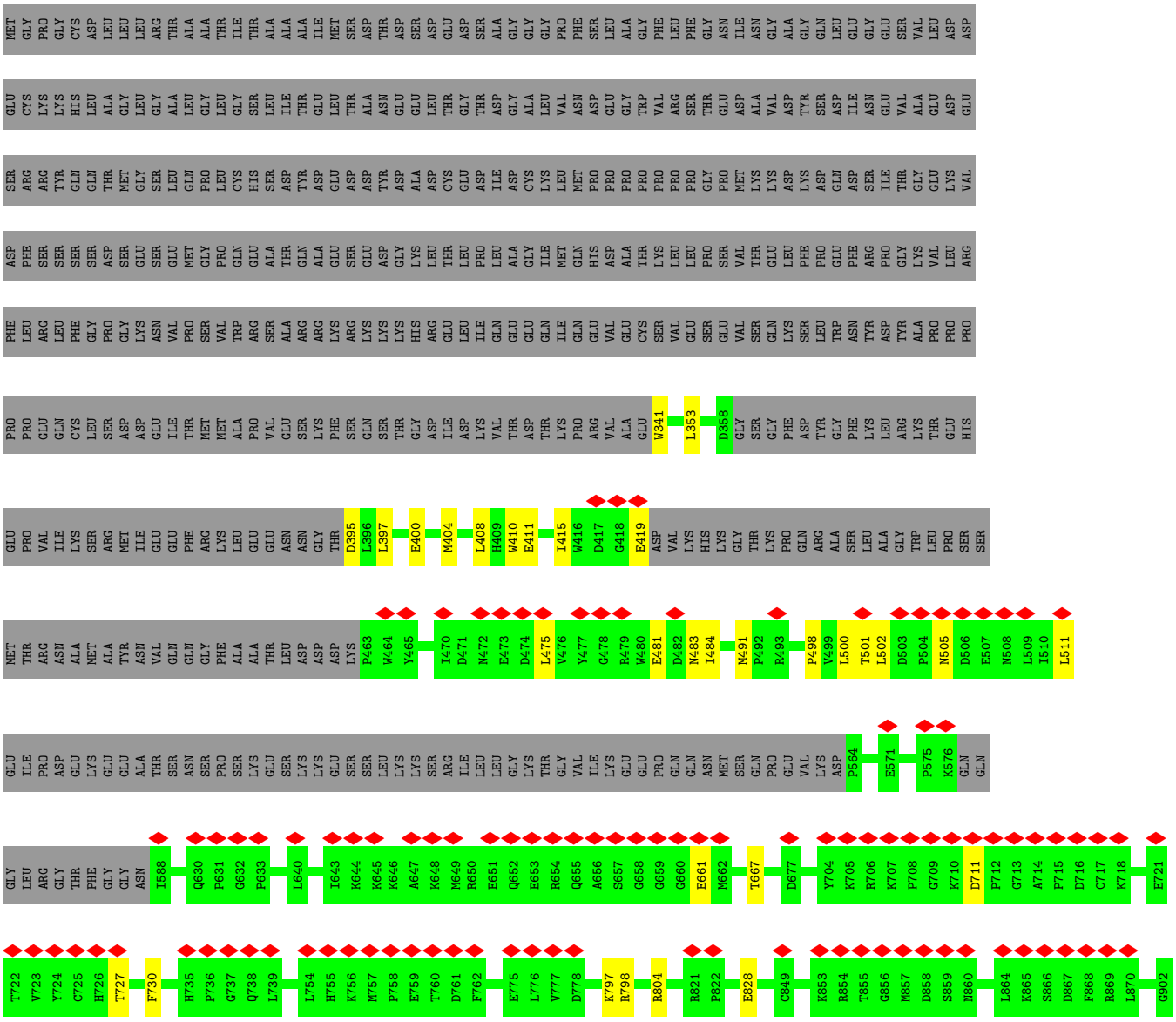
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
37	o	1	1	1	0

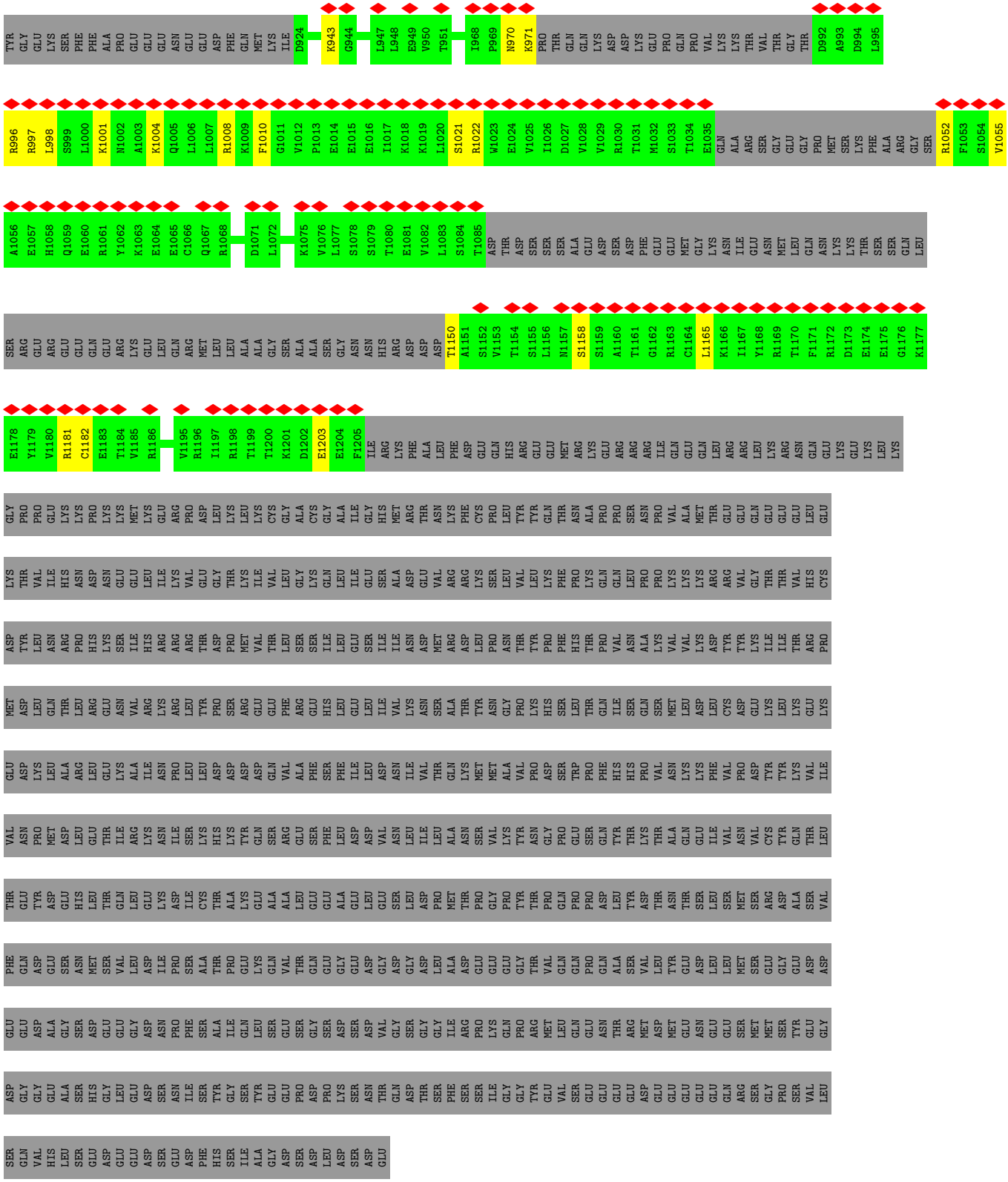
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Transcription initiation factor TFIID subunit 1

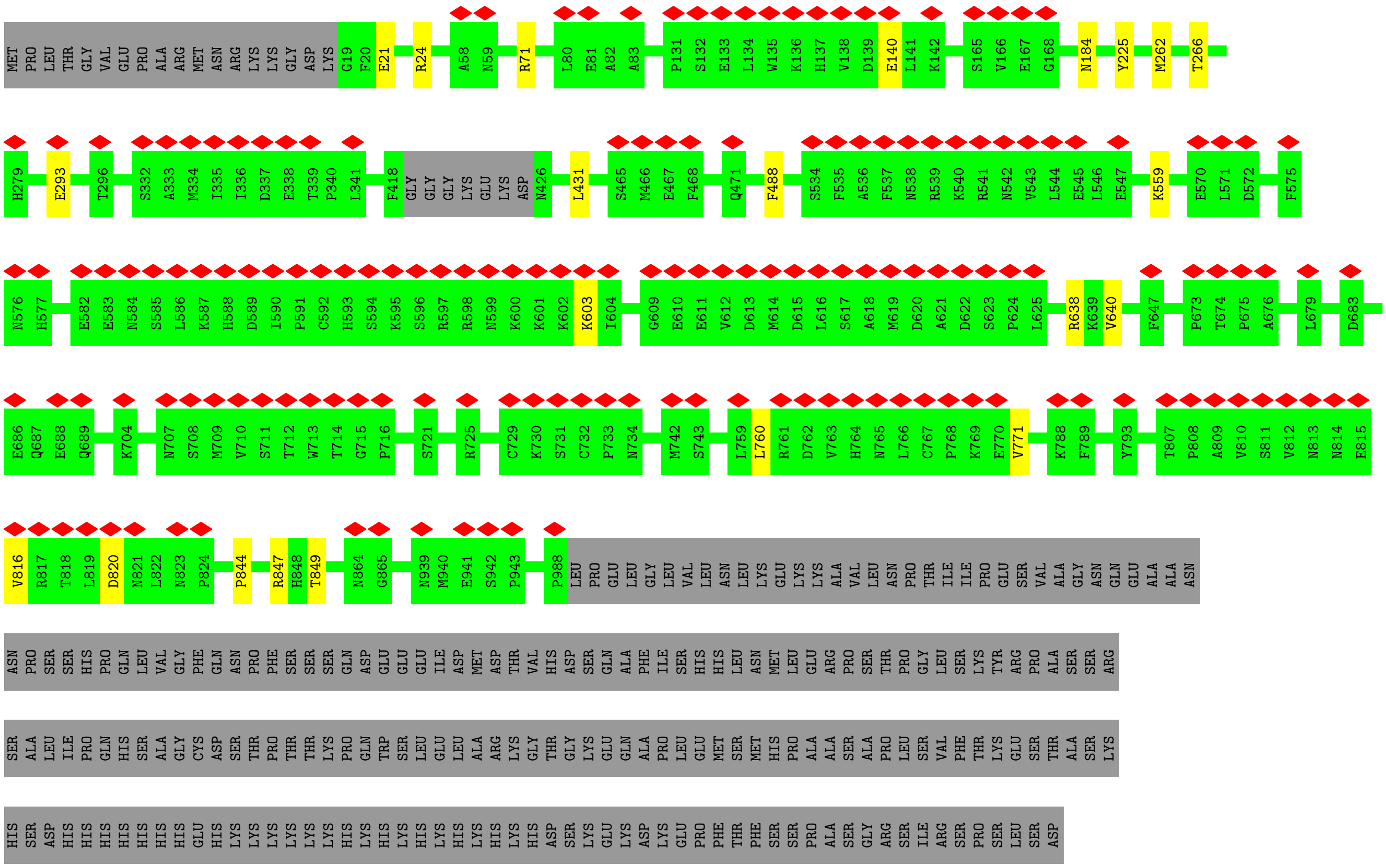
Chain A:





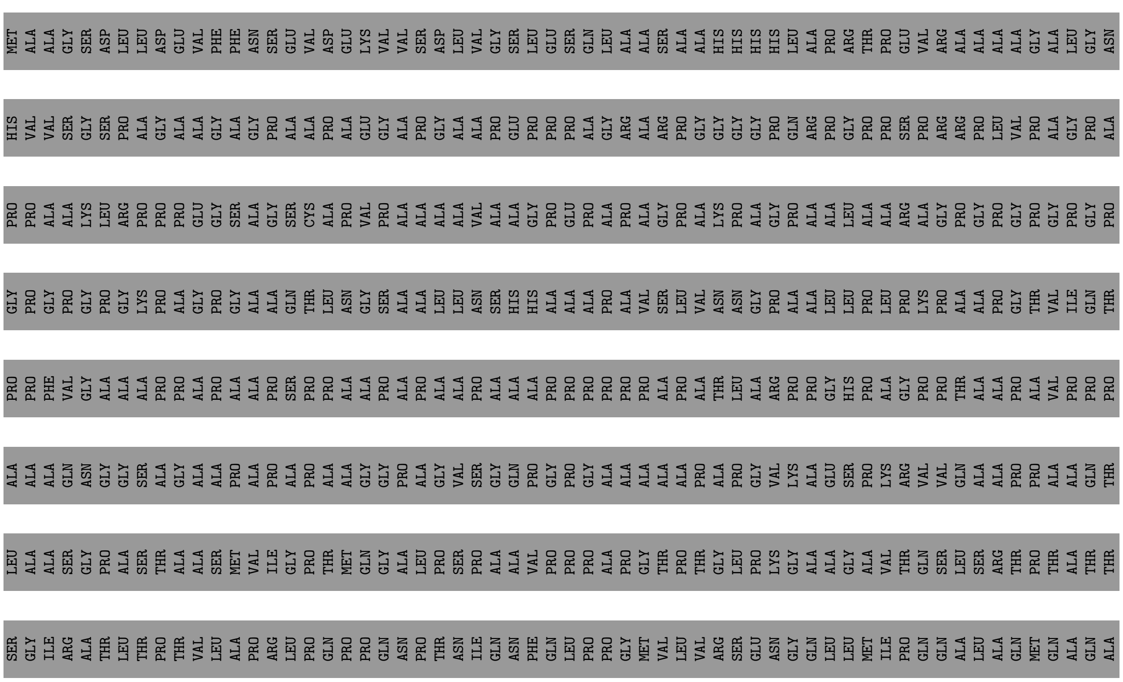
- Molecule 2: Transcription initiation factor TFIID subunit 2

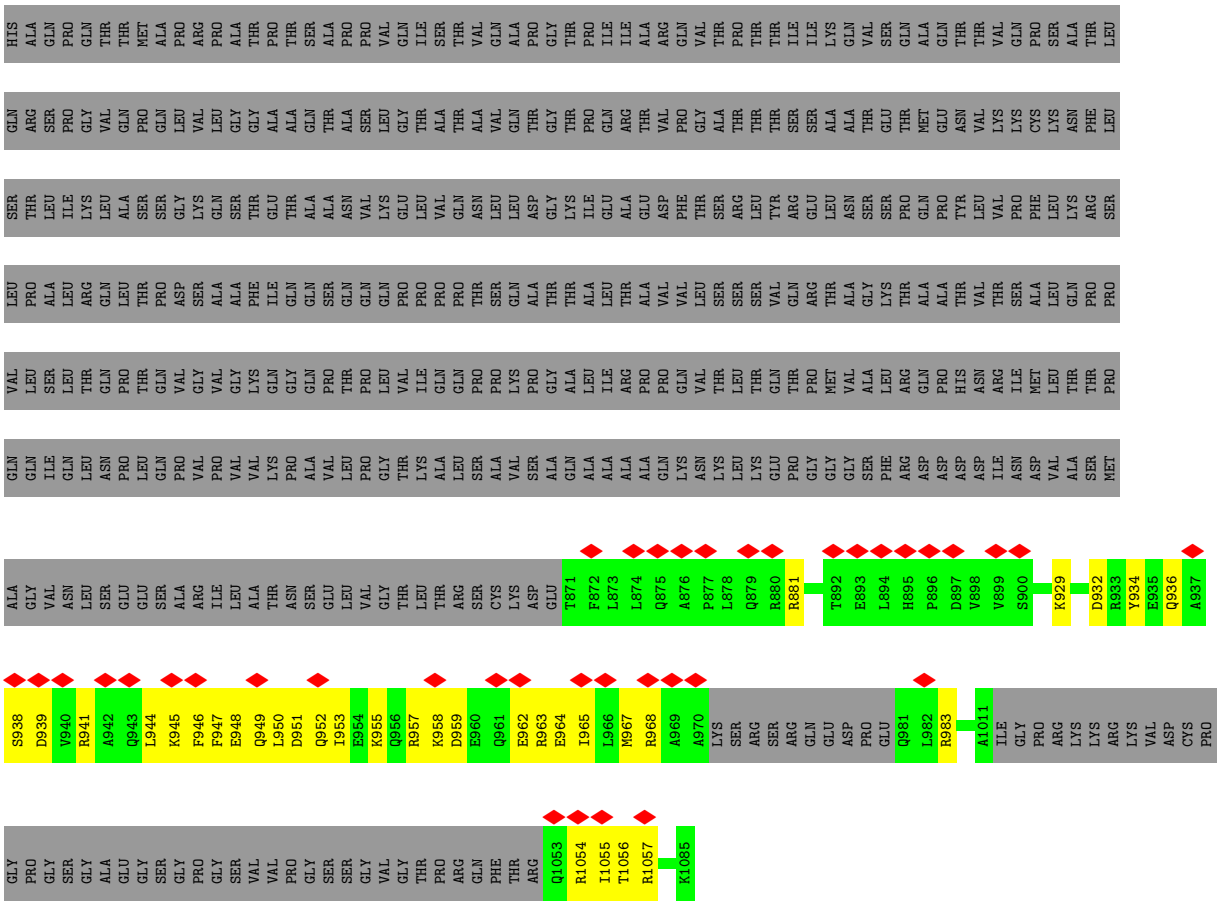
Chain B:



• Molecule 3: Transcription initiation factor TFIID subunit 4

Chain D:





- Molecule 3: Transcription initiation factor TFIID subunit 4

Chain d:

HIS ALA GLN PRO GLN THR THR MET ALA PRO ARG PRO ALA THR PRO THR SER 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 THR VAL GLN PRO SER ALA THR LEU

GLN ARG SER PRO GLY VAL GLN PRO GLN LEU LEU VAL LEU GLY GLY ALA ALA GLN THR ALA SER LEU 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 SER PRO GLN PRO TYR LEU VAL PRO PHE LEU LYS ARG SER

LEU PRO ALA LEU ARG GLN LEU LEU THR PRO ASP SER ALA ALA PHE ILE GLN GLN SER GLN GLN GLN PRO PRO PRO PRO PRO PRO THR SER GLN ALA THR THR ALA ALA VAL VAL LEU SER SER VAL GLN ARG THR THR VAL PRO PHE LEU LYS GLN PRO PRO

VAL LEU SER LEU THR GLN PRO THR GLN VAL GLY VAL GLY LYS GLN GLY GLN PRO THR PRO LEU VAL ILE 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 PRO VAL VAL LYS PRO ALA VAL LEU PRO GLY THR LYS ALA LEU SER ALA VAL SER ALA LYS GLN 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 V843 N844 L845 S846 E847 E848 S849 A850 R851 I852 L853 A854 T855 N856 S857 E858 L859 V860 G861 T862 L863 T864 R865 S866 C867 K868 D869 E870 T871 F872 L873 L874 Q875 A876 P877 L878 Q879 R880 R881 I882 L883 E884 I885 G886 K887 K888 H889 G890 I891 T892 E893 L894 H895 P896 D897 V898 V899 S900

Y901 V902 S903 H904 A905 T906 Q907 Q908 R909 L910 Q911 N912 L913 V914 E915 K916 I917 S918 E919 T920 A921 Q922 Q923 K924 N925 F926 S927 Y928 K929 D930 D931 D932 R933 Y934 E935 Q936 A937 S938 D939 V940 R941 A942 Q943 L944 K945 F946 F947 E948 Q949 L950 D951 Q952 I953 E954 K955 Q956 R957 K958 D959 E960

Q961 E962 R963 E964 I965 L966 M967 R968 ALA ALA LYS SER ARG SER ARG GLN GLU ASP PRO GLU GLN GLN LEU ARG LEU LYS GLN LYS ALA LYS GLU MET GLN GLN GLN GLU LEU ALA GLN MET ARG GLN ARG ASP ALA ASN LEU 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 R1054 I1055 T1056 R1057 V1058 N1059 L1060 R1061 D1062 L1063 I1064 F1065 C1066 L1067 E1068 N1069 E1070 R1071 E1072 T1073 S1074 H1075 S1076 L1077 L1078 L1079 Y1080

K1081 A1082 F1083 L1084 K1085

- Molecule 4: Transcription initiation factor TFIID subunit 5

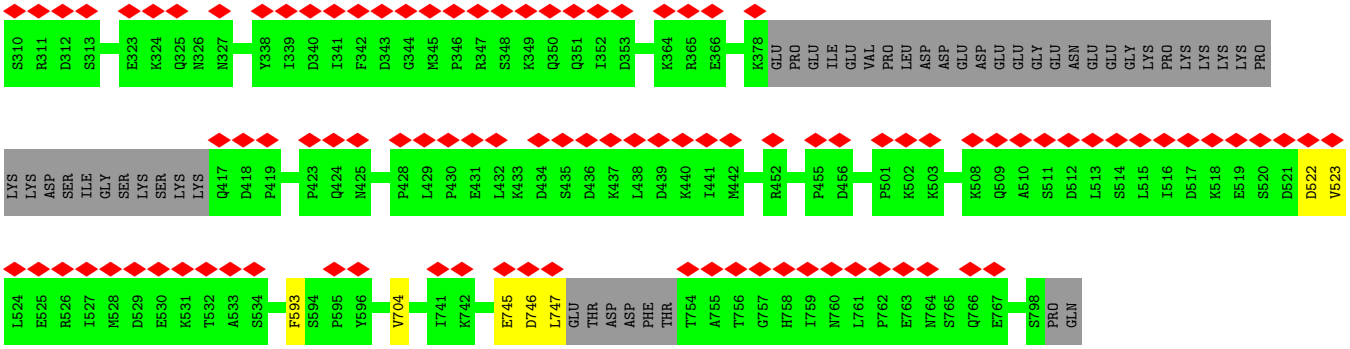
Chain E: 16% 67% • 32%

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

GLY GLY THR PRO LYS PRO THR VAL ALA VAL SER ALA ALA ALA PRO ALA GLY ALA ALA PRO VAL PRO ALA ALA PRO HIS ASP ALA ARG GLN THR LEU LEU ALA VAL LEU GLN PHE LEU ARG GLN SER LYS LEU ARG GLU ALA GLU GLU ALA LEU ARG ARG GLU ALA

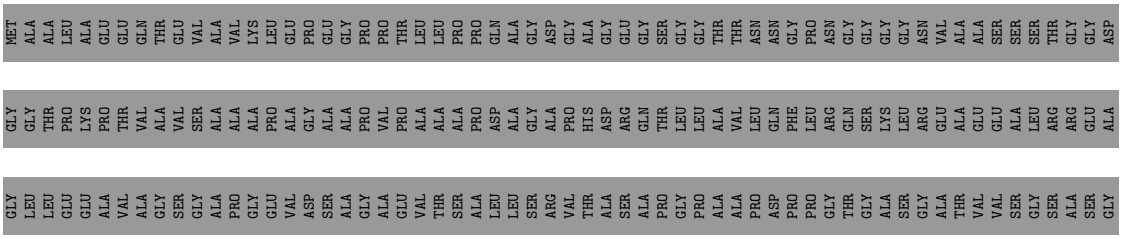
GLY LEU LEU GLU GLU ALA VAL ALA GLY SER GLY ALA ALA PRO GLY GLU VAL ASP SER ALA GLY ALA GLU VAL ALA THR SER ALA LEU LEU SER ARG VAL THR ALA SER ALA PRO GLY PRO ALA ALA PRO ASP PRO PRO GLY THR GLY ALA SER GLY ALA THR VAL VAL SER GLY SER ALA SER GLY

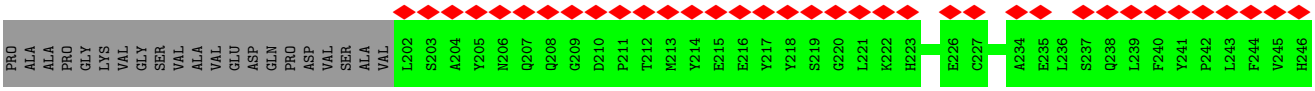
PRO ALA ALA PRO GLY LYS VAL GLY SER VAL ALA VAL GLU ASP GLN PRO ASP VAL SER ALA VAL LEU SER ALA TYR ASN GLN GLN G209 D210 P211 T212 M213 E216 H223 E226 C227 S228 L229 D230 C231 H232 R233 A234 E235 E272 C273 T302 S303 K304 F305 V306 L307 R308 I309

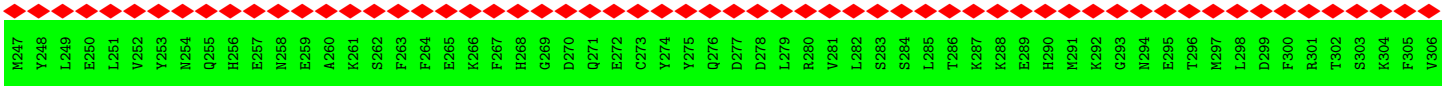


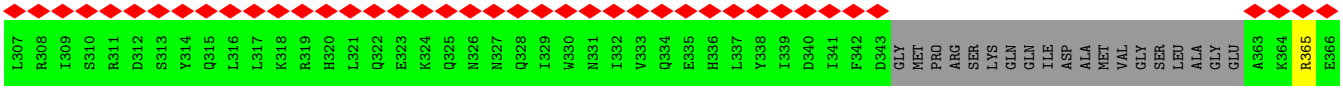
- Molecule 4: Transcription initiation factor TFIID subunit 5

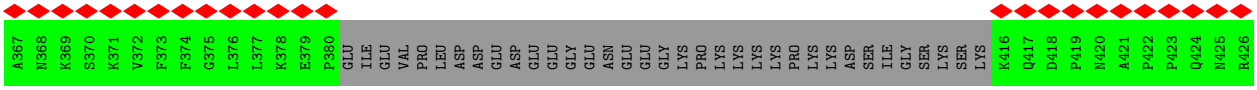
Chain e:

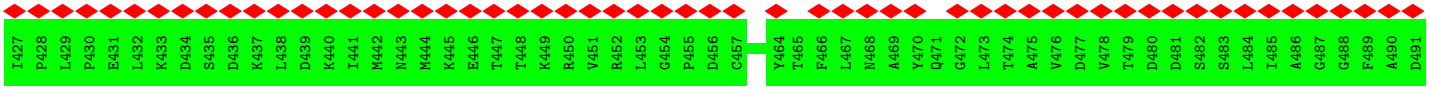


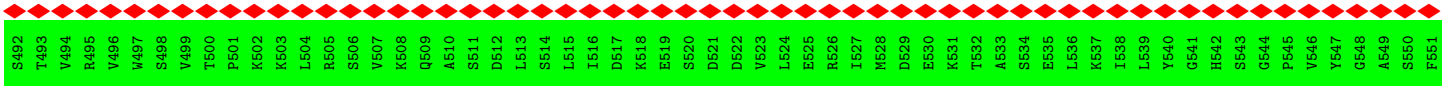


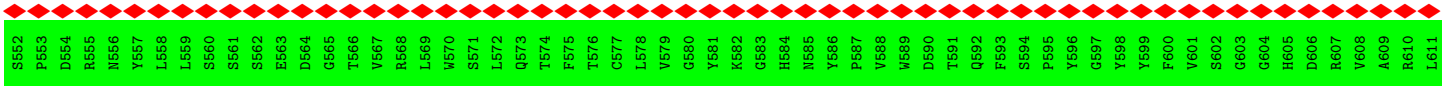


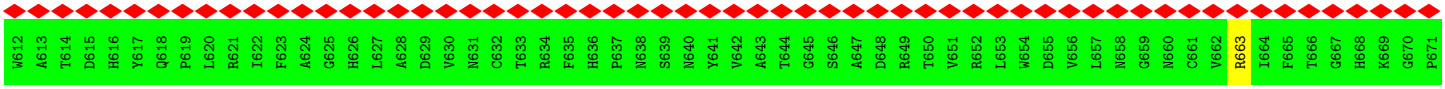






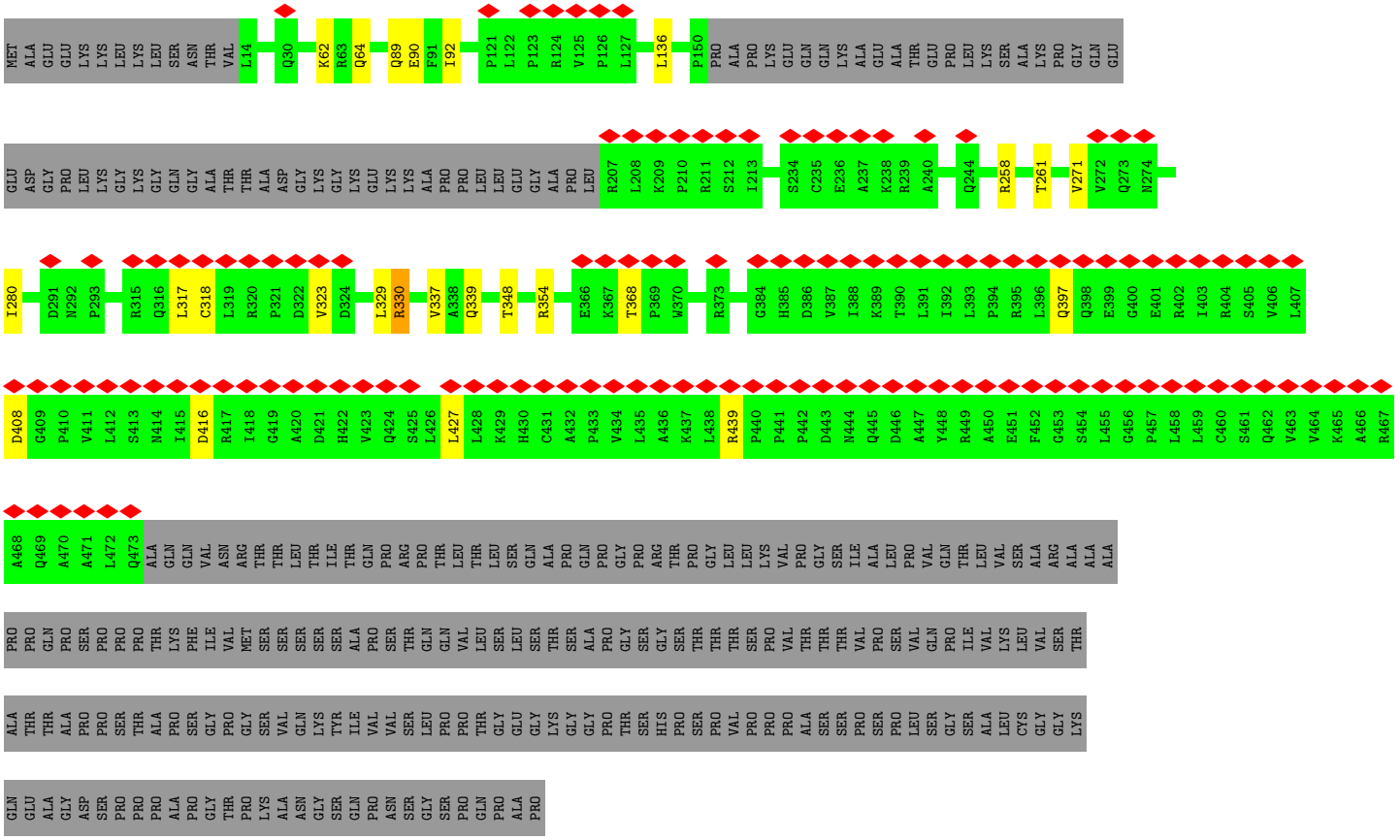






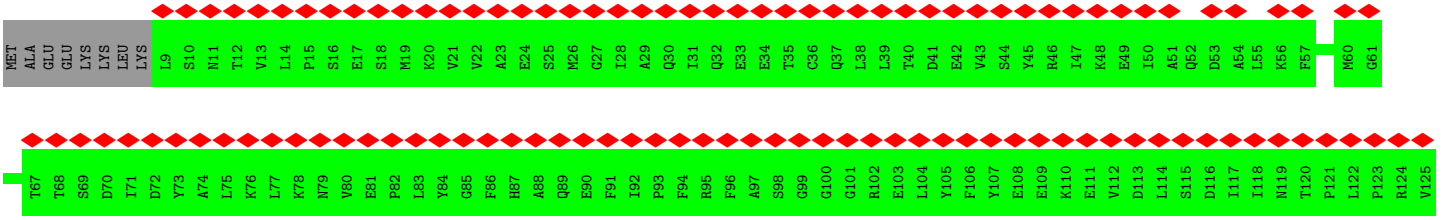
• Molecule 5: Transcription initiation factor TFIID subunit 6

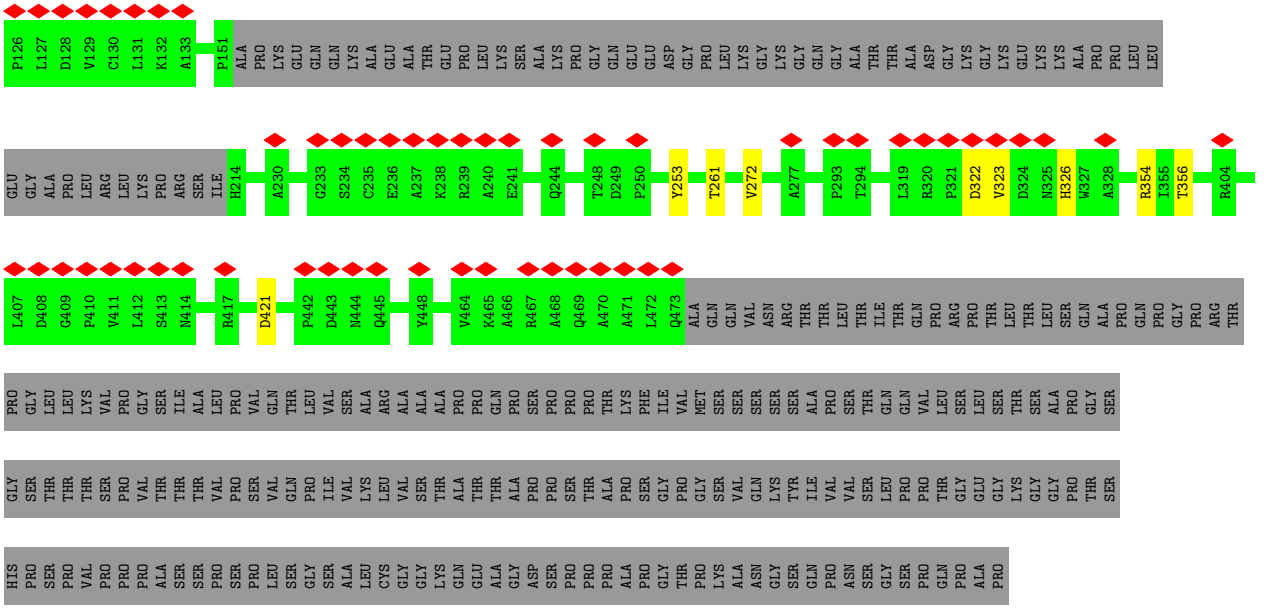
Chain F:



• Molecule 5: Transcription initiation factor TFIID subunit 6

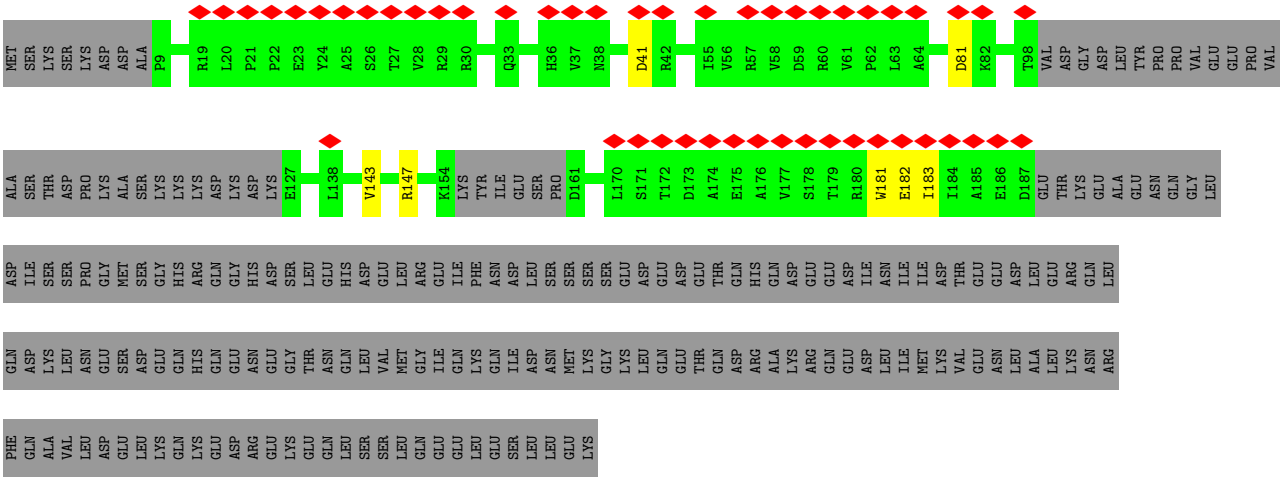
Chain f:





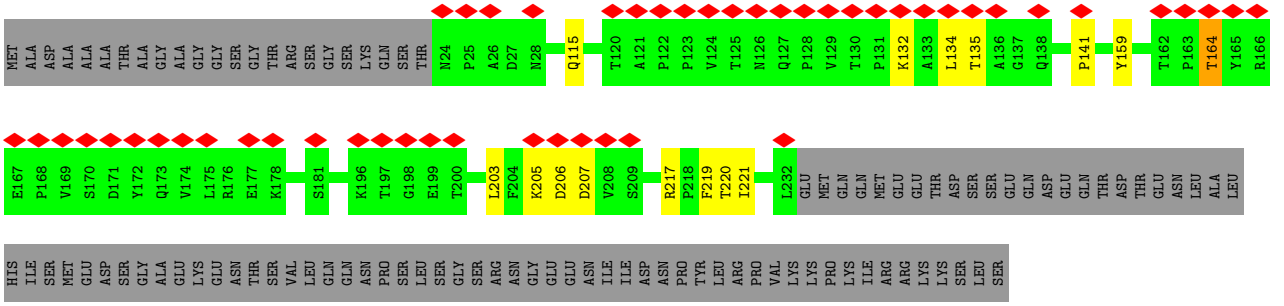
- Molecule 6: Transcription initiation factor TFIID subunit 7

Chain G:



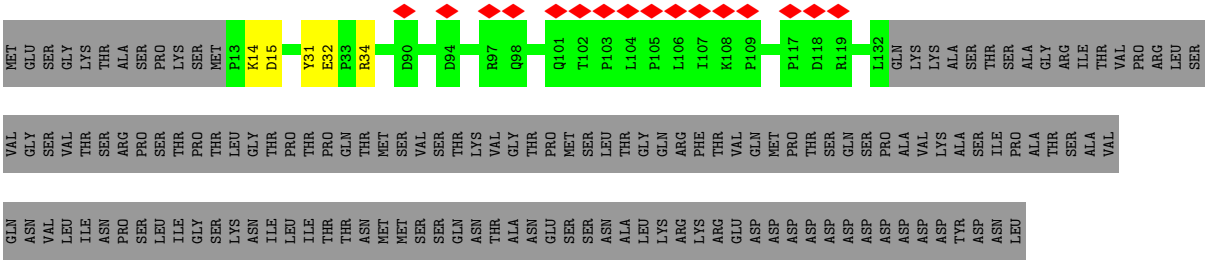
- Molecule 7: Transcription initiation factor TFIID subunit 8

Chain H:



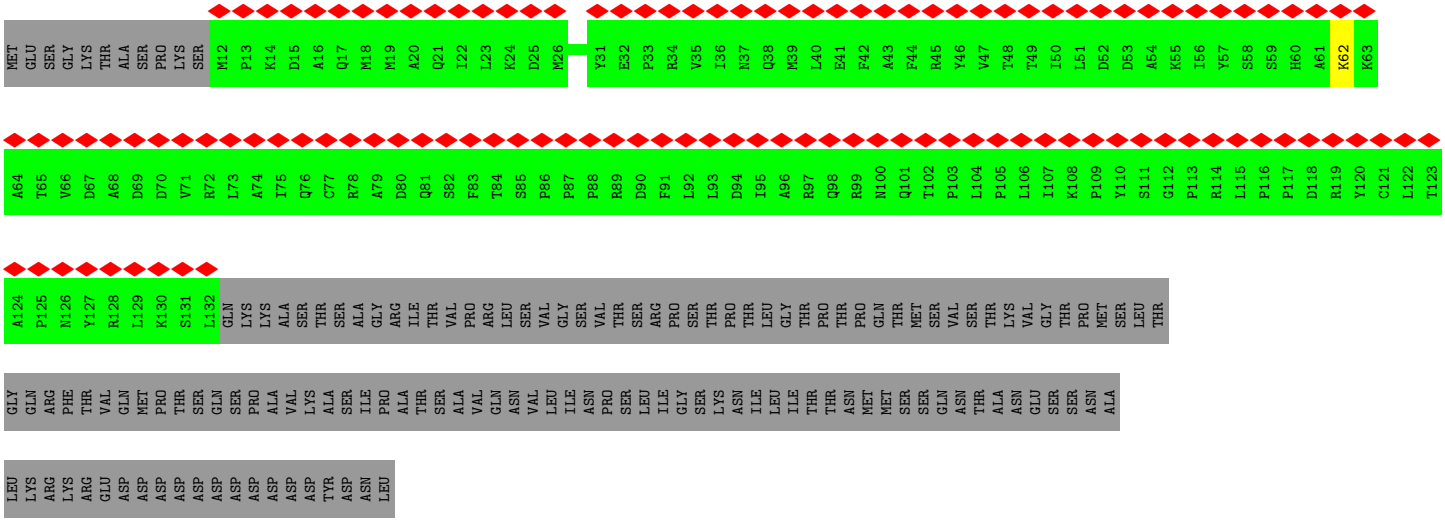
• Molecule 8: Transcription initiation factor TFIID subunit 9

Chain I:



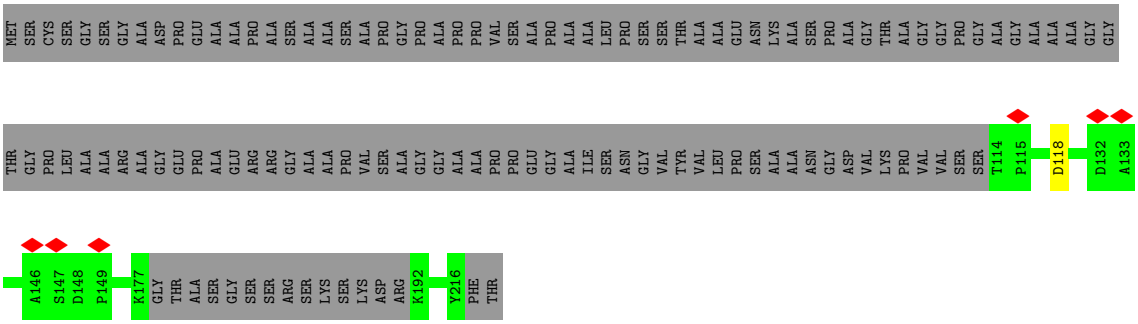
• Molecule 8: Transcription initiation factor TFIID subunit 9

Chain i:



• Molecule 9: Transcription initiation factor TFIID subunit 10

Chain J:



• Molecule 9: Transcription initiation factor TFIID subunit 10

Chain j:

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

THR GLY PRO LEU ALA ALA ARG ALA GLY GLU PRO ALA GLU ARG ARG GLY ALA ALA PRO VAL SER ALA GLY GLY ALA ALA PRO PRO GLU GLY ALA ALA ILE SER ASN GLY VAL TYR VAL LEU PRO SER ALA ALA ASN GLY ASP VAL LYS PRO VAL VAL SER SER T114 P115 L116 V117 D118 F119 L120

M121 Q122 L123 E124 D125 Y126 T127 P128 T129 I130 P131 D132 A133 V134 T135 G136 Y137 Y138 L139 N140 R141 A142 G143 F144 E145 A146 S147 D148 P149 R150 I151 I152 R153 L154 I155 S156 L157 A158 A159 Q160 K161 F162 I163 S164 D165 I166 A167 N168 D169 A170 L171 Q172 H173 C174 K175 M176 K177 G178 THR ALA

SER GLY SER SER ARG SER LYS SER K189 D190 R191 K192 Y193 T194 L195 T196 M197 E198 D199 L200 T201 P202 A203 L204 S205 E206 Y207 G208 I209 N210 V211 K212 K213 P214 H215 Y216 F217 T218

- Molecule 10: Transcription initiation factor TFIID subunit 12

Chain L:

MET ASN GLN PHE GLY PRO SER ALA LEU ILE ASN LEU SER ASN PHE SER SER ILE LYS PRO GLU PRO ALA SER THR PRO PRO GLN GLY SER MET ALA ASN SER THR ALA VAL VAL LYS ILE PRO GLY THR PRO GLY ALA GLY GLY ARG LEU SER PRO GLU ASN N55 Q56 T59 K60 K61

K62 L63 Q64 D65 R68 E69 V70 D71 P72 N73 E74 Q75 L76 D77 E78 D79 V80 E81 E82 L85 Q86 I87 K107 S108 S109 T110 G130 PHE GLY SER GLU GLU ILE ARG PRO TYR LYS LYS ALA CYS THR THR GLU ALA HIS LYS GLN ARG MET ALA LEU ILE ARG LYS THR THR

LYS LYS

- Molecule 10: Transcription initiation factor TFIID subunit 12

Chain l:

MET ASN GLN PHE GLY PRO SER ALA LEU ILE ASN LEU SER ASN PHE SER SER ILE LYS PRO GLU PRO ALA SER THR PRO PRO GLN GLY SER MET ALA ASN SER THR ALA VAL VAL LYS ILE PRO GLY THR PRO GLY ALA GLY GLY ARG LEU SER PRO GLU ASN N55 Q56 V57 L58 T59 K60

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

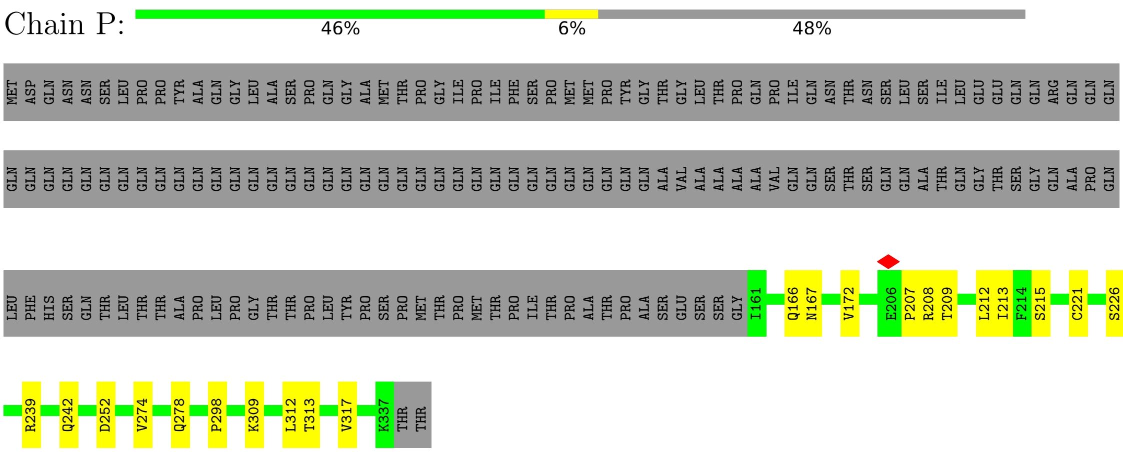
E121 R122 Q123 W124 N125 M126 W127 I128 P129 G130 F131 G132 S133 E134 E135 I136 R137 P138 Y139 K140 K141 A142 C143 T144 T145 E146 A147 H148 K149 Q150 R151 M152 A153 L154 I155 R156 K157 T158 T159 K160 K161

- Molecule 11: Transcription initiation factor IIA subunit 2

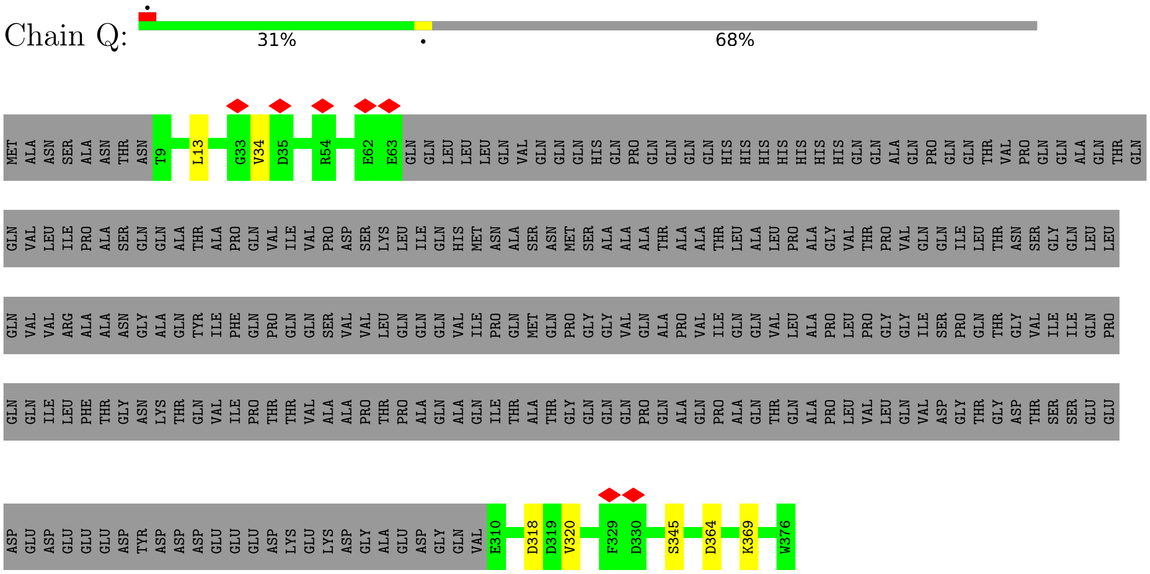
Chain O:

MET ALA Y3 Q24 S25 Q26 P30 Q31 V52 R53 N54 N57 F58 R59 L76 V84 D99 GLY LYS ASN THR GLY SER ASN THR THR GLU

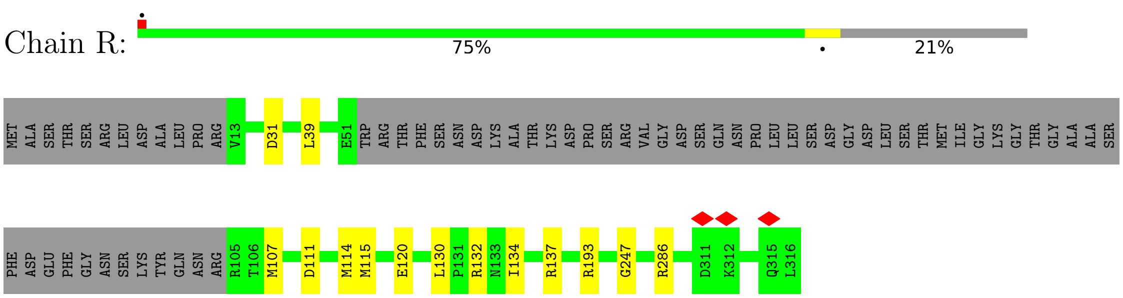
- Molecule 12: TATA-box-binding protein



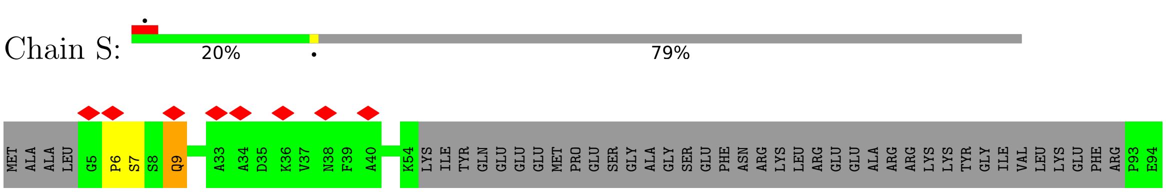
• Molecule 13: Transcription initiation factor IIA subunit 1

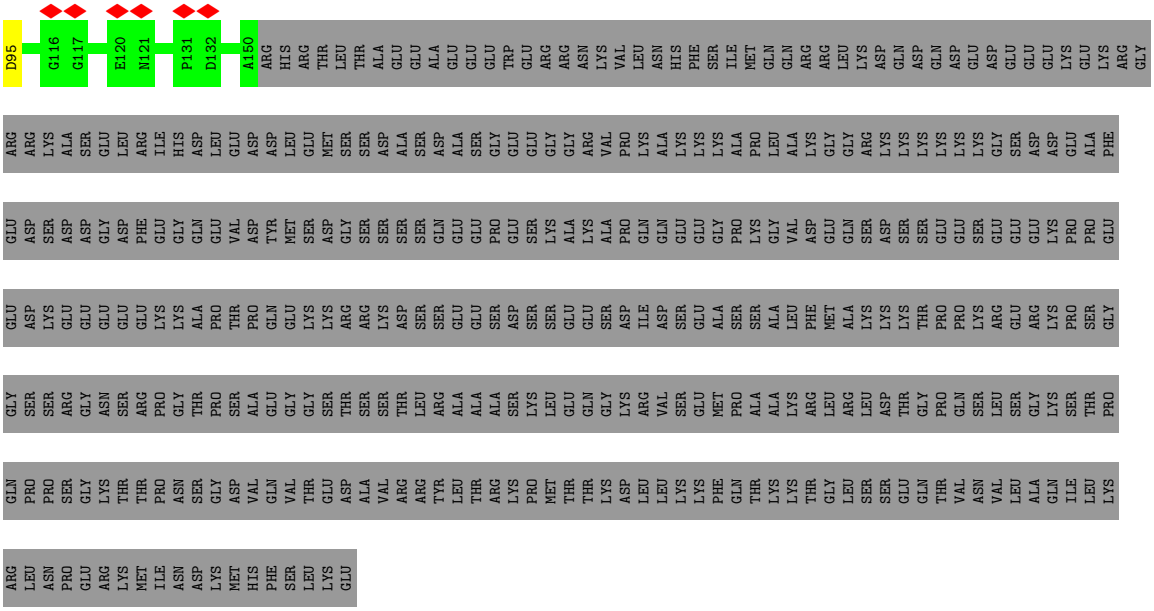


• Molecule 14: Transcription initiation factor IIB



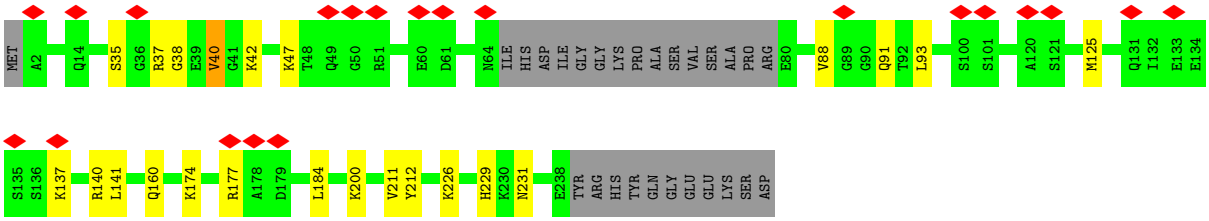
• Molecule 15: General transcription factor IIF subunit 1





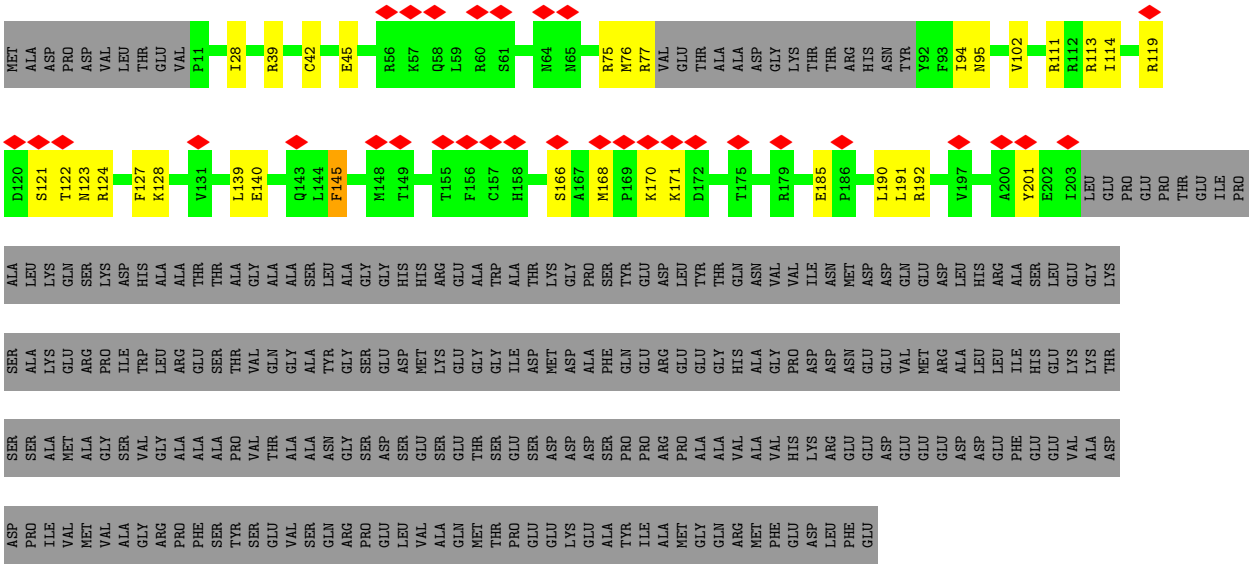
- Molecule 16: General transcription factor IIF subunit 2

Chain T:



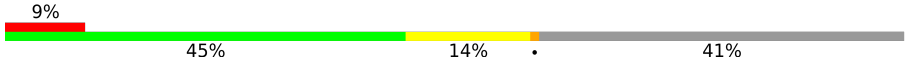
- Molecule 17: General transcription factor IIE subunit 1

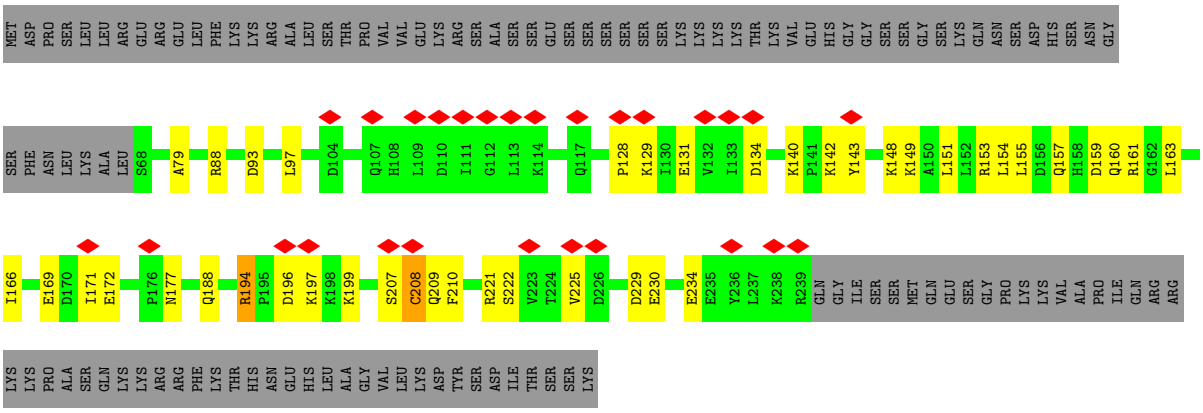
Chain U:



- Molecule 18: Transcription initiation factor IIE subunit beta

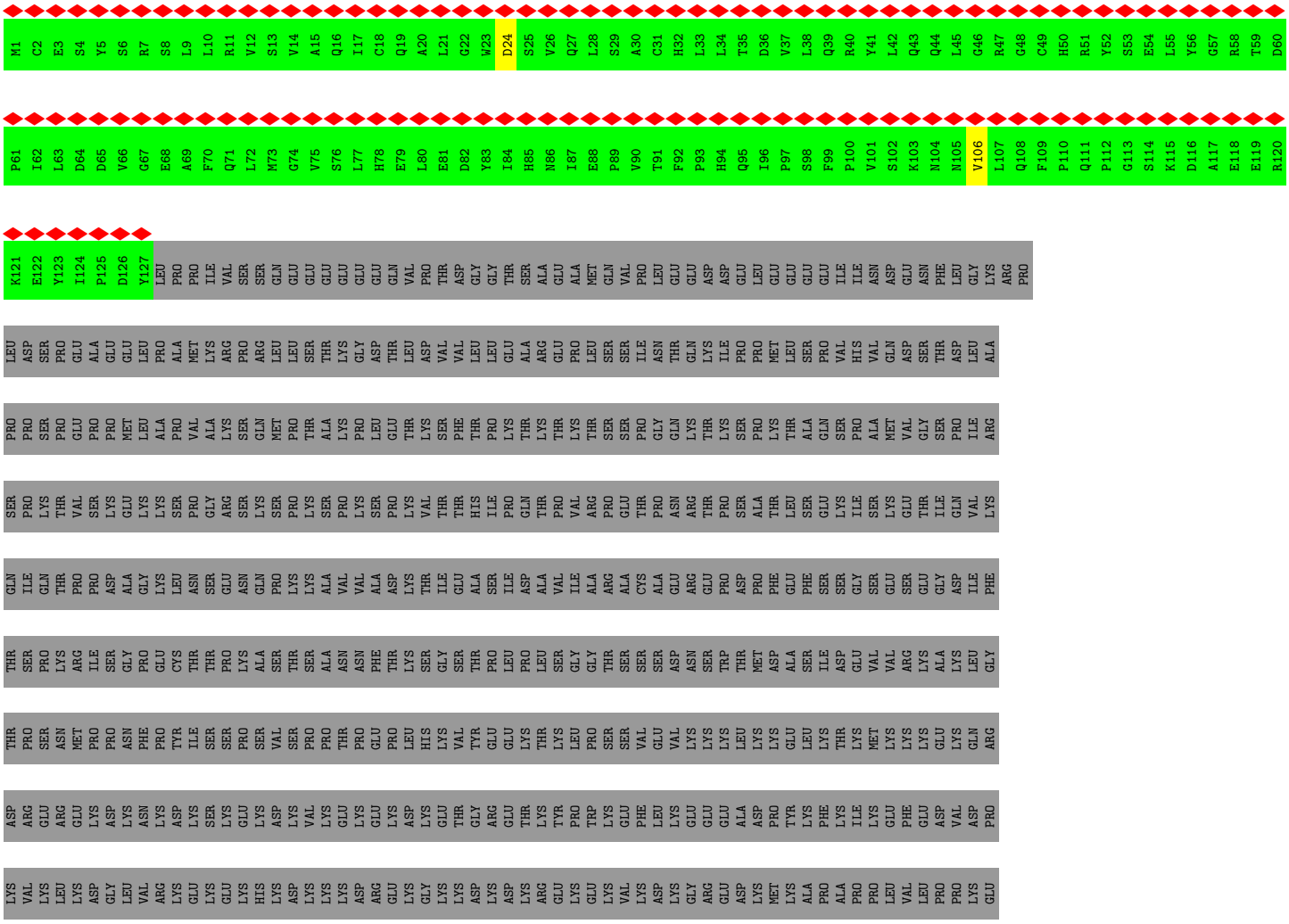
Chain V:





- Molecule 19: Transcription initiation factor TFIID subunit 3

Chain c:



LEU ALA LEU PRO LEU PHE SER PRO ALA THR ALA SER ARG VAL PRO ALA MET LEU PRO SER LEU LEU PRO VAL LEU PRO GLU LYS LEU PHE GLU GLU LYS GLU LYS VAL LYS GLU LYS GLU LYS LYS LYS ASP LYS LYS GLU LYS GLU LYS LYS LYS LYS GLU LYS GLU

LYS GLU ARG GLU LYS GLU LYS ARG GLU ARG GLU LYS ARG GLU LYS GLU LYS HIS HIS HIS HIS GLU LYS ILE LYS VAL GLU PRO VAL ALA LEU ALA PRO SER PRO VAL ILE PRO ARG LEU THR LEU ARG VAL GLY ALA GLY GLN ASP LYS ILE VAL ILE SER LYS VAL VAL PRO ALA

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

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

PRO PRO GLU GLU MET GLN TRP PHE CYS PRO LYS CYS ALA ASN LYS LYS LYS ASP LYS LYS HIS LYS LYS ARG LYS HIS ARG ALA HIS

- Molecule 20: Transcription initiation factor TFIID subunit 11

Chain k:

MET ASP ASP ALA HIS GLU SER PRO SER ASP LYS GLY GLY GLU THR GLY GLU SER ASP GLU THR ALA ALA VAL PRO GLY ASP PRO GLY ALA THR ASP THR ASP GLY ILE PRO GLU GLU GLU THR ASP GLY ASP ALA ASP VAL ASP LEU LYS GLU ALA ALA ALA GLU GLU GLY GLU LEU GLU SER

GLN ASP VAL SER ASP LEU THR THR VAL GLU ARG GLU ASP SER SER LEU LEU ASN PRO ALA ALA LYS LYS LEU LYS ILE ASP THR LYS GLU LYS LYS GLU LYS LYS GLN LYS VAL ASP GLU ASP GLU ILE GLN LYS MET GLN ILE LEU VAL SER SER PHE S114 E115 E116 Q117 L118 N119 R120

Y121 E122 M123 Y124 R125 R126 S127 A128 F129 P130 K131 A132 A133 I134 K135 R136 L137 I138 Q139 S140 I141 T142 G143 T144 S145 V146 S147 Q148 N149 V150 V151 I152 A153 M154 S155 G156 I157 S158 K159 V160 F161 V162 G163 E164 V165 V166 E167 E168 A169 L170 D171 V172 C173 E174 K175 W176 G177 E178 M179 P180

P181 L182 Q183 P184 K185 H186 M187 R188 E189 A190 V191 R192 R193 L194 K195 S196 K197 G198 Q199 I200 P201 M202 S203 K204 H205 K206 K207 I208 I209 F210 F211

- Molecule 21: Transcription initiation factor TFIID subunit 13

Chain m:

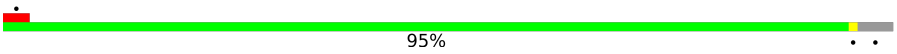
MET ALA ASP GLU GLU GLU ASP PRO THR PHE GLU GLU GLU ASN GLU GLU ILE GLY GLY GLY ALA GLU GLY GLY GLN GLY LYS R28 K29 R30 L31 F32 S33 K34 E35 L36 R37 C38 M39 M40 Y41 G42 F43 G44 D45 D46 Q47 N48 P49 Y50 T51 E52 S53 V54 D55 I56 L57 E58 D59 L60

V61 I62 E63 F64 I65 T66 E67 M68 T69 H70 K71 A72 M73 S74 I75 G76 R77 Q78 G79 R80 V81 Q82 V83 E84 D85 I86 V87 F88 L89 I90 R91 K92 D93 P94 R95 K96 F97 A98 R99 V100 K101 D102 L103 L104 T105 M106 N107 E108 E109 L110 K111 R112 A113 R114 LYS ALA PHE ASP GLU ALA

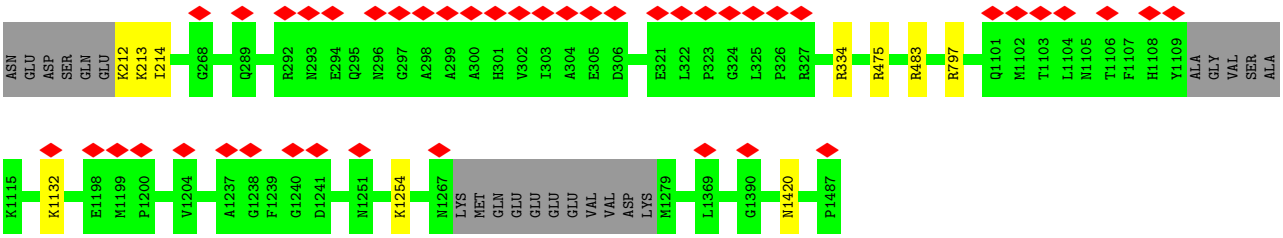
ASN TYR GLY SER

- Molecule 22: DNA-directed RNA polymerase subunit

Chain o:

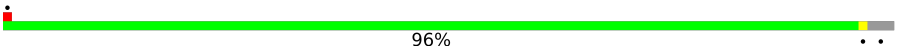


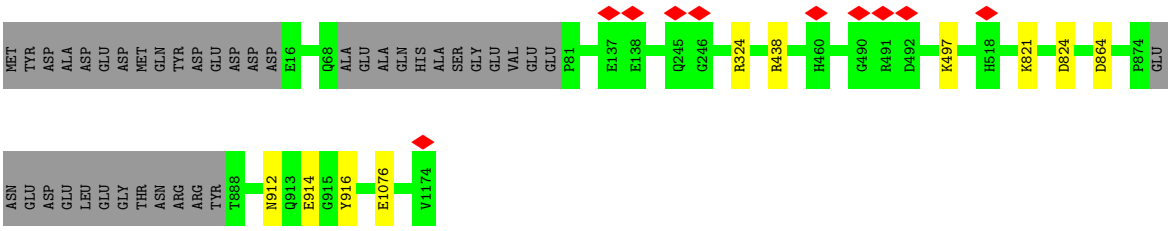
MET HIS GLY GLY GLY PRO PRO SER GLY ASP S11 G49 A131 K132 S133 K134 G135 K138 K149 G150 E155 GLY GLY GLU GLU MET ASP ASN LYS PHE GLY VAL GLU GLN PRO GLU GLY ASP GLU ASP LEU THR LYS GLU LYS GLY H181 R192 R193 W202 LYS HIS VAL



• Molecule 23: DNA-directed RNA polymerase subunit beta

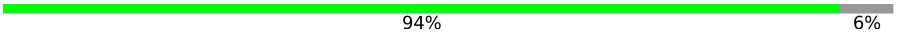
Chain p:





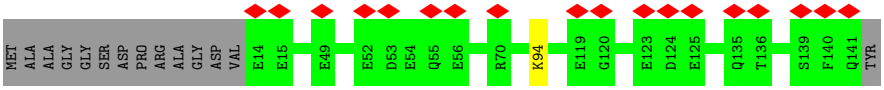
• Molecule 24: DNA-directed RNA polymerase II subunit RPB3

Chain q:



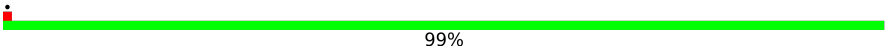
• Molecule 25: DNA-directed RNA polymerase II subunit RPB4

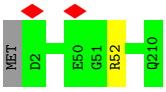
Chain r:



• Molecule 26: DNA-directed RNA polymerase II subunit E

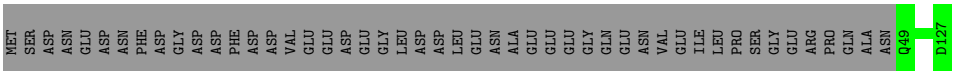
Chain s:





• Molecule 27: DNA-directed RNA polymerase II subunit F

Chain t:

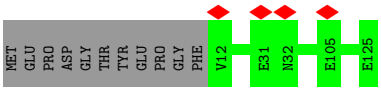


• Molecule 28: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain v: 99%

• Molecule 29: DNA-directed RNA polymerase II subunit RPB9

Chain w: 91% 9%



• Molecule 30: RPB10

Chain x: 100%

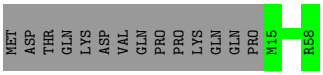
There are no outlier residues recorded for this chain.

• Molecule 31: RNA_pol_L_2 domain-containing protein

Chain y: 100%

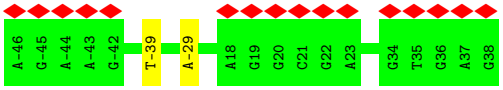
• Molecule 32: RPB12

Chain z: 76% 24%



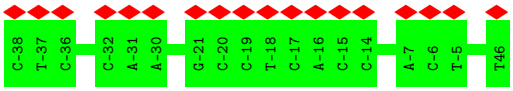
• Molecule 33: DNA (85-MER)

Chain X: 19% 98%



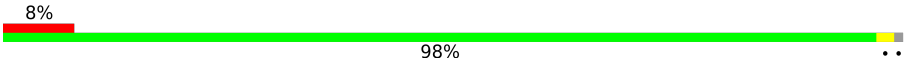
• Molecule 34: DNA (85-MER)

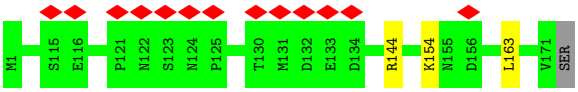
Chain Y: 21% 100%



• Molecule 35: DNA-directed RNA polymerase II subunit RPB7

Chain u:


8%
98%


M1
S115
E116
P121
N122
S123
N124
P125
T130
M131
D132
E133
D134
R144
K154
N155
D156
L163
V171
SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21692	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 ($e^-/Å^2$)	50.0	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	0.114	Depositor
Minimum map value	-0.069	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0085	Depositor
Map size (Å)	508.8, 508.8, 508.8	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.52	0/5046	0.64	0/6810
2	B	0.47	0/7993	0.61	0/10836
3	D	0.47	0/1379	0.61	1/1843 (0.1%)
3	d	0.28	0/1321	0.49	0/1772
4	E	0.35	0/4469	0.55	0/6050
4	e	0.33	0/4433	0.55	0/6004
5	F	0.51	0/3139	0.71	2/4264 (0.0%)
5	f	0.40	0/3140	0.63	0/4268
6	G	0.51	0/1199	0.63	0/1612
7	H	0.41	0/1673	0.59	0/2285
8	I	0.32	0/981	0.50	0/1332
8	i	0.31	0/989	0.46	0/1343
9	J	0.31	0/724	0.53	1/982 (0.1%)
9	j	0.30	0/775	0.52	0/1049
10	L	0.32	0/630	0.57	1/852 (0.1%)
10	l	0.37	0/888	0.56	1/1194 (0.1%)
11	O	0.52	0/781	0.76	0/1061
12	P	0.62	0/1438	0.72	0/1935
13	Q	0.46	0/1013	0.61	0/1366
14	R	0.34	0/1967	0.55	0/2656
15	S	0.36	0/896	0.55	0/1213
16	T	0.54	0/1817	0.66	0/2445
17	U	0.50	1/1499 (0.1%)	0.77	4/2012 (0.2%)
18	V	0.49	0/1428	0.68	0/1917
19	c	0.40	0/1035	0.54	0/1406
20	k	0.30	0/799	0.48	0/1070
21	m	0.31	0/733	0.51	0/977
22	o	0.34	0/11516	0.50	0/15548
23	p	0.38	0/9243	0.47	0/12475
24	q	0.39	0/2102	0.46	0/2857
25	r	0.27	0/1019	0.47	0/1374
26	s	0.30	0/1751	0.45	0/2366

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
27	t	0.37	0/645	0.47	0/871
28	v	0.37	0/1207	0.49	0/1628
29	w	0.30	0/948	0.46	0/1284
30	x	0.43	0/516	0.45	0/696
31	y	0.35	0/956	0.44	0/1294
32	z	0.38	0/377	0.45	0/500
33	X	0.78	2/1966 (0.1%)	1.00	1/3034 (0.0%)
34	Y	0.64	0/1942	0.90	0/2993
35	u	0.33	0/1382	0.53	0/1874
All	All	0.42	3/87755 (0.0%)	0.59	11/119348 (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
15	S	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	U	123	ASN	C-N	5.62	1.47	1.34
33	X	-29	DA	O3'-P	5.45	1.67	1.61
33	X	-39	DT	C1'-N1	5.02	1.55	1.49

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	U	127	PHE	CB-CA-C	8.11	126.62	110.40
3	D	881	ARG	CB-CA-C	-6.21	97.99	110.40
17	U	123	ASN	O-C-N	5.99	132.29	122.70
17	U	140	GLU	CB-CA-C	-5.37	99.66	110.40
10	L	79	ASP	CB-CG-OD2	5.29	123.06	118.30
33	X	-29	DA	C3'-C2'-C1'	-5.26	96.19	102.50
5	F	330	ARG	CG-CD-NE	-5.23	100.82	111.80
9	J	118	ASP	CB-CG-OD2	5.22	123.00	118.30
10	l	79	ASP	CB-CG-OD2	5.18	122.96	118.30
5	F	330	ARG	CB-CA-C	-5.15	100.10	110.40
17	U	128	LYS	N-CA-CB	5.01	119.61	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	S	6	PRO	Mainchain

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	584/1872 (31%)	552 (94%)	30 (5%)	2 (0%)	41 75
2	B	959/1199 (80%)	914 (95%)	45 (5%)	0	100 100
3	D	158/1085 (15%)	142 (90%)	15 (10%)	1 (1%)	25 63
3	d	154/1085 (14%)	150 (97%)	4 (3%)	0	100 100
4	E	540/800 (68%)	507 (94%)	30 (6%)	3 (1%)	25 63
4	e	531/800 (66%)	484 (91%)	47 (9%)	0	100 100
5	F	400/677 (59%)	375 (94%)	21 (5%)	4 (1%)	15 52
5	f	399/677 (59%)	380 (95%)	19 (5%)	0	100 100
6	G	139/349 (40%)	137 (99%)	2 (1%)	0	100 100
7	H	207/310 (67%)	186 (90%)	18 (9%)	3 (1%)	11 45
8	I	118/264 (45%)	115 (98%)	3 (2%)	0	100 100
8	i	119/264 (45%)	115 (97%)	4 (3%)	0	100 100
9	J	85/218 (39%)	82 (96%)	3 (4%)	0	100 100
9	j	91/218 (42%)	89 (98%)	2 (2%)	0	100 100
10	L	74/161 (46%)	67 (90%)	7 (10%)	0	100 100
10	l	105/161 (65%)	100 (95%)	5 (5%)	0	100 100
11	O	95/109 (87%)	83 (87%)	9 (10%)	3 (3%)	4 30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	P	175/339 (52%)	166 (95%)	7 (4%)	2 (1%)	14	50
13	Q	118/376 (31%)	107 (91%)	10 (8%)	1 (1%)	19	58
14	R	247/316 (78%)	237 (96%)	9 (4%)	1 (0%)	34	71
15	S	104/517 (20%)	99 (95%)	3 (3%)	2 (2%)	8	39
16	T	218/249 (88%)	197 (90%)	15 (7%)	6 (3%)	5	32
17	U	175/439 (40%)	154 (88%)	18 (10%)	3 (2%)	9	42
18	V	170/291 (58%)	131 (77%)	29 (17%)	10 (6%)	1	19
19	c	125/929 (14%)	116 (93%)	9 (7%)	0	100	100
20	k	96/211 (46%)	91 (95%)	5 (5%)	0	100	100
21	m	85/124 (68%)	79 (93%)	6 (7%)	0	100	100
22	o	1417/1487 (95%)	1304 (92%)	113 (8%)	0	100	100
23	p	1128/1174 (96%)	1050 (93%)	77 (7%)	1 (0%)	51	84
24	q	253/273 (93%)	226 (89%)	27 (11%)	0	100	100
25	r	126/142 (89%)	119 (94%)	7 (6%)	0	100	100
26	s	207/210 (99%)	196 (95%)	11 (5%)	0	100	100
27	t	77/127 (61%)	74 (96%)	3 (4%)	0	100	100
28	v	146/150 (97%)	133 (91%)	13 (9%)	0	100	100
29	w	112/125 (90%)	103 (92%)	9 (8%)	0	100	100
30	x	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
31	y	115/117 (98%)	109 (95%)	6 (5%)	0	100	100
32	z	42/58 (72%)	38 (90%)	4 (10%)	0	100	100
35	u	169/172 (98%)	156 (92%)	12 (7%)	1 (1%)	25	63
All	All	10125/18139 (56%)	9423 (93%)	659 (6%)	43 (0%)	38	71

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1158	SER
5	F	323	VAL
7	H	141	PRO
11	O	52	VAL
15	S	9	GLN
16	T	140	ARG
16	T	174	LYS

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Mol	Chain	Res	Type
17	U	124	ARG
18	V	177	ASN
35	u	154	LYS
4	E	522	ASP
4	E	704	VAL
11	O	26	GLN
18	V	79	ALA
18	V	128	PRO
18	V	171	ILE
18	V	208	CYS
3	D	934	TYR
5	F	64	GLN
12	P	207	PRO
16	T	231	ASN
18	V	134	ASP
18	V	196	ASP
18	V	207	SER
5	F	439	ARG
11	O	84	VAL
13	Q	320	VAL
15	S	7	SER
16	T	226	LYS
17	U	121	SER
17	U	145	PHE
18	V	194	ARG
18	V	225	VAL
5	F	318	CYS
7	H	134	LEU
7	H	164	THR
16	T	38	GLY
23	p	912	ASN
12	P	298	PRO
14	R	247	GLY
4	E	523	VAL
16	T	40	VAL
1	A	498	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	536/1665 (32%)	487 (91%)	49 (9%)	9	33
2	B	876/1083 (81%)	854 (98%)	22 (2%)	47	68
3	D	147/815 (18%)	116 (79%)	31 (21%)	1	6
3	d	146/815 (18%)	146 (100%)	0	100	100
4	E	478/657 (73%)	474 (99%)	4 (1%)	81	88
4	e	475/657 (72%)	473 (100%)	2 (0%)	91	94
5	F	320/574 (56%)	299 (93%)	21 (7%)	16	44
5	f	322/574 (56%)	313 (97%)	9 (3%)	43	65
6	G	133/322 (41%)	126 (95%)	7 (5%)	22	51
7	H	181/270 (67%)	168 (93%)	13 (7%)	14	42
8	I	106/235 (45%)	101 (95%)	5 (5%)	26	53
8	i	107/235 (46%)	106 (99%)	1 (1%)	78	87
9	J	78/154 (51%)	78 (100%)	0	100	100
9	j	83/154 (54%)	83 (100%)	0	100	100
10	L	71/141 (50%)	69 (97%)	2 (3%)	43	65
10	l	98/141 (70%)	95 (97%)	3 (3%)	40	63
11	O	84/98 (86%)	78 (93%)	6 (7%)	14	42
12	P	153/293 (52%)	134 (88%)	19 (12%)	4	22
13	Q	111/324 (34%)	105 (95%)	6 (5%)	22	50
14	R	214/268 (80%)	201 (94%)	13 (6%)	18	47
15	S	93/448 (21%)	91 (98%)	2 (2%)	52	71
16	T	196/218 (90%)	178 (91%)	18 (9%)	9	32
17	U	163/373 (44%)	137 (84%)	26 (16%)	2	15
18	V	155/261 (59%)	121 (78%)	34 (22%)	1	6
19	c	113/833 (14%)	111 (98%)	2 (2%)	59	77
20	k	87/182 (48%)	87 (100%)	0	100	100
21	m	80/106 (76%)	79 (99%)	1 (1%)	69	81
22	o	1257/1306 (96%)	1243 (99%)	14 (1%)	73	84
23	p	993/1027 (97%)	984 (99%)	9 (1%)	78	87
24	q	234/250 (94%)	234 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	r	106/126 (84%)	105 (99%)	1 (1%)	78	87
26	s	191/192 (100%)	190 (100%)	1 (0%)	88	93
27	t	69/111 (62%)	69 (100%)	0	100	100
28	v	129/131 (98%)	129 (100%)	0	100	100
29	w	103/112 (92%)	103 (100%)	0	100	100
30	x	53/53 (100%)	53 (100%)	0	100	100
31	y	106/106 (100%)	106 (100%)	0	100	100
32	z	41/55 (74%)	41 (100%)	0	100	100
35	u	152/153 (99%)	150 (99%)	2 (1%)	69	81
All	All	9040/15518 (58%)	8717 (96%)	323 (4%)	38	60

All (323) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	341	TRP
1	A	353	LEU
1	A	395	ASP
1	A	397	LEU
1	A	400	GLU
1	A	404	MET
1	A	408	LEU
1	A	410	TRP
1	A	411	GLU
1	A	415	ILE
1	A	419	GLU
1	A	475	LEU
1	A	481	GLU
1	A	483	ASN
1	A	484	ILE
1	A	491	MET
1	A	500	LEU
1	A	501	THR
1	A	502	LEU
1	A	505	ASN
1	A	511	LEU
1	A	661	GLU
1	A	667	THR
1	A	711	ASP
1	A	727	THR

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Mol	Chain	Res	Type
1	A	730	PHE
1	A	797	LYS
1	A	798	ARG
1	A	804	ARG
1	A	828	GLU
1	A	943	LYS
1	A	970	ASN
1	A	971	LYS
1	A	996	ARG
1	A	997	ARG
1	A	998	LEU
1	A	1001	LYS
1	A	1004	LYS
1	A	1008	ARG
1	A	1010	PHE
1	A	1021	SER
1	A	1022	ARG
1	A	1052	ARG
1	A	1055	VAL
1	A	1150	THR
1	A	1165	LEU
1	A	1181	ARG
1	A	1182	CYS
1	A	1203	GLU
2	B	21	GLU
2	B	24	ARG
2	B	71	ARG
2	B	140	GLU
2	B	184	ASN
2	B	225	TYR
2	B	262	MET
2	B	266	THR
2	B	293	GLU
2	B	431	LEU
2	B	488	PHE
2	B	559	LYS
2	B	603	LYS
2	B	638	ARG
2	B	640	VAL
2	B	760	LEU
2	B	771	VAL
2	B	816	VAL

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Mol	Chain	Res	Type
2	B	820	ASP
2	B	844	PRO
2	B	847	ARG
2	B	849	THR
3	D	929	LYS
3	D	932	ASP
3	D	936	GLN
3	D	938	SER
3	D	939	ASP
3	D	941	ARG
3	D	944	LEU
3	D	945	LYS
3	D	946	PHE
3	D	947	PHE
3	D	948	GLU
3	D	949	GLN
3	D	950	LEU
3	D	951	ASP
3	D	952	GLN
3	D	953	ILE
3	D	955	LYS
3	D	957	ARG
3	D	958	LYS
3	D	959	ASP
3	D	962	GLU
3	D	963	ARG
3	D	964	GLU
3	D	965	ILE
3	D	967	MET
3	D	968	ARG
3	D	983	ARG
3	D	1054	ARG
3	D	1055	ILE
3	D	1056	THR
3	D	1057	ARG
4	E	593	PHE
4	E	745	GLU
4	E	746	ASP
4	E	747	LEU
5	F	62	LYS
5	F	89	GLN
5	F	90	GLU

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Mol	Chain	Res	Type
5	F	92	ILE
5	F	136	LEU
5	F	258	ARG
5	F	261	THR
5	F	271	VAL
5	F	280	ILE
5	F	317	LEU
5	F	329	LEU
5	F	330	ARG
5	F	337	VAL
5	F	339	GLN
5	F	348	THR
5	F	354	ARG
5	F	368	THR
5	F	397	GLN
5	F	408	ASP
5	F	416	ASP
5	F	427	LEU
6	G	41	ASP
6	G	81	ASP
6	G	143	VAL
6	G	147	ARG
6	G	181	TRP
6	G	182	GLU
6	G	183	ILE
7	H	115	GLN
7	H	132	LYS
7	H	135	THR
7	H	159	TYR
7	H	164	THR
7	H	203	LEU
7	H	205	LYS
7	H	206	ASP
7	H	207	ASP
7	H	217	ARG
7	H	219	PHE
7	H	220	THR
7	H	221	ILE
8	I	14	LYS
8	I	15	ASP
8	I	31	TYR
8	I	32	GLU

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Mol	Chain	Res	Type
8	I	34	ARG
10	L	85	LEU
10	L	87	ILE
11	O	24	GLN
11	O	52	VAL
11	O	54	ASN
11	O	57	ASN
11	O	59	ARG
11	O	76	LEU
12	P	166	GLN
12	P	167	ASN
12	P	172	VAL
12	P	208	ARG
12	P	209	THR
12	P	212	LEU
12	P	213	ILE
12	P	215	SER
12	P	221	CYS
12	P	226	SER
12	P	239	ARG
12	P	242	GLN
12	P	252	ASP
12	P	274	VAL
12	P	278	GLN
12	P	309	LYS
12	P	312	LEU
12	P	313	THR
12	P	317	VAL
13	Q	13	LEU
13	Q	34	VAL
13	Q	318	ASP
13	Q	345	SER
13	Q	364	ASP
13	Q	369	LYS
14	R	31	ASP
14	R	39	LEU
14	R	107	MET
14	R	111	ASP
14	R	114	MET
14	R	115	MET
14	R	120	GLU
14	R	130	LEU

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Mol	Chain	Res	Type
14	R	132	ARG
14	R	134	ILE
14	R	137	ARG
14	R	193	ARG
14	R	286	ARG
15	S	9	GLN
15	S	95	ASP
16	T	35	SER
16	T	37	ARG
16	T	40	VAL
16	T	42	LYS
16	T	47	LYS
16	T	88	VAL
16	T	91	GLN
16	T	93	LEU
16	T	125	MET
16	T	137	LYS
16	T	141	LEU
16	T	160	GLN
16	T	177	ARG
16	T	184	LEU
16	T	200	LYS
16	T	211	VAL
16	T	212	TYR
16	T	229	HIS
17	U	28	ILE
17	U	39	ARG
17	U	42	CYS
17	U	45	GLU
17	U	75	ARG
17	U	76	MET
17	U	77	ARG
17	U	94	ILE
17	U	95	ASN
17	U	102	VAL
17	U	111	ARG
17	U	113	ARG
17	U	114	ILE
17	U	119	ARG
17	U	122	THR
17	U	139	LEU
17	U	145	PHE

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Mol	Chain	Res	Type
17	U	166	SER
17	U	168	MET
17	U	170	LYS
17	U	171	LYS
17	U	185	GLU
17	U	190	LEU
17	U	191	LEU
17	U	192	ARG
17	U	201	TYR
18	V	88	ARG
18	V	93	ASP
18	V	97	LEU
18	V	129	LYS
18	V	131	GLU
18	V	140	LYS
18	V	142	LYS
18	V	143	TYR
18	V	148	LYS
18	V	149	LYS
18	V	151	LEU
18	V	153	ARG
18	V	154	LEU
18	V	155	LEU
18	V	157	GLN
18	V	159	ASP
18	V	160	GLN
18	V	161	ARG
18	V	163	LEU
18	V	166	ILE
18	V	169	GLU
18	V	172	GLU
18	V	188	GLN
18	V	194	ARG
18	V	197	LYS
18	V	199	LYS
18	V	208	CYS
18	V	209	GLN
18	V	210	PHE
18	V	221	ARG
18	V	222	SER
18	V	229	ASP
18	V	230	GLU

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Mol	Chain	Res	Type
18	V	234	GLU
19	c	24	ASP
19	c	106	VAL
4	e	365	ARG
4	e	663	ARG
5	f	253	TYR
5	f	261	THR
5	f	272	VAL
5	f	322	ASP
5	f	323	VAL
5	f	326	HIS
5	f	354	ARG
5	f	356	THR
5	f	421	ASP
8	i	62	LYS
10	l	83	MET
10	l	104	ARG
10	l	106	ARG
21	m	31	LEU
22	o	132	LYS
22	o	138	LYS
22	o	192	ARG
22	o	193	ARG
22	o	212	LYS
22	o	213	LYS
22	o	214	ILE
22	o	334	ARG
22	o	475	ARG
22	o	483	ARG
22	o	797	ARG
22	o	1132	LYS
22	o	1254	LYS
22	o	1420	ASN
23	p	324	ARG
23	p	438	ARG
23	p	497	LYS
23	p	821	LYS
23	p	824	ASP
23	p	864	ASP
23	p	914	GLU
23	p	916	TYR
23	p	1076	GLU

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Mol	Chain	Res	Type
25	r	94	LYS
26	s	52	ARG
35	u	144	ARG
35	u	163	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (122) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	401	ASN
1	A	472	ASN
1	A	489	GLN
1	A	569	ASN
1	A	860	ASN
1	A	896	GLN
1	A	1073	GLN
2	B	30	HIS
2	B	176	HIS
2	B	183	GLN
2	B	184	ASN
2	B	235	HIS
2	B	348	GLN
2	B	432	HIS
2	B	439	HIS
2	B	450	GLN
2	B	509	ASN
2	B	745	GLN
2	B	750	GLN
2	B	765	ASN
2	B	813	ASN
2	B	908	GLN
2	B	916	ASN
3	D	875	GLN
3	D	936	GLN
4	E	254	ASN
4	E	268	HIS
4	E	327	ASN
4	E	351	GLN
4	E	616	HIS
4	E	640	ASN
5	F	52	GLN
5	F	119	ASN
5	F	221	GLN

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Mol	Chain	Res	Type
5	F	270	ASN
5	F	273	GLN
5	F	274	ASN
5	F	275	ASN
5	F	316	GLN
5	F	352	GLN
6	G	48	HIS
7	H	145	HIS
7	H	201	GLN
8	I	21	GLN
8	I	38	GLN
8	I	60	HIS
8	I	98	GLN
9	J	160	GLN
9	J	173	HIS
10	L	105	HIS
10	L	117	GLN
11	O	8	ASN
11	O	13	ASN
11	O	27	GLN
11	O	31	GLN
11	O	57	ASN
13	Q	60	HIS
13	Q	352	HIS
13	Q	361	ASN
16	T	91	GLN
16	T	158	ASN
16	T	181	GLN
17	U	40	ASN
17	U	95	ASN
17	U	181	ASN
18	V	89	HIS
18	V	95	HIS
18	V	117	GLN
18	V	126	ASN
19	c	104	ASN
3	d	912	ASN
3	d	1069	ASN
4	e	294	ASN
4	e	320	HIS
4	e	336	HIS
4	e	616	HIS

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Mol	Chain	Res	Type
5	f	325	ASN
8	i	81	GLN
20	k	186	HIS
10	l	73	ASN
10	l	105	HIS
21	m	107	ASN
22	o	123	ASN
22	o	278	HIS
22	o	289	GLN
22	o	296	ASN
22	o	301	HIS
22	o	311	GLN
22	o	330	GLN
22	o	372	ASN
22	o	507	GLN
22	o	620	HIS
22	o	721	HIS
22	o	731	ASN
22	o	739	ASN
22	o	809	HIS
22	o	913	ASN
22	o	950	ASN
22	o	1005	HIS
22	o	1230	GLN
22	o	1248	ASN
22	o	1332	GLN
22	o	1397	HIS
22	o	1445	HIS
22	o	1462	GLN
23	p	56	GLN
23	p	111	ASN
23	p	139	GLN
23	p	287	HIS
23	p	525	ASN
23	p	570	ASN
23	p	749	HIS
23	p	1021	HIS
23	p	1094	GLN
23	p	1117	HIS
23	p	1120	ASN
25	r	19	GLN
26	s	133	GLN

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Mol	Chain	Res	Type
28	v	131	ASN
31	y	2	ASN
31	y	29	ASN
35	u	60	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 11 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 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.

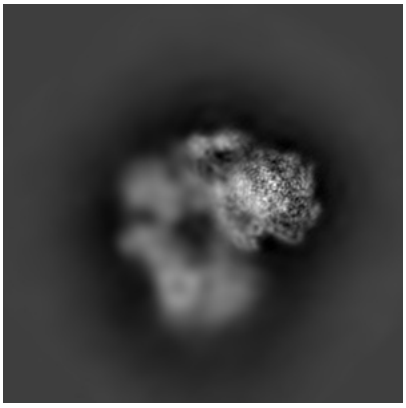
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-31110. These allow visual inspection of the internal detail of the map and identification of artifacts.

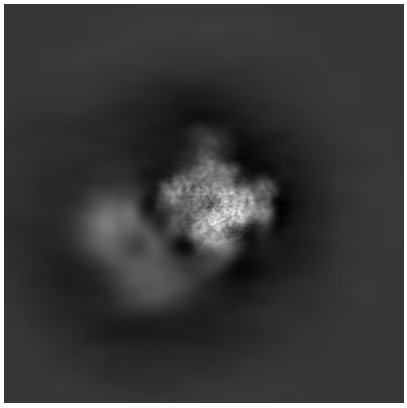
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

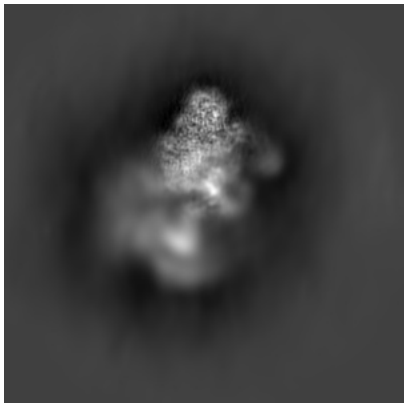
6.1.1 Primary map



X



Y

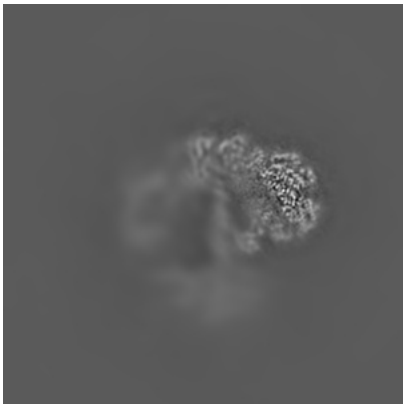


Z

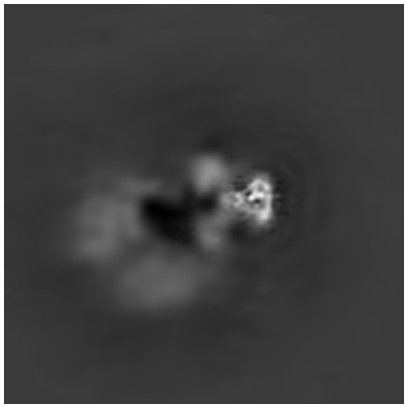
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

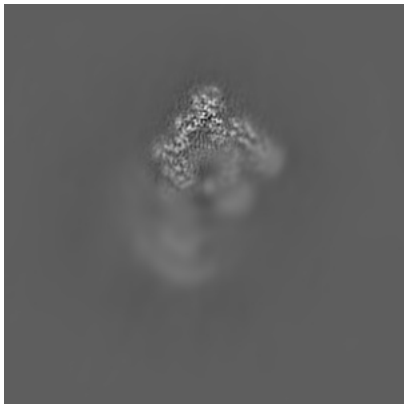
6.2.1 Primary map



X Index: 240



Y Index: 240

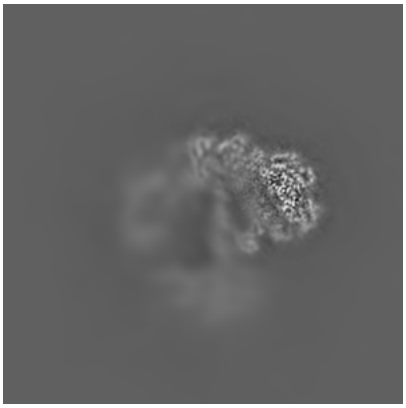


Z Index: 240

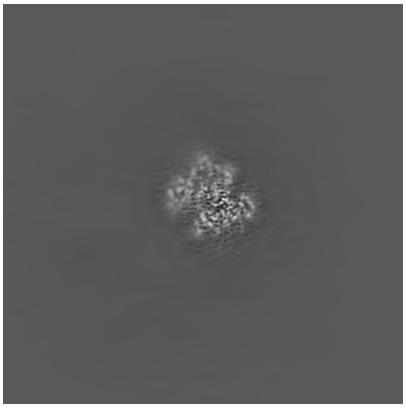
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

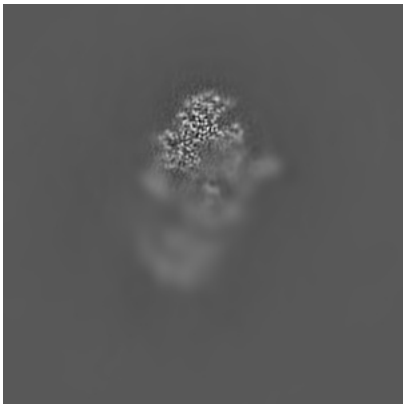
6.3.1 Primary map



X Index: 239



Y Index: 330

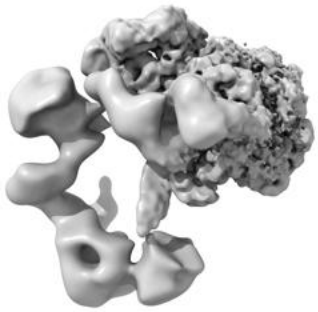


Z Index: 264

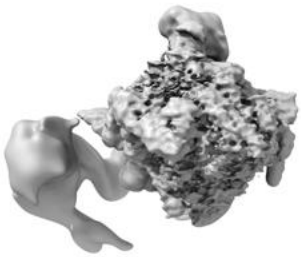
The images above show the largest variance slices of the map in three orthogonal directions.

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 0.0085. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

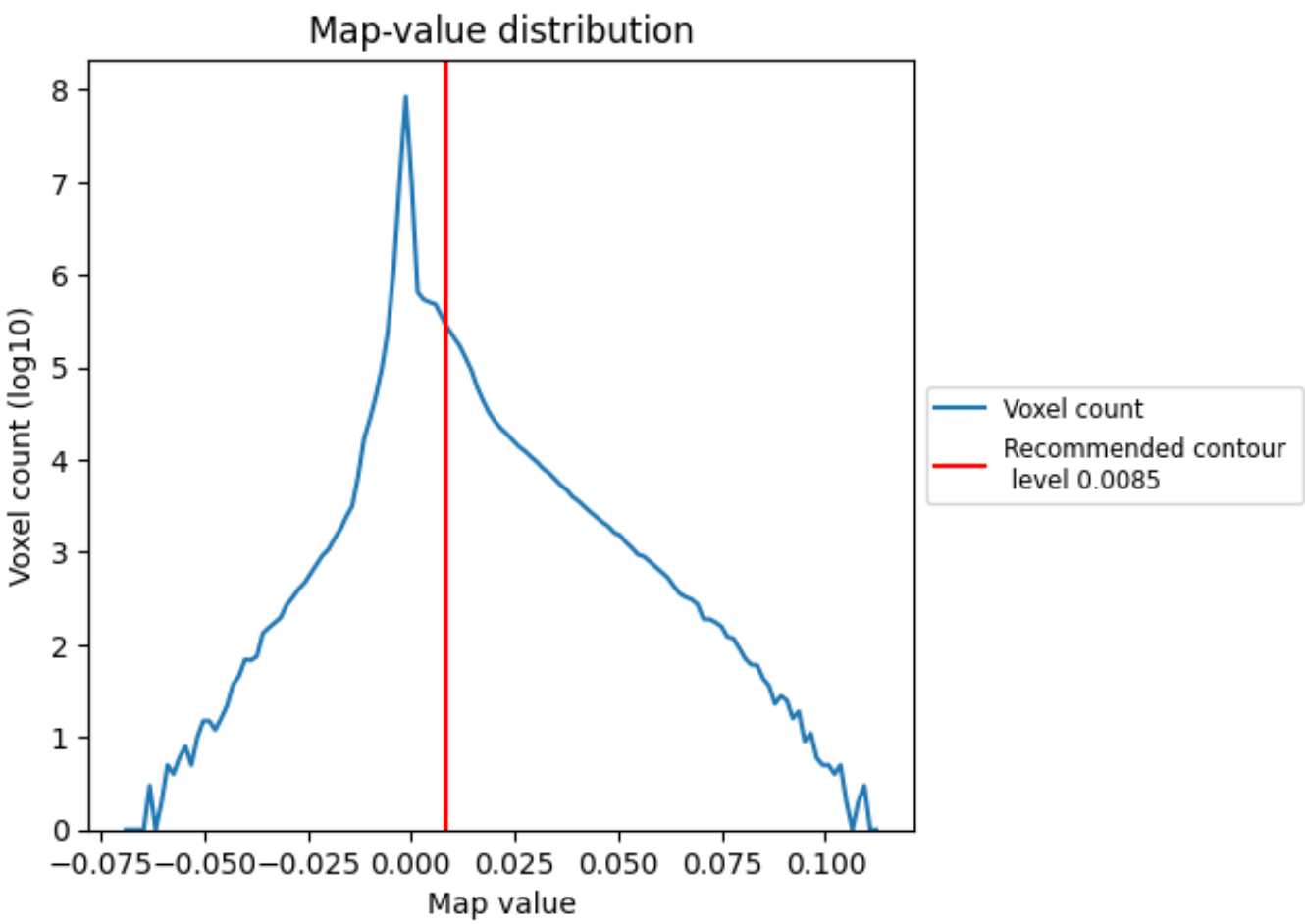
6.5 Mask visualisation (i)

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

7 Map analysis (i)

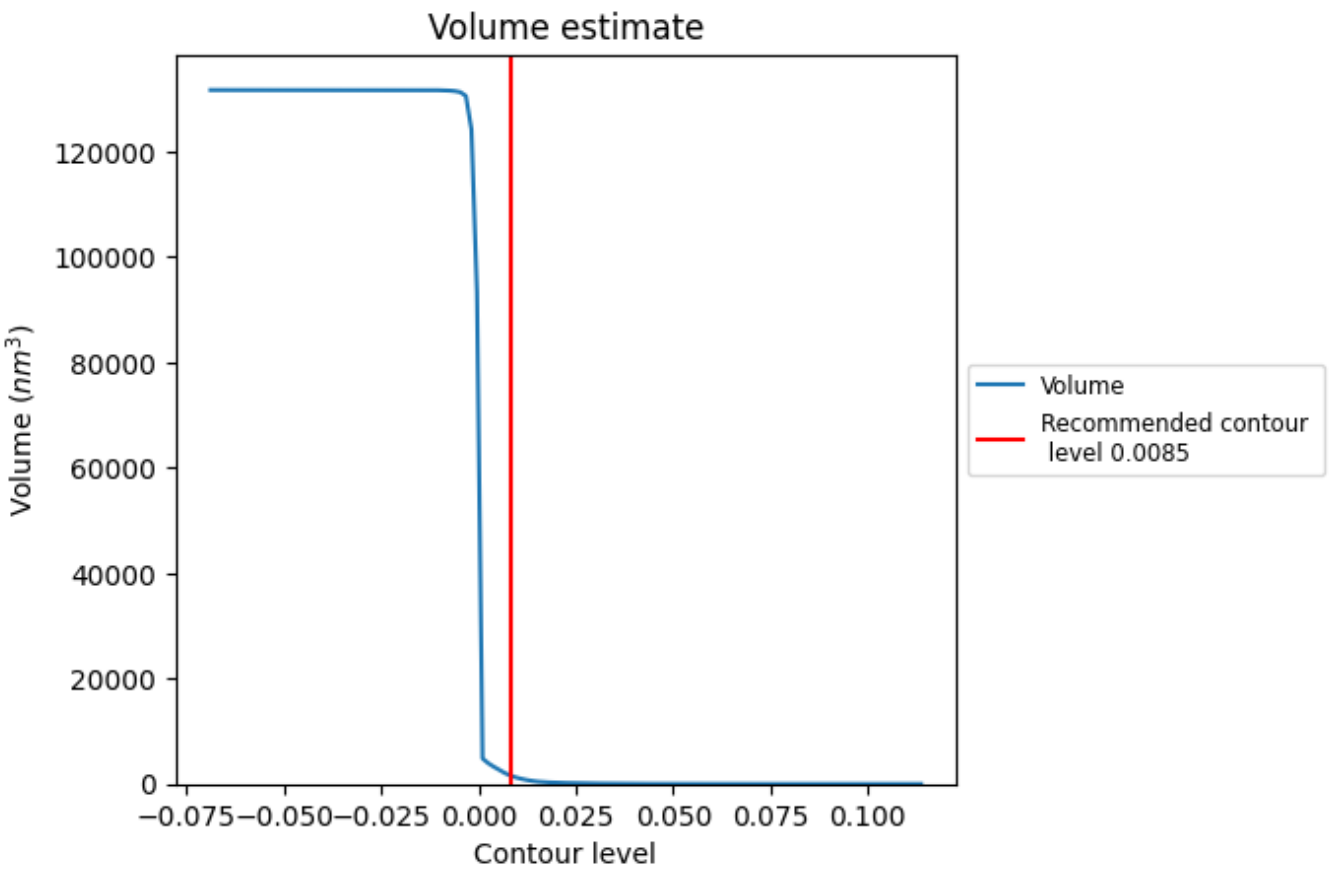
This section contains the results of statistical analysis of the map.

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.

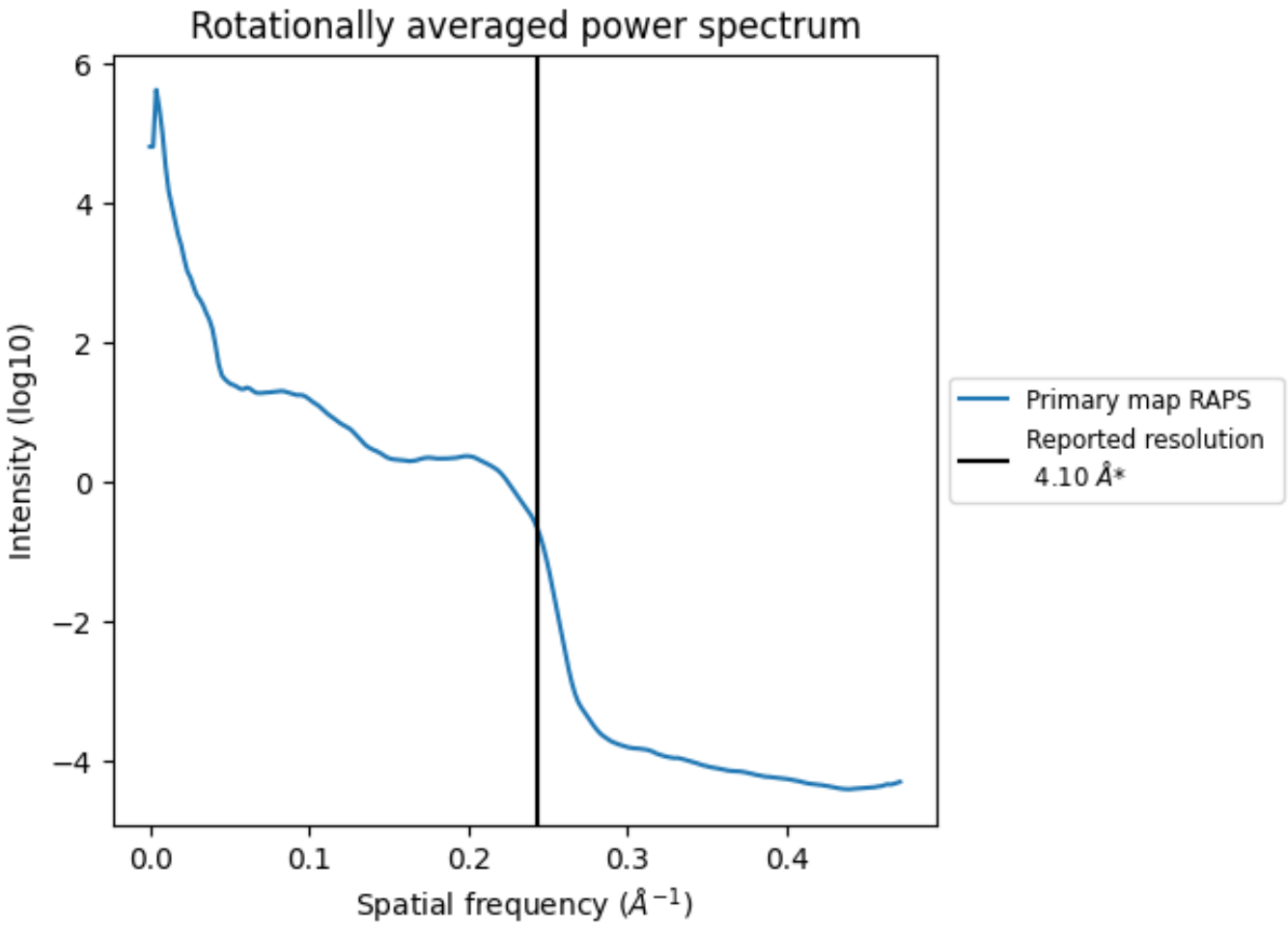
7.2 Volume estimate (i)



The volume at the recommended contour level is 1522 nm^3; this corresponds to an approximate mass of 1374 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 0.244 Å^{-1}

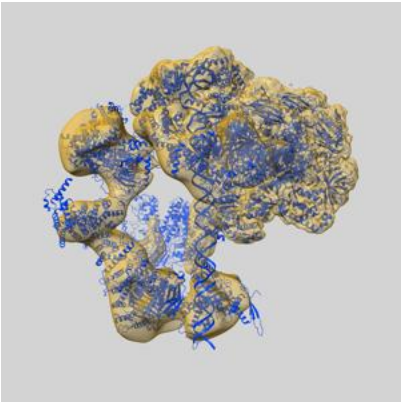
8 Fourier-Shell correlation (i)

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

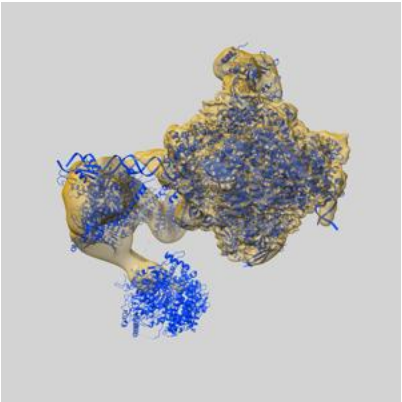
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-31110 and PDB model 7EGA. Per-residue inclusion information can be found in section 3 on page 11.

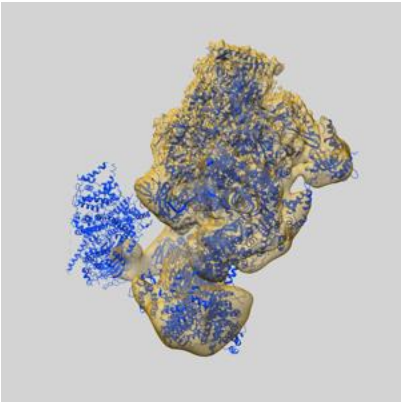
9.1 Map-model overlay (i)



X



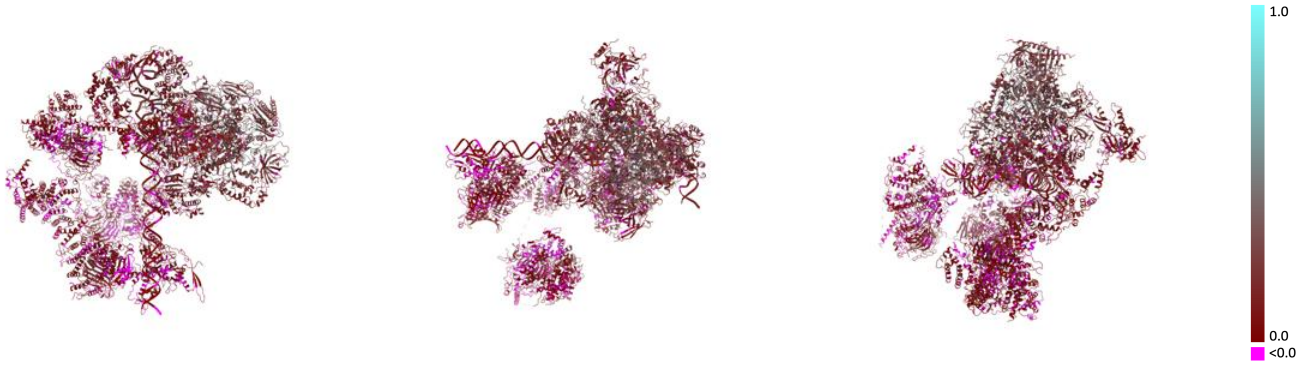
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0085 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.

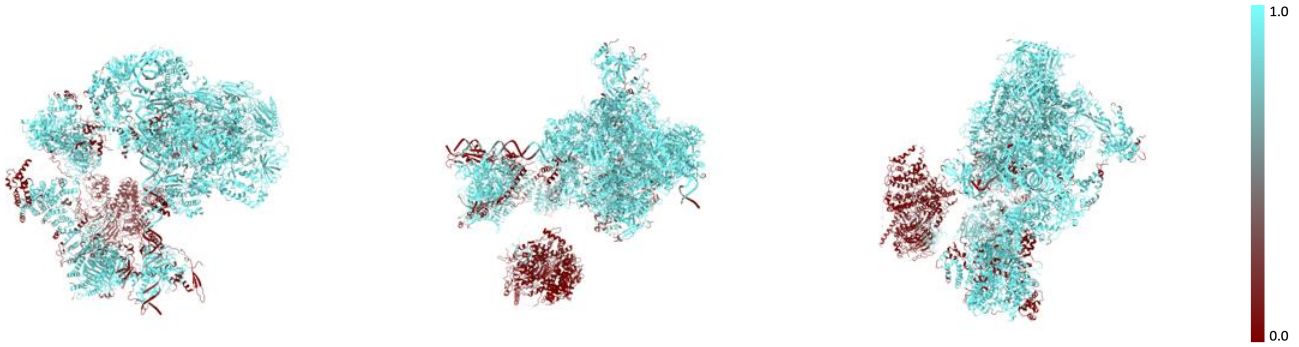
9.2 Q-score mapped to coordinate model (i)



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.

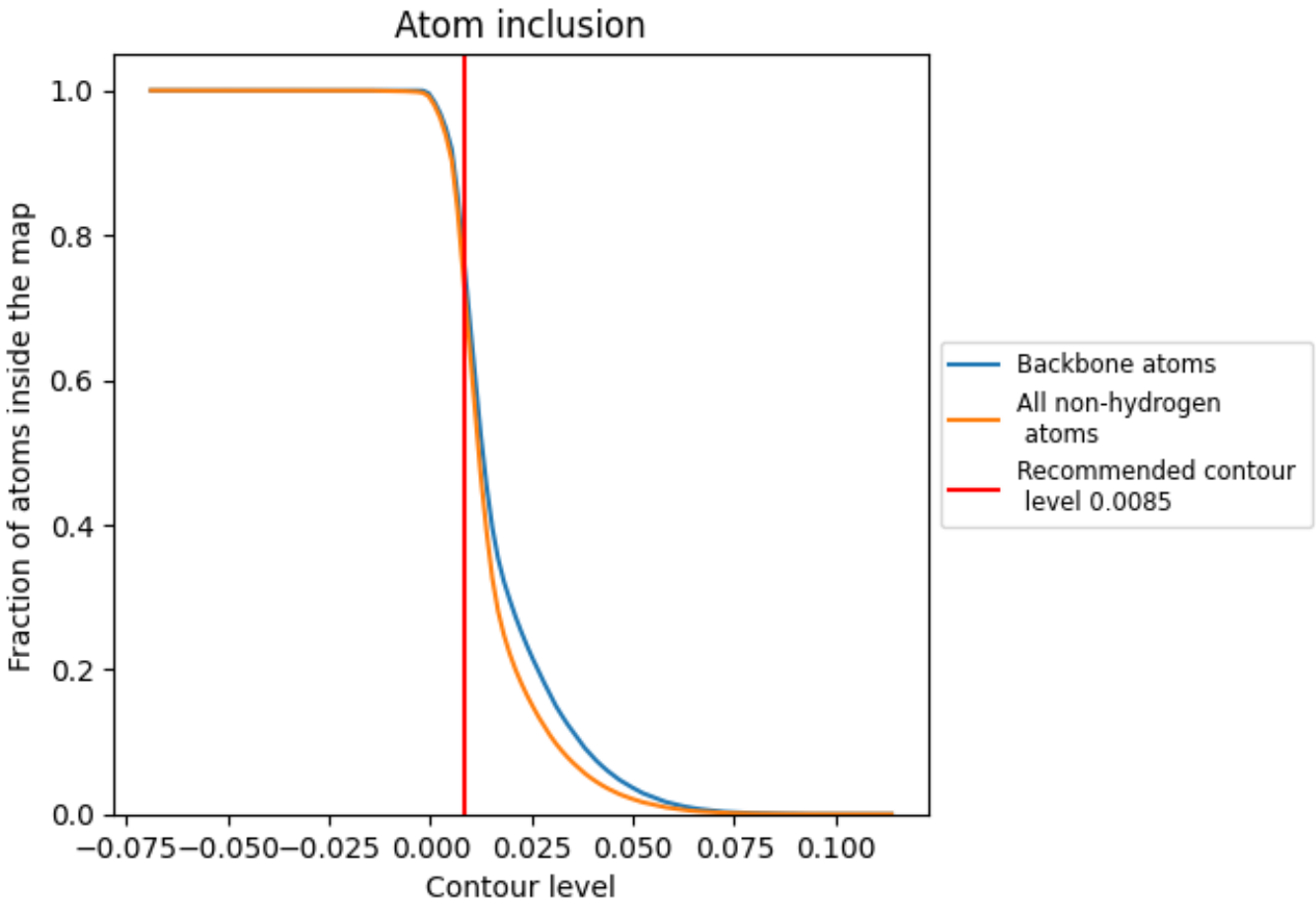
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0085).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 72% 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 (0.0085) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7222	0.1220
A	0.6006	0.0360
B	0.8155	0.0470
D	0.7177	0.0730
E	0.7491	0.0490
F	0.6917	0.0420
G	0.6330	0.0590
H	0.7351	0.0450
I	0.8449	0.0430
J	0.9283	0.0530
L	0.6422	0.0560
O	0.9379	0.1050
P	0.9644	0.1320
Q	0.9084	0.1150
R	0.9267	0.1760
S	0.8712	0.0910
T	0.8620	0.1020
U	0.7799	0.0840
V	0.8175	0.0700
X	0.7270	0.1100
Y	0.7151	0.1110
c	0.0000	0.0100
d	0.0000	0.0160
e	0.1298	0.0380
f	0.5795	0.0480
i	0.0339	0.0210
j	0.0000	0.0050
k	0.0000	0.0400
l	0.0000	0.0300
m	0.0000	0.0290
o	0.8977	0.2140
p	0.9000	0.2790
q	0.9376	0.2910
r	0.8485	0.1080
s	0.9327	0.1680

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Chain	Atom inclusion	Q-score
t	0.9286	0.2370
u	0.8866	0.1280
v	0.9422	0.2110
w	0.8778	0.1930
x	0.9212	0.3030
y	0.9203	0.2620
z	0.9129	0.2670