Full wwPDB EM Validation Report (i)

Oct 1, 2024 – 12:29 PM JST

PDB ID	:	7EG7
EMDB ID	:	EMD-31107
Title	:	TFIID-based core PIC on SCP promoter
Authors	:	Chen, X.; Qi, Y.; Hou, H.; Wang, X.; Wu, Z.; Li, J.; Xu, Y.
Deposited on	:	2021-03-24
Resolution	:	6.20 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 (i) 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 (i)) were used in the production of this report:

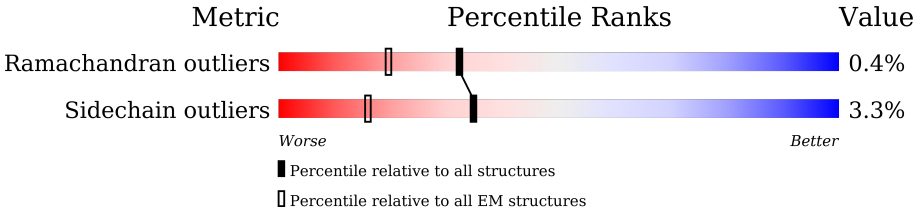
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 6.20 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	A	1872	12% 29% • 68%
2	B	1199	10% 79% • 20%
3	D	1085	• 13% • 85%
3	d	1085	14% 15% 85%
4	E	800	6% 67% • 32%
4	e	800	64% 67% 33%
5	F	677	17% 56% • 40%
5	f	677	30% 58% • 40%
6	G	349	17% 38% • 58%

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Mol	Chain	Length	Quality of chain
7	H	310	11% 65% 33%
8	I	264	5% 45% 55%
8	i	264	46% 46% 54%
9	J	218	6% 41% 59%
9	j	218	36% 44% 56%
10	L	161	16% 42% 6% 53%
10	l	161	66% 65% 34%
11	O	109	7% 77% 11% 11%
12	P	339	49% 48%
13	Q	376	31% 68%
14	R	316	72% 6% 22%
15	S	517	24% 74%
16	T	249	8% 43% 55%
17	X	79	25% 49% 41% 10%
18	Y	79	28% 58% 32% 10%
19	c	929	10% 13% 86%
20	k	211	46% 46% 54%
21	m	124	70% 69% 30%
22	o	1970	70% 28%
23	p	1174	95%
24	q	275	93% 7%
25	r	142	18% 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	91% 9%
30	x	67	96%
31	y	117	6% 100%
32	z	58	76% 24%
33	u	172	10% 98%

2 Entry composition (i)

There are 35 unique types of molecules in this entry. The entry contains 81525 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
			Total	C	N	O	S		
1	A	599	4909	3132	855	894	28	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	963	7795	5011	1315	1411	58	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	165	1377	858	257	258	4	0	0
3	d	158	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
			Total	C	N	O	S		
4	E	546	4364	2766	757	820	21	0	0
4	e	539	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
			Total	C	N	O	S		
5	F	404	3081	1954	537	572	18	0	0
5	f	403	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
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
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
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
			Total	C	N	O	S		
12	P	177	1412	918	249	238	7	0	0

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

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

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

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

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

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

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

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

- Molecule 17 is a DNA chain called DNA (79-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
17	X	71	1469	691	287	420	71	0	0

- Molecule 18 is a DNA chain called DNA (79-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
18	Y	71	1442	684	255	432	71	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
			Total	C	N	O	S		
26	s	209	1720	1089	300	323	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	t	79	635	406	108	116	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
			Total	C	N	O	S		
28	v	148	1186	750	194	237	5	0	0

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

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

- Molecule 30 is a protein called RPB10.

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

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

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

- Molecule 32 is a protein called RPB12.

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

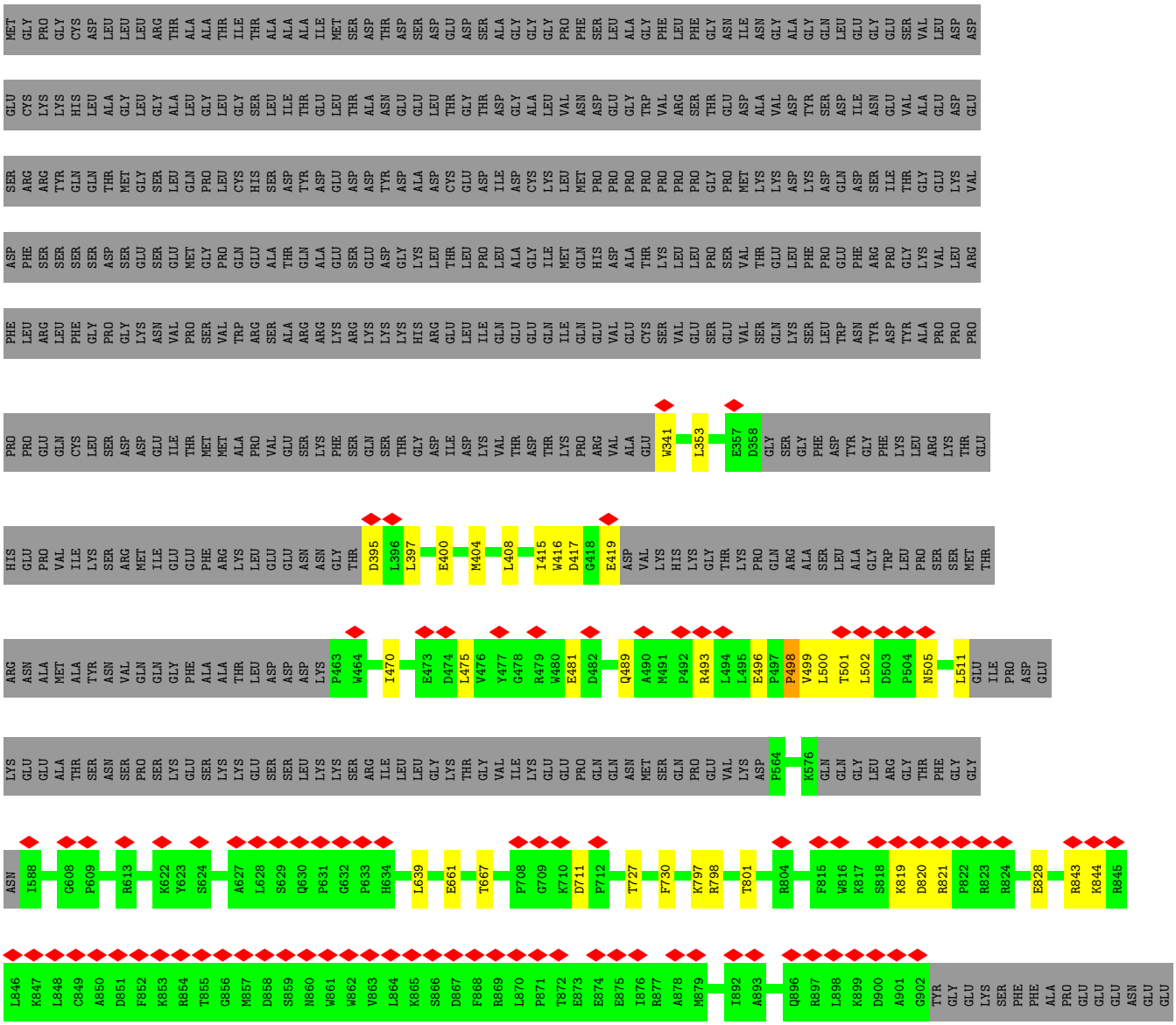
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
35	o	1	1	1	0

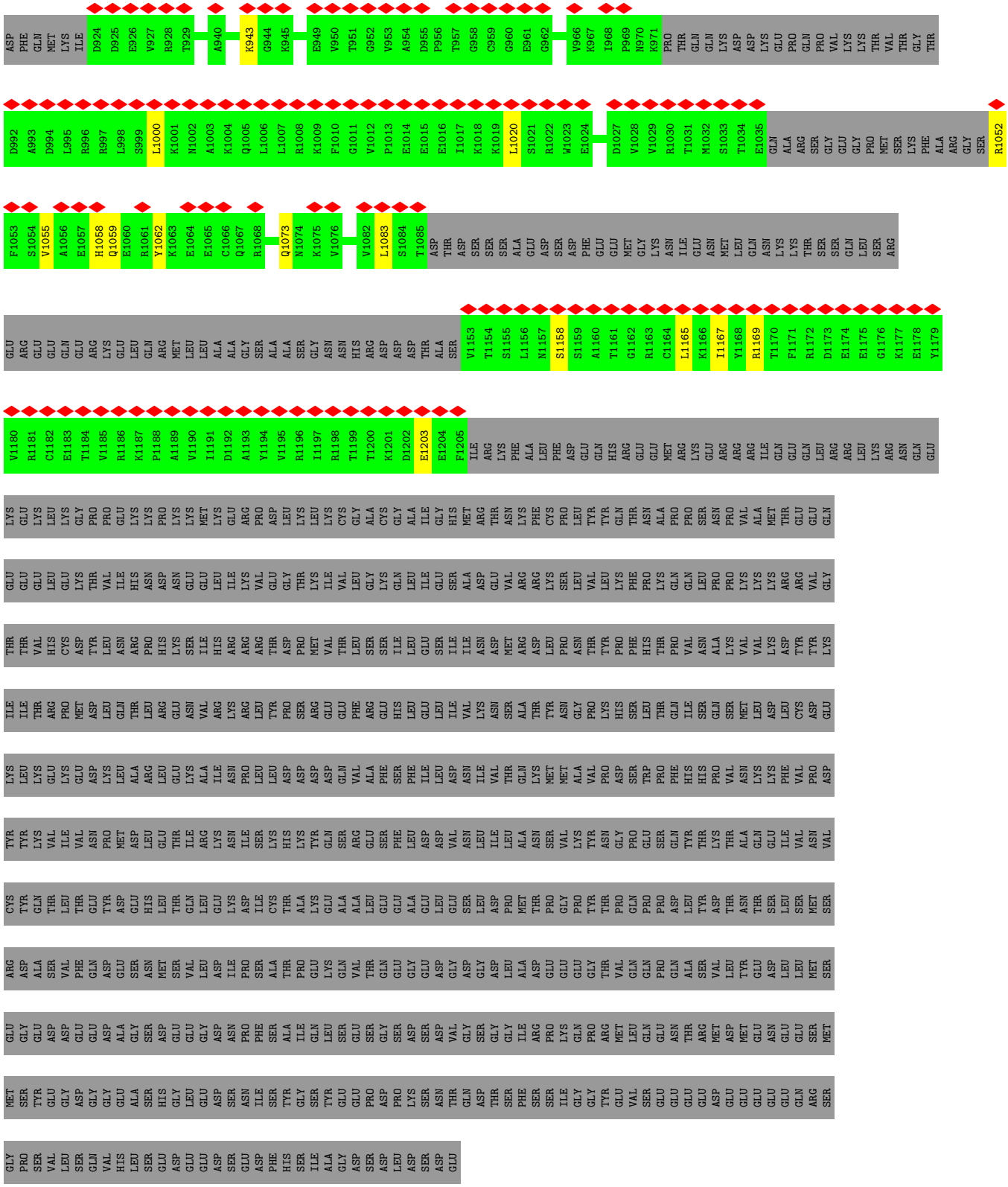
3 Residue-property plots (i)

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: Transcription initiation factor TFIID subunit 1

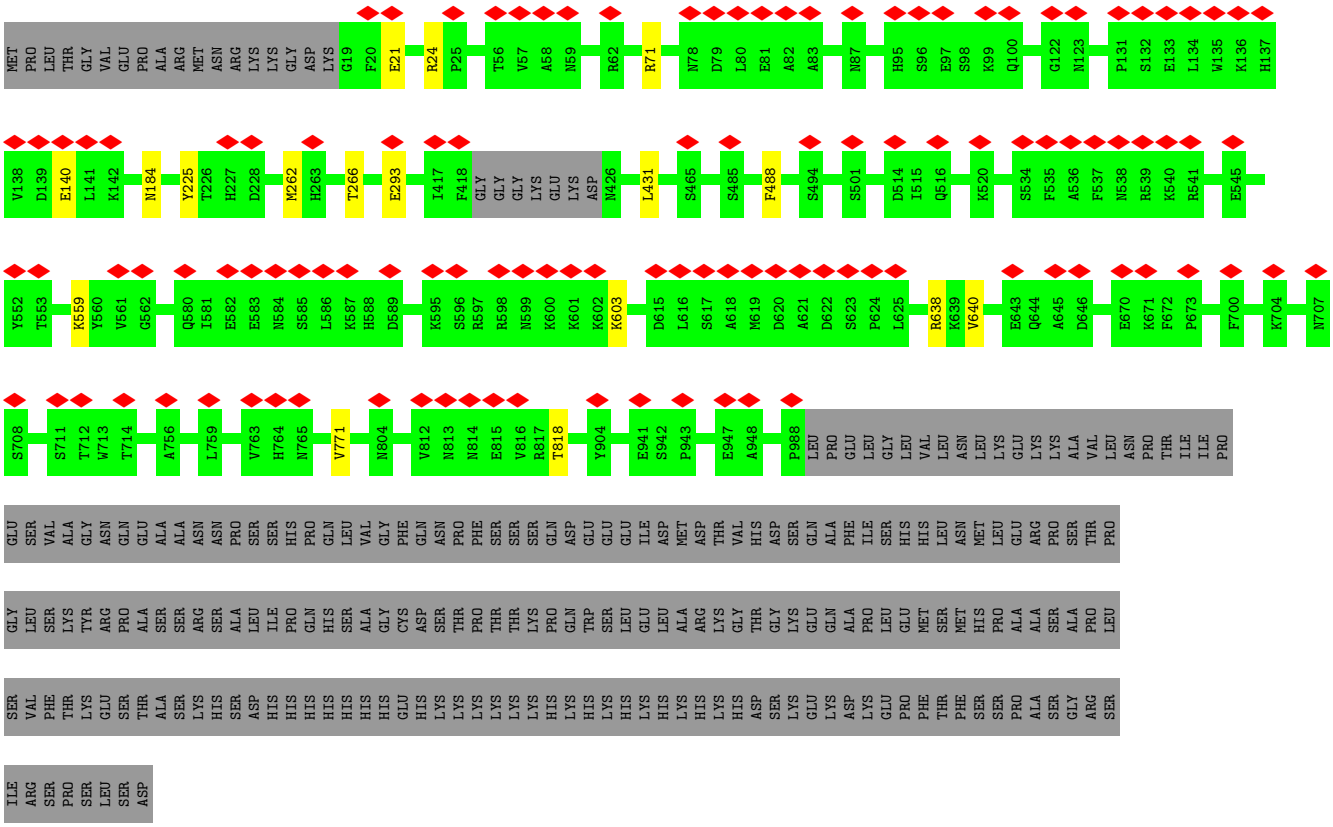
Chain A:





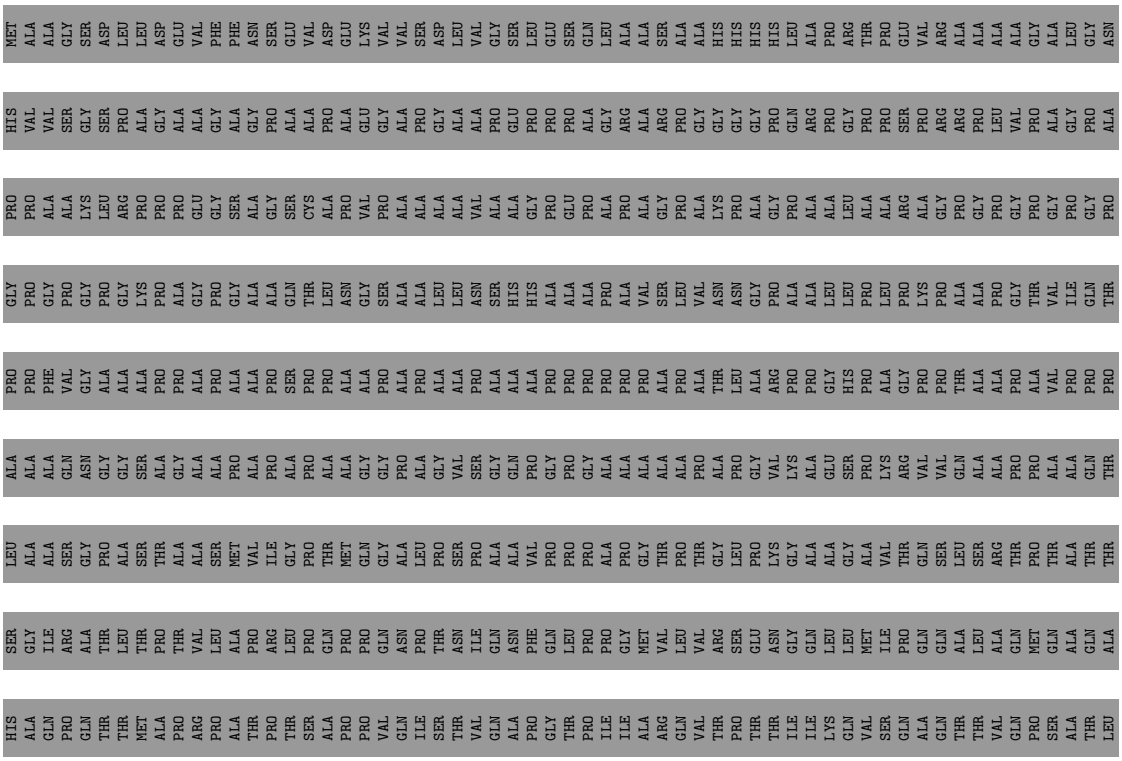
- Molecule 2: Transcription initiation factor TFIID subunit 2

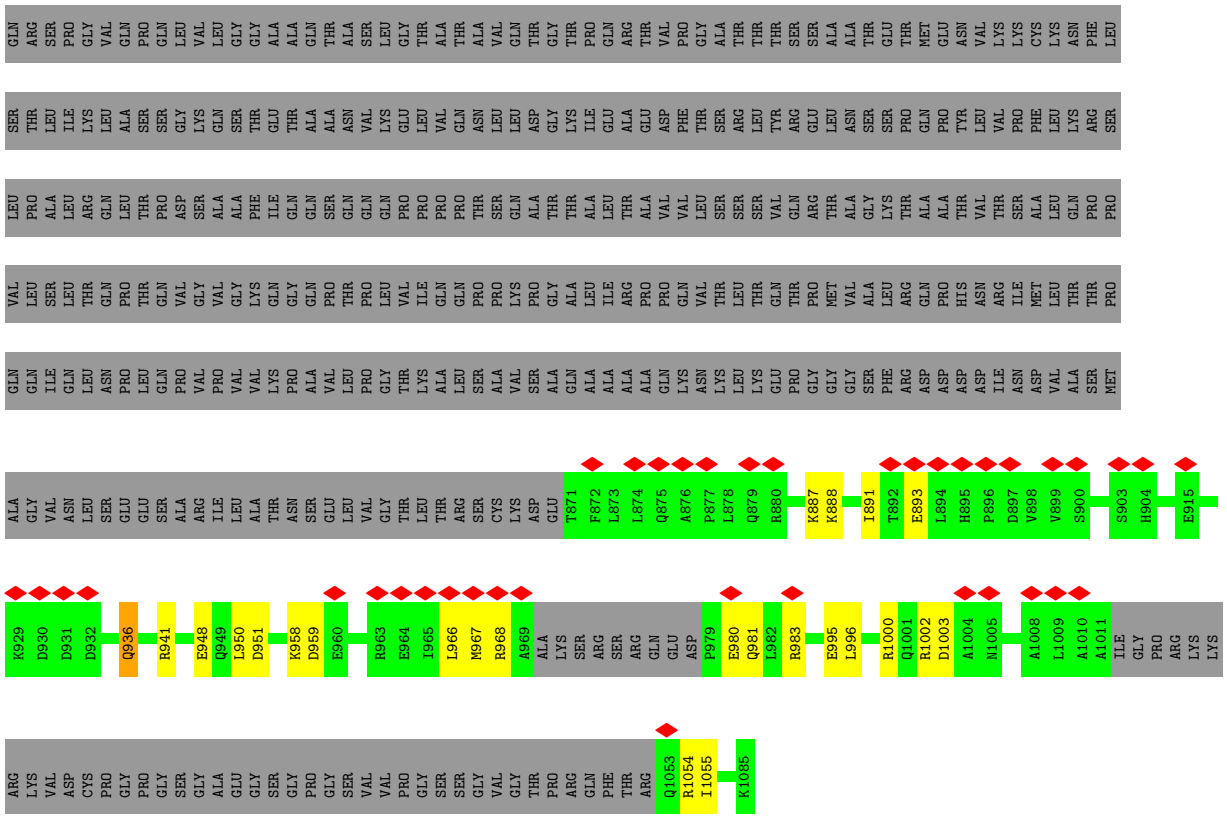
Chain B:



- Molecule 3: Transcription initiation factor TFIID subunit 4

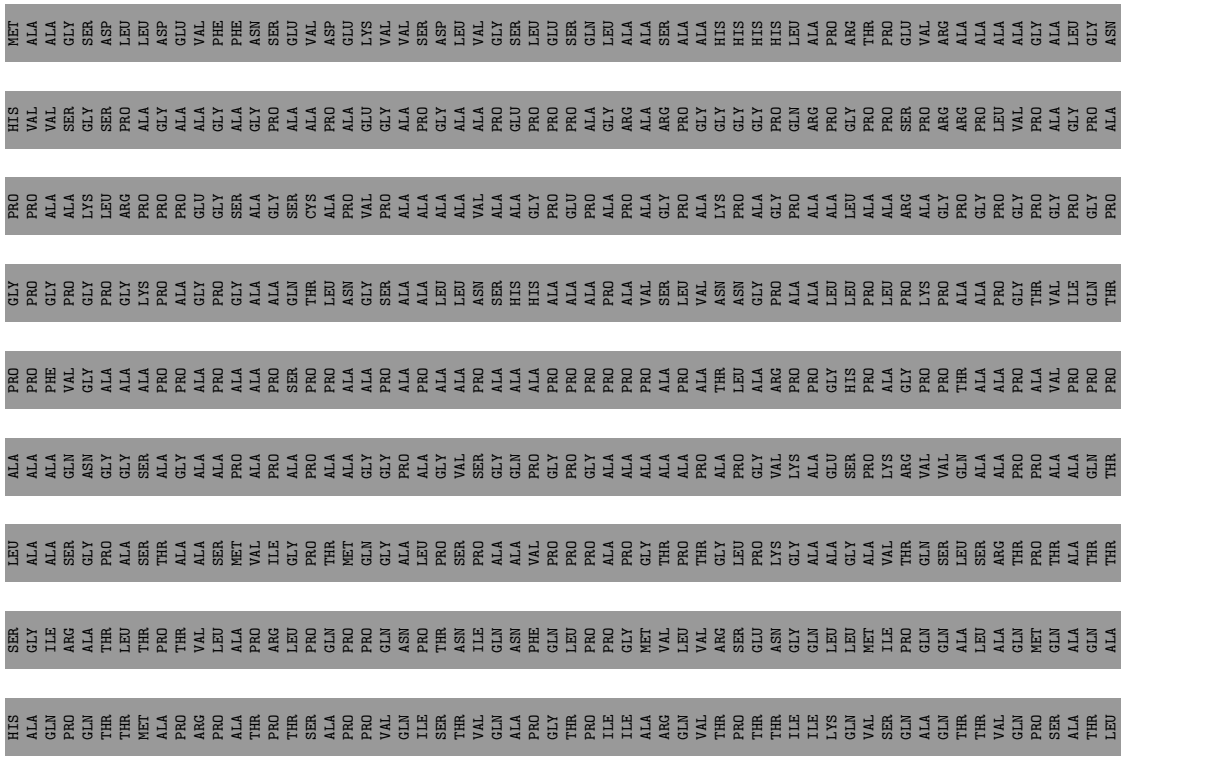
Chain D:

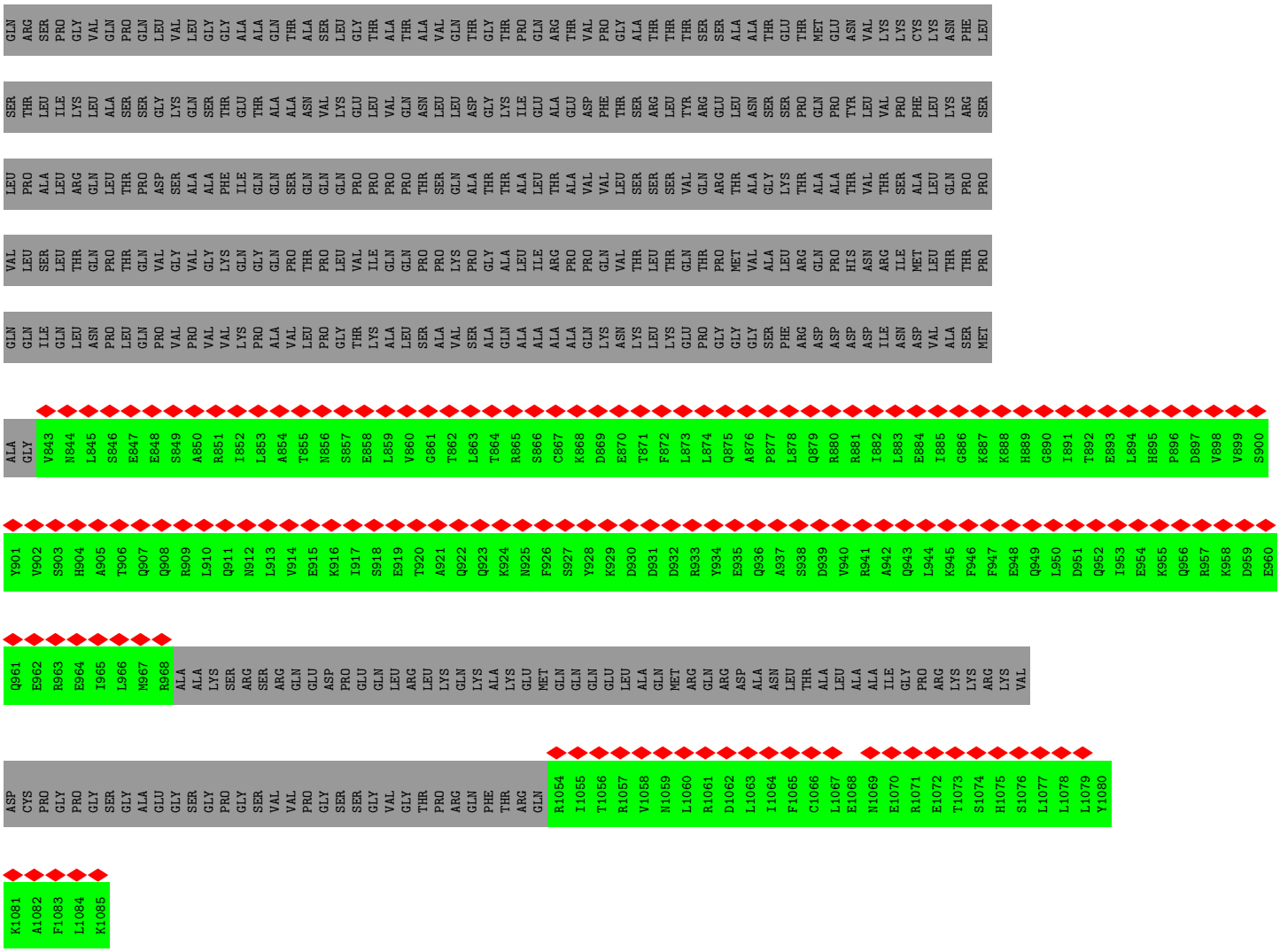




- Molecule 3: Transcription initiation factor TFIID subunit 4

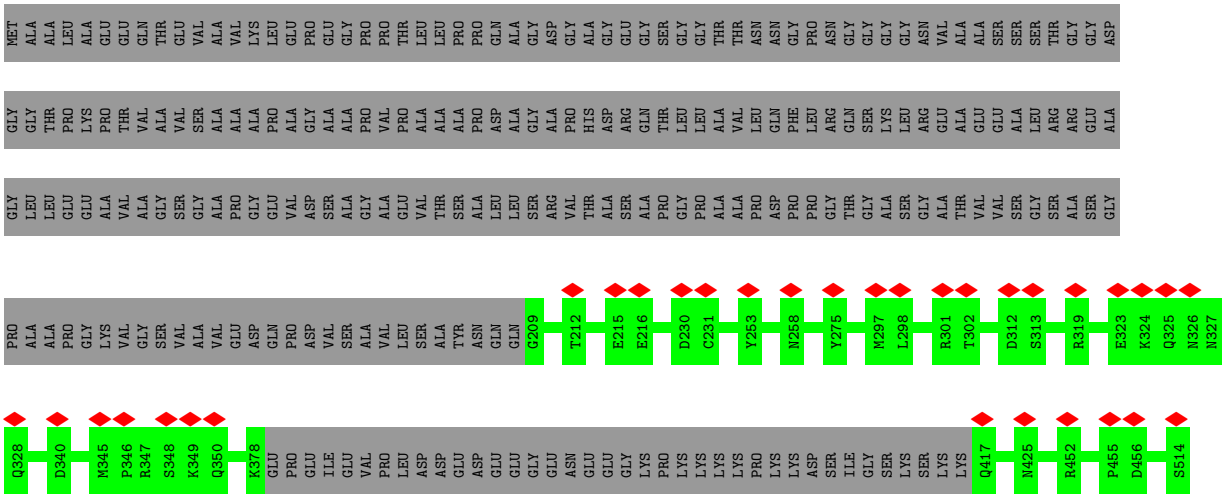
Chain d:





- Molecule 4: Transcription initiation factor TFIID subunit 5

Chain E:



L515 I516 D517 K518 E519 S520 D521 D522 V523 L524 E525 R526 K531 F593 L702 M703 V704 K742 E745 D746 L747 GLU THR ASP ASP PHE THR T754 I759 N760 L761 P762 E763 Q766 E767 S798 PRO GLN

- Molecule 4: Transcription initiation factor TFIID subunit 5

Chain e: 64% 67% 33%

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

GLY GLY THR PRO LYS PRO THR VAL ALA VAL SER ALA ALA ALA PRO ALA GLY ALA ALA PRO VAL PRO ALA ALA ALA PRO ASP ALA GLY ALA PRO HIS ASP ARG GLN THR LEU LEU ALA VAL LEU GLN PHE LEU ARG GLN SER LYS LEU ARG GLU ALA GLU GLU ALA LEU ARG ARG GLU ALA

GLY LEU LEU GLU GLU ALA VAL ALA GLY SER GLY ALA PRO GLY GLU VAL ASP SER ALA GLY ALA GLU VAL THR SER ALA LEU LEU SER ARG VAL THR ALA SER ALA PRO GLY PRO ALA ALA PRO ASP PRO PRO GLY THR GLY ALA SER GLY ALA THR VAL VAL SER GLY SER ALA SER GLY

PRO ALA ALA PRO GLY LYS VAL GLY SER VAL ALA VAL GLU ASP GLN PRO ASP VAL SER ALA VAL L202 S203 A204 Y205 N206 Q207 Q208 G209 D210 P211 T212 M213 Y214 E215 E216 Y217 Y218 S219 G220 L221 K222 H223 F224 I225 E226 C227 S228 L229 D230 C231 H232 R233 A234 E235 L236 S237 Q238 L239 F240

Y241 P242 L243 F244 V245 H246 M247 Y248 L249 E250 L251 V252 Y253 N254 Q255 H256 E257 N258 E259 A260 K261 S262 F263 F264 E265 K266 F267 H268 G269 D270 Q271 E272 C273 Y274 Y275 Q276 D277 D278 L279 R280 V281 L282 S283 S284 L285 T286 K287 K288 E289 H290 M291 K292 G293 N294 E295 T296 M297 L298 D299 F300

R301 T302 S303 K304 F305 V306 L307 R308 I309 S310 R311 D312 S313 Y314 Q315 L316 L317 K318 R319 H320 L321 Q322 E323 K324 Q325 N326 N327 Q328 I329 W330 N331 I332 V333 Q334 E335 H336 L337 Y338 I339 D340 I341 F342 D343 GLY MET PRO ARG SER LYS GLN GLN ILE ASP ALA MET VAL GLY SER LEU ALA

GLY GLU A363 K364 R365 E366 A367 N368 K369 S370 K371 V372 F373 F374 G375 L376 L377 K378 E379 P380 GLU ILE GLU VAL PRO LEU ASP ASP GLU ASP GLU GLU GLY GLU ASN GLU GLU GLY LYS PRO LYS LYS LYS LYS PRO LYS LYS ASP SER ILE GLY SER LYS SER LYS K416 Q417 D418 P419 N420

A421 P422 P423 Q424 N425 R426 I427 P428 L429 P430 E431 L432 K433 D434 S435 D436 K437 L438 D439 K440 I441 M442 N443 M444 K445 E446 T447 T448 K449 R450 V451 R452 L453 G454 P455 D456 C457 L458 P459 S460 I461 C462 F463 Y464 T465 F466 L467 M468 A469 Y470 Q471 G472 L473 T474 A475 V476 D477 V478 T479 D480

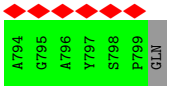
D481 S482 S483 L484 I485 A486 G487 G488 F489 A490 D491 S492 T493 V494 R495 V496 W497 S498 V499 T500 P501 K502 K503 L504 R505 S506 V507 K508 Q509 A510 S511 D512 L513 S514 L515 I516 D517 K518 E519 S520 D521 D522 V523 L524 E525 R526 I527 M528 D529 E530 K531 T532 A533 S534 E535 L536 K537 I538 G541

H542 P545 V546 Y547 S550 F551 S552 P553 D554 R555 N556 Y557 L558 L559 S560 S561 S562 E563 R568 L569 W570 S571 L572 Q573 T574 F575 T576 C577 L578 K582 G583 H584 N585 Y586 W589 D590 F593 S594 P595 Y596 G597 Y598 Y599 F600 V601 S602 G603 G604 H605 D606 R607 V608 L611

W612 A613 T614 D615 H616 Y617 Q618 P619 L620 R621 I622 F623 A624 G625 H626 L627 V630 M631 C632 T633 R634 F635 H636 P637 N638 S639 N640 Y641 V642 A643 T644 G645 S646 A647 D648 R649 R652 L653 W654 D655 V656 L657 N658 G659 N660 C661 V662 R663 I664 F665 T666 G667 H668 K669 G670 P671 I672 H673

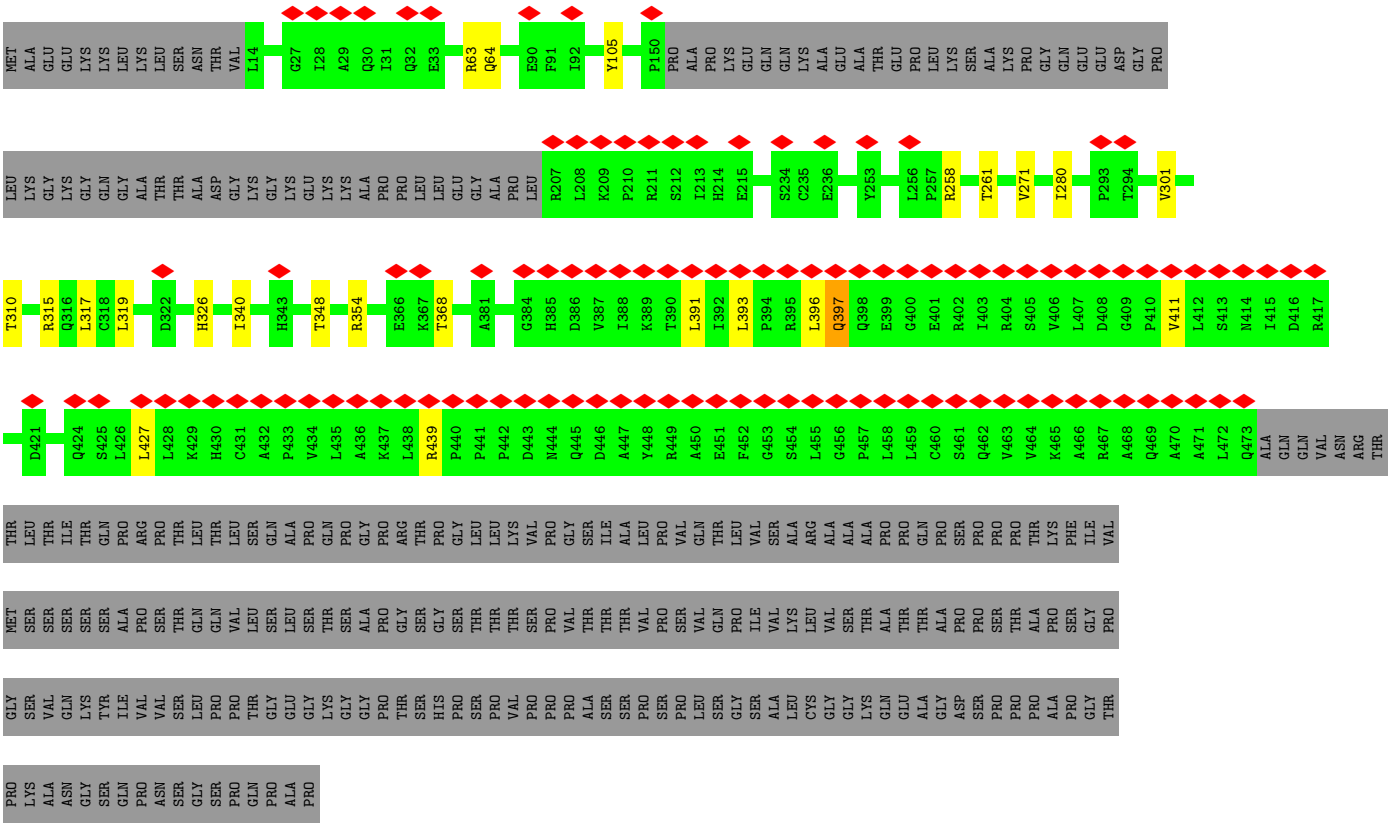
S674 L675 T676 F677 S678 P679 N680 G681 R682 F683 L684 A685 T686 G687 A688 T689 D690 G691 R692 V693 L694 L695 W696 D697 I698 G699 H700 G701 L702 M703 V704 G705 E706 L707 K708 G709 H710 T711 D712 T713 V714 C715 S716 L717 R718 F719 S720 R721 D722 G723 E724 I725 L726 A727 S728 G729 S730 M731 D732 N733

T734 V735 R736 L737 W738 D739 A740 I741 K742 A743 F744 E745 D746 L747 E748 THR ASP ASP PHE THR T754 A755 T756 G757 H758 I759 N760 L761 P762 E763 N764 S765 Q766 E767 L768 L769 L770 G771 T772 Y773 M774 T775 K776 S777 T778 P779 V780 V781 H782 L783 H784 F785 T786 R787 R788 N789 L790 V791 L792 A793



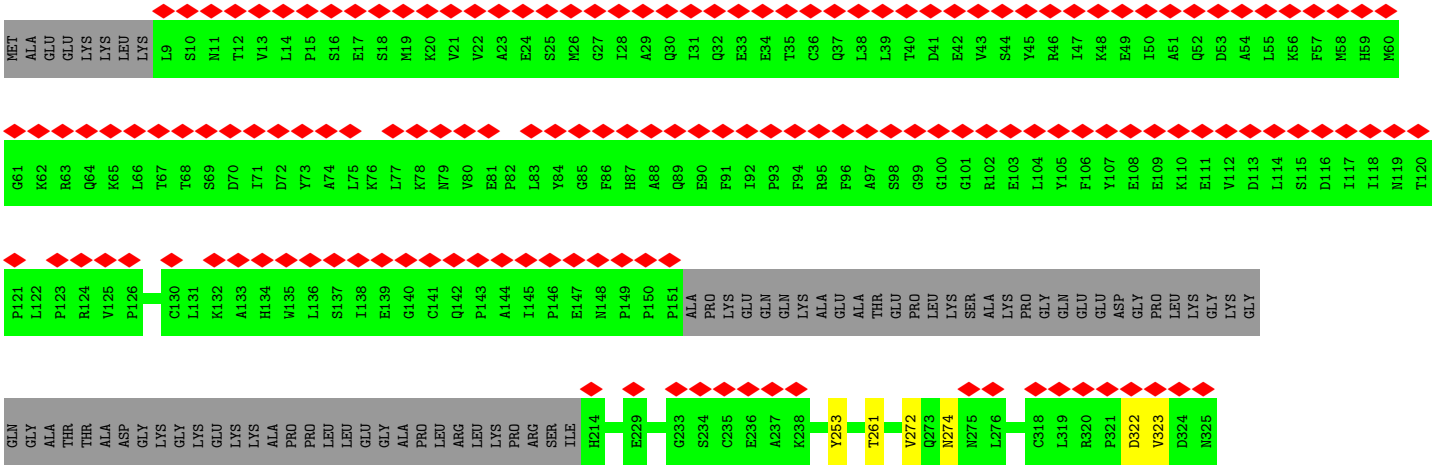
• Molecule 5: Transcription initiation factor TFIID subunit 6

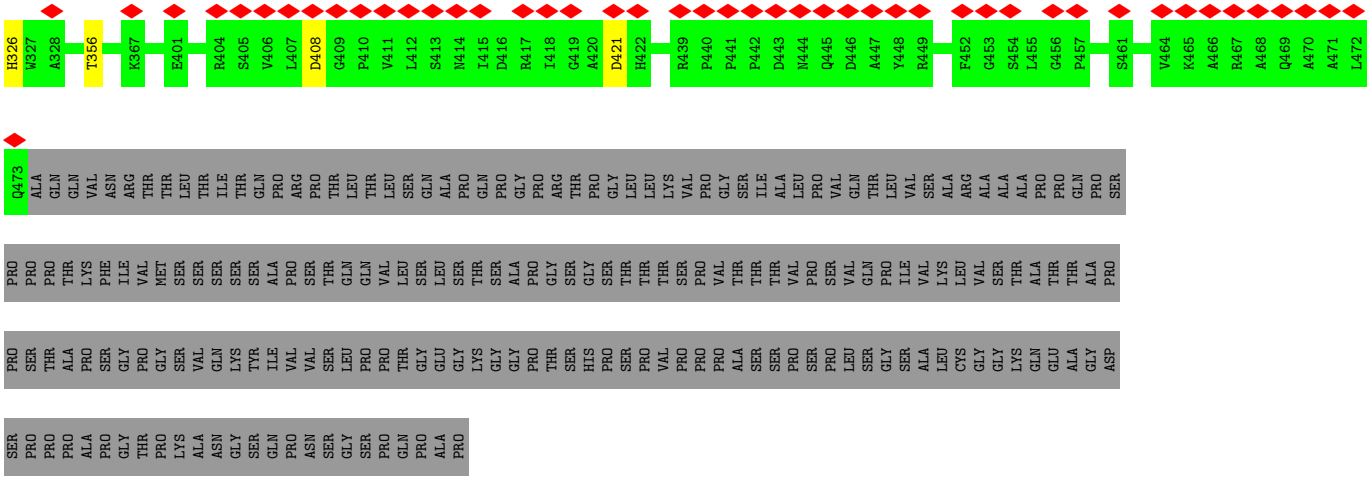
Chain F:



• Molecule 5: Transcription initiation factor TFIID subunit 6

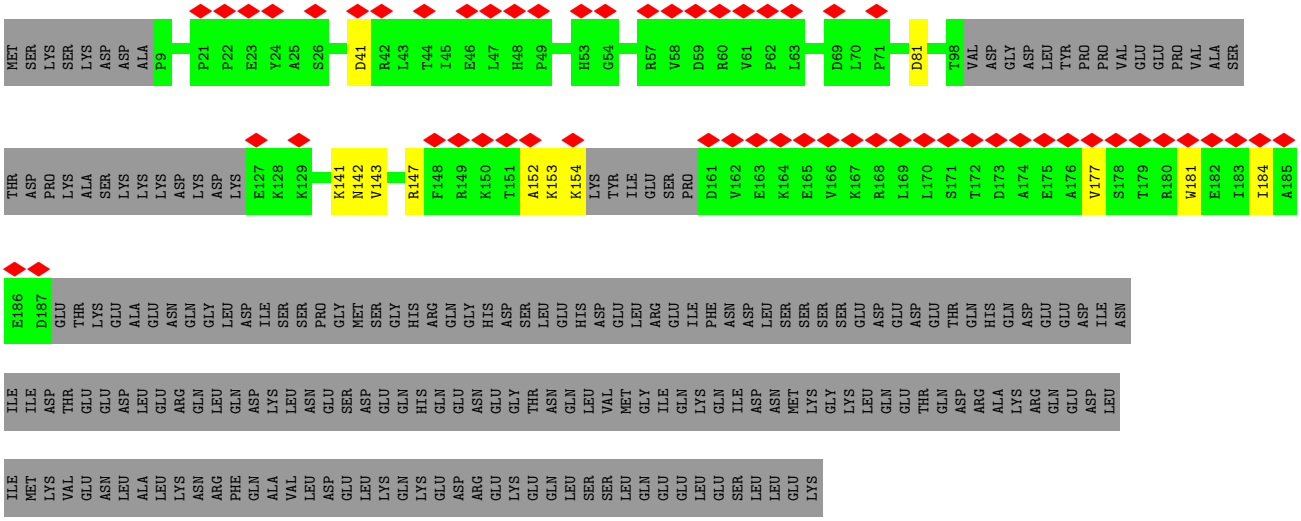
Chain f:





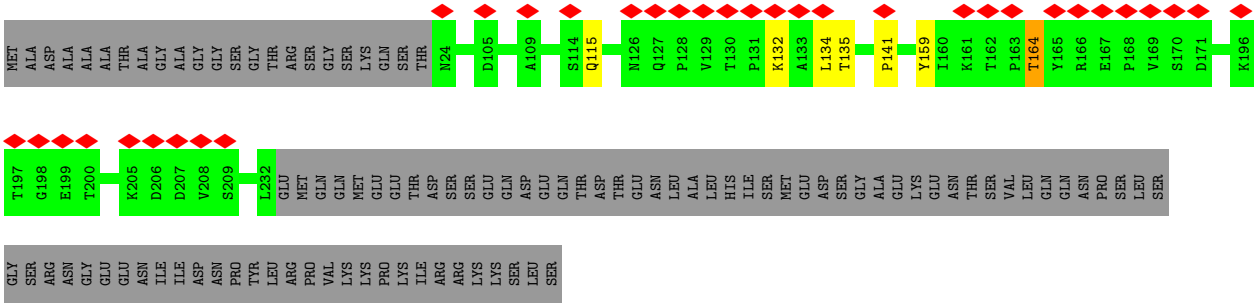
- Molecule 6: Transcription initiation factor TFIID subunit 7

Chain G:



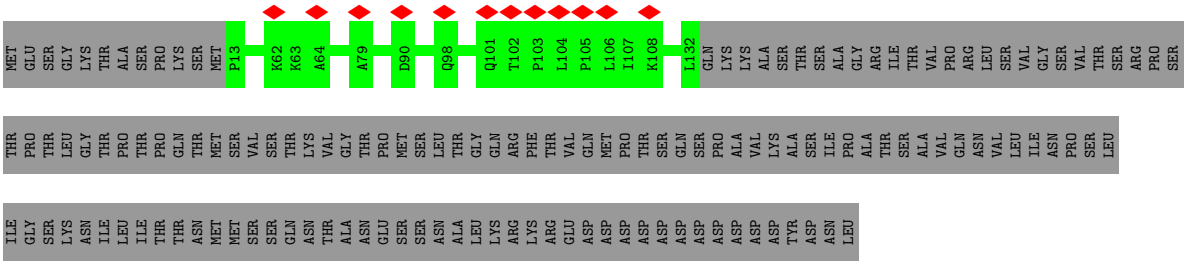
- Molecule 7: Transcription initiation factor TFIID subunit 8

Chain H:



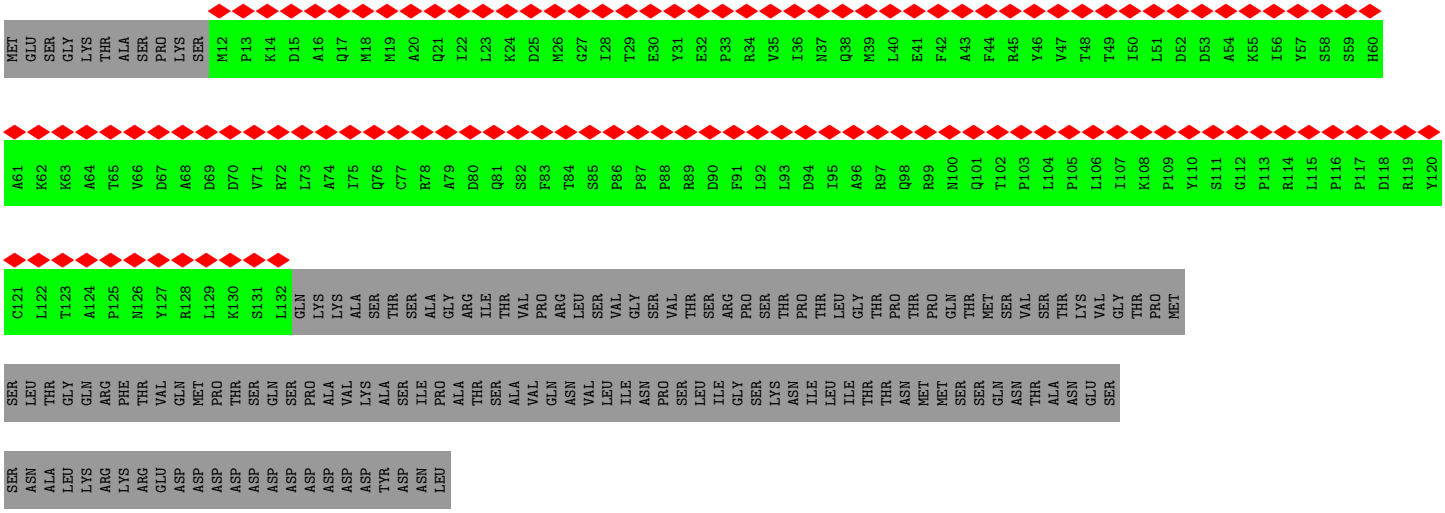
- Molecule 8: Transcription initiation factor TFIID subunit 9

Chain I:



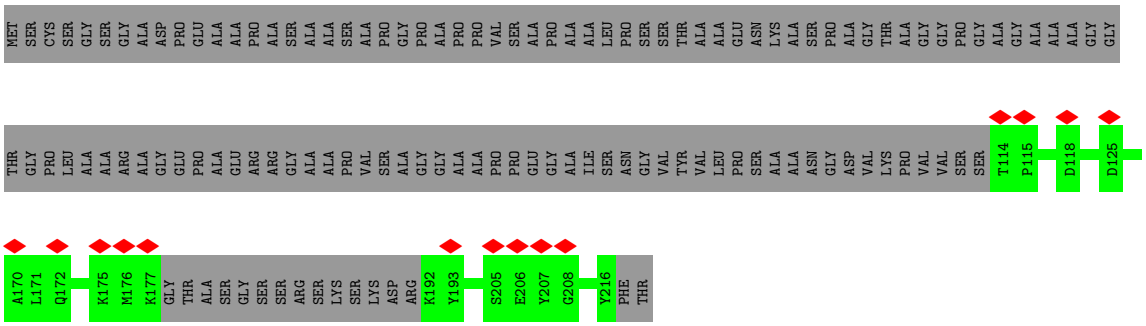
- Molecule 8: Transcription initiation factor TFIID subunit 9

Chain i:



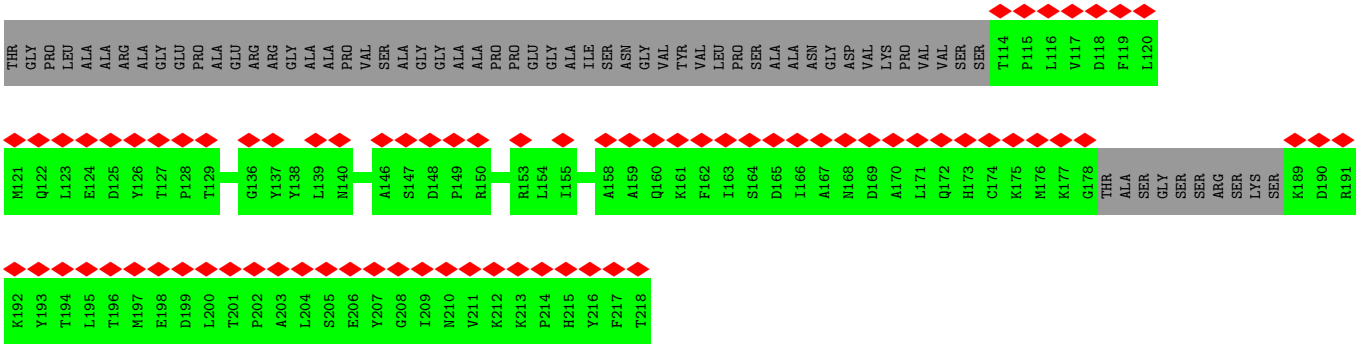
- Molecule 9: Transcription initiation factor TFIID subunit 10

Chain J:

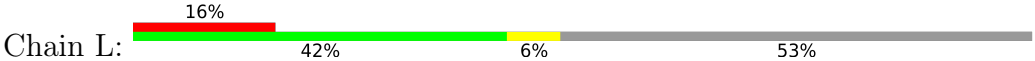


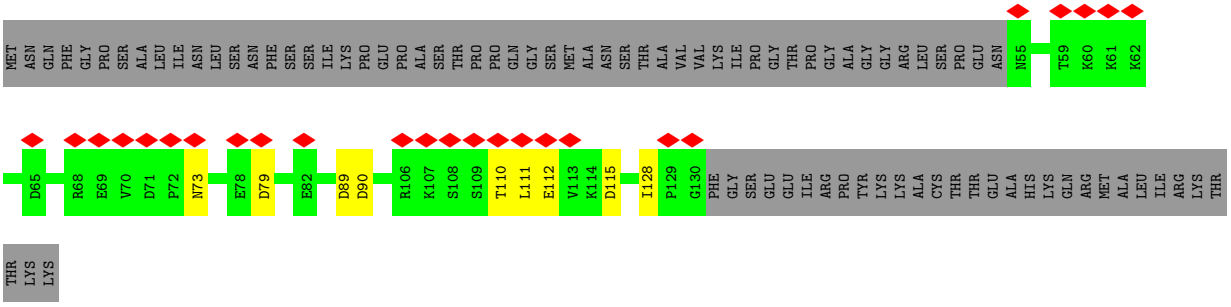
- Molecule 9: Transcription initiation factor TFIID subunit 10

Chain j:

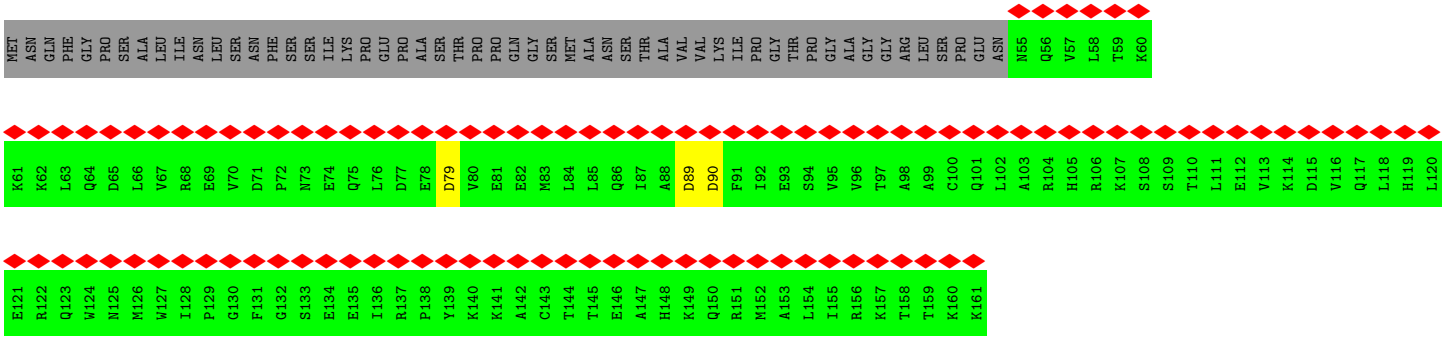


• Molecule 10: Transcription initiation factor TFIID subunit 12

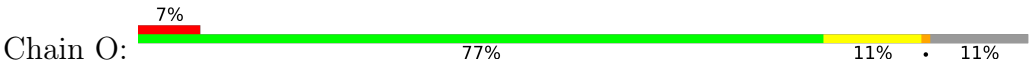


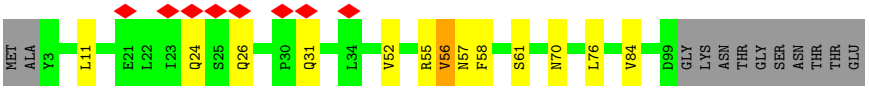


• Molecule 10: Transcription initiation factor TFIID subunit 12

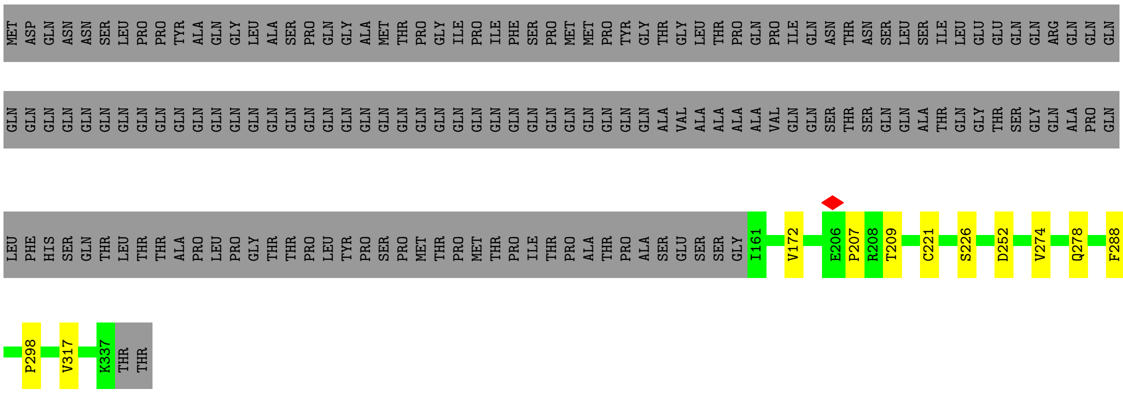


• Molecule 11: Transcription initiation factor IIA subunit 2



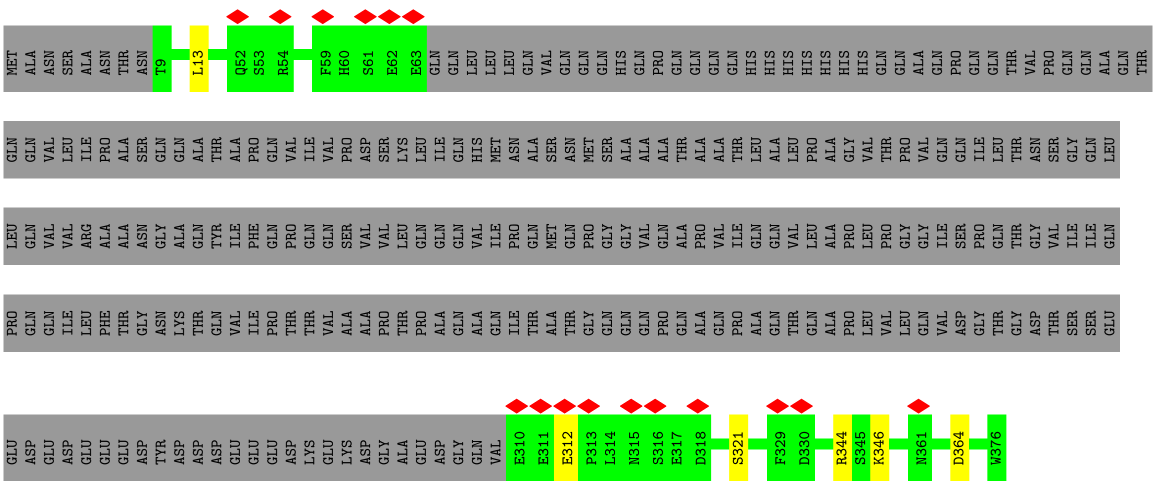


• Molecule 12: TATA-box-binding protein



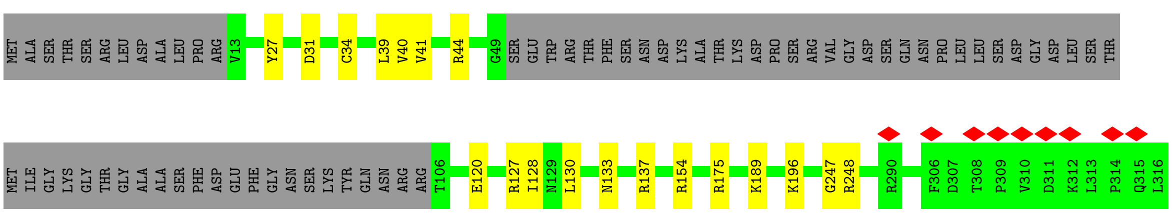
• Molecule 13: Transcription initiation factor IIA subunit 1

Chain Q:



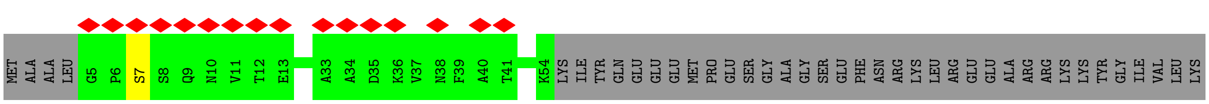
• Molecule 14: Transcription initiation factor IIB

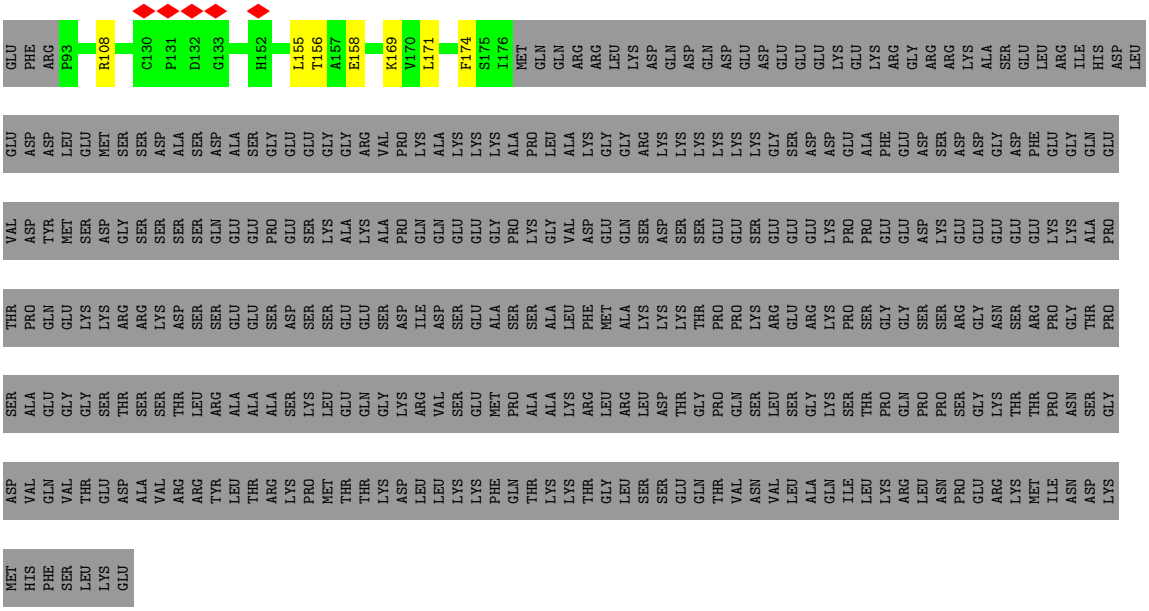
Chain R:



• Molecule 15: General transcription factor IIF subunit 1

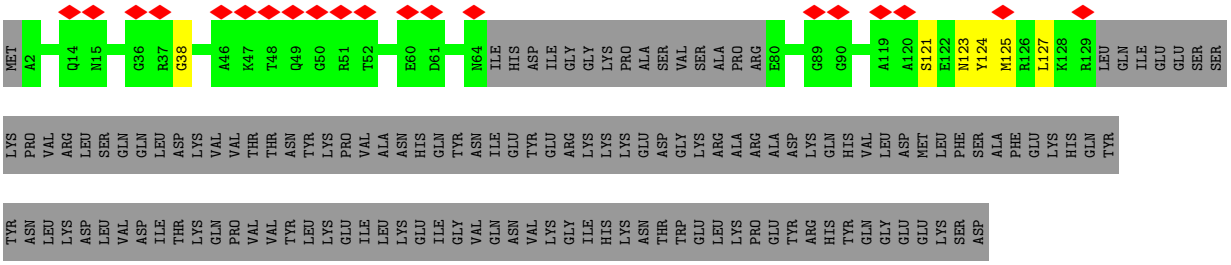
Chain S:





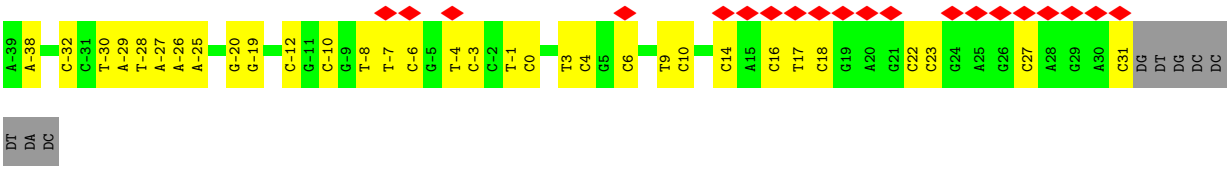
- Molecule 16: General transcription factor IIF subunit 2

Chain T:



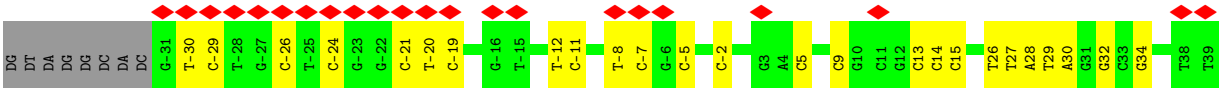
- Molecule 17: DNA (79-MER)

Chain X:



- Molecule 18: DNA (79-MER)

Chain Y:



- Molecule 19: Transcription initiation factor TFIID subunit 3

Chain c: 10% 13% 86%

M1 S6 R7 S8 V12 S13 V14 A15 Q16 I17 C18 Q19 A20 L21 C22 W23 D24 S25 V26 Q27 L28 S29 A30 C31 H32 L33 L34 T35 D36 V37 R40 R47 H50 R51 Y52 L55 Y56 G57 R58 T59 I62 L63 D64 D65 V66 G67 E68 A69 F70 Q71 L72 M73 G74

V75 S76 L77 H78 E79 L80 E81 D82 Y83 I84 H85 N86 I87 E88 P89 V90 T91 F92 P93 H94 Q95 I96 P97 V101 S102 K103 N104 N105 V106 L107 Q108 F109 P110 Q111 P112 G113 S114 K115 D116 A117 E118 E119 R120 K121 E122 Y123 I124 P125 D126 Y127 LEU PRO PRO ILE VAL SER SER GLN GLU

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

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

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

SER PRO LYS SER PRO LYS SER PRO LYS VAL THR THR HIS ILE PRO GLN THR PRO VAL ARG PRO GLU THR PRO ASN ARG THR PRO SER ALA THR LEU SER GLU LYS ILE SER LYS GLU THR ILE GLN VAL LYS GLN ILE GLN THR PRO PRO ASP ALA GLY LYS GLU ASN GLN

PRO LYS LYS ALA VAL VAL ALA ASP LYS THR ILE GLU ALA SER ILE ASP ALA VAL ILE ALA ARG ALA CYS ALA GLU ARG GLU PRO ASP PRO PHE GLU PHE SER SER GLY SER GLU SER GLU GLY ASP ILE PHE THR SER PRO LYS ARG ILE SER GLY PRO GLU CYS THR THR PRO LYS ALA

SER THR SER ALA ASN ASN PHE THR LYS SER GLY SER THR PRO LEU PRO LEU SER GLY GLY THR SER SER SER SER ASP ASN SER TRP THR MET ASP ALA SER ILE ASP GLU VAL VAL ARG LYS ALA LYS LEU GLY THR PRO SER ASN MET PRO PRO ASN PHE PRO TYR ILE SER SER PRO SER

VAL SER PRO PRO THR PRO GLU PRO LEU HIS LYS VAL TYR GLU GLU LYS THR LYS LEU PRO SER SER VAL GLU VAL LYS LYS LYS LYS LEU LYS LYS THR LYS MET LYS LYS LYS GLU GLU LYS GLN ARG ASP ARG GLU ARG GLU LYS ASP LYS ASN LYS ASP LYS GLU LYS LYS

ASP LYS VAL LYS GLU LYS GLU LYS ASP LYS GLU THR GLY ARG GLU THR LYS TYR PRO TRP LYS GLU PHE LEU LYS GLU GLU GLU ALA ASP PRO TYR LYS PHE LYS ILE LYS GLU PHE GLU ASP VAL ASP PRO LYS VAL LYS LEU LYS ASP GLY LEU VAL ARG LYS GLU LYS GLU LYS HIS

LYS ASP LYS LYS LYS ASP ARG GLU LYS GLY LYS LYS ASP LYS ASP LYS GLU LYS GLY ARG GLU ASP LYS MET LYS ALA PRO ALA PRO PRO LEU VAL LEU PRO PRO LYS GLU LEU ALA LEU PRO LEU PHE SER PRO ALA THR ALA SER ARG VAL PRO ALA

MET LEU PRO SER LEU LEU PRO VAL LEU PRO GLU LYS LEU PHE GLU GLU LYS GLU LYS VAL LYS GLU LYS LYS LYS ASP LYS LYS GLU LYS LYS LYS LYS LYS GLU LYS LYS LYS GLU LYS GLU LYS GLU LYS GLU ARG GLU LYS LYS GLU LYS ARG GLU LYS GLU

LYS GLU LYS HIS LYS HIS GLU LYS ILE LYS VAL GLU PRO VAL ALA LEU ALA PRO SER PRO VAL ILE PRO ARG LEU THR LEU ARG VAL GLY ALA GLY GLN ASP LYS ILE VAL ILE SER LYS VAL VAL PRO ALA PRO GLU ALA LYS PRO VAL ALA PRO SER GLN ASN ARG PRO LYS THR PRO PRO

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

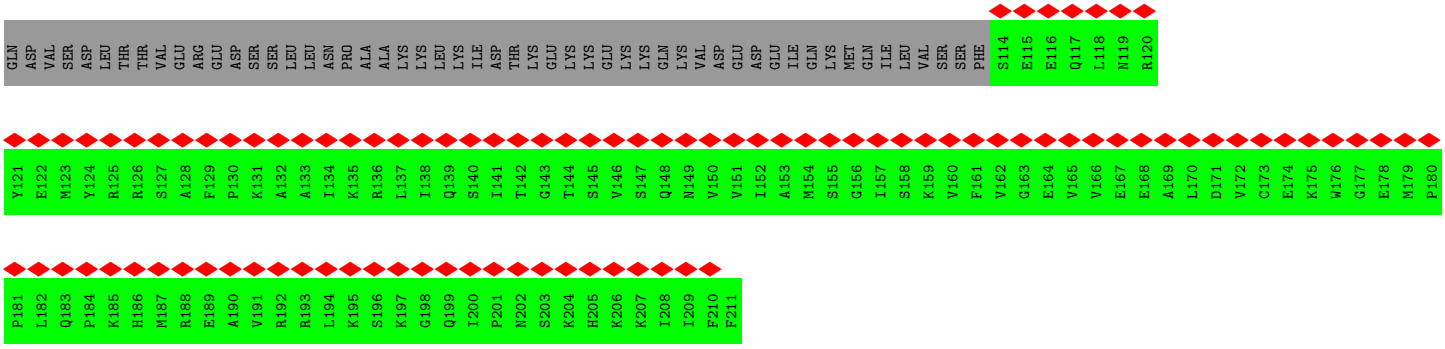
ILE ARG ASP GLU TRP GLY ASN GLN ILE TRP ILE CYS PRO GLY CYS ASN LYS PRO ASP ASP GLY SER PRO MET ILE GLY CYS ASP ASP CYS ASP ASP TRP TYR HIS TRP PRO GLY PRO ALA ALA SER GLY ILE MET THR ALA PRO PRO GLU GLU MET GLN TRP PHE CYS PRO LYS CYS ALA ASN LYS LYS

LYS ASP LYS LYS HIS LYS LYS ARG LYS HIS ARG ALA HIS

- Molecule 20: Transcription initiation factor TFIID subunit 11

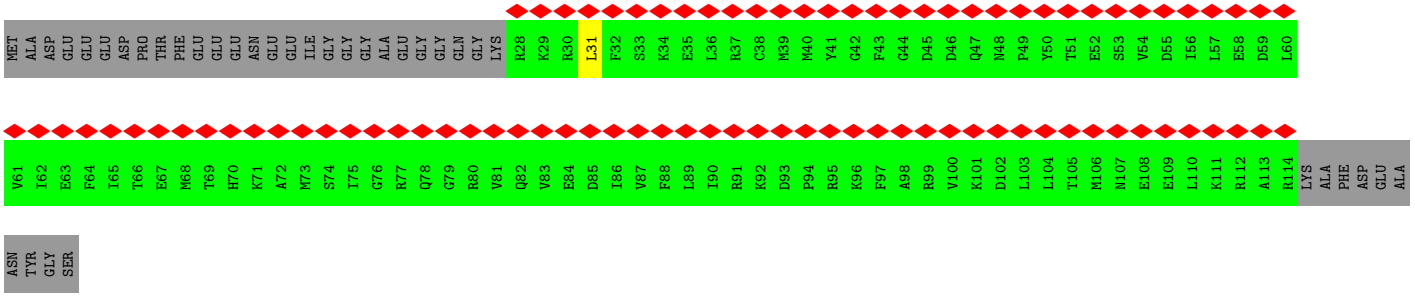
Chain k: 46% 46% 54%

MET ASP ASP ALA HIS GLU SER PRO SER ASP LYS GLY GLY GLU THR GLY GLU SER ASP GLU THR ALA ALA VAL PRO GLY GLY ASP PRO GLY ALA THR ASP THR ASP GLY ILE PRO GLU GLU THR ASP GLY ASP ALA ASP VAL ASP LEU LYS GLU ALA ALA ALA GLU GLU GLY GLU LEU GLU SER



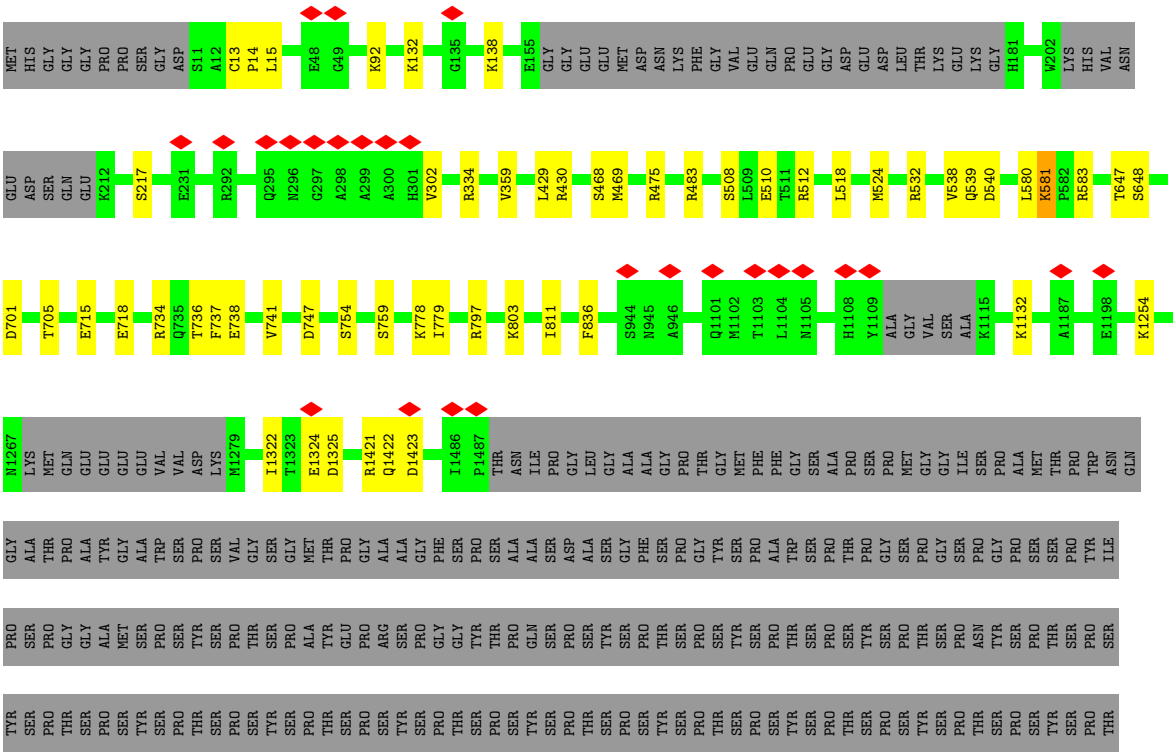
- Molecule 21: Transcription initiation factor TFIID subunit 13

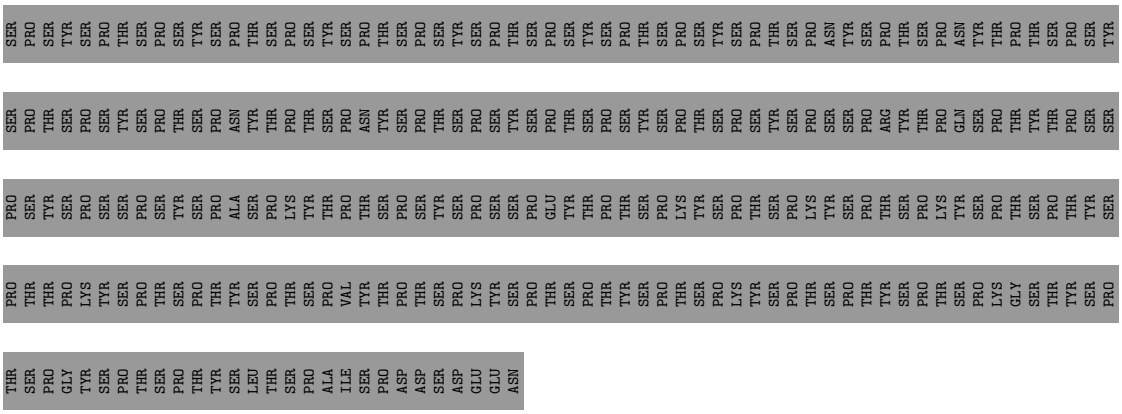
Chain m:



- Molecule 22: RPB1

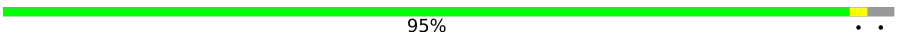
Chain o:

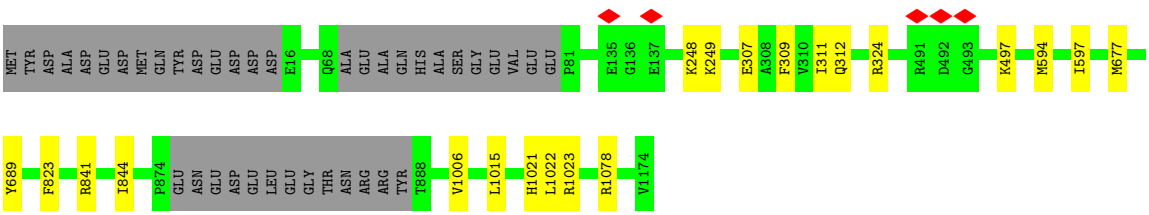




• Molecule 23: DNA-directed RNA polymerase subunit beta

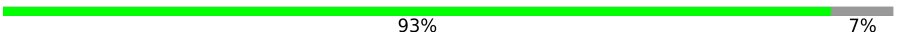
Chain p:

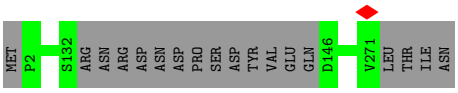




• Molecule 24: DNA-directed RNA polymerase II subunit RPB3

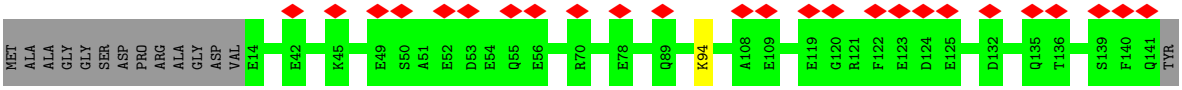
Chain q:





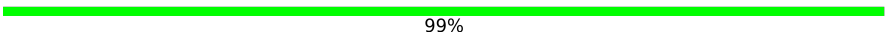
• Molecule 25: DNA-directed RNA polymerase II subunit RPB4

Chain r:



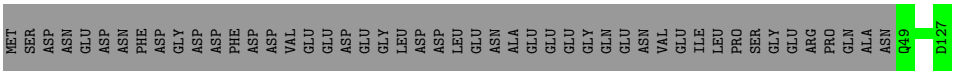
• Molecule 26: DNA-directed RNA polymerase II subunit E

Chain s:



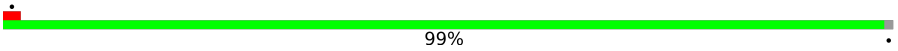
• Molecule 27: DNA-directed RNA polymerase II subunit F

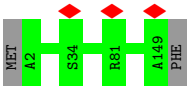
Chain t:



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

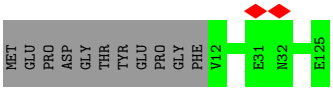
Chain v:





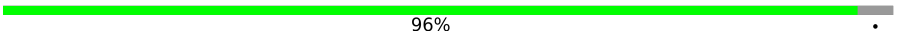
• Molecule 29: DNA-directed RNA polymerase II subunit RPB9

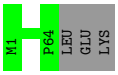
Chain w:



• Molecule 30: RPB10

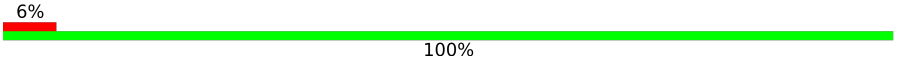
Chain x:

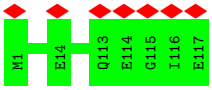




• Molecule 31: RNA_pol_L_2 domain-containing protein

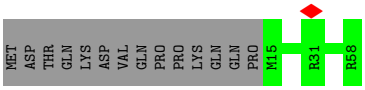
Chain y:





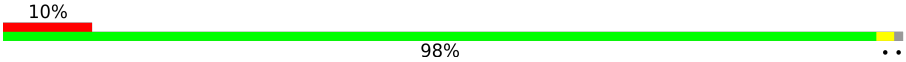
• Molecule 32: RPB12

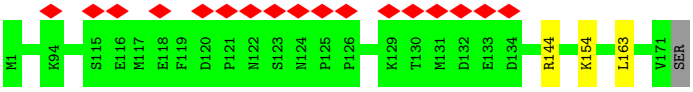
Chain z:



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

Chain u:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	72012	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 ($e^-/Å^2$)	50.0	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	0.034	Depositor
Minimum map value	-0.006	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	488.15997, 488.15997, 488.15997	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.356, 1.356, 1.356	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0/5028	0.70	1/6785 (0.0%)
2	B	0.46	0/7992	0.60	0/10835
3	D	0.49	0/1391	0.59	0/1859
3	d	0.28	0/1321	0.49	0/1772
4	E	0.35	0/4469	0.54	0/6050
4	e	0.33	0/4433	0.55	0/6004
5	F	0.48	0/3139	0.69	0/4264
5	f	0.41	0/3140	0.63	0/4268
6	G	0.52	0/1199	0.66	0/1612
7	H	0.39	0/1673	0.59	0/2285
8	I	0.30	0/981	0.49	0/1332
8	i	0.29	0/989	0.46	0/1343
9	J	0.30	0/724	0.50	0/982
9	j	0.30	0/775	0.52	0/1049
10	L	0.34	0/630	0.63	4/852 (0.5%)
10	l	0.30	0/888	0.56	3/1194 (0.3%)
11	O	0.51	0/781	0.74	0/1061
12	P	0.61	0/1438	0.74	0/1935
13	Q	0.42	0/1013	0.64	0/1366
14	R	0.33	0/1941	0.60	1/2622 (0.0%)
15	S	0.37	0/1130	0.53	0/1528
16	T	0.26	0/887	0.54	0/1193
17	X	1.09	28/1652 (1.7%)	1.38	7/2550 (0.3%)
18	Y	1.04	20/1612 (1.2%)	1.35	11/2483 (0.4%)
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	0.43	0/11516	0.56	0/15548
23	p	0.39	0/9243	0.51	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	0.30	0/948	0.45	0/1284
30	x	0.42	0/516	0.45	0/696
31	y	0.36	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	0.45	48/83455 (0.1%)	0.63	27/113444 (0.0%)

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	Y	32	DG	C1'-N9	-7.51	1.36	1.47
18	Y	34	DG	C1'-N9	-6.84	1.37	1.47
17	X	-20	DG	C1'-N9	-6.59	1.38	1.47
17	X	-12	DC	C1'-N1	6.22	1.57	1.49
17	X	-8	DT	C1'-N1	6.19	1.57	1.49
17	X	16	DC	C1'-N1	6.18	1.57	1.49
18	Y	-29	DC	C1'-N1	6.17	1.57	1.49
17	X	-1	DT	C1'-N1	6.16	1.57	1.49
18	Y	-19	DC	C1'-N1	6.15	1.57	1.49
17	X	22	DC	C1'-N1	6.09	1.57	1.49
18	Y	-7	DC	C1'-N1	6.04	1.57	1.49
17	X	-19	DG	C1'-N9	-5.97	1.38	1.47
17	X	-38	DA	C1'-N9	-5.89	1.39	1.47
17	X	-28	DT	C4'-O4'	-5.72	1.39	1.45
18	Y	-20	DT	C1'-N1	5.25	1.56	1.49
17	X	9	DT	C1'-N1	5.24	1.56	1.49
18	Y	5	DC	C1'-N1	5.23	1.56	1.49
18	Y	15	DC	C1'-N1	5.23	1.56	1.49
17	X	23	DC	C1'-N1	5.22	1.56	1.49
18	Y	-2	DC	C1'-N1	5.22	1.56	1.49
17	X	-7	DT	C1'-N1	5.21	1.56	1.49
18	Y	-11	DC	C1'-N1	5.21	1.56	1.49
17	X	17	DT	C1'-N1	5.20	1.56	1.49
18	Y	-26	DC	C1'-N1	5.20	1.56	1.49
17	X	6	DC	C1'-N1	5.19	1.55	1.49
17	X	10	DC	C1'-N1	5.19	1.55	1.49
18	Y	-8	DT	C1'-N1	5.19	1.55	1.49
18	Y	-24	DC	C1'-N1	5.18	1.55	1.49
17	X	-10	DC	C1'-N1	5.18	1.55	1.49
17	X	4	DC	C1'-N1	5.18	1.55	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	Y	-30	DT	C1'-N1	5.18	1.55	1.49
17	X	-6	DC	C1'-N1	5.17	1.55	1.49
18	Y	9	DC	C1'-N1	5.17	1.55	1.49
17	X	27	DC	C1'-N1	5.16	1.55	1.49
18	Y	-21	DC	C1'-N1	5.16	1.55	1.49
17	X	-32	DC	C1'-N1	5.14	1.55	1.49
17	X	31	DC	C1'-N1	5.13	1.55	1.49
17	X	-27	DA	C4'-O4'	-5.12	1.40	1.45
17	X	-3	DC	C1'-N1	5.12	1.55	1.49
17	X	3	DT	C1'-N1	5.12	1.55	1.49
17	X	14	DC	C1'-N1	5.12	1.55	1.49
18	Y	13	DC	C1'-N1	5.11	1.55	1.49
18	Y	14	DC	C1'-N1	5.11	1.55	1.49
17	X	0	DC	C1'-N1	5.10	1.55	1.49
17	X	-4	DT	C1'-N1	5.09	1.55	1.49
18	Y	-12	DT	C1'-N1	5.07	1.55	1.49
18	Y	-5	DC	C1'-N1	5.07	1.55	1.49
17	X	18	DC	C1'-N1	5.00	1.55	1.49

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	Y	32	DG	O4'-C1'-C2'	-11.13	97.00	105.90
17	X	-27	DA	O4'-C4'-C3'	-9.33	100.40	106.00
17	X	-26	DA	O4'-C4'-C3'	-8.89	100.66	106.00
18	Y	30	DA	O4'-C1'-C2'	-7.20	100.14	105.90
14	R	44	ARG	CB-CA-C	6.90	124.19	110.40
18	Y	27	DT	C6-C5-C7	-6.74	118.86	122.90
1	A	498	PRO	N-CA-CB	6.69	111.33	103.30
17	X	-28	DT	C4-C5-C6	6.21	121.72	118.00
17	X	-26	DA	P-O3'-C3'	6.12	127.04	119.70
17	X	-25	DA	P-O3'-C3'	5.57	126.39	119.70
17	X	-30	DT	C6-C5-C7	-5.57	119.56	122.90
18	Y	28	DA	P-O3'-C3'	5.52	126.33	119.70
18	Y	27	DT	C1'-O4'-C4'	-5.28	104.82	110.10
18	Y	26	DT	O4'-C1'-N1	-5.25	104.32	108.00
18	Y	29	DT	O4'-C4'-C3'	-5.24	102.40	104.50
10	L	89	ASP	CB-CG-OD2	5.20	122.98	118.30
10	l	90	ASP	CB-CG-OD2	5.20	122.98	118.30
10	l	79	ASP	CB-CG-OD2	5.18	122.97	118.30
10	l	89	ASP	CB-CG-OD2	5.18	122.97	118.30
18	Y	26	DT	C6-C5-C7	-5.18	119.79	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	L	90	ASP	CB-CG-OD2	5.18	122.96	118.30
10	L	115	ASP	CB-CG-OD2	5.16	122.94	118.30
10	L	79	ASP	CB-CG-OD2	5.15	122.94	118.30
18	Y	32	DG	O4'-C1'-N9	5.13	111.59	108.00
18	Y	26	DT	C4-C5-C6	5.05	121.03	118.00
17	X	-29	DA	C5'-C4'-C3'	-5.04	105.03	114.10
18	Y	30	DA	C1'-O4'-C4'	-5.03	105.07	110.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	581/1872 (31%)	543 (94%)	35 (6%)	3 (0%)	25 65
2	B	959/1199 (80%)	912 (95%)	47 (5%)	0	100 100
3	D	159/1085 (15%)	151 (95%)	7 (4%)	1 (1%)	22 61
3	d	154/1085 (14%)	150 (97%)	4 (3%)	0	100 100
4	E	540/800 (68%)	502 (93%)	36 (7%)	2 (0%)	30 68
4	e	531/800 (66%)	484 (91%)	47 (9%)	0	100 100
5	F	400/677 (59%)	376 (94%)	18 (4%)	6 (2%)	8 40
5	f	399/677 (59%)	377 (94%)	22 (6%)	0	100 100
6	G	139/349 (40%)	133 (96%)	5 (4%)	1 (1%)	19 57
7	H	207/310 (67%)	189 (91%)	15 (7%)	3 (1%)	9 40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	I	118/264 (45%)	114 (97%)	4 (3%)	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%)	72 (97%)	2 (3%)	0	100	100
10	l	105/161 (65%)	101 (96%)	4 (4%)	0	100	100
11	O	95/109 (87%)	79 (83%)	12 (13%)	4 (4%)	2	17
12	P	175/339 (52%)	168 (96%)	5 (3%)	2 (1%)	12	47
13	Q	118/376 (31%)	106 (90%)	10 (8%)	2 (2%)	7	36
14	R	244/316 (77%)	233 (96%)	10 (4%)	1 (0%)	30	68
15	S	130/517 (25%)	126 (97%)	4 (3%)	0	100	100
16	T	109/249 (44%)	102 (94%)	4 (4%)	3 (3%)	4	24
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%)	1303 (92%)	110 (8%)	4 (0%)	37	73
23	p	1128/1174 (96%)	1050 (93%)	77 (7%)	1 (0%)	48	83
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%)	103 (92%)	9 (8%)	0	100	100
30	x	62/67 (92%)	60 (97%)	2 (3%)	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%)	22	61
All	All	9692/17897 (54%)	9057 (93%)	601 (6%)	34 (0%)	32	68

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1000	LEU

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Mol	Chain	Res	Type
1	A	1158	SER
4	E	704	VAL
5	F	396	LEU
7	H	141	PRO
11	O	52	VAL
13	Q	321	SER
16	T	124	TYR
22	o	14	PRO
22	o	539	GLN
22	o	581	LYS
23	p	1021	HIS
33	u	154	LYS
1	A	498	PRO
4	E	521	ASP
5	F	397	GLN
5	F	411	VAL
6	G	152	ALA
11	O	26	GLN
16	T	121	SER
3	D	936	GLN
12	P	207	PRO
5	F	393	LEU
5	F	439	ARG
11	O	56	VAL
11	O	84	VAL
16	T	38	GLY
5	F	64	GLN
7	H	134	LEU
7	H	164	THR
22	o	469	MET
12	P	298	PRO
14	R	247	GLY
13	Q	312	GLU

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	A	534/1665 (32%)	483 (90%)	51 (10%)	7	22
2	B	875/1083 (81%)	858 (98%)	17 (2%)	52	69
3	D	149/815 (18%)	125 (84%)	24 (16%)	2	10
3	d	146/815 (18%)	146 (100%)	0	100	100
4	E	478/657 (73%)	469 (98%)	9 (2%)	52	69
4	e	475/657 (72%)	473 (100%)	2 (0%)	89	91
5	F	320/574 (56%)	301 (94%)	19 (6%)	16	37
5	f	322/574 (56%)	312 (97%)	10 (3%)	35	54
6	G	133/322 (41%)	122 (92%)	11 (8%)	9	27
7	H	181/270 (67%)	176 (97%)	5 (3%)	38	57
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%)	66 (93%)	5 (7%)	12	32
10	l	98/141 (70%)	98 (100%)	0	100	100
11	O	84/98 (86%)	74 (88%)	10 (12%)	4	16
12	P	153/293 (52%)	144 (94%)	9 (6%)	16	37
13	Q	111/324 (34%)	107 (96%)	4 (4%)	30	50
14	R	211/268 (79%)	194 (92%)	17 (8%)	9	28
15	S	117/448 (26%)	109 (93%)	8 (7%)	13	34
16	T	94/218 (43%)	91 (97%)	3 (3%)	34	53
19	c	113/833 (14%)	111 (98%)	2 (2%)	54	71
20	k	87/182 (48%)	87 (100%)	0	100	100
21	m	80/106 (76%)	79 (99%)	1 (1%)	65	77
22	o	1257/1748 (72%)	1204 (96%)	53 (4%)	25	46
23	p	993/1027 (97%)	973 (98%)	20 (2%)	50	68
24	q	234/252 (93%)	234 (100%)	0	100	100
25	r	106/126 (84%)	105 (99%)	1 (1%)	75	83
26	s	191/192 (100%)	190 (100%)	1 (0%)	86	89
27	t	69/111 (62%)	69 (100%)	0	100	100
28	v	129/131 (98%)	129 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	w	103/112 (92%)	103 (100%)	0	100	100
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%)	65	77
All	All	8640/15331 (56%)	8356 (97%)	284 (3%)	35	52

All (284) 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	408	LEU
1	A	415	ILE
1	A	416	TRP
1	A	417	ASP
1	A	419	GLU
1	A	470	ILE
1	A	475	LEU
1	A	481	GLU
1	A	489	GLN
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	797	LYS

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Mol	Chain	Res	Type
1	A	798	ARG
1	A	801	THR
1	A	819	LYS
1	A	820	ASP
1	A	821	ARG
1	A	828	GLU
1	A	843	ARG
1	A	844	LYS
1	A	943	LYS
1	A	1020	LEU
1	A	1052	ARG
1	A	1055	VAL
1	A	1058	HIS
1	A	1059	GLN
1	A	1062	TYR
1	A	1073	GLN
1	A	1083	LEU
1	A	1165	LEU
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
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	887	LYS
3	D	888	LYS
3	D	891	ILE
3	D	893	GLU

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Mol	Chain	Res	Type
3	D	936	GLN
3	D	941	ARG
3	D	948	GLU
3	D	950	LEU
3	D	951	ASP
3	D	958	LYS
3	D	959	ASP
3	D	966	LEU
3	D	967	MET
3	D	968	ARG
3	D	980	GLU
3	D	981	GLN
3	D	983	ARG
3	D	995	GLU
3	D	996	LEU
3	D	1000	ARG
3	D	1002	ARG
3	D	1003	ASP
3	D	1054	ARG
3	D	1055	ILE
4	E	522	ASP
4	E	593	PHE
4	E	702	LEU
4	E	704	VAL
4	E	745	GLU
4	E	746	ASP
4	E	747	LEU
4	E	761	LEU
4	E	763	GLU
5	F	63	ARG
5	F	105	TYR
5	F	258	ARG
5	F	261	THR
5	F	271	VAL
5	F	280	ILE
5	F	301	VAL
5	F	310	THR
5	F	315	ARG
5	F	317	LEU
5	F	319	LEU
5	F	326	HIS
5	F	340	ILE

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Mol	Chain	Res	Type
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	153	LYS
6	G	154	LYS
6	G	177	VAL
6	G	181	TRP
6	G	184	ILE
7	H	115	GLN
7	H	132	LYS
7	H	135	THR
7	H	159	TYR
7	H	164	THR
10	L	73	ASN
10	L	110	THR
10	L	111	LEU
10	L	112	GLU
10	L	128	ILE
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	70	ASN
11	O	76	LEU
12	P	172	VAL
12	P	209	THR
12	P	221	CYS
12	P	226	SER
12	P	252	ASP

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Mol	Chain	Res	Type
12	P	274	VAL
12	P	278	GLN
12	P	288	PHE
12	P	317	VAL
13	Q	13	LEU
13	Q	344	ARG
13	Q	346	LYS
13	Q	364	ASP
14	R	27	TYR
14	R	31	ASP
14	R	34	CYS
14	R	39	LEU
14	R	40	VAL
14	R	41	VAL
14	R	120	GLU
14	R	127	ARG
14	R	128	ILE
14	R	130	LEU
14	R	133	ASN
14	R	137	ARG
14	R	154	ARG
14	R	175	ARG
14	R	189	LYS
14	R	196	LYS
14	R	248	ARG
15	S	7	SER
15	S	108	ARG
15	S	155	LEU
15	S	156	THR
15	S	158	GLU
15	S	169	LYS
15	S	171	LEU
15	S	174	PHE
16	T	123	ASN
16	T	125	MET
16	T	127	LEU
19	c	24	ASP
19	c	106	VAL
4	e	365	ARG
4	e	663	ARG
5	f	253	TYR
5	f	261	THR

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Mol	Chain	Res	Type
5	f	272	VAL
5	f	274	ASN
5	f	322	ASP
5	f	323	VAL
5	f	326	HIS
5	f	356	THR
5	f	408	ASP
5	f	421	ASP
21	m	31	LEU
22	o	13	CYS
22	o	15	LEU
22	o	92	LYS
22	o	132	LYS
22	o	138	LYS
22	o	217	SER
22	o	302	VAL
22	o	334	ARG
22	o	359	VAL
22	o	429	LEU
22	o	430	ARG
22	o	468	SER
22	o	475	ARG
22	o	483	ARG
22	o	508	SER
22	o	510	GLU
22	o	512	ARG
22	o	518	LEU
22	o	524	MET
22	o	532	ARG
22	o	538	VAL
22	o	540	ASP
22	o	580	LEU
22	o	581	LYS
22	o	583	ARG
22	o	647	THR
22	o	648	SER
22	o	701	ASP
22	o	705	THR
22	o	715	GLU
22	o	718	GLU
22	o	734	ARG
22	o	736	THR

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Mol	Chain	Res	Type
22	o	737	PHE
22	o	738	GLU
22	o	741	VAL
22	o	747	ASP
22	o	754	SER
22	o	759	SER
22	o	778	LYS
22	o	779	ILE
22	o	797	ARG
22	o	803	LYS
22	o	811	ILE
22	o	836	PHE
22	o	1132	LYS
22	o	1254	LYS
22	o	1322	ILE
22	o	1324	GLU
22	o	1325	ASP
22	o	1421	ARG
22	o	1422	GLN
22	o	1423	ASP
23	p	248	LYS
23	p	249	LYS
23	p	307	GLU
23	p	309	PHE
23	p	311	ILE
23	p	312	GLN
23	p	324	ARG
23	p	497	LYS
23	p	594	MET
23	p	597	ILE
23	p	677	MET
23	p	689	TYR
23	p	823	PHE
23	p	841	ARG
23	p	844	ILE
23	p	1006	VAL
23	p	1015	LEU
23	p	1022	LEU
23	p	1023	ARG
23	p	1078	ARG
25	r	94	LYS
26	s	52	ARG

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Mol	Chain	Res	Type
33	u	144	ARG
33	u	163	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (113) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	401	ASN
1	A	409	HIS
1	A	569	ASN
1	A	800	ASN
1	A	860	ASN
1	A	896	GLN
1	A	1058	HIS
2	B	30	HIS
2	B	137	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	580	GLN
2	B	644	GLN
2	B	652	GLN
2	B	745	GLN
2	B	750	GLN
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	327	ASN
4	E	351	GLN

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Mol	Chain	Res	Type
4	E	616	HIS
4	E	640	ASN
5	F	119	ASN
5	F	221	GLN
5	F	270	ASN
5	F	273	GLN
5	F	275	ASN
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	119	HIS
11	O	13	ASN
11	O	57	ASN
12	P	189	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
21	m	107	ASN
22	o	123	ASN
22	o	278	HIS
22	o	289	GLN
22	o	296	ASN
22	o	330	GLN
22	o	576	GLN
22	o	620	HIS

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Mol	Chain	Res	Type
22	o	703	GLN
22	o	721	HIS
22	o	731	ASN
22	o	739	ASN
22	o	757	GLN
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	254	GLN
23	p	287	HIS
23	p	370	HIS
23	p	525	ASN
23	p	570	ASN
23	p	749	HIS
23	p	777	ASN
23	p	1073	GLN
23	p	1117	HIS
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 (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 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.

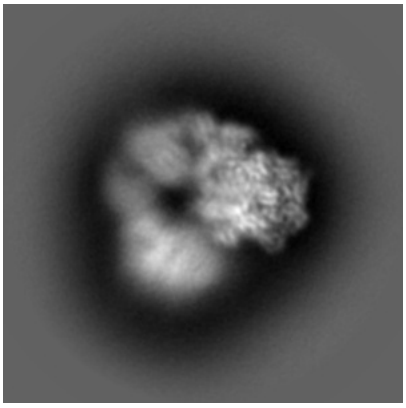
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-31107. These allow visual inspection of the internal detail of the map and identification of artifacts.

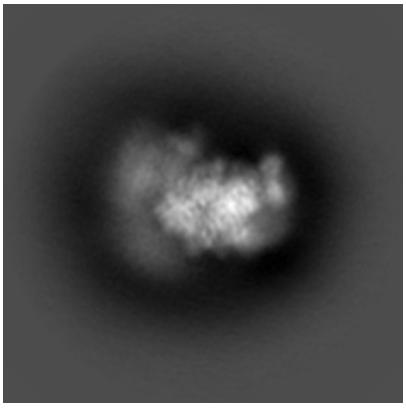
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

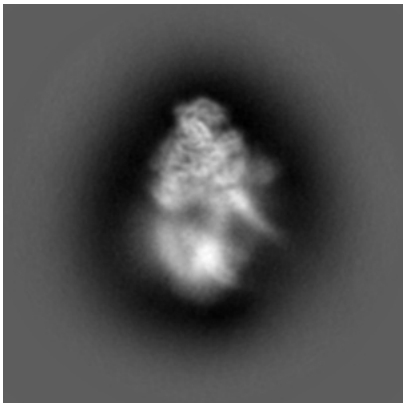
6.1.1 Primary map



X



Y

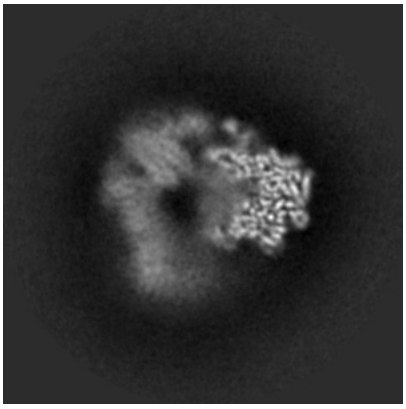


Z

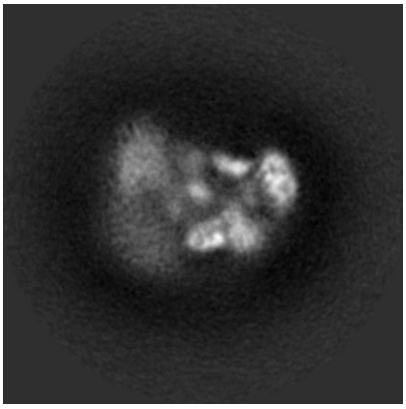
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

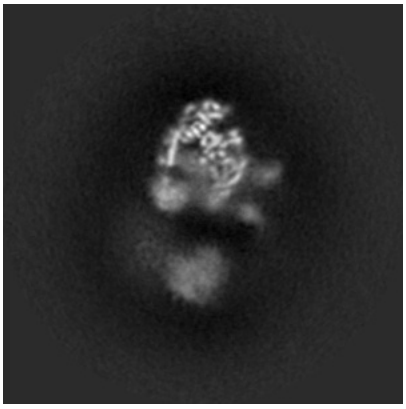
6.2.1 Primary map



X Index: 180



Y Index: 180

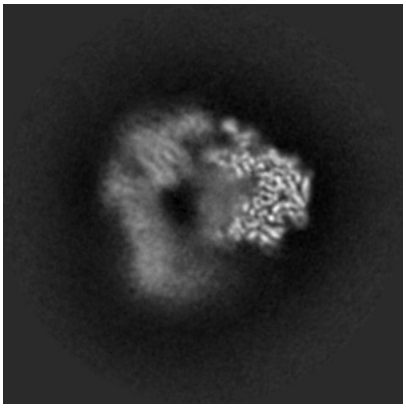


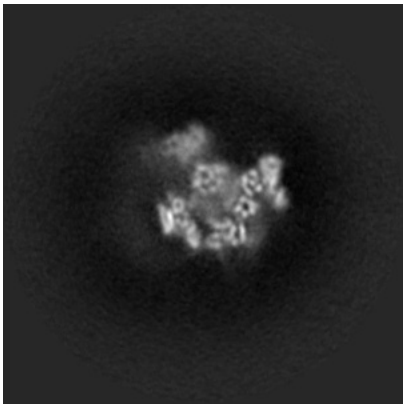
Z Index: 180

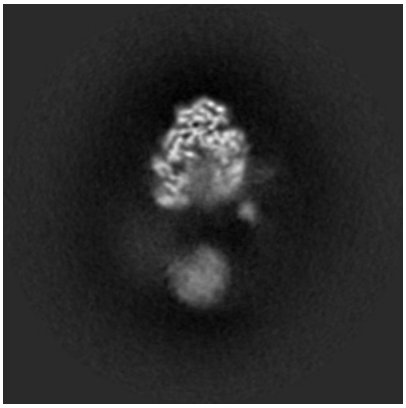
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 182

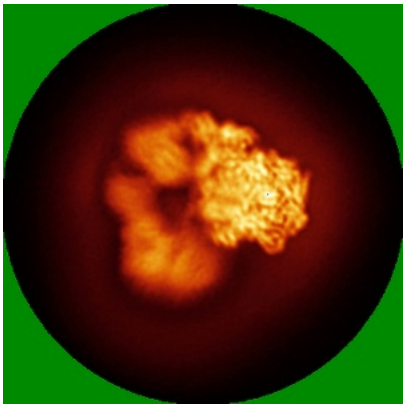

Y Index: 206

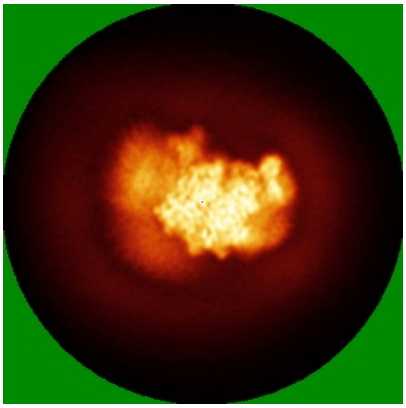

Z Index: 189

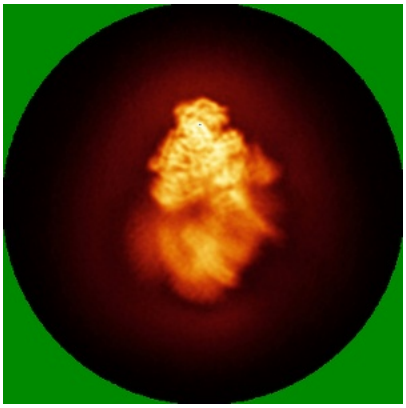
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map


X

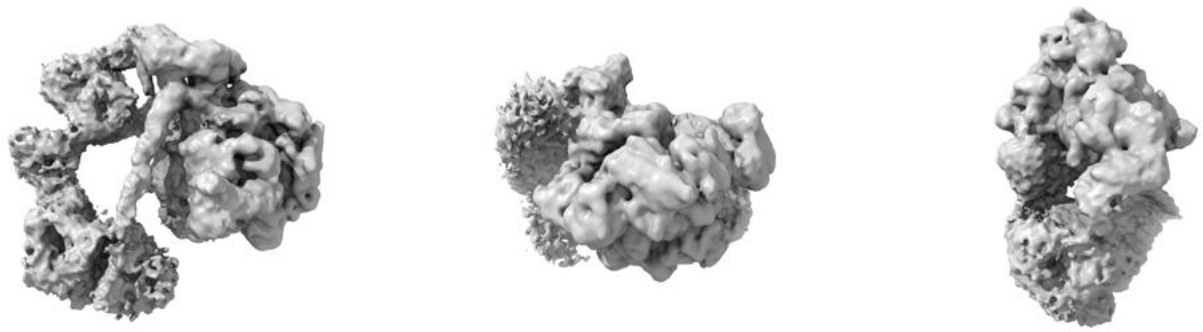

Y


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

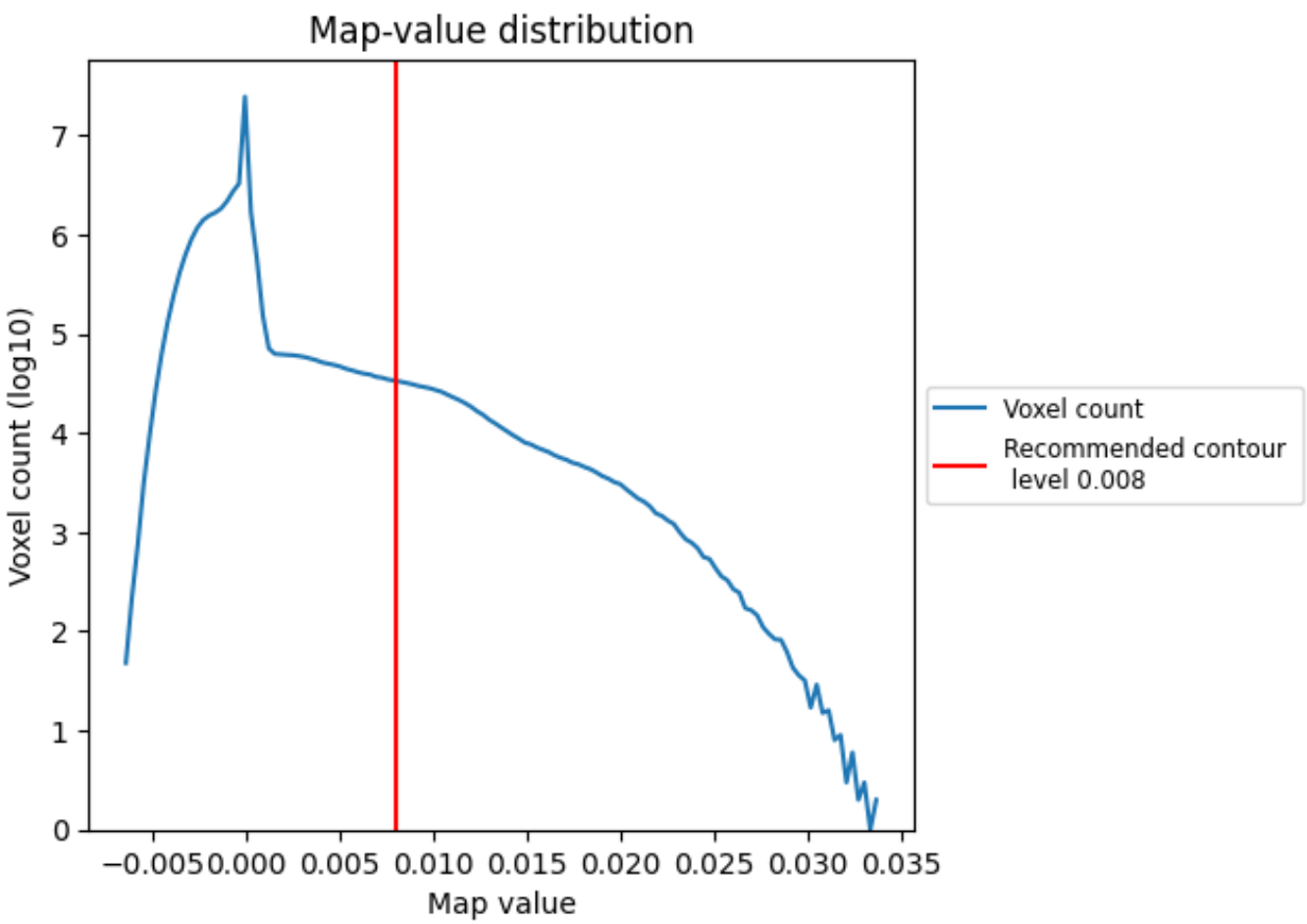
6.6 Mask visualisation (i)

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

7 Map analysis (i)

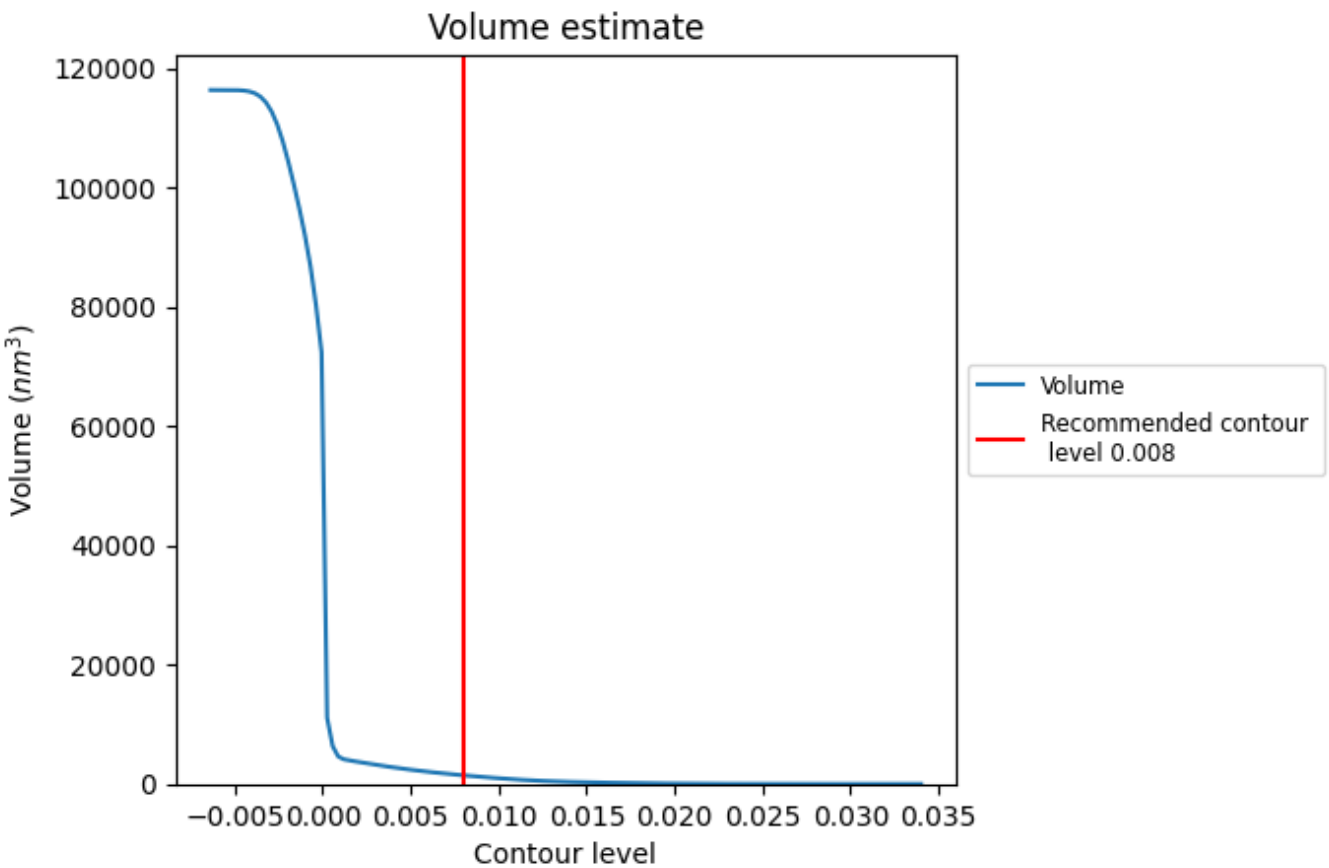
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

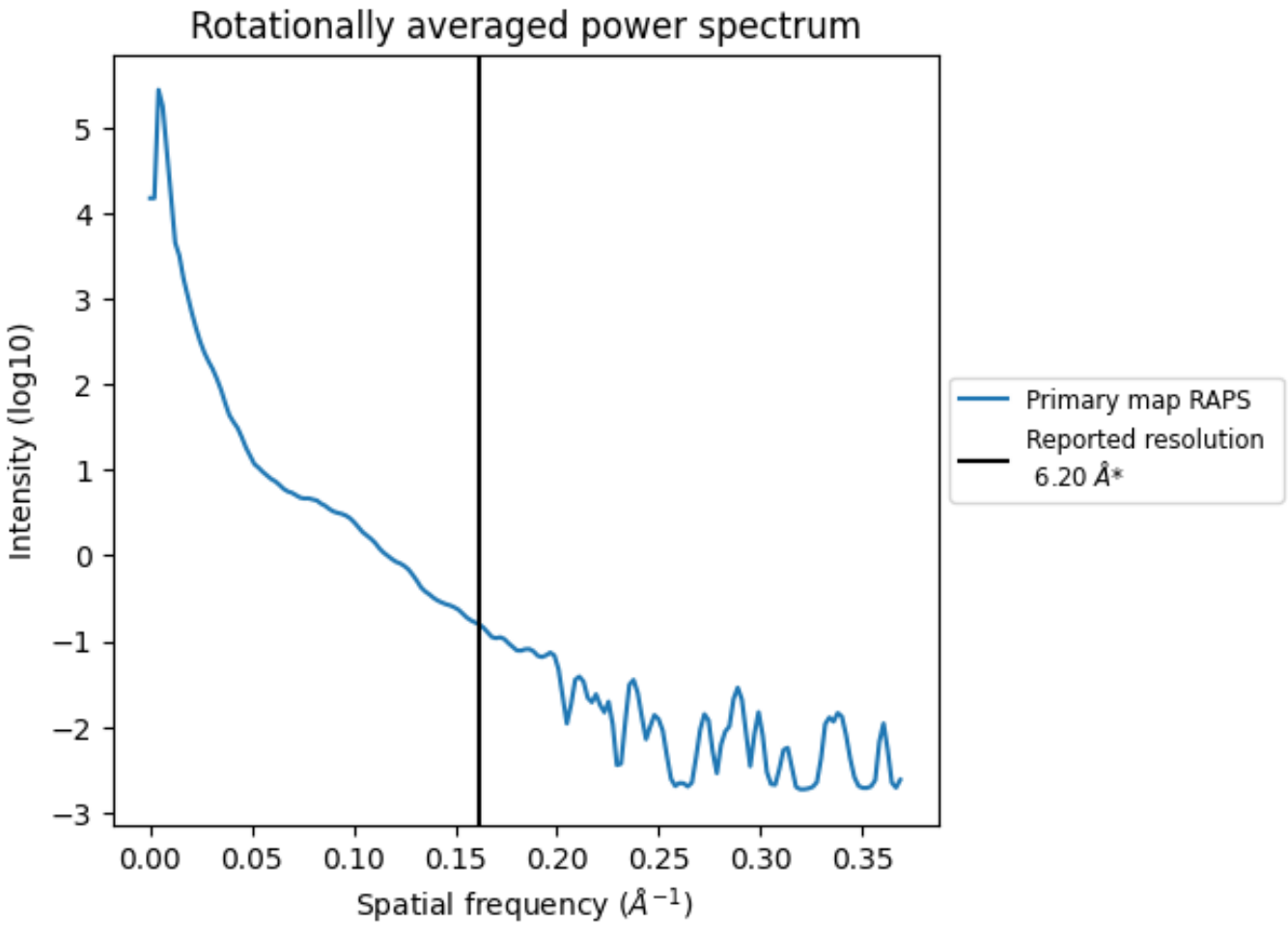
7.2 Volume estimate (i)



The volume at the recommended contour level is 1445 nm^3; this corresponds to an approximate mass of 1305 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 0.161 Å^{-1}

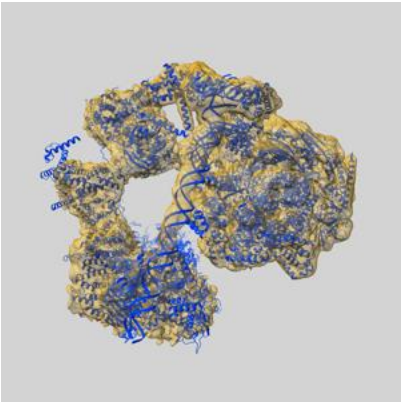
8 Fourier-Shell correlation (i)

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

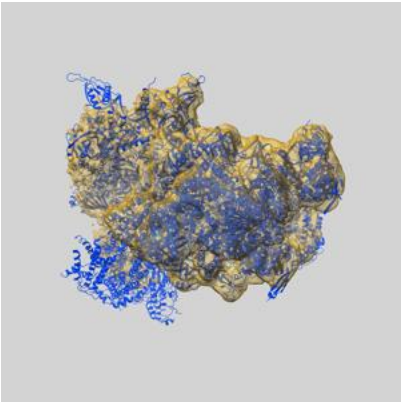
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-31107 and PDB model 7EG7. Per-residue inclusion information can be found in section 3 on page 11.

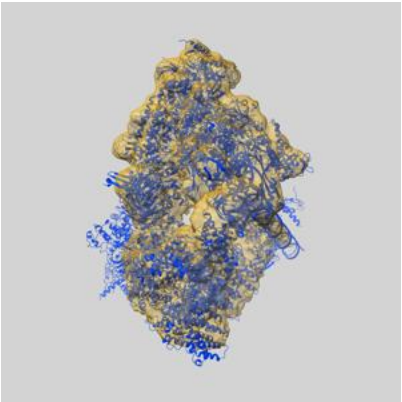
9.1 Map-model overlay (i)



X



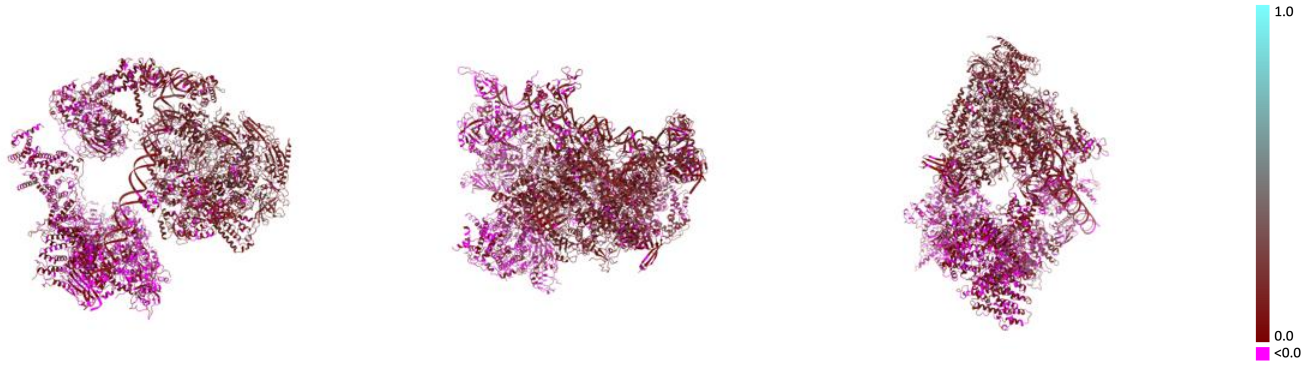
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.008 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.

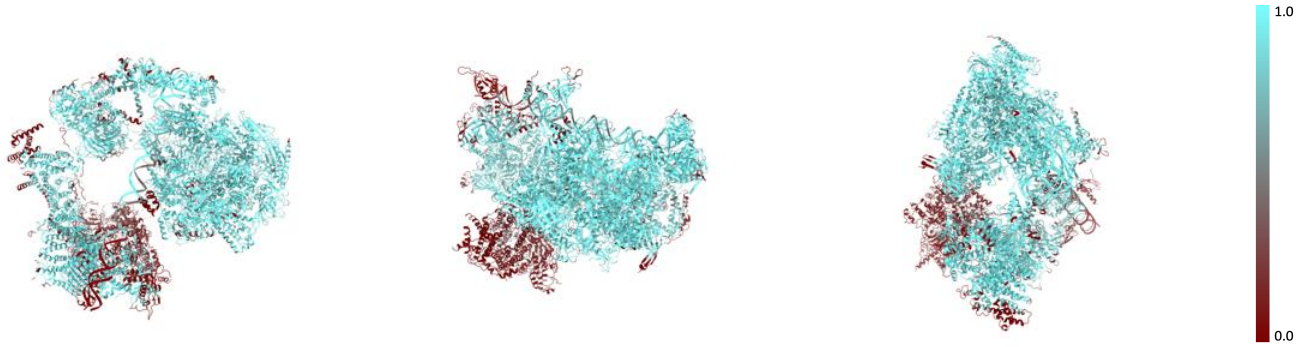
9.2 Q-score mapped to coordinate model (i)



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.

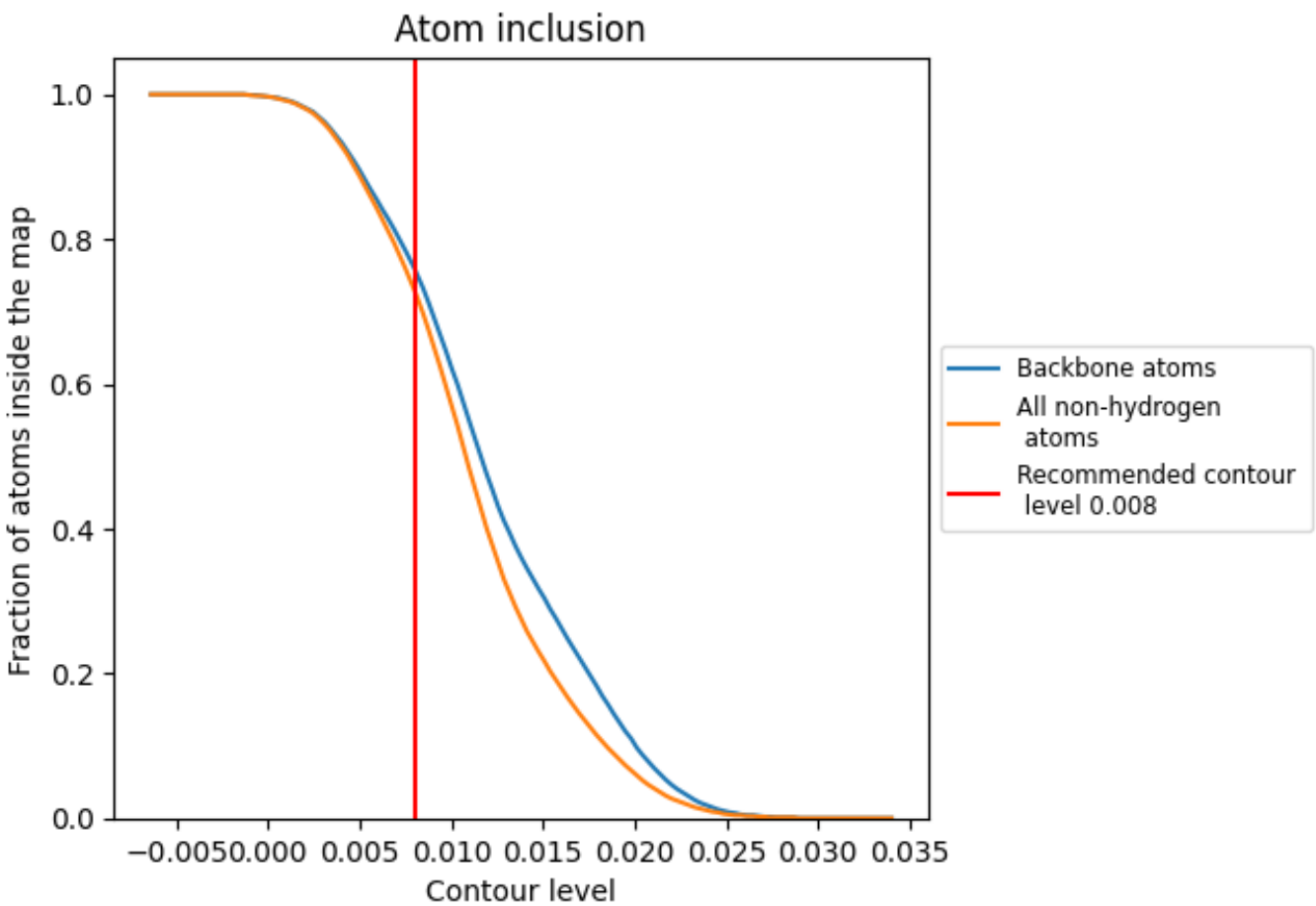
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.008).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7290	0.0920
A	0.5890	0.0280
B	0.8520	0.0460
D	0.6930	0.0990
E	0.8650	0.0630
F	0.7070	0.0540
G	0.5640	0.0300
H	0.8190	0.0590
I	0.8570	0.0830
J	0.8090	0.0350
L	0.6230	0.0530
O	0.8630	0.1070
P	0.9540	0.1200
Q	0.8390	0.0920
R	0.9130	0.1560
S	0.8360	0.1030
T	0.7780	0.0750
X	0.6380	0.1080
Y	0.5990	0.1090
c	0.2220	0.0200
d	0.0170	0.0020
e	0.0500	0.0130
f	0.5080	0.0280
i	0.0040	0.0090
j	0.1450	0.0020
k	0.0170	-0.0090
l	0.0000	-0.0020
m	0.0000	0.0330
o	0.9420	0.1540
p	0.9530	0.1540
q	0.9360	0.1750
r	0.7540	0.0880
s	0.9610	0.1650
t	0.9820	0.1850
u	0.8520	0.1080

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Chain	Atom inclusion	Q-score
v	0.9250	0.1720
w	0.9320	0.1570
x	0.9660	0.1700
y	0.8880	0.1760
z	0.9690	0.1810