Full wwPDB EM Validation Report ⓘ

Nov 4, 2024 – 07:22 AM JST

PDB ID	:	7ENA
EMDB ID	:	EMD-31204
Title	:	TFIID-based PIC-Mediator holo-complex in pre-assembled state (pre-hPIC-MED)
Authors	:	Chen, X.; Qi, Y.; Wang, X.; Wu, Z.; Yin, X.; Li, J.; Liu, W.; Xu, Y.
Deposited on	:	2021-04-16
Resolution	:	4.07 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:

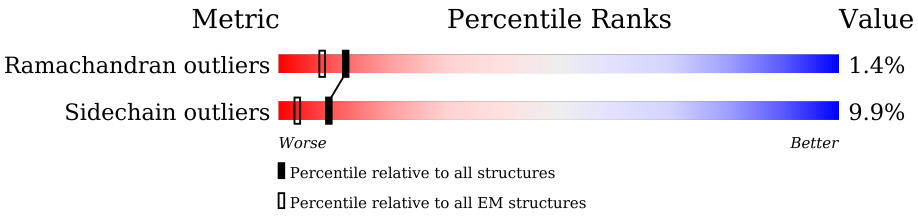
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance

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

The reported resolution of this entry is 4.07 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	309	17% 83% 16%
2	8	346	8% 64% 23% 14%
3	9	323	33% 65% 24% 11%
4	DO	109	75% 14% 11%
5	DP	339	49% 48%
6	DQ	307	6% 34% 6% 60%
7	BA	316	75% 5% 19%
8	FA	517	25% 74%
9	FB	249	5% 74% 15% 11%

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Mol	Chain	Length	Quality of chain
10	PA	1970	61% 13% 25%
11	PB	1174	79% 17%
12	PC	275	76% 17% 7%
13	PD	142	75% 16% 9%
14	PE	210	83% 17%
15	PF	127	48% 14% 38%
16	PG	172	77% 21%
17	PH	150	83% 15%
18	PI	125	72% 18% 9%
19	PJ	67	81% 13%
20	PK	117	81% 19%
21	PL	58	55% 19% 24%
22	DA	1872	5% 29% 68%
23	DB	1199	8% 79% 20%
24	DD	1085	13% 85%
24	Dd	1085	15% 15% 85%
25	DE	800	10% 66% 32%
25	De	800	67% 67% 33%
26	DF	677	14% 50% 10% 40%
26	Df	677	34% 56% 40%
27	DG	349	5% 39% 58%
28	DH	310	10% 59% 8% 33%
29	DI	264	7% 39% 7% 55%
29	Di	264	46% 46% 54%
30	DJ	218	36% 5% 59%

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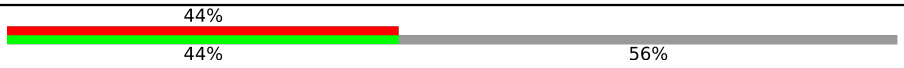
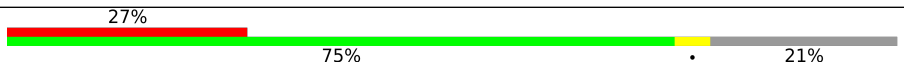
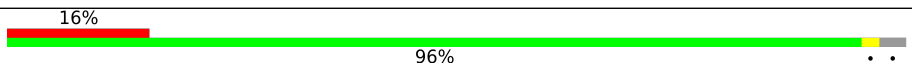
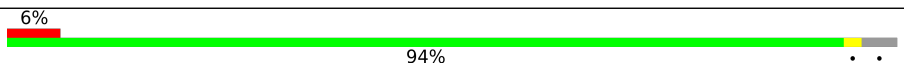
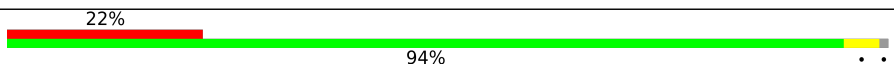
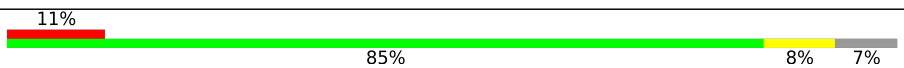
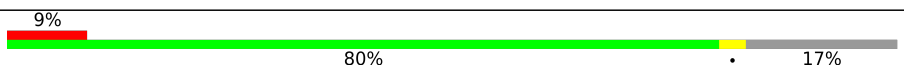
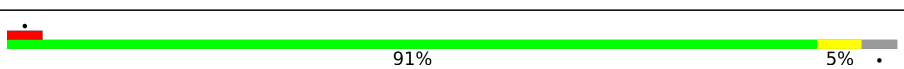
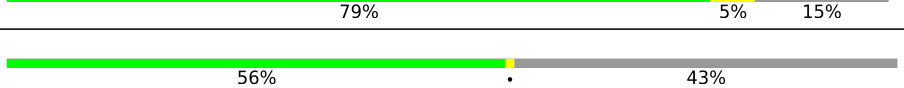
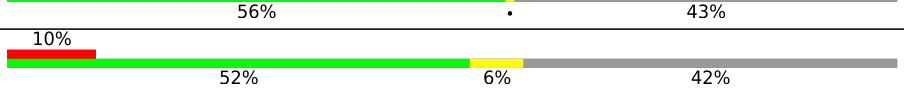
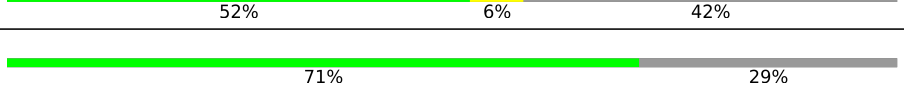
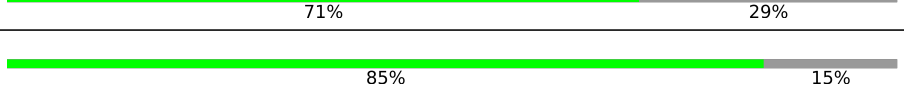
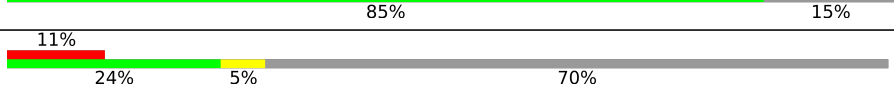
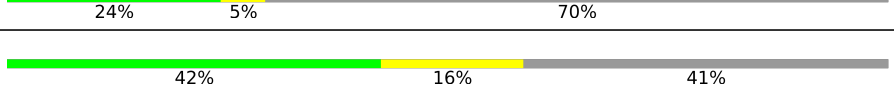
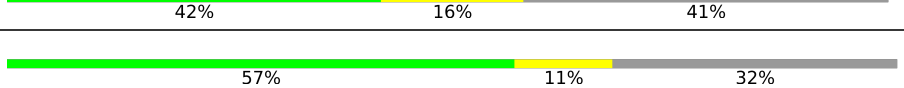
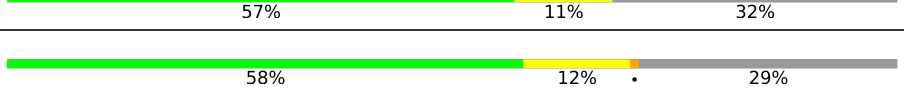
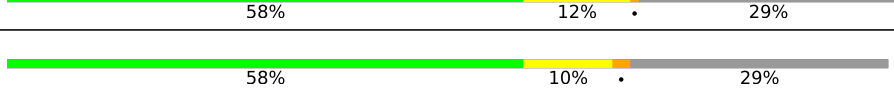
Mol	Chain	Length	Quality of chain
30	Dj	218	
31	DL	161	
31	Dl	161	
32	Dc	929	
33	Dk	211	
34	Dm	124	
35	EA	439	
36	EB	291	
37	1	548	
38	2	395	
39	3	308	
40	4	462	
41	5	71	
42	6	782	
43	7	760	
44	c	311	
45	e	178	
46	b	200	
47	l	178	
48	m	131	
49	a	1581	
50	d	270	
51	f	246	
52	g	233	
53	h	268	

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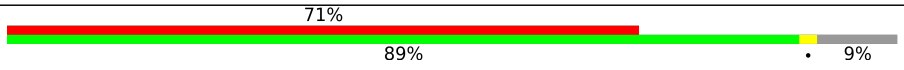
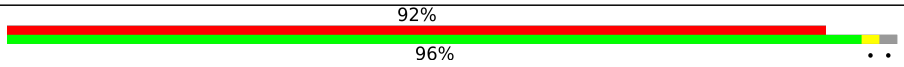
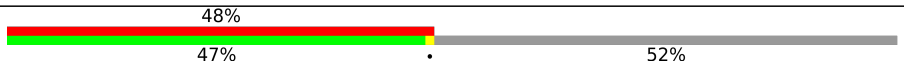
Mol	Chain	Length	Quality of chain
54	i	146	
55	j	135	
56	k	117	
57	n	1454	
58	o	788	
59	q	651	
60	r	208	
61	s	244	
62	t	212	
63	u	144	
64	v	200	
65	z	600	
66	x	989	
67	w	1368	
68	p	841	
69	X	69	
70	Y	69	

2 Entry composition

There are 73 unique types of molecules in this entry. The entry contains 173965 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called CDK-activating kinase assembly factor MAT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	306	2255	1404	399	441	11	0	0

- Molecule 2 is a protein called Cyclin-dependent kinase 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	8	299	2378	1535	406	426	11	0	0

- Molecule 3 is a protein called Cyclin-H.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	9	287	2307	1477	398	417	15	0	0

- Molecule 4 is a protein called Transcription initiation factor IIA subunit 2.

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

- Molecule 5 is a protein called TATA-box-binding protein.

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

- Molecule 6 is a protein called TFIIA-a.

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

- Molecule 7 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	BA	255	Total	C	N	O	S	0	0
			1959	1226	348	368	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	FA	134	Total	C	N	O	S	0	0
			1101	698	199	202	2		

- Molecule 9 is a protein called General transcription factor IIF subunit 2.

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

- Molecule 10 is a protein called RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	PA	1475	Total	C	N	O	S	0	0
			11662	7336	2071	2183	72		

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

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

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB3.

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

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	PD	129	Total	C	N	O	S	0	0
			1021	643	174	200	4		

- Molecule 14 is a protein called DNA-directed RNA polymerase II subunit E.

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

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

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

- Molecule 16 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	PG	171	Total	C	N	O	S	0	0
			1334	867	216	243	8		

- Molecule 17 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 18 is a protein called DNA-directed RNA polymerase II subunit RPB9.

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

- Molecule 19 is a protein called RPB10.

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

- Molecule 20 is a protein called RNA_pol_L_2 domain-containing protein.

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

- Molecule 21 is a protein called RPB12.

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

- Molecule 22 is a protein called Transcription initiation factor TFIID subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	DA	600	Total	C	N	O	S	0	0
			4918	3135	858	897	28		

- Molecule 23 is a protein called Transcription initiation factor TFIID subunit 2.

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

- Molecule 24 is a protein called Transcription initiation factor TFIID subunit 4.

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

- Molecule 25 is a protein called Transcription initiation factor TFIID subunit 5.

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

- Molecule 26 is a protein called Transcription initiation factor TFIID subunit 6.

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

- Molecule 27 is a protein called Transcription initiation factor TFIID subunit 7.

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

- Molecule 28 is a protein called Transcription initiation factor TFIID subunit 8.

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

- Molecule 29 is a protein called Transcription initiation factor TFIID subunit 9.

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

- Molecule 30 is a protein called Transcription initiation factor TFIID subunit 10.

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

- Molecule 31 is a protein called Transcription initiation factor TFIID subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	DL	75	Total	C	N	O	S	0	0
			614	384	107	120	3		
31	Dl	107	Total	C	N	O	S	0	0
			876	547	158	166	5		

- Molecule 32 is a protein called Transcription initiation factor TFIID subunit 3.

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

- Molecule 33 is a protein called Transcription initiation factor TFIID subunit 11.

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

- Molecule 34 is a protein called Transcription initiation factor TFIID subunit 13.

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

- Molecule 35 is a protein called General transcription factor IIE subunit 1.

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

- Molecule 36 is a protein called Transcription initiation factor IIE subunit beta.

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

- Molecule 37 is a protein called General transcription factor IIH subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	1	433	Total	C	N	O	S	0	0
			3436	2153	602	664	17		

- Molecule 38 is a protein called General transcription factor IIH subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	2	385	Total	C	N	O	S	0	0
			3024	1909	524	564	27		

- Molecule 39 is a protein called General transcription factor IIH subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	3	295	Total	C	N	O	S	0	0
			2306	1477	384	426	19		

- Molecule 40 is a protein called General transcription factor IIH subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	4	457	Total	C	N	O	S	0	0
			3644	2341	641	648	14		

- Molecule 41 is a protein called General transcription factor IIH subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	5	66	Total	C	N	O	S	0	0
			522	336	83	100	3		

- Molecule 42 is a protein called General transcription and DNA repair factor IIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	6	652	Total	C	N	O	S	0	0
			5255	3345	898	980	32		

- Molecule 43 is a protein called General transcription and DNA repair factor IIH helicase subunit XPD.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	7	732	Total	C	N	O	S	0	0
			5861	3742	1023	1068	28		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
44	c	263	Total	C	N	O	S	0	0
			2108	1337	378	382	11		

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

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

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

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

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

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

- Molecule 48 is a protein called Mediator of RNA polymerase II transcription subunit 31.

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

- Molecule 49 is a protein called Mediator of RNA polymerase II transcription subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	a	469	Total	C	N	O	S	0	0
			3585	2283	615	663	24		

- Molecule 50 is a protein called Mediator of RNA polymerase II transcription subunit 4.

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

- Molecule 51 is a protein called Mediator of RNA polymerase II transcription subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	f	167	Total	C	N	O	S	0	0
			1329	851	231	242	5		

- Molecule 52 is a protein called Mediator of RNA polymerase II transcription subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	g	166	Total	C	N	O	S	0	0
			1382	880	244	248	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	11	LEU	PRO	conflict	UNP O43513

- Molecule 53 is a protein called Isoform 2 of Mediator of RNA polymerase II transcription subunit 8.

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

- Molecule 54 is a protein called Mediator of RNA polymerase II transcription subunit 9.

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

- Molecule 55 is a protein called Mediator of RNA polymerase II transcription subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	j	122	Total	C	N	O	S	0	0
			1001	636	174	187	4		

- Molecule 56 is a protein called Mediator of RNA polymerase II transcription subunit 11.

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

- Molecule 57 is a protein called Mediator of RNA polymerase II transcription subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	n	994	Total	C	N	O	S	0	0
			7241	4576	1293	1334	38		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	133	LEU	ALA	conflict	UNP O60244

- Molecule 58 is a protein called Mediator of RNA polymerase II transcription subunit 15.

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

- Molecule 59 is a protein called Mediator of RNA polymerase II transcription subunit 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	q	555	Total	C	N	O	S	0	0
			4276	2700	767	792	17		

- Molecule 60 is a protein called Mediator of RNA polymerase II transcription subunit 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	r	206	Total	C	N	O	S	0	0
			1630	1033	285	294	18		

- Molecule 61 is a protein called Mediator of RNA polymerase II transcription subunit 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	s	81	Total	C	N	O	S	0	0
			505	312	91	100	2		

- Molecule 62 is a protein called Mediator of RNA polymerase II transcription subunit 20.

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

- Molecule 63 is a protein called Mediator of RNA polymerase II transcription subunit 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	u	107	Total	C	N	O	S	0	0
			792	492	132	165	3		

- Molecule 64 is a protein called Mediator of RNA polymerase II transcription subunit 22.

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

- Molecule 65 is a protein called Mediator of RNA polymerase II transcription subunit 26.

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

- Molecule 66 is a protein called Mediator of RNA polymerase II transcription subunit 24.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	x	896	Total	C	N	O	S	0	0
			7050	4516	1188	1292	54		

- Molecule 67 is a protein called Mediator of RNA polymerase II transcription subunit 23.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	w	1334	Total	C	N	O	S	0	0
			10772	6965	1827	1909	71		

- Molecule 68 is a protein called Isoform 2 of Mediator of RNA polymerase II transcription subunit 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	p	406	Total	C	N	O	S	0	0
			3124	1982	536	585	21		

- Molecule 69 is a DNA chain called DNA (69-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
69	X	69	Total	C	N	O	P	0	0
			1429	672	279	409	69		

- Molecule 70 is a DNA chain called DNA(69-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Y	69	Total	C	N	O	P	0	0
			1400	664	248	419	69		

- Molecule 71 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
71	0	2	Total	Zn	0
			2	2	
71	BA	1	Total	Zn	0
			1	1	
71	PA	2	Total	Zn	0
			2	2	
71	PB	1	Total	Zn	0
			1	1	
71	PC	1	Total	Zn	0
			1	1	
71	PI	2	Total	Zn	0
			2	2	

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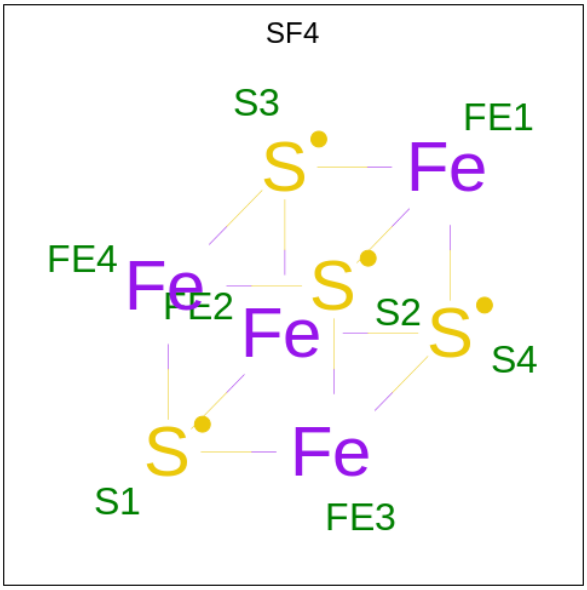
Mol	Chain	Residues	Atoms	AltConf
71	PJ	1	Total Zn 1 1	0
71	PL	1	Total Zn 1 1	0
71	EA	1	Total Zn 1 1	0
71	2	3	Total Zn 3 3	0
71	3	1	Total Zn 1 1	0

- Molecule 72 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 73 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



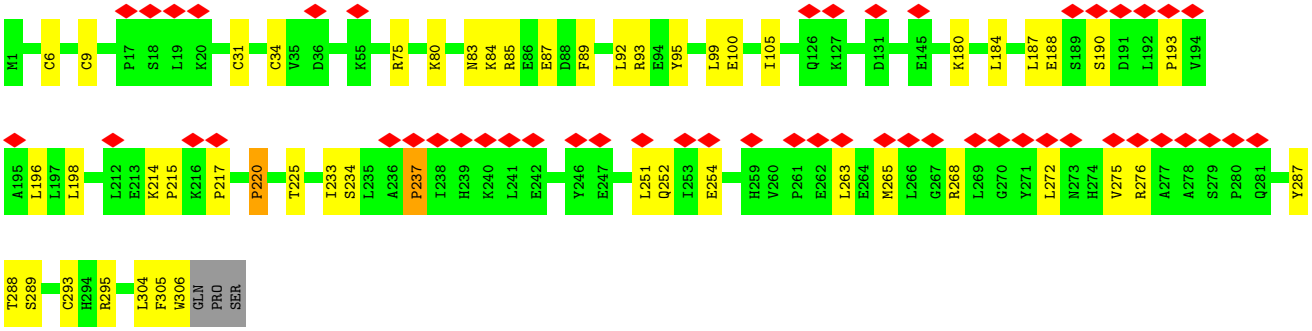
Mol	Chain	Residues	Atoms	AltConf
73	7	1	Total Fe S 8 4 4	0

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.

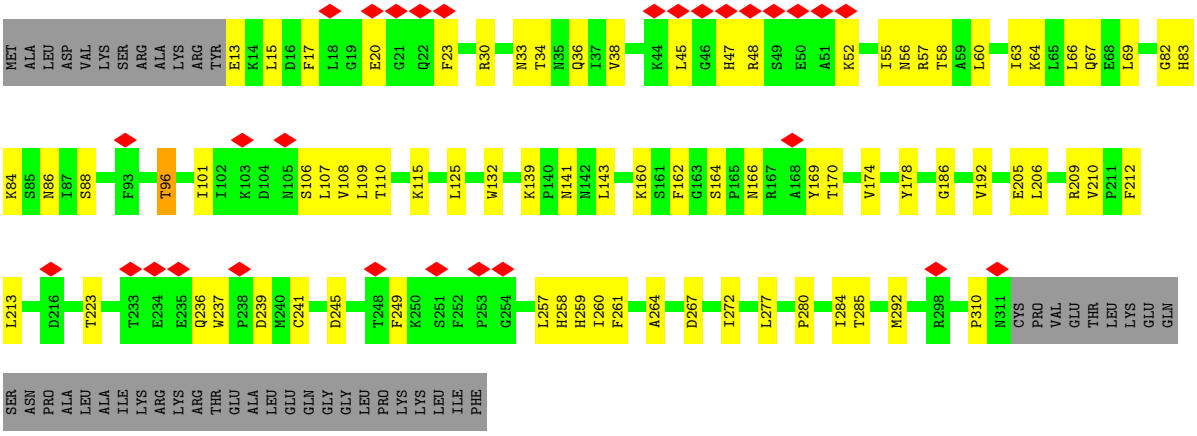
• Molecule 1: CDK-activating kinase assembly factor MAT1

Chain 0:



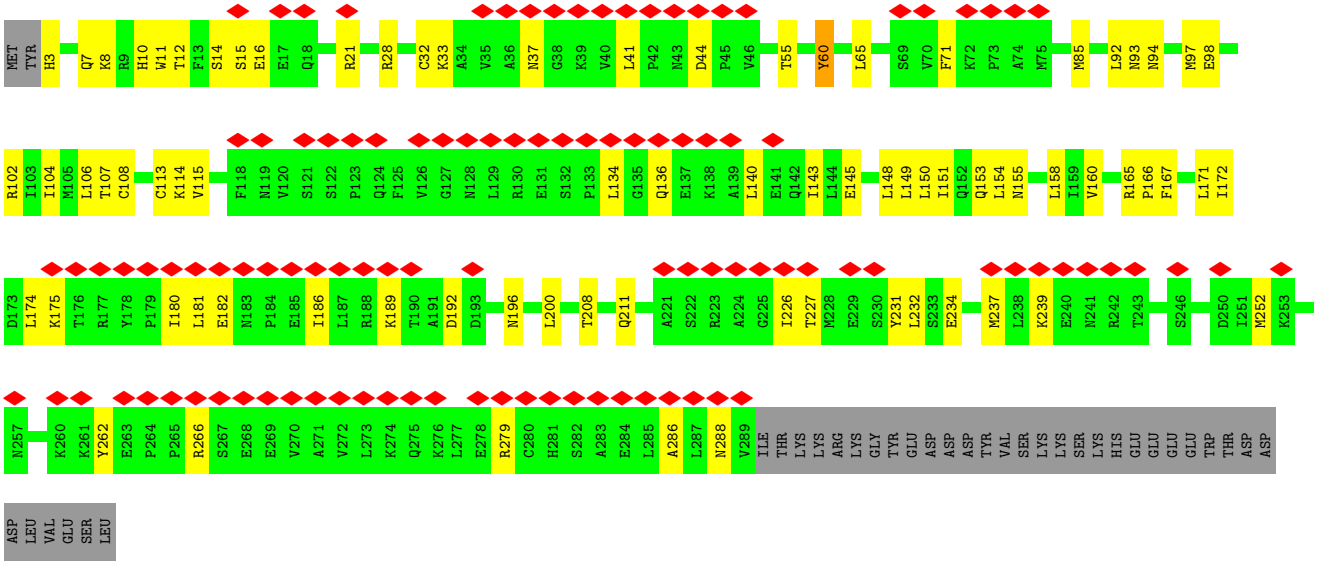
• Molecule 2: Cyclin-dependent kinase 7

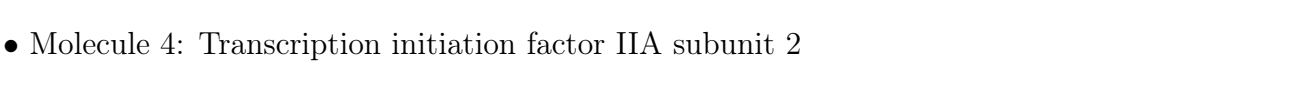
Chain 8:



• Molecule 3: Cyclin-H

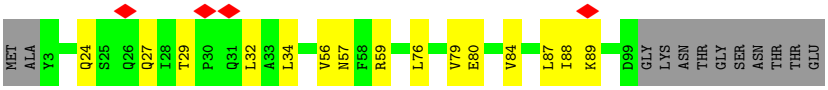
Chain 9:





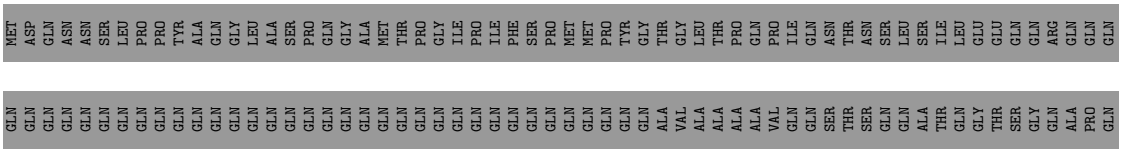
• Molecule 4: Transcription initiation factor IIA subunit 2

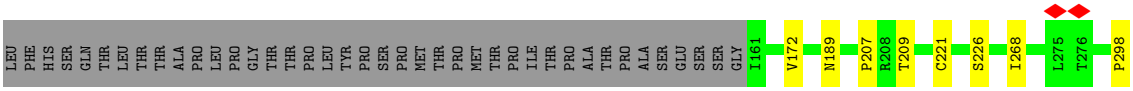
Chain DO:



• Molecule 5: TATA-box-binding protein

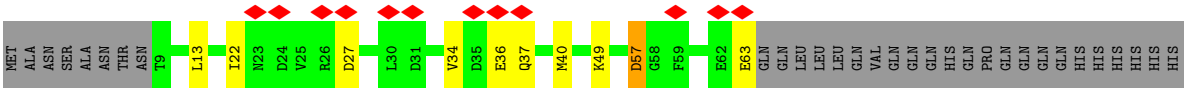
Chain DP:

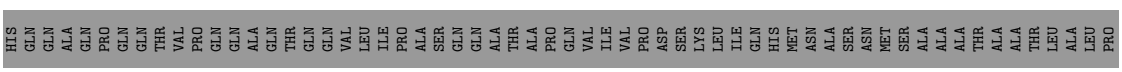


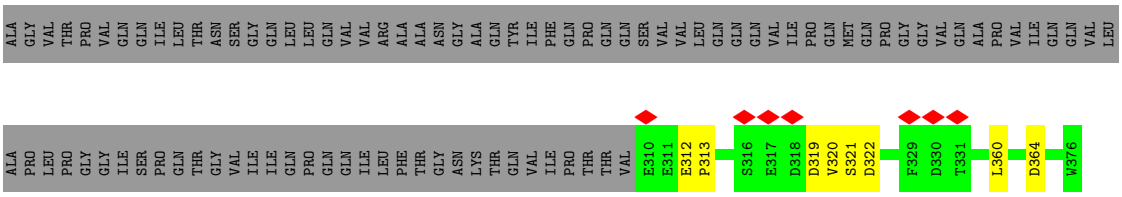


• Molecule 6: TFIIA-a

Chain DQ:

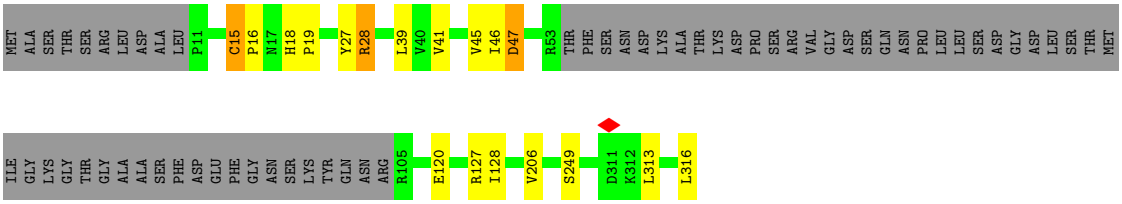






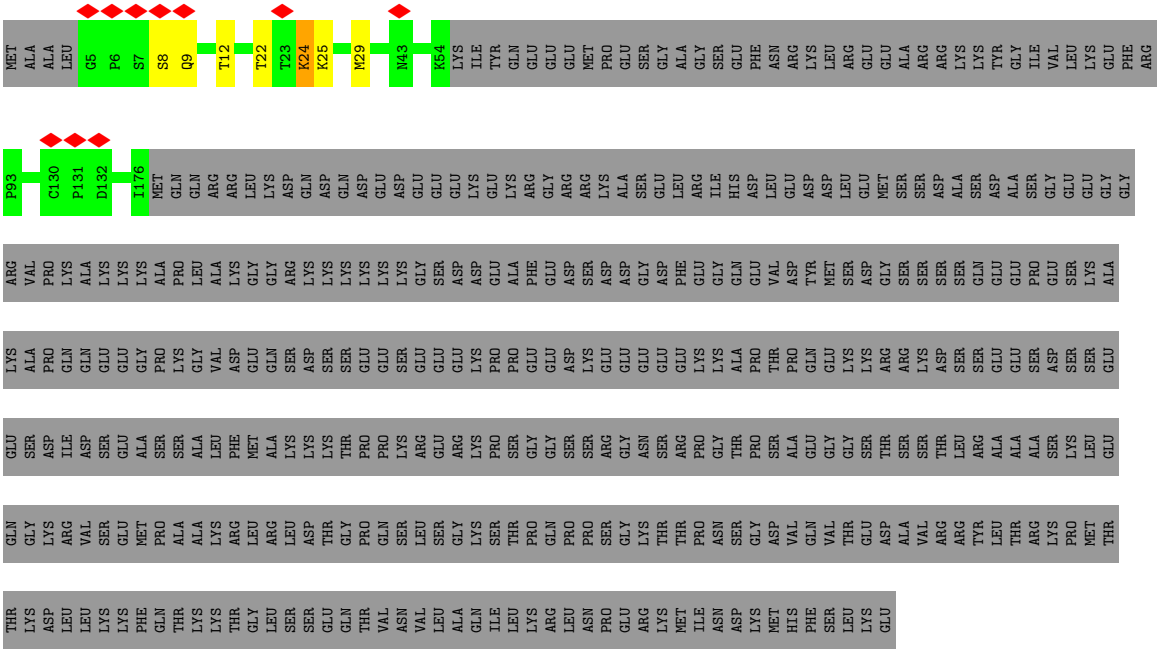
• Molecule 7: Transcription initiation factor IIB

Chain BA:



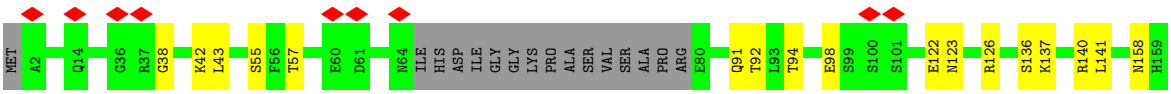
• Molecule 8: General transcription factor IIF subunit 1

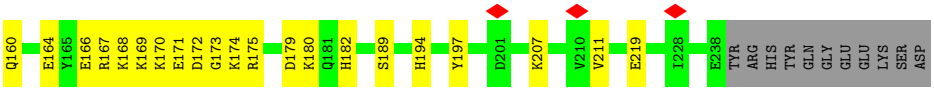
Chain FA:



• Molecule 9: General transcription factor IIF subunit 2

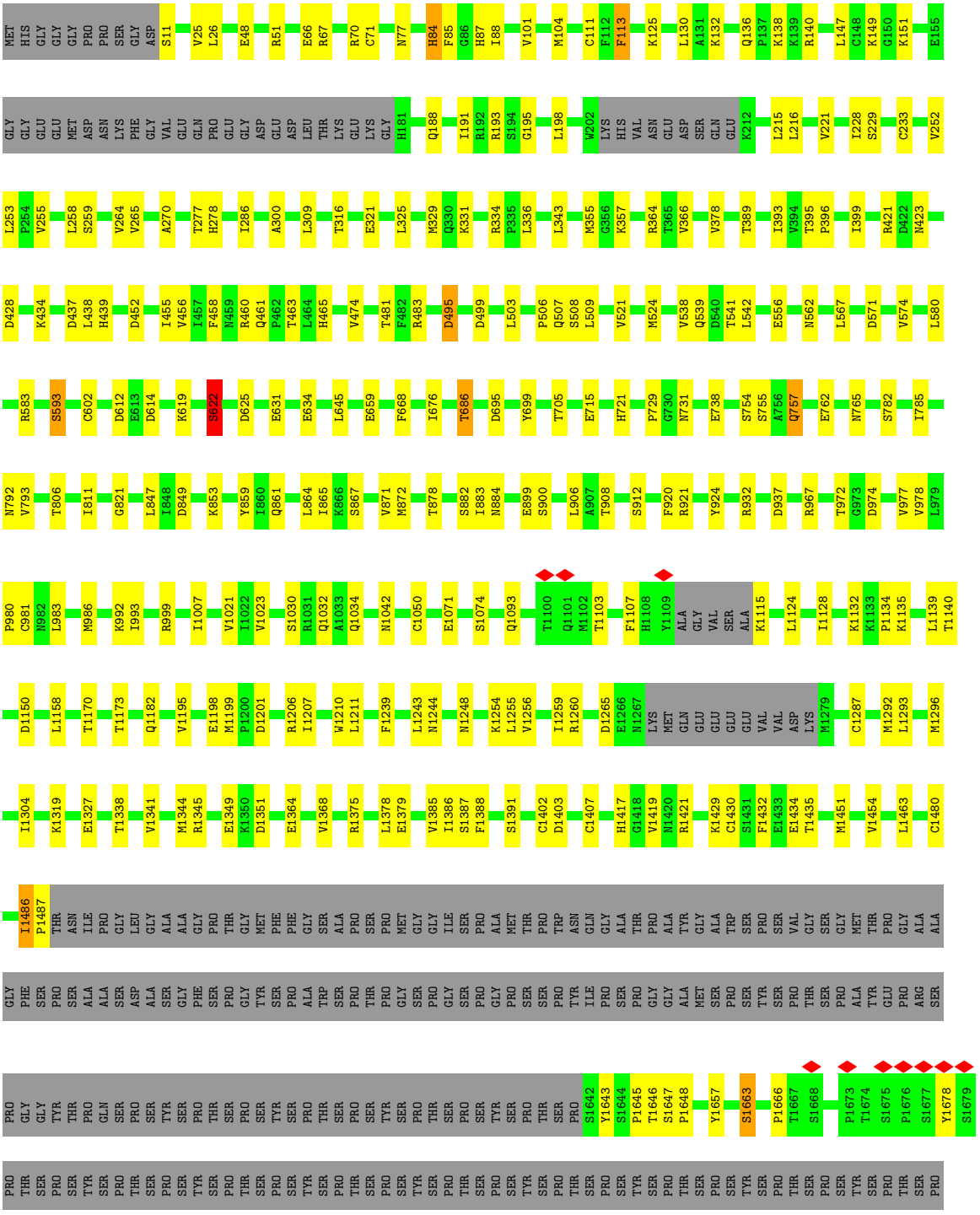
Chain FB:

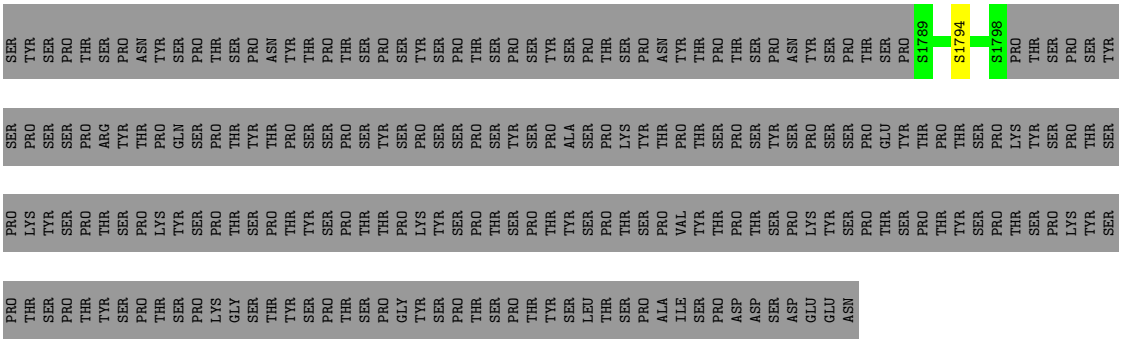




• Molecule 10: RPB1

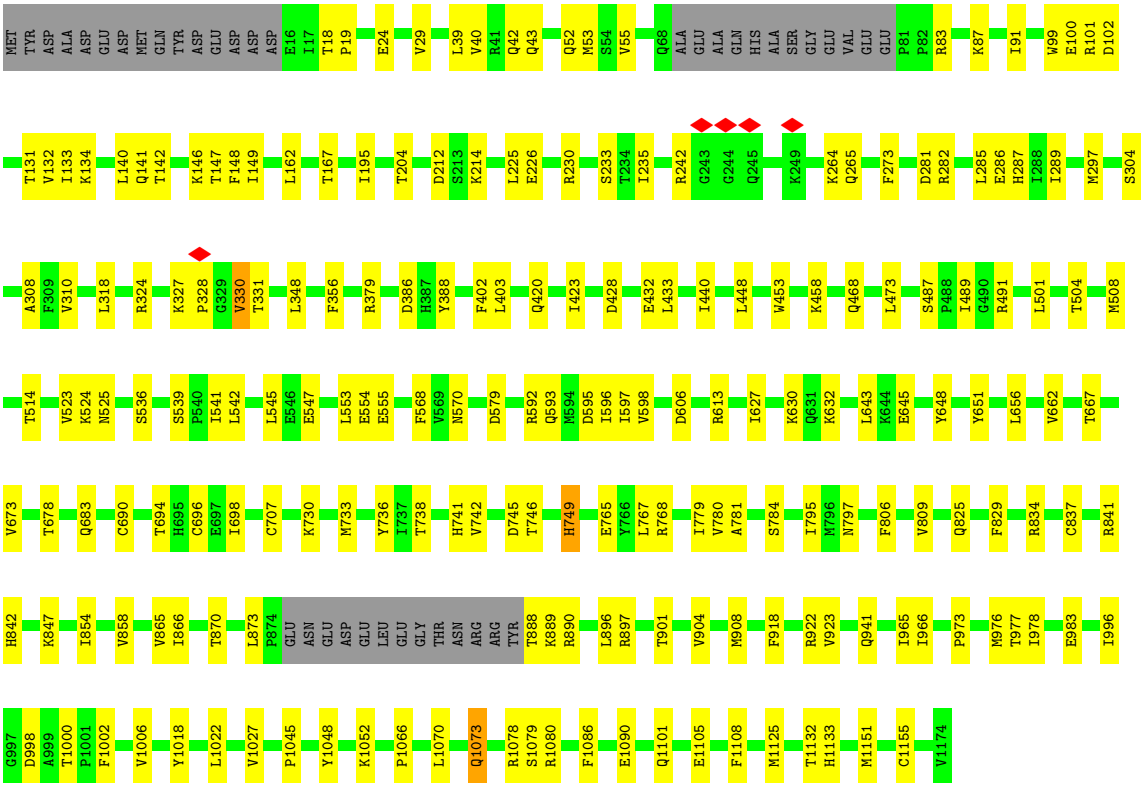
Chain PA:





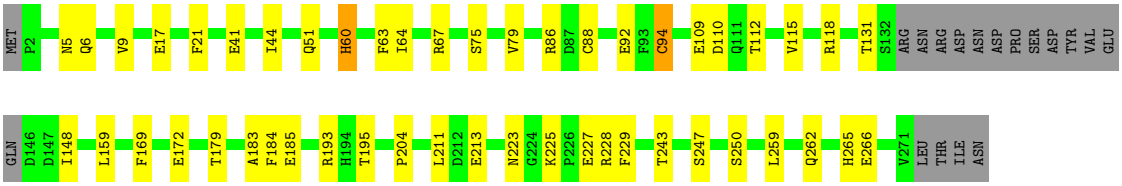
• Molecule 11: DNA-directed RNA polymerase subunit beta

Chain PB:



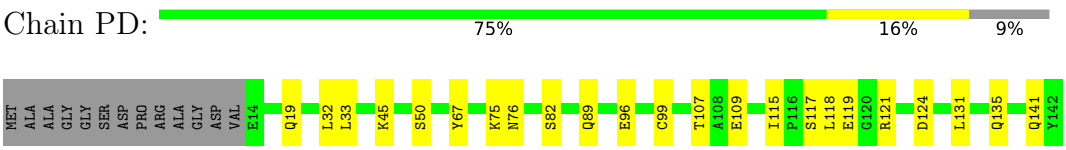
• Molecule 12: DNA-directed RNA polymerase II subunit RPB3

Chain PC:



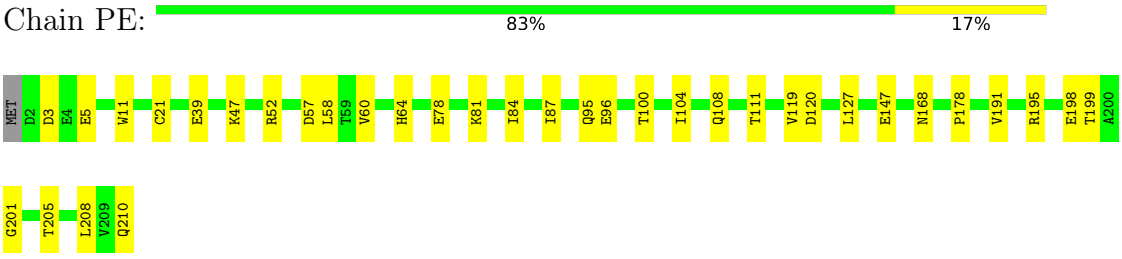
• Molecule 13: DNA-directed RNA polymerase II subunit RPB4

Chain PD:



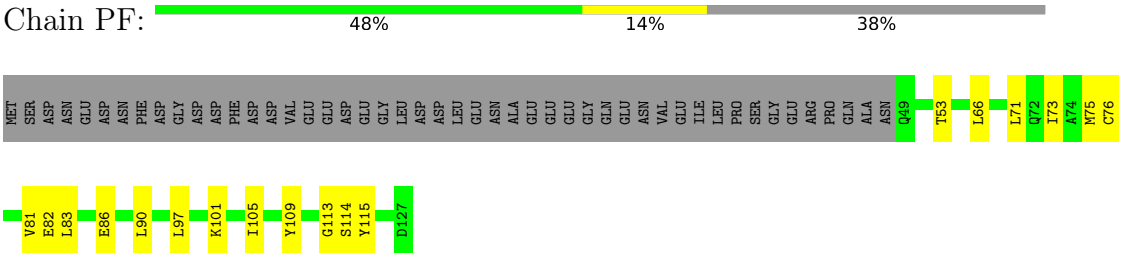
• Molecule 14: DNA-directed RNA polymerase II subunit E

Chain PE:



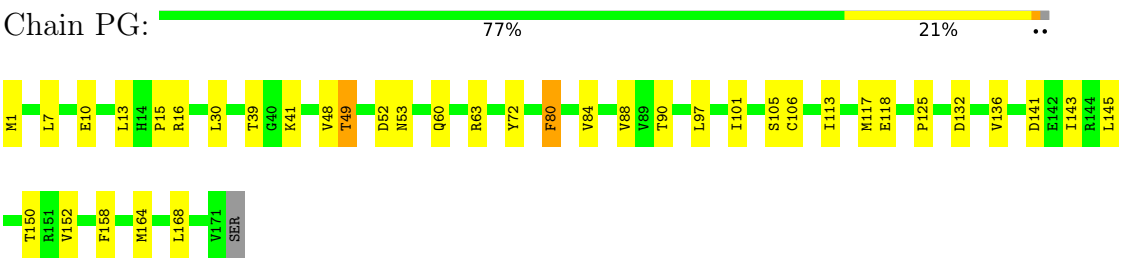
• Molecule 15: DNA-directed RNA polymerase II subunit F

Chain PF:



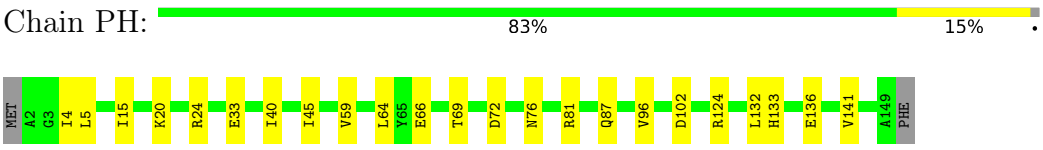
• Molecule 16: DNA-directed RNA polymerase II subunit RPB7

Chain PG:



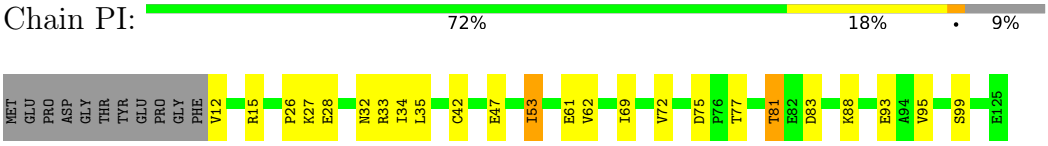
• Molecule 17: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain PH:



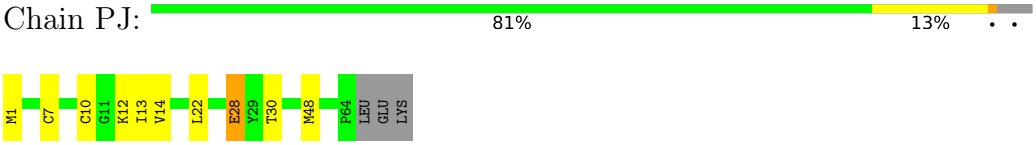
• Molecule 18: DNA-directed RNA polymerase II subunit RPB9

Chain PI:



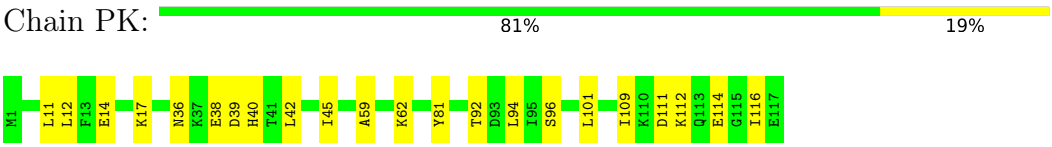
• Molecule 19: RPB10

Chain PJ:



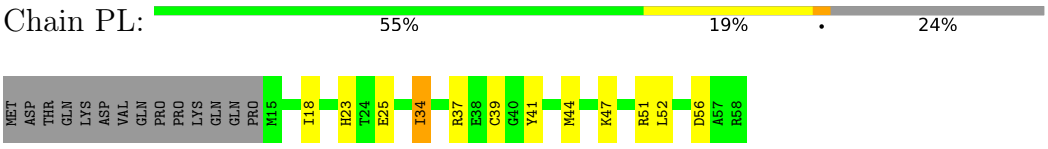
• Molecule 20: RNA_pol_L_2 domain-containing protein

Chain PK:



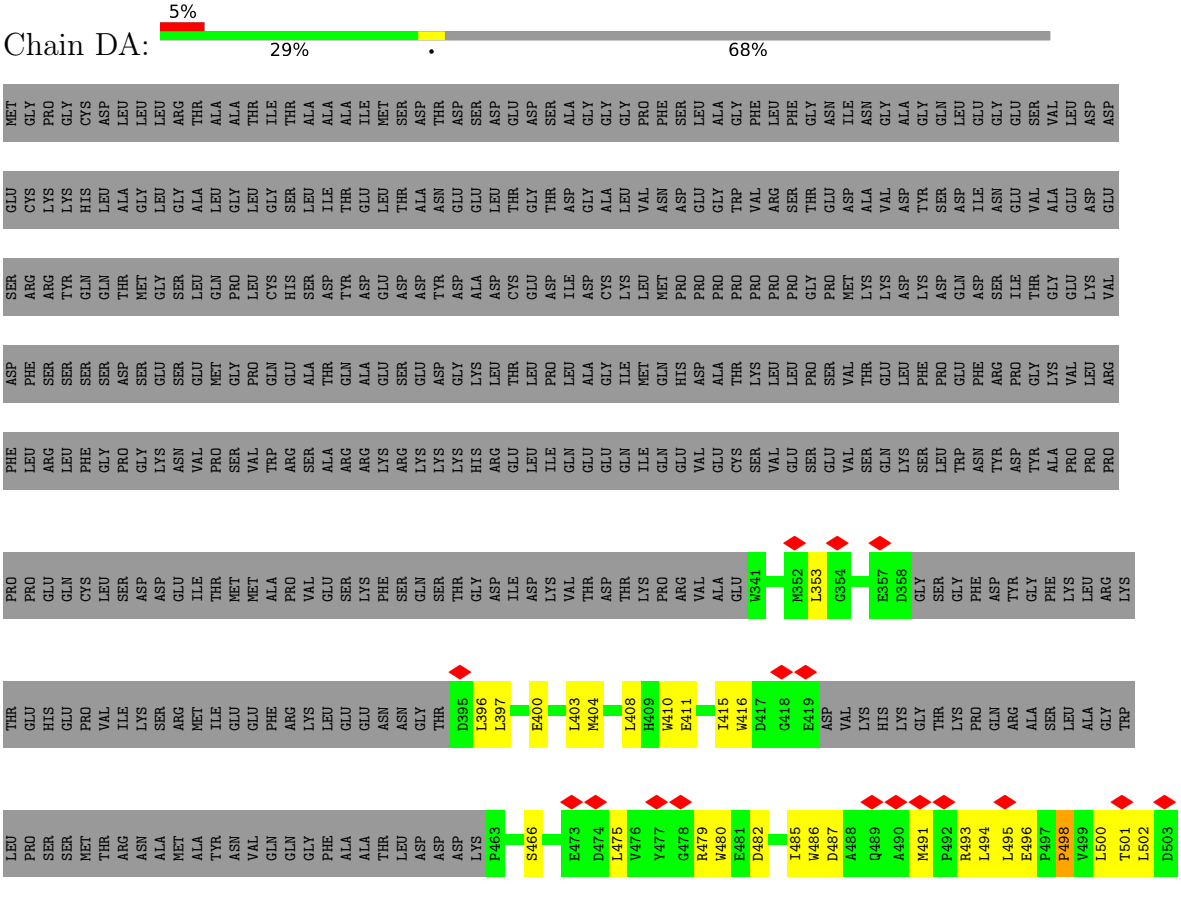
• Molecule 21: RPB12

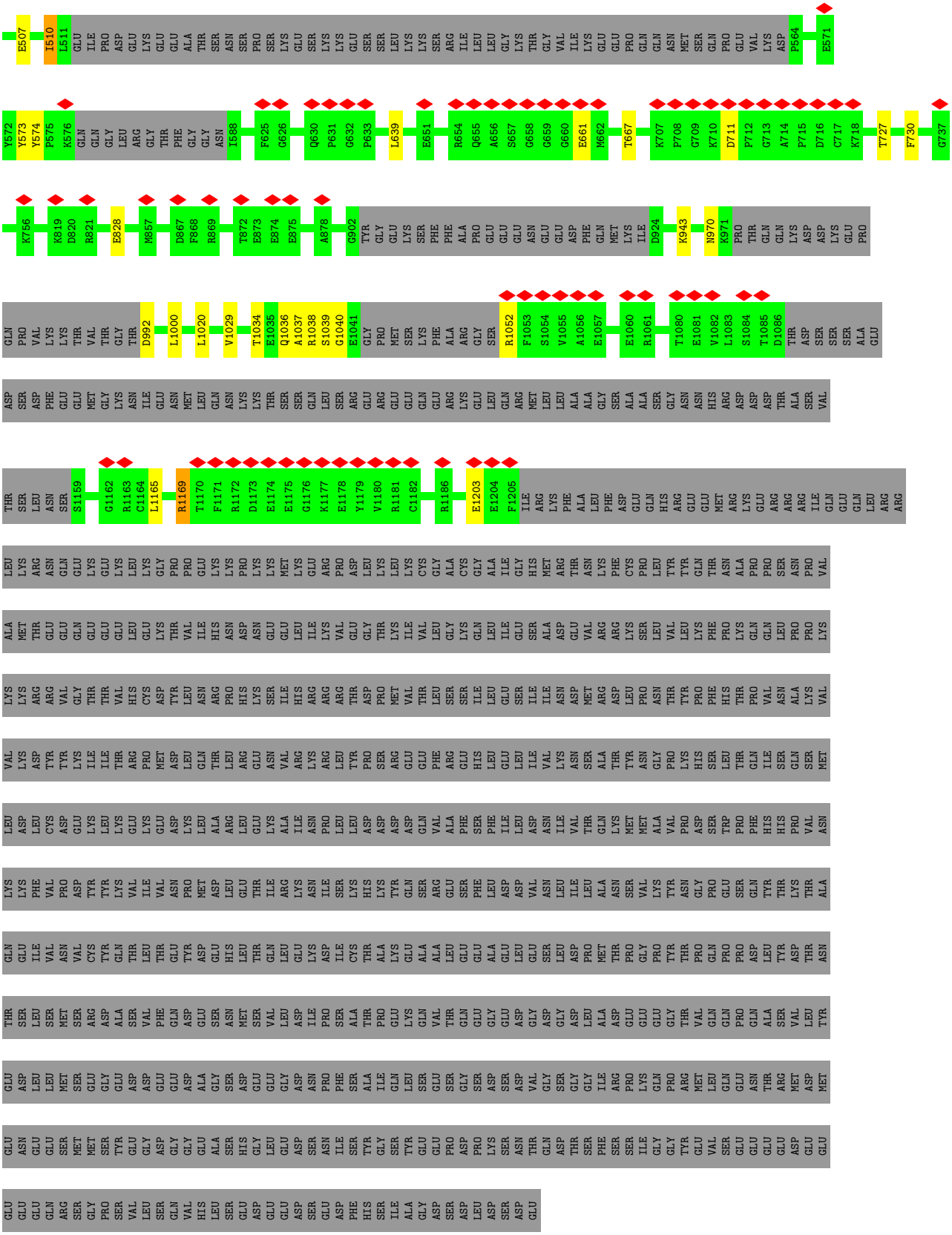
Chain PL:



• Molecule 22: Transcription initiation factor TFIID subunit 1

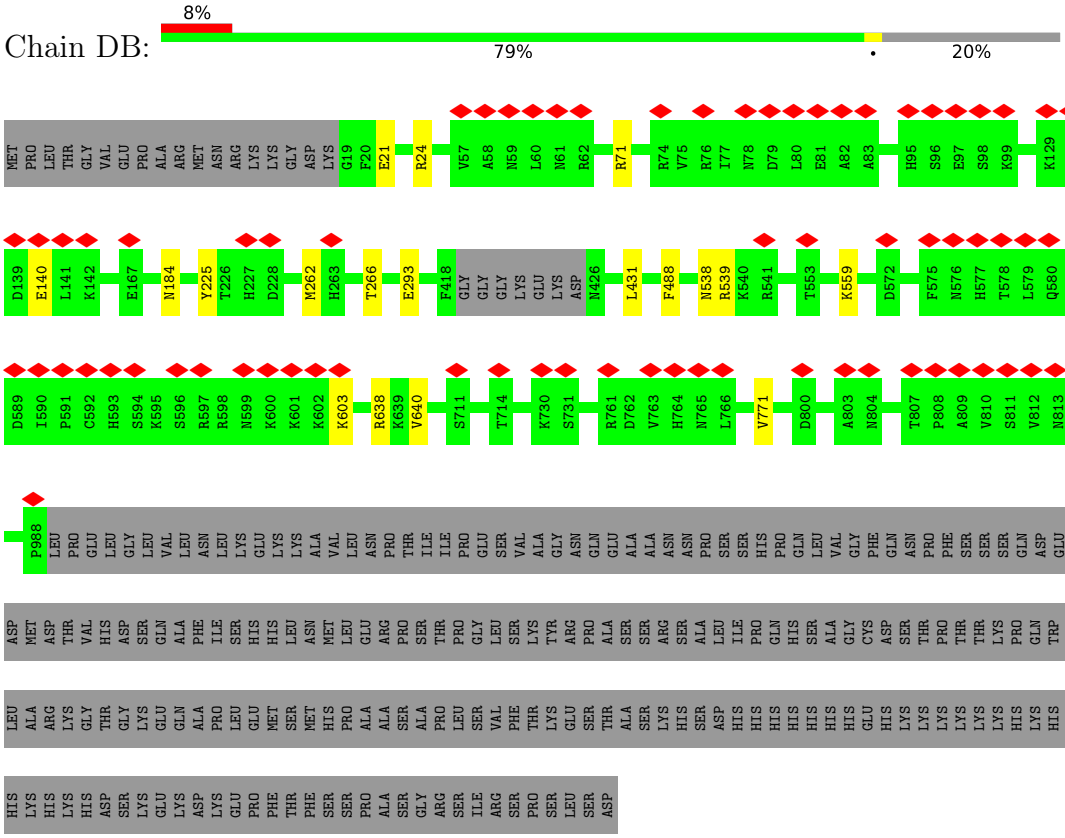
Chain DA:





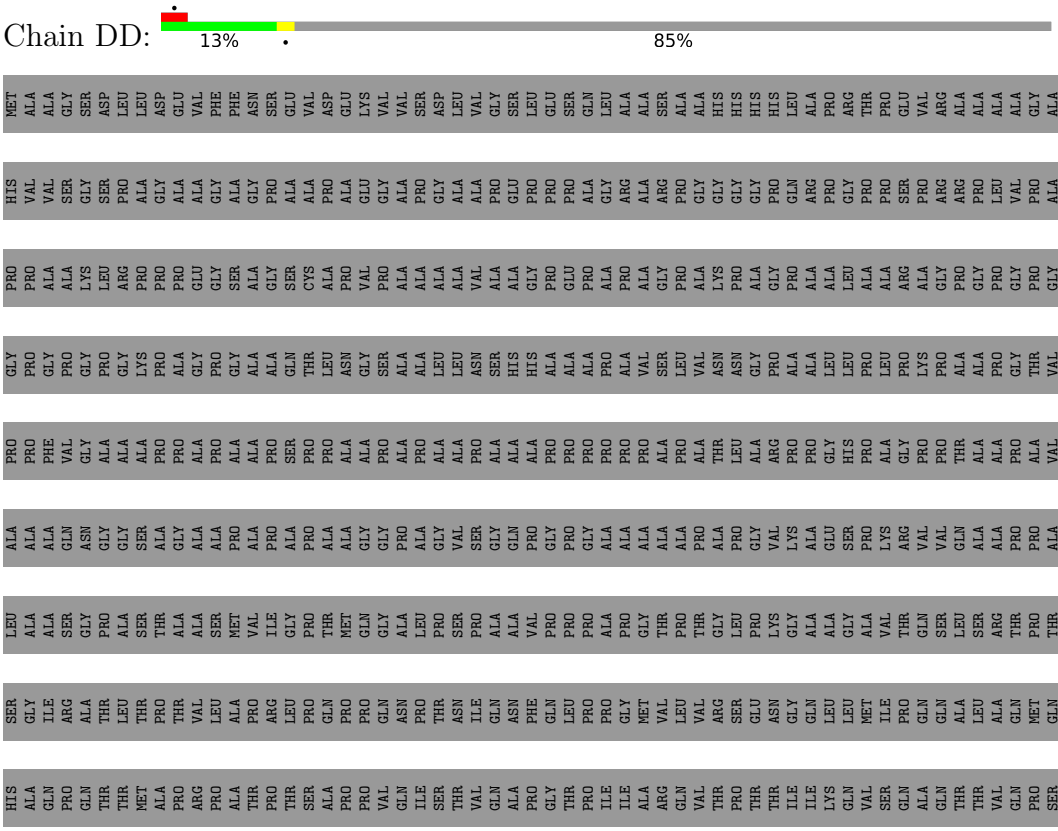
• Molecule 23: Transcription initiation factor TFIID subunit 2

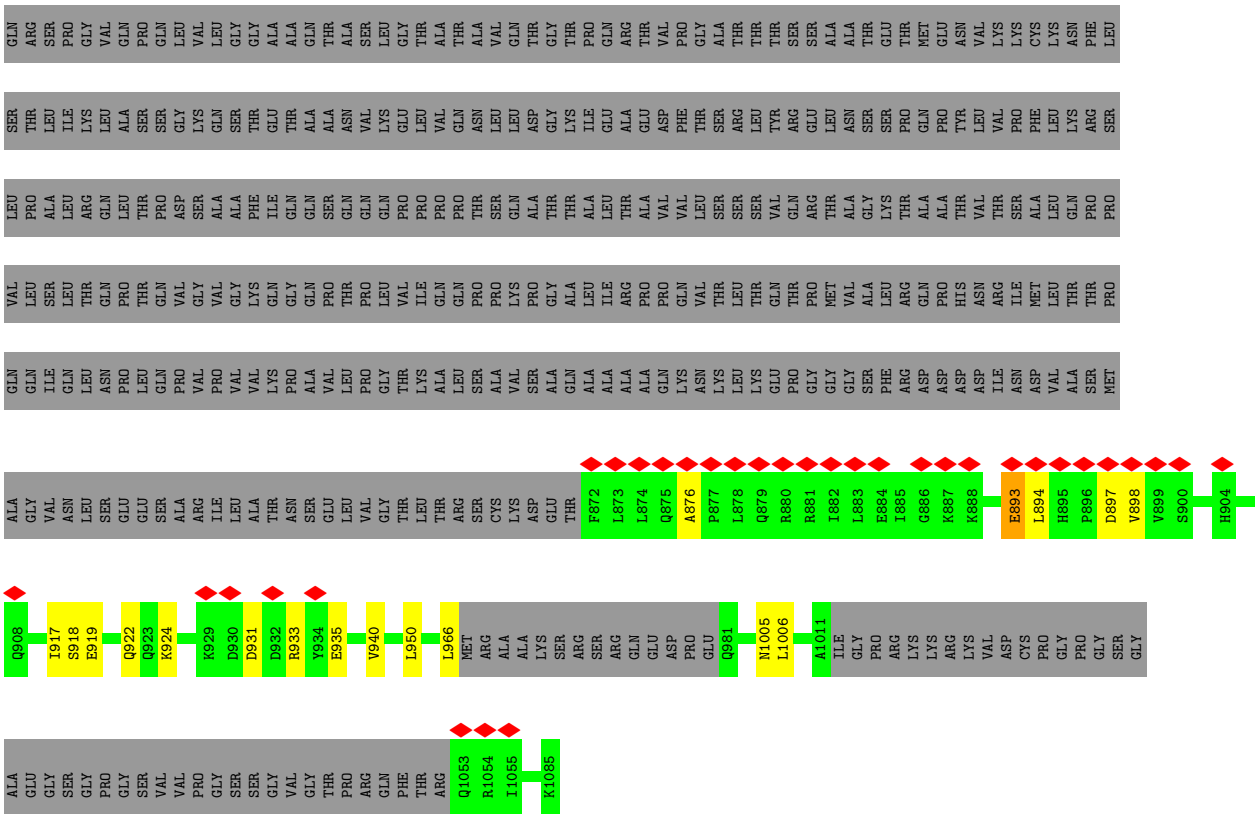
Chain DB:



• Molecule 24: Transcription initiation factor TFIID subunit 4

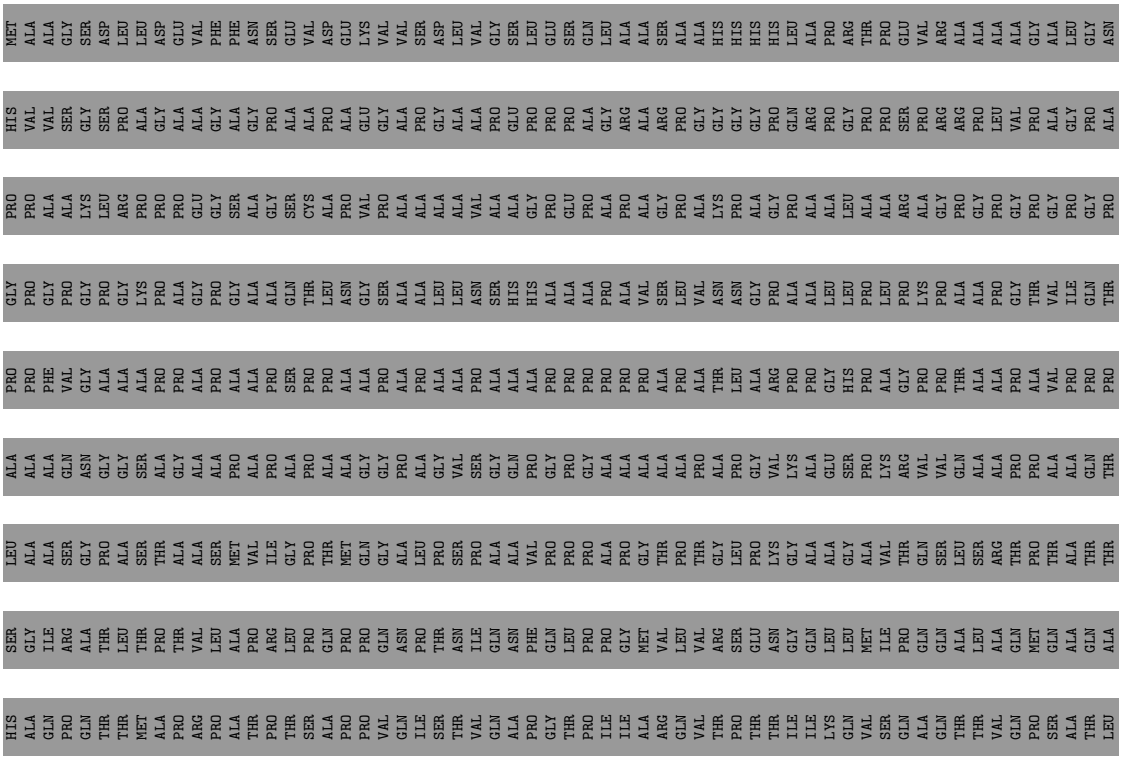
Chain DD:

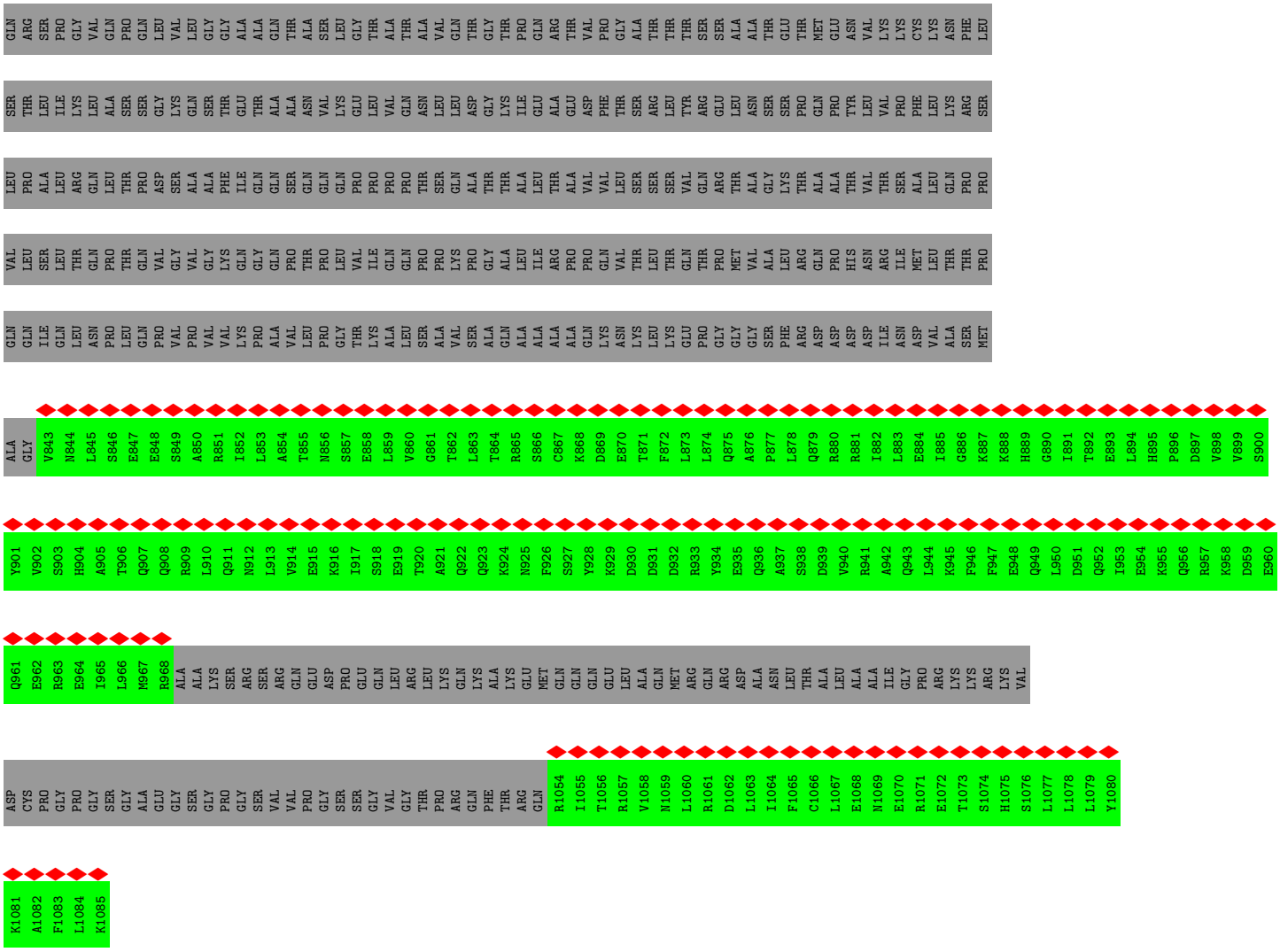




• Molecule 24: Transcription initiation factor TFIID subunit 4

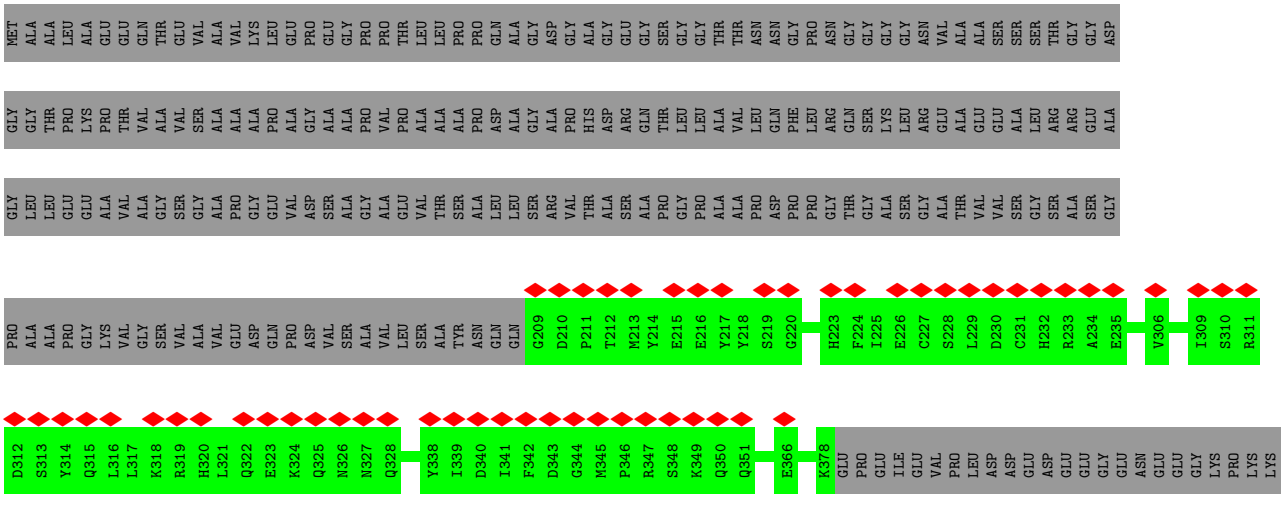
Chain Dd:

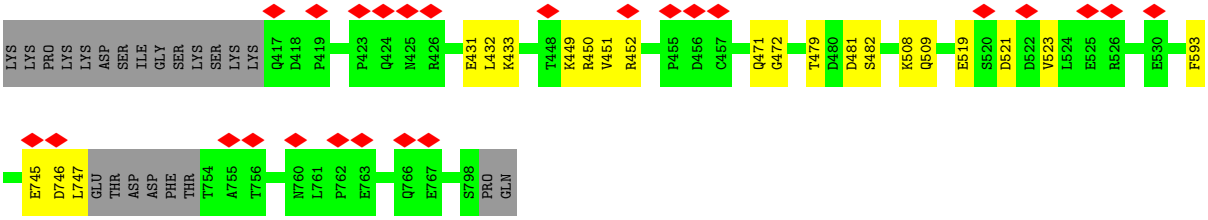




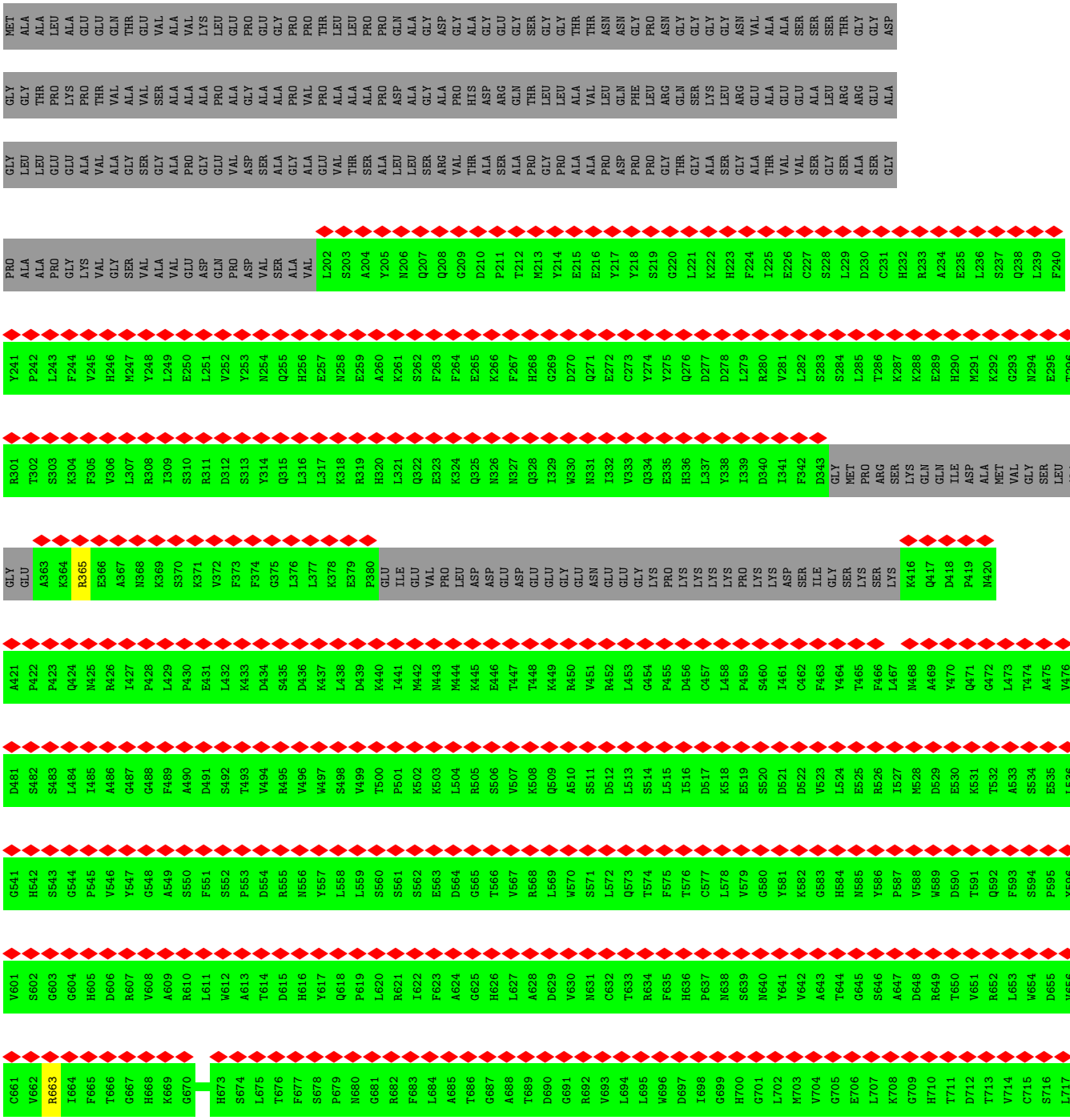
• Molecule 25: Transcription initiation factor TFIID subunit 5

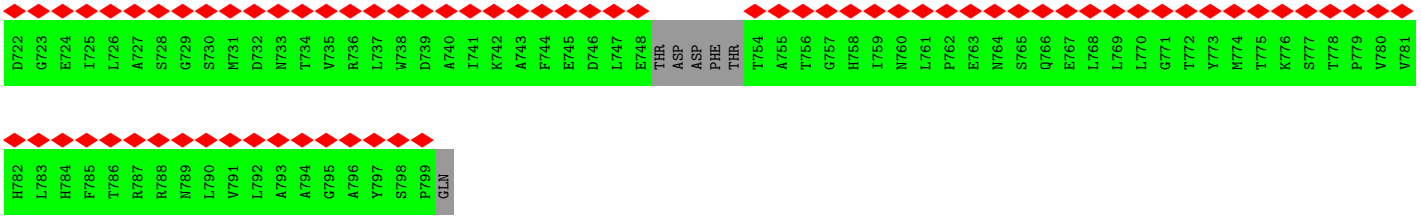
Chain DE:



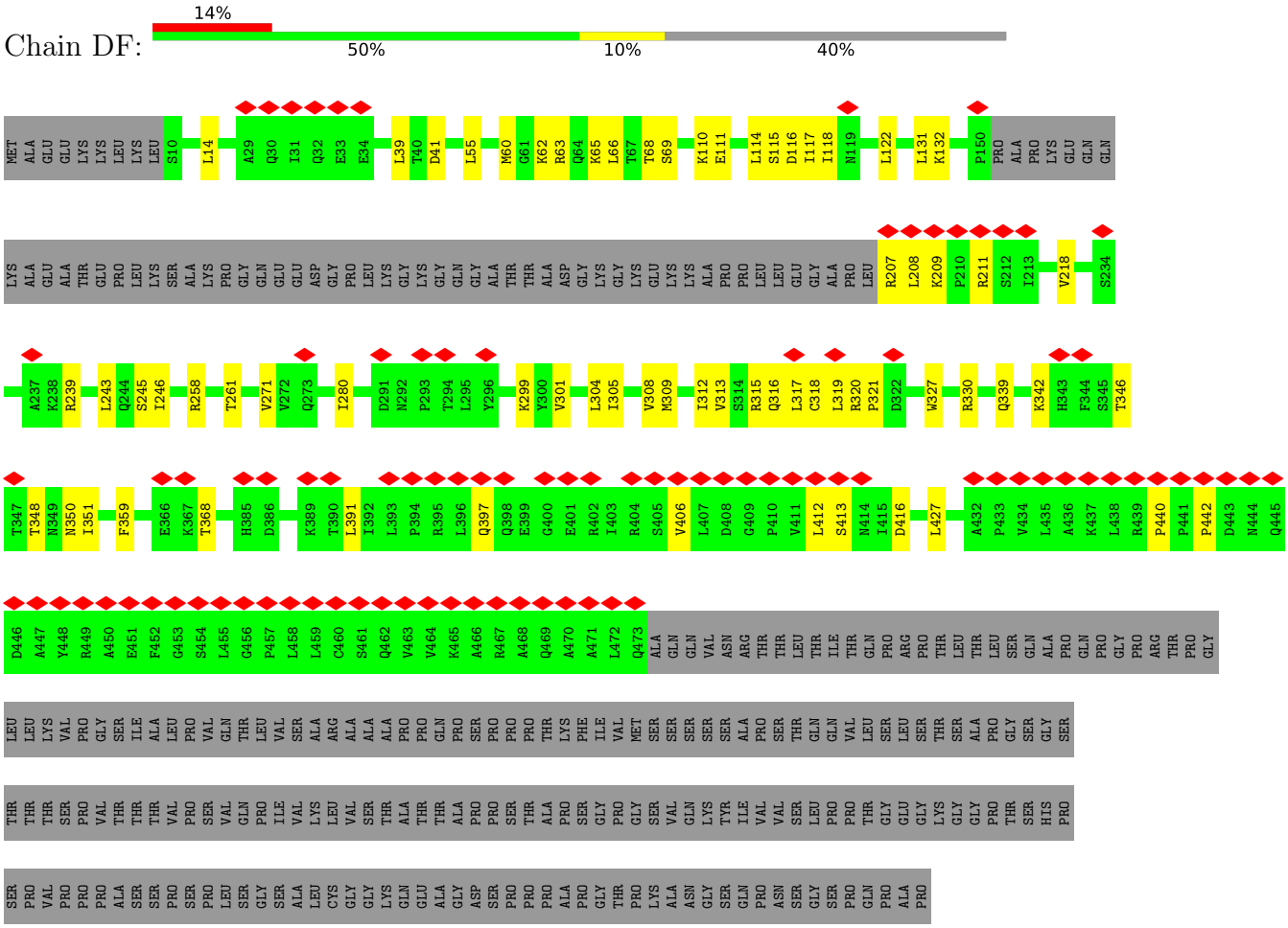


• Molecule 25: Transcription initiation factor TFIID subunit 5

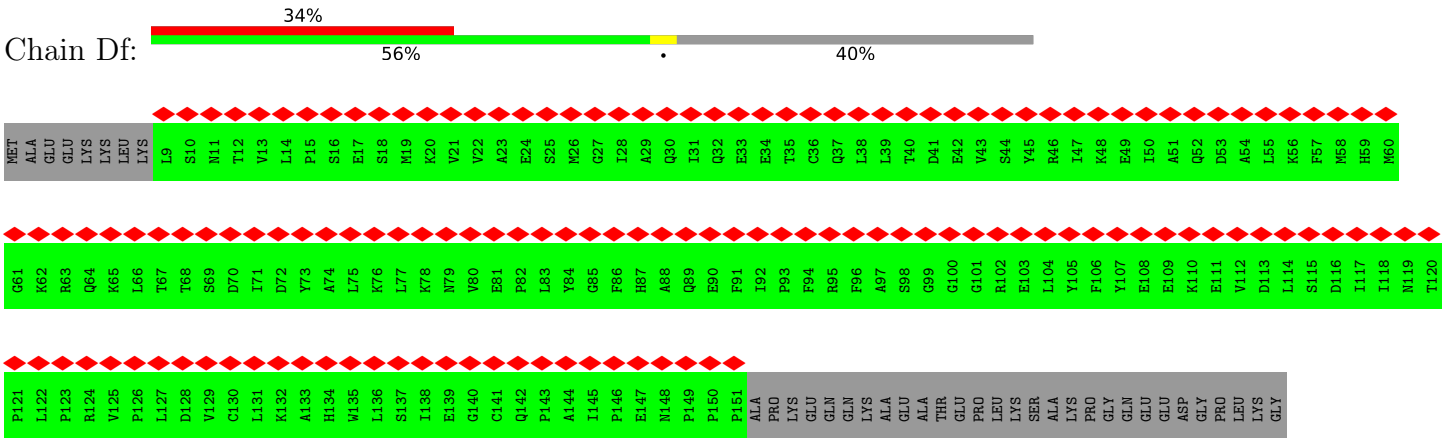


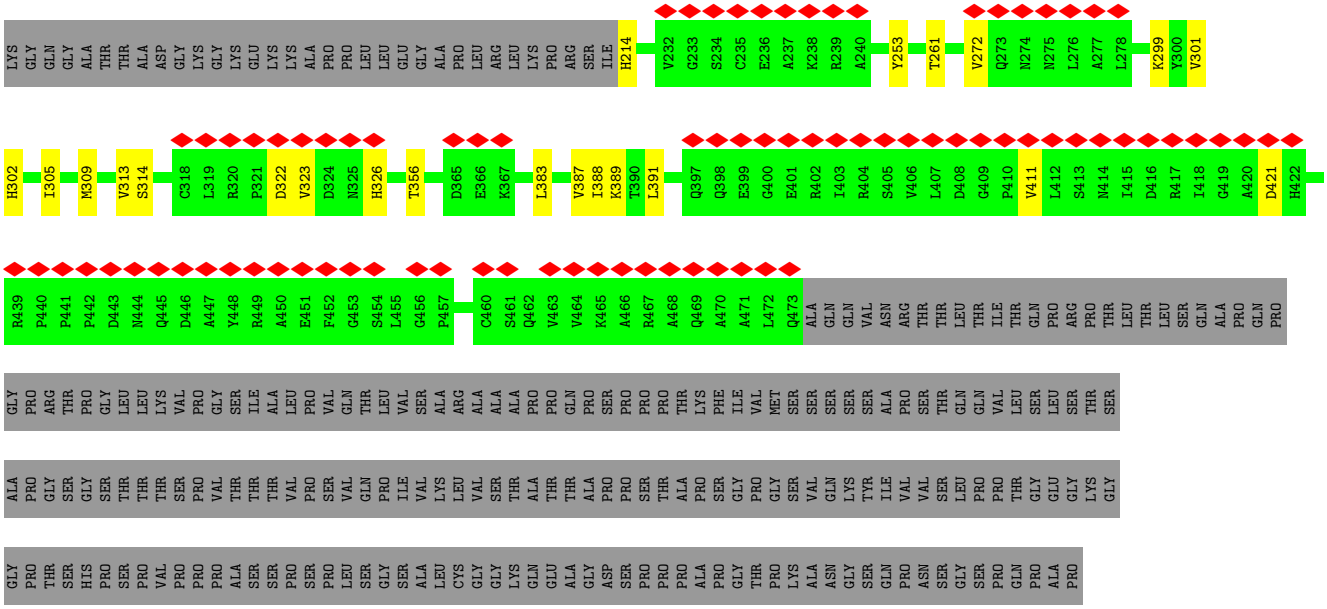


• Molecule 26: Transcription initiation factor TFIID subunit 6



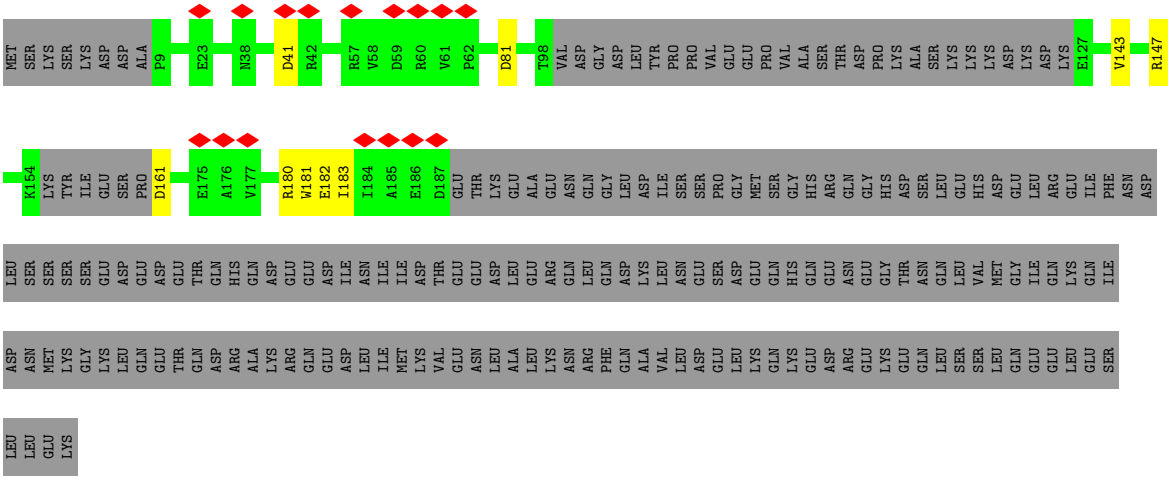
• Molecule 26: Transcription initiation factor TFIID subunit 6





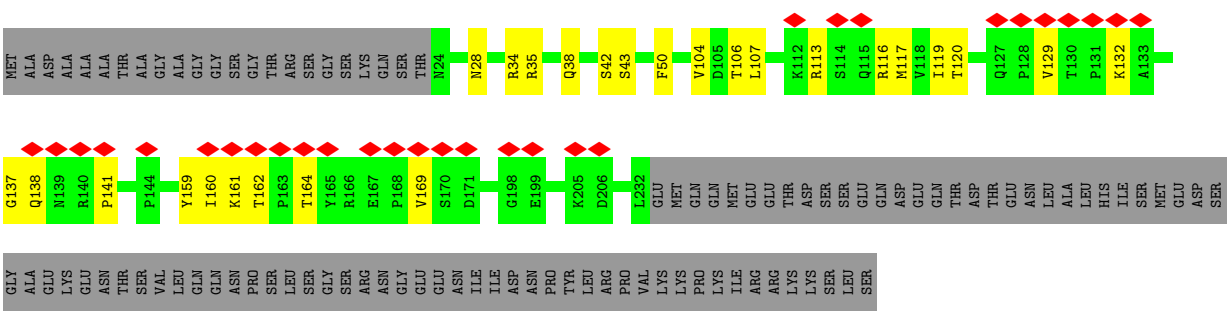
• Molecule 27: Transcription initiation factor TFIID subunit 7

Chain DG:



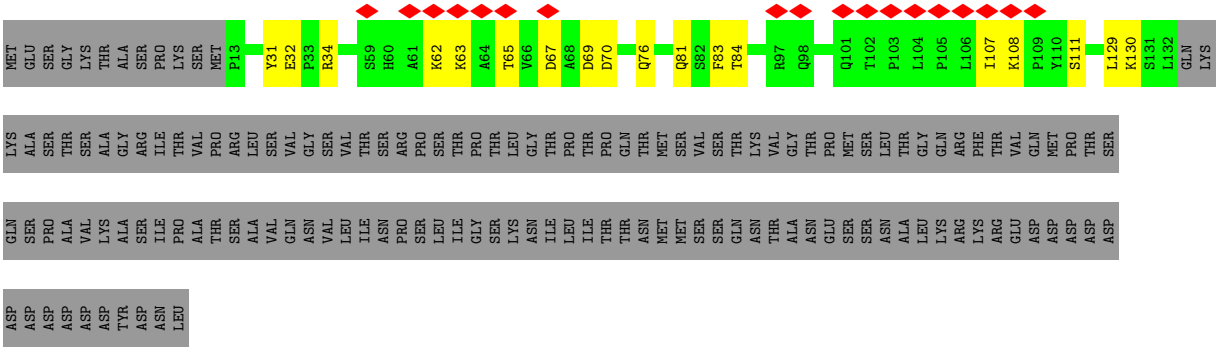
• Molecule 28: Transcription initiation factor TFIID subunit 8

Chain DH:



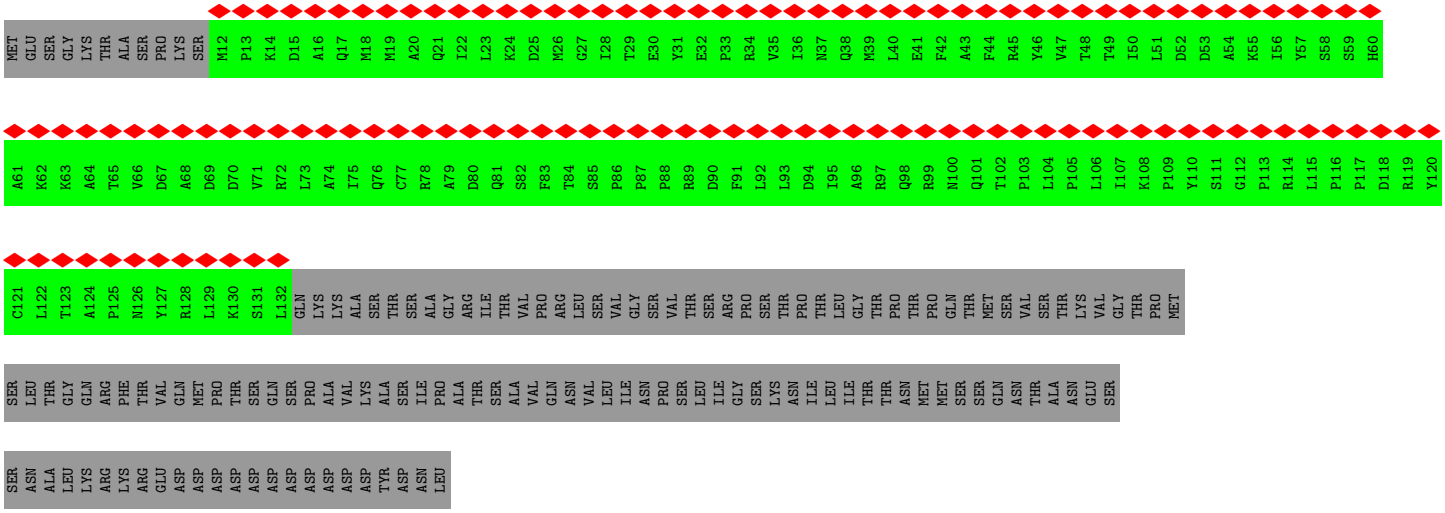
• Molecule 29: Transcription initiation factor TFIID subunit 9

Chain DI:



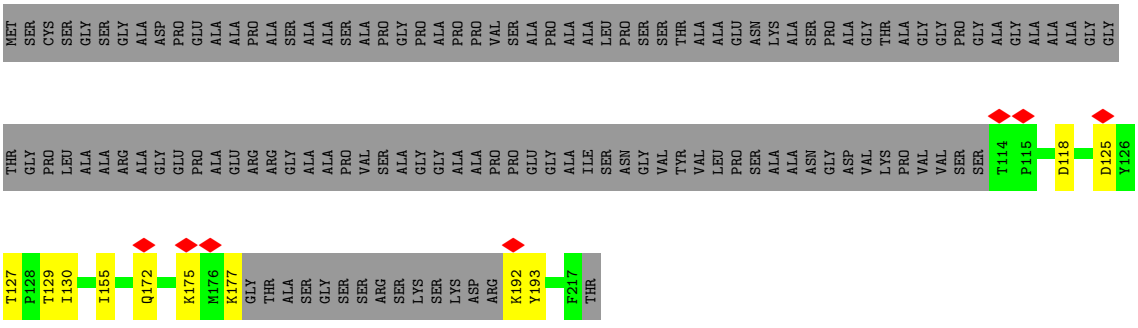
• Molecule 29: Transcription initiation factor TFIID subunit 9

Chain Di:



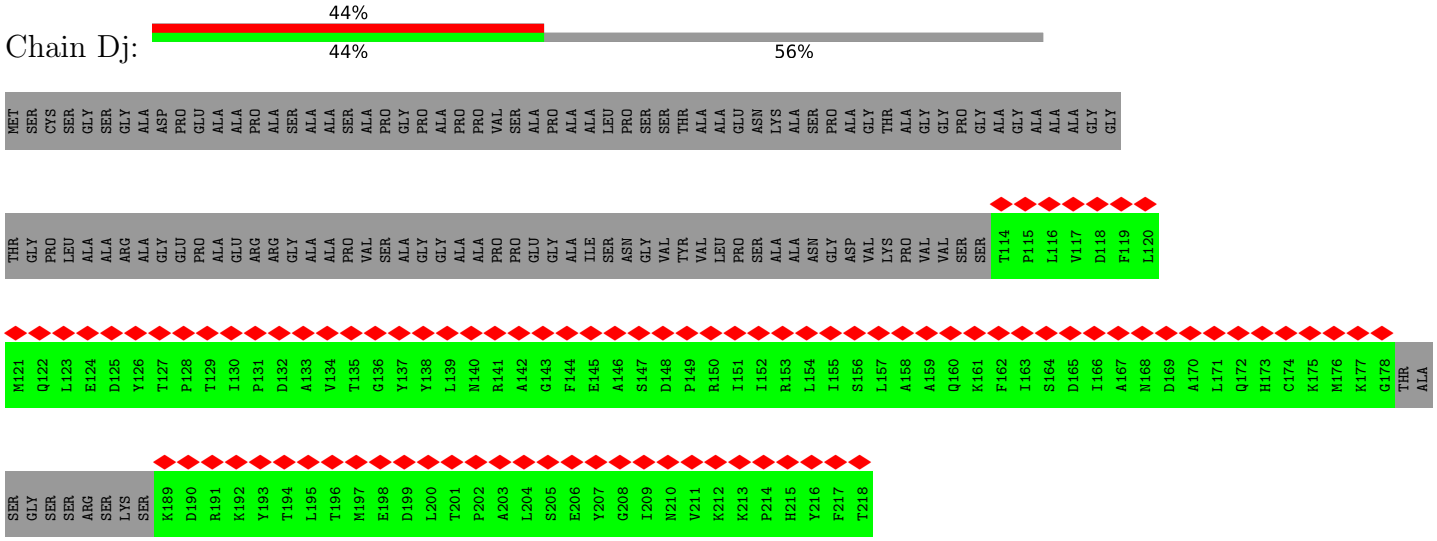
• Molecule 30: Transcription initiation factor TFIID subunit 10

Chain DJ:



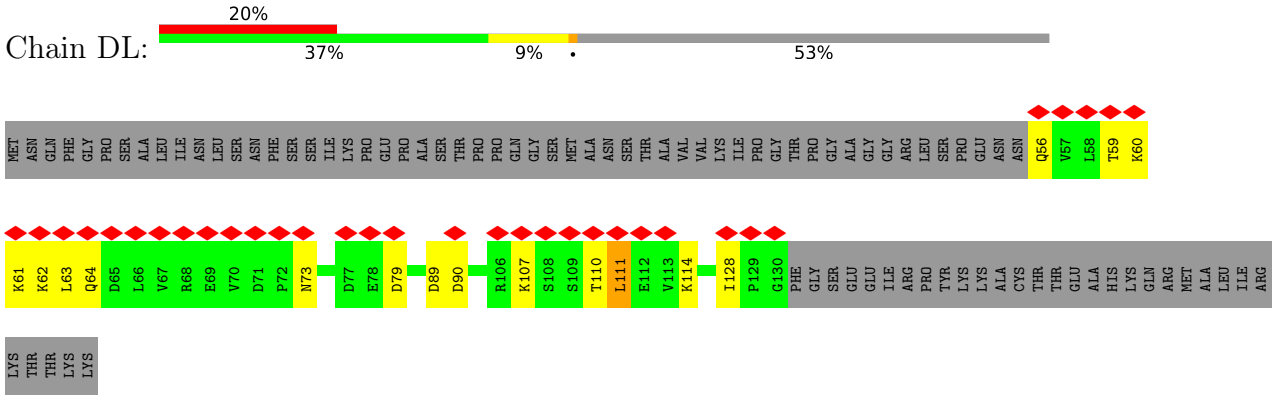
• Molecule 30: Transcription initiation factor TFIID subunit 10

Chain Dj:



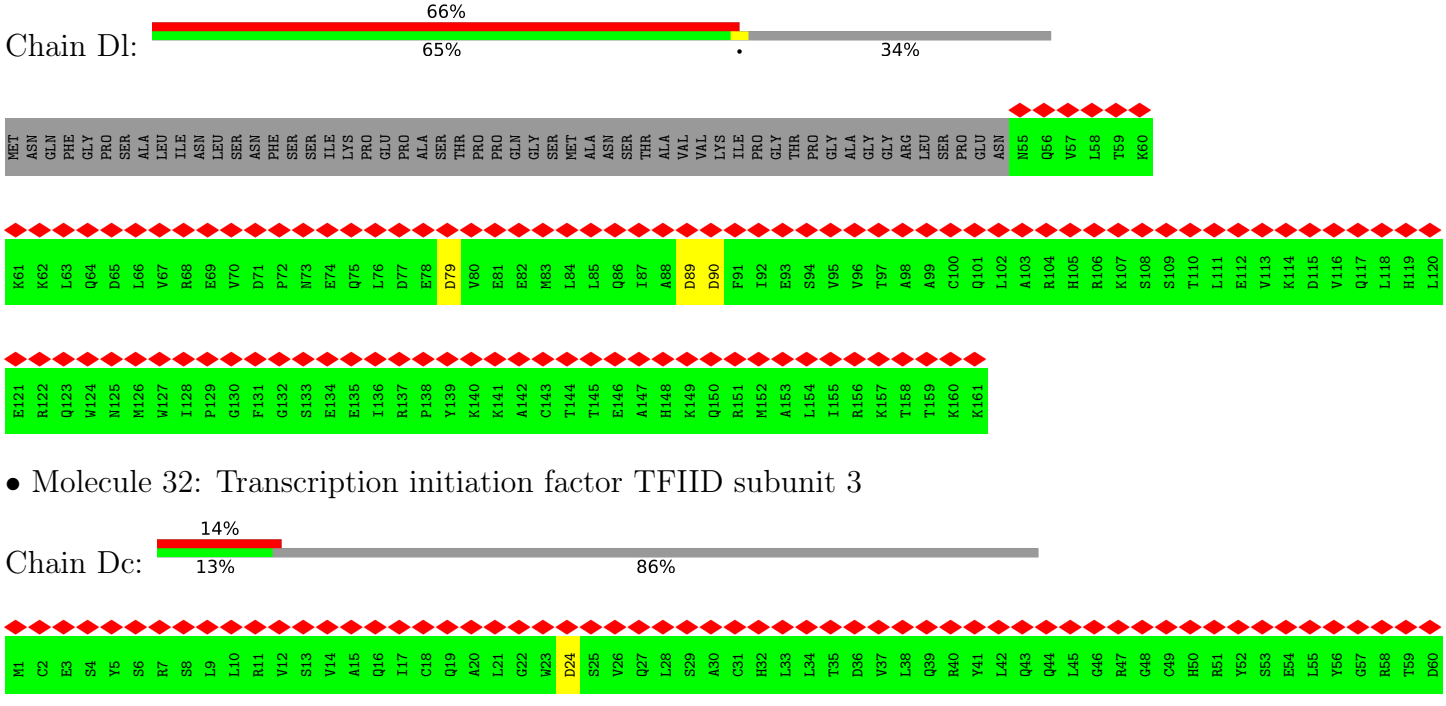
• Molecule 31: Transcription initiation factor TFIID subunit 12

Chain DL:



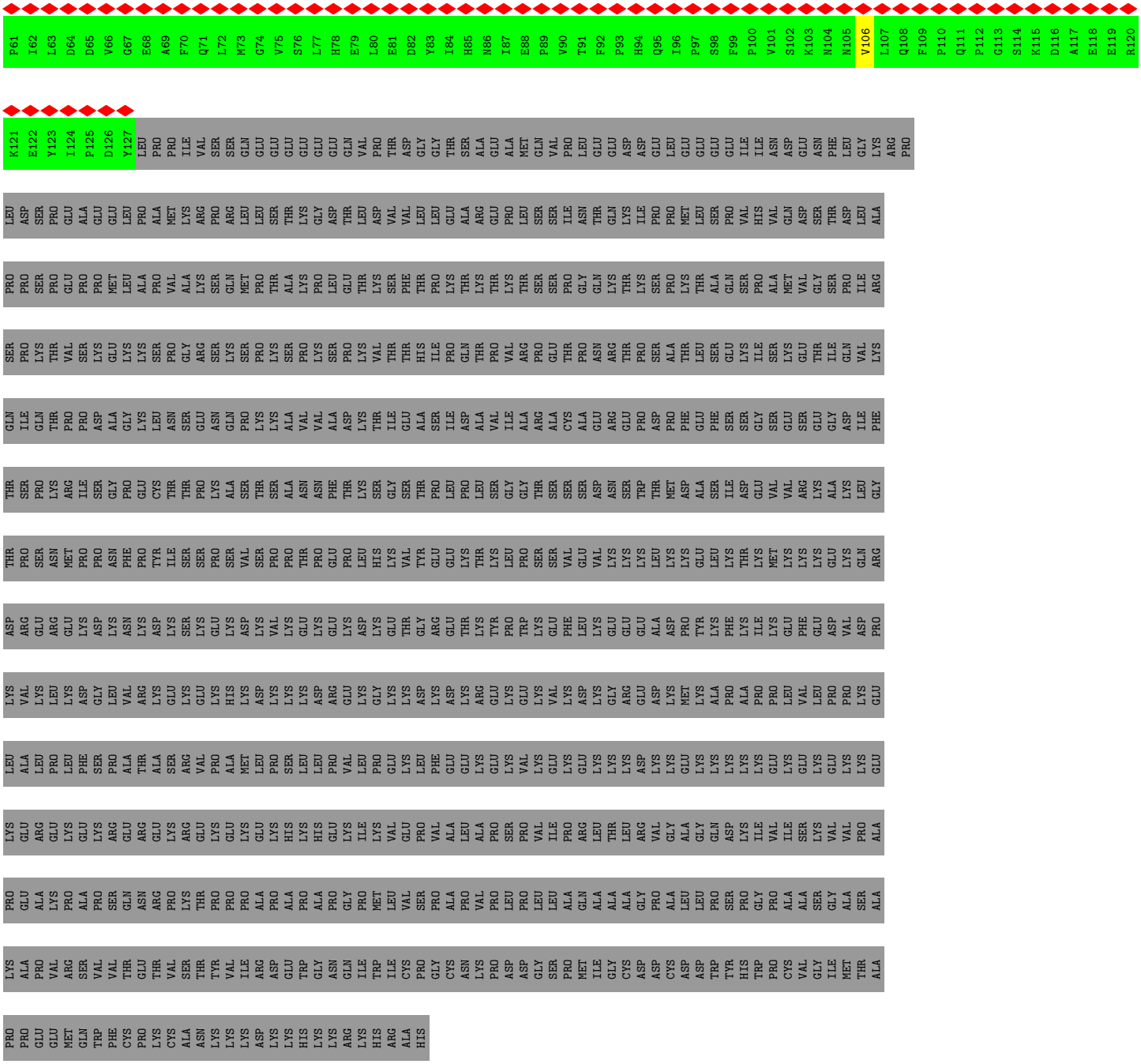
• Molecule 31: Transcription initiation factor TFIID subunit 12

Chain Dl:



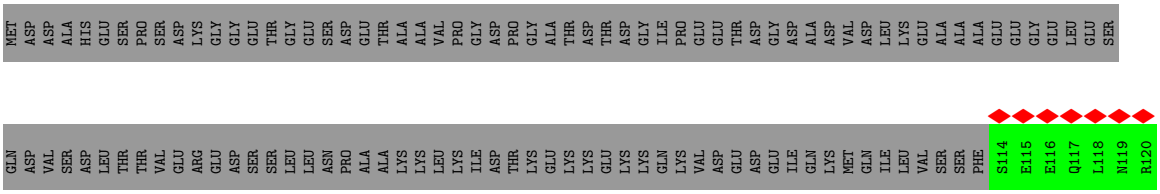
• Molecule 32: Transcription initiation factor TFIID subunit 3

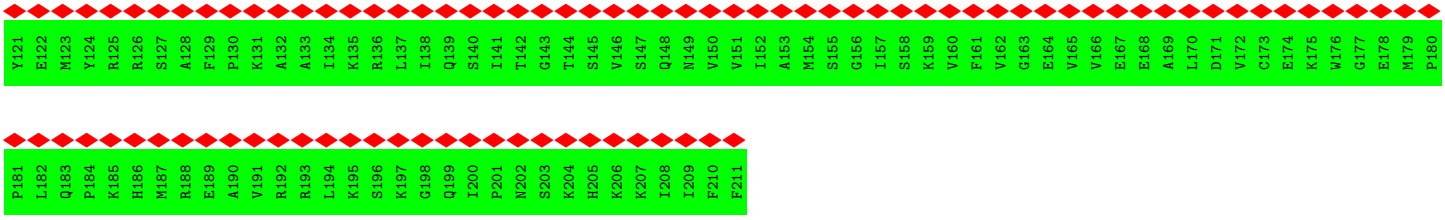
Chain Dc:



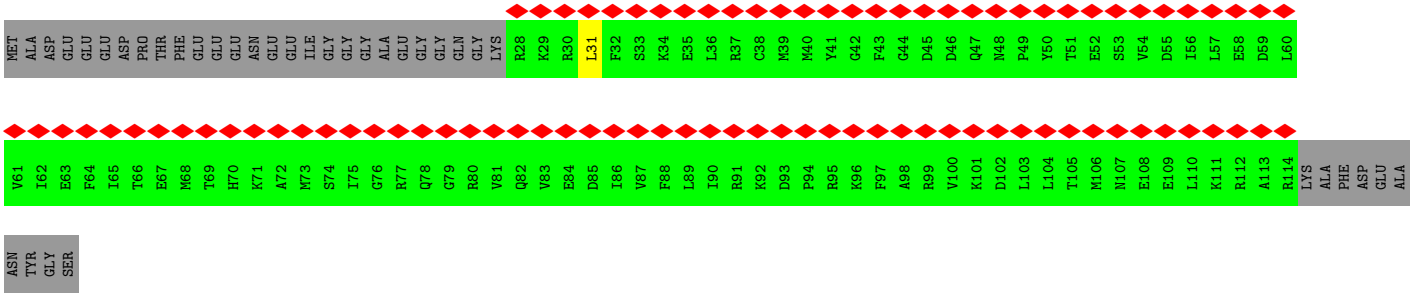
• Molecule 33: Transcription initiation factor TFIID subunit 11

Chain Dk:

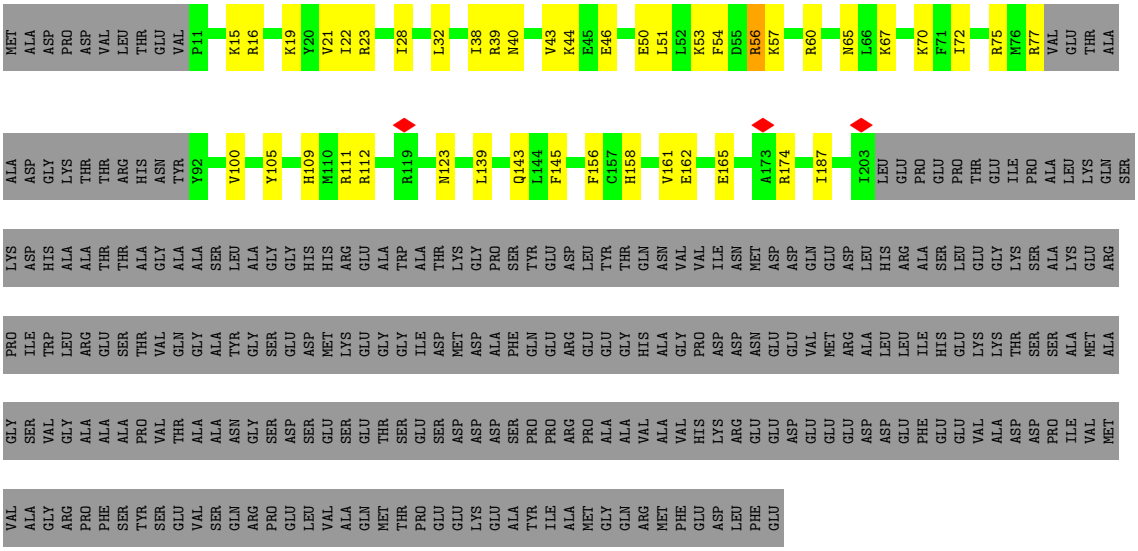




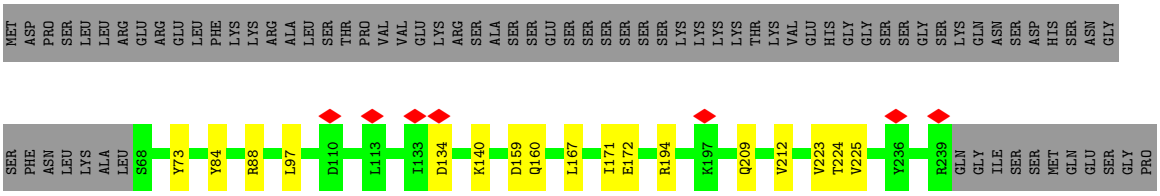
• Molecule 34: Transcription initiation factor TFIID subunit 13



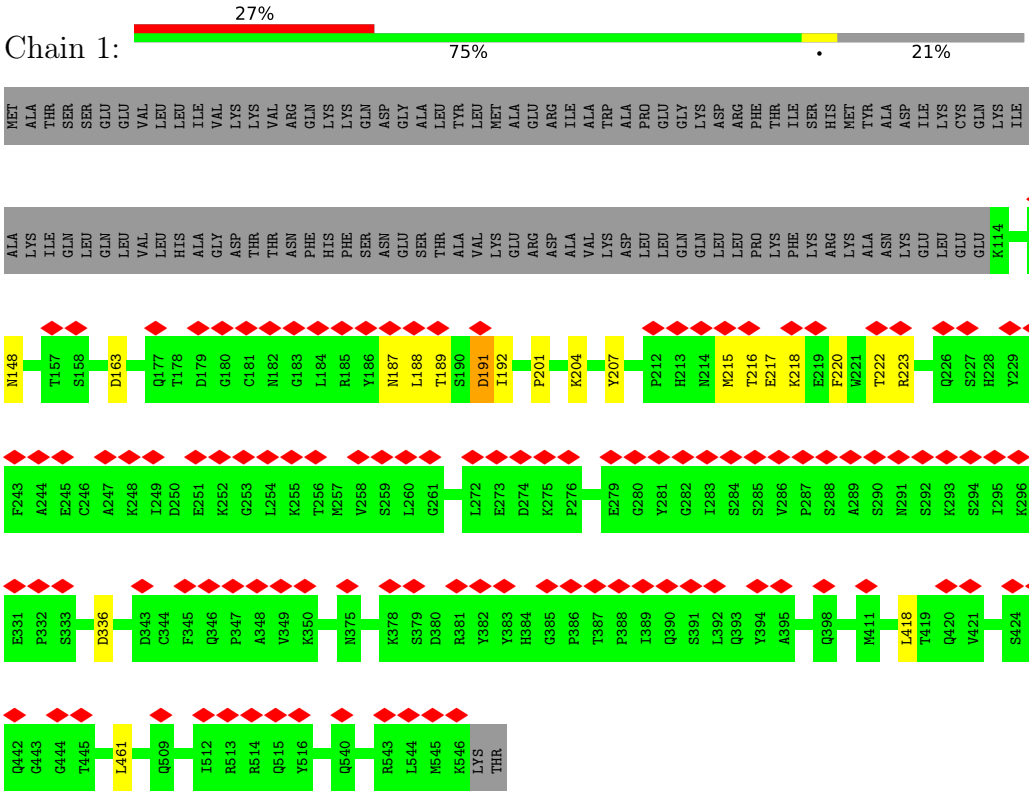
• Molecule 35: General transcription factor IIE subunit 1



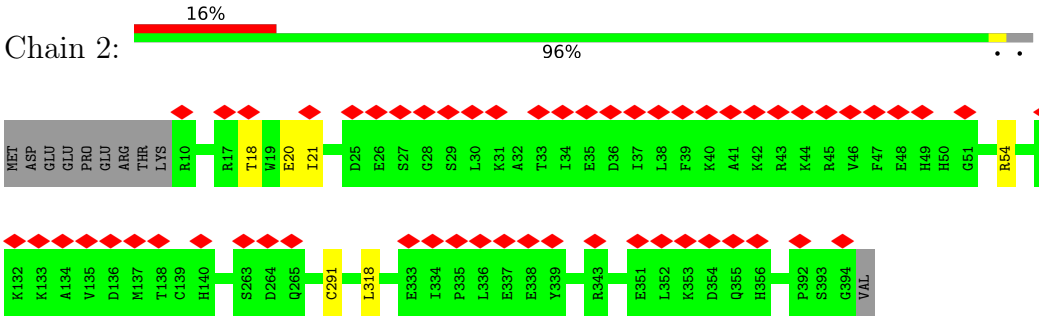
• Molecule 36: Transcription initiation factor IIE subunit beta



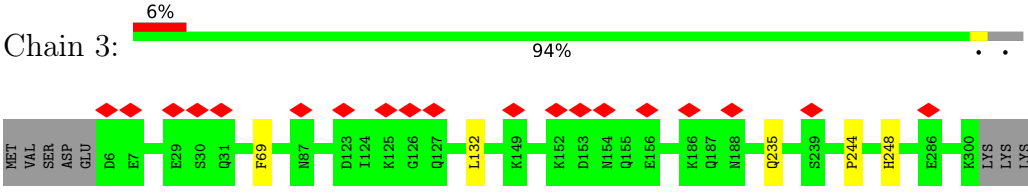
• Molecule 37: General transcription factor IIH subunit 1



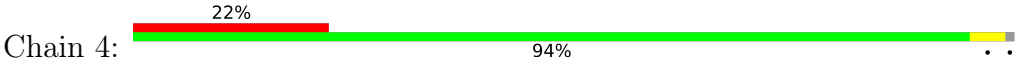
• Molecule 38: General transcription factor IIH subunit 2

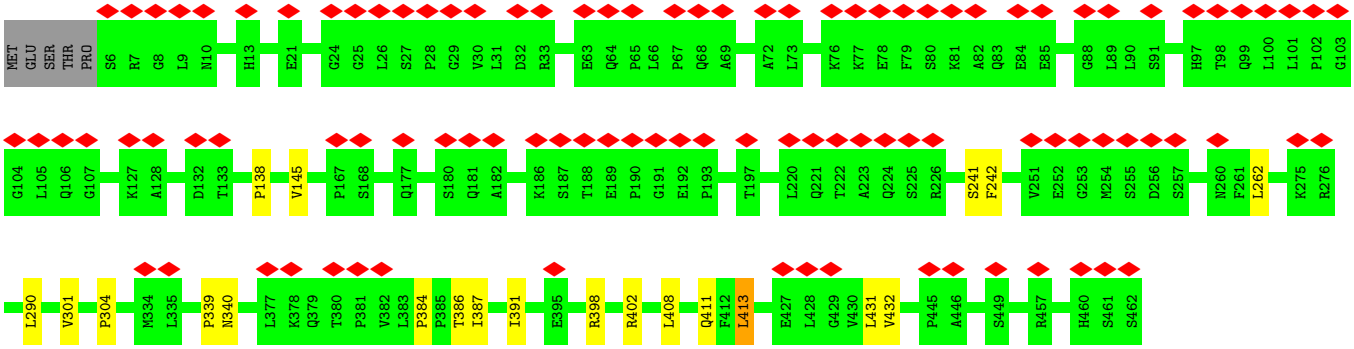


• Molecule 39: General transcription factor IIH subunit 3

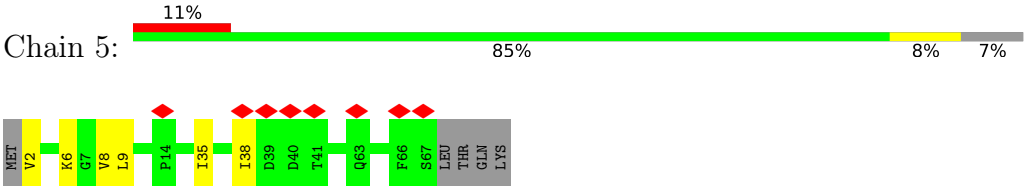


• Molecule 40: General transcription factor IIH subunit 4

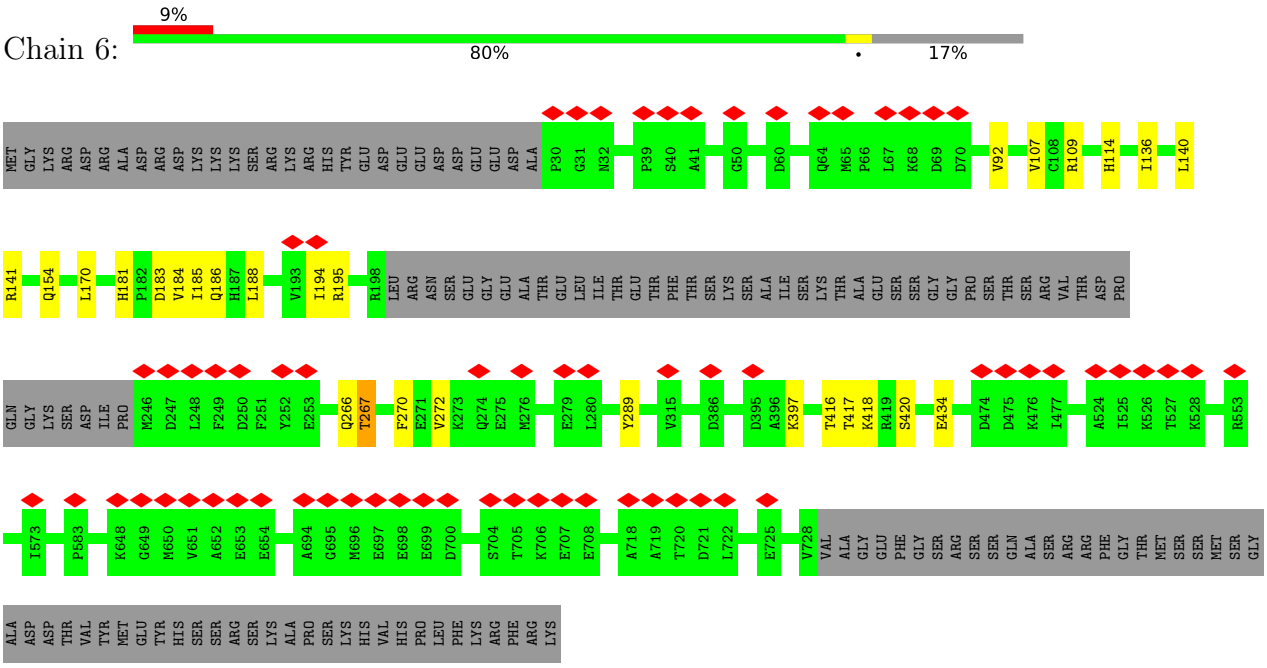




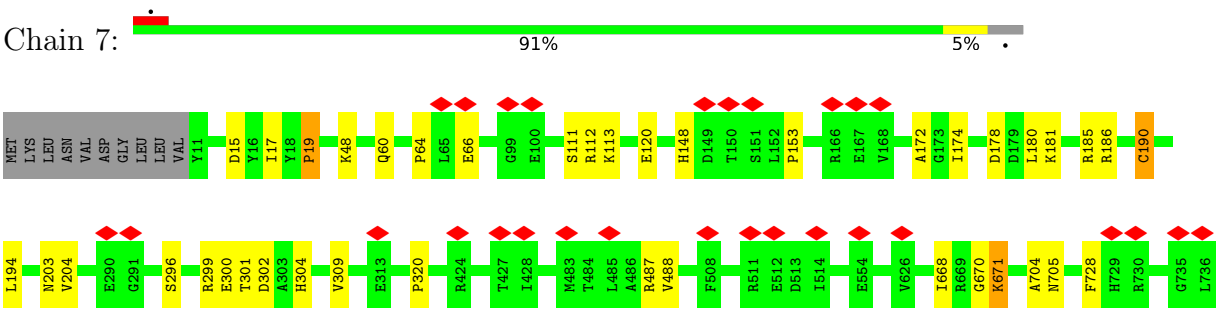
• Molecule 41: General transcription factor IIH subunit 5

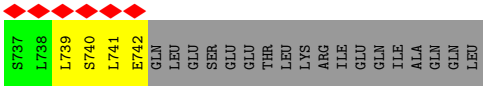


• Molecule 42: General transcription and DNA repair factor IIH helicase subunit XPB

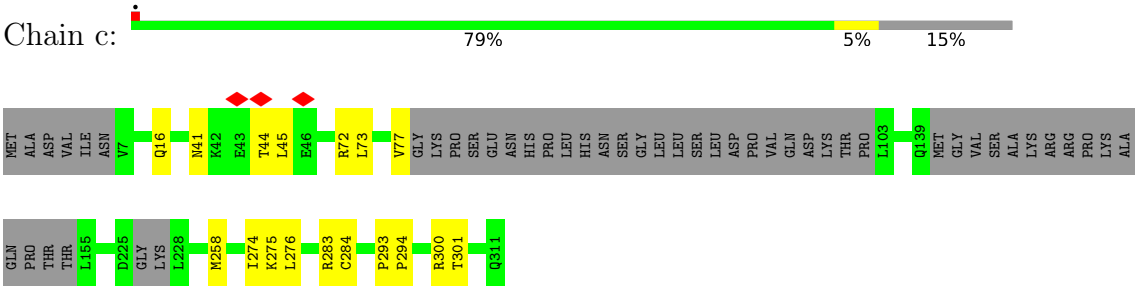


• Molecule 43: General transcription and DNA repair factor IIH helicase subunit XPD

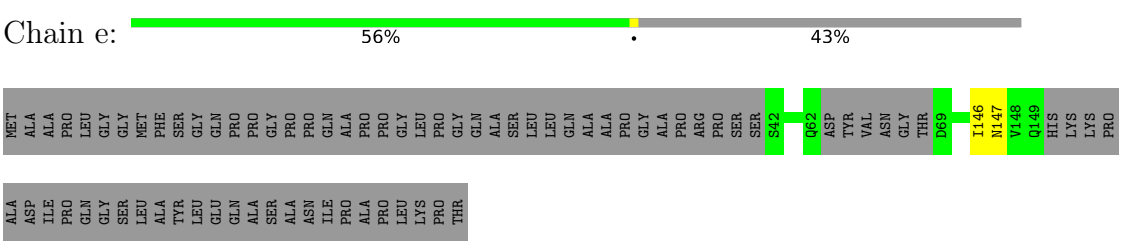




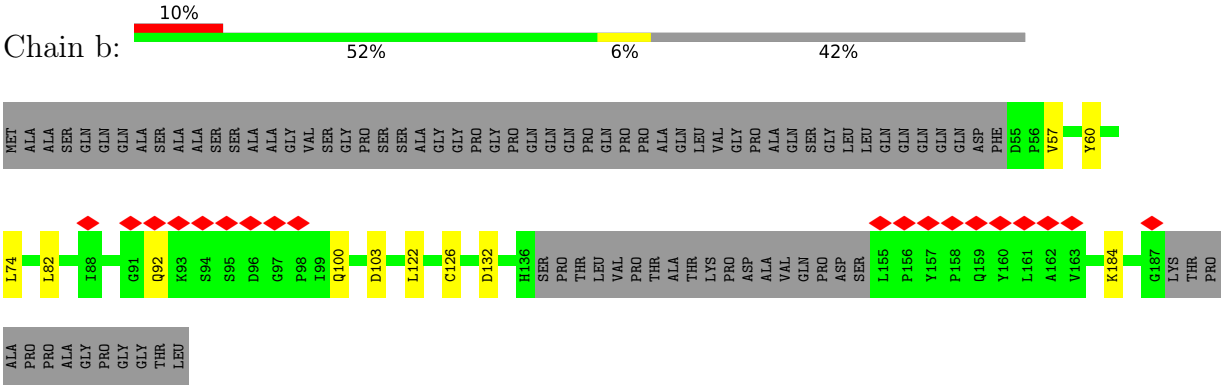
• Molecule 44: Mediator of RNA polymerase II transcription subunit 27



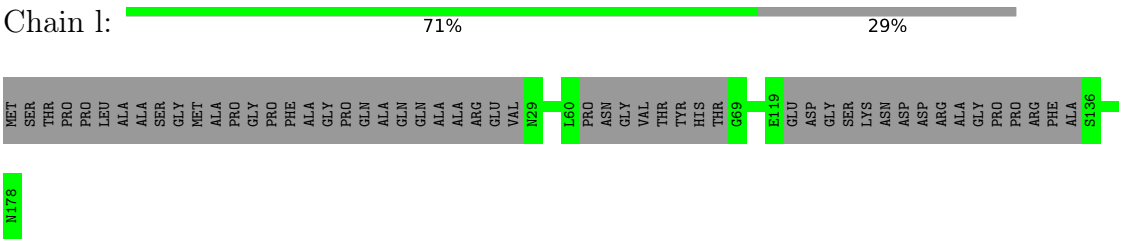
• Molecule 45: Mediator of RNA polymerase II transcription subunit 28



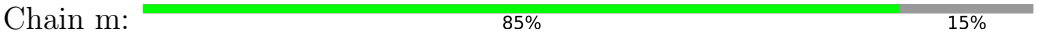
• Molecule 46: Mediator of RNA polymerase II transcription subunit 29

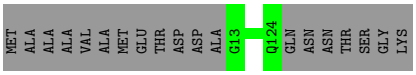


• Molecule 47: Mediator of RNA polymerase II transcription subunit 30



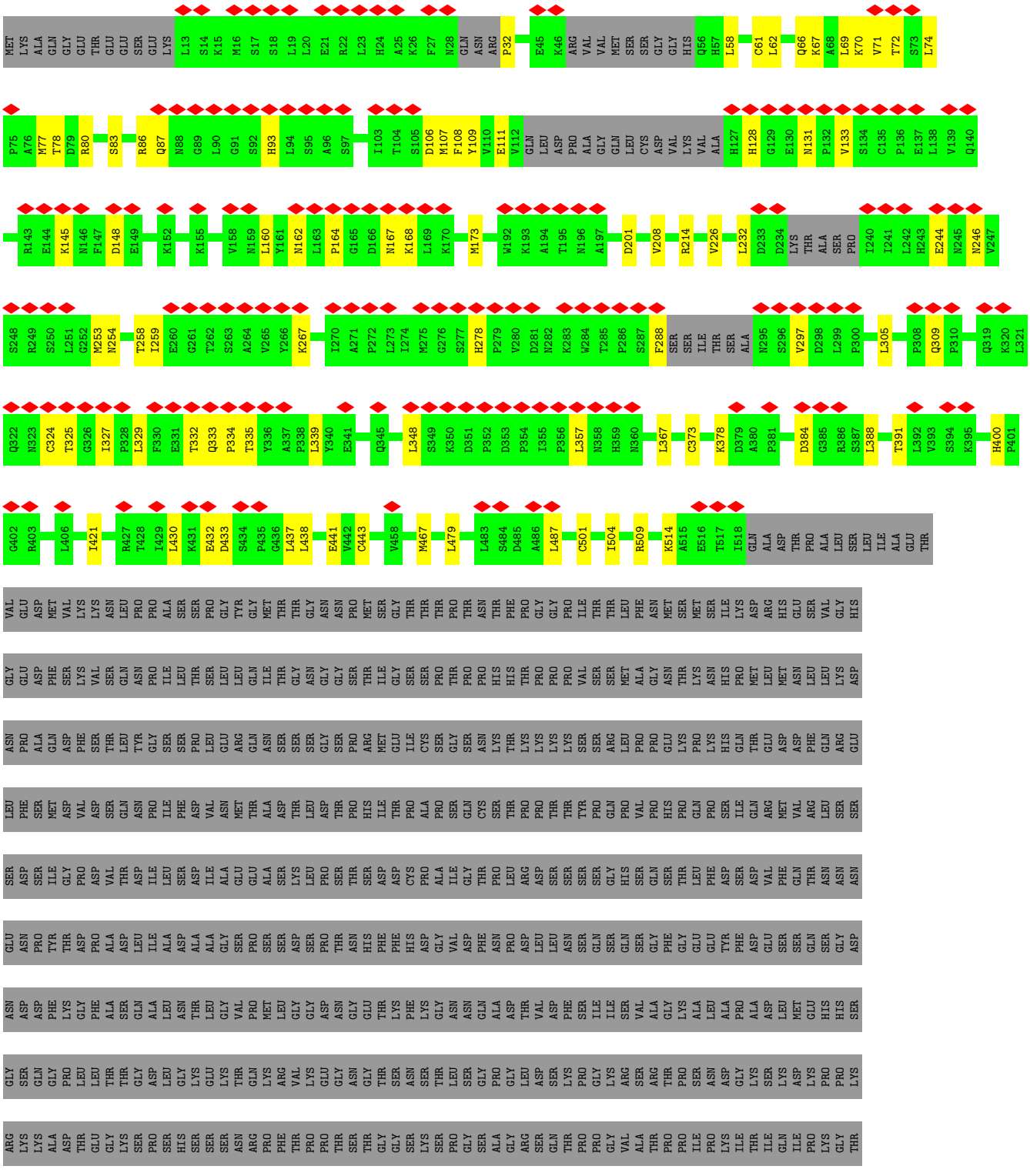
• Molecule 48: Mediator of RNA polymerase II transcription subunit 31

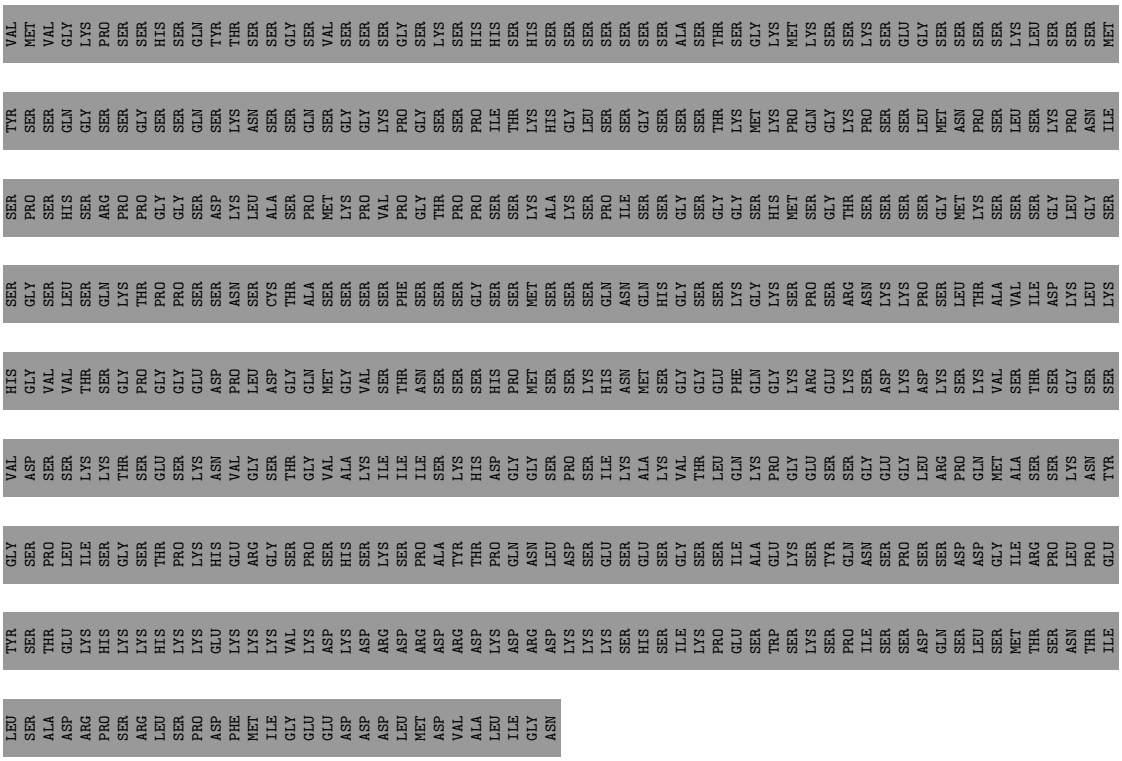




• Molecule 49: Mediator of RNA polymerase II transcription subunit 1

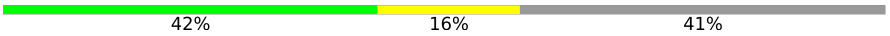
Chain a:

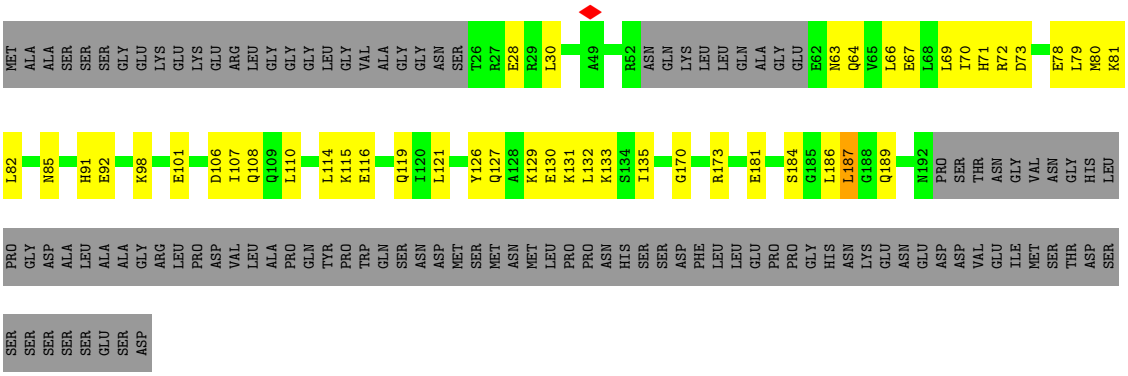




• Molecule 50: Mediator of RNA polymerase II transcription subunit 4

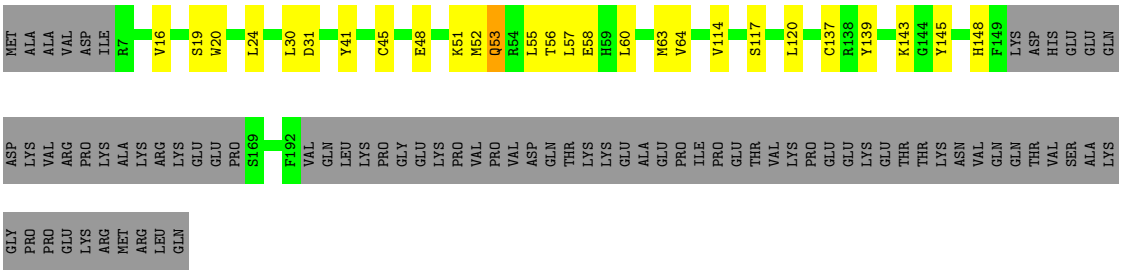
Chain d:





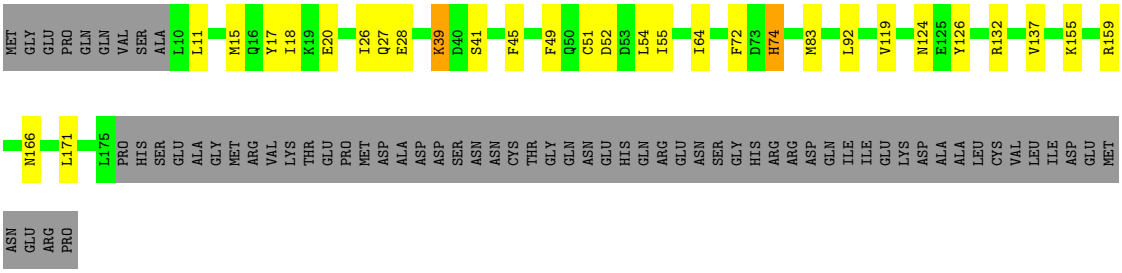
• Molecule 51: Mediator of RNA polymerase II transcription subunit 6

Chain f:



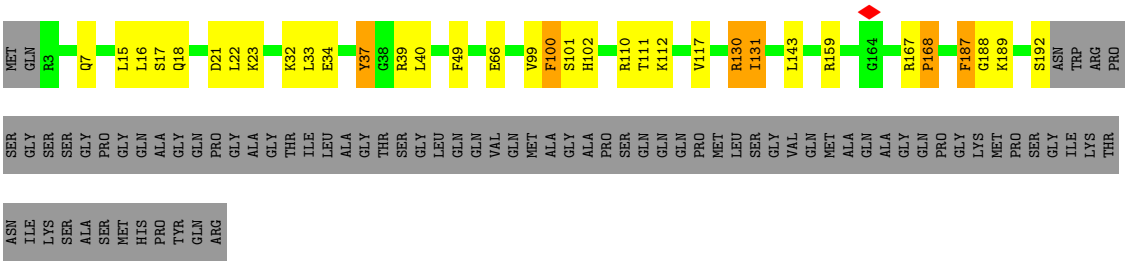
• Molecule 52: Mediator of RNA polymerase II transcription subunit 7

Chain g:



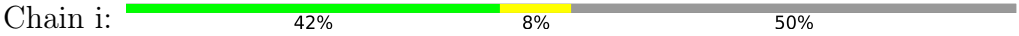
• Molecule 53: Isoform 2 of Mediator of RNA polymerase II transcription subunit 8

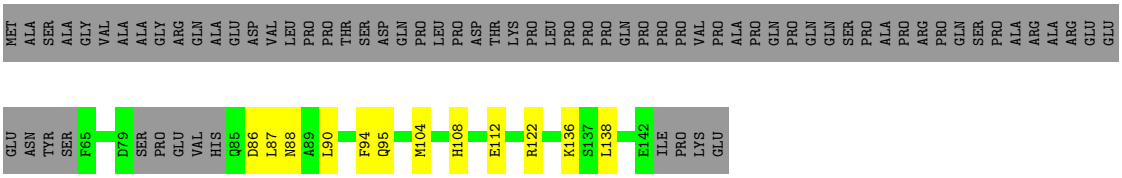
Chain h:



• Molecule 54: Mediator of RNA polymerase II transcription subunit 9

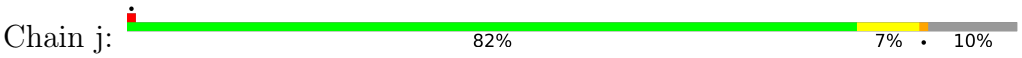
Chain i:





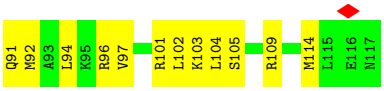
• Molecule 55: Mediator of RNA polymerase II transcription subunit 10

Chain j:

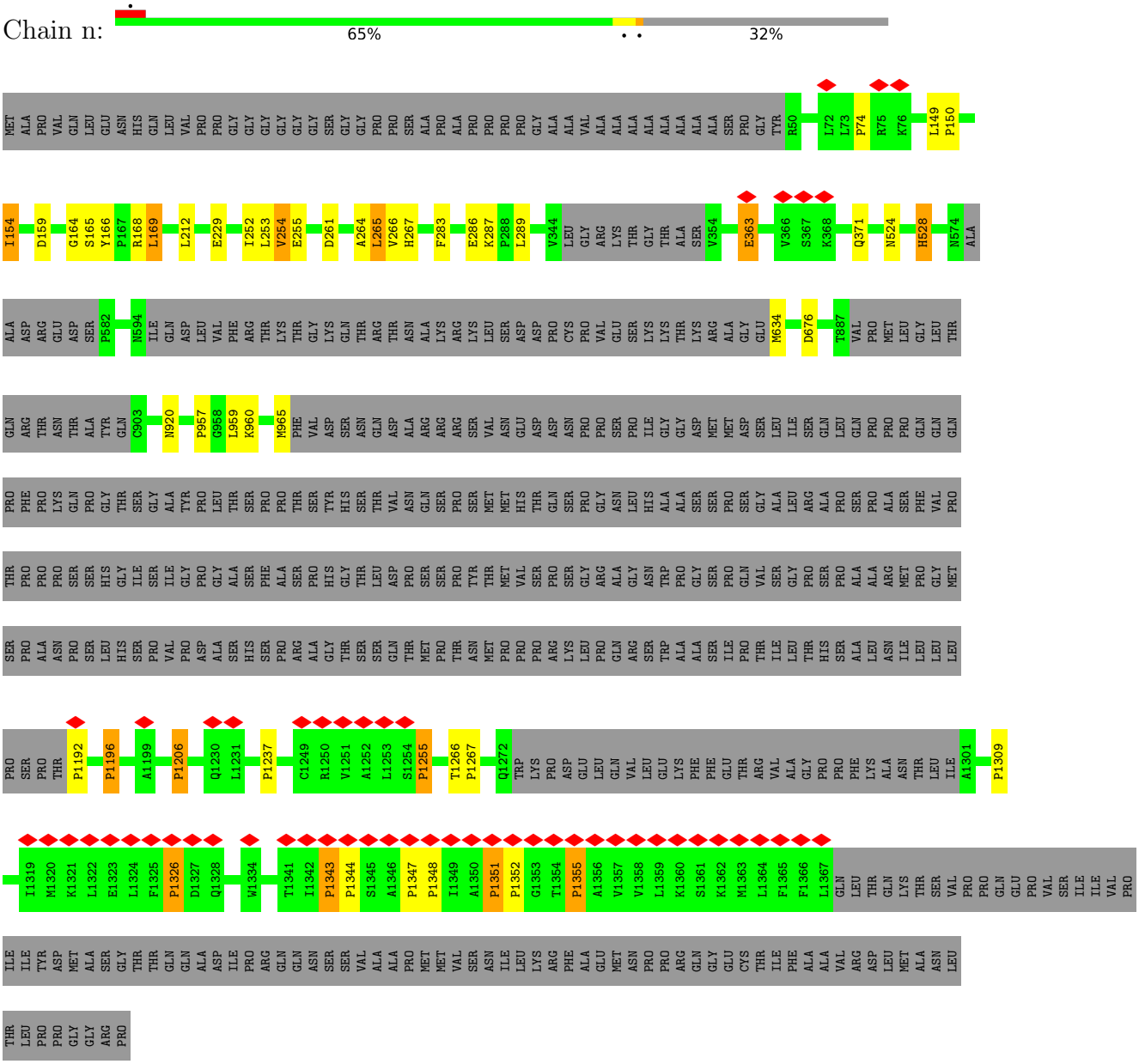


• Molecule 56: Mediator of RNA polymerase II transcription subunit 11

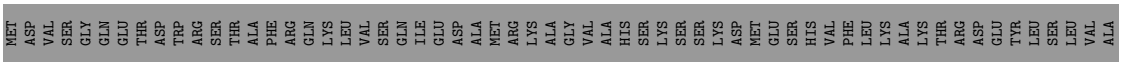
Chain k:

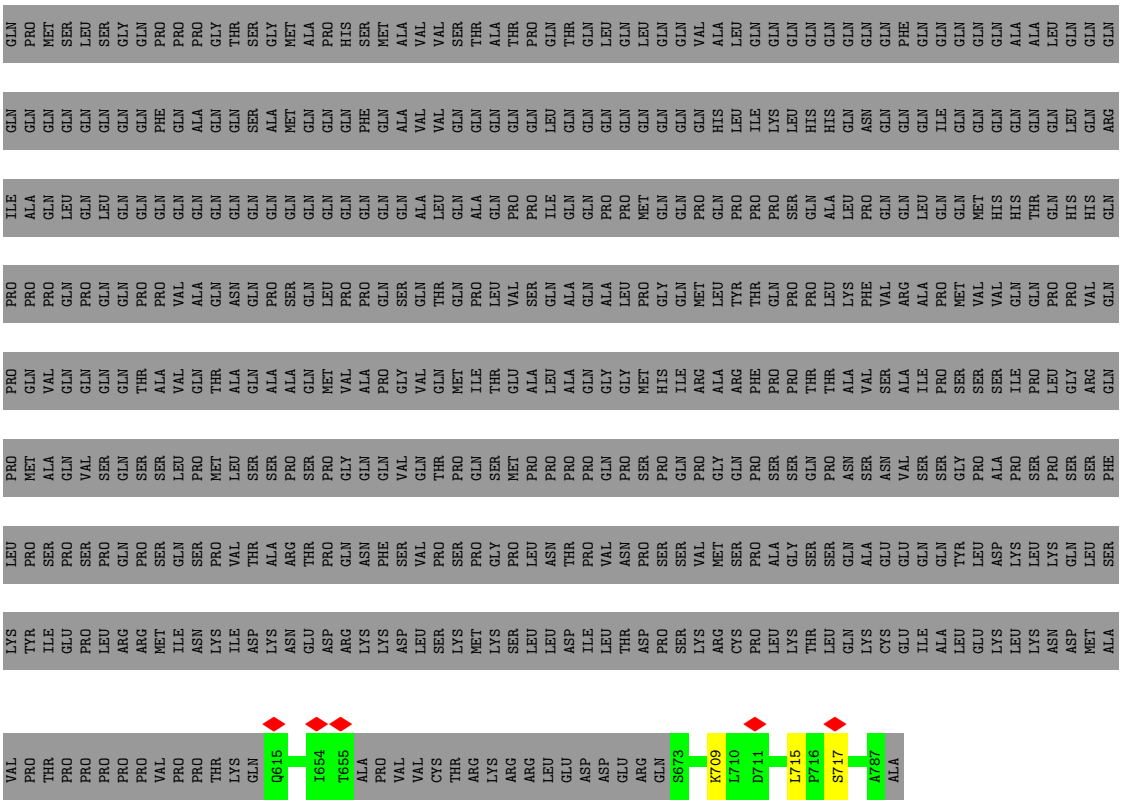


• Molecule 57: Mediator of RNA polymerase II transcription subunit 14



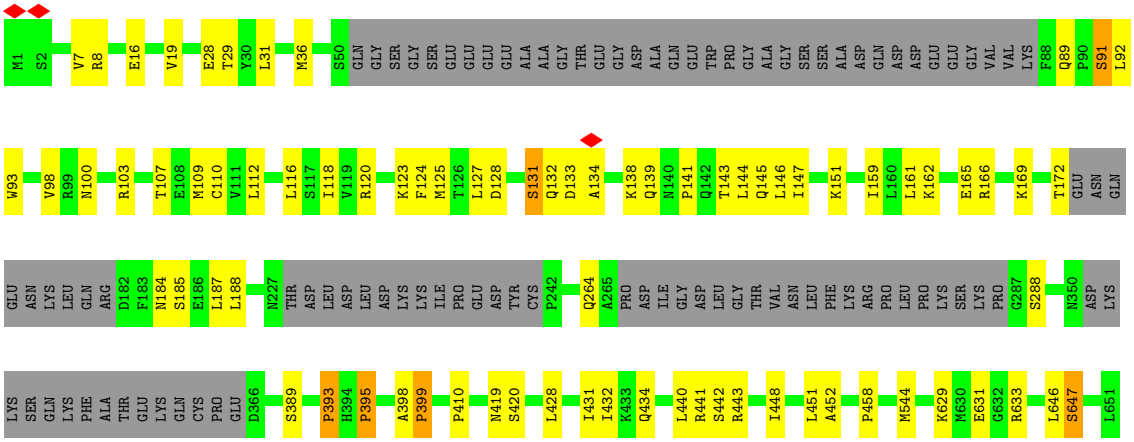
• Molecule 58: Mediator of RNA polymerase II transcription subunit 15





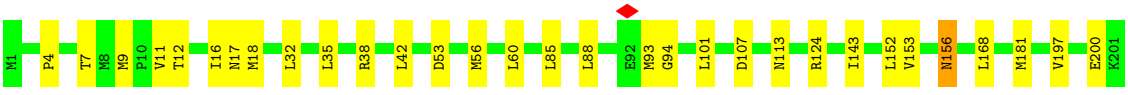
• Molecule 59: Mediator of RNA polymerase II transcription subunit 17

Chain q:



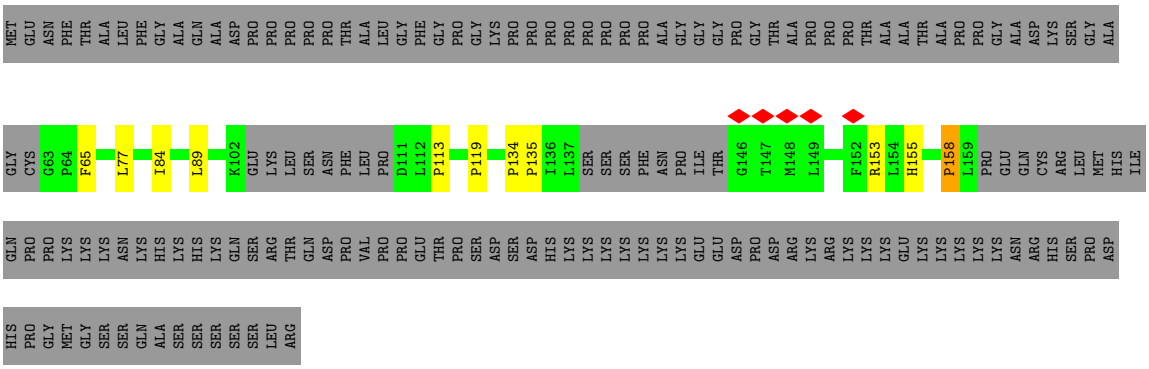
• Molecule 60: Mediator of RNA polymerase II transcription subunit 18

Chain r:



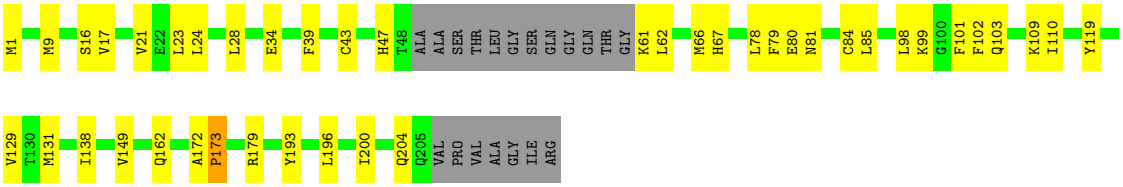
• Molecule 61: Mediator of RNA polymerase II transcription subunit 19

Chain s:



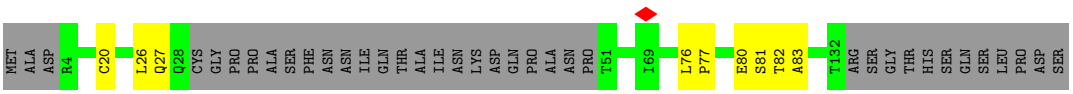
• Molecule 62: Mediator of RNA polymerase II transcription subunit 20

Chain t:



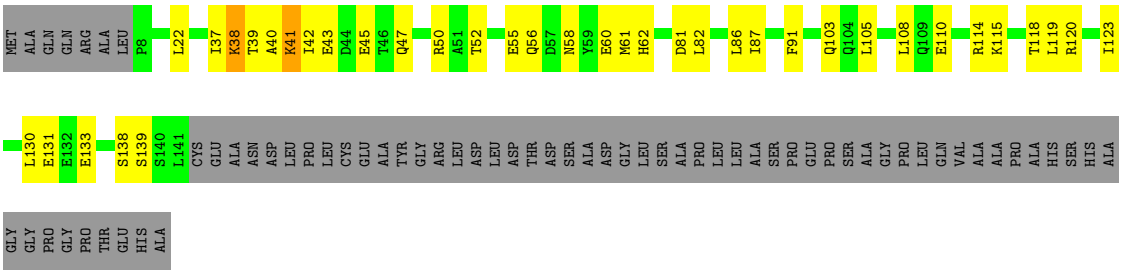
• Molecule 63: Mediator of RNA polymerase II transcription subunit 21

Chain u:



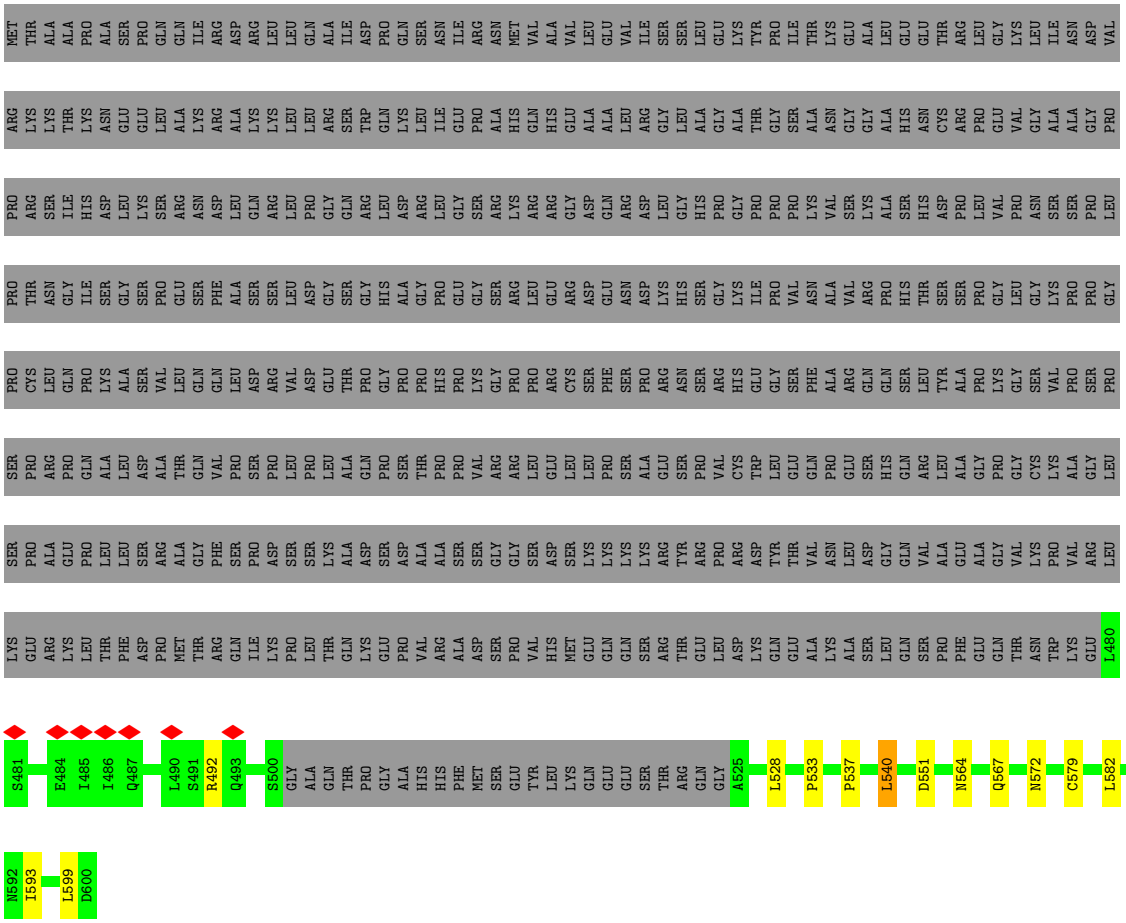
• Molecule 64: Mediator of RNA polymerase II transcription subunit 22

Chain v:



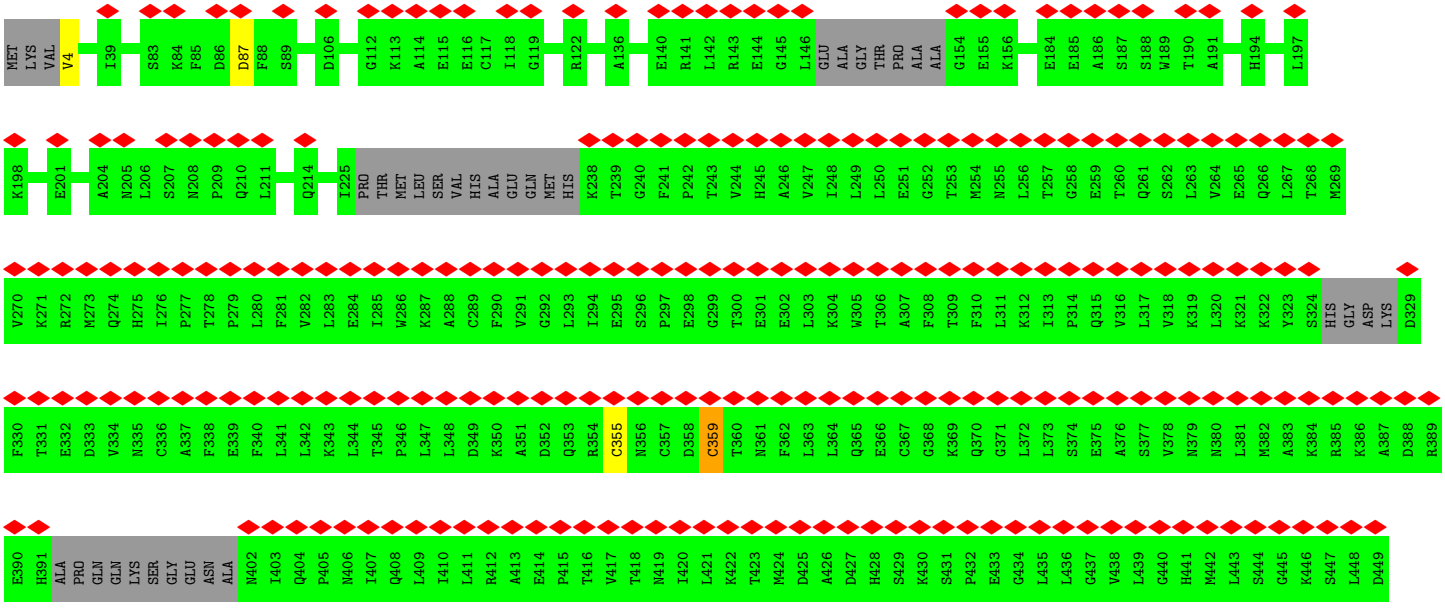
• Molecule 65: Mediator of RNA polymerase II transcription subunit 26

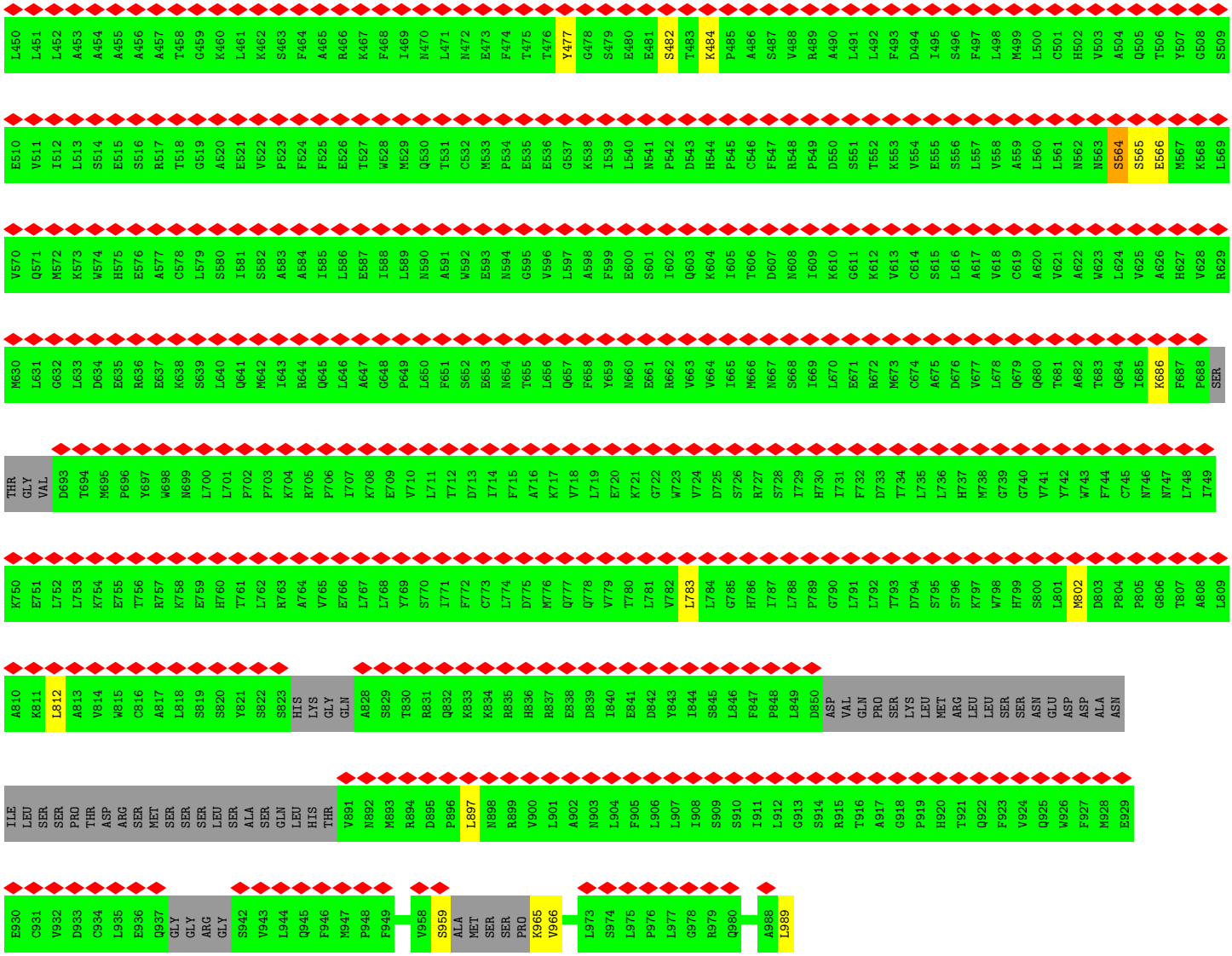
Chain z:



• Molecule 66: Mediator of RNA polymerase II transcription subunit 24

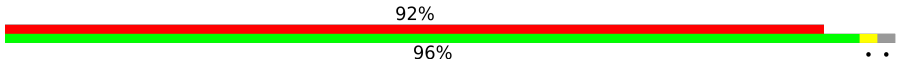
Chain x:

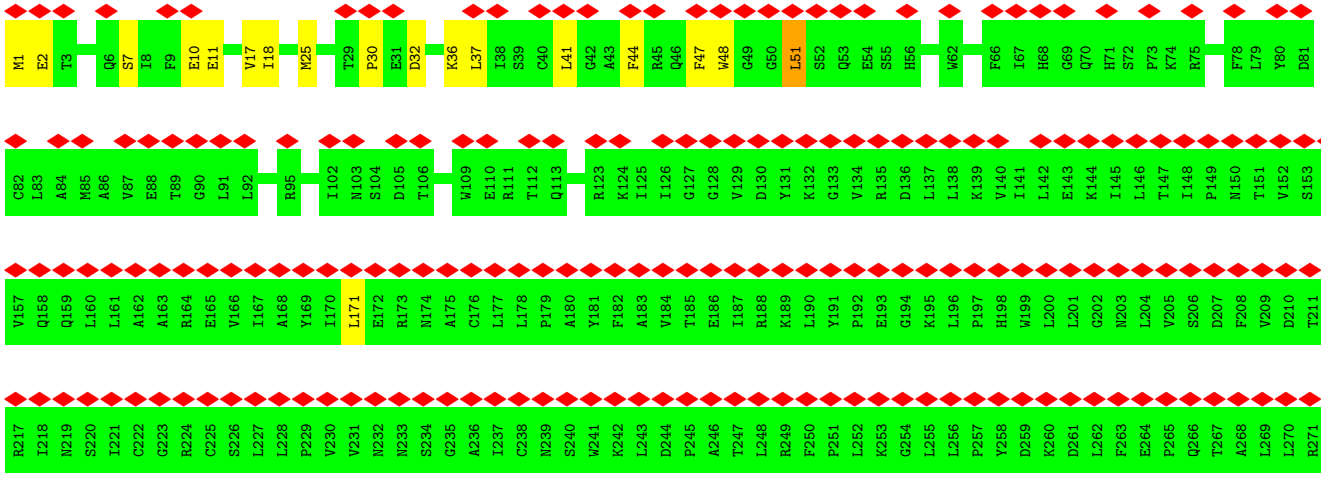


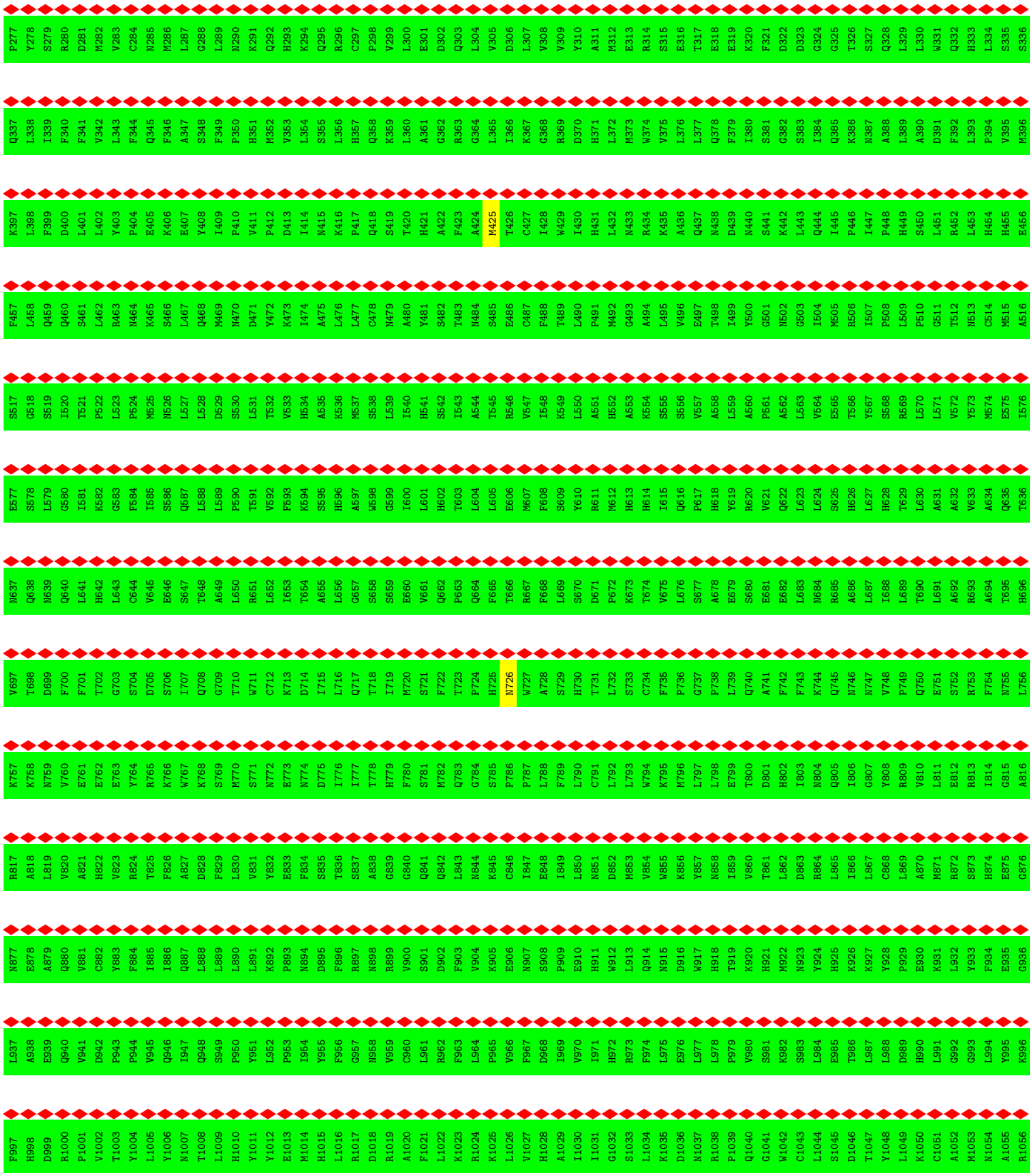


• Molecule 67: Mediator of RNA polymerase II transcription subunit 23

Chain w:






P277 Y278 S279 R280 D281 M282 V283 C284 N285 M286 L287 G288 L289 N290 K291 Q292 H293 K294 Q295 R296 C297 P298 V299 L300 E301 D302 Q303 L304 V305 D306 L307 V308 V309 Y310 A311 M312 E313 R314 S315 E316 T317 E318 E319 K320 F321 D322 D323 G324 G325 T326 S327 Q328 L329 L330 W331 Q332 H333 L334 S335 S336
Q337 L338 I339 F340 F341 V342 L343 F344 Q345 F346 A347 S348 F349 P350 H351 M352 V353 L354 S355 L356 H357 Q358 K359 L360 A361 G362 R363 G364 L365 I366 K367 G368 R369 D370 H371 L372 M373 W374 V375 L376 L377 Q378 F379 I380 S381 G382 S383 I384 Q385 K386 N387 A388 L389 A390 D391 F392 L393 P394 V395 M396
K397 L398 F399 D400 L401 L402 Y403 P404 E405 K406 E407 Y408 I409 P410 V411 P412 D413 I414 N415 K416 P417 Q418 S419 T420 H421 A422 F423 A424 M425 T426 C427 I428 W429 I430 H431 L432 N433 R434 K435 A436 Q437 N438 D439 N440 S441 K442 L443 Q444 I445 P446 I447 P448 H449 S450 L451 R452 L453 H454 H455 E456
F457 L458 Q459 Q460 S461 L462 R463 N464 K465 S466 L467 Q468 M469 N470 D471 Y472 K473 I474 A475 L476 L477 C478 N479 A480 Y481 S482 T483 N484 S485 E486 C487 F488 T489 L490 P491 M492 G493 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 D529 S530 L531 T532 V533 H534 A535 K536 M537 S538 L539 I540 H541 S542 I543 A544 T545 R546 V547 I548 K549 L550 A551 H552 A553 K554 S555 S556 V557 A558 L559 A560 P561 A562 L563 V564 E565 T566 Y567 S568 R569 L570 L571 V572 Y573 M574 E575 I576
E577 S578 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 H614 I615 Q616 P617 H618 Y619 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 I653 T654 A655 L656 G657 S658 S659 E660 V661 Q662 P663 Q664 F665 T666 R667 F668 L669 S670 D671 P672 K673 T674 V675 L676 S677 A678 E679 S680 E681 E682 L683 N684 R685 A686 L687 I688 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 T723 P724 H725 N726 W727 A728 S729 H730 T731 L732 S733 C734 F735 P736 G737 P738 L739 Q740 A741 F742 F743 K744 Q745 N746 N747 V748 P749 Q750 E751 S752 R753 F754 N755 L756
K757 K758 N759 V760 E761 E762 E763 Y764 R765 K766 W767 K768 S769 M770 S771 N772 E773 N774 D775 I776 I777 T778 H779 F780 S781 M782 Q783 G784 S785 P786 P787 L788 F789 L790 C791 L792 L793 W794 K795 M796 L797 L798 E799 T800 D801 H802 I803 N804 Q805 I806 G807 Y808 R809 V810 L811 E812 R813 I814 G815 A816
R817 A818 L819 V820 A821 H822 V823 R824 T825 F826 A827 D828 F829 L830 V831 Y832 E833 F834 S835 T836 S837 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 I866 L867 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 C960 L961 R962 F963 L964 P965 V966 F967 D968 I969 V970 I971 H972 R973 F974 L975 E976 L977 L978 P979 V980 S981 K982 S983 L984 E985 T986 L987 I988 D989 H990 L991 G992 G993 L994 Y995 K996
F997 H998 D999 R1000 P1001 V1002 T1003 Y1004 L1005 Y1006 N1007 T1008 L1009 H1010 Y1011 Y1012 E1013 M1014 H1015 L1016 R1017 D1018 R1019 A1020 F1021 L1022 K1023 R1024 K1025 L1026 V1027 H1028 A1029 I1030 I1031 G1032 S1033 L1034 K1035 D1036 N1037 R1038 P1039 Q1040 G1041 W1042 C1043 L1044 S1045 D1046 T1047 Y1048 L1049 K1050 C1051 A1052 M1053 N1054 A1055 R1056

E1057 E1058 N1059 P1060 W1061 V1062 P1063 D1064 D1065 T1066 Y1067 Y1068 C1069 R1070 L1071 I1072 G1073 R1074 L1075 V1076 D1077 T1078 M1079 A1080 G1081 K1082 S1083 P1084 G1085 P1086 F1087 P1088 N1089 C1090 D1091 W1092 R1093 F1094 N1095 E1096 F1097 P1098 N1099 P1100 A1101 A1102 H1103 A1104 L1105 H1106 V1107 T1108 C1109 V1110 E1111 L1112 M1113 A1114 L1115 A1116

V1117 S1118 G1119 K1120 E1121 V1122 G1123 N1124 A1125 L1126 L1127 N1128 V1129 V1130 L1131 K1132 S1133 Q1134 P1135 L1136 V1137 P1138 R1139 E1140 N1141 I1142 T1143 A1144 W1145 M1146 N1147 A1148 I1149 G1150 L1151 I1152 I1153 T1154 A1155 L1156 P1157 E1158 P1159 Y1160 W1161 I1162 V1163 L1164 H1165 D1166 R1167 I1168 V1169 S1170 V1171 I1172 S1173 S1174 P1175 S1176

L1177 T1178 S1179 E1180 T1181 E1182 W1183 V1184 G1185 Y1186 P1187 F1188 R1189 L1190 F1191 D1192 F1193 T1194 A1195 C1196 H1197 Q1198 S1199 Y1200 S1201 E1202 M1203 S1204 C1205 S1206 Y1207 T1208 L1209 A1210 L1211 A1212 H1213 A1214 V1215 W1216 H1217 H1218 S1219 S1220 I1221 G1222 Q1223 L1224 S1225 L1226 I1227 P1228 K1229 F1230 L1231 T1232 E1233 V1234 L1235 L1236

P1237 I1238 V1239 K1240 T1241 E1242 F1243 Q1244 L1245 L1246 Y1247 V1248 Y1249 H1250 L1251 V1252 G1253 P1254 F1255 L1256 Q1257 R1258 F1259 Q1260 Q1261 E1262 R1263 T1264 R1265 C1266 M1267 I1268 E1269 I1270 G1271 V1272 A1273 F1274 Y1275 D1276 M1277 L1278 L1279 N1280 V1281 D1282 Q1283 C1284 S1285 T1286 H1287 L1288 N1289 Y1290 M1291 D1292 P1293 I1294 C1295 D1296

F1297 L1298 Y1299 H1300 M1301 K1302 Y1303 M1304 F1305 T1306 G1307 D1308 S1309 V1310 K1311 E1312 Q1313 V1314 E1315 K1316 I1317 I1318 C1319 N1320 L1321 K1322 P1323 A1324 L1325 K1326 L1327 R1328 L1329 R1330 F1331 I1332 T1333 H1334 ILE SER LYS MET GLU PRO ALA ALA VAL PRO PRO GLN ALA MET ASN SER GLY SER PRO ALA PRO GLN

SER ASN GLN VAL PRO VAL SER LEU PRO VAL THR GLN

• Molecule 68: Isoform 2 of Mediator of RNA polymerase II transcription subunit 16

Chain p:

MET CYS ASP LEU ARG ARG PRO ALA ALA GLY GLY MET M13 D14 L15 A16 Y17 V18 C19 E20 W21 E22 K23 W24 S25 K26 S27 T28 H29 C30 P31 S32 V33 P34 L35 A36 C37 A38 W39 S40 C41 R42 N43 L44 I45 A46 F47 T48 M49 D50 L51 R52 S53 D54 D55 Q56 D57 L58 T59 R60

M61 I62 H63 I64 L65 D66 T67 E68 H69 P70 W71 D72 L73 H74 S75 I76 P77 S78 E79 H80 H81 E82 A83 I84 T85 C86 L87 E88 W89 D90 Q91 S92 G93 S94 R95 L96 L97 S98 A99 D100 A101 D102 G103 Q104 I105 K106 C107 W108 S109 M110 A111 D112 H113 L114 A115 N116 S117 W118 E119 S120

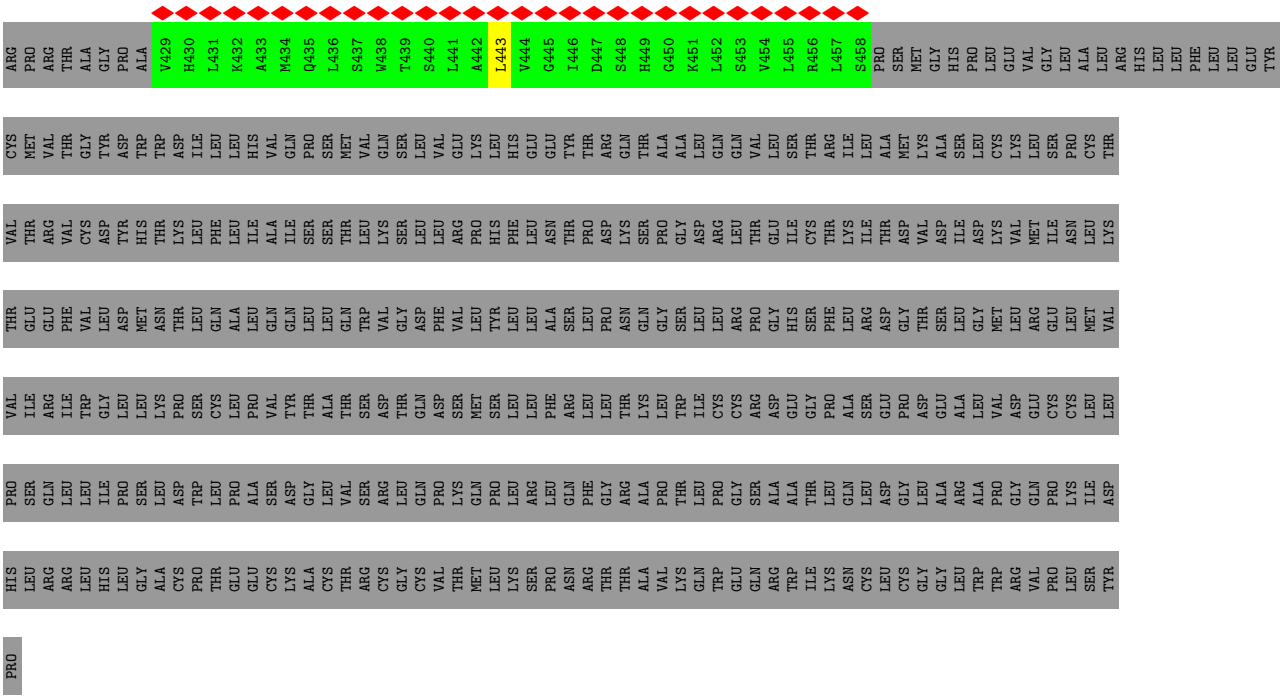
S121 V122 G123 S124 L125 V126 E127 G128 D129 P130 I131 V132 A133 L134 S135 W136 L137 H138 N139 G140 V141 K142 L143 A144 L145 H146 V147 E148 K149 S150 G151 A152 S153 S154 F155 G156 E157 K158 F159 S160 R161 V162 K163 F164 S165 P166 S167 L168 T169 L170 F171 G172 G173 K174 P175 M176 E177 G178 W179 I180

A181 V182 T183 V184 S185 G186 L187 V188 T189 V190 S191 L192 L193 K194 P195 S196 G197 Q198 V199 L200 T201 S202 T203 E204 S205 L206 C207 R208 L209 R210 G211 R212 V213 A214 L215 A216 D217 I218 A219 P220 T221 G222 G223 G224 N225 I226 V227 V228 A229 T230 A231 D232 G233 S234 S235 A236 S237 P238 V239 Q240

F241 Y242 K243 V244 C245 V246 S247 V248 V249 S250 E251 K252 C253 R254 I255 D256 T257 E258 I259 L260 P261 S262 L263 F264 M265 R266 C267 T268 T269 D270 L271 N272 R273 K274 D275 K276 F277 P278 A279 I280 T281 H282 L283 K284 F285 L286 A287 R288 D289 M290 S291 E292 Q293 V294 L295 L296 C297 A298 S299 S300

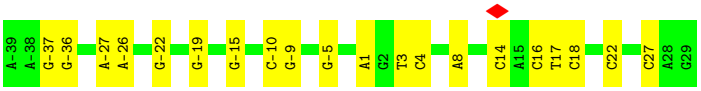
Q301 T302 S303 S304 I305 V306 E307 C308 W309 S310 L311 R312 K313 E314 GLY LEU PRO VAL ASN ASN ILE PHE GLN GLN ILE SER PRO VAL VAL GLY ASP LYS GLN PRO T335 I336 L337 K338 W339 R340 I341 L342 S343 A344 T345 N346 D347 L348 D349 R350 V351 S352 A353 V354 A355 L356 P357 K358 L359 P360

I361 S362 L363 T364 N365 T366 D367 L368 K369 V370 A371 S372 D373 T374 Q375 F376 Y377 P378 G379 L380 G381 L382 A383 L384 A385 F386 H387 D388 G389 S390 V391 H392 I393 V394 H395 R396 L397 S398 L399 Q400 T401 M402 A403 V404 F405 Y406 S407 S408 ALA ALA PRO ARG PRO VAL ASP GLU PRO ALA MET LYS



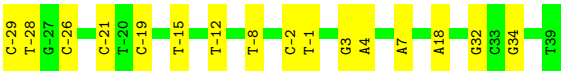
- Molecule 69: DNA (69-MER)

Chain X:



- Molecule 70: DNA(69-MER)

Chain Y:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	48654	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	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	8.884	Depositor
Minimum map value	-4.573	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.113	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	674.56, 674.56, 674.56	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3175, 1.3175, 1.3175	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SF4, 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	0.61	0/2288	0.81	4/3101 (0.1%)
2	8	0.66	0/2437	0.97	0/3306
3	9	0.73	0/2356	0.97	1/3185 (0.0%)
4	DO	0.56	0/781	0.75	0/1061
5	DP	0.62	0/1438	0.73	0/1935
6	DQ	0.54	0/1013	0.64	0/1366
7	BA	0.46	0/1987	0.75	2/2684 (0.1%)
8	FA	0.47	0/1130	0.57	0/1528
9	FB	0.55	0/1817	0.66	0/2445
10	PA	0.73	6/11888 (0.1%)	1.00	13/16066 (0.1%)
11	PB	0.77	1/9243 (0.0%)	1.01	15/12475 (0.1%)
12	PC	0.86	0/2102	1.19	7/2857 (0.2%)
13	PD	0.63	0/1036	0.97	0/1397
14	PE	0.58	0/1751	0.90	0/2366
15	PF	0.83	1/645 (0.2%)	1.07	1/871 (0.1%)
16	PG	0.65	0/1365	1.06	4/1853 (0.2%)
17	PH	0.67	0/1207	1.05	1/1628 (0.1%)
18	PI	0.62	0/948	1.06	1/1284 (0.1%)
19	PJ	0.86	0/516	1.19	0/696
20	PK	0.81	0/956	1.07	3/1294 (0.2%)
21	PL	0.70	0/377	0.95	0/500
22	DA	0.50	0/5037	0.65	2/6794 (0.0%)
23	DB	0.47	0/7993	0.61	0/10836
24	DD	0.58	0/1343	0.70	0/1795
24	Dd	0.29	0/1321	0.49	0/1772
25	DE	0.43	0/4469	0.58	0/6050
25	De	0.34	0/4433	0.55	0/6004
26	DF	0.55	0/3167	0.71	0/4303
26	Df	0.44	0/3140	0.64	0/4268
27	DG	0.53	0/1199	0.63	0/1612
28	DH	0.46	0/1673	0.60	0/2285
29	DI	0.46	0/981	0.57	0/1332

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
29	Di	0.31	0/989	0.46	0/1343
30	DJ	0.48	0/736	0.60	1/998 (0.1%)
30	Dj	0.31	0/775	0.52	0/1049
31	DL	0.43	0/622	0.69	3/841 (0.4%)
31	Dl	0.30	0/888	0.56	3/1194 (0.3%)
32	Dc	0.40	0/1035	0.54	0/1406
33	Dk	0.31	0/799	0.48	0/1070
34	Dm	0.32	0/733	0.52	0/977
35	EA	0.61	0/1499	0.74	0/2012
36	EB	0.64	0/1428	0.64	0/1917
37	1	0.36	0/3502	0.65	0/4731
38	2	0.42	0/3094	0.67	0/4188
39	3	0.44	0/2353	0.74	0/3187
40	4	0.49	0/3729	0.73	0/5053
41	5	0.50	0/528	0.70	0/713
42	6	0.42	0/5365	0.68	0/7247
43	7	0.46	0/5984	0.69	0/8104
44	c	0.46	0/2146	0.62	0/2899
45	e	0.26	0/840	0.36	0/1128
46	b	0.51	0/911	0.62	0/1229
47	l	0.26	0/1048	0.41	0/1405
48	m	0.26	0/1010	0.37	0/1359
49	a	0.62	0/3660	0.75	1/4971 (0.0%)
50	d	0.62	0/1281	0.65	0/1718
51	f	0.57	0/1359	0.69	1/1845 (0.1%)
52	g	0.58	0/1411	0.81	0/1901
53	h	0.62	0/1485	0.72	1/2008 (0.0%)
54	i	0.67	0/612	0.71	0/815
55	j	0.41	0/1016	0.64	5/1363 (0.4%)
56	k	0.66	0/885	0.60	0/1190
57	n	0.34	0/7371	0.55	17/10037 (0.2%)
58	o	0.36	0/1256	0.62	0/1724
59	q	0.48	2/4351 (0.0%)	0.55	4/5886 (0.1%)
60	r	0.60	0/1663	0.79	1/2241 (0.0%)
61	s	0.59	0/510	0.77	5/694 (0.7%)
62	t	0.71	1/1530 (0.1%)	0.89	0/2066
63	u	0.38	0/797	0.52	0/1082
64	v	0.66	0/1092	0.73	0/1468
65	z	0.64	0/781	0.81	0/1067
66	x	0.59	0/7179	0.63	3/9712 (0.0%)
67	w	0.57	0/11053	0.62	2/15018 (0.0%)
68	p	0.71	0/3191	0.73	4/4333 (0.1%)
69	X	1.00	16/1607 (1.0%)	1.16	8/2481 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
70	Y	1.00	15/1565 (1.0%)	1.10	2/2410 (0.1%)
All	All	0.57	42/177706 (0.0%)	0.75	115/241029 (0.0%)

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	q	264	GLN	C-N	7.96	1.52	1.34
69	X	-26	DA	C1'-N9	-7.92	1.36	1.47
69	X	-27	DA	C1'-N9	-7.66	1.36	1.47
69	X	-19	DG	C1'-N9	-7.58	1.36	1.47
69	X	-36	DG	C1'-N9	-7.06	1.37	1.47
69	X	-5	DG	C1'-N9	-6.85	1.37	1.47
70	Y	34	DG	C1'-N9	-6.69	1.37	1.47
70	Y	4	DA	C1'-N9	-6.68	1.37	1.47
70	Y	7	DA	C1'-N9	-6.68	1.38	1.47
70	Y	32	DG	C1'-N9	-6.66	1.38	1.47
69	X	-22	DG	C1'-N9	-6.66	1.38	1.47
69	X	-15	DG	C1'-N9	-6.64	1.38	1.47
69	X	-37	DG	C1'-N9	-6.54	1.38	1.47
70	Y	18	DA	C1'-N9	-6.48	1.38	1.47
70	Y	-29	DC	C1'-N1	6.42	1.57	1.49
62	t	119	TYR	C-N	6.40	1.48	1.34
69	X	8	DA	C1'-N9	-6.35	1.38	1.47
69	X	1	DA	C1'-N9	-6.22	1.38	1.47
70	Y	-19	DC	C1'-N1	6.15	1.57	1.49
69	X	22	DC	C1'-N1	6.07	1.57	1.49
70	Y	-26	DC	C1'-N1	6.03	1.57	1.49
70	Y	3	DG	O3'-P	5.72	1.68	1.61
10	PA	593	SER	CA-CB	-5.65	1.44	1.52
59	q	452	ALA	C-N	5.61	1.47	1.34
69	X	18	DC	C1'-N1	5.36	1.56	1.49
10	PA	1387	SER	CA-CB	-5.35	1.45	1.52
69	X	17	DT	C1'-N1	5.34	1.56	1.49
10	PA	622	SER	CA-CB	-5.31	1.45	1.52
70	Y	-12	DT	C1'-N1	5.31	1.56	1.49
70	Y	-1	DT	C1'-N1	5.21	1.56	1.49
70	Y	-8	DT	C1'-N1	5.21	1.56	1.49
70	Y	-15	DT	C1'-N1	5.15	1.55	1.49
69	X	27	DC	C1'-N1	5.14	1.55	1.49
69	X	16	DC	C1'-N1	5.12	1.55	1.49
69	X	14	DC	C1'-N1	5.12	1.55	1.49
10	PA	782	SER	CA-CB	-5.11	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
70	Y	-28	DT	C1'-N1	5.08	1.55	1.49
70	Y	-21	DC	C1'-N1	5.06	1.55	1.49
10	PA	508	SER	CA-CB	-5.05	1.45	1.52
15	PF	114	SER	CA-CB	-5.02	1.45	1.52
11	PB	797	ASN	C-O	-5.00	1.13	1.23
10	PA	456	VAL	C-O	-5.00	1.13	1.23

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
69	X	3	DT	P-O3'-C3'	-13.62	103.35	119.70
69	X	-10	DC	O5'-P-OP2	-9.57	97.08	105.70
70	Y	-2	DC	P-O3'-C3'	8.34	129.71	119.70
57	n	1355	PRO	N-CA-CB	6.88	111.55	103.30
67	w	47	PHE	CB-CA-C	6.87	124.14	110.40
57	n	1343	PRO	N-CA-CB	6.83	111.50	103.30
69	X	3	DT	O3'-P-O5'	-6.79	91.09	104.00
69	X	4	DC	P-O3'-C3'	6.79	127.85	119.70
57	n	1351	PRO	N-CA-CB	6.64	111.27	103.30
57	n	1237	PRO	N-CA-CB	6.62	111.24	103.30
57	n	1196	PRO	N-CA-CB	6.42	111.00	103.30
57	n	1255	PRO	N-CA-CB	6.22	110.77	103.30
57	n	1326	PRO	N-CA-CB	6.17	110.70	103.30
69	X	3	DT	OP2-P-O3'	6.17	118.77	105.20
69	X	-9	DG	C3'-C2'-C1'	-6.14	95.13	102.50
57	n	1267	PRO	N-CA-CB	6.11	110.63	103.30
57	n	1347	PRO	N-CA-CB	6.06	110.57	103.30
68	p	97	LEU	CB-CG-CD1	-6.03	100.74	111.00
11	PB	736	TYR	CA-CB-CG	5.98	124.75	113.40
67	w	30	PRO	N-CA-CB	5.96	110.45	103.30
57	n	1192	PRO	N-CA-CB	5.95	110.44	103.30
57	n	1352	PRO	N-CA-CB	5.94	110.42	103.30
57	n	1344	PRO	N-CA-CB	5.93	110.42	103.30
16	PG	49	THR	CB-CA-C	5.91	127.57	111.60
10	PA	619	LYS	CB-CA-C	-5.91	98.59	110.40
18	PI	81	THR	CB-CA-C	-5.88	95.72	111.60
11	PB	1073	GLN	CB-CA-C	5.83	122.07	110.40
61	s	135	PRO	N-CA-CB	5.81	110.28	103.30
17	PH	124	ARG	CB-CA-C	-5.75	98.91	110.40
10	PA	84	HIS	CB-CA-C	5.74	121.88	110.40
11	PB	781	ALA	N-CA-CB	-5.73	102.08	110.10
20	PK	36	ASN	CB-CA-C	-5.73	98.94	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	PB	941	GLN	CB-CA-C	-5.72	98.95	110.40
57	n	1206	PRO	N-CA-CB	5.71	110.15	103.30
61	s	134	PRO	N-CA-CB	5.68	110.12	103.30
11	PB	1132	THR	CB-CA-C	-5.64	96.37	111.60
59	q	410	PRO	N-CA-CB	5.64	110.07	103.30
69	X	-9	DG	C1'-O4'-C4'	-5.64	104.46	110.10
59	q	395	PRO	N-CA-CB	5.62	110.05	103.30
10	PA	113	PHE	CB-CA-C	5.62	121.64	110.40
11	PB	749	HIS	CB-CA-C	-5.62	99.16	110.40
57	n	1309	PRO	N-CA-CB	5.61	110.04	103.30
57	n	1348	PRO	N-CA-CB	5.60	110.02	103.30
68	p	443	LEU	CA-CB-CG	5.60	128.18	115.30
12	PC	67	ARG	CB-CA-C	5.59	121.57	110.40
1	0	220	PRO	N-CA-CB	5.57	109.98	103.30
61	s	113	PRO	N-CA-CB	5.57	109.98	103.30
11	PB	1105	GLU	CB-CA-C	-5.55	99.29	110.40
61	s	119	PRO	N-CA-CB	5.55	109.96	103.30
12	PC	184	PHE	CB-CA-C	5.54	121.48	110.40
57	n	74	PRO	N-CA-CB	5.52	109.93	103.30
10	PA	495	ASP	N-CA-C	-5.51	96.11	111.00
59	q	393	PRO	N-CA-CB	5.51	109.92	103.30
11	PB	1108	PHE	CB-CA-C	-5.50	99.40	110.40
16	PG	125	PRO	N-CA-C	-5.48	97.86	112.10
16	PG	15	PRO	N-CA-C	-5.44	97.96	112.10
10	PA	602	CYS	CB-CA-C	-5.43	99.54	110.40
22	DA	498	PRO	N-CA-CB	5.43	109.81	103.30
1	0	237	PRO	N-CA-CB	5.42	109.81	103.30
11	PB	596	ILE	CB-CA-C	-5.42	100.76	111.60
49	a	32	PRO	N-CA-CB	5.42	109.80	103.30
1	0	215	PRO	N-CA-CB	5.40	109.78	103.30
7	BA	15	CYS	CB-CA-C	-5.39	99.62	110.40
7	BA	16	PRO	N-CA-CB	-5.39	96.67	102.60
53	h	168	PRO	N-CA-CB	5.37	109.75	103.30
59	q	399	PRO	N-CA-CB	5.37	109.75	103.30
10	PA	631	GLU	CB-CA-C	-5.37	99.66	110.40
10	PA	686	THR	CB-CA-C	-5.37	97.11	111.60
1	0	217	PRO	N-CA-CB	5.36	109.73	103.30
70	Y	3	DG	P-O3'-C3'	5.35	126.12	119.70
12	PC	265	HIS	CB-CA-C	5.34	121.09	110.40
22	DA	1169	ARG	CG-CD-NE	5.31	122.96	111.80
66	x	783	LEU	CA-CB-CG	5.31	127.52	115.30
66	x	359	CYS	CA-CB-SG	5.31	123.55	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	PA	428	ASP	CB-CA-C	-5.31	99.79	110.40
31	DL	90	ASP	CB-CG-OD2	5.30	123.07	118.30
55	j	72	ASP	CB-CG-OD2	5.29	123.06	118.30
10	PA	524	MET	CB-CG-SD	-5.27	96.59	112.40
30	DJ	118	ASP	CB-CG-OD2	5.27	123.04	118.30
31	DL	79	ASP	CB-CG-OD2	5.26	123.04	118.30
12	PC	51	GLN	CB-CA-C	-5.25	99.89	110.40
31	Dl	79	ASP	CB-CG-OD2	5.25	123.03	118.30
31	Dl	90	ASP	CB-CG-OD2	5.25	123.03	118.30
55	j	120	ASP	CB-CG-OD2	5.24	123.02	118.30
55	j	60	ASP	CB-CG-OD2	5.24	123.02	118.30
31	DL	89	ASP	CB-CG-OD2	5.23	123.01	118.30
68	p	14	ASP	CB-CG-OD2	5.23	123.01	118.30
10	PA	659	GLU	CB-CA-C	-5.22	99.96	110.40
55	j	28	ASP	CB-CG-OD2	5.22	122.99	118.30
10	PA	765	ASN	CB-CA-C	5.20	120.81	110.40
11	PB	765	GLU	CB-CA-C	-5.20	99.99	110.40
68	p	275	ASP	CB-CG-OD2	5.20	122.98	118.30
3	9	60	TYR	CB-CA-C	5.20	120.80	110.40
15	PF	109	TYR	CB-CA-C	-5.18	100.03	110.40
55	j	100	ASP	CB-CG-OD2	5.17	122.96	118.30
31	Dl	89	ASP	CB-CG-OD2	5.17	122.95	118.30
61	s	158	PRO	N-CA-CB	5.17	109.50	103.30
16	PG	72	TYR	CB-CA-C	-5.16	100.07	110.40
11	PB	977	THR	CB-CA-C	-5.16	97.67	111.60
51	f	31	ASP	CB-CG-OD2	5.15	122.94	118.30
11	PB	1045	PRO	N-CA-CB	-5.15	96.93	102.60
69	X	-10	DC	O5'-P-OP1	5.14	116.87	110.70
11	PB	504	THR	CB-CA-C	-5.14	97.73	111.60
10	PA	757	GLN	CB-CA-C	5.13	120.66	110.40
11	PB	1066	PRO	N-CA-CB	-5.13	96.96	102.60
57	n	676	ASP	CB-CG-OD2	5.12	122.91	118.30
12	PC	115	VAL	N-CA-C	-5.09	97.25	111.00
60	r	4	PRO	N-CA-C	-5.08	98.89	112.10
20	PK	62	LYS	N-CA-CB	5.08	119.74	110.60
11	PB	1018	TYR	CB-CA-C	5.07	120.54	110.40
12	PC	183	ALA	N-CA-CB	-5.06	103.01	110.10
20	PK	59	ALA	N-CA-CB	-5.04	103.04	110.10
10	PA	465	HIS	CB-CA-C	5.04	120.47	110.40
66	x	355	CYS	CA-CB-SG	5.03	123.05	114.00
12	PC	229	PHE	N-CA-CB	-5.00	101.59	110.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	0	304/309 (98%)	242 (80%)	51 (17%)	11 (4%)	3 24
2	8	297/346 (86%)	266 (90%)	20 (7%)	11 (4%)	2 23
3	9	285/323 (88%)	268 (94%)	14 (5%)	3 (1%)	12 46
4	DO	95/109 (87%)	83 (87%)	11 (12%)	1 (1%)	12 46
5	DP	175/339 (52%)	166 (95%)	7 (4%)	2 (1%)	12 46
6	DQ	118/307 (38%)	105 (89%)	8 (7%)	5 (4%)	2 21
7	BA	251/316 (79%)	237 (94%)	10 (4%)	4 (2%)	8 39
8	FA	130/517 (25%)	117 (90%)	12 (9%)	1 (1%)	16 53
9	FB	218/249 (88%)	200 (92%)	13 (6%)	5 (2%)	5 32
10	PA	1461/1970 (74%)	1363 (93%)	81 (6%)	17 (1%)	11 44
11	PB	1128/1174 (96%)	1029 (91%)	83 (7%)	16 (1%)	9 41
12	PC	253/275 (92%)	229 (90%)	18 (7%)	6 (2%)	5 31
13	PD	127/142 (89%)	123 (97%)	3 (2%)	1 (1%)	16 53
14	PE	207/210 (99%)	201 (97%)	5 (2%)	1 (0%)	25 62
15	PF	77/127 (61%)	72 (94%)	3 (4%)	2 (3%)	4 29
16	PG	169/172 (98%)	159 (94%)	8 (5%)	2 (1%)	11 44
17	PH	146/150 (97%)	129 (88%)	16 (11%)	1 (1%)	19 56
18	PI	112/125 (90%)	102 (91%)	8 (7%)	2 (2%)	7 36
19	PJ	62/67 (92%)	59 (95%)	2 (3%)	1 (2%)	8 39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
20	PK	115/117 (98%)	106 (92%)	8 (7%)	1 (1%)	14 50
21	PL	42/58 (72%)	38 (90%)	3 (7%)	1 (2%)	5 31
22	DA	582/1872 (31%)	539 (93%)	33 (6%)	10 (2%)	7 37
23	DB	959/1199 (80%)	912 (95%)	47 (5%)	0	100 100
24	DD	153/1085 (14%)	144 (94%)	6 (4%)	3 (2%)	6 34
24	Dd	154/1085 (14%)	150 (97%)	4 (3%)	0	100 100
25	DE	540/800 (68%)	500 (93%)	36 (7%)	4 (1%)	19 56
25	De	531/800 (66%)	484 (91%)	47 (9%)	0	100 100
26	DF	404/677 (60%)	369 (91%)	29 (7%)	6 (2%)	8 40
26	Df	399/677 (59%)	371 (93%)	27 (7%)	1 (0%)	37 71
27	DG	139/349 (40%)	135 (97%)	4 (3%)	0	100 100
28	DH	207/310 (67%)	183 (88%)	20 (10%)	4 (2%)	6 35
29	DI	118/264 (45%)	103 (87%)	14 (12%)	1 (1%)	16 53
29	Di	119/264 (45%)	115 (97%)	4 (3%)	0	100 100
30	DJ	86/218 (39%)	82 (95%)	4 (5%)	0	100 100
30	Dj	91/218 (42%)	89 (98%)	2 (2%)	0	100 100
31	DL	73/161 (45%)	65 (89%)	5 (7%)	3 (4%)	2 21
31	Dl	105/161 (65%)	101 (96%)	4 (4%)	0	100 100
32	Dc	125/929 (14%)	116 (93%)	9 (7%)	0	100 100
33	Dk	96/211 (46%)	91 (95%)	5 (5%)	0	100 100
34	Dm	85/124 (68%)	79 (93%)	6 (7%)	0	100 100
35	EA	175/439 (40%)	160 (91%)	12 (7%)	3 (2%)	7 37
36	EB	170/291 (58%)	160 (94%)	6 (4%)	4 (2%)	5 31
37	1	431/548 (79%)	350 (81%)	73 (17%)	8 (2%)	6 35
38	2	383/395 (97%)	311 (81%)	72 (19%)	0	100 100
39	3	293/308 (95%)	238 (81%)	51 (17%)	4 (1%)	9 41
40	4	455/462 (98%)	374 (82%)	70 (15%)	11 (2%)	5 31
41	5	64/71 (90%)	57 (89%)	6 (9%)	1 (2%)	8 39
42	6	648/782 (83%)	514 (79%)	123 (19%)	11 (2%)	7 37
43	7	730/760 (96%)	600 (82%)	112 (15%)	18 (2%)	4 30
44	c	255/311 (82%)	235 (92%)	17 (7%)	3 (1%)	11 44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
45	e	98/178 (55%)	92 (94%)	4 (4%)	2 (2%)	6 34
46	b	111/200 (56%)	109 (98%)	1 (1%)	1 (1%)	14 50
47	l	120/178 (67%)	115 (96%)	5 (4%)	0	100 100
48	m	110/131 (84%)	106 (96%)	4 (4%)	0	100 100
49	a	457/1581 (29%)	421 (92%)	31 (7%)	5 (1%)	12 46
50	d	154/270 (57%)	143 (93%)	9 (6%)	2 (1%)	10 43
51	f	163/246 (66%)	145 (89%)	13 (8%)	5 (3%)	3 26
52	g	164/233 (70%)	150 (92%)	11 (7%)	3 (2%)	7 36
53	h	188/268 (70%)	163 (87%)	15 (8%)	10 (5%)	1 18
54	i	69/146 (47%)	65 (94%)	2 (3%)	2 (3%)	3 27
55	j	120/135 (89%)	107 (89%)	9 (8%)	4 (3%)	3 25
56	k	110/117 (94%)	98 (89%)	10 (9%)	2 (2%)	7 36
57	n	980/1454 (67%)	876 (89%)	83 (8%)	21 (2%)	5 33
58	o	152/788 (19%)	138 (91%)	13 (9%)	1 (1%)	19 56
59	q	543/651 (83%)	476 (88%)	53 (10%)	14 (3%)	4 29
60	r	204/208 (98%)	190 (93%)	10 (5%)	4 (2%)	6 34
61	s	75/244 (31%)	64 (85%)	7 (9%)	4 (5%)	1 18
62	t	189/212 (89%)	168 (89%)	17 (9%)	4 (2%)	5 33
63	u	103/144 (72%)	99 (96%)	0	4 (4%)	2 22
64	v	132/200 (66%)	117 (89%)	9 (7%)	6 (4%)	2 20
65	z	93/600 (16%)	84 (90%)	6 (6%)	3 (3%)	3 26
66	x	876/989 (89%)	824 (94%)	50 (6%)	2 (0%)	44 76
67	w	1332/1368 (97%)	1266 (95%)	62 (5%)	4 (0%)	37 71
68	p	400/841 (48%)	366 (92%)	33 (8%)	1 (0%)	37 71
All	All	21285/34555 (62%)	19303 (91%)	1689 (8%)	293 (1%)	12 41

All (293) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	214	LYS
1	0	220	PRO
1	0	237	PRO
10	PA	539	GLN
10	PA	980	PRO

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Mol	Chain	Res	Type
10	PA	1666	PRO
11	PB	630	LYS
12	PC	228	ARG
19	PJ	28	GLU
20	PK	39	ASP
22	DA	466	SER
22	DA	498	PRO
22	DA	1000	LEU
22	DA	1034	THR
24	DD	876	ALA
25	DE	452	ARG
25	DE	509	GLN
26	DF	68	THR
26	DF	69	SER
26	DF	350	ASN
26	DF	442	PRO
28	DH	141	PRO
31	DL	73	ASN
35	EA	123	ASN
36	EB	172	GLU
37	1	191	ASP
40	4	340	ASN
40	4	402	ARG
42	6	267	THR
43	7	19	PRO
43	7	64	PRO
43	7	153	PRO
43	7	671	LYS
44	c	283	ARG
44	c	293	PRO
44	c	294	PRO
50	d	187	LEU
51	f	145	TYR
51	f	148	HIS
53	h	100	PHE
53	h	130	ARG
53	h	167	ARG
53	h	168	PRO
55	j	29	PHE
55	j	61	ILE
57	n	150	PRO
57	n	154	ILE

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Mol	Chain	Res	Type
57	n	363	GLU
57	n	1196	PRO
57	n	1255	PRO
57	n	1266	THR
57	n	1326	PRO
59	q	131	SER
59	q	288	SER
59	q	393	PRO
59	q	398	ALA
59	q	399	PRO
62	t	173	PRO
63	u	81	SER
64	v	91	PHE
66	x	566	GLU
67	w	51	LEU
1	0	233	ILE
1	0	234	SER
2	8	96	THR
2	8	192	VAL
2	8	236	GLN
2	8	239	ASP
2	8	310	PRO
6	DQ	57	ASP
6	DQ	320	VAL
10	PA	538	VAL
10	PA	1645	PRO
10	PA	1663	SER
11	PB	226	GLU
11	PB	310	VAL
11	PB	673	VAL
11	PB	806	PHE
12	PC	41	GLU
13	PD	75	LYS
14	PE	201	GLY
15	PF	76	CYS
16	PG	16	ARG
22	DA	495	LEU
22	DA	510	ILE
24	DD	893	GLU
24	DD	898	VAL
28	DH	129	VAL
29	DI	83	PHE

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Mol	Chain	Res	Type
31	DL	111	LEU
31	DL	114	LYS
36	EB	134	ASP
37	1	163	ASP
37	1	187	ASN
37	1	192	ILE
37	1	201	PRO
37	1	336	ASP
37	1	418	LEU
40	4	301	VAL
42	6	92	VAL
43	7	15	ASP
43	7	148	HIS
43	7	704	ALA
43	7	739	LEU
45	e	146	ILE
49	a	164	PRO
49	a	334	PRO
49	a	430	LEU
53	h	37	TYR
53	h	131	ILE
54	i	108	HIS
54	i	138	LEU
55	j	78	GLN
57	n	169	LEU
57	n	254	VAL
57	n	920	ASN
57	n	957	PRO
57	n	1351	PRO
59	q	395	PRO
59	q	419	ASN
62	t	99	LYS
64	v	40	ALA
64	v	41	LYS
64	v	42	ILE
64	v	139	SER
67	w	32	ASP
67	w	1196	CYS
1	0	289	SER
2	8	106	SER
2	8	277	LEU
3	9	237	MET

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Mol	Chain	Res	Type
5	DP	207	PRO
6	DQ	319	ASP
9	FB	136	SER
9	FB	172	ASP
10	PA	921	ARG
10	PA	1134	PRO
10	PA	1206	ARG
10	PA	1486	ILE
11	PB	308	ALA
11	PB	973	PRO
12	PC	185	GLU
16	PG	80	PHE
22	DA	1037	ALA
36	EB	212	VAL
37	1	148	ASN
39	3	244	PRO
40	4	242	PHE
40	4	339	PRO
40	4	411	GLN
41	5	6	LYS
42	6	289	TYR
42	6	397	LYS
49	a	487	LEU
50	d	170	GLY
52	g	39	LYS
52	g	41	SER
53	h	159	ARG
55	j	60	ASP
57	n	1206	PRO
58	o	709	LYS
59	q	91	SER
59	q	420	SER
59	q	458	PRO
60	r	156	ASN
61	s	77	LEU
61	s	158	PRO
64	v	38	LYS
66	x	564	SER
67	w	1203	MET
68	p	249	VAL
1	0	198	LEU
2	8	264	ALA

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Mol	Chain	Res	Type
3	9	286	ALA
4	DO	84	VAL
7	BA	28	ARG
7	BA	46	ILE
7	BA	47	ASP
9	FB	38	GLY
9	FB	140	ARG
10	PA	195	GLY
10	PA	270	ALA
10	PA	300	ALA
10	PA	622	SER
11	PB	19	PRO
11	PB	730	LYS
12	PC	92	GLU
22	DA	1036	GLN
25	DE	482	SER
26	DF	321	PRO
35	EA	54	PHE
35	EA	56	ARG
36	EB	225	VAL
39	3	235	GLN
39	3	248	HIS
40	4	241	SER
40	4	384	PRO
40	4	413	LEU
42	6	114	HIS
42	6	266	GLN
43	7	66	GLU
43	7	113	LYS
43	7	487	ARG
43	7	670	GLY
45	e	147	ASN
46	b	100	GLN
49	a	208	VAL
57	n	165	SER
57	n	265	LEU
57	n	1355	PRO
59	q	127	LEU
59	q	134	ALA
60	r	113	ASN
61	s	155	HIS
62	t	172	ALA

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Mol	Chain	Res	Type
65	z	533	PRO
1	0	89	PHE
1	0	225	THR
1	0	265	MET
3	9	16	GLU
8	FA	24	LYS
10	PA	821	GLY
10	PA	884	ASN
11	PB	328	PRO
11	PB	428	ASP
11	PB	978	ILE
17	PH	69	THR
18	PI	53	ILE
22	DA	1038	ARG
26	DF	440	PRO
28	DH	138	GLN
40	4	304	PRO
42	6	418	LYS
42	6	434	GLU
43	7	111	SER
43	7	172	ALA
43	7	740	SER
51	f	53	GLN
51	f	55	LEU
51	f	143	LYS
52	g	74	HIS
56	k	79	HIS
56	k	81	GLY
57	n	264	ALA
57	n	524	ASN
57	n	1343	PRO
61	s	153	ARG
62	t	129	VAL
63	u	82	THR
63	u	83	ALA
65	z	540	LEU
2	8	82	GLY
2	8	212	PHE
5	DP	298	PRO
6	DQ	312	GLU
7	BA	19	PRO
11	PB	1079	SER

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Mol	Chain	Res	Type
12	PC	60	HIS
22	DA	1040	GLY
28	DH	137	GLY
26	Df	411	VAL
39	3	69	PHE
42	6	181	HIS
42	6	417	THR
43	7	190	CYS
53	h	187	PHE
57	n	164	GLY
59	q	89	GLN
59	q	647	SER
25	DE	472	GLY
40	4	138	PRO
60	r	94	GLY
60	r	153	VAL
65	z	537	PRO
9	FB	173	GLY
11	PB	779	ILE
53	h	188	GLY
57	n	528	HIS
63	u	77	PRO
1	0	193	PRO
2	8	186	GLY
6	DQ	313	PRO
10	PA	1648	PRO
21	PL	34	ILE
43	7	204	VAL
53	h	99	VAL
15	PF	113	GLY
42	6	109	ARG
43	7	320	PRO
11	PB	330	VAL
11	PB	858	VAL
12	PC	94	CYS
18	PI	26	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	209/283 (74%)	172 (82%)	37 (18%)	1 10
2	8	259/299 (87%)	190 (73%)	69 (27%)	0 3
3	9	252/296 (85%)	177 (70%)	75 (30%)	0 2
4	DO	84/98 (86%)	70 (83%)	14 (17%)	2 11
5	DP	153/293 (52%)	145 (95%)	8 (5%)	19 43
6	DQ	111/269 (41%)	97 (87%)	14 (13%)	3 18
7	BA	214/268 (80%)	199 (93%)	15 (7%)	12 35
8	FA	117/448 (26%)	110 (94%)	7 (6%)	16 39
9	FB	196/218 (90%)	163 (83%)	33 (17%)	1 11
10	PA	1305/1748 (75%)	1060 (81%)	245 (19%)	1 8
11	PB	993/1027 (97%)	817 (82%)	176 (18%)	1 10
12	PC	234/252 (93%)	196 (84%)	38 (16%)	2 12
13	PD	108/126 (86%)	86 (80%)	22 (20%)	1 6
14	PE	191/192 (100%)	157 (82%)	34 (18%)	1 10
15	PF	69/111 (62%)	55 (80%)	14 (20%)	1 6
16	PG	147/153 (96%)	113 (77%)	34 (23%)	0 4
17	PH	129/131 (98%)	108 (84%)	21 (16%)	2 12
18	PI	103/112 (92%)	80 (78%)	23 (22%)	1 5
19	PJ	53/56 (95%)	43 (81%)	10 (19%)	1 8
20	PK	106/106 (100%)	88 (83%)	18 (17%)	1 11
21	PL	41/55 (74%)	29 (71%)	12 (29%)	0 2
22	DA	532/1665 (32%)	486 (91%)	46 (9%)	8 29
23	DB	876/1083 (81%)	855 (98%)	21 (2%)	44 63
24	DD	144/815 (18%)	128 (89%)	16 (11%)	5 20
24	Dd	146/815 (18%)	146 (100%)	0	100 100
25	DE	478/657 (73%)	461 (96%)	17 (4%)	30 53
25	De	475/657 (72%)	473 (100%)	2 (0%)	89 91
26	DF	324/574 (56%)	262 (81%)	62 (19%)	1 8
26	Df	322/574 (56%)	301 (94%)	21 (6%)	14 37
27	DG	133/322 (41%)	124 (93%)	9 (7%)	13 36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
28	DH	181/270 (67%)	159 (88%)	22 (12%)	4 18
29	DI	106/235 (45%)	89 (84%)	17 (16%)	2 13
29	Di	107/235 (46%)	107 (100%)	0	100 100
30	DJ	79/154 (51%)	69 (87%)	10 (13%)	3 17
30	Dj	83/154 (54%)	83 (100%)	0	100 100
31	DL	70/141 (50%)	59 (84%)	11 (16%)	2 13
31	Dl	98/141 (70%)	98 (100%)	0	100 100
32	Dc	113/833 (14%)	111 (98%)	2 (2%)	54 72
33	Dk	87/182 (48%)	87 (100%)	0	100 100
34	Dm	80/106 (76%)	79 (99%)	1 (1%)	65 77
35	EA	163/373 (44%)	122 (75%)	41 (25%)	0 3
36	EB	155/261 (59%)	142 (92%)	13 (8%)	9 30
37	1	384/484 (79%)	367 (96%)	17 (4%)	24 47
38	2	342/352 (97%)	336 (98%)	6 (2%)	54 72
39	3	259/272 (95%)	258 (100%)	1 (0%)	89 91
40	4	394/399 (99%)	383 (97%)	11 (3%)	38 60
41	5	59/64 (92%)	54 (92%)	5 (8%)	8 30
42	6	576/688 (84%)	558 (97%)	18 (3%)	35 56
43	7	630/664 (95%)	601 (95%)	29 (5%)	23 46
44	c	231/280 (82%)	217 (94%)	14 (6%)	15 39
45	e	94/152 (62%)	94 (100%)	0	100 100
46	b	102/163 (63%)	92 (90%)	10 (10%)	6 23
47	l	116/155 (75%)	116 (100%)	0	100 100
48	m	102/115 (89%)	102 (100%)	0	100 100
49	a	393/1391 (28%)	315 (80%)	78 (20%)	1 7
50	d	139/230 (60%)	95 (68%)	44 (32%)	0 2
51	f	144/223 (65%)	122 (85%)	22 (15%)	2 13
52	g	157/216 (73%)	128 (82%)	29 (18%)	1 9
53	h	161/225 (72%)	132 (82%)	29 (18%)	1 9
54	i	71/133 (53%)	61 (86%)	10 (14%)	3 16
55	j	113/124 (91%)	110 (97%)	3 (3%)	40 61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
56	k	94/98 (96%)	48 (51%)	46 (49%)	0 0
57	n	689/1272 (54%)	662 (96%)	27 (4%)	27 50
58	o	141/697 (20%)	139 (99%)	2 (1%)	62 76
59	q	461/577 (80%)	396 (86%)	65 (14%)	3 16
60	r	180/183 (98%)	151 (84%)	29 (16%)	2 12
61	s	31/208 (15%)	28 (90%)	3 (10%)	6 24
62	t	166/178 (93%)	128 (77%)	38 (23%)	0 4
63	u	78/119 (66%)	73 (94%)	5 (6%)	14 37
64	v	122/173 (70%)	88 (72%)	34 (28%)	0 3
65	z	89/512 (17%)	77 (86%)	12 (14%)	3 16
66	x	787/864 (91%)	771 (98%)	16 (2%)	50 68
67	w	1202/1232 (98%)	1185 (99%)	17 (1%)	62 76
68	p	353/736 (48%)	346 (98%)	7 (2%)	50 68
All	All	18686/29967 (62%)	16829 (90%)	1857 (10%)	9 23

All (1857) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	6	CYS
1	0	9	CYS
1	0	31	CYS
1	0	34	CYS
1	0	75	ARG
1	0	80	LYS
1	0	83	ASN
1	0	84	LYS
1	0	85	ARG
1	0	87	GLU
1	0	92	LEU
1	0	93	ARG
1	0	95	TYR
1	0	99	LEU
1	0	100	GLU
1	0	105	ILE
1	0	180	LYS
1	0	184	LEU
1	0	187	LEU

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Mol	Chain	Res	Type
1	0	188	GLU
1	0	190	SER
1	0	196	LEU
1	0	251	LEU
1	0	252	GLN
1	0	254	GLU
1	0	263	LEU
1	0	268	ARG
1	0	272	LEU
1	0	275	VAL
1	0	276	ARG
1	0	287	TYR
1	0	288	THR
1	0	293	CYS
1	0	295	ARG
1	0	304	LEU
1	0	305	PHE
1	0	306	TRP
2	8	13	GLU
2	8	15	LEU
2	8	17	PHE
2	8	20	GLU
2	8	23	PHE
2	8	30	ARG
2	8	33	ASN
2	8	34	THR
2	8	36	GLN
2	8	38	VAL
2	8	45	LEU
2	8	47	HIS
2	8	48	ARG
2	8	52	LYS
2	8	55	ILE
2	8	56	ASN
2	8	57	ARG
2	8	58	THR
2	8	60	LEU
2	8	63	ILE
2	8	64	LYS
2	8	66	LEU
2	8	67	GLN
2	8	69	LEU

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Mol	Chain	Res	Type
2	8	83	HIS
2	8	84	LYS
2	8	86	ASN
2	8	88	SER
2	8	96	THR
2	8	101	ILE
2	8	107	LEU
2	8	108	VAL
2	8	109	LEU
2	8	110	THR
2	8	115	LYS
2	8	125	LEU
2	8	132	TRP
2	8	139	LYS
2	8	141	ASN
2	8	143	LEU
2	8	160	LYS
2	8	162	PHE
2	8	164	SER
2	8	166	ASN
2	8	169	TYR
2	8	170	THR
2	8	174	VAL
2	8	178	TYR
2	8	205	GLU
2	8	206	LEU
2	8	209	ARG
2	8	210	VAL
2	8	213	LEU
2	8	223	THR
2	8	237	TRP
2	8	241	CYS
2	8	245	ASP
2	8	249	PHE
2	8	257	LEU
2	8	258	HIS
2	8	259	HIS
2	8	260	ILE
2	8	261	PHE
2	8	267	ASP
2	8	272	ILE
2	8	280	PRO

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Mol	Chain	Res	Type
2	8	284	ILE
2	8	285	THR
2	8	292	MET
3	9	3	HIS
3	9	7	GLN
3	9	8	LYS
3	9	10	HIS
3	9	11	TRP
3	9	12	THR
3	9	14	SER
3	9	15	SER
3	9	21	ARG
3	9	28	ARG
3	9	32	CYS
3	9	33	LYS
3	9	37	ASN
3	9	41	LEU
3	9	44	ASP
3	9	55	THR
3	9	60	TYR
3	9	65	LEU
3	9	71	PHE
3	9	85	MET
3	9	92	LEU
3	9	93	ASN
3	9	94	ASN
3	9	97	MET
3	9	98	GLU
3	9	102	ARG
3	9	104	ILE
3	9	106	LEU
3	9	107	THR
3	9	108	CYS
3	9	113	CYS
3	9	114	LYS
3	9	115	VAL
3	9	134	LEU
3	9	136	GLN
3	9	140	LEU
3	9	143	ILE
3	9	145	GLU
3	9	148	LEU

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Mol	Chain	Res	Type
3	9	149	LEU
3	9	150	LEU
3	9	151	ILE
3	9	153	GLN
3	9	154	LEU
3	9	155	ASN
3	9	158	LEU
3	9	160	VAL
3	9	165	ARG
3	9	166	PRO
3	9	167	PHE
3	9	171	LEU
3	9	172	ILE
3	9	174	LEU
3	9	175	LYS
3	9	180	ILE
3	9	181	LEU
3	9	182	GLU
3	9	186	ILE
3	9	189	LYS
3	9	192	ASP
3	9	196	ASN
3	9	200	LEU
3	9	208	THR
3	9	211	GLN
3	9	226	ILE
3	9	227	THR
3	9	231	TYR
3	9	232	LEU
3	9	234	GLU
3	9	239	LYS
3	9	252	MET
3	9	262	TYR
3	9	266	ARG
3	9	279	ARG
3	9	288	ASN
4	DO	24	GLN
4	DO	27	GLN
4	DO	29	THR
4	DO	32	LEU
4	DO	34	LEU
4	DO	56	VAL

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Mol	Chain	Res	Type
4	DO	57	ASN
4	DO	59	ARG
4	DO	76	LEU
4	DO	79	VAL
4	DO	80	GLU
4	DO	87	LEU
4	DO	88	ILE
4	DO	89	LYS
5	DP	172	VAL
5	DP	189	ASN
5	DP	209	THR
5	DP	221	CYS
5	DP	226	SER
5	DP	268	ILE
5	DP	303	LEU
5	DP	317	VAL
6	DQ	13	LEU
6	DQ	22	ILE
6	DQ	27	ASP
6	DQ	34	VAL
6	DQ	36	GLU
6	DQ	37	GLN
6	DQ	40	MET
6	DQ	49	LYS
6	DQ	57	ASP
6	DQ	63	GLU
6	DQ	321	SER
6	DQ	322	ASP
6	DQ	360	LEU
6	DQ	364	ASP
7	BA	15	CYS
7	BA	18	HIS
7	BA	27	TYR
7	BA	28	ARG
7	BA	39	LEU
7	BA	41	VAL
7	BA	45	VAL
7	BA	47	ASP
7	BA	120	GLU
7	BA	127	ARG
7	BA	128	ILE
7	BA	206	VAL

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Mol	Chain	Res	Type
7	BA	249	SER
7	BA	313	LEU
7	BA	316	LEU
8	FA	8	SER
8	FA	9	GLN
8	FA	12	THR
8	FA	22	THR
8	FA	24	LYS
8	FA	25	LYS
8	FA	29	MET
9	FB	42	LYS
9	FB	43	LEU
9	FB	55	SER
9	FB	57	THR
9	FB	91	GLN
9	FB	92	THR
9	FB	94	THR
9	FB	98	GLU
9	FB	122	GLU
9	FB	123	ASN
9	FB	126	ARG
9	FB	137	LYS
9	FB	141	LEU
9	FB	158	ASN
9	FB	160	GLN
9	FB	164	GLU
9	FB	166	GLU
9	FB	167	ARG
9	FB	168	LYS
9	FB	169	LYS
9	FB	170	LYS
9	FB	171	GLU
9	FB	174	LYS
9	FB	175	ARG
9	FB	179	ASP
9	FB	180	LYS
9	FB	182	HIS
9	FB	189	SER
9	FB	194	HIS
9	FB	197	TYR
9	FB	207	LYS
9	FB	211	VAL

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Mol	Chain	Res	Type
9	FB	219	GLU
10	PA	11	SER
10	PA	25	VAL
10	PA	26	LEU
10	PA	48	GLU
10	PA	51	ARG
10	PA	66	GLU
10	PA	67	ARG
10	PA	70	ARG
10	PA	71	CYS
10	PA	77	ASN
10	PA	84	HIS
10	PA	85	PHE
10	PA	87	HIS
10	PA	88	ILE
10	PA	101	VAL
10	PA	104	MET
10	PA	111	CYS
10	PA	113	PHE
10	PA	125	LYS
10	PA	130	LEU
10	PA	132	LYS
10	PA	136	GLN
10	PA	138	LYS
10	PA	140	ARG
10	PA	147	LEU
10	PA	149	LYS
10	PA	151	LYS
10	PA	188	GLN
10	PA	191	ILE
10	PA	193	ARG
10	PA	198	LEU
10	PA	215	LEU
10	PA	216	LEU
10	PA	221	VAL
10	PA	228	ILE
10	PA	229	SER
10	PA	233	CYS
10	PA	252	VAL
10	PA	253	LEU
10	PA	255	VAL
10	PA	258	LEU

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Mol	Chain	Res	Type
10	PA	259	SER
10	PA	264	VAL
10	PA	265	VAL
10	PA	277	THR
10	PA	278	HIS
10	PA	286	ILE
10	PA	309	LEU
10	PA	316	THR
10	PA	321	GLU
10	PA	325	LEU
10	PA	329	MET
10	PA	331	LYS
10	PA	334	ARG
10	PA	336	LEU
10	PA	343	LEU
10	PA	355	MET
10	PA	357	LYS
10	PA	364	ARG
10	PA	366	VAL
10	PA	378	VAL
10	PA	389	THR
10	PA	393	ILE
10	PA	395	THR
10	PA	396	PRO
10	PA	399	ILE
10	PA	421	ARG
10	PA	423	ASN
10	PA	434	LYS
10	PA	437	ASP
10	PA	438	LEU
10	PA	439	HIS
10	PA	452	ASP
10	PA	455	ILE
10	PA	458	PHE
10	PA	460	ARG
10	PA	461	GLN
10	PA	463	THR
10	PA	474	VAL
10	PA	481	THR
10	PA	483	ARG
10	PA	495	ASP
10	PA	499	ASP

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Mol	Chain	Res	Type
10	PA	503	LEU
10	PA	506	PRO
10	PA	507	GLN
10	PA	509	LEU
10	PA	521	VAL
10	PA	541	THR
10	PA	542	LEU
10	PA	556	GLU
10	PA	562	ASN
10	PA	567	LEU
10	PA	571	ASP
10	PA	574	VAL
10	PA	580	LEU
10	PA	583	ARG
10	PA	593	SER
10	PA	612	ASP
10	PA	614	ASP
10	PA	622	SER
10	PA	625	ASP
10	PA	634	GLU
10	PA	645	LEU
10	PA	668	PHE
10	PA	676	ILE
10	PA	686	THR
10	PA	695	ASP
10	PA	699	TYR
10	PA	705	THR
10	PA	715	GLU
10	PA	721	HIS
10	PA	729	PRO
10	PA	731	ASN
10	PA	738	GLU
10	PA	754	SER
10	PA	755	SER
10	PA	757	GLN
10	PA	762	GLU
10	PA	785	ILE
10	PA	792	ASN
10	PA	793	VAL
10	PA	806	THR
10	PA	811	ILE
10	PA	847	LEU

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Mol	Chain	Res	Type
10	PA	849	ASP
10	PA	853	LYS
10	PA	859	TYR
10	PA	861	GLN
10	PA	864	LEU
10	PA	865	ILE
10	PA	867	SER
10	PA	871	VAL
10	PA	872	MET
10	PA	878	THR
10	PA	882	SER
10	PA	883	ILE
10	PA	899	GLU
10	PA	900	SER
10	PA	906	LEU
10	PA	908	THR
10	PA	912	SER
10	PA	920	PHE
10	PA	924	TYR
10	PA	932	ARG
10	PA	937	ASP
10	PA	967	ARG
10	PA	972	THR
10	PA	974	ASP
10	PA	977	VAL
10	PA	978	VAL
10	PA	981	CYS
10	PA	983	LEU
10	PA	986	MET
10	PA	992	LYS
10	PA	993	ILE
10	PA	999	ARG
10	PA	1007	ILE
10	PA	1021	VAL
10	PA	1023	VAL
10	PA	1030	SER
10	PA	1032	GLN
10	PA	1034	GLN
10	PA	1042	ASN
10	PA	1050	CYS
10	PA	1071	GLU
10	PA	1074	SER

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Mol	Chain	Res	Type
10	PA	1093	GLN
10	PA	1103	THR
10	PA	1107	PHE
10	PA	1115	LYS
10	PA	1124	LEU
10	PA	1128	ILE
10	PA	1132	LYS
10	PA	1135	LYS
10	PA	1139	LEU
10	PA	1140	THR
10	PA	1150	ASP
10	PA	1158	LEU
10	PA	1170	THR
10	PA	1173	THR
10	PA	1182	GLN
10	PA	1195	VAL
10	PA	1198	GLU
10	PA	1199	MET
10	PA	1201	ASP
10	PA	1207	ILE
10	PA	1210	TRP
10	PA	1211	LEU
10	PA	1239	PHE
10	PA	1243	LEU
10	PA	1244	ASN
10	PA	1248	ASN
10	PA	1254	LYS
10	PA	1255	LEU
10	PA	1256	VAL
10	PA	1259	ILE
10	PA	1260	ARG
10	PA	1265	ASP
10	PA	1287	CYS
10	PA	1292	MET
10	PA	1293	LEU
10	PA	1296	MET
10	PA	1304	ILE
10	PA	1319	LYS
10	PA	1327	GLU
10	PA	1338	THR
10	PA	1341	VAL
10	PA	1344	MET

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Mol	Chain	Res	Type
10	PA	1345	ARG
10	PA	1349	GLU
10	PA	1351	ASP
10	PA	1364	GLU
10	PA	1368	VAL
10	PA	1375	ARG
10	PA	1378	LEU
10	PA	1379	GLU
10	PA	1385	VAL
10	PA	1386	ILE
10	PA	1388	PHE
10	PA	1391	SER
10	PA	1402	CYS
10	PA	1403	ASP
10	PA	1407	CYS
10	PA	1417	HIS
10	PA	1419	VAL
10	PA	1421	ARG
10	PA	1429	LYS
10	PA	1430	CYS
10	PA	1432	PHE
10	PA	1434	GLU
10	PA	1435	THR
10	PA	1451	MET
10	PA	1454	VAL
10	PA	1463	LEU
10	PA	1480	CYS
10	PA	1486	ILE
10	PA	1487	PRO
10	PA	1643	TYR
10	PA	1646	THR
10	PA	1647	SER
10	PA	1657	TYR
10	PA	1663	SER
10	PA	1678	TYR
10	PA	1794	SER
11	PB	18	THR
11	PB	24	GLU
11	PB	29	VAL
11	PB	39	LEU
11	PB	40	VAL
11	PB	42	GLN

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Mol	Chain	Res	Type
11	PB	43	GLN
11	PB	52	GLN
11	PB	53	MET
11	PB	55	VAL
11	PB	83	ARG
11	PB	87	LYS
11	PB	91	ILE
11	PB	99	TRP
11	PB	100	GLU
11	PB	101	ARG
11	PB	102	ASP
11	PB	131	THR
11	PB	132	VAL
11	PB	133	ILE
11	PB	134	LYS
11	PB	140	LEU
11	PB	141	GLN
11	PB	142	THR
11	PB	146	LYS
11	PB	147	THR
11	PB	148	PHE
11	PB	149	ILE
11	PB	162	LEU
11	PB	167	THR
11	PB	195	ILE
11	PB	204	THR
11	PB	212	ASP
11	PB	214	LYS
11	PB	225	LEU
11	PB	230	ARG
11	PB	233	SER
11	PB	235	ILE
11	PB	242	ARG
11	PB	264	LYS
11	PB	265	GLN
11	PB	273	PHE
11	PB	281	ASP
11	PB	282	ARG
11	PB	285	LEU
11	PB	286	GLU
11	PB	287	HIS
11	PB	289	ILE

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Mol	Chain	Res	Type
11	PB	297	MET
11	PB	304	SER
11	PB	318	LEU
11	PB	324	ARG
11	PB	327	LYS
11	PB	330	VAL
11	PB	331	THR
11	PB	348	LEU
11	PB	356	PHE
11	PB	379	ARG
11	PB	386	ASP
11	PB	388	TYR
11	PB	402	PHE
11	PB	403	LEU
11	PB	420	GLN
11	PB	423	ILE
11	PB	432	GLU
11	PB	433	LEU
11	PB	440	ILE
11	PB	448	LEU
11	PB	453	TRP
11	PB	458	LYS
11	PB	468	GLN
11	PB	473	LEU
11	PB	487	SER
11	PB	489	ILE
11	PB	491	ARG
11	PB	501	LEU
11	PB	508	MET
11	PB	514	THR
11	PB	523	VAL
11	PB	524	LYS
11	PB	525	ASN
11	PB	536	SER
11	PB	539	SER
11	PB	541	ILE
11	PB	542	LEU
11	PB	545	LEU
11	PB	547	GLU
11	PB	553	LEU
11	PB	554	GLU
11	PB	555	GLU

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Mol	Chain	Res	Type
11	PB	568	PHE
11	PB	570	ASN
11	PB	579	ASP
11	PB	592	ARG
11	PB	593	GLN
11	PB	595	ASP
11	PB	597	ILE
11	PB	598	VAL
11	PB	606	ASP
11	PB	613	ARG
11	PB	627	ILE
11	PB	632	LYS
11	PB	643	LEU
11	PB	645	GLU
11	PB	648	TYR
11	PB	651	TYR
11	PB	656	LEU
11	PB	662	VAL
11	PB	667	THR
11	PB	678	THR
11	PB	683	GLN
11	PB	690	CYS
11	PB	694	THR
11	PB	696	CYS
11	PB	698	ILE
11	PB	707	CYS
11	PB	733	MET
11	PB	738	THR
11	PB	741	HIS
11	PB	742	VAL
11	PB	745	ASP
11	PB	746	THR
11	PB	749	HIS
11	PB	767	LEU
11	PB	768	ARG
11	PB	780	VAL
11	PB	784	SER
11	PB	795	ILE
11	PB	809	VAL
11	PB	825	GLN
11	PB	829	PHE
11	PB	834	ARG

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Mol	Chain	Res	Type
11	PB	837	CYS
11	PB	841	ARG
11	PB	842	HIS
11	PB	847	LYS
11	PB	854	ILE
11	PB	865	VAL
11	PB	866	ILE
11	PB	870	THR
11	PB	873	LEU
11	PB	888	THR
11	PB	889	LYS
11	PB	890	ARG
11	PB	896	LEU
11	PB	897	ARG
11	PB	901	THR
11	PB	904	VAL
11	PB	908	MET
11	PB	918	PHE
11	PB	922	ARG
11	PB	923	VAL
11	PB	965	ILE
11	PB	966	ILE
11	PB	976	MET
11	PB	983	GLU
11	PB	996	ILE
11	PB	998	ASP
11	PB	1000	THR
11	PB	1002	PHE
11	PB	1006	VAL
11	PB	1022	LEU
11	PB	1027	VAL
11	PB	1048	TYR
11	PB	1052	LYS
11	PB	1070	LEU
11	PB	1073	GLN
11	PB	1078	ARG
11	PB	1080	ARG
11	PB	1086	PHE
11	PB	1090	GLU
11	PB	1101	GLN
11	PB	1125	MET
11	PB	1133	HIS

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Mol	Chain	Res	Type
11	PB	1151	MET
11	PB	1155	CYS
12	PC	5	ASN
12	PC	6	GLN
12	PC	9	VAL
12	PC	17	GLU
12	PC	21	PHE
12	PC	44	ILE
12	PC	60	HIS
12	PC	63	PHE
12	PC	64	ILE
12	PC	75	SER
12	PC	79	VAL
12	PC	86	ARG
12	PC	88	CYS
12	PC	94	CYS
12	PC	109	GLU
12	PC	110	ASP
12	PC	112	THR
12	PC	118	ARG
12	PC	131	THR
12	PC	148	ILE
12	PC	159	LEU
12	PC	169	PHE
12	PC	172	GLU
12	PC	179	THR
12	PC	193	ARG
12	PC	195	THR
12	PC	204	PRO
12	PC	211	LEU
12	PC	213	GLU
12	PC	223	ASN
12	PC	225	LYS
12	PC	227	GLU
12	PC	243	THR
12	PC	247	SER
12	PC	250	SER
12	PC	259	LEU
12	PC	262	GLN
12	PC	266	GLU
13	PD	19	GLN
13	PD	32	LEU

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Mol	Chain	Res	Type
13	PD	33	LEU
13	PD	45	LYS
13	PD	50	SER
13	PD	67	TYR
13	PD	76	ASN
13	PD	82	SER
13	PD	89	GLN
13	PD	96	GLU
13	PD	99	CYS
13	PD	107	THR
13	PD	109	GLU
13	PD	115	ILE
13	PD	117	SER
13	PD	118	LEU
13	PD	119	GLU
13	PD	121	ARG
13	PD	124	ASP
13	PD	131	LEU
13	PD	135	GLN
13	PD	141	GLN
14	PE	3	ASP
14	PE	5	GLU
14	PE	11	TRP
14	PE	21	CYS
14	PE	39	GLU
14	PE	47	LYS
14	PE	52	ARG
14	PE	57	ASP
14	PE	58	LEU
14	PE	60	VAL
14	PE	64	HIS
14	PE	78	GLU
14	PE	81	LYS
14	PE	84	ILE
14	PE	87	ILE
14	PE	95	GLN
14	PE	96	GLU
14	PE	100	THR
14	PE	104	ILE
14	PE	108	GLN
14	PE	111	THR
14	PE	119	VAL

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Mol	Chain	Res	Type
14	PE	120	ASP
14	PE	127	LEU
14	PE	147	GLU
14	PE	168	ASN
14	PE	178	PRO
14	PE	191	VAL
14	PE	195	ARG
14	PE	198	GLU
14	PE	199	THR
14	PE	205	THR
14	PE	208	LEU
14	PE	210	GLN
15	PF	53	THR
15	PF	66	LEU
15	PF	71	LEU
15	PF	73	ILE
15	PF	75	MET
15	PF	81	VAL
15	PF	82	GLU
15	PF	83	LEU
15	PF	86	GLU
15	PF	90	LEU
15	PF	97	LEU
15	PF	101	LYS
15	PF	105	ILE
15	PF	115	TYR
16	PG	1	MET
16	PG	7	LEU
16	PG	10	GLU
16	PG	13	LEU
16	PG	30	LEU
16	PG	39	THR
16	PG	41	LYS
16	PG	48	VAL
16	PG	49	THR
16	PG	52	ASP
16	PG	53	ASN
16	PG	60	GLN
16	PG	63	ARG
16	PG	80	PHE
16	PG	84	VAL
16	PG	88	VAL

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Mol	Chain	Res	Type
16	PG	90	THR
16	PG	97	LEU
16	PG	101	ILE
16	PG	105	SER
16	PG	106	CYS
16	PG	113	ILE
16	PG	117	MET
16	PG	118	GLU
16	PG	132	ASP
16	PG	136	VAL
16	PG	141	ASP
16	PG	143	ILE
16	PG	145	LEU
16	PG	150	THR
16	PG	152	VAL
16	PG	158	PHE
16	PG	164	MET
16	PG	168	LEU
17	PH	4	ILE
17	PH	5	LEU
17	PH	15	ILE
17	PH	20	LYS
17	PH	24	ARG
17	PH	33	GLU
17	PH	40	ILE
17	PH	45	ILE
17	PH	59	VAL
17	PH	64	LEU
17	PH	66	GLU
17	PH	72	ASP
17	PH	76	ASN
17	PH	81	ARG
17	PH	87	GLN
17	PH	96	VAL
17	PH	102	ASP
17	PH	132	LEU
17	PH	133	HIS
17	PH	136	GLU
17	PH	141	VAL
18	PI	12	VAL
18	PI	15	ARG
18	PI	27	LYS

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Mol	Chain	Res	Type
18	PI	28	GLU
18	PI	32	ASN
18	PI	33	ARG
18	PI	34	ILE
18	PI	35	LEU
18	PI	42	CYS
18	PI	47	GLU
18	PI	53	ILE
18	PI	61	GLU
18	PI	62	VAL
18	PI	69	ILE
18	PI	72	VAL
18	PI	75	ASP
18	PI	77	THR
18	PI	81	THR
18	PI	83	ASP
18	PI	88	LYS
18	PI	93	GLU
18	PI	95	VAL
18	PI	99	SER
19	PJ	1	MET
19	PJ	7	CYS
19	PJ	10	CYS
19	PJ	12	LYS
19	PJ	13	ILE
19	PJ	14	VAL
19	PJ	22	LEU
19	PJ	28	GLU
19	PJ	30	THR
19	PJ	48	MET
20	PK	11	LEU
20	PK	12	LEU
20	PK	14	GLU
20	PK	17	LYS
20	PK	38	GLU
20	PK	40	HIS
20	PK	42	LEU
20	PK	45	ILE
20	PK	81	TYR
20	PK	92	THR
20	PK	94	LEU
20	PK	96	SER

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Mol	Chain	Res	Type
20	PK	101	LEU
20	PK	109	ILE
20	PK	111	ASP
20	PK	112	LYS
20	PK	114	GLU
20	PK	116	ILE
21	PL	18	ILE
21	PL	23	HIS
21	PL	25	GLU
21	PL	34	ILE
21	PL	37	ARG
21	PL	39	CYS
21	PL	41	TYR
21	PL	44	MET
21	PL	47	LYS
21	PL	51	ARG
21	PL	52	LEU
21	PL	56	ASP
22	DA	353	LEU
22	DA	396	LEU
22	DA	397	LEU
22	DA	400	GLU
22	DA	403	LEU
22	DA	404	MET
22	DA	408	LEU
22	DA	410	TRP
22	DA	411	GLU
22	DA	415	ILE
22	DA	416	TRP
22	DA	475	LEU
22	DA	479	ARG
22	DA	480	TRP
22	DA	482	ASP
22	DA	485	ILE
22	DA	486	TRP
22	DA	487	ASP
22	DA	491	MET
22	DA	493	ARG
22	DA	494	LEU
22	DA	496	GLU
22	DA	500	LEU
22	DA	501	THR

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Mol	Chain	Res	Type
22	DA	502	LEU
22	DA	507	GLU
22	DA	510	ILE
22	DA	573	TYR
22	DA	574	TYR
22	DA	639	LEU
22	DA	661	GLU
22	DA	667	THR
22	DA	711	ASP
22	DA	727	THR
22	DA	730	PHE
22	DA	828	GLU
22	DA	943	LYS
22	DA	970	ASN
22	DA	992	ASP
22	DA	1020	LEU
22	DA	1029	VAL
22	DA	1039	SER
22	DA	1052	ARG
22	DA	1165	LEU
22	DA	1169	ARG
22	DA	1203	GLU
23	DB	21	GLU
23	DB	24	ARG
23	DB	71	ARG
23	DB	140	GLU
23	DB	184	ASN
23	DB	225	TYR
23	DB	262	MET
23	DB	266	THR
23	DB	293	GLU
23	DB	431	LEU
23	DB	488	PHE
23	DB	538	ASN
23	DB	539	ARG
23	DB	559	LYS
23	DB	603	LYS
23	DB	638	ARG
23	DB	640	VAL
23	DB	771	VAL
23	DB	818	THR
23	DB	942	SER

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Mol	Chain	Res	Type
23	DB	945	CYS
24	DD	893	GLU
24	DD	894	LEU
24	DD	897	ASP
24	DD	917	ILE
24	DD	918	SER
24	DD	919	GLU
24	DD	922	GLN
24	DD	924	LYS
24	DD	931	ASP
24	DD	933	ARG
24	DD	935	GLU
24	DD	940	VAL
24	DD	950	LEU
24	DD	966	LEU
24	DD	1005	ASN
24	DD	1006	LEU
25	DE	431	GLU
25	DE	432	LEU
25	DE	433	LYS
25	DE	449	LYS
25	DE	450	ARG
25	DE	451	VAL
25	DE	471	GLN
25	DE	479	THR
25	DE	481	ASP
25	DE	508	LYS
25	DE	519	GLU
25	DE	521	ASP
25	DE	523	VAL
25	DE	593	PHE
25	DE	745	GLU
25	DE	746	ASP
25	DE	747	LEU
26	DF	14	LEU
26	DF	39	LEU
26	DF	41	ASP
26	DF	55	LEU
26	DF	60	MET
26	DF	62	LYS
26	DF	63	ARG
26	DF	65	LYS

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Mol	Chain	Res	Type
26	DF	66	LEU
26	DF	110	LYS
26	DF	111	GLU
26	DF	114	LEU
26	DF	115	SER
26	DF	116	ASP
26	DF	117	ILE
26	DF	118	ILE
26	DF	122	LEU
26	DF	131	LEU
26	DF	132	LYS
26	DF	207	ARG
26	DF	208	LEU
26	DF	209	LYS
26	DF	211	ARG
26	DF	218	VAL
26	DF	239	ARG
26	DF	243	LEU
26	DF	245	SER
26	DF	246	ILE
26	DF	258	ARG
26	DF	261	THR
26	DF	271	VAL
26	DF	280	ILE
26	DF	299	LYS
26	DF	301	VAL
26	DF	304	LEU
26	DF	305	ILE
26	DF	308	VAL
26	DF	309	MET
26	DF	312	ILE
26	DF	313	VAL
26	DF	315	ARG
26	DF	316	GLN
26	DF	317	LEU
26	DF	318	CYS
26	DF	319	LEU
26	DF	320	ARG
26	DF	327	TRP
26	DF	330	ARG
26	DF	339	GLN
26	DF	342	LYS

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Mol	Chain	Res	Type
26	DF	346	THR
26	DF	348	THR
26	DF	351	ILE
26	DF	359	PHE
26	DF	368	THR
26	DF	391	LEU
26	DF	397	GLN
26	DF	406	VAL
26	DF	412	LEU
26	DF	413	SER
26	DF	416	ASP
26	DF	427	LEU
27	DG	41	ASP
27	DG	81	ASP
27	DG	143	VAL
27	DG	147	ARG
27	DG	161	ASP
27	DG	180	ARG
27	DG	181	TRP
27	DG	182	GLU
27	DG	183	ILE
28	DH	28	ASN
28	DH	34	ARG
28	DH	35	ARG
28	DH	38	GLN
28	DH	42	SER
28	DH	43	SER
28	DH	50	PHE
28	DH	104	VAL
28	DH	106	THR
28	DH	107	LEU
28	DH	113	ARG
28	DH	116	ARG
28	DH	117	MET
28	DH	119	ILE
28	DH	120	THR
28	DH	132	LYS
28	DH	159	TYR
28	DH	160	ILE
28	DH	161	LYS
28	DH	162	THR
28	DH	164	THR

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Mol	Chain	Res	Type
28	DH	169	VAL
29	DI	31	TYR
29	DI	32	GLU
29	DI	34	ARG
29	DI	62	LYS
29	DI	63	LYS
29	DI	65	THR
29	DI	67	ASP
29	DI	69	ASP
29	DI	70	ASP
29	DI	76	GLN
29	DI	81	GLN
29	DI	84	THR
29	DI	107	ILE
29	DI	108	LYS
29	DI	111	SER
29	DI	129	LEU
29	DI	130	LYS
30	DJ	125	ASP
30	DJ	127	THR
30	DJ	129	THR
30	DJ	130	ILE
30	DJ	155	ILE
30	DJ	172	GLN
30	DJ	175	LYS
30	DJ	177	LYS
30	DJ	192	LYS
30	DJ	193	TYR
31	DL	56	GLN
31	DL	59	THR
31	DL	60	LYS
31	DL	61	LYS
31	DL	62	LYS
31	DL	63	LEU
31	DL	64	GLN
31	DL	107	LYS
31	DL	110	THR
31	DL	111	LEU
31	DL	128	ILE
32	Dc	24	ASP
32	Dc	106	VAL
25	De	365	ARG

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Mol	Chain	Res	Type
25	De	663	ARG
26	Df	214	HIS
26	Df	253	TYR
26	Df	261	THR
26	Df	272	VAL
26	Df	299	LYS
26	Df	301	VAL
26	Df	302	HIS
26	Df	305	ILE
26	Df	309	MET
26	Df	313	VAL
26	Df	314	SER
26	Df	322	ASP
26	Df	323	VAL
26	Df	326	HIS
26	Df	356	THR
26	Df	383	LEU
26	Df	387	VAL
26	Df	388	ILE
26	Df	389	LYS
26	Df	391	LEU
26	Df	421	ASP
34	Dm	31	LEU
35	EA	15	LYS
35	EA	16	ARG
35	EA	19	LYS
35	EA	21	VAL
35	EA	22	ILE
35	EA	23	ARG
35	EA	28	ILE
35	EA	32	LEU
35	EA	38	ILE
35	EA	39	ARG
35	EA	40	ASN
35	EA	43	VAL
35	EA	44	LYS
35	EA	46	GLU
35	EA	50	GLU
35	EA	51	LEU
35	EA	53	LYS
35	EA	56	ARG
35	EA	57	LYS

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Mol	Chain	Res	Type
35	EA	60	ARG
35	EA	65	ASN
35	EA	67	LYS
35	EA	70	LYS
35	EA	72	ILE
35	EA	75	ARG
35	EA	77	ARG
35	EA	100	VAL
35	EA	105	TYR
35	EA	109	HIS
35	EA	111	ARG
35	EA	112	ARG
35	EA	139	LEU
35	EA	143	GLN
35	EA	145	PHE
35	EA	156	PHE
35	EA	158	HIS
35	EA	161	VAL
35	EA	162	GLU
35	EA	165	GLU
35	EA	174	ARG
35	EA	187	ILE
36	EB	73	TYR
36	EB	84	TYR
36	EB	88	ARG
36	EB	97	LEU
36	EB	140	LYS
36	EB	159	ASP
36	EB	160	GLN
36	EB	167	LEU
36	EB	171	ILE
36	EB	194	ARG
36	EB	209	GLN
36	EB	223	VAL
36	EB	224	THR
37	1	188	LEU
37	1	189	THR
37	1	191	ASP
37	1	204	LYS
37	1	207	TYR
37	1	215	MET
37	1	216	THR

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Mol	Chain	Res	Type
37	1	217	GLU
37	1	218	LYS
37	1	220	PHE
37	1	222	THR
37	1	223	ARG
37	1	237	THR
37	1	239	SER
37	1	240	LYS
37	1	242	LEU
37	1	461	LEU
38	2	18	THR
38	2	20	GLU
38	2	21	ILE
38	2	54	ARG
38	2	291	CYS
38	2	318	LEU
39	3	132	LEU
40	4	145	VAL
40	4	262	LEU
40	4	290	LEU
40	4	386	THR
40	4	387	ILE
40	4	391	ILE
40	4	398	ARG
40	4	408	LEU
40	4	413	LEU
40	4	431	LEU
40	4	432	VAL
41	5	2	VAL
41	5	8	VAL
41	5	9	LEU
41	5	35	ILE
41	5	38	ILE
42	6	107	VAL
42	6	136	ILE
42	6	140	LEU
42	6	141	ARG
42	6	154	GLN
42	6	170	LEU
42	6	183	ASP
42	6	184	VAL
42	6	185	ILE

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Mol	Chain	Res	Type
42	6	186	GLN
42	6	188	LEU
42	6	194	ILE
42	6	195	ARG
42	6	267	THR
42	6	270	PHE
42	6	272	VAL
42	6	416	THR
42	6	420	SER
43	7	17	ILE
43	7	19	PRO
43	7	48	LYS
43	7	60	GLN
43	7	112	ARG
43	7	120	GLU
43	7	174	ILE
43	7	178	ASP
43	7	180	LEU
43	7	181	LYS
43	7	185	ARG
43	7	186	ARG
43	7	190	CYS
43	7	194	LEU
43	7	203	ASN
43	7	296	SER
43	7	299	ARG
43	7	300	GLU
43	7	301	THR
43	7	302	ASP
43	7	304	HIS
43	7	309	VAL
43	7	488	VAL
43	7	668	ILE
43	7	671	LYS
43	7	705	ASN
43	7	728	PHE
43	7	741	LEU
43	7	742	GLU
44	c	16	GLN
44	c	41	ASN
44	c	44	THR
44	c	45	LEU

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Mol	Chain	Res	Type
44	c	72	ARG
44	c	73	LEU
44	c	77	VAL
44	c	258	MET
44	c	274	ILE
44	c	275	LYS
44	c	276	LEU
44	c	284	CYS
44	c	300	ARG
44	c	301	THR
46	b	57	VAL
46	b	60	TYR
46	b	74	LEU
46	b	82	LEU
46	b	92	GLN
46	b	103	ASP
46	b	122	LEU
46	b	126	CYS
46	b	132	ASP
46	b	184	LYS
49	a	58	LEU
49	a	61	CYS
49	a	62	LEU
49	a	66	GLN
49	a	67	LYS
49	a	69	LEU
49	a	70	LYS
49	a	71	VAL
49	a	72	THR
49	a	74	LEU
49	a	77	MET
49	a	78	THR
49	a	80	ARG
49	a	83	SER
49	a	86	ARG
49	a	87	GLN
49	a	93	HIS
49	a	106	ASP
49	a	107	MET
49	a	108	PHE
49	a	109	TYR
49	a	111	GLU

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Mol	Chain	Res	Type
49	a	128	HIS
49	a	131	ASN
49	a	133	VAL
49	a	145	LYS
49	a	148	ASP
49	a	160	LEU
49	a	162	ASN
49	a	167	ASN
49	a	168	LYS
49	a	173	MET
49	a	201	ASP
49	a	214	ARG
49	a	226	VAL
49	a	232	LEU
49	a	244	GLU
49	a	246	ASN
49	a	253	MET
49	a	254	ASN
49	a	258	THR
49	a	259	ILE
49	a	267	LYS
49	a	278	HIS
49	a	288	PHE
49	a	297	VAL
49	a	305	LEU
49	a	309	GLN
49	a	324	CYS
49	a	325	THR
49	a	327	ILE
49	a	329	LEU
49	a	332	THR
49	a	333	GLN
49	a	335	THR
49	a	339	LEU
49	a	348	LEU
49	a	357	LEU
49	a	367	LEU
49	a	373	CYS
49	a	378	LYS
49	a	384	ASP
49	a	388	LEU
49	a	391	THR

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Mol	Chain	Res	Type
49	a	400	HIS
49	a	421	ILE
49	a	432	GLU
49	a	433	ASP
49	a	437	LEU
49	a	438	LEU
49	a	441	GLU
49	a	443	CYS
49	a	467	MET
49	a	479	LEU
49	a	501	CYS
49	a	504	ILE
49	a	509	ARG
49	a	514	LYS
50	d	28	GLU
50	d	30	LEU
50	d	63	ASN
50	d	64	GLN
50	d	66	LEU
50	d	67	GLU
50	d	69	LEU
50	d	70	ILE
50	d	71	HIS
50	d	72	ARG
50	d	73	ASP
50	d	78	GLU
50	d	79	LEU
50	d	80	MET
50	d	81	LYS
50	d	82	LEU
50	d	85	ASN
50	d	91	HIS
50	d	92	GLU
50	d	98	LYS
50	d	101	GLU
50	d	106	ASP
50	d	107	ILE
50	d	108	GLN
50	d	110	LEU
50	d	114	LEU
50	d	115	LYS
50	d	116	GLU

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Mol	Chain	Res	Type
50	d	119	GLN
50	d	121	LEU
50	d	126	TYR
50	d	127	GLN
50	d	129	LYS
50	d	130	GLU
50	d	131	LYS
50	d	132	LEU
50	d	133	LYS
50	d	135	ILE
50	d	173	ARG
50	d	181	GLU
50	d	184	SER
50	d	186	LEU
50	d	187	LEU
50	d	189	GLN
51	f	16	VAL
51	f	19	SER
51	f	20	TRP
51	f	24	LEU
51	f	30	LEU
51	f	41	TYR
51	f	45	CYS
51	f	48	GLU
51	f	51	LYS
51	f	52	MET
51	f	53	GLN
51	f	56	THR
51	f	57	LEU
51	f	58	GLU
51	f	60	LEU
51	f	63	MET
51	f	64	VAL
51	f	114	VAL
51	f	117	SER
51	f	120	LEU
51	f	137	CYS
51	f	139	TYR
52	g	11	LEU
52	g	15	MET
52	g	17	TYR
52	g	18	ILE

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Mol	Chain	Res	Type
52	g	20	GLU
52	g	26	ILE
52	g	27	GLN
52	g	28	GLU
52	g	39	LYS
52	g	45	PHE
52	g	49	PHE
52	g	51	CYS
52	g	52	ASP
52	g	54	LEU
52	g	55	ILE
52	g	64	ILE
52	g	72	PHE
52	g	74	HIS
52	g	83	MET
52	g	92	LEU
52	g	119	VAL
52	g	124	ASN
52	g	126	TYR
52	g	132	ARG
52	g	137	VAL
52	g	155	LYS
52	g	159	ARG
52	g	166	ASN
52	g	171	LEU
53	h	7	GLN
53	h	15	LEU
53	h	16	LEU
53	h	17	SER
53	h	18	GLN
53	h	21	ASP
53	h	22	LEU
53	h	23	LYS
53	h	32	LYS
53	h	33	LEU
53	h	34	GLU
53	h	37	TYR
53	h	39	ARG
53	h	40	LEU
53	h	49	PHE
53	h	66	GLU
53	h	100	PHE

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Mol	Chain	Res	Type
53	h	101	SER
53	h	102	HIS
53	h	110	ARG
53	h	111	THR
53	h	112	LYS
53	h	117	VAL
53	h	130	ARG
53	h	131	ILE
53	h	143	LEU
53	h	187	PHE
53	h	189	LYS
53	h	192	SER
54	i	86	ASP
54	i	87	LEU
54	i	88	ASN
54	i	90	LEU
54	i	94	PHE
54	i	95	GLN
54	i	104	MET
54	i	112	GLU
54	i	122	ARG
54	i	136	LYS
55	j	52	ASP
55	j	53	LYS
55	j	62	THR
56	k	8	ASN
56	k	10	ARG
56	k	11	LEU
56	k	12	ARG
56	k	14	LEU
56	k	15	GLU
56	k	18	GLU
56	k	19	ARG
56	k	26	GLN
56	k	32	ILE
56	k	33	LEU
56	k	34	GLU
56	k	35	LEU
56	k	36	SER
56	k	37	LYS
56	k	40	THR
56	k	42	GLU

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Mol	Chain	Res	Type
56	k	43	ARG
56	k	44	LEU
56	k	45	LEU
56	k	52	PHE
56	k	57	GLN
56	k	58	HIS
56	k	60	GLU
56	k	69	TYR
56	k	70	LEU
56	k	72	GLN
56	k	75	THR
56	k	82	SER
56	k	83	SER
56	k	86	SER
56	k	87	ARG
56	k	88	LYS
56	k	90	CYS
56	k	91	GLN
56	k	92	MET
56	k	94	LEU
56	k	96	ARG
56	k	97	VAL
56	k	101	ARG
56	k	102	LEU
56	k	103	LYS
56	k	104	LEU
56	k	105	SER
56	k	109	ARG
56	k	114	MET
57	n	149	LEU
57	n	154	ILE
57	n	159	ASP
57	n	166	TYR
57	n	168	ARG
57	n	169	LEU
57	n	212	LEU
57	n	229	GLU
57	n	252	ILE
57	n	253	LEU
57	n	254	VAL
57	n	255	GLU
57	n	261	ASP

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Mol	Chain	Res	Type
57	n	265	LEU
57	n	266	VAL
57	n	267	HIS
57	n	283	PHE
57	n	286	GLU
57	n	287	LYS
57	n	289	LEU
57	n	363	GLU
57	n	371	GLN
57	n	528	HIS
57	n	634	MET
57	n	959	LEU
57	n	960	LYS
57	n	965	MET
58	o	715	LEU
58	o	717	SER
59	q	7	VAL
59	q	8	ARG
59	q	16	GLU
59	q	19	VAL
59	q	28	GLU
59	q	29	THR
59	q	31	LEU
59	q	36	MET
59	q	91	SER
59	q	92	LEU
59	q	93	TRP
59	q	98	VAL
59	q	100	ASN
59	q	103	ARG
59	q	107	THR
59	q	109	MET
59	q	110	CYS
59	q	112	LEU
59	q	116	LEU
59	q	118	ILE
59	q	120	ARG
59	q	123	LYS
59	q	124	PHE
59	q	125	MET
59	q	128	ASP
59	q	131	SER

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Mol	Chain	Res	Type
59	q	132	GLN
59	q	133	ASP
59	q	138	LYS
59	q	139	GLN
59	q	141	PRO
59	q	143	THR
59	q	144	LEU
59	q	145	GLN
59	q	146	LEU
59	q	147	ILE
59	q	151	LYS
59	q	159	ILE
59	q	161	LEU
59	q	162	LYS
59	q	165	GLU
59	q	166	ARG
59	q	169	LYS
59	q	172	THR
59	q	184	ASN
59	q	185	SER
59	q	187	LEU
59	q	188	LEU
59	q	389	SER
59	q	428	LEU
59	q	431	ILE
59	q	432	ILE
59	q	434	GLN
59	q	440	LEU
59	q	441	ARG
59	q	442	SER
59	q	443	ARG
59	q	448	ILE
59	q	451	LEU
59	q	544	MET
59	q	629	LYS
59	q	631	GLU
59	q	633	ARG
59	q	646	LEU
59	q	647	SER
60	r	7	THR
60	r	9	MET
60	r	11	VAL

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Mol	Chain	Res	Type
60	r	12	THR
60	r	16	ILE
60	r	17	ASN
60	r	18	MET
60	r	32	LEU
60	r	35	LEU
60	r	38	ARG
60	r	42	LEU
60	r	53	ASP
60	r	56	MET
60	r	60	LEU
60	r	85	LEU
60	r	88	LEU
60	r	93	MET
60	r	101	LEU
60	r	107	ASP
60	r	124	ARG
60	r	143	ILE
60	r	152	LEU
60	r	156	ASN
60	r	168	LEU
60	r	181	MET
60	r	197	VAL
60	r	200	GLU
60	r	202	ILE
60	r	206	ARG
61	s	65	PHE
61	s	84	ILE
61	s	89	LEU
62	t	1	MET
62	t	9	MET
62	t	16	SER
62	t	17	VAL
62	t	21	VAL
62	t	23	LEU
62	t	24	LEU
62	t	28	LEU
62	t	34	GLU
62	t	39	PHE
62	t	43	CYS
62	t	47	HIS
62	t	61	LYS

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Mol	Chain	Res	Type
62	t	62	LEU
62	t	66	MET
62	t	67	HIS
62	t	78	LEU
62	t	79	PHE
62	t	80	GLU
62	t	81	ASN
62	t	84	CYS
62	t	85	LEU
62	t	98	LEU
62	t	101	PHE
62	t	102	PHE
62	t	103	GLN
62	t	109	LYS
62	t	110	ILE
62	t	131	MET
62	t	138	ILE
62	t	149	VAL
62	t	162	GLN
62	t	173	PRO
62	t	179	ARG
62	t	193	TYR
62	t	196	LEU
62	t	200	ILE
62	t	204	GLN
63	u	20	CYS
63	u	26	LEU
63	u	27	GLN
63	u	76	LEU
63	u	80	GLU
64	v	22	LEU
64	v	37	ILE
64	v	38	LYS
64	v	39	THR
64	v	41	LYS
64	v	43	GLU
64	v	45	GLU
64	v	47	GLN
64	v	50	ARG
64	v	52	THR
64	v	55	GLU
64	v	56	GLN

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Mol	Chain	Res	Type
64	v	58	ASN
64	v	60	GLU
64	v	61	MET
64	v	62	HIS
64	v	81	ASP
64	v	82	LEU
64	v	86	LEU
64	v	87	ILE
64	v	103	GLN
64	v	105	LEU
64	v	108	LEU
64	v	110	GLU
64	v	114	ARG
64	v	115	LYS
64	v	118	THR
64	v	119	LEU
64	v	120	ARG
64	v	123	ILE
64	v	130	LEU
64	v	131	GLU
64	v	133	GLU
64	v	138	SER
65	z	492	ARG
65	z	528	LEU
65	z	540	LEU
65	z	551	ASP
65	z	564	ASN
65	z	567	GLN
65	z	572	ASN
65	z	579	CYS
65	z	582	LEU
65	z	591	LEU
65	z	593	ILE
65	z	599	LEU
66	x	4	VAL
66	x	87	ASP
66	x	359	CYS
66	x	477	TYR
66	x	482	SER
66	x	484	LYS
66	x	564	SER
66	x	565	SER

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Mol	Chain	Res	Type
66	x	686	LYS
66	x	802	MET
66	x	812	LEU
66	x	897	LEU
66	x	959	SER
66	x	965	LYS
66	x	966	VAL
66	x	989	LEU
67	w	1	MET
67	w	2	GLU
67	w	7	SER
67	w	10	GLU
67	w	11	GLU
67	w	17	VAL
67	w	18	ILE
67	w	25	MET
67	w	36	LYS
67	w	37	LEU
67	w	41	LEU
67	w	44	PHE
67	w	48	TRP
67	w	51	LEU
67	w	171	LEU
67	w	425	MET
67	w	726	ASN
68	p	162	VAL
68	p	170	LEU
68	p	232	ASP
68	p	249	VAL
68	p	252	LYS
68	p	289	ASP
68	p	401	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (381) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	200	GLN
1	0	294	HIS
1	0	298	GLN
2	8	56	ASN
2	8	67	GLN
2	8	83	HIS

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Mol	Chain	Res	Type
2	8	86	ASN
2	8	131	HIS
2	8	135	HIS
2	8	166	ASN
2	8	171	HIS
3	9	7	GLN
3	9	37	ASN
3	9	100	HIS
3	9	128	ASN
3	9	211	GLN
3	9	275	GLN
3	9	288	ASN
4	DO	8	ASN
4	DO	13	ASN
4	DO	57	ASN
5	DP	173	ASN
5	DP	278	GLN
6	DQ	352	HIS
6	DQ	359	ASN
7	BA	129	ASN
7	BA	139	ASN
9	FB	91	GLN
9	FB	143	GLN
9	FB	152	ASN
9	FB	158	ASN
9	FB	229	HIS
9	FB	231	ASN
10	PA	77	ASN
10	PA	87	HIS
10	PA	123	ASN
10	PA	267	GLN
10	PA	272	ASN
10	PA	353	ASN
10	PA	403	GLN
10	PA	410	ASN
10	PA	441	GLN
10	PA	507	GLN
10	PA	531	ASN
10	PA	601	ASN
10	PA	671	ASN
10	PA	678	ASN
10	PA	703	GLN

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Mol	Chain	Res	Type
10	PA	721	HIS
10	PA	731	ASN
10	PA	739	ASN
10	PA	740	GLN
10	PA	780	ASN
10	PA	792	ASN
10	PA	997	ASN
10	PA	1044	HIS
10	PA	1101	GLN
10	PA	1267	ASN
10	PA	1332	GLN
10	PA	1462	GLN
11	PB	43	GLN
11	PB	90	GLN
11	PB	139	GLN
11	PB	143	GLN
11	PB	227	ASN
11	PB	245	GLN
11	PB	452	ASN
11	PB	468	GLN
11	PB	577	HIS
11	PB	585	ASN
11	PB	593	GLN
11	PB	639	HIS
11	PB	650	ASN
11	PB	717	ASN
11	PB	731	GLN
11	PB	749	HIS
11	PB	906	GLN
11	PB	941	GLN
11	PB	1021	HIS
11	PB	1025	ASN
11	PB	1030	ASN
11	PB	1094	GLN
11	PB	1120	ASN
11	PB	1133	HIS
11	PB	1142	ASN
12	PC	6	GLN
12	PC	83	GLN
12	PC	114	HIS
12	PC	157	GLN
12	PC	177	ASN

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Mol	Chain	Res	Type
12	PC	262	GLN
12	PC	268	GLN
13	PD	34	ASN
13	PD	47	GLN
13	PD	48	ASN
13	PD	89	GLN
13	PD	129	GLN
13	PD	135	GLN
14	PE	92	GLN
14	PE	95	GLN
14	PE	107	GLN
14	PE	108	GLN
14	PE	116	GLN
14	PE	210	GLN
16	PG	139	GLN
17	PH	29	HIS
17	PH	126	GLN
18	PI	84	HIS
18	PI	91	HIS
19	PJ	26	GLN
20	PK	2	ASN
20	PK	29	ASN
20	PK	40	HIS
22	DA	401	ASN
22	DA	569	ASN
22	DA	860	ASN
22	DA	896	GLN
22	DA	1058	HIS
23	DB	30	HIS
23	DB	176	HIS
23	DB	183	GLN
23	DB	184	ASN
23	DB	235	HIS
23	DB	272	GLN
23	DB	348	GLN
23	DB	432	HIS
23	DB	439	HIS
23	DB	450	GLN
23	DB	509	ASN
23	DB	745	GLN
23	DB	750	GLN
23	DB	813	ASN

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Mol	Chain	Res	Type
23	DB	908	GLN
23	DB	916	ASN
24	DD	912	ASN
24	DD	922	GLN
24	DD	925	ASN
24	DD	1053	GLN
24	DD	1075	HIS
25	DE	268	HIS
25	DE	327	ASN
25	DE	351	GLN
25	DE	471	GLN
25	DE	616	HIS
25	DE	640	ASN
26	DF	244	GLN
26	DF	270	ASN
26	DF	273	GLN
26	DF	275	ASN
26	DF	349	ASN
27	DG	48	HIS
28	DH	145	HIS
28	DH	173	GLN
29	DI	21	GLN
29	DI	38	GLN
29	DI	60	HIS
29	DI	76	GLN
29	DI	81	GLN
29	DI	98	GLN
30	DJ	160	GLN
30	DJ	173	HIS
31	DL	105	HIS
31	DL	117	GLN
24	Dd	912	ASN
24	Dd	1069	ASN
25	De	294	ASN
25	De	320	HIS
25	De	336	HIS
25	De	424	GLN
25	De	616	HIS
26	Df	325	ASN
29	Di	81	GLN
31	Dl	73	ASN
31	Dl	105	HIS

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Mol	Chain	Res	Type
34	Dm	107	ASN
35	EA	142	ASN
36	EB	95	HIS
36	EB	193	ASN
36	EB	204	ASN
36	EB	209	GLN
37	1	187	ASN
37	1	210	ASN
37	1	298	ASN
37	1	300	ASN
37	1	328	GLN
37	1	384	HIS
37	1	393	GLN
37	1	501	GLN
37	1	520	ASN
37	1	534	ASN
38	2	49	HIS
38	2	234	HIS
38	2	275	HIS
38	2	323	HIS
38	2	365	ASN
38	2	376	HIS
39	3	92	ASN
39	3	148	ASN
39	3	235	GLN
39	3	237	GLN
40	4	54	ASN
40	4	64	GLN
40	4	117	ASN
40	4	211	GLN
40	4	239	GLN
40	4	289	ASN
40	4	458	GLN
41	5	3	ASN
41	5	36	GLN
41	5	64	ASN
42	6	320	GLN
42	6	330	ASN
42	6	433	GLN
42	6	497	GLN
42	6	665	GLN
43	7	164	HIS

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Mol	Chain	Res	Type
43	7	241	ASN
43	7	304	HIS
43	7	347	GLN
43	7	522	ASN
43	7	613	HIS
44	c	10	ASN
44	c	41	ASN
44	c	237	GLN
44	c	306	HIS
44	c	311	GLN
45	e	97	GLN
45	e	105	GLN
45	e	132	HIS
45	e	140	GLN
46	b	66	GLN
46	b	129	GLN
46	b	136	HIS
47	l	72	GLN
47	l	102	ASN
47	l	151	GLN
48	m	26	GLN
48	m	50	ASN
48	m	80	GLN
48	m	90	ASN
48	m	106	GLN
48	m	116	GLN
49	a	66	GLN
49	a	87	GLN
49	a	131	ASN
49	a	146	ASN
49	a	254	ASN
49	a	333	GLN
49	a	359	HIS
49	a	413	HIS
49	a	459	ASN
50	d	63	ASN
50	d	64	GLN
50	d	71	HIS
50	d	85	ASN
50	d	90	HIS
50	d	94	GLN
50	d	111	GLN

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Mol	Chain	Res	Type
50	d	113	GLN
50	d	119	GLN
50	d	127	GLN
51	f	72	HIS
51	f	84	GLN
51	f	87	GLN
51	f	107	GLN
51	f	127	GLN
52	g	47	ASN
52	g	50	GLN
52	g	74	HIS
52	g	88	ASN
52	g	124	ASN
53	h	18	GLN
53	h	60	ASN
53	h	102	HIS
54	i	70	HIS
54	i	85	GLN
54	i	108	HIS
54	i	117	GLN
55	j	11	HIS
55	j	38	ASN
55	j	56	GLN
56	k	41	ASN
56	k	66	GLN
56	k	77	GLN
56	k	79	HIS
56	k	91	GLN
57	n	267	HIS
57	n	304	GLN
57	n	311	GLN
57	n	330	HIS
57	n	411	GLN
57	n	507	GLN
57	n	521	GLN
57	n	532	ASN
57	n	590	GLN
57	n	668	HIS
57	n	841	ASN
57	n	880	ASN
57	n	909	GLN
58	o	701	ASN

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Mol	Chain	Res	Type
58	o	705	HIS
59	q	139	GLN
59	q	262	GLN
59	q	264	GLN
59	q	290	HIS
59	q	292	GLN
59	q	340	GLN
59	q	367	HIS
59	q	437	HIS
59	q	461	GLN
59	q	496	ASN
59	q	506	HIS
59	q	533	GLN
59	q	547	GLN
59	q	565	ASN
59	q	626	GLN
59	q	634	ASN
60	r	156	ASN
60	r	192	GLN
61	s	82	ASN
62	t	8	GLN
62	t	103	GLN
62	t	178	ASN
63	u	7	GLN
63	u	18	GLN
63	u	21	ASN
63	u	86	GLN
63	u	97	ASN
64	v	16	GLN
64	v	32	ASN
64	v	62	HIS
64	v	103	GLN
65	z	483	ASN
65	z	527	GLN
65	z	549	GLN
65	z	556	GLN
65	z	567	GLN
65	z	585	HIS
65	z	592	ASN
66	x	8	GLN
66	x	49	GLN
66	x	111	HIS

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Mol	Chain	Res	Type
66	x	217	GLN
66	x	361	ASN
66	x	380	ASN
66	x	402	ASN
66	x	404	GLN
66	x	472	ASN
66	x	502	HIS
66	x	544	HIS
67	w	46	GLN
67	w	113	GLN
67	w	293	HIS
67	w	295	GLN
67	w	357	HIS
67	w	358	GLN
67	w	378	GLN
67	w	421	HIS
67	w	513	ASN
67	w	726	ASN
67	w	783	GLN
67	w	805	GLN
67	w	822	HIS
67	w	851	ASN
67	w	874	HIS
67	w	921	HIS
67	w	923	ASN
67	w	925	HIS
67	w	972	HIS
67	w	1059	ASN
67	w	1134	GLN
67	w	1300	HIS
67	w	1320	ASN
68	p	63	HIS
68	p	80	HIS
68	p	225	ASN
68	p	272	ASN
68	p	282	HIS
68	p	387	HIS
68	p	400	GLN
68	p	435	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
73	SF4	7	801	43	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
73	SF4	7	801	43	-	-	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.

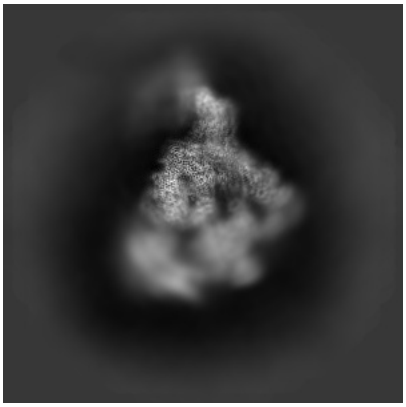
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-31204. These allow visual inspection of the internal detail of the map and identification of artifacts.

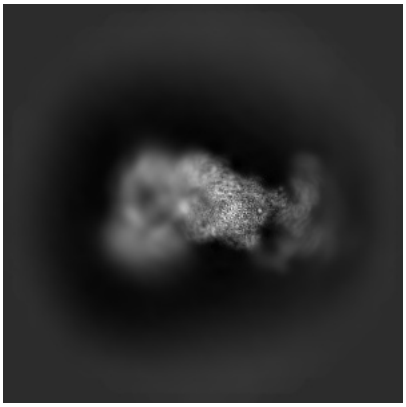
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

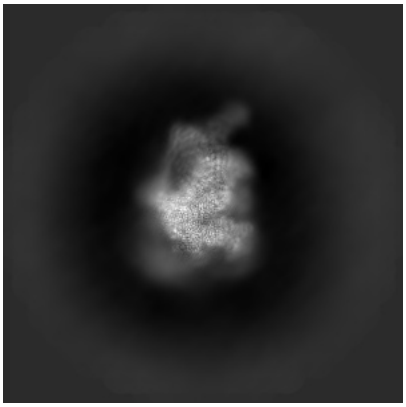
6.1.1 Primary map



X



Y

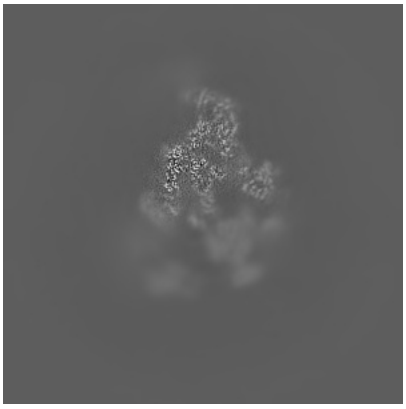


Z

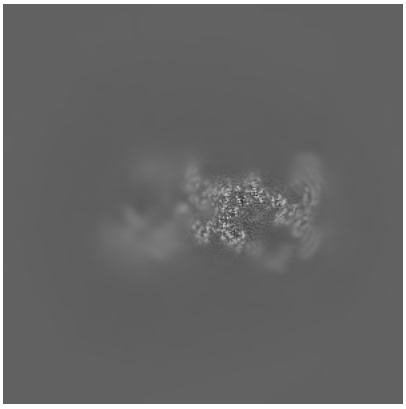
The images above show the map projected in three orthogonal directions.

6.2 Central slices

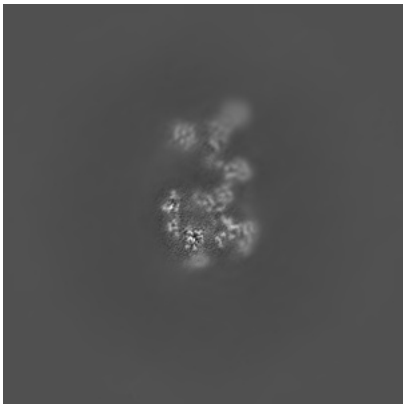
6.2.1 Primary map



X Index: 256



Y Index: 256

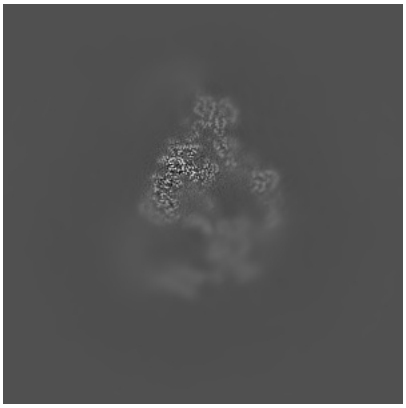


Z Index: 256

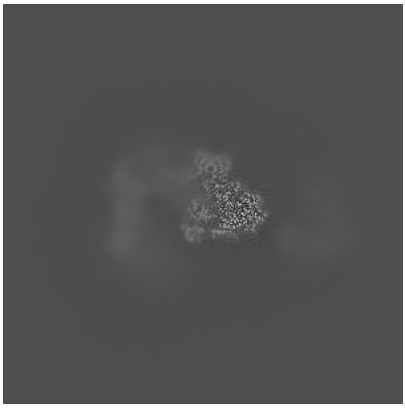
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

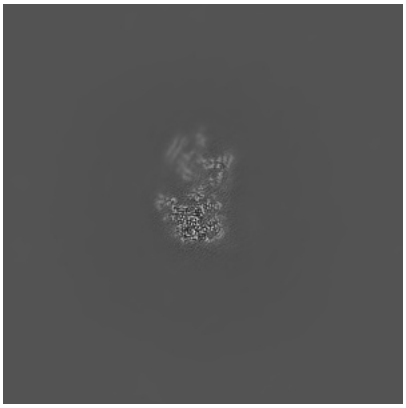
6.3.1 Primary map



X Index: 245



Y Index: 219

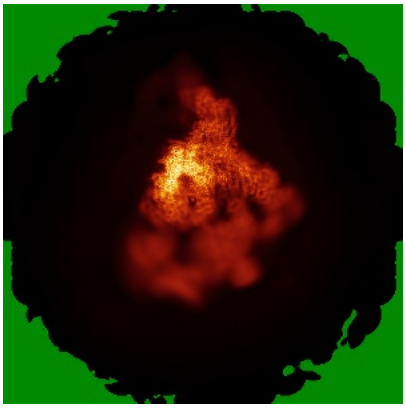


Z Index: 301

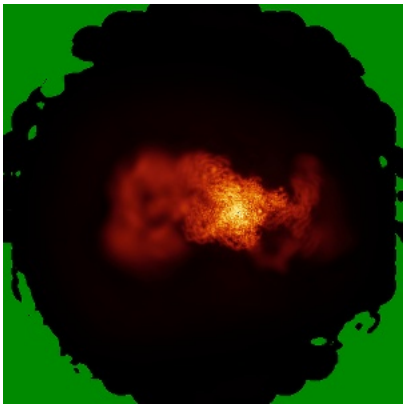
The images above show the largest variance slices of the map in three orthogonal directions.

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

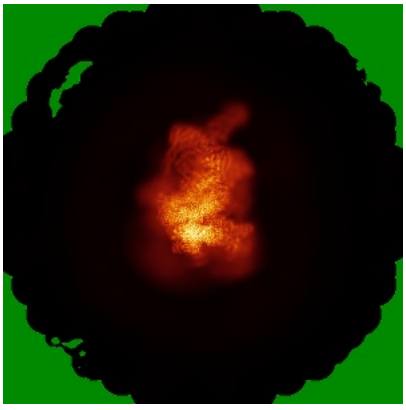
6.4.1 Primary map



X



Y

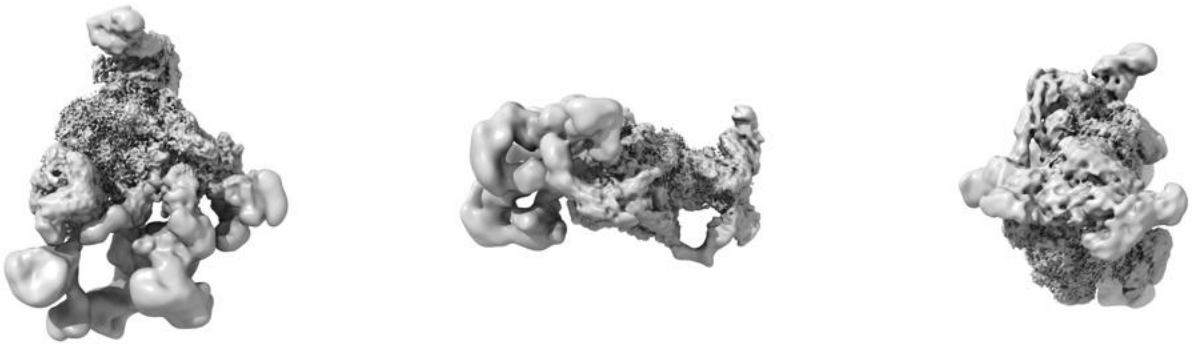


Z

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

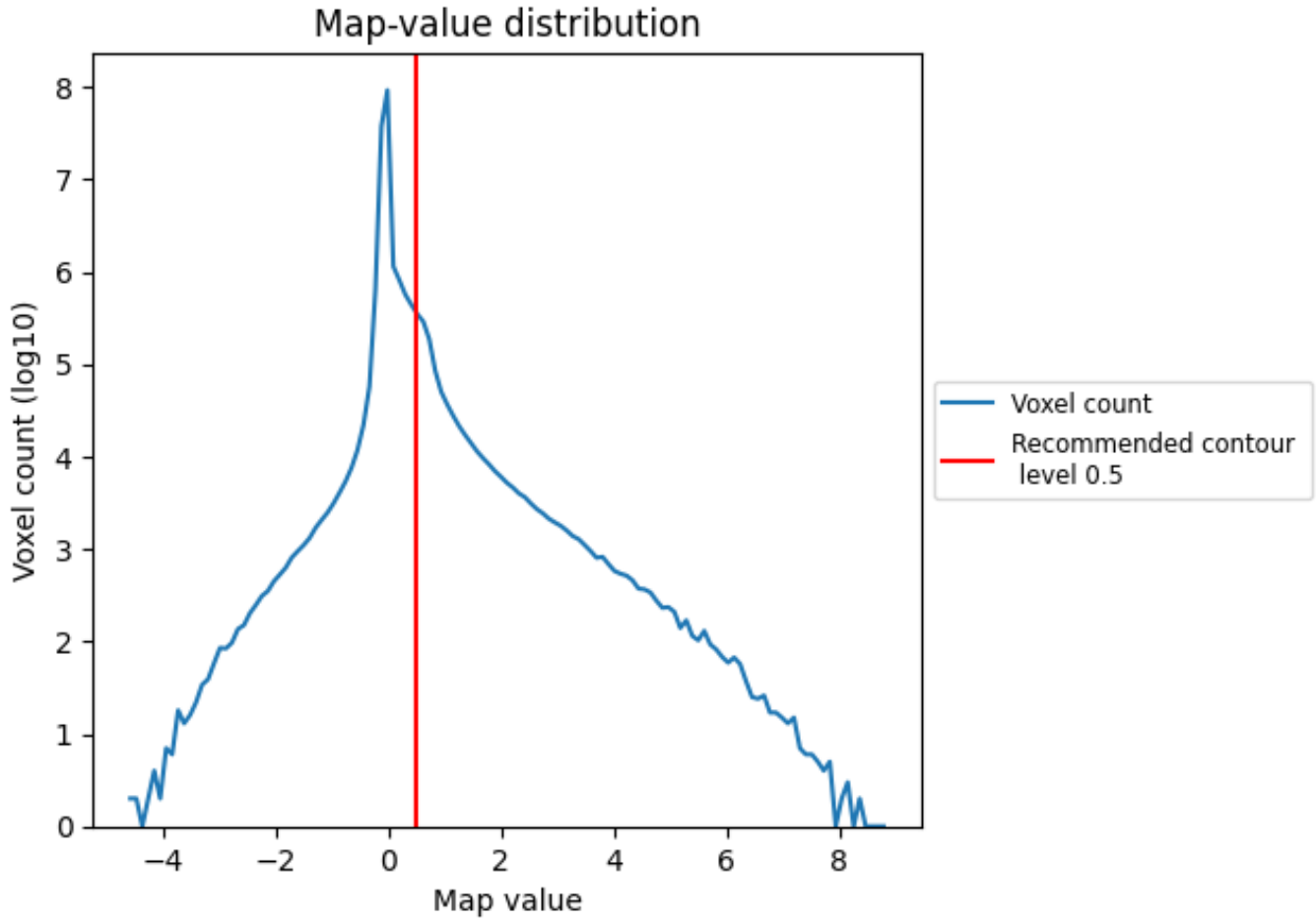
6.6 Mask visualisation (i)

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

7 Map analysis

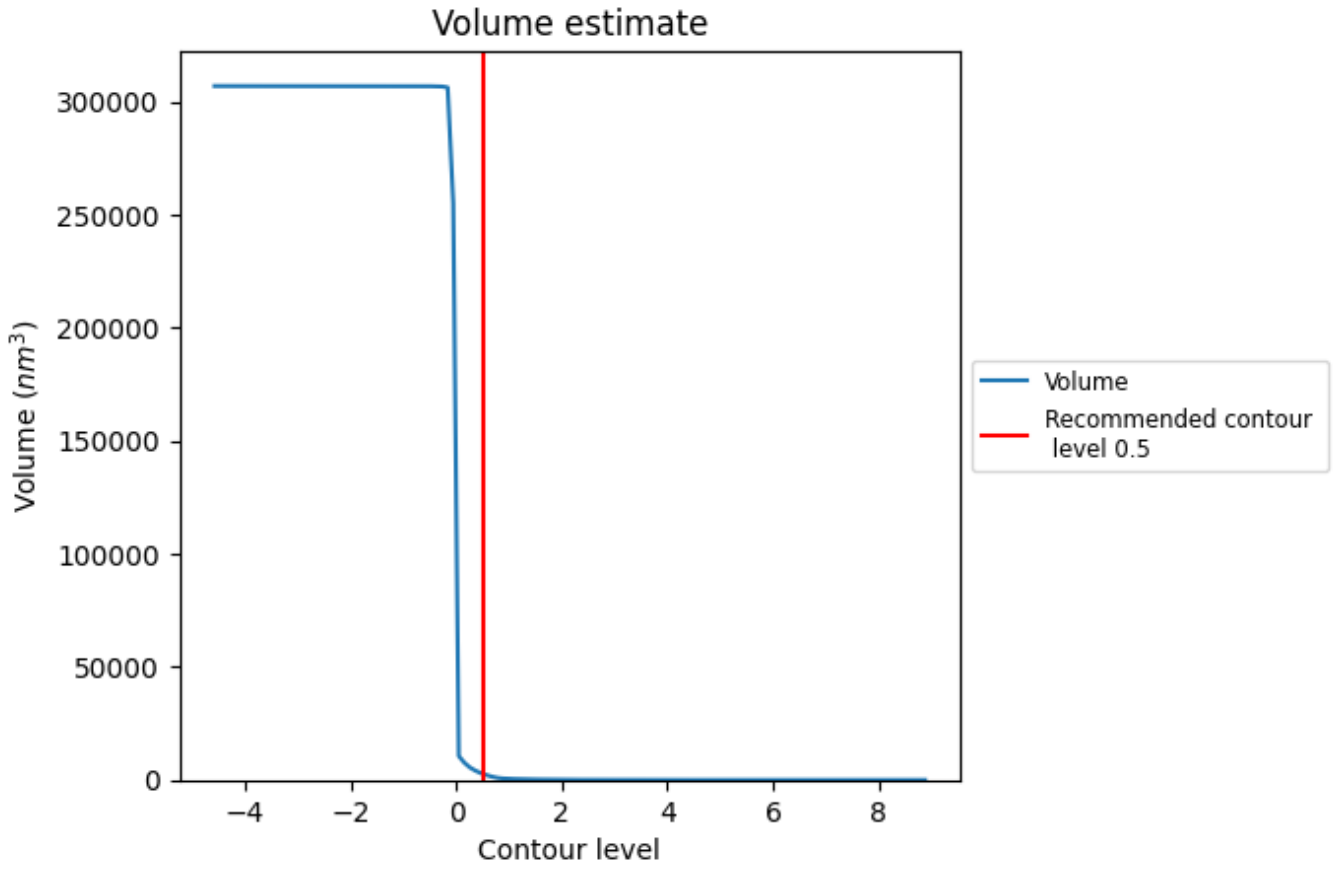
This section contains the results of statistical analysis of the map.

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.

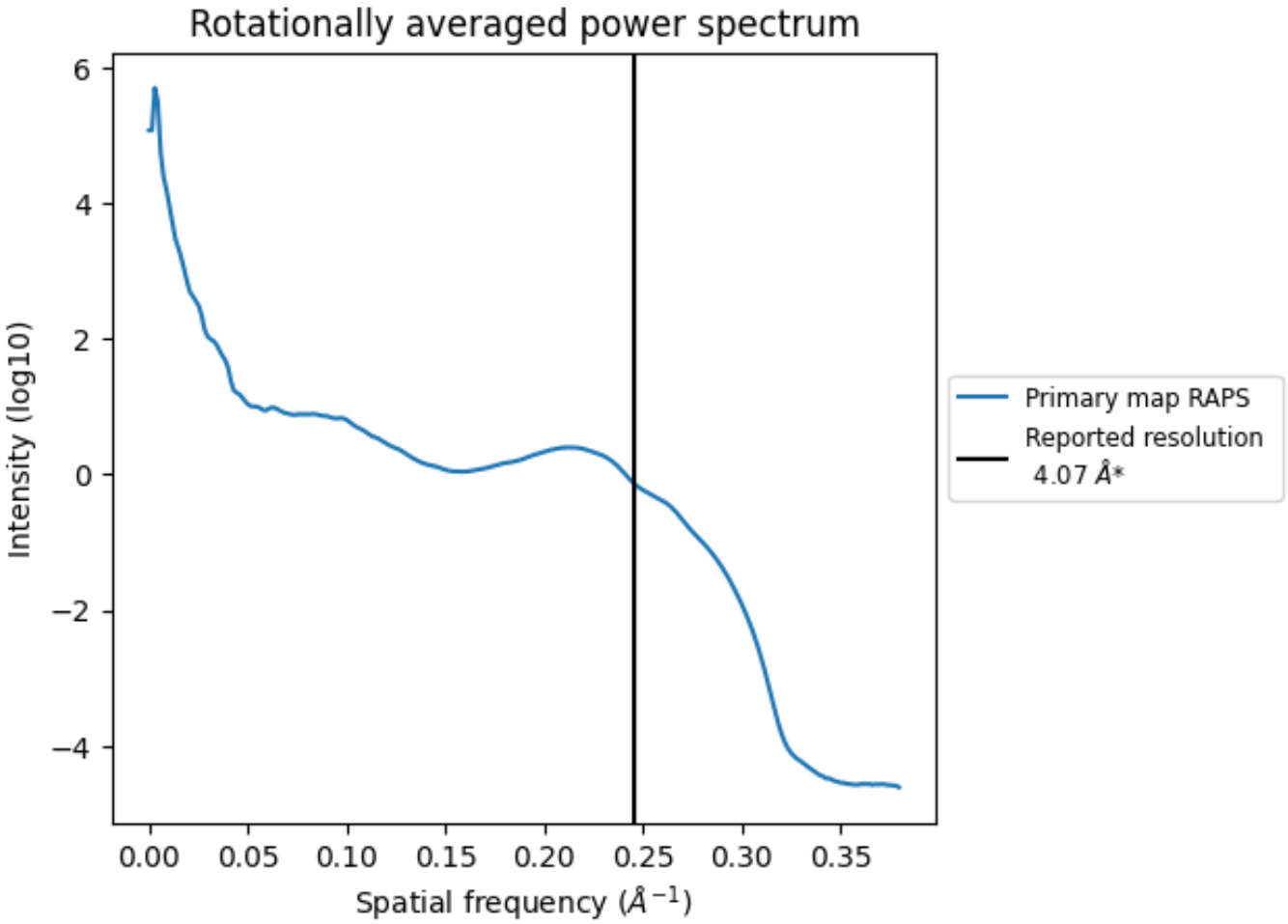
7.2 Volume estimate



The volume at the recommended contour level is 2784 nm^3; this corresponds to an approximate mass of 2515 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 0.246 Å^{-1}

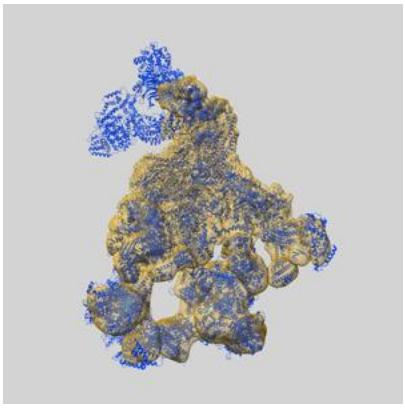
8 Fourier-Shell correlation

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

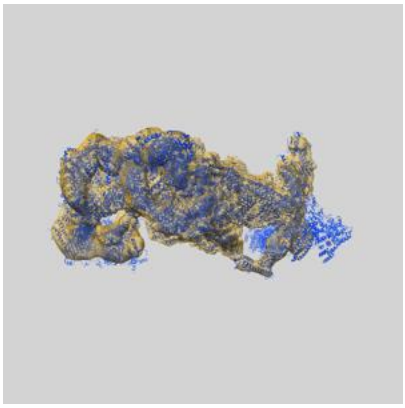
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-31204 and PDB model 7ENA. Per-residue inclusion information can be found in section 3 on page 18.

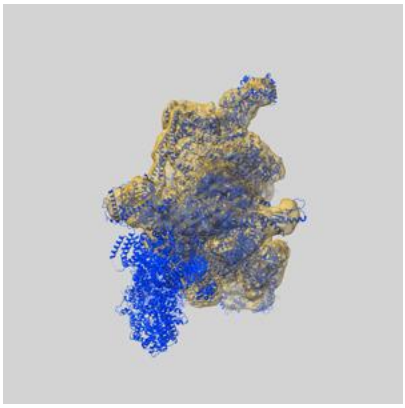
9.1 Map-model overlay



X



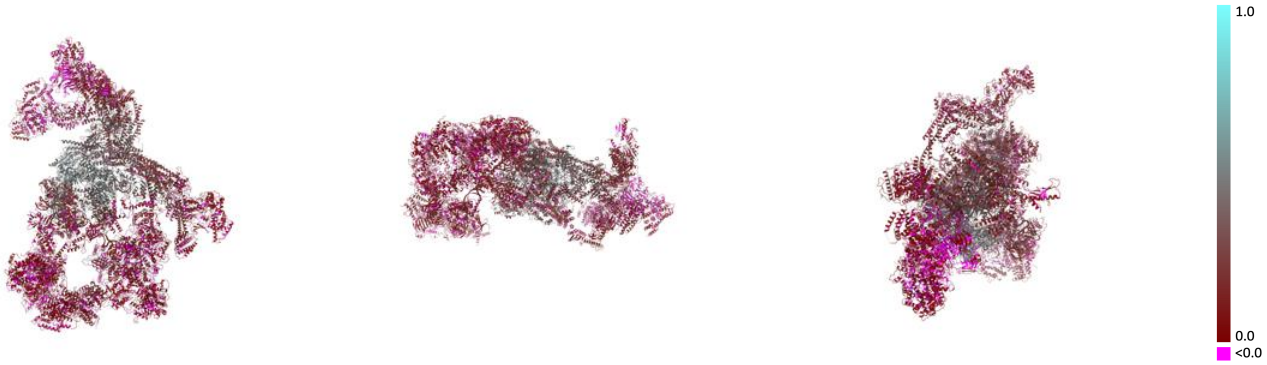
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5 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.

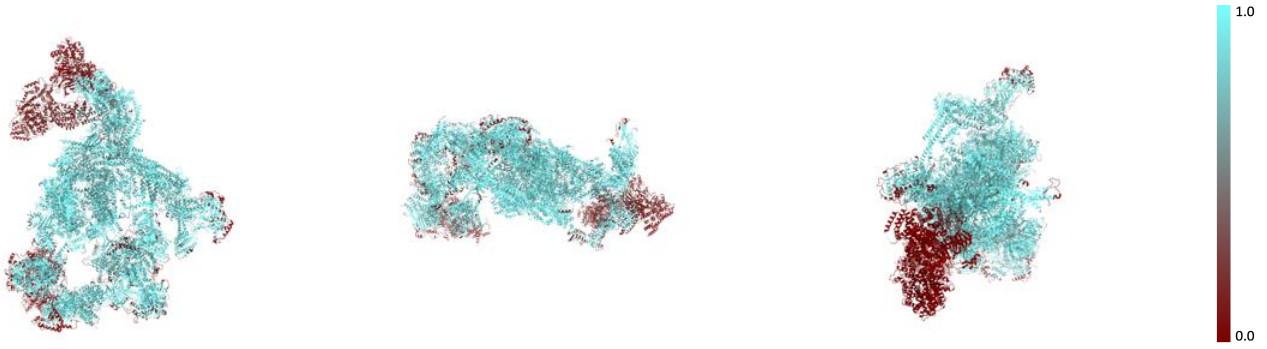
9.2 Q-score mapped to coordinate model (i)



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.

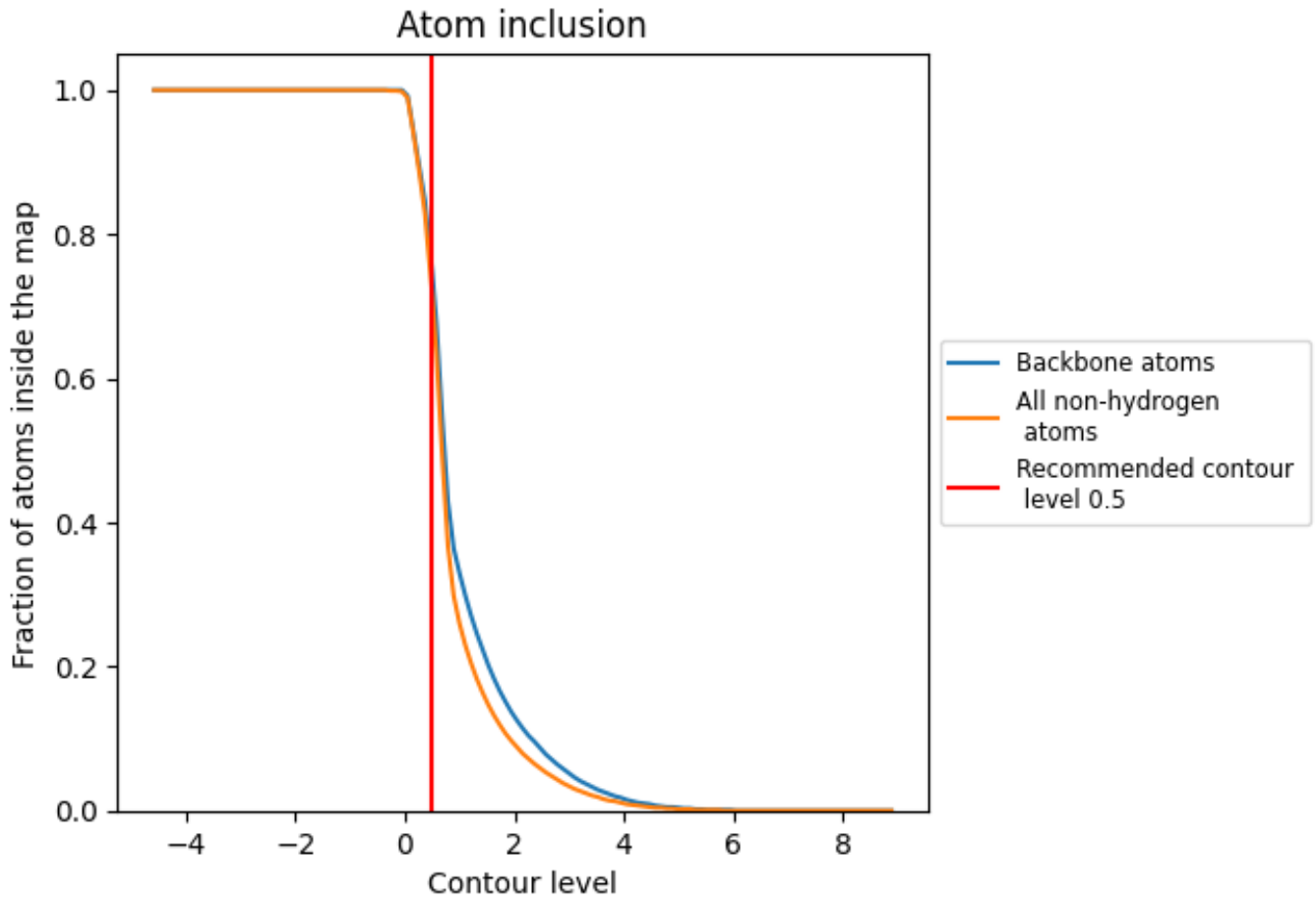
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.5).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7170	0.1680
0	0.7760	0.1210
1	0.6320	0.0350
2	0.8070	0.0600
3	0.9160	0.0610
4	0.7590	0.0700
5	0.8320	0.0600
6	0.8640	0.0830
7	0.9110	0.1070
8	0.8330	0.1070
9	0.6160	0.0680
BA	0.9210	0.2770
DA	0.8310	0.0650
DB	0.8880	0.0600
DD	0.7420	0.0830
DE	0.8120	0.0650
DF	0.7670	0.0520
DG	0.8530	0.0550
DH	0.8340	0.0500
DI	0.8170	0.0540
DJ	0.8740	0.0580
DL	0.5260	0.0640
DO	0.9130	0.1060
DP	0.9510	0.1750
DQ	0.7990	0.1050
Dc	0.0000	0.0350
Dd	0.0000	0.0350
De	0.0040	0.0330
Df	0.4390	0.0530
Di	0.0000	0.0290
Dj	0.0000	0.0260
Dk	0.0000	0.0420
Dl	0.0000	0.0460
Dm	0.0000	0.0440
EA	0.9470	0.1860

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Chain	Atom inclusion	Q-score
EB	0.9150	0.1040
FA	0.8960	0.0700
FB	0.8840	0.1080
PA	0.9540	0.4180
PB	0.9500	0.4520
PC	0.9630	0.4890
PD	0.9350	0.4060
PE	0.9720	0.3600
PF	0.9770	0.5210
PG	0.9610	0.4380
PH	0.9610	0.4530
PI	0.9710	0.3540
PJ	0.9740	0.5150
PK	0.9360	0.4430
PL	0.9580	0.4470
X	0.9510	0.1560
Y	0.9660	0.1760
a	0.5990	0.0940
b	0.7900	0.1460
c	0.8980	0.2830
d	0.9100	0.1440
e	0.8860	0.1890
f	0.9330	0.2460
g	0.9520	0.1380
h	0.8910	0.2730
i	0.9110	0.1540
j	0.9320	0.1050
k	0.9320	0.2870
l	0.9220	0.1950
m	0.9190	0.1730
n	0.8870	0.1890
o	0.9030	0.1670
p	0.0000	-0.0140
q	0.9170	0.3040
r	0.9260	0.3830
s	0.9400	0.1130
t	0.8860	0.3610
u	0.9390	0.1550
v	0.9140	0.3410
w	0.0420	0.0510
x	0.1950	0.0640
z	0.8980	0.1220