Full wwPDB EM Validation Report ⓘ

Oct 6, 2024 – 08:47 PM EDT

PDB ID	:	7LBM
EMDB ID	:	EMD-23255
Title	:	Structure of the human Mediator-bound transcription pre-initiation complex
Authors	:	Abdella, R.; Talyzina, A.; He, Y.
Deposited on	:	2021-01-08
Resolution	:	4.80 Å(reported)

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

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

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

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

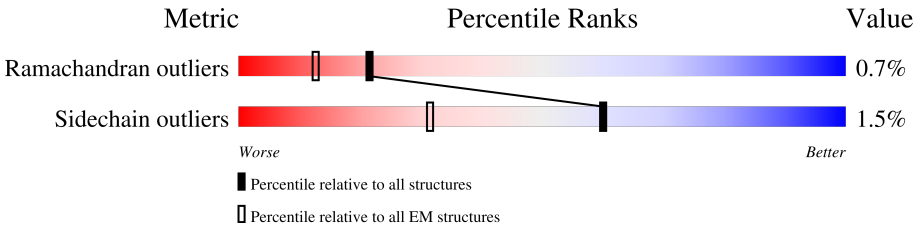
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 4.80 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	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	841	14% 85% 5% 11%
2	1	1368	48% 96%
3	2	989	31% 89% 9%
4	3	747	10% 24% 74%
5	A	1970	73% 26%
6	B	1174	97%
7	C	275	10% 97%
8	D	142	8% 89% 9%
9	E	210	100%

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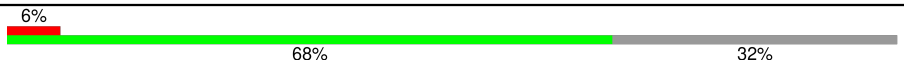
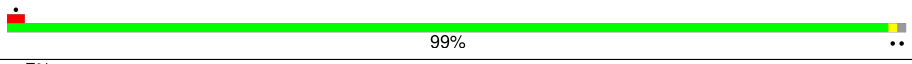
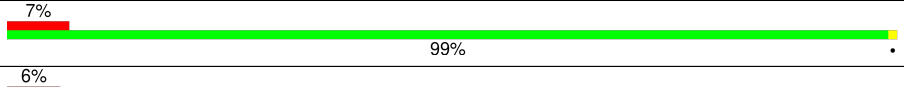
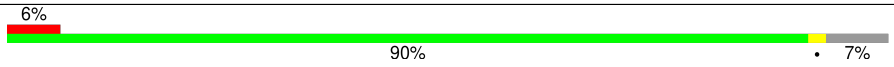
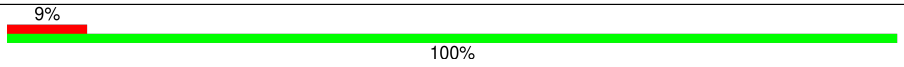
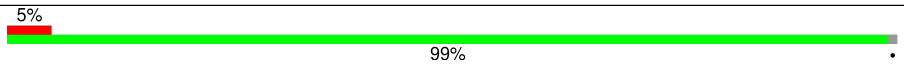
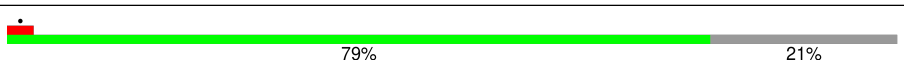
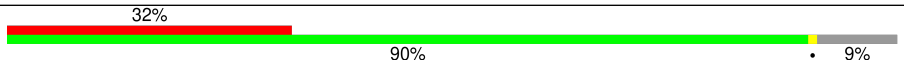
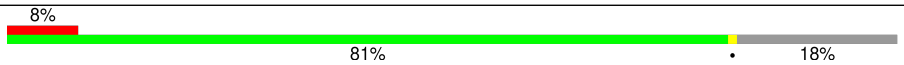
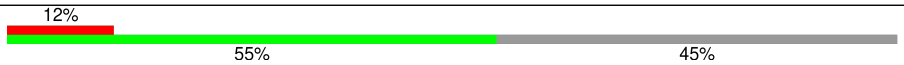
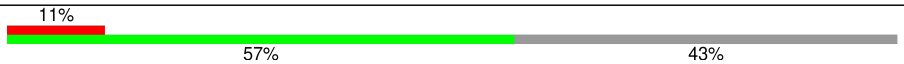
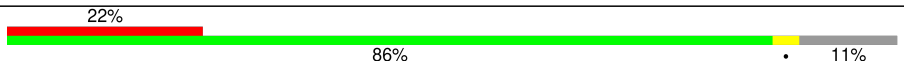
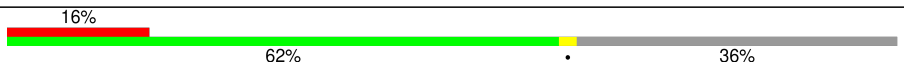
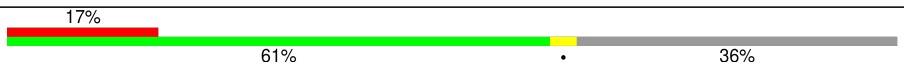
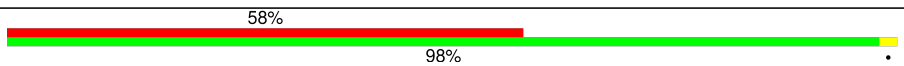
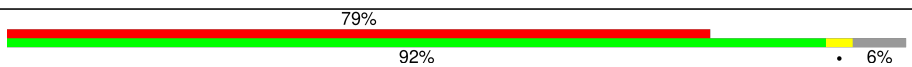
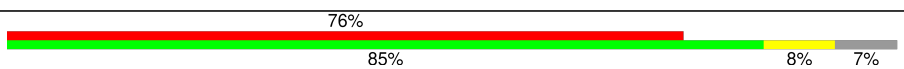
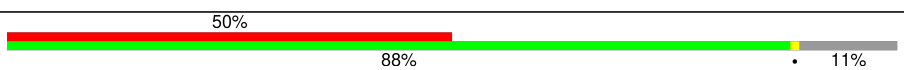
Mol	Chain	Length	Quality of chain
10	F	127	
11	G	172	
12	H	150	
13	I	125	
14	J	67	
15	K	117	
16	L	58	
17	M	376	
18	N	109	
19	O	316	
20	P	339	
21	Q	439	
22	R	291	
23	S	517	
24	T	249	
25	U	100	
26	V	100	
27	W	782	
28	X	760	
29	Y	548	
30	Z	462	
31	a	395	
32	b	308	
33	c	71	
34	d	309	

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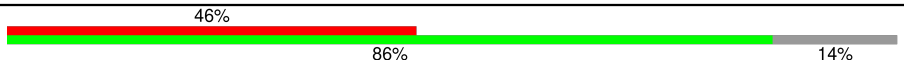
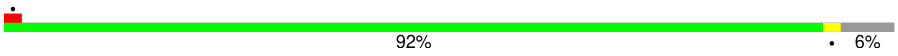
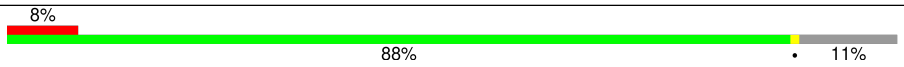
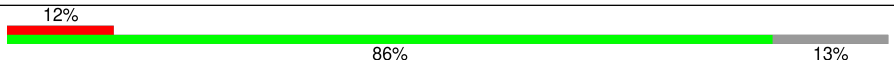
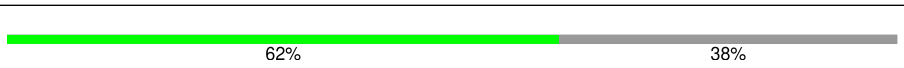
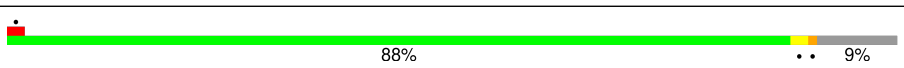
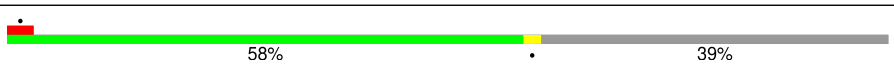
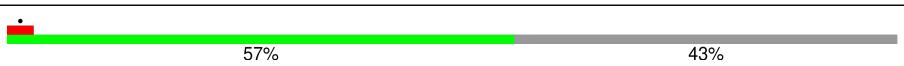
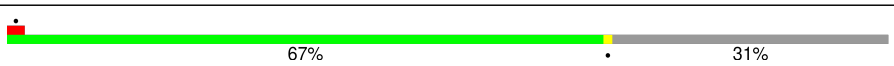
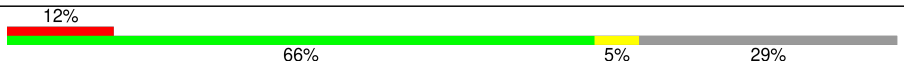
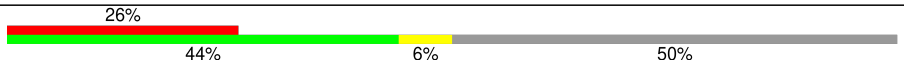
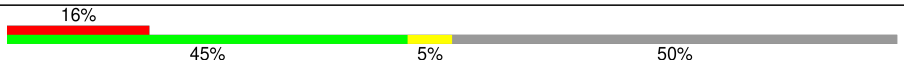
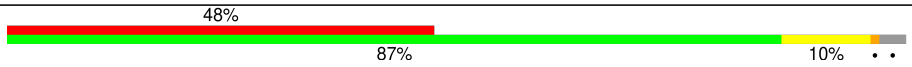
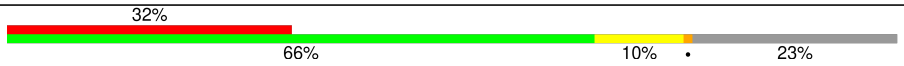
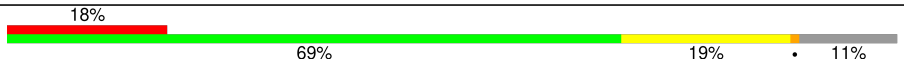
Mol	Chain	Length	Quality of chain
35	e	346	
36	f	323	
37	g	246	
38	h	268	
39	i	117	
40	j	651	
41	k	208	
42	l	212	
43	m	200	
44	n	311	
45	o	178	
46	p	200	
47	q	178	
48	r	1454	
49	s	270	
50	t	233	
51	u	146	
52	v	135	
53	w	244	
54	x	144	
55	y	131	
56	z	788	

2 Entry composition (i)

There are 59 unique types of molecules in this entry. The entry contains 129277 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Isoform 2 of Mediator of RNA polymerase II transcription subunit 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	752	5864	3744	1005	1068	47	0	0

- Molecule 2 is a protein called Mediator of RNA polymerase II transcription subunit 23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	1317	10636	6878	1809	1880	69	0	0

- Molecule 3 is a protein called Mediator of RNA polymerase II transcription subunit 24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	897	7007	4487	1180	1284	56	0	0

- Molecule 4 is a protein called Mediator of RNA polymerase II transcription subunit 25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	195	1504	969	249	277	9	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	A	1455	11519	7241	2052	2154	72	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	B	1142	9129	5769	1604	1692	64	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	267	Total	C	N	O	S	0	0
			2147	1344	370	426	7		

- Molecule 8 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	129	Total	C	N	O	S	0	0
			1062	665	179	214	4		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	210	Total	C	N	O	S	0	0
			1723	1088	301	325	9		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	86	Total	C	N	O	S	0	0
			689	437	120	127	5		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB7.

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

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	150	Total	C	N	O	S	0	0
			1205	764	196	239	6		

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	116	Total	C	N	O	S	0	0
			942	582	168	181	11		

- Molecule 14 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 15 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	116	Total	C	N	O	S	0	0
			928	599	153	174	2		

- Molecule 16 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	46	Total	C	N	O	S	0	0
			388	241	75	66	6		

- Molecule 17 is a protein called Transcription initiation factor IIA subunit 1.

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

- Molecule 18 is a protein called Transcription initiation factor IIA subunit 2.

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

- Molecule 19 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	260	Total	C	N	O	S	0	0
			2018	1265	360	376	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	185	Total	C	N	O	S	0	0
			1462	946	257	252	7		

- Molecule 21 is a protein called General transcription factor IIE subunit 1.

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

- Molecule 22 is a protein called Transcription initiation factor IIE subunit beta.

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

- Molecule 23 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	127	Total	C	N	O	S	0	0
			1059	671	196	189	3		

- Molecule 24 is a protein called General transcription factor IIF subunit 2.

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

- Molecule 25 is a DNA chain called super core promoter sense strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	64	Total	C	N	O	P	0	0
			1321	623	256	379	63		

- Molecule 26 is a DNA chain called super core promoter antisense strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	V	64	Total	C	N	O	P	0	0
			1300	616	233	387	64		

- Molecule 27 is a protein called TFIIH basal transcription factor complex helicase XPB subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	W	574	Total	C	N	O	S	0	0
			4645	2973	807	835	30		

- Molecule 28 is a protein called TFIIH basal transcription factor complex helicase XPD subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	760	Total	C	N	O	S	0	0
			6109	3899	1066	1115	29		

- Molecule 29 is a protein called General transcription factor IIH subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	218	Total	C	N	O	S	0	0
			1631	1028	290	305	8		

- Molecule 30 is a protein called General transcription factor IIH subunit 4, p52.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Z	436	Total	C	N	O	S	0	0
			3473	2239	609	611	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	331	Total	C	N	O	S	0	0
			2580	1628	443	482	27		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	b	263	Total	C	N	O	S	0	0
			2065	1323	344	379	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	c	66	Total	C	N	O	S	0	0
			522	336	83	100	3		

- Molecule 34 is a protein called CDK-activating kinase assembly factor MAT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	d	275	Total	C	N	O	S	0	0
			2104	1315	368	410	11		

- Molecule 35 is a protein called Cyclin-dependent kinase 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	e	298	Total	C	N	O	S	0	0
			2376	1537	404	423	12		

- Molecule 36 is a protein called Cyclin-H.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	f	281	Total	C	N	O	S	0	0
			2293	1465	394	416	18		

- Molecule 37 is a protein called Mediator of RNA polymerase II transcription subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	130	Total	C	N	O	S	0	0
			1035	664	174	192	5		

- Molecule 38 is a protein called Mediator of RNA polymerase II transcription subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	158	Total	C	N	O	S	0	0
			1230	767	214	246	3		

- Molecule 39 is a protein called Mediator of RNA polymerase II transcription subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	110	Total	C	N	O	S	0	0
			863	527	160	172	4		

- Molecule 40 is a protein called Mediator of RNA polymerase II transcription subunit 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	504	Total	C	N	O	S	0	0
			4005	2530	719	739	17		

- Molecule 41 is a protein called Mediator of RNA polymerase II transcription subunit 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	k	185	Total	C	N	O	S	0	0
			1484	942	259	268	15		

- Molecule 42 is a protein called Mediator of RNA polymerase II transcription subunit 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	l	184	Total	C	N	O	S	0	0
			1425	907	235	267	16		

- Molecule 43 is a protein called Mediator of RNA polymerase II transcription subunit 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	125	Total	C	N	O	S	0	0
			1024	632	175	213	4		

- Molecule 44 is a protein called Mediator of RNA polymerase II transcription subunit 27.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	n	283	Total	C	N	O	S	0	0
			2279	1445	406	417	11		

- Molecule 45 is a protein called Mediator of RNA polymerase II transcription subunit 28.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	o	108	Total	C	N	O	S	0	0
			887	553	155	176	3		

- Molecule 46 is a protein called Mediator of RNA polymerase II transcription subunit 29.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	p	114	Total	C	N	O	S	0	0
			893	559	154	171	9		

- Molecule 47 is a protein called Mediator of RNA polymerase II transcription subunit 30.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	q	122	Total	C	N	O	S	0	0
			1007	628	188	182	9		

- Molecule 48 is a protein called Mediator of RNA polymerase II transcription subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	r	1034	Total	C	N	O	S	0	0
			8174	5239	1427	1461	47		

- Molecule 49 is a protein called Mediator of RNA polymerase II transcription subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	s	135	Total	C	N	O	S	0	0
			1084	676	191	212	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	t	116	Total	C	N	O	S	0	0
			975	621	175	173	6		

- Molecule 51 is a protein called Mediator of RNA polymerase II transcription subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	u	60	Total	C	N	O	S	0	0
			501	314	93	90	4		

- Molecule 52 is a protein called Mediator of RNA polymerase II transcription subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	v	131	Total	C	N	O	S	0	0
			1067	676	182	204	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
53	w	39	Total	C	N	O	S	0	0
			309	198	52	57	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
54	x	111	Total	C	N	O	S	0	0
			852	528	142	178	4		

- Molecule 55 is a protein called Mediator of RNA polymerase II transcription subunit 31.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	y	116	Total	C	N	O	S	0	0
			1003	649	177	172	5		

- Molecule 56 is a protein called Mediator of RNA polymerase II transcription subunit 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	z	149	Total	C	N	O	S	0	0
			1168	747	204	210	7		

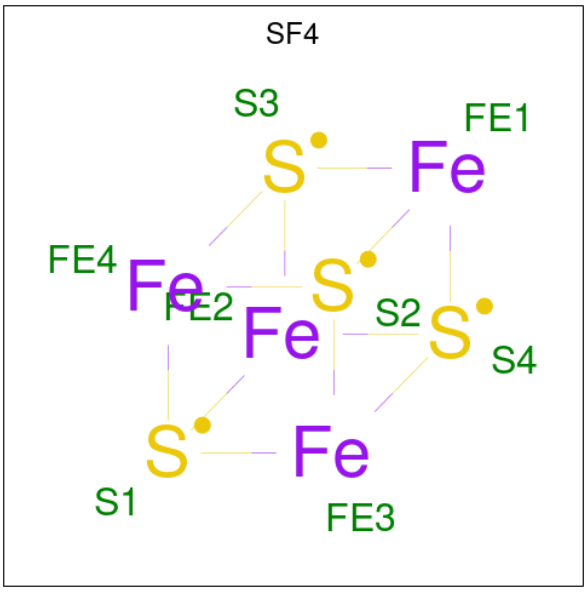
- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	A	2	Total	Mg	0
			2	2	

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
58	A	2	Total	Zn	0
			2	2	
58	B	1	Total	Zn	0
			1	1	
58	C	1	Total	Zn	0
			1	1	
58	I	2	Total	Zn	0
			2	2	
58	J	1	Total	Zn	0
			1	1	
58	L	1	Total	Zn	0
			1	1	
58	O	1	Total	Zn	0
			1	1	
58	Q	1	Total	Zn	0
			1	1	
58	a	3	Total	Zn	0
			3	3	
58	b	1	Total	Zn	0
			1	1	
58	d	2	Total	Zn	0
			2	2	

- Molecule 59 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



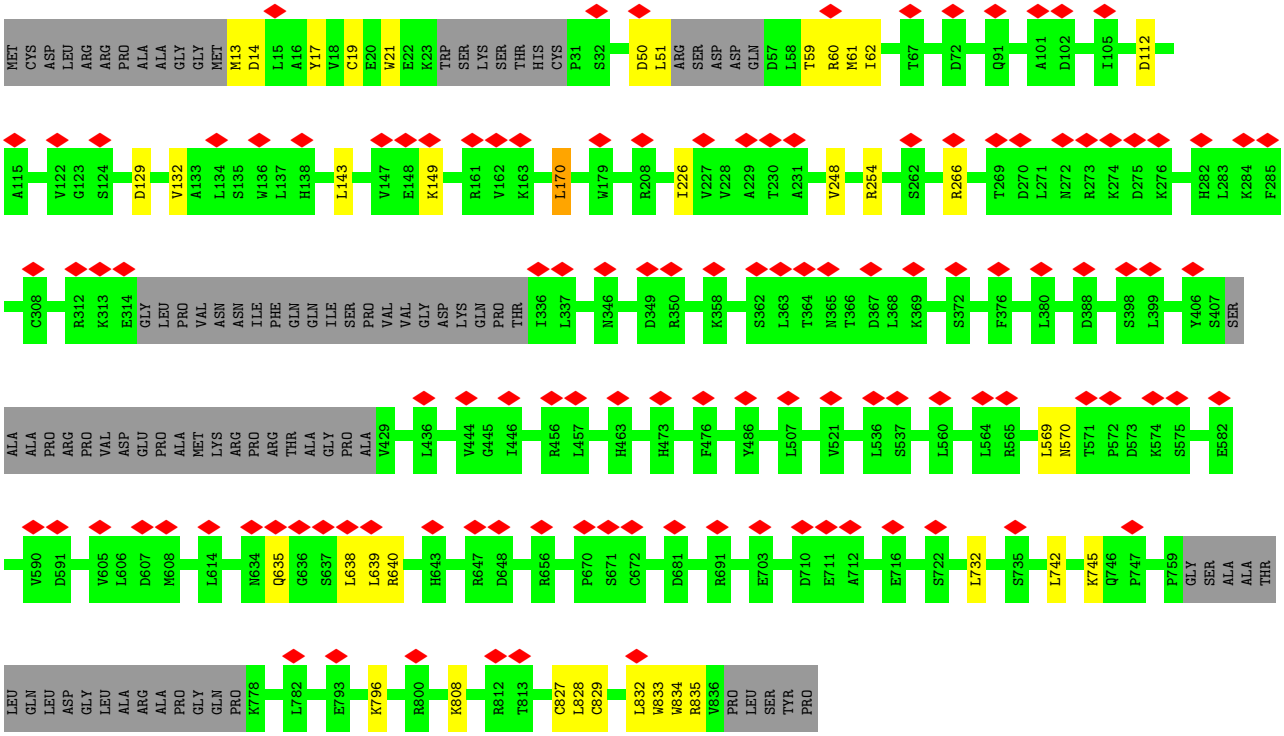
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
59	X	1	8	4	4	0

3 Residue-property plots (i)

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

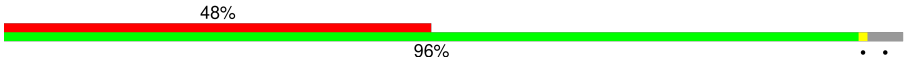
• Molecule 1: Isoform 2 of Mediator of RNA polymerase II transcription subunit 16

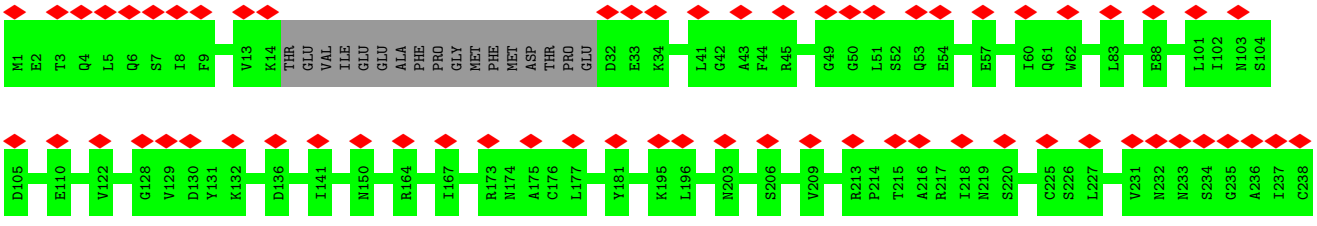
Chain 0:

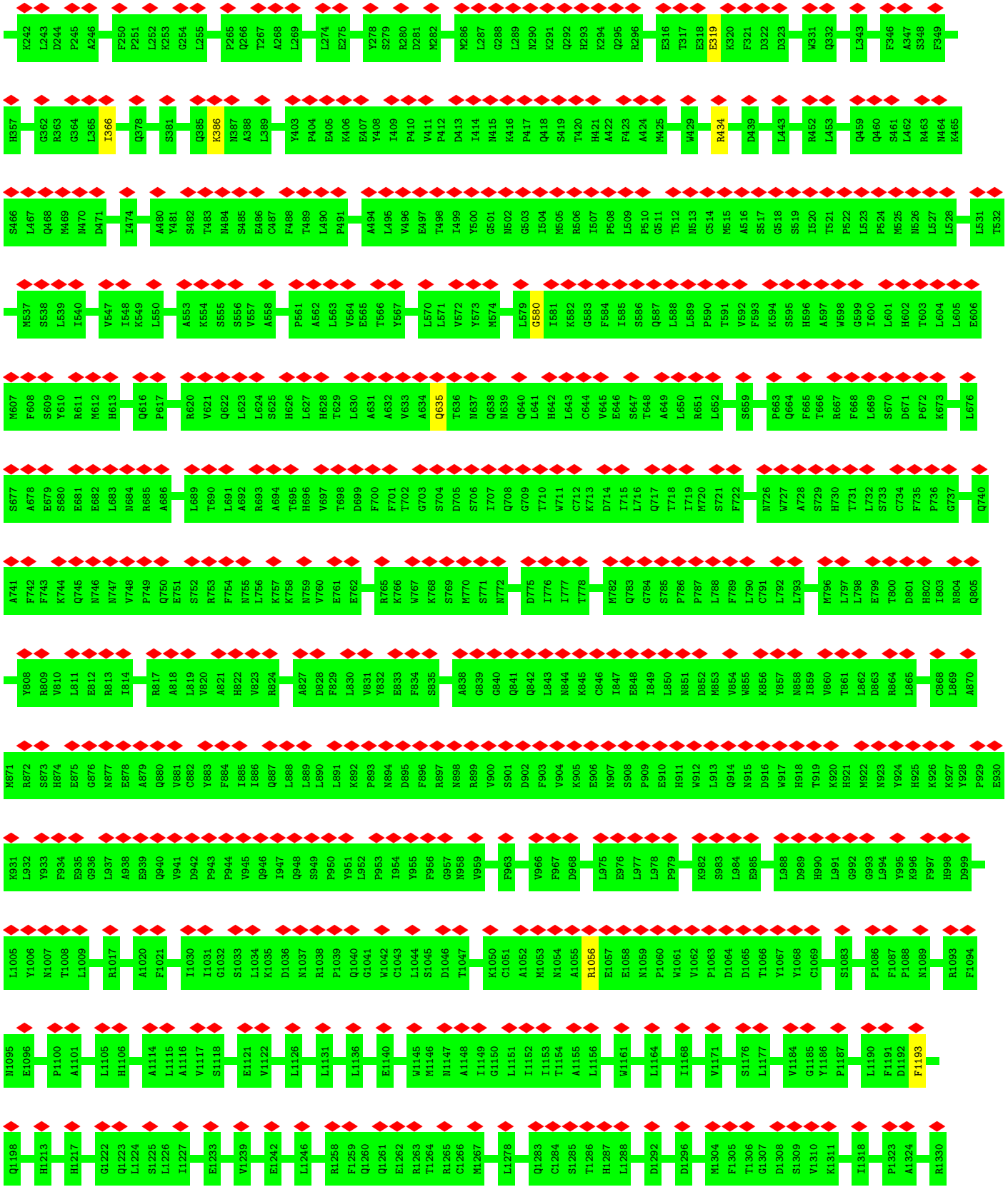


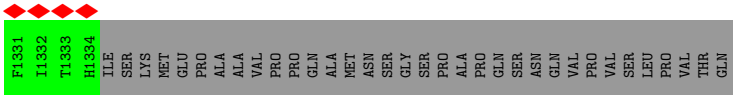
• Molecule 2: Mediator of RNA polymerase II transcription subunit 23

Chain 1:



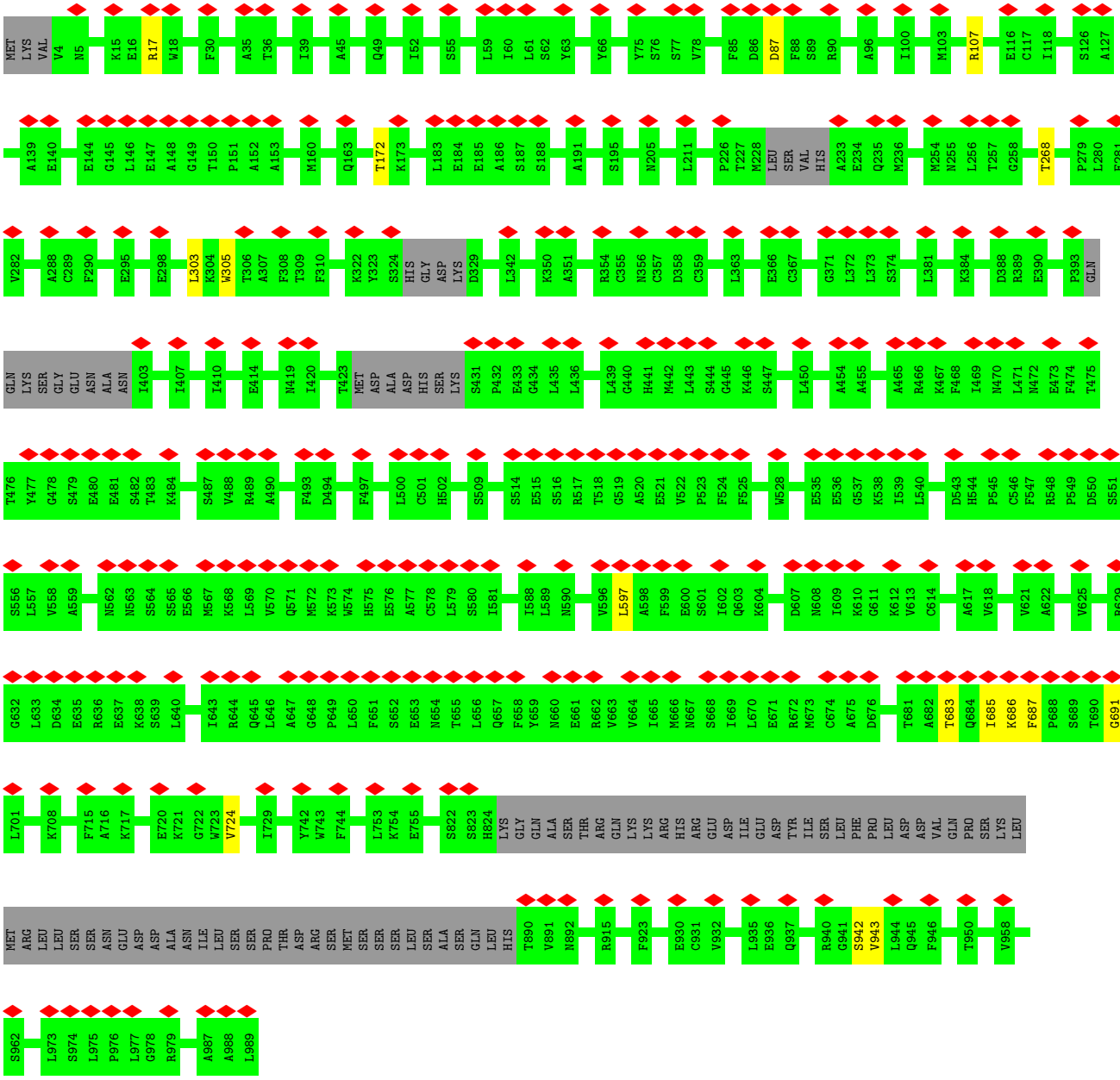



K242 L243 D244 P245 A246 F250 P251 L252 K253 G254 L255 P265 Q266 T267 A268 L269 L274 E275 Y278 S279 R280 D281 M282 M286 L287 G288 L289 N290 K291 Q292 H293 K294 Q295 R296 E316 T317 E318 E319 K320 F321 D322 D323 W331 Q332 L343 F346 A347 S348 F349
H357 G362 R363 G364 L365 I366 Q378 S381 Q385 K386 N387 A388 L389 Y403 P404 E405 K406 E407 Y408 I409 P410 V411 P412 D413 I414 N415 K416 P417 Q418 S419 T420 H421 A422 F423 A424 N425 W429 R434 D439 L443 R452 L453 Q459 Q460 S461 L462 R463 N464 K465
S466 L467 Q468 M469 N470 D471 I474 A480 Y481 S482 T483 N484 S485 E486 C487 F488 T489 L490 P491 A494 L495 V496 E497 T498 I499 Y500 G501 N502 G503 I504 M505 R506 I507 P508 L509 P510 G511 T512 N513 C514 M515 A516 S517 G518 S519 I520 T521 P522 L523 P524 M525 N526 L527 L528 L531 T532
M537 S538 L539 I540 V547 I548 K549 L550 A553 K554 S555 S556 V557 A558 P561 A562 L563 V564 E565 T566 Y567 L570 L571 V572 Y573 M574 L579 G580 I581 K582 G583 F584 I585 S586 Q587 L588 L589 P590 T591 V592 F593 K594 S595 H596 A597 W598 G599 I600 L601 H602 T603 L604 L605 E606
M607 F608 S609 Y610 R611 M612 H613 Q616 P617 R620 V621 Q622 L623 L624 S625 H626 L627 H628 T629 L630 A631 A632 V633 A634 Q635 T636 N637 Q638 N639 Q640 L641 H642 L643 C644 V645 E646 S647 T648 A649 L650 R651 L652 S659 P663 Q664 F665 T666 R667 F668 L669 S670 D671 P672 K673 L676
S677 A678 E679 S680 E681 E682 L683 N684 R685 A686 L689 T690 L691 A692 R693 A694 T695 H696 V697 T698 D699 F700 F701 T702 G703 S704 D705 S706 I707 Q708 G709 T710 W711 C712 K713 D714 I715 L716 Q717 T718 I719 M720 S721 F722 W726 W727 A728 S729 H730 T731 L732 S733 C734 F735 P736 G737 Q740
A741 F742 F743 K744 Q745 N746 N747 V748 P749 Q750 E751 S752 R753 F754 N755 L756 K757 K758 N759 V760 E761 E762 R765 K766 W767 K768 S769 M770 S771 N772 D775 I776 I777 T778 M782 Q783 G784 S785 P786 P787 L788 F789 L790 C791 L792 L793 M796 L797 L798 E799 T800 D801 H802 I803 N804 Q805
Y808 R809 V810 L811 E812 R813 I814 R817 A818 L819 V820 A821 H822 V823 R824 A827 D828 F829 L830 V831 Y832 E833 F834 S835 A838 G839 G840 Q841 Q842 L843 N844 K845 C846 I847 E848 I849 L850 N851 D852 M853 V854 W855 K856 Y857 N858 I859 V860 T861 L862 D863 R864 L865 C868 L869 A870
M871 R872 S873 H874 E875 G876 N877 E878 A879 Q880 V881 C882 Y883 F884 I885 I886 Q887 L888 L889 L890 L891 K892 P893 N894 D895 F896 R897 N898 R899 V900 S901 D902 F903 V904 K905 E906 N907 S908 P909 E910 H911 W912 L913 Q914 N915 D916 W917 H918 T919 K920 H921 M922 N923 Y924 H925 K926 K927 Y928 P929 E930
K931 L932 Y933 F934 E935 G936 L937 A938 E939 Q940 V941 D942 P943 P944 V945 Q946 I947 Q948 S949 P950 Y951 L952 P953 I954 Y955 F956 G957 N958 V959 F963 V966 F967 D968 L975 E976 L977 L978 P979 K982 S983 L984 E985 L988 D989 H990 L991 G992 G993 L994 Y995 K996 F997 H998 D999
L1005 Y1006 N1007 T1008 L1009 R1017 A1020 F1021 I1030 I1031 G1032 S1033 L1034 K1035 D1036 N1037 R1038 P1039 Q1040 G1041 W1042 C1043 L1044 S1045 D1046 T1047 K1050 C1051 A1052 M1053 N1054 A1055 R1056 E1057 E1058 N1059 P1060 W1061 V1062 P1063 D1064 D1065 T1066 Y1067 Y1068 C1069 S1083 P1086 F1087 P1088 N1089 R1093 F1094
N1095 E1096 P1100 A1101 L1105 H1106 A1114 L1115 A1116 V1117 S1118 E1121 V1122 L1126 L1131 L1136 E1140 W1145 M1146 N1147 A1148 I1149 G1150 L1151 I1152 I1153 T1154 A1155 L1156 W1161 L1164 I1168 V1171 S1176 L1177 V1184 G1185 Y1186 P1187 L1190 F1191 D1192 F1193
Q1198 H1213 H1217 G1222 Q1223 L1224 S1225 L1226 I1227 E1233 V1239 E1242 L1246 R1258 F1259 Q1260 Q1261 E1262 R1263 T1264 R1265 C1266 M1267 L1278 Q1283 C1284 S1285 T1286 H1287 L1288 D1292 D1296 M1304 F1305 T1306 G1307 D1308 S1309 V1310 K1311 I1318 P1323 A1324 R1330



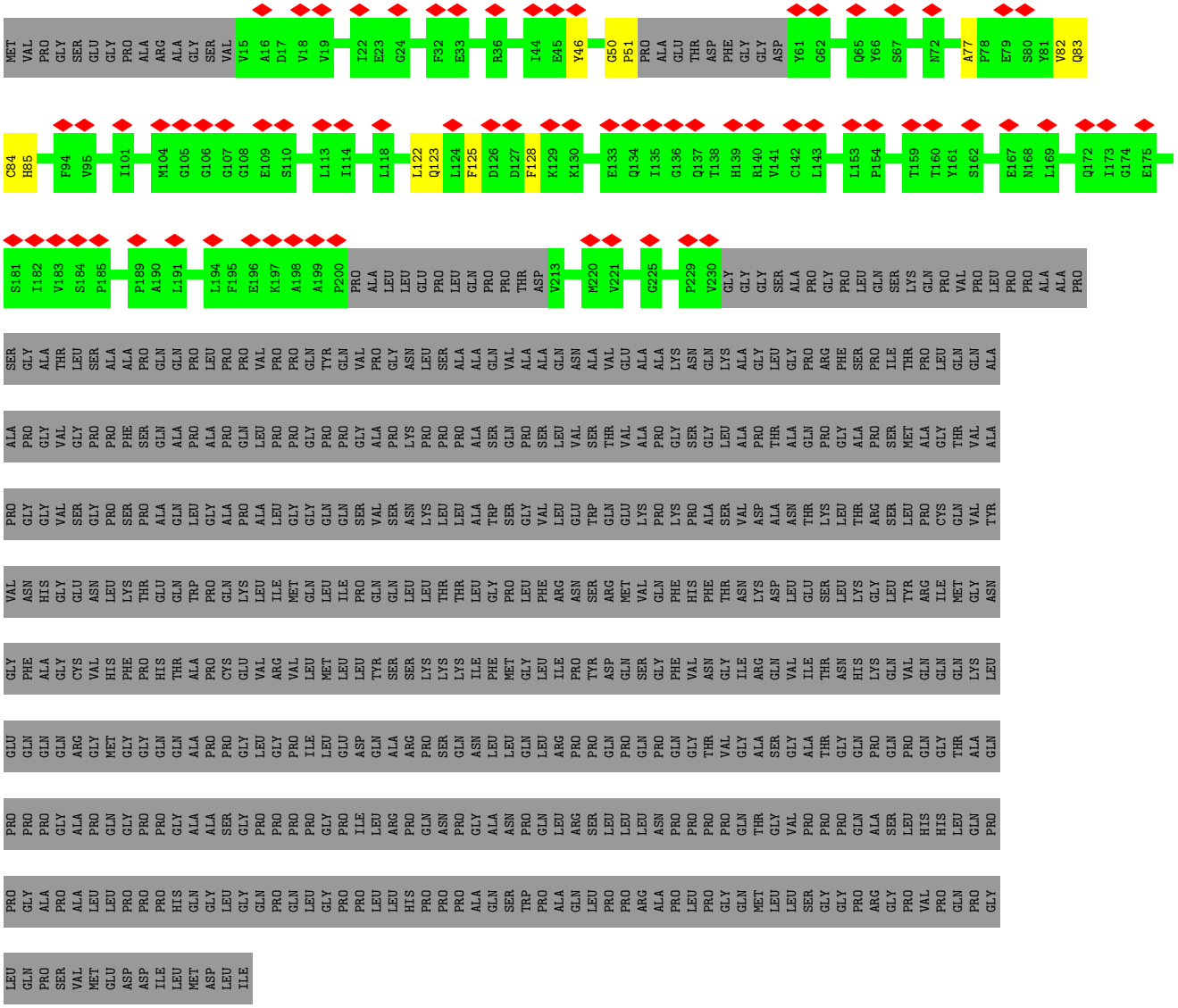
• Molecule 3: Mediator of RNA polymerase II transcription subunit 24

Chain 2:



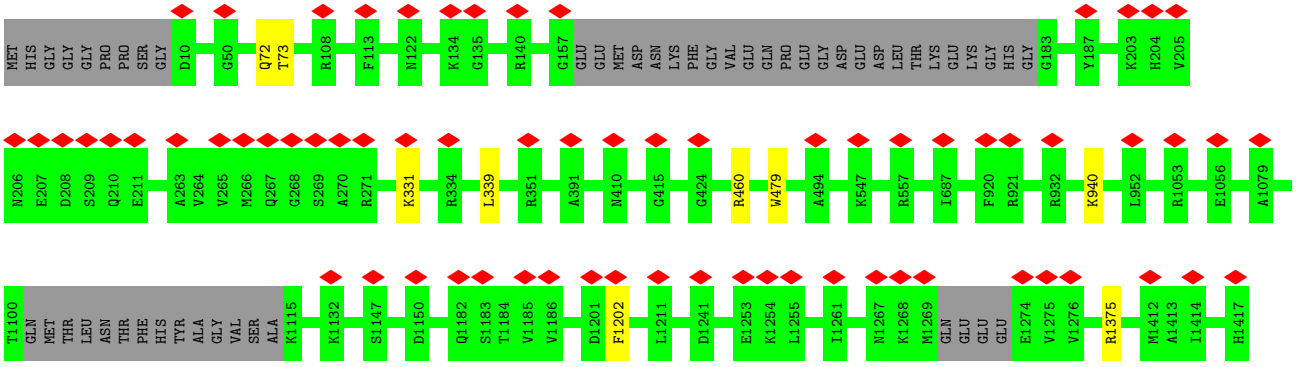
• Molecule 4: Mediator of RNA polymerase II transcription subunit 25

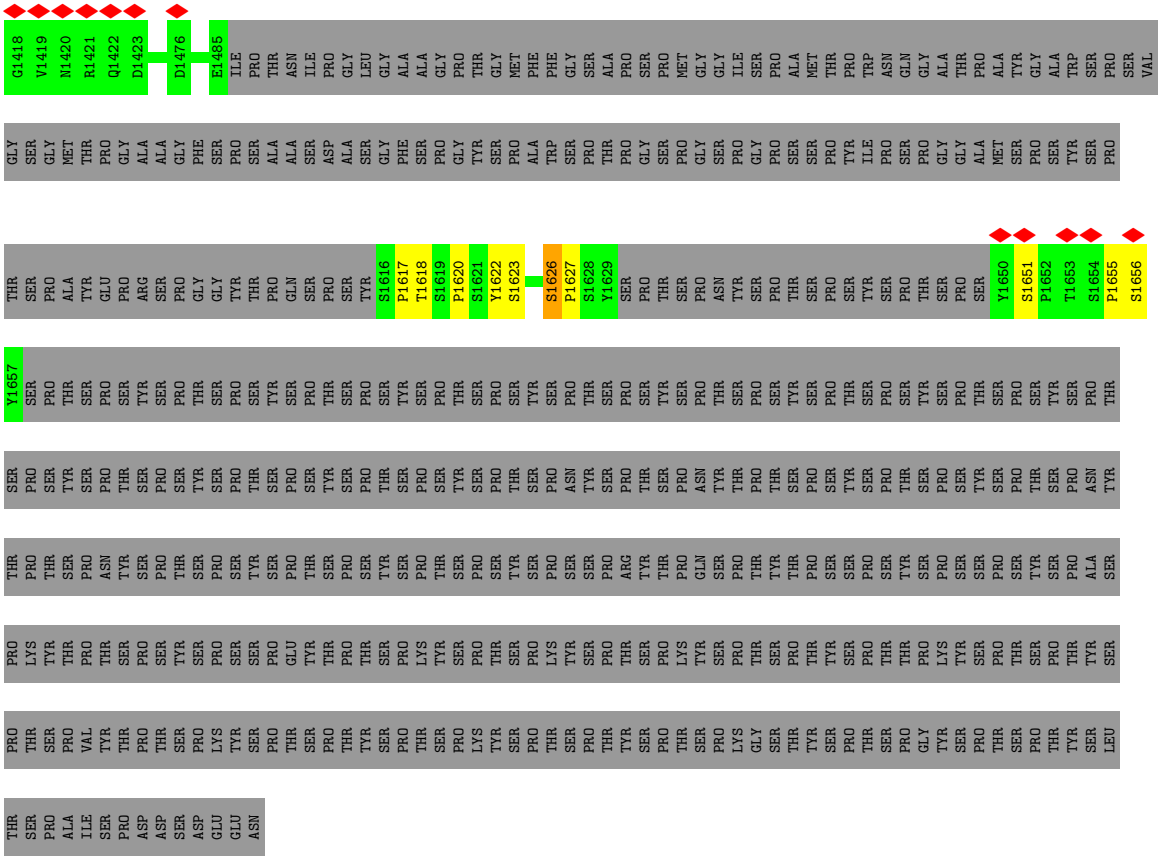
Chain 3:



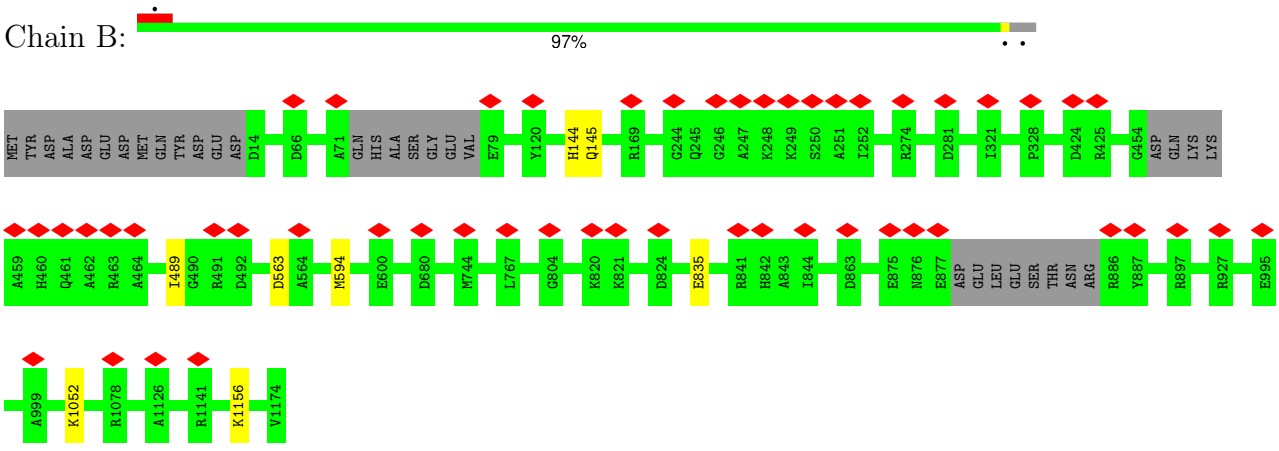
• Molecule 5: DNA-directed RNA polymerase II subunit RPB1

Chain A:

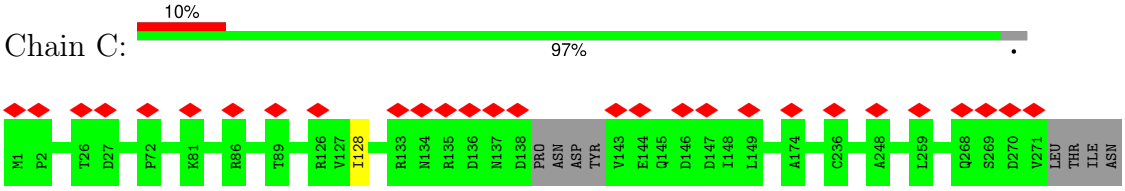




• Molecule 6: DNA-directed RNA polymerase II subunit RPB2

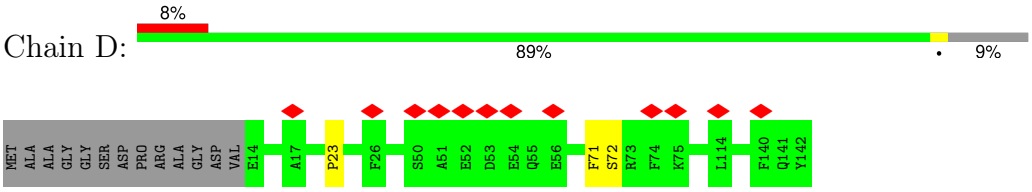


• Molecule 7: DNA-directed RNA polymerase II subunit RPB3



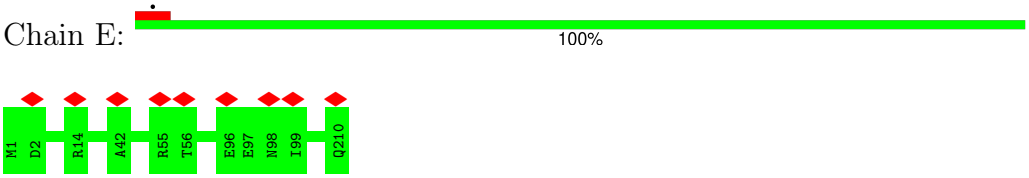
• Molecule 8: DNA-directed RNA polymerase II subunit RPB4

Chain D:



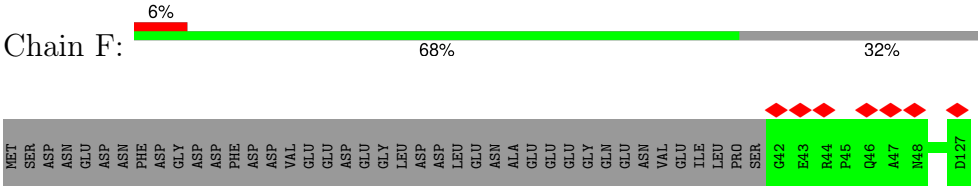
• Molecule 9: DNA-directed RNA polymerase II subunit RPB5

Chain E:



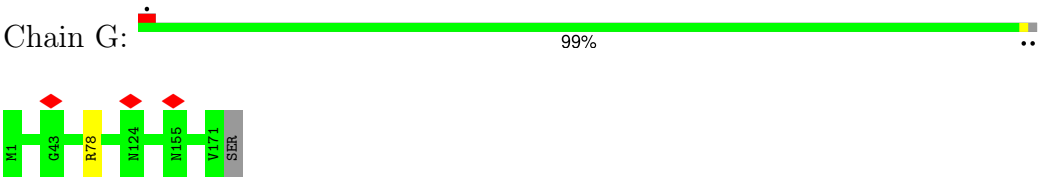
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:



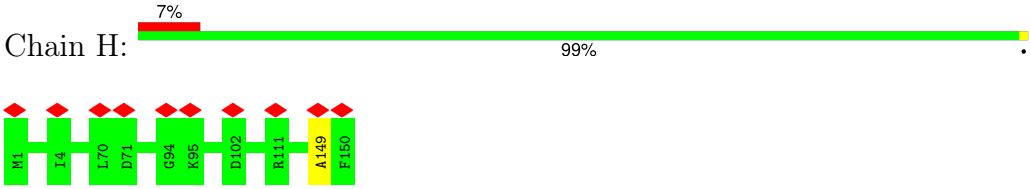
• Molecule 11: DNA-directed RNA polymerase II subunit RPB7

Chain G:



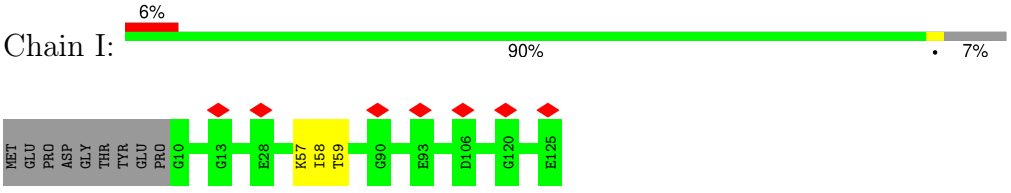
• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



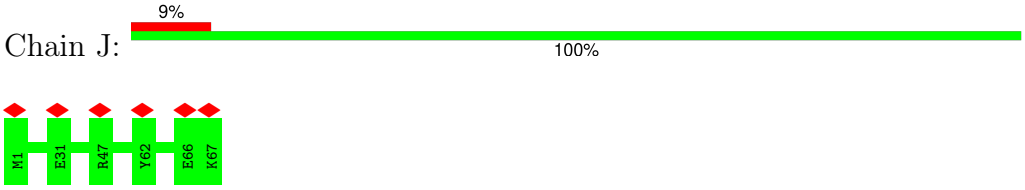
• Molecule 13: DNA-directed RNA polymerase II subunit RPB9

Chain I:



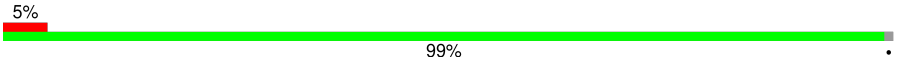
• Molecule 14: DNA-directed RNA polymerases I, II, and III subunit RPABC5

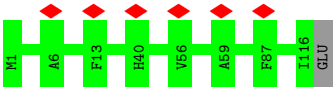
Chain J:



• Molecule 15: DNA-directed RNA polymerase II subunit RPB11-a

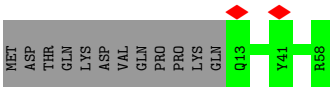
Chain K:





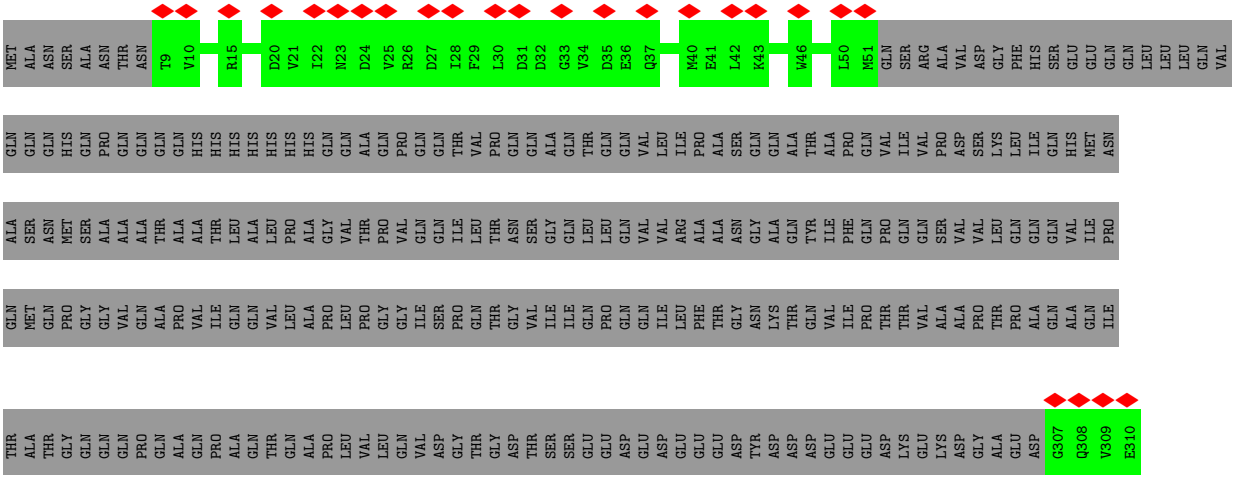
• Molecule 16: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:



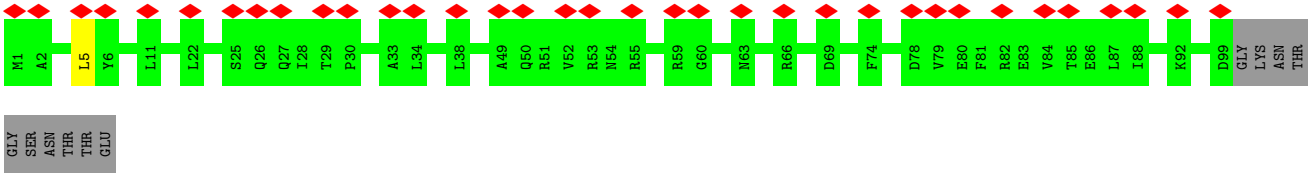
• Molecule 17: Transcription initiation factor IIA subunit 1

Chain M:



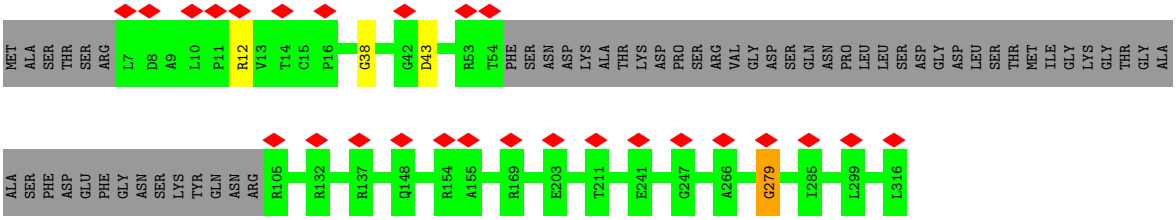
• Molecule 18: Transcription initiation factor IIA subunit 2

Chain N:



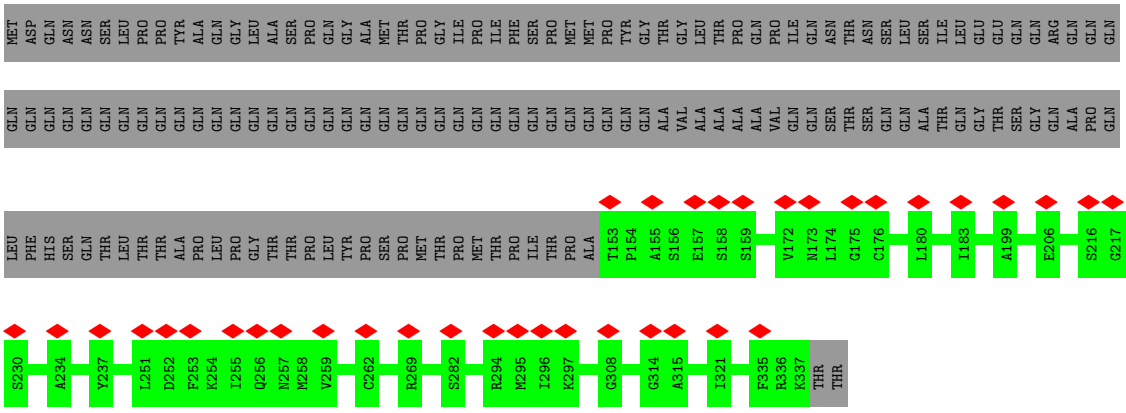
• Molecule 19: Transcription initiation factor IIB

Chain O:



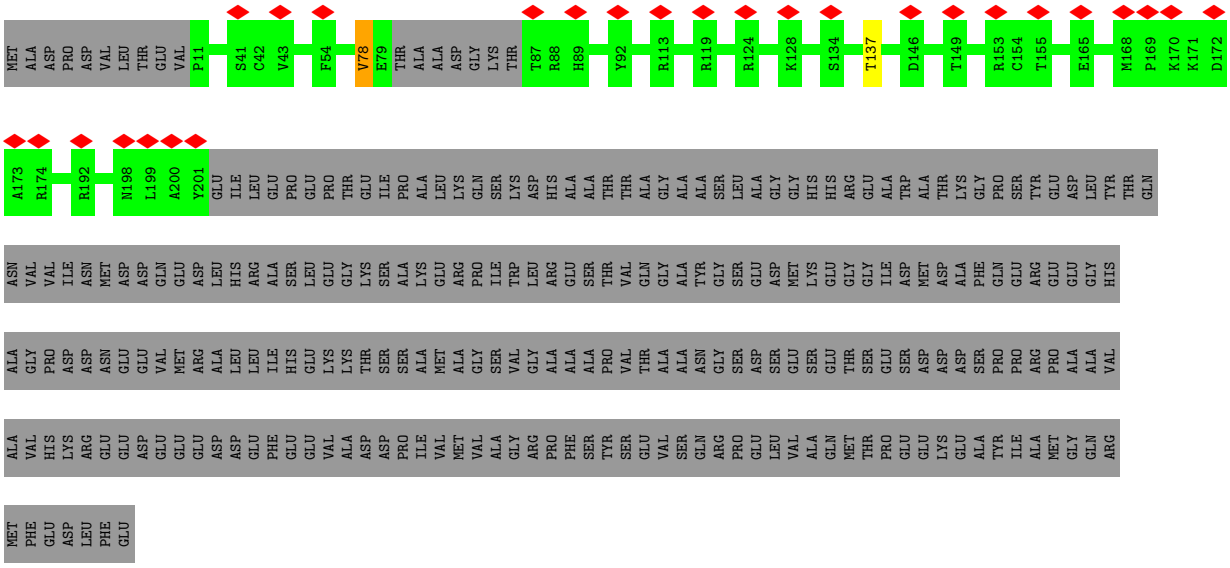
• Molecule 20: TATA-box-binding protein

Chain P:



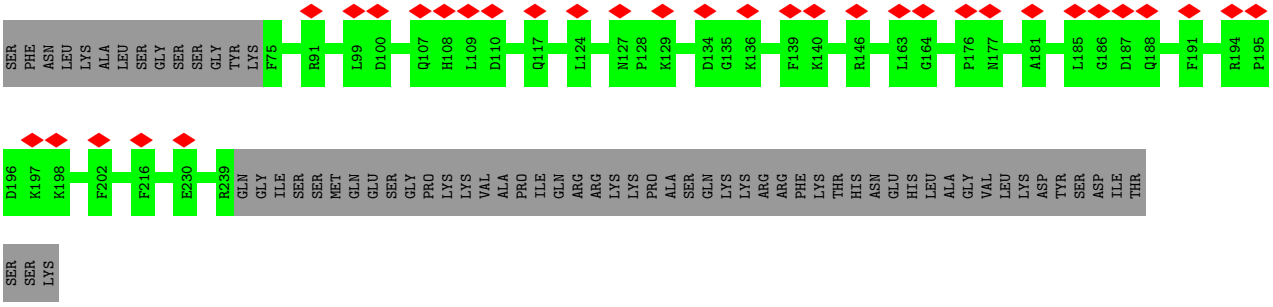
• Molecule 21: General transcription factor IIE subunit 1

Chain Q:



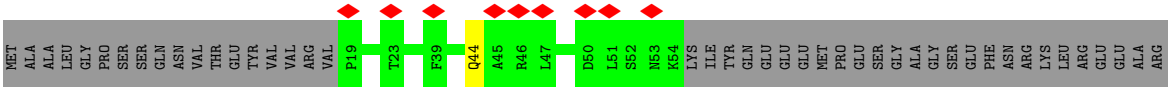
• Molecule 22: Transcription initiation factor IIE subunit beta

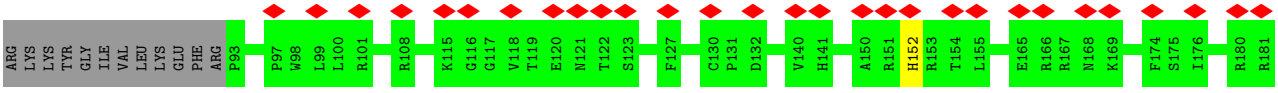
Chain R:

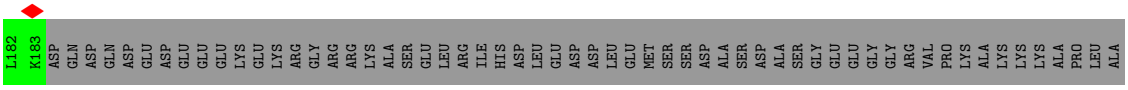


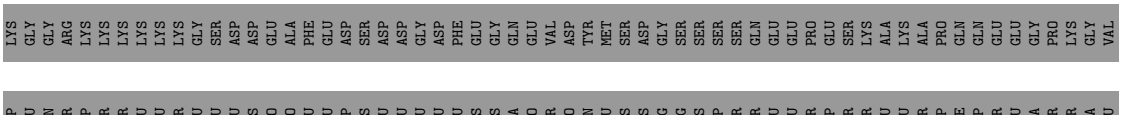
• Molecule 23: General transcription factor IIF subunit 1

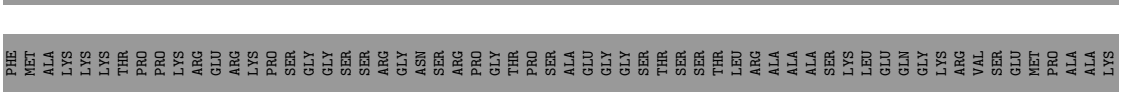
Chain S:

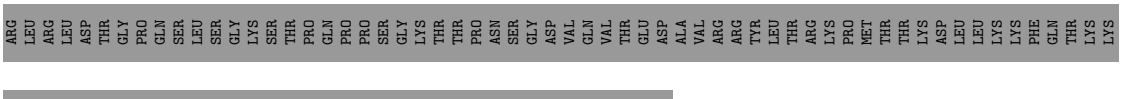


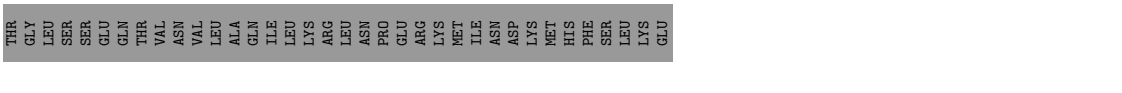


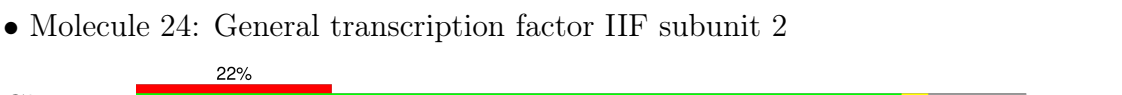


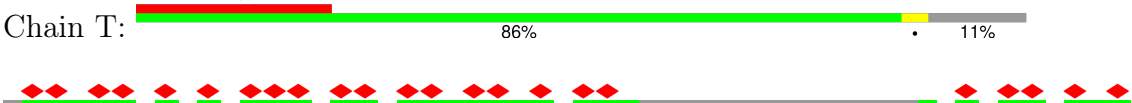


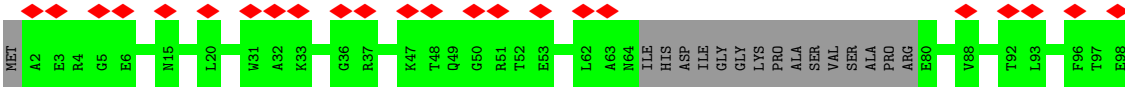


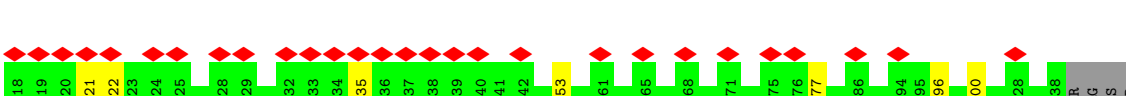


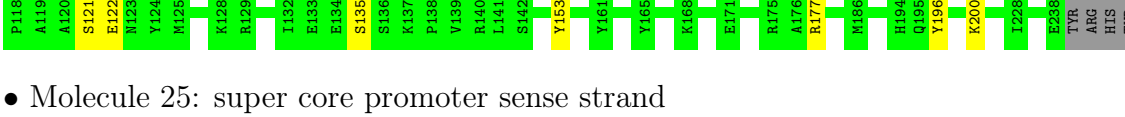


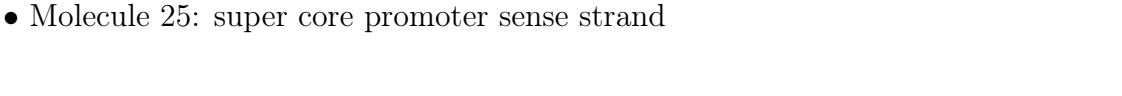










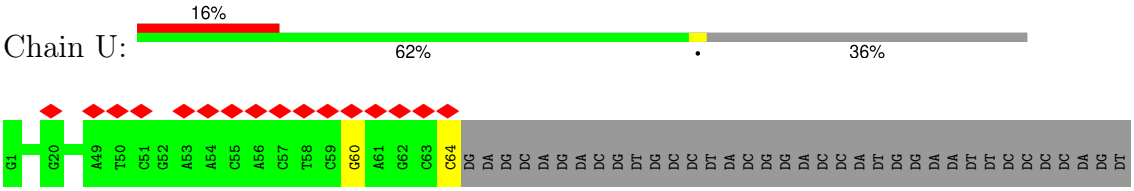


• Molecule 24: General transcription factor IIF subunit 2

Chain T:

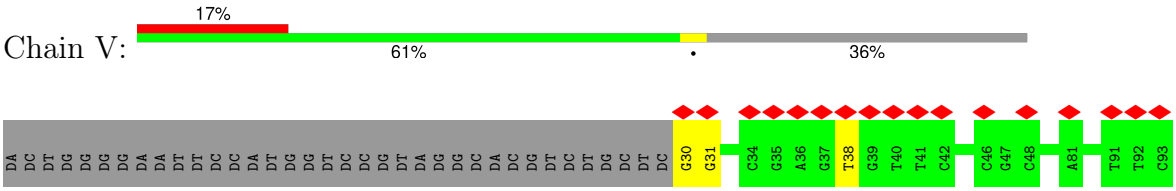
• Molecule 25: super core promoter sense strand

Chain U:



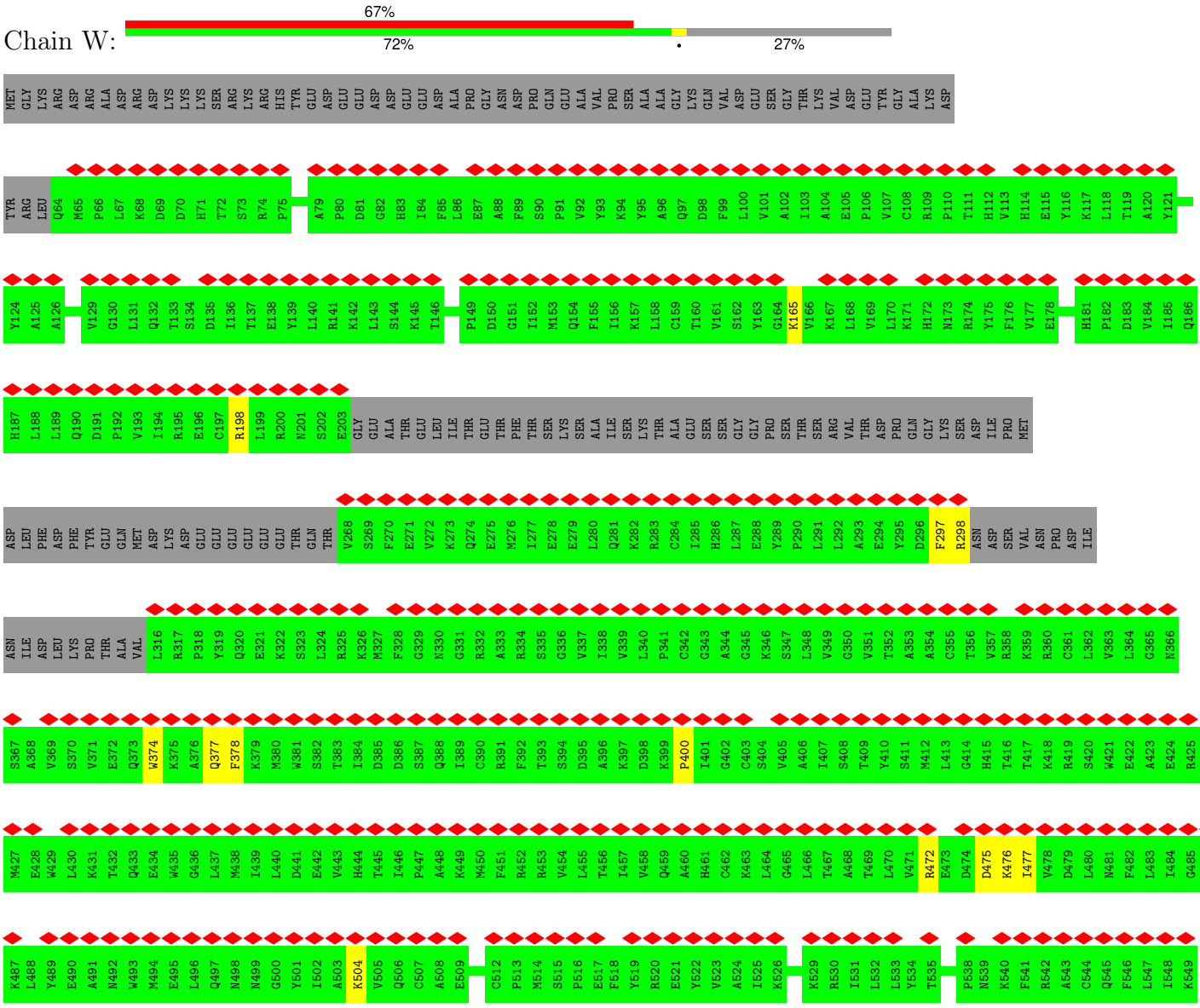
• Molecule 26: super core promoter antisense strand

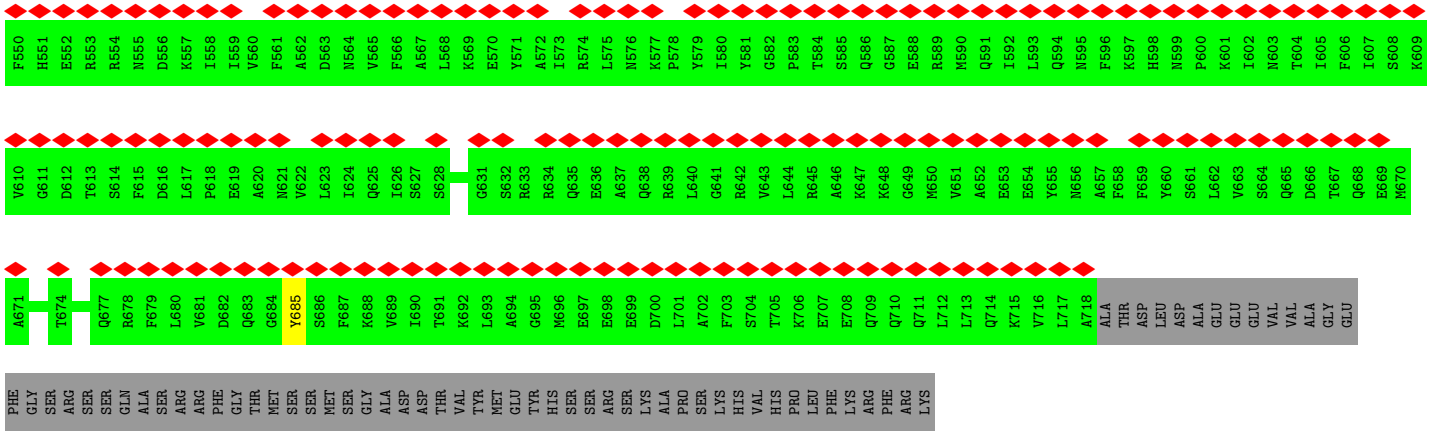
Chain V:



• Molecule 27: TFIIH basal transcription factor complex helicase XPB subunit

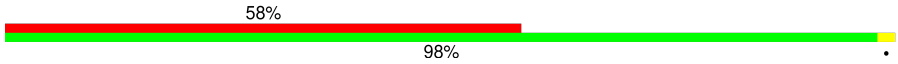
Chain W:

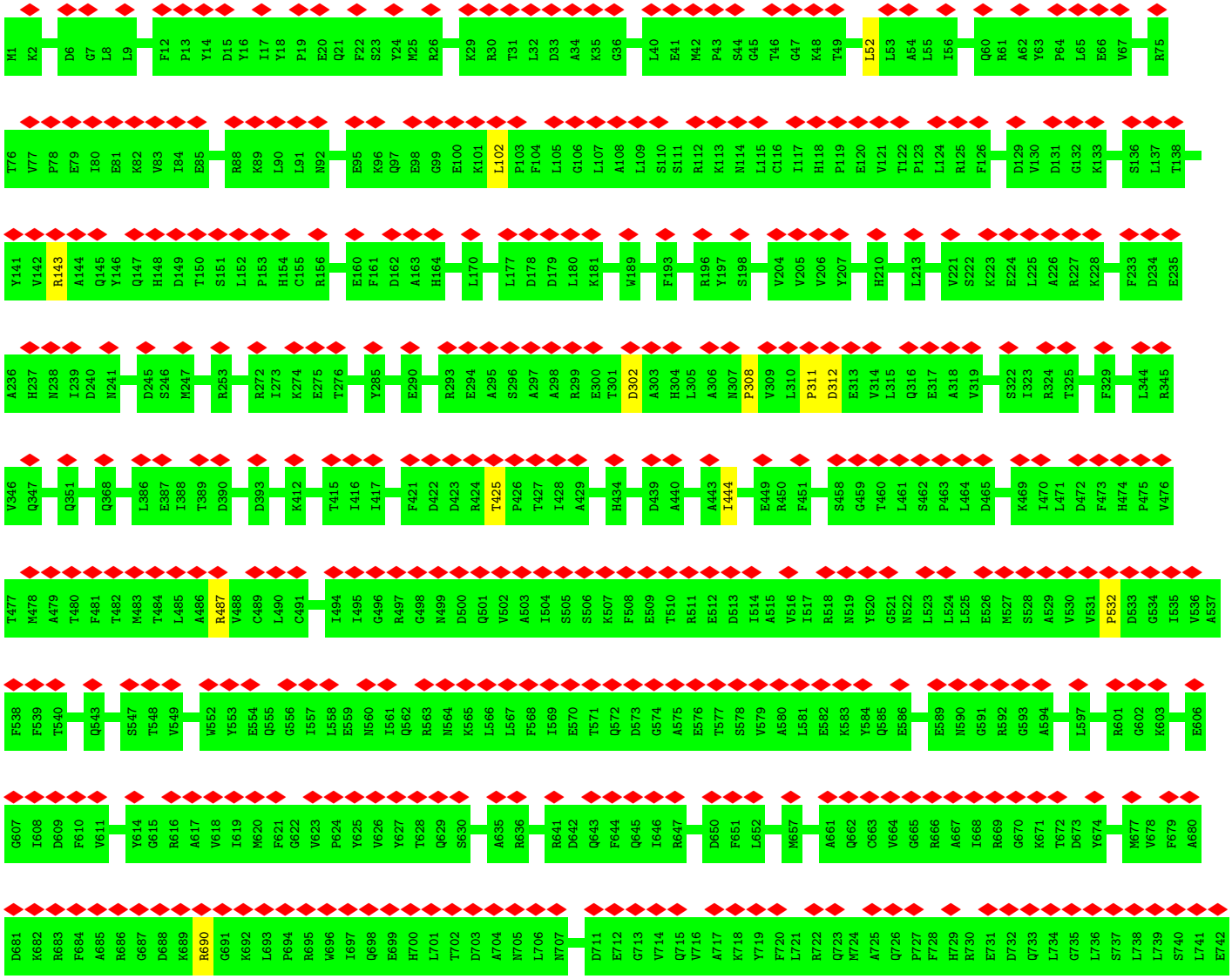


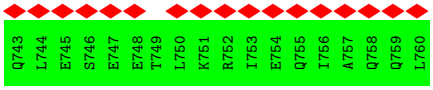


• Molecule 28: TFIIH basal transcription factor complex helicase XPD subunit

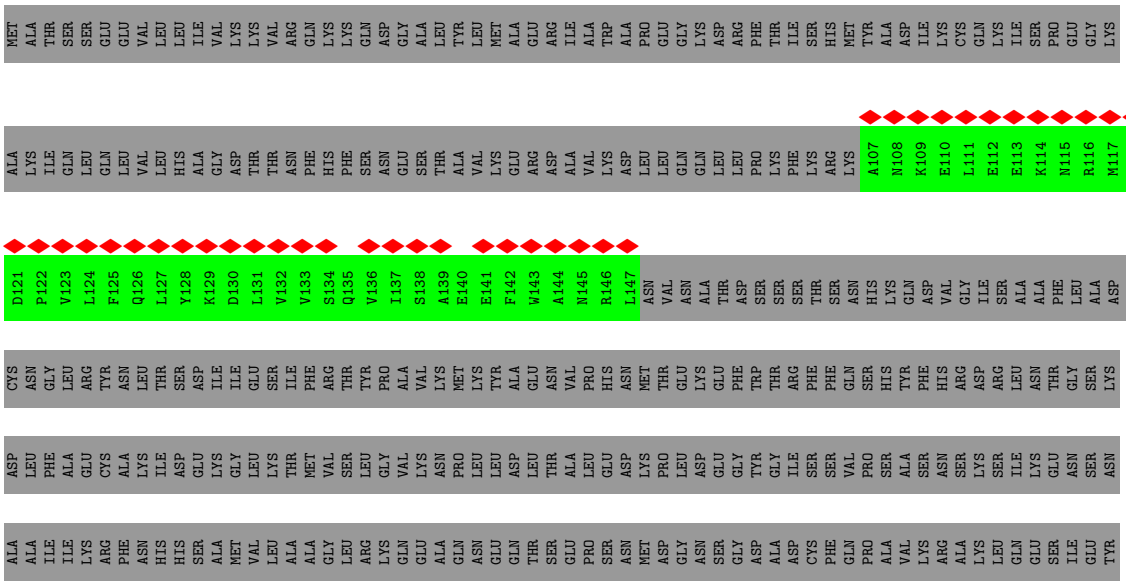
Chain X:

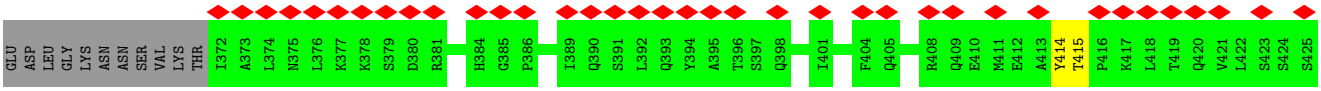


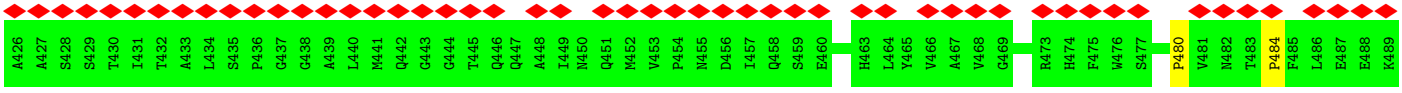


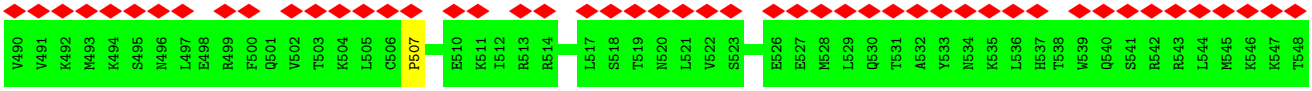


• Molecule 29: General transcription factor IIH subunit 1

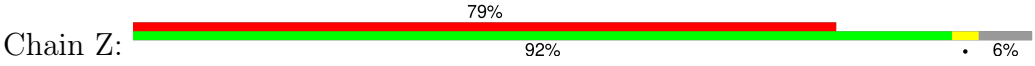


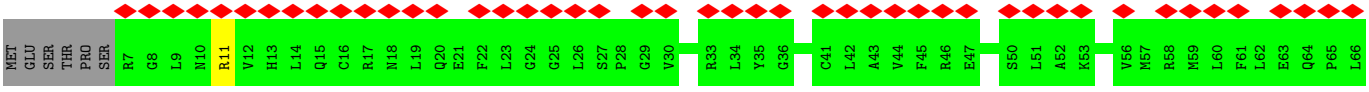


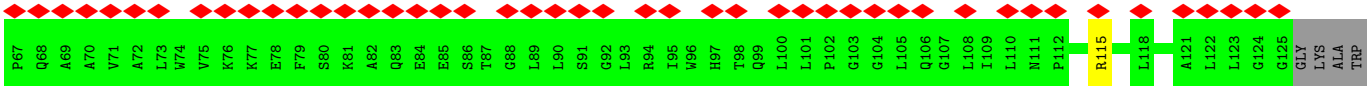


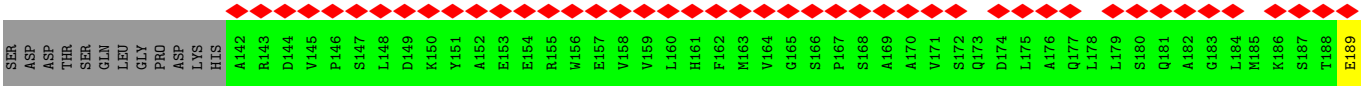


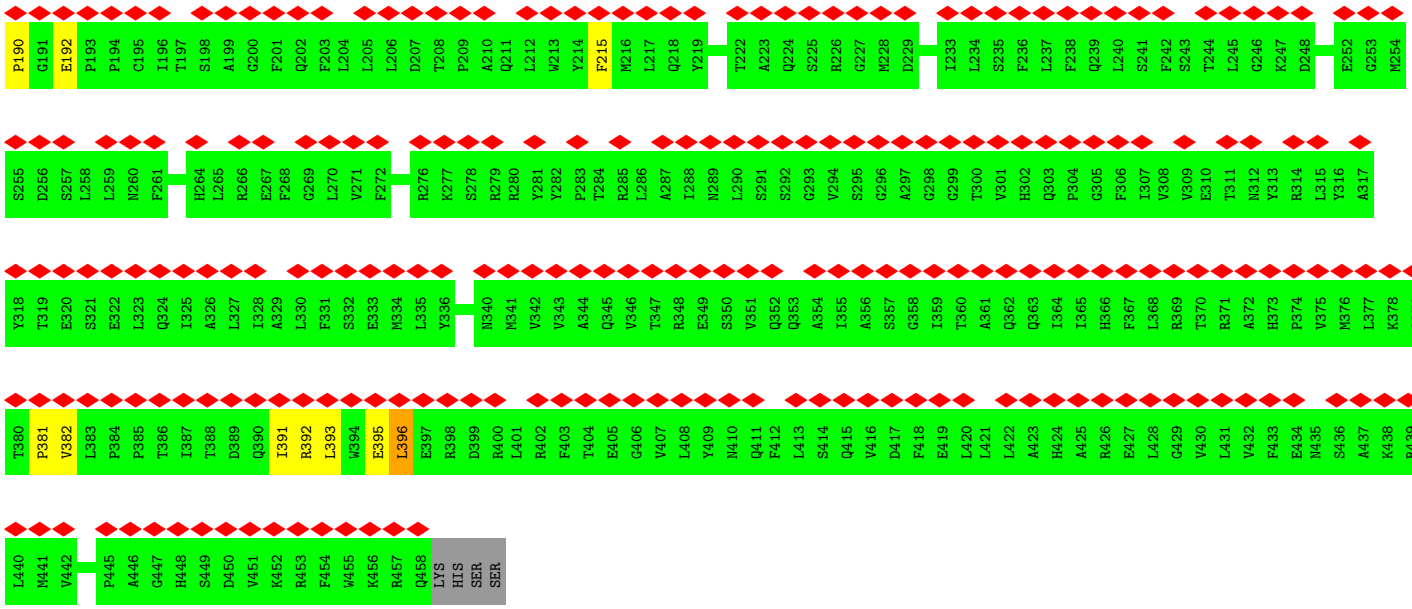
• Molecule 30: General transcription factor IIH subunit 4, p52





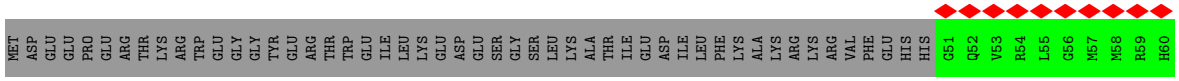


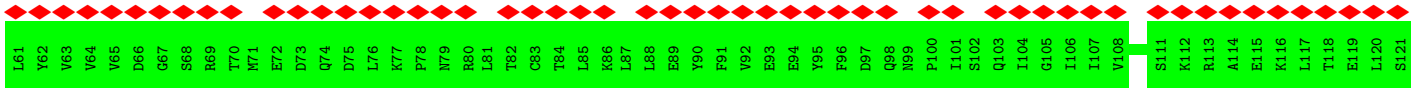


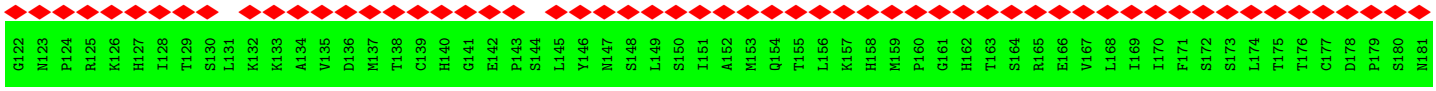


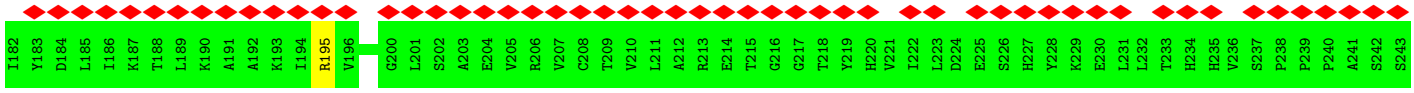
• Molecule 31: General transcription factor IIH subunit 2

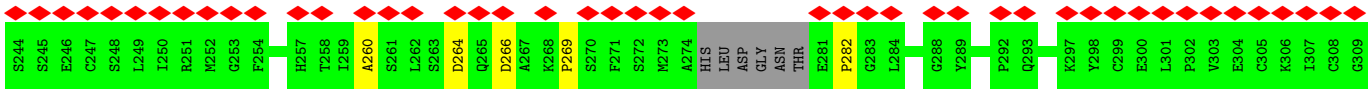
Chain a:

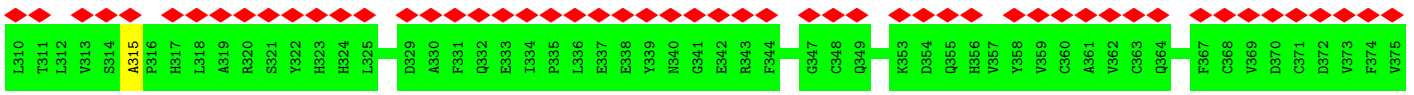


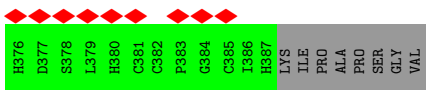






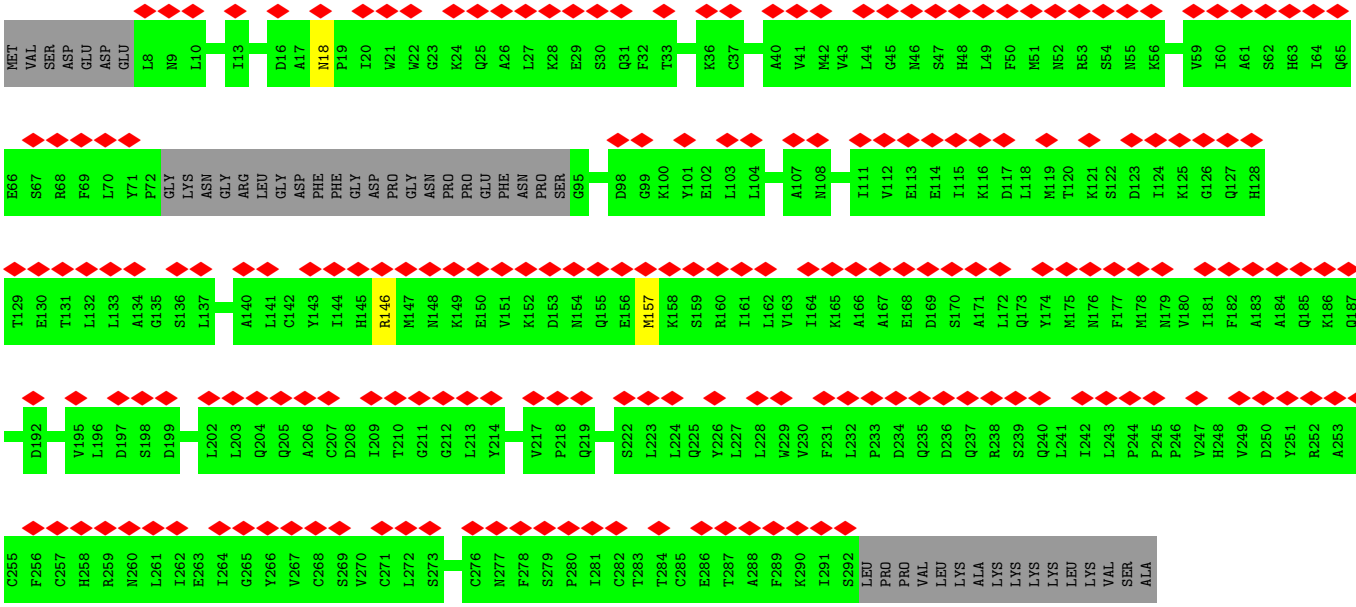






• Molecule 32: General transcription factor IIH subunit 3

Chain b:

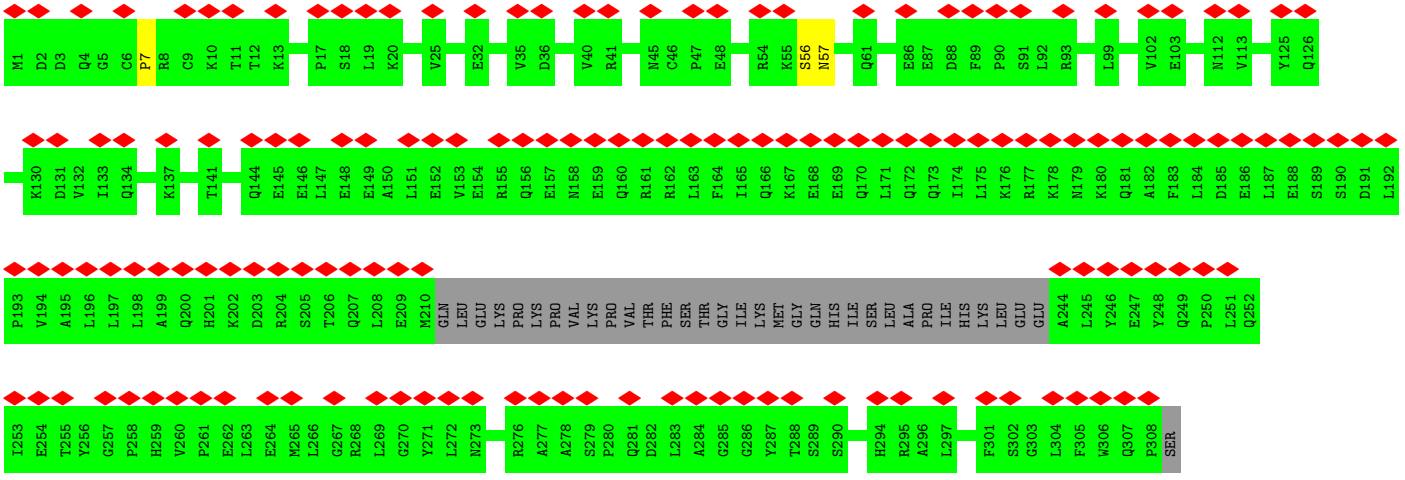


• Molecule 33: General transcription factor IIH subunit 5

Chain c:

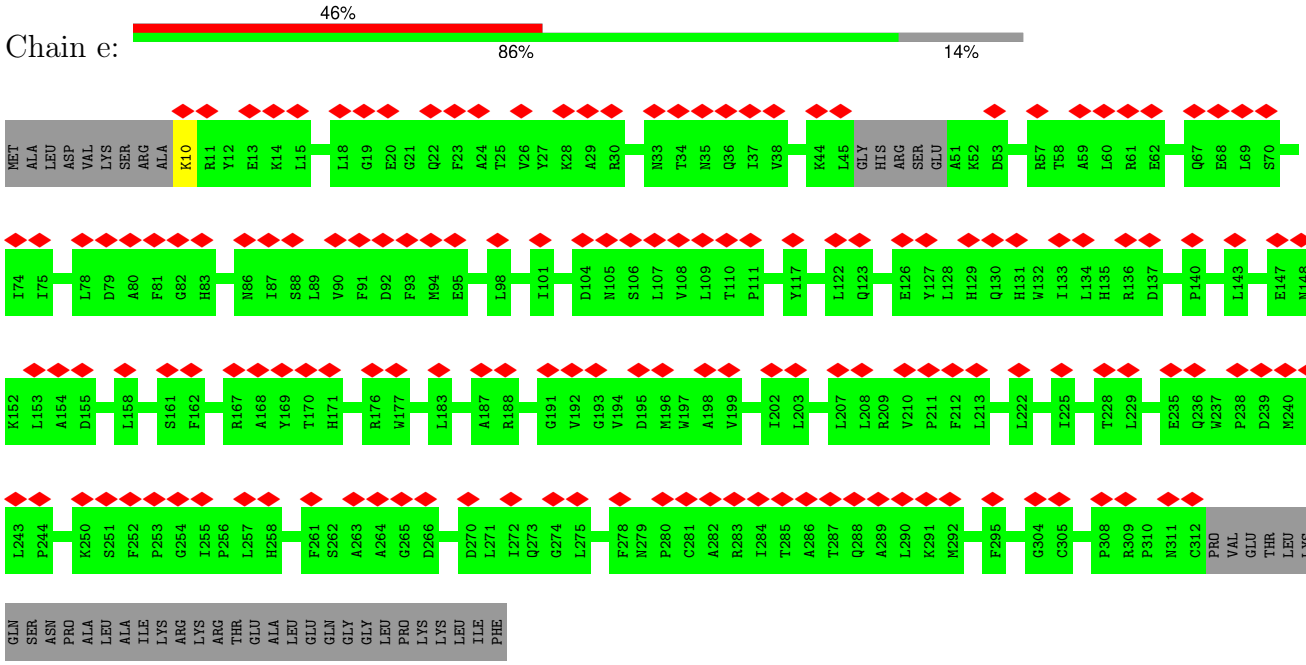
• Molecule 34: CDK-activating kinase assembly factor MAT1

Chain d:



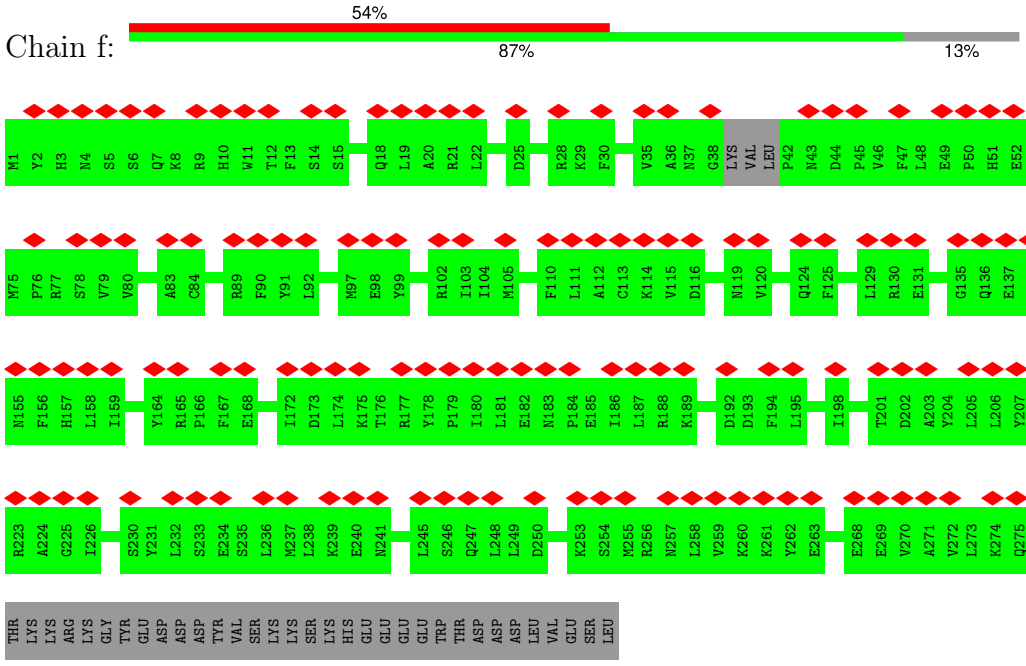
• Molecule 35: Cyclin-dependent kinase 7

Chain e:



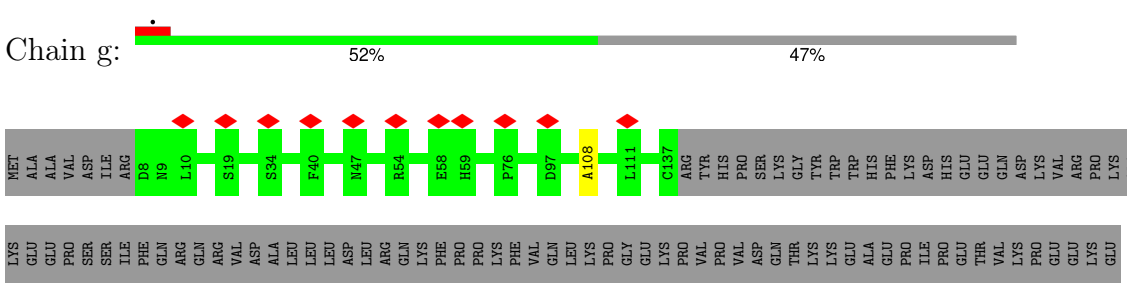
• Molecule 36: Cyclin-H

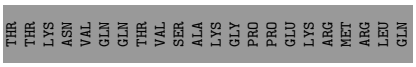
Chain f:



• Molecule 37: Mediator of RNA polymerase II transcription subunit 6

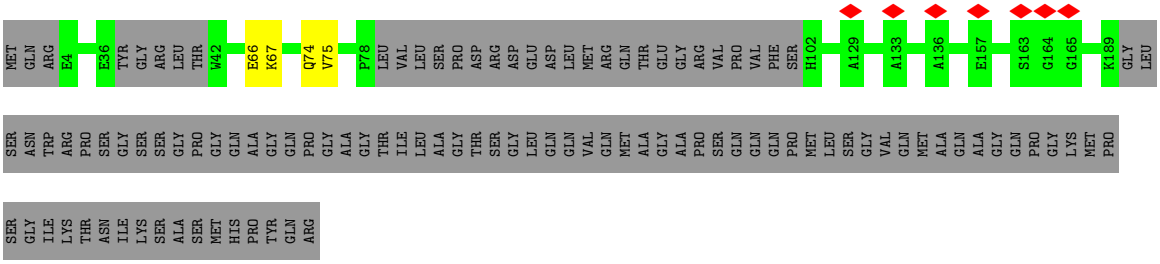
Chain g:





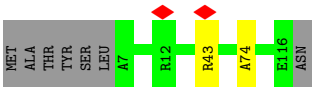
• Molecule 38: Mediator of RNA polymerase II transcription subunit 8

Chain h:



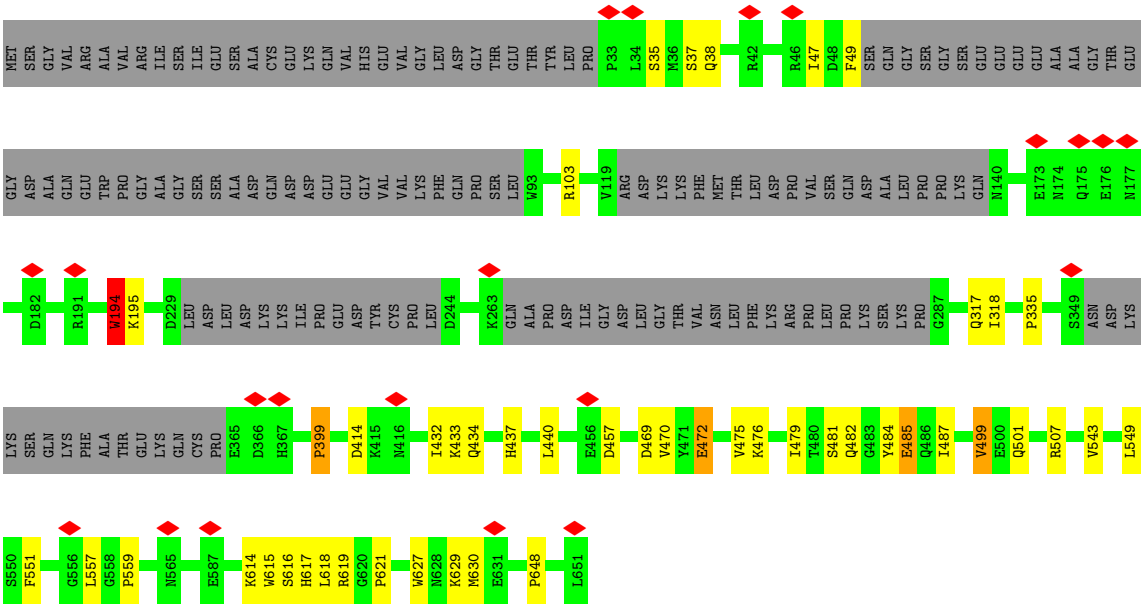
• Molecule 39: Mediator of RNA polymerase II transcription subunit 11

Chain i:



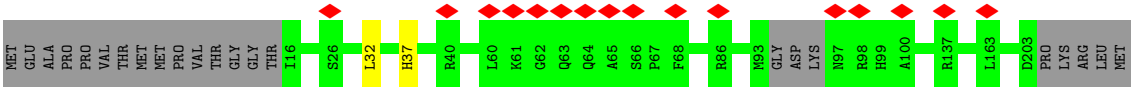
• Molecule 40: Mediator of RNA polymerase II transcription subunit 17

Chain j:

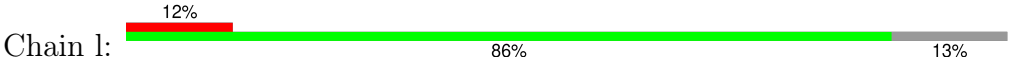


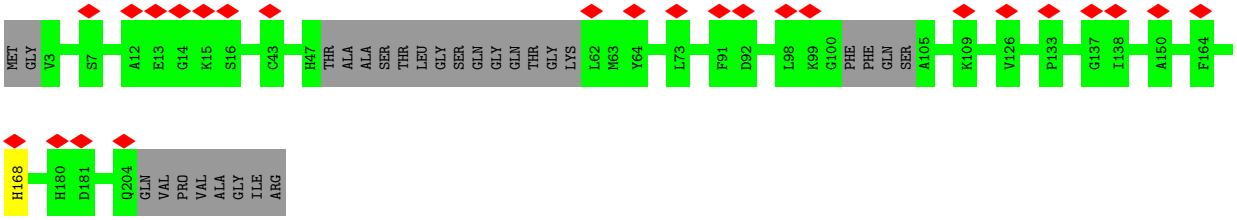
• Molecule 41: Mediator of RNA polymerase II transcription subunit 18

Chain k:

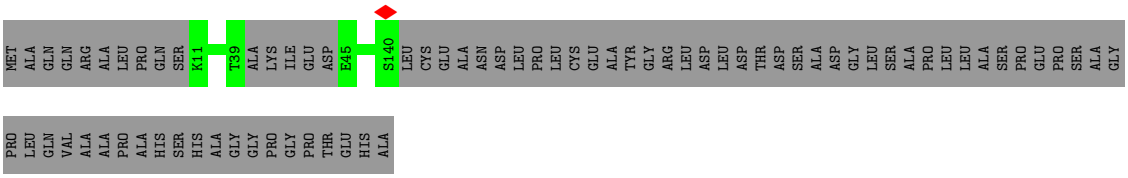


• Molecule 42: Mediator of RNA polymerase II transcription subunit 20

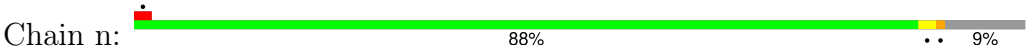


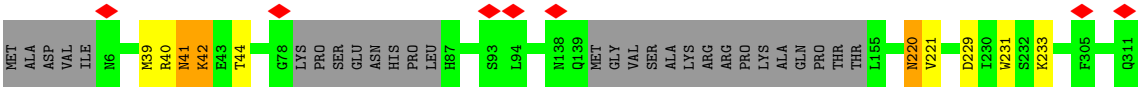


• Molecule 43: Mediator of RNA polymerase II transcription subunit 22

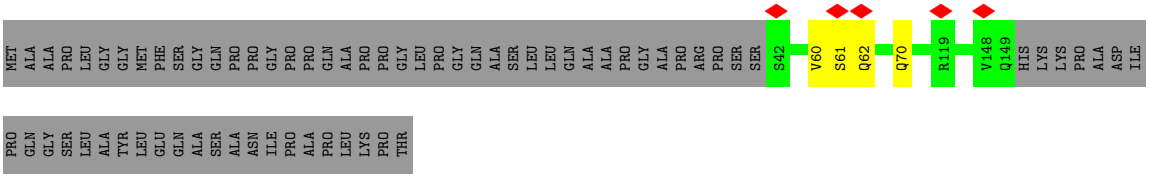


• Molecule 44: Mediator of RNA polymerase II transcription subunit 27

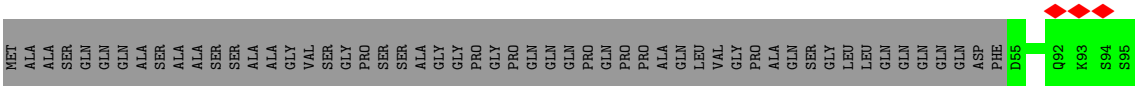


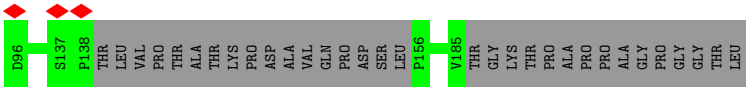


• Molecule 45: Mediator of RNA polymerase II transcription subunit 28



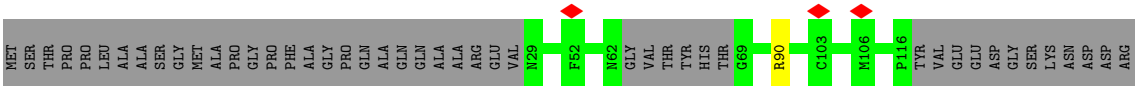
• Molecule 46: Mediator of RNA polymerase II transcription subunit 29





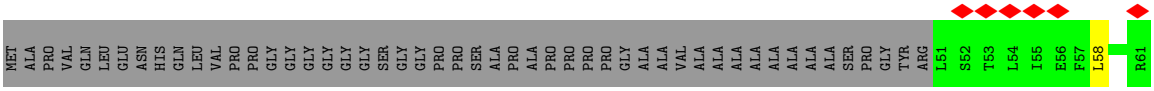
• Molecule 47: Mediator of RNA polymerase II transcription subunit 30

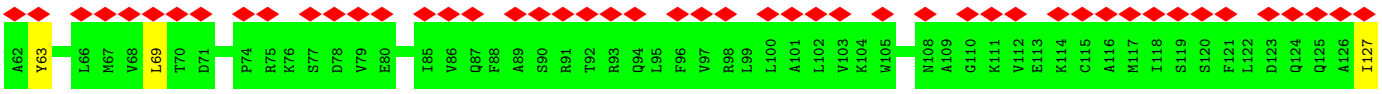
Chain q:

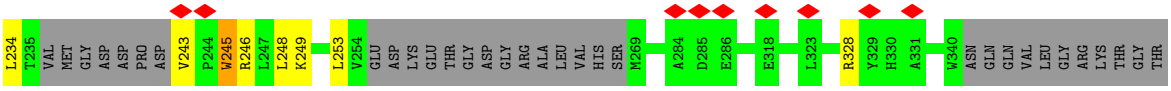


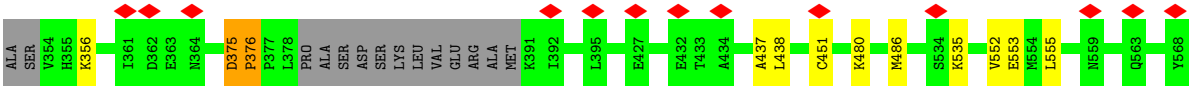
• Molecule 48: Mediator of RNA polymerase II transcription subunit 14

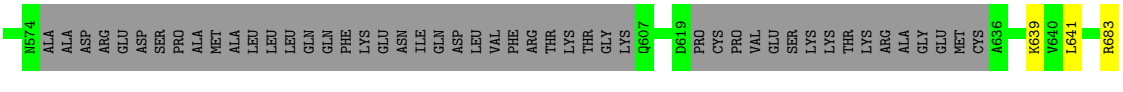
Chain r:

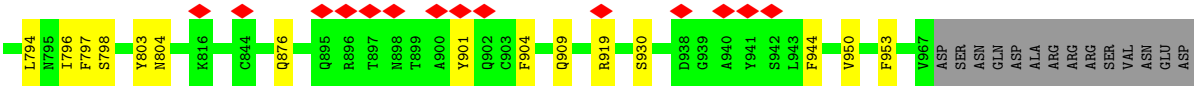


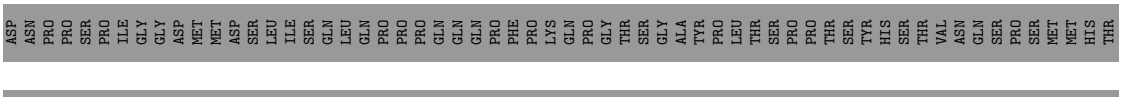


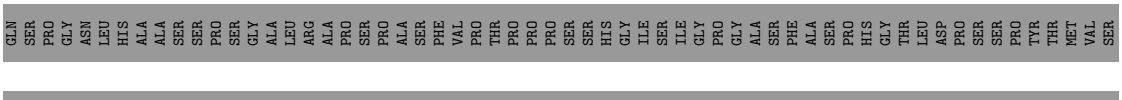


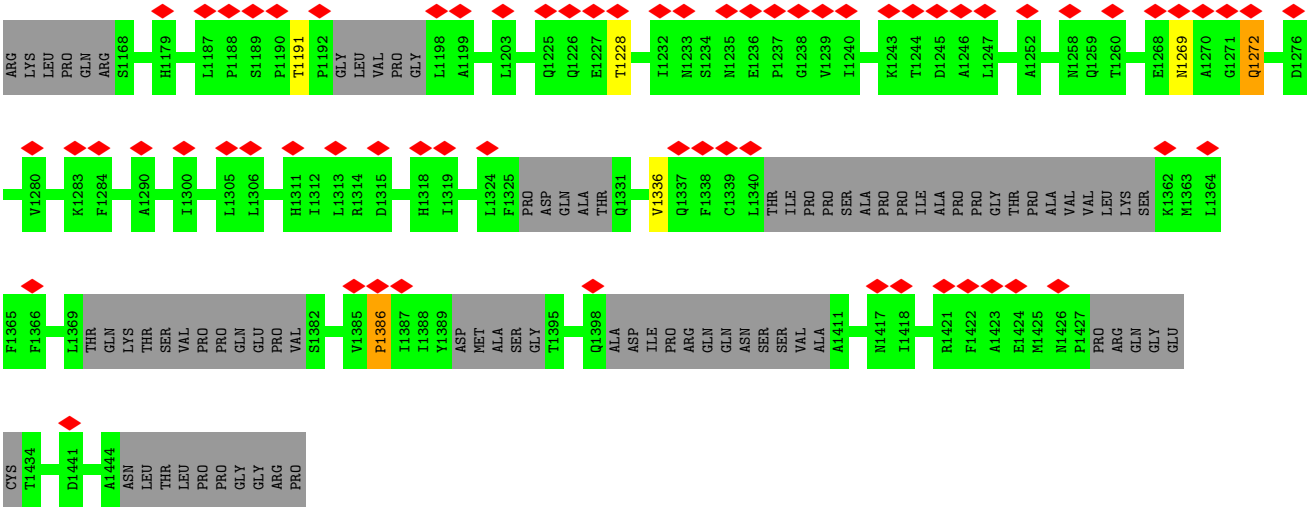






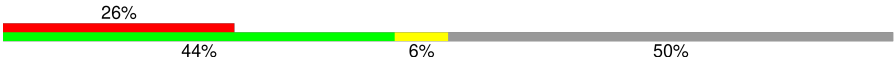


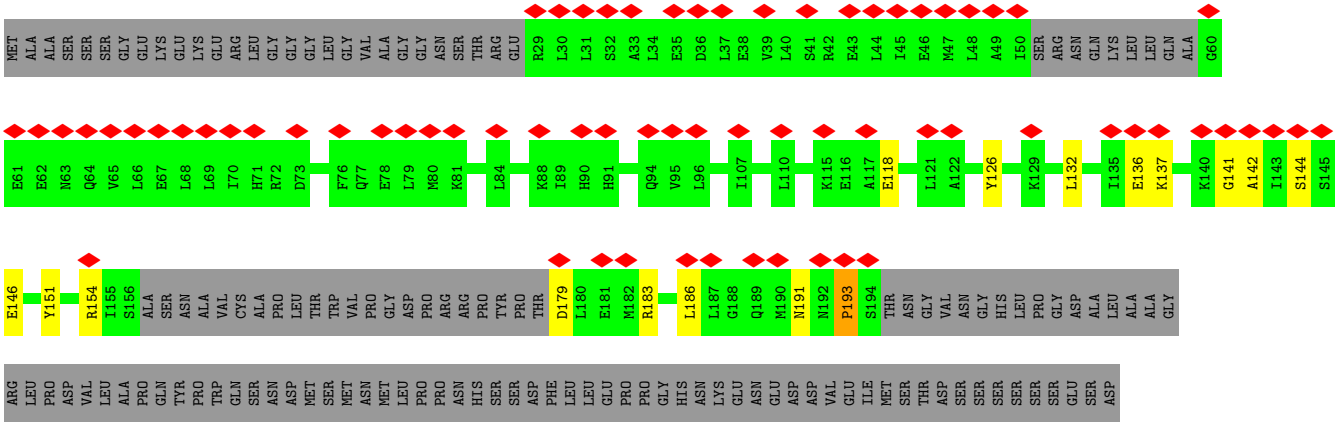




• Molecule 49: Mediator of RNA polymerase II transcription subunit 4

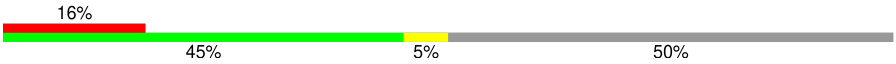
Chain s:

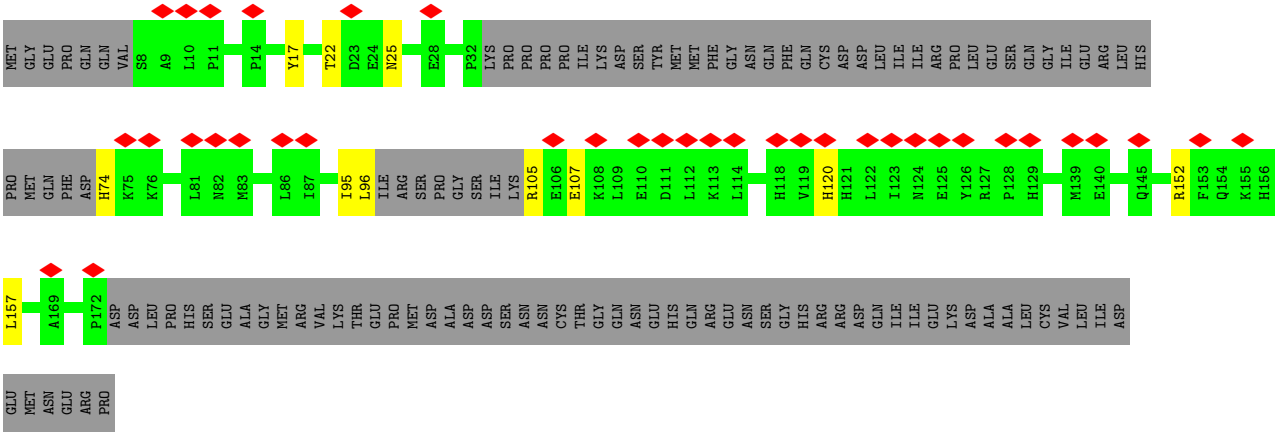




• Molecule 50: Mediator of RNA polymerase II transcription subunit 7

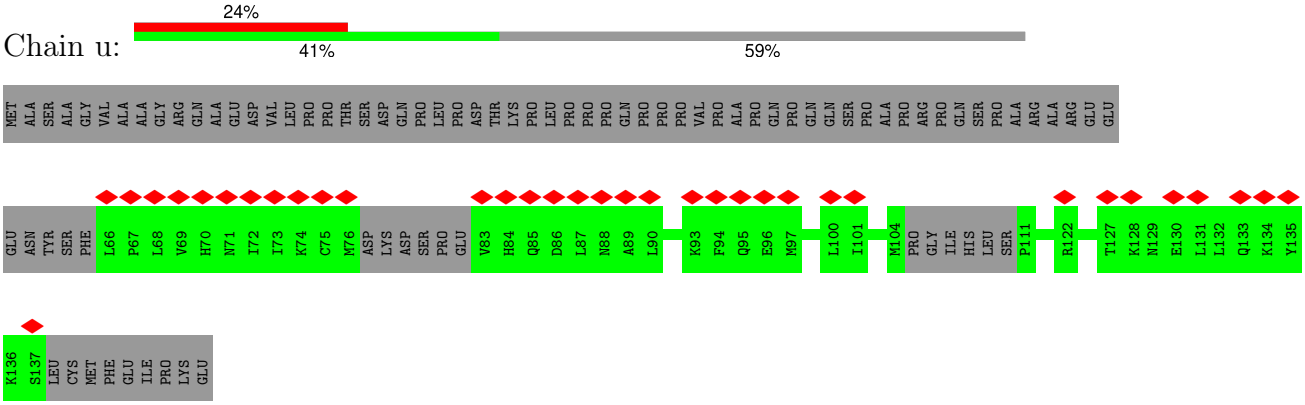
Chain t:





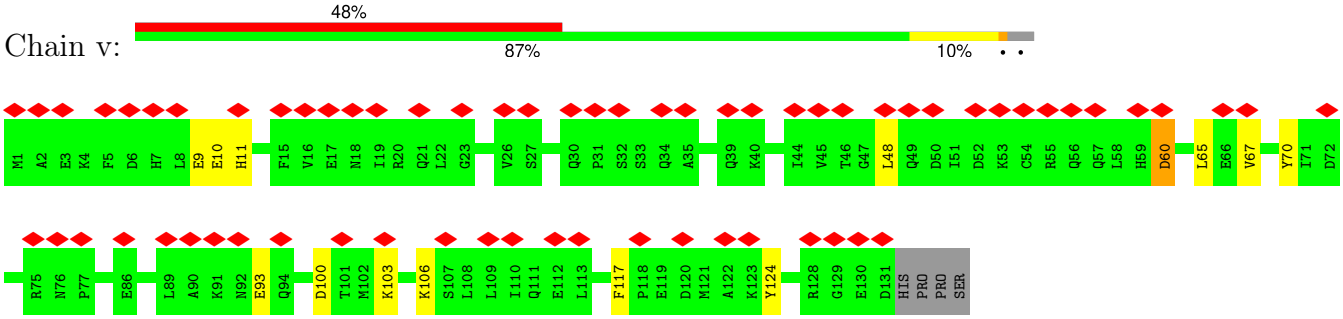
• Molecule 51: Mediator of RNA polymerase II transcription subunit 9

Chain u:



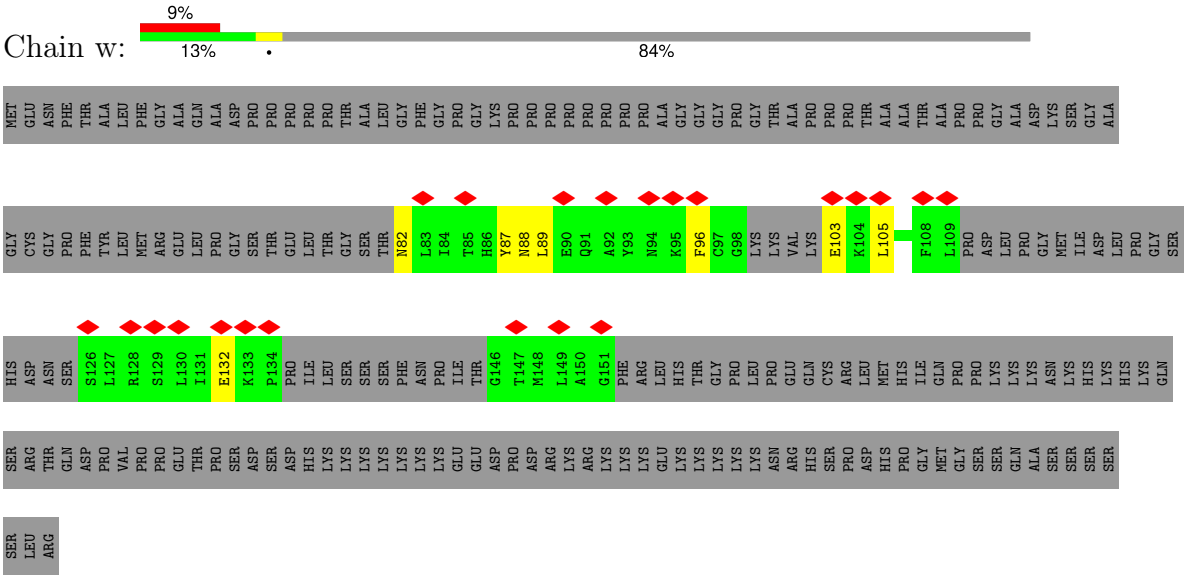
• Molecule 52: Mediator of RNA polymerase II transcription subunit 10

Chain v:



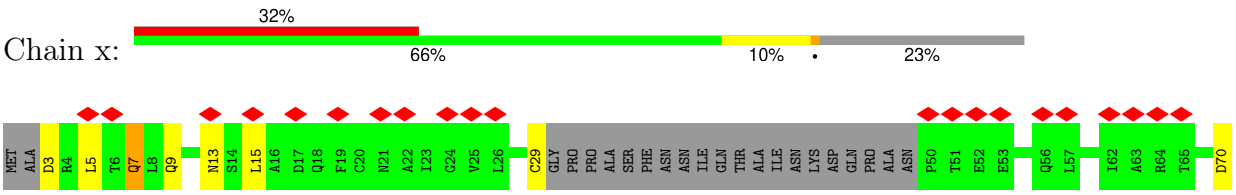
• Molecule 53: Mediator of RNA polymerase II transcription subunit 19

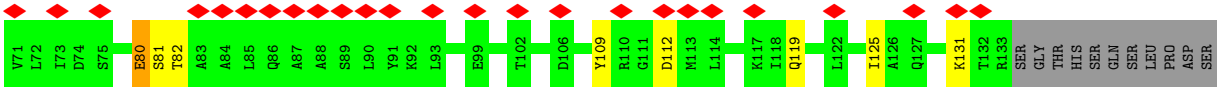
Chain w:



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

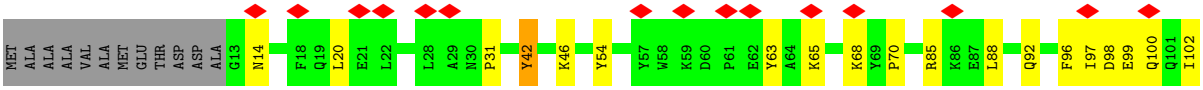
Chain x:

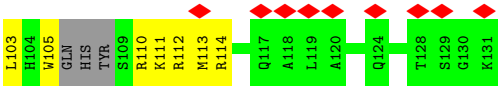




• Molecule 55: Mediator of RNA polymerase II transcription subunit 31

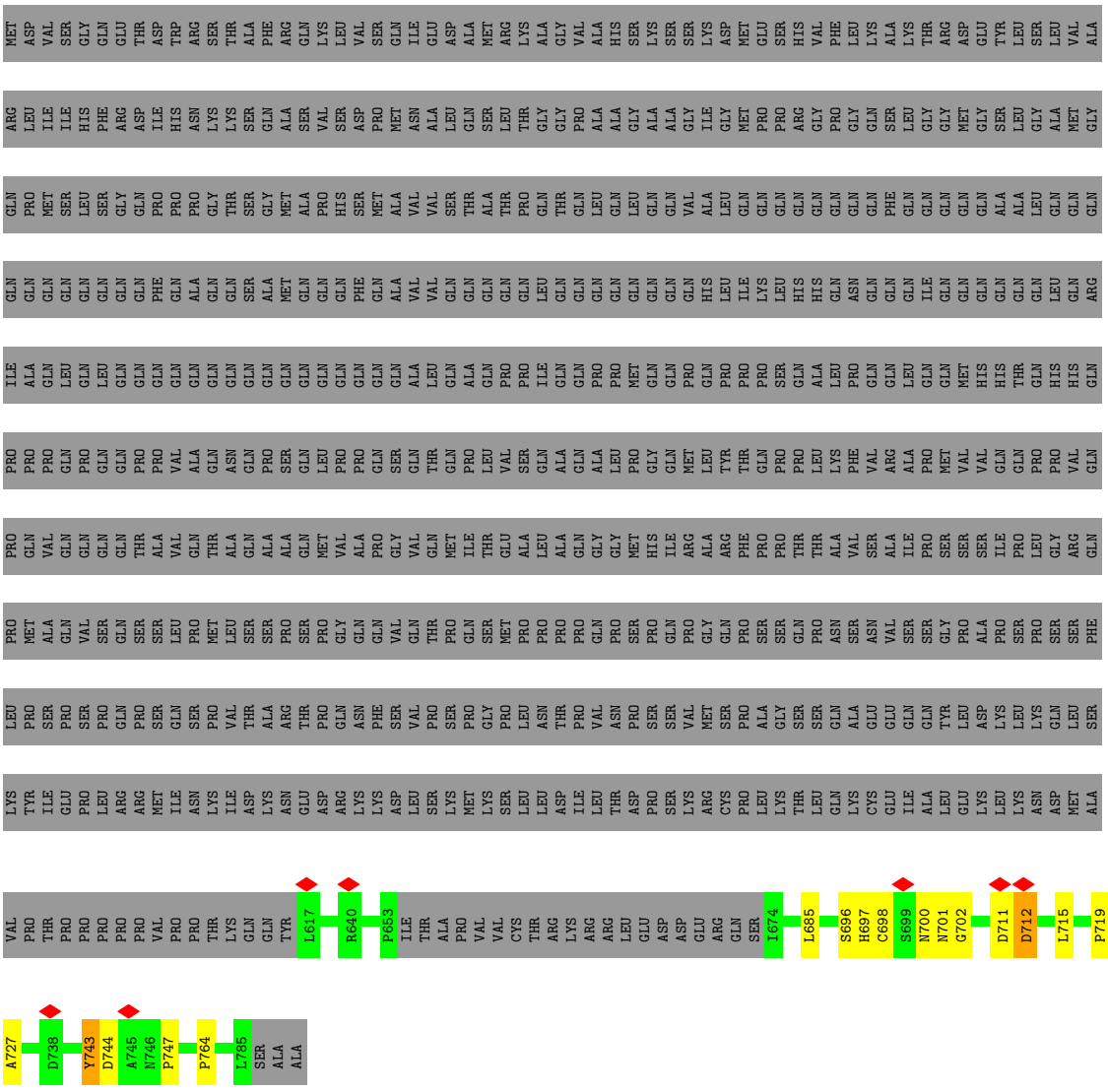
Chain y:





• Molecule 56: Mediator of RNA polymerase II transcription subunit 15

Chain z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	156383	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	31.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.116	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	444.78, 444.78, 444.78	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	0	0.67	12/5990 (0.2%)	0.62	3/8137 (0.0%)
2	1	0.40	0/10913	0.47	0/14828
3	2	0.45	2/7141 (0.0%)	0.53	1/9672 (0.0%)
4	3	0.62	0/1540	0.63	1/2093 (0.0%)
5	A	0.37	0/11733	0.53	3/15844 (0.0%)
6	B	0.39	0/9310	0.49	0/12567
7	C	0.40	0/2190	0.51	0/2975
8	D	0.29	0/1077	0.49	0/1446
9	E	0.34	0/1753	0.47	0/2368
10	F	0.39	0/700	0.48	0/946
11	G	0.34	0/1382	0.49	0/1874
12	H	0.39	0/1227	0.52	0/1654
13	I	0.34	0/964	0.53	0/1305
14	J	0.45	0/542	0.51	0/730
15	K	0.37	0/947	0.48	0/1282
16	L	0.38	0/394	0.50	0/524
17	M	0.27	0/945	0.53	0/1274
18	N	0.27	0/816	0.54	0/1105
19	O	0.33	0/2049	0.49	0/2769
20	P	0.30	0/1489	0.50	0/2005
21	Q	0.28	0/1545	0.51	0/2075
22	R	0.27	0/1380	0.53	0/1854
23	S	0.29	0/1086	0.55	0/1461
24	T	0.28	0/1817	0.55	0/2445
25	U	0.58	2/1485 (0.1%)	0.84	0/2293
26	V	0.59	3/1454 (0.2%)	0.87	0/2239
27	W	0.40	0/4744	0.60	0/6402
28	X	0.45	0/6236	0.68	6/8444 (0.1%)
29	Y	0.37	0/1660	0.66	4/2253 (0.2%)
30	Z	0.40	0/3552	0.62	1/4814 (0.0%)
31	a	0.43	0/2637	0.68	4/3572 (0.1%)
32	b	0.39	0/2102	0.56	0/2844

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	c	0.33	0/528	0.63	0/713
34	d	0.35	0/2137	0.55	0/2890
35	e	0.38	0/2434	0.55	0/3300
36	f	0.40	0/2342	0.48	0/3159
37	g	0.30	0/1058	0.50	0/1441
38	h	0.33	0/1245	0.52	0/1679
39	i	0.34	0/869	0.45	0/1168
40	j	0.69	3/4079 (0.1%)	0.72	5/5504 (0.1%)
41	k	0.40	0/1512	0.53	0/2034
42	l	0.41	0/1453	0.53	0/1963
43	m	0.43	0/1032	0.49	0/1385
44	n	0.61	2/2324 (0.1%)	0.60	2/3143 (0.1%)
45	o	0.41	0/897	0.51	0/1208
46	p	0.42	0/906	0.46	0/1222
47	q	0.40	0/1015	0.52	0/1360
48	r	0.60	3/8336 (0.0%)	0.69	8/11299 (0.1%)
49	s	0.85	3/1089 (0.3%)	0.93	3/1450 (0.2%)
50	t	1.02	3/991 (0.3%)	0.98	4/1331 (0.3%)
51	u	0.49	0/504	0.61	0/668
52	v	0.99	5/1082 (0.5%)	0.91	5/1450 (0.3%)
53	w	0.75	0/311	0.94	2/412 (0.5%)
54	x	0.92	1/858 (0.1%)	0.98	3/1161 (0.3%)
55	y	0.93	1/1027 (0.1%)	0.80	1/1379 (0.1%)
56	z	0.77	2/1202 (0.2%)	0.83	6/1650 (0.4%)
All	All	0.48	42/132031 (0.0%)	0.59	62/179063 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	4
3	2	0	5
4	3	0	2
5	A	0	1
6	B	0	3
7	C	0	1
8	D	0	2
13	I	0	2
17	M	0	1
19	O	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
21	Q	0	1
23	S	0	1
27	W	0	3
28	X	0	3
29	Y	0	1
30	Z	0	2
31	a	0	2
34	d	0	1
37	g	0	1
38	h	0	1
39	i	0	1
40	j	0	9
44	n	0	4
45	o	0	2
48	r	0	13
49	s	0	5
50	t	0	3
52	v	0	1
53	w	0	4
54	x	0	5
55	y	0	1
56	z	0	1
All	All	0	88

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	n	231	TRP	CB-CG	-11.19	1.30	1.50
1	0	834	TRP	CB-CG	-10.76	1.30	1.50
1	0	833	TRP	CB-CG	-10.23	1.31	1.50
40	j	615	TRP	CB-CG	-10.02	1.32	1.50
1	0	833	TRP	CG-CD1	-9.55	1.23	1.36
48	r	245	TRP	C-N	8.54	1.53	1.34
52	v	93	GLU	CB-CG	-8.35	1.36	1.52
52	v	124	TYR	CB-CG	-7.78	1.40	1.51
50	t	17	TYR	CD1-CE1	-7.69	1.27	1.39
1	0	829	CYS	CB-SG	-7.69	1.69	1.82
1	0	833	TRP	CD2-CE2	-7.60	1.32	1.41
1	0	834	TRP	CG-CD1	-6.64	1.27	1.36
52	v	124	TYR	CD2-CE2	-6.64	1.29	1.39
52	v	70	TYR	CD2-CE2	-6.54	1.29	1.39
44	n	231	TRP	CG-CD1	-6.39	1.27	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	v	117	PHE	C-N	-6.38	1.22	1.34
1	0	17	TYR	CE1-CZ	-6.28	1.30	1.38
3	2	305	TRP	CG-CD1	-6.24	1.28	1.36
1	0	21	TRP	CD2-CE2	-6.18	1.33	1.41
54	x	80	GLU	CB-CG	6.06	1.63	1.52
48	r	944	PHE	CG-CD1	-5.90	1.29	1.38
50	t	17	TYR	CE1-CZ	-5.77	1.31	1.38
1	0	21	TRP	CB-CG	-5.71	1.40	1.50
26	V	31	DG	C1'-N9	-5.67	1.39	1.47
49	s	191	ASN	CB-CG	-5.58	1.38	1.51
25	U	60	DG	C1'-N9	-5.52	1.39	1.47
56	z	719	PRO	CA-C	-5.42	1.42	1.52
26	V	30	DG	C1'-N9	-5.39	1.39	1.47
1	0	833	TRP	CE2-CZ2	-5.37	1.30	1.39
3	2	305	TRP	CE2-CZ2	-5.37	1.30	1.39
40	j	615	TRP	CG-CD1	-5.33	1.29	1.36
48	r	175	ASP	CB-CG	-5.33	1.40	1.51
55	y	42	TYR	CB-CG	-5.32	1.43	1.51
26	V	38	DT	C1'-N1	5.29	1.56	1.49
1	0	21	TRP	CG-CD1	-5.23	1.29	1.36
40	j	440	LEU	CA-C	-5.20	1.39	1.52
1	0	834	TRP	CE2-CZ2	-5.16	1.30	1.39
50	t	17	TYR	CG-CD2	-5.15	1.32	1.39
49	s	126	TYR	CE2-CZ	-5.14	1.31	1.38
56	z	743	TYR	CE1-CZ	-5.11	1.31	1.38
25	U	64	DC	C1'-N1	5.03	1.55	1.49
49	s	151	TYR	CE2-CZ	-5.00	1.32	1.38

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	z	715	LEU	C-N-CD	-10.26	98.04	120.60
29	Y	480	PRO	CA-N-CD	-9.33	98.44	111.50
29	Y	484	PRO	CA-N-CD	-8.89	99.05	111.50
29	Y	507	PRO	CA-N-CD	-8.56	99.52	111.50
31	a	282	PRO	CA-N-CD	-8.37	99.78	111.50
28	X	308	PRO	CA-N-CD	-8.36	99.79	111.50
31	a	269	PRO	CA-N-CD	-8.36	99.79	111.50
28	X	311	PRO	CA-N-CD	-8.29	99.89	111.50
48	r	245	TRP	C-N-CA	-7.65	102.58	121.70
48	r	641	LEU	CA-CB-CG	-7.53	97.98	115.30
50	t	96	LEU	CA-CB-CG	7.44	132.40	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	x	112	ASP	CB-CG-OD1	-7.40	111.64	118.30
49	s	154	ARG	NE-CZ-NH1	7.18	123.89	120.30
52	v	60	ASP	CB-CG-OD1	6.98	124.58	118.30
48	r	63	TYR	CA-CB-CG	6.81	126.34	113.40
56	z	685	LEU	CB-CG-CD2	-6.74	99.54	111.00
1	0	829	CYS	CB-CA-C	-6.44	97.51	110.40
56	z	715	LEU	C-N-CA	6.43	149.00	122.00
48	r	58	LEU	CA-CB-CG	6.25	129.67	115.30
30	Z	396	LEU	N-CA-C	6.22	127.79	111.00
40	j	194	TRP	N-CA-C	6.14	127.58	111.00
28	X	444	ILE	CG1-CB-CG2	-6.09	98.00	111.40
40	j	499	VAL	CB-CA-C	-5.98	100.03	111.40
28	X	52	LEU	CA-CB-CG	5.96	129.01	115.30
3	2	303	LEU	CA-CB-CG	-5.96	101.59	115.30
54	x	119	GLN	CA-CB-CG	-5.91	100.40	113.40
44	n	231	TRP	N-CA-C	5.82	126.72	111.00
50	t	96	LEU	N-CA-C	-5.82	95.30	111.00
40	j	484	TYR	CB-CG-CD1	-5.74	117.56	121.00
52	v	65	LEU	CA-CB-CG	5.73	128.49	115.30
48	r	248	LEU	CA-CB-CG	-5.70	102.20	115.30
52	v	100	ASP	CB-CG-OD1	-5.66	113.20	118.30
54	x	7	GLN	O-C-N	-5.65	113.66	122.70
29	Y	414	TYR	C-N-CA	5.62	135.75	121.70
55	y	68	LYS	C-N-CA	-5.58	107.75	121.70
49	s	132	LEU	CA-CB-CG	5.44	127.80	115.30
1	0	62	ILE	CB-CA-C	-5.40	100.81	111.60
4	3	50	GLY	C-N-CD	-5.40	108.73	120.60
53	w	89	LEU	CA-CB-CG	5.38	127.67	115.30
31	a	266	ASP	CB-CG-OD2	5.34	123.11	118.30
49	s	186	LEU	CA-CB-CG	5.32	127.53	115.30
48	r	555	LEU	CA-CB-CG	5.31	127.52	115.30
5	A	1655	PRO	C-N-CA	5.30	134.95	121.70
50	t	107	GLU	CA-CB-CG	5.29	125.04	113.40
56	z	712	ASP	CB-CG-OD2	5.24	123.02	118.30
48	r	177	ILE	CG1-CB-CG2	-5.24	99.88	111.40
28	X	302	ASP	CB-CG-OD2	5.24	123.01	118.30
56	z	685	LEU	CA-CB-CG	-5.22	103.28	115.30
53	w	105	LEU	CA-CB-CG	5.21	127.28	115.30
56	z	697	HIS	N-CA-CB	5.21	119.97	110.60
31	a	264	ASP	CB-CG-OD2	5.19	122.97	118.30
52	v	70	TYR	CA-CB-CG	5.17	123.23	113.40
48	r	1386	PRO	N-CA-CB	5.17	109.50	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	j	484	TYR	CA-CB-CG	-5.16	103.59	113.40
52	v	70	TYR	CB-CG-CD2	-5.14	117.92	121.00
44	n	231	TRP	N-CA-CB	-5.12	101.39	110.60
5	A	1623	SER	C-N-CD	-5.07	109.45	120.60
50	t	157	LEU	CA-CB-CG	5.04	126.90	115.30
5	A	1656	SER	CA-C-N	5.03	128.27	117.20
1	0	19	CYS	CA-CB-SG	-5.02	104.96	114.00
40	j	619	ARG	NE-CZ-NH1	-5.02	117.79	120.30
28	X	312	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (88) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	112	ASP	Peptide
1	0	170	LEU	Peptide
1	0	569	LEU	Peptide
1	0	732	LEU	Peptide
3	2	597	LEU	Peptide
3	2	685	ILE	Peptide
3	2	686	LYS	Peptide
3	2	691	GLY	Peptide
3	2	942	SER	Peptide
4	3	46	TYR	Mainchain
4	3	77	ALA	Peptide
5	A	1202	PHE	Peptide
6	B	563	ASP	Peptide
6	B	594	MET	Peptide
6	B	835	GLU	Peptide
7	C	128	ILE	Peptide
8	D	71	PHE	Peptide
8	D	72	SER	Peptide
13	I	57	LYS	Peptide
13	I	59	THR	Peptide
17	M	316	SER	Peptide
19	O	279	GLY	Peptide
19	O	38	GLY	Peptide
21	Q	78	VAL	Peptide
23	S	44	GLN	Peptide
27	W	400	PRO	Peptide
27	W	475	ASP	Peptide
27	W	476	LYS	Peptide

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Mol	Chain	Res	Type	Group
28	X	102	LEU	Peptide
28	X	425	THR	Peptide
28	X	532	PRO	Peptide
29	Y	415	THR	Peptide
30	Z	189	GLU	Peptide
30	Z	192	GLU	Peptide
31	a	260	ALA	Peptide
31	a	315	ALA	Peptide
34	d	56	SER	Peptide
37	g	108	ALA	Peptide
38	h	66	GLU	Peptide
39	i	74	ALA	Peptide
40	j	194	TRP	Peptide
40	j	317	GLN	Peptide
40	j	399	PRO	Peptide
40	j	414	ASP	Peptide
40	j	457	ASP	Peptide
40	j	485	GLU	Mainchain
40	j	543	VAL	Peptide
40	j	549	LEU	Peptide
40	j	629	LYS	Peptide
44	n	220	ASN	Peptide
44	n	39	MET	Peptide
44	n	41	ASN	Peptide
44	n	42	LYS	Peptide
45	o	60	VAL	Peptide
45	o	62	GLN	Peptide
48	r	1228	THR	Peptide
48	r	147	ALA	Peptide
48	r	148	ARG	Peptide
48	r	163	THR	Peptide
48	r	164	GLY	Peptide
48	r	178	ILE	Peptide
48	r	228	GLY	Peptide
48	r	375	ASP	Peptide
48	r	376	PRO	Peptide
48	r	486	MET	Peptide
48	r	803	TYR	Peptide
48	r	909	GLN	Peptide
48	r	930	SER	Peptide
49	s	137	LYS	Peptide
49	s	141	GLY	Peptide

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Mol	Chain	Res	Type	Group
49	s	142	ALA	Peptide
49	s	179	ASP	Peptide
49	s	193	PRO	Peptide
50	t	105	ARG	Peptide
50	t	22	THR	Peptide
50	t	95	ILE	Peptide
52	v	60	ASP	Peptide
53	w	103	GLU	Peptide
53	w	82	ASN	Peptide
53	w	87	TYR	Peptide
53	w	96	PHE	Peptide
54	x	3	ASP	Peptide
54	x	7	GLN	Mainchain
54	x	80	GLU	Peptide
54	x	81	SER	Peptide
54	x	82	THR	Peptide
55	y	42	TYR	Peptide
56	z	764	PRO	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	0	740/841 (88%)	619 (84%)	114 (15%)	7 (1%)	14 50
2	1	1313/1368 (96%)	1201 (92%)	108 (8%)	4 (0%)	37 72
3	2	885/989 (90%)	774 (88%)	105 (12%)	6 (1%)	19 56
4	3	189/747 (25%)	167 (88%)	22 (12%)	0	100 100
5	A	1443/1970 (73%)	1316 (91%)	119 (8%)	8 (1%)	22 59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
6	B	1134/1174 (97%)	1028 (91%)	103 (9%)	3 (0%)	37 72
7	C	263/275 (96%)	240 (91%)	23 (9%)	0	100 100
8	D	127/142 (89%)	114 (90%)	12 (9%)	1 (1%)	16 53
9	E	208/210 (99%)	190 (91%)	18 (9%)	0	100 100
10	F	84/127 (66%)	80 (95%)	4 (5%)	0	100 100
11	G	169/172 (98%)	154 (91%)	15 (9%)	0	100 100
12	H	148/150 (99%)	134 (90%)	13 (9%)	1 (1%)	19 56
13	I	114/125 (91%)	95 (83%)	18 (16%)	1 (1%)	14 50
14	J	65/67 (97%)	61 (94%)	4 (6%)	0	100 100
15	K	114/117 (97%)	108 (95%)	6 (5%)	0	100 100
16	L	44/58 (76%)	37 (84%)	7 (16%)	0	100 100
17	M	109/376 (29%)	91 (84%)	18 (16%)	0	100 100
18	N	97/109 (89%)	83 (86%)	14 (14%)	0	100 100
19	O	256/316 (81%)	232 (91%)	21 (8%)	3 (1%)	11 44
20	P	183/339 (54%)	178 (97%)	5 (3%)	0	100 100
21	Q	180/439 (41%)	153 (85%)	25 (14%)	2 (1%)	12 46
22	R	163/291 (56%)	139 (85%)	24 (15%)	0	100 100
23	S	123/517 (24%)	97 (79%)	25 (20%)	1 (1%)	16 53
24	T	218/249 (88%)	182 (84%)	33 (15%)	3 (1%)	9 40
27	W	568/782 (73%)	518 (91%)	49 (9%)	1 (0%)	44 78
28	X	758/760 (100%)	666 (88%)	92 (12%)	0	100 100
29	Y	214/548 (39%)	179 (84%)	35 (16%)	0	100 100
30	Z	432/462 (94%)	391 (90%)	39 (9%)	2 (0%)	25 64
31	a	327/395 (83%)	287 (88%)	40 (12%)	0	100 100
32	b	259/308 (84%)	244 (94%)	15 (6%)	0	100 100
33	c	64/71 (90%)	60 (94%)	4 (6%)	0	100 100
34	d	271/309 (88%)	236 (87%)	33 (12%)	2 (1%)	19 56
35	e	294/346 (85%)	277 (94%)	17 (6%)	0	100 100
36	f	277/323 (86%)	268 (97%)	9 (3%)	0	100 100
37	g	128/246 (52%)	111 (87%)	17 (13%)	0	100 100
38	h	152/268 (57%)	133 (88%)	16 (10%)	3 (2%)	6 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
39	i	108/117 (92%)	103 (95%)	5 (5%)	0	100 100
40	j	492/651 (76%)	409 (83%)	72 (15%)	11 (2%)	5 29
41	k	181/208 (87%)	159 (88%)	22 (12%)	0	100 100
42	l	178/212 (84%)	150 (84%)	27 (15%)	1 (1%)	22 59
43	m	121/200 (60%)	118 (98%)	3 (2%)	0	100 100
44	n	277/311 (89%)	225 (81%)	46 (17%)	6 (2%)	5 29
45	o	106/178 (60%)	95 (90%)	9 (8%)	2 (2%)	6 32
46	p	110/200 (55%)	106 (96%)	4 (4%)	0	100 100
47	q	116/178 (65%)	107 (92%)	9 (8%)	0	100 100
48	r	1004/1454 (69%)	819 (82%)	165 (16%)	20 (2%)	6 31
49	s	129/270 (48%)	98 (76%)	27 (21%)	4 (3%)	3 22
50	t	110/233 (47%)	76 (69%)	32 (29%)	2 (2%)	7 34
51	u	54/146 (37%)	49 (91%)	5 (9%)	0	100 100
52	v	129/135 (96%)	92 (71%)	35 (27%)	2 (2%)	8 37
53	w	31/244 (13%)	21 (68%)	9 (29%)	1 (3%)	3 21
54	x	107/144 (74%)	81 (76%)	26 (24%)	0	100 100
55	y	112/131 (86%)	71 (63%)	36 (32%)	5 (4%)	2 17
56	z	145/788 (18%)	126 (87%)	14 (10%)	5 (3%)	3 20
All	All	15623/21786 (72%)	13748 (88%)	1768 (11%)	107 (1%)	21 56

All (107) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	170	LEU
1	0	570	ASN
3	2	687	PHE
5	A	1617	PRO
5	A	1620	PRO
5	A	1622	TYR
24	T	122	GLU
38	h	75	VAL
40	j	318	ILE
48	r	1336	VAL
48	r	1386	PRO
52	v	9	GLU
56	z	702	GLY

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Mol	Chain	Res	Type
1	0	143	LEU
2	1	319	GLU
3	2	87	ASP
5	A	72	GLN
6	B	489	ILE
23	S	152	HIS
34	d	57	ASN
40	j	35	SER
45	o	61	SER
48	r	437	ALA
48	r	438	LEU
48	r	553	GLU
52	v	10	GLU
55	y	65	LYS
56	z	727	ALA
1	0	248	VAL
1	0	266	ARG
5	A	339	LEU
5	A	1626	SER
6	B	145	GLN
13	I	58	ILE
19	O	43	ASP
40	j	195	LYS
40	j	501	GLN
40	j	630	MET
44	n	40	ARG
44	n	229	ASP
48	r	128	LEU
48	r	249	LYS
48	r	804	ASN
48	r	1272	GLN
55	y	70	PRO
56	z	700	ASN
2	1	366	ILE
5	A	73	THR
6	B	144	HIS
12	H	149	ALA
24	T	135	SER
30	Z	381	PRO
38	h	74	GLN
44	n	41	ASN
45	o	70	GLN

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Mol	Chain	Res	Type
48	r	155	PRO
48	r	451	CYS
48	r	798	SER
50	t	25	ASN
1	0	742	LEU
3	2	172	THR
3	2	683	THR
8	D	23	PRO
19	O	12	ARG
34	d	7	PRO
40	j	335	PRO
40	j	472	GLU
44	n	42	LYS
44	n	220	ASN
44	n	221	VAL
48	r	69	LEU
48	r	376	PRO
49	s	118	GLU
49	s	144	SER
49	s	146	GLU
53	w	88	ASN
55	y	14	ASN
55	y	88	LEU
2	1	635	GLN
21	Q	78	VAL
21	Q	137	THR
24	T	121	SER
38	h	67	LYS
42	l	168	HIS
48	r	127	ILE
50	t	120	HIS
56	z	712	ASP
19	O	279	GLY
40	j	621	PRO
48	r	552	VAL
2	1	580	GLY
3	2	943	VAL
40	j	399	PRO
48	r	170	PRO
48	r	375	ASP
49	s	193	PRO
56	z	747	PRO

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Mol	Chain	Res	Type
1	0	226	ILE
5	A	1627	PRO
40	j	648	PRO
48	r	182	PRO
55	y	31	PRO
3	2	724	VAL
27	W	477	ILE
30	Z	190	PRO
48	r	950	VAL
40	j	559	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	0	666/736 (90%)	644 (97%)	22 (3%)	33 53
2	1	1187/1232 (96%)	1183 (100%)	4 (0%)	91 92
3	2	780/864 (90%)	777 (100%)	3 (0%)	89 91
4	3	165/601 (28%)	156 (94%)	9 (6%)	18 40
5	A	1285/1748 (74%)	1277 (99%)	8 (1%)	84 88
6	B	999/1028 (97%)	997 (100%)	2 (0%)	92 94
7	C	244/252 (97%)	244 (100%)	0	100 100
8	D	119/126 (94%)	119 (100%)	0	100 100
9	E	192/192 (100%)	192 (100%)	0	100 100
10	F	74/111 (67%)	74 (100%)	0	100 100
11	G	152/153 (99%)	151 (99%)	1 (1%)	81 87
12	H	131/131 (100%)	131 (100%)	0	100 100
13	I	104/112 (93%)	104 (100%)	0	100 100
14	J	56/56 (100%)	56 (100%)	0	100 100
15	K	105/106 (99%)	105 (100%)	0	100 100
16	L	43/55 (78%)	43 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
17	M	105/324 (32%)	104 (99%)	1 (1%)	73 82
18	N	90/98 (92%)	89 (99%)	1 (1%)	70 80
19	O	222/268 (83%)	222 (100%)	0	100 100
20	P	159/293 (54%)	159 (100%)	0	100 100
21	Q	167/373 (45%)	167 (100%)	0	100 100
22	R	150/261 (58%)	150 (100%)	0	100 100
23	S	111/448 (25%)	111 (100%)	0	100 100
24	T	196/218 (90%)	192 (98%)	4 (2%)	50 69
27	W	508/688 (74%)	498 (98%)	10 (2%)	50 69
28	X	661/664 (100%)	658 (100%)	3 (0%)	86 90
29	Y	162/484 (34%)	162 (100%)	0	100 100
30	Z	372/399 (93%)	363 (98%)	9 (2%)	44 63
31	a	296/352 (84%)	295 (100%)	1 (0%)	91 92
32	b	234/272 (86%)	231 (99%)	3 (1%)	65 77
33	c	59/64 (92%)	53 (90%)	6 (10%)	6 21
34	d	210/283 (74%)	210 (100%)	0	100 100
35	e	259/299 (87%)	258 (100%)	1 (0%)	89 91
36	f	256/296 (86%)	256 (100%)	0	100 100
37	g	115/223 (52%)	115 (100%)	0	100 100
38	h	139/225 (62%)	139 (100%)	0	100 100
39	i	92/98 (94%)	91 (99%)	1 (1%)	70 80
40	j	452/577 (78%)	423 (94%)	29 (6%)	14 36
41	k	164/183 (90%)	162 (99%)	2 (1%)	67 79
42	l	158/178 (89%)	158 (100%)	0	100 100
43	m	118/173 (68%)	118 (100%)	0	100 100
44	n	256/280 (91%)	254 (99%)	2 (1%)	79 85
45	o	102/152 (67%)	102 (100%)	0	100 100
46	p	102/163 (63%)	102 (100%)	0	100 100
47	q	114/155 (74%)	112 (98%)	2 (2%)	54 71
48	r	905/1271 (71%)	869 (96%)	36 (4%)	27 48
49	s	119/230 (52%)	117 (98%)	2 (2%)	56 72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
50	t	110/216 (51%)	108 (98%)	2 (2%)	54 71
51	u	59/133 (44%)	59 (100%)	0	100 100
52	v	119/124 (96%)	114 (96%)	5 (4%)	25 47
53	w	34/208 (16%)	33 (97%)	1 (3%)	37 57
54	x	92/119 (77%)	83 (90%)	9 (10%)	6 22
55	y	105/115 (91%)	86 (82%)	19 (18%)	1 8
56	z	135/697 (19%)	129 (96%)	6 (4%)	24 46
All	All	14009/19107 (73%)	13805 (98%)	204 (2%)	60 75

All (204) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	13	MET
1	0	14	ASP
1	0	50	ASP
1	0	51	LEU
1	0	59	THR
1	0	60	ARG
1	0	61	MET
1	0	129	ASP
1	0	132	VAL
1	0	149	LYS
1	0	254	ARG
1	0	635	GLN
1	0	638	LEU
1	0	639	LEU
1	0	640	ARG
1	0	745	LYS
1	0	796	LYS
1	0	808	LYS
1	0	827	CYS
1	0	828	LEU
1	0	832	LEU
1	0	835	ARG
2	1	386	LYS
2	1	434	ARG
2	1	1056	ARG
2	1	1193	PHE
3	2	17	ARG
3	2	107	ARG

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Mol	Chain	Res	Type
3	2	268	THR
4	3	51	PRO
4	3	82	VAL
4	3	83	GLN
4	3	84	CYS
4	3	85	HIS
4	3	122	LEU
4	3	123	GLN
4	3	125	PHE
4	3	128	PHE
5	A	331	LYS
5	A	460	ARG
5	A	479	TRP
5	A	940	LYS
5	A	1375	ARG
5	A	1618	THR
5	A	1626	SER
5	A	1651	SER
6	B	1052	LYS
6	B	1156	LYS
11	G	78	ARG
17	M	341	LYS
18	N	5	LEU
24	T	153	TYR
24	T	177	ARG
24	T	196	TYR
24	T	200	LYS
27	W	165	LYS
27	W	198	ARG
27	W	297	PHE
27	W	298	ARG
27	W	374	TRP
27	W	377	GLN
27	W	378	PHE
27	W	472	ARG
27	W	504	LYS
27	W	685	TYR
28	X	143	ARG
28	X	487	ARG
28	X	690	ARG
30	Z	11	ARG
30	Z	115	ARG

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Mol	Chain	Res	Type
30	Z	215	PHE
30	Z	382	VAL
30	Z	391	ILE
30	Z	392	ARG
30	Z	393	LEU
30	Z	395	GLU
30	Z	396	LEU
31	a	195	ARG
32	b	18	ASN
32	b	146	ARG
32	b	157	MET
33	c	2	VAL
33	c	3	ASN
33	c	4	VAL
33	c	5	LEU
33	c	6	LYS
33	c	44	PHE
35	e	10	LYS
39	i	43	ARG
40	j	37	SER
40	j	38	GLN
40	j	47	ILE
40	j	49	PHE
40	j	103	ARG
40	j	194	TRP
40	j	432	ILE
40	j	433	LYS
40	j	434	GLN
40	j	437	HIS
40	j	469	ASP
40	j	470	VAL
40	j	472	GLU
40	j	475	VAL
40	j	476	LYS
40	j	479	ILE
40	j	481	SER
40	j	482	GLN
40	j	485	GLU
40	j	487	ILE
40	j	499	VAL
40	j	507	ARG
40	j	551	PHE

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Mol	Chain	Res	Type
40	j	557	LEU
40	j	614	LYS
40	j	616	SER
40	j	617	HIS
40	j	618	LEU
40	j	627	TRP
41	k	32	LEU
41	k	37	HIS
44	n	44	THR
44	n	233	LYS
47	q	90	ARG
47	q	140	ARG
48	r	142	ASP
48	r	168	ARG
48	r	175	ASP
48	r	184	THR
48	r	185	LYS
48	r	187	GLU
48	r	188	LYS
48	r	221	ARG
48	r	222	VAL
48	r	226	VAL
48	r	227	GLU
48	r	229	GLU
48	r	231	GLU
48	r	233	THR
48	r	234	LEU
48	r	243	VAL
48	r	245	TRP
48	r	246	ARG
48	r	253	LEU
48	r	328	ARG
48	r	356	LYS
48	r	480	LYS
48	r	535	LYS
48	r	639	LYS
48	r	683	ARG
48	r	794	LEU
48	r	796	ILE
48	r	797	PHE
48	r	876	GLN
48	r	901	TYR

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Mol	Chain	Res	Type
48	r	904	PHE
48	r	919	ARG
48	r	953	PHE
48	r	1191	THR
48	r	1269	ASN
48	r	1272	GLN
49	s	136	GLU
49	s	183	ARG
50	t	74	HIS
50	t	152	ARG
52	v	11	HIS
52	v	48	LEU
52	v	67	VAL
52	v	103	LYS
52	v	106	LYS
53	w	132	GLU
54	x	5	LEU
54	x	9	GLN
54	x	13	ASN
54	x	15	LEU
54	x	29	CYS
54	x	70	ASP
54	x	109	TYR
54	x	125	ILE
54	x	131	LYS
55	y	20	LEU
55	y	46	LYS
55	y	54	TYR
55	y	63	TYR
55	y	85	ARG
55	y	92	GLN
55	y	96	PHE
55	y	97	ILE
55	y	98	ASP
55	y	99	GLU
55	y	100	GLN
55	y	102	ILE
55	y	103	LEU
55	y	105	TRP
55	y	110	ARG
55	y	111	LYS
55	y	112	ARG

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Mol	Chain	Res	Type
55	y	113	MET
55	y	114	ARG
56	z	696	SER
56	z	698	CYS
56	z	701	ASN
56	z	711	ASP
56	z	743	TYR
56	z	744	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (285) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	43	ASN
1	0	63	HIS
1	0	104	GLN
1	0	392	HIS
1	0	395	HIS
1	0	635	GLN
1	0	643	HIS
1	0	683	GLN
1	0	743	GLN
1	0	821	GLN
2	1	158	GLN
2	1	292	GLN
2	1	303	GLN
2	1	332	GLN
2	1	358	GLN
2	1	415	ASN
2	1	433	ASN
2	1	460	GLN
2	1	526	ASN
2	1	541	HIS
2	1	622	GLN
2	1	628	HIS
2	1	696	HIS
2	1	759	ASN
2	1	907	ASN
2	1	1198	GLN
2	1	1250	HIS
2	1	1300	HIS
3	2	22	GLN
3	2	174	ASN

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Mol	Chain	Res	Type
3	2	217	GLN
3	2	261	GLN
3	2	266	GLN
3	2	370	GLN
3	2	530	GLN
3	2	541	ASN
3	2	645	GLN
3	2	799	HIS
3	2	898	ASN
3	2	925	GLN
4	3	123	GLN
4	3	139	HIS
4	3	179	HIS
4	3	219	HIS
5	A	122	ASN
5	A	204	HIS
5	A	267	GLN
5	A	273	GLN
5	A	288	ASN
5	A	296	ASN
5	A	311	GLN
5	A	330	GLN
5	A	353	ASN
5	A	432	HIS
5	A	461	GLN
5	A	502	ASN
5	A	539	GLN
5	A	606	HIS
5	A	609	HIS
5	A	620	HIS
5	A	654	HIS
5	A	678	ASN
5	A	685	HIS
5	A	746	ASN
5	A	757	GLN
5	A	765	ASN
5	A	792	ASN
5	A	905	ASN
5	A	982	ASN
5	A	1220	HIS
5	A	1397	HIS
5	A	1410	HIS

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Mol	Chain	Res	Type
5	A	1422	GLN
5	A	1462	GLN
6	B	90	GLN
6	B	111	ASN
6	B	117	ASN
6	B	139	GLN
6	B	245	GLN
6	B	312	GLN
6	B	314	GLN
6	B	344	GLN
6	B	370	HIS
6	B	503	ASN
6	B	650	ASN
6	B	683	GLN
6	B	718	GLN
6	B	755	GLN
6	B	790	GLN
6	B	825	GLN
6	B	876	ASN
6	B	913	GLN
6	B	941	GLN
6	B	992	ASN
6	B	1013	ASN
6	B	1025	ASN
6	B	1060	HIS
6	B	1117	HIS
6	B	1142	ASN
7	C	32	ASN
7	C	60	HIS
7	C	217	GLN
8	D	43	HIS
8	D	135	GLN
9	E	148	HIS
10	F	46	GLN
11	G	14	HIS
11	G	93	ASN
12	H	29	HIS
12	H	131	ASN
13	I	41	ASN
13	I	60	HIS
13	I	98	GLN
13	I	100	HIS

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Mol	Chain	Res	Type
16	L	23	HIS
17	M	48	ASN
17	M	359	ASN
18	N	8	ASN
18	N	39	GLN
19	O	17	ASN
19	O	271	GLN
20	P	164	GLN
20	P	167	ASN
20	P	173	ASN
20	P	257	ASN
20	P	327	ASN
21	Q	64	ASN
21	Q	142	ASN
22	R	83	ASN
22	R	90	GLN
22	R	117	GLN
22	R	157	GLN
22	R	160	GLN
23	S	173	HIS
24	T	143	GLN
24	T	158	ASN
24	T	195	GLN
24	T	198	ASN
24	T	229	HIS
27	W	112	HIS
27	W	187	HIS
27	W	377	GLN
27	W	459	GLN
27	W	591	GLN
27	W	595	ASN
27	W	683	GLN
28	X	118	HIS
28	X	237	HIS
28	X	238	ASN
28	X	328	HIS
28	X	402	ASN
28	X	452	GLN
28	X	562	GLN
28	X	613	HIS
28	X	726	GLN
29	Y	384	HIS

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Mol	Chain	Res	Type
29	Y	442	GLN
29	Y	501	GLN
29	Y	520	ASN
29	Y	524	HIS
30	Z	97	HIS
30	Z	181	GLN
30	Z	424	HIS
31	a	235	HIS
31	a	256	GLN
31	a	340	ASN
32	b	18	ASN
32	b	248	HIS
33	c	3	ASN
33	c	42	HIS
33	c	54	GLN
33	c	64	ASN
34	d	117	ASN
34	d	307	GLN
35	e	130	GLN
35	e	288	GLN
36	f	3	HIS
36	f	7	GLN
36	f	18	GLN
36	f	247	GLN
37	g	53	GLN
37	g	59	HIS
37	g	62	GLN
37	g	116	ASN
37	g	127	GLN
38	h	35	ASN
38	h	65	HIS
38	h	139	GLN
39	i	27	ASN
39	i	48	GLN
39	i	58	HIS
39	i	79	HIS
40	j	38	GLN
40	j	142	GLN
40	j	329	ASN
40	j	374	ASN
40	j	394	HIS
40	j	419	ASN

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Mol	Chain	Res	Type
40	j	461	GLN
40	j	463	HIS
40	j	492	GLN
40	j	517	GLN
40	j	528	GLN
40	j	532	HIS
40	j	547	GLN
40	j	565	ASN
40	j	617	HIS
41	k	30	HIS
41	k	37	HIS
41	k	84	HIS
41	k	127	HIS
41	k	134	HIS
42	l	19	GLN
42	l	90	ASN
43	m	58	ASN
43	m	67	ASN
43	m	104	GLN
44	n	59	ASN
44	n	68	ASN
44	n	109	GLN
44	n	220	ASN
44	n	245	HIS
44	n	252	HIS
45	o	70	GLN
45	o	79	GLN
45	o	101	GLN
45	o	105	GLN
45	o	109	GLN
46	p	81	ASN
46	p	84	GLN
46	p	92	GLN
46	p	124	HIS
47	q	29	ASN
47	q	53	GLN
47	q	154	GLN
47	q	171	ASN
47	q	178	ASN
48	r	211	GLN
48	r	214	ASN
48	r	276	GLN

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Mol	Chain	Res	Type
48	r	304	GLN
48	r	459	HIS
48	r	464	GLN
48	r	521	GLN
48	r	528	HIS
48	r	532	ASN
48	r	536	ASN
48	r	607	GLN
48	r	669	GLN
48	r	698	GLN
48	r	717	ASN
48	r	744	HIS
48	r	849	ASN
48	r	898	ASN
48	r	913	HIS
48	r	946	ASN
48	r	1426	ASN
49	s	64	GLN
49	s	108	GLN
49	s	109	GLN
50	t	74	HIS
50	t	120	HIS
50	t	142	GLN
50	t	154	GLN
51	u	70	HIS
51	u	116	GLN
51	u	129	ASN
52	v	11	HIS
52	v	21	GLN
52	v	56	GLN
52	v	76	ASN
54	x	18	GLN
54	x	27	GLN
54	x	86	GLN
54	x	119	GLN
54	x	127	GLN
54	x	129	GLN
55	y	127	ASN
56	z	628	ASN
56	z	636	HIS
56	z	697	HIS
56	z	701	ASN

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Mol	Chain	Res	Type
56	z	705	HIS
56	z	732	GLN
56	z	753	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 18 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	$\#\|Z\| > 2$
59	SF4	X	1000	28	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
59	SF4	X	1000	28	-	-	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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

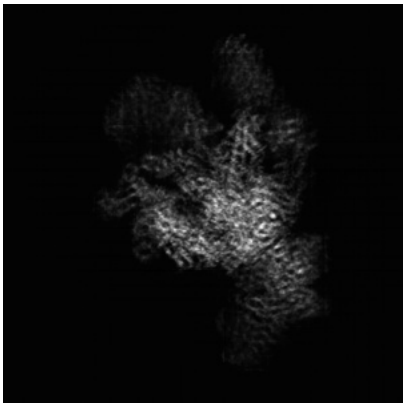
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23255. These allow visual inspection of the internal detail of the map and identification of artifacts.

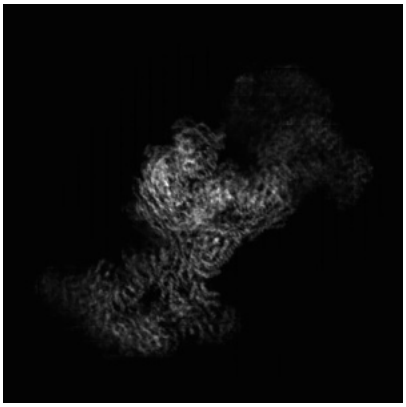
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

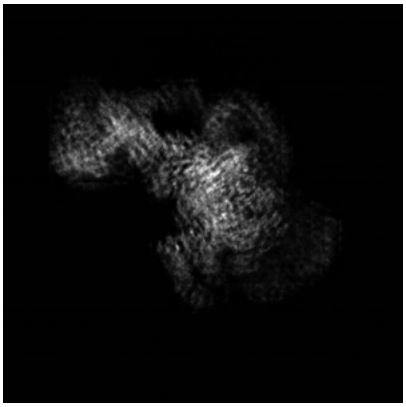
6.1.1 Primary map



X



Y

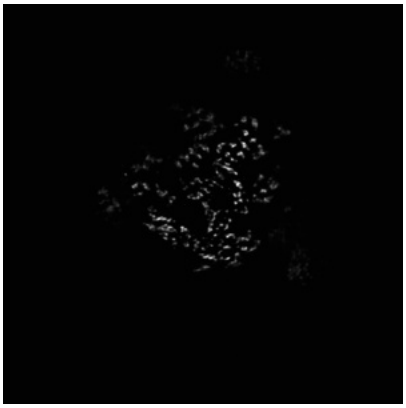


Z

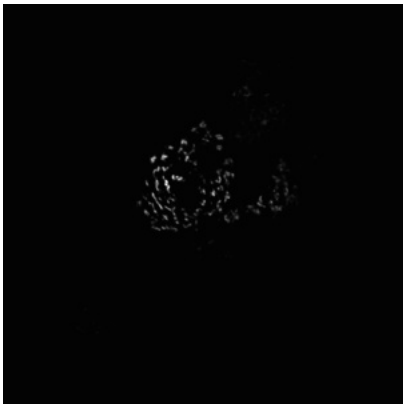
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map



X Index: 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 (i)

6.3.1 Primary map

X Index: 221

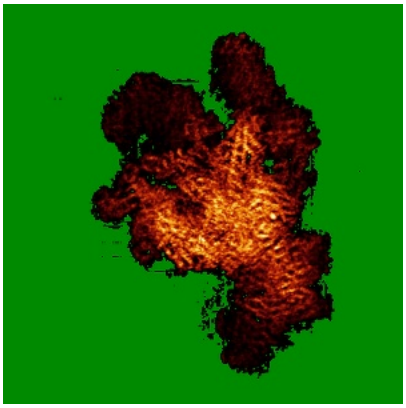
Y Index: 254

Z Index: 182

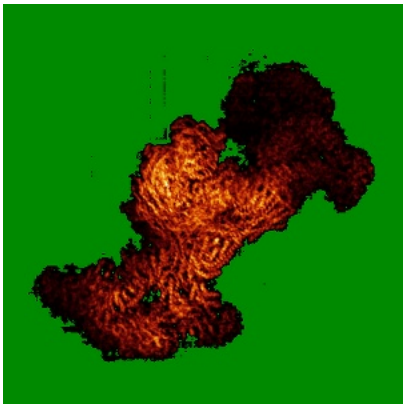
The images above show the largest variance slices of the map in three orthogonal directions.

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

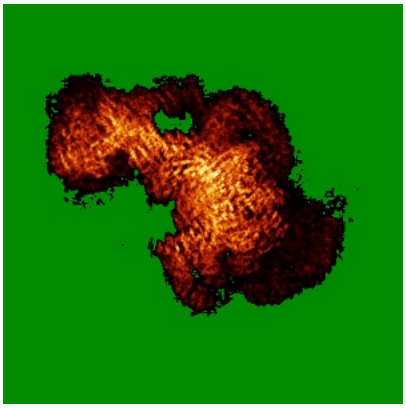
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

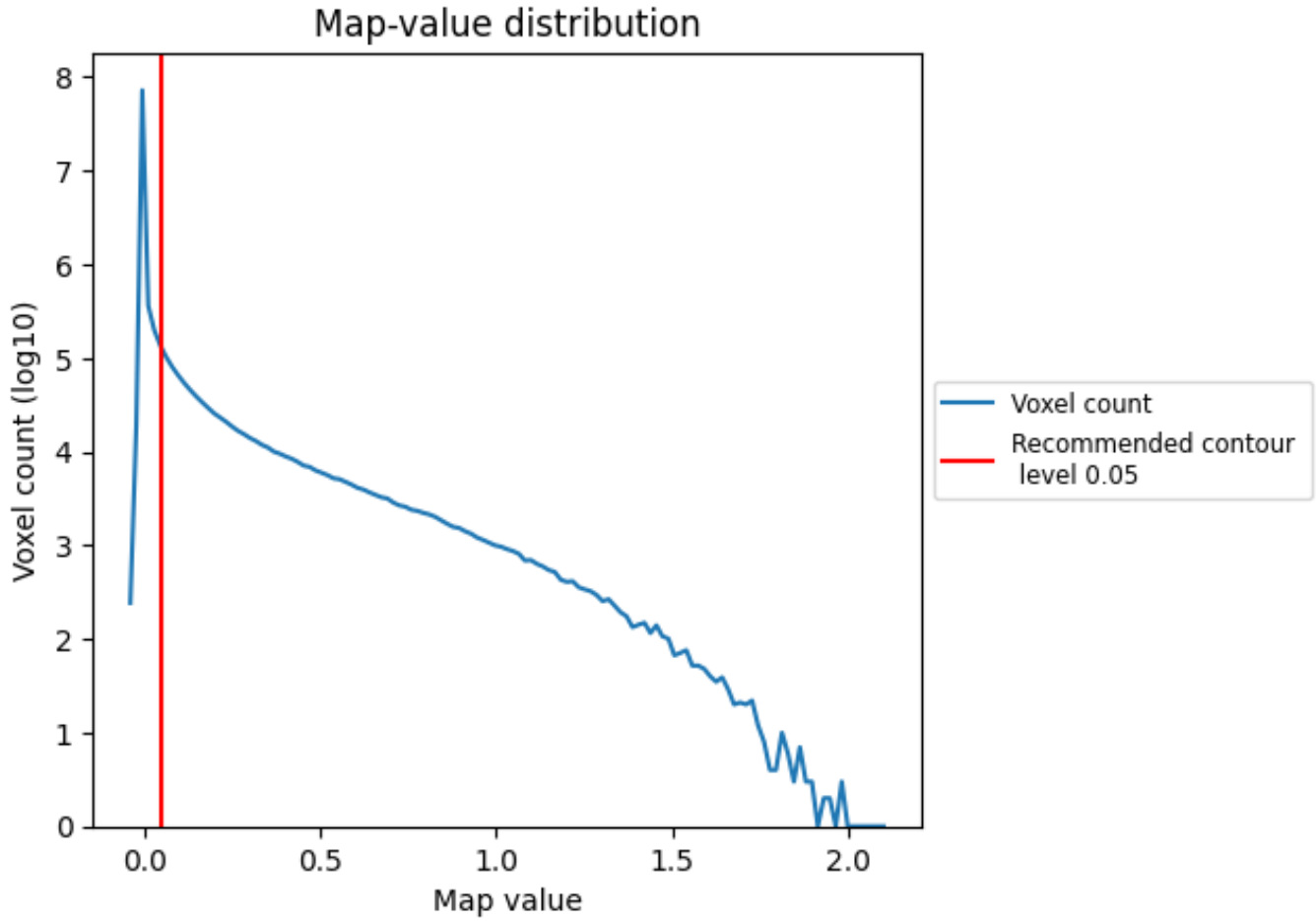
6.6 Mask visualisation (i)

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

7 Map analysis

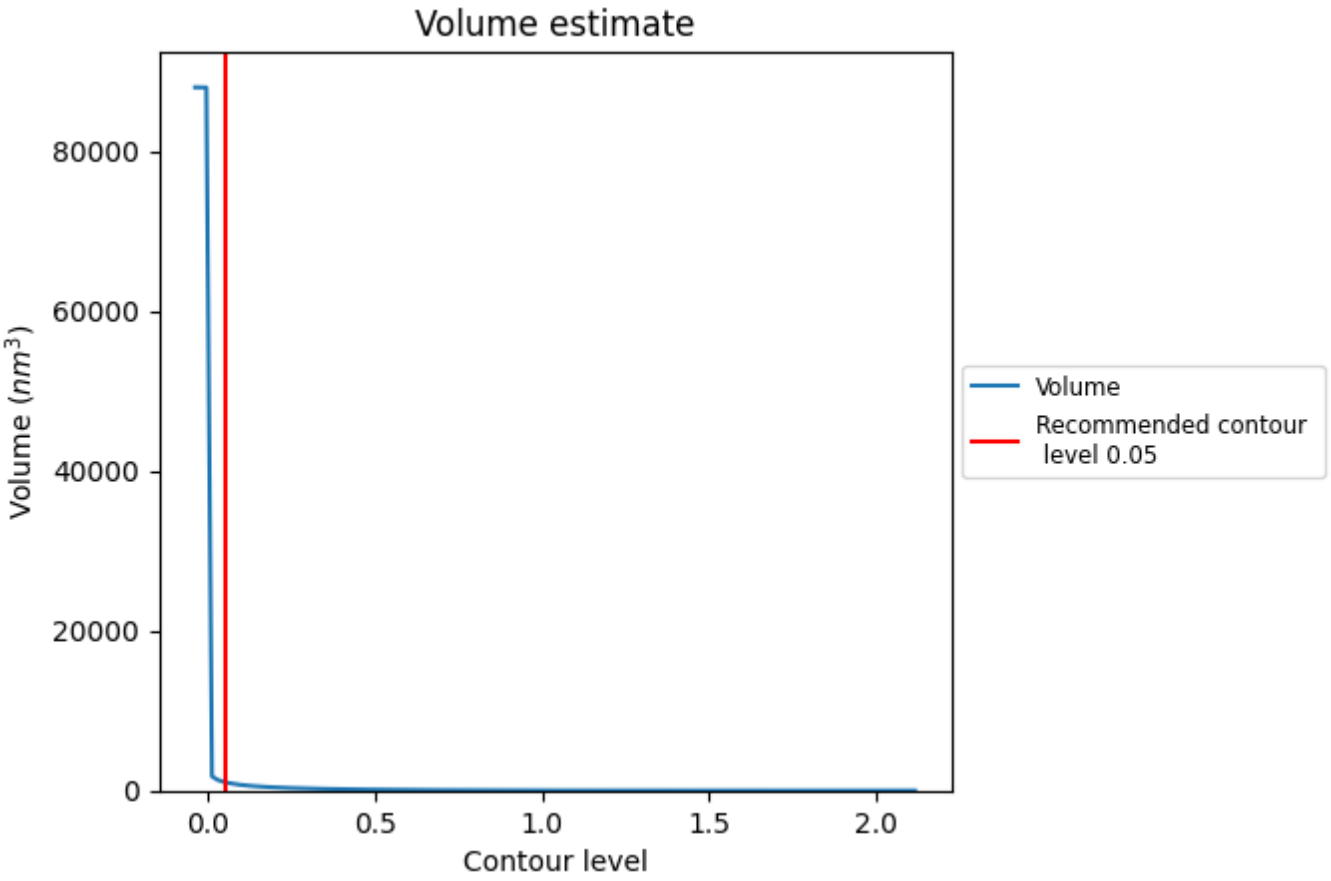
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

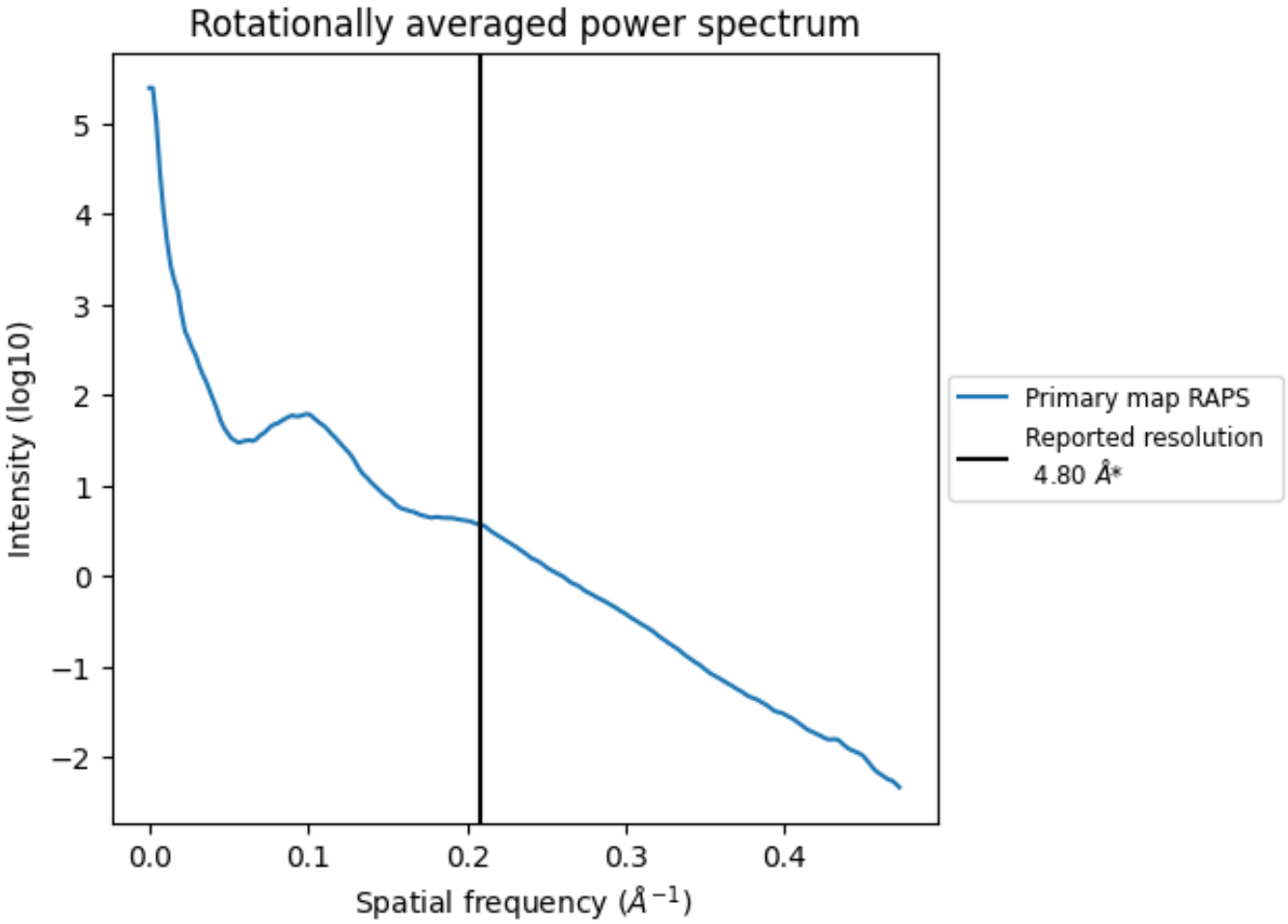
7.2 Volume estimate



The volume at the recommended contour level is 1055 nm^3; this corresponds to an approximate mass of 953 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.208 Å^{-1}

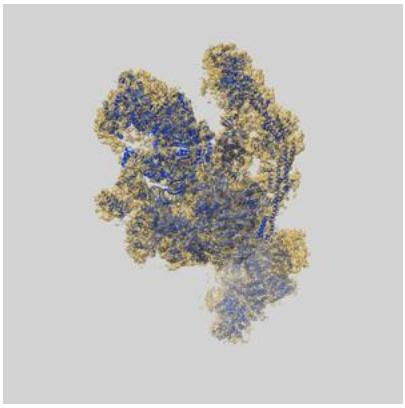
8 Fourier-Shell correlation

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

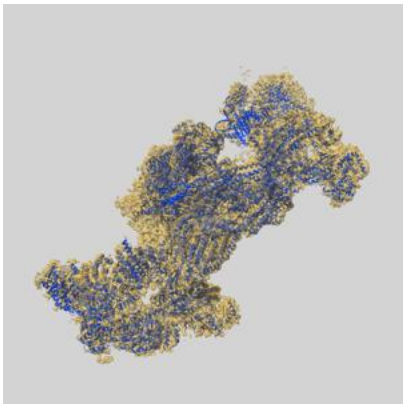
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23255 and PDB model 7LBM. Per-residue inclusion information can be found in section 3 on page 15.

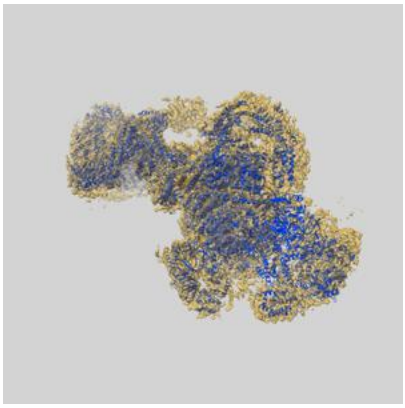
9.1 Map-model overlay



X



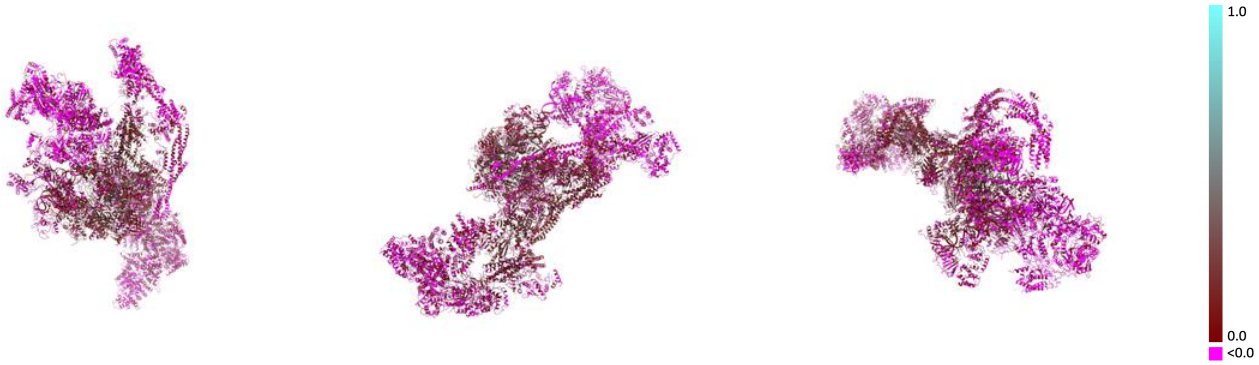
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

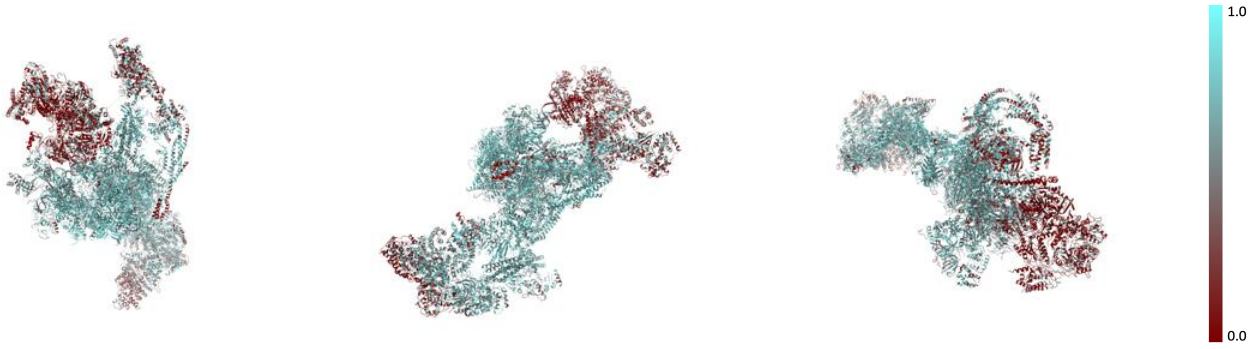
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

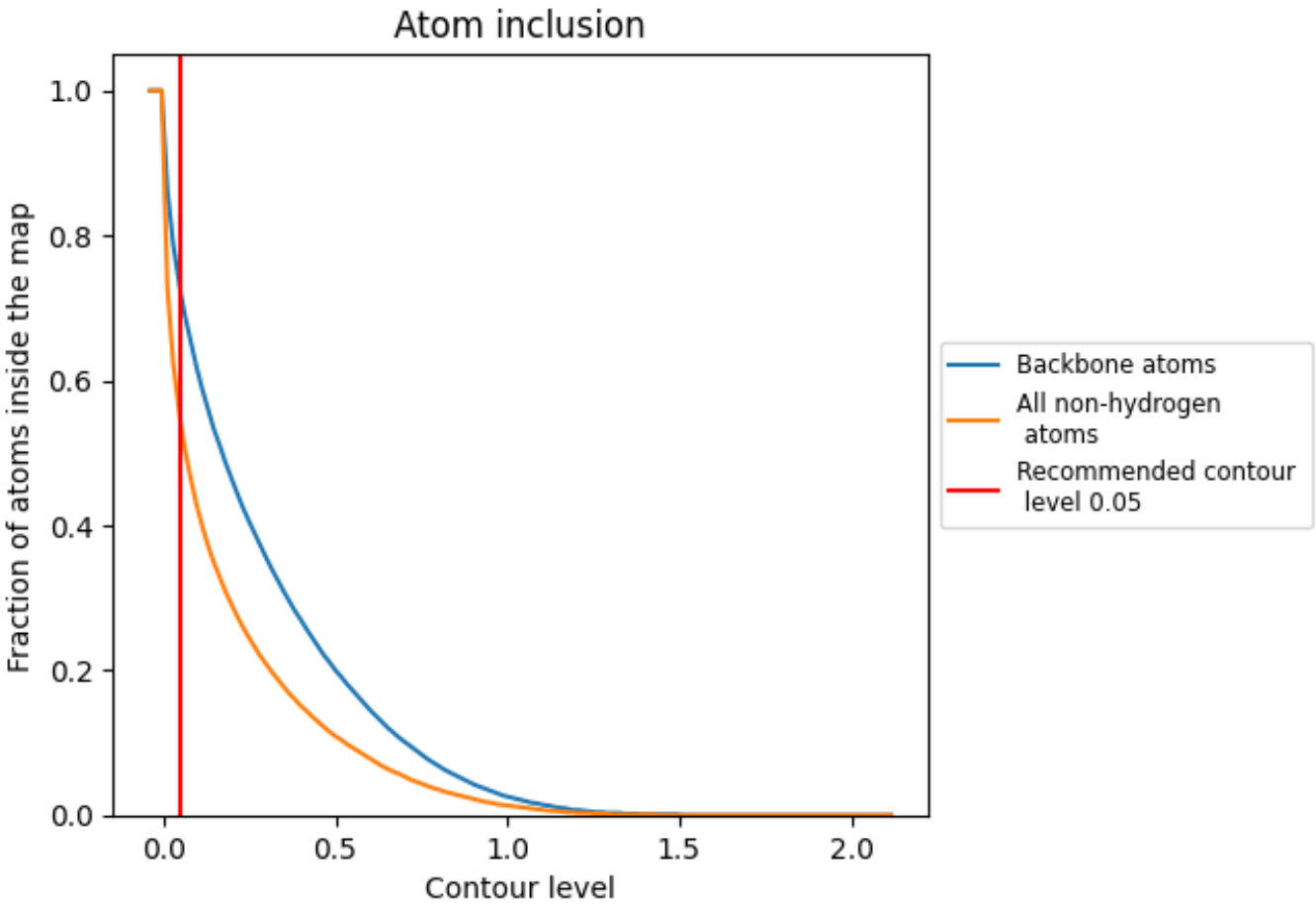
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

9.4 Atom inclusion (i)



At the recommended contour level, 72% of all backbone atoms, 54% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5400	0.0740
0	0.6280	0.0650
1	0.4060	-0.0060
2	0.5140	0.0300
3	0.5240	0.0330
A	0.7150	0.1930
B	0.7240	0.2010
C	0.6720	0.1450
D	0.6640	0.1400
E	0.7060	0.1630
F	0.7070	0.2010
G	0.7280	0.1730
H	0.6740	0.1380
I	0.7120	0.1510
J	0.6810	0.1180
K	0.6870	0.1510
L	0.7020	0.1860
M	0.4900	-0.0110
N	0.4860	0.0020
O	0.6640	0.1200
P	0.6060	0.0650
Q	0.6220	0.0780
R	0.6070	0.0470
S	0.5410	0.0520
T	0.5720	0.0580
U	0.5970	0.0640
V	0.5890	0.0520
W	0.0960	-0.0490
X	0.3510	-0.0060
Y	0.2250	-0.0660
Z	0.1720	-0.0670
a	0.1290	-0.0590
b	0.2200	-0.0550
c	0.1850	-0.0860
d	0.3580	-0.0120

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Chain	Atom inclusion	Q-score
e	0.3920	-0.0170
f	0.3390	-0.0590
g	0.6910	0.0790
h	0.7060	0.1450
i	0.7250	0.1740
j	0.7350	0.1960
k	0.6540	0.1170
l	0.6410	0.1080
m	0.7310	0.2080
n	0.7070	0.1790
o	0.6650	0.1300
p	0.6440	0.1040
q	0.6880	0.1560
r	0.6350	0.1010
s	0.4180	0.0040
t	0.5380	0.0180
u	0.3480	-0.0210
v	0.4240	-0.0400
w	0.3930	-0.0220
x	0.5280	0.0110
y	0.6030	0.0470
z	0.7130	0.1360