Full wwPDB EM Validation Report ⓘ

Oct 26, 2022 – 01:28 PM JST

PDB ID	:	8GXS
EMDB ID	:	EMD-34360
Title	:	PIC-Mediator in complex with +1 nucleosome (T40N) in H-binding state
Authors	:	Chen, X.; Wang, X.; Liu, W.; Ren, Y.; Qu, X.; Li, J.; Yin, X.
Deposited on	:	2022-09-21
Resolution	:	4.16 Å(reported)

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

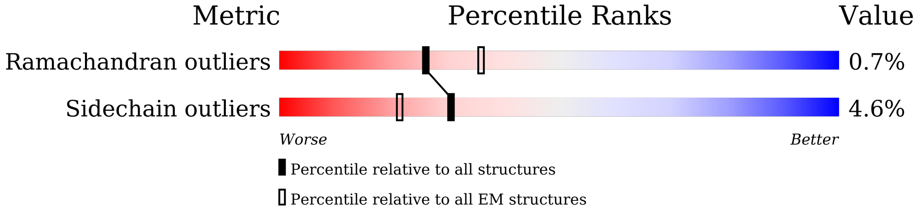
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

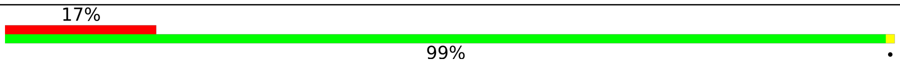
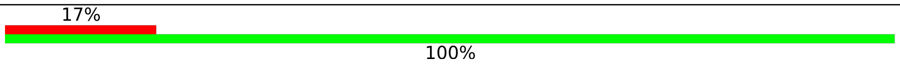
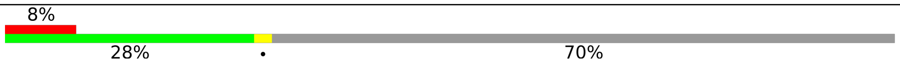
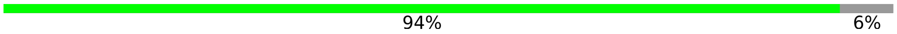
The reported resolution of this entry is 4.16 Å.

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	X	228	
2	Y	228	
3	NX	162	
4	NY	162	
5	BA	316	
6	DA	1872	
7	EA	439	
8	FA	517	
9	HA	760	

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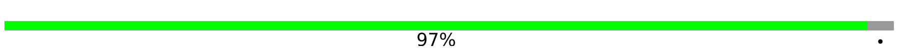
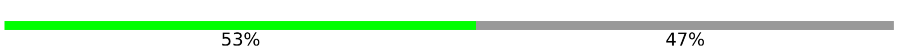
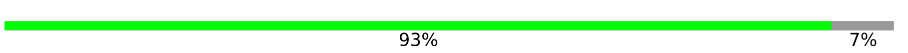
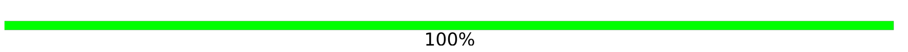
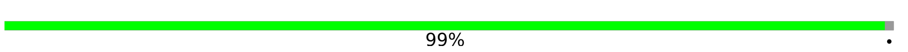
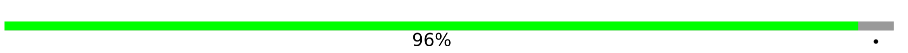
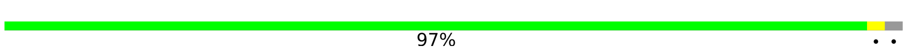
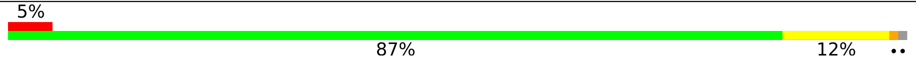
Mol	Chain	Length	Quality of chain
10	NA	136	
10	NE	136	
11	PA	1970	
12	DB	1199	
13	EB	291	
14	FB	249	
15	HB	548	
16	NB	103	
16	NF	103	
17	PB	1174	
18	HC	462	
19	DO	109	
20	DP	339	
21	DQ	376	
22	PC	275	
23	PE	210	
24	PF	127	
25	PH	150	
26	PI	125	
27	PJ	67	
28	PK	117	
29	PL	58	
30	HD	309	
31	HG	395	
32	HE	308	

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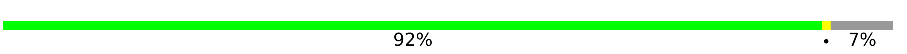
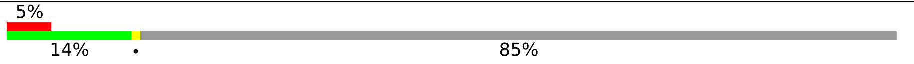
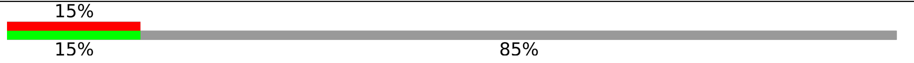
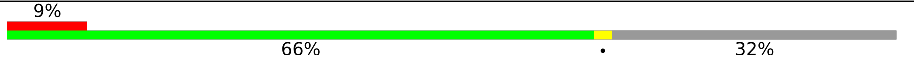
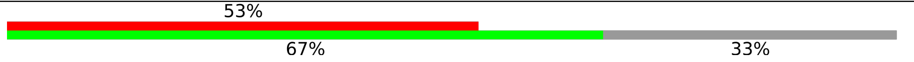
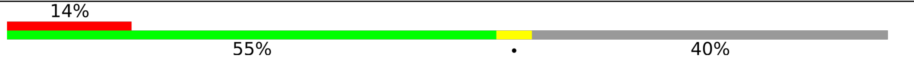
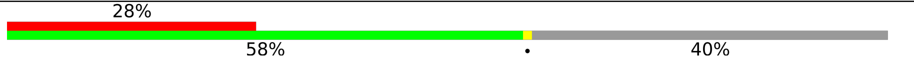
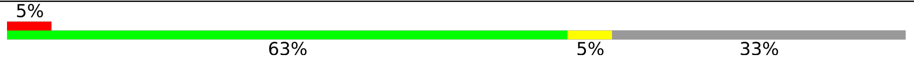
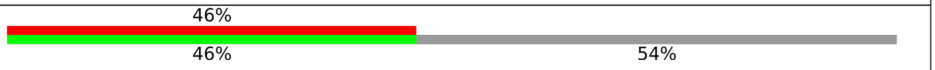
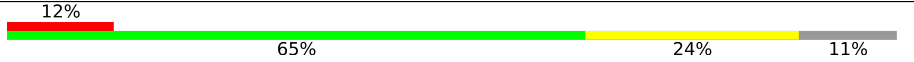
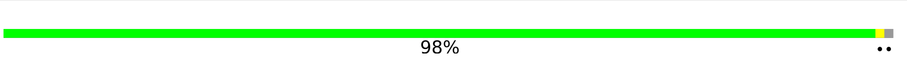
Mol	Chain	Length	Quality of chain
33	HF	71	
34	HH	782	
35	DD	1085	
35	Dd	1085	
36	DE	800	
36	De	800	
37	DF	677	
37	Df	677	
38	DG	349	
39	DH	310	
40	DI	264	
40	Di	264	
41	DL	161	
41	Dl	161	
42	Dc	929	
43	DJ	218	
43	Dj	218	
44	Dk	211	
45	Dm	124	
46	HI	346	
47	HJ	323	
48	PD	142	
49	PG	172	
50	g	233	
51	j	135	

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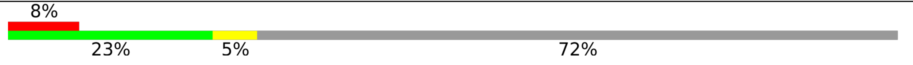
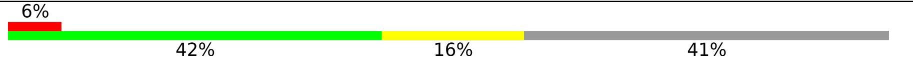
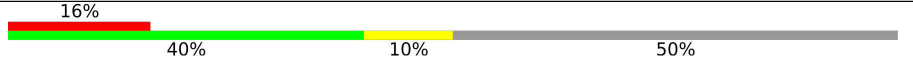
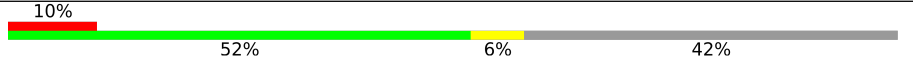
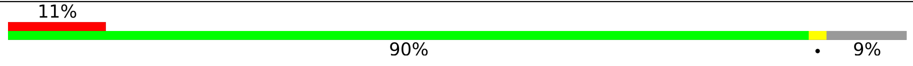
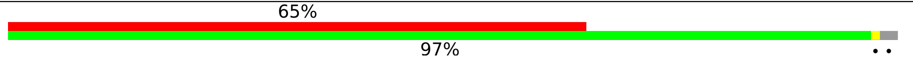
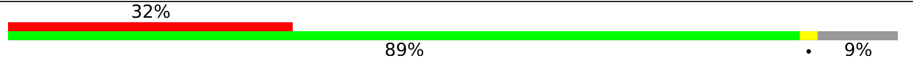
Mol	Chain	Length	Quality of chain
52	n	1454	
53	s	244	
54	u	144	
55	a	1581	
56	d	270	
57	f	246	
58	i	146	
59	m	131	
60	q	651	
61	z	600	
62	b	200	
63	c	311	
64	e	178	
65	l	178	
66	o	788	
67	h	268	
68	k	117	
69	r	208	
70	t	212	
71	v	200	
72	p	841	
73	w	1368	
74	x	989	
75	y	747	
76	NC	128	

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Mol	Chain	Length	Quality of chain
76	NG	128	
77	ND	126	
77	NH	126	

2 Entry composition

There are 80 unique types of molecules in this entry. The entry contains 185972 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 DNA chain called DNA (228-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	X	67	Total	C	N	O	P	0	0
			1387	652	275	394	66		

- Molecule 2 is a DNA chain called DNA (228-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Y	67	Total	C	N	O	P	0	0
			1357	643	239	408	67		

- Molecule 3 is a DNA chain called DNA (162-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	NX	162	Total	C	N	O	P	0	0
			3078	1458	486	972	162		

- Molecule 4 is a DNA chain called DNA (162-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	NY	162	Total	C	N	O	P	0	0
			3561	1620	810	970	161		

- Molecule 5 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	BA	252	Total	C	N	O	S	0	0
			1953	1224	346	366	17		

- Molecule 6 is a protein called Transcription initiation factor TFIID subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	DA	558	Total	C	N	O	S	0	0
			4563	2913	791	832	27		

- Molecule 7 is a protein called General transcription factor IIE subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	EA	187	1535	964	275	285	11	0	0

- Molecule 8 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	FA	138	1138	719	208	208	3	0	0

- Molecule 9 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		
9	HA	714	5751	3683	999	1040	29	0	0

- Molecule 10 is a protein called Histone H3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	NA	100	498	298	100	100	0	0
			Total	C	N	O		
10	NE	103	511	305	103	103	0	0

- Molecule 11 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	PA	1471	11628	7314	2064	2178	72	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	DB	963	7796	5011	1315	1412	58	0	0

- Molecule 13 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	EB	171	1403	895	243	261	4	0	0

- Molecule 14 is a protein called General transcription factor IIF subunit 2.

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

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

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

- Molecule 16 is a protein called Histone H4.

Mol	Chain	Residues	Atoms	AltConf	Trace
16	NB	80	Total C N O 391 231 80 80	0	0
16	NF	86	Total C N O 421 249 86 86	0	0

- Molecule 17 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms	AltConf	Trace
17	PB	1136	Total C N O S 9076 5739 1597 1676 64	0	0

- Molecule 18 is a protein called General transcription factor IIH subunit 4.

Mol	Chain	Residues	Atoms	AltConf	Trace
18	HC	390	Total C N O S 3158 2050 545 551 12	0	0

- Molecule 19 is a protein called Transcription initiation factor IIA subunit 2.

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

- Molecule 20 is a protein called TATA-box-binding protein.

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

- Molecule 21 is a protein called Transcription initiation factor IIA subunit 1.

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

- Molecule 22 is a protein called DNA-directed RNA polymerase II subunit RPB3.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	PE	209	Total 1721	C 1089	N 300	O 324	S 8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	PF	79	Total 636	C 406	N 108	O 117	S 5	0	0

- Molecule 25 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 26 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	PI	114	Total 928	C 571	N 166	O 180	S 11	0	0

- Molecule 27 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 28 is a protein called RNA_pol_L_2 domain-containing protein.

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

- Molecule 29 is a protein called RPB12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	PL	44	373	231	72	64	6	0	0

- Molecule 30 is a protein called CDK-activating kinase assembly factor MAT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	HD	306	2400	1498	424	465	13	0	0

- Molecule 31 is a protein called General transcription factor IIH subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	HG	347	2732	1726	471	508	27	0	0

- Molecule 32 is a protein called General transcription factor IIH subunit 3.

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

- Molecule 33 is a protein called General transcription factor IIH subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	HF	66	523	337	83	100	3	0	0

- Molecule 34 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		
34	HH	605	4890	3127	848	885	30	0	0

- Molecule 35 is a protein called Transcription initiation factor TFIID subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	DD	159	Total 1330	C 830	N 248	O 249	S 3	0	0
35	Dd	158	Total 1307	C 814	N 238	O 252	S 3	0	0

- Molecule 36 is a protein called Transcription initiation factor TFIID subunit 5.

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

- Molecule 37 is a protein called Transcription initiation factor TFIID subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	DF	408	Total 3109	C 1970	N 542	O 579	S 18	0	0
37	Df	403	Total 3081	C 1954	N 533	O 576	S 18	0	0

- Molecule 38 is a protein called Transcription initiation factor TFIID subunit 7.

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

- Molecule 39 is a protein called Transcription initiation factor TFIID subunit 8.

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

- Molecule 40 is a protein called Transcription initiation factor TFIID subunit 9.

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

- Molecule 41 is a protein called Transcription initiation factor TFIID subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	DL	74	Total 605	C 379	N 105	O 118	S 3	0	0
41	Dl	107	Total 876	C 547	N 158	O 166	S 5	0	0

- Molecule 42 is a protein called Transcription initiation factor TFIID subunit 3.

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

- Molecule 43 is a protein called Transcription initiation factor TFIID subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Dj	95	Total 759	C 488	N 124	O 143	S 4	0	0
43	DJ	90	Total 720	C 466	N 115	O 135	S 4	0	0

- Molecule 44 is a protein called Transcription initiation factor TFIID subunit 11.

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

- Molecule 45 is a protein called Transcription initiation factor TFIID subunit 13.

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

- Molecule 46 is a protein called Cyclin-dependent kinase 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	HI	299	Total 2374	C 1532	N 405	O 426	S 11	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
HI	41	ALA	LYS	engineered mutation	UNP P50613

- Molecule 47 is a protein called Cyclin-H.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	HJ	287	Total 2307	C 1477	N 398	O 417	S 15	0	0

- Molecule 48 is a protein called DNA-directed RNA polymerase II subunit RPB4.

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

- Molecule 49 is a protein called DNA-directed RNA polymerase II subunit RPB7.

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

- Molecule 50 is a protein called Mediator of RNA polymerase II transcription subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	g	106	Total 898	C 569	N 166	O 157	S 6	0	0

- Molecule 51 is a protein called Mediator of RNA polymerase II transcription subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	j	122	Total 840	C 527	N 151	O 159	S 3	0	0

- Molecule 52 is a protein called Mediator of RNA polymerase II transcription subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	n	1015	Total 7751	C 4941	N 1363	O 1405	S 42	0	0

- Molecule 53 is a protein called Mediator of RNA polymerase II transcription subunit 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	s	93	Total 723	C 463	N 121	O 135	S 4	0	0

- Molecule 54 is a protein called Mediator of RNA polymerase II transcription subunit 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	u	117	886	552	146	184	4	0	0

- Molecule 55 is a protein called Mediator of RNA polymerase II transcription subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	a	438	3430	2190	584	632	24	0	0

- Molecule 56 is a protein called Mediator of RNA polymerase II transcription subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	d	158	1268	791	228	243	6	0	0

- Molecule 57 is a protein called Mediator of RNA polymerase II transcription subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	f	167	1365	882	235	243	5	0	0

- Molecule 58 is a protein called Mediator of RNA polymerase II transcription subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	i	73	605	382	107	110	6	0	0

- Molecule 59 is a protein called Mediator of RNA polymerase II transcription subunit 31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	m	112	983	641	172	165	5	0	0

- Molecule 60 is a protein called Mediator of RNA polymerase II transcription subunit 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	q	555	4373	2765	783	805	20	0	0

- Molecule 61 is a protein called Mediator of RNA polymerase II transcription subunit 26.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	z	97	Total 765	C 472	N 136	O 154	S 3	0	0

- Molecule 62 is a protein called Mediator of RNA polymerase II transcription subunit 29.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	b	115	Total 899	C 563	N 155	O 172	S 9	0	0

- Molecule 63 is a protein called Mediator of RNA polymerase II transcription subunit 27.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	c	263	Total 2131	C 1356	N 379	O 385	S 11	0	0

- Molecule 64 is a protein called Mediator of RNA polymerase II transcription subunit 28.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	e	102	Total 832	C 520	N 146	O 163	S 3	0	0

- Molecule 65 is a protein called Mediator of RNA polymerase II transcription subunit 30.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	l	126	Total 1040	C 649	N 191	O 193	S 7	0	0

- Molecule 66 is a protein called Mediator of RNA polymerase II transcription subunit 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	o	156	Total 1221	C 780	N 212	O 222	S 7	0	0

- Molecule 67 is a protein called Isoform 2 of Mediator of RNA polymerase II transcription subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	h	190	Total 1465	C 913	N 259	O 289	S 4	0	0

- Molecule 68 is a protein called Mediator of RNA polymerase II transcription subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
68	k	112	879	537	163	175	4	0	0

- Molecule 69 is a protein called Mediator of RNA polymerase II transcription subunit 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
69	r	192	1535	973	271	276	15	0	0

- Molecule 70 is a protein called Mediator of RNA polymerase II transcription subunit 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
70	t	193	1499	955	247	280	17	0	0

- Molecule 71 is a protein called Mediator of RNA polymerase II transcription subunit 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
71	v	134	1083	668	185	226	4	0	0

- Molecule 72 is a protein called Isoform 2 of Mediator of RNA polymerase II transcription subunit 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
72	p	766	5983	3816	1026	1092	49	0	0

- Molecule 73 is a protein called Mediator of RNA polymerase II transcription subunit 23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
73	w	1334	10774	6967	1827	1909	71	0	0

- Molecule 74 is a protein called Mediator of RNA polymerase II transcription subunit 24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
74	x	897	7061	4524	1190	1293	54	0	0

- Molecule 75 is a protein called Mediator of RNA polymerase II transcription subunit 25.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	y	210	Total 1605	C 1030	N 264	O 302	S 9	0	0

- Molecule 76 is a protein called HISTONE H2A.Z.

Mol	Chain	Residues	Atoms				AltConf	Trace
76	NC	103	Total 506	C 300	N 103	O 103	0	0
76	NG	107	Total 524	C 310	N 107	O 107	0	0

- Molecule 77 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms				AltConf	Trace
77	ND	95	Total 471	C 281	N 95	O 95	0	0
77	NH	95	Total 471	C 281	N 95	O 95	0	0

- Molecule 78 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
78	BA	1	Total 1	Zn 1	0
78	EA	1	Total 1	Zn 1	0
78	PA	2	Total 2	Zn 2	0
78	PB	1	Total 1	Zn 1	0
78	PC	1	Total 1	Zn 1	0
78	PI	2	Total 2	Zn 2	0
78	PJ	1	Total 1	Zn 1	0
78	PL	1	Total 1	Zn 1	0
78	HD	2	Total 2	Zn 2	0
78	HG	3	Total 3	Zn 3	0

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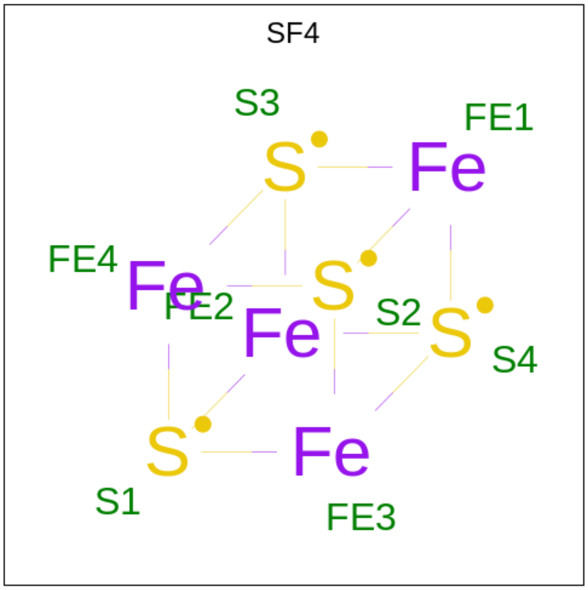
Mol	Chain	Residues	Atoms		AltConf
78	HE	2	Total 2	Zn 2	0
78	c	1	Total 1	Zn 1	0
78	p	1	Total 1	Zn 1	0

- Molecule 79 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
79	HA	1	Total 8	Fe 4	S 4	0

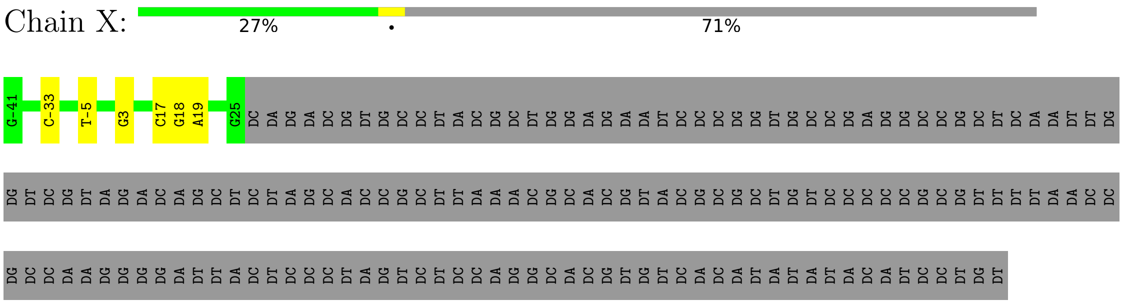
- Molecule 80 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
80	PA	1	Total 1	Mg 1	0

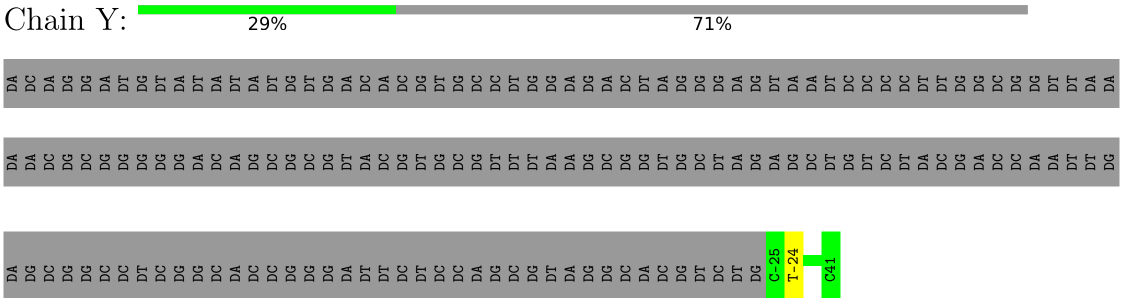
3 Residue-property plots ⓘ

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.

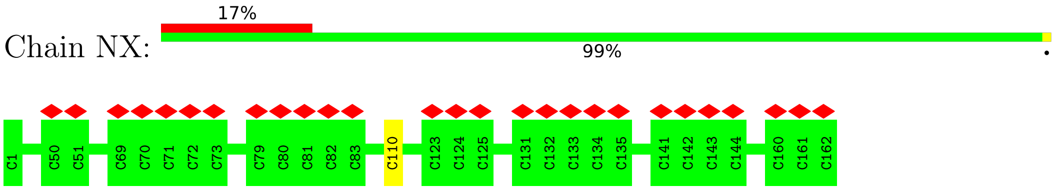
- Molecule 1: DNA (228-mer)



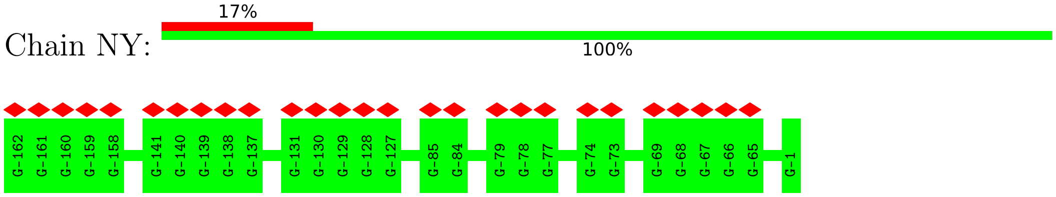
- Molecule 2: DNA (228-mer)



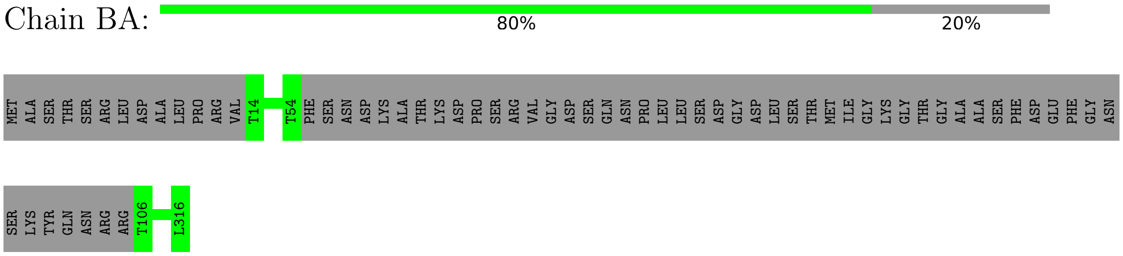
- Molecule 3: DNA (162-mer)



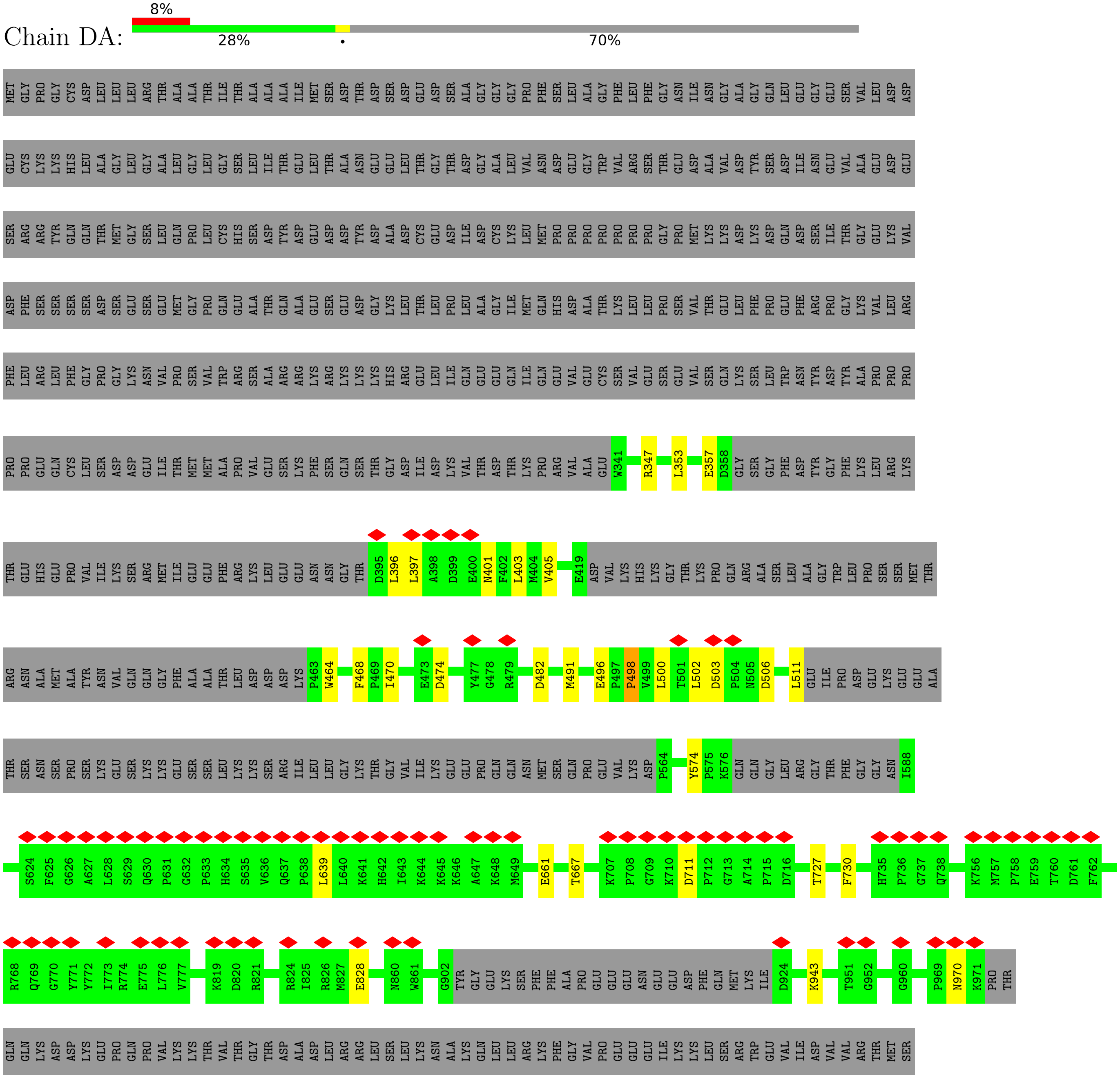
- Molecule 4: DNA (162-mer)

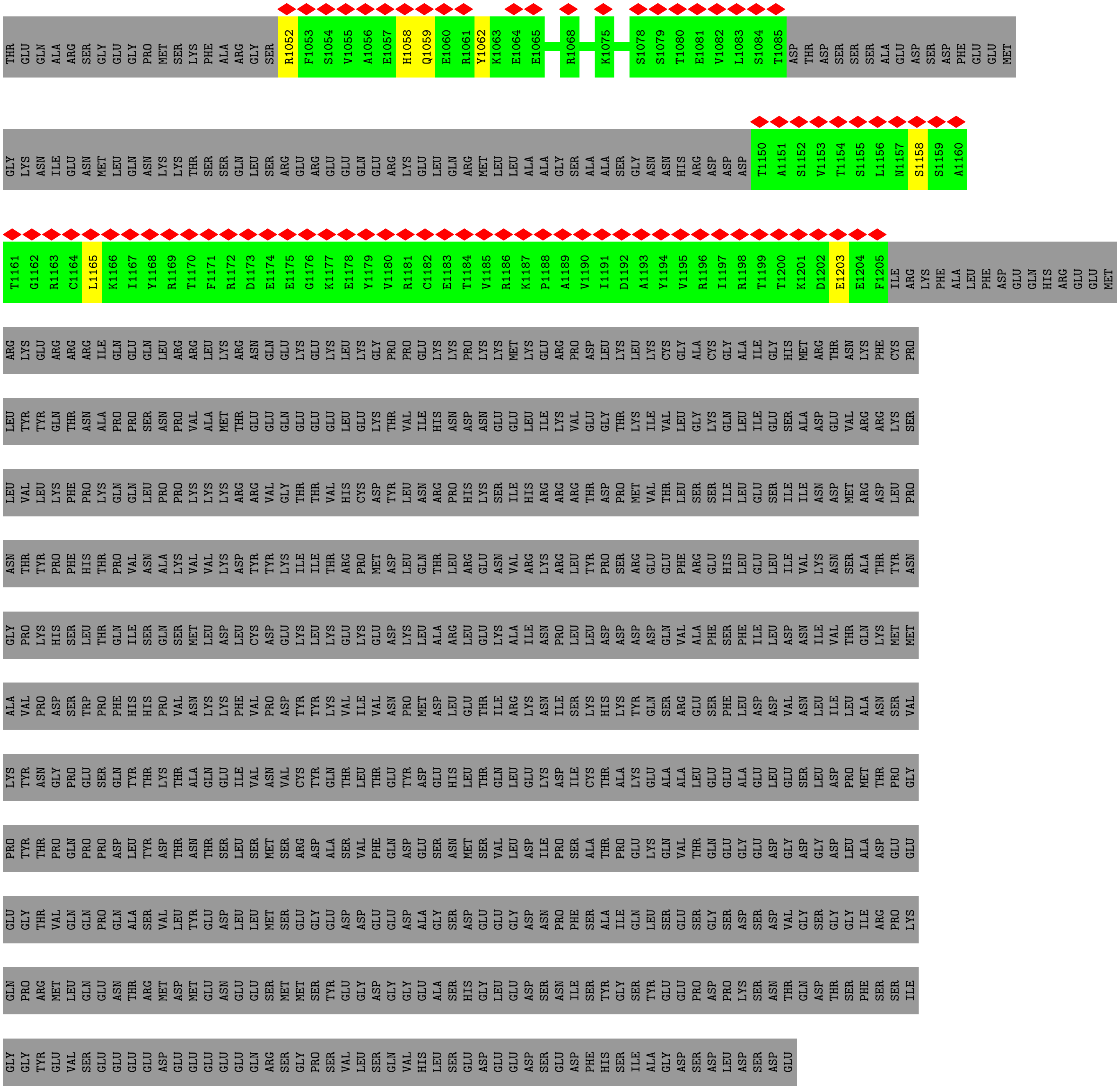


- Molecule 5: Transcription initiation factor IIB



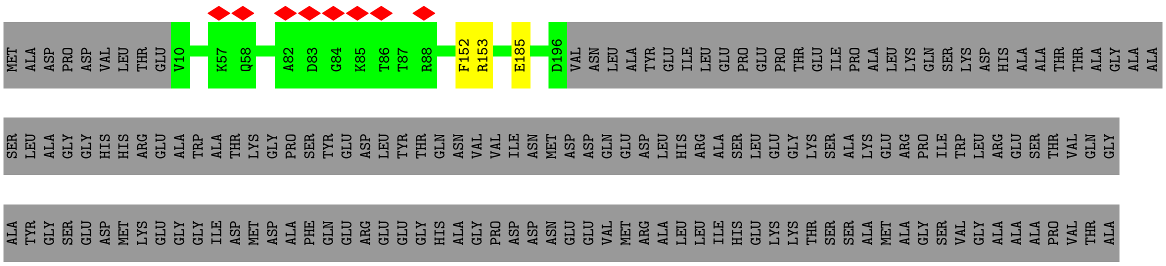
- Molecule 6: Transcription initiation factor TFIID subunit 1

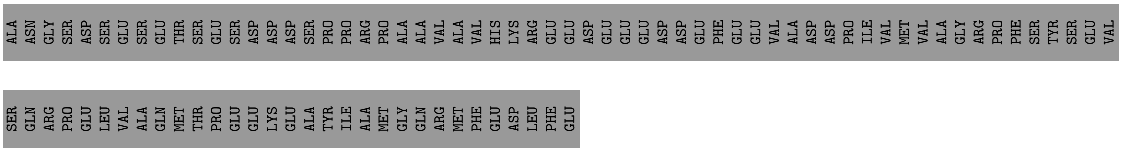




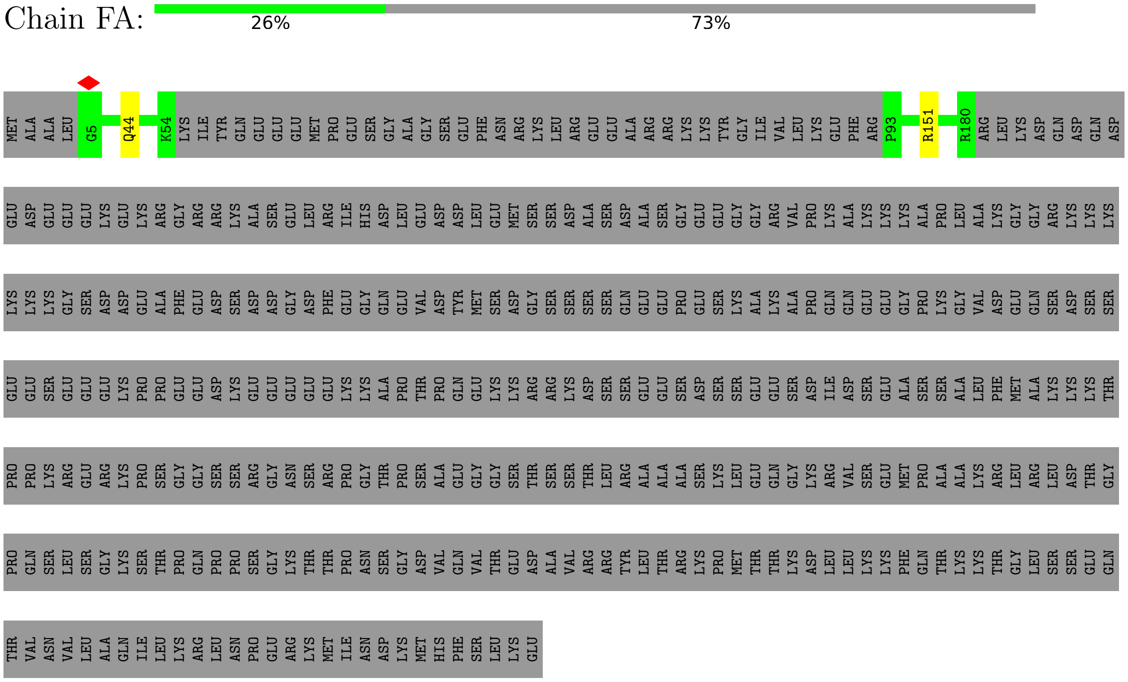
- Molecule 7: General transcription factor IIE subunit 1

Chain EA:

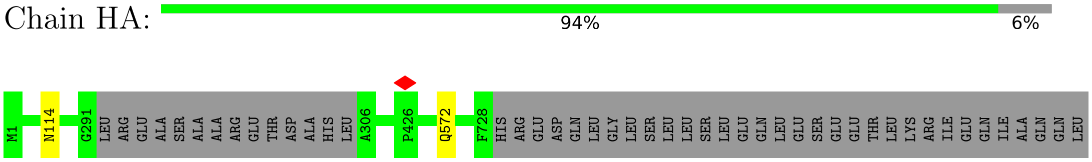




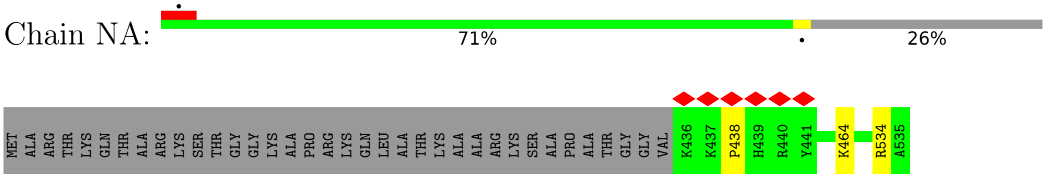
- Molecule 8: General transcription factor IIF subunit 1



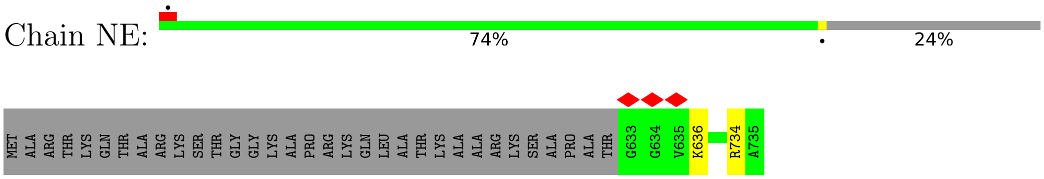
- Molecule 9: General transcription and DNA repair factor IIH helicase subunit XPD



- Molecule 10: Histone H3

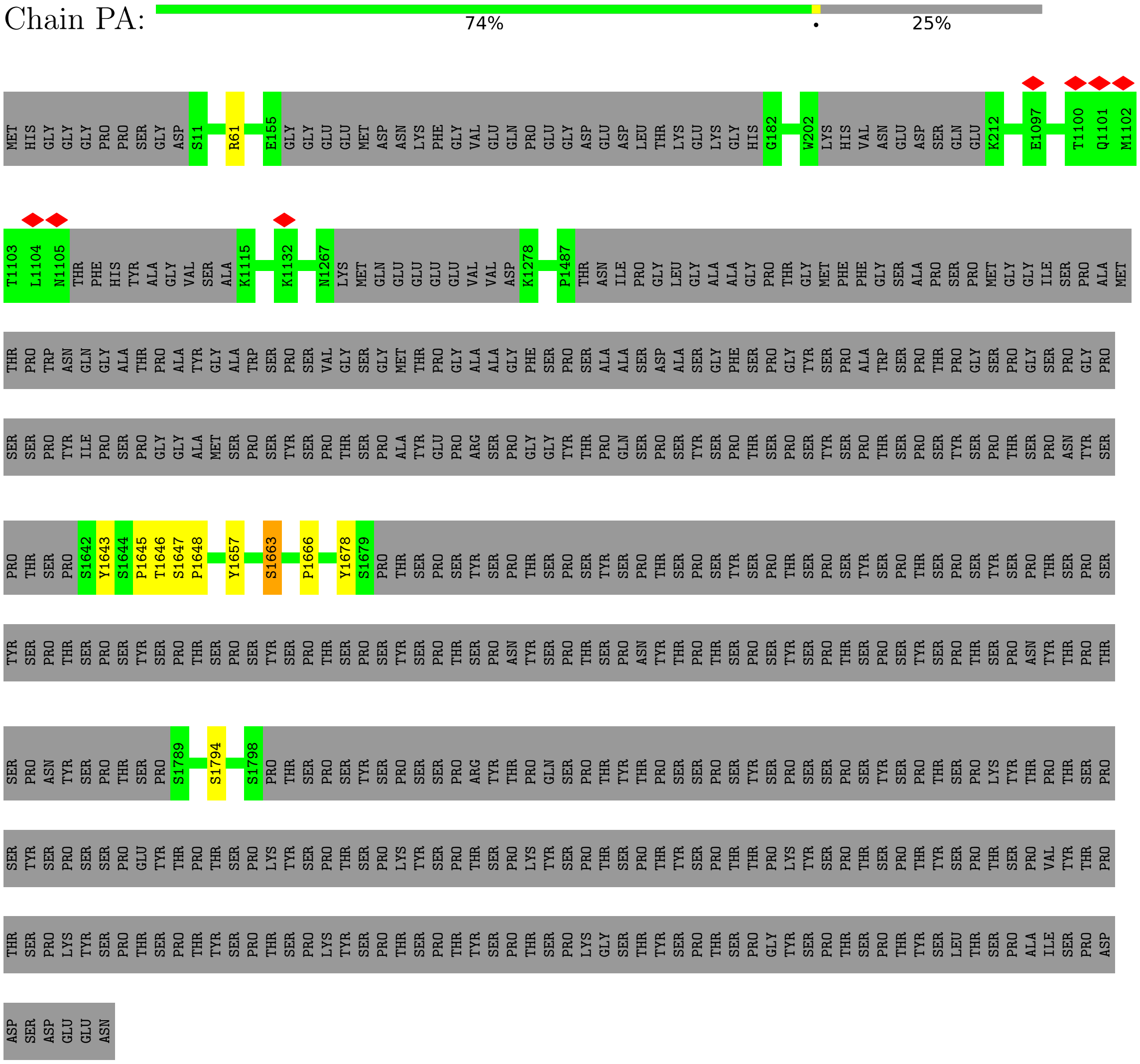


- Molecule 10: Histone H3



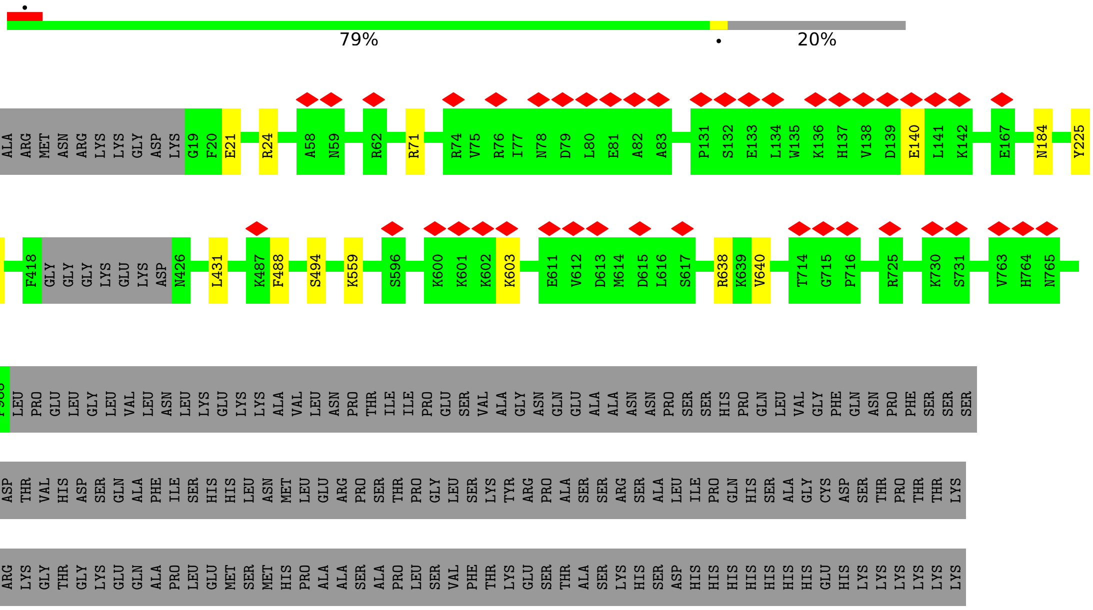
- Molecule 11: DNA-directed RNA polymerase subunit

Chain PA:



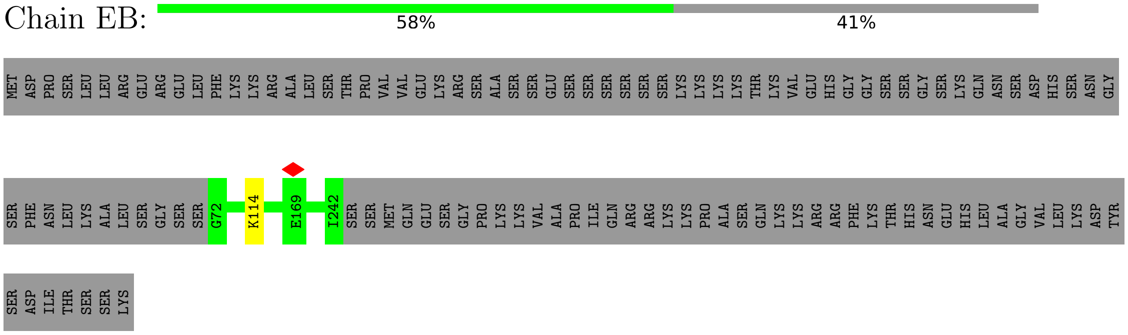
- Molecule 12: Transcription initiation factor TFIID subunit 2

Chain DB:



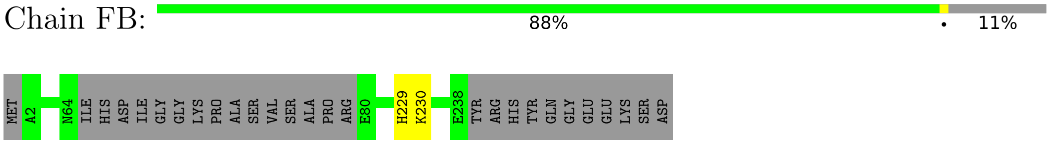
- Molecule 13: Transcription initiation factor IIE subunit beta

Chain EB:



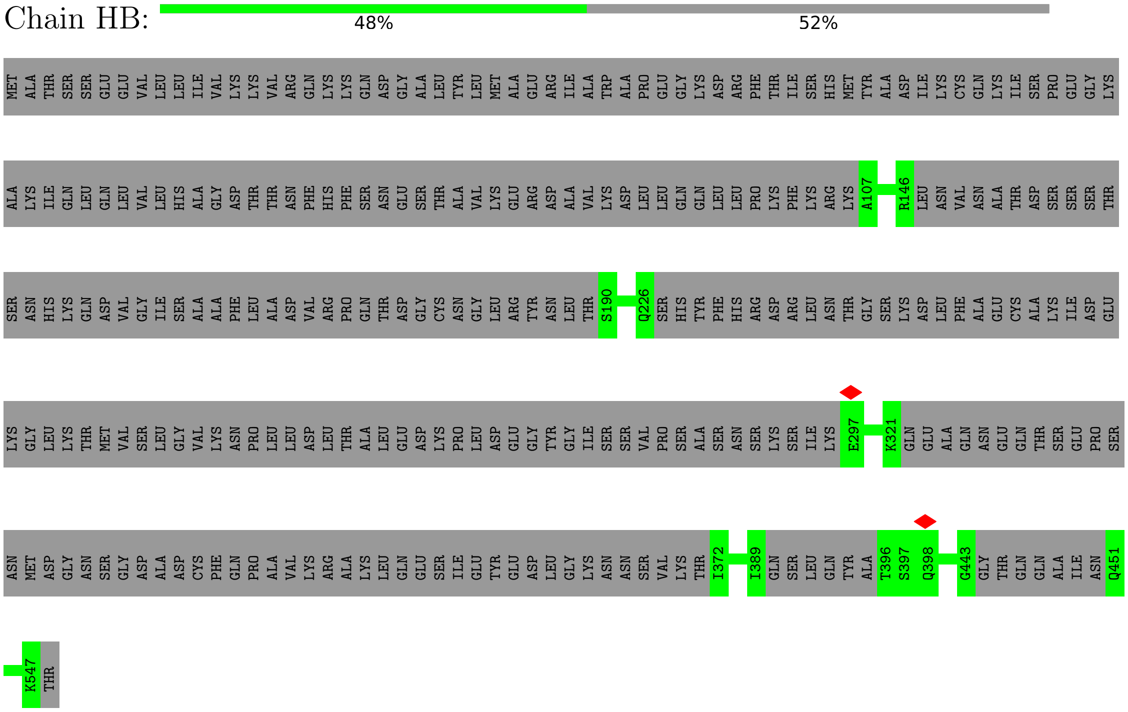
- Molecule 14: General transcription factor IIF subunit 2

Chain FB:



- Molecule 15: General transcription factor IIH subunit 1

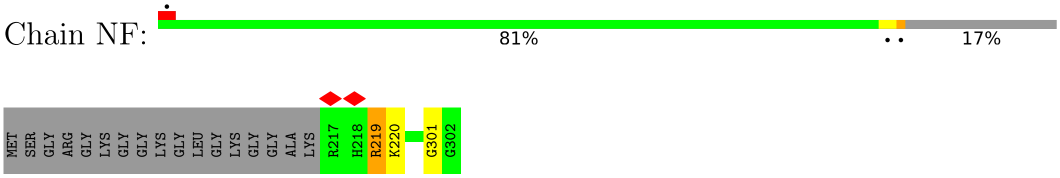
Chain HB:



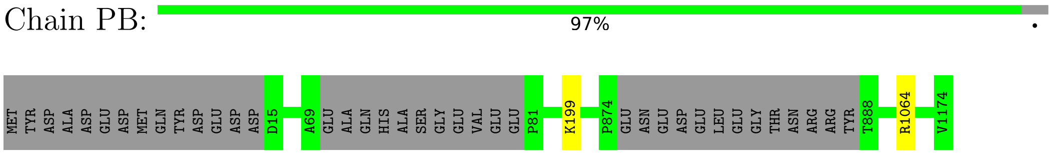
- Molecule 16: Histone H4

Chain NB:

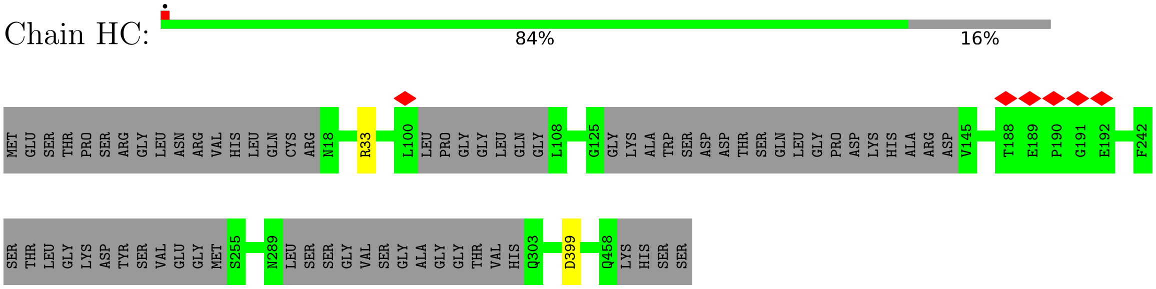
- Molecule 16: Histone H4



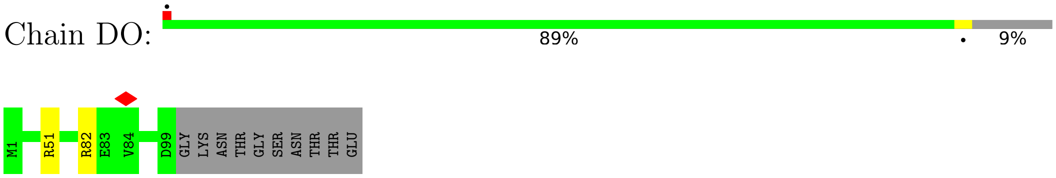
- Molecule 17: DNA-directed RNA polymerase subunit beta



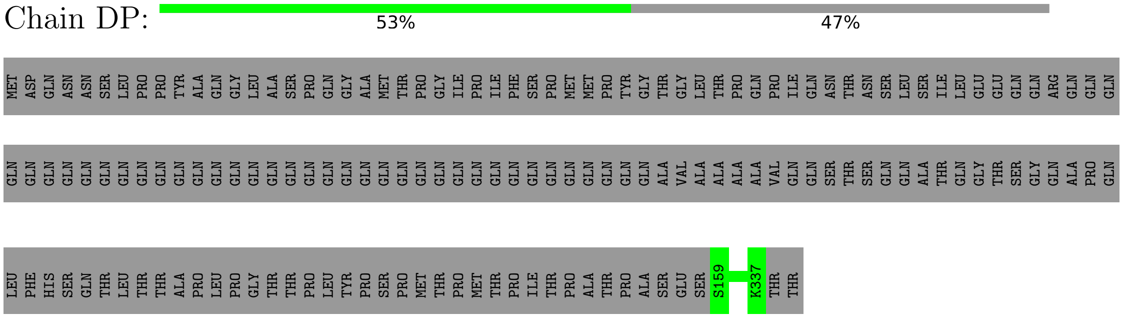
- Molecule 18: General transcription factor IIH subunit 4



- Molecule 19: Transcription initiation factor IIA subunit 2

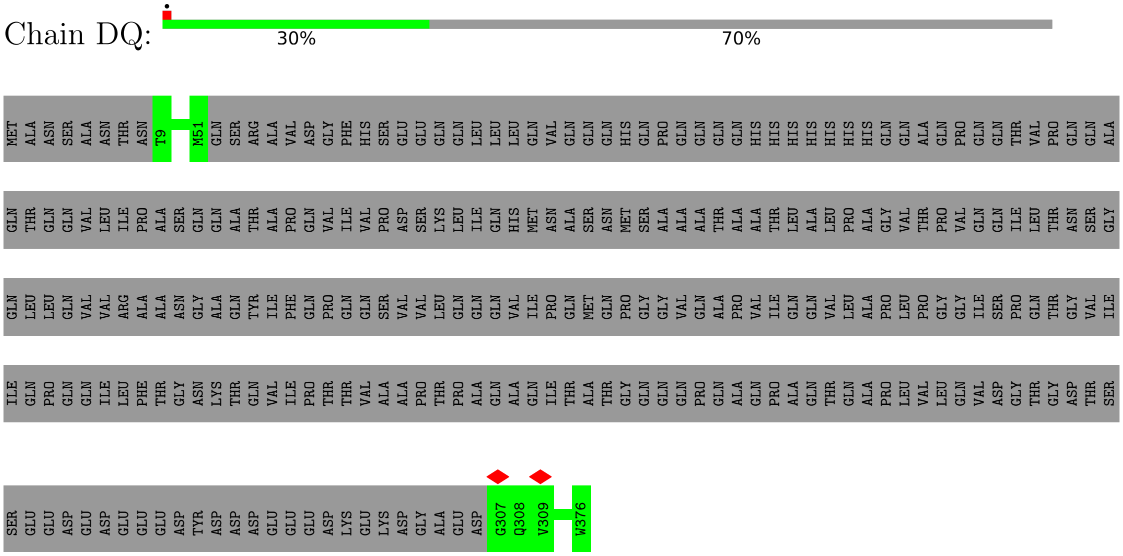


- Molecule 20: TATA-box-binding protein



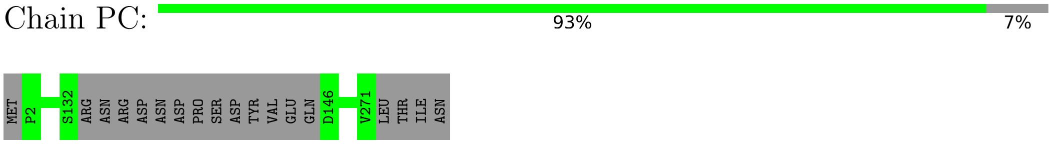
- Molecule 21: Transcription initiation factor IIA subunit 1

Chain DQ:



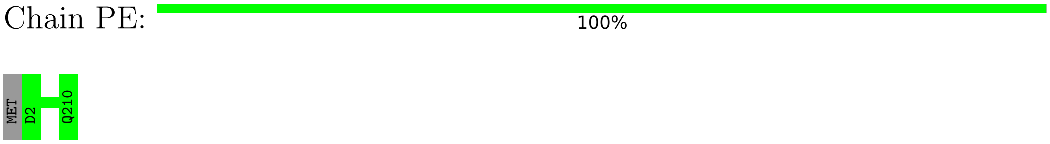
- Molecule 22: DNA-directed RNA polymerase II subunit RPB3

Chain PC:



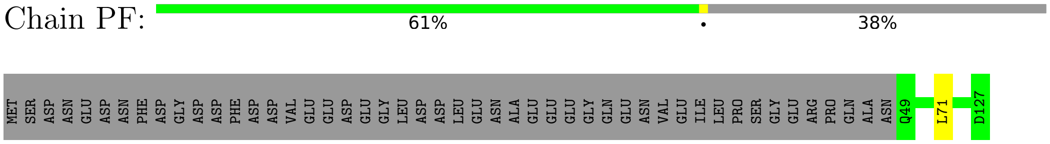
- Molecule 23: DNA-directed RNA polymerase II subunit E

Chain PE:



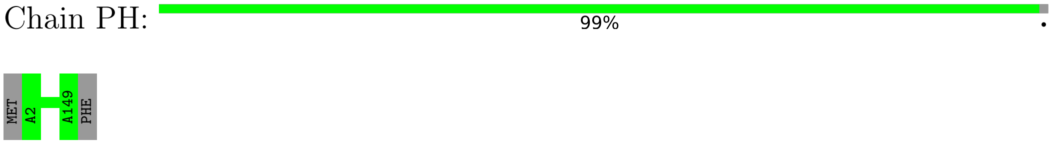
- Molecule 24: DNA-directed RNA polymerase II subunit F

Chain PF:



- Molecule 25: DNA-directed RNA polymerases I, II, and III subunit RPABC3

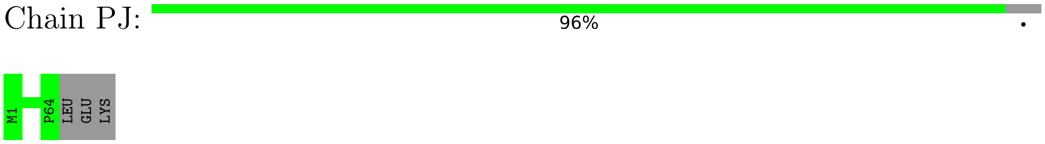
Chain PH:



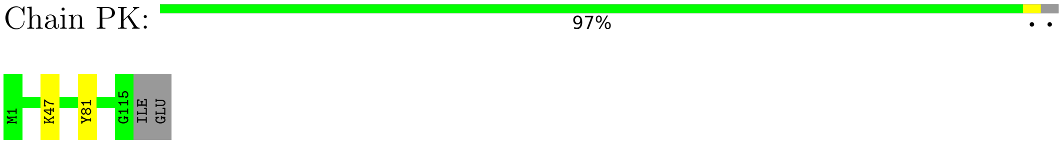
- Molecule 26: DNA-directed RNA polymerase II subunit RPB9

Chain PI:

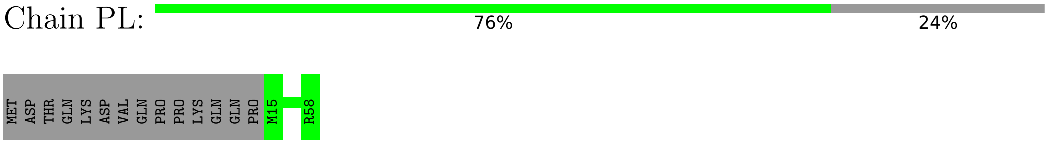
- Molecule 27: DNA-directed RNA polymerases I, II, and III subunit RPABC5



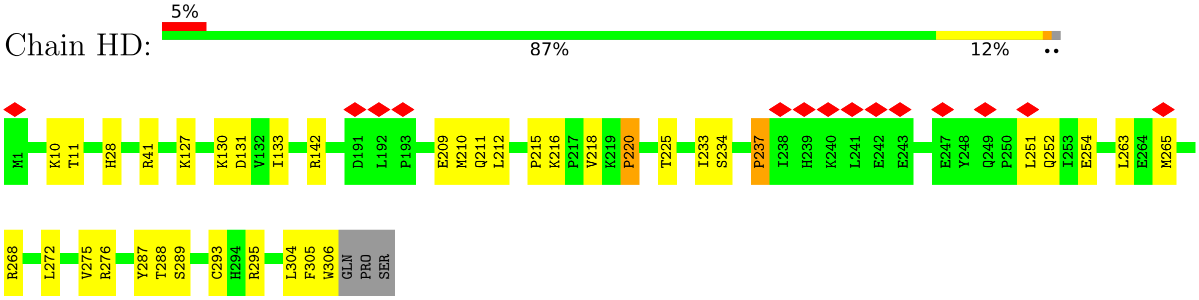
- Molecule 28: RNA_pol_L_2 domain-containing protein



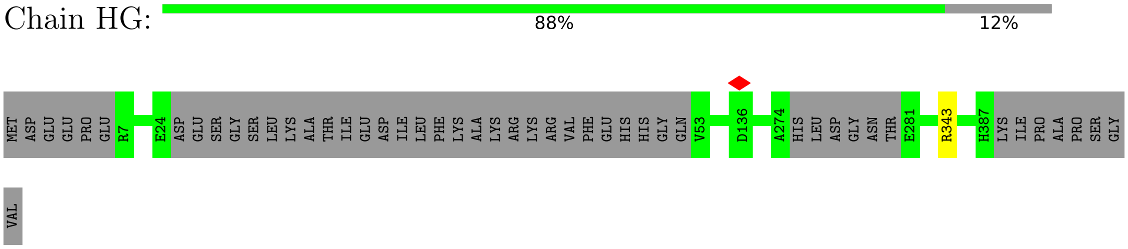
- Molecule 29: RPB12



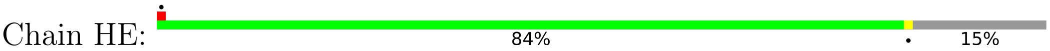
- Molecule 30: CDK-activating kinase assembly factor MAT1



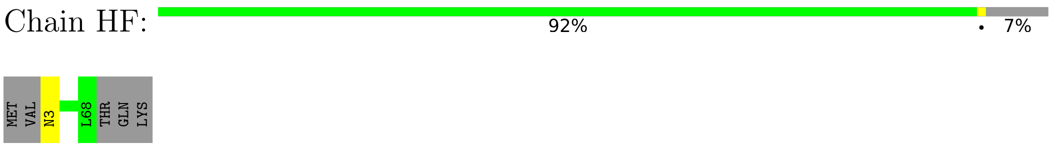
- Molecule 31: General transcription factor IIH subunit 2



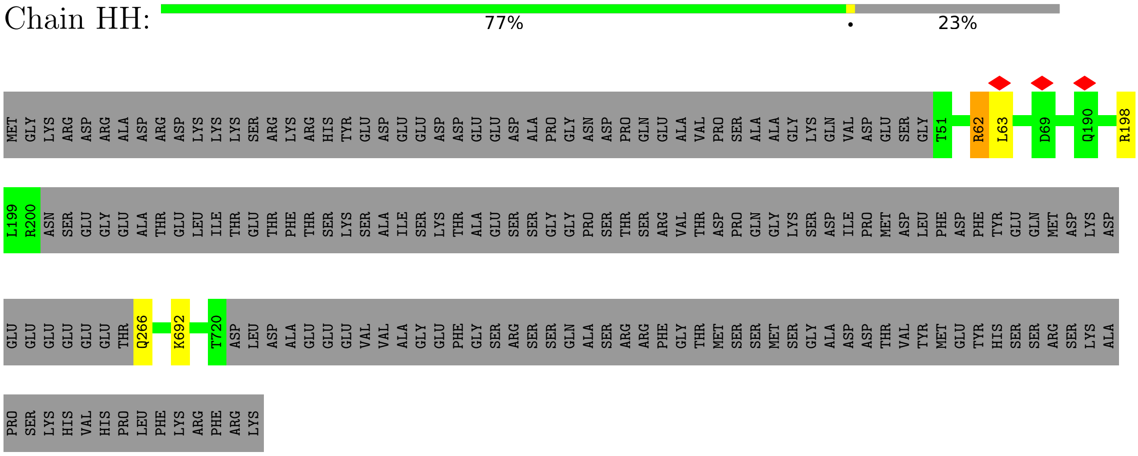
- Molecule 32: General transcription factor IIH subunit 3



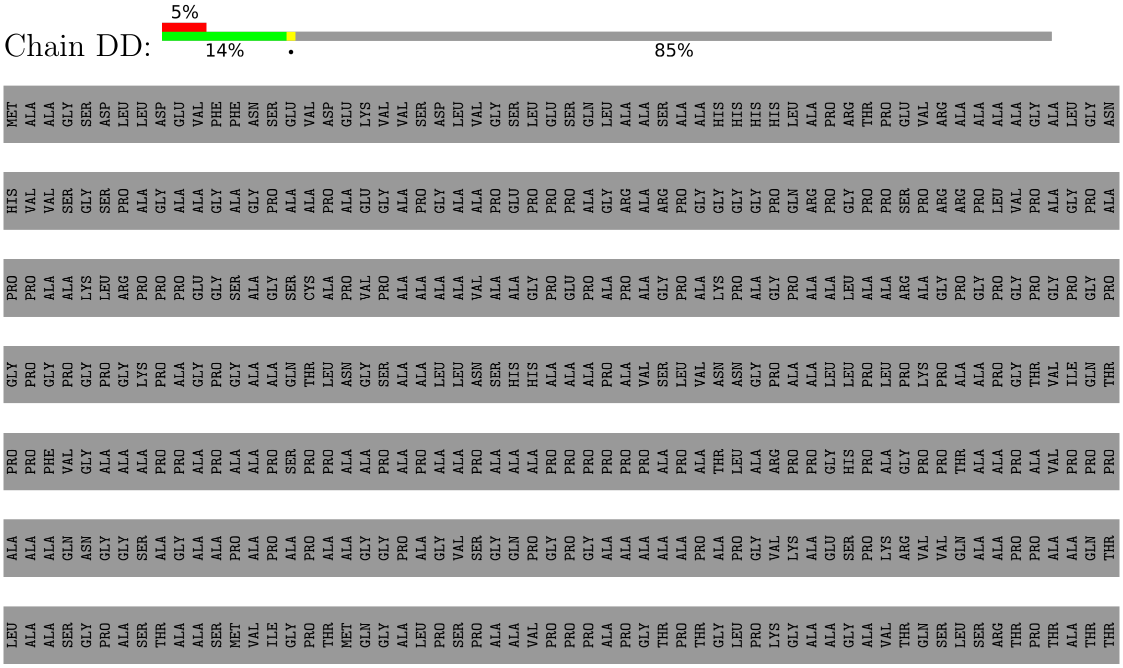
- Molecule 33: General transcription factor IIH subunit 5

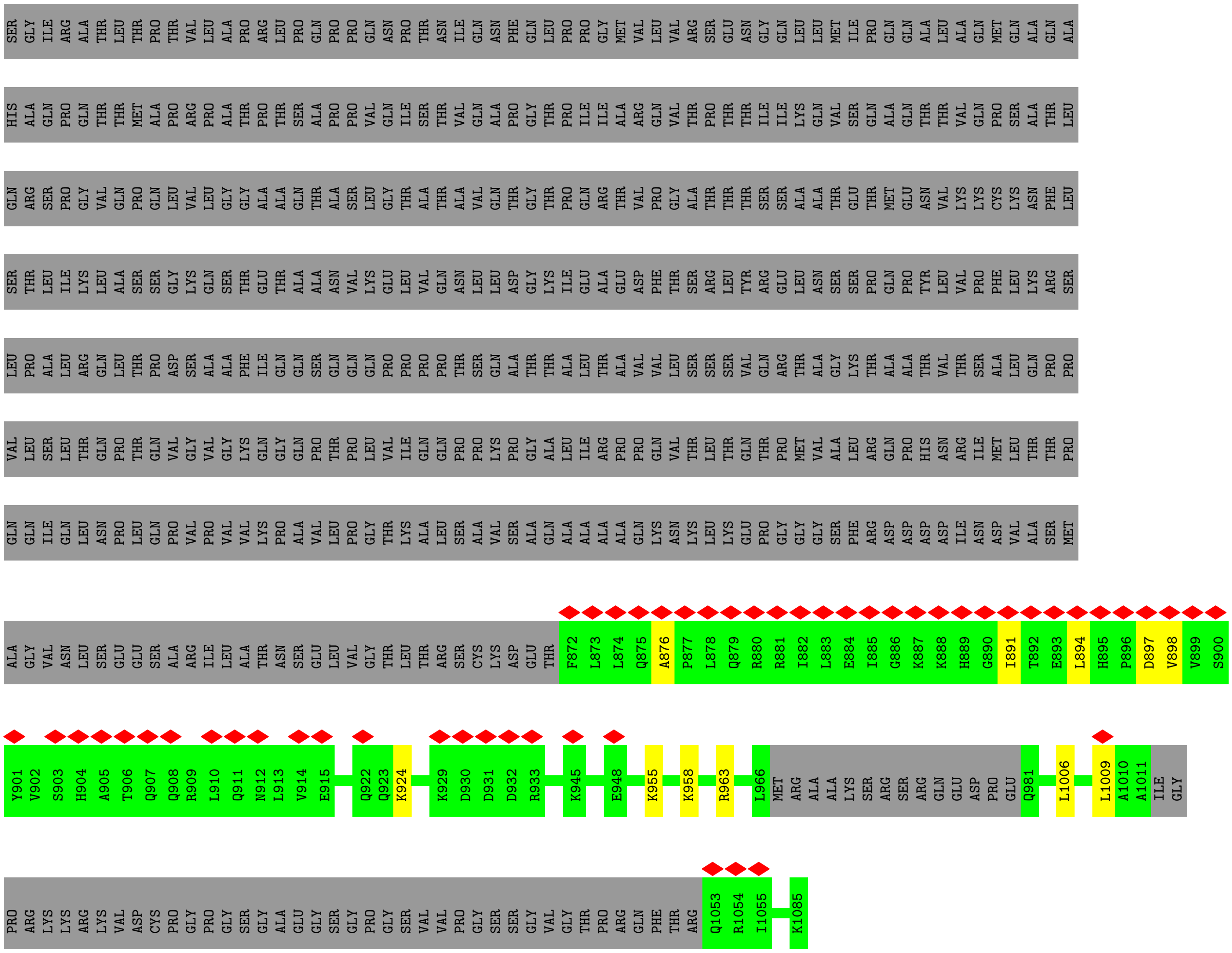


- Molecule 34: General transcription and DNA repair factor IIH helicase subunit XPB



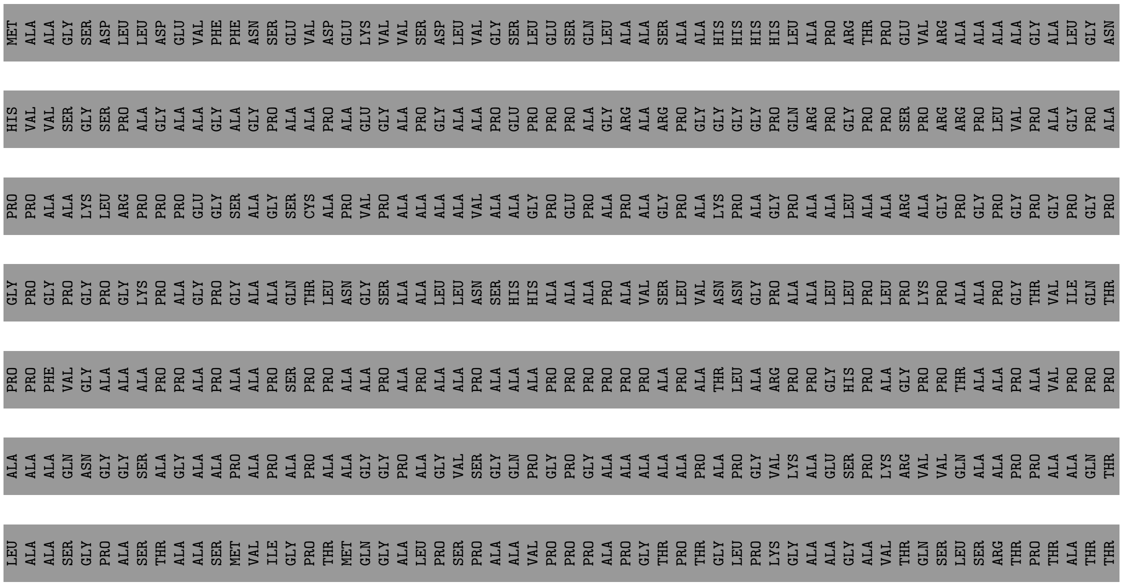
- Molecule 35: Transcription initiation factor TFIID subunit 4

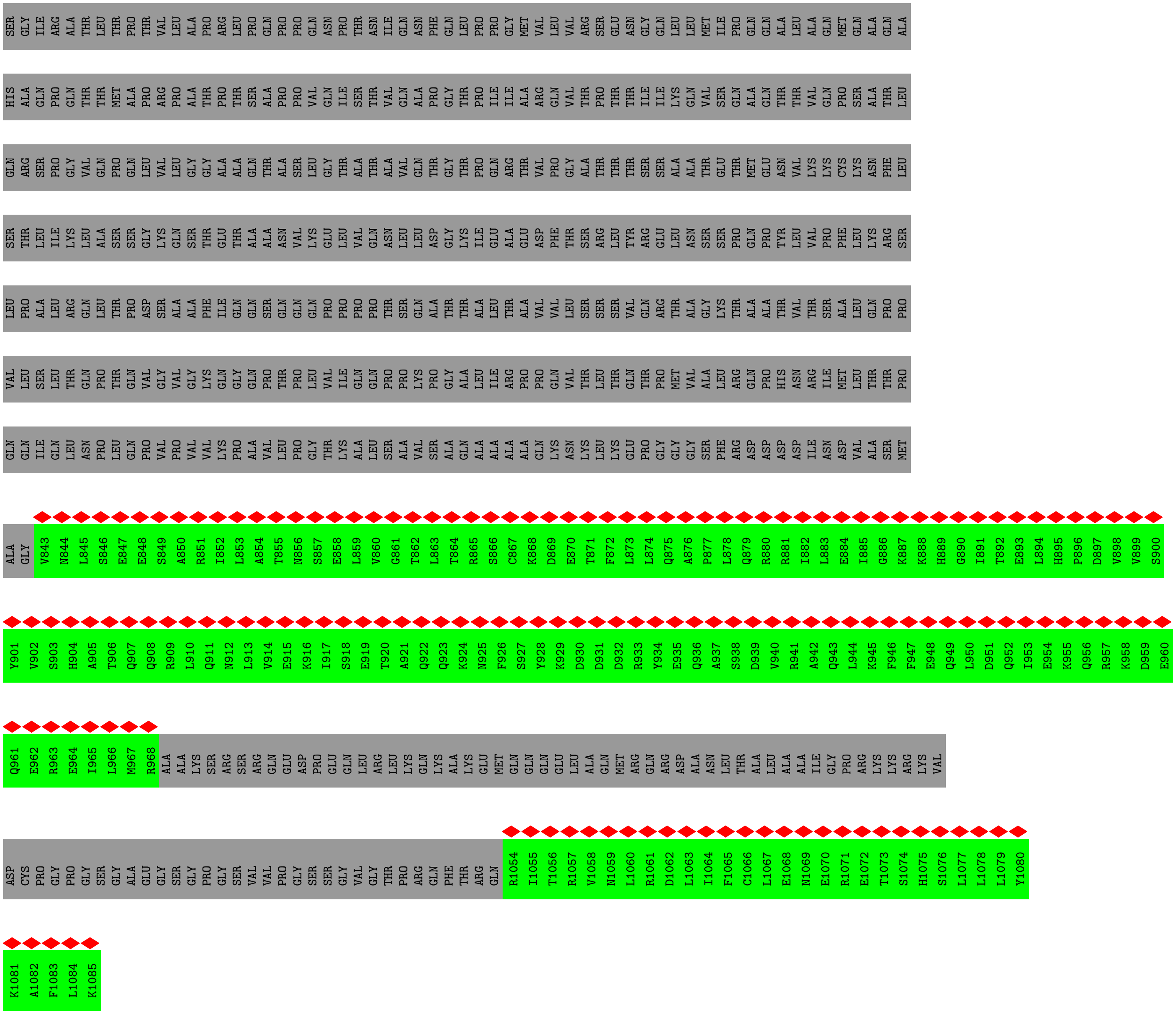




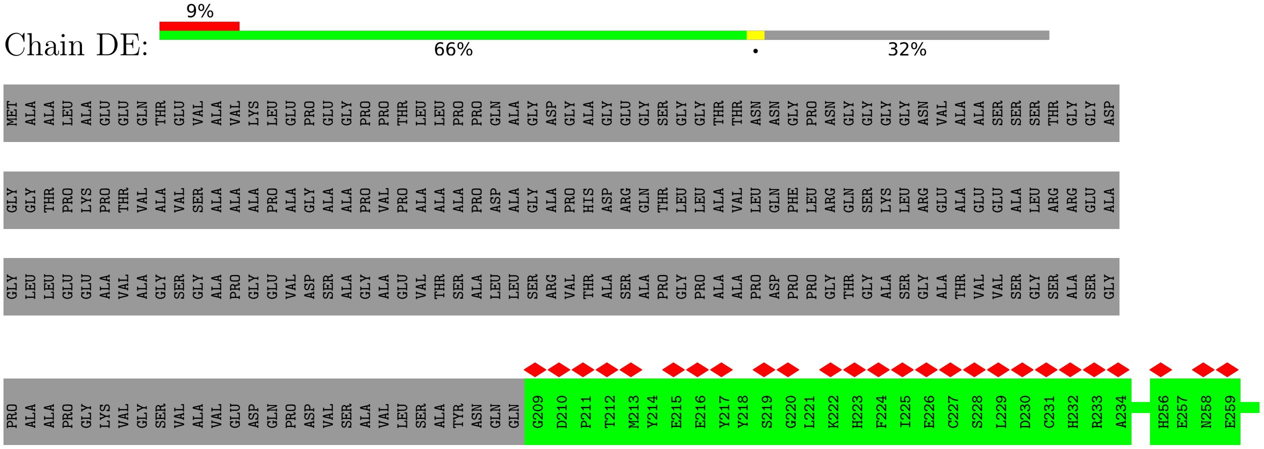
- Molecule 35: Transcription initiation factor TFIID subunit 4

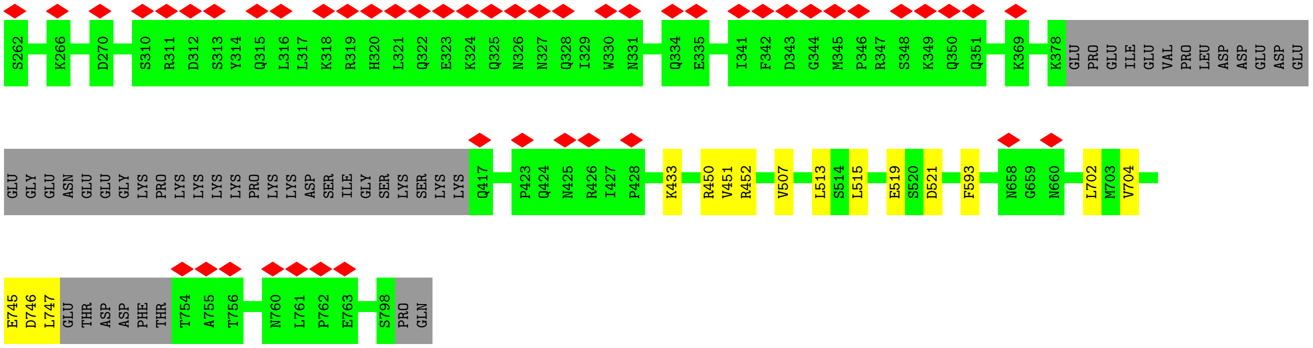
Chain Dd:





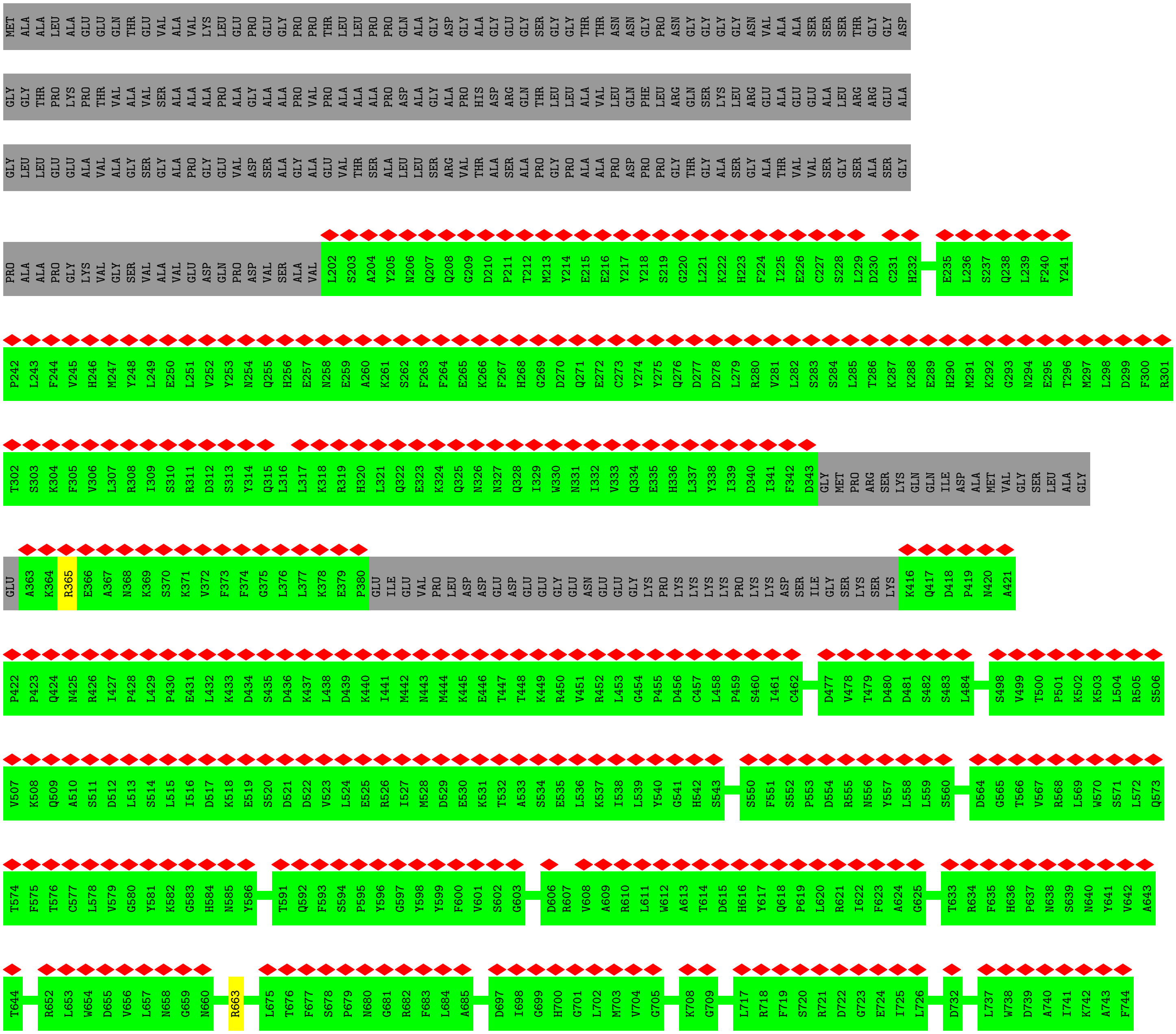
- Molecule 36: Transcription initiation factor TFIID subunit 5

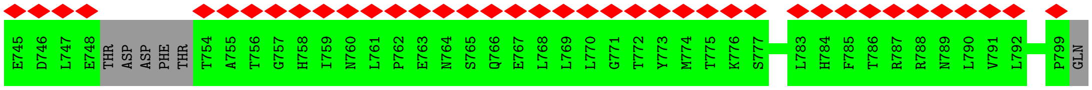




- Molecule 36: Transcription initiation factor TFIID subunit 5

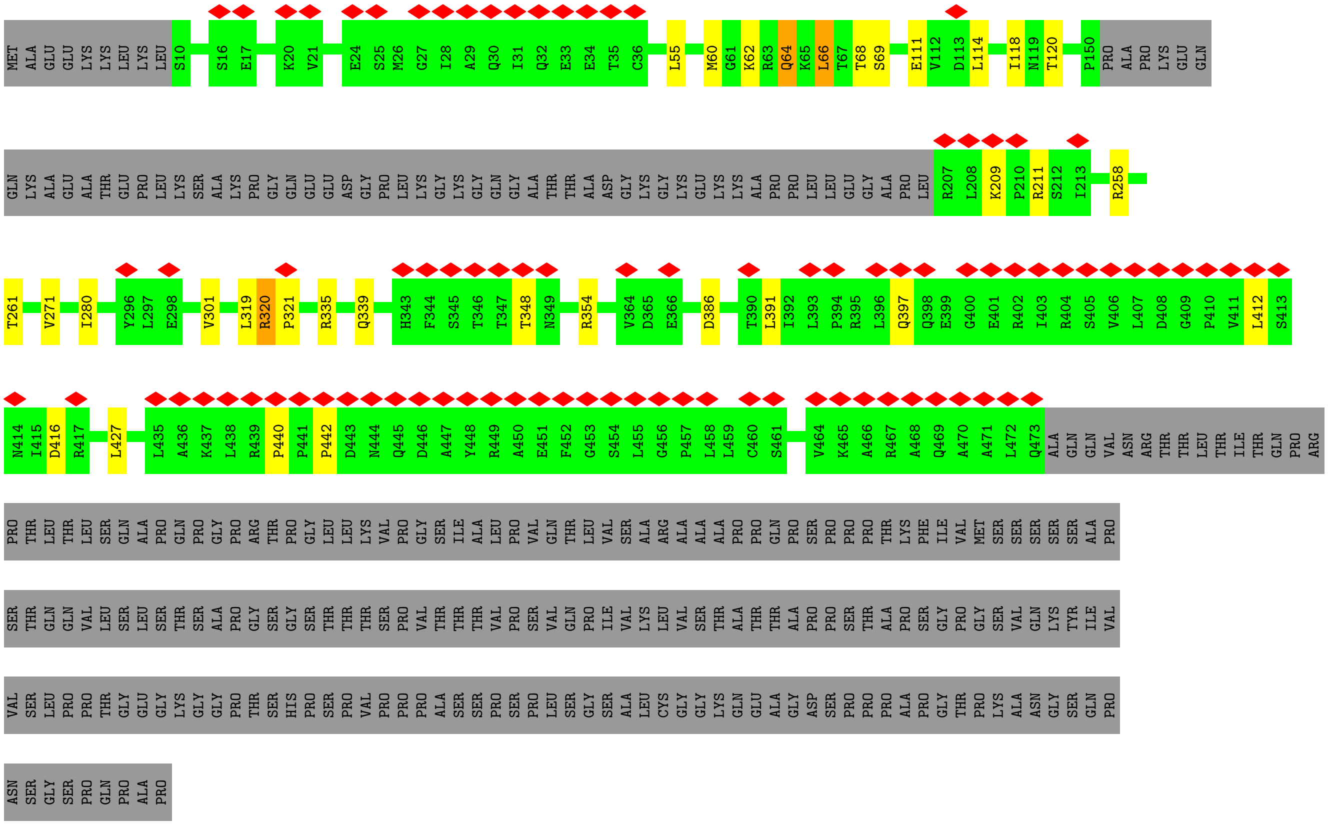
Chain De:





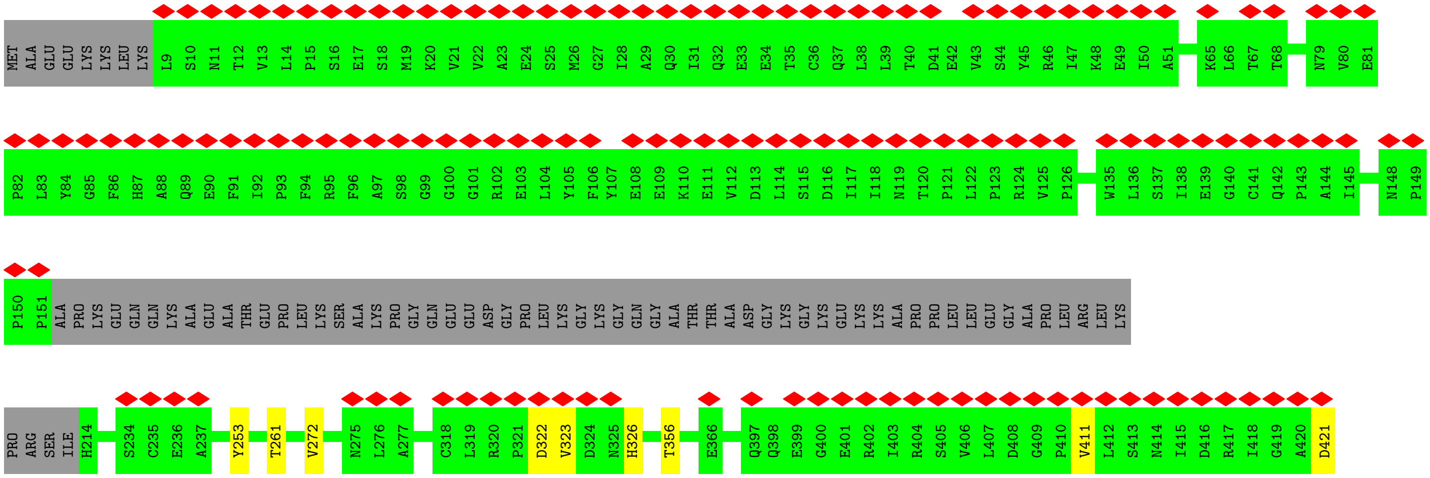
- Molecule 37: Transcription initiation factor TFIID subunit 6

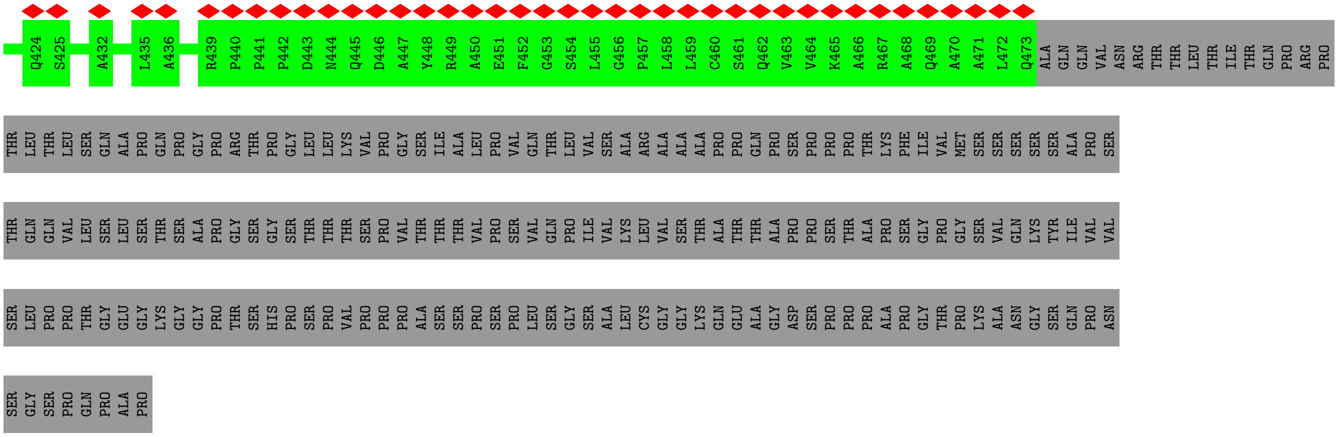
Chain DF:



- Molecule 37: Transcription initiation factor TFIID subunit 6

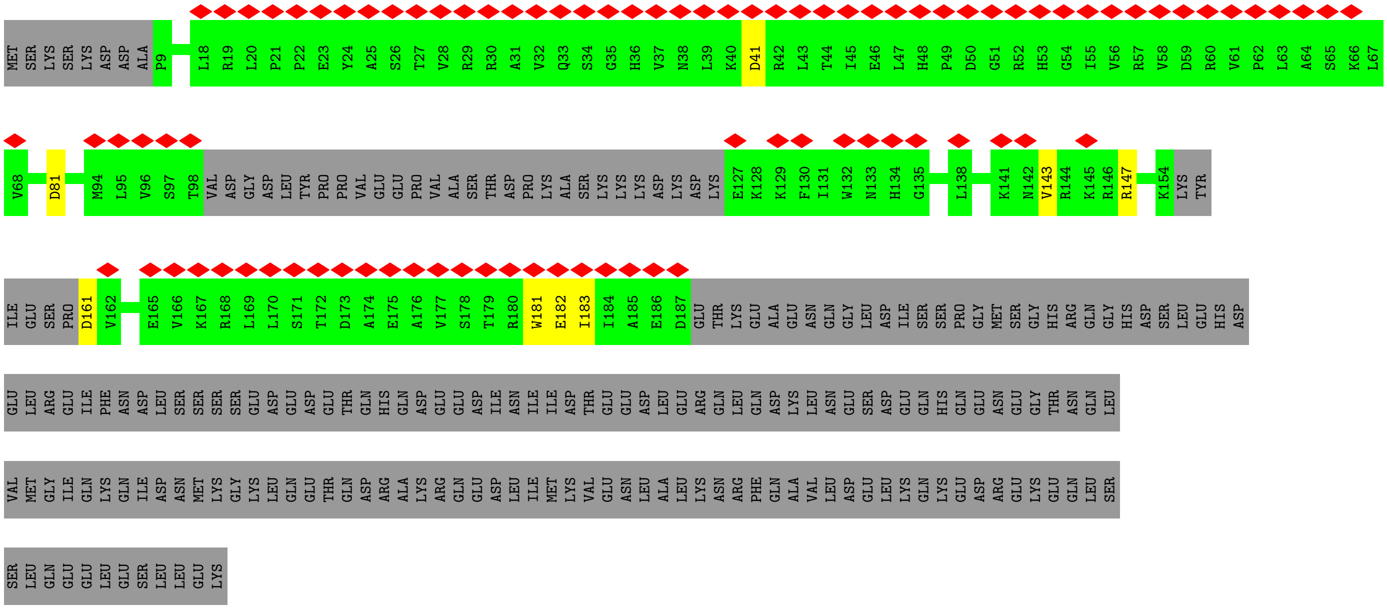
Chain Df:





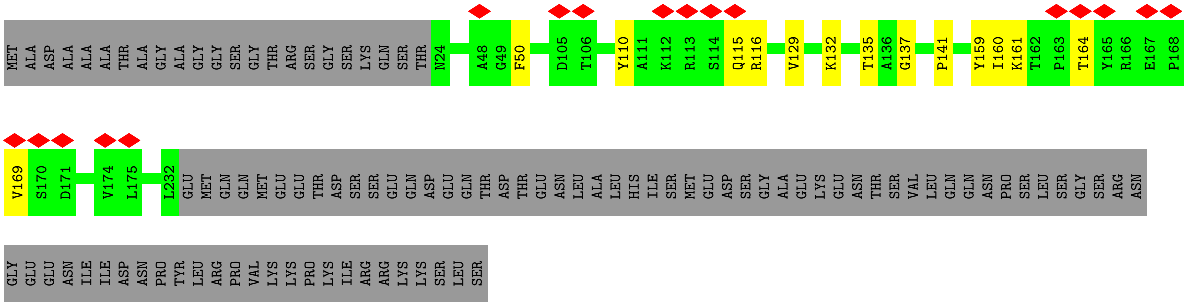
- Molecule 38: Transcription initiation factor TFIID subunit 7

Chain DG:

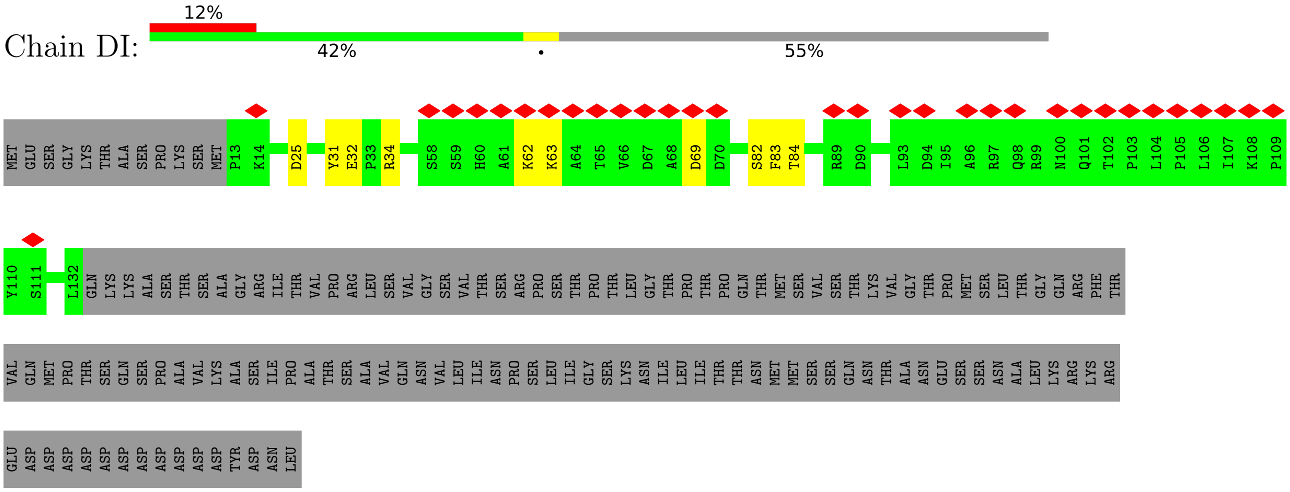


- Molecule 39: Transcription initiation factor TFIID subunit 8

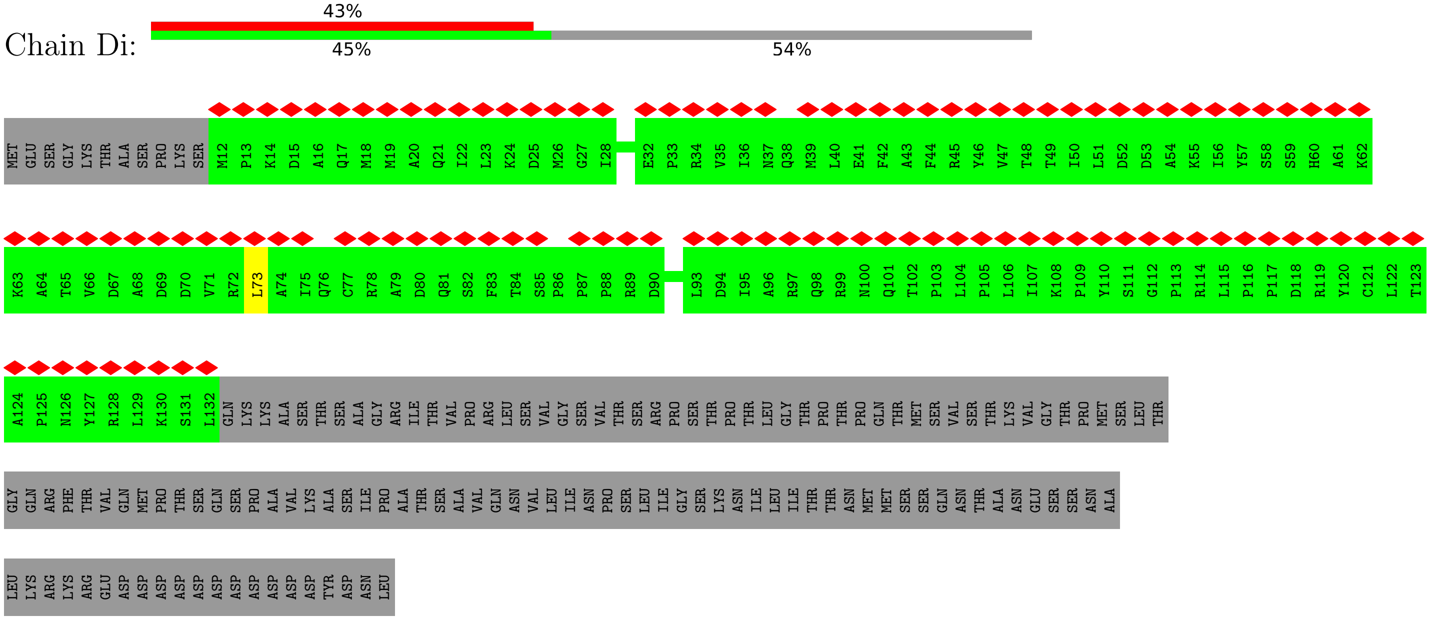
Chain DH:



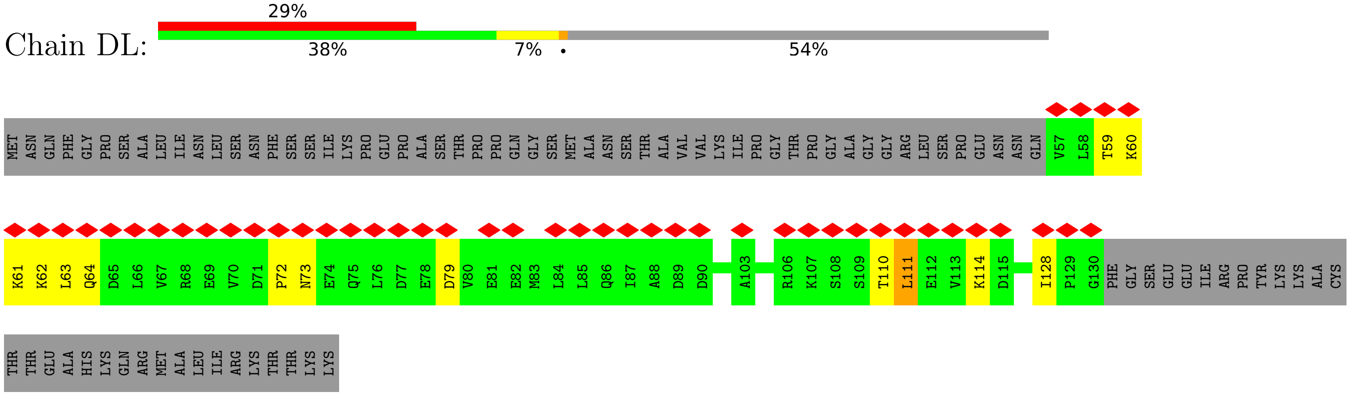
- Molecule 40: Transcription initiation factor TFIID subunit 9



- Molecule 40: Transcription initiation factor TFIID subunit 9

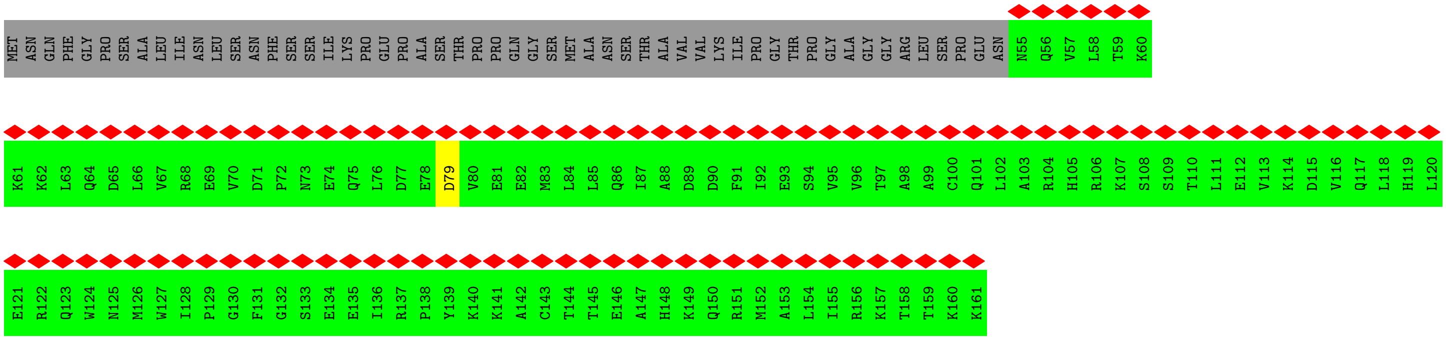


- Molecule 41: Transcription initiation factor TFIID subunit 12



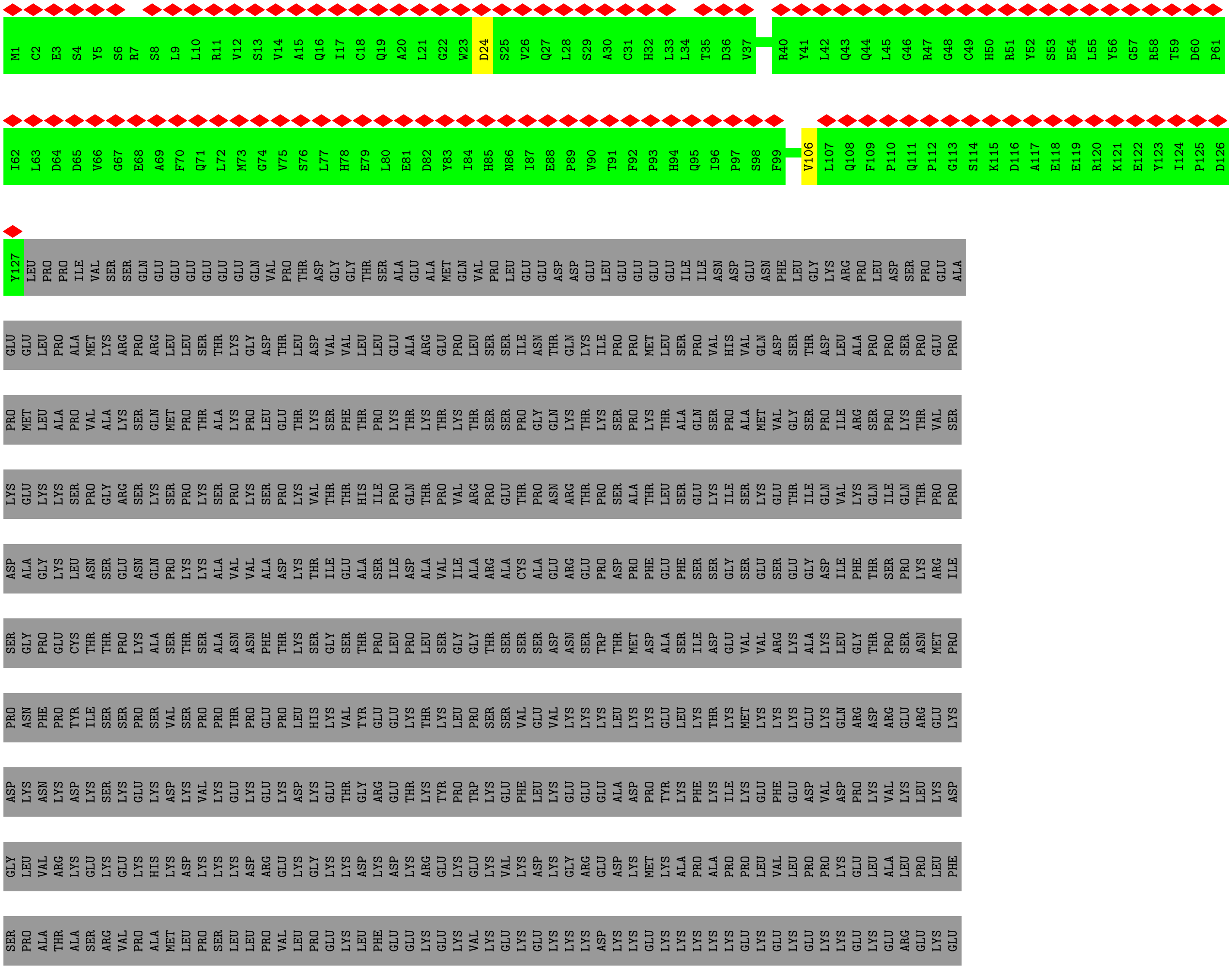
- Molecule 41: Transcription initiation factor TFIID subunit 12

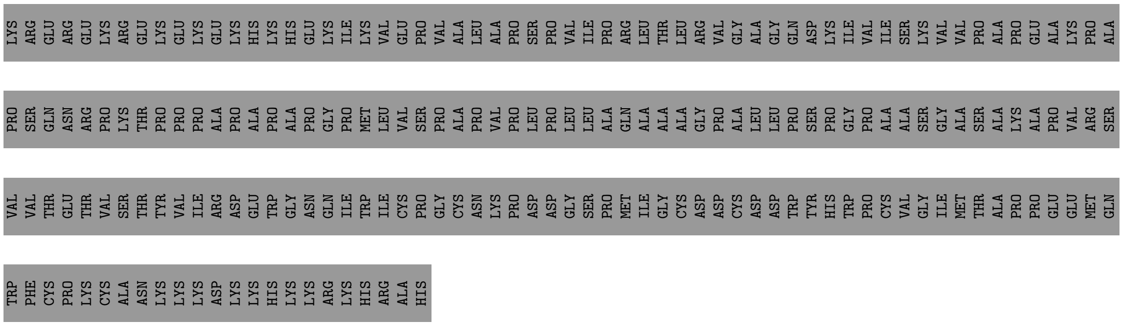
Chain Dl:



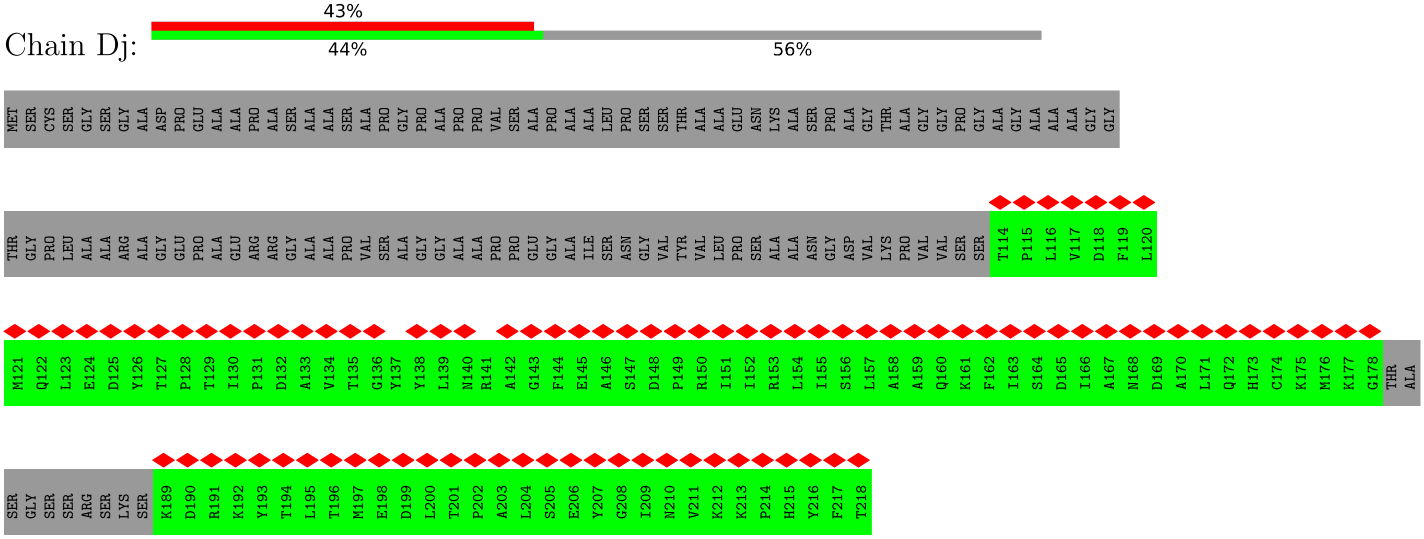
- Molecule 42: Transcription initiation factor TFIID subunit 3

Chain Dc:

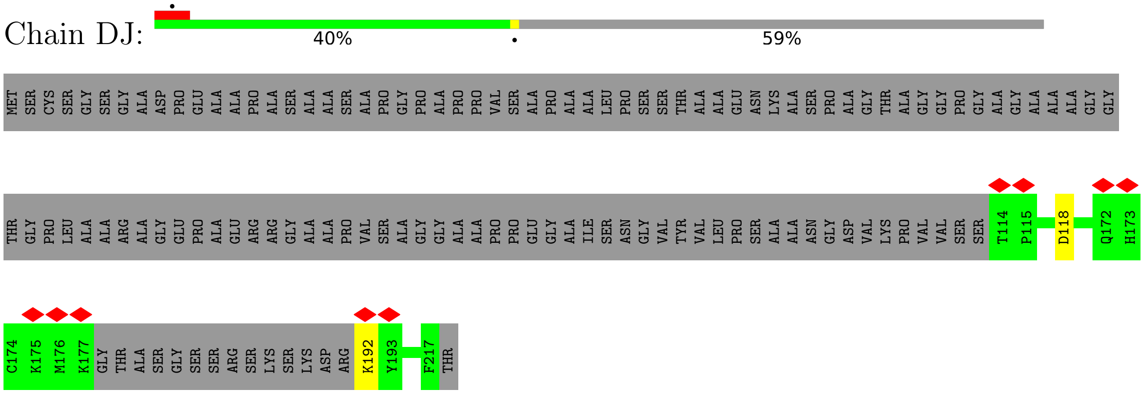




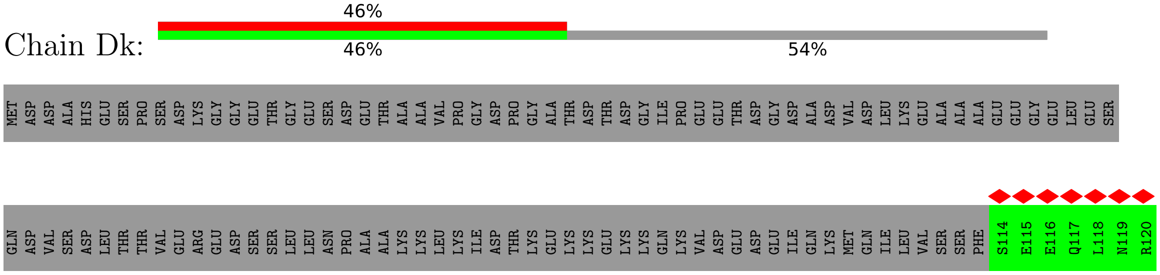
- Molecule 43: Transcription initiation factor TFIID subunit 10

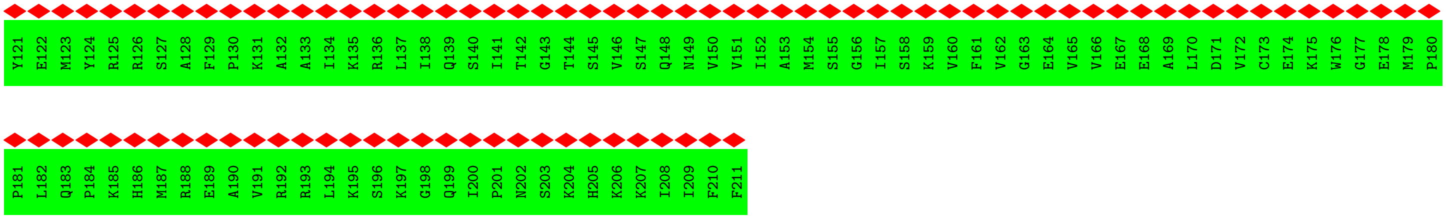


- Molecule 43: Transcription initiation factor TFIID subunit 10



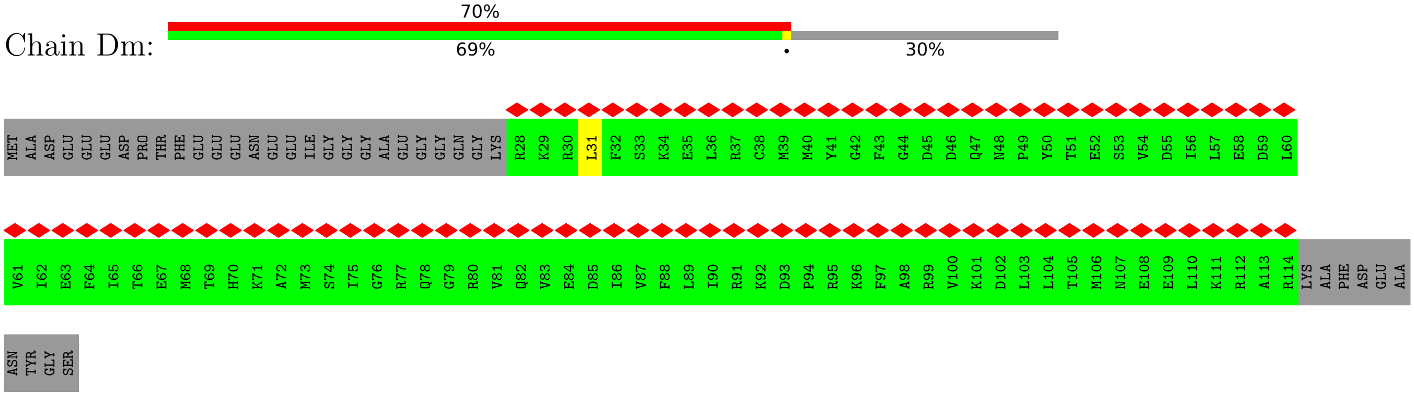
- Molecule 44: Transcription initiation factor TFIID subunit 11





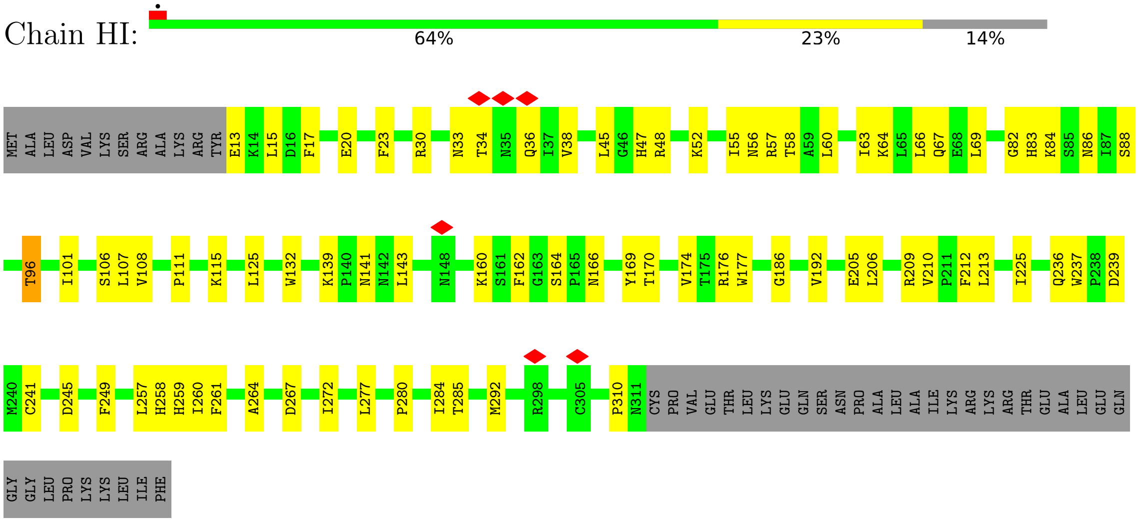
- Molecule 45: Transcription initiation factor TFIID subunit 13

Chain Dm:



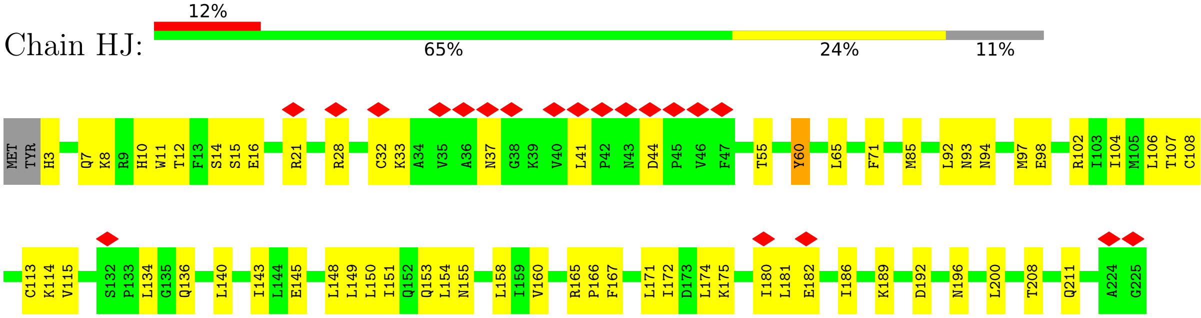
- Molecule 46: Cyclin-dependent kinase 7

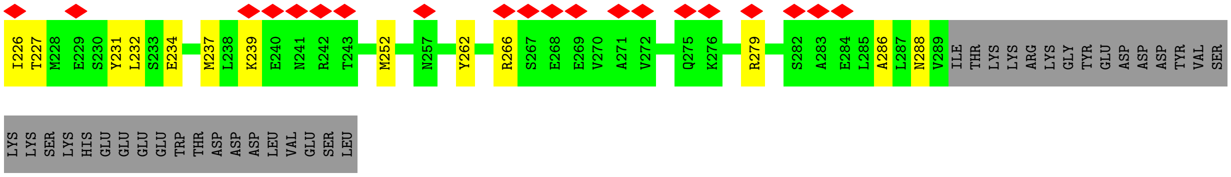
Chain HI:



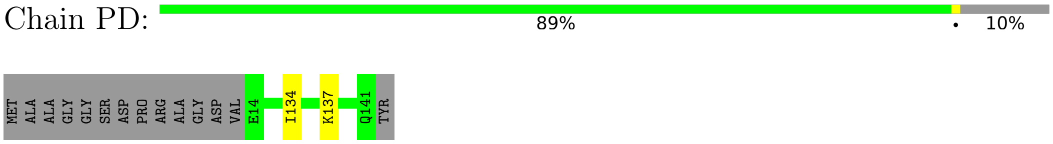
- Molecule 47: Cyclin-H

Chain HJ:

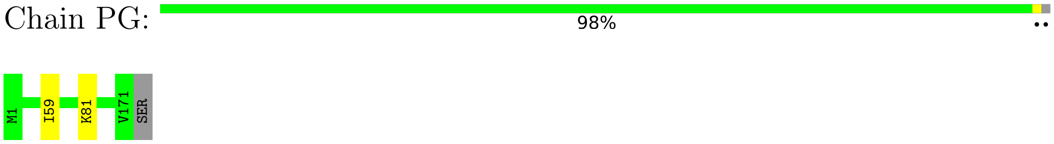




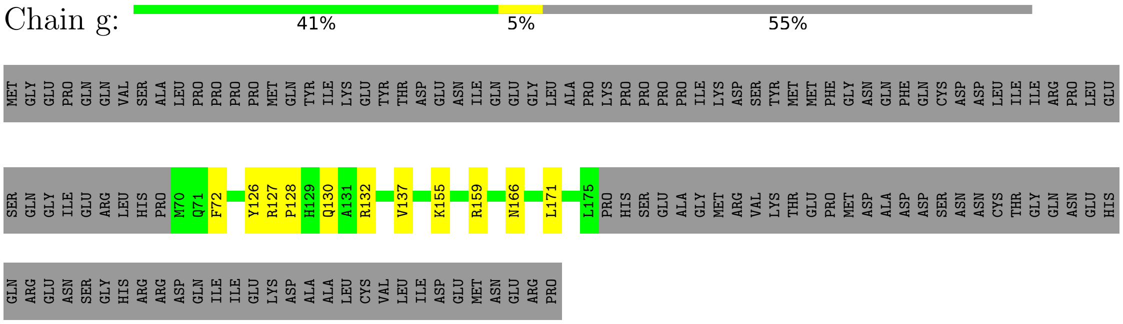
- Molecule 48: DNA-directed RNA polymerase II subunit RPB4



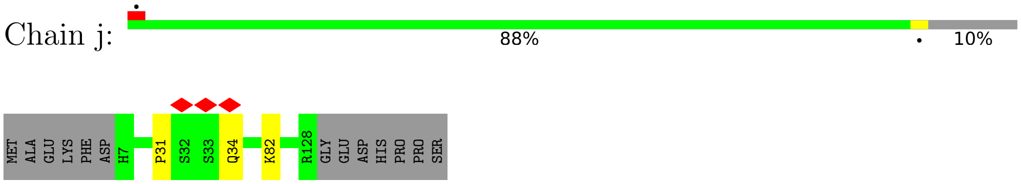
- Molecule 49: DNA-directed RNA polymerase II subunit RPB7



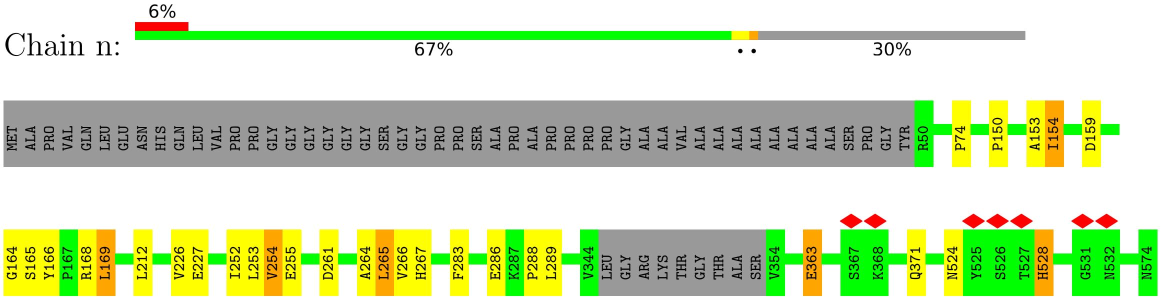
- Molecule 50: Mediator of RNA polymerase II transcription subunit 7

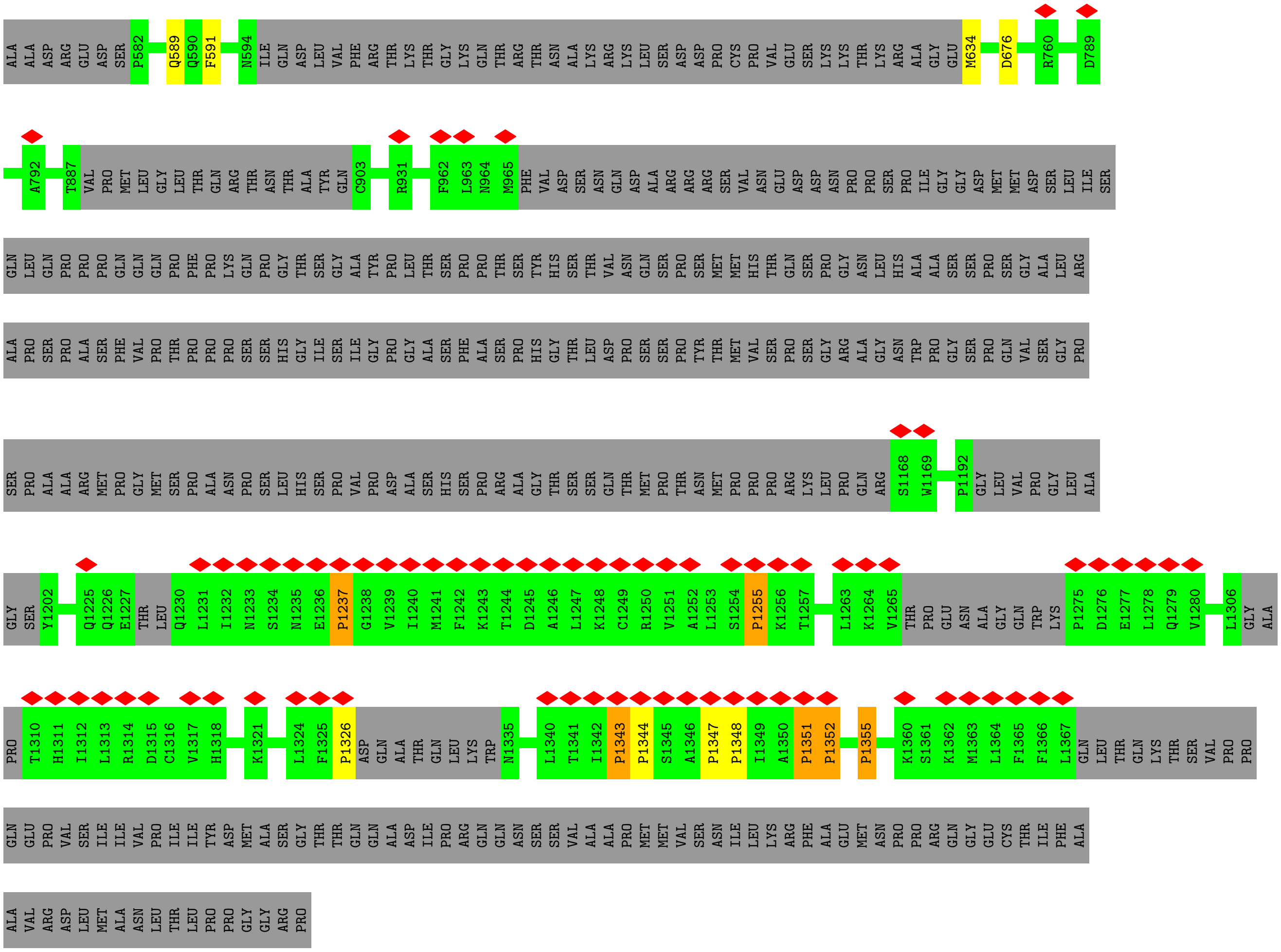


- Molecule 51: Mediator of RNA polymerase II transcription subunit 10

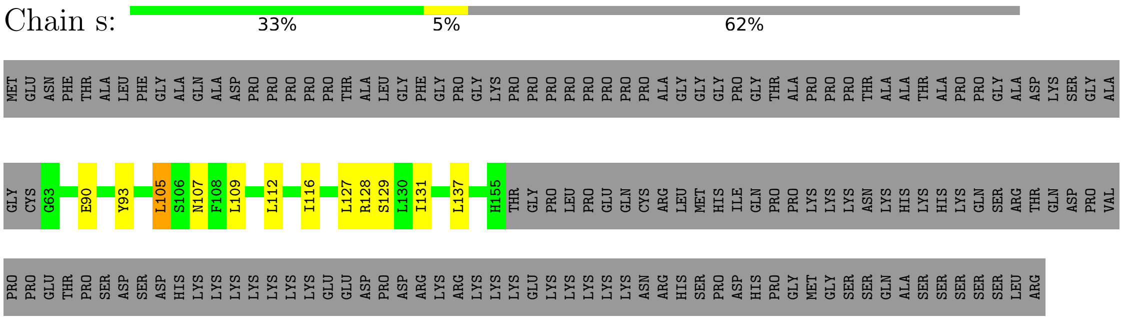


- Molecule 52: Mediator of RNA polymerase II transcription subunit 14

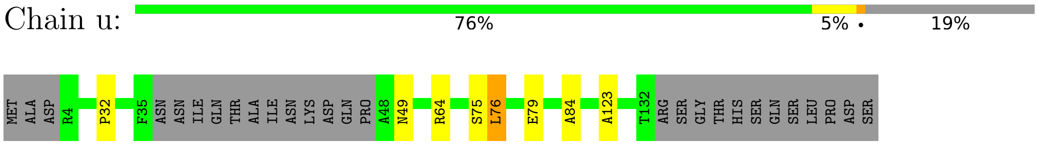




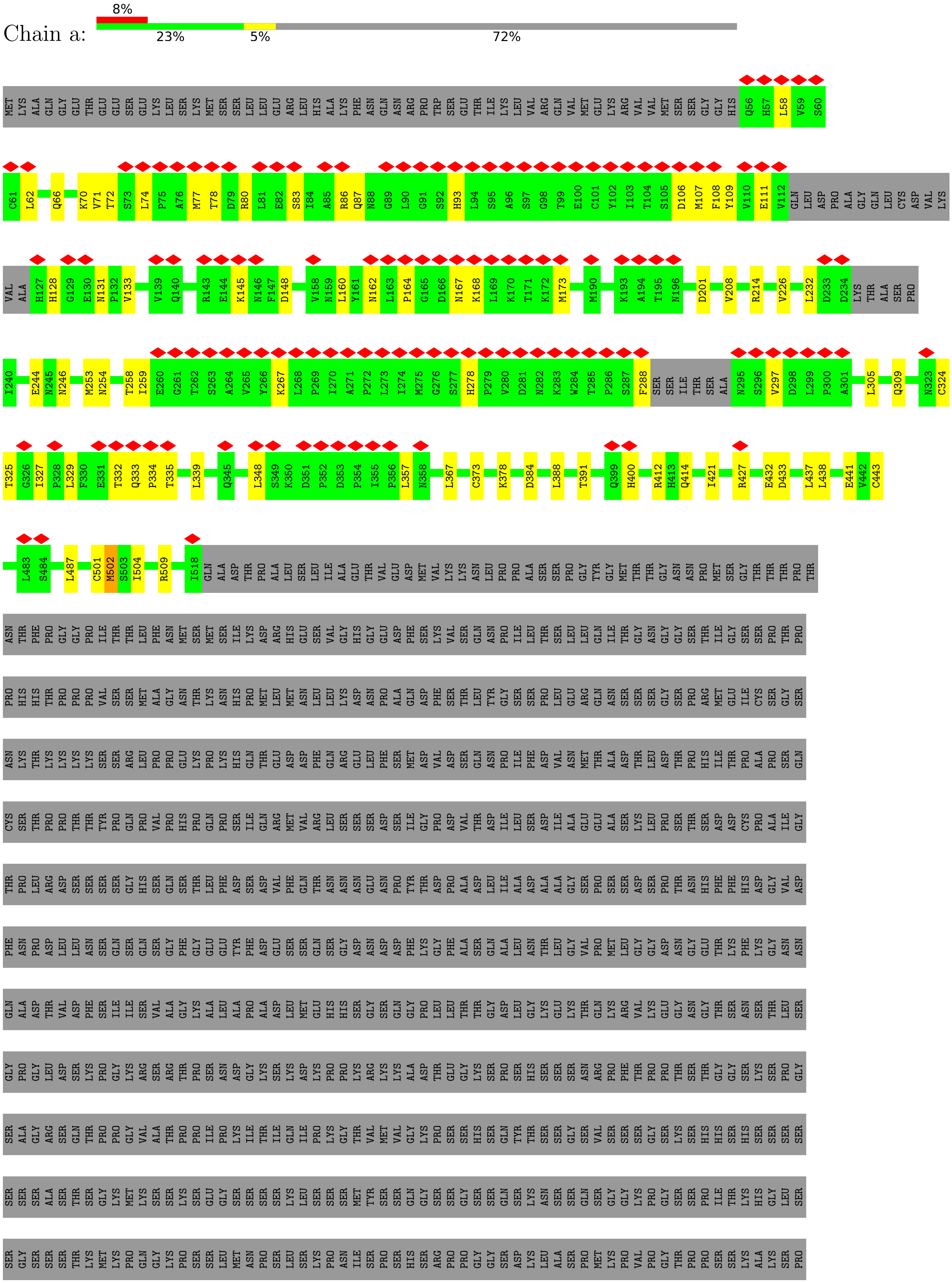
- Molecule 53: Mediator of RNA polymerase II transcription subunit 19



- Molecule 54: Mediator of RNA polymerase II transcription subunit 21



- Molecule 55: Mediator of RNA polymerase II transcription subunit 1


8%
Chain a:
23%
5%
72%
MET LYS ALA GLN GLY GLU THR GLU GLU SER GLU LYS LEU SER LYS MET SER SER LEU LEU GLU ARG LEU HIS ALA LYS PHE ASN GLN ASN ARG PRO TRP SER GLU THR ILE LYS LEU VAL ARG GLN VAL MET GLU LYS ARG VAL VAL MET SER SER GLY GLY HIS Q56 H57 L58 V59 S60
C61 L62 Q66 K70 V71 T72 S73 L74 P75 A76 M77 T78 D79 R80 L81 E82 S83 I84 A85 R86 Q87 N88 G89 L90 G91 S92 H93 L94 S95 A96 S97 G98 T99 E100 C101 Y102 I103 T104 S105 D106 M107 F108 Y109 V110 E111 V112 GLN LEU ASP PRO ALA GLY GLN LEU CYS ASP VAL LYS
VAL ALA H127 H128 G129 E130 N131 P132 V133 V139 Q140 R143 E144 K145 N146 F147 D148 V158 N159 L160 Y161 N162 L163 P164 G165 D166 N167 K168 L169 K170 T171 K172 M173 M190 K193 A194 T195 N196 D201 V208 R214 V226 L232 D233 D234 LYS THR ALA SER PRO
I240 E244 N245 N246 M253 N254 T258 I259 E260 G261 T262 S263 A264 V265 Y266 K267 L268 P269 I270 A271 P272 L273 I274 M275 G276 S277 H278 P279 V280 D281 N282 K283 W284 T285 P286 S287 F288 SER SER ILE THR SER ALA N295 S296 V297 D298 L299 P300 A301 L305 Q309 N323 C324
T325 G326 I327 P328 L329 F330 E331 T332 Q333 P334 T335 L339 Q345 L348 S349 K350 D351 P352 D353 P354 I355 P356 L357 N358 L367 C373 K378 D384 L388 T391 Q399 H400 R412 H413 Q414 I421 R427 E432 D433 L437 L438 E441 V442 C443
L483 S484 L487 C501 M502 S503 I504 R509 I518 GLN ALA ASP THR PRO ALA LEU SER LEU ILE ALA GLU THR VAL GLU ASP MET VAL LYS LYS ASN LEU PRO PRO ALA SER SER PRO GLY TYR GLY MET THR THR GLY ASN PRO MET SER GLY THR THR THR PRO THR
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GLN ALA ASP THR VAL ASP PHE SER ILE ILE SER VAL ALA GLY LYS ALA LEU ALA PRO ALA ASP LEU MET GLU HIS HIS SER GLY SER GLN GLY PRO LEU LEU THR THR GLY ASP LEU GLY LYS GLU LYS THR GLN LYS ARG VAL LYS GLU GLY ASN GLY THR SER ASN SER THR LEU SER
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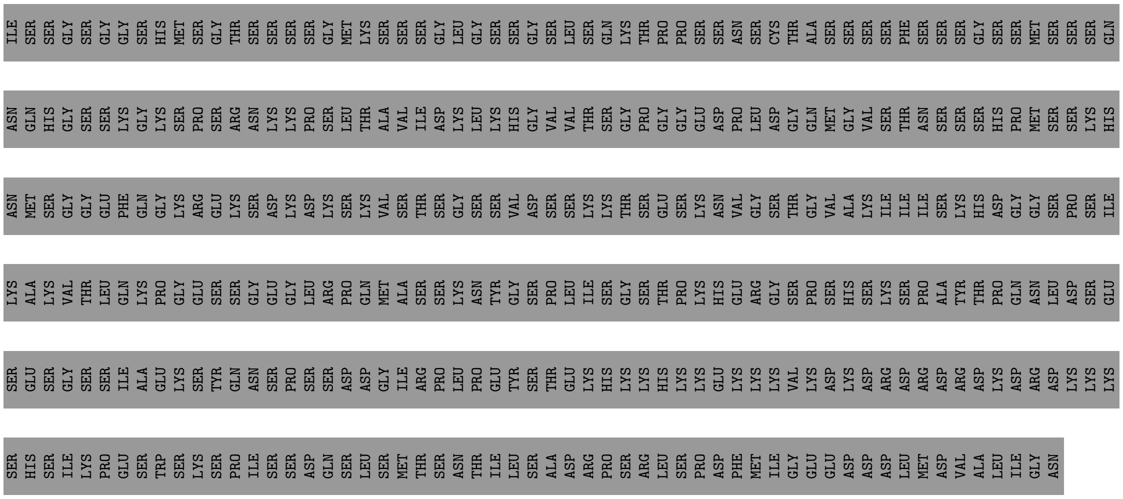
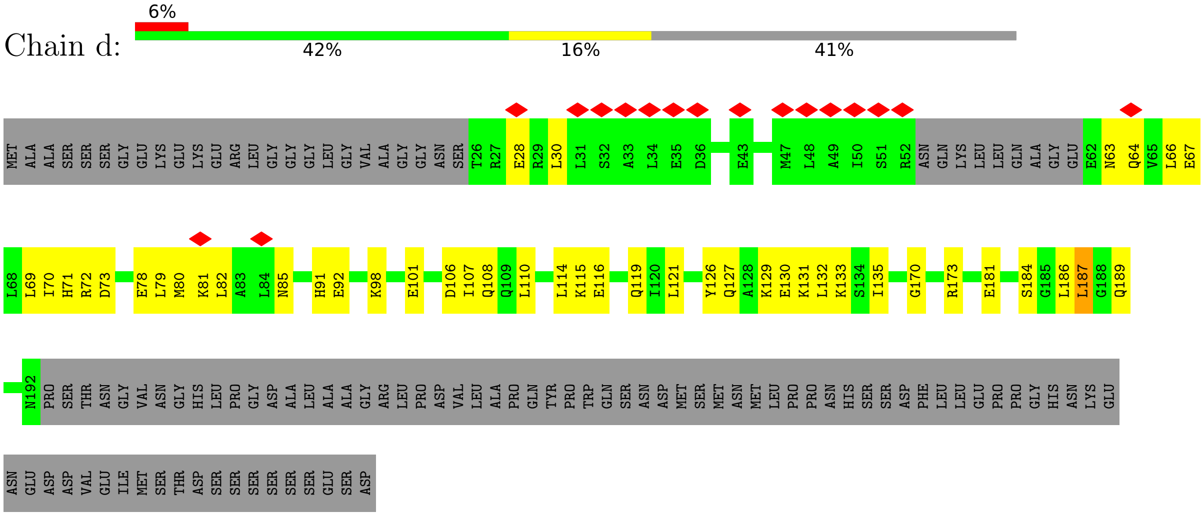
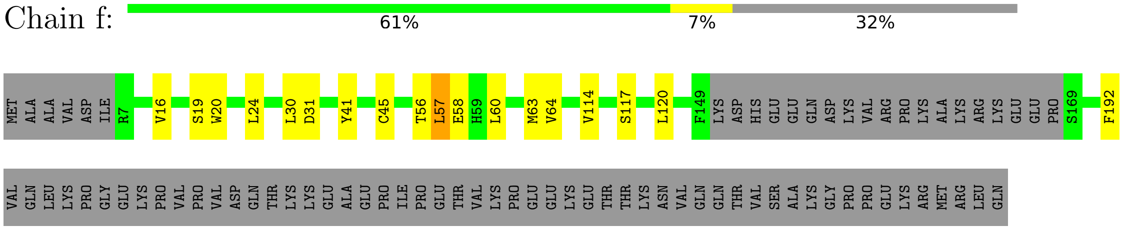


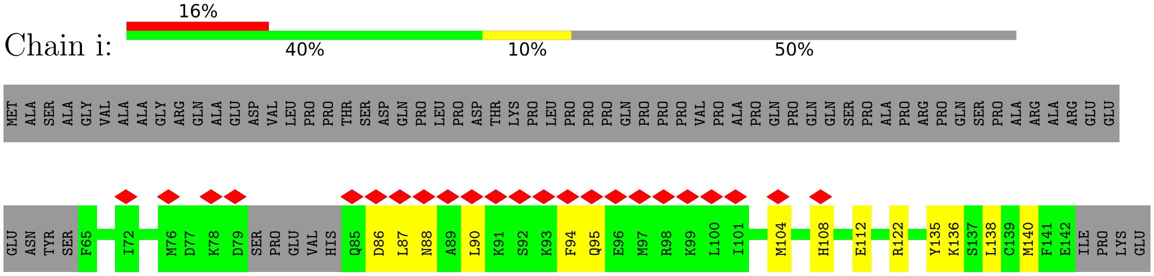
- Molecule 56: Mediator of RNA polymerase II transcription subunit 4



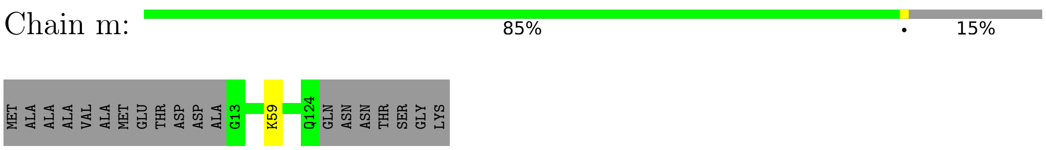
- Molecule 57: Mediator of RNA polymerase II transcription subunit 6



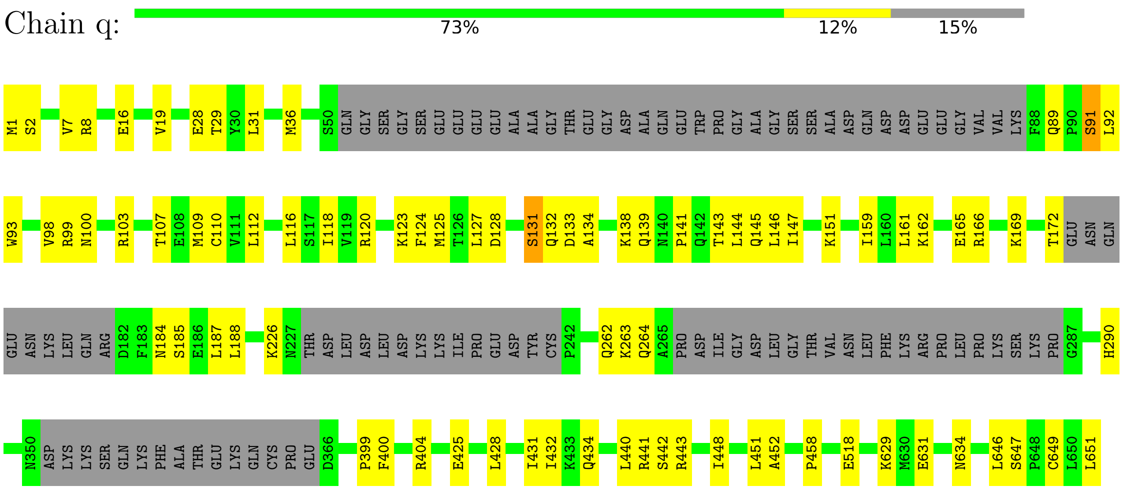
- Molecule 58: Mediator of RNA polymerase II transcription subunit 9



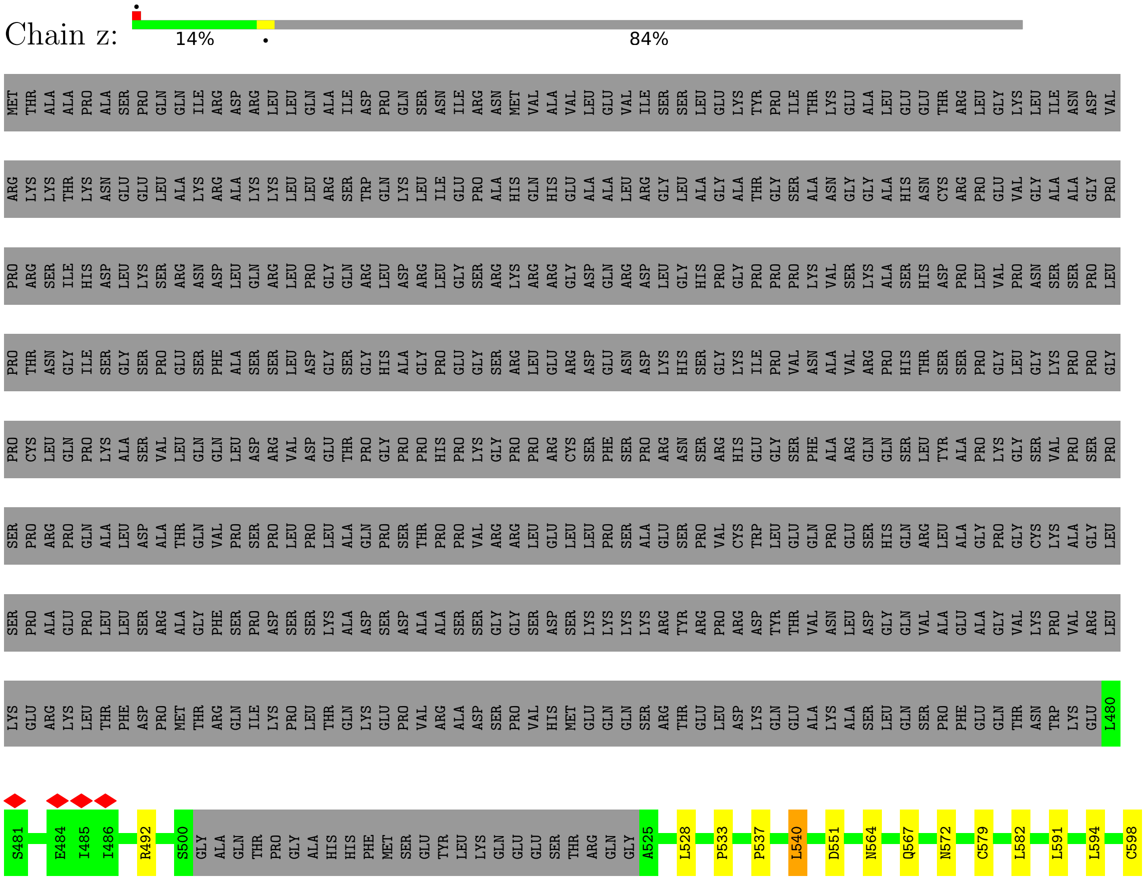
- Molecule 59: Mediator of RNA polymerase II transcription subunit 31



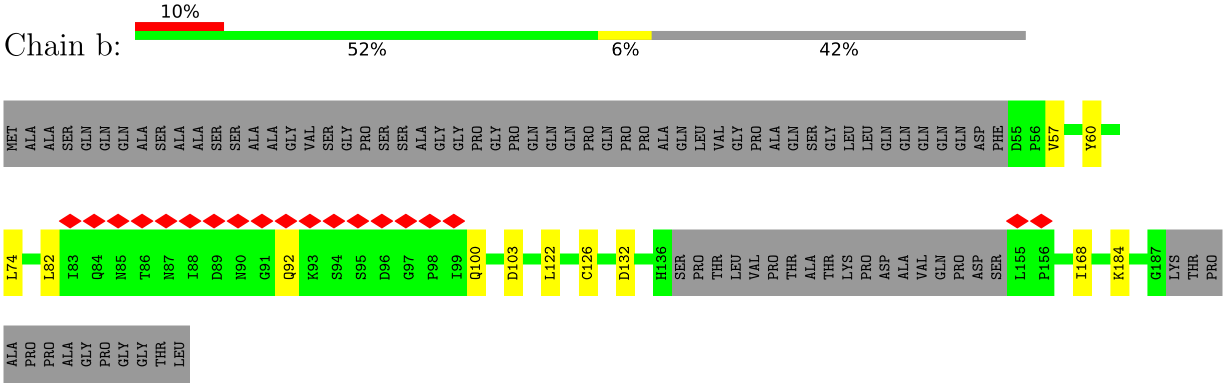
- Molecule 60: Mediator of RNA polymerase II transcription subunit 17



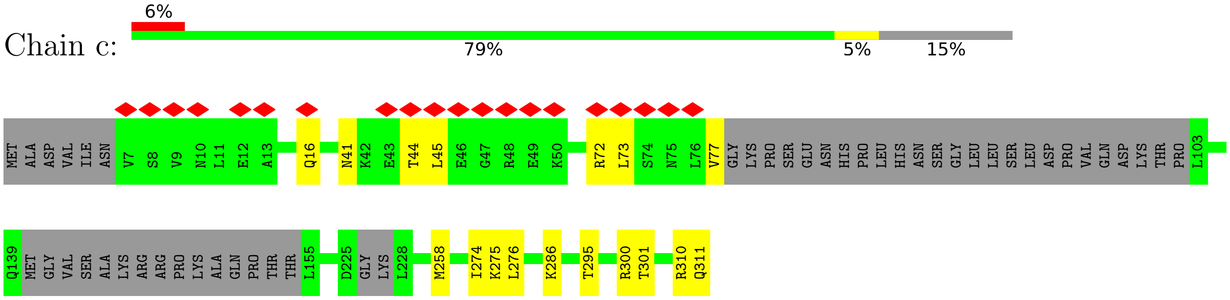
- Molecule 61: Mediator of RNA polymerase II transcription subunit 26



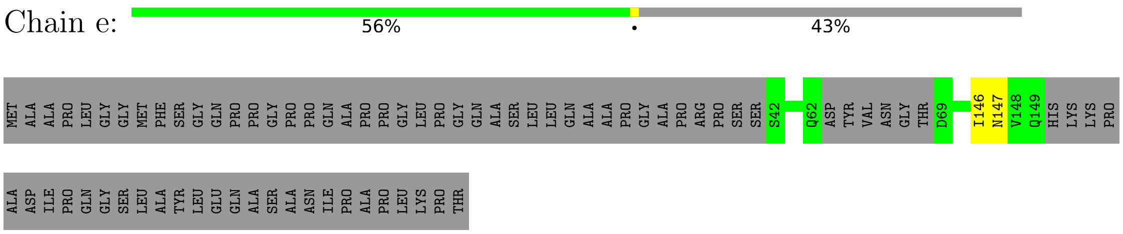
- Molecule 62: Mediator of RNA polymerase II transcription subunit 29



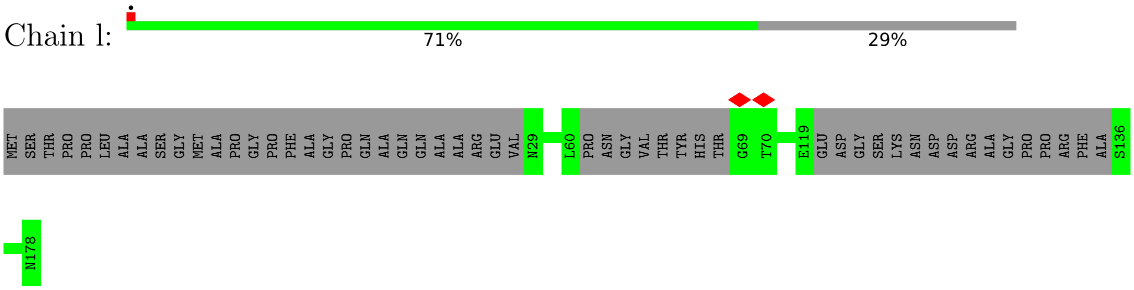
- Molecule 63: Mediator of RNA polymerase II transcription subunit 27



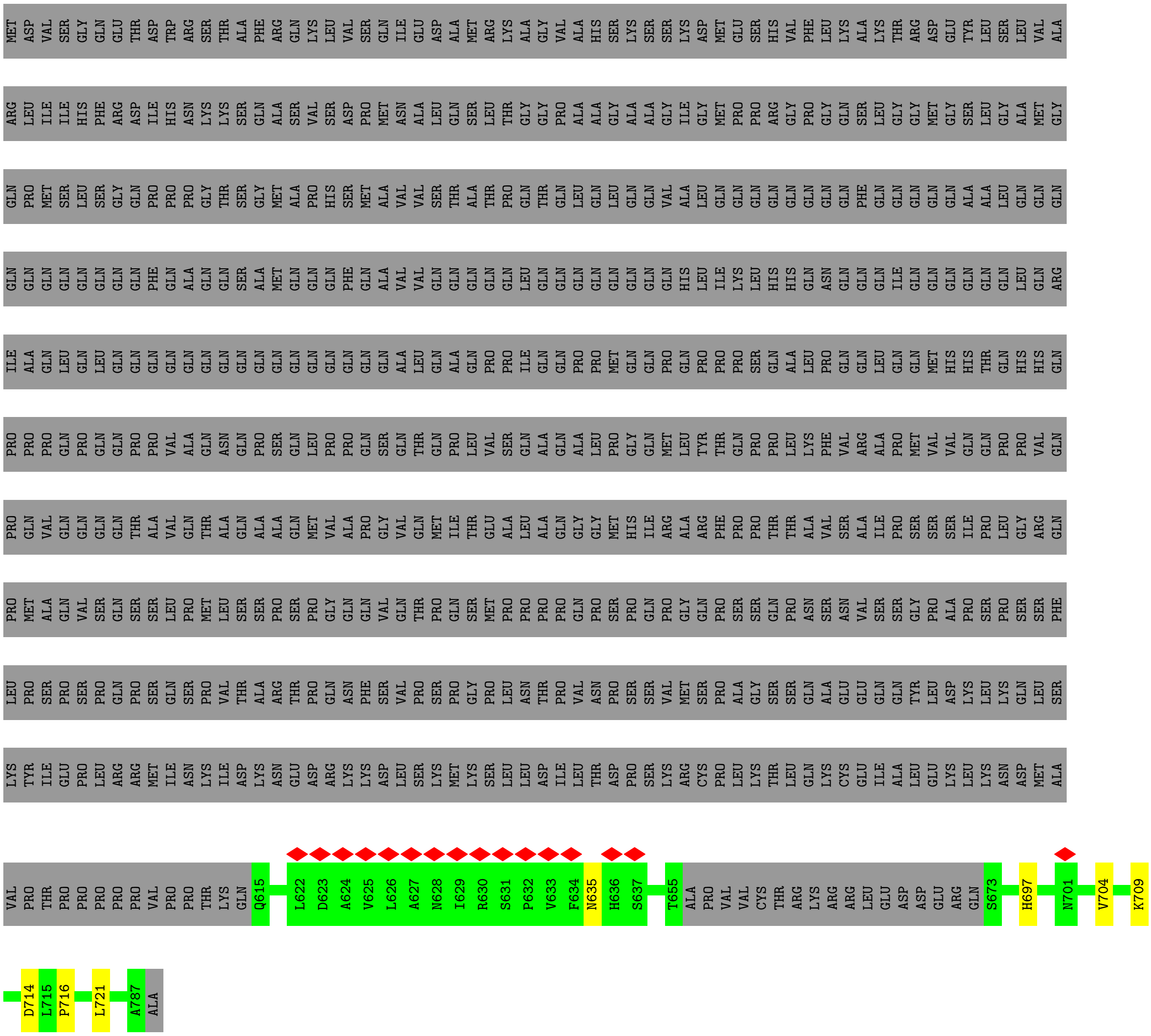
- Molecule 64: Mediator of RNA polymerase II transcription subunit 28



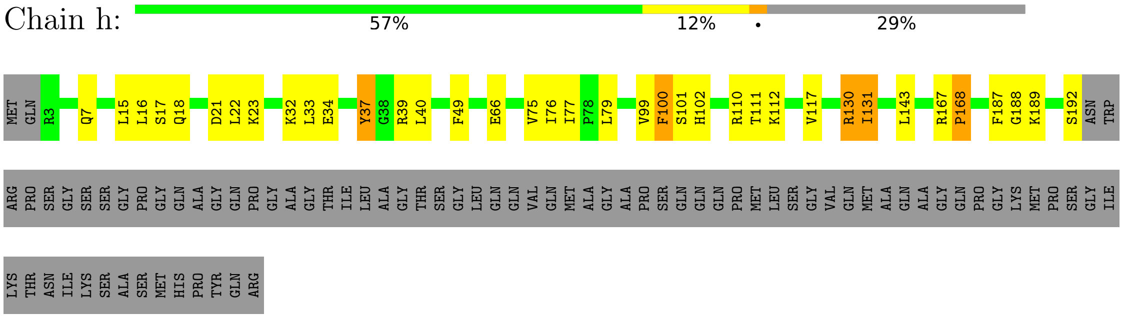
- Molecule 65: Mediator of RNA polymerase II transcription subunit 30



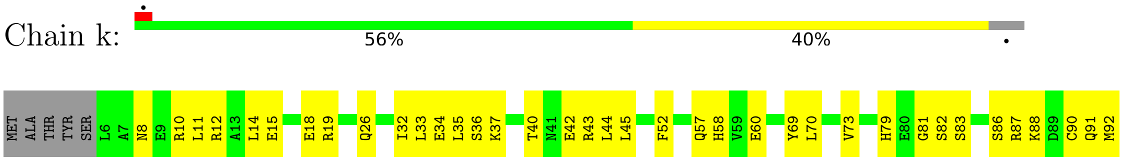
- Molecule 66: Mediator of RNA polymerase II transcription subunit 15

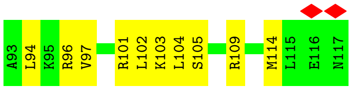


- Molecule 67: Isoform 2 of Mediator of RNA polymerase II transcription subunit 8



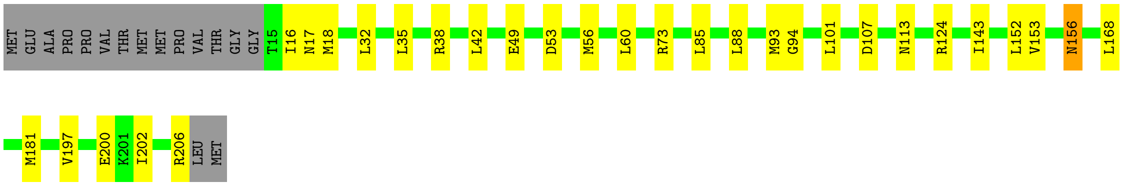
- Molecule 68: Mediator of RNA polymerase II transcription subunit 11





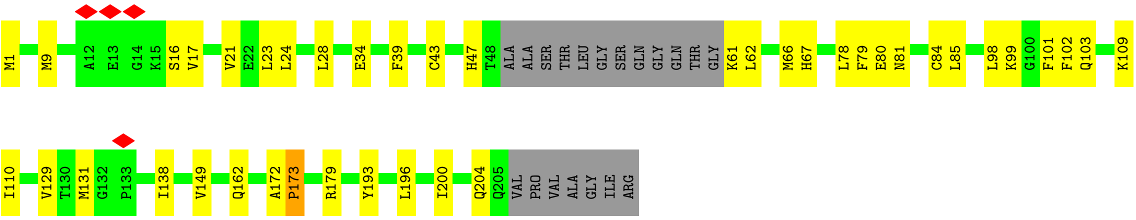
- Molecule 69: Mediator of RNA polymerase II transcription subunit 18

Chain r:



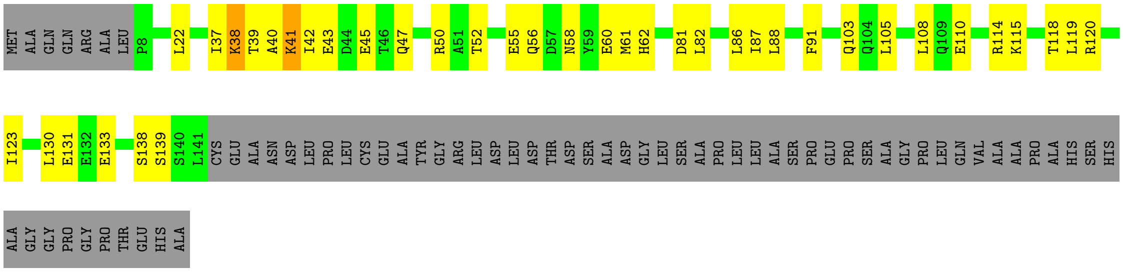
- Molecule 70: Mediator of RNA polymerase II transcription subunit 20

Chain t:



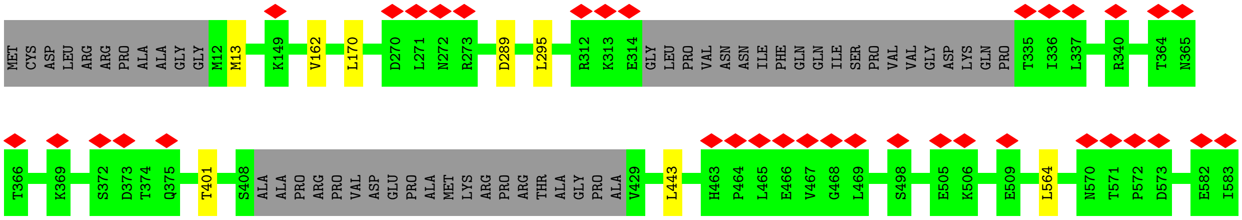
- Molecule 71: Mediator of RNA polymerase II transcription subunit 22

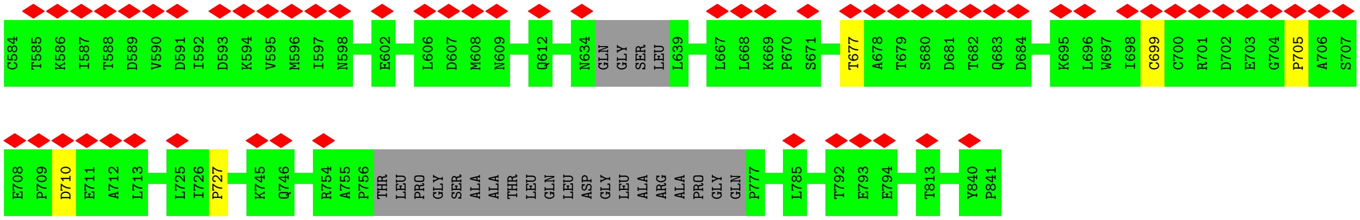
Chain v:



- Molecule 72: Isoform 2 of Mediator of RNA polymerase II transcription subunit 16

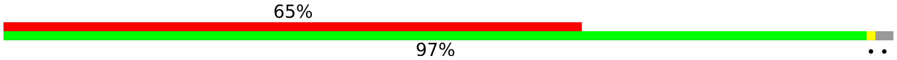
Chain p:

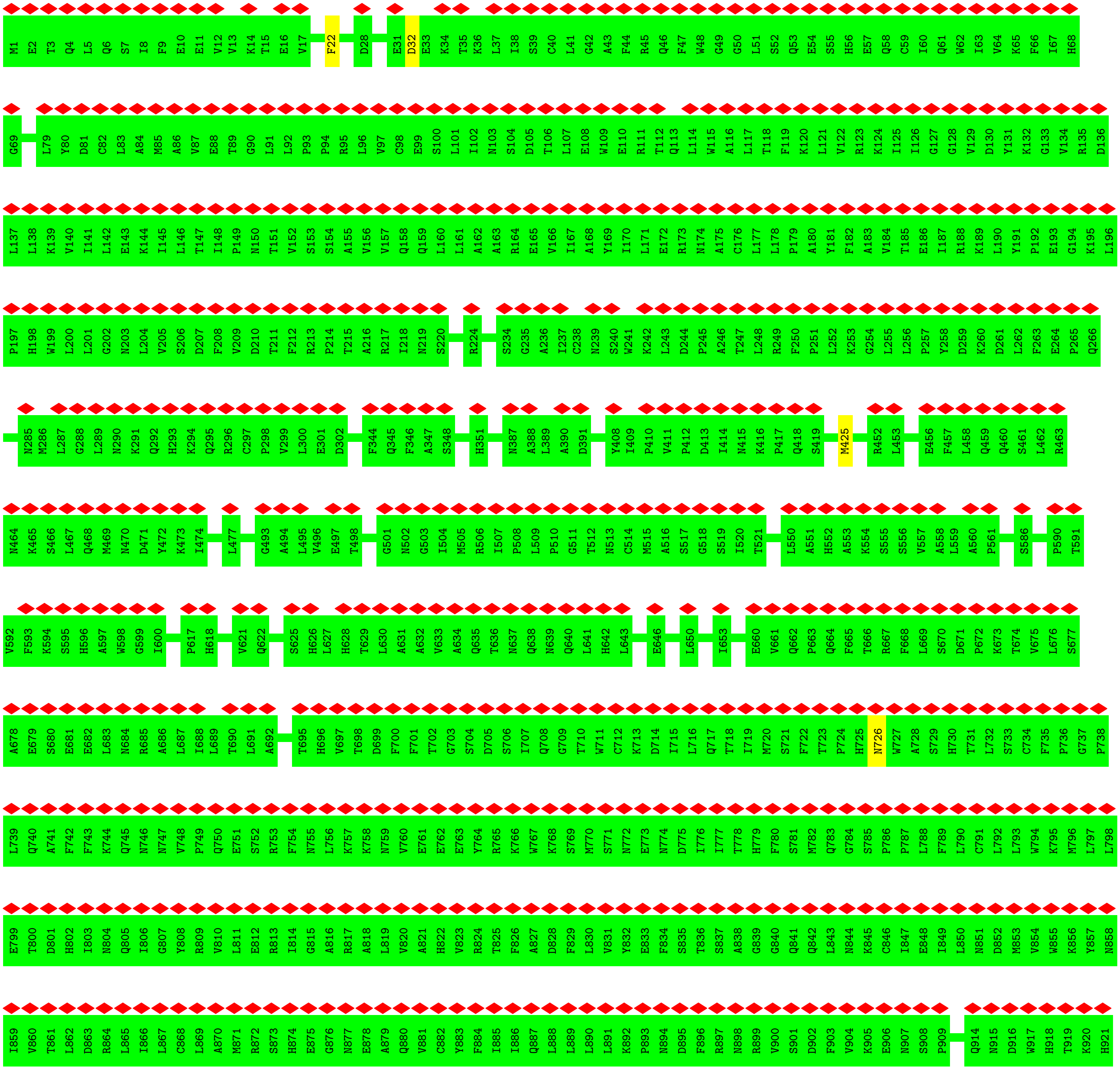


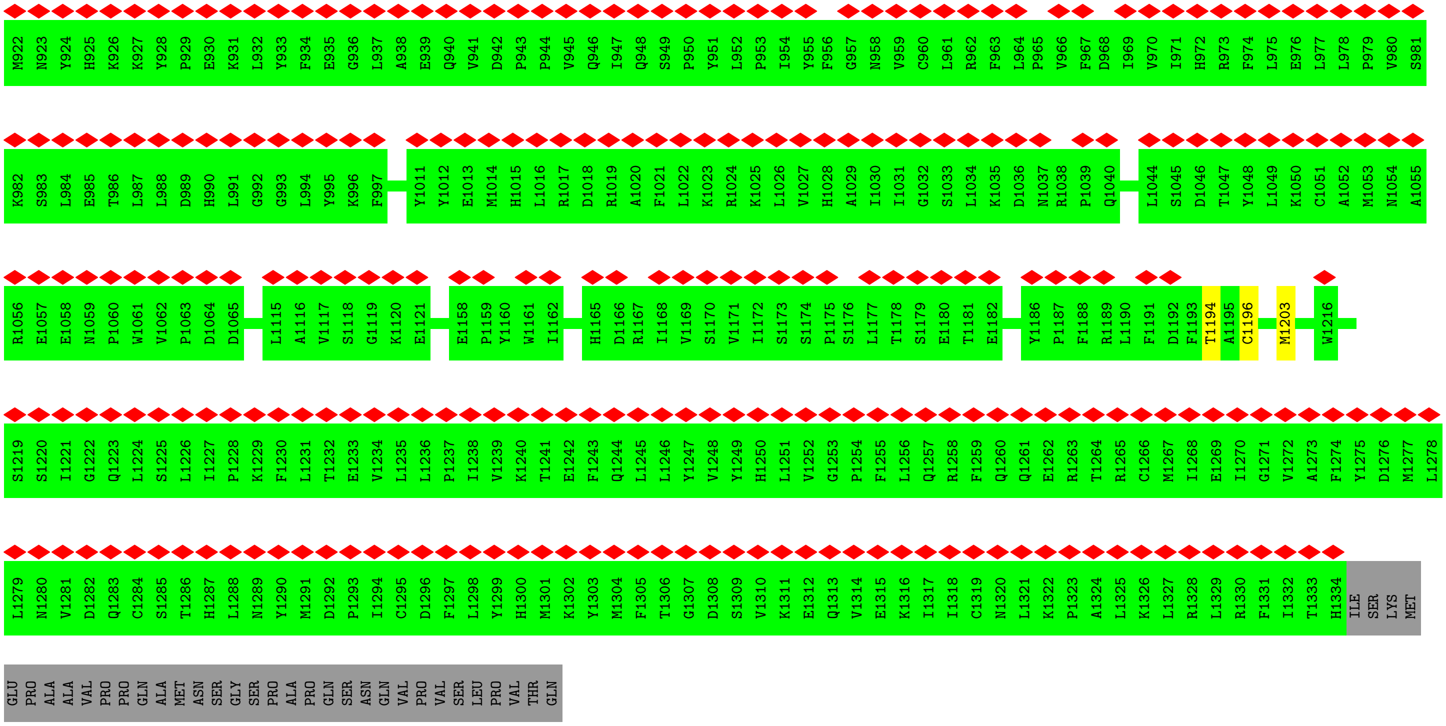


- Molecule 73: Mediator of RNA polymerase II transcription subunit 23

Chain w:

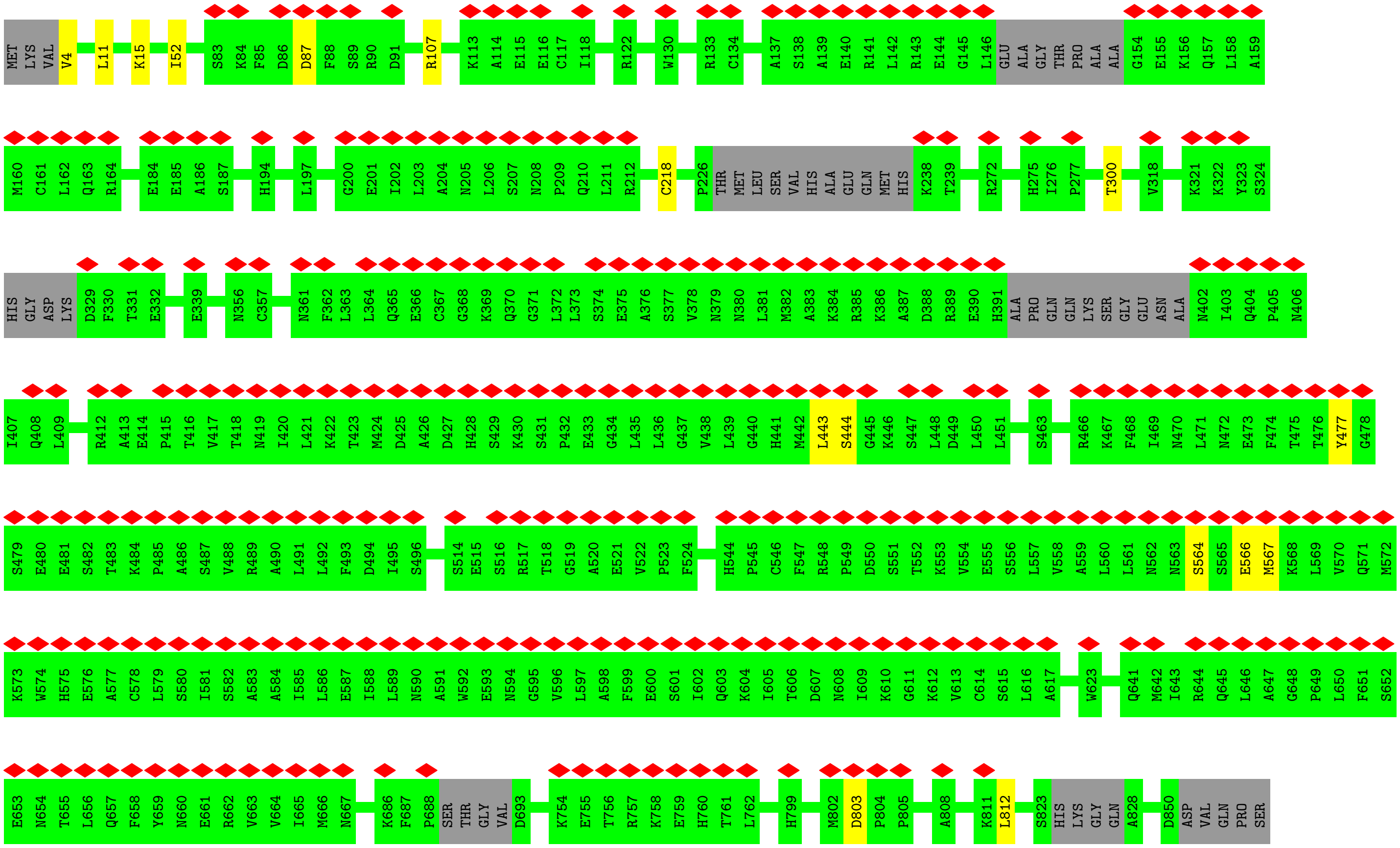


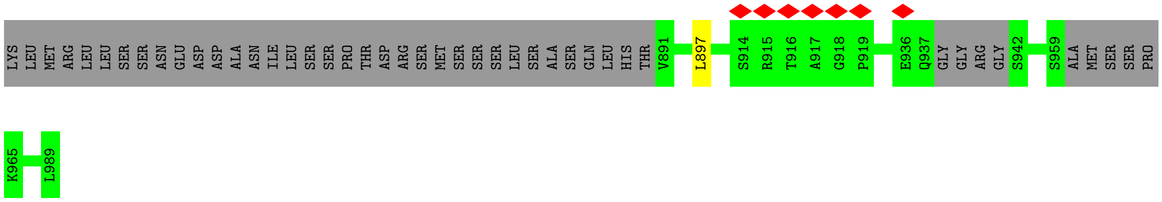




- Molecule 74: Mediator of RNA polymerase II transcription subunit 24

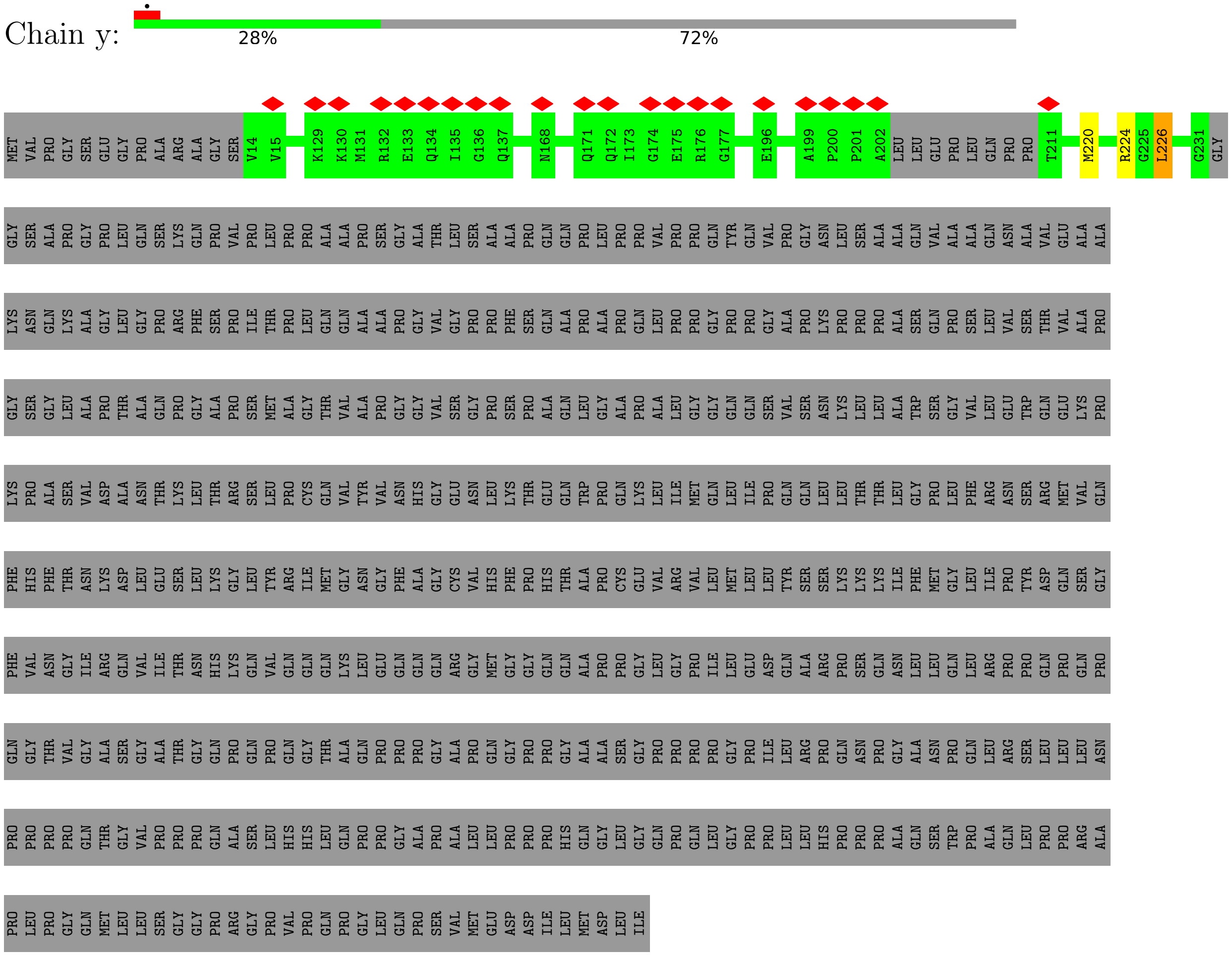
Chain x:





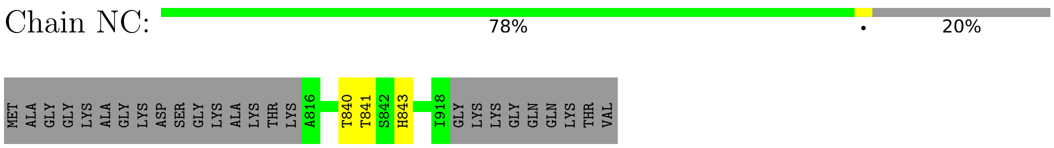
- Molecule 75: Mediator of RNA polymerase II transcription subunit 25

Chain y:



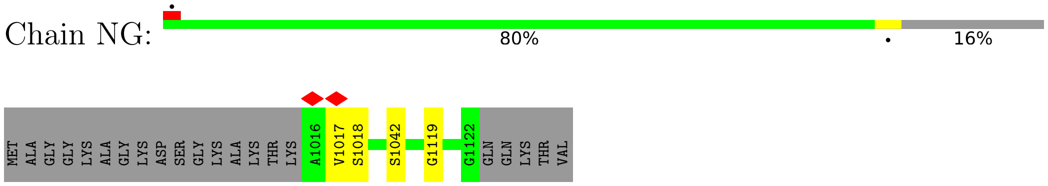
- Molecule 76: HISTONE H2A.Z

Chain NC:

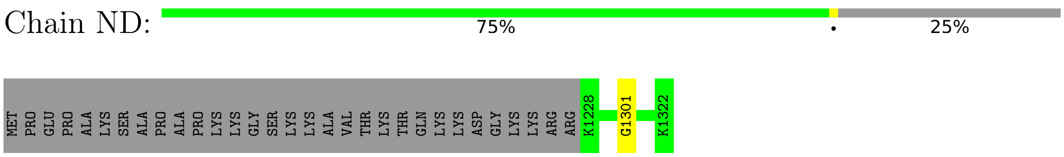


- Molecule 76: HISTONE H2A.Z

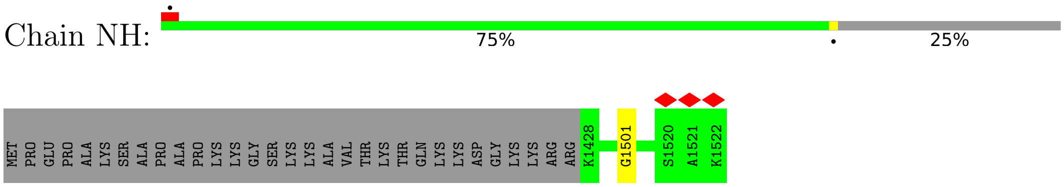
Chain NG:



- Molecule 77: Histone H2B



- Molecule 77: Histone H2B



4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	29473	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	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.762	Depositor
Minimum map value	-1.277	Depositor
Average map value	0.015	Depositor
Map value standard deviation	0.075	Depositor
Recommended contour level	0.205	Depositor
Map size (Å)	560.27997, 560.27997, 560.27997	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3339999, 1.3339999, 1.3339999	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: MG, ZN, SF4

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	X	0.63	5/1561 (0.3%)	0.83	1/2411 (0.0%)
2	Y	0.67	1/1516 (0.1%)	0.92	0/2334
3	NX	0.34	1/3401 (0.0%)	0.82	0/5180
4	NY	0.38	0/4046	0.76	0/6310
5	BA	0.25	0/1983	0.41	0/2679
6	DA	0.51	0/4679	0.62	1/6320 (0.0%)
7	EA	0.34	0/1560	0.51	0/2097
8	FA	0.25	0/1167	0.41	0/1576
9	HA	0.26	0/5875	0.41	0/7955
10	NA	0.68	0/497	0.82	1/693 (0.1%)
10	NE	0.76	0/510	0.88	0/710
11	PA	0.28	0/11851	0.44	0/16014
12	DB	0.47	1/7993 (0.0%)	0.61	0/10836
13	EB	0.28	0/1427	0.46	0/1916
14	FB	0.26	0/1817	0.41	0/2445
15	HB	0.25	0/2210	0.40	0/2975
16	NB	0.76	0/390	0.84	0/539
16	NF	0.85	0/420	0.97	1/581 (0.2%)
17	PB	0.25	0/9257	0.42	0/12493
18	HC	0.28	0/3230	0.43	0/4376
19	DO	0.25	0/816	0.43	0/1105
20	DP	0.25	0/1448	0.42	0/1948
21	DQ	0.25	0/945	0.42	0/1274
22	PC	0.24	0/2102	0.42	0/2857
23	PE	0.25	0/1752	0.41	0/2366
24	PF	0.28	0/646	0.42	0/871
25	PH	0.24	0/1207	0.43	0/1628
26	PI	0.25	0/949	0.44	0/1284
27	PJ	0.26	0/516	0.41	0/696
28	PK	0.26	0/939	0.40	0/1271
29	PL	0.26	0/378	0.41	0/500
30	HD	0.50	0/2436	0.67	2/3286 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
31	HG	0.25	0/2793	0.42	0/3780
32	HE	0.31	0/2103	0.46	0/2846
33	HF	0.27	0/529	0.49	1/714 (0.1%)
34	HH	0.25	0/4994	0.41	0/6745
35	DD	0.42	0/1343	0.52	0/1795
35	Dd	0.29	0/1321	0.49	0/1772
36	DE	0.39	0/4469	0.56	0/6050
36	De	0.33	0/4433	0.55	0/6004
37	DF	0.51	0/3167	0.69	1/4303 (0.0%)
37	Df	0.42	0/3140	0.63	0/4268
38	DG	0.52	0/1199	0.63	0/1612
39	DH	0.37	0/1673	0.58	1/2285 (0.0%)
40	DI	0.43	0/981	0.58	0/1332
40	Di	0.31	0/989	0.48	0/1343
41	DL	0.44	0/613	0.65	1/829 (0.1%)
41	Dl	0.41	0/888	0.54	1/1194 (0.1%)
42	Dc	0.40	0/1035	0.54	0/1406
43	DJ	0.30	0/736	0.49	1/998 (0.1%)
43	Dj	0.30	0/775	0.52	0/1049
44	Dk	0.31	0/799	0.48	0/1070
45	Dm	0.32	0/733	0.52	0/977
46	HI	0.67	0/2433	0.96	0/3302
47	HJ	0.74	0/2356	0.97	1/3185 (0.0%)
48	PD	0.29	0/1064	0.44	0/1428
49	PG	0.27	0/1382	0.44	0/1874
50	g	0.57	0/911	0.86	2/1219 (0.2%)
51	j	0.37	0/849	0.54	0/1150
52	n	0.36	0/7901	0.57	14/10731 (0.1%)
53	s	0.64	0/741	0.76	1/1002 (0.1%)
54	u	0.54	0/895	0.75	2/1215 (0.2%)
55	a	0.62	0/3507	0.78	1/4760 (0.0%)
56	d	0.62	0/1281	0.65	0/1718
57	f	0.56	0/1402	0.68	1/1905 (0.1%)
58	i	0.68	0/612	0.76	1/815 (0.1%)
59	m	0.28	0/1010	0.38	0/1359
60	q	0.49	1/4456 (0.0%)	0.56	0/6019
61	z	0.64	0/781	0.86	0/1067
62	b	0.51	0/911	0.63	0/1229
63	c	0.43	0/2172	0.58	1/2935 (0.0%)
64	e	0.29	0/840	0.40	0/1128
65	l	0.26	0/1048	0.43	0/1405
66	o	0.41	0/1256	0.65	0/1724
67	h	0.63	0/1485	0.73	1/2008 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
68	k	0.66	0/885	0.67	0/1190
69	r	0.60	0/1565	0.73	0/2106
70	t	0.70	0/1530	0.87	0/2066
71	v	0.66	0/1092	0.74	0/1468
72	p	0.65	0/6116	0.69	0/8311
73	w	0.57	0/11056	0.60	0/15023
74	x	0.58	0/7191	0.64	0/9728
75	y	0.57	0/1645	0.64	0/2240
76	NC	0.80	0/505	0.86	0/700
76	NG	0.68	0/523	0.90	1/724 (0.1%)
77	ND	0.76	0/470	0.83	0/654
77	NH	0.65	0/470	0.85	0/654
All	All	0.45	9/190578 (0.0%)	0.60	38/259940 (0.0%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	q	452	ALA	C-N	5.60	1.47	1.34
1	X	3	DG	O3'-P	5.58	1.67	1.61
1	X	17	DC	O3'-P	5.55	1.67	1.61
1	X	19	DA	O3'-P	5.46	1.67	1.61
1	X	-33	DC	O3'-P	5.28	1.67	1.61
2	Y	-24	DT	O3'-P	5.25	1.67	1.61
3	NX	110	DC	C1'-N1	5.02	1.55	1.49
12	DB	494	SER	CA-CB	-5.01	1.45	1.52
1	X	-5	DT	C1'-N1	5.01	1.55	1.49

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	g	128	PRO	N-CA-C	-7.63	92.27	112.10
50	g	128	PRO	CA-N-CD	-7.39	101.15	111.50
52	n	1351	PRO	N-CA-CB	7.36	112.14	103.30
52	n	1343	PRO	N-CA-CB	7.25	112.01	103.30
52	n	1355	PRO	N-CA-CB	6.89	111.57	103.30
37	DF	320	ARG	CB-CG-CD	6.74	129.13	111.60
1	X	18	DG	C3'-C2'-C1'	-6.43	94.78	102.50
52	n	1352	PRO	N-CA-CB	6.34	110.91	103.30
52	n	1326	PRO	N-CA-CB	6.16	110.69	103.30
55	a	412	ARG	CB-CA-C	6.00	122.40	110.40
6	DA	498	PRO	N-CA-CB	5.93	110.42	103.30
53	s	107	ASN	N-CA-C	-5.88	95.13	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	n	1255	PRO	N-CA-CB	5.85	110.32	103.30
52	n	1237	PRO	N-CA-CB	5.79	110.24	103.30
76	NG	1119	GLY	N-CA-C	5.77	127.53	113.10
52	n	288	PRO	N-CA-C	5.76	127.07	112.10
52	n	1348	PRO	N-CA-CB	5.76	110.21	103.30
52	n	1344	PRO	N-CA-CB	5.75	110.20	103.30
54	u	64	ARG	CB-CA-C	-5.75	98.91	110.40
52	n	74	PRO	N-CA-CB	5.74	110.19	103.30
39	DH	110	TYR	CB-CA-C	-5.70	99.00	110.40
33	HF	3	ASN	CB-CA-C	-5.62	99.16	110.40
30	HD	220	PRO	N-CA-CB	5.57	109.99	103.30
52	n	1347	PRO	N-CA-CB	5.43	109.82	103.30
30	HD	237	PRO	N-CA-CB	5.36	109.73	103.30
67	h	168	PRO	N-CA-CB	5.34	109.71	103.30
63	c	311	GLN	CA-CB-CG	5.29	125.04	113.40
52	n	591	PHE	CB-CA-C	5.27	120.94	110.40
47	HJ	60	TYR	CB-CA-C	5.23	120.86	110.40
52	n	676	ASP	CB-CG-OD2	5.22	123.00	118.30
16	NF	219	ARG	N-CA-C	5.19	125.02	111.00
43	DJ	118	ASP	CB-CG-OD2	5.11	122.90	118.30
41	Dl	79	ASP	CB-CG-OD2	5.11	122.89	118.30
41	DL	79	ASP	CB-CG-OD2	5.10	122.89	118.30
58	i	135	TYR	CB-CA-C	5.09	120.58	110.40
54	u	75	SER	N-CA-CB	-5.08	102.88	110.50
57	f	31	ASP	CB-CG-OD2	5.06	122.86	118.30
10	NA	464	LYS	N-CA-C	5.03	124.58	111.00

There are no chirality outliers.

There are no planarity outliers.

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	
5	BA	248/316 (78%)	246 (99%)	2 (1%)	0	100	100
6	DA	542/1872 (29%)	524 (97%)	15 (3%)	3 (1%)	25	64
7	EA	185/439 (42%)	183 (99%)	1 (0%)	1 (0%)	29	68
8	FA	134/517 (26%)	129 (96%)	5 (4%)	0	100	100
9	HA	710/760 (93%)	682 (96%)	28 (4%)	0	100	100
10	NA	98/136 (72%)	94 (96%)	2 (2%)	2 (2%)	7	40
10	NE	101/136 (74%)	96 (95%)	3 (3%)	2 (2%)	7	40
11	PA	1457/1970 (74%)	1406 (96%)	47 (3%)	4 (0%)	41	76
12	DB	959/1199 (80%)	910 (95%)	49 (5%)	0	100	100
13	EB	169/291 (58%)	164 (97%)	5 (3%)	0	100	100
14	FB	218/249 (88%)	213 (98%)	4 (2%)	1 (0%)	29	68
15	HB	253/548 (46%)	245 (97%)	8 (3%)	0	100	100
16	NB	78/103 (76%)	78 (100%)	0	0	100	100
16	NF	84/103 (82%)	77 (92%)	4 (5%)	3 (4%)	3	29
17	PB	1130/1174 (96%)	1093 (97%)	37 (3%)	0	100	100
18	HC	380/462 (82%)	363 (96%)	17 (4%)	0	100	100
19	DO	97/109 (89%)	95 (98%)	2 (2%)	0	100	100
20	DP	177/339 (52%)	175 (99%)	2 (1%)	0	100	100
21	DQ	109/376 (29%)	102 (94%)	7 (6%)	0	100	100
22	PC	253/275 (92%)	241 (95%)	12 (5%)	0	100	100
23	PE	207/210 (99%)	203 (98%)	4 (2%)	0	100	100
24	PF	77/127 (61%)	76 (99%)	1 (1%)	0	100	100
25	PH	146/150 (97%)	143 (98%)	3 (2%)	0	100	100
26	PI	112/125 (90%)	104 (93%)	8 (7%)	0	100	100
27	PJ	62/67 (92%)	60 (97%)	2 (3%)	0	100	100
28	PK	113/117 (97%)	112 (99%)	1 (1%)	0	100	100
29	PL	42/58 (72%)	40 (95%)	2 (5%)	0	100	100
30	HD	304/309 (98%)	265 (87%)	29 (10%)	10 (3%)	4	30
31	HG	341/395 (86%)	329 (96%)	12 (4%)	0	100	100
32	HE	259/308 (84%)	253 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	HF	64/71 (90%)	62 (97%)	2 (3%)	0	100	100
34	HH	601/782 (77%)	573 (95%)	27 (4%)	1 (0%)	47	80
35	DD	153/1085 (14%)	146 (95%)	5 (3%)	2 (1%)	12	48
35	Dd	154/1085 (14%)	150 (97%)	4 (3%)	0	100	100
36	DE	540/800 (68%)	506 (94%)	32 (6%)	2 (0%)	34	71
36	De	531/800 (66%)	484 (91%)	47 (9%)	0	100	100
37	DF	404/677 (60%)	377 (93%)	20 (5%)	7 (2%)	9	44
37	Df	399/677 (59%)	378 (95%)	20 (5%)	1 (0%)	41	76
38	DG	139/349 (40%)	135 (97%)	4 (3%)	0	100	100
39	DH	207/310 (67%)	191 (92%)	12 (6%)	4 (2%)	8	41
40	DI	118/264 (45%)	113 (96%)	4 (3%)	1 (1%)	19	59
40	Di	119/264 (45%)	115 (97%)	4 (3%)	0	100	100
41	DL	72/161 (45%)	62 (86%)	6 (8%)	4 (6%)	2	21
41	Dl	105/161 (65%)	101 (96%)	4 (4%)	0	100	100
42	Dc	125/929 (14%)	116 (93%)	9 (7%)	0	100	100
43	DJ	86/218 (39%)	82 (95%)	4 (5%)	0	100	100
43	Dj	91/218 (42%)	89 (98%)	2 (2%)	0	100	100
44	Dk	96/211 (46%)	91 (95%)	5 (5%)	0	100	100
45	Dm	85/124 (68%)	79 (93%)	6 (7%)	0	100	100
46	HI	297/346 (86%)	265 (89%)	20 (7%)	12 (4%)	3	26
47	HJ	285/323 (88%)	268 (94%)	14 (5%)	3 (1%)	14	52
48	PD	126/142 (89%)	122 (97%)	4 (3%)	0	100	100
49	PG	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
50	g	104/233 (45%)	99 (95%)	4 (4%)	1 (1%)	15	53
51	j	120/135 (89%)	117 (98%)	1 (1%)	2 (2%)	9	44
52	n	993/1454 (68%)	894 (90%)	80 (8%)	19 (2%)	8	41
53	s	91/244 (37%)	81 (89%)	8 (9%)	2 (2%)	6	38
54	u	113/144 (78%)	104 (92%)	5 (4%)	4 (4%)	3	29
55	a	430/1581 (27%)	387 (90%)	38 (9%)	5 (1%)	13	50
56	d	154/270 (57%)	143 (93%)	9 (6%)	2 (1%)	12	48
57	f	163/246 (66%)	150 (92%)	12 (7%)	1 (1%)	25	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
58	i	69/146 (47%)	65 (94%)	2 (3%)	2 (3%)	4	33
59	m	110/131 (84%)	106 (96%)	4 (4%)	0	100	100
60	q	543/651 (83%)	486 (90%)	50 (9%)	7 (1%)	12	48
61	z	93/600 (16%)	83 (89%)	7 (8%)	3 (3%)	4	31
62	b	111/200 (56%)	109 (98%)	1 (1%)	1 (1%)	17	56
63	c	255/311 (82%)	239 (94%)	15 (6%)	1 (0%)	34	71
64	e	98/178 (55%)	92 (94%)	4 (4%)	2 (2%)	7	40
65	l	120/178 (67%)	115 (96%)	5 (4%)	0	100	100
66	o	152/788 (19%)	135 (89%)	13 (9%)	4 (3%)	5	35
67	h	188/268 (70%)	165 (88%)	15 (8%)	8 (4%)	2	25
68	k	110/117 (94%)	96 (87%)	12 (11%)	2 (2%)	8	42
69	r	190/208 (91%)	180 (95%)	6 (3%)	4 (2%)	7	39
70	t	189/212 (89%)	169 (89%)	16 (8%)	4 (2%)	7	39
71	v	132/200 (66%)	116 (88%)	10 (8%)	6 (4%)	2	25
72	p	756/841 (90%)	707 (94%)	47 (6%)	2 (0%)	41	76
73	w	1332/1368 (97%)	1262 (95%)	66 (5%)	4 (0%)	41	76
74	x	877/989 (89%)	828 (94%)	44 (5%)	5 (1%)	25	64
75	y	206/747 (28%)	196 (95%)	9 (4%)	1 (0%)	29	68
76	NC	101/128 (79%)	93 (92%)	5 (5%)	3 (3%)	4	32
76	NG	105/128 (82%)	94 (90%)	8 (8%)	3 (3%)	4	33
77	ND	93/126 (74%)	91 (98%)	1 (1%)	1 (1%)	14	52
77	NH	93/126 (74%)	89 (96%)	3 (3%)	1 (1%)	14	52
All	All	22102/36357 (61%)	20863 (94%)	1076 (5%)	163 (1%)	26	62

All (163) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	DA	498	PRO
6	DA	1158	SER
10	NA	534	ARG
11	PA	1666	PRO
14	FB	229	HIS
30	HD	215	PRO
30	HD	220	PRO

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Mol	Chain	Res	Type
30	HD	237	PRO
34	HH	62	ARG
35	DD	876	ALA
36	DE	452	ARG
37	DF	68	THR
37	DF	69	SER
37	DF	442	PRO
39	DH	115	GLN
39	DH	141	PRO
41	DL	73	ASN
51	j	31	PRO
52	n	154	ILE
52	n	363	GLU
52	n	1351	PRO
52	n	1355	PRO
55	a	502	MET
56	d	187	LEU
60	q	131	SER
63	c	310	ARG
67	h	100	PHE
67	h	130	ARG
67	h	167	ARG
67	h	168	PRO
70	t	173	PRO
71	v	91	PHE
72	p	705	PRO
74	x	15	LYS
74	x	567	MET
76	NC	841	THR
77	ND	1301	GLY
10	NE	636	LYS
76	NG	1017	VAL
77	NH	1501	GLY
11	PA	1645	PRO
11	PA	1663	SER
30	HD	233	ILE
30	HD	234	SER
35	DD	898	VAL
36	DE	704	VAL
39	DH	129	VAL
41	DL	111	LEU
41	DL	114	LYS

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Mol	Chain	Res	Type
46	HI	96	THR
46	HI	111	PRO
46	HI	192	VAL
46	HI	236	GLN
46	HI	239	ASP
46	HI	310	PRO
52	n	169	LEU
52	n	254	VAL
52	n	1343	PRO
54	u	32	PRO
54	u	76	LEU
55	a	164	PRO
55	a	334	PRO
58	i	108	HIS
58	i	138	LEU
60	q	399	PRO
64	e	146	ILE
66	o	714	ASP
67	h	37	TYR
67	h	131	ILE
70	t	99	LYS
71	v	40	ALA
71	v	41	LYS
71	v	42	ILE
71	v	139	SER
72	p	727	PRO
73	w	1196	CYS
74	x	444	SER
74	x	564	SER
76	NC	843	HIS
30	HD	289	SER
37	DF	321	PRO
46	HI	106	SER
46	HI	277	LEU
47	HJ	237	MET
52	n	150	PRO
52	n	153	ALA
52	n	165	SER
52	n	1237	PRO
53	s	105	LEU
53	s	129	SER
54	u	84	ALA

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Mol	Chain	Res	Type
54	u	123	ALA
55	a	487	LEU
56	d	170	GLY
60	q	91	SER
60	q	458	PRO
66	o	709	LYS
69	r	156	ASN
71	v	38	LYS
73	w	1203	MET
74	x	566	GLU
76	NC	840	THR
37	DF	66	LEU
40	DI	62	LYS
46	HI	264	ALA
47	HJ	286	ALA
51	j	34	GLN
52	n	265	LEU
52	n	1255	PRO
55	a	208	VAL
60	q	127	LEU
60	q	134	ALA
61	z	533	PRO
62	b	100	GLN
64	e	147	ASN
68	k	81	GLY
69	r	113	ASN
70	t	172	ALA
75	y	226	LEU
16	NF	220	LYS
16	NF	301	GLY
76	NG	1042	SER
7	EA	153	ARG
10	NA	438	PRO
30	HD	218	VAL
30	HD	225	THR
30	HD	265	MET
37	DF	64	GLN
37	DF	440	PRO
39	DH	137	GLY
47	HJ	16	GLU
50	g	127	ARG
52	n	264	ALA

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Mol	Chain	Res	Type
52	n	286	GLU
52	n	524	ASN
52	n	1352	PRO
57	f	57	LEU
61	z	540	LEU
66	o	721	LEU
68	k	79	HIS
70	t	129	VAL
73	w	32	ASP
76	NG	1018	SER
6	DA	506	ASP
41	DL	72	PRO
37	Df	411	VAL
46	HI	82	GLY
46	HI	212	PHE
52	n	164	GLY
60	q	89	GLN
67	h	188	GLY
73	w	1194	THR
10	NE	734	ARG
16	NF	219	ARG
61	z	537	PRO
69	r	94	GLY
69	r	153	VAL
52	n	528	HIS
11	PA	1648	PRO
46	HI	186	GLY
66	o	716	PRO
67	h	99	VAL
30	HD	216	LYS

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	
5	BA	215/268 (80%)	215 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	DA	495/1665 (30%)	460 (93%)	35 (7%)	14	41
7	EA	169/373 (45%)	167 (99%)	2 (1%)	71	83
8	FA	121/448 (27%)	119 (98%)	2 (2%)	60	78
9	HA	624/664 (94%)	622 (100%)	2 (0%)	92	95
11	PA	1302/1749 (74%)	1294 (99%)	8 (1%)	86	92
12	DB	876/1083 (81%)	859 (98%)	17 (2%)	57	74
13	EB	154/261 (59%)	153 (99%)	1 (1%)	86	92
14	FB	196/218 (90%)	195 (100%)	1 (0%)	88	93
15	HB	241/484 (50%)	241 (100%)	0	100	100
17	PB	994/1027 (97%)	992 (100%)	2 (0%)	93	96
18	HC	342/399 (86%)	340 (99%)	2 (1%)	86	92
19	DO	90/98 (92%)	88 (98%)	2 (2%)	52	70
20	DP	154/293 (53%)	154 (100%)	0	100	100
21	DQ	105/324 (32%)	105 (100%)	0	100	100
22	PC	234/252 (93%)	234 (100%)	0	100	100
23	PE	191/192 (100%)	191 (100%)	0	100	100
24	PF	69/111 (62%)	68 (99%)	1 (1%)	67	80
25	PH	129/131 (98%)	129 (100%)	0	100	100
26	PI	103/112 (92%)	103 (100%)	0	100	100
27	PJ	53/56 (95%)	53 (100%)	0	100	100
28	PK	104/106 (98%)	102 (98%)	2 (2%)	57	74
29	PL	41/55 (74%)	41 (100%)	0	100	100
30	HD	251/283 (89%)	223 (89%)	28 (11%)	6	25
31	HG	311/352 (88%)	310 (100%)	1 (0%)	92	95
32	HE	234/272 (86%)	230 (98%)	4 (2%)	60	78
33	HF	59/64 (92%)	59 (100%)	0	100	100
34	HH	536/688 (78%)	531 (99%)	5 (1%)	78	88
35	DD	144/815 (18%)	135 (94%)	9 (6%)	18	45
35	Dd	146/815 (18%)	146 (100%)	0	100	100
36	DE	478/657 (73%)	465 (97%)	13 (3%)	44	66
36	De	475/657 (72%)	473 (100%)	2 (0%)	91	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	DF	324/574 (56%)	296 (91%)	28 (9%)	10	35
37	Df	322/574 (56%)	314 (98%)	8 (2%)	47	68
38	DG	133/322 (41%)	125 (94%)	8 (6%)	19	46
39	DH	181/270 (67%)	172 (95%)	9 (5%)	24	51
40	DI	106/235 (45%)	97 (92%)	9 (8%)	10	36
40	Di	107/235 (46%)	106 (99%)	1 (1%)	78	88
41	DL	69/141 (49%)	60 (87%)	9 (13%)	4	21
41	Dl	98/141 (70%)	98 (100%)	0	100	100
42	Dc	113/833 (14%)	111 (98%)	2 (2%)	59	76
43	DJ	79/154 (51%)	78 (99%)	1 (1%)	69	82
43	Dj	83/154 (54%)	83 (100%)	0	100	100
44	Dk	87/182 (48%)	87 (100%)	0	100	100
45	Dm	80/106 (76%)	79 (99%)	1 (1%)	69	82
46	HI	258/298 (87%)	190 (74%)	68 (26%)	0	3
47	HJ	252/296 (85%)	177 (70%)	75 (30%)	0	2
48	PD	118/126 (94%)	116 (98%)	2 (2%)	60	78
49	PG	152/153 (99%)	150 (99%)	2 (1%)	69	82
50	g	102/216 (47%)	93 (91%)	9 (9%)	10	34
51	j	66/124 (53%)	65 (98%)	1 (2%)	65	79
52	n	807/1271 (64%)	784 (97%)	23 (3%)	42	64
53	s	83/208 (40%)	73 (88%)	10 (12%)	5	23
54	u	95/119 (80%)	92 (97%)	3 (3%)	39	62
55	a	393/1391 (28%)	318 (81%)	75 (19%)	1	9
56	d	139/230 (60%)	95 (68%)	44 (32%)	0	2
57	f	149/223 (67%)	132 (89%)	17 (11%)	5	24
58	i	71/133 (53%)	60 (84%)	11 (16%)	2	16
59	m	102/115 (89%)	101 (99%)	1 (1%)	76	86
60	q	491/577 (85%)	414 (84%)	77 (16%)	2	16
61	z	89/512 (17%)	76 (85%)	13 (15%)	3	18
62	b	102/163 (63%)	91 (89%)	11 (11%)	6	26
63	c	238/280 (85%)	223 (94%)	15 (6%)	18	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
64	e	94/152 (62%)	94 (100%)	0	100	100
65	l	116/155 (75%)	116 (100%)	0	100	100
66	o	141/697 (20%)	138 (98%)	3 (2%)	53	71
67	h	161/225 (72%)	128 (80%)	33 (20%)	1	7
68	k	94/98 (96%)	49 (52%)	45 (48%)	0	0
69	r	169/183 (92%)	142 (84%)	27 (16%)	2	15
70	t	166/178 (93%)	128 (77%)	38 (23%)	1	5
71	v	122/173 (70%)	87 (71%)	35 (29%)	0	3
72	p	681/736 (92%)	670 (98%)	11 (2%)	62	79
73	w	1203/1232 (98%)	1200 (100%)	3 (0%)	93	96
74	x	789/864 (91%)	777 (98%)	12 (2%)	65	79
75	y	175/601 (29%)	172 (98%)	3 (2%)	60	78
All	All	19036/30622 (62%)	18154 (95%)	882 (5%)	31	53

All (882) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	DA	347	ARG
6	DA	353	LEU
6	DA	357	GLU
6	DA	396	LEU
6	DA	397	LEU
6	DA	401	ASN
6	DA	403	LEU
6	DA	405	VAL
6	DA	464	TRP
6	DA	468	PHE
6	DA	470	ILE
6	DA	474	ASP
6	DA	482	ASP
6	DA	491	MET
6	DA	496	GLU
6	DA	500	LEU
6	DA	502	LEU
6	DA	503	ASP
6	DA	511	LEU
6	DA	574	TYR
6	DA	639	LEU

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Mol	Chain	Res	Type
6	DA	661	GLU
6	DA	667	THR
6	DA	711	ASP
6	DA	727	THR
6	DA	730	PHE
6	DA	828	GLU
6	DA	943	LYS
6	DA	970	ASN
6	DA	1052	ARG
6	DA	1058	HIS
6	DA	1059	GLN
6	DA	1062	TYR
6	DA	1165	LEU
6	DA	1203	GLU
7	EA	152	PHE
7	EA	185	GLU
8	FA	44	GLN
8	FA	151	ARG
9	HA	114	ASN
9	HA	572	GLN
11	PA	61	ARG
11	PA	1643	TYR
11	PA	1646	THR
11	PA	1647	SER
11	PA	1657	TYR
11	PA	1663	SER
11	PA	1678	TYR
11	PA	1794	SER
12	DB	21	GLU
12	DB	24	ARG
12	DB	71	ARG
12	DB	140	GLU
12	DB	184	ASN
12	DB	225	TYR
12	DB	262	MET
12	DB	266	THR
12	DB	293	GLU
12	DB	431	LEU
12	DB	488	PHE
12	DB	559	LYS
12	DB	603	LYS
12	DB	638	ARG

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Mol	Chain	Res	Type
12	DB	640	VAL
12	DB	771	VAL
12	DB	818	THR
13	EB	114	LYS
14	FB	230	LYS
17	PB	199	LYS
17	PB	1064	ARG
18	HC	33	ARG
18	HC	399	ASP
19	DO	51	ARG
19	DO	82	ARG
24	PF	71	LEU
28	PK	47	LYS
28	PK	81	TYR
30	HD	10	LYS
30	HD	11	THR
30	HD	28	HIS
30	HD	41	ARG
30	HD	127	LYS
30	HD	130	LYS
30	HD	131	ASP
30	HD	133	ILE
30	HD	142	ARG
30	HD	209	GLU
30	HD	210	MET
30	HD	211	GLN
30	HD	212	LEU
30	HD	251	LEU
30	HD	252	GLN
30	HD	254	GLU
30	HD	263	LEU
30	HD	268	ARG
30	HD	272	LEU
30	HD	275	VAL
30	HD	276	ARG
30	HD	287	TYR
30	HD	288	THR
30	HD	293	CYS
30	HD	295	ARG
30	HD	304	LEU
30	HD	305	PHE
30	HD	306	TRP

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Mol	Chain	Res	Type
31	HG	343	ARG
32	HE	62	SER
32	HE	222	SER
32	HE	257	CYS
32	HE	258	HIS
34	HH	62	ARG
34	HH	63	LEU
34	HH	198	ARG
34	HH	266	GLN
34	HH	692	LYS
35	DD	891	ILE
35	DD	894	LEU
35	DD	897	ASP
35	DD	924	LYS
35	DD	955	LYS
35	DD	958	LYS
35	DD	963	ARG
35	DD	1006	LEU
35	DD	1009	LEU
36	DE	433	LYS
36	DE	450	ARG
36	DE	451	VAL
36	DE	507	VAL
36	DE	513	LEU
36	DE	515	LEU
36	DE	519	GLU
36	DE	521	ASP
36	DE	593	PHE
36	DE	702	LEU
36	DE	745	GLU
36	DE	746	ASP
36	DE	747	LEU
37	DF	55	LEU
37	DF	60	MET
37	DF	62	LYS
37	DF	64	GLN
37	DF	66	LEU
37	DF	111	GLU
37	DF	114	LEU
37	DF	118	ILE
37	DF	120	THR
37	DF	209	LYS

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Mol	Chain	Res	Type
37	DF	211	ARG
37	DF	258	ARG
37	DF	261	THR
37	DF	271	VAL
37	DF	280	ILE
37	DF	301	VAL
37	DF	319	LEU
37	DF	320	ARG
37	DF	335	ARG
37	DF	339	GLN
37	DF	348	THR
37	DF	354	ARG
37	DF	386	ASP
37	DF	391	LEU
37	DF	397	GLN
37	DF	412	LEU
37	DF	416	ASP
37	DF	427	LEU
38	DG	41	ASP
38	DG	81	ASP
38	DG	143	VAL
38	DG	147	ARG
38	DG	161	ASP
38	DG	181	TRP
38	DG	182	GLU
38	DG	183	ILE
39	DH	50	PHE
39	DH	116	ARG
39	DH	132	LYS
39	DH	135	THR
39	DH	159	TYR
39	DH	160	ILE
39	DH	161	LYS
39	DH	164	THR
39	DH	169	VAL
40	DI	25	ASP
40	DI	31	TYR
40	DI	32	GLU
40	DI	34	ARG
40	DI	63	LYS
40	DI	69	ASP
40	DI	82	SER

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Mol	Chain	Res	Type
40	DI	83	PHE
40	DI	84	THR
41	DL	59	THR
41	DL	60	LYS
41	DL	61	LYS
41	DL	62	LYS
41	DL	63	LEU
41	DL	64	GLN
41	DL	110	THR
41	DL	111	LEU
41	DL	128	ILE
42	Dc	24	ASP
42	Dc	106	VAL
36	De	365	ARG
36	De	663	ARG
37	Df	253	TYR
37	Df	261	THR
37	Df	272	VAL
37	Df	322	ASP
37	Df	323	VAL
37	Df	326	HIS
37	Df	356	THR
37	Df	421	ASP
40	Di	73	LEU
45	Dm	31	LEU
46	HI	13	GLU
46	HI	15	LEU
46	HI	17	PHE
46	HI	20	GLU
46	HI	23	PHE
46	HI	30	ARG
46	HI	33	ASN
46	HI	34	THR
46	HI	36	GLN
46	HI	38	VAL
46	HI	45	LEU
46	HI	47	HIS
46	HI	48	ARG
46	HI	52	LYS
46	HI	55	ILE
46	HI	56	ASN
46	HI	57	ARG

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Mol	Chain	Res	Type
46	HI	58	THR
46	HI	60	LEU
46	HI	63	ILE
46	HI	64	LYS
46	HI	66	LEU
46	HI	67	GLN
46	HI	69	LEU
46	HI	83	HIS
46	HI	84	LYS
46	HI	86	ASN
46	HI	88	SER
46	HI	96	THR
46	HI	101	ILE
46	HI	107	LEU
46	HI	108	VAL
46	HI	115	LYS
46	HI	125	LEU
46	HI	132	TRP
46	HI	139	LYS
46	HI	141	ASN
46	HI	143	LEU
46	HI	160	LYS
46	HI	162	PHE
46	HI	164	SER
46	HI	166	ASN
46	HI	169	TYR
46	HI	170	THR
46	HI	174	VAL
46	HI	176	ARG
46	HI	177	TRP
46	HI	205	GLU
46	HI	206	LEU
46	HI	209	ARG
46	HI	210	VAL
46	HI	213	LEU
46	HI	225	ILE
46	HI	237	TRP
46	HI	241	CYS
46	HI	245	ASP
46	HI	249	PHE
46	HI	257	LEU
46	HI	258	HIS

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Mol	Chain	Res	Type
46	HI	259	HIS
46	HI	260	ILE
46	HI	261	PHE
46	HI	267	ASP
46	HI	272	ILE
46	HI	280	PRO
46	HI	284	ILE
46	HI	285	THR
46	HI	292	MET
47	HJ	3	HIS
47	HJ	7	GLN
47	HJ	8	LYS
47	HJ	10	HIS
47	HJ	11	TRP
47	HJ	12	THR
47	HJ	14	SER
47	HJ	15	SER
47	HJ	21	ARG
47	HJ	28	ARG
47	HJ	32	CYS
47	HJ	33	LYS
47	HJ	37	ASN
47	HJ	41	LEU
47	HJ	44	ASP
47	HJ	55	THR
47	HJ	60	TYR
47	HJ	65	LEU
47	HJ	71	PHE
47	HJ	85	MET
47	HJ	92	LEU
47	HJ	93	ASN
47	HJ	94	ASN
47	HJ	97	MET
47	HJ	98	GLU
47	HJ	102	ARG
47	HJ	104	ILE
47	HJ	106	LEU
47	HJ	107	THR
47	HJ	108	CYS
47	HJ	113	CYS
47	HJ	114	LYS
47	HJ	115	VAL

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Mol	Chain	Res	Type
47	HJ	134	LEU
47	HJ	136	GLN
47	HJ	140	LEU
47	HJ	143	ILE
47	HJ	145	GLU
47	HJ	148	LEU
47	HJ	149	LEU
47	HJ	150	LEU
47	HJ	151	ILE
47	HJ	153	GLN
47	HJ	154	LEU
47	HJ	155	ASN
47	HJ	158	LEU
47	HJ	160	VAL
47	HJ	165	ARG
47	HJ	166	PRO
47	HJ	167	PHE
47	HJ	171	LEU
47	HJ	172	ILE
47	HJ	174	LEU
47	HJ	175	LYS
47	HJ	180	ILE
47	HJ	181	LEU
47	HJ	182	GLU
47	HJ	186	ILE
47	HJ	189	LYS
47	HJ	192	ASP
47	HJ	196	ASN
47	HJ	200	LEU
47	HJ	208	THR
47	HJ	211	GLN
47	HJ	226	ILE
47	HJ	227	THR
47	HJ	231	TYR
47	HJ	232	LEU
47	HJ	234	GLU
47	HJ	239	LYS
47	HJ	252	MET
47	HJ	262	TYR
47	HJ	266	ARG
47	HJ	279	ARG
47	HJ	288	ASN

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Mol	Chain	Res	Type
48	PD	134	ILE
48	PD	137	LYS
49	PG	59	ILE
49	PG	81	LYS
50	g	72	PHE
50	g	126	TYR
50	g	130	GLN
50	g	132	ARG
50	g	137	VAL
50	g	155	LYS
50	g	159	ARG
50	g	166	ASN
50	g	171	LEU
51	j	82	LYS
52	n	154	ILE
52	n	159	ASP
52	n	166	TYR
52	n	168	ARG
52	n	169	LEU
52	n	212	LEU
52	n	226	VAL
52	n	227	GLU
52	n	252	ILE
52	n	253	LEU
52	n	254	VAL
52	n	255	GLU
52	n	261	ASP
52	n	265	LEU
52	n	266	VAL
52	n	267	HIS
52	n	283	PHE
52	n	289	LEU
52	n	363	GLU
52	n	371	GLN
52	n	528	HIS
52	n	589	GLN
52	n	634	MET
53	s	90	GLU
53	s	93	TYR
53	s	105	LEU
53	s	109	LEU
53	s	112	LEU

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Mol	Chain	Res	Type
53	s	116	ILE
53	s	127	LEU
53	s	128	ARG
53	s	131	ILE
53	s	137	LEU
54	u	49	ASN
54	u	76	LEU
54	u	79	GLU
55	a	58	LEU
55	a	62	LEU
55	a	66	GLN
55	a	70	LYS
55	a	71	VAL
55	a	72	THR
55	a	74	LEU
55	a	77	MET
55	a	78	THR
55	a	80	ARG
55	a	83	SER
55	a	86	ARG
55	a	87	GLN
55	a	93	HIS
55	a	106	ASP
55	a	107	MET
55	a	108	PHE
55	a	109	TYR
55	a	111	GLU
55	a	128	HIS
55	a	131	ASN
55	a	133	VAL
55	a	145	LYS
55	a	148	ASP
55	a	160	LEU
55	a	162	ASN
55	a	167	ASN
55	a	168	LYS
55	a	173	MET
55	a	201	ASP
55	a	214	ARG
55	a	226	VAL
55	a	232	LEU
55	a	244	GLU

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Mol	Chain	Res	Type
55	a	246	ASN
55	a	253	MET
55	a	254	ASN
55	a	258	THR
55	a	259	ILE
55	a	267	LYS
55	a	278	HIS
55	a	288	PHE
55	a	297	VAL
55	a	305	LEU
55	a	309	GLN
55	a	324	CYS
55	a	325	THR
55	a	327	ILE
55	a	329	LEU
55	a	332	THR
55	a	333	GLN
55	a	335	THR
55	a	339	LEU
55	a	348	LEU
55	a	357	LEU
55	a	367	LEU
55	a	373	CYS
55	a	378	LYS
55	a	384	ASP
55	a	388	LEU
55	a	391	THR
55	a	400	HIS
55	a	414	GLN
55	a	421	ILE
55	a	427	ARG
55	a	432	GLU
55	a	433	ASP
55	a	437	LEU
55	a	438	LEU
55	a	441	GLU
55	a	443	CYS
55	a	501	CYS
55	a	502	MET
55	a	504	ILE
55	a	509	ARG
56	d	28	GLU

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Mol	Chain	Res	Type
56	d	30	LEU
56	d	63	ASN
56	d	64	GLN
56	d	66	LEU
56	d	67	GLU
56	d	69	LEU
56	d	70	ILE
56	d	71	HIS
56	d	72	ARG
56	d	73	ASP
56	d	78	GLU
56	d	79	LEU
56	d	80	MET
56	d	81	LYS
56	d	82	LEU
56	d	85	ASN
56	d	91	HIS
56	d	92	GLU
56	d	98	LYS
56	d	101	GLU
56	d	106	ASP
56	d	107	ILE
56	d	108	GLN
56	d	110	LEU
56	d	114	LEU
56	d	115	LYS
56	d	116	GLU
56	d	119	GLN
56	d	121	LEU
56	d	126	TYR
56	d	127	GLN
56	d	129	LYS
56	d	130	GLU
56	d	131	LYS
56	d	132	LEU
56	d	133	LYS
56	d	135	ILE
56	d	173	ARG
56	d	181	GLU
56	d	184	SER
56	d	186	LEU
56	d	187	LEU

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Mol	Chain	Res	Type
56	d	189	GLN
57	f	16	VAL
57	f	19	SER
57	f	20	TRP
57	f	24	LEU
57	f	30	LEU
57	f	41	TYR
57	f	45	CYS
57	f	56	THR
57	f	57	LEU
57	f	58	GLU
57	f	60	LEU
57	f	63	MET
57	f	64	VAL
57	f	114	VAL
57	f	117	SER
57	f	120	LEU
57	f	192	PHE
58	i	86	ASP
58	i	87	LEU
58	i	88	ASN
58	i	90	LEU
58	i	94	PHE
58	i	95	GLN
58	i	104	MET
58	i	112	GLU
58	i	122	ARG
58	i	136	LYS
58	i	140	MET
59	m	59	LYS
60	q	1	MET
60	q	2	SER
60	q	7	VAL
60	q	8	ARG
60	q	16	GLU
60	q	19	VAL
60	q	28	GLU
60	q	29	THR
60	q	31	LEU
60	q	36	MET
60	q	91	SER
60	q	92	LEU

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Mol	Chain	Res	Type
60	q	93	TRP
60	q	98	VAL
60	q	99	ARG
60	q	100	ASN
60	q	103	ARG
60	q	107	THR
60	q	109	MET
60	q	110	CYS
60	q	112	LEU
60	q	116	LEU
60	q	118	ILE
60	q	120	ARG
60	q	123	LYS
60	q	124	PHE
60	q	125	MET
60	q	128	ASP
60	q	131	SER
60	q	132	GLN
60	q	133	ASP
60	q	138	LYS
60	q	139	GLN
60	q	141	PRO
60	q	143	THR
60	q	144	LEU
60	q	145	GLN
60	q	146	LEU
60	q	147	ILE
60	q	151	LYS
60	q	159	ILE
60	q	161	LEU
60	q	162	LYS
60	q	165	GLU
60	q	166	ARG
60	q	169	LYS
60	q	172	THR
60	q	184	ASN
60	q	185	SER
60	q	187	LEU
60	q	188	LEU
60	q	226	LYS
60	q	262	GLN
60	q	263	LYS

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Mol	Chain	Res	Type
60	q	264	GLN
60	q	290	HIS
60	q	400	PHE
60	q	404	ARG
60	q	425	GLU
60	q	428	LEU
60	q	431	ILE
60	q	432	ILE
60	q	434	GLN
60	q	440	LEU
60	q	441	ARG
60	q	442	SER
60	q	443	ARG
60	q	448	ILE
60	q	451	LEU
60	q	518	GLU
60	q	629	LYS
60	q	631	GLU
60	q	634	ASN
60	q	646	LEU
60	q	647	SER
60	q	649	CYS
60	q	651	LEU
61	z	492	ARG
61	z	528	LEU
61	z	540	LEU
61	z	551	ASP
61	z	564	ASN
61	z	567	GLN
61	z	572	ASN
61	z	579	CYS
61	z	582	LEU
61	z	591	LEU
61	z	594	LEU
61	z	598	CYS
61	z	599	LEU
62	b	57	VAL
62	b	60	TYR
62	b	74	LEU
62	b	82	LEU
62	b	92	GLN
62	b	103	ASP

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Mol	Chain	Res	Type
62	b	122	LEU
62	b	126	CYS
62	b	132	ASP
62	b	168	ILE
62	b	184	LYS
63	c	16	GLN
63	c	41	ASN
63	c	44	THR
63	c	45	LEU
63	c	72	ARG
63	c	73	LEU
63	c	77	VAL
63	c	258	MET
63	c	274	ILE
63	c	275	LYS
63	c	276	LEU
63	c	286	LYS
63	c	295	THR
63	c	300	ARG
63	c	301	THR
66	o	635	ASN
66	o	697	HIS
66	o	704	VAL
67	h	7	GLN
67	h	15	LEU
67	h	16	LEU
67	h	17	SER
67	h	18	GLN
67	h	21	ASP
67	h	22	LEU
67	h	23	LYS
67	h	32	LYS
67	h	33	LEU
67	h	34	GLU
67	h	37	TYR
67	h	39	ARG
67	h	40	LEU
67	h	49	PHE
67	h	66	GLU
67	h	75	VAL
67	h	76	ILE
67	h	77	ILE

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Mol	Chain	Res	Type
67	h	79	LEU
67	h	100	PHE
67	h	101	SER
67	h	102	HIS
67	h	110	ARG
67	h	111	THR
67	h	112	LYS
67	h	117	VAL
67	h	130	ARG
67	h	131	ILE
67	h	143	LEU
67	h	187	PHE
67	h	189	LYS
67	h	192	SER
68	k	8	ASN
68	k	10	ARG
68	k	11	LEU
68	k	12	ARG
68	k	14	LEU
68	k	15	GLU
68	k	18	GLU
68	k	19	ARG
68	k	26	GLN
68	k	32	ILE
68	k	33	LEU
68	k	34	GLU
68	k	35	LEU
68	k	36	SER
68	k	37	LYS
68	k	40	THR
68	k	42	GLU
68	k	43	ARG
68	k	44	LEU
68	k	45	LEU
68	k	52	PHE
68	k	57	GLN
68	k	58	HIS
68	k	60	GLU
68	k	69	TYR
68	k	70	LEU
68	k	73	VAL
68	k	82	SER

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Mol	Chain	Res	Type
68	k	83	SER
68	k	86	SER
68	k	87	ARG
68	k	88	LYS
68	k	90	CYS
68	k	91	GLN
68	k	92	MET
68	k	94	LEU
68	k	96	ARG
68	k	97	VAL
68	k	101	ARG
68	k	102	LEU
68	k	103	LYS
68	k	104	LEU
68	k	105	SER
68	k	109	ARG
68	k	114	MET
69	r	16	ILE
69	r	17	ASN
69	r	18	MET
69	r	32	LEU
69	r	35	LEU
69	r	38	ARG
69	r	42	LEU
69	r	49	GLU
69	r	53	ASP
69	r	56	MET
69	r	60	LEU
69	r	73	ARG
69	r	85	LEU
69	r	88	LEU
69	r	93	MET
69	r	101	LEU
69	r	107	ASP
69	r	124	ARG
69	r	143	ILE
69	r	152	LEU
69	r	156	ASN
69	r	168	LEU
69	r	181	MET
69	r	197	VAL
69	r	200	GLU

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Mol	Chain	Res	Type
69	r	202	ILE
69	r	206	ARG
70	t	1	MET
70	t	9	MET
70	t	16	SER
70	t	17	VAL
70	t	21	VAL
70	t	23	LEU
70	t	24	LEU
70	t	28	LEU
70	t	34	GLU
70	t	39	PHE
70	t	43	CYS
70	t	47	HIS
70	t	61	LYS
70	t	62	LEU
70	t	66	MET
70	t	67	HIS
70	t	78	LEU
70	t	79	PHE
70	t	80	GLU
70	t	81	ASN
70	t	84	CYS
70	t	85	LEU
70	t	98	LEU
70	t	101	PHE
70	t	102	PHE
70	t	103	GLN
70	t	109	LYS
70	t	110	ILE
70	t	131	MET
70	t	138	ILE
70	t	149	VAL
70	t	162	GLN
70	t	173	PRO
70	t	179	ARG
70	t	193	TYR
70	t	196	LEU
70	t	200	ILE
70	t	204	GLN
71	v	22	LEU
71	v	37	ILE

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Mol	Chain	Res	Type
71	v	38	LYS
71	v	39	THR
71	v	41	LYS
71	v	43	GLU
71	v	45	GLU
71	v	47	GLN
71	v	50	ARG
71	v	52	THR
71	v	55	GLU
71	v	56	GLN
71	v	58	ASN
71	v	60	GLU
71	v	61	MET
71	v	62	HIS
71	v	81	ASP
71	v	82	LEU
71	v	86	LEU
71	v	87	ILE
71	v	88	LEU
71	v	103	GLN
71	v	105	LEU
71	v	108	LEU
71	v	110	GLU
71	v	114	ARG
71	v	115	LYS
71	v	118	THR
71	v	119	LEU
71	v	120	ARG
71	v	123	ILE
71	v	130	LEU
71	v	131	GLU
71	v	133	GLU
71	v	138	SER
72	p	13	MET
72	p	162	VAL
72	p	170	LEU
72	p	289	ASP
72	p	295	LEU
72	p	401	THR
72	p	443	LEU
72	p	564	LEU
72	p	677	THR

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Mol	Chain	Res	Type
72	p	699	CYS
72	p	710	ASP
73	w	22	PHE
73	w	425	MET
73	w	726	ASN
74	x	4	VAL
74	x	11	LEU
74	x	52	ILE
74	x	87	ASP
74	x	107	ARG
74	x	218	CYS
74	x	300	THR
74	x	443	LEU
74	x	477	TYR
74	x	803	ASP
74	x	812	LEU
74	x	897	LEU
75	y	220	MET
75	y	224	ARG
75	y	226	LEU
43	DJ	192	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (254) such sidechains are listed below:

Mol	Chain	Res	Type
6	DA	401	ASN
6	DA	409	HIS
6	DA	860	ASN
6	DA	896	GLN
6	DA	1073	GLN
7	EA	142	ASN
7	EA	181	ASN
12	DB	30	HIS
12	DB	176	HIS
12	DB	183	GLN
12	DB	184	ASN
12	DB	235	HIS
12	DB	272	GLN
12	DB	348	GLN
12	DB	432	HIS
12	DB	439	HIS
12	DB	450	GLN

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Mol	Chain	Res	Type
12	DB	509	ASN
12	DB	576	ASN
12	DB	750	GLN
12	DB	813	ASN
12	DB	908	GLN
12	DB	916	ASN
13	EB	89	HIS
14	FB	229	HIS
17	PB	1101	GLN
18	HC	352	GLN
18	HC	410	ASN
18	HC	415	GLN
30	HD	129	ASN
30	HD	136	ASN
30	HD	294	HIS
30	HD	298	GLN
33	HF	36	GLN
34	HH	629	HIS
35	DD	922	GLN
35	DD	925	ASN
35	DD	936	GLN
35	DD	1053	GLN
35	DD	1075	HIS
36	DE	254	ASN
36	DE	268	HIS
36	DE	327	ASN
36	DE	351	GLN
36	DE	509	GLN
36	DE	616	HIS
36	DE	636	HIS
36	DE	640	ASN
37	DF	119	ASN
37	DF	214	HIS
37	DF	270	ASN
37	DF	273	GLN
37	DF	275	ASN
37	DF	316	GLN
37	DF	326	HIS
38	DG	48	HIS
39	DH	145	HIS
39	DH	173	GLN
40	DI	21	GLN

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Mol	Chain	Res	Type
40	DI	38	GLN
40	DI	81	GLN
40	DI	98	GLN
41	DL	117	GLN
41	DL	123	GLN
35	Dd	912	ASN
35	Dd	1069	ASN
36	De	294	ASN
36	De	320	HIS
36	De	336	HIS
36	De	424	GLN
36	De	616	HIS
37	Df	325	ASN
40	Di	81	GLN
44	Dk	186	HIS
41	Dl	73	ASN
41	Dl	105	HIS
45	Dm	107	ASN
46	HI	56	ASN
46	HI	67	GLN
46	HI	83	HIS
46	HI	86	ASN
46	HI	131	HIS
46	HI	135	HIS
46	HI	166	ASN
46	HI	171	HIS
47	HJ	7	GLN
47	HJ	37	ASN
47	HJ	100	HIS
47	HJ	128	ASN
47	HJ	211	GLN
47	HJ	275	GLN
47	HJ	288	ASN
48	PD	66	ASN
48	PD	76	ASN
49	PG	124	ASN
50	g	120	HIS
50	g	130	GLN
51	j	92	ASN
52	n	201	HIS
52	n	211	GLN
52	n	267	HIS

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Mol	Chain	Res	Type
52	n	330	HIS
52	n	411	GLN
52	n	507	GLN
52	n	521	GLN
52	n	532	ASN
52	n	651	ASN
52	n	668	HIS
52	n	841	ASN
52	n	880	ASN
52	n	909	GLN
53	s	82	ASN
53	s	88	ASN
54	u	49	ASN
54	u	56	GLN
54	u	86	GLN
54	u	97	ASN
55	a	87	GLN
55	a	131	ASN
55	a	146	ASN
55	a	254	ASN
55	a	333	GLN
55	a	359	HIS
55	a	377	ASN
55	a	413	HIS
55	a	439	GLN
55	a	459	ASN
56	d	63	ASN
56	d	64	GLN
56	d	71	HIS
56	d	85	ASN
56	d	111	GLN
56	d	113	GLN
56	d	119	GLN
56	d	127	GLN
56	d	191	ASN
57	f	59	HIS
57	f	84	GLN
57	f	107	GLN
57	f	127	GLN
58	i	70	HIS
58	i	85	GLN
58	i	108	HIS

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Mol	Chain	Res	Type
58	i	117	GLN
59	m	80	GLN
59	m	90	ASN
59	m	106	GLN
59	m	116	GLN
60	q	139	GLN
60	q	262	GLN
60	q	310	GLN
60	q	321	GLN
60	q	402	HIS
60	q	411	GLN
60	q	434	GLN
60	q	437	HIS
60	q	461	GLN
60	q	496	ASN
60	q	506	HIS
60	q	519	GLN
60	q	533	GLN
60	q	539	GLN
60	q	547	GLN
60	q	565	ASN
60	q	611	GLN
60	q	626	GLN
61	z	527	GLN
61	z	529	HIS
61	z	549	GLN
61	z	556	GLN
61	z	567	GLN
61	z	585	HIS
61	z	592	ASN
62	b	66	GLN
62	b	92	GLN
62	b	129	GLN
62	b	136	HIS
63	c	10	ASN
63	c	41	ASN
63	c	237	GLN
63	c	245	HIS
63	c	306	HIS
64	e	97	GLN
64	e	132	HIS
64	e	140	GLN

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Mol	Chain	Res	Type
65	l	72	GLN
65	l	102	ASN
65	l	151	GLN
66	o	697	HIS
66	o	746	ASN
66	o	753	HIS
66	o	778	GLN
67	h	18	GLN
67	h	60	ASN
67	h	65	HIS
67	h	102	HIS
67	h	171	GLN
68	k	41	ASN
68	k	66	GLN
68	k	77	GLN
68	k	79	HIS
68	k	91	GLN
69	r	156	ASN
70	t	8	GLN
70	t	103	GLN
70	t	178	ASN
70	t	204	GLN
71	v	16	GLN
71	v	32	ASN
71	v	62	HIS
71	v	103	GLN
72	p	63	HIS
72	p	80	HIS
72	p	225	ASN
72	p	272	ASN
72	p	282	HIS
72	p	387	HIS
72	p	400	GLN
72	p	435	GLN
72	p	598	ASN
72	p	619	GLN
72	p	751	GLN
73	w	203	ASN
73	w	378	GLN
73	w	421	HIS
73	w	513	ASN
73	w	726	ASN

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Mol	Chain	Res	Type
73	w	783	GLN
73	w	822	HIS
73	w	851	ASN
73	w	874	HIS
73	w	921	HIS
73	w	923	ASN
73	w	925	HIS
73	w	972	HIS
73	w	1059	ASN
73	w	1134	GLN
73	w	1300	HIS
73	w	1320	ASN
74	x	8	GLN
74	x	49	GLN
74	x	179	HIS
74	x	217	GLN
74	x	356	ASN
74	x	361	ASN
74	x	380	ASN
74	x	402	ASN
74	x	404	GLN
74	x	472	ASN
74	x	502	HIS
74	x	544	HIS
75	y	134	GLN
43	DJ	160	GLN
43	DJ	173	HIS

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 ⓘ

Of 21 ligands modelled in this entry, 20 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	$\#\|Z\| > 2$
79	SF4	HA	1000	9	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**
79	SF4	HA	1000	9	-	-	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.

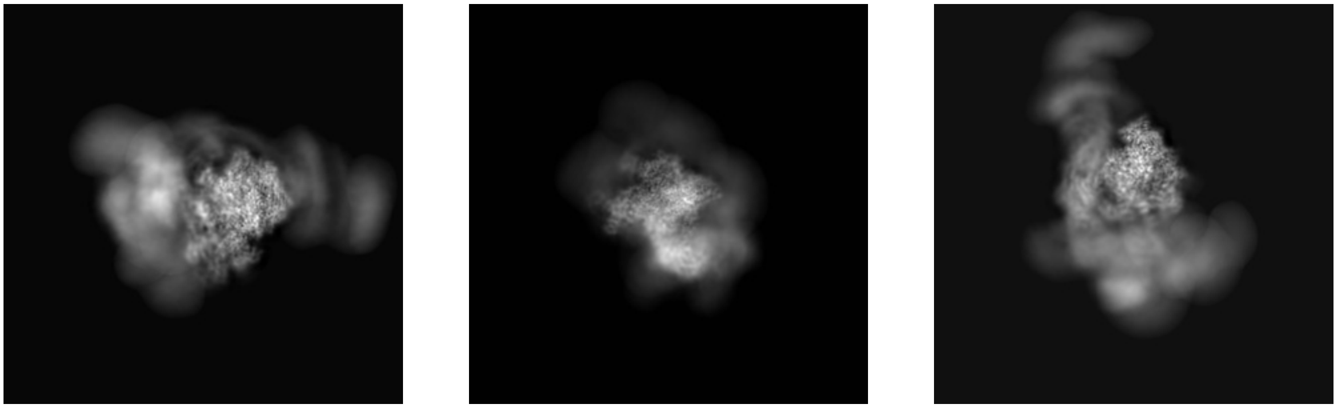
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-34360. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

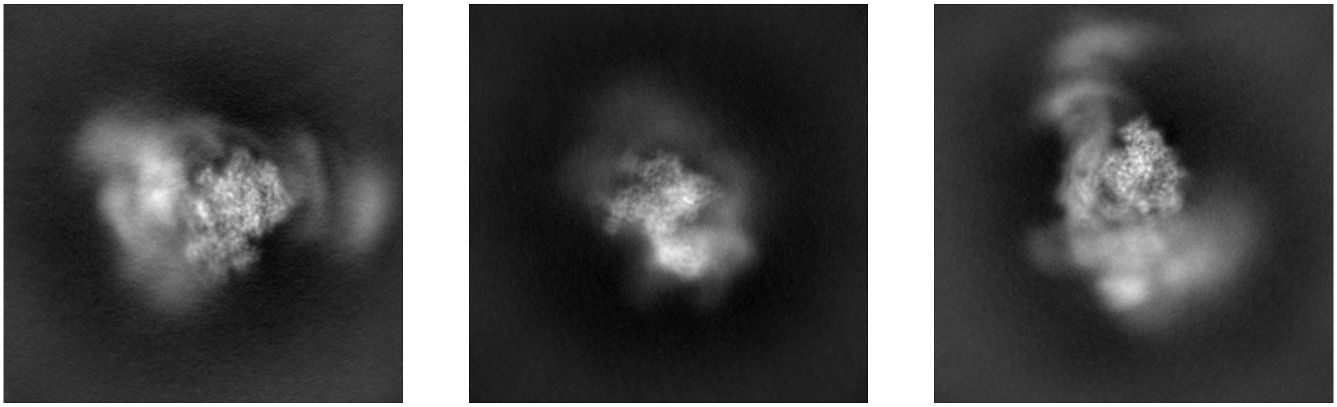
6.1 Orthogonal projections ⓘ

6.1.1 Primary map



X Y Z

6.1.2 Raw map

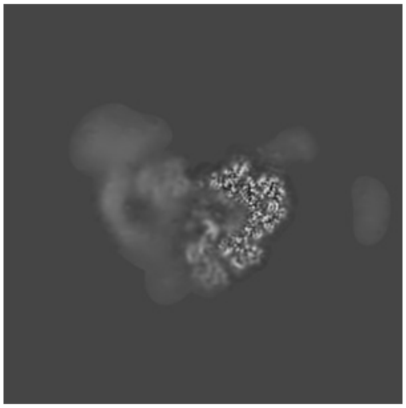


X Y Z

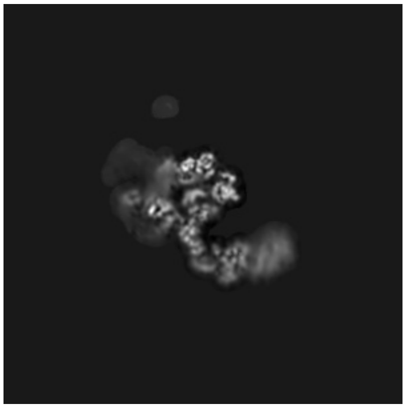
The images above show the map projected in three orthogonal directions.

6.2 Central slices

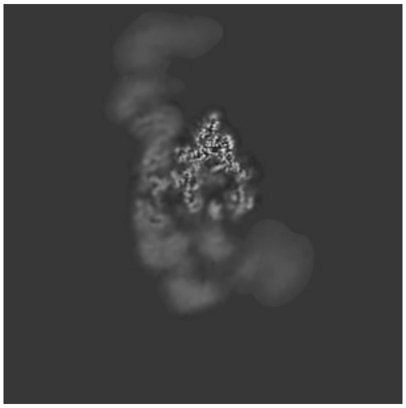
6.2.1 Primary map



X Index: 210

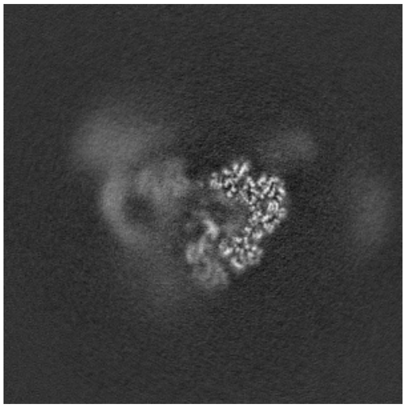


Y Index: 210

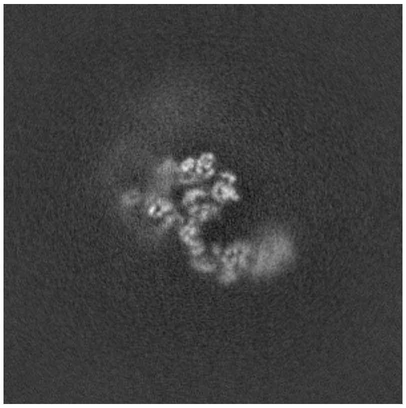


Z Index: 210

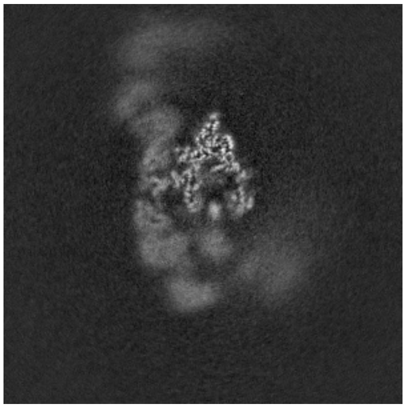
6.2.2 Raw map



X Index: 210



Y Index: 210

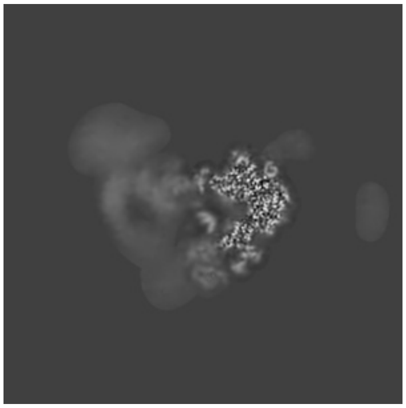


Z Index: 210

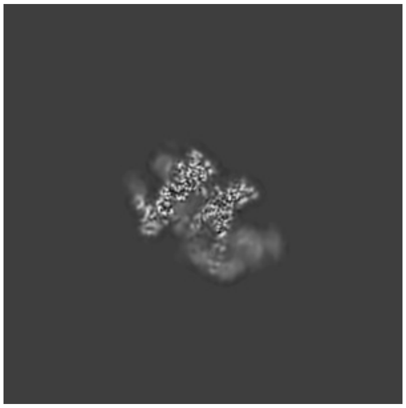
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ

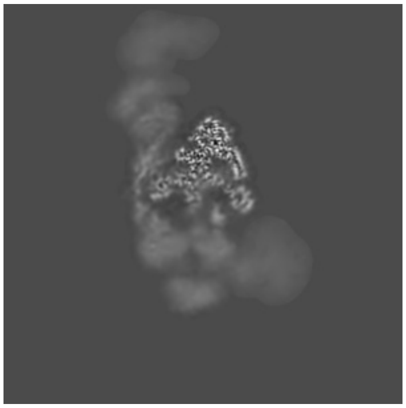
6.3.1 Primary map



X Index: 215

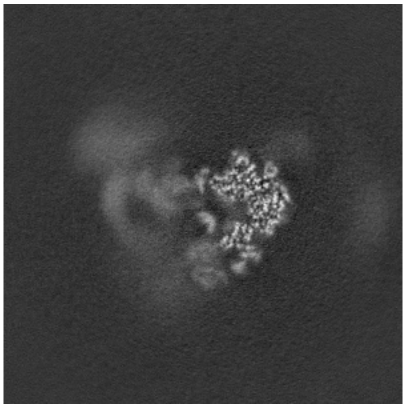


Y Index: 246

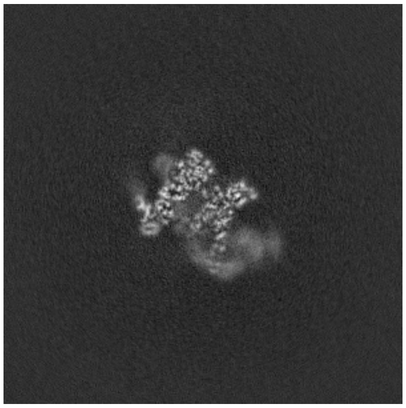


Z Index: 217

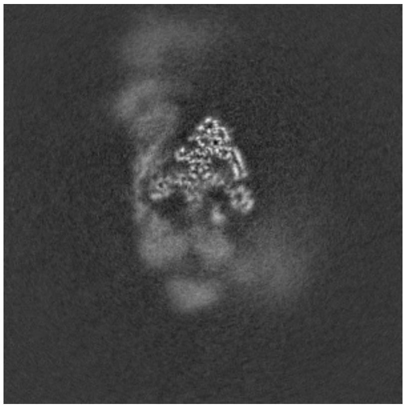
6.3.2 Raw map



X Index: 215



Y Index: 245

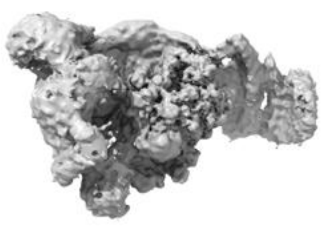


Z Index: 217

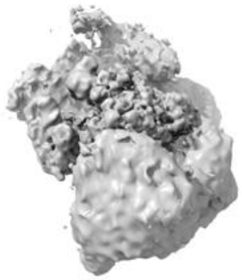
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.2 Raw map

X

Y

Z

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

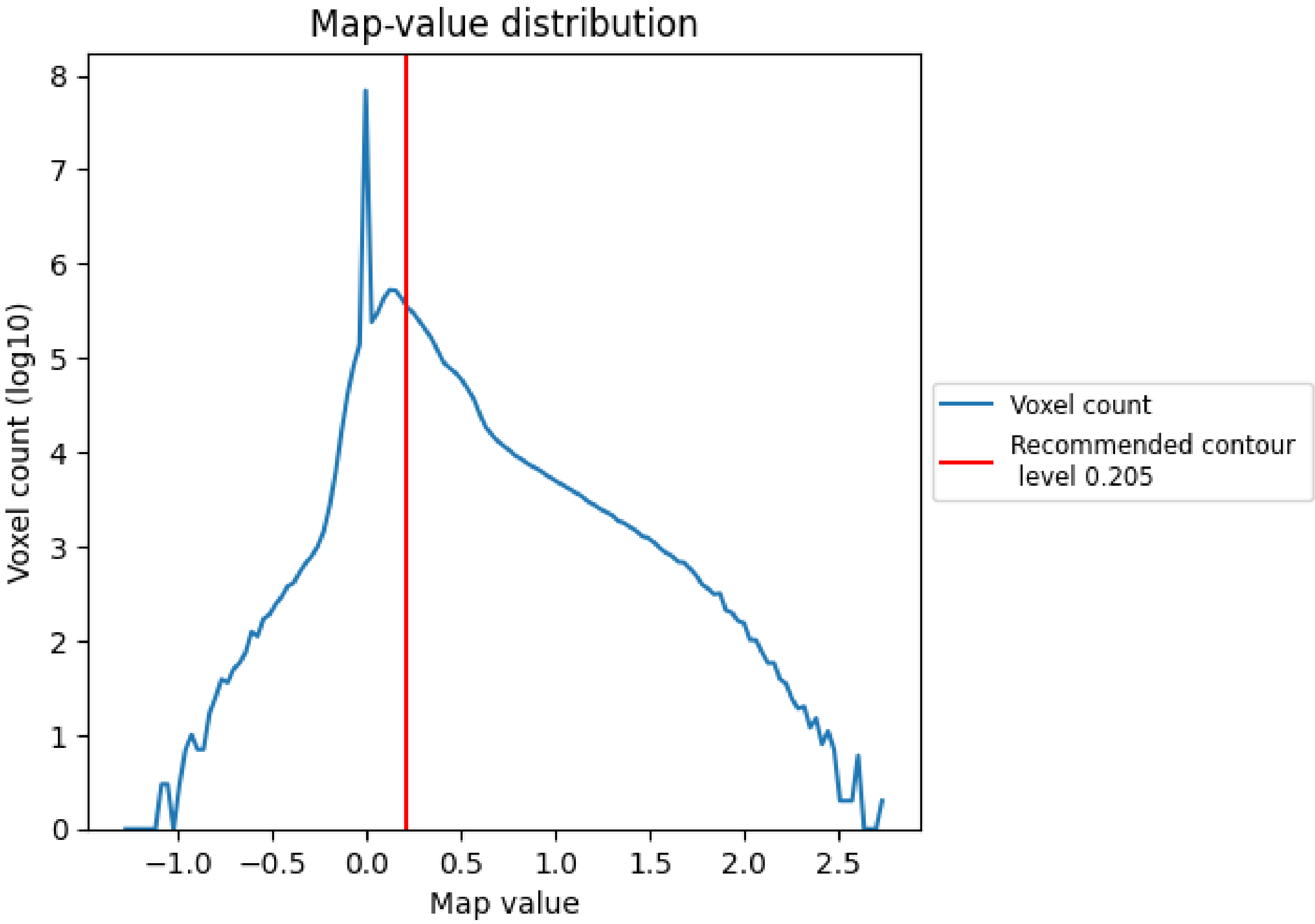
6.5 Mask visualisation

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

7 Map analysis ⓘ

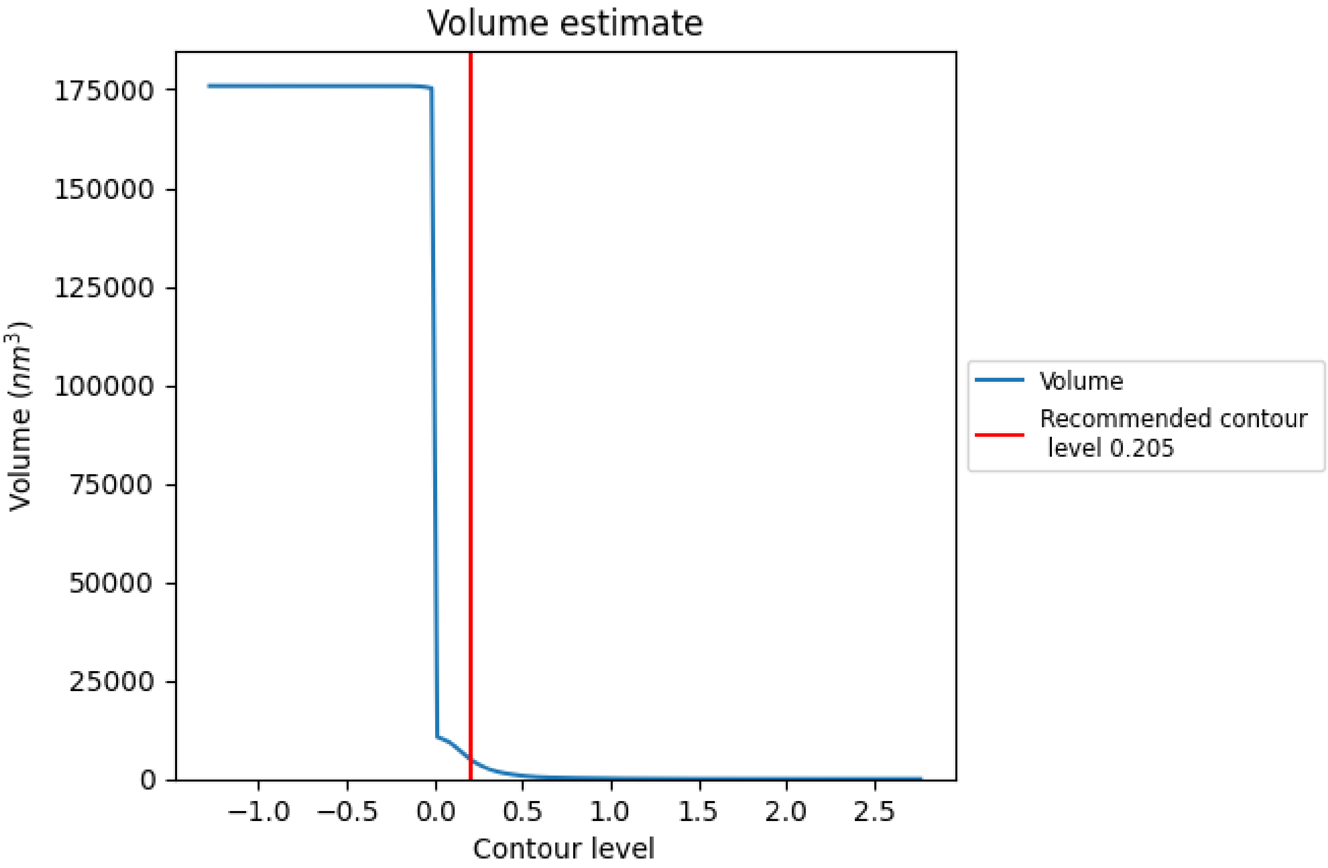
This section contains the results of statistical analysis of the map.

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.

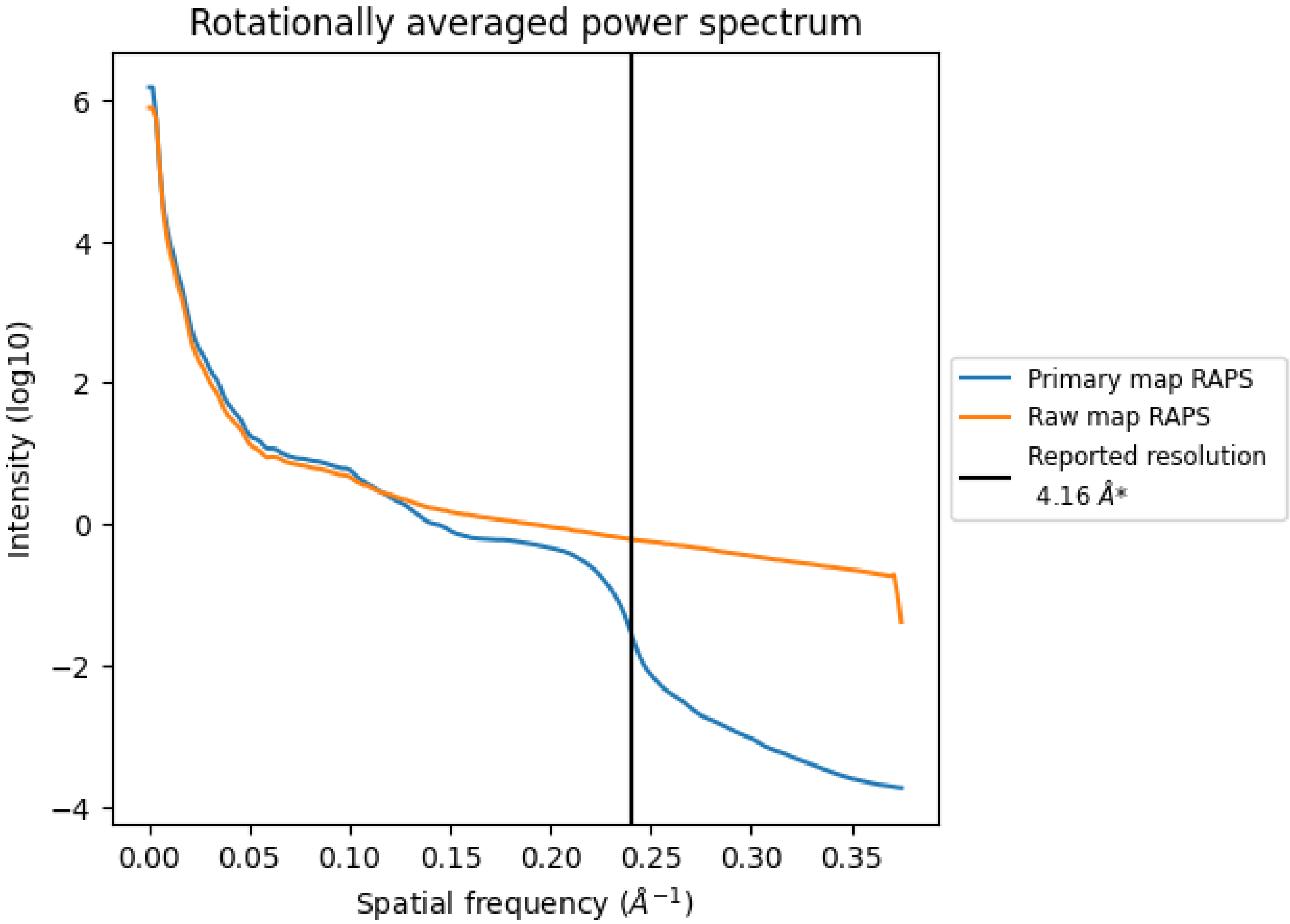
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 4986 nm^3; this corresponds to an approximate mass of 4504 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 ⓘ

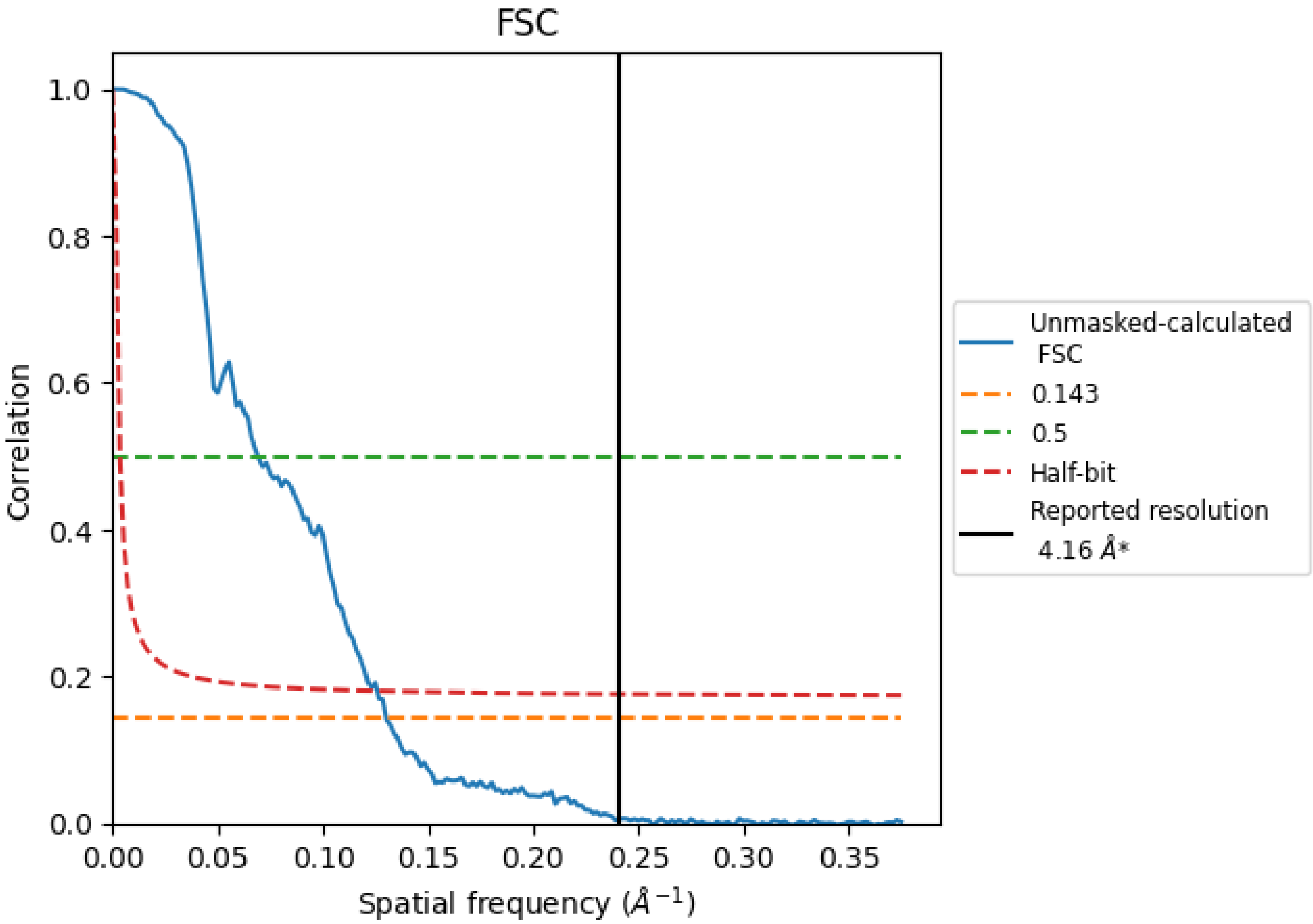


*Reported resolution corresponds to spatial frequency of 0.240 $Å^{-1}$

8 Fourier-Shell correlation ⓘ

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC ⓘ



*Reported resolution corresponds to spatial frequency of 0.240 $Å^{-1}$

8.2 Resolution estimates ⓘ

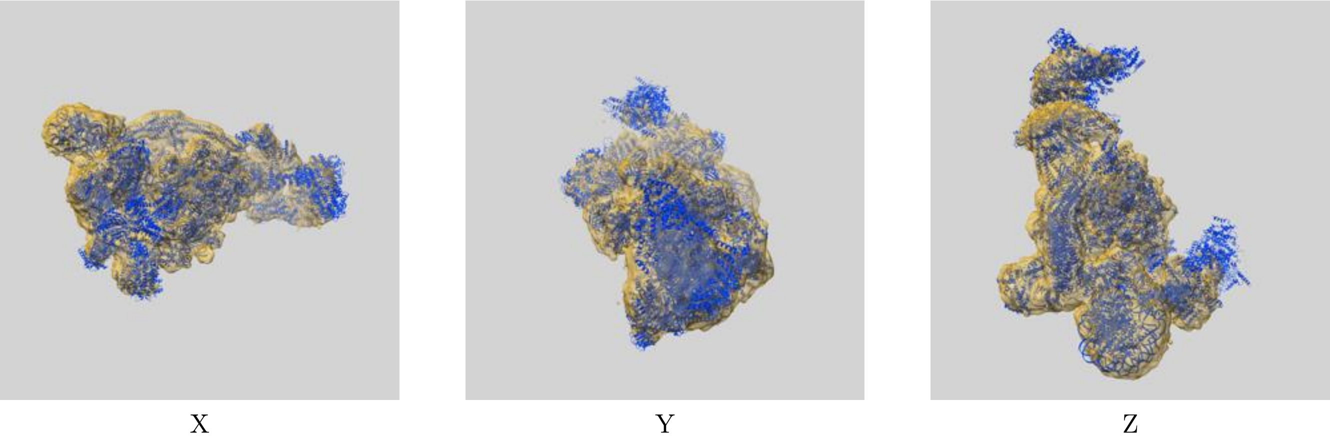
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	4.16	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.68	14.47	7.94

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.68 differs from the reported value 4.16 by more than 10 %

9 Map-model fit ⓘ

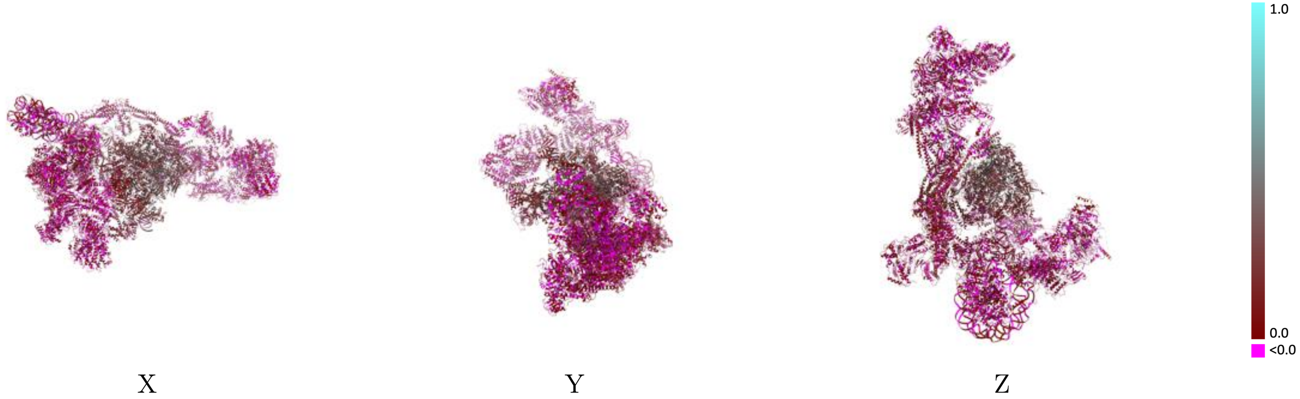
This section contains information regarding the fit between EMDB map EMD-34360 and PDB model 8GXS. Per-residue inclusion information can be found in section 3 on page 20.

9.1 Map-model overlay ⓘ



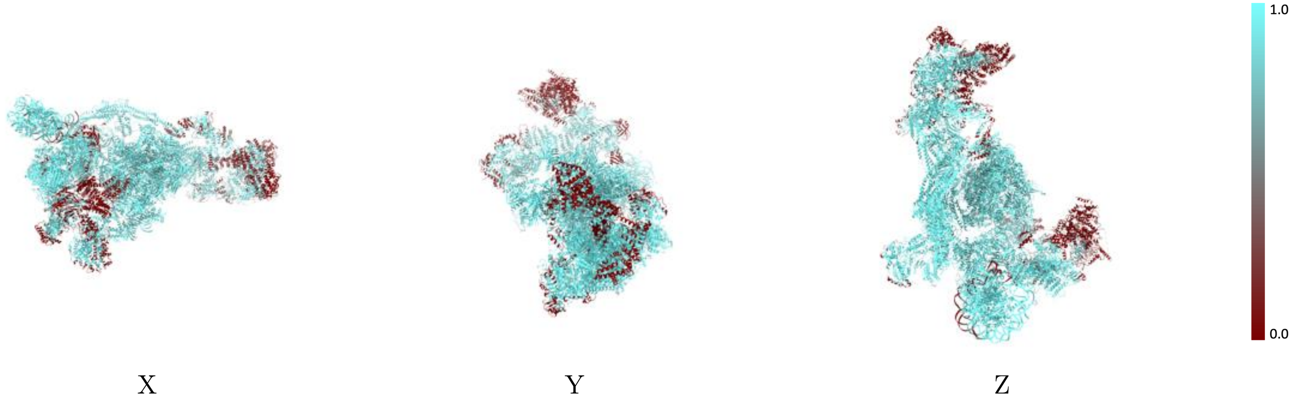
The images above show the 3D surface view of the map at the recommended contour level 0.205 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ



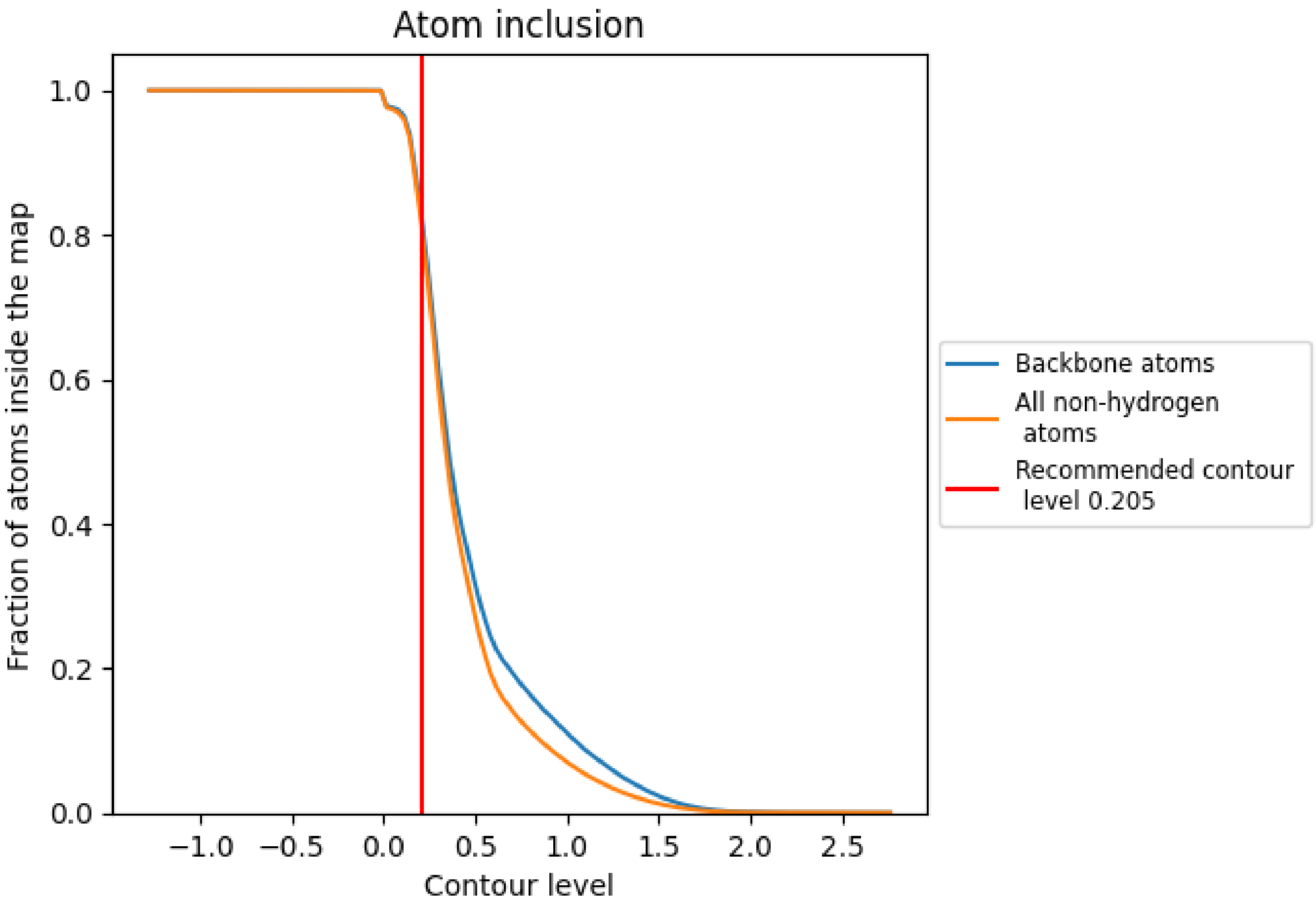
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 ⓘ



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 (0.205).

9.4 Atom inclusion ⓘ



At the recommended contour level, 83% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.205) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8181	0.0930
BA	0.9696	0.2280
DA	0.7095	0.0220
DB	0.9433	0.0400
DD	0.6541	0.0380
DE	0.8404	0.0360
DF	0.7872	0.0420
DG	0.3757	0.0250
DH	0.9105	0.0420
DI	0.7219	0.0330
DJ	0.8814	0.0270
DL	0.3731	0.0400
DO	0.9518	0.1340
DP	0.9856	0.1680
DQ	0.9410	0.1180
Dc	0.0646	0.0310
Dd	0.0016	0.0010
De	0.1898	0.0150
Df	0.5497	0.0330
Di	0.0594	0.0290
Dj	0.0174	0.0500
Dk	0.0000	-0.0140
Dl	0.0000	-0.0070
Dm	0.0000	-0.0090
EA	0.9344	0.1170
EB	0.9761	0.1150
FA	0.9711	0.1500
FB	0.9778	0.1680
HA	0.9893	0.0880
HB	0.9873	0.0480
HC	0.9825	0.0680
HD	0.9190	0.1020
HE	0.9824	0.0530
HF	1.0000	0.0510
HG	0.9892	0.0560

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Chain	Atom inclusion	Q-score
HH	🟦 0.9900	🟥 0.0720
HI	🟦 0.9666	🟥 0.0600
HJ	🟦 0.8512	🟥 0.0620
NA	🟦 0.9418	🟥 0.0310
NB	🟦 1.0000	🟥 0.0490
NC	🟦 1.0000	🟥 0.0050
ND	🟦 1.0000	🟥 0.0090
NE	🟦 0.9765	🟥 0.0330
NF	🟦 0.9715	🟥 0.0480
NG	🟦 0.9847	🟥 0.0410
NH	🟦 0.9639	🟥 0.0380
NX	🟦 0.8070	🟥 0.0300
NY	🟦 0.7947	🟥 0.0250
PA	🟦 0.9581	🟥 0.2510
PB	🟦 0.9667	🟥 0.3080
PC	🟦 0.9742	🟥 0.3060
PD	🟦 0.9710	🟥 0.1790
PE	🟦 0.9607	🟥 0.2250
PF	🟦 0.9287	🟥 0.2910
PG	🟦 0.9767	🟥 0.1770
PH	🟦 0.9741	🟥 0.2790
PI	🟦 0.9769	🟥 0.2320
PJ	🟦 0.9717	🟥 0.3180
PK	🟦 0.9572	🟥 0.3000
PL	🟦 0.9636	🟥 0.3100
X	🟦 0.9993	🟥 0.1960
Y	🟦 0.9971	🟥 0.2010
a	🟦 0.6862	🟥 0.0430
b	🟦 0.8335	🟥 0.0330
c	🟦 0.9131	🟥 0.0440
d	🟦 0.8599	🟥 0.0710
e	🟦 0.9866	🟥 0.0840
f	🟦 0.9925	🟥 0.1270
g	🟦 1.0000	🟥 0.0910
h	🟦 0.9848	🟥 0.1250
i	🟦 0.6572	🟥 0.0630
j	🟦 0.9783	🟥 0.0830
k	🟦 0.9755	🟥 0.1280
l	🟦 0.9911	🟥 0.0600
m	🟦 1.0000	🟥 0.0720
n	🟦 0.9281	🟥 0.0510
o	🟦 0.8827	🟥 0.0320

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Chain	Atom inclusion	Q-score
p	🟦 0.8586	🟥 0.0390
q	🟦 0.9981	🟥 0.0750
r	🟦 0.9914	🟥 0.0850
s	🟦 0.9916	🟥 0.0460
t	🟦 0.9648	🟥 0.0660
u	🟦 1.0000	🟥 0.0740
v	🟦 0.9849	🟥 0.1190
w	🟫 0.3203	🟥 0.0150
x	🟦 0.6378	🟥 0.0290
y	🟦 0.8771	🟥 0.0350
z	🟦 0.9317	🟥 0.0350