Full wwPDB EM Validation Report ⓘ

Nov 22, 2022 – 12:19 PM JST

PDB ID	:	7EDX
EMDB ID	:	EMD-31075
Title	:	p53-bound TFIID-based core PIC on HDM2 promoter
Authors	:	Chen, X.; Qi, Y.; Hou, H.; Wang, X.; Wu, Z.; Li, J.; Xu, Y.
Deposited on	:	2021-03-17
Resolution	:	4.50 Å(reported)

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

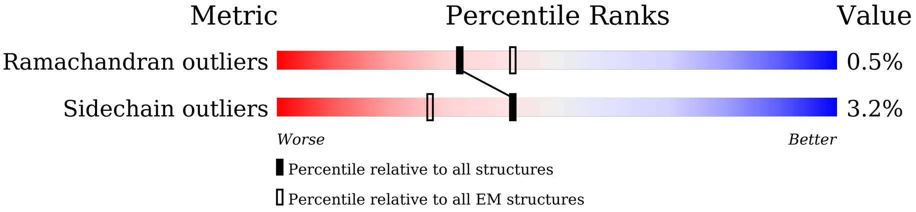
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance

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

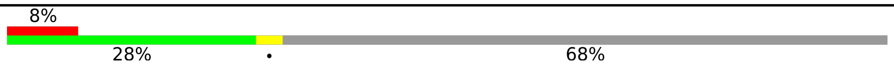
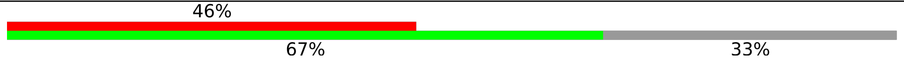
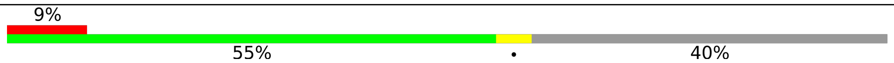
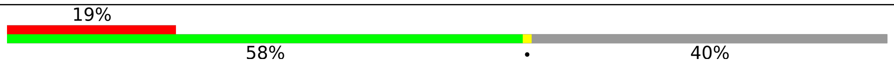
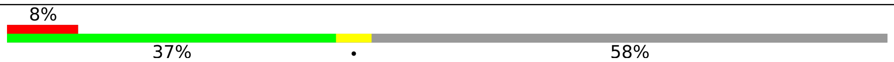
The reported resolution of this entry is 4.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	1872	
2	B	1199	
3	D	1085	
3	d	1085	
4	E	800	
4	e	800	
5	F	677	
5	f	677	
6	G	349	

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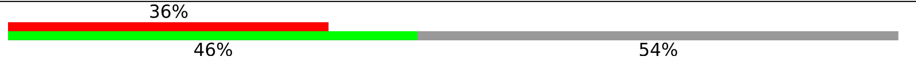
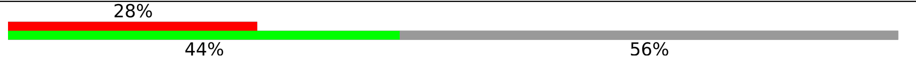
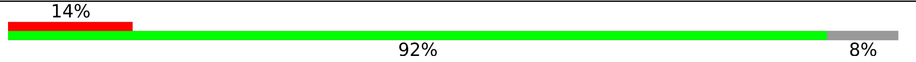
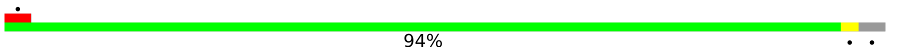
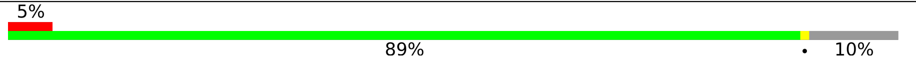
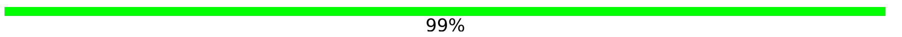
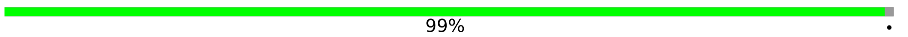
Mol	Chain	Length	Quality of chain
7	H	310	 6% 65% • 33%
8	I	264	 • 45% 55%
8	i	264	 36% 46% 54%
9	J	218	 41% 59%
9	j	218	 28% 44% 56%
10	L	161	 47% • 53%
10	l	161	 57% 65% • 34%
11	O	109	 76% 12% • 11%
12	P	339	 48% • 48%
13	Q	376	 • 30% • 68%
14	R	316	 74% • 22%
15	S	517	 • 24% • 74%
16	T	249	 • 43% • 55%
17	X	84	 10% 90% • 8%
18	Y	84	 14% 92% 8%
19	c	929	 8% 13% 86%
20	k	211	 40% 46% 54%
21	m	124	 70% 69% • 30%
22	o	1970	 • 71% • 28%
23	p	1174	 • 94% • •
24	q	275	 93% 7%
25	r	142	 5% 89% • 10%
26	s	210	 99%
27	t	127	 62% 38%
28	v	150	 99% •

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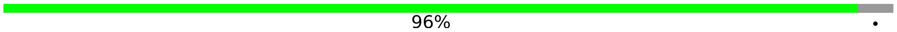
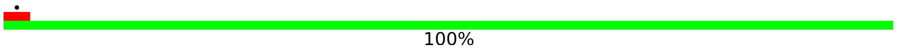
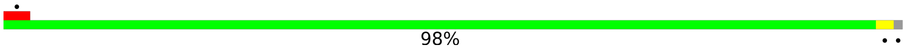
Mol	Chain	Length	Quality of chain
29	w	125	
30	x	67	
31	y	117	
32	z	58	
33	u	172	

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 81790 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 Transcription initiation factor TFIID subunit 1.

Mol	Chain	Residues	Atoms	AltConf	Trace
1	A	602	Total C N O S 4927 3142 858 899 28	0	0

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

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

- Molecule 3 is a protein called Transcription initiation factor TFIID subunit 4.

Mol	Chain	Residues	Atoms	AltConf	Trace
3	D	165	Total C N O S 1377 858 257 258 4	0	0
3	d	158	Total C N O S 1307 814 238 252 3	0	0

- Molecule 4 is a protein called Transcription initiation factor TFIID subunit 5.

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

- Molecule 5 is a protein called Transcription initiation factor TFIID subunit 6.

Mol	Chain	Residues	Atoms	AltConf	Trace
5	F	404	Total C N O S 3081 1954 537 572 18	0	0
5	f	403	Total C N O S 3081 1954 533 576 18	0	0

- Molecule 6 is a protein called Transcription initiation factor TFIID subunit 7.

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

- Molecule 7 is a protein called Transcription initiation factor TFIID subunit 8.

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

- Molecule 8 is a protein called Transcription initiation factor TFIID subunit 9.

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

- Molecule 9 is a protein called Transcription initiation factor TFIID subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	J	89	709	457	114	134	4	0	0
			Total	C	N	O	S		
9	j	95	759	488	124	143	4	0	0

- Molecule 10 is a protein called Transcription initiation factor TFIID subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	L	76	622	388	109	122	3	0	0
			Total	C	N	O	S		
10	l	107	876	547	158	166	5	0	0

- Molecule 11 is a protein called Transcription initiation factor IIA subunit 2.

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

- Molecule 12 is a protein called TATA-box-binding protein.

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

- Molecule 13 is a protein called Transcription initiation factor IIA subunit 1.

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

- Molecule 14 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	R	248	Total 1913	C 1200	N 338	O 358	S 17	0	0

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

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

- Molecule 16 is a protein called General transcription factor IIF subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	113	Total 876	C 545	N 160	O 169	S 2	0	0

- Molecule 17 is a DNA chain called DNA (84-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
17	X	77	Total 1582	C 752	N 283	O 470	P 77	0	0

- Molecule 18 is a DNA chain called DNA (84-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Y	77	Total 1575	C 747	N 297	O 454	P 77	0	0

- Molecule 19 is a protein called Transcription initiation factor TFIID subunit 3.

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

- Molecule 20 is a protein called Transcription initiation factor TFIID subunit 11.

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

- Molecule 21 is a protein called Transcription initiation factor TFIID subunit 13.

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

- Molecule 22 is a protein called RPB1.

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

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

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

- Molecule 24 is a protein called DNA-directed RNA polymerase II subunit RPB3.

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

- Molecule 25 is a protein called DNA-directed RNA polymerase II subunit RPB4.

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

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

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

- Molecule 27 is a protein called DNA-directed RNA polymerase II subunit F.

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

- Molecule 28 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 29 is a protein called DNA-directed RNA polymerase II subunit RPB9.

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

- Molecule 30 is a protein called RPB10.

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

- Molecule 31 is a protein called RNA_pol_L_2 domain-containing protein.

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

- Molecule 32 is a protein called RPB12.

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

- Molecule 33 is a protein called DNA-directed RNA polymerase II subunit RPB7.

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

- Molecule 34 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 35 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

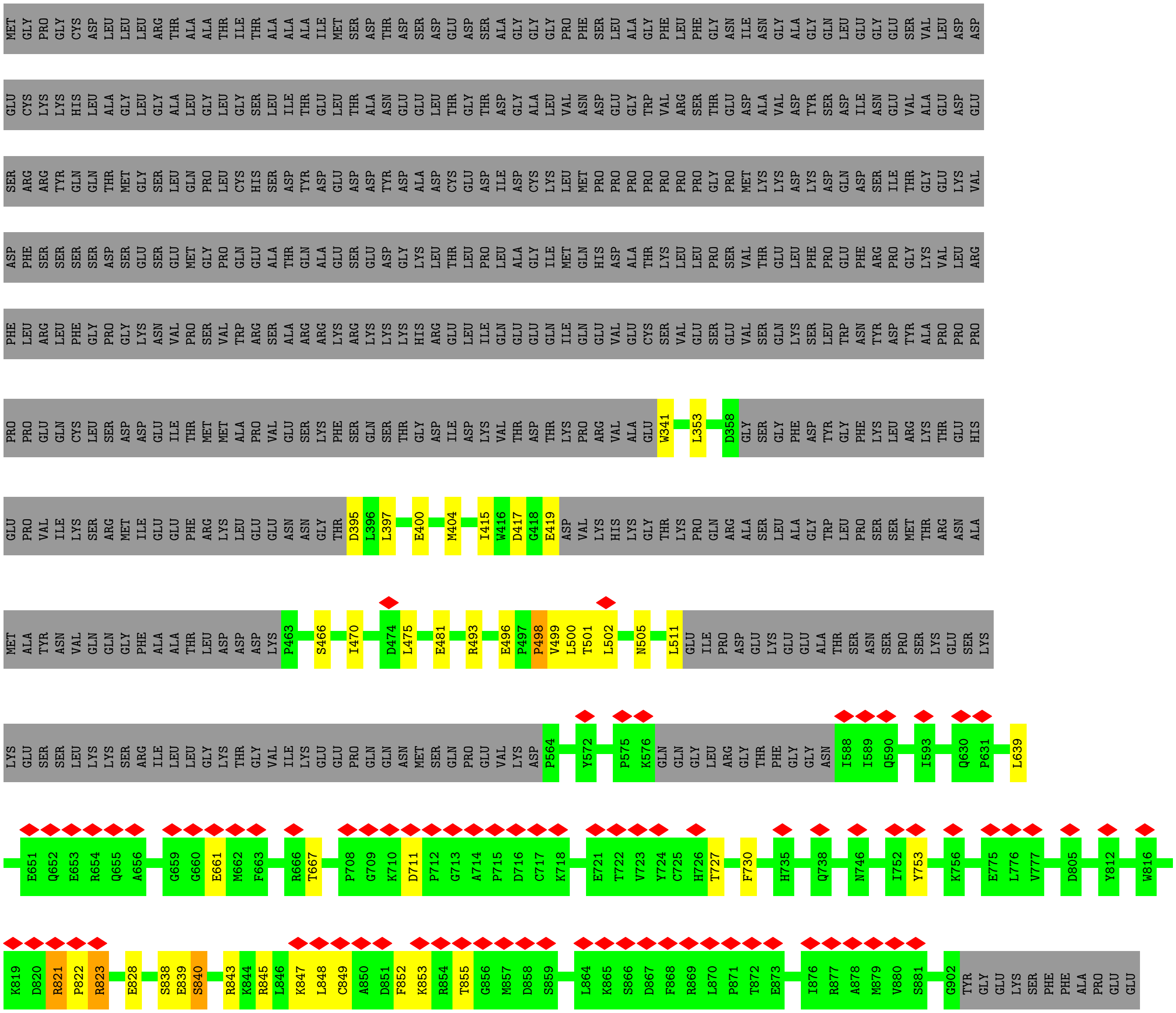
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
35	o	1	1	1	0

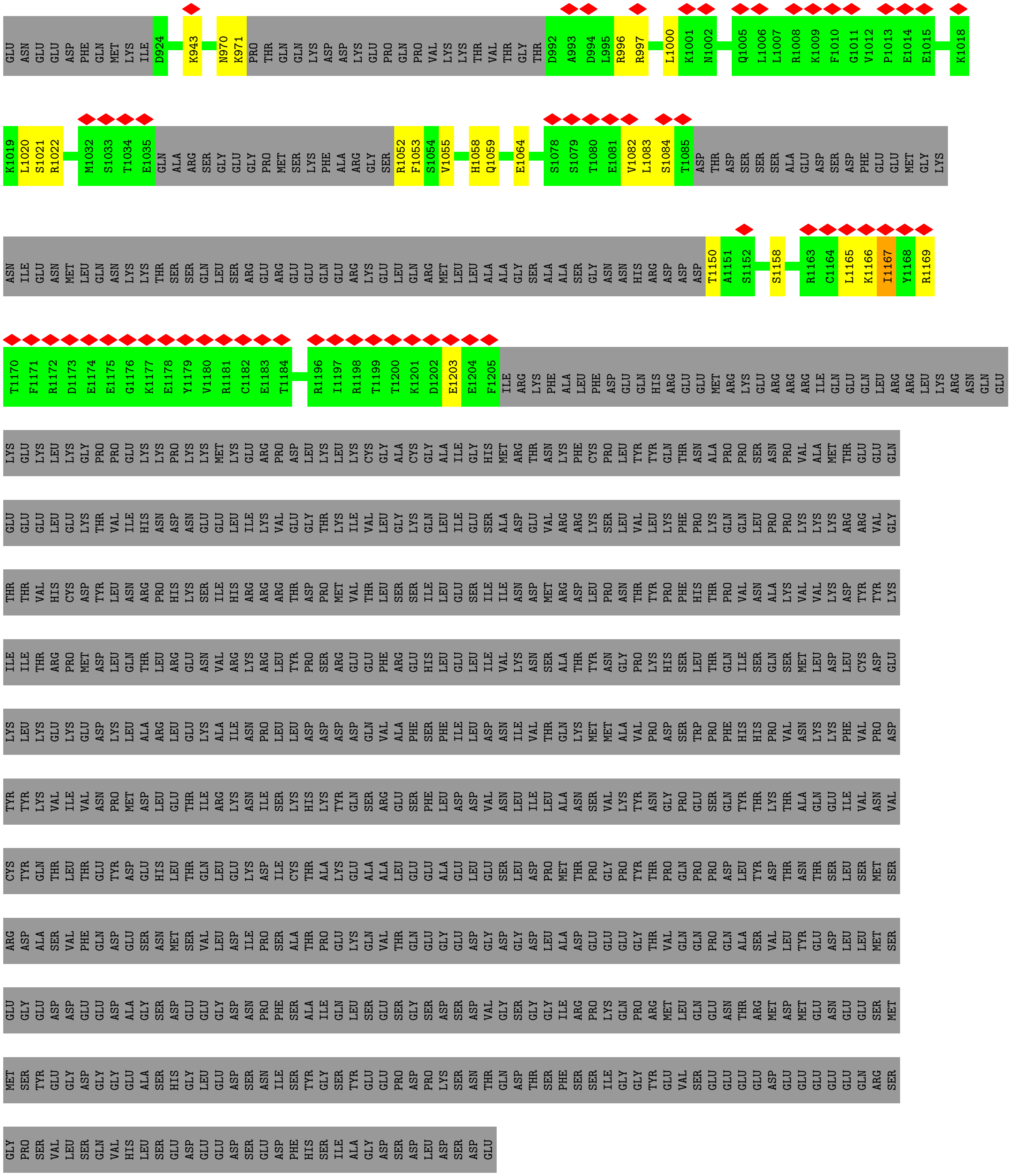
3 Residue-property plots ⓘ

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

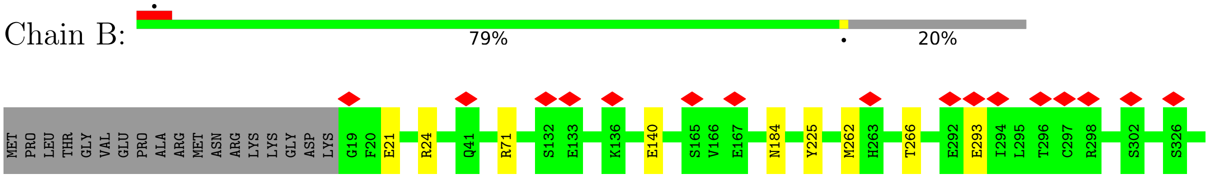
- Molecule 1: Transcription initiation factor TFIID subunit 1

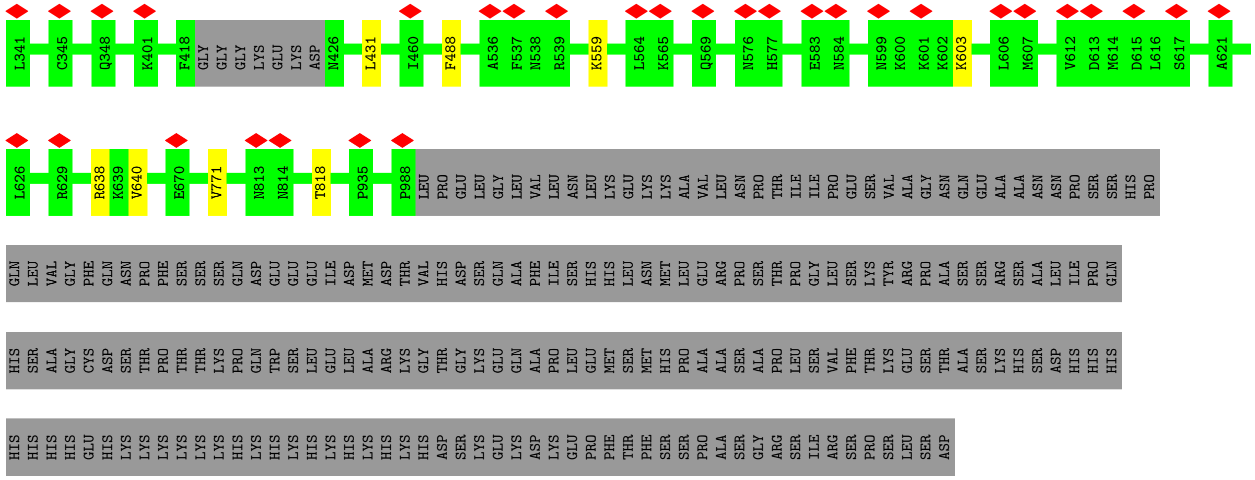
Chain A:





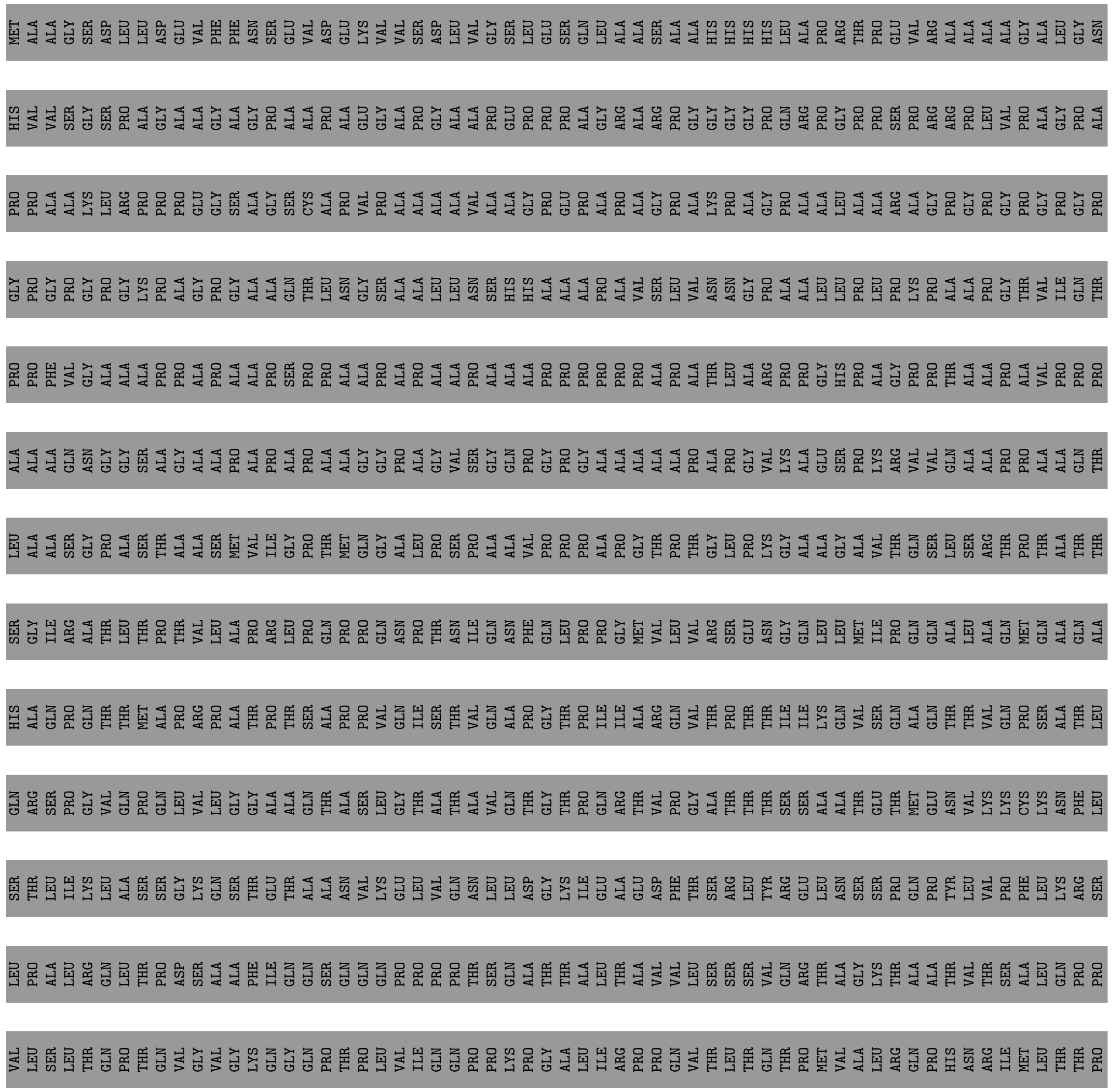
- Molecule 2: Transcription initiation factor TFIID subunit 2

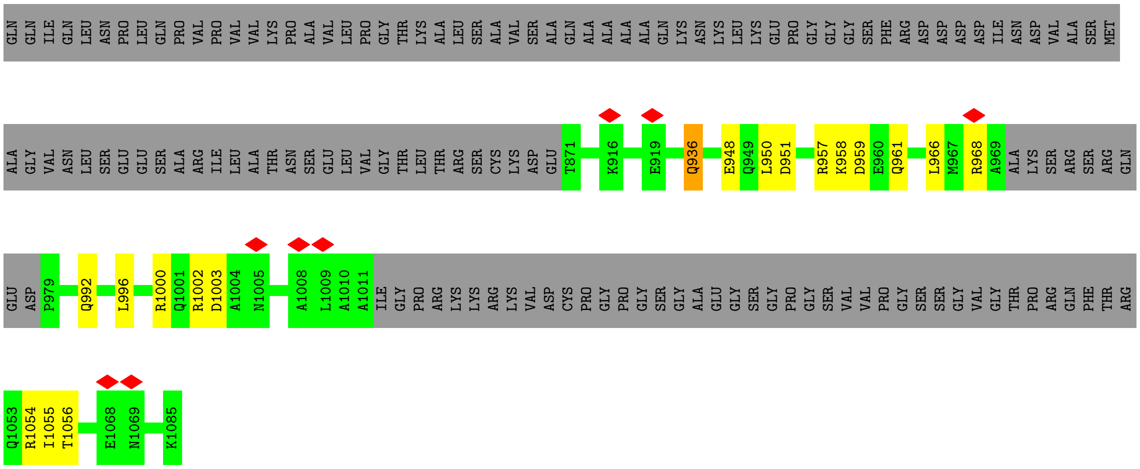




- Molecule 3: Transcription initiation factor TFIID subunit 4

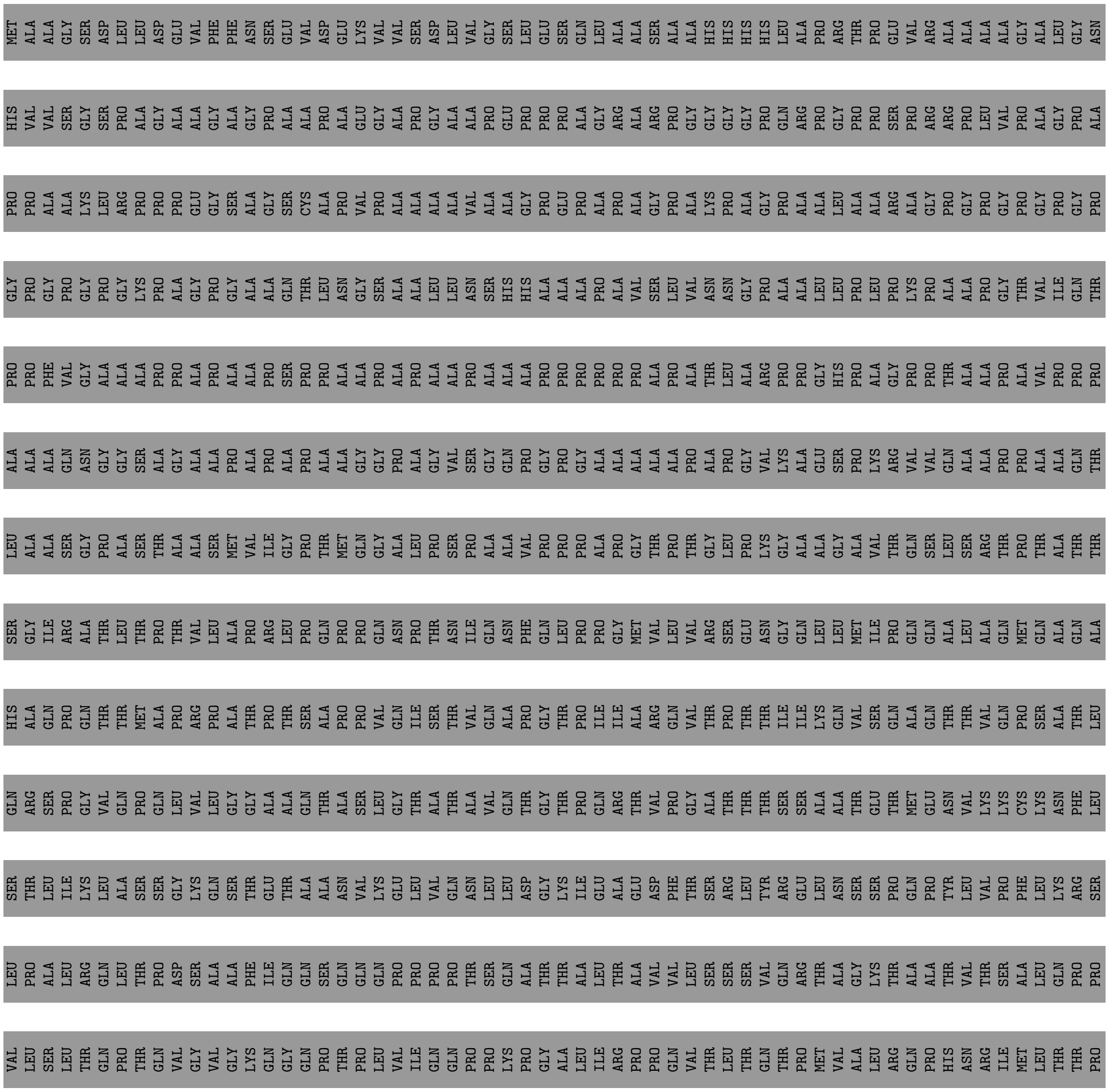
Chain D:

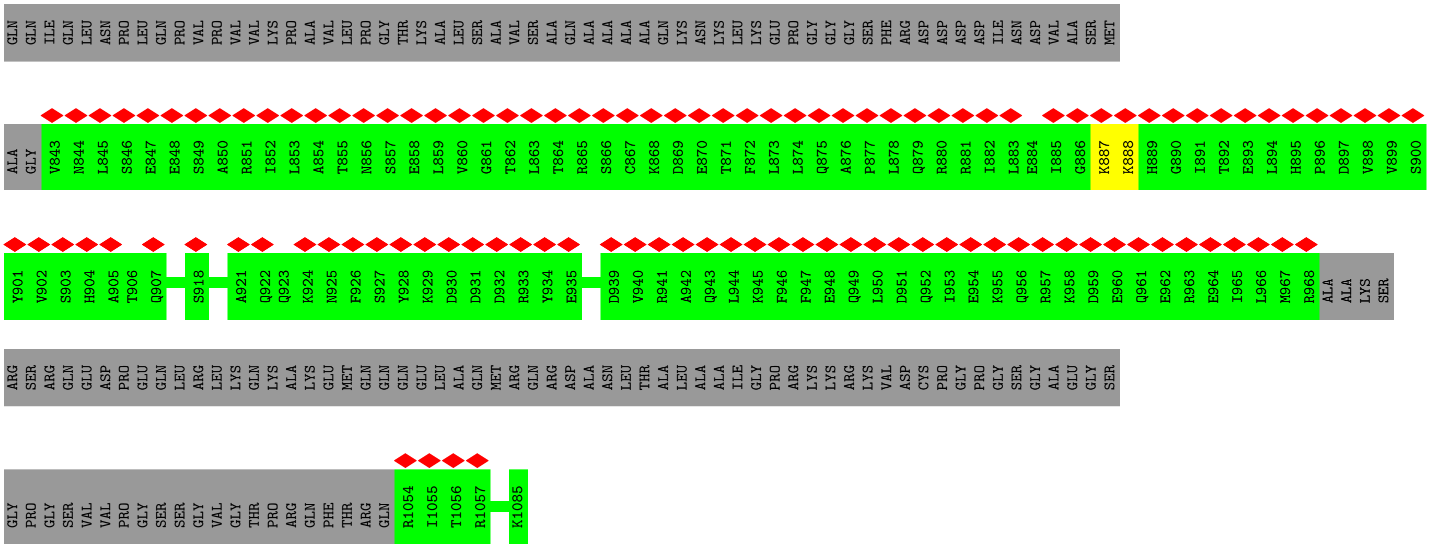




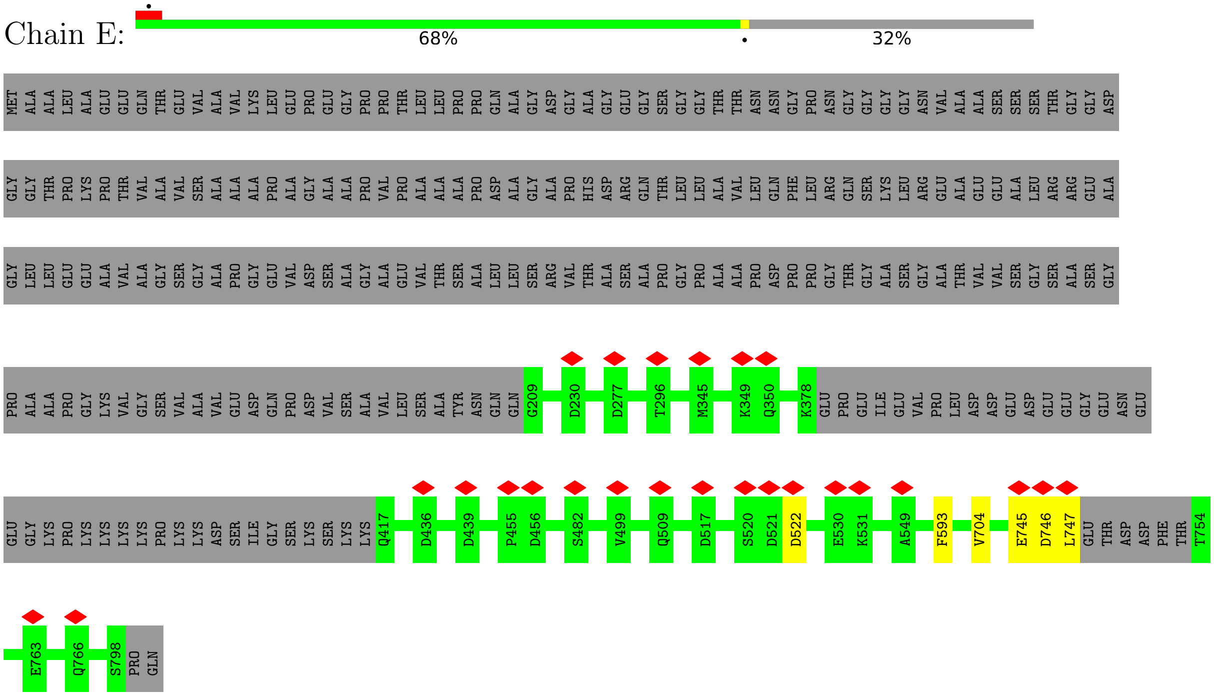
- Molecule 3: Transcription initiation factor TFIID subunit 4

Chain d:

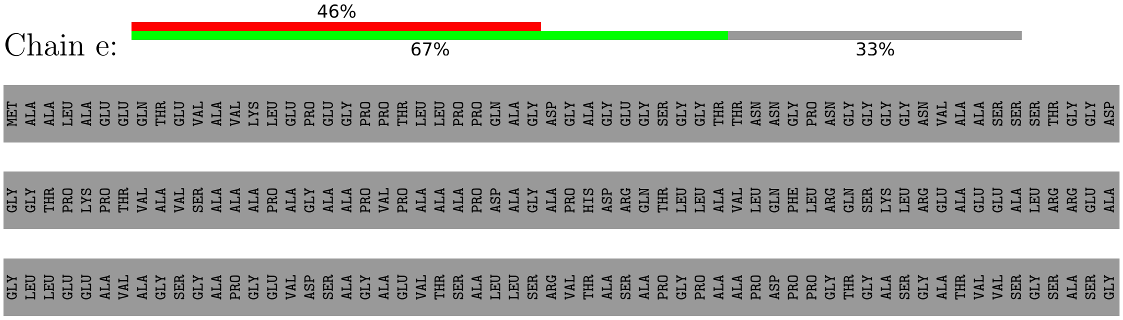


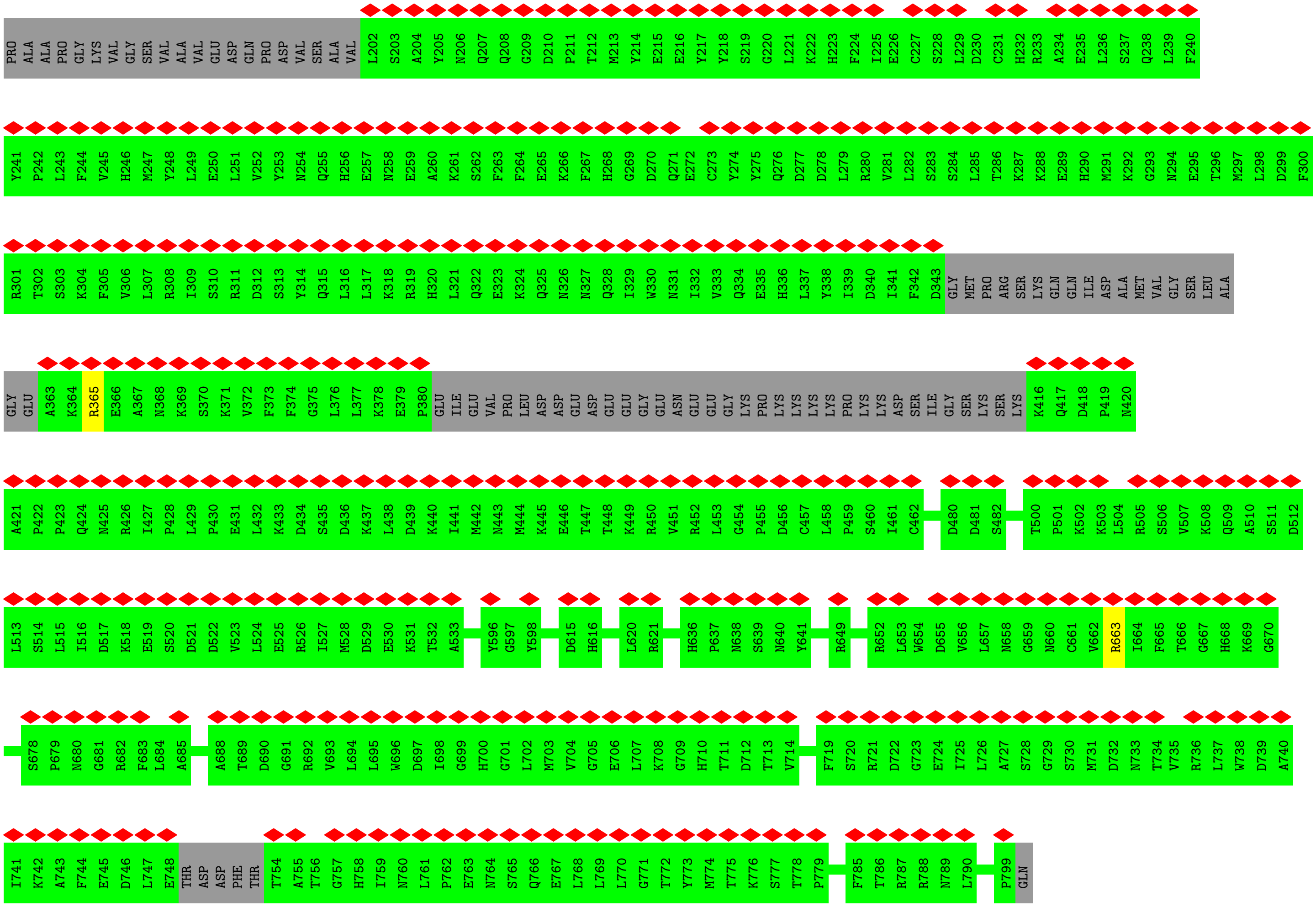


- Molecule 4: Transcription initiation factor TFIID subunit 5



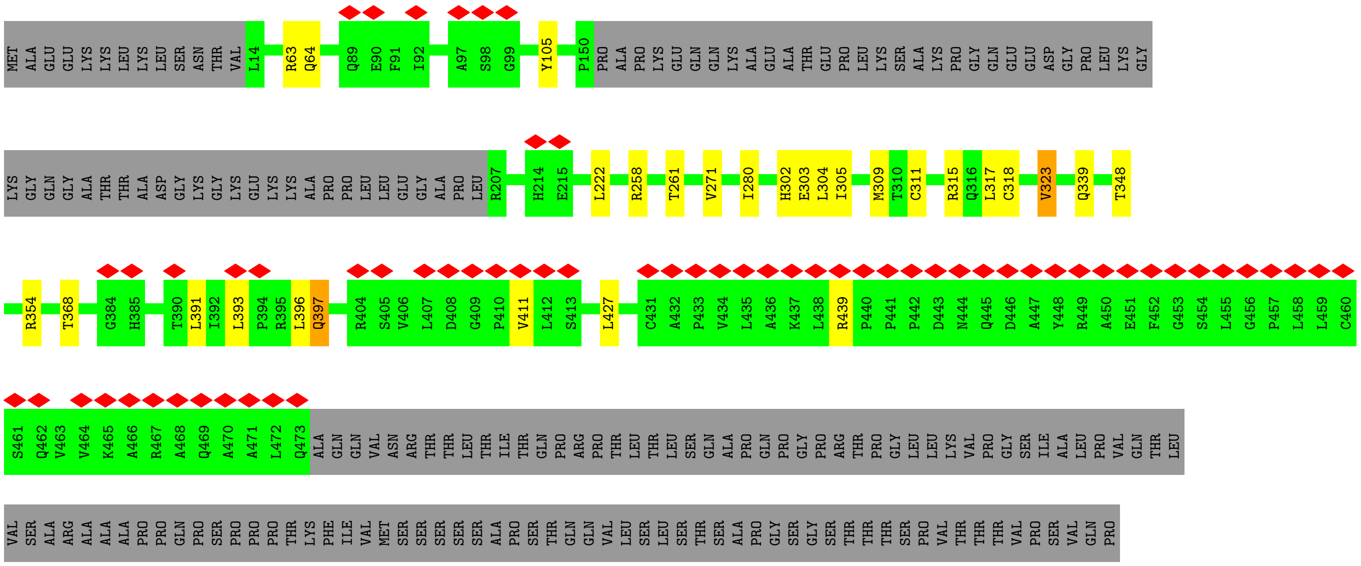
- Molecule 4: Transcription initiation factor TFIID subunit 5

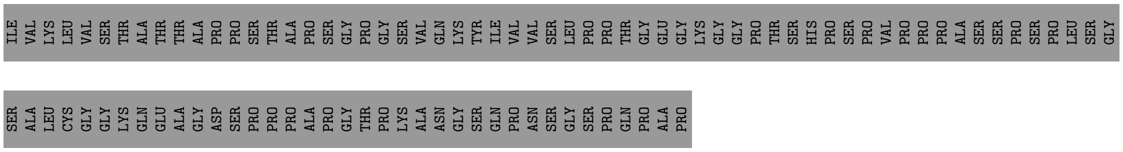




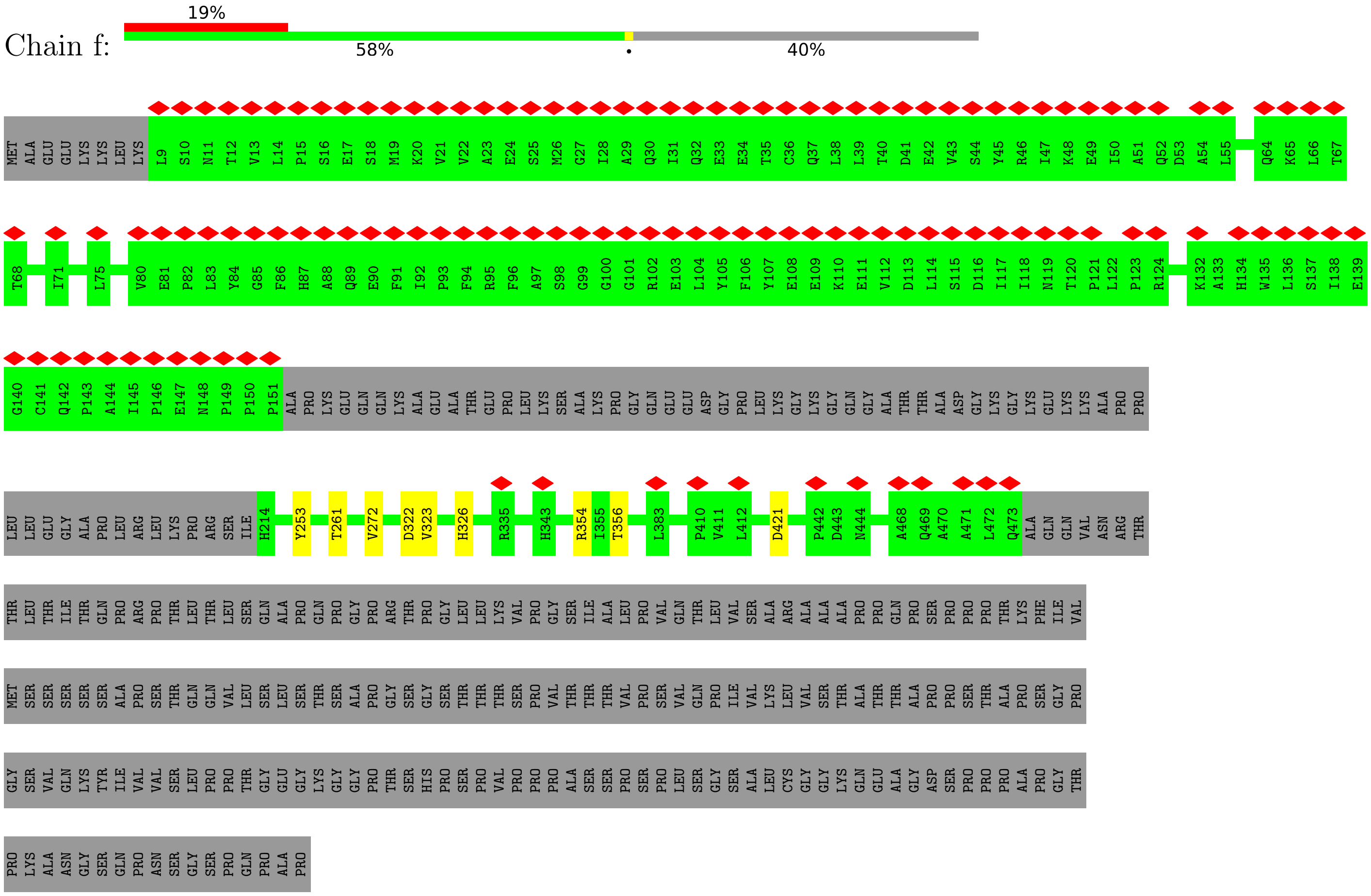
- Molecule 5: Transcription initiation factor TFIID subunit 6

Chain F:

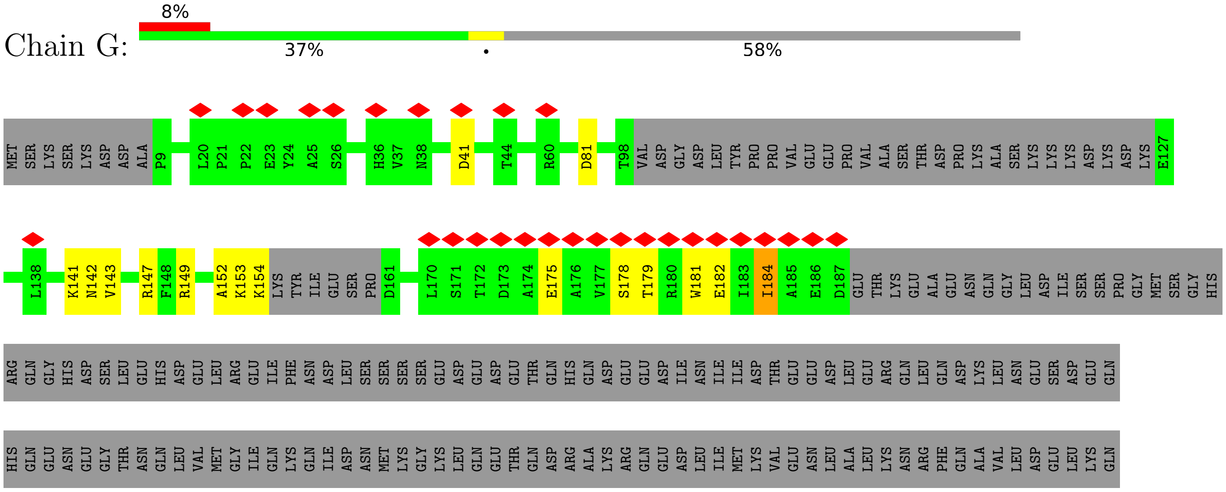




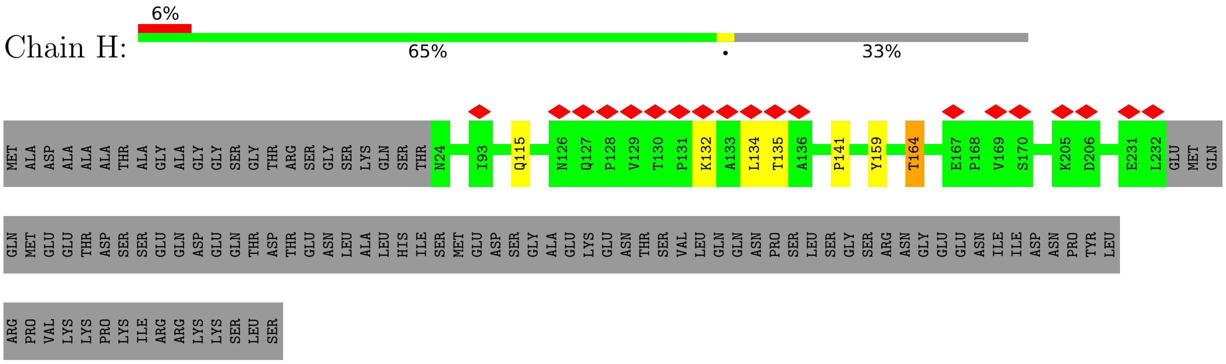
- Molecule 5: Transcription initiation factor TFIID subunit 6



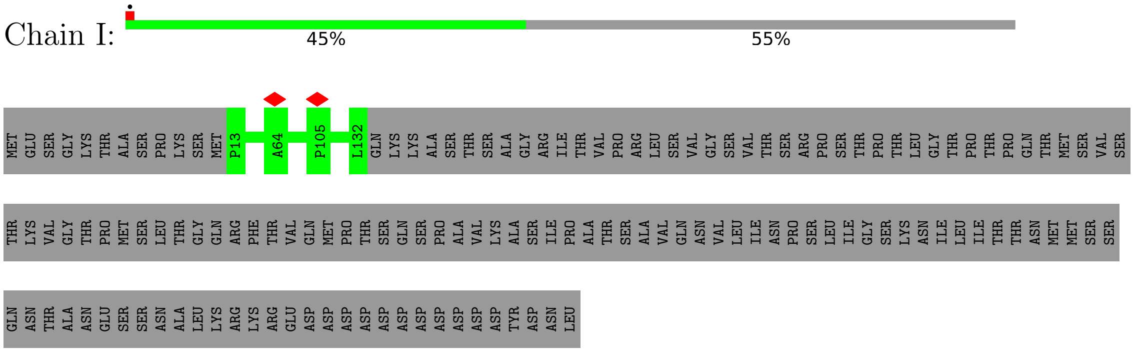
- Molecule 6: Transcription initiation factor TFIID subunit 7



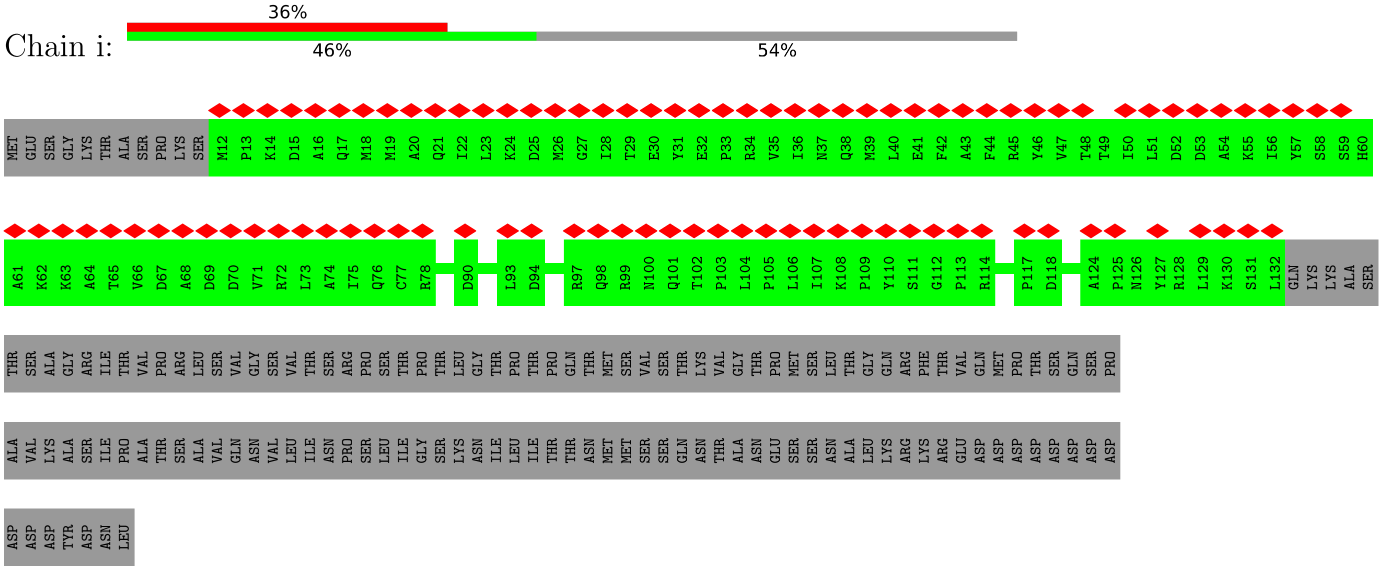
- Molecule 7: Transcription initiation factor TFIID subunit 8



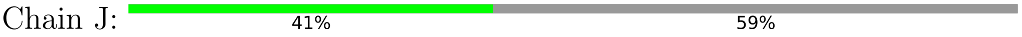
- Molecule 8: Transcription initiation factor TFIID subunit 9

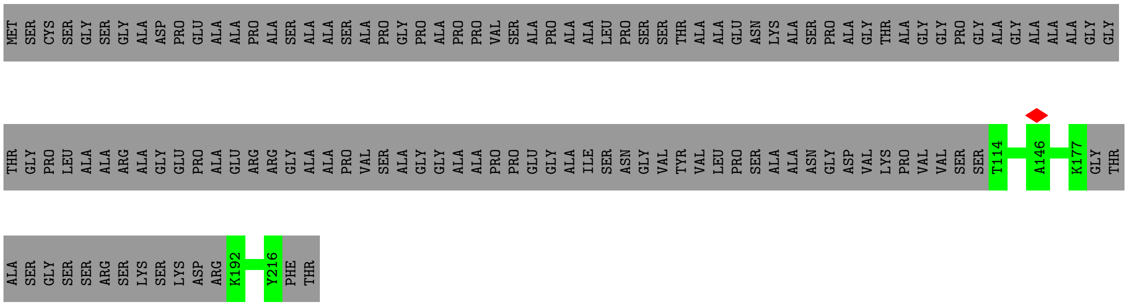


- Molecule 8: Transcription initiation factor TFIID subunit 9



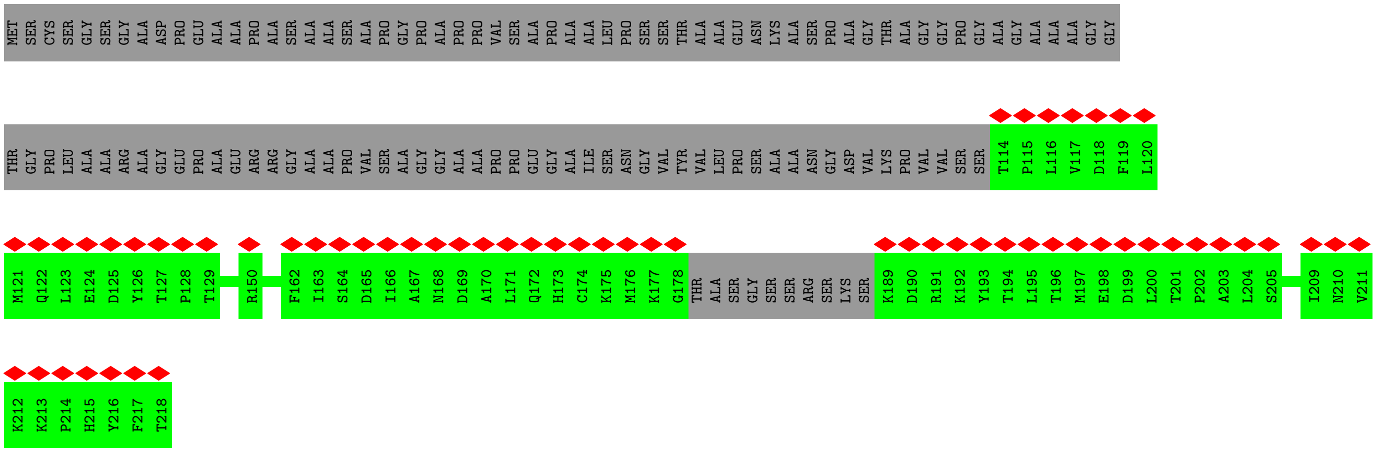
- Molecule 9: Transcription initiation factor TFIID subunit 10





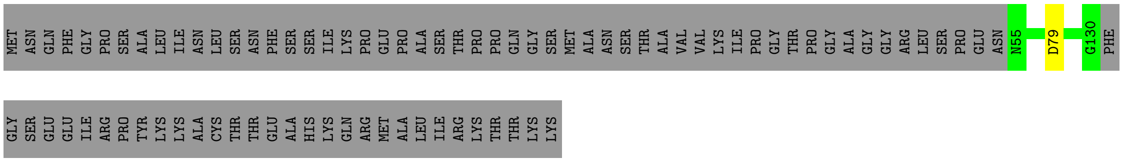
- Molecule 9: Transcription initiation factor TFIID subunit 10

Chain j:



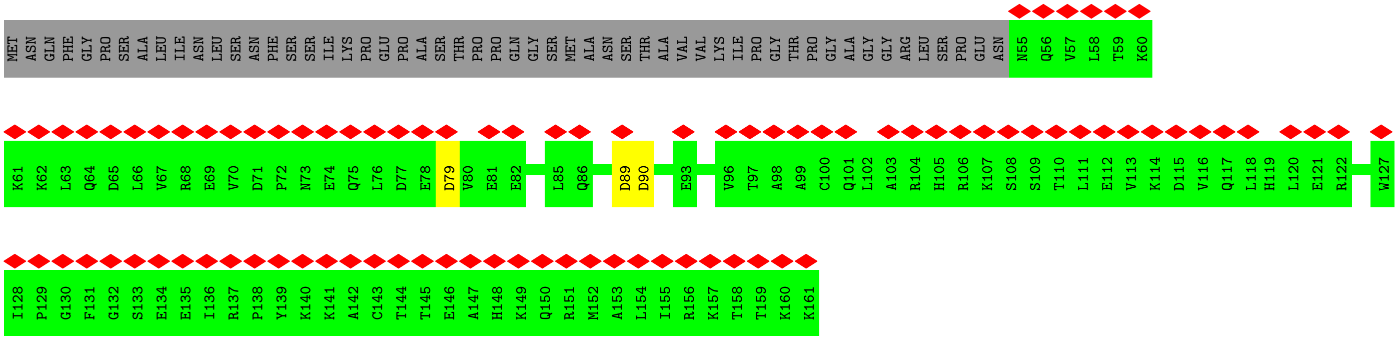
- Molecule 10: Transcription initiation factor TFIID subunit 12

Chain L:

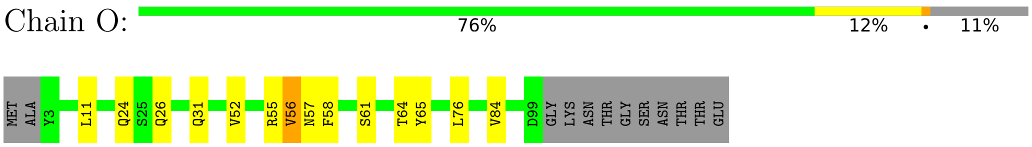


- Molecule 10: Transcription initiation factor TFIID subunit 12

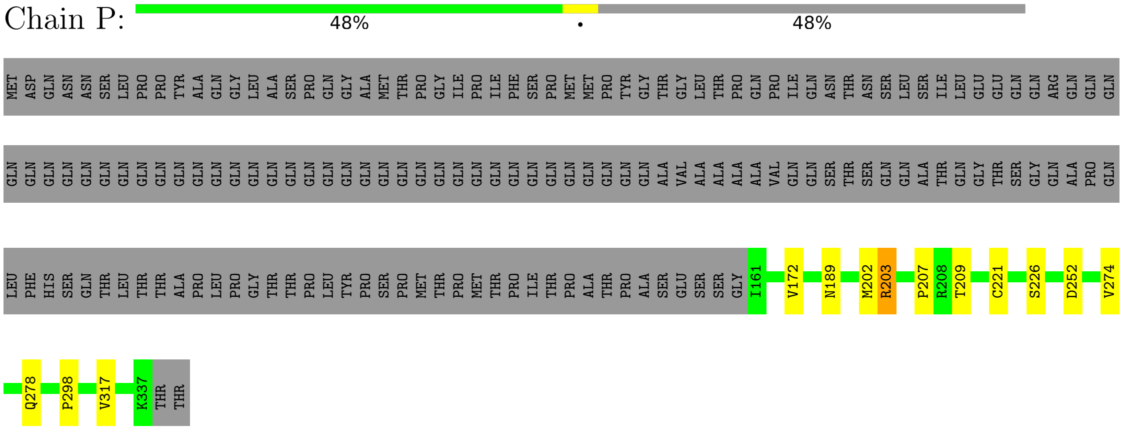
Chain l:



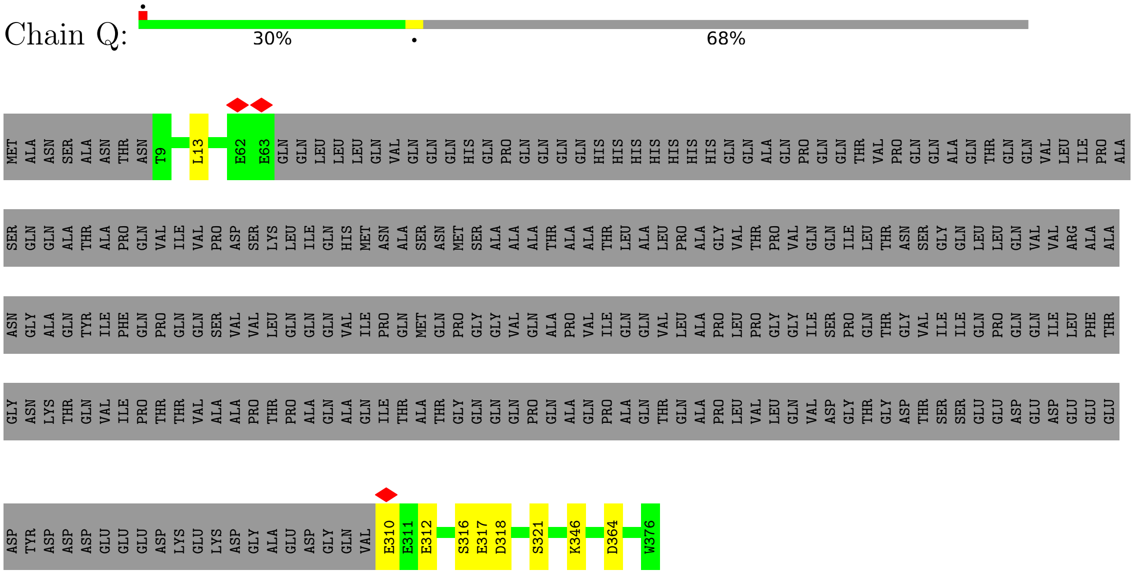
- Molecule 11: Transcription initiation factor IIA subunit 2



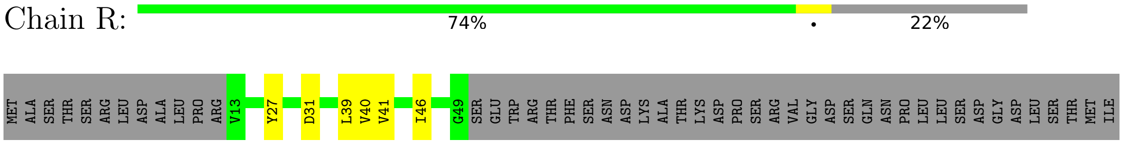
- Molecule 12: TATA-box-binding protein

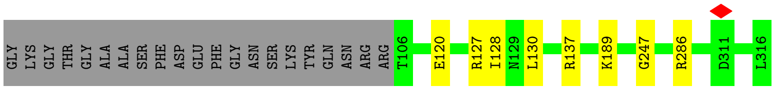


- Molecule 13: Transcription initiation factor IIA subunit 1

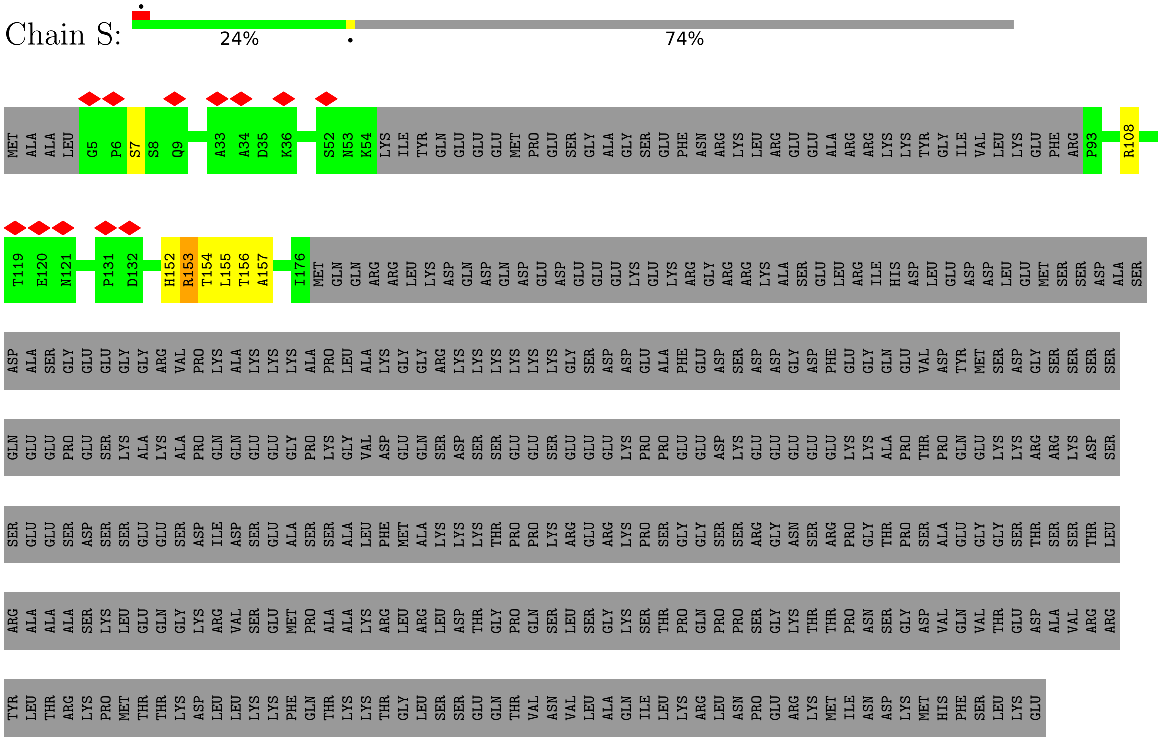


- Molecule 14: Transcription initiation factor IIB

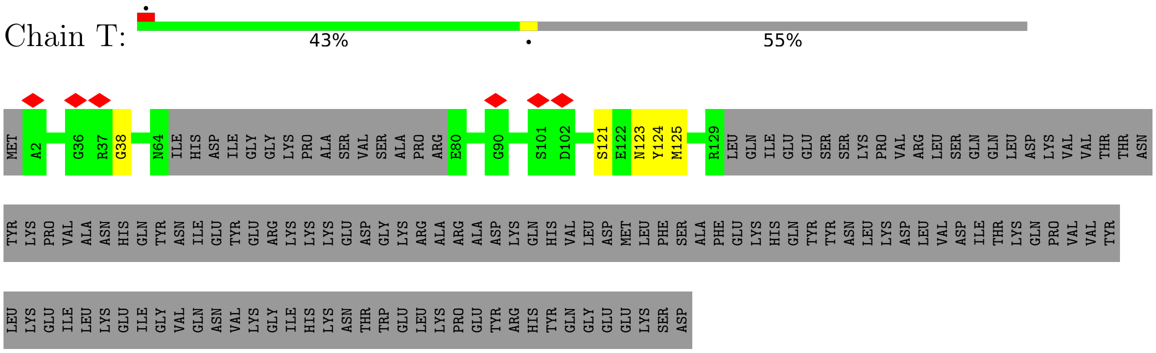




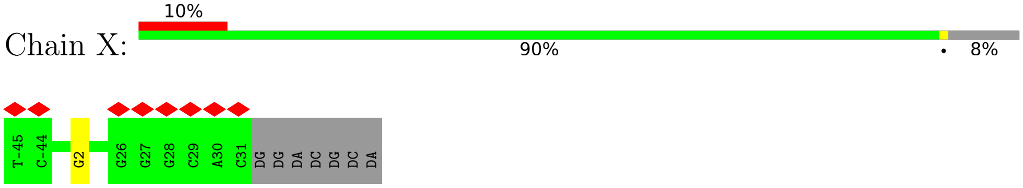
- Molecule 15: General transcription factor IIF subunit 1



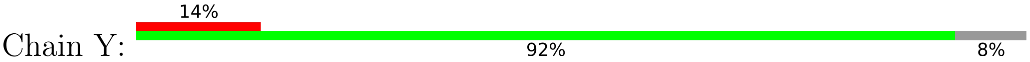
- Molecule 16: General transcription factor IIF subunit 2

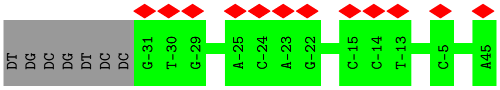


- Molecule 17: DNA (84-mer)



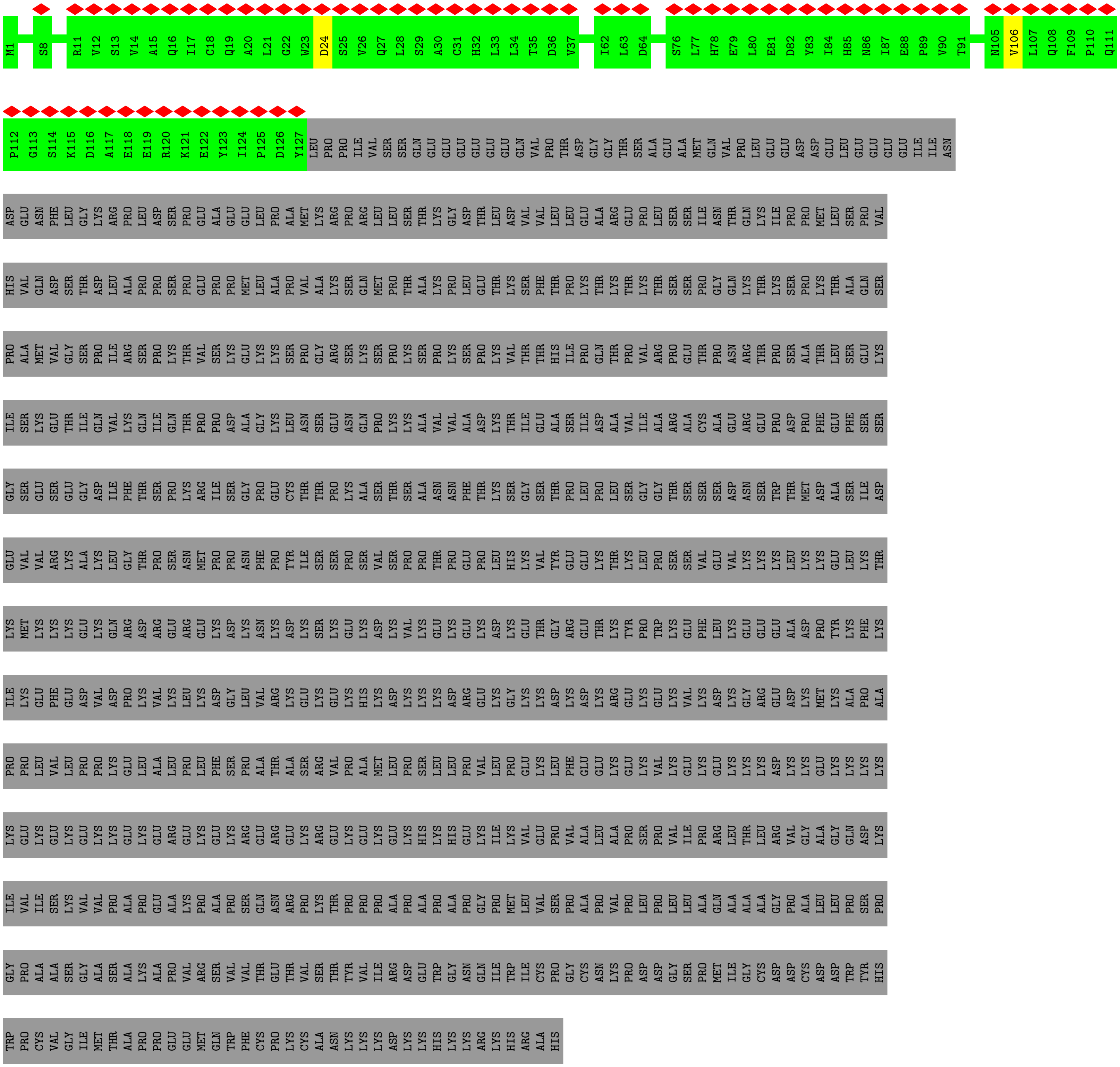
- Molecule 18: DNA (84-mer)





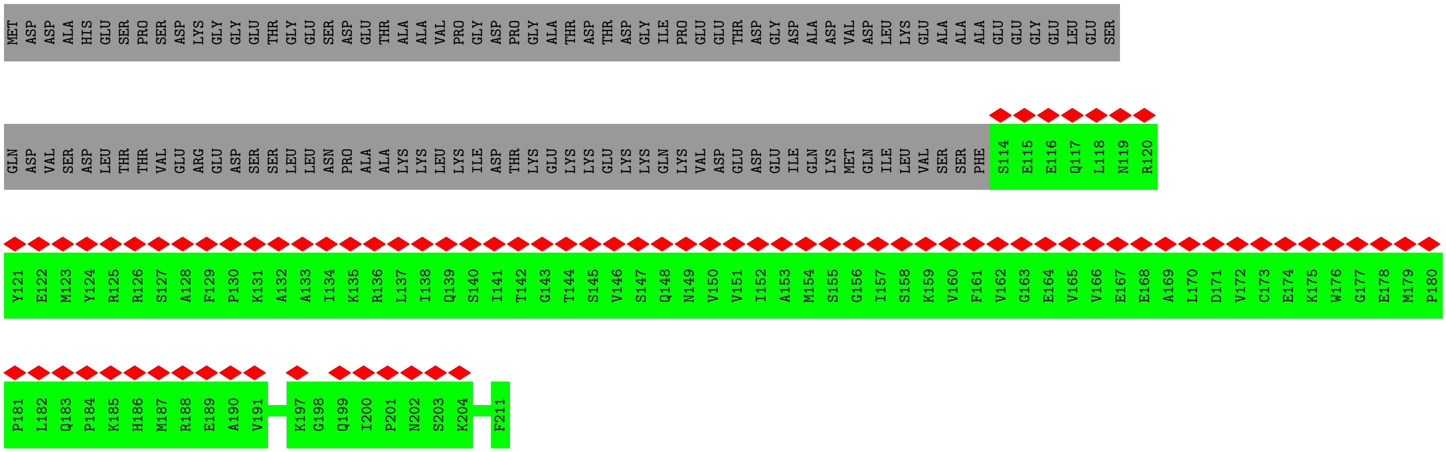
- Molecule 19: Transcription initiation factor TFIID subunit 3

Chain c:



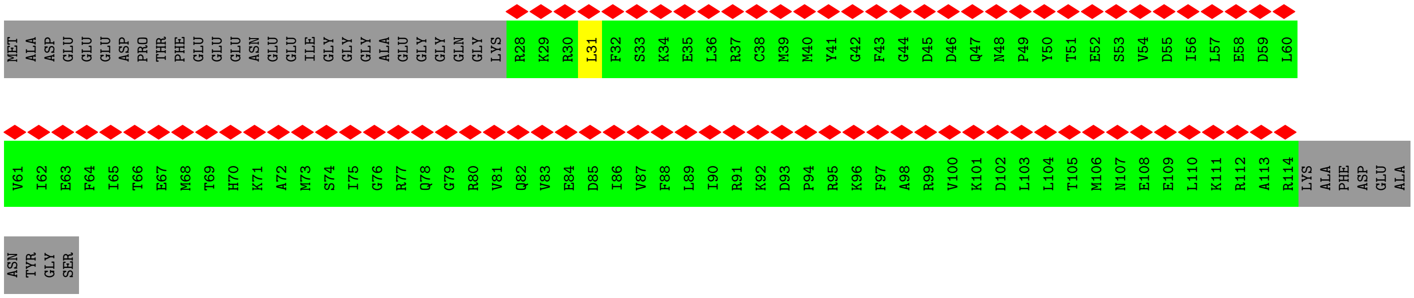
- Molecule 20: Transcription initiation factor TFIID subunit 11

Chain k:



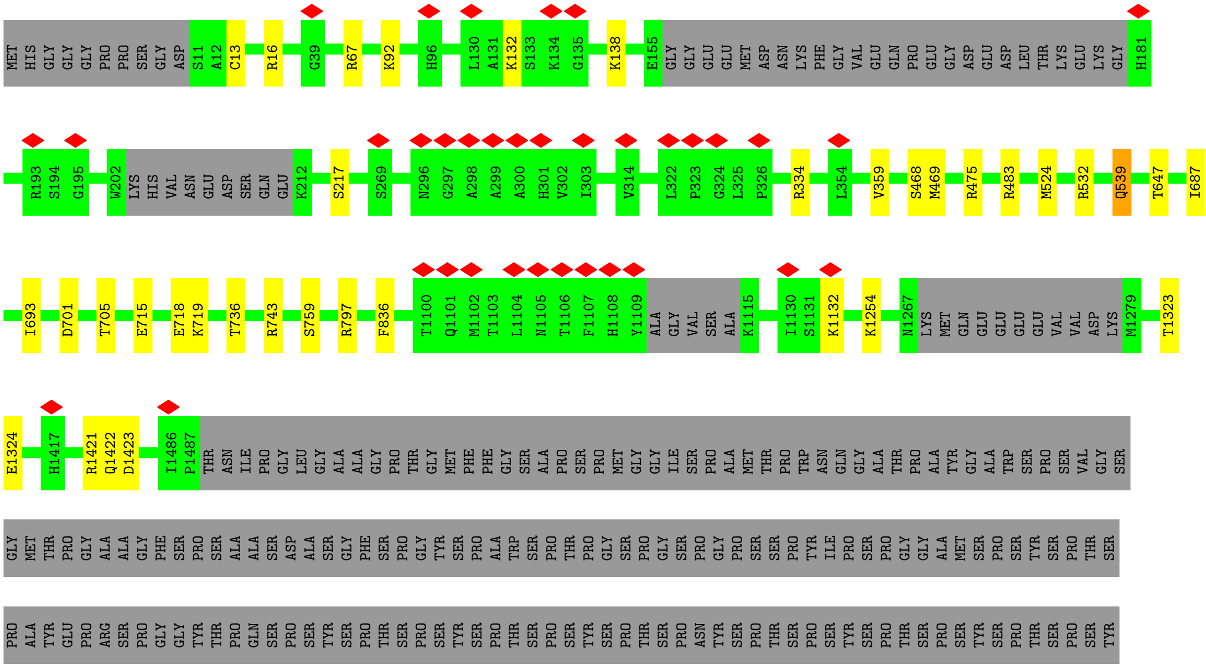
- Molecule 21: Transcription initiation factor TFIID subunit 13

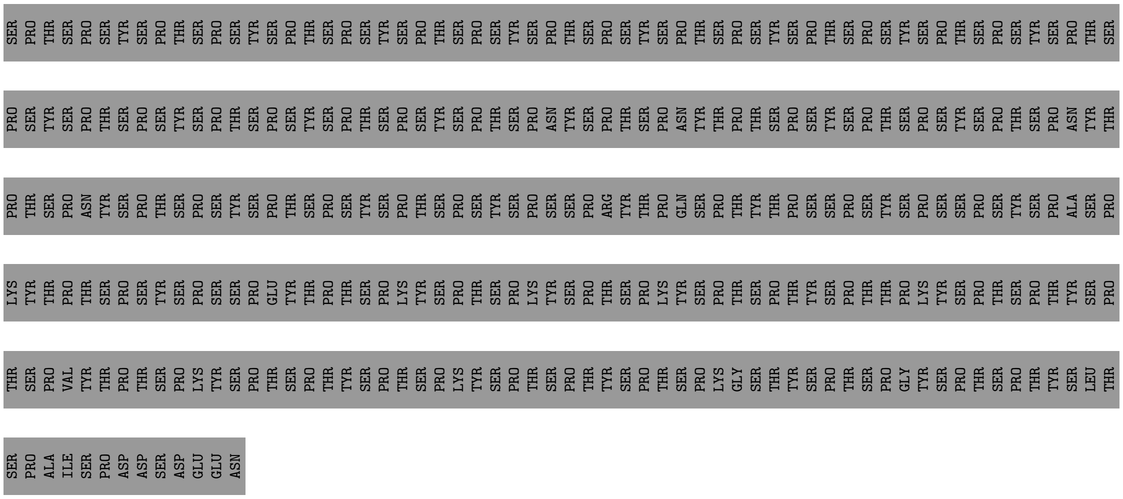
Chain m:



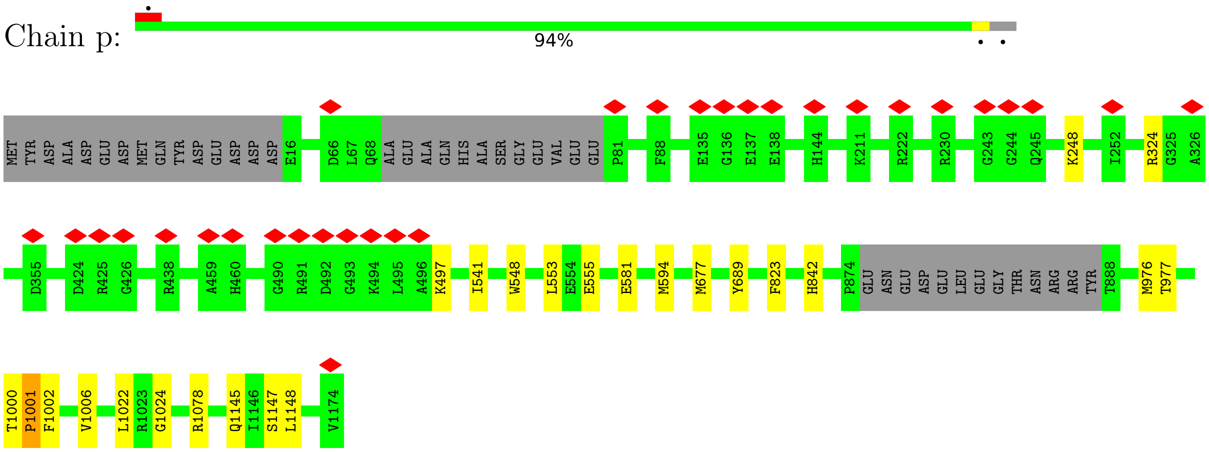
- Molecule 22: RPB1

Chain o:

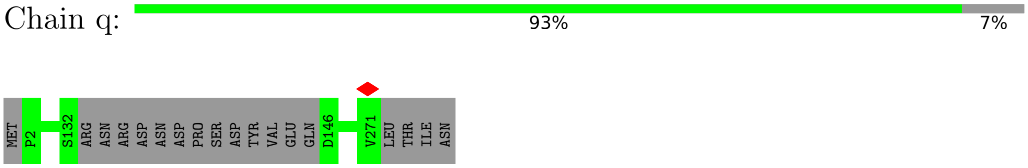




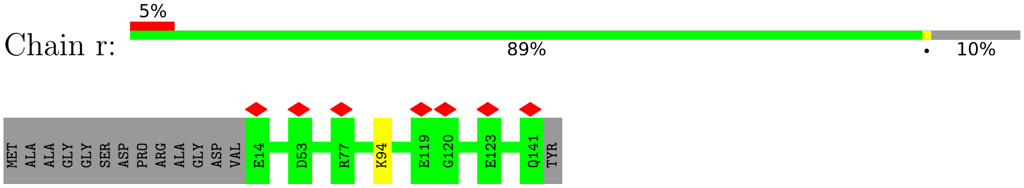
- Molecule 23: DNA-directed RNA polymerase subunit beta



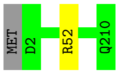
- Molecule 24: DNA-directed RNA polymerase II subunit RPB3



- Molecule 25: DNA-directed RNA polymerase II subunit RPB4

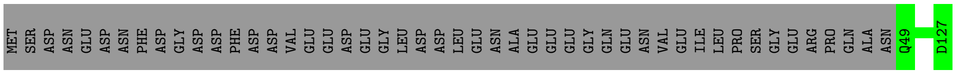


- Molecule 26: DNA-directed RNA polymerase II subunit E

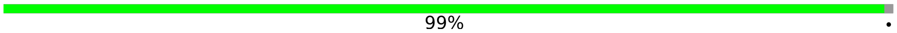


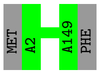
- Molecule 27: DNA-directed RNA polymerase II subunit F

Chain t:

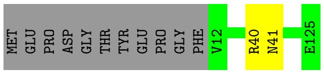
- Molecule 28: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain v:


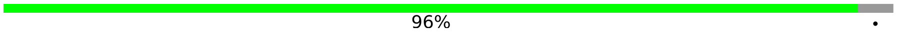


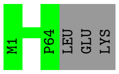
- Molecule 29: DNA-directed RNA polymerase II subunit RPB9

Chain w:

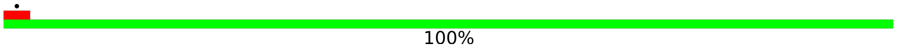



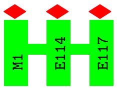
- Molecule 30: RPB10

Chain x:




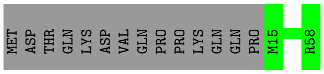
- Molecule 31: RNA_pol_L_2 domain-containing protein

Chain y:


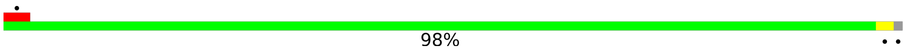


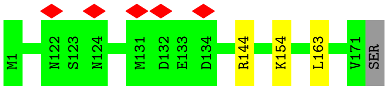
- Molecule 32: RPB12

Chain z:

- Molecule 33: DNA-directed RNA polymerase II subunit RPB7

Chain u:



M1
N122
S123
N124
M131
D132
E133
D134
R144
K154
L163
V171
SER

4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	99580	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	50.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.612	Depositor
Minimum map value	-0.877	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	508.8, 508.8, 508.8	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.50	0/5046	0.66	1/6810 (0.0%)
2	B	0.46	0/7993	0.60	0/10836
3	D	0.51	0/1391	0.62	0/1859
3	d	0.29	0/1321	0.50	0/1772
4	E	0.34	0/4469	0.54	0/6050
4	e	0.32	0/4433	0.55	0/6004
5	F	0.51	0/3139	0.71	0/4264
5	f	0.41	0/3140	0.63	0/4268
6	G	0.53	0/1199	0.66	0/1612
7	H	0.39	0/1673	0.59	0/2285
8	I	0.28	0/981	0.47	0/1332
8	i	0.29	0/989	0.46	0/1343
9	J	0.31	0/724	0.50	0/982
9	j	0.30	0/775	0.52	0/1049
10	L	0.32	0/630	0.58	1/852 (0.1%)
10	l	0.29	0/888	0.56	3/1194 (0.3%)
11	O	0.52	0/781	0.73	0/1061
12	P	0.62	0/1438	0.80	2/1935 (0.1%)
13	Q	0.43	0/1013	0.67	0/1366
14	R	0.31	0/1941	0.54	0/2622
15	S	0.35	0/1130	0.53	0/1528
16	T	0.26	0/887	0.52	0/1193
17	X	0.66	1/1772 (0.1%)	1.11	0/2735
18	Y	0.66	0/1768	1.14	0/2724
19	c	0.39	0/1035	0.54	0/1406
20	k	0.30	0/799	0.47	0/1070
21	m	0.31	0/733	0.51	0/977
22	o	0.40	0/11516	0.54	0/15548
23	p	0.40	0/9243	0.50	0/12475
24	q	0.38	0/2102	0.46	0/2857
25	r	0.27	0/1019	0.47	0/1374
26	s	0.30	0/1751	0.45	0/2366

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
27	t	0.37	0/645	0.46	0/871
28	v	0.37	0/1207	0.49	0/1628
29	w	0.31	0/948	0.47	0/1284
30	x	0.42	0/516	0.45	0/696
31	y	0.35	0/956	0.44	0/1294
32	z	0.38	0/377	0.45	0/500
33	u	0.33	0/1382	0.53	0/1874
All	All	0.42	1/83750 (0.0%)	0.60	7/113896 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
23	p	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	X	2	DG	O3'-P	5.29	1.67	1.61

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	P	203	ARG	CB-CA-C	10.12	130.65	110.40
1	A	498	PRO	N-CA-CB	6.71	111.36	103.30
12	P	202	MET	C-N-CA	-5.74	107.34	121.70
10	l	90	ASP	CB-CG-OD2	5.24	123.02	118.30
10	l	79	ASP	CB-CG-OD2	5.21	122.99	118.30
10	L	79	ASP	CB-CG-OD2	5.11	122.90	118.30
10	l	89	ASP	CB-CG-OD2	5.09	122.88	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	821	ARG	Peptide
23	p	1000	THR	Mainchain

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	A	584/1872 (31%)	543 (93%)	32 (6%)	9 (2%)	10	46
2	B	959/1199 (80%)	911 (95%)	48 (5%)	0	100	100
3	D	159/1085 (15%)	147 (92%)	9 (6%)	3 (2%)	8	41
3	d	154/1085 (14%)	150 (97%)	4 (3%)	0	100	100
4	E	540/800 (68%)	505 (94%)	33 (6%)	2 (0%)	34	72
4	e	531/800 (66%)	484 (91%)	47 (9%)	0	100	100
5	F	400/677 (59%)	374 (94%)	18 (4%)	8 (2%)	7	40
5	f	399/677 (59%)	378 (95%)	21 (5%)	0	100	100
6	G	139/349 (40%)	132 (95%)	5 (4%)	2 (1%)	11	47
7	H	207/310 (67%)	189 (91%)	15 (7%)	3 (1%)	11	47
8	I	118/264 (45%)	115 (98%)	3 (2%)	0	100	100
8	i	119/264 (45%)	115 (97%)	4 (3%)	0	100	100
9	J	85/218 (39%)	82 (96%)	3 (4%)	0	100	100
9	j	91/218 (42%)	89 (98%)	2 (2%)	0	100	100
10	L	74/161 (46%)	69 (93%)	5 (7%)	0	100	100
10	l	105/161 (65%)	101 (96%)	4 (4%)	0	100	100
11	O	95/109 (87%)	81 (85%)	10 (10%)	4 (4%)	3	25
12	P	175/339 (52%)	169 (97%)	4 (2%)	2 (1%)	14	52
13	Q	118/376 (31%)	108 (92%)	9 (8%)	1 (1%)	19	60
14	R	244/316 (77%)	235 (96%)	8 (3%)	1 (0%)	34	72
15	S	130/517 (25%)	124 (95%)	4 (3%)	2 (2%)	10	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	T	109/249 (44%)	102 (94%)	4 (4%)	3 (3%)	5	33
19	c	125/929 (14%)	116 (93%)	9 (7%)	0	100	100
20	k	96/211 (46%)	91 (95%)	5 (5%)	0	100	100
21	m	85/124 (68%)	79 (93%)	6 (7%)	0	100	100
22	o	1417/1970 (72%)	1305 (92%)	110 (8%)	2 (0%)	51	85
23	p	1128/1174 (96%)	1051 (93%)	75 (7%)	2 (0%)	47	81
24	q	253/275 (92%)	226 (89%)	27 (11%)	0	100	100
25	r	126/142 (89%)	119 (94%)	7 (6%)	0	100	100
26	s	207/210 (99%)	196 (95%)	11 (5%)	0	100	100
27	t	77/127 (61%)	74 (96%)	3 (4%)	0	100	100
28	v	146/150 (97%)	132 (90%)	14 (10%)	0	100	100
29	w	112/125 (90%)	102 (91%)	9 (8%)	1 (1%)	17	56
30	x	62/67 (92%)	59 (95%)	3 (5%)	0	100	100
31	y	115/117 (98%)	109 (95%)	6 (5%)	0	100	100
32	z	42/58 (72%)	38 (90%)	4 (10%)	0	100	100
33	u	169/172 (98%)	157 (93%)	11 (6%)	1 (1%)	25	65
All	All	9695/17897 (54%)	9057 (93%)	592 (6%)	46 (0%)	32	68

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1000	LEU
1	A	1158	SER
3	D	958	LYS
5	F	323	VAL
5	F	396	LEU
7	H	141	PRO
11	O	52	VAL
13	Q	321	SER
15	S	157	ALA
16	T	124	TYR
23	p	1001	PRO
33	u	154	LYS
1	A	498	PRO
4	E	522	ASP
4	E	704	VAL

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Mol	Chain	Res	Type
5	F	397	GLN
5	F	411	VAL
6	G	152	ALA
6	G	184	ILE
11	O	26	GLN
16	T	121	SER
22	o	539	GLN
23	p	1024	GLY
3	D	936	GLN
3	D	957	ARG
12	P	207	PRO
1	A	823	ARG
1	A	839	GLU
5	F	393	LEU
5	F	439	ARG
11	O	56	VAL
11	O	84	VAL
16	T	38	GLY
1	A	822	PRO
5	F	64	GLN
7	H	134	LEU
7	H	164	THR
15	S	153	ARG
22	o	469	MET
29	w	41	ASN
1	A	838	SER
1	A	840	SER
5	F	318	CYS
12	P	298	PRO
14	R	247	GLY
1	A	1167	ILE

5.3.2 Protein sidechains ⓘ

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	536/1665 (32%)	473 (88%)	63 (12%)	5	23
2	B	876/1083 (81%)	859 (98%)	17 (2%)	57	75
3	D	149/815 (18%)	133 (89%)	16 (11%)	6	26
3	d	146/815 (18%)	144 (99%)	2 (1%)	67	81
4	E	478/657 (73%)	474 (99%)	4 (1%)	81	89
4	e	475/657 (72%)	473 (100%)	2 (0%)	91	94
5	F	320/574 (56%)	297 (93%)	23 (7%)	14	41
5	f	322/574 (56%)	313 (97%)	9 (3%)	43	65
6	G	133/322 (41%)	118 (89%)	15 (11%)	6	24
7	H	181/270 (67%)	176 (97%)	5 (3%)	43	65
8	I	106/235 (45%)	106 (100%)	0	100	100
8	i	107/235 (46%)	107 (100%)	0	100	100
9	J	78/154 (51%)	78 (100%)	0	100	100
9	j	83/154 (54%)	83 (100%)	0	100	100
10	L	71/141 (50%)	71 (100%)	0	100	100
10	l	98/141 (70%)	98 (100%)	0	100	100
11	O	84/98 (86%)	73 (87%)	11 (13%)	4	20
12	P	153/293 (52%)	143 (94%)	10 (6%)	17	44
13	Q	111/324 (34%)	103 (93%)	8 (7%)	14	41
14	R	211/268 (79%)	198 (94%)	13 (6%)	18	45
15	S	117/448 (26%)	110 (94%)	7 (6%)	19	46
16	T	94/218 (43%)	92 (98%)	2 (2%)	53	72
19	c	113/833 (14%)	111 (98%)	2 (2%)	59	77
20	k	87/182 (48%)	87 (100%)	0	100	100
21	m	80/106 (76%)	79 (99%)	1 (1%)	69	82
22	o	1257/1748 (72%)	1222 (97%)	35 (3%)	43	65
23	p	993/1027 (97%)	970 (98%)	23 (2%)	50	70
24	q	234/252 (93%)	234 (100%)	0	100	100
25	r	106/126 (84%)	105 (99%)	1 (1%)	78	87
26	s	191/192 (100%)	190 (100%)	1 (0%)	88	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	t	69/111 (62%)	69 (100%)	0	100	100
28	v	129/131 (98%)	129 (100%)	0	100	100
29	w	103/112 (92%)	102 (99%)	1 (1%)	76	86
30	x	53/56 (95%)	53 (100%)	0	100	100
31	y	106/106 (100%)	106 (100%)	0	100	100
32	z	41/55 (74%)	41 (100%)	0	100	100
33	u	152/153 (99%)	150 (99%)	2 (1%)	69	82
All	All	8643/15331 (56%)	8370 (97%)	273 (3%)	42	62

All (273) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	341	TRP
1	A	353	LEU
1	A	395	ASP
1	A	397	LEU
1	A	400	GLU
1	A	404	MET
1	A	415	ILE
1	A	417	ASP
1	A	419	GLU
1	A	466	SER
1	A	470	ILE
1	A	475	LEU
1	A	481	GLU
1	A	493	ARG
1	A	496	GLU
1	A	499	VAL
1	A	500	LEU
1	A	501	THR
1	A	502	LEU
1	A	505	ASN
1	A	511	LEU
1	A	639	LEU
1	A	661	GLU
1	A	667	THR
1	A	711	ASP
1	A	727	THR
1	A	730	PHE
1	A	753	TYR

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Mol	Chain	Res	Type
1	A	821	ARG
1	A	823	ARG
1	A	828	GLU
1	A	840	SER
1	A	843	ARG
1	A	845	ARG
1	A	847	LYS
1	A	848	LEU
1	A	849	CYS
1	A	852	PHE
1	A	853	LYS
1	A	855	THR
1	A	943	LYS
1	A	970	ASN
1	A	971	LYS
1	A	996	ARG
1	A	997	ARG
1	A	1020	LEU
1	A	1021	SER
1	A	1022	ARG
1	A	1052	ARG
1	A	1053	PHE
1	A	1055	VAL
1	A	1058	HIS
1	A	1059	GLN
1	A	1064	GLU
1	A	1082	VAL
1	A	1083	LEU
1	A	1084	SER
1	A	1150	THR
1	A	1165	LEU
1	A	1166	LYS
1	A	1167	ILE
1	A	1169	ARG
1	A	1203	GLU
2	B	21	GLU
2	B	24	ARG
2	B	71	ARG
2	B	140	GLU
2	B	184	ASN
2	B	225	TYR
2	B	262	MET

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Mol	Chain	Res	Type
2	B	266	THR
2	B	293	GLU
2	B	431	LEU
2	B	488	PHE
2	B	559	LYS
2	B	603	LYS
2	B	638	ARG
2	B	640	VAL
2	B	771	VAL
2	B	818	THR
3	D	936	GLN
3	D	948	GLU
3	D	950	LEU
3	D	951	ASP
3	D	959	ASP
3	D	961	GLN
3	D	966	LEU
3	D	968	ARG
3	D	992	GLN
3	D	996	LEU
3	D	1000	ARG
3	D	1002	ARG
3	D	1003	ASP
3	D	1054	ARG
3	D	1055	ILE
3	D	1056	THR
4	E	593	PHE
4	E	745	GLU
4	E	746	ASP
4	E	747	LEU
5	F	63	ARG
5	F	105	TYR
5	F	222	LEU
5	F	258	ARG
5	F	261	THR
5	F	271	VAL
5	F	280	ILE
5	F	302	HIS
5	F	303	GLU
5	F	304	LEU
5	F	305	ILE
5	F	309	MET

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Mol	Chain	Res	Type
5	F	311	CYS
5	F	315	ARG
5	F	317	LEU
5	F	323	VAL
5	F	339	GLN
5	F	348	THR
5	F	354	ARG
5	F	368	THR
5	F	391	LEU
5	F	397	GLN
5	F	427	LEU
6	G	41	ASP
6	G	81	ASP
6	G	141	LYS
6	G	142	ASN
6	G	143	VAL
6	G	147	ARG
6	G	149	ARG
6	G	153	LYS
6	G	154	LYS
6	G	175	GLU
6	G	178	SER
6	G	179	THR
6	G	181	TRP
6	G	182	GLU
6	G	184	ILE
7	H	115	GLN
7	H	132	LYS
7	H	135	THR
7	H	159	TYR
7	H	164	THR
11	O	11	LEU
11	O	24	GLN
11	O	31	GLN
11	O	55	ARG
11	O	56	VAL
11	O	57	ASN
11	O	58	PHE
11	O	61	SER
11	O	64	THR
11	O	65	TYR
11	O	76	LEU

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Mol	Chain	Res	Type
12	P	172	VAL
12	P	189	ASN
12	P	203	ARG
12	P	209	THR
12	P	221	CYS
12	P	226	SER
12	P	252	ASP
12	P	274	VAL
12	P	278	GLN
12	P	317	VAL
13	Q	13	LEU
13	Q	310	GLU
13	Q	312	GLU
13	Q	316	SER
13	Q	317	GLU
13	Q	318	ASP
13	Q	346	LYS
13	Q	364	ASP
14	R	27	TYR
14	R	31	ASP
14	R	39	LEU
14	R	40	VAL
14	R	41	VAL
14	R	46	ILE
14	R	120	GLU
14	R	127	ARG
14	R	128	ILE
14	R	130	LEU
14	R	137	ARG
14	R	189	LYS
14	R	286	ARG
15	S	7	SER
15	S	108	ARG
15	S	152	HIS
15	S	153	ARG
15	S	154	THR
15	S	155	LEU
15	S	156	THR
16	T	123	ASN
16	T	125	MET
19	c	24	ASP
19	c	106	VAL

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Mol	Chain	Res	Type
3	d	887	LYS
3	d	888	LYS
4	e	365	ARG
4	e	663	ARG
5	f	253	TYR
5	f	261	THR
5	f	272	VAL
5	f	322	ASP
5	f	323	VAL
5	f	326	HIS
5	f	354	ARG
5	f	356	THR
5	f	421	ASP
21	m	31	LEU
22	o	13	CYS
22	o	16	ARG
22	o	67	ARG
22	o	92	LYS
22	o	132	LYS
22	o	138	LYS
22	o	217	SER
22	o	334	ARG
22	o	359	VAL
22	o	468	SER
22	o	475	ARG
22	o	483	ARG
22	o	524	MET
22	o	532	ARG
22	o	539	GLN
22	o	647	THR
22	o	687	ILE
22	o	693	ILE
22	o	701	ASP
22	o	705	THR
22	o	715	GLU
22	o	718	GLU
22	o	719	LYS
22	o	736	THR
22	o	743	ARG
22	o	759	SER
22	o	797	ARG
22	o	836	PHE

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Mol	Chain	Res	Type
22	o	1132	LYS
22	o	1254	LYS
22	o	1323	THR
22	o	1324	GLU
22	o	1421	ARG
22	o	1422	GLN
22	o	1423	ASP
23	p	248	LYS
23	p	324	ARG
23	p	497	LYS
23	p	541	ILE
23	p	548	TRP
23	p	553	LEU
23	p	555	GLU
23	p	581	GLU
23	p	594	MET
23	p	677	MET
23	p	689	TYR
23	p	823	PHE
23	p	842	HIS
23	p	976	MET
23	p	977	THR
23	p	1001	PRO
23	p	1002	PHE
23	p	1006	VAL
23	p	1022	LEU
23	p	1078	ARG
23	p	1145	GLN
23	p	1147	SER
23	p	1148	LEU
25	r	94	LYS
26	s	52	ARG
29	w	40	ARG
33	u	144	ARG
33	u	163	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (123) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	401	ASN
1	A	569	ASN
1	A	860	ASN

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Mol	Chain	Res	Type
1	A	896	GLN
1	A	1073	GLN
1	A	1074	ASN
2	B	30	HIS
2	B	176	HIS
2	B	183	GLN
2	B	184	ASN
2	B	235	HIS
2	B	348	GLN
2	B	432	HIS
2	B	439	HIS
2	B	450	GLN
2	B	509	ASN
2	B	521	GLN
2	B	580	GLN
2	B	644	GLN
2	B	652	GLN
2	B	745	GLN
2	B	750	GLN
2	B	765	ASN
2	B	813	ASN
2	B	908	GLN
2	B	916	ASN
3	D	875	GLN
3	D	936	GLN
3	D	943	GLN
3	D	956	GLN
3	D	1075	HIS
4	E	238	GLN
4	E	254	ASN
4	E	268	HIS
4	E	315	GLN
4	E	327	ASN
4	E	351	GLN
4	E	616	HIS
4	E	640	ASN
5	F	119	ASN
5	F	214	HIS
5	F	221	GLN
5	F	270	ASN
5	F	273	GLN
5	F	274	ASN

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Mol	Chain	Res	Type
5	F	275	ASN
5	F	316	GLN
5	F	343	HIS
6	G	48	HIS
7	H	145	HIS
8	I	21	GLN
8	I	60	HIS
8	I	98	GLN
9	J	160	GLN
9	J	173	HIS
9	J	210	ASN
10	L	105	HIS
10	L	117	GLN
11	O	13	ASN
11	O	57	ASN
13	Q	60	HIS
13	Q	352	HIS
13	Q	361	ASN
15	S	44	GLN
3	d	912	ASN
3	d	1069	ASN
4	e	294	ASN
4	e	320	HIS
4	e	336	HIS
4	e	616	HIS
5	f	325	ASN
8	i	60	HIS
8	i	81	GLN
10	l	73	ASN
10	l	105	HIS
21	m	107	ASN
22	o	123	ASN
22	o	278	HIS
22	o	289	GLN
22	o	296	ASN
22	o	507	GLN
22	o	539	GLN
22	o	576	GLN
22	o	620	HIS
22	o	703	GLN
22	o	721	HIS
22	o	731	ASN

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Mol	Chain	Res	Type
22	o	739	ASN
22	o	913	ASN
22	o	950	ASN
22	o	1005	HIS
22	o	1230	GLN
22	o	1248	ASN
22	o	1332	GLN
22	o	1397	HIS
22	o	1445	HIS
22	o	1462	GLN
23	p	111	ASN
23	p	139	GLN
23	p	287	HIS
23	p	370	HIS
23	p	525	ASN
23	p	537	GLN
23	p	570	ASN
23	p	582	GLN
23	p	585	ASN
23	p	593	GLN
23	p	749	HIS
23	p	777	ASN
23	p	790	GLN
23	p	1009	GLN
23	p	1021	HIS
23	p	1073	GLN
23	p	1120	ASN
24	q	5	ASN
24	q	60	HIS
25	r	19	GLN
26	s	133	GLN
28	v	131	ASN
29	w	98	GLN
31	y	2	ASN
31	y	29	ASN
33	u	60	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

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.

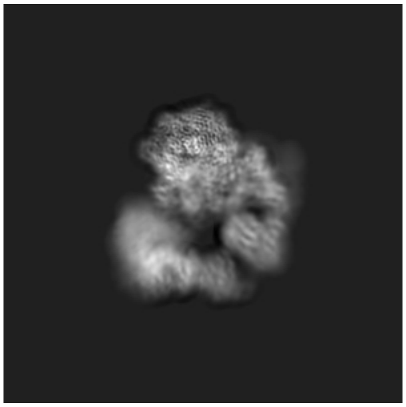
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-31075. These allow visual inspection of the internal detail of the map and identification of artifacts.

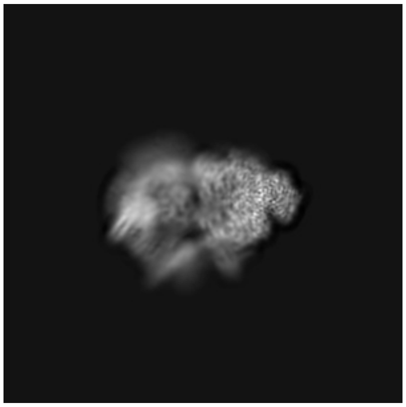
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

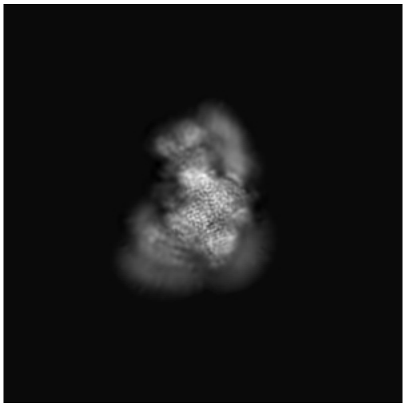
6.1.1 Primary map



X



Y

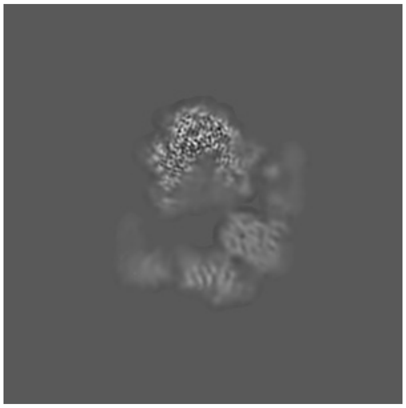


Z

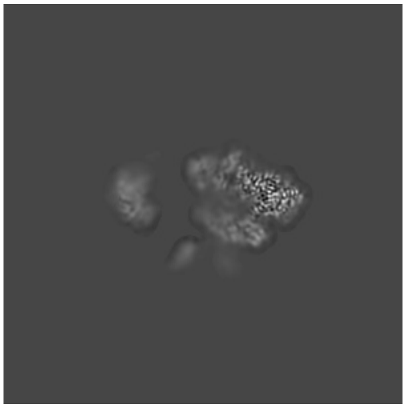
The images above show the map projected in three orthogonal directions.

6.2 Central slices

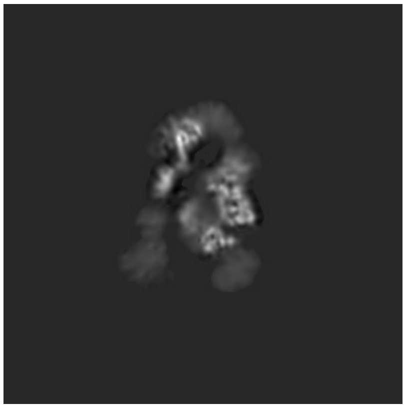
6.2.1 Primary map



X Index: 240



Y Index: 240



Z Index: 240

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

6.3 Largest variance slices

6.3.1 Primary map

X Index: 241 Y Index: 230 Z Index: 307

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

6.4 Orthogonal surface views

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

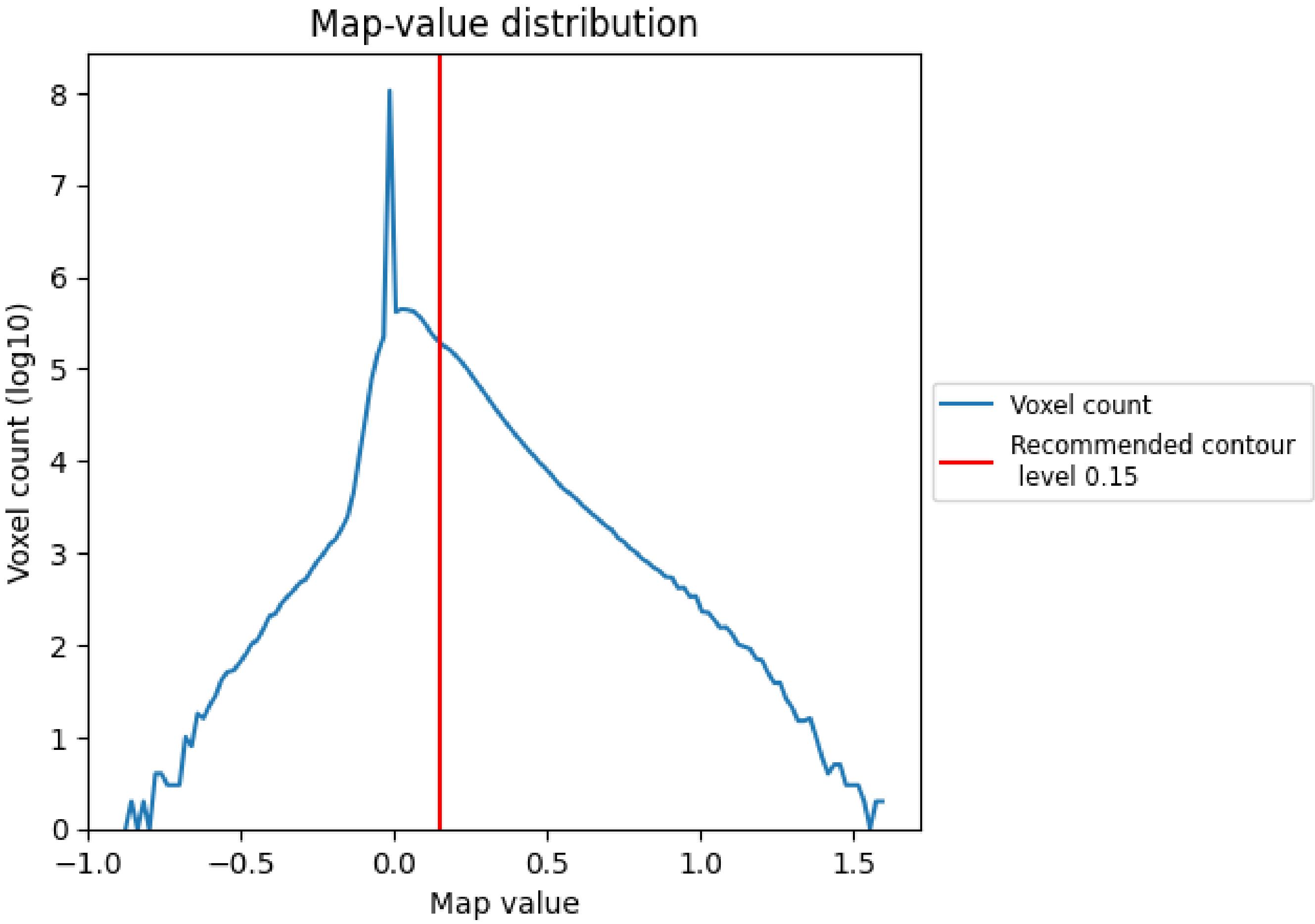
6.5 Mask visualisation ⓘ

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

7 Map analysis ⓘ

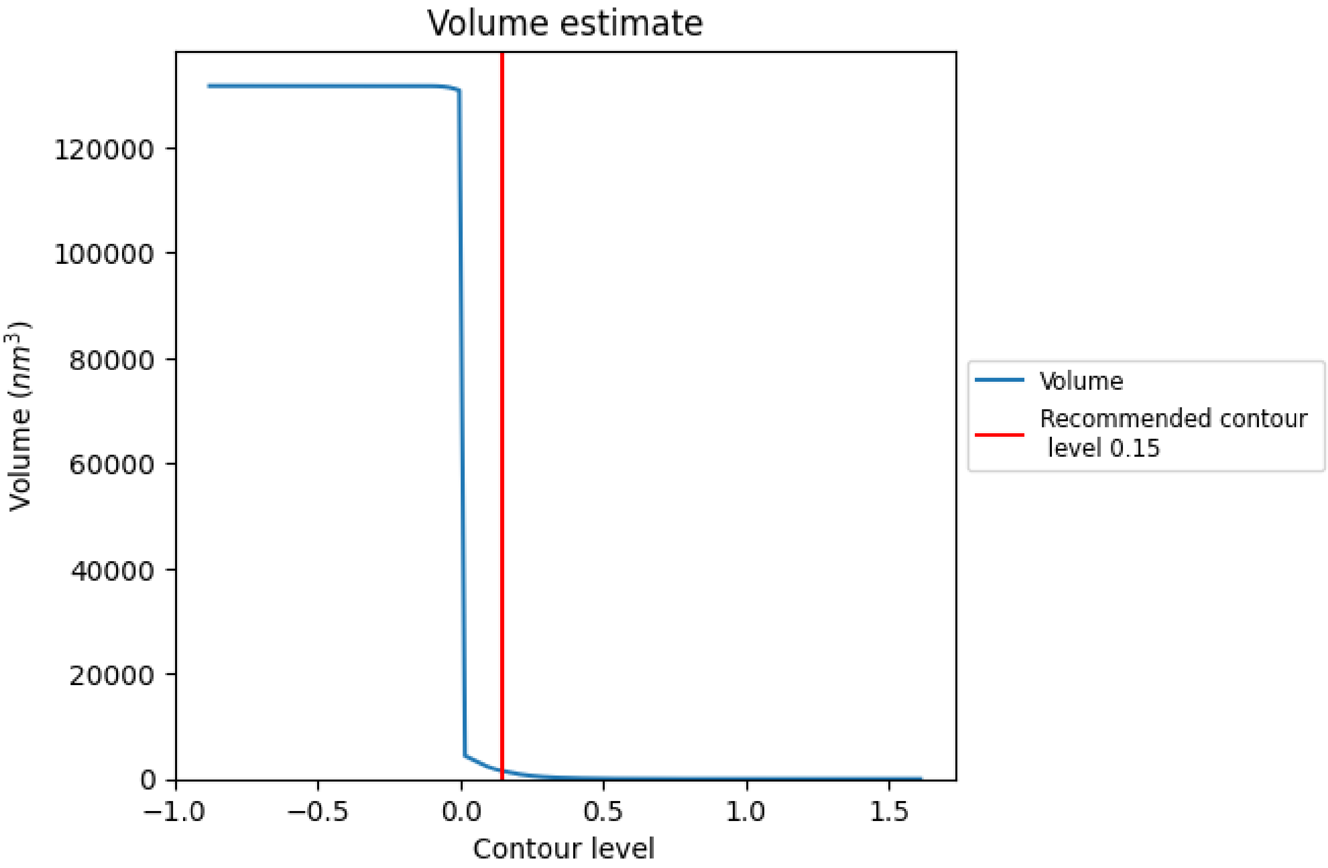
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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

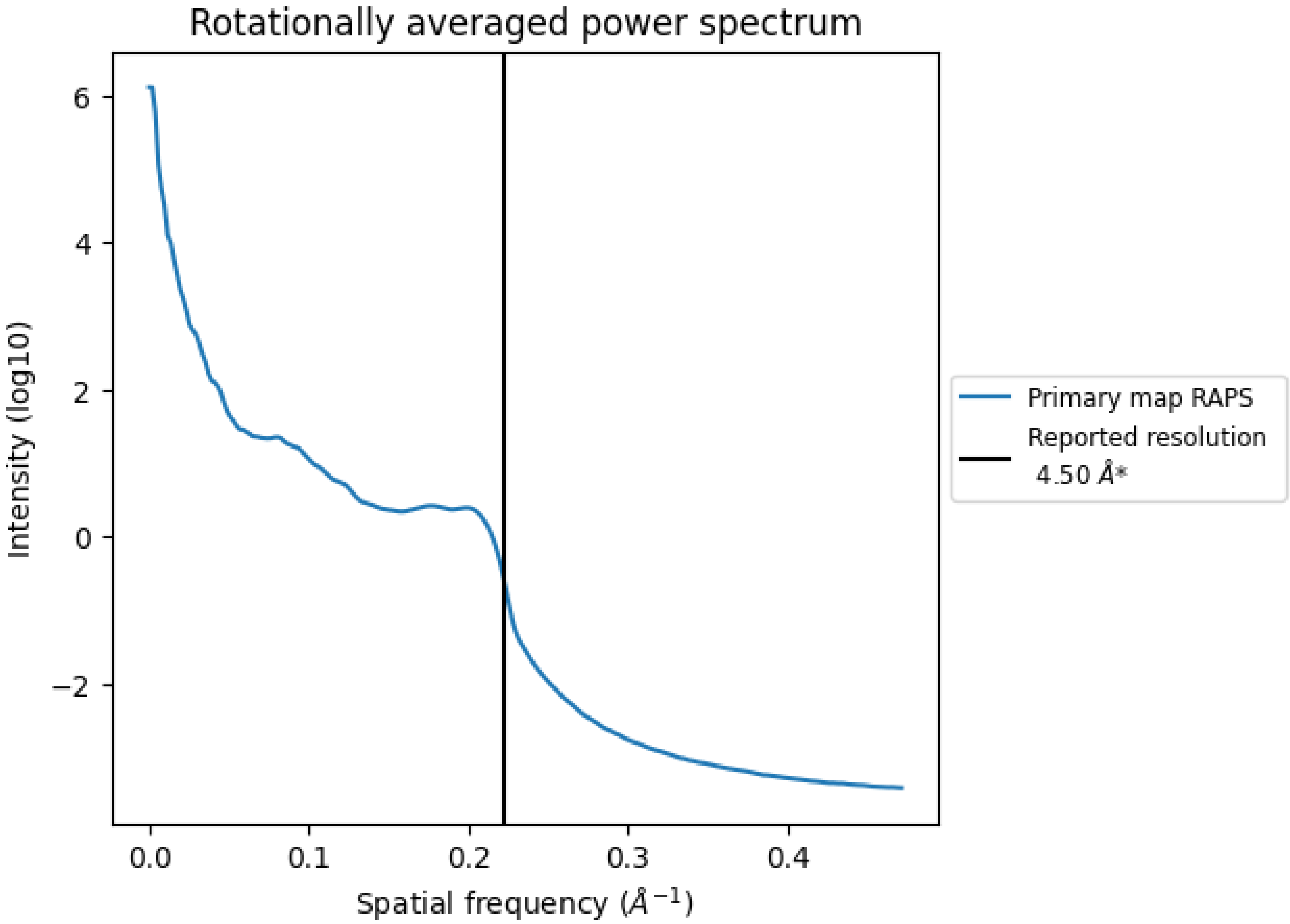
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 1509 nm^3; this corresponds to an approximate mass of 1363 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.222 $Å^{-1}$

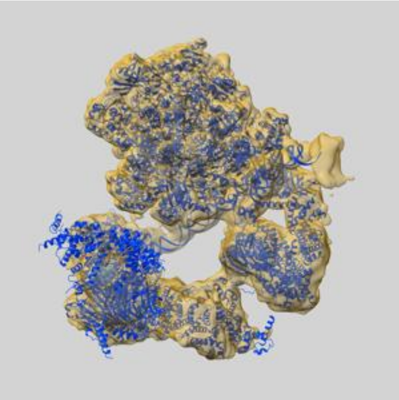
8 Fourier-Shell correlation

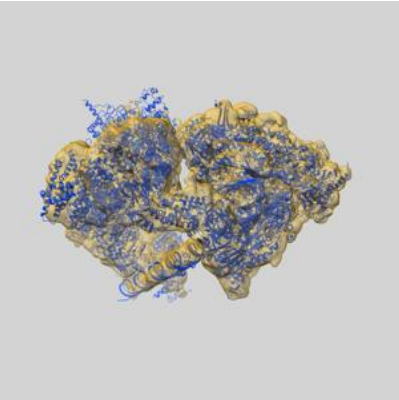
This section was not generated. No FSC curve or half-maps provided.

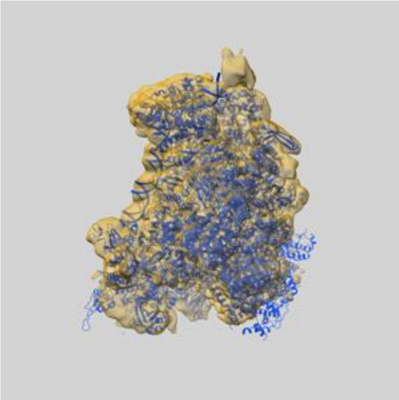
9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-31075 and PDB model 7EDX. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay ⓘ

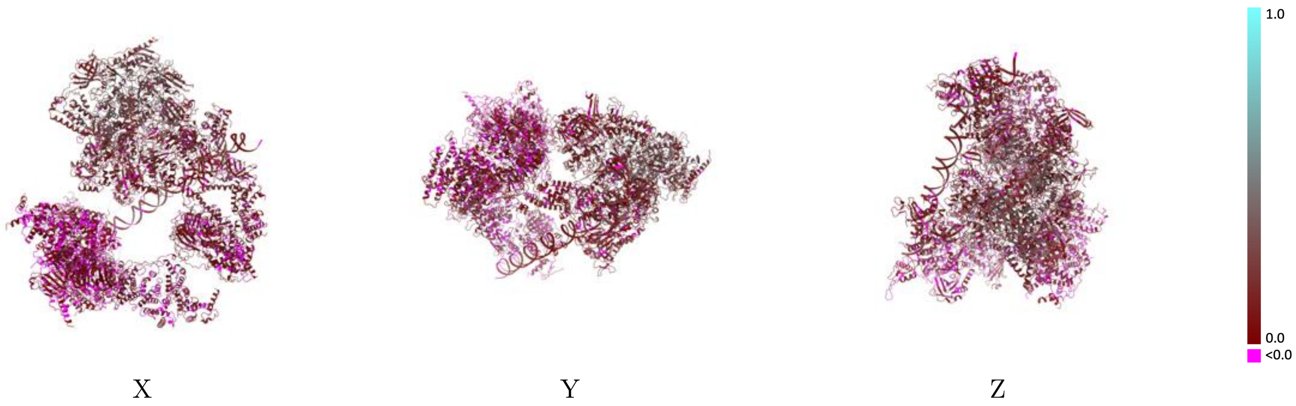

X


Y


Z

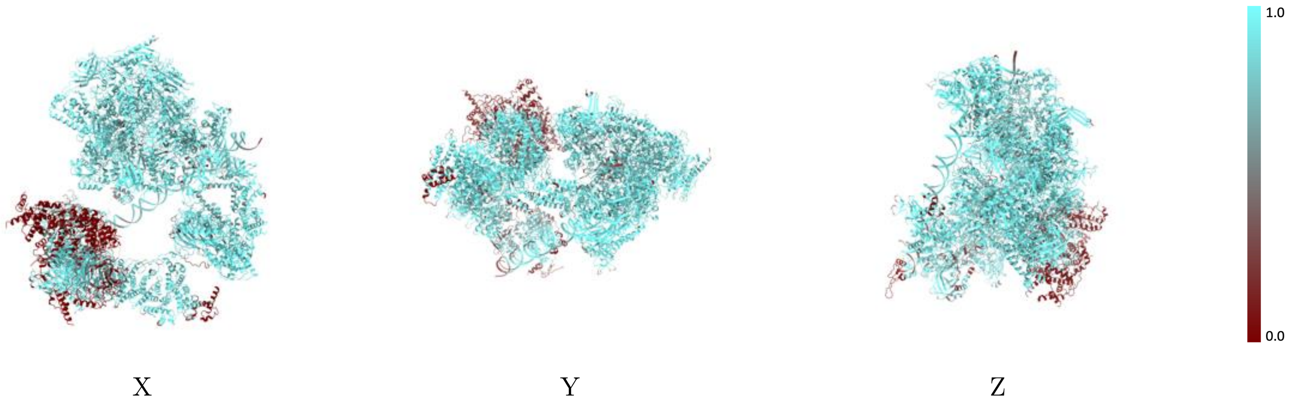
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ



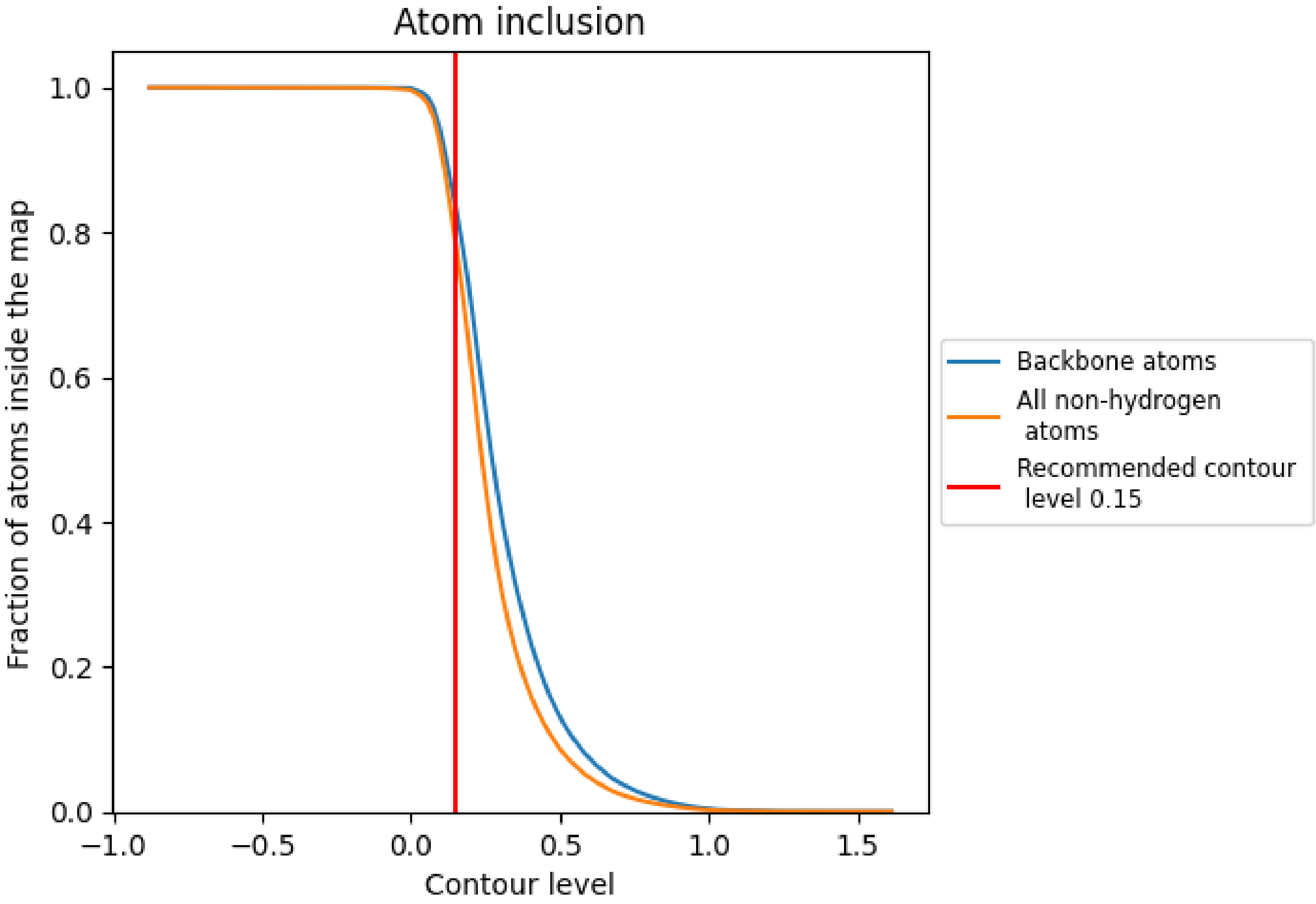
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model ⓘ



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

9.4 Atom inclusion ⓘ



At the recommended contour level, 84% of all backbone atoms, 78% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7849	0.1300
A	0.7315	0.0490
B	0.8956	0.0780
D	0.8660	0.1150
E	0.9057	0.0940
F	0.8202	0.0910
G	0.7496	0.0360
H	0.8654	0.0890
I	0.9401	0.0780
J	0.9684	0.0620
L	0.9199	0.1140
O	0.9287	0.1400
P	0.9702	0.1260
Q	0.9277	0.0970
R	0.9028	0.1670
S	0.8557	0.0980
T	0.8914	0.1130
X	0.7990	0.1150
Y	0.7752	0.1120
c	0.4455	0.0240
d	0.2816	0.0290
e	0.3019	0.0310
f	0.6412	0.0430
i	0.2248	0.0250
j	0.3383	0.0260
k	0.1276	0.0230
l	0.1281	0.0200
m	0.0057	0.0120
o	0.8917	0.2240
p	0.8561	0.2220
q	0.9415	0.2680
r	0.8687	0.1400
s	0.9303	0.2020
t	0.9286	0.2630
u	0.9354	0.1370

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Chain	Atom inclusion	Q-score
v	🟦 0.9085	🟫 0.2410
w	🟦 0.9405	🟫 0.1850
x	🟦 0.9455	🟫 0.3130
y	🟦 0.8934	🟫 0.2800
z	🟦 0.9551	🟫 0.2230