Full wwPDB EM Validation Report ⓘ

Nov 22, 2022 – 01:16 PM JST

PDB ID	:	7EGC
EMDB ID	:	EMD-31112
Title	:	p53-bound TFIID-based holo PIC on HDM2 promoter
Authors	:	Chen, X.; Wu, Z.; Hou, H.; Qi, Y.; Wang, X.; Li, J.; Xu, Y.
Deposited on	:	2021-03-24
Resolution	:	3.90 Å(reported)

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

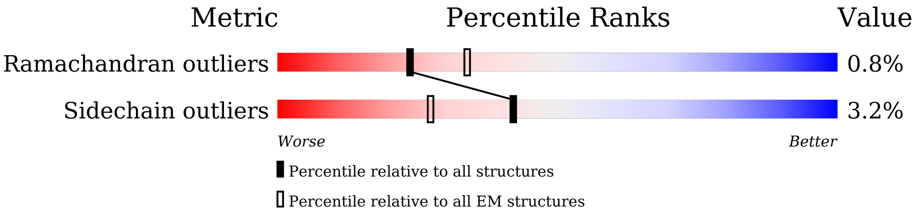
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance ⓘ

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

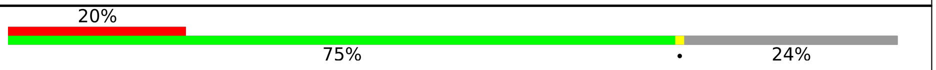
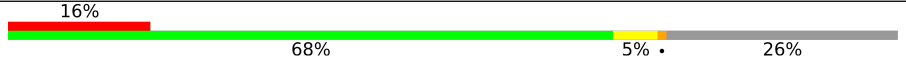
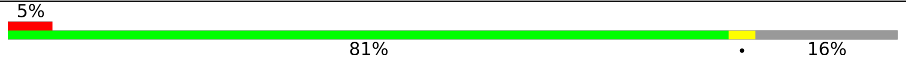
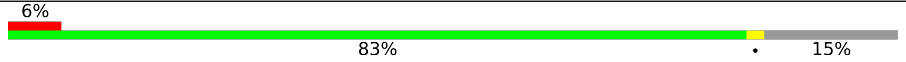
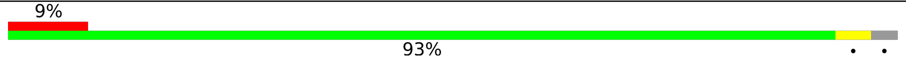
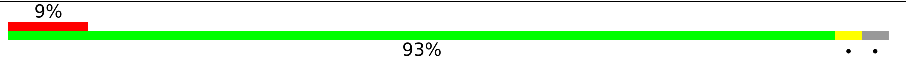
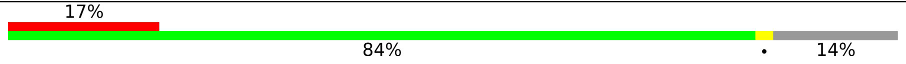
The reported resolution of this entry is 3.90 Å.

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	0	309	
2	1	548	
3	2	395	
4	3	308	
5	4	462	
6	5	71	
7	6	782	
8	7	760	
9	8	346	

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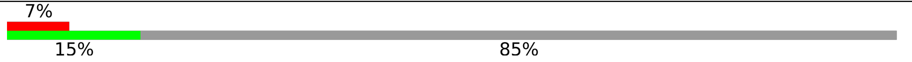
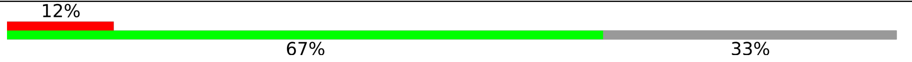
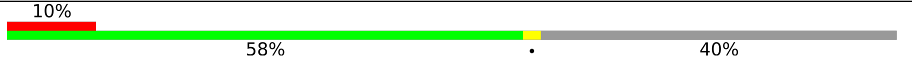
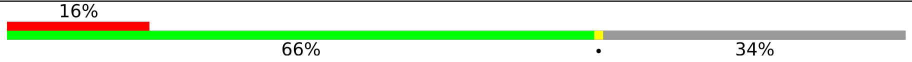
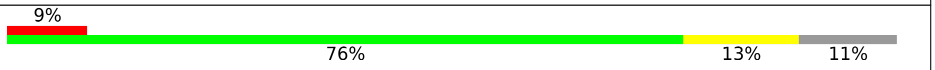
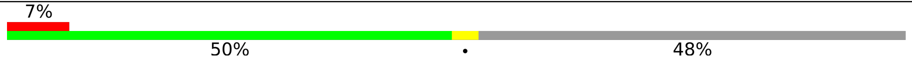
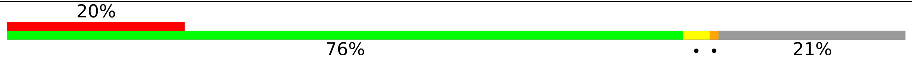
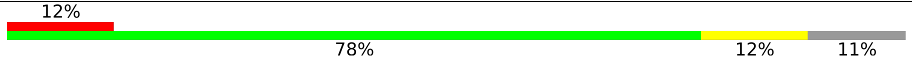
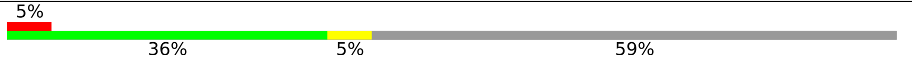
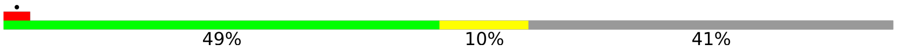
Mol	Chain	Length	Quality of chain
10	9	323	
11	A	1872	
12	B	1199	
13	D	1085	
13	d	1085	
14	E	800	
14	e	800	
15	F	677	
15	f	677	
16	G	349	
17	H	310	
18	I	264	
18	i	264	
19	J	218	
19	j	218	
20	L	161	
20	l	161	
21	O	109	
22	P	339	
23	Q	376	
24	R	316	
25	S	517	
26	T	249	
27	U	439	
28	V	291	

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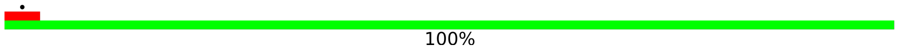
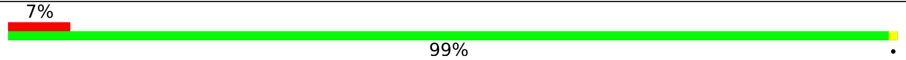
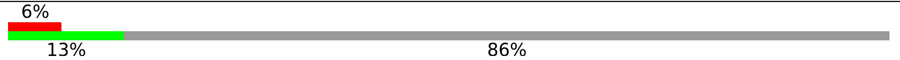
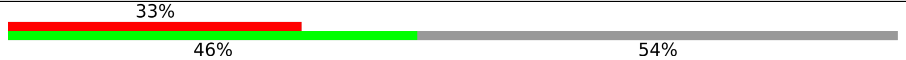
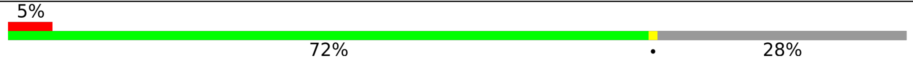
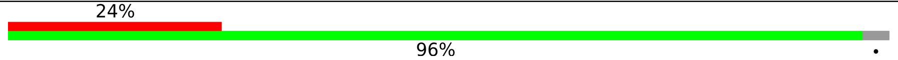
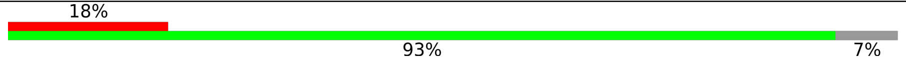
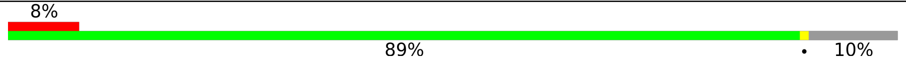
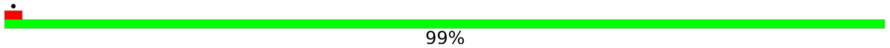
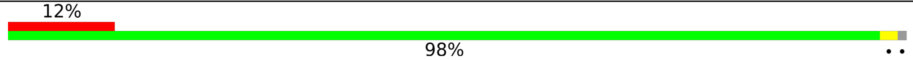
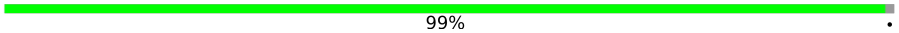
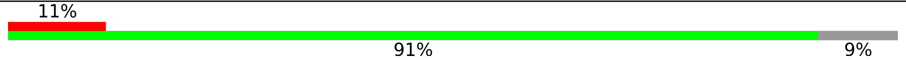
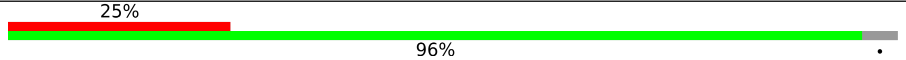
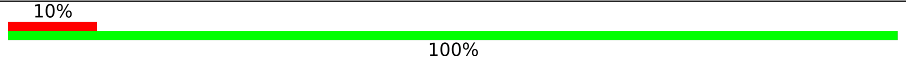
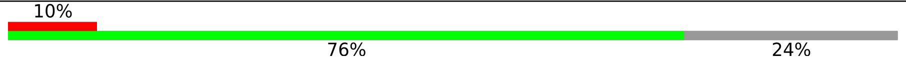
Mol	Chain	Length	Quality of chain
29	X	71	
30	Y	71	
31	c	929	
32	k	211	
33	m	124	
34	o	1970	
35	p	1174	
36	q	275	
37	r	142	
38	s	210	
39	t	127	
40	u	172	
41	v	150	
42	w	125	
43	x	67	
44	y	117	
45	z	58	

2 Entry composition

There are 48 unique types of molecules in this entry. The entry contains 113129 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	234	1774	1108	309	347	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	405	2634	1640	486	501	7	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	331	2534	1597	441	470	26	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	2065	1323	344	379	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	449	3579	2303	624	638	14	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
			Total	C	N	O	S		
7	6	606	4880	3117	849	884	30	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	7	734	5833	3727	1022	1055	29	0	0

- Molecule 9 is a protein called Cyclin-dependent kinase 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	8	298	2370	1531	404	424	11	0	0

- Molecule 10 is a protein called Cyclin-H.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	9	287	2334	1493	402	422	17	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	A	550	4511	2882	782	820	27	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	D	158	1322	824	247	248	3	0	0

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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	546	Total 4364	C 2766	N 757	O 820	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	408	Total 3109	C 1970	N 542	O 579	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	145	Total 1180	C 748	N 217	O 211	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	75	Total 614	C 384	N 107	O 120	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	97	Total 771	C 491	N 133	O 145	S 2	0	0

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

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

- Molecule 23 is a protein called Transcription initiation factor IIA subunit 1.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R	250	Total 1929	C 1209	N 343	O 360	S 17	0	0

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

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

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

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

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

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

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

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

- Molecule 29 is a DNA chain called DNA (71-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
29	X	71	1464	695	265	433	71	0	0

- Molecule 30 is a DNA chain called DNA (71-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
30	Y	71	1447	687	270	419	71	0	0

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

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

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

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

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

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

- Molecule 34 is a protein called DNA-directed RNA polymerase II subunit RPB1.

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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 1186	C 750	N 194	O 237	S 5	0	0

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

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

- Molecule 43 is a protein called RPB10.

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

- Molecule 44 is a protein called RNA_pol_L_2 domain-containing protein.

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

- Molecule 45 is a protein called RPB12.

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

- Molecule 46 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
46	0	2	Total 2	Zn 2	0
46	2	3	Total 3	Zn 3	0
46	3	1	Total 1	Zn 1	0

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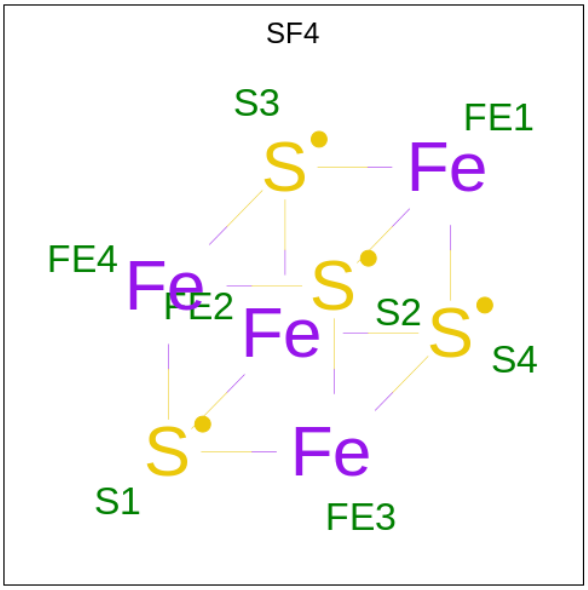
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
46	R	1	1	1	0
46	U	1	Total 1	Zn 1	0
46	o	2	Total 2	Zn 2	0
46	p	1	Total 1	Zn 1	0
46	q	1	Total 1	Zn 1	0
46	w	2	Total 2	Zn 2	0
46	x	1	Total 1	Zn 1	0
46	z	1	Total 1	Zn 1	0

- Molecule 47 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 48 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

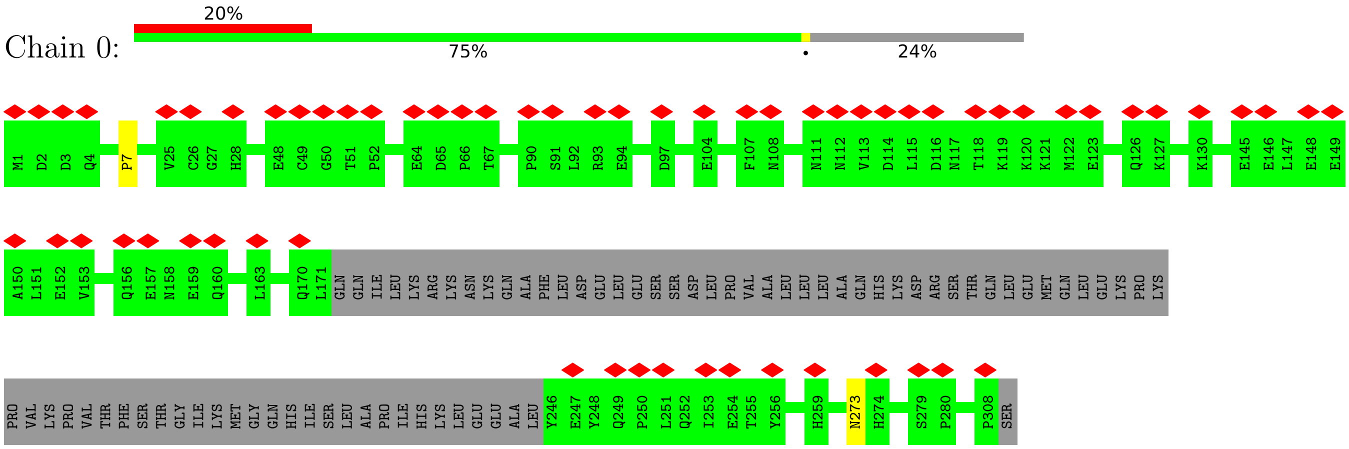
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
48	o	1	1	1	0

3 Residue-property plots ⓘ

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.

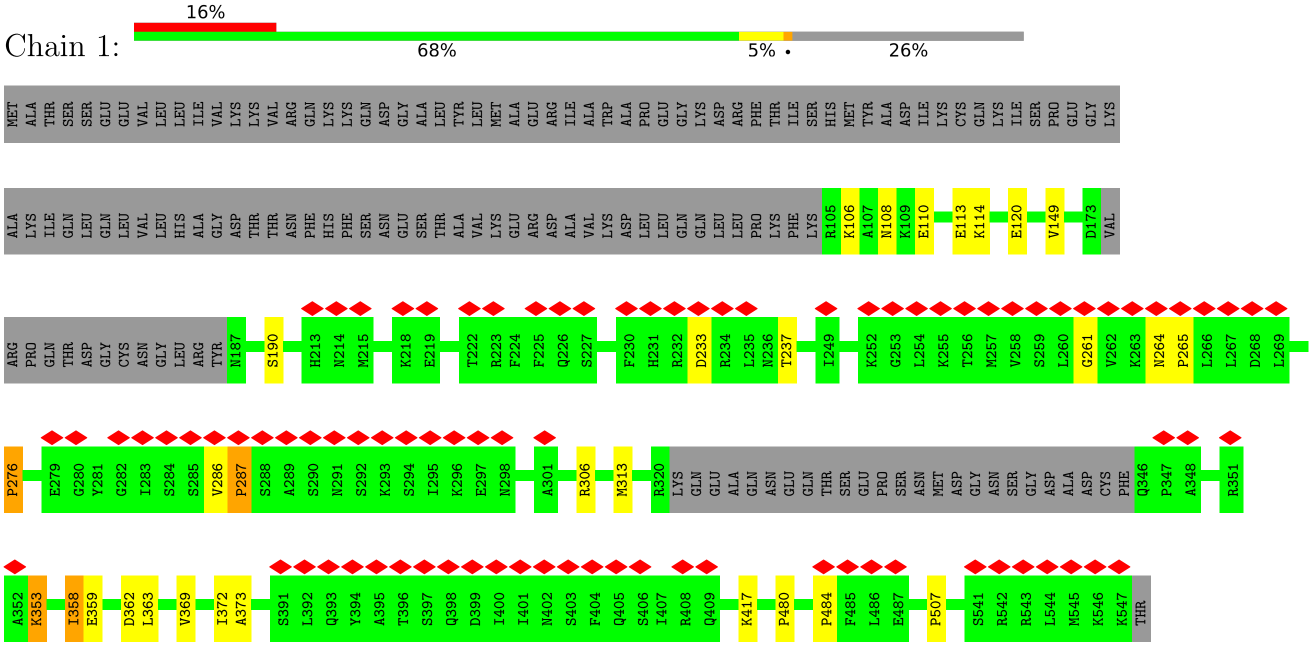
- Molecule 1: CDK-activating kinase assembly factor MAT1

Chain 0:

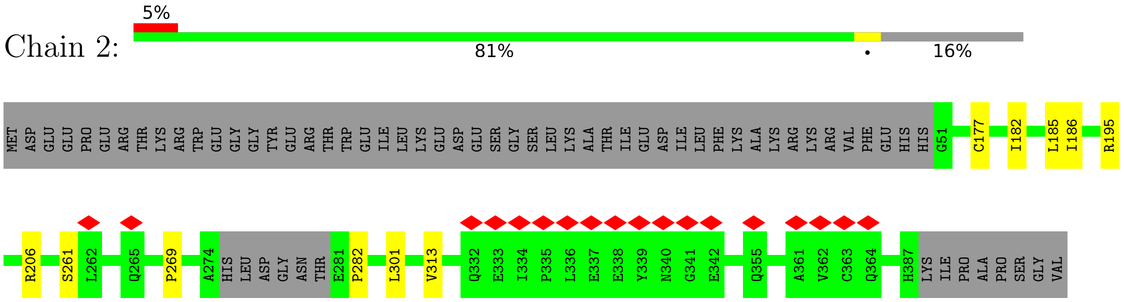


- Molecule 2: General transcription factor IIH subunit 1

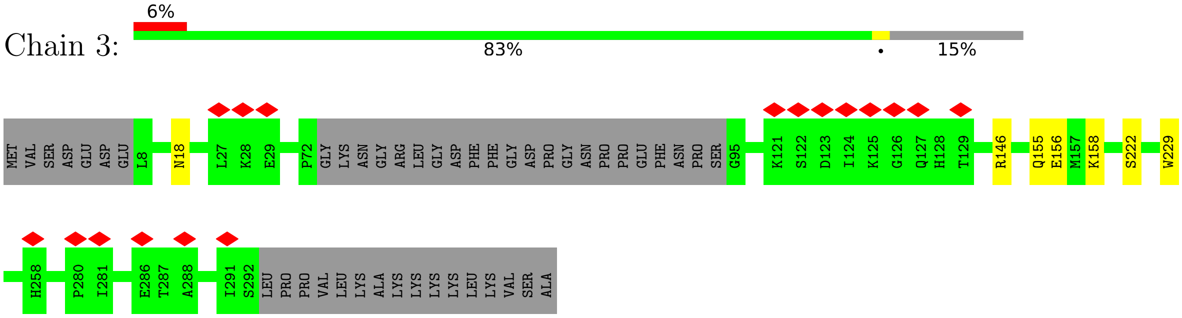
Chain 1:



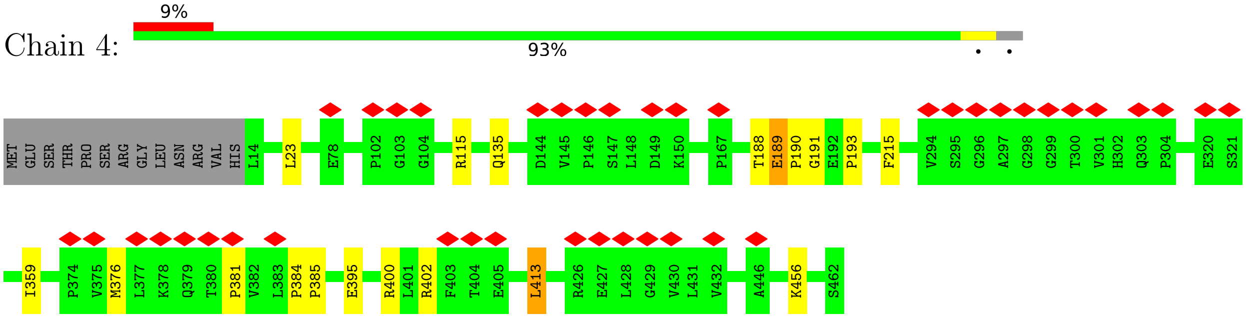
- Molecule 3: General transcription factor IIH subunit 2



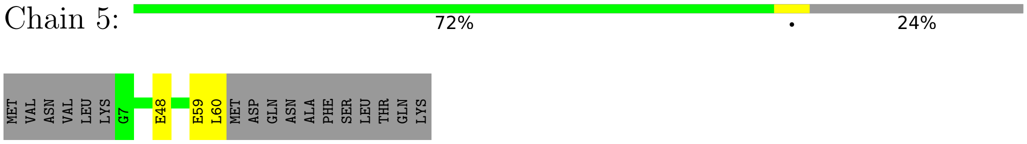
- Molecule 4: General transcription factor IIH subunit 3



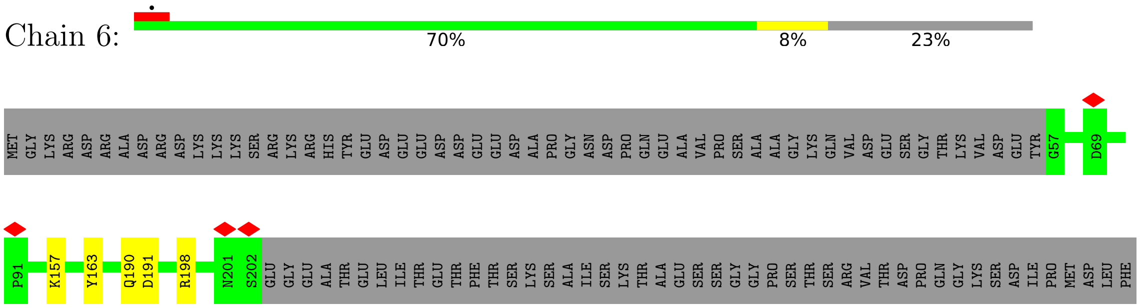
- Molecule 5: General transcription factor IIH subunit 4

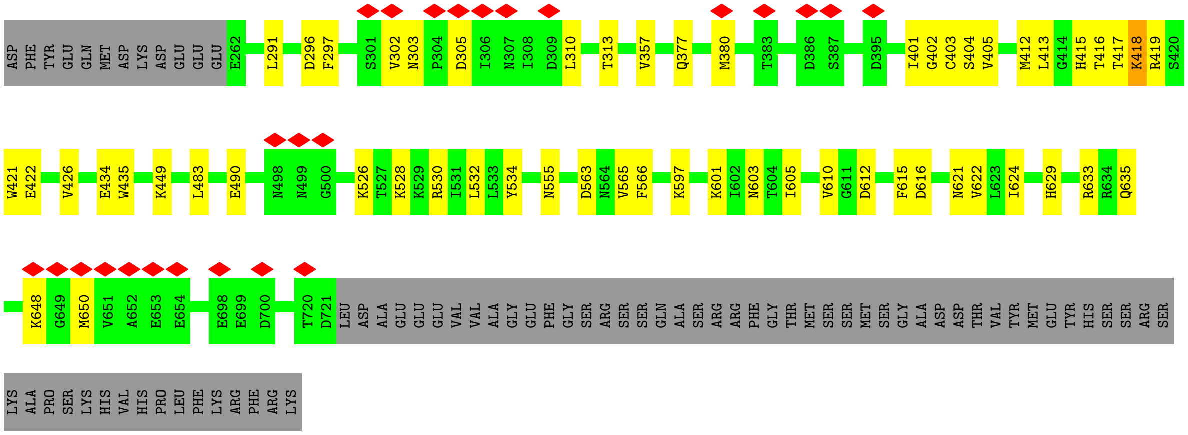


- Molecule 6: General transcription factor IIH subunit 5



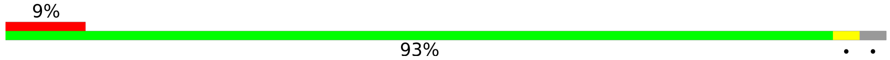
- Molecule 7: General transcription and DNA repair factor IIH helicase subunit XPB

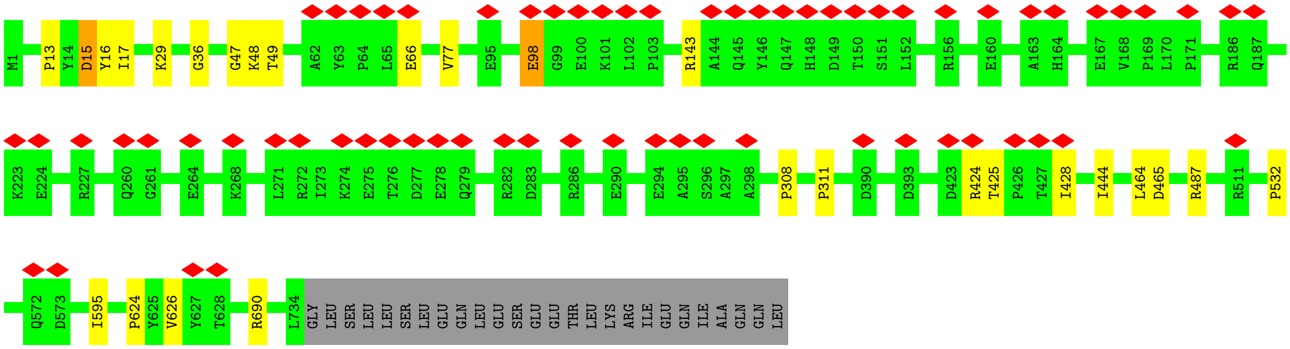




- Molecule 8: General transcription and DNA repair factor IIH helicase subunit XPD

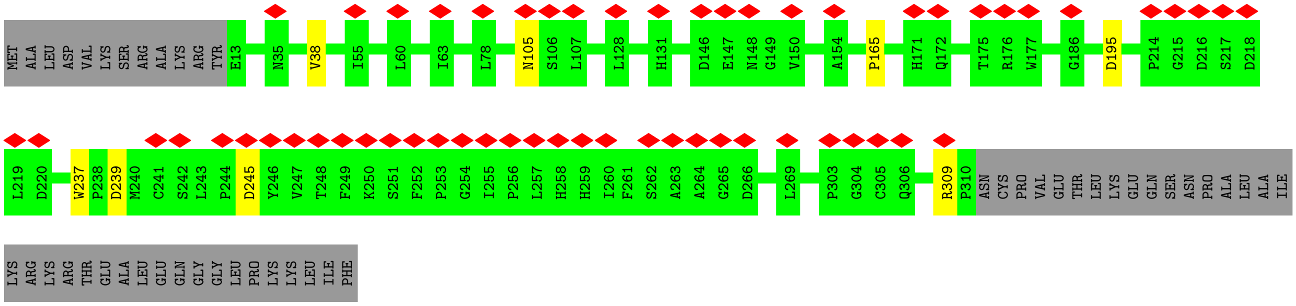
Chain 7:





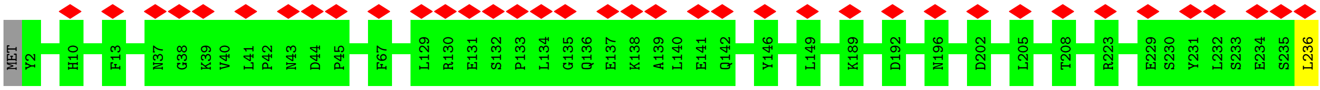
- Molecule 9: Cyclin-dependent kinase 7

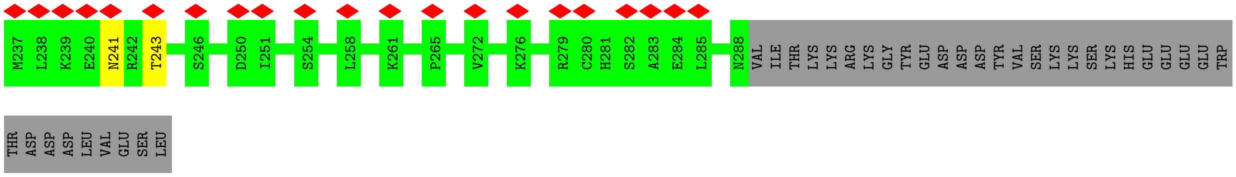
Chain 8:



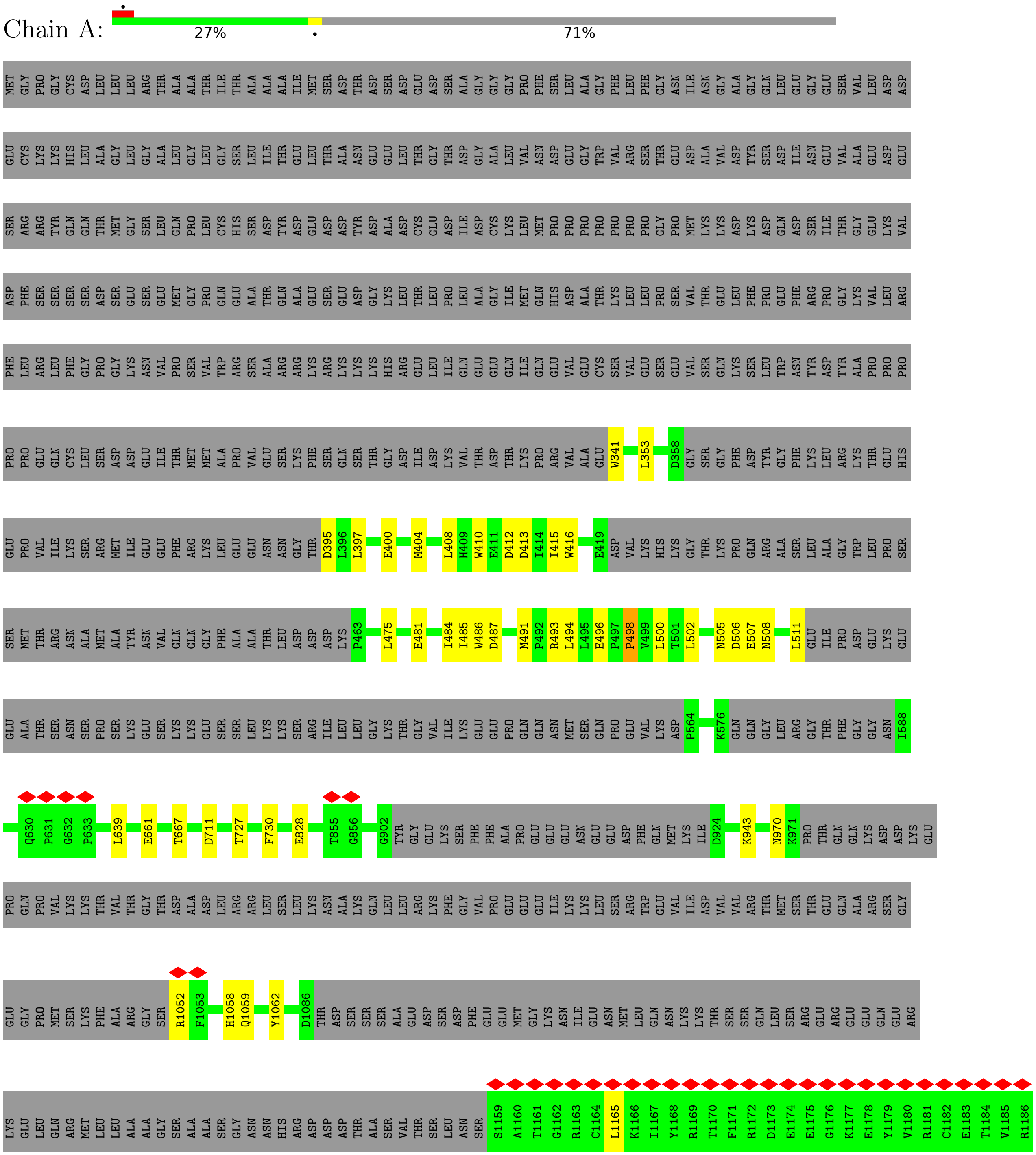
- Molecule 10: Cyclin-H

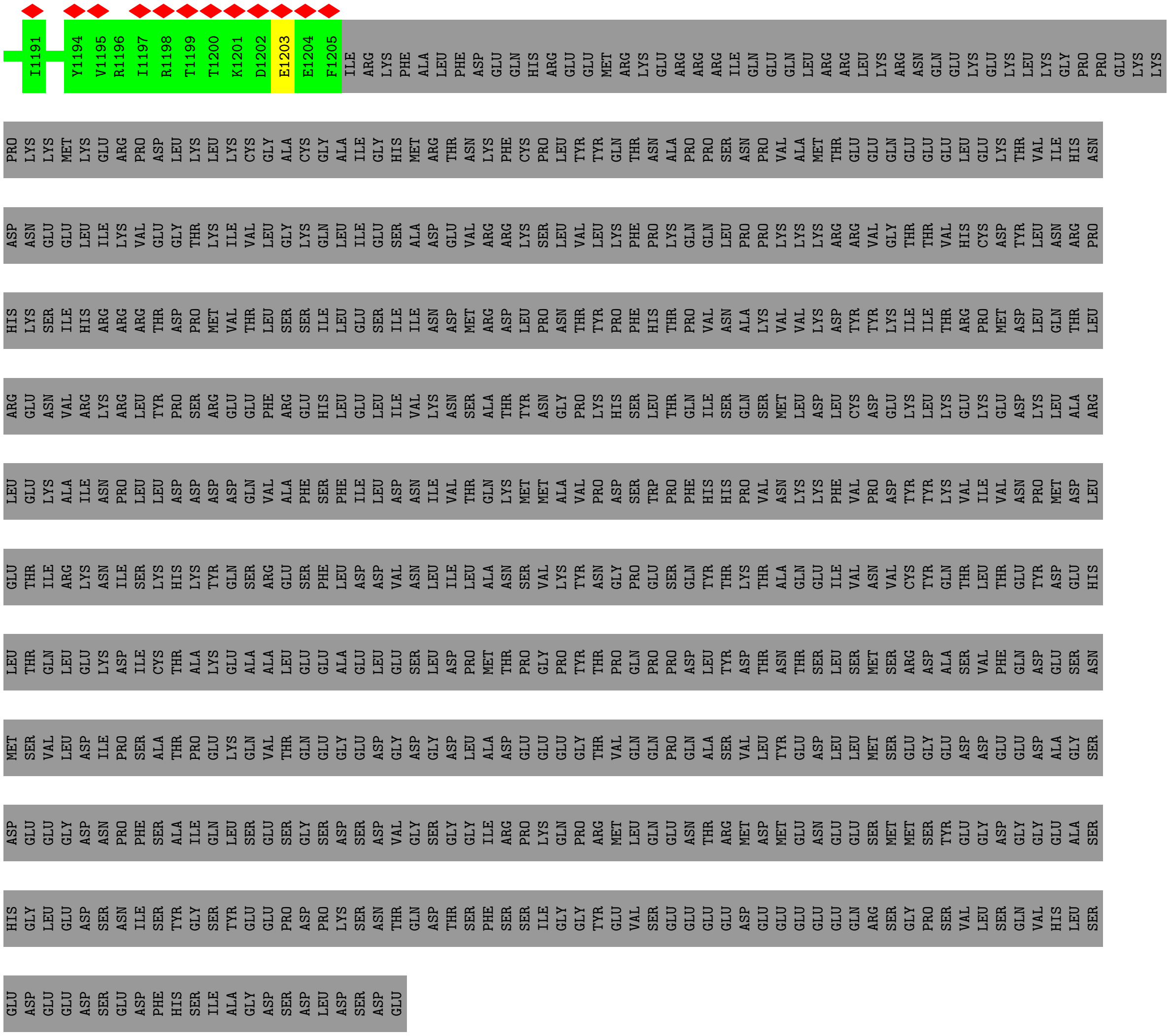
Chain 9:



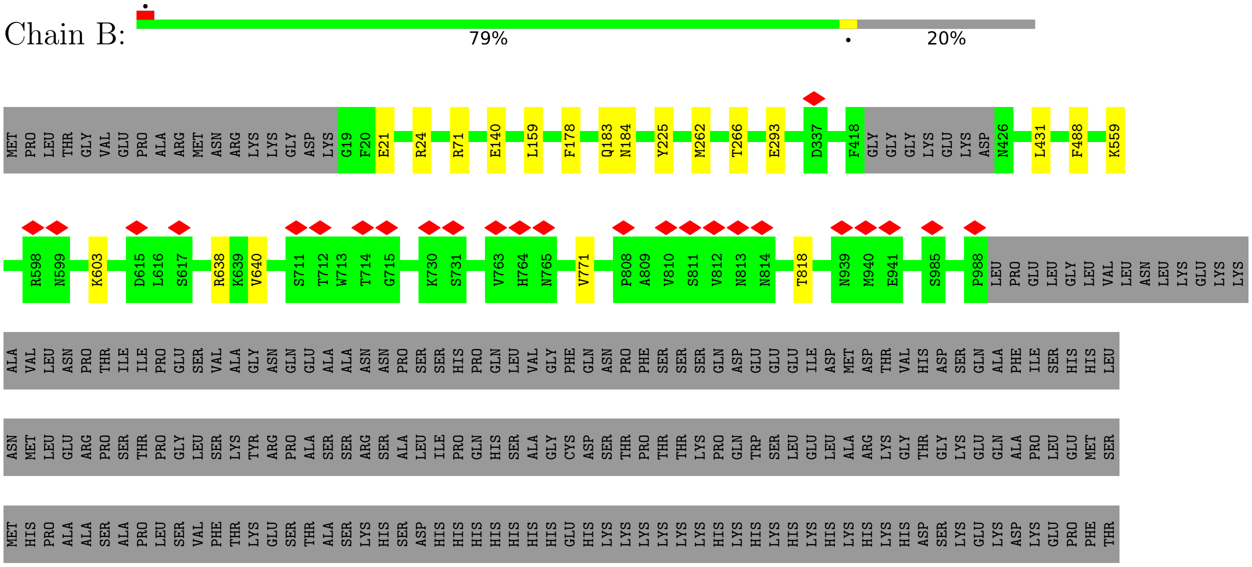


- Molecule 11: Transcription initiation factor TFIID subunit 1



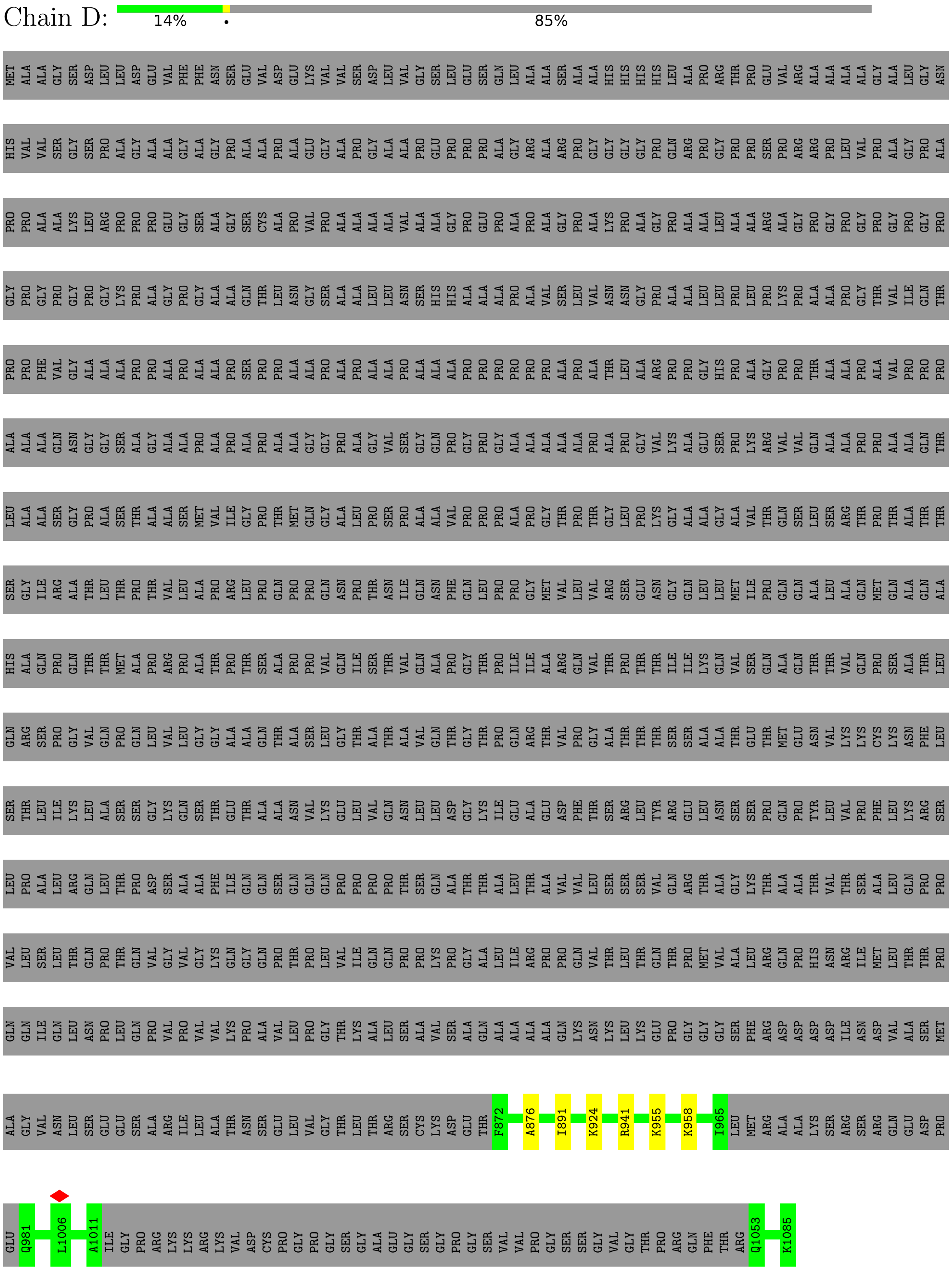


- Molecule 12: Transcription initiation factor TFIID subunit 2



PHE SER SER PRO ALA SER GLY ARG SER ILE ARG SER PRO SER LEU SER ASP

- Molecule 13: Transcription initiation factor TFIID subunit 4



Chain D:

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

HIS VAL VAL SER GLY SER PRO ALA GLY ALA ALA GLY ALA GLY PRO ALA ALA PRO ALA GLU GLY ALA PRO GLY ALA ALA PRO GLU PRO PRO ALA GLY ARG ALA ARG PRO GLY GLY GLY PRO GLN ARG PRO GLY PRO PRO SER PRO ARG ARG PRO LEU VAL PRO ALA GLY PRO ALA

PRO PRO ALA ALA LYS LEU ARG PRO PRO PRO GLU GLY SER ALA GLY SER CYS ALA PRO VAL PRO ALA ALA ALA ALA VAL ALA ALA GLY PRO GLU PRO ALA PRO ALA GLY PRO ALA LYS PRO ALA GLY PRO ALA ALA LEU ALA ALA ARG ALA GLY PRO GLY PRO GLY PRO GLY PRO GLY PRO

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

PRO PRO PHE VAL GLY ALA ALA ALA PRO PRO ALA PRO ALA ALA PRO SER PRO PRO ALA ALA PRO ALA PRO ALA ALA PRO ALA ALA ALA PRO PRO PRO PRO PRO PRO ALA PRO ALA THR LEU ALA ARG PRO PRO GLY HIS PRO ALA GLY PRO PRO THR ALA ALA PRO ALA VAL PRO PRO PRO

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

LEU ALA ALA SER GLY PRO ALA SER THR ALA ALA SER MET VAL ILE GLY PRO THR MET GLN GLY ALA LEU PRO SER PRO ALA ALA VAL PRO PRO PRO ALA PRO GLY THR PRO THR GLY LEU PRO LYS GLY ALA ALA GLY ALA VAL THR GLN SER LEU SER ARG THR PRO THR ALA THR THR

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

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

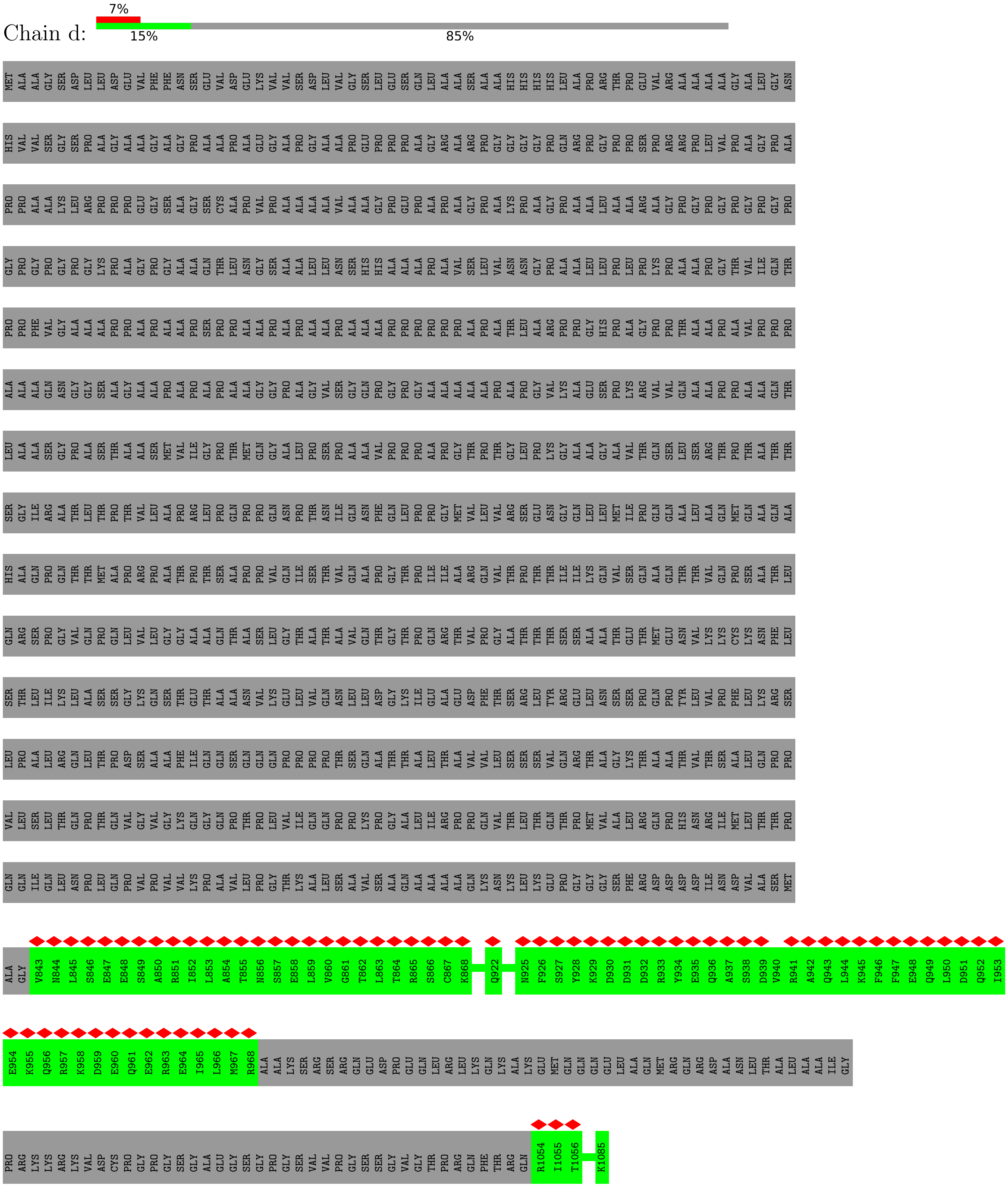
VAL LEU SER LEU THR GLN PRO THR GLN VAL GLY VAL GLY LYS GLN GLY GLN PRO THR PRO LEU VAL ILE GLN GLN PRO PRO LYS PRO GLY ALA LEU ILE ARG PRO PRO GLN VAL THR LEU THR GLN THR PRO MET VAL ALA LEU ARG GLN PRO HIS ASN ARG ILE MET LEU THR THR PRO

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

ALA GLY VAL ASN LEU SER GLU GLU SER ALA ARG ILE LEU ALA THR ASN SER GLU LEU VAL GLY THR LEU THR ARG SER CYS LYS ASP GLU THR F872 A876 I891 K924 R941 K955 K958 I965 LEU MET ARG ALA ALA LYS SER ARG SER ARG GLN GLU ASP PRO

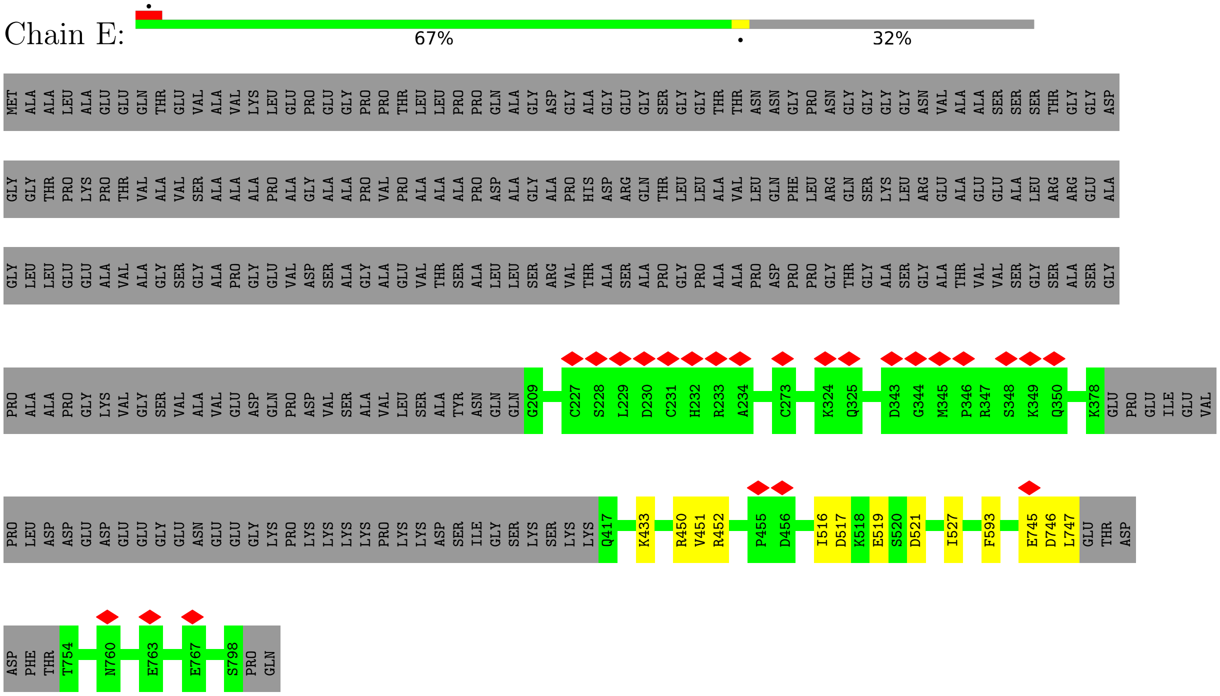
GLU Q981 L1006 A1011 ILE GLY PRO ARG LYS LYS ARG LYS VAL ASP CYS PRO GLY PRO GLY SER GLY ALA GLU GLY SER GLY PRO GLY SER VAL VAL PRO GLY SER SER GLY VAL GLY THR PRO ARG GLN PHE THR ARG Q1053 K1085

- Molecule 13: Transcription initiation factor TFIID subunit 4



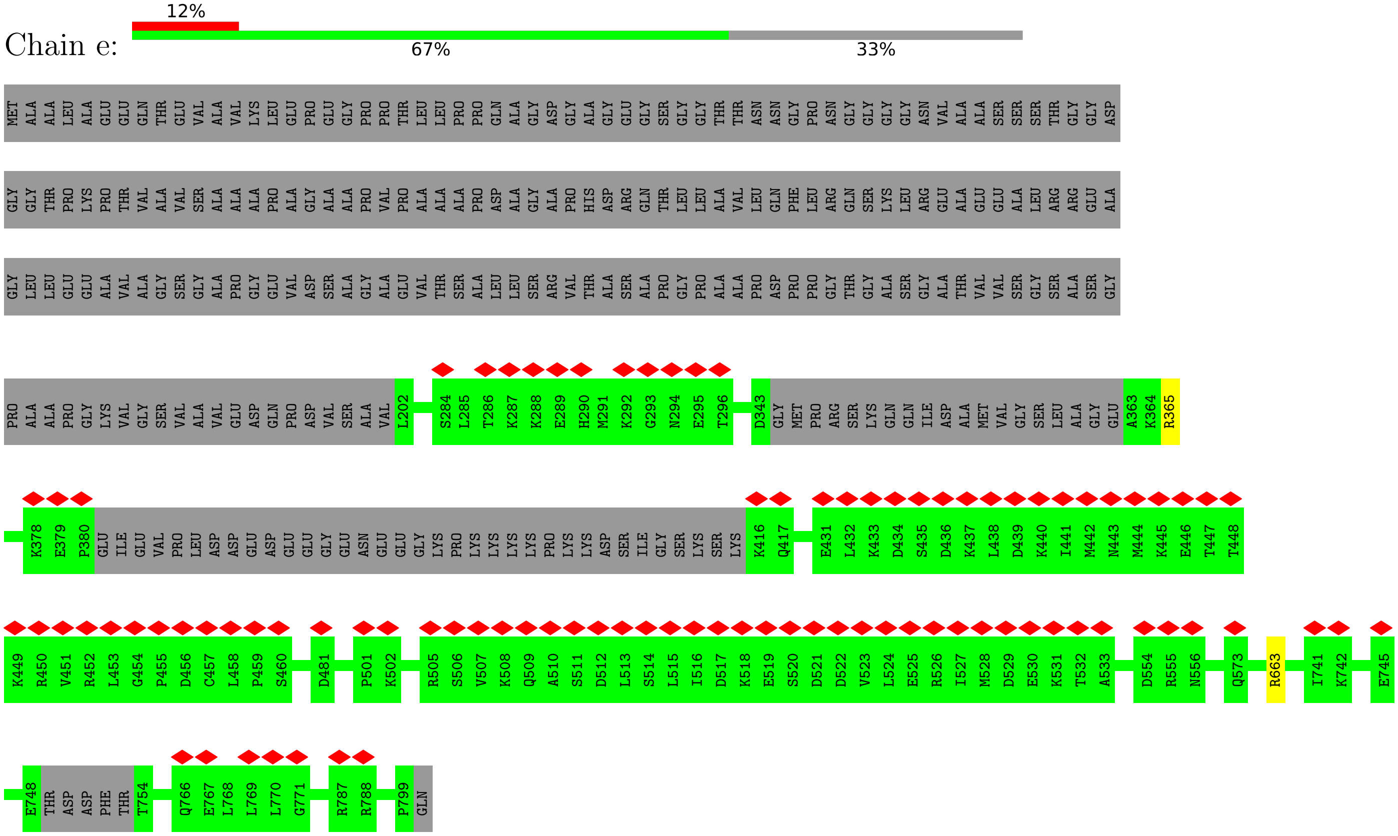
- Molecule 14: Transcription initiation factor TFIID subunit 5

Chain E:



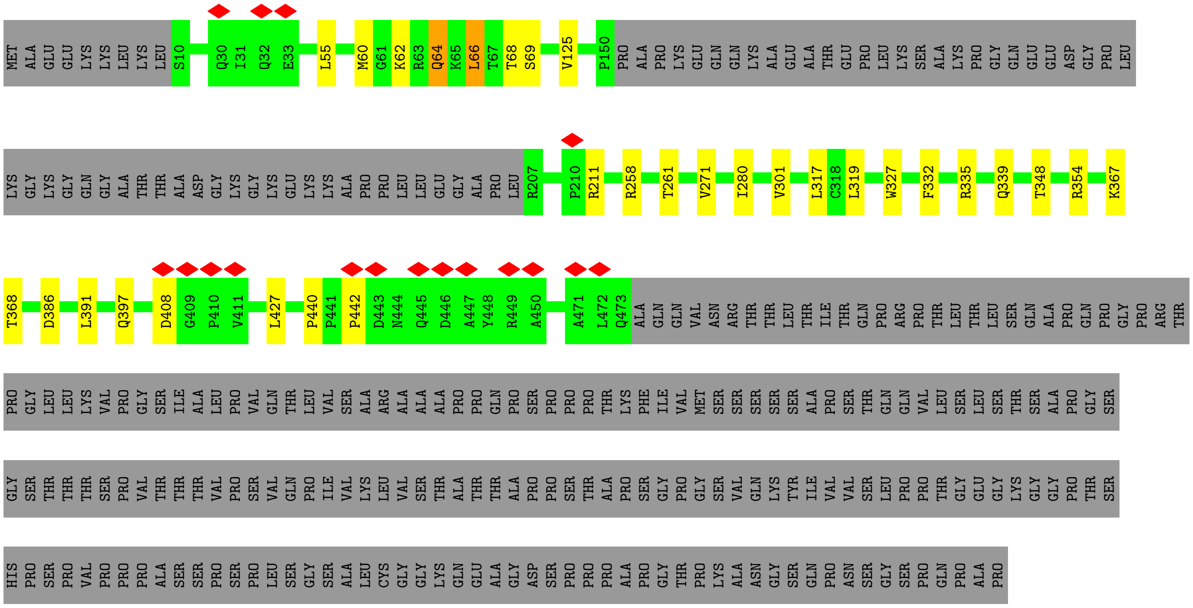
- Molecule 14: Transcription initiation factor TFIID subunit 5

Chain e:



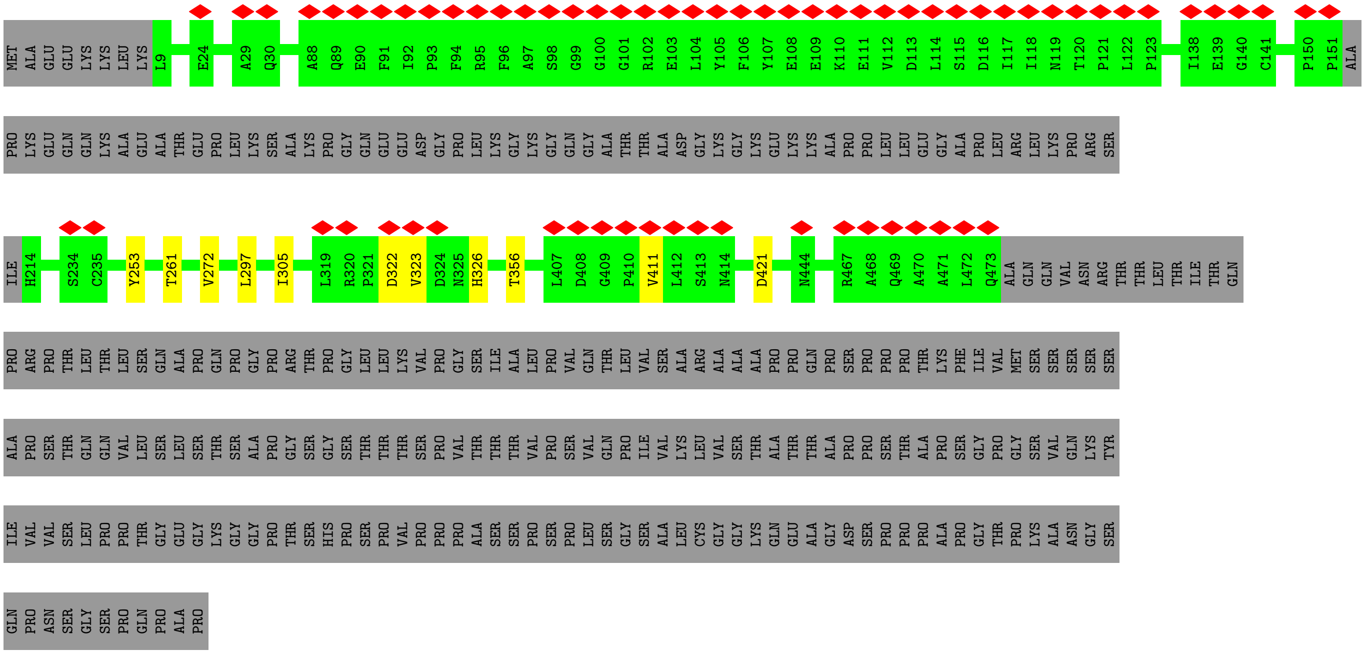
- Molecule 15: Transcription initiation factor TFIID subunit 6

Chain F:



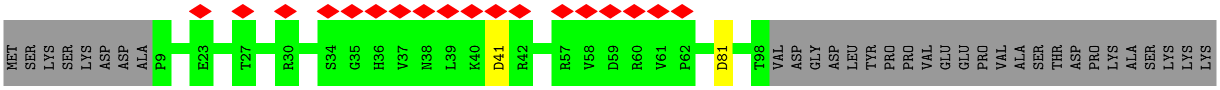
- Molecule 15: Transcription initiation factor TFIID subunit 6

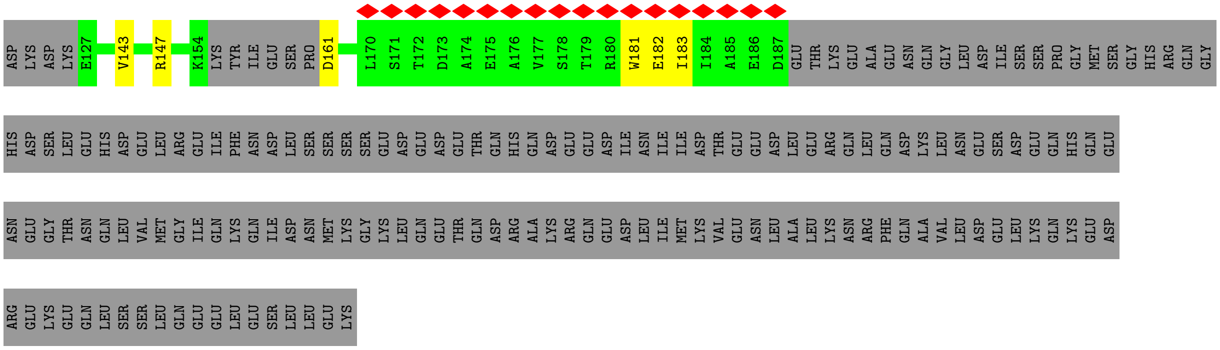
Chain f:



- Molecule 16: Transcription initiation factor TFIID subunit 7

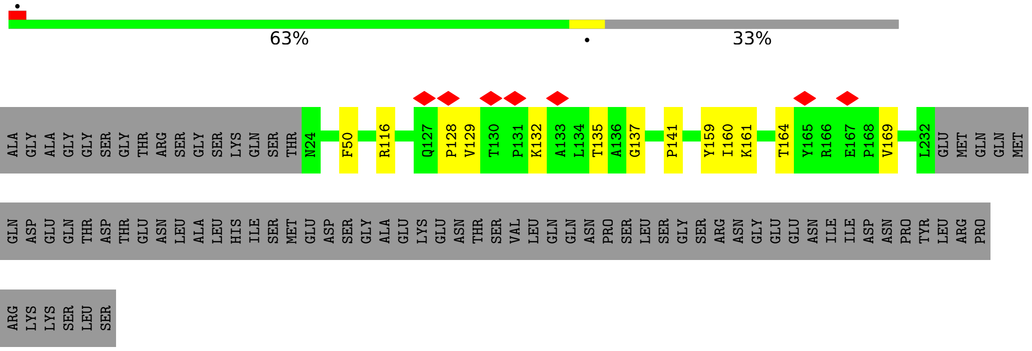
Chain G:





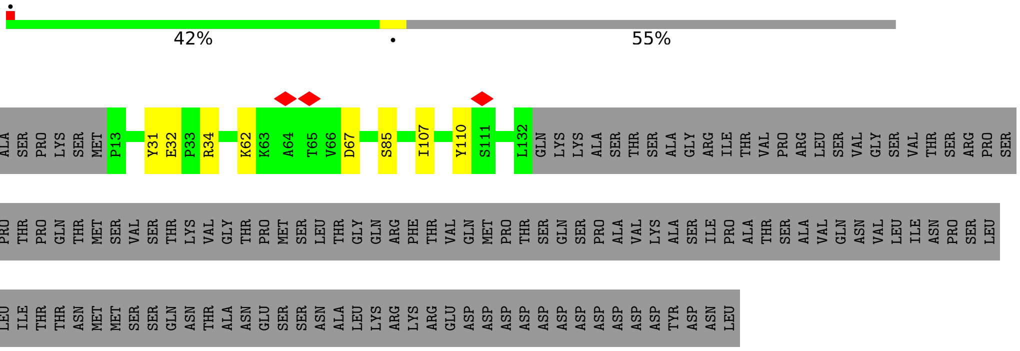
- Molecule 17: Transcription initiation factor TFIID subunit 8

Chain H:



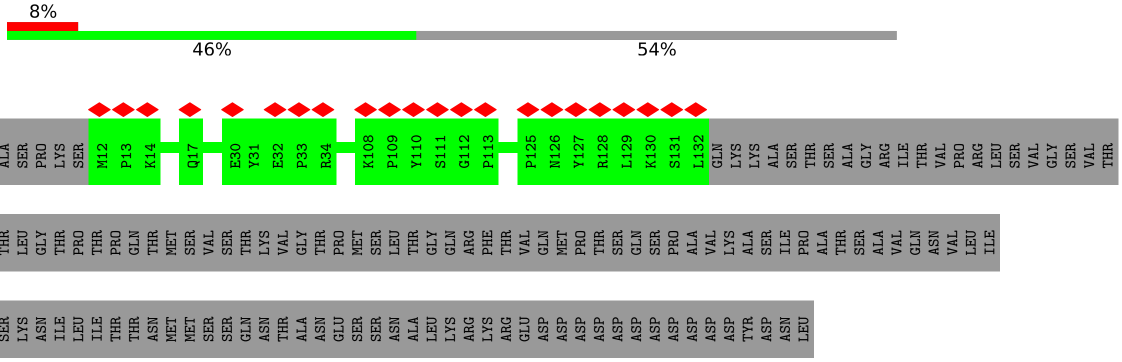
- Molecule 18: Transcription initiation factor TFIID subunit 9

Chain I:



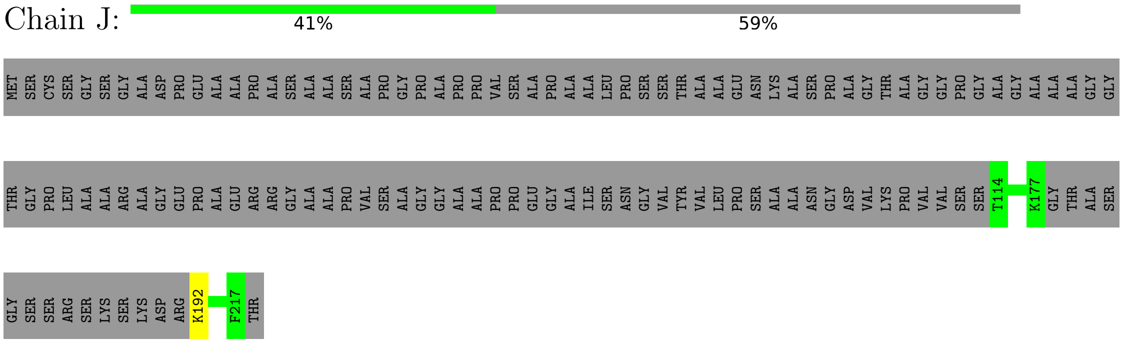
- Molecule 18: Transcription initiation factor TFIID subunit 9

Chain i:



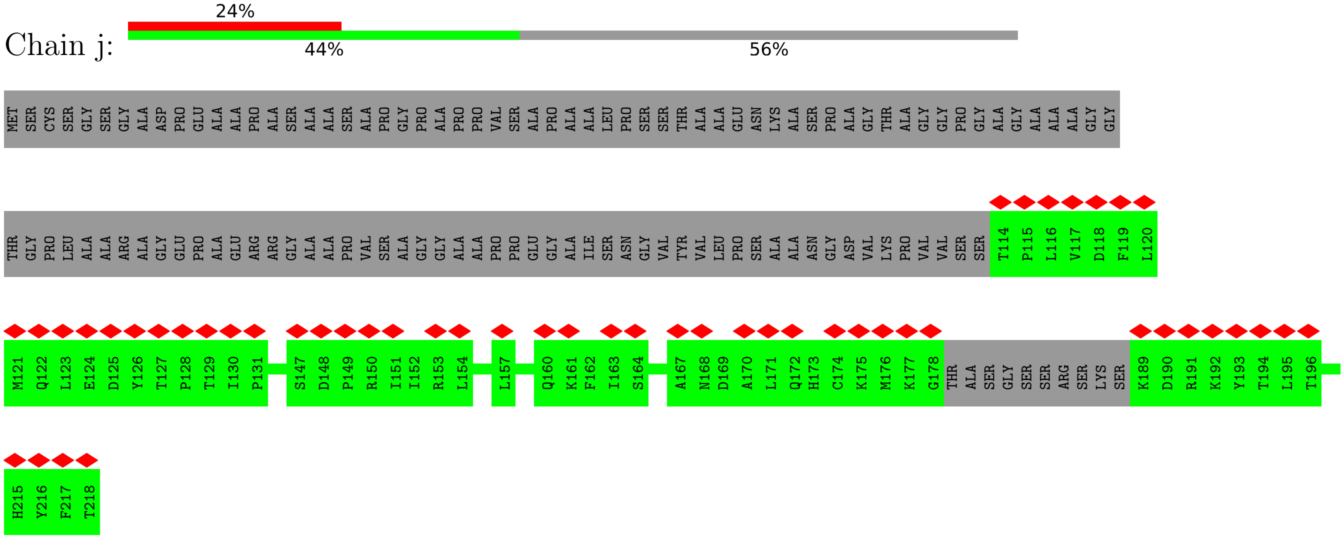
- Molecule 19: Transcription initiation factor TFIID subunit 10

Chain J:



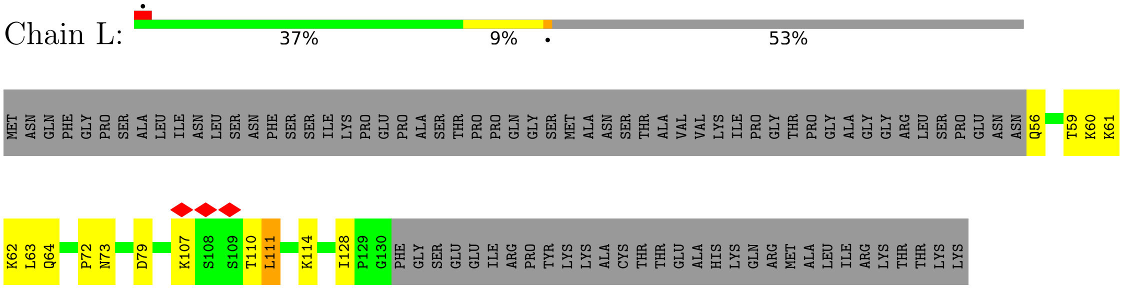
- Molecule 19: Transcription initiation factor TFIID subunit 10

Chain j:



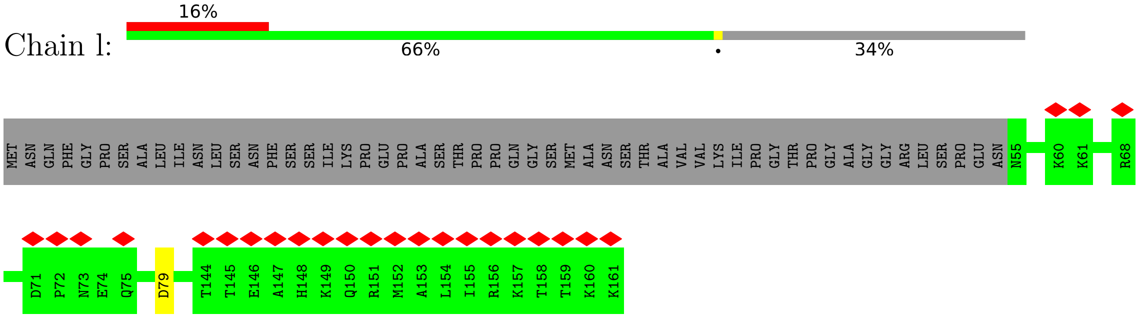
- Molecule 20: Transcription initiation factor TFIID subunit 12

Chain L:

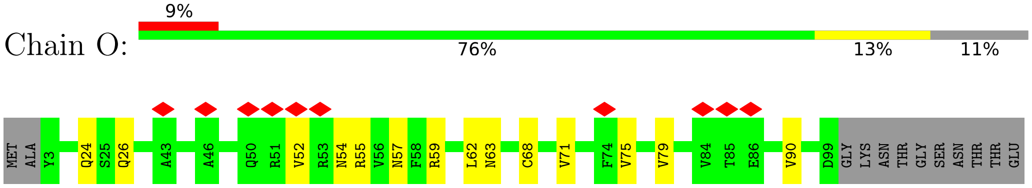


- Molecule 20: Transcription initiation factor TFIID subunit 12

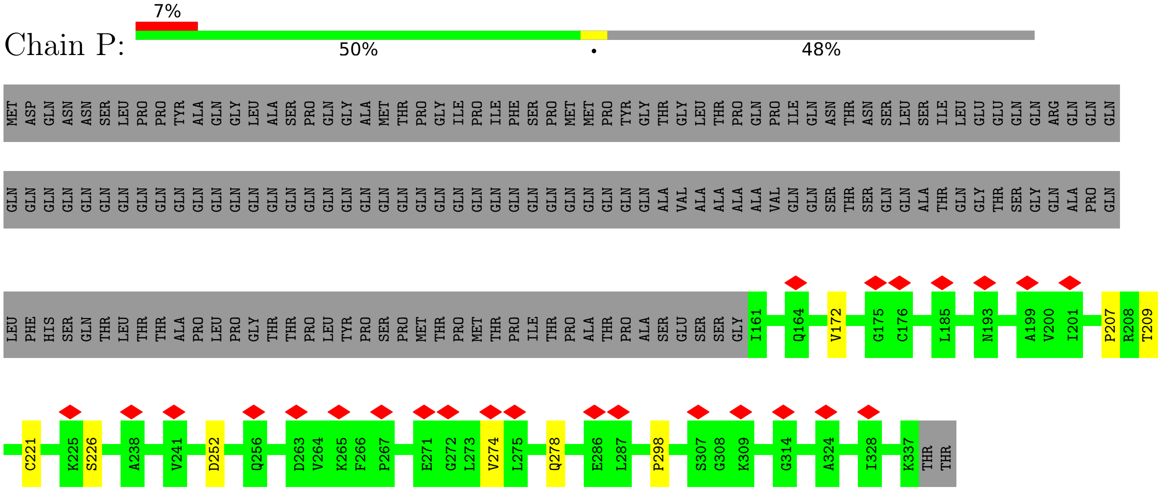
Chain l:



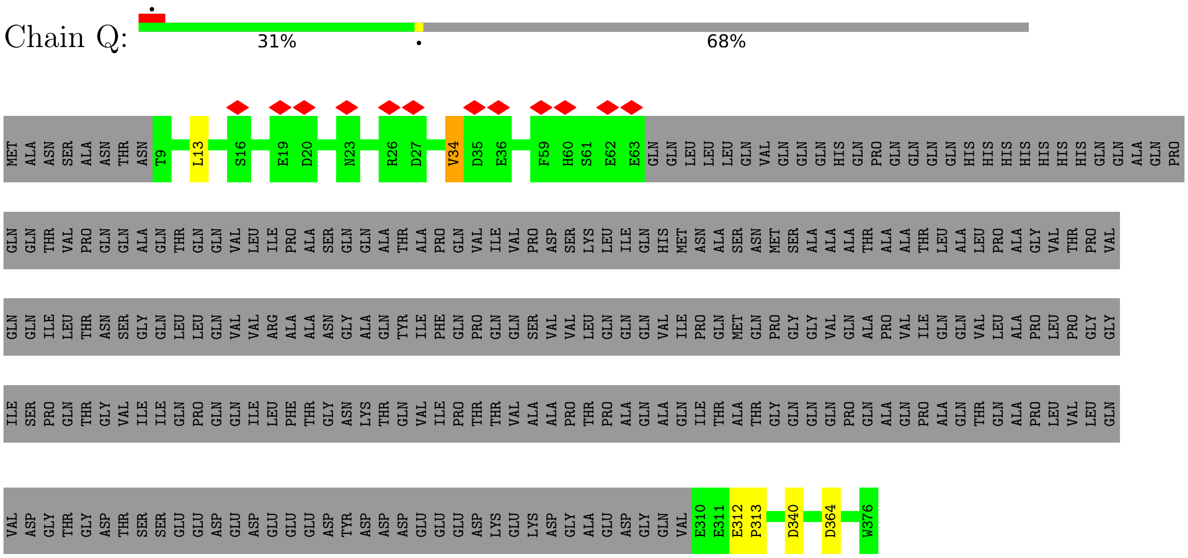
- Molecule 21: Transcription initiation factor IIA subunit 2



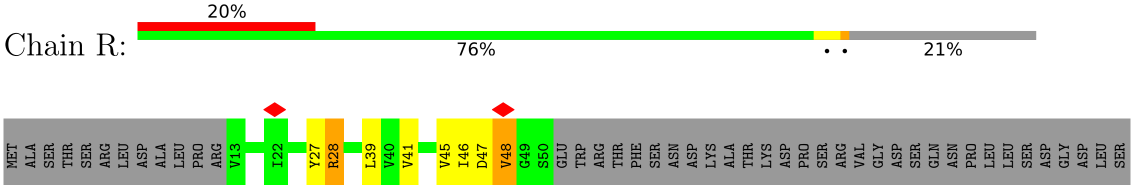
- Molecule 22: TATA-box-binding protein

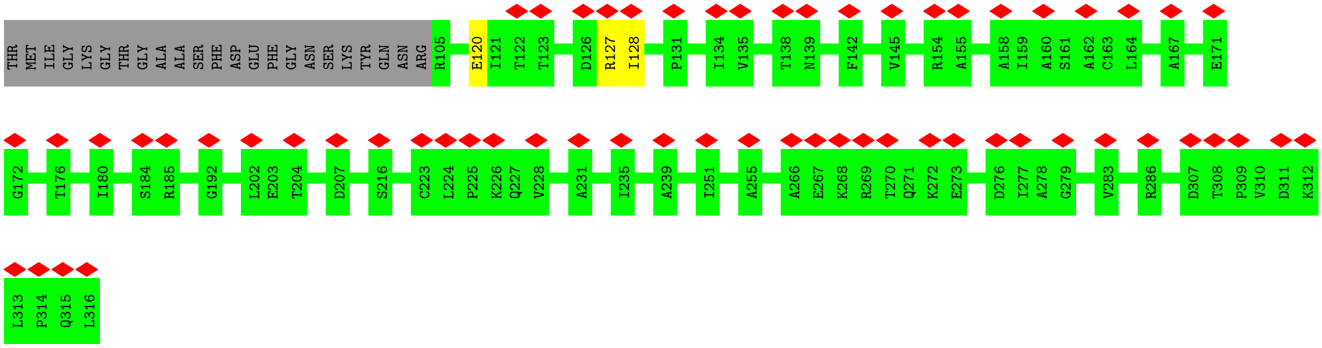


- Molecule 23: Transcription initiation factor IIA subunit 1

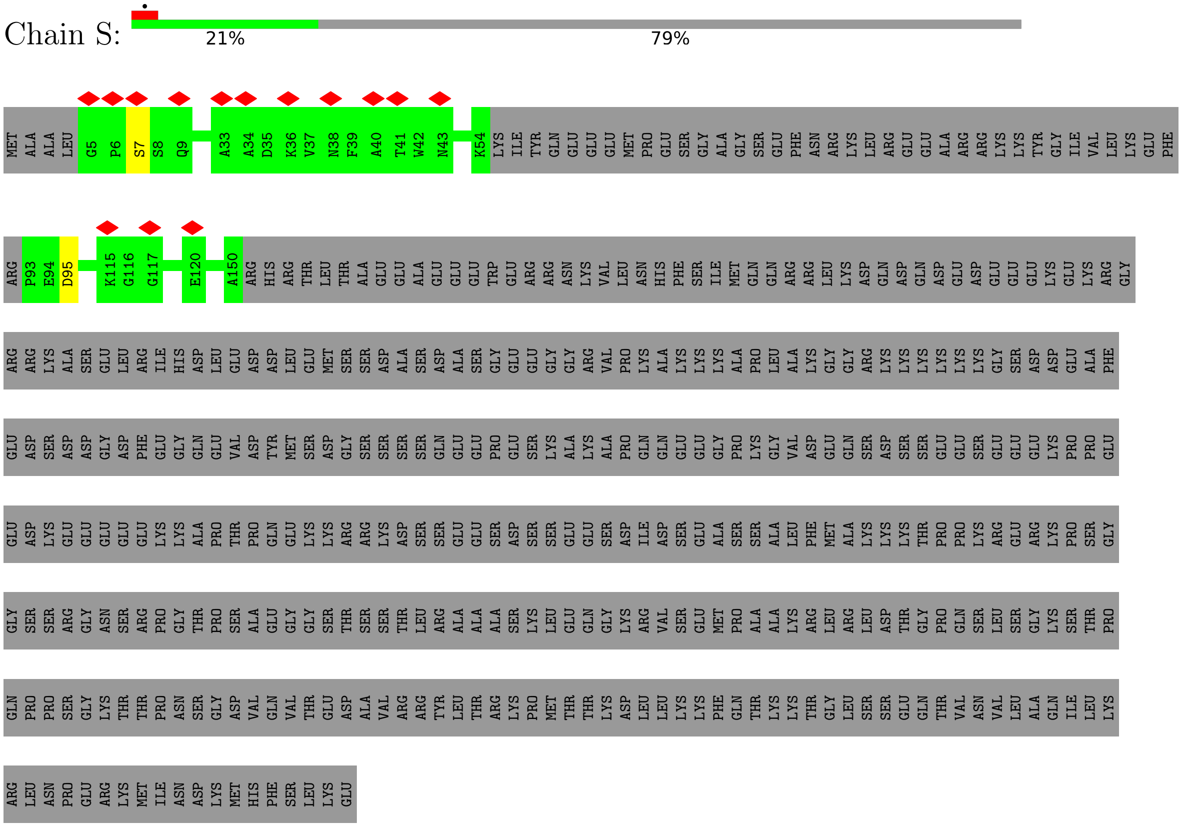


- Molecule 24: Transcription initiation factor IIB

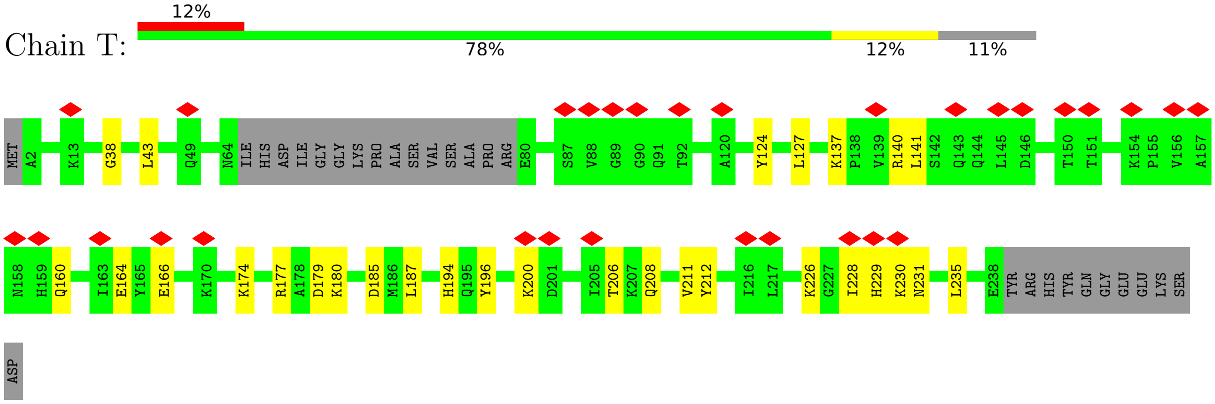




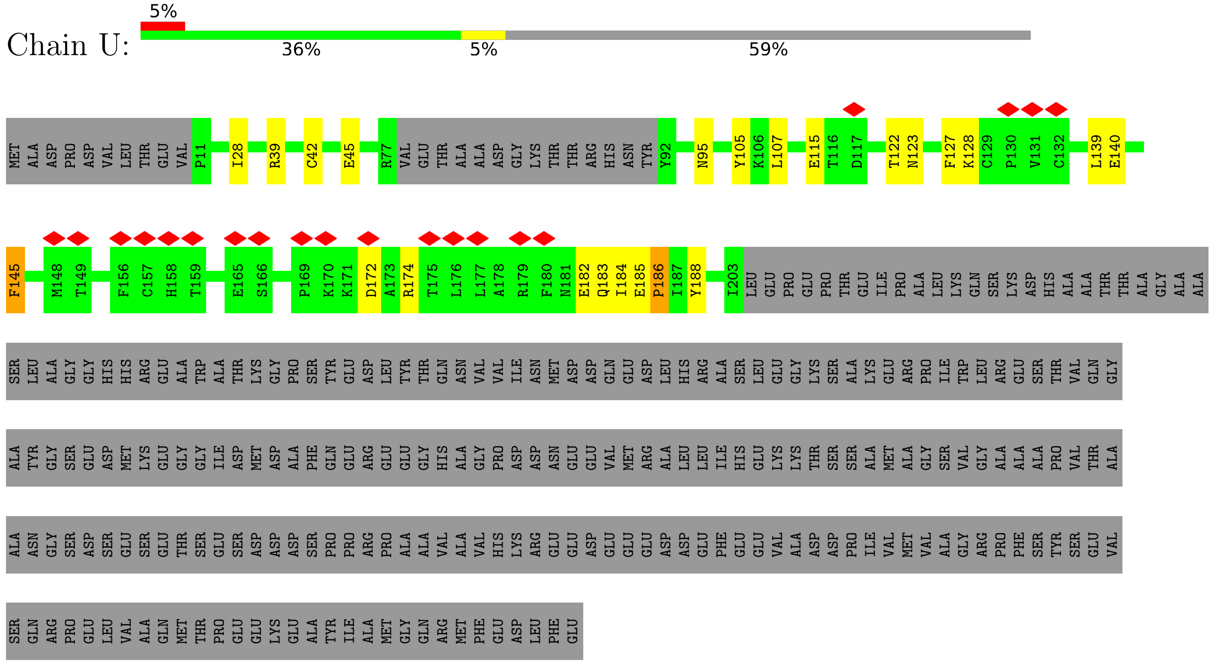
- Molecule 25: General transcription factor IIF subunit 1



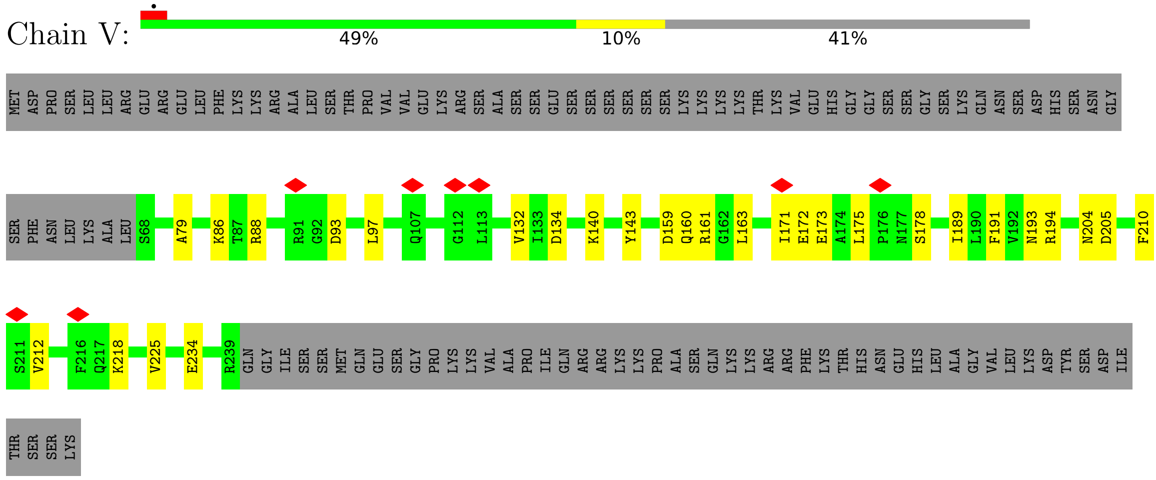
- Molecule 26: General transcription factor IIF subunit 2



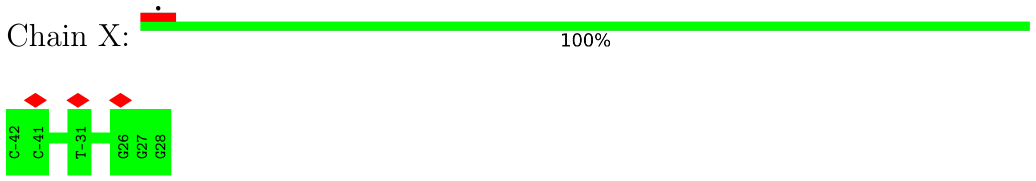
- Molecule 27: General transcription factor IIE subunit 1



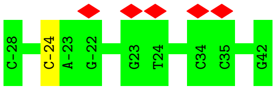
- Molecule 28: Transcription initiation factor IIE subunit beta



- Molecule 29: DNA (71-MER)

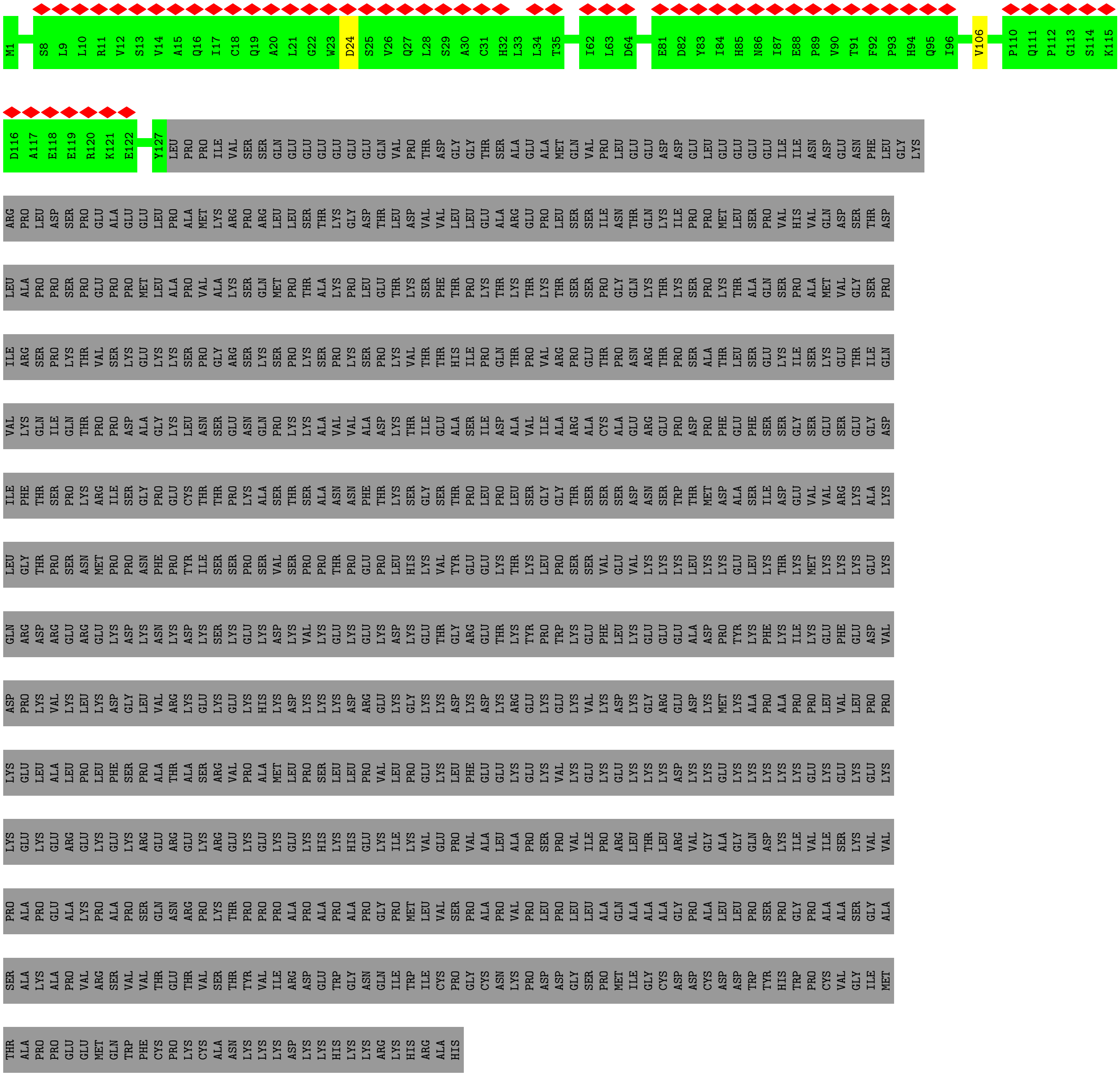


- Molecule 30: DNA (71-MER)



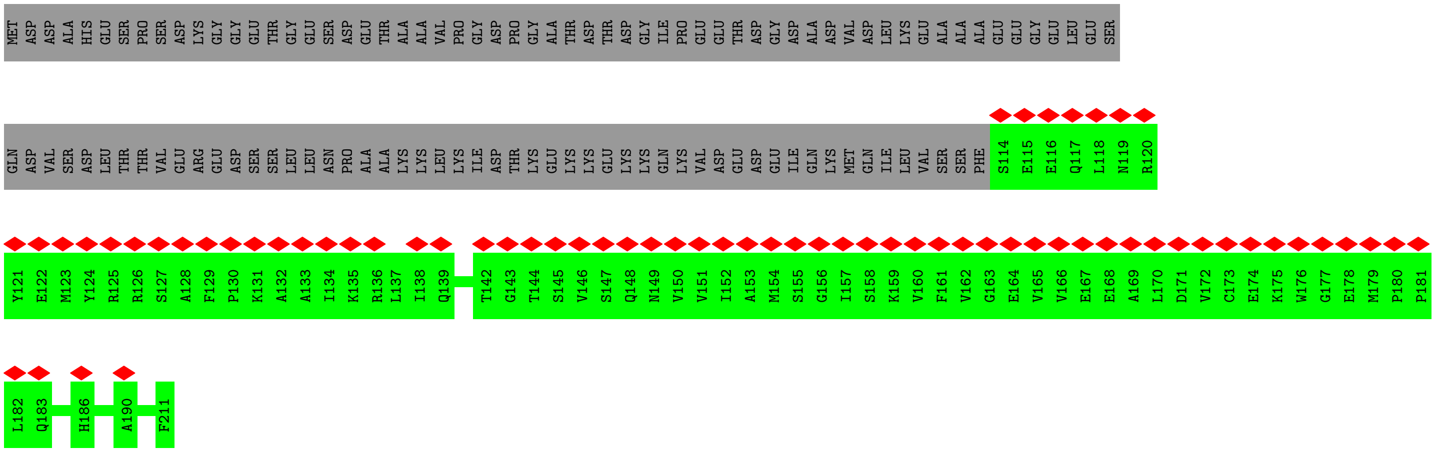
- Molecule 31: Transcription initiation factor TFIID subunit 3

Chain c:



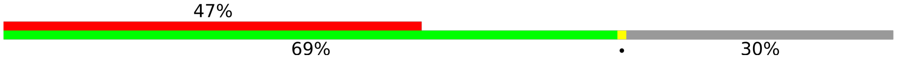
- Molecule 32: Transcription initiation factor TFIID subunit 11

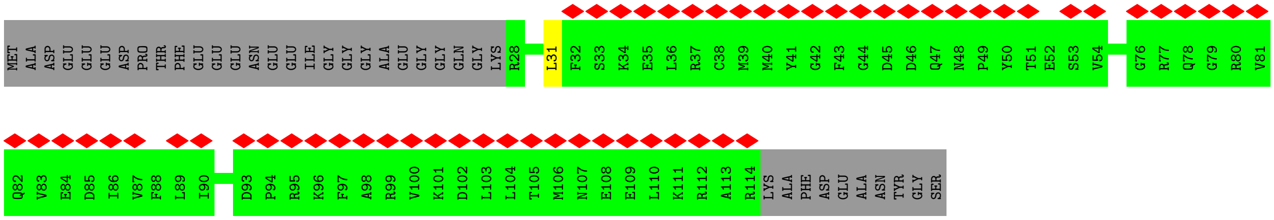
Chain k:



• Molecule 33: Transcription initiation factor TFIID subunit 13

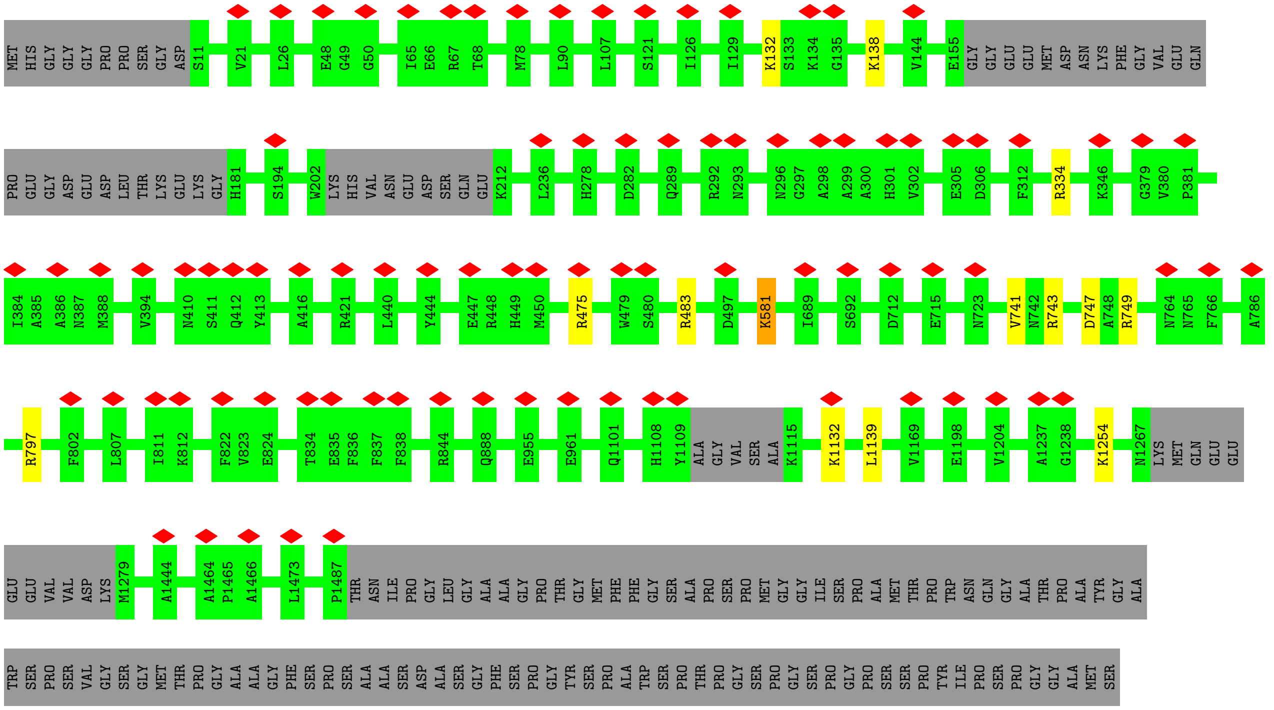
Chain m:

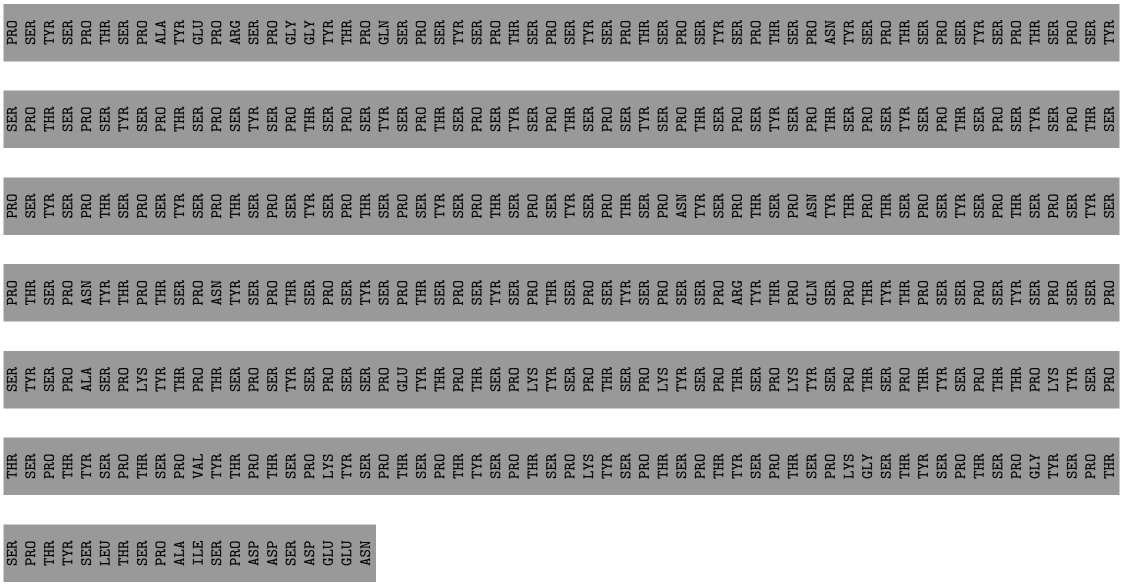




• Molecule 34: DNA-directed RNA polymerase II subunit RPB1

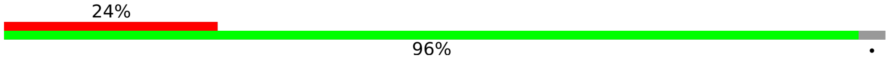
Chain o:

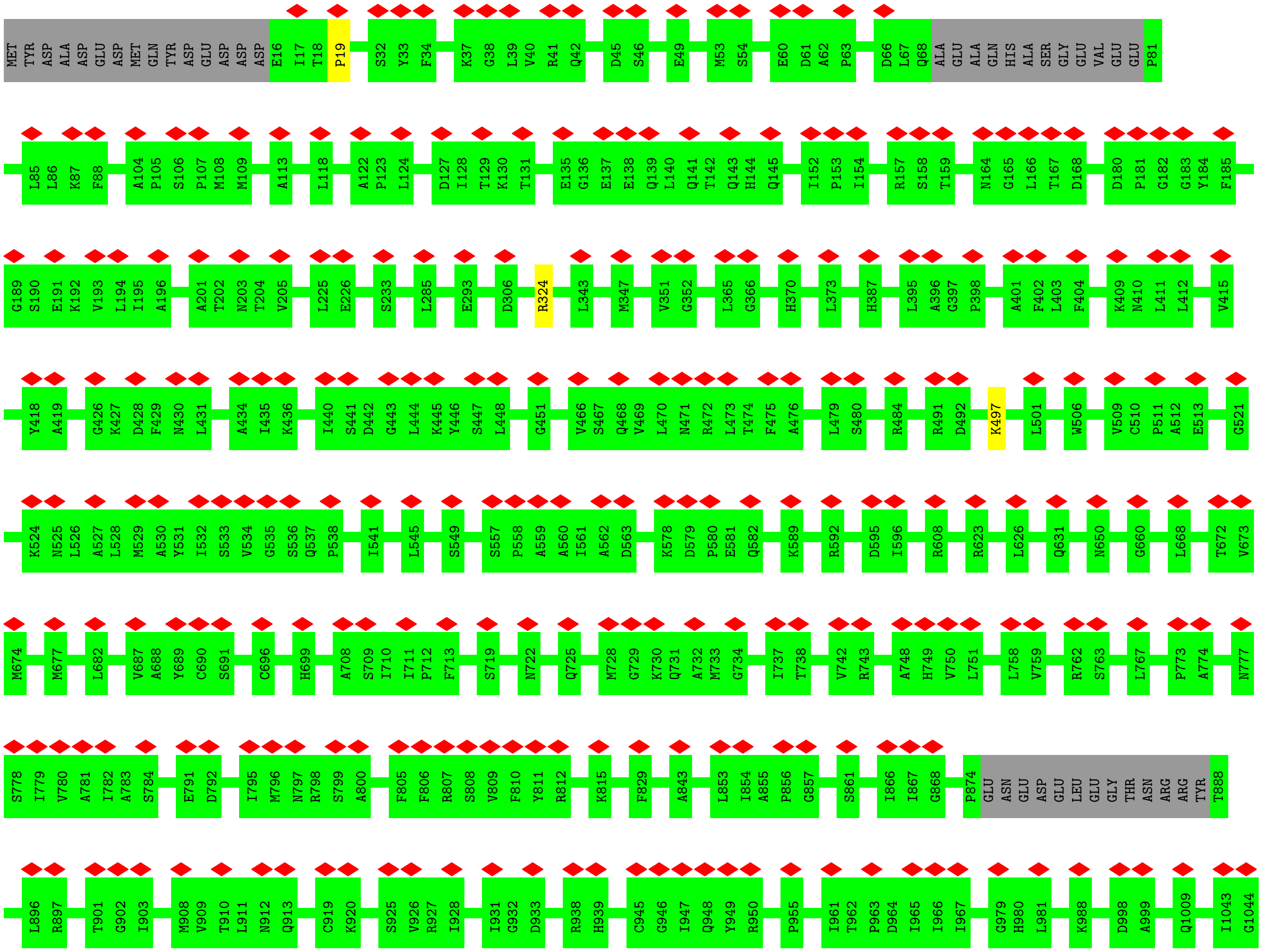


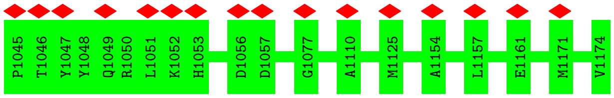


- Molecule 35: DNA-directed RNA polymerase subunit beta

Chain p:

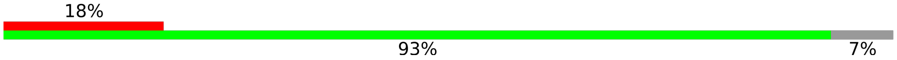


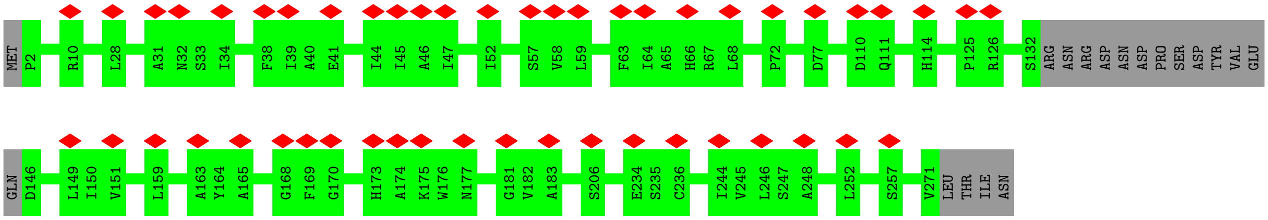




- Molecule 36: DNA-directed RNA polymerase II subunit RPB3

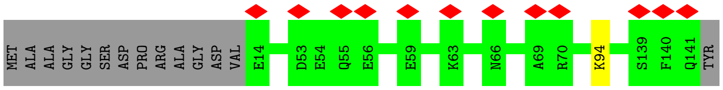
Chain q:





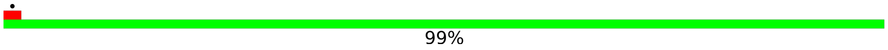
- Molecule 37: DNA-directed RNA polymerase II subunit RPB4

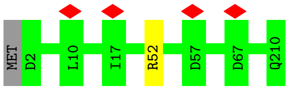
Chain r:



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

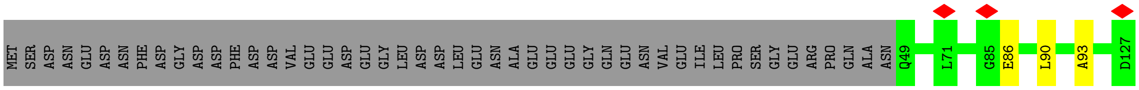
Chain s:





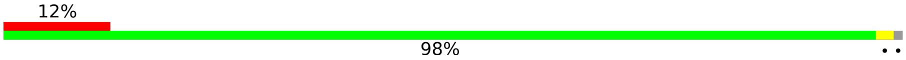
- Molecule 39: DNA-directed RNA polymerase II subunit F

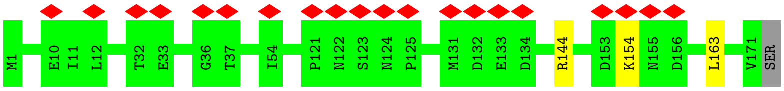
Chain t:



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

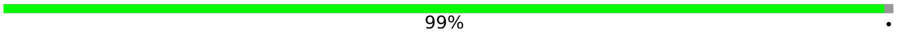
Chain u:

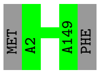




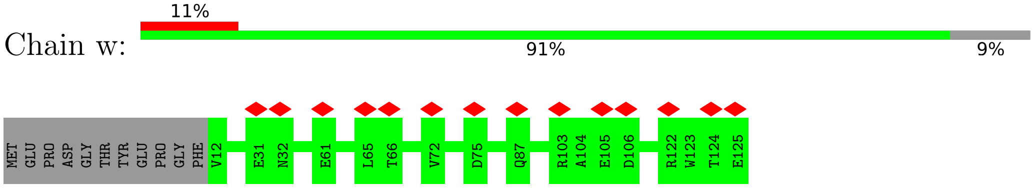
- Molecule 41: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain v:

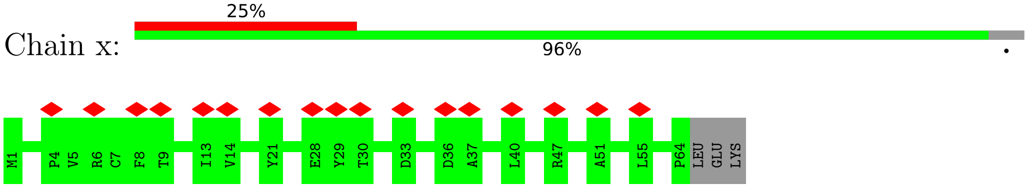




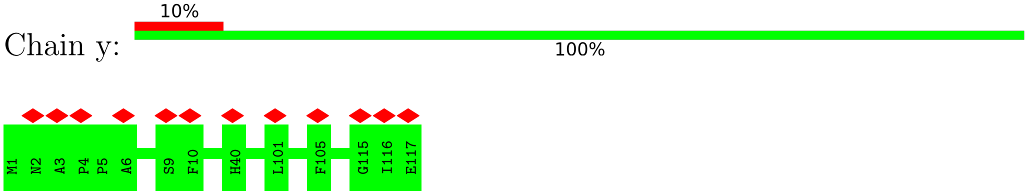
- Molecule 42: DNA-directed RNA polymerase II subunit RPB9



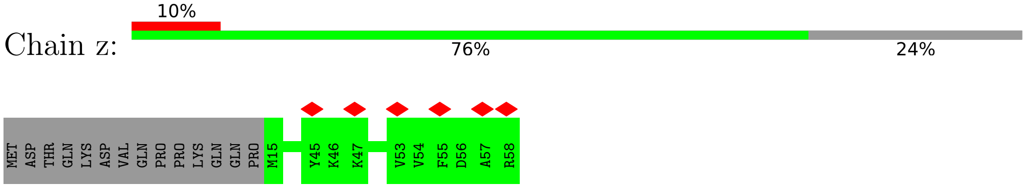
- Molecule 43: RPB10



- Molecule 44: RNA_pol_L_2 domain-containing protein



- Molecule 45: RPB12



4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	42939	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 ($e^-/\text{Å}^2$)	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	0.212	Depositor
Minimum map value	-0.116	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0051	Depositor
Map size (Å)	542.72, 542.72, 542.72	wwPDB
Map dimensions	512, 512, 512	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: SF4, 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	0	0.36	0/1804	0.57	0/2443
2	1	0.44	0/2674	0.65	7/3660 (0.2%)
3	2	0.45	0/2588	0.66	2/3509 (0.1%)
4	3	0.43	0/2102	0.61	0/2844
5	4	0.44	0/3663	0.63	0/4965
6	5	0.37	0/433	0.54	0/585
7	6	0.45	0/4983	0.61	0/6731
8	7	0.46	0/5957	0.66	2/8071 (0.0%)
9	8	0.55	0/2429	0.69	0/3295
10	9	0.54	0/2384	0.61	0/3220
11	A	0.48	0/4627	0.65	1/6248 (0.0%)
12	B	0.47	0/7993	0.61	0/10836
13	D	0.39	0/1335	0.51	0/1784
13	d	0.28	0/1321	0.49	0/1772
14	E	0.37	0/4469	0.55	0/6050
14	e	0.33	0/4433	0.55	0/6004
15	F	0.50	0/3167	0.69	0/4303
15	f	0.42	0/3140	0.64	0/4268
16	G	0.52	0/1199	0.63	0/1612
17	H	0.36	0/1673	0.53	0/2285
18	I	0.50	0/981	0.59	0/1332
18	i	0.30	0/989	0.46	0/1343
19	J	0.29	0/736	0.46	0/998
19	j	0.30	0/775	0.52	0/1049
20	L	0.41	0/622	0.63	1/841 (0.1%)
20	l	0.35	0/888	0.52	1/1194 (0.1%)
21	O	0.53	0/781	0.71	0/1061
22	P	0.67	0/1438	0.79	0/1935
23	Q	0.43	0/1013	0.62	0/1366
24	R	0.35	0/1957	0.64	0/2643
25	S	0.32	0/896	0.49	0/1213
26	T	0.51	0/1817	0.73	0/2445

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
27	U	0.52	1/1499 (0.1%)	0.81	5/2012 (0.2%)
28	V	0.46	0/1428	0.61	0/1917
29	X	0.76	0/1641	0.96	0/2534
30	Y	0.79	1/1623 (0.1%)	0.98	0/2499
31	c	0.39	0/1035	0.54	0/1406
32	k	0.30	0/799	0.48	0/1070
33	m	0.31	0/733	0.51	0/977
34	o	0.35	0/11516	0.52	0/15548
35	p	0.38	0/9243	0.49	0/12475
36	q	0.38	0/2102	0.46	0/2857
37	r	0.27	0/1019	0.47	0/1374
38	s	0.31	0/1751	0.47	0/2366
39	t	0.49	0/645	0.65	0/871
40	u	0.32	0/1382	0.53	0/1874
41	v	0.37	0/1207	0.49	0/1628
42	w	0.30	0/948	0.46	0/1284
43	x	0.42	0/516	0.45	0/696
44	y	0.35	0/956	0.44	0/1294
45	z	0.38	0/377	0.44	0/500
All	All	0.43	2/115687 (0.0%)	0.60	19/157087 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	Y	-24	DC	C1'-N1	5.96	1.56	1.49
27	U	183	GLN	C-O	5.40	1.33	1.23

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	U	186	PRO	CA-N-CD	-12.85	93.52	111.50
27	U	127	PHE	CB-CA-C	8.09	126.58	110.40
2	1	276	PRO	N-CA-CB	7.81	112.67	103.30
2	1	353	LYS	CB-CA-C	6.44	123.29	110.40
8	7	311	PRO	N-CA-CB	6.08	110.60	103.30
3	2	282	PRO	N-CA-CB	6.06	110.57	103.30
2	1	507	PRO	N-CA-CB	5.94	110.43	103.30
3	2	269	PRO	N-CA-CB	5.82	110.28	103.30
11	A	498	PRO	N-CA-CB	5.81	110.28	103.30
8	7	308	PRO	N-CA-CB	5.68	110.11	103.30
2	1	484	PRO	N-CA-CB	5.46	109.85	103.30
2	1	287	PRO	N-CA-CB	5.40	109.78	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	U	140	GLU	CB-CA-C	-5.38	99.63	110.40
27	U	115	GLU	C-N-CA	-5.31	108.42	121.70
20	L	79	ASP	CB-CG-OD2	5.22	122.99	118.30
20	l	79	ASP	CB-CG-OD2	5.17	122.95	118.30
2	1	480	PRO	N-CA-CB	5.05	109.36	103.30
27	U	128	LYS	N-CA-CB	5.03	119.65	110.60
2	1	265	PRO	N-CA-CB	5.02	109.33	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	230/309 (74%)	199 (86%)	29 (13%)	2 (1%)	17	54
2	1	399/548 (73%)	311 (78%)	70 (18%)	18 (4%)	2	25
3	2	327/395 (83%)	288 (88%)	37 (11%)	2 (1%)	25	63
4	3	259/308 (84%)	243 (94%)	16 (6%)	0	100	100
5	4	447/462 (97%)	399 (89%)	38 (8%)	10 (2%)	6	38
6	5	52/71 (73%)	47 (90%)	4 (8%)	1 (2%)	8	41
7	6	602/782 (77%)	512 (85%)	79 (13%)	11 (2%)	8	42
8	7	732/760 (96%)	649 (89%)	74 (10%)	9 (1%)	13	49
9	8	296/346 (86%)	261 (88%)	33 (11%)	2 (1%)	22	60
10	9	285/323 (88%)	270 (95%)	14 (5%)	1 (0%)	34	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	A	534/1872 (28%)	505 (95%)	26 (5%)	3 (1%)	25	63
12	B	959/1199 (80%)	912 (95%)	47 (5%)	0	100	100
13	D	152/1085 (14%)	146 (96%)	5 (3%)	1 (1%)	22	60
13	d	154/1085 (14%)	150 (97%)	4 (3%)	0	100	100
14	E	540/800 (68%)	506 (94%)	33 (6%)	1 (0%)	47	79
14	e	531/800 (66%)	484 (91%)	47 (9%)	0	100	100
15	F	404/677 (60%)	380 (94%)	17 (4%)	7 (2%)	9	43
15	f	399/677 (59%)	378 (95%)	20 (5%)	1 (0%)	41	75
16	G	139/349 (40%)	135 (97%)	4 (3%)	0	100	100
17	H	207/310 (67%)	190 (92%)	13 (6%)	4 (2%)	8	41
18	I	118/264 (45%)	111 (94%)	5 (4%)	2 (2%)	9	43
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%)	89 (98%)	2 (2%)	0	100	100
20	L	73/161 (45%)	64 (88%)	4 (6%)	5 (7%)	1	18
20	l	105/161 (65%)	101 (96%)	4 (4%)	0	100	100
21	O	95/109 (87%)	82 (86%)	8 (8%)	5 (5%)	2	22
22	P	175/339 (52%)	168 (96%)	5 (3%)	2 (1%)	14	51
23	Q	118/376 (31%)	106 (90%)	9 (8%)	3 (2%)	5	36
24	R	246/316 (78%)	234 (95%)	10 (4%)	2 (1%)	19	57
25	S	104/517 (20%)	102 (98%)	2 (2%)	0	100	100
26	T	218/249 (88%)	204 (94%)	11 (5%)	3 (1%)	11	46
27	U	175/439 (40%)	165 (94%)	9 (5%)	1 (1%)	25	63
28	V	170/291 (58%)	144 (85%)	17 (10%)	9 (5%)	2	22
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%)	79 (93%)	6 (7%)	0	100	100
34	o	1417/1970 (72%)	1310 (92%)	106 (8%)	1 (0%)	51	84
35	p	1128/1174 (96%)	1054 (93%)	73 (6%)	1 (0%)	51	84
36	q	253/275 (92%)	225 (89%)	28 (11%)	0	100	100
37	r	126/142 (89%)	119 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	s	207/210 (99%)	195 (94%)	12 (6%)	0	100	100
39	t	77/127 (61%)	73 (95%)	3 (4%)	1 (1%)	12	48
40	u	169/172 (98%)	156 (92%)	12 (7%)	1 (1%)	25	63
41	v	146/150 (97%)	132 (90%)	14 (10%)	0	100	100
42	w	112/125 (90%)	103 (92%)	9 (8%)	0	100	100
43	x	62/67 (92%)	59 (95%)	3 (5%)	0	100	100
44	y	115/117 (98%)	109 (95%)	6 (5%)	0	100	100
45	z	42/58 (72%)	38 (90%)	4 (10%)	0	100	100
All	All	13701/22931 (60%)	12591 (92%)	1001 (7%)	109 (1%)	24	57

All (109) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	1	106	LYS
2	1	108	ASN
2	1	110	GLU
2	1	114	LYS
2	1	120	GLU
2	1	237	THR
2	1	264	ASN
2	1	276	PRO
2	1	287	PRO
2	1	358	ILE
2	1	359	GLU
2	1	373	ALA
3	2	261	SER
5	4	193	PRO
5	4	381	PRO
5	4	395	GLU
6	5	48	GLU
7	6	405	VAL
7	6	418	LYS
7	6	421	TRP
7	6	449	LYS
7	6	605	ILE
7	6	622	VAL
8	7	15	ASP
8	7	624	PRO
9	8	105	ASN

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Mol	Chain	Res	Type
11	A	498	PRO
11	A	508	ASN
13	D	876	ALA
14	E	452	ARG
15	F	68	THR
15	F	69	SER
15	F	442	PRO
17	H	141	PRO
18	I	85	SER
20	L	73	ASN
20	L	107	LYS
23	Q	34	VAL
28	V	212	VAL
39	t	93	ALA
40	u	154	LYS
1	0	273	ASN
2	1	113	GLU
5	4	135	GLN
7	6	401	ILE
7	6	555	ASN
7	6	610	VAL
17	H	129	VAL
20	L	111	LEU
20	L	114	LYS
21	O	26	GLN
26	T	229	HIS
28	V	79	ALA
28	V	171	ILE
28	V	178	SER
35	p	19	PRO
2	1	286	VAL
3	2	206	ARG
5	4	190	PRO
7	6	629	HIS
8	7	465	ASP
10	9	236	LEU
22	P	207	PRO
28	V	134	ASP
1	0	7	PRO
2	1	233	ASP
2	1	261	GLY
2	1	369	VAL

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Mol	Chain	Res	Type
5	4	384	PRO
5	4	413	LEU
8	7	36	GLY
8	7	98	GLU
11	A	505	ASN
15	F	66	LEU
15	F	367	LYS
18	I	62	LYS
21	O	52	VAL
21	O	63	ASN
24	R	28	ARG
26	T	140	ARG
27	U	145	PHE
28	V	86	LYS
28	V	225	VAL
34	o	581	LYS
5	4	385	PRO
15	F	64	GLN
15	F	440	PRO
17	H	137	GLY
20	L	72	PRO
26	T	38	GLY
5	4	191	GLY
8	7	532	PRO
8	7	595	ILE
9	8	165	PRO
22	P	298	PRO
23	Q	312	GLU
24	R	48	VAL
15	f	411	VAL
8	7	13	PRO
7	6	402	GLY
21	O	71	VAL
28	V	189	ILE
5	4	189	GLU
8	7	47	GLY
21	O	75	VAL
28	V	140	LYS
2	1	149	VAL
17	H	128	PRO
23	Q	313	PRO

5.3.2 Protein sidechains ⓘ

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	173/283 (61%)	173 (100%)	0	100	100
2	1	176/484 (36%)	167 (95%)	9 (5%)	24	53
3	2	279/352 (79%)	272 (98%)	7 (2%)	47	69
4	3	234/272 (86%)	227 (97%)	7 (3%)	41	64
5	4	387/399 (97%)	376 (97%)	11 (3%)	43	66
6	5	48/64 (75%)	46 (96%)	2 (4%)	30	57
7	6	533/688 (78%)	482 (90%)	51 (10%)	8	32
8	7	616/664 (93%)	598 (97%)	18 (3%)	42	65
9	8	258/299 (86%)	252 (98%)	6 (2%)	50	71
10	9	259/296 (88%)	257 (99%)	2 (1%)	81	89
11	A	488/1665 (29%)	446 (91%)	42 (9%)	10	38
12	B	876/1083 (81%)	856 (98%)	20 (2%)	50	71
13	D	143/815 (18%)	138 (96%)	5 (4%)	36	62
13	d	146/815 (18%)	146 (100%)	0	100	100
14	E	478/657 (73%)	466 (98%)	12 (2%)	47	69
14	e	475/657 (72%)	473 (100%)	2 (0%)	91	94
15	F	324/574 (56%)	298 (92%)	26 (8%)	12	41
15	f	322/574 (56%)	312 (97%)	10 (3%)	40	64
16	G	133/322 (41%)	125 (94%)	8 (6%)	19	49
17	H	181/270 (67%)	172 (95%)	9 (5%)	24	53
18	I	106/235 (45%)	100 (94%)	6 (6%)	20	50
18	i	107/235 (46%)	107 (100%)	0	100	100
19	J	79/154 (51%)	78 (99%)	1 (1%)	69	82
19	j	83/154 (54%)	83 (100%)	0	100	100
20	L	70/141 (50%)	60 (86%)	10 (14%)	3	20
20	l	98/141 (70%)	98 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	O	84/98 (86%)	75 (89%)	9 (11%)	6	29
22	P	153/293 (52%)	146 (95%)	7 (5%)	27	55
23	Q	111/324 (34%)	107 (96%)	4 (4%)	35	61
24	R	212/268 (79%)	201 (95%)	11 (5%)	23	53
25	S	93/448 (21%)	91 (98%)	2 (2%)	52	71
26	T	196/218 (90%)	170 (87%)	26 (13%)	4	22
27	U	163/373 (44%)	145 (89%)	18 (11%)	6	28
28	V	155/261 (59%)	135 (87%)	20 (13%)	4	23
31	c	113/833 (14%)	111 (98%)	2 (2%)	59	77
32	k	87/182 (48%)	87 (100%)	0	100	100
33	m	80/106 (76%)	79 (99%)	1 (1%)	69	82
34	o	1257/1748 (72%)	1243 (99%)	14 (1%)	73	84
35	p	993/1027 (97%)	991 (100%)	2 (0%)	93	96
36	q	234/252 (93%)	234 (100%)	0	100	100
37	r	106/126 (84%)	105 (99%)	1 (1%)	78	87
38	s	191/192 (100%)	190 (100%)	1 (0%)	88	93
39	t	69/111 (62%)	67 (97%)	2 (3%)	42	65
40	u	152/153 (99%)	150 (99%)	2 (1%)	69	82
41	v	129/131 (98%)	129 (100%)	0	100	100
42	w	103/112 (92%)	103 (100%)	0	100	100
43	x	53/56 (95%)	53 (100%)	0	100	100
44	y	106/106 (100%)	106 (100%)	0	100	100
45	z	41/55 (74%)	41 (100%)	0	100	100
All	All	11953/19766 (60%)	11567 (97%)	386 (3%)	42	63

All (386) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	190	SER
2	1	306	ARG
2	1	313	MET
2	1	353	LYS
2	1	358	ILE
2	1	362	ASP

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Mol	Chain	Res	Type
2	1	363	LEU
2	1	372	ILE
2	1	417	LYS
3	2	177	CYS
3	2	182	ILE
3	2	185	LEU
3	2	186	ILE
3	2	195	ARG
3	2	301	LEU
3	2	313	VAL
4	3	18	ASN
4	3	146	ARG
4	3	155	GLN
4	3	156	GLU
4	3	158	LYS
4	3	222	SER
4	3	229	TRP
5	4	23	LEU
5	4	115	ARG
5	4	188	THR
5	4	189	GLU
5	4	215	PHE
5	4	359	ILE
5	4	376	MET
5	4	400	ARG
5	4	402	ARG
5	4	413	LEU
5	4	456	LYS
6	5	59	GLU
6	5	60	LEU
7	6	157	LYS
7	6	163	TYR
7	6	190	GLN
7	6	191	ASP
7	6	198	ARG
7	6	291	LEU
7	6	296	ASP
7	6	297	PHE
7	6	302	VAL
7	6	303	ASN
7	6	305	ASP
7	6	310	LEU

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Mol	Chain	Res	Type
7	6	313	THR
7	6	357	VAL
7	6	377	GLN
7	6	380	MET
7	6	403	CYS
7	6	404	SER
7	6	412	MET
7	6	413	LEU
7	6	415	HIS
7	6	416	THR
7	6	417	THR
7	6	418	LYS
7	6	419	ARG
7	6	422	GLU
7	6	426	VAL
7	6	434	GLU
7	6	435	TRP
7	6	483	LEU
7	6	490	GLU
7	6	526	LYS
7	6	528	LYS
7	6	530	ARG
7	6	532	LEU
7	6	534	TYR
7	6	563	ASP
7	6	565	VAL
7	6	566	PHE
7	6	597	LYS
7	6	601	LYS
7	6	603	ASN
7	6	612	ASP
7	6	615	PHE
7	6	616	ASP
7	6	621	ASN
7	6	624	ILE
7	6	633	ARG
7	6	635	GLN
7	6	648	LYS
7	6	650	MET
8	7	15	ASP
8	7	16	TYR
8	7	17	ILE

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Mol	Chain	Res	Type
8	7	29	LYS
8	7	48	LYS
8	7	49	THR
8	7	66	GLU
8	7	77	VAL
8	7	98	GLU
8	7	143	ARG
8	7	424	ARG
8	7	425	THR
8	7	428	ILE
8	7	444	ILE
8	7	464	LEU
8	7	487	ARG
8	7	626	VAL
8	7	690	ARG
9	8	38	VAL
9	8	195	ASP
9	8	237	TRP
9	8	239	ASP
9	8	245	ASP
9	8	309	ARG
10	9	241	ASN
10	9	243	THR
11	A	341	TRP
11	A	353	LEU
11	A	395	ASP
11	A	397	LEU
11	A	400	GLU
11	A	404	MET
11	A	408	LEU
11	A	410	TRP
11	A	412	ASP
11	A	413	ASP
11	A	415	ILE
11	A	416	TRP
11	A	475	LEU
11	A	481	GLU
11	A	484	ILE
11	A	485	ILE
11	A	486	TRP
11	A	487	ASP
11	A	491	MET

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Mol	Chain	Res	Type
11	A	493	ARG
11	A	494	LEU
11	A	496	GLU
11	A	500	LEU
11	A	502	LEU
11	A	506	ASP
11	A	507	GLU
11	A	511	LEU
11	A	639	LEU
11	A	661	GLU
11	A	667	THR
11	A	711	ASP
11	A	727	THR
11	A	730	PHE
11	A	828	GLU
11	A	943	LYS
11	A	970	ASN
11	A	1052	ARG
11	A	1058	HIS
11	A	1059	GLN
11	A	1062	TYR
11	A	1165	LEU
11	A	1203	GLU
12	B	21	GLU
12	B	24	ARG
12	B	71	ARG
12	B	140	GLU
12	B	159	LEU
12	B	178	PHE
12	B	183	GLN
12	B	184	ASN
12	B	225	TYR
12	B	262	MET
12	B	266	THR
12	B	293	GLU
12	B	431	LEU
12	B	488	PHE
12	B	559	LYS
12	B	603	LYS
12	B	638	ARG
12	B	640	VAL
12	B	771	VAL

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Mol	Chain	Res	Type
12	B	818	THR
13	D	891	ILE
13	D	924	LYS
13	D	941	ARG
13	D	955	LYS
13	D	958	LYS
14	E	433	LYS
14	E	450	ARG
14	E	451	VAL
14	E	516	ILE
14	E	517	ASP
14	E	519	GLU
14	E	521	ASP
14	E	527	ILE
14	E	593	PHE
14	E	745	GLU
14	E	746	ASP
14	E	747	LEU
15	F	55	LEU
15	F	60	MET
15	F	62	LYS
15	F	64	GLN
15	F	66	LEU
15	F	125	VAL
15	F	211	ARG
15	F	258	ARG
15	F	261	THR
15	F	271	VAL
15	F	280	ILE
15	F	301	VAL
15	F	317	LEU
15	F	319	LEU
15	F	327	TRP
15	F	332	PHE
15	F	335	ARG
15	F	339	GLN
15	F	348	THR
15	F	354	ARG
15	F	368	THR
15	F	386	ASP
15	F	391	LEU
15	F	397	GLN

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Mol	Chain	Res	Type
15	F	408	ASP
15	F	427	LEU
16	G	41	ASP
16	G	81	ASP
16	G	143	VAL
16	G	147	ARG
16	G	161	ASP
16	G	181	TRP
16	G	182	GLU
16	G	183	ILE
17	H	50	PHE
17	H	116	ARG
17	H	132	LYS
17	H	135	THR
17	H	159	TYR
17	H	160	ILE
17	H	161	LYS
17	H	164	THR
17	H	169	VAL
18	I	31	TYR
18	I	32	GLU
18	I	34	ARG
18	I	67	ASP
18	I	107	ILE
18	I	110	TYR
19	J	192	LYS
20	L	56	GLN
20	L	59	THR
20	L	60	LYS
20	L	61	LYS
20	L	62	LYS
20	L	63	LEU
20	L	64	GLN
20	L	110	THR
20	L	111	LEU
20	L	128	ILE
21	O	24	GLN
21	O	54	ASN
21	O	55	ARG
21	O	57	ASN
21	O	59	ARG
21	O	62	LEU

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Mol	Chain	Res	Type
21	O	68	CYS
21	O	79	VAL
21	O	90	VAL
22	P	172	VAL
22	P	209	THR
22	P	221	CYS
22	P	226	SER
22	P	252	ASP
22	P	274	VAL
22	P	278	GLN
23	Q	13	LEU
23	Q	34	VAL
23	Q	340	ASP
23	Q	364	ASP
24	R	27	TYR
24	R	28	ARG
24	R	39	LEU
24	R	41	VAL
24	R	45	VAL
24	R	46	ILE
24	R	47	ASP
24	R	48	VAL
24	R	120	GLU
24	R	127	ARG
24	R	128	ILE
25	S	7	SER
25	S	95	ASP
26	T	43	LEU
26	T	124	TYR
26	T	127	LEU
26	T	137	LYS
26	T	141	LEU
26	T	160	GLN
26	T	164	GLU
26	T	166	GLU
26	T	174	LYS
26	T	177	ARG
26	T	179	ASP
26	T	180	LYS
26	T	185	ASP
26	T	187	LEU
26	T	194	HIS

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Mol	Chain	Res	Type
26	T	196	TYR
26	T	200	LYS
26	T	206	THR
26	T	208	GLN
26	T	211	VAL
26	T	212	TYR
26	T	226	LYS
26	T	228	ILE
26	T	230	LYS
26	T	231	ASN
26	T	235	LEU
27	U	28	ILE
27	U	39	ARG
27	U	42	CYS
27	U	45	GLU
27	U	95	ASN
27	U	105	TYR
27	U	107	LEU
27	U	122	THR
27	U	123	ASN
27	U	139	LEU
27	U	145	PHE
27	U	172	ASP
27	U	174	ARG
27	U	182	GLU
27	U	184	ILE
27	U	185	GLU
27	U	186	PRO
27	U	188	TYR
28	V	88	ARG
28	V	93	ASP
28	V	97	LEU
28	V	132	VAL
28	V	143	TYR
28	V	159	ASP
28	V	160	GLN
28	V	161	ARG
28	V	163	LEU
28	V	172	GLU
28	V	173	GLU
28	V	175	LEU
28	V	191	PHE

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Mol	Chain	Res	Type
28	V	193	ASN
28	V	194	ARG
28	V	204	ASN
28	V	205	ASP
28	V	210	PHE
28	V	218	LYS
28	V	234	GLU
31	c	24	ASP
31	c	106	VAL
14	e	365	ARG
14	e	663	ARG
15	f	253	TYR
15	f	261	THR
15	f	272	VAL
15	f	297	LEU
15	f	305	ILE
15	f	322	ASP
15	f	323	VAL
15	f	326	HIS
15	f	356	THR
15	f	421	ASP
33	m	31	LEU
34	o	132	LYS
34	o	138	LYS
34	o	334	ARG
34	o	475	ARG
34	o	483	ARG
34	o	581	LYS
34	o	741	VAL
34	o	743	ARG
34	o	747	ASP
34	o	749	ARG
34	o	797	ARG
34	o	1132	LYS
34	o	1139	LEU
34	o	1254	LYS
35	p	324	ARG
35	p	497	LYS
37	r	94	LYS
38	s	52	ARG
39	t	86	GLU
39	t	90	LEU

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Mol	Chain	Res	Type
40	u	144	ARG
40	u	163	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (176) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	28	HIS
1	0	117	ASN
1	0	259	HIS
2	1	384	HIS
2	1	524	HIS
3	2	235	HIS
3	2	317	HIS
3	2	340	ASN
4	3	18	ASN
4	3	108	ASN
4	3	179	ASN
4	3	248	HIS
5	4	54	ASN
5	4	181	GLN
5	4	312	ASN
5	4	352	GLN
5	4	366	HIS
5	4	373	HIS
5	4	390	GLN
5	4	458	GLN
5	4	460	HIS
7	6	97	GLN
7	6	112	HIS
7	6	172	HIS
7	6	187	HIS
7	6	320	GLN
7	6	377	GLN
7	6	444	HIS
7	6	461	HIS
7	6	497	GLN
7	6	551	HIS
7	6	595	ASN
7	6	629	HIS
7	6	638	GLN
8	7	118	HIS
8	7	237	HIS

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Mol	Chain	Res	Type
8	7	238	ASN
8	7	328	HIS
8	7	562	GLN
8	7	726	GLN
8	7	733	GLN
9	8	36	GLN
9	8	73	ASN
9	8	131	HIS
10	9	94	ASN
10	9	100	HIS
10	9	153	GLN
10	9	183	ASN
10	9	241	ASN
11	A	489	GLN
11	A	569	ASN
11	A	860	ASN
11	A	896	GLN
11	A	1073	GLN
12	B	30	HIS
12	B	137	HIS
12	B	160	HIS
12	B	183	GLN
12	B	184	ASN
12	B	235	HIS
12	B	272	GLN
12	B	348	GLN
12	B	432	HIS
12	B	450	GLN
12	B	509	ASN
12	B	644	GLN
12	B	652	GLN
12	B	745	GLN
12	B	750	GLN
12	B	813	ASN
12	B	908	GLN
12	B	916	ASN
13	D	922	GLN
13	D	925	ASN
13	D	936	GLN
13	D	1053	GLN
13	D	1075	HIS
14	E	254	ASN

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Mol	Chain	Res	Type
14	E	268	HIS
14	E	290	HIS
14	E	327	ASN
14	E	351	GLN
14	E	616	HIS
14	E	640	ASN
15	F	119	ASN
15	F	214	HIS
15	F	270	ASN
15	F	273	GLN
15	F	275	ASN
15	F	302	HIS
15	F	316	GLN
16	G	48	HIS
17	H	145	HIS
17	H	173	GLN
18	I	21	GLN
18	I	38	GLN
18	I	60	HIS
18	I	81	GLN
18	I	98	GLN
19	J	160	GLN
19	J	173	HIS
20	L	105	HIS
20	L	117	GLN
21	O	8	ASN
21	O	13	ASN
21	O	27	GLN
21	O	54	ASN
21	O	57	ASN
21	O	70	ASN
21	O	77	ASN
22	P	167	ASN
23	Q	60	HIS
23	Q	361	ASN
24	R	129	ASN
26	T	152	ASN
26	T	158	ASN
26	T	181	GLN
26	T	195	GLN
26	T	208	GLN
27	U	123	ASN

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Mol	Chain	Res	Type
28	V	95	HIS
28	V	117	GLN
28	V	193	ASN
31	c	104	ASN
13	d	912	ASN
13	d	1069	ASN
14	e	294	ASN
14	e	320	HIS
14	e	336	HIS
14	e	616	HIS
15	f	325	ASN
18	i	60	HIS
18	i	81	GLN
20	l	73	ASN
20	l	105	HIS
33	m	107	ASN
34	o	123	ASN
34	o	278	HIS
34	o	289	GLN
34	o	296	ASN
34	o	301	HIS
34	o	311	GLN
34	o	330	GLN
34	o	372	ASN
34	o	507	GLN
34	o	620	HIS
34	o	721	HIS
34	o	723	ASN
34	o	731	ASN
34	o	739	ASN
34	o	780	ASN
34	o	913	ASN
34	o	950	ASN
34	o	1005	HIS
34	o	1230	GLN
34	o	1248	ASN
34	o	1332	GLN
34	o	1397	HIS
34	o	1445	HIS
34	o	1462	GLN
35	p	111	ASN
35	p	139	GLN

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Mol	Chain	Res	Type
35	p	287	HIS
35	p	370	HIS
35	p	525	ASN
35	p	570	ASN
35	p	749	HIS
35	p	1021	HIS
35	p	1094	GLN
35	p	1117	HIS
35	p	1120	ASN
37	r	19	GLN
40	u	60	GLN
41	v	131	ASN
44	y	2	ASN
44	y	29	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
47	SF4	7	1000	8	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	SF4	7	1000	8	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

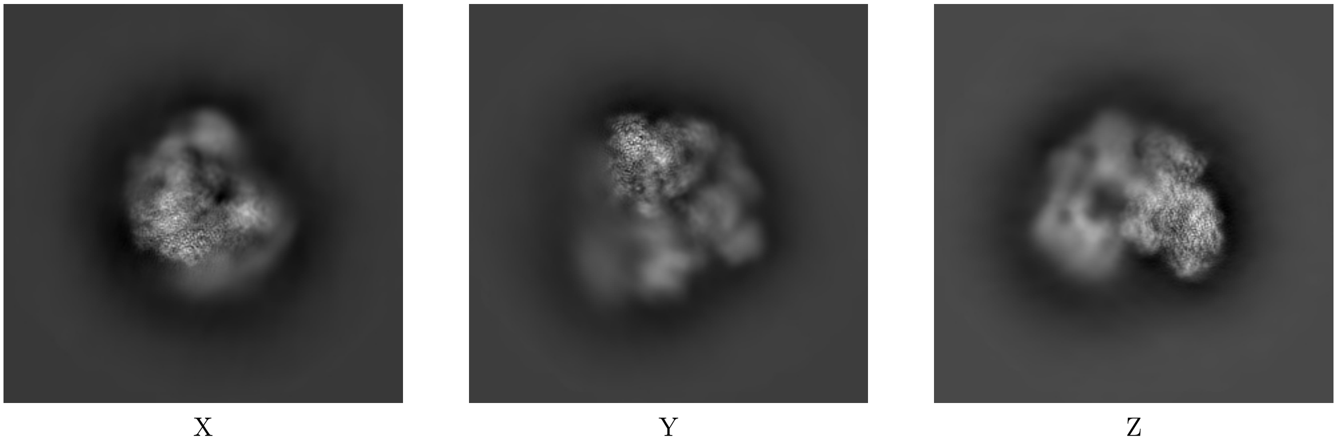
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-31112. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections ⓘ

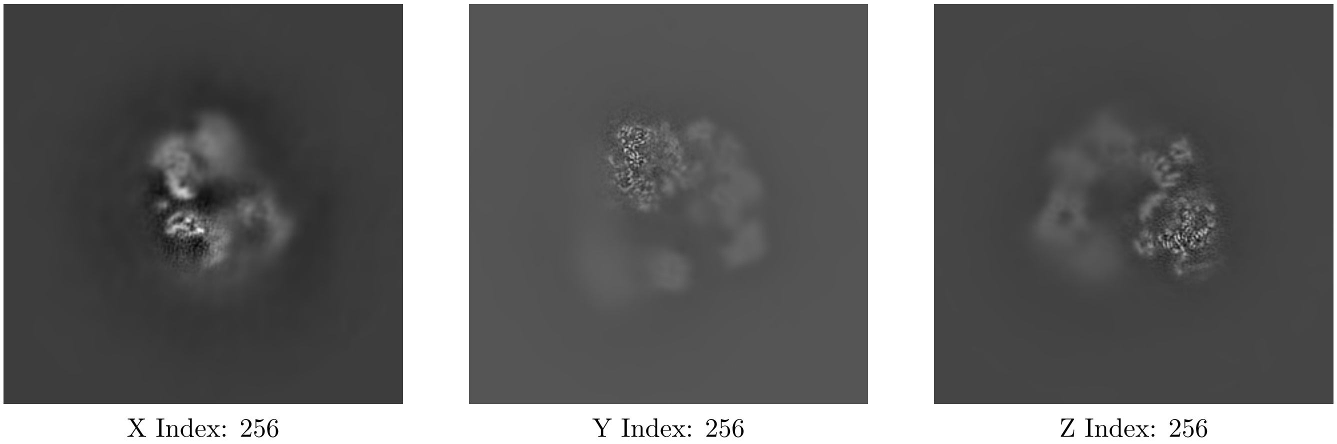
6.1.1 Primary map


X Y Z

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

6.2 Central slices ⓘ

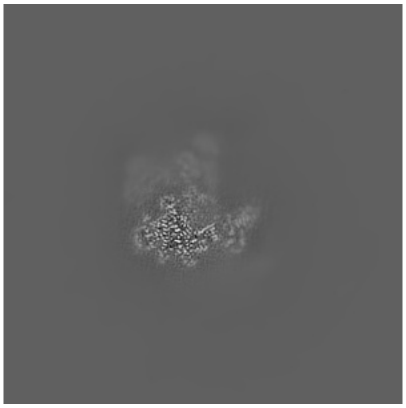
6.2.1 Primary map

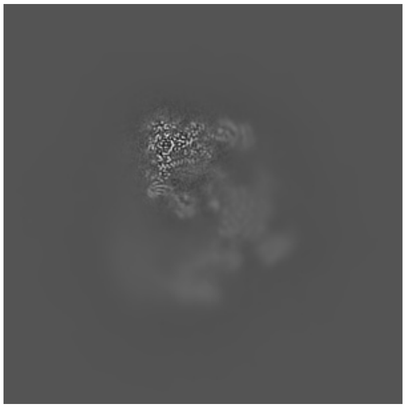

X Index: 256 Y Index: 256 Z Index: 256

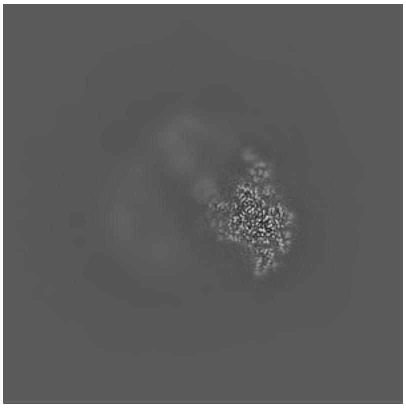
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ

6.3.1 Primary map


X Index: 334

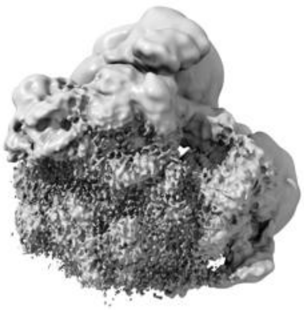

Y Index: 228

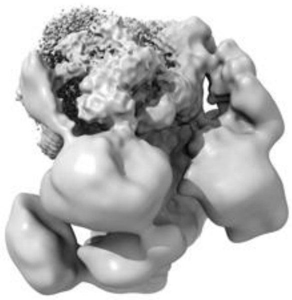

Z Index: 209

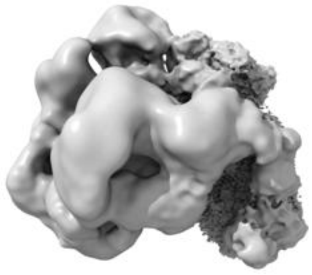
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map


X


Y


Z

The images above show the 3D surface view of the map at the recommended contour level 0.0051. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

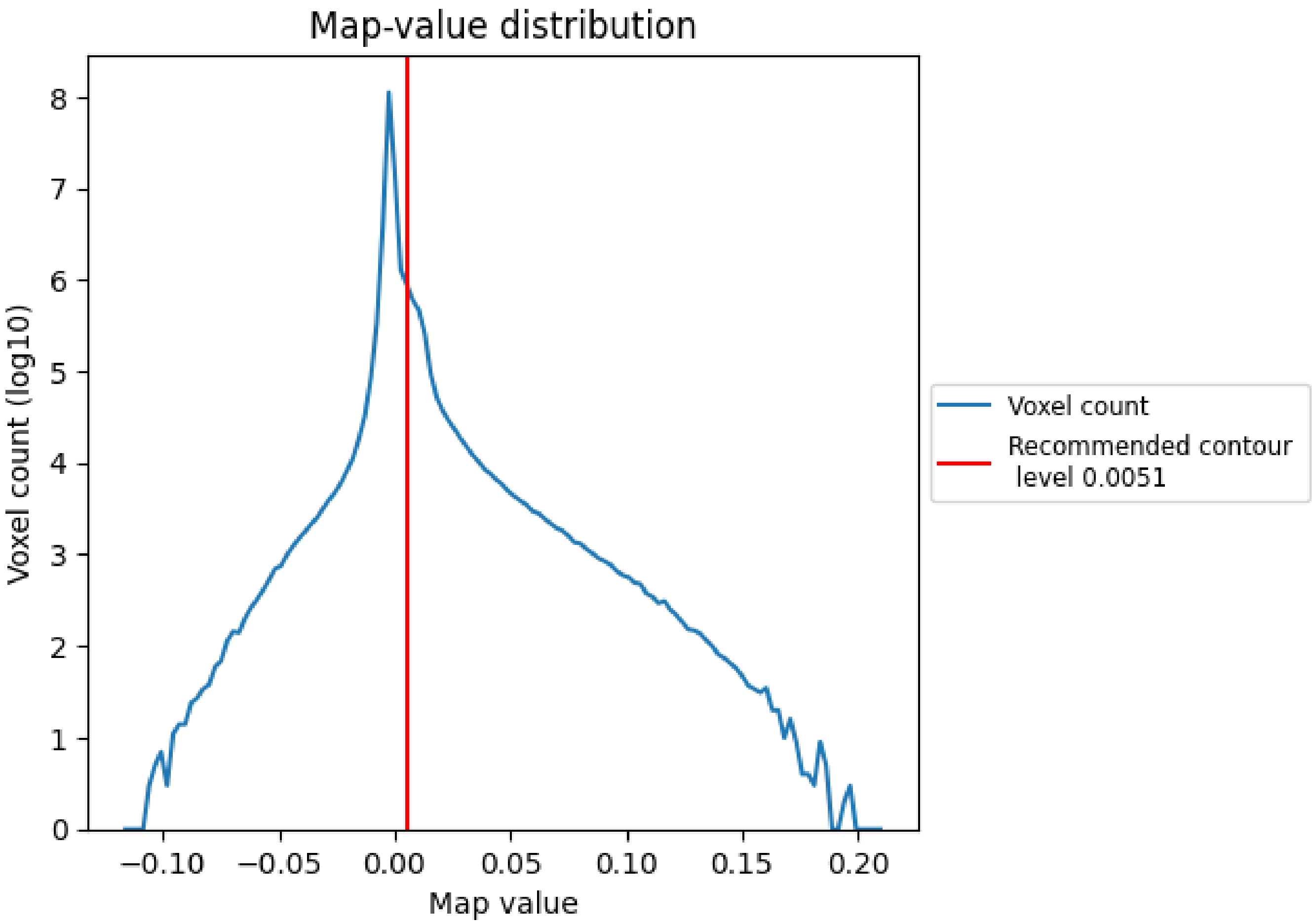
6.5 Mask visualisation ⓘ

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

7 Map analysis ⓘ

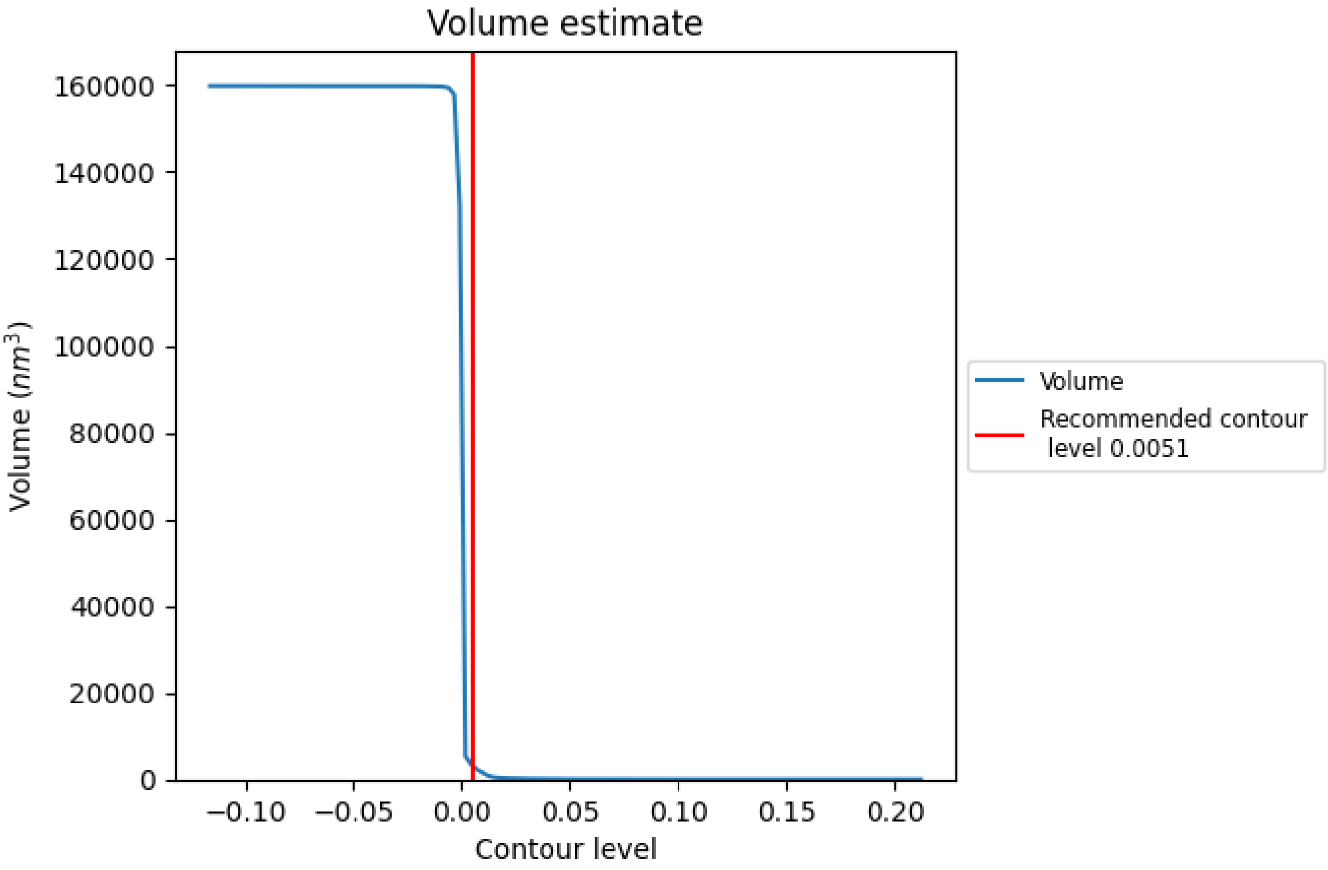
This section contains the results of statistical analysis of the map.

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.

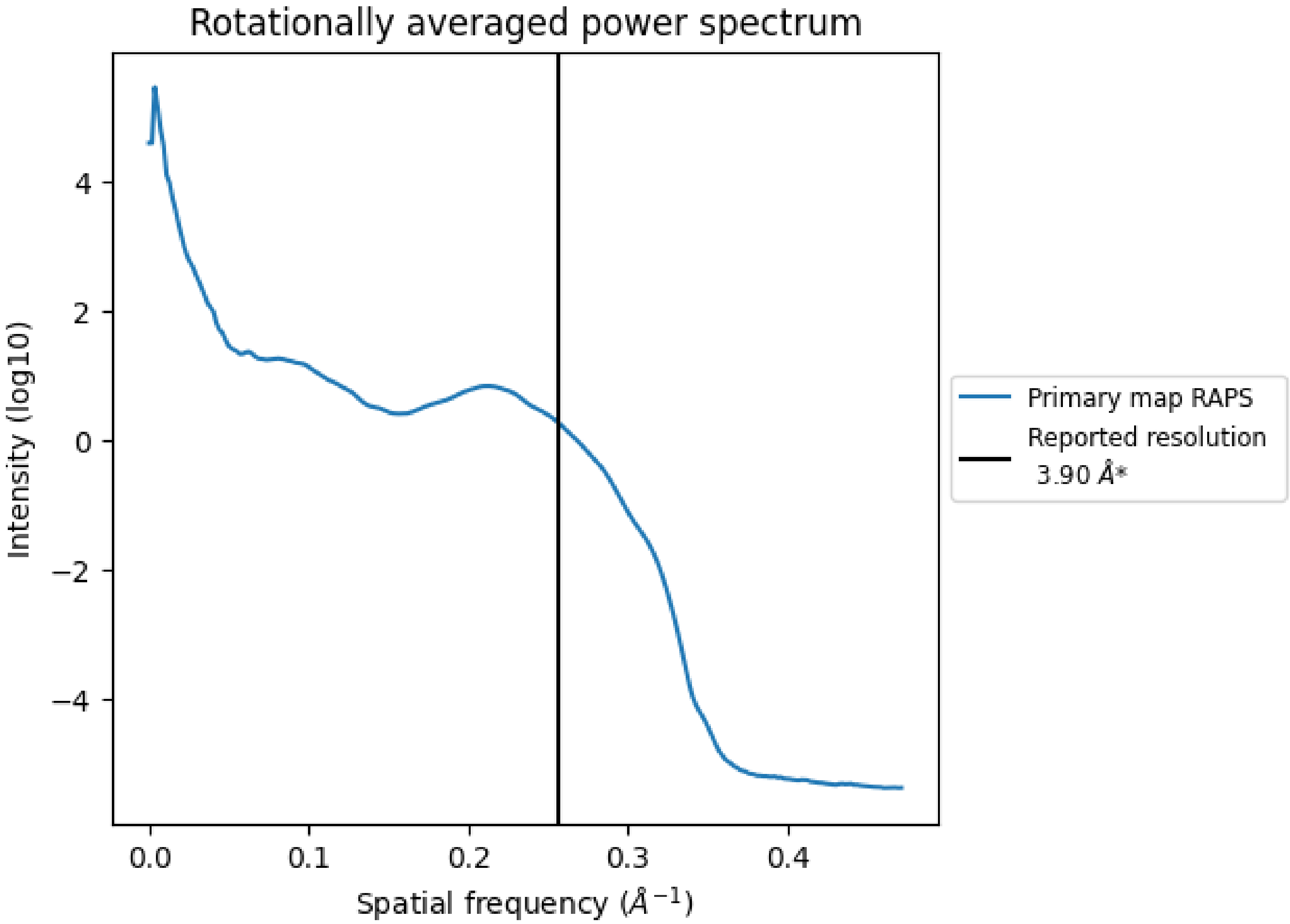
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 3205 nm^3; this corresponds to an approximate mass of 2895 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

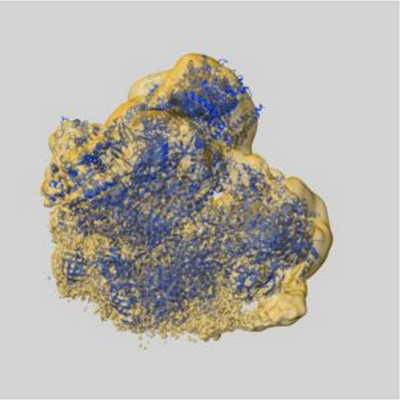
8 Fourier-Shell correlation ⓘ

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

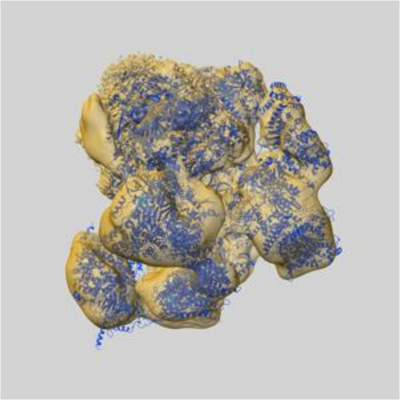
9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-31112 and PDB model 7EGC. Per-residue inclusion information can be found in section 3 on page 14.

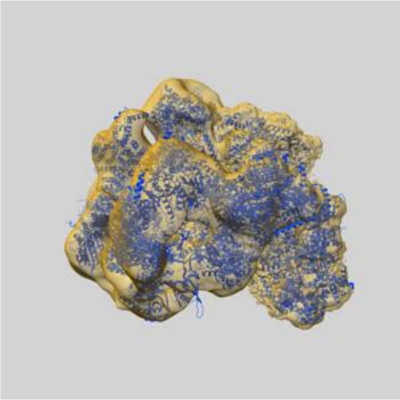
9.1 Map-model overlay ⓘ



X



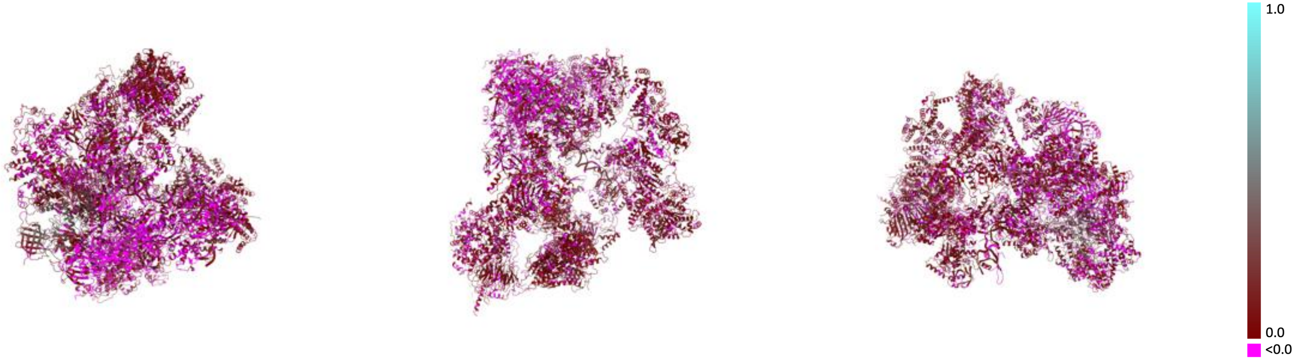
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0051 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

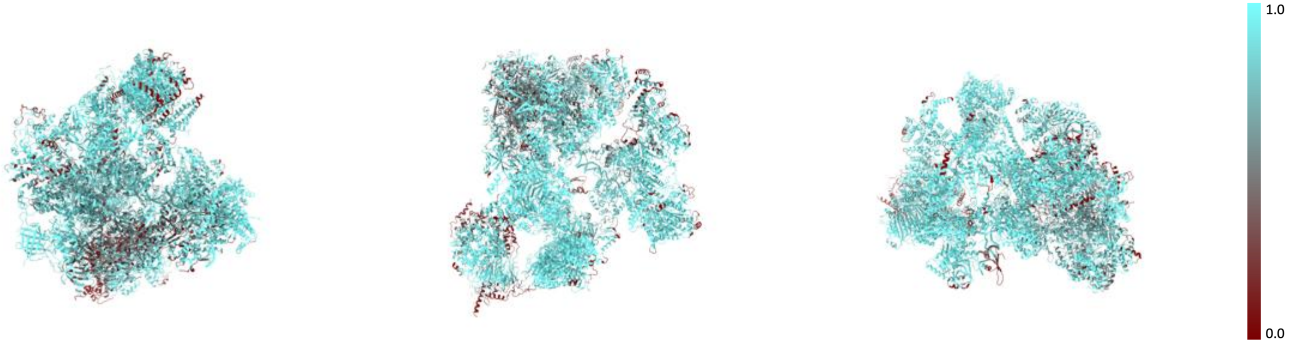
9.2 Q-score mapped to coordinate model ⓘ



X Y Z

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

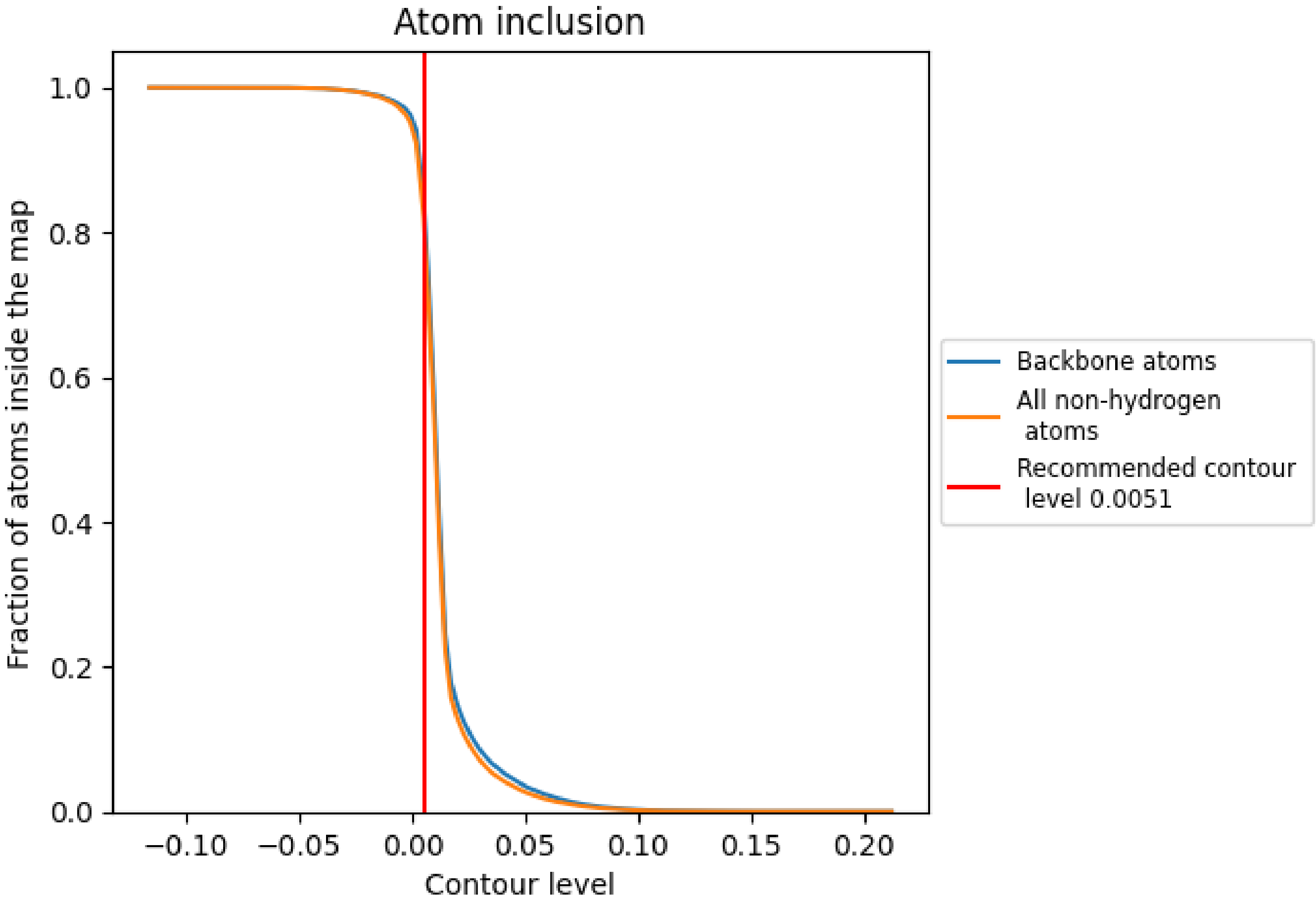
9.3 Atom inclusion mapped to coordinate model ⓘ



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0051).

9.4 Atom inclusion ⓘ



At the recommended contour level, 85% of all backbone atoms, 82% 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 (0.0051) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8209	0.0510
0	0.6777	0.0570
1	0.7753	0.0270
2	0.9403	0.0590
3	0.9285	0.0540
4	0.8883	0.0660
5	0.9294	0.0540
6	0.9351	0.0560
7	0.8985	0.0570
8	0.7652	0.0310
9	0.7138	0.0580
A	0.9051	0.0510
B	0.9607	0.0590
D	0.9574	0.0370
E	0.9473	0.0620
F	0.9623	0.0700
G	0.7487	0.0490
H	0.9537	0.0570
I	0.9497	0.0490
J	1.0000	0.0740
L	0.9603	0.0400
O	0.8666	0.0250
P	0.7910	-0.0350
Q	0.8340	0.0430
R	0.6575	-0.0250
S	0.8677	0.0190
T	0.7946	0.0260
U	0.8712	0.0620
V	0.9124	0.0630
X	0.8320	0.0580
Y	0.8245	0.0620
c	0.5152	0.0220
d	0.5318	0.0350
e	0.8142	0.0440
f	0.8272	0.0520

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Chain	Atom inclusion	Q-score
i	■ 0.7932	■ 0.0320
j	■ 0.4242	■ 0.0270
k	■ 0.2969	■ 0.0090
l	■ 0.7299	■ 0.0210
m	■ 0.3462	■ 0.0180
o	■ 0.8151	■ 0.1210
p	■ 0.6112	■ -0.0170
q	■ 0.6789	■ -0.0350
r	■ 0.8939	■ 0.0770
s	■ 0.8654	■ 0.1030
t	■ 0.7922	■ 0.1140
u	■ 0.8393	■ 0.0330
v	■ 0.9310	■ 0.2230
w	■ 0.7753	■ 0.0030
x	■ 0.5758	■ -0.0350
y	■ 0.7793	■ 0.1080
z	■ 0.6404	■ -0.0420