



wwPDB EM Validation Summary Report ⓘ

Nov 16, 2022 – 10:27 PM EST

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

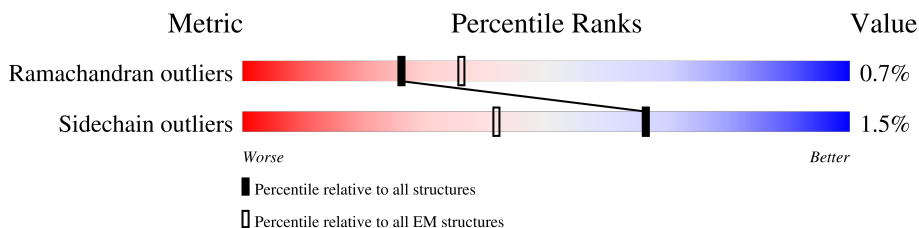
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al.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

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.80 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	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	<div style="display: flex; align-items: center;"> <div style="width: 14%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 85%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: grey;"></div> </div>
2	1	1368	<div style="display: flex; align-items: center;"> <div style="width: 48%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 96%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div>
3	2	989	<div style="display: flex; align-items: center;"> <div style="width: 31%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 89%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: grey;"></div> </div>
4	3	747	<div style="display: flex; align-items: center;"> <div style="width: 10%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 24%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 74%; height: 10px; background-color: grey;"></div> </div>
5	A	1970	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 73%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 26%; height: 10px; background-color: grey;"></div> </div>
6	B	1174	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 97%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div>
7	C	275	<div style="display: flex; align-items: center;"> <div style="width: 10%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 97%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div>
8	D	142	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 89%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: grey;"></div> </div>
9	E	210	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 100%; height: 10px; background-color: green; margin-right: 5px;"></div> </div>

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Mol	Chain	Length	Quality of chain
10	F	127	6% 68% 32%
11	G	172	99% ..
12	H	150	7% 99% .
13	I	125	6% 90% 7%
14	J	67	9% 100%
15	K	117	5% 99% .
16	L	58	79% 21%
17	M	376	12% 30% 70%
18	N	109	32% 90% 9%
19	O	316	8% 81% 18%
20	P	339	12% 55% 45%
21	Q	439	6% 41% 58%
22	R	291	11% 57% 43%
23	S	517	8% 24% 75%
24	T	249	22% 86% 11%
25	U	100	16% 62% 36%
26	V	100	17% 61% 36%
27	W	782	67% 72% 27%
28	X	760	58% 98% .
29	Y	548	32% 39% 60%
30	Z	462	79% 92% 6%
31	a	395	72% 82% 16%
32	b	308	66% 84% 15%
33	c	71	76% 85% 8% 7%
34	d	309	50% 88% 11%

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Mol	Chain	Length	Quality of chain
35	e	346	46% 86% 14%
36	f	323	54% 87% 13%
37	g	246	52% 47%
38	h	268	57% 41%
39	i	117	92% 6%
40	j	651	70% 7% 23%
41	k	208	8% 88% 11%
42	l	212	12% 86% 13%
43	m	200	62% 38%
44	n	311	88% 9%
45	o	178	58% 39%
46	p	200	57% 43%
47	q	178	67% 31%
48	r	1454	12% 66% 5% 29%
49	s	270	26% 44% 6% 50%
50	t	233	16% 45% 5% 50%
51	u	146	24% 41% 59%
52	v	135	48% 87% 10%
53	w	244	9% 13% 84%
54	x	144	32% 66% 10% 23%
55	y	131	18% 69% 19% 11%
56	z	788	17% 81%

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	Total	C	N	O	S	0	0
			5864	3744	1005	1068	47		

- 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	Total	C	N	O	S	0	0
			10636	6878	1809	1880	69		

- 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	Total	C	N	O	S	0	0
			7007	4487	1180	1284	56		

- 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	Total	C	N	O	S	0	0
			1504	969	249	277	9		

- 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	Total	C	N	O	S	0	0
			11519	7241	2052	2154	72		

- 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	Total	C	N	O	S	0	0
			9129	5769	1604	1692	64		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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
			Total	C	N	O	S		
21	Q	184	1520	957	272	280	11	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 36 is a protein called Cyclin-H.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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		

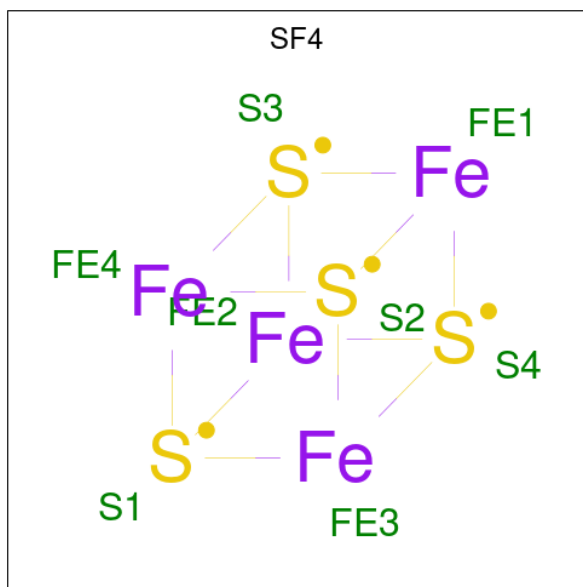
- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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: Fe₄S₄).

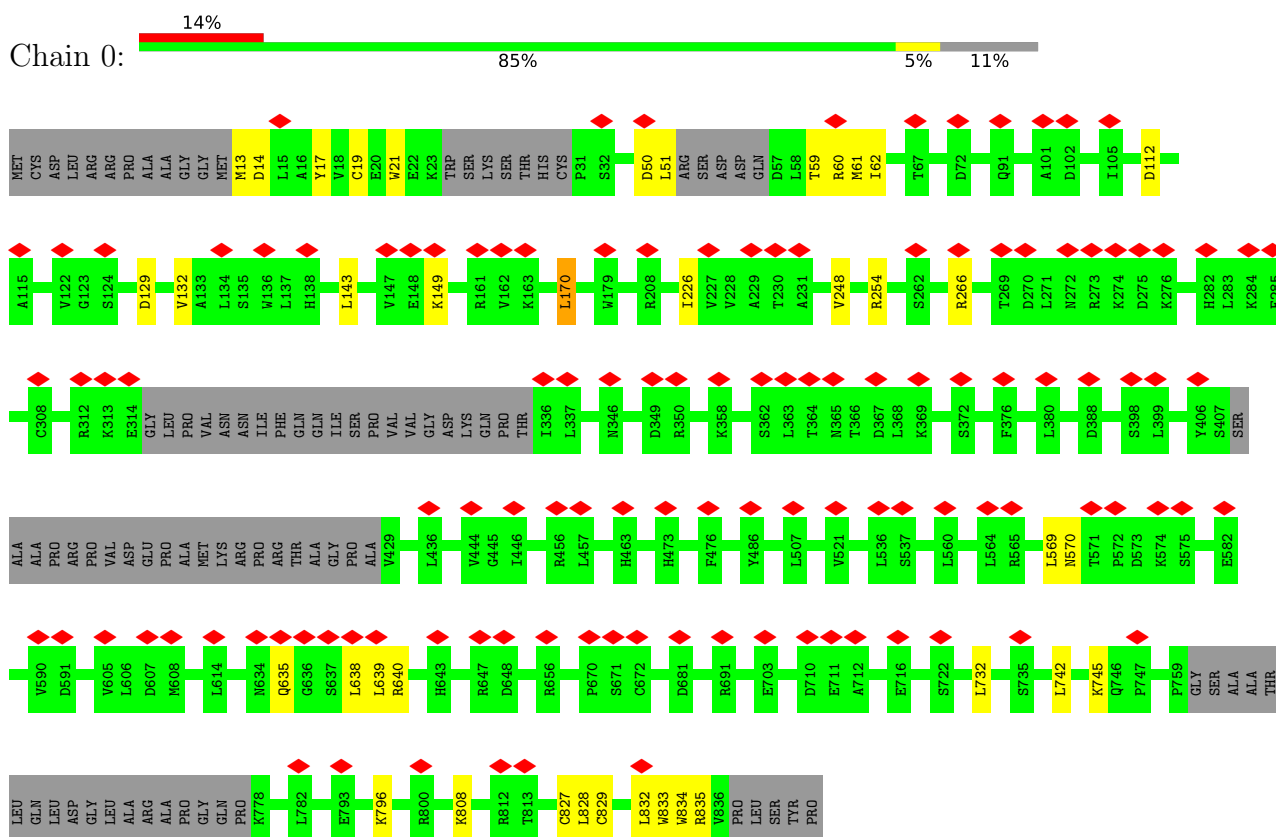


Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
59	X	1	8	4	4	0

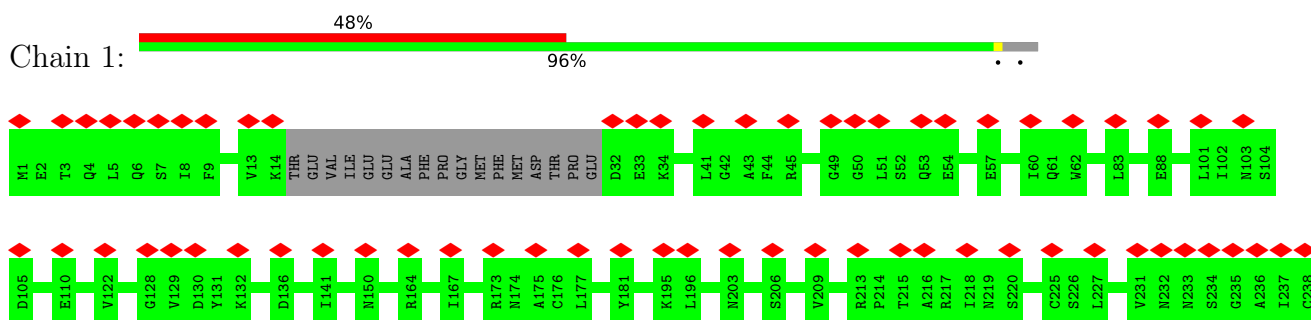
3 Residue-property plots

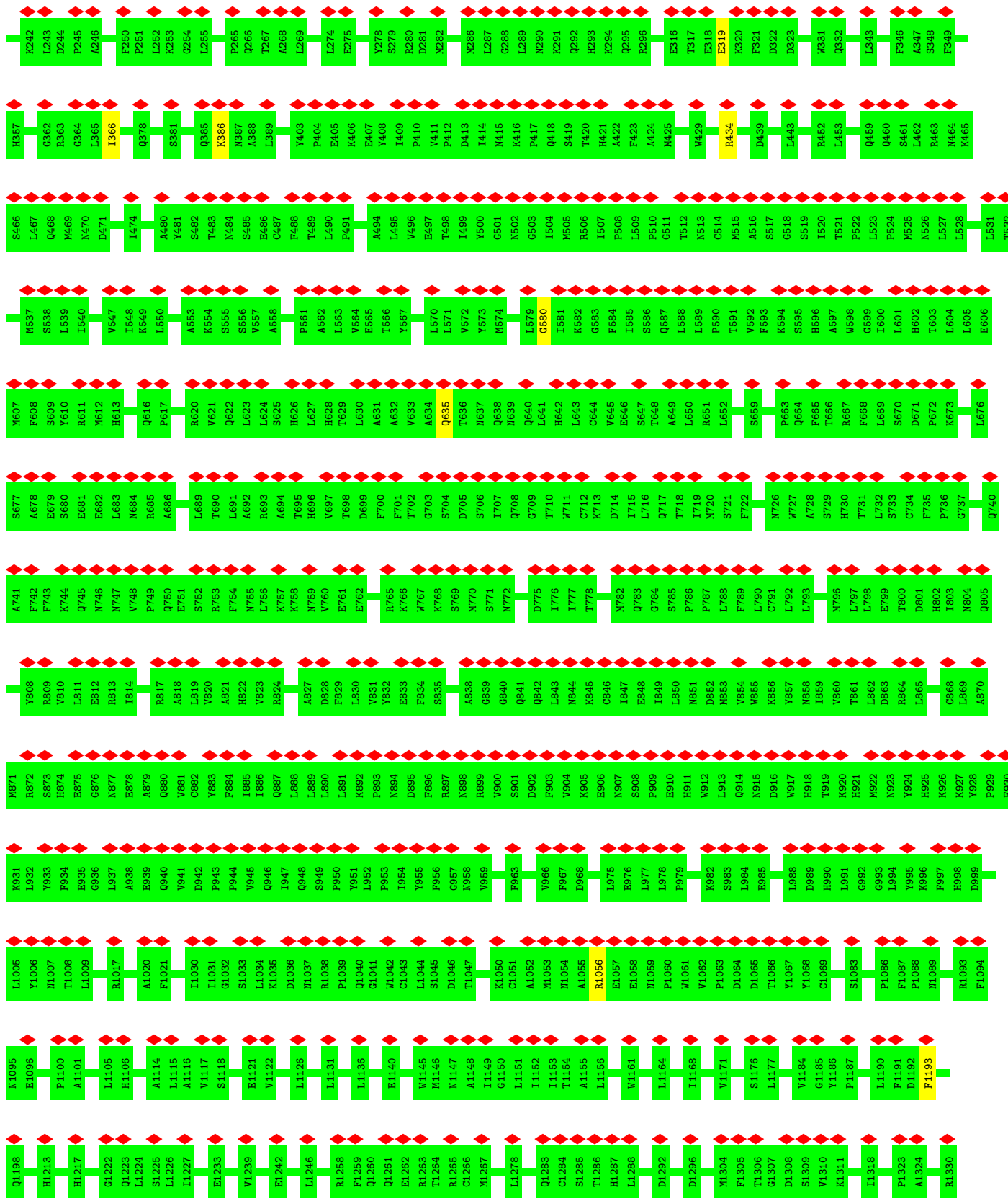
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

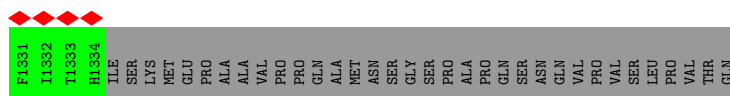
- Molecule 1: Isoform 2 of Mediator of RNA polymerase II transcription subunit 16



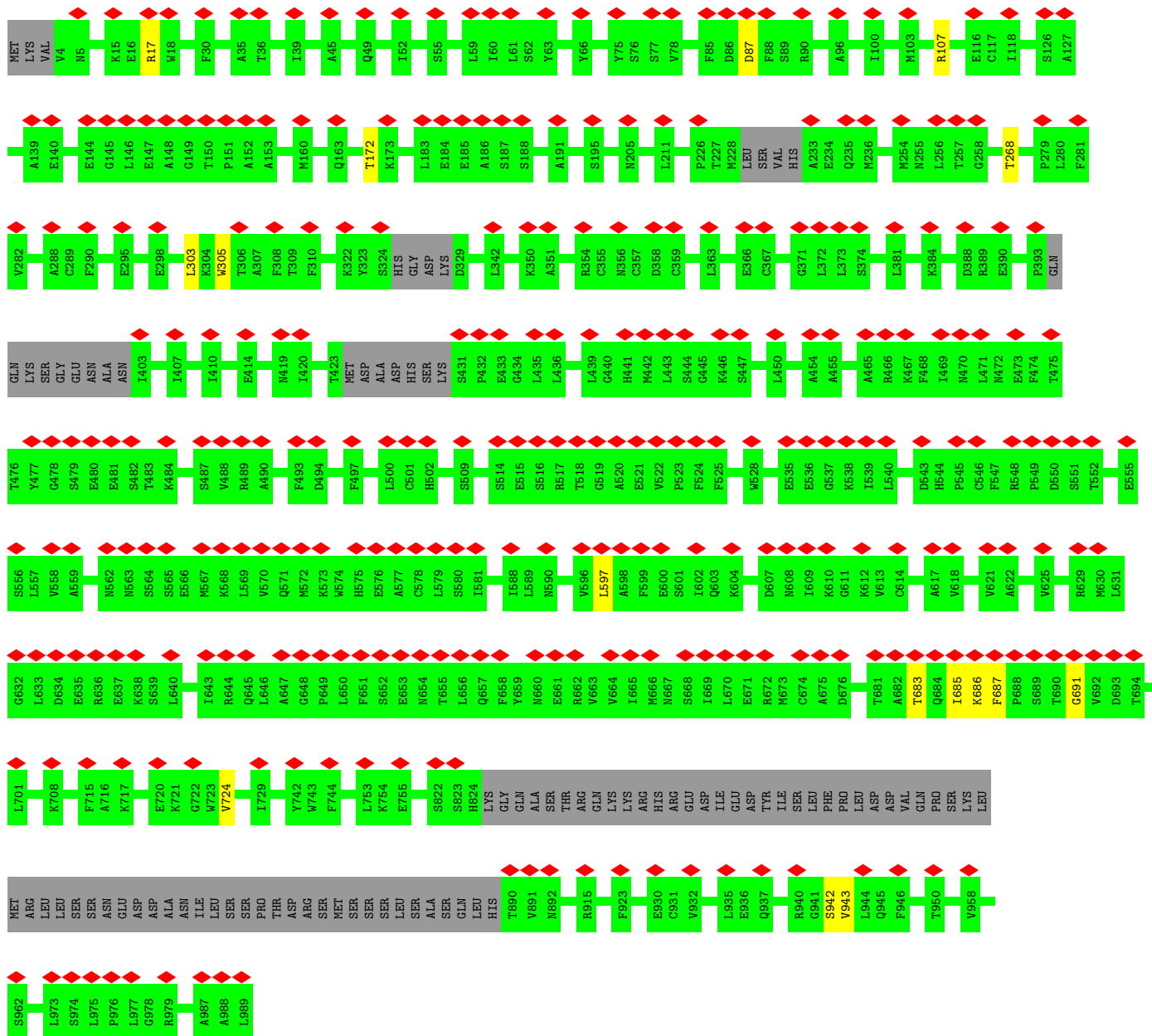
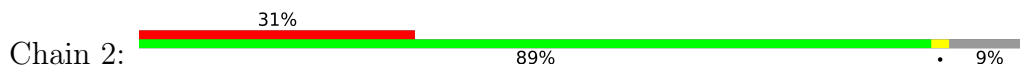
- Molecule 2: Mediator of RNA polymerase II transcription subunit 23





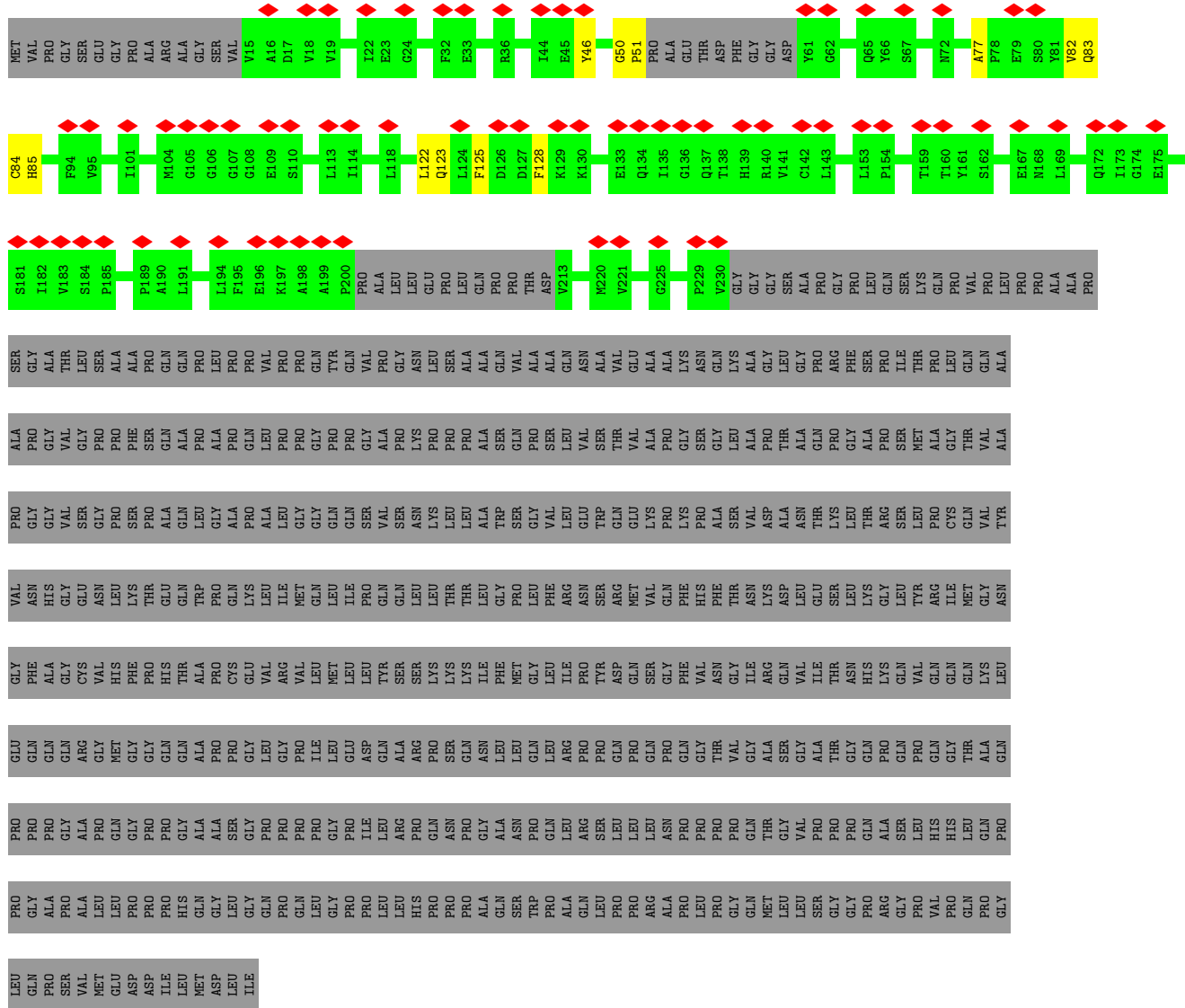


• Molecule 3: Mediator of RNA polymerase II transcription subunit 24

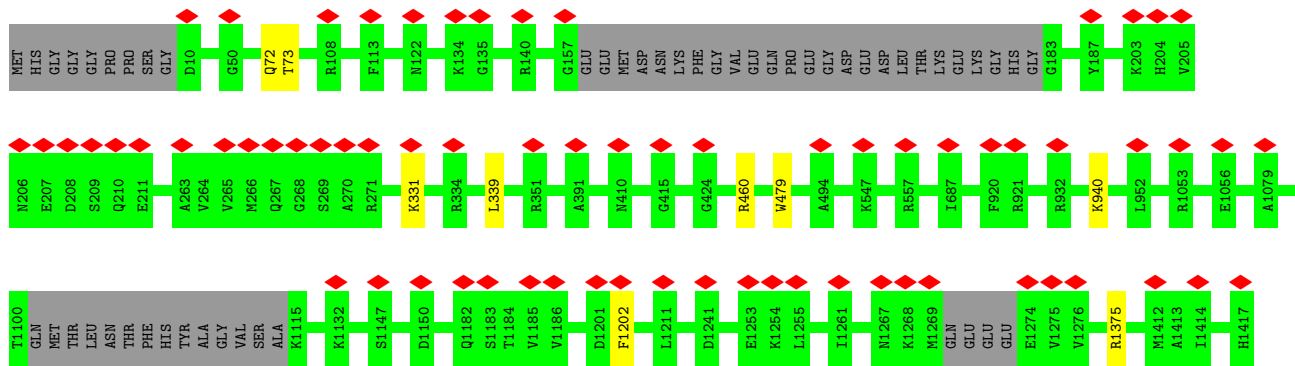
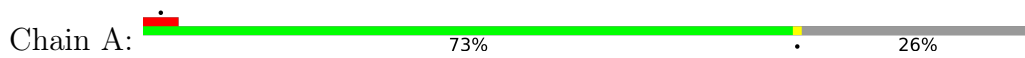


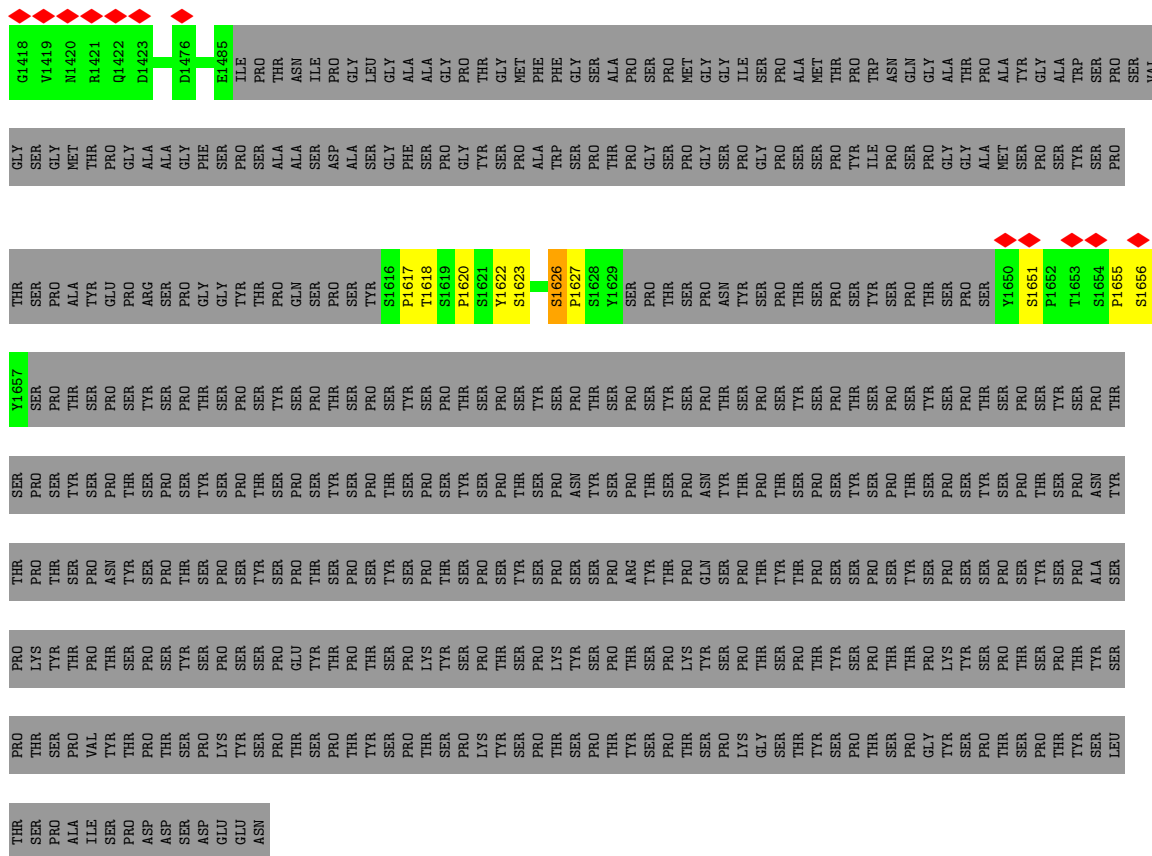
• Molecule 4: Mediator of RNA polymerase II transcription subunit 25



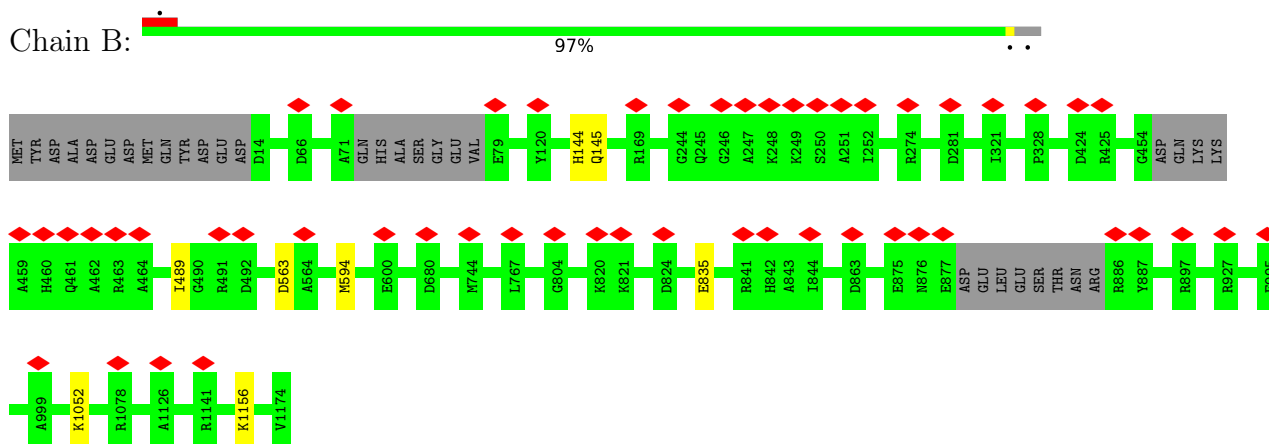


● Molecule 5: DNA-directed RNA polymerase II subunit RPB1

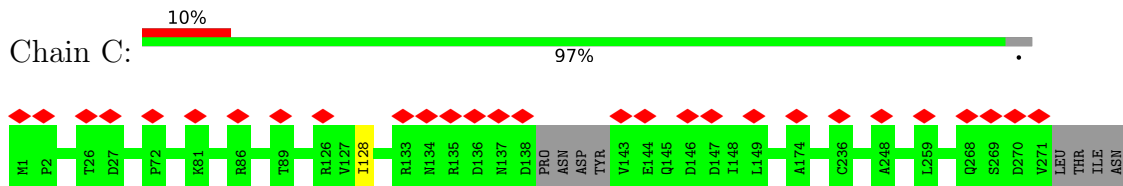




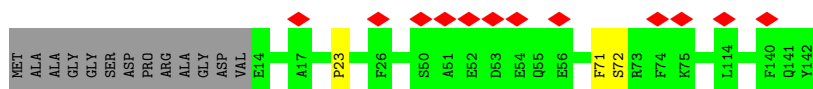
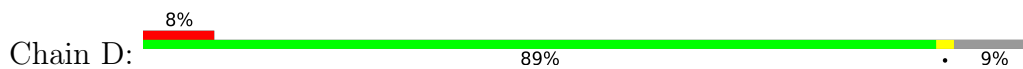
• Molecule 6: DNA-directed RNA polymerase II subunit RPB2



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



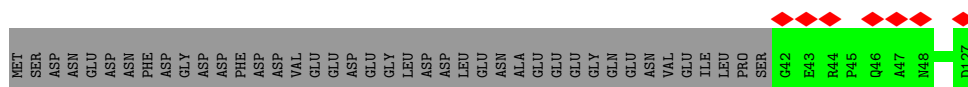
• Molecule 8: DNA-directed RNA polymerase II subunit RPB4



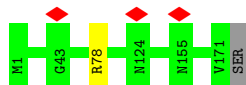
- Molecule 9: DNA-directed RNA polymerase II subunit RPB5



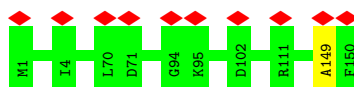
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC2



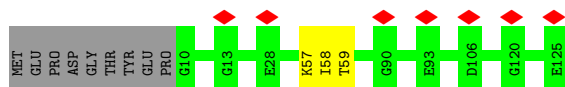
- Molecule 11: DNA-directed RNA polymerase II subunit RPB7



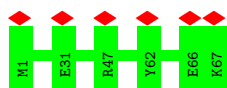
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC3



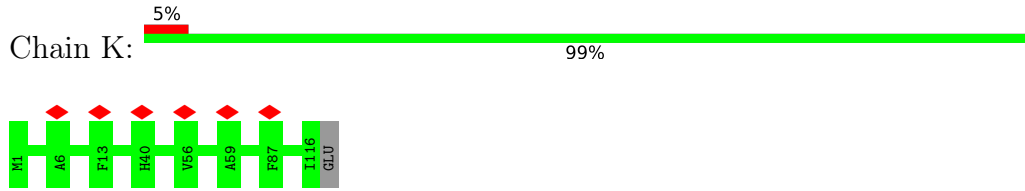
- Molecule 13: DNA-directed RNA polymerase II subunit RPB9



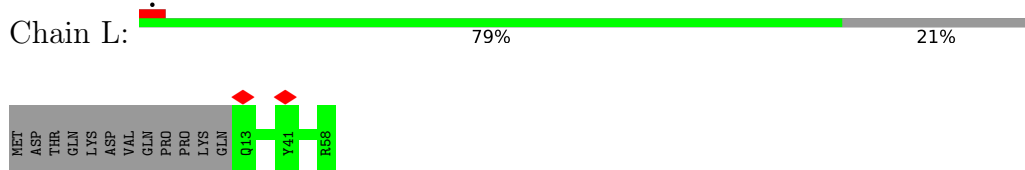
- Molecule 14: DNA-directed RNA polymerases I, II, and III subunit RPABC5



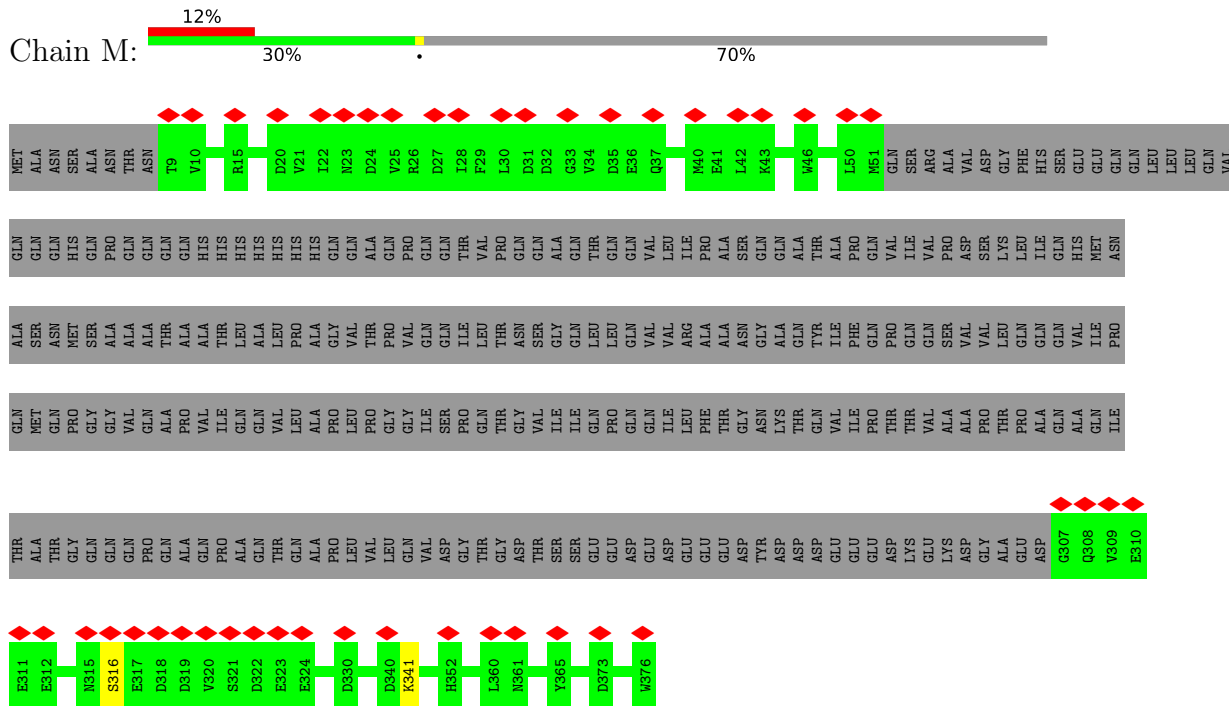
- Molecule 15: DNA-directed RNA polymerase II subunit RPB11-a



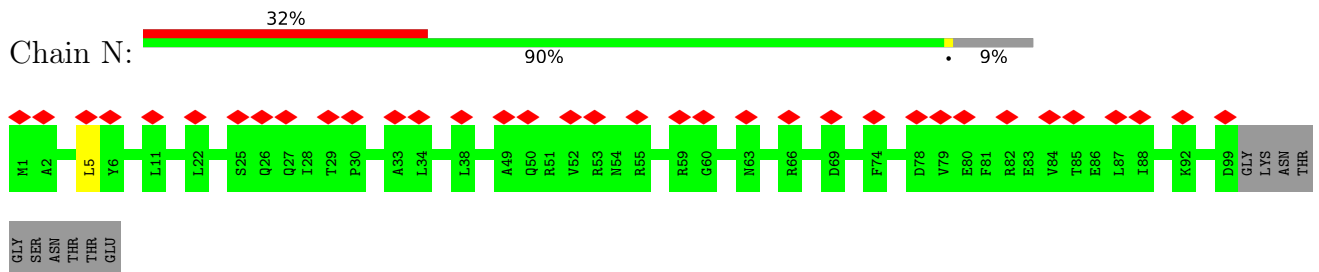
- Molecule 16: DNA-directed RNA polymerases I, II, and III subunit RPABC4



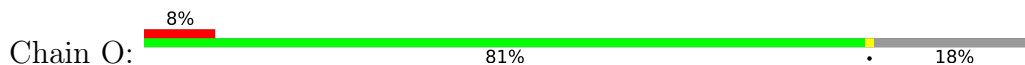
- Molecule 17: Transcription initiation factor IIA subunit 1

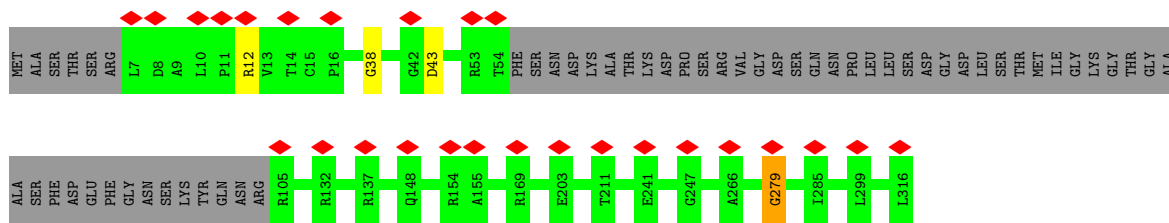


- Molecule 18: Transcription initiation factor IIA subunit 2

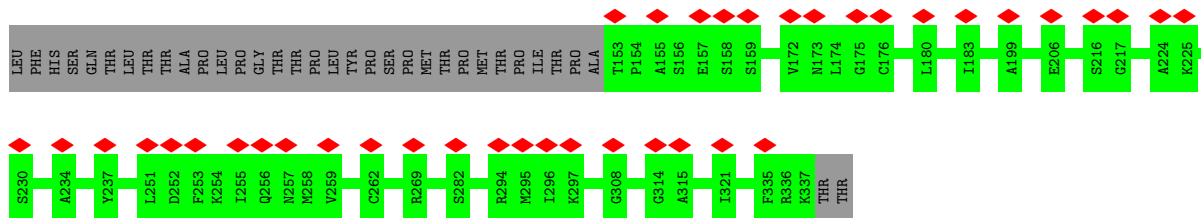
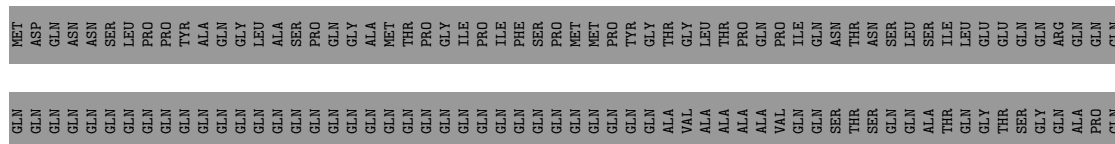


- Molecule 19: Transcription initiation factor IIB

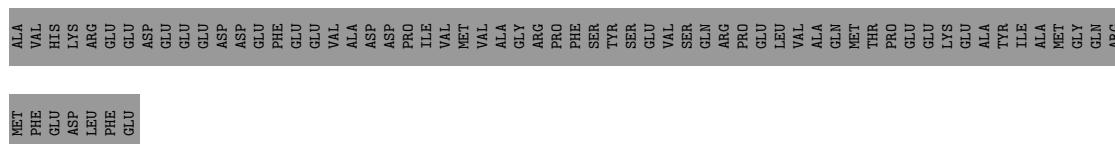
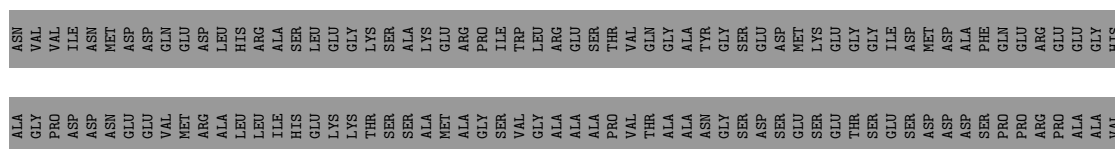
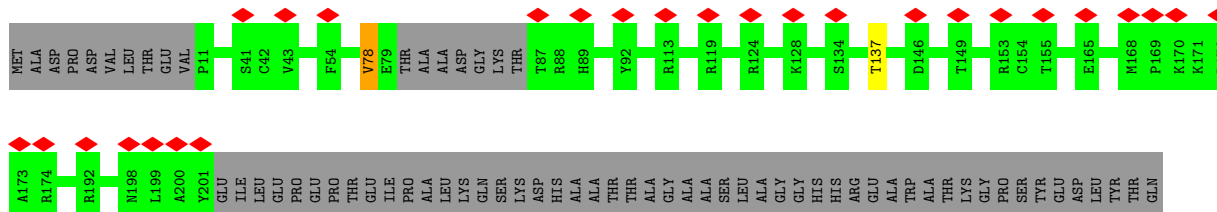




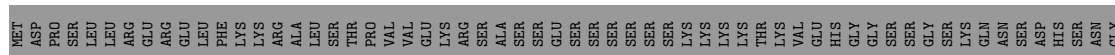
• Molecule 20: TATA-box-binding protein

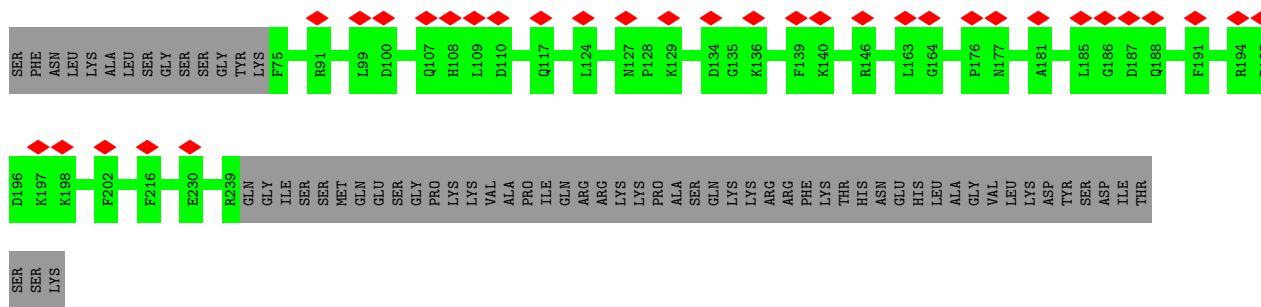


• Molecule 21: General transcription factor IIE subunit 1

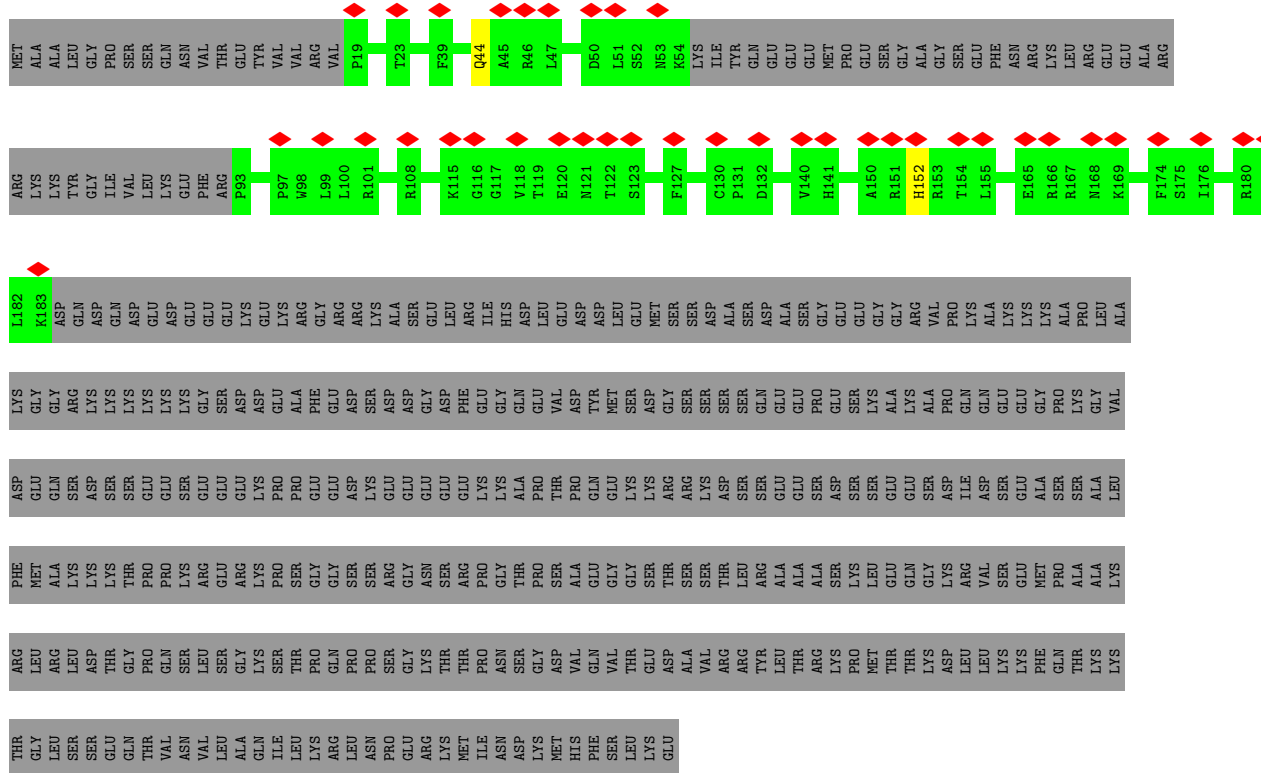


• Molecule 22: Transcription initiation factor IIE subunit beta

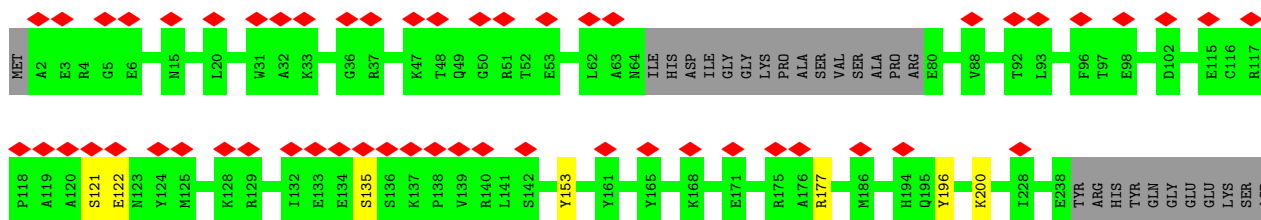
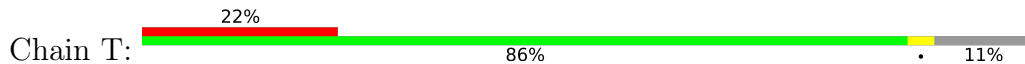




● Molecule 23: General transcription factor IIF subunit 1



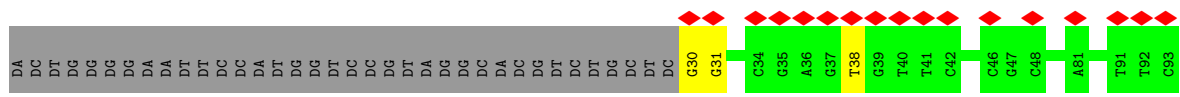
● Molecule 24: General transcription factor IIF subunit 2



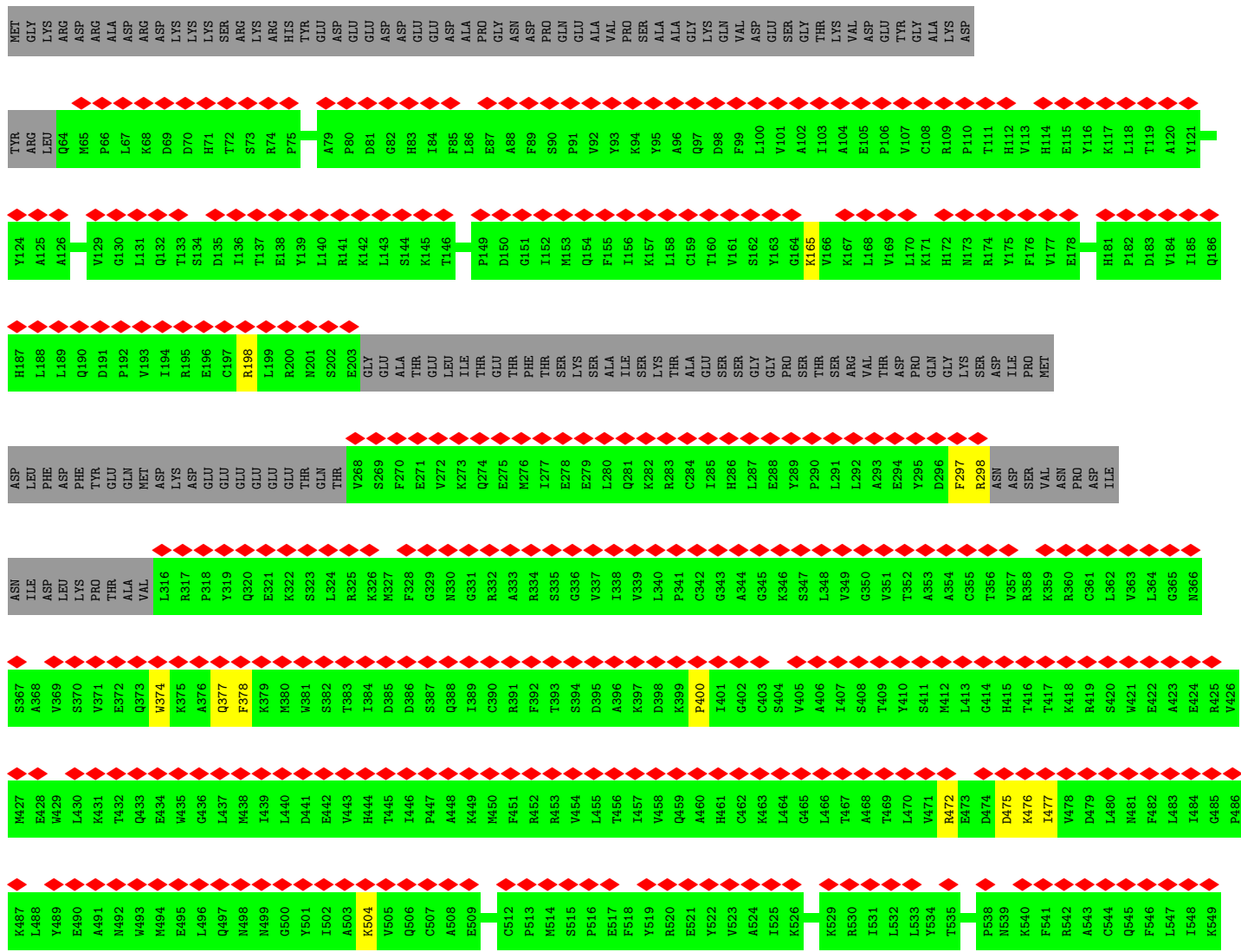
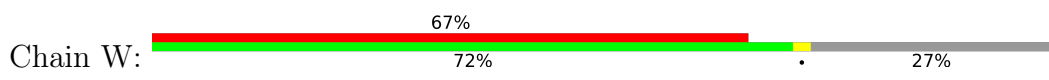
● Molecule 25: super core promoter sense strand

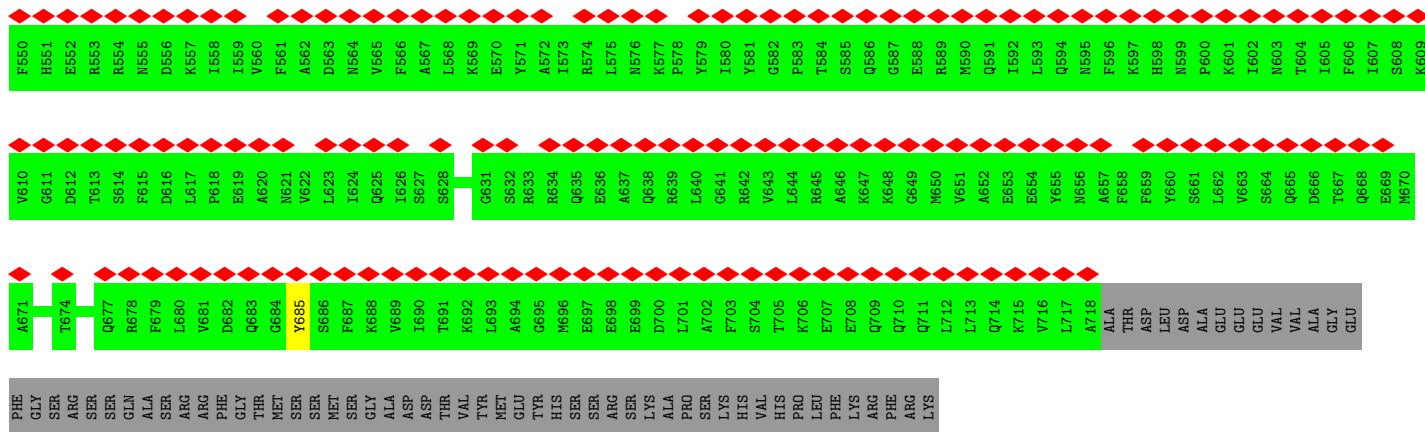


• Molecule 26: super core promoter antisense strand

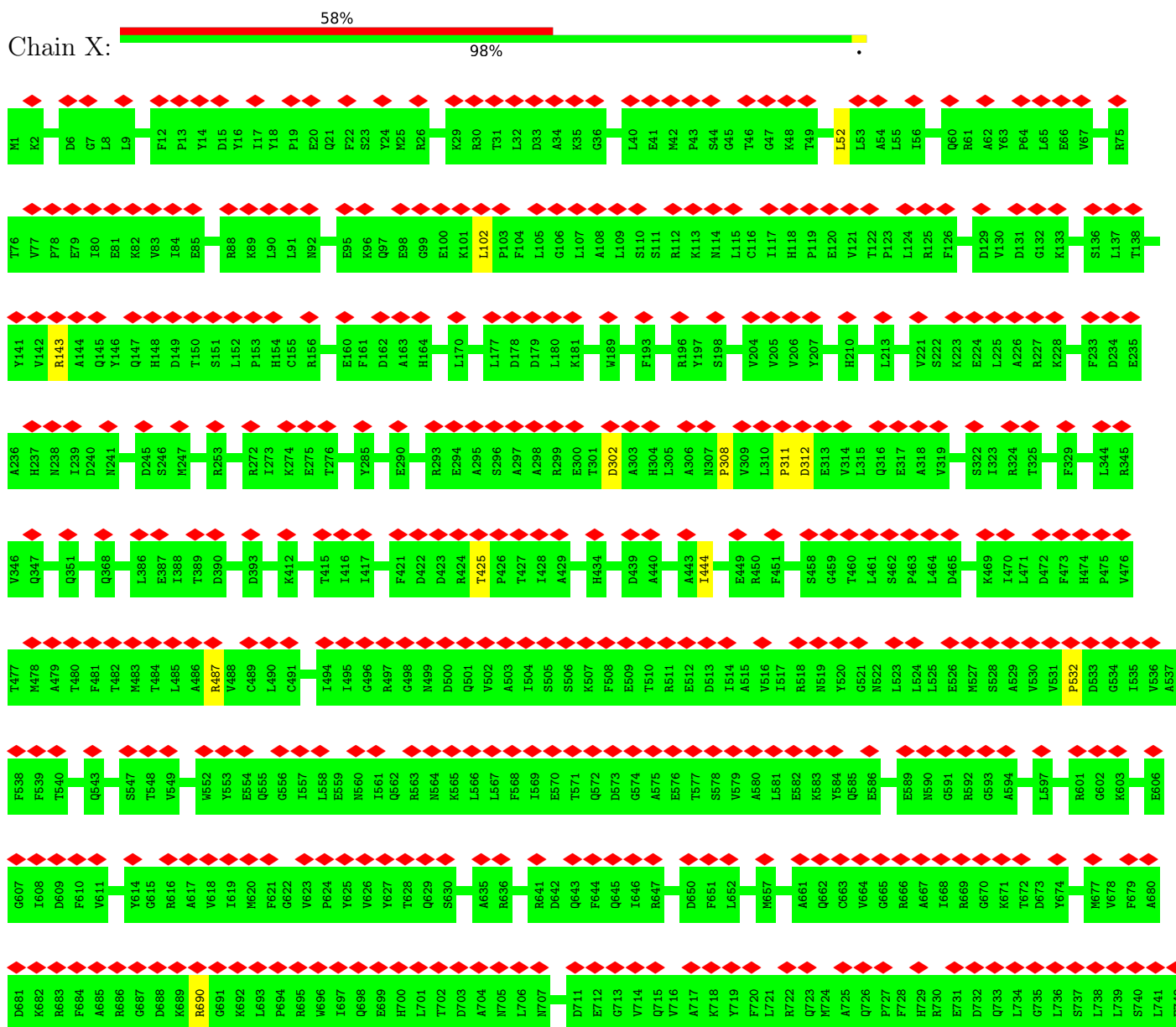


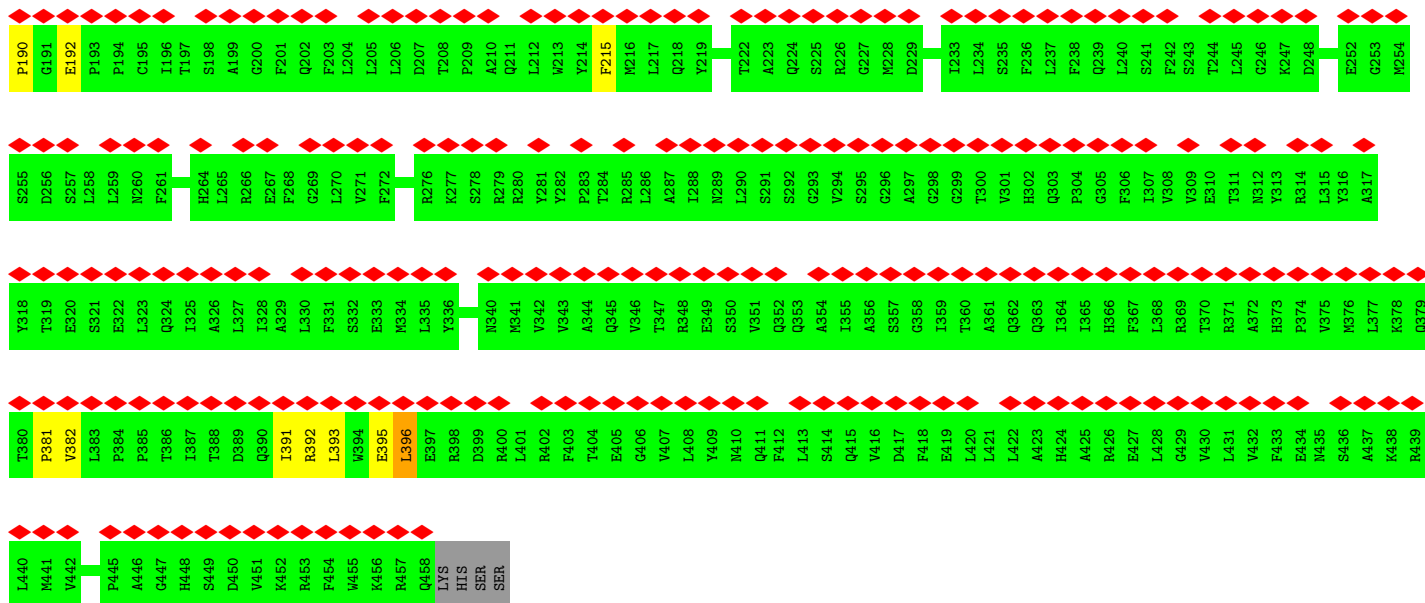
• Molecule 27: TFIIF basal transcription factor complex helicase XPB subunit



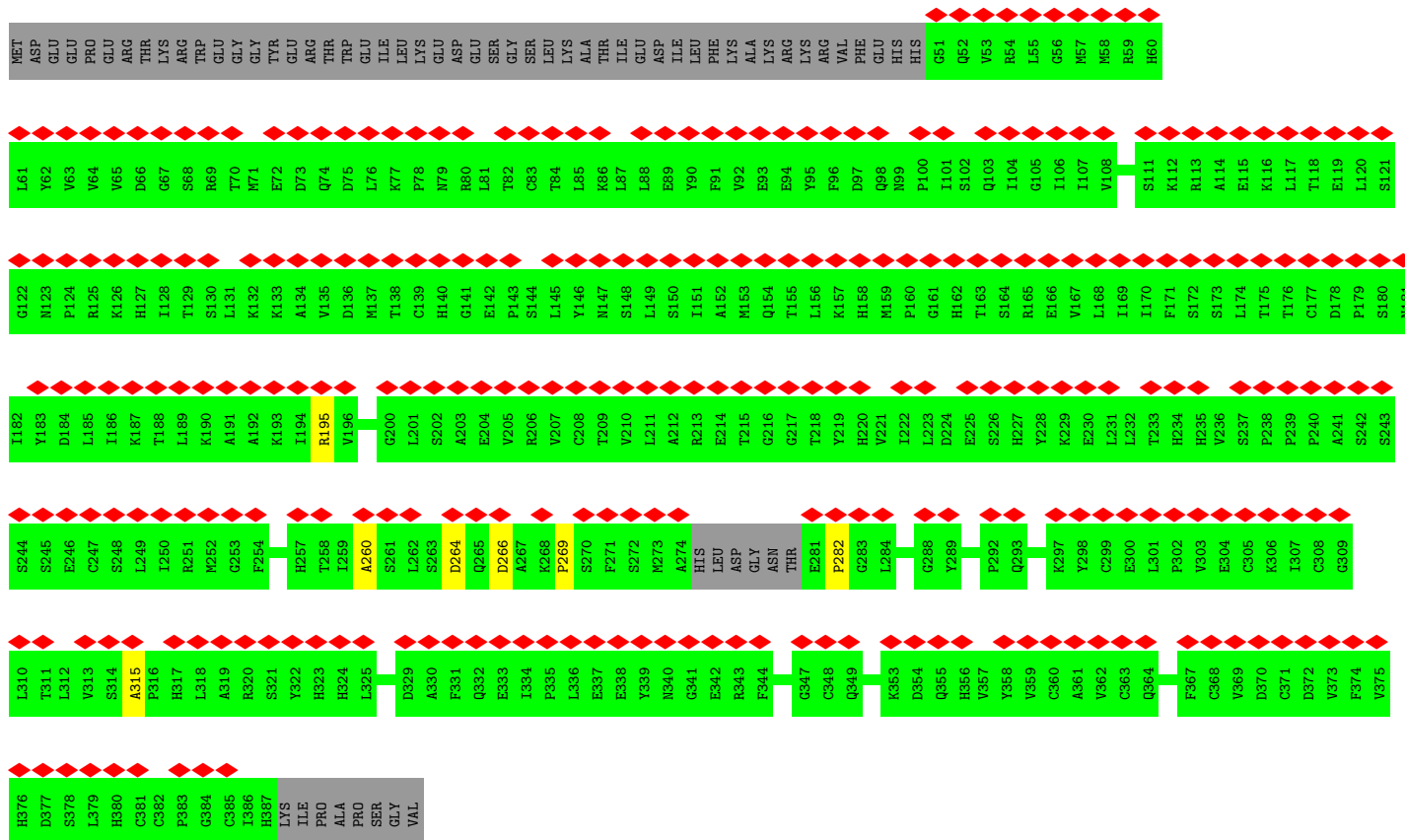
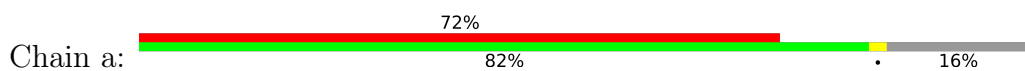


● Molecule 28: TFIIF basal transcription factor complex helicase XPD subunit

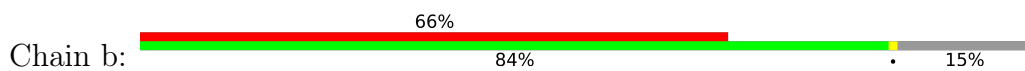


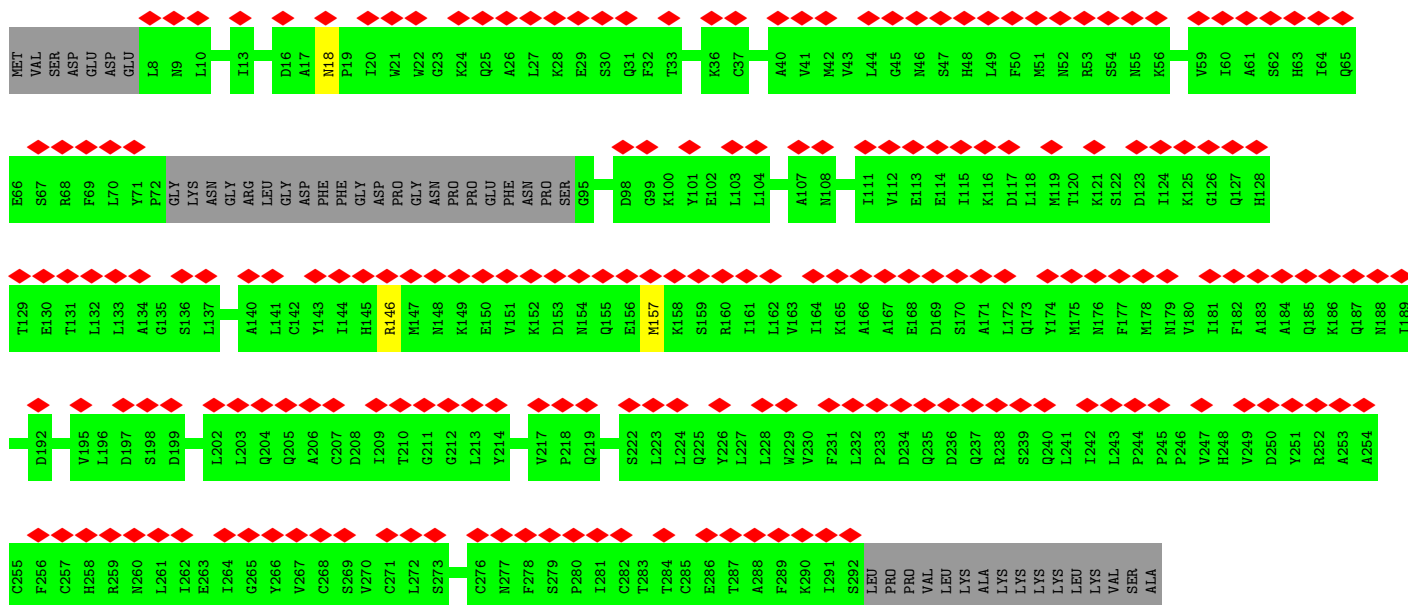


• Molecule 31: General transcription factor IIH subunit 2

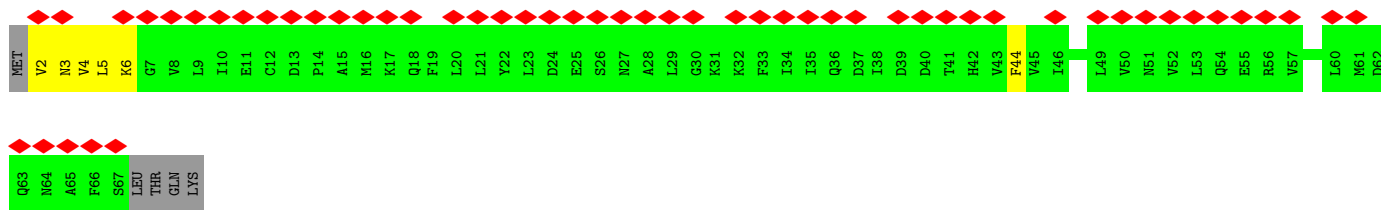
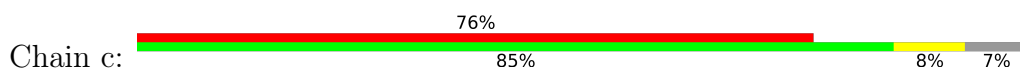


• Molecule 32: General transcription factor IIH subunit 3

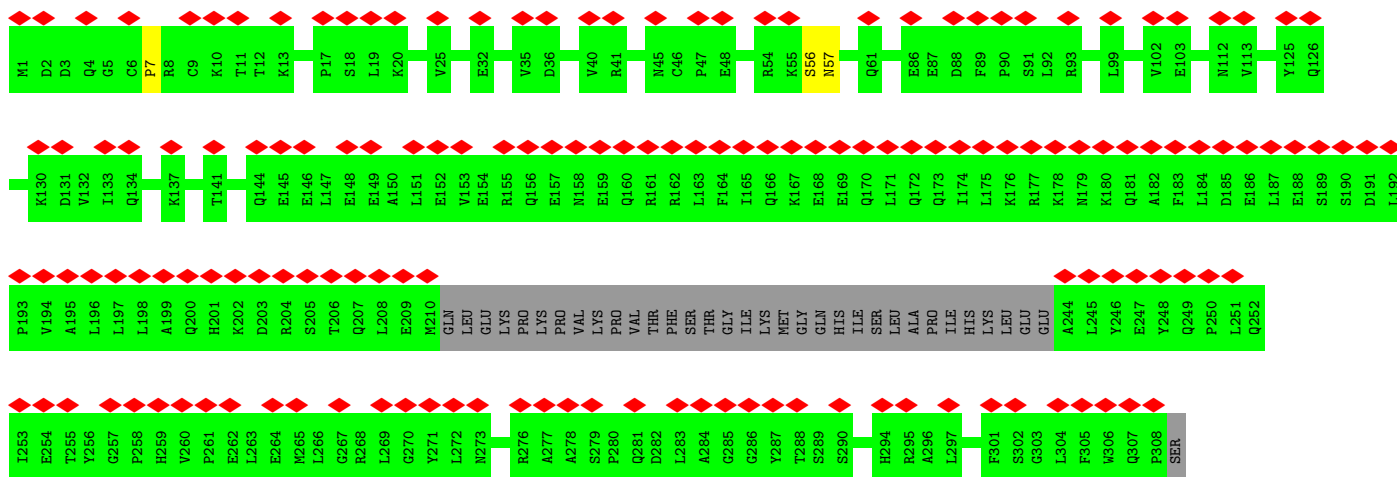
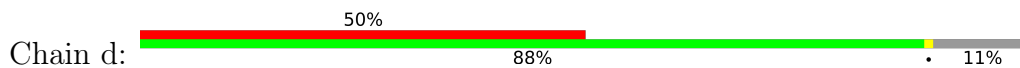




• Molecule 33: General transcription factor IIH subunit 5



• Molecule 34: CDK-activating kinase assembly factor MAT1



• Molecule 35: Cyclin-dependent kinase 7

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

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

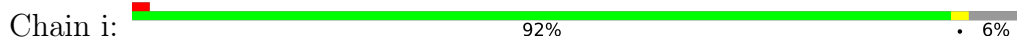


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GLN
ARG
E4
E36
TYR
GLY
ARG
LEU
SER
THR
W42
E66
K67
Q74
V75
P76
LEU
VAL
LEU
SER
PRO
ASP
ASP
ASP
ASP
LEU
MET
ARG
GLN
MET
GLN
THR
GLY
GLY
ALA
ARG
VAL
PRO
PHE
VAL
SER
MET
H102
A129
A133
A136
E157
S163
G164
G165
K189
GLY
LEU

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

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

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



MET
ALA
THR
TYR
SER
LEU
A7
R12
R43
A74
E116
ASN

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



MET
SER
GLY
VAL
ARG
ALA
VAL
ARG
ILE
SER
ILE
GLU
SER
ALA
CYS
GLU
LYS
GLN
VAL
HIS
GLU
VAL
GLY
LEU
ASP
GLY
THR
GLU
TYR
LEU
PRO
P33
L34
S35
M36
S37
Q38
R42
R46
I47
F49
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GLU
GLU
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ALA
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GLY
THR
GLU

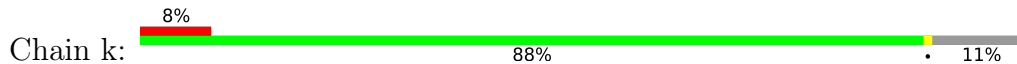
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VAL
PHE
GLN
PRO
SER
LEU
W93
R103
V119
ARG
ASP
LYS
LYS
PHE
MET
THR
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M174
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E176
M177

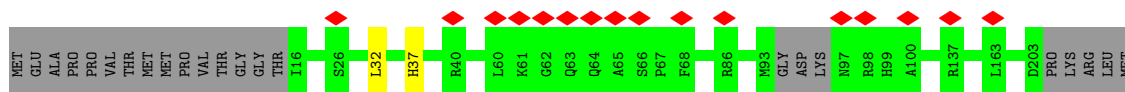
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CYS
PRO
LEU
D244
K263
GLN
ALA
PRO
ASP
ILE
GLY
ASP
LEU
GLY
THR
VAL
ASN
SER
PHE
LYS
ARG
PRO
PRO
LEU
LEU
P287
Q317
I318
P335
S349
ASN
ASP
LYS

LYS
SER
GLN
LYS
PHE
THR
GLU
GLN
CYS
PRO
E365
D366
H367
P399
D414
K415
M416
I432
K433
Q434
H437
L440
E456
D457
D469
V470
V471
E472
V475
K476
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Q501
R507
V543
L549

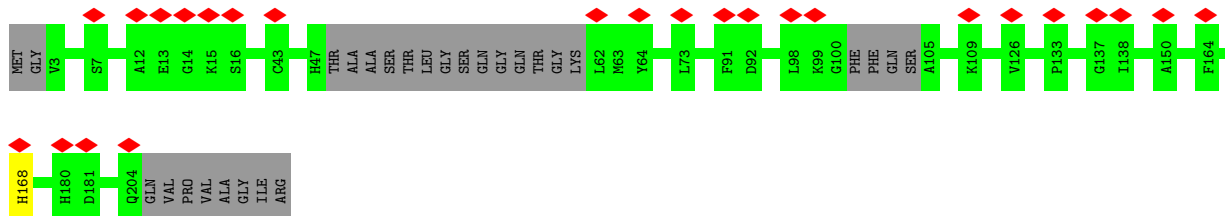
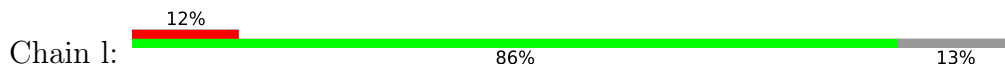
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L557
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P559
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E587
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W615
S616
H617
L618
R619
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P621
W627
N628
K629
M630
E631
P648
L651

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

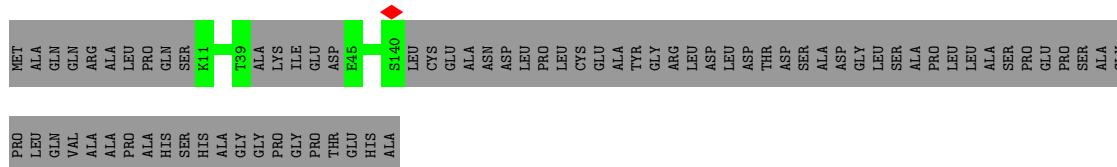




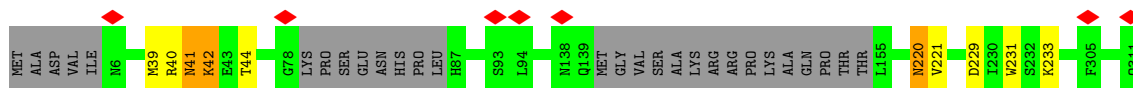
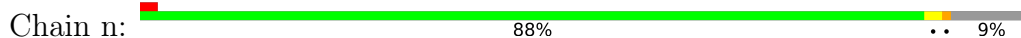
• Molecule 42: Mediator of RNA polymerase II transcription subunit 20



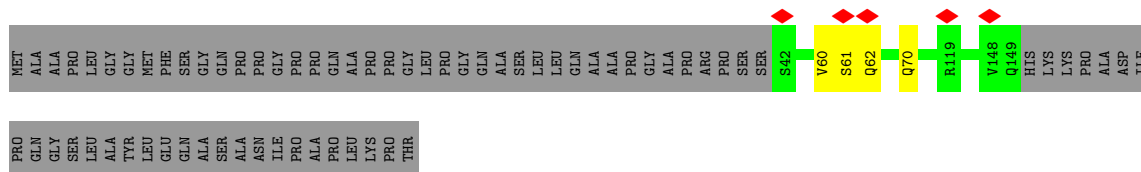
• Molecule 43: Mediator of RNA polymerase II transcription subunit 22



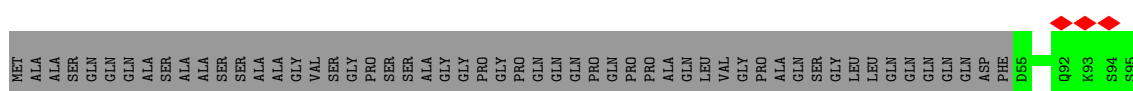
• Molecule 44: Mediator of RNA polymerase II transcription subunit 27



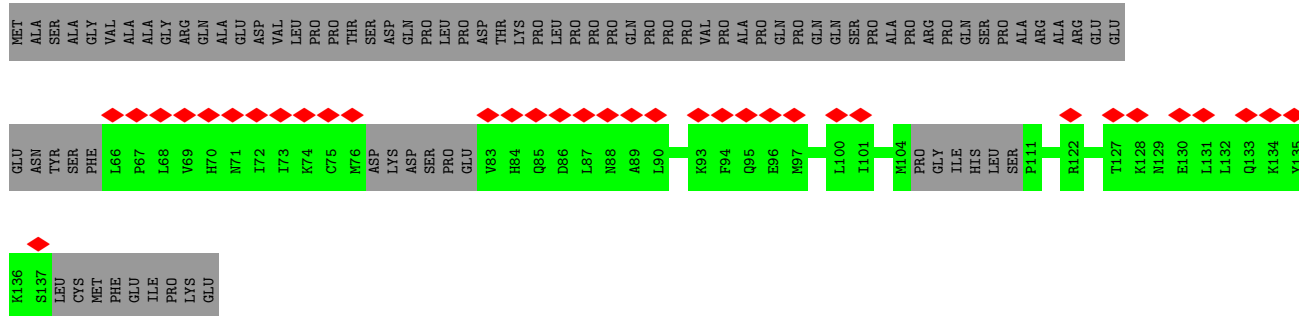
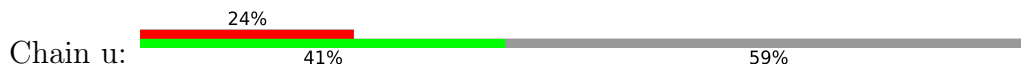
• Molecule 45: Mediator of RNA polymerase II transcription subunit 28



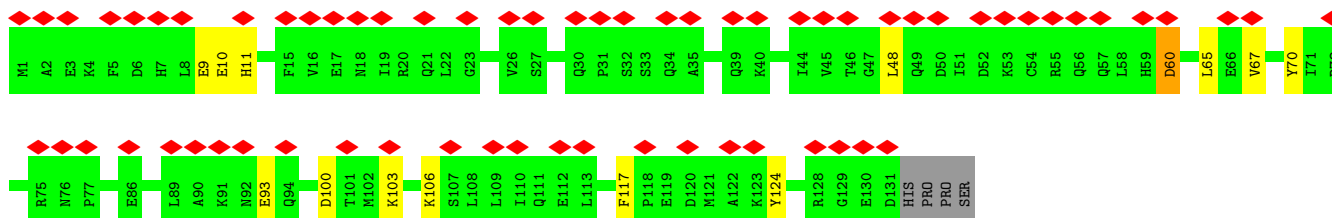
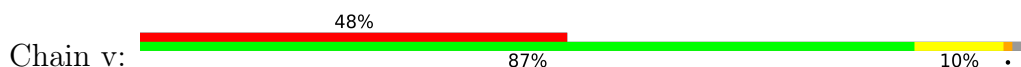
• Molecule 46: Mediator of RNA polymerase II transcription subunit 29



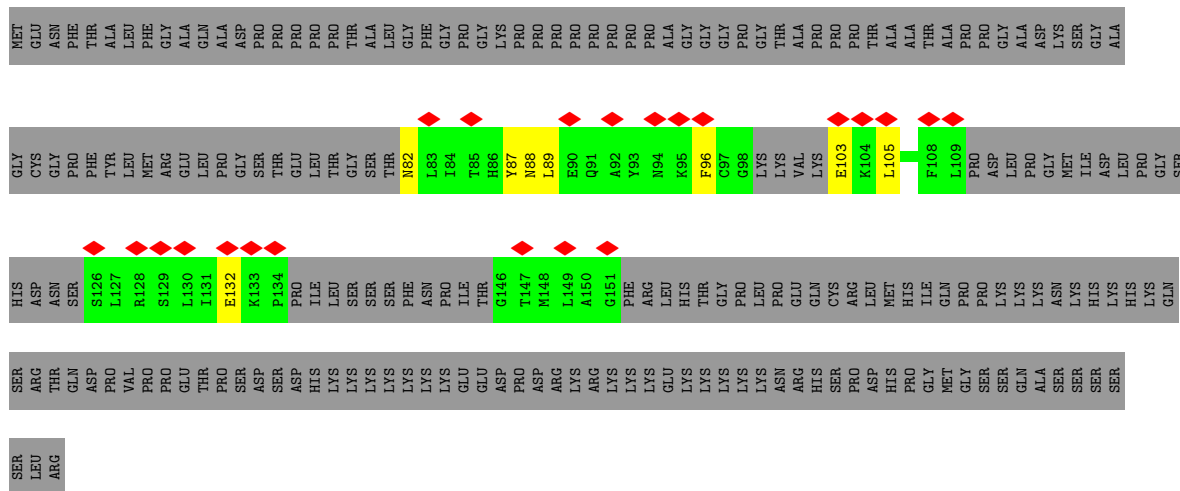
• Molecule 51: Mediator of RNA polymerase II transcription subunit 9



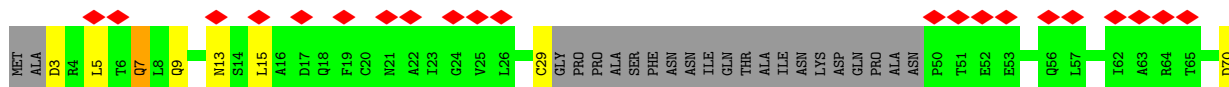
• Molecule 52: Mediator of RNA polymerase II transcription subunit 10

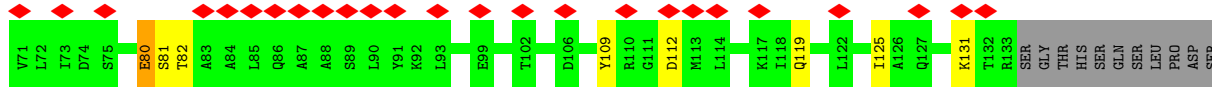


• Molecule 53: Mediator of RNA polymerase II transcription subunit 19

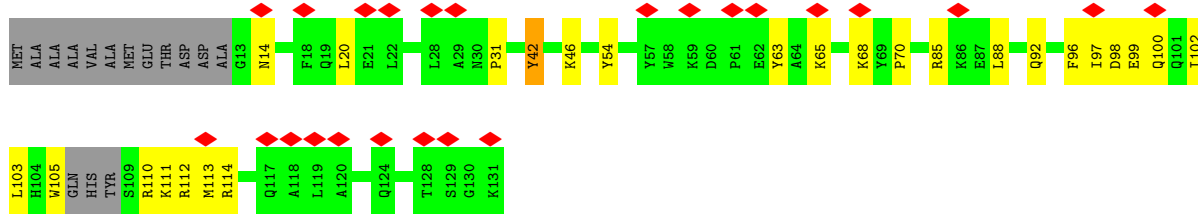


• Molecule 54: Mediator of RNA polymerase II transcription subunit 21

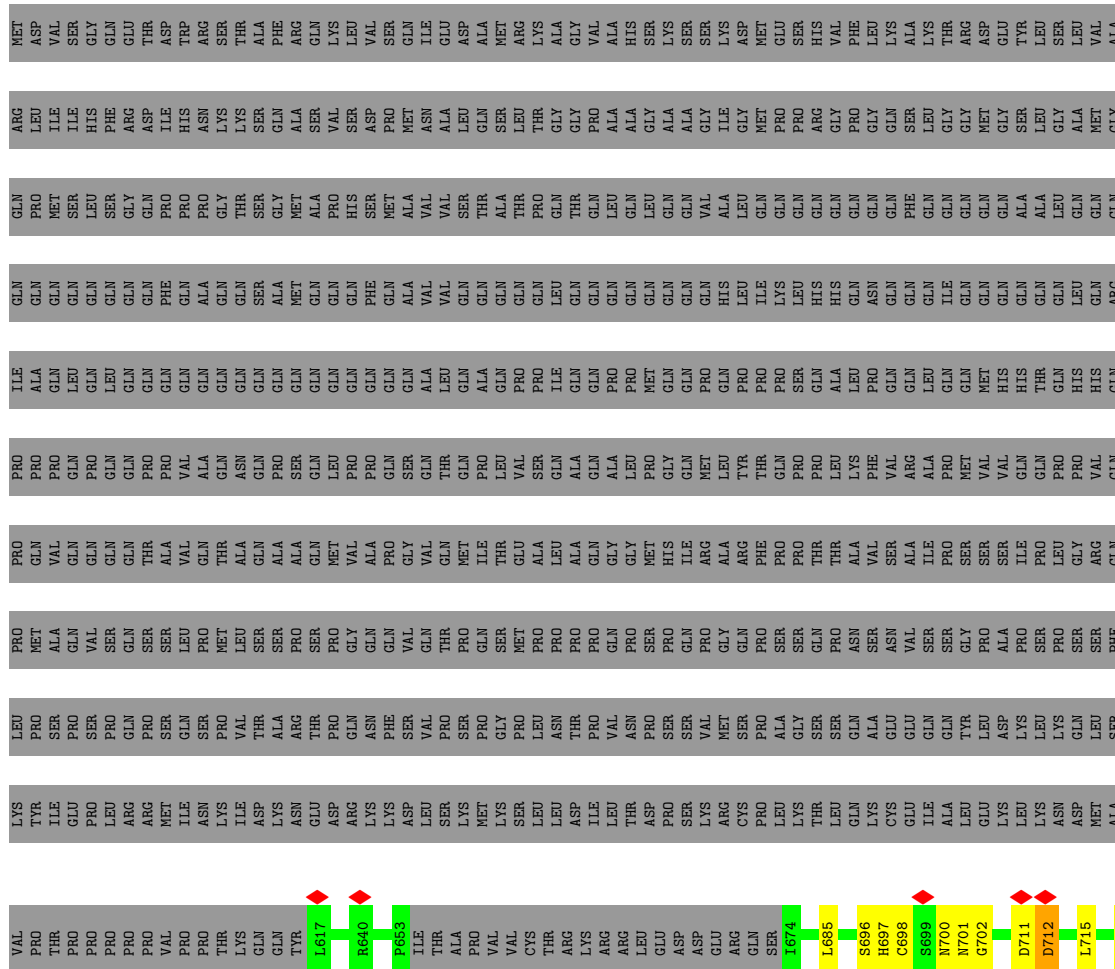




• Molecule 55: Mediator of RNA polymerase II transcription subunit 31



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



4 Experimental information

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 ($e^-/\text{\AA}^2$)	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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.67	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

The worst 5 of 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

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

There are no chirality outliers.

5 of 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

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%)	17	56
2	1	1313/1368 (96%)	1201 (92%)	108 (8%)	4 (0%)	41	76
3	2	885/989 (90%)	774 (88%)	105 (12%)	6 (1%)	22	62
4	3	189/747 (25%)	167 (88%)	22 (12%)	0	100	100
5	A	1443/1970 (73%)	1316 (91%)	119 (8%)	8 (1%)	25	65
6	B	1134/1174 (97%)	1028 (91%)	103 (9%)	3 (0%)	41	76
7	C	263/275 (96%)	240 (91%)	23 (9%)	0	100	100
8	D	127/142 (89%)	114 (90%)	12 (9%)	1 (1%)	19	59
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%)	22	62
13	I	114/125 (91%)	95 (83%)	18 (16%)	1 (1%)	17	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	13	50
20	P	183/339 (54%)	178 (97%)	5 (3%)	0	100	100
21	Q	180/439 (41%)	153 (85%)	25 (14%)	2 (1%)	14	51
22	R	163/291 (56%)	139 (85%)	24 (15%)	0	100	100
23	S	123/517 (24%)	97 (79%)	25 (20%)	1 (1%)	19	59
24	T	218/249 (88%)	182 (84%)	33 (15%)	3 (1%)	11	46
27	W	568/782 (73%)	518 (91%)	49 (9%)	1 (0%)	47	81
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%)	29	68
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%)	22	62
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%)	7	39
39	i	108/117 (92%)	103 (95%)	5 (5%)	0	100	100
40	j	492/651 (76%)	409 (83%)	72 (15%)	11 (2%)	6	37
41	k	181/208 (87%)	159 (88%)	22 (12%)	0	100	100
42	l	178/212 (84%)	150 (84%)	27 (15%)	1 (1%)	25	65
43	m	121/200 (60%)	118 (98%)	3 (2%)	0	100	100
44	n	277/311 (89%)	225 (81%)	46 (17%)	6 (2%)	6	37
45	o	106/178 (60%)	95 (90%)	9 (8%)	2 (2%)	8	40
46	p	110/200 (55%)	106 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	q	116/178 (65%)	107 (92%)	9 (8%)	0	100	100
48	r	1004/1454 (69%)	819 (82%)	165 (16%)	20 (2%)	7	39
49	s	129/270 (48%)	98 (76%)	27 (21%)	4 (3%)	4	30
50	t	110/233 (47%)	76 (69%)	32 (29%)	2 (2%)	8	41
51	u	54/146 (37%)	49 (91%)	5 (9%)	0	100	100
52	v	129/135 (96%)	92 (71%)	35 (27%)	2 (2%)	9	44
53	w	31/244 (13%)	21 (68%)	9 (29%)	1 (3%)	4	30
54	x	107/144 (74%)	81 (76%)	26 (24%)	0	100	100
55	y	112/131 (86%)	71 (63%)	36 (32%)	5 (4%)	2	24
56	z	145/788 (18%)	126 (87%)	14 (10%)	5 (3%)	3	29
All	All	15623/21786 (72%)	13748 (88%)	1768 (11%)	107 (1%)	26	62

5 of 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

5.3.2 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%)	38	61
2	1	1187/1232 (96%)	1183 (100%)	4 (0%)	92	95
3	2	780/864 (90%)	777 (100%)	3 (0%)	91	94
4	3	165/601 (28%)	156 (94%)	9 (6%)	21	49
5	A	1285/1748 (74%)	1277 (99%)	8 (1%)	86	92
6	B	999/1028 (97%)	997 (100%)	2 (0%)	93	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	84	90
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
17	M	105/324 (32%)	104 (99%)	1 (1%)	76	86
18	N	90/98 (92%)	89 (99%)	1 (1%)	73	85
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%)	55	73
27	W	508/688 (74%)	498 (98%)	10 (2%)	55	73
28	X	661/664 (100%)	658 (100%)	3 (0%)	88	93
29	Y	162/484 (34%)	162 (100%)	0	100	100
30	Z	372/399 (93%)	363 (98%)	9 (2%)	49	69
31	a	296/352 (84%)	295 (100%)	1 (0%)	92	95
32	b	234/272 (86%)	231 (99%)	3 (1%)	69	82
33	c	59/64 (92%)	53 (90%)	6 (10%)	7	27
34	d	210/283 (74%)	210 (100%)	0	100	100
35	e	259/299 (87%)	258 (100%)	1 (0%)	91	94
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%)	73	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	j	452/577 (78%)	423 (94%)	29 (6%)	17	44
41	k	164/183 (90%)	162 (99%)	2 (1%)	71	84
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%)	81	89
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%)	59	77
48	r	905/1271 (71%)	869 (96%)	36 (4%)	31	56
49	s	119/230 (52%)	117 (98%)	2 (2%)	60	78
50	t	110/216 (51%)	108 (98%)	2 (2%)	59	77
51	u	59/133 (44%)	59 (100%)	0	100	100
52	v	119/124 (96%)	114 (96%)	5 (4%)	30	55
53	w	34/208 (16%)	33 (97%)	1 (3%)	42	64
54	x	92/119 (77%)	83 (90%)	9 (10%)	8	28
55	y	105/115 (91%)	86 (82%)	19 (18%)	1	11
56	z	135/697 (19%)	129 (96%)	6 (4%)	28	54
All	All	14009/19107 (73%)	13805 (98%)	204 (2%)	66	80

5 of 204 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
40	j	617	HIS
48	r	328	ARG
56	z	698	CYS
41	k	37	HIS
48	r	188	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 285 such sidechains are listed below:

Mol	Chain	Res	Type
46	p	124	HIS
48	r	214	ASN
50	t	74	HIS
6	B	1117	HIS

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Mol	Chain	Res	Type
6	B	1013	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

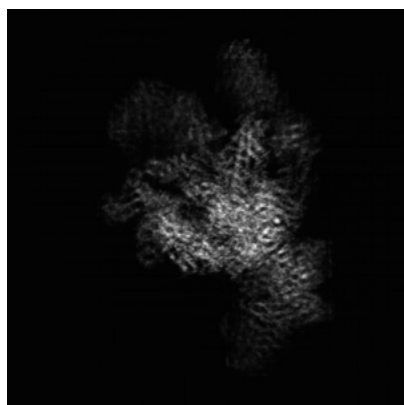
6 Map visualisation [i](#)

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.

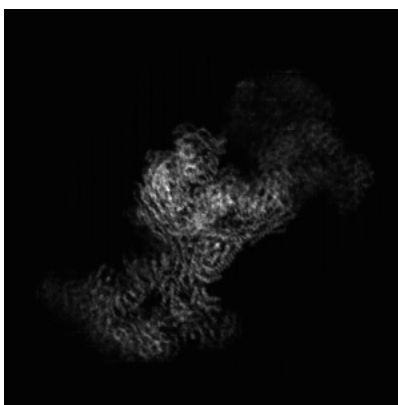
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

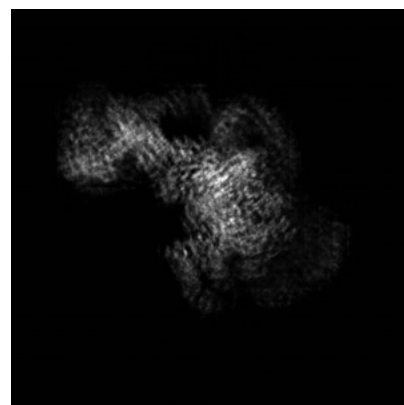
6.1.1 Primary map



X



Y

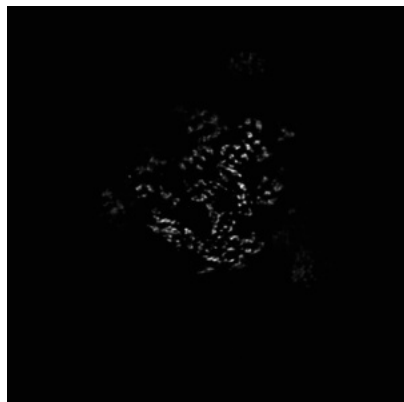


Z

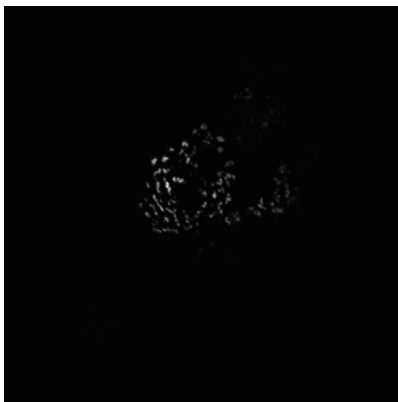
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 210



Y Index: 210

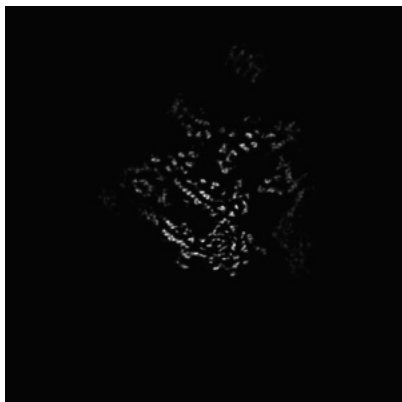


Z Index: 210

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

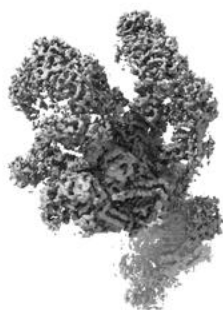


Z Index: 182

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

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

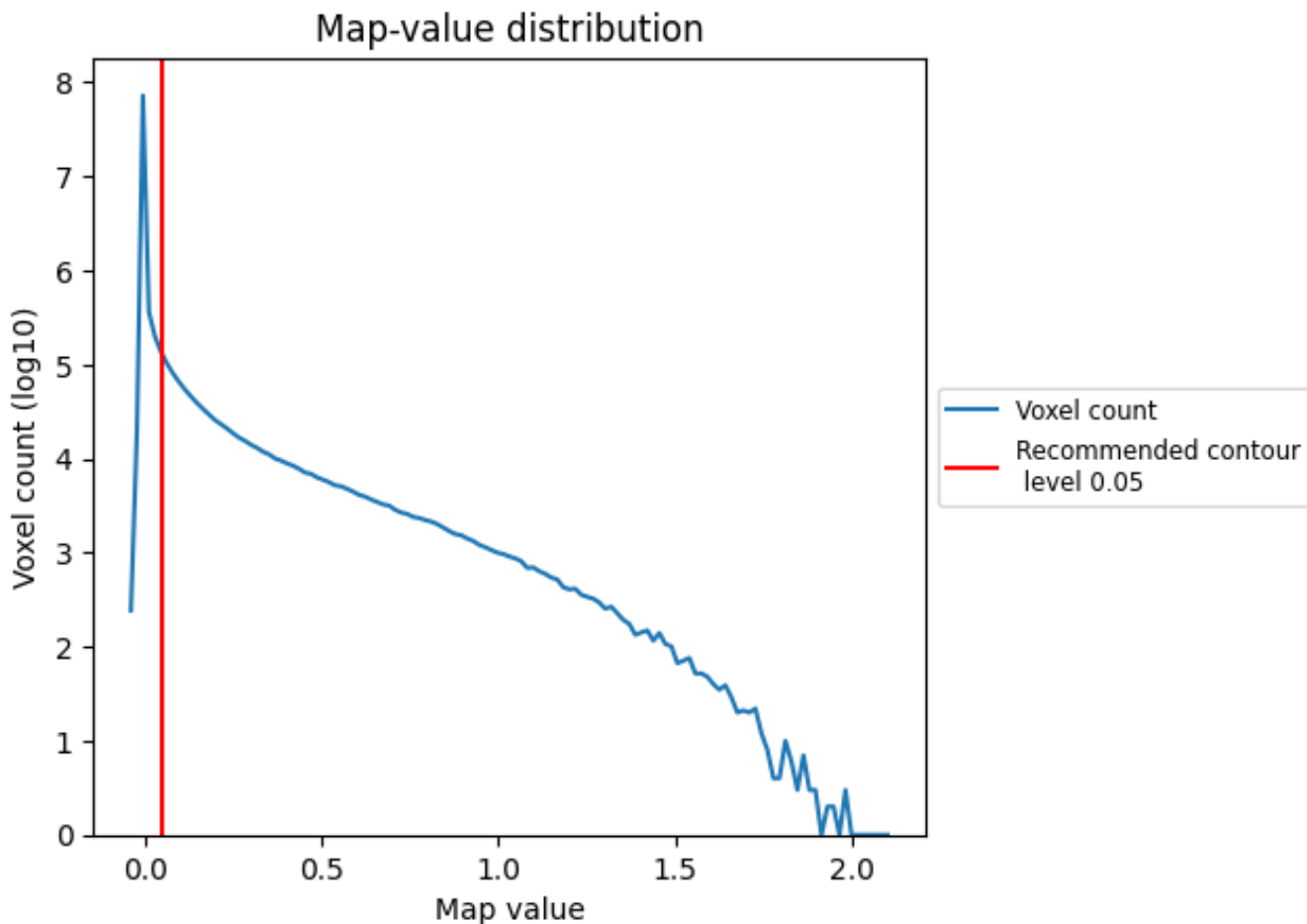
6.5 Mask visualisation

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

7 Map analysis [i](#)

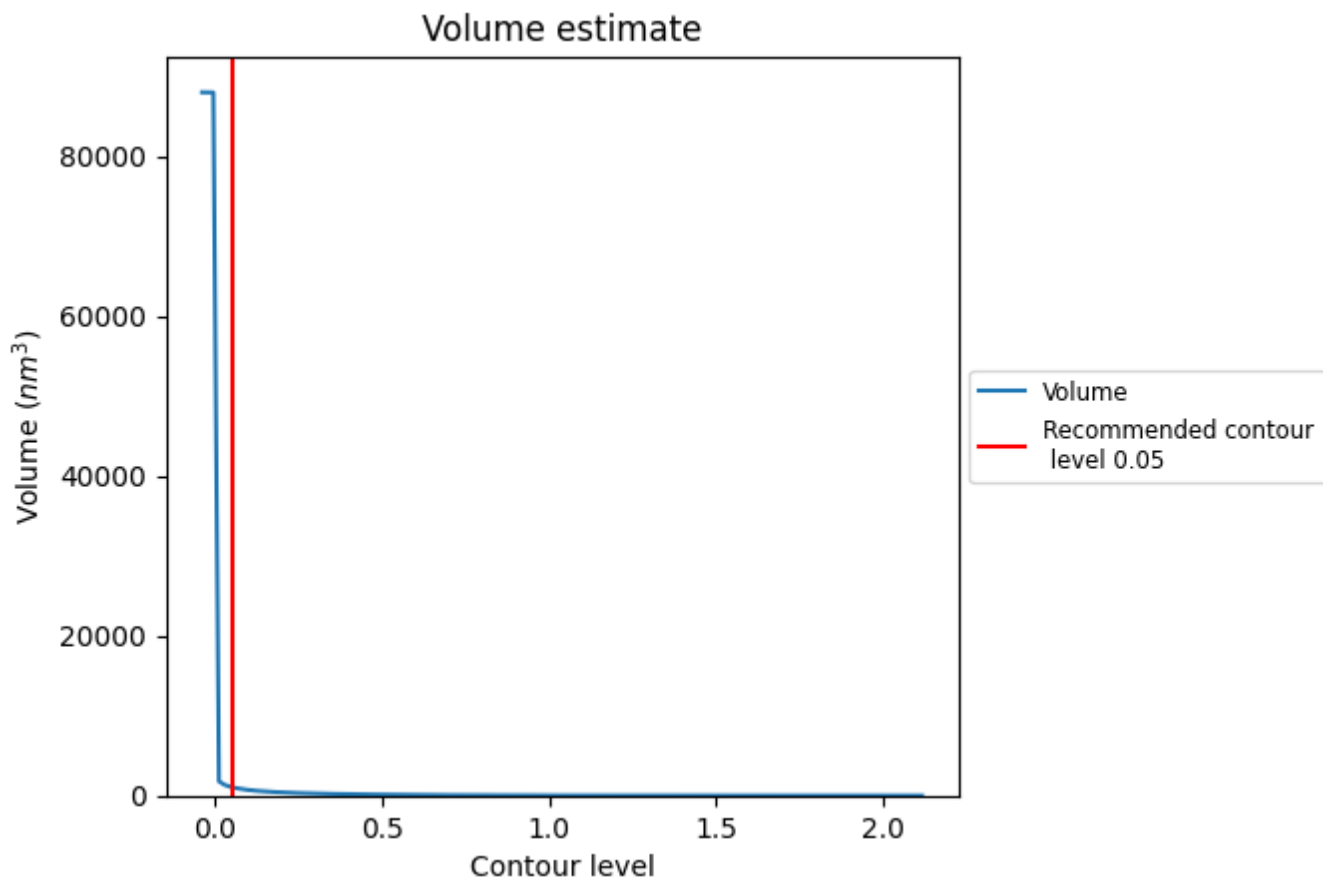
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

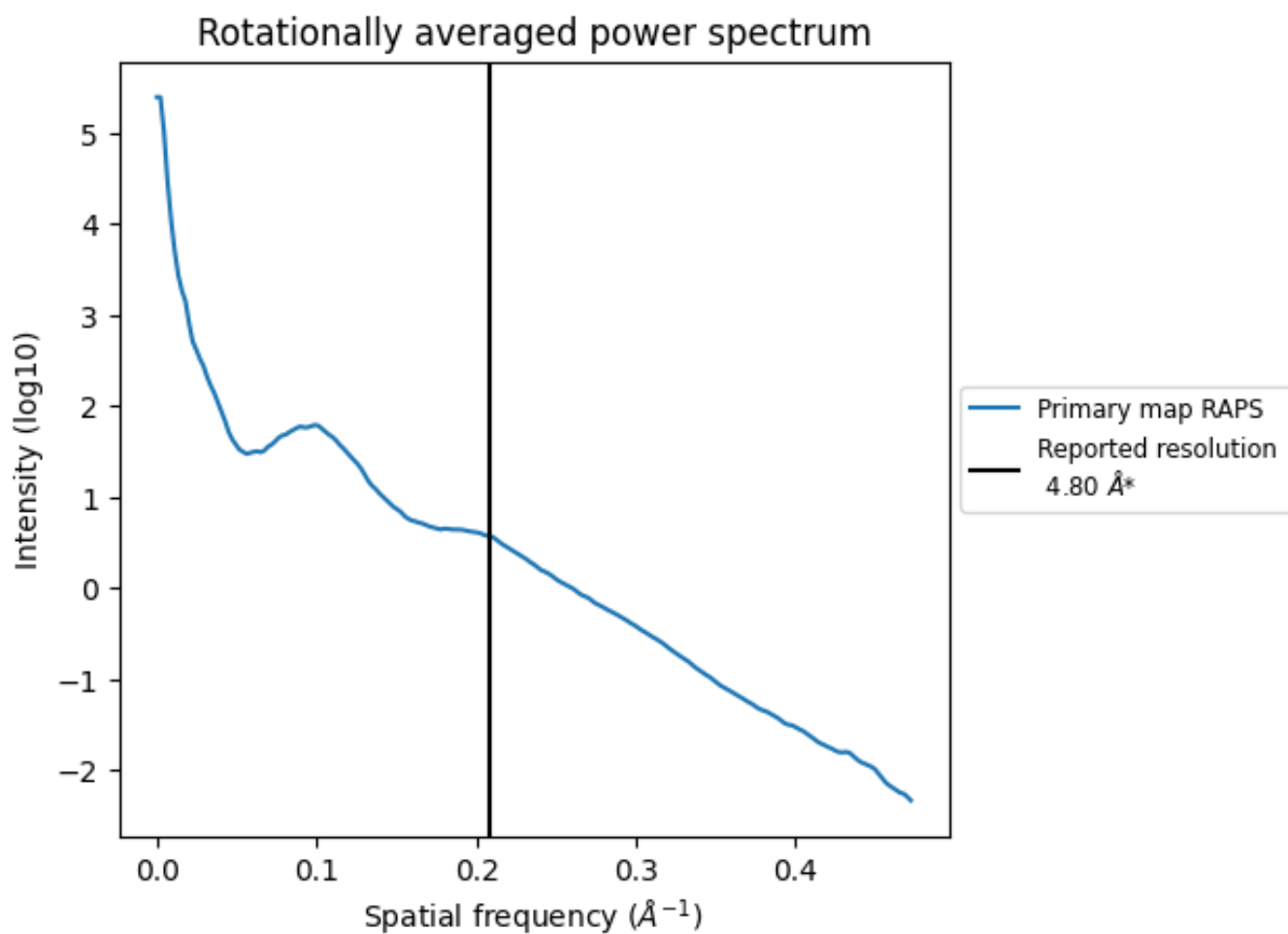
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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

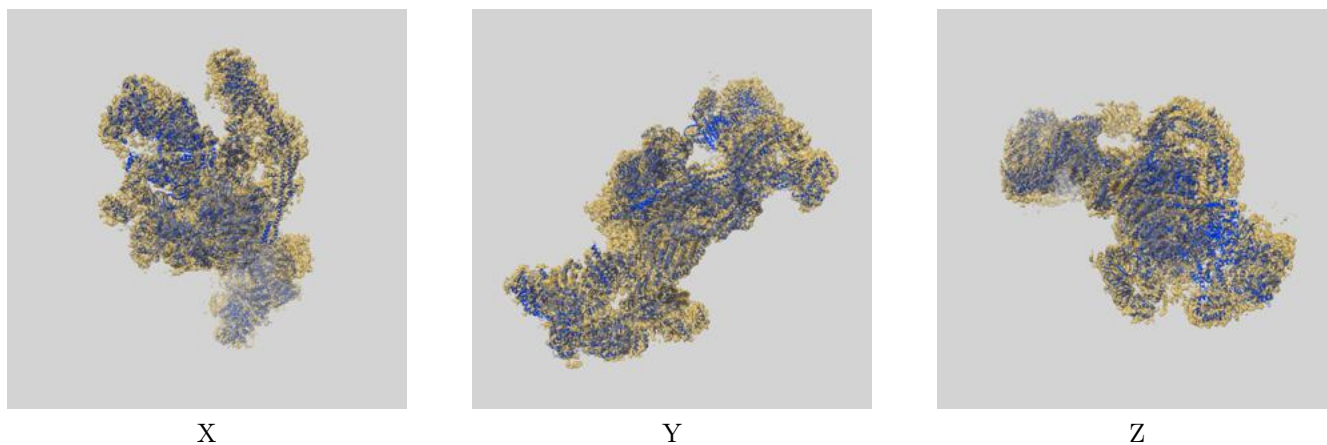
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

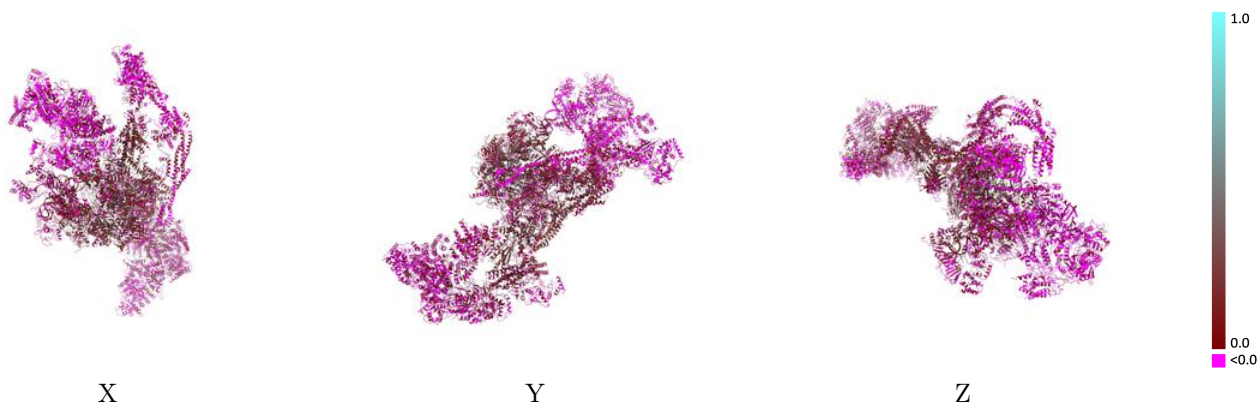
This section contains information regarding the fit between EMDB map EMD-23255 and PDB model 7LBM. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



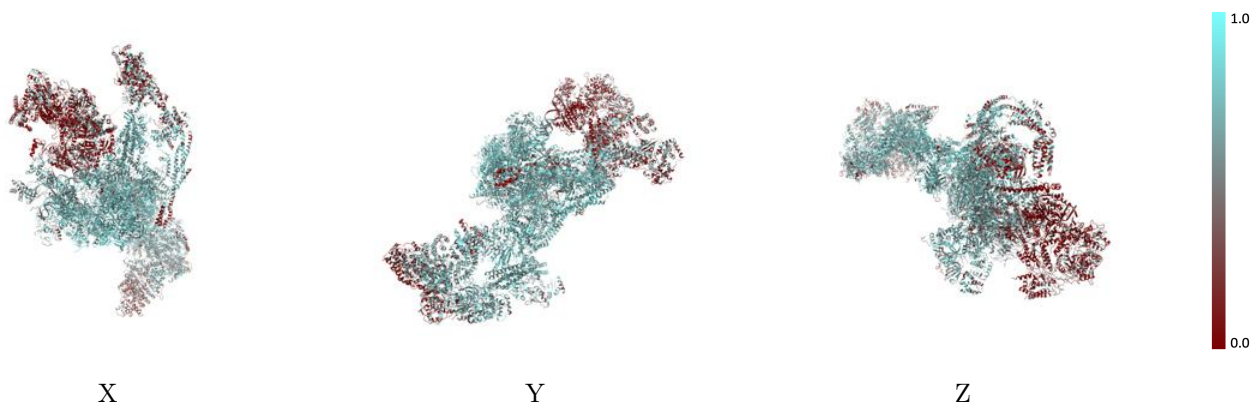
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [\(i\)](#)



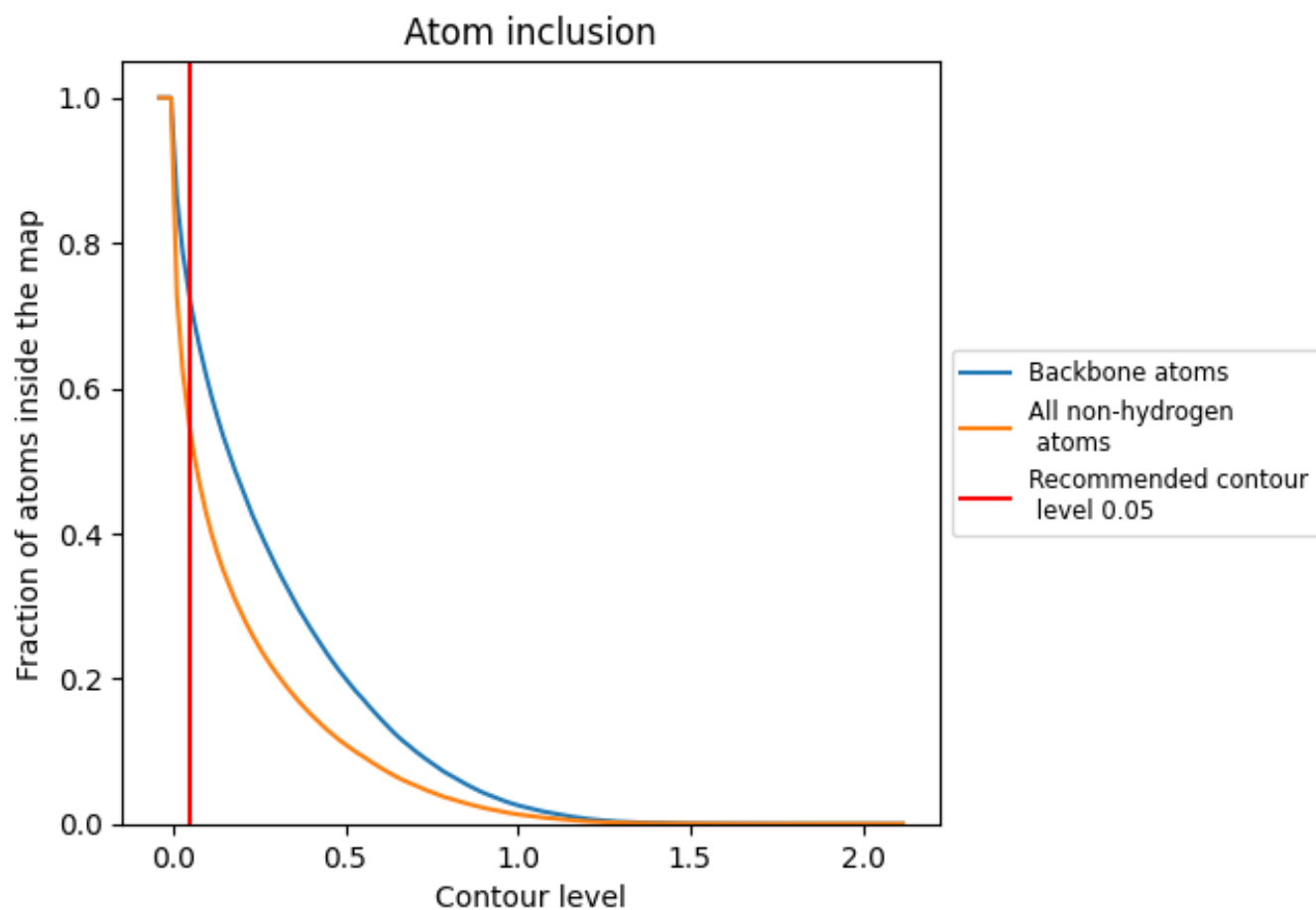
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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	 0.5398	 0.0740
0	 0.6279	 0.0650
1	 0.4063	 -0.0060
2	 0.5137	 0.0300
3	 0.5237	 0.0330
A	 0.7146	 0.1930
B	 0.7235	 0.2010
C	 0.6722	 0.1450
D	 0.6644	 0.1400
E	 0.7057	 0.1630
F	 0.7066	 0.2010
G	 0.7275	 0.1730
H	 0.6740	 0.1380
I	 0.7118	 0.1510
J	 0.6814	 0.1180
K	 0.6870	 0.1510
L	 0.7016	 0.1860
M	 0.4902	 -0.0110
N	 0.4860	 0.0020
O	 0.6640	 0.1200
P	 0.6057	 0.0650
Q	 0.6222	 0.0780
R	 0.6067	 0.0470
S	 0.5412	 0.0520
T	 0.5716	 0.0580
U	 0.5965	 0.0640
V	 0.5885	 0.0520
W	 0.0964	 -0.0490
X	 0.3513	 -0.0060
Y	 0.2254	 -0.0660
Z	 0.1725	 -0.0670
a	 0.1286	 -0.0590
b	 0.2200	 -0.0550
c	 0.1850	 -0.0860
d	 0.3584	 -0.0120



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Chain	Atom inclusion	Q-score
e	 0.3923	 -0.0170
f	 0.3387	 -0.0590
g	 0.6913	 0.0790
h	 0.7063	 0.1450
i	 0.7250	 0.1740
j	 0.7353	 0.1960
k	 0.6543	 0.1170
l	 0.6410	 0.1080
m	 0.7308	 0.2080
n	 0.7067	 0.1790
o	 0.6655	 0.1300
p	 0.6444	 0.1040
q	 0.6881	 0.1560
r	 0.6351	 0.1010
s	 0.4176	 0.0040
t	 0.5377	 0.0180
u	 0.3482	 -0.0210
v	 0.4240	 -0.0400
w	 0.3934	 -0.0220
x	 0.5279	 0.0110
y	 0.6033	 0.0470
z	 0.7130	 0.1360