wwPDB EM Validation Summary Report (i)

Nov 14, 2022 – 02:43 PM JST

PDB ID	:	6J2X
EMDB ID	:	EMD-9772
Title	:	Yeast proteasome in resting state (C1-a)
Authors	:	Cong, Y.
Deposited on	:	2019-01-03
Resolution	:	3.80 Å(reported)

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

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

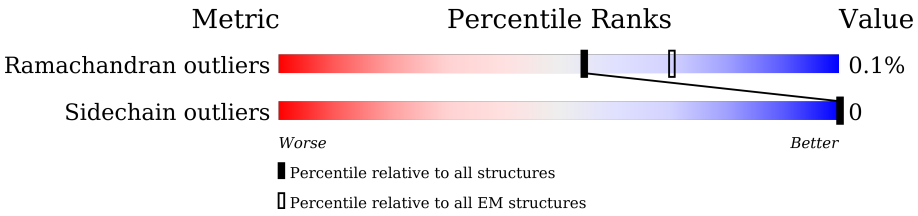
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	1	215	11% 95% 5%
1	b	215	12% 95% 5%
2	2	261	85% 15%
2	i	261	85% 15%
3	3	205	6% 100%
3	h	205	8% 100%
4	4	198	12% 100%
4	g	198	10% 100%
5	5	287	5% 74% 26%

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Mol	Chain	Length	Quality of chain
5	f	287	74% 26%
6	6	241	9% 92% 8%
6	e	241	6% 92% 8%
7	7	266	88% 12%
7	a	266	6% 88% 12%
8	A	252	10% 96%
8	c	252	6% 96%
9	B	250	10% 100%
9	j	250	5% 100%
10	C	258	10% 95% 5%
10	d	258	5% 95% 5%
11	D	254	7% 95% 5%
11	n	254	5% 95% 5%
12	E	260	9% 93% 7%
12	m	260	8% 93% 7%
13	F	234	7% 100%
13	l	234	8% 100%
14	G	288	7% 84% 16%
14	k	288	5% 85% 15%
15	H	467	19% 76% 24%
16	I	437	20% 83% 17%
17	J	405	27% 92% 8%
18	K	428	25% 88% 11%
19	L	437	22% 85% 15%
20	M	434	22% 84% 15%

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Mol	Chain	Length	Quality of chain
21	N	945	42% 90% 10%
22	O	393	57% 98%
23	P	445	27% 97%
24	Q	434	24% 99%
25	R	429	28% 93% 7%
26	S	523	50% 91% 9%
27	T	274	73% 99%
28	U	338	22% 75% 25%
29	V	306	28% 84% 16%
30	W	268	48% 74% 26%
31	X	156	71% 71% 29%
32	Y	89	12% 29% 70%
33	Z	993	80% 82% 18%

2 Entry composition (i)

There are 33 unique types of molecules in this entry. The entry contains 106176 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 Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	205	Total	C	N	O	S	0	0
			1576	996	261	312	7		
1	b	205	Total	C	N	O	S	0	0
			1576	996	261	312	7		

- Molecule 2 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	222	Total	C	N	O	S	0	0
			1684	1061	293	323	7		
2	i	222	Total	C	N	O	S	0	0
			1684	1061	293	323	7		

- Molecule 3 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	204	Total	C	N	O	S	0	0
			1581	1010	258	305	8		
3	h	204	Total	C	N	O	S	0	0
			1581	1010	258	305	8		

- Molecule 4 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	198	Total	C	N	O	S	0	0
			1585	1005	269	305	6		
4	g	198	Total	C	N	O	S	0	0
			1585	1005	269	305	6		

- Molecule 5 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	212	Total	C	N	O	S	0	0
			1644	1045	280	312	7		
5	f	212	Total	C	N	O	S	0	0
			1644	1045	280	312	7		

- Molecule 6 is a protein called PROTEASOME COMPONENT C5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	222	Total	C	N	O	S	0	0
			1757	1115	303	335	4		
6	e	222	Total	C	N	O	S	0	0
			1757	1115	303	335	4		

- Molecule 7 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	233	Total	C	N	O	S	0	0
			1824	1154	312	351	7		
7	a	233	Total	C	N	O	S	0	0
			1824	1154	312	351	7		

- Molecule 8 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	243	Total	C	N	O	S	0	0
			1921	1221	322	370	8		
8	c	243	Total	C	N	O	S	0	0
			1921	1221	322	370	8		

- Molecule 9 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	250	Total	C	N	O	S	0	0
			1915	1219	315	377	4		
9	j	250	Total	C	N	O	S	0	0
			1915	1219	315	377	4		

- Molecule 10 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	244	Total	C	N	O	S	0	0
			1904	1201	321	379	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	d	244	Total	C	N	O	S	0	0
			1904	1201	321	379	3		

- Molecule 11 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	241	Total	C	N	O	S	0	0
			1890	1181	331	374	4		
11	n	241	Total	C	N	O	S	0	0
			1890	1181	331	374	4		

- Molecule 12 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	242	Total	C	N	O	S	0	0
			1861	1162	314	378	7		
12	m	242	Total	C	N	O	S	0	0
			1861	1162	314	378	7		

- Molecule 13 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	233	Total	C	N	O	S	0	0
			1795	1129	312	350	4		
13	l	233	Total	C	N	O	S	0	0
			1795	1129	312	350	4		

- Molecule 14 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	243	Total	C	N	O	S	0	0
			1888	1201	328	355	4		
14	k	244	Total	C	N	O	S	0	0
			1896	1205	330	357	4		

- Molecule 15 is a protein called 26S proteasome regulatory subunit 7 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	355	Total	C	N	O	S	0	0
			2787	1755	500	515	17		

- Molecule 16 is a protein called 26S PROTEASE REGULATORY SUBUNIT 4 HOMOLOG.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	362	Total	C	N	O	S	0	0
			2822	1773	471	563	15		

- Molecule 17 is a protein called 26S proteasome regulatory subunit 8 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	373	Total	C	N	O	S	0	0
			2928	1837	527	547	17		

- Molecule 18 is a protein called 26S proteasome regulatory subunit 6B homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	381	Total	C	N	O	S	0	0
			3019	1898	530	581	10		

- Molecule 19 is a protein called 26S proteasome subunit RPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	371	Total	C	N	O	S	0	0
			2937	1852	519	554	12		

- Molecule 20 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	M	367	Total	C	N	O	S	0	0
			2866	1799	503	553	11		

- Molecule 21 is a protein called 26S proteasome regulatory subunit RPN2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	N	849	Total	C	N	O	S	0	0
			6562	4174	1099	1261	28		

- Molecule 22 is a protein called 26S proteasome regulatory subunit RPN9.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	O	387	Total	C	N	O	S	0	0
			3182	2047	520	606	9		

- Molecule 23 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN5.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	P	432	Total	C	N	O	S	0	0
			3545	2260	592	684	9		

- Molecule 24 is a protein called 26S proteasome regulatory subunit RPN6.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Q	431	Total	C	N	O	S	0	0
			3471	2205	574	676	16		

- Molecule 25 is a protein called 26S proteasome regulatory subunit RPN7.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	R	400	Total	C	N	O	S	0	0
			3218	2051	527	630	10		

- Molecule 26 is a protein called 26S proteasome regulatory subunit RPN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	S	475	Total	C	N	O	S	0	0
			3894	2488	653	738	15		

- Molecule 27 is a protein called 26S proteasome regulatory subunit RPN12.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	T	272	Total	C	N	O	S	0	0
			2235	1432	355	441	7		

- Molecule 28 is a protein called 26S proteasome regulatory subunit RPN8.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	U	255	Total	C	N	O	S	0	0
			2061	1312	352	391	6		

- Molecule 29 is a protein called Ubiquitin carboxyl-terminal hydrolase RPN11.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	V	258	Total	C	N	O	S	0	0
			2025	1273	344	395	13		

- Molecule 30 is a protein called 26S proteasome regulatory subunit RPN10.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	W	197	Total	C	N	O	S	0	0
			1534	962	269	300	3		

- Molecule 31 is a protein called 26S proteasome regulatory subunit RPN13.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	X	111	Total	C	N	O	S	0	0
			906	586	148	169	3		

- Molecule 32 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	Y	27	Total	C	N	O	0	0
			236	143	39	54		

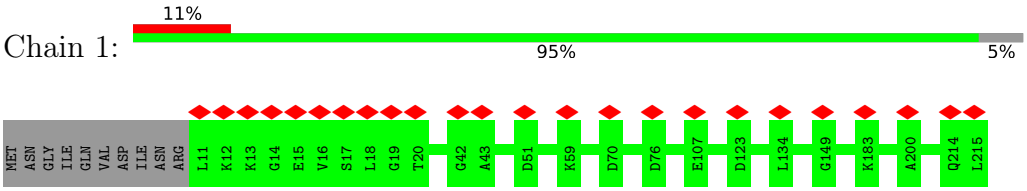
- Molecule 33 is a protein called 26S proteasome regulatory subunit RPN1.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Z	813	Total	C	N	O	S	0	0
			6290	3995	1029	1237	29		

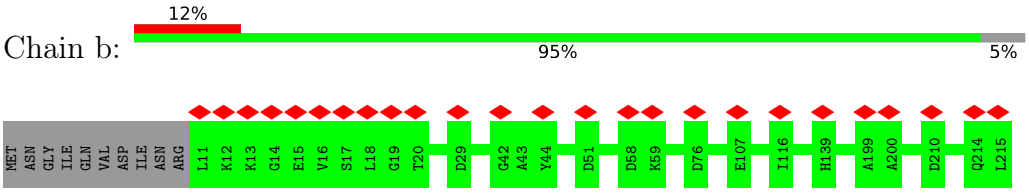
3 Residue-property plots (i)

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.

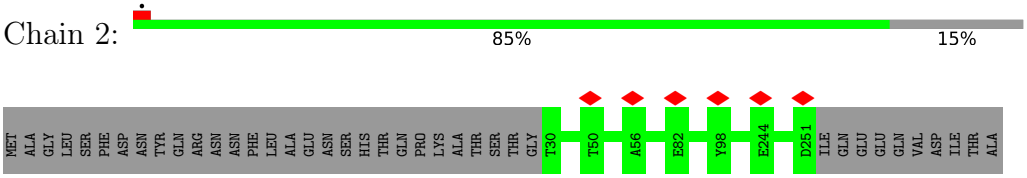
• Molecule 1: Proteasome subunit beta type-1



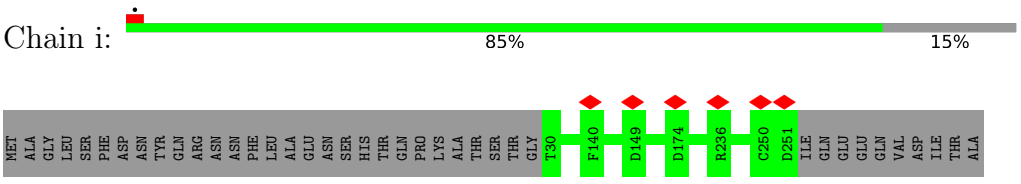
• Molecule 1: Proteasome subunit beta type-1



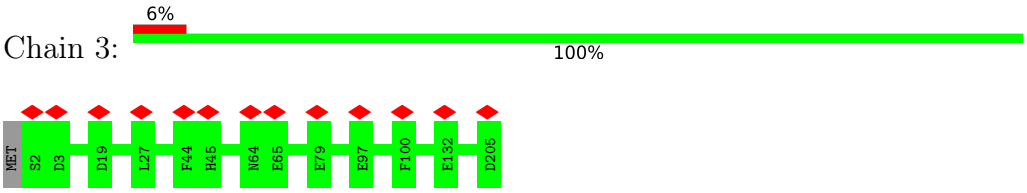
• Molecule 2: Proteasome subunit beta type-2



• Molecule 2: Proteasome subunit beta type-2

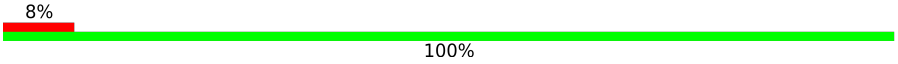


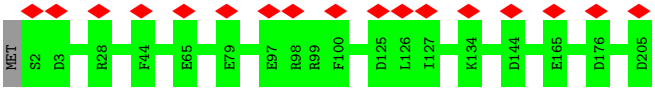
• Molecule 3: Proteasome subunit beta type-3



• Molecule 3: Proteasome subunit beta type-3

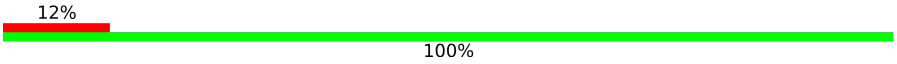
Chain h:

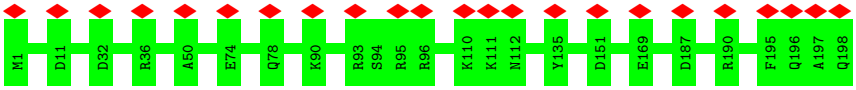




• Molecule 4: Proteasome subunit beta type-4

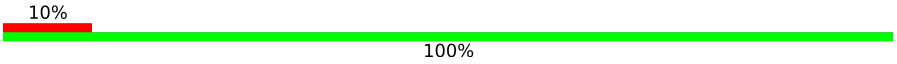
Chain 4:

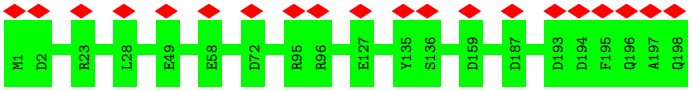




• Molecule 4: Proteasome subunit beta type-4

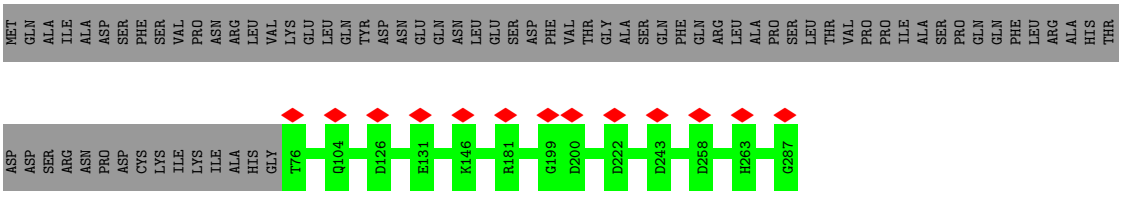
Chain g:





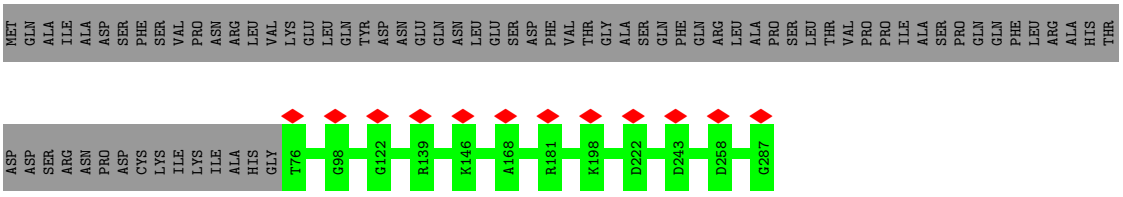
• Molecule 5: Proteasome subunit beta type-5

Chain 5:



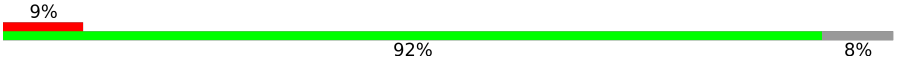
• Molecule 5: Proteasome subunit beta type-5

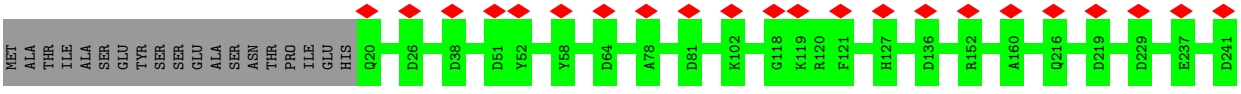
Chain f:



• Molecule 6: PROTEASOME COMPONENT C5

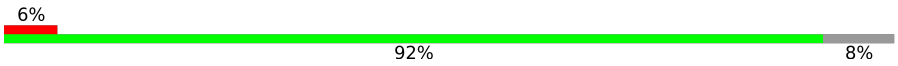
Chain 6:

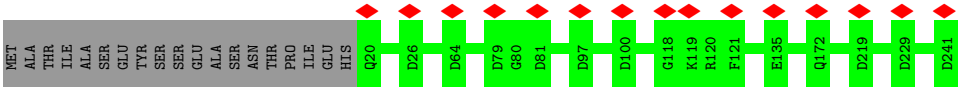




• Molecule 6: PROTEASOME COMPONENT C5

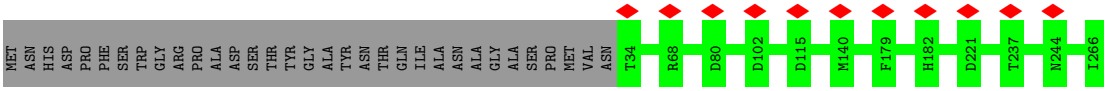
Chain e:





• Molecule 7: Proteasome subunit beta type-7

Chain 7:



• Molecule 7: Proteasome subunit beta type-7

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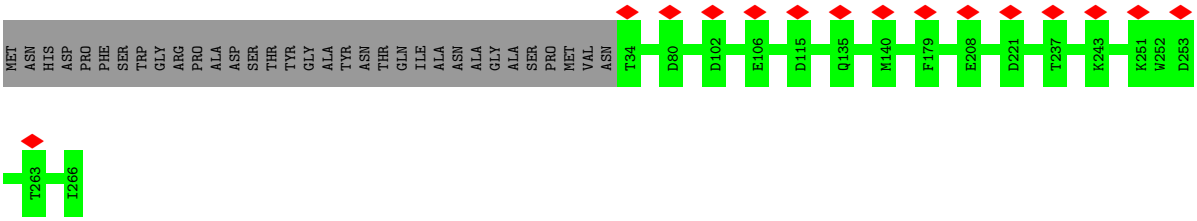
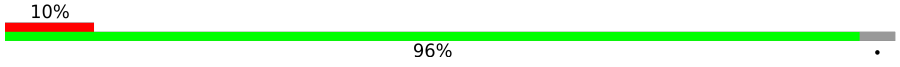
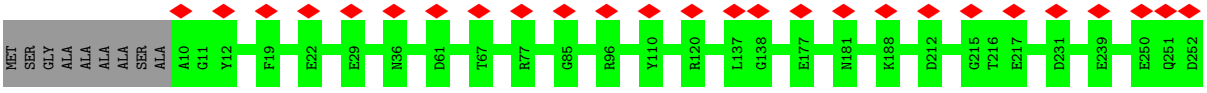


• Molecule 8: Proteasome subunit alpha type-1

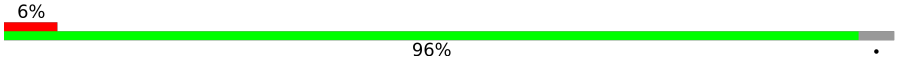
Chain A:

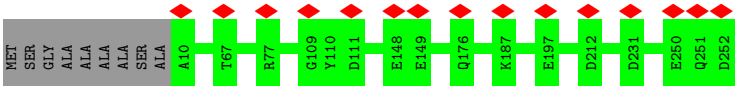




• Molecule 8: Proteasome subunit alpha type-1

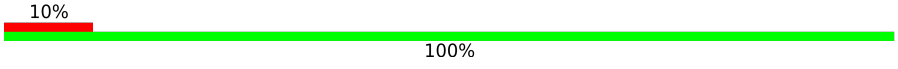
Chain c:

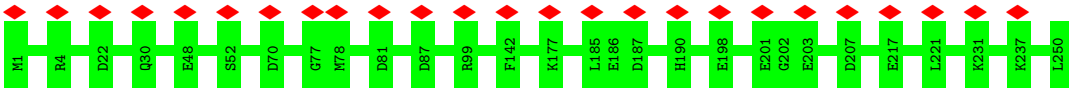




• Molecule 9: Proteasome subunit alpha type-2

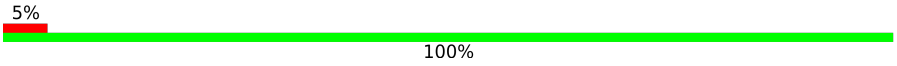
Chain B:

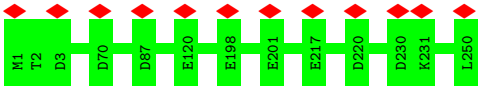




• Molecule 9: Proteasome subunit alpha type-2

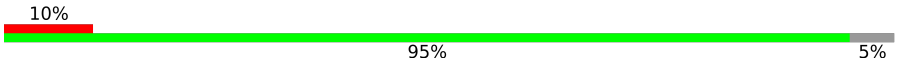
Chain j:

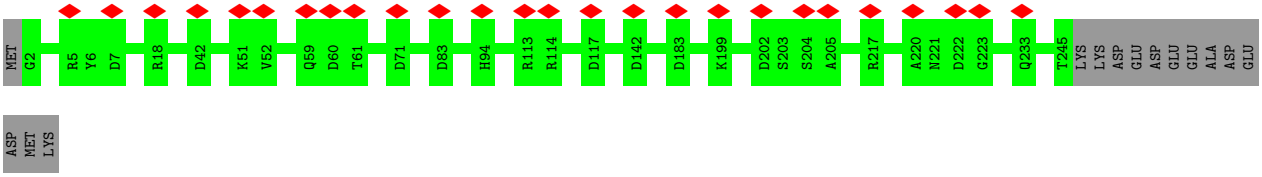




• Molecule 10: Proteasome subunit alpha type-3

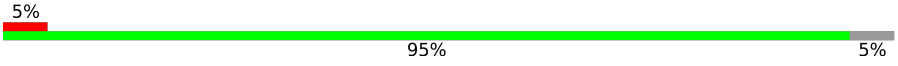
Chain C:

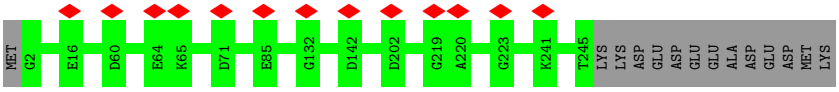




• Molecule 10: Proteasome subunit alpha type-3

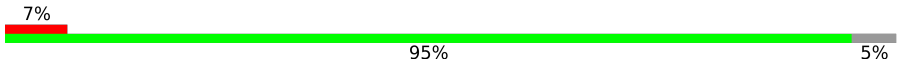
Chain d:

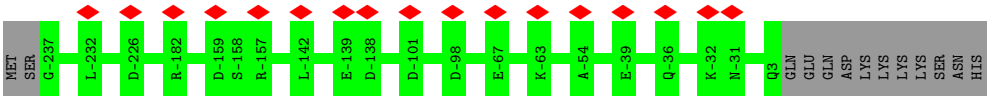




• Molecule 11: Proteasome subunit alpha type-4

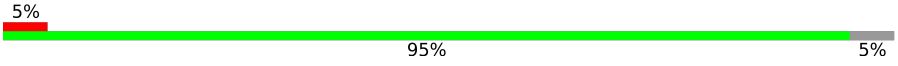
Chain D:

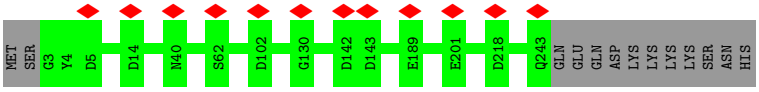




• Molecule 11: Proteasome subunit alpha type-4

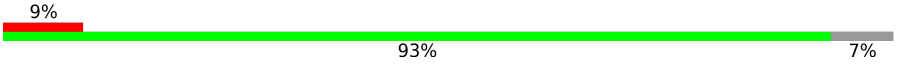
Chain n:

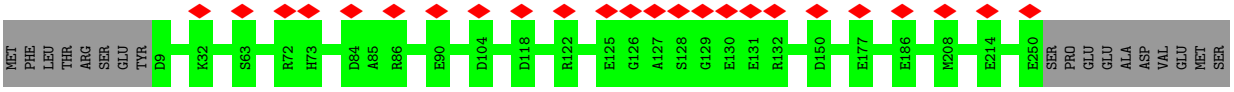




• Molecule 12: Proteasome subunit alpha type-5

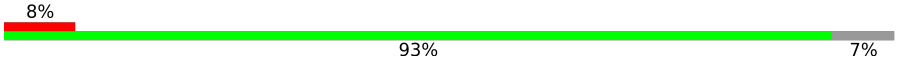
Chain E:

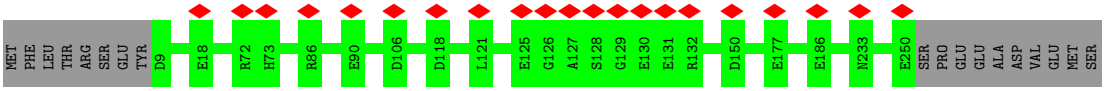




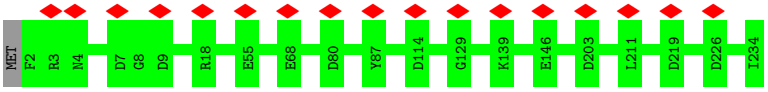
• Molecule 12: Proteasome subunit alpha type-5

Chain m:

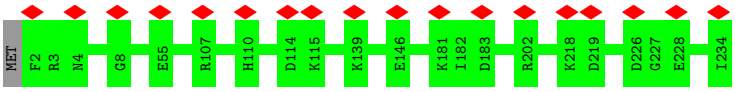




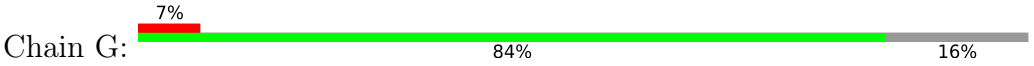
• Molecule 13: Proteasome subunit alpha type-6

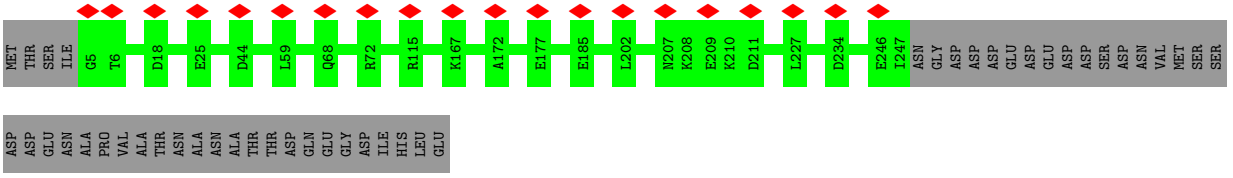


• Molecule 13: Proteasome subunit alpha type-6

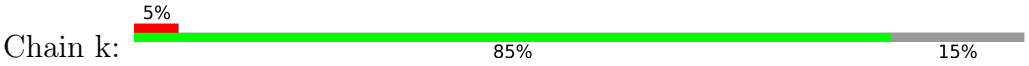


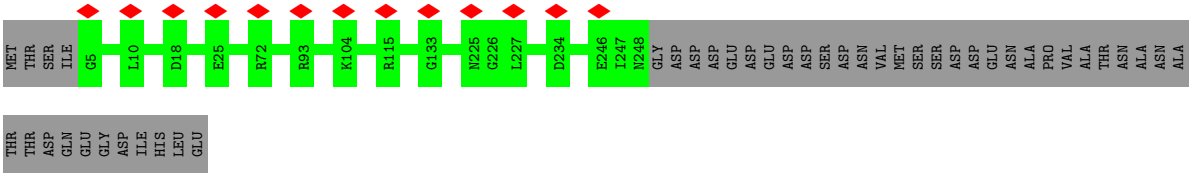
• Molecule 14: Probable proteasome subunit alpha type-7



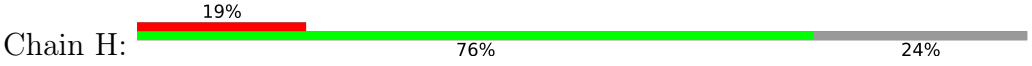


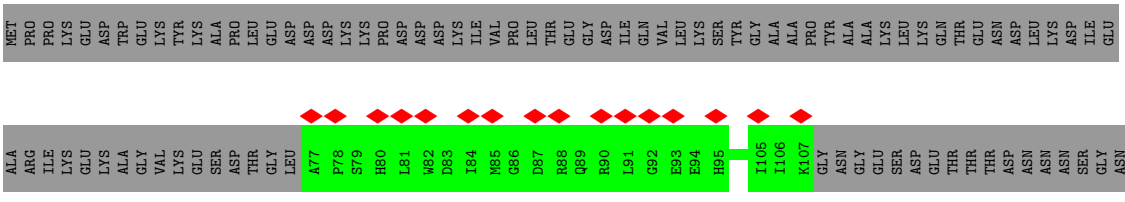
• Molecule 14: Probable proteasome subunit alpha type-7

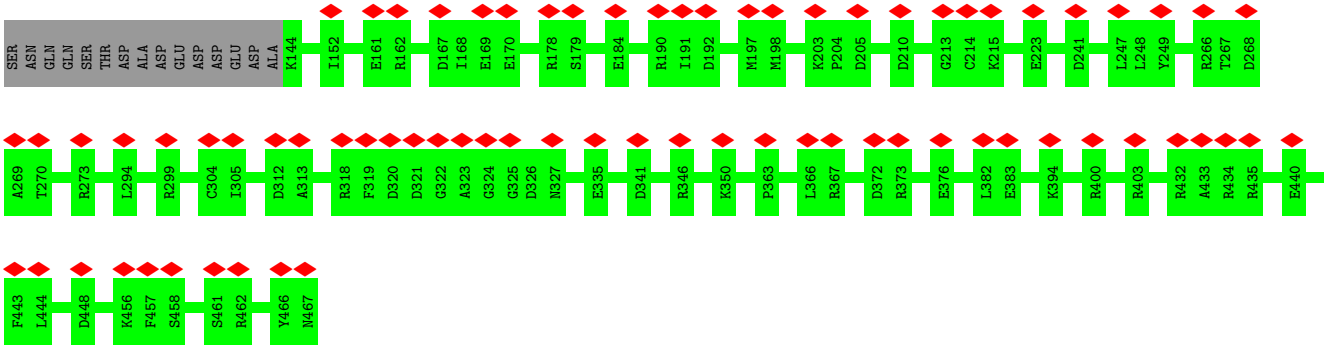




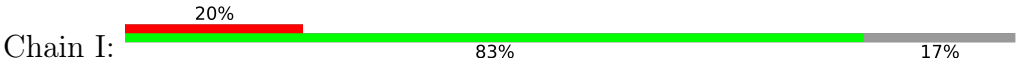
• Molecule 15: 26S proteasome regulatory subunit 7 homolog

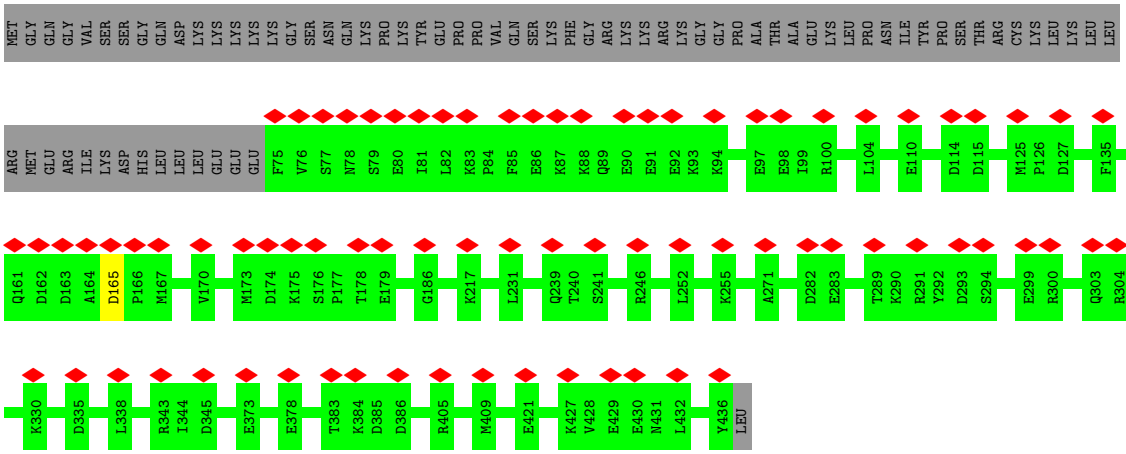




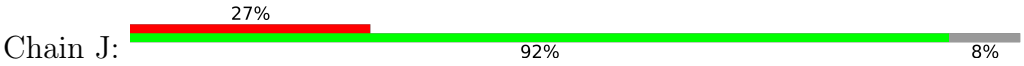


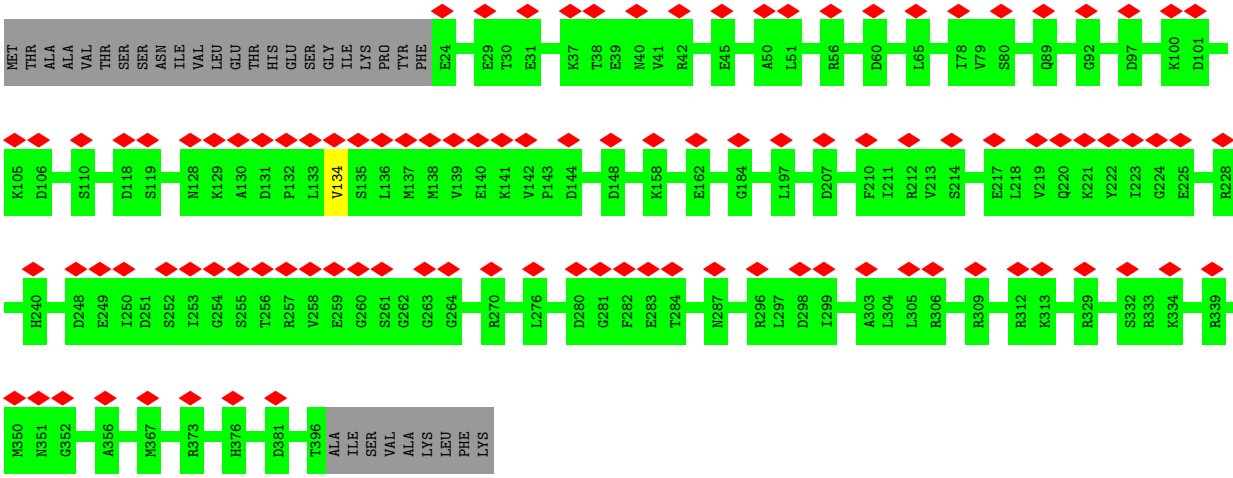
• Molecule 16: 26S PROTEASE REGULATORY SUBUNIT 4 HOMOLOG



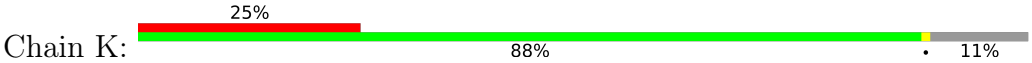


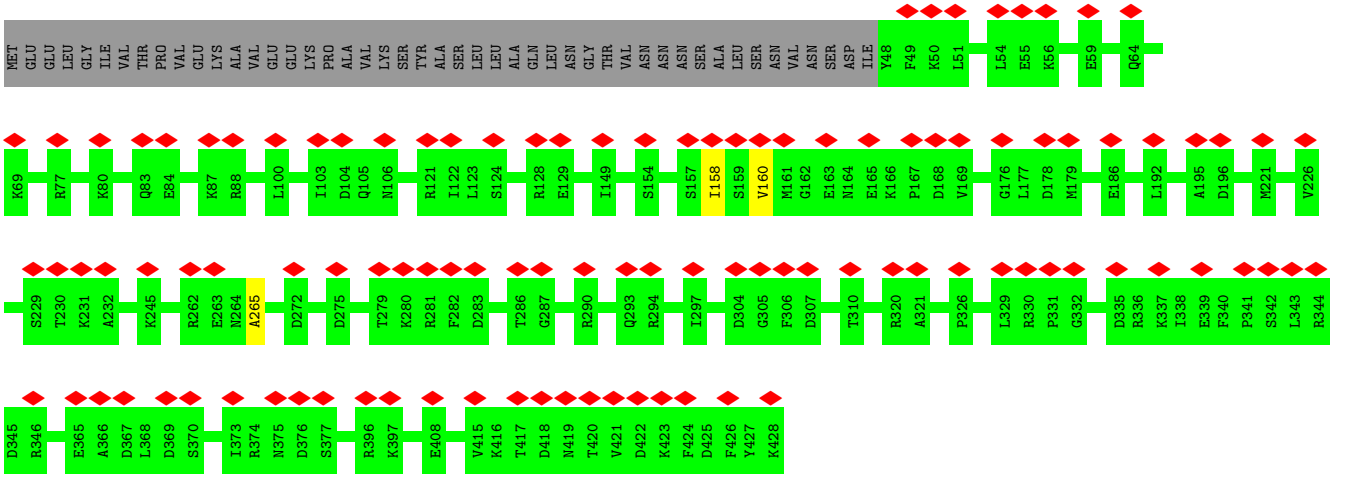
• Molecule 17: 26S proteasome regulatory subunit 8 homolog



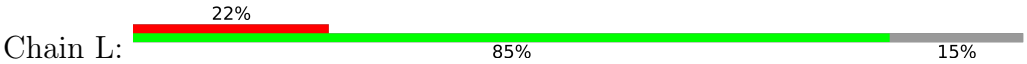


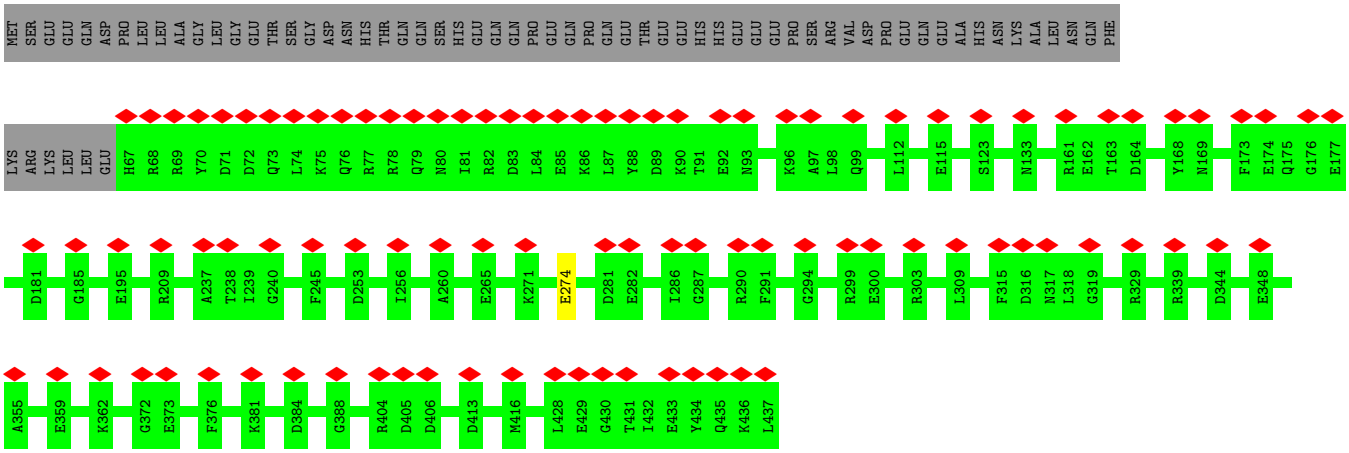
• Molecule 18: 26S proteasome regulatory subunit 6B homolog



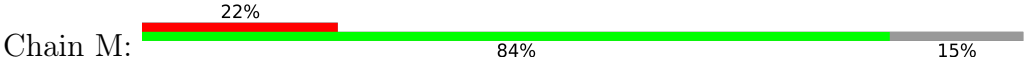


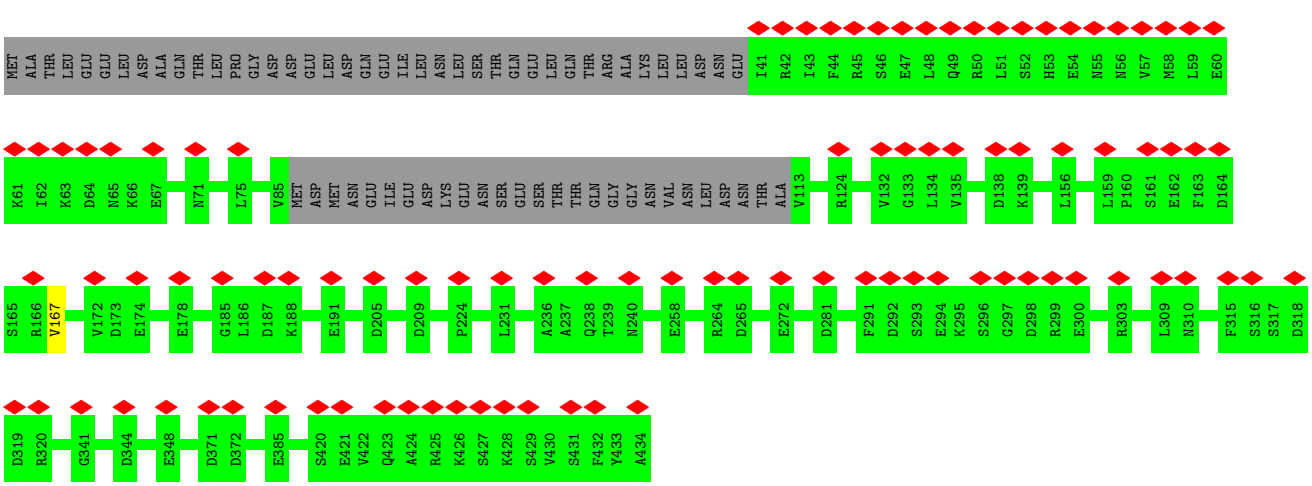
• Molecule 19: 26S proteasome subunit RPT4





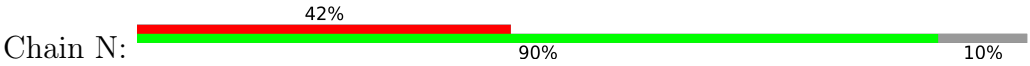
• Molecule 20: 26S proteasome regulatory subunit 6A

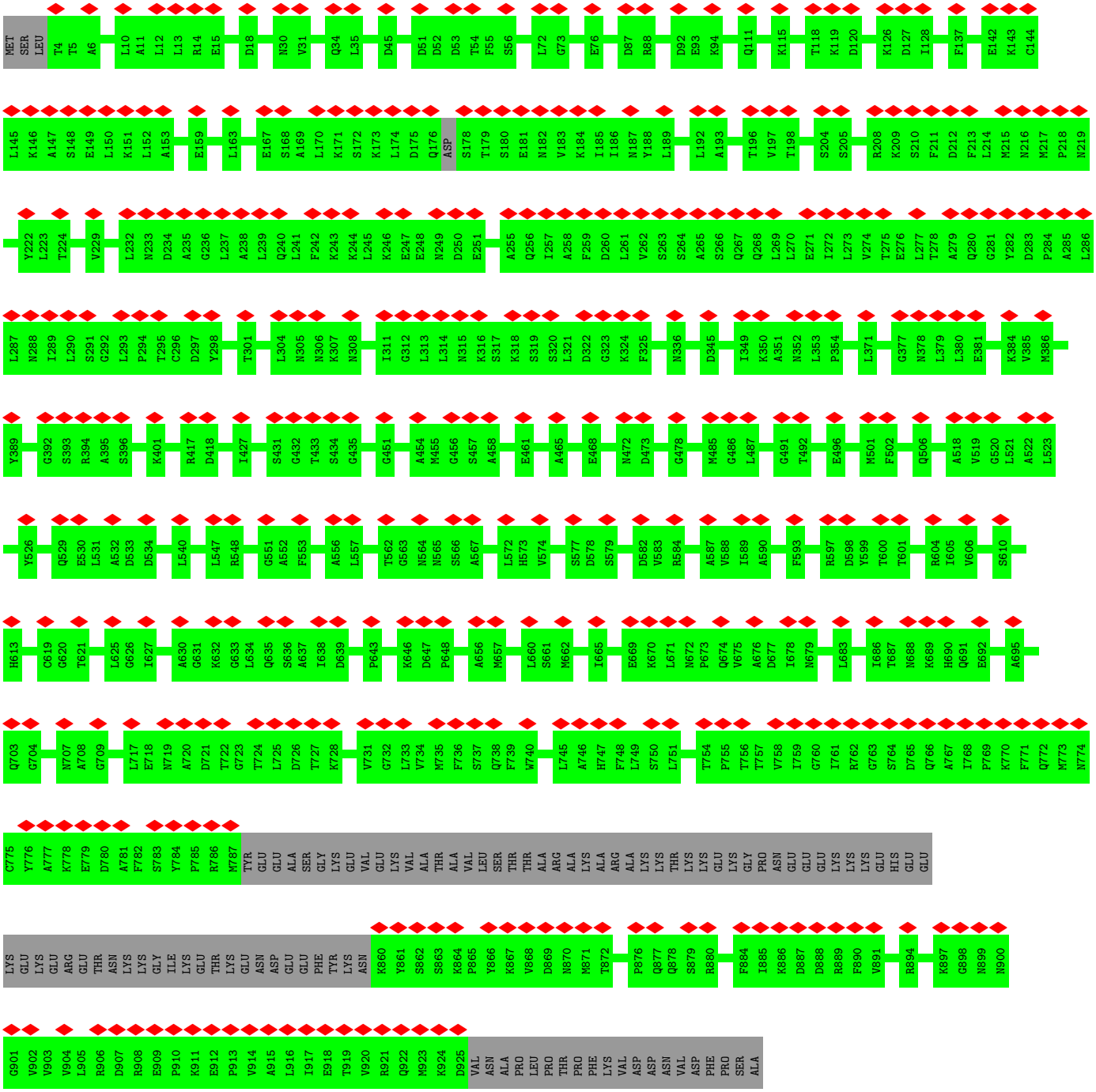




• Molecule 21: 26S proteasome regulatory subunit RPN2

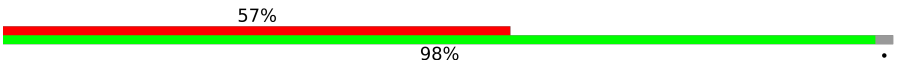
Chain N:

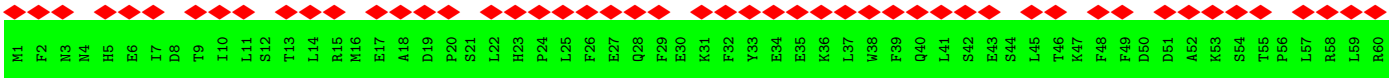


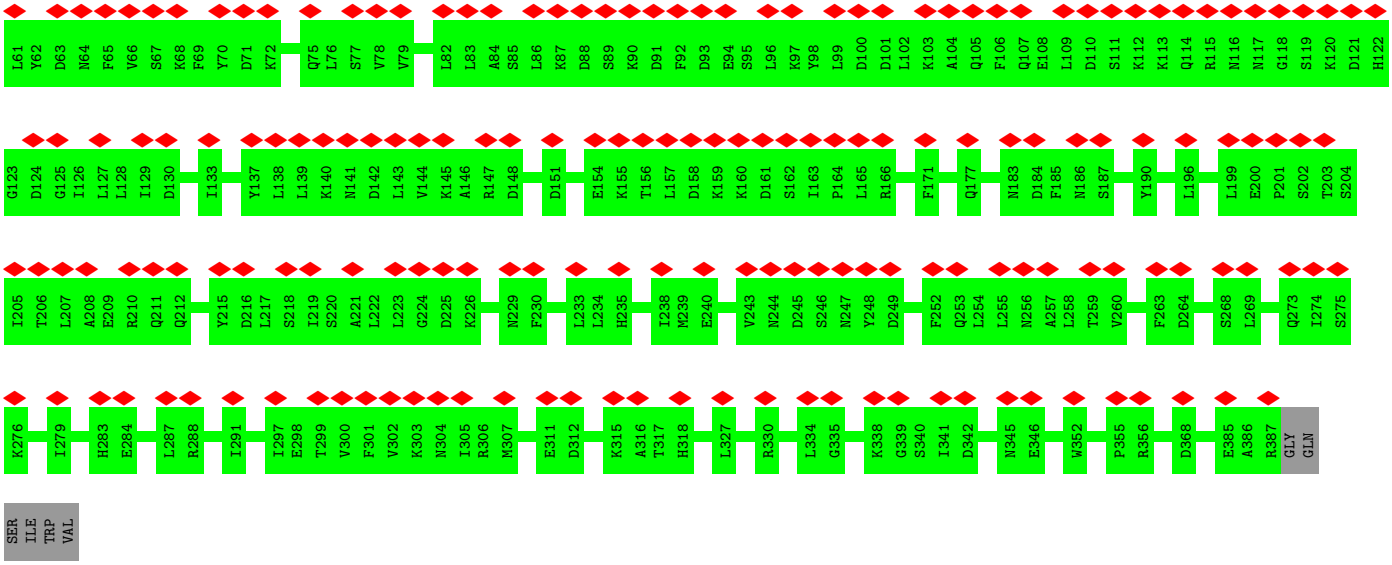


• Molecule 22: 26S proteasome regulatory subunit RPN9

Chain O:

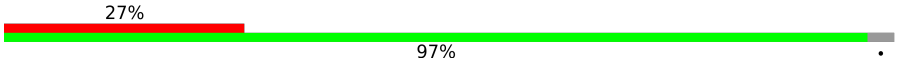


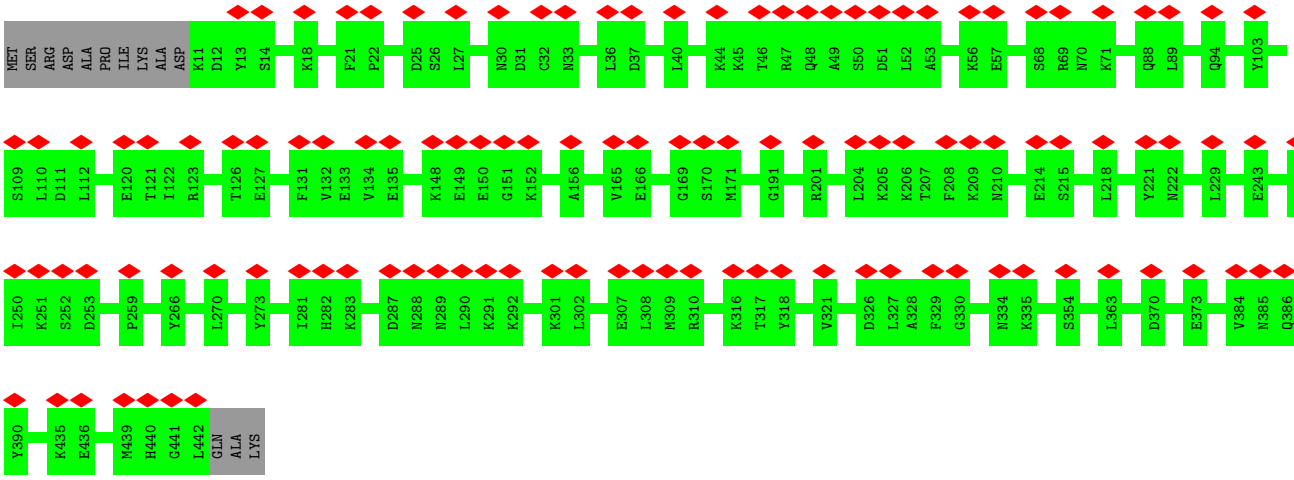




• Molecule 23: 26S PROTEASOME REGULATORY SUBUNIT RPN5

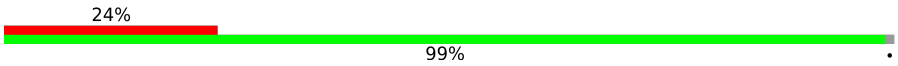
Chain P:

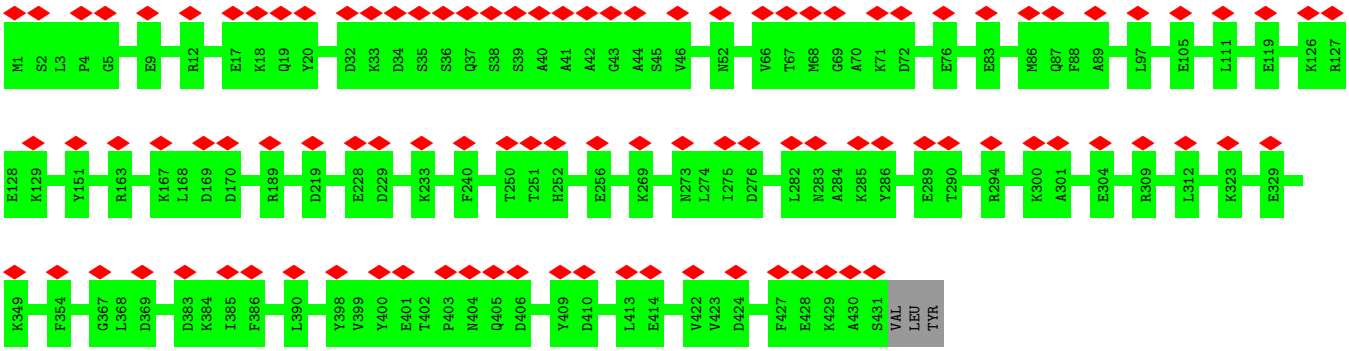




• Molecule 24: 26S proteasome regulatory subunit RPN6

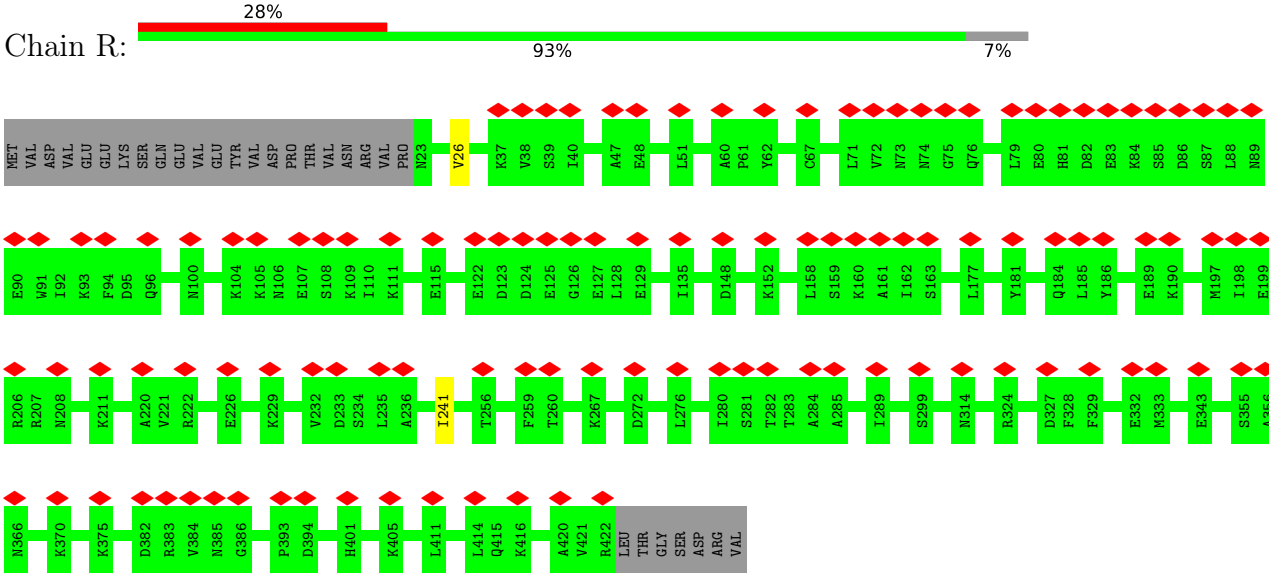
Chain Q:





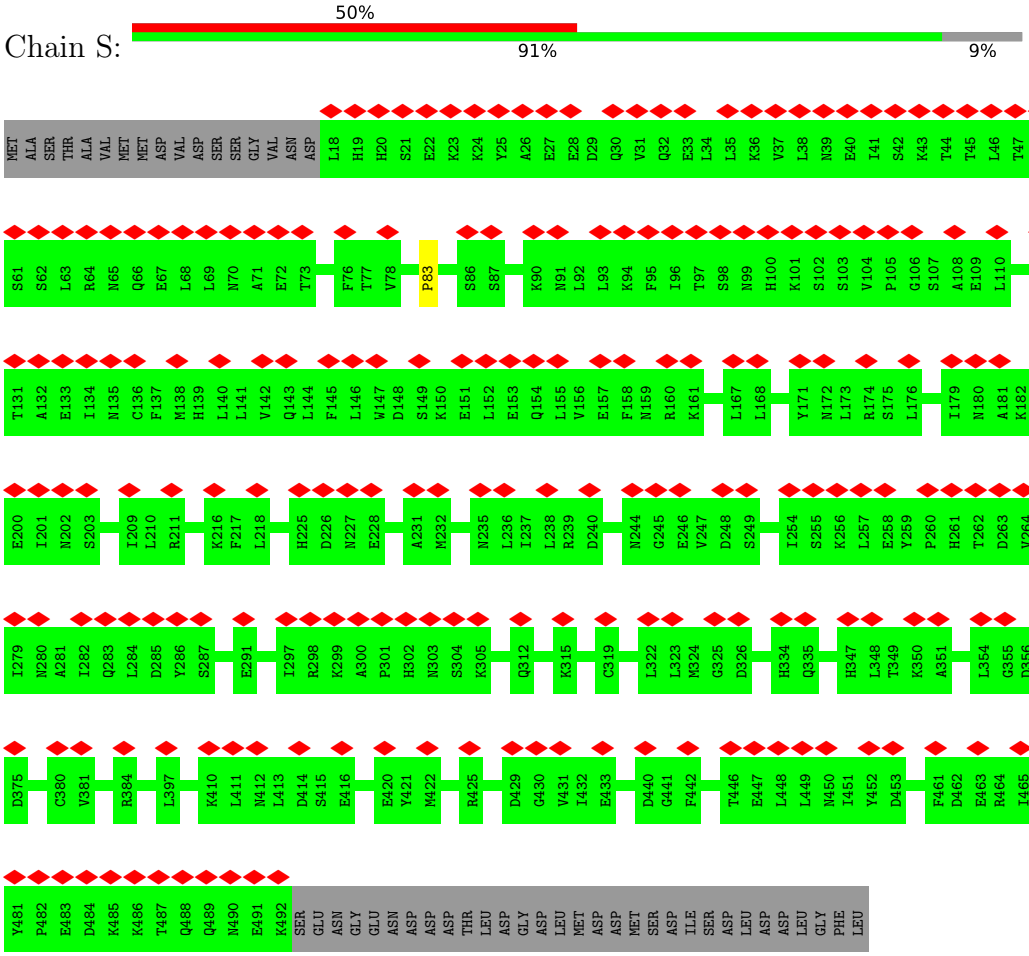
• Molecule 25: 26S proteasome regulatory subunit RPN7

Chain R:



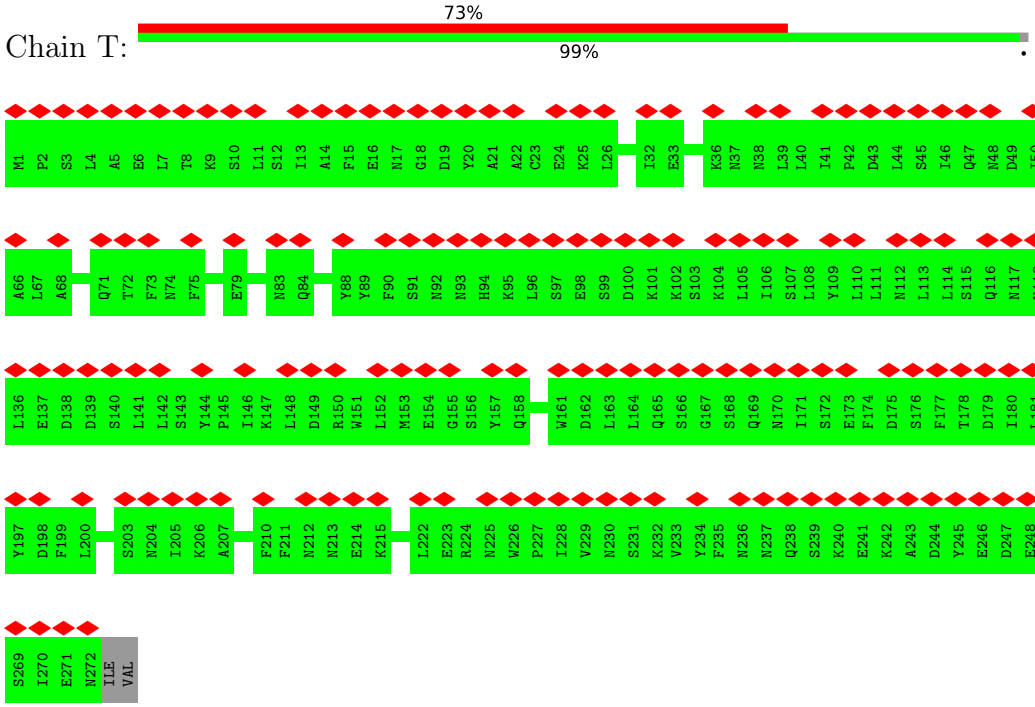
• Molecule 26: 26S proteasome regulatory subunit RPN3

Chain S:



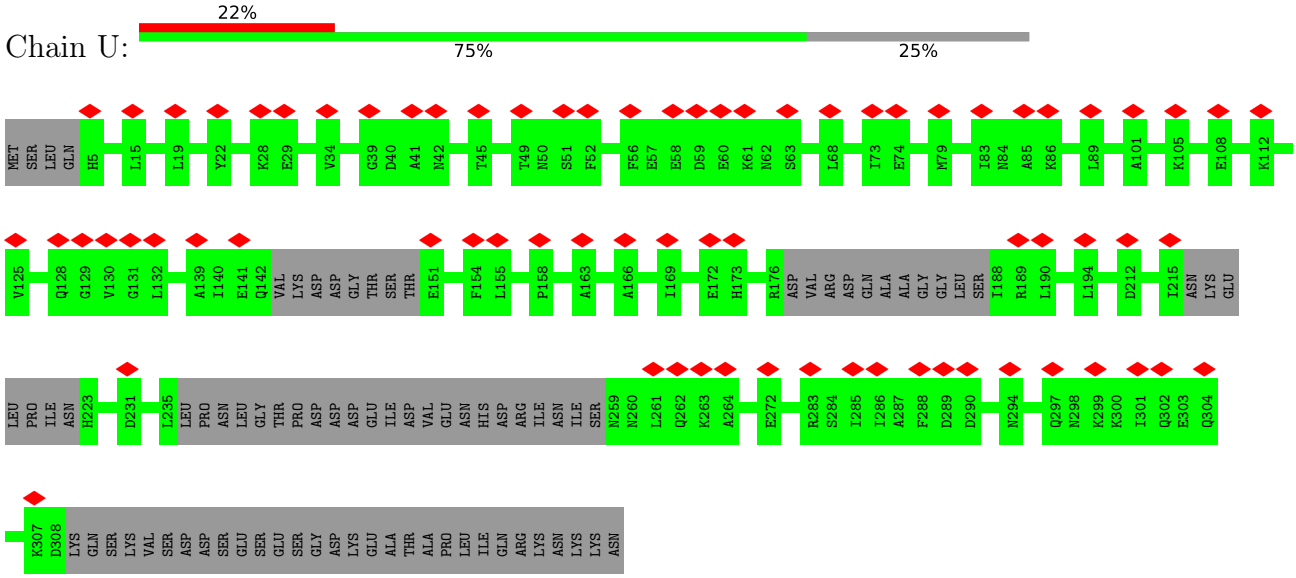
• Molecule 27: 26S proteasome regulatory subunit RPN12

Chain T:



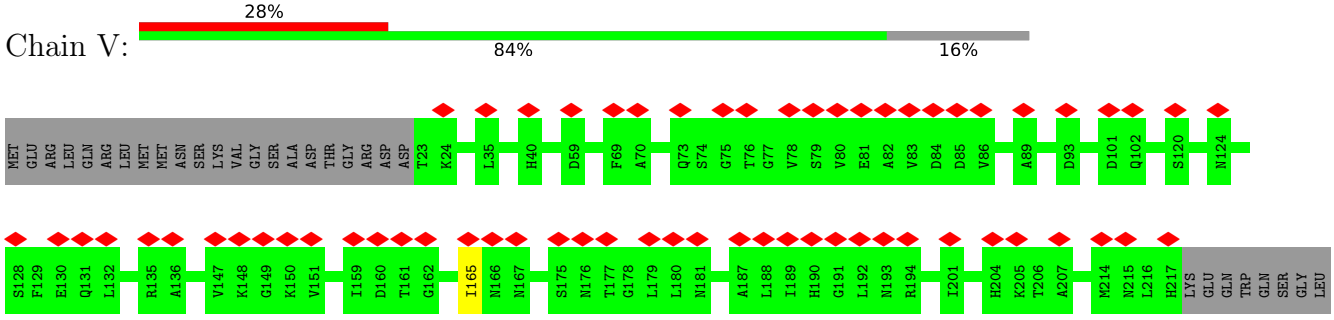
• Molecule 28: 26S proteasome regulatory subunit RPN8

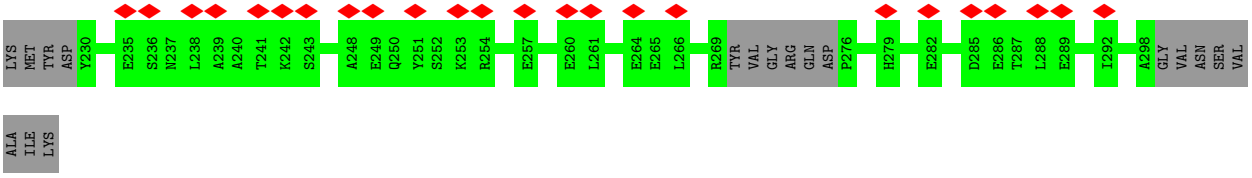
Chain U:



• Molecule 29: Ubiquitin carboxyl-terminal hydrolase RPN11

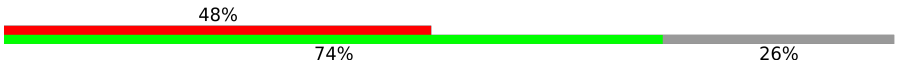
Chain V:

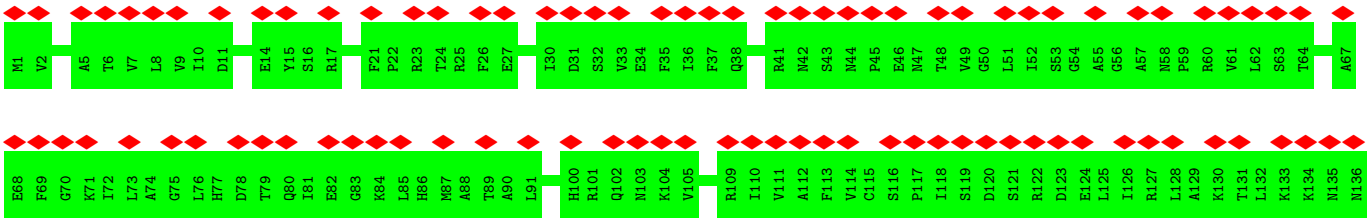




• Molecule 30: 26S proteasome regulatory subunit RPN10

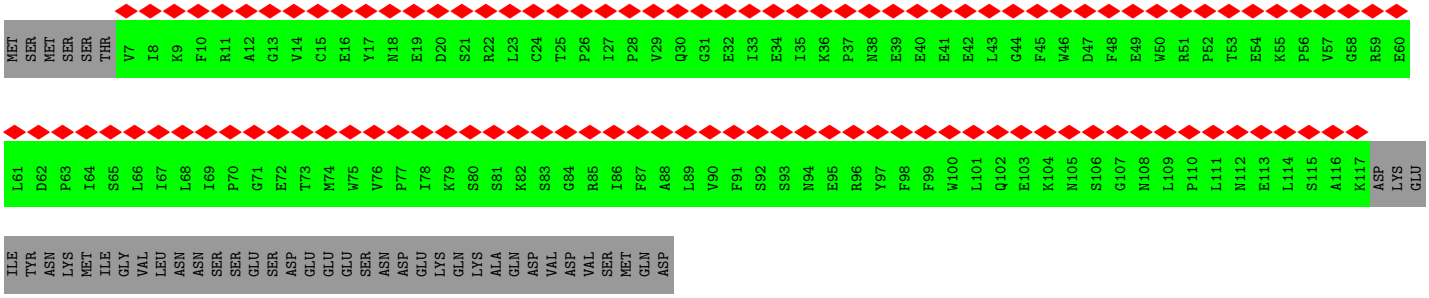
Chain W:





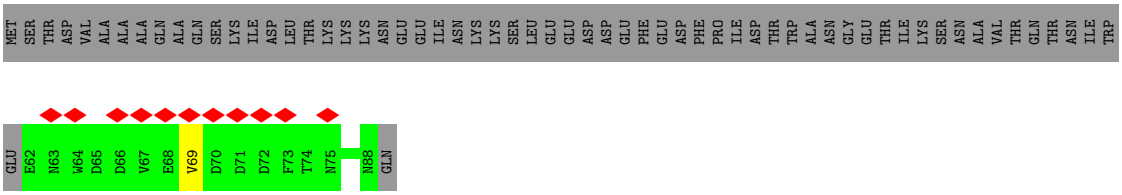
• Molecule 31: 26S proteasome regulatory subunit RPN13

Chain X:



• Molecule 32: 26S proteasome complex subunit SEM1

Chain Y:



• Molecule 33: 26S proteasome regulatory subunit RPN1

Chain Z:

MET VAL ASP GLU SER ASP LYS LYS GLN GLN THR ILE ASP GLU GLN SER GLN ILE SER PRO GLU LYS GLN THR PRO ASN LYS LYS ASP LYS LYS GLU GLU GLU GLU GLN LEU SER GLU GLU ASP ALA LYS LEU LYS THR ASP L49 E50 L51 L52 V53 E54 R55 L56 K57 E58 D59 D60

S61 S62 L63 Y64 E65 A66 S67 L68 N69 A70 L71 K72 E73 S74 I75 K76 N77 S78 T79 S80 S81 M82 T83 A84 V85 P86 K87 P88 L89 K90 F91 L92 R93 P94 T95 Y96 P97 D98 L99 C100 S101 I102 Y103 D104 K105 W106 T107 D108 P109 N110 L111 K112 S113 S114 L115 A116 D117 V118 L119 S120

I121 L122 A123 M124 T125 Y126 S127 E128 N129 G130 K131 H132 D133 S134 L135 R136 Y137 R138 L139 L140 S141 D142 V143 S144 D145 F146 E147 G148 W149 G150 H151 E152 Y153 I154 R155 H156 L157 A158 L159 E160 I161 G162 E163 V164 Y165 N166 D167 Q168 V169 E170 K171 D172 A173 E174 D175 E176 T177 S178 S179 D180

G181 S182 K183 S184 D185 G186 S187 A188 A189 T190 S191 G192 F193 E194 F195 S196 K197 E198 D199 T200 L201 R202 L203 C204 L205 D206 I207 Y208 P209 Y210 F211 L212 K213 H214 N215 G216 E217 E218 D219 A220 V221 D222 L223 L224 L225 E226 I227 E228 S229 I230 D231 K232 L233 P234 Q235 F236 V237 D238 E239 N240

T241 F242 Q243 R244 V245 C246 Q247 Y248 M249 V250 A251 C252 V253 P254 L255 L256 P257 P258 P259 E260 D261 V262 A263 F264 L265 K266 T267 A268 Y269 S270 I271 Y272 L273 S274 Q275 N276 E277 L278 T279 D280 A281 I282 A283 L284 A285 V286 R287 L288 G289 E290 E291 D292 M293 I294 R295 F298 D299 S302

D303 P304 V305 M306 H307 K308 Q309 L310 A311 Y312 I313 L314 A315 A316 Q317 K318 T319 S320 F321 E322 Y323 E324 G325 V326 Q327 D328 I329 I330 G331 N332 G333 K334 L335 S336 E337 H338 F339 L340 Y341 L342 A343 K344 E345 L346 N347 L348 T349 G350 P351 K352 V353 P354 E355 D356 I357 Y358 K359 S360 H361 L362

D363 N364 S365 K366 S367 V368 F369 S370 S371 A372 G373 L374 D375 S376 A377 Q378 Q379 N380 L381 A382 S383 S384 F385 V386 N387 G388 F389 L390 N391 L392 G393 Y394 C395 N396 D397 K398 L399 I400 V401 D402 N403 D404 N405 W406 V407 Y408 K409 T410 K411 G412 D413 G414 M415 T416 S417 A418 V419 A420 S421 I422

G423 S424 I425 Y426 Q427 W428 N429 L430 D431 G432 L433 Q434 Q435 L436 D437 K438 Y439 L440 Y441 V442 D443 E444 P445 E446 V447 K448 A449 G450 A451 L452 L453 G454 I455 G456 I457 S458 A459 S460 G461 V462 H463 D464 G465 E466 V467 E468 P469 A470 L471 L472 L473 L474 Q475 D476 Y477 V478 T479 N480 P481 D482

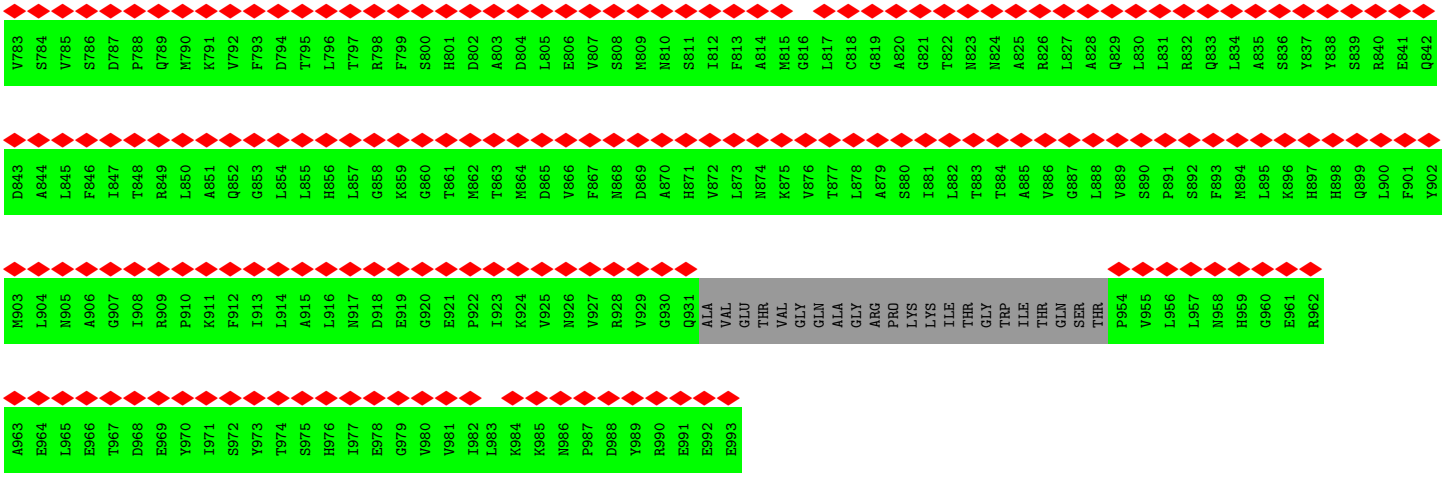
T483 K484 I485 S486 S487 A488 A489 I490 L491 G492 L493 G494 I495 A496 F497 A498 G499 S500 K501 N502 D503 E504 V505 L506 G507 L508 L509 L510 P511 I512 A513 A514 S515 T516 D517 L518 P519 I520 E521 T522 A523 A524 M525 A526 S527 L528 A529 L530 A531 H532 V533 F534 V535 G536 T537 C538 N539 G540 D541 I542

T543 T544 S545 I546 M547 D548 N549 F550 L551 E552 R553 T554 A555 I556 E557 L558 K559 T560 D561 W562 V563 R564 F565 L566 A567 L568 A569 L570 G571 I572 L573 Y574 M575 G576 Q577 G578 E579 Q580 V581 D582 D583 V584 L585 E586 A587 I588 S589 A590 I591 E592 H593 P594 M595 T596 S597 A598 I599 E600 V601 L602

V603 G604 S605 C606 A607 Y608 T609 G610 T611 G612 D613 V614 L615 L616 I617 Q618 D619 L620 L621 H622 R623 L624 T625 PRO LYS ASN VAL LYS GLY GLU GLU ASP ALA ASP GLU GLU GLU THR ALA GLU GLY GLN THR ASN SER ILE SER ASP PHE LEU GLY GLU GLN VAL ASN GLU PRO THR LYS ASN

GLU GLU ALA GLU ILE GLU VAL ASP GLU MET GLU VAL ASP ALA GLU GLY GLU GLU VAL GLU VAL LYS ALA GLU ILE LEU GLU SER LEU GLU GLY GLU GLU ILE LYS GLU GLU LYS LYS GLY LYS SER SER ASP LYS ASP ALA THR THR ASP GLY LYS ASN ASP

ASP GLU GLU GLU GLU LYS GLU ALA GLY ILE VAL ASP GLU L736 A737 Y738 A739 V740 L741 G742 I743 A744 L745 I746 A747 L748 G749 E750 D751 I752 G753 K754 E755 M756 S757 L758 R759 H760 F761 G762 H763 L764 M765 H766 Y767 G768 N769 E770 H771 I772 R773 R774 M775 V776 P777 L778 A779 M780 G781 I782


V783 S784 V785 S786 D787 P788 Q789 M790 K791 V792 F793 D794 T795 L796 T797 R798 F799 S800 H801 D802 A803 D804 L805 E806 V807 S808 M809 N810 S811 I812 F813 A814 M815 G816 L817 C818 G819 A820 G821 T822 N823 N824 A825 R826 L827 A828 Q829 L830 L831 R832 Q833 L834 A835 S836 Y837 Y838 S839 R840 E841 Q842
D843 A844 L845 F846 I847 T848 R849 L850 A851 Q852 G853 L854 L855 H856 L857 G858 K859 G860 T861 M862 T863 M864 D865 V866 F867 N868 D869 A870 H871 V872 L873 N874 K875 V876 T877 L878 A879 S880 I881 L882 T883 T884 A885 V886 G887 L888 V889 S890 P891 S892 F893 M894 L895 K896 H897 H898 Q899 L900 F901 Y902
M903 L904 N905 A906 G907 I908 R909 P910 K911 F912 I913 L914 A915 L916 N917 D918 E919 G920 E921 P922 I923 K924 V925 N926 V927 R928 V929 G930 Q931 ALA VAL GLU THR VAL GLY GLN ALA GLY ARG PRO LYS LYS ILE THR GLY TRP ILE THR GLN SER THR P954 V955 L956 L957 N958 H959 G960 E961 R962
A963 E964 L965 E966 T967 D968 E969 Y970 I971 S972 Y973 T974 S975 H976 I977 E978 G979 V980 V981 I982 L983 K984 K985 N986 P987 D988 Y989 R990 E991 E992 E993

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	49507	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	38	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.766	Depositor
Minimum map value	-1.268	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.098	Depositor
Recommended contour level	0.704	Depositor
Map size (Å)	474.47998, 474.47998, 474.47998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.318, 1.318, 1.318	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	1	0.24	0/1605	0.42	0/2171
1	b	0.23	0/1605	0.43	0/2171
2	2	0.23	0/1715	0.42	0/2326
2	i	0.23	0/1715	0.42	0/2326
3	3	0.24	0/1611	0.40	0/2174
3	h	0.24	0/1611	0.41	0/2174
4	4	0.23	0/1613	0.39	0/2173
4	g	0.23	0/1613	0.39	0/2173
5	5	0.23	0/1681	0.39	0/2274
5	f	0.23	0/1681	0.40	0/2274
6	6	0.24	0/1795	0.40	0/2420
6	e	0.24	0/1795	0.40	0/2420
7	7	0.24	0/1855	0.42	0/2514
7	a	0.24	0/1855	0.41	0/2514
8	A	0.24	0/1959	0.39	0/2652
8	c	0.24	0/1959	0.39	0/2652
9	B	0.24	0/1952	0.41	0/2642
9	j	0.24	0/1952	0.40	0/2642
10	C	0.23	0/1934	0.40	0/2618
10	d	0.24	0/1934	0.40	0/2618
11	D	0.22	0/1919	0.39	0/2598
11	n	0.23	0/1919	0.39	0/2598
12	E	0.23	0/1886	0.39	0/2541
12	m	0.23	0/1886	0.40	0/2541
13	F	0.24	0/1823	0.41	0/2463
13	l	0.24	0/1823	0.43	0/2463
14	G	0.24	0/1928	0.39	0/2603
14	k	0.23	0/1936	0.39	0/2614
15	H	0.24	0/2834	0.40	0/3816
16	I	0.26	1/2860 (0.0%)	0.41	0/3856
17	J	0.23	0/2964	0.39	0/3981
18	K	0.33	1/3062 (0.0%)	0.41	0/4132
19	L	0.32	1/2981 (0.0%)	0.40	0/4008
20	M	0.24	0/2903	0.41	0/3909

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
21	N	0.23	0/6670	0.39	0/9023
22	O	0.23	0/3243	0.39	0/4374
23	P	0.23	0/3599	0.38	0/4854
24	Q	0.23	0/3527	0.36	0/4748
25	R	0.23	0/3272	0.38	0/4412
26	S	0.23	0/3966	0.37	0/5355
27	T	0.23	0/2279	0.38	0/3077
28	U	0.23	0/2087	0.37	0/2811
29	V	0.23	0/2054	0.42	0/2770
30	W	0.23	0/1557	0.40	0/2111
31	X	0.23	0/931	0.40	0/1262
32	Y	0.22	0/239	0.37	0/322
33	Z	0.23	0/6404	0.39	0/8686
All	All	0.24	3/107992 (0.0%)	0.40	0/145856

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	K	265	ALA	C-N	12.60	1.58	1.34
19	L	274	GLU	C-N	11.88	1.56	1.34
16	I	165	ASP	C-N	6.37	1.46	1.34

There are no bond angle outliers.

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	1	203/215 (94%)	194 (96%)	9 (4%)	0	100	100
1	b	203/215 (94%)	191 (94%)	12 (6%)	0	100	100
2	2	220/261 (84%)	214 (97%)	6 (3%)	0	100	100
2	i	220/261 (84%)	211 (96%)	9 (4%)	0	100	100
3	3	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
3	h	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
4	4	196/198 (99%)	187 (95%)	9 (5%)	0	100	100
4	g	196/198 (99%)	190 (97%)	6 (3%)	0	100	100
5	5	210/287 (73%)	200 (95%)	10 (5%)	0	100	100
5	f	210/287 (73%)	201 (96%)	9 (4%)	0	100	100
6	6	220/241 (91%)	213 (97%)	7 (3%)	0	100	100
6	e	220/241 (91%)	212 (96%)	8 (4%)	0	100	100
7	7	231/266 (87%)	219 (95%)	12 (5%)	0	100	100
7	a	231/266 (87%)	226 (98%)	5 (2%)	0	100	100
8	A	241/252 (96%)	235 (98%)	6 (2%)	0	100	100
8	c	241/252 (96%)	234 (97%)	7 (3%)	0	100	100
9	B	248/250 (99%)	240 (97%)	8 (3%)	0	100	100
9	j	248/250 (99%)	239 (96%)	9 (4%)	0	100	100
10	C	242/258 (94%)	233 (96%)	9 (4%)	0	100	100
10	d	242/258 (94%)	234 (97%)	8 (3%)	0	100	100
11	D	239/254 (94%)	232 (97%)	7 (3%)	0	100	100
11	n	239/254 (94%)	231 (97%)	8 (3%)	0	100	100
12	E	240/260 (92%)	230 (96%)	10 (4%)	0	100	100
12	m	240/260 (92%)	230 (96%)	10 (4%)	0	100	100
13	F	231/234 (99%)	222 (96%)	9 (4%)	0	100	100
13	l	231/234 (99%)	217 (94%)	14 (6%)	0	100	100
14	G	241/288 (84%)	232 (96%)	9 (4%)	0	100	100
14	k	242/288 (84%)	233 (96%)	9 (4%)	0	100	100
15	H	351/467 (75%)	313 (89%)	38 (11%)	0	100	100
16	I	360/437 (82%)	324 (90%)	36 (10%)	0	100	100
17	J	371/405 (92%)	344 (93%)	26 (7%)	1 (0%)	41	74
18	K	379/428 (89%)	338 (89%)	39 (10%)	2 (0%)	29	66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
19	L	369/437 (84%)	339 (92%)	30 (8%)	0	100 100
20	M	363/434 (84%)	325 (90%)	37 (10%)	1 (0%)	41 74
21	N	843/945 (89%)	810 (96%)	33 (4%)	0	100 100
22	O	385/393 (98%)	342 (89%)	43 (11%)	0	100 100
23	P	430/445 (97%)	395 (92%)	35 (8%)	0	100 100
24	Q	429/434 (99%)	404 (94%)	25 (6%)	0	100 100
25	R	398/429 (93%)	355 (89%)	41 (10%)	2 (0%)	29 66
26	S	473/523 (90%)	452 (96%)	20 (4%)	1 (0%)	47 79
27	T	270/274 (98%)	245 (91%)	25 (9%)	0	100 100
28	U	245/338 (72%)	238 (97%)	7 (3%)	0	100 100
29	V	252/306 (82%)	231 (92%)	20 (8%)	1 (0%)	34 70
30	W	195/268 (73%)	183 (94%)	12 (6%)	0	100 100
31	X	109/156 (70%)	96 (88%)	13 (12%)	0	100 100
32	Y	25/89 (28%)	20 (80%)	4 (16%)	1 (4%)	3 28
33	Z	807/993 (81%)	753 (93%)	53 (7%)	1 (0%)	51 83
All	All	13383/15139 (88%)	12596 (94%)	777 (6%)	10 (0%)	54 83

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	J	134	VAL
18	K	158	ILE
18	K	160	VAL
20	M	167	VAL
25	R	26	VAL

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	1	169/178 (95%)	169 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	b	169/178 (95%)	169 (100%)	0	100	100
2	2	181/214 (85%)	181 (100%)	0	100	100
2	i	181/214 (85%)	181 (100%)	0	100	100
3	3	172/173 (99%)	172 (100%)	0	100	100
3	h	172/173 (99%)	172 (100%)	0	100	100
4	4	175/175 (100%)	175 (100%)	0	100	100
4	g	175/175 (100%)	175 (100%)	0	100	100
5	5	169/235 (72%)	169 (100%)	0	100	100
5	f	169/235 (72%)	169 (100%)	0	100	100
6	6	185/201 (92%)	185 (100%)	0	100	100
6	e	185/201 (92%)	185 (100%)	0	100	100
7	7	199/224 (89%)	199 (100%)	0	100	100
7	a	199/224 (89%)	199 (100%)	0	100	100
8	A	207/210 (99%)	207 (100%)	0	100	100
8	c	207/210 (99%)	207 (100%)	0	100	100
9	B	209/209 (100%)	209 (100%)	0	100	100
9	j	209/209 (100%)	209 (100%)	0	100	100
10	C	203/216 (94%)	203 (100%)	0	100	100
10	d	203/216 (94%)	203 (100%)	0	100	100
11	D	213/226 (94%)	213 (100%)	0	100	100
11	n	213/226 (94%)	213 (100%)	0	100	100
12	E	198/215 (92%)	198 (100%)	0	100	100
12	m	198/215 (92%)	198 (100%)	0	100	100
13	F	192/193 (100%)	192 (100%)	0	100	100
13	l	192/193 (100%)	192 (100%)	0	100	100
14	G	200/239 (84%)	200 (100%)	0	100	100
14	k	201/239 (84%)	201 (100%)	0	100	100
15	H	303/399 (76%)	303 (100%)	0	100	100
16	I	319/385 (83%)	319 (100%)	0	100	100
17	J	325/352 (92%)	325 (100%)	0	100	100
18	K	334/374 (89%)	334 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	L	317/377 (84%)	317 (100%)	0	100	100
20	M	315/375 (84%)	315 (100%)	0	100	100
21	N	713/797 (90%)	713 (100%)	0	100	100
22	O	363/368 (99%)	363 (100%)	0	100	100
23	P	405/415 (98%)	405 (100%)	0	100	100
24	Q	388/391 (99%)	388 (100%)	0	100	100
25	R	351/379 (93%)	351 (100%)	0	100	100
26	S	447/489 (91%)	447 (100%)	0	100	100
27	T	254/256 (99%)	254 (100%)	0	100	100
28	U	234/308 (76%)	234 (100%)	0	100	100
29	V	227/268 (85%)	227 (100%)	0	100	100
30	W	171/230 (74%)	171 (100%)	0	100	100
31	X	101/144 (70%)	101 (100%)	0	100	100
32	Y	26/81 (32%)	26 (100%)	0	100	100
33	Z	692/850 (81%)	692 (100%)	0	100	100
All	All	11630/13054 (89%)	11630 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 100 such sidechains are listed below:

Mol	Chain	Res	Type
21	N	738	GLN
25	R	73	ASN
33	Z	976	HIS
22	O	122	HIS
24	Q	106	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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.

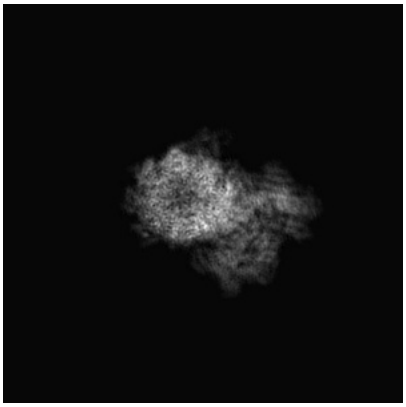
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9772. These allow visual inspection of the internal detail of the map and identification of artifacts.

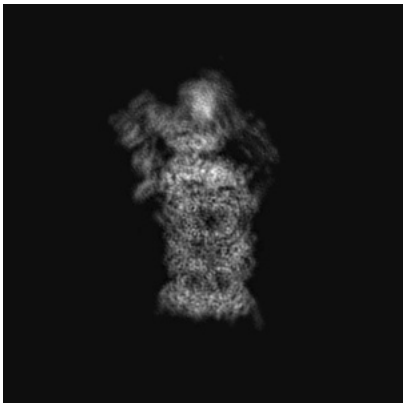
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

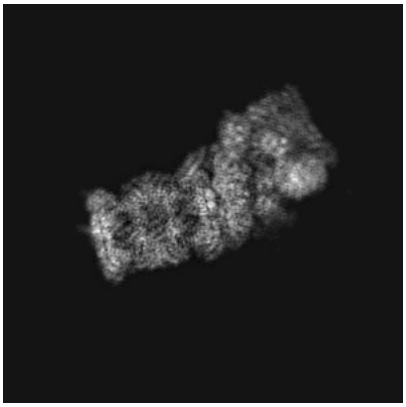
6.1.1 Primary map



X



Y

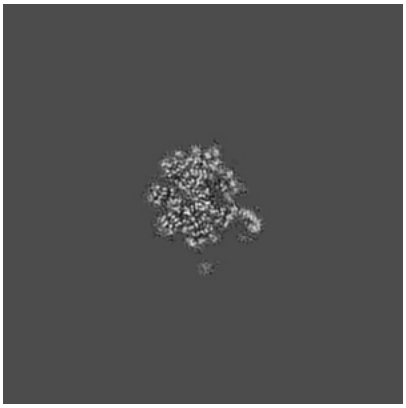


Z

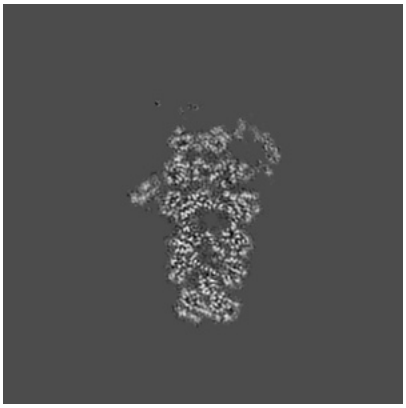
The images above show the map projected in three orthogonal directions.

6.2 Central slices

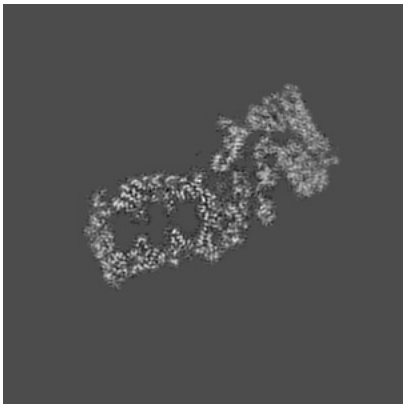
6.2.1 Primary map



X Index: 180



Y Index: 180

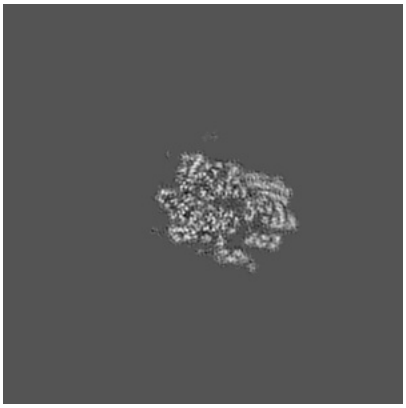


Z Index: 180

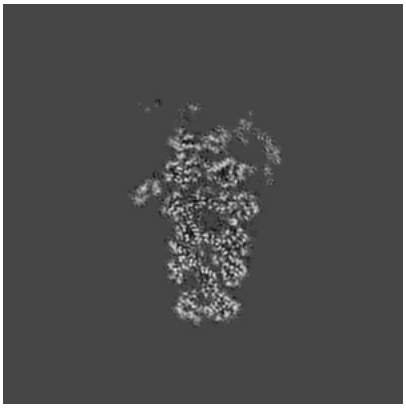
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

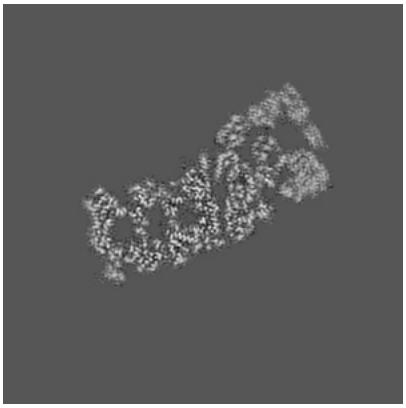
6.3.1 Primary map



X Index: 204



Y Index: 182



Z Index: 172

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.704. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

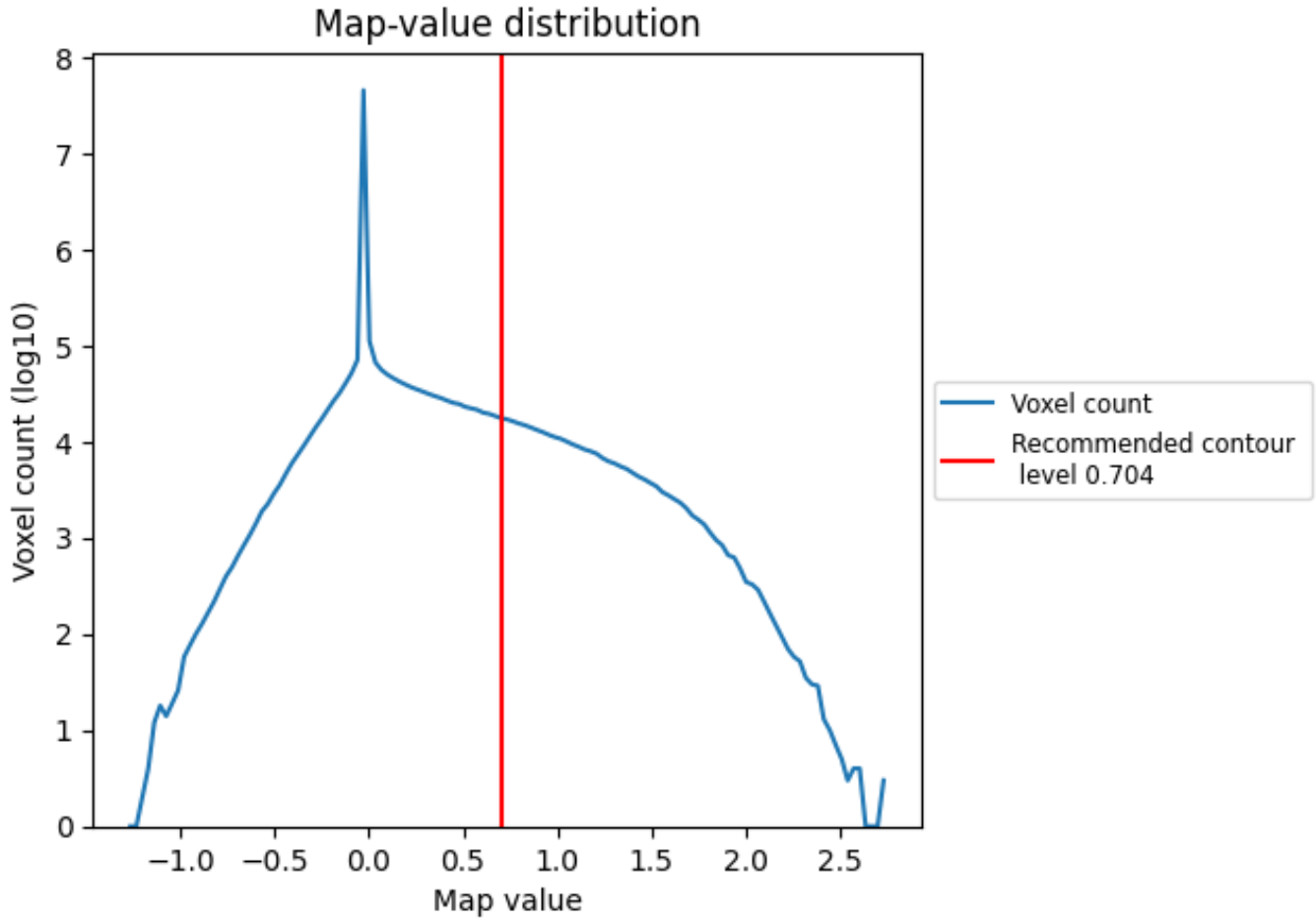
6.5 Mask visualisation (i)

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

7 Map analysis

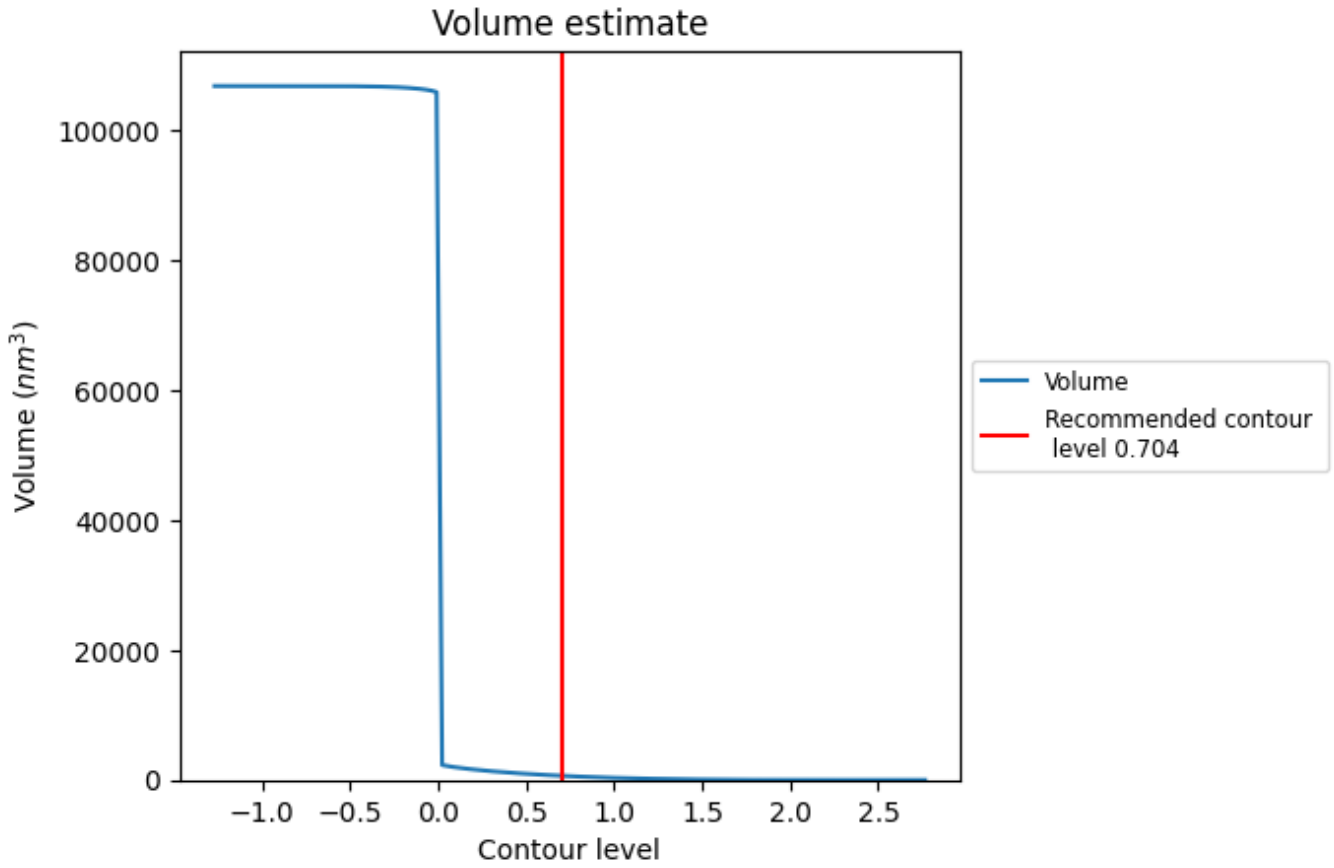
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

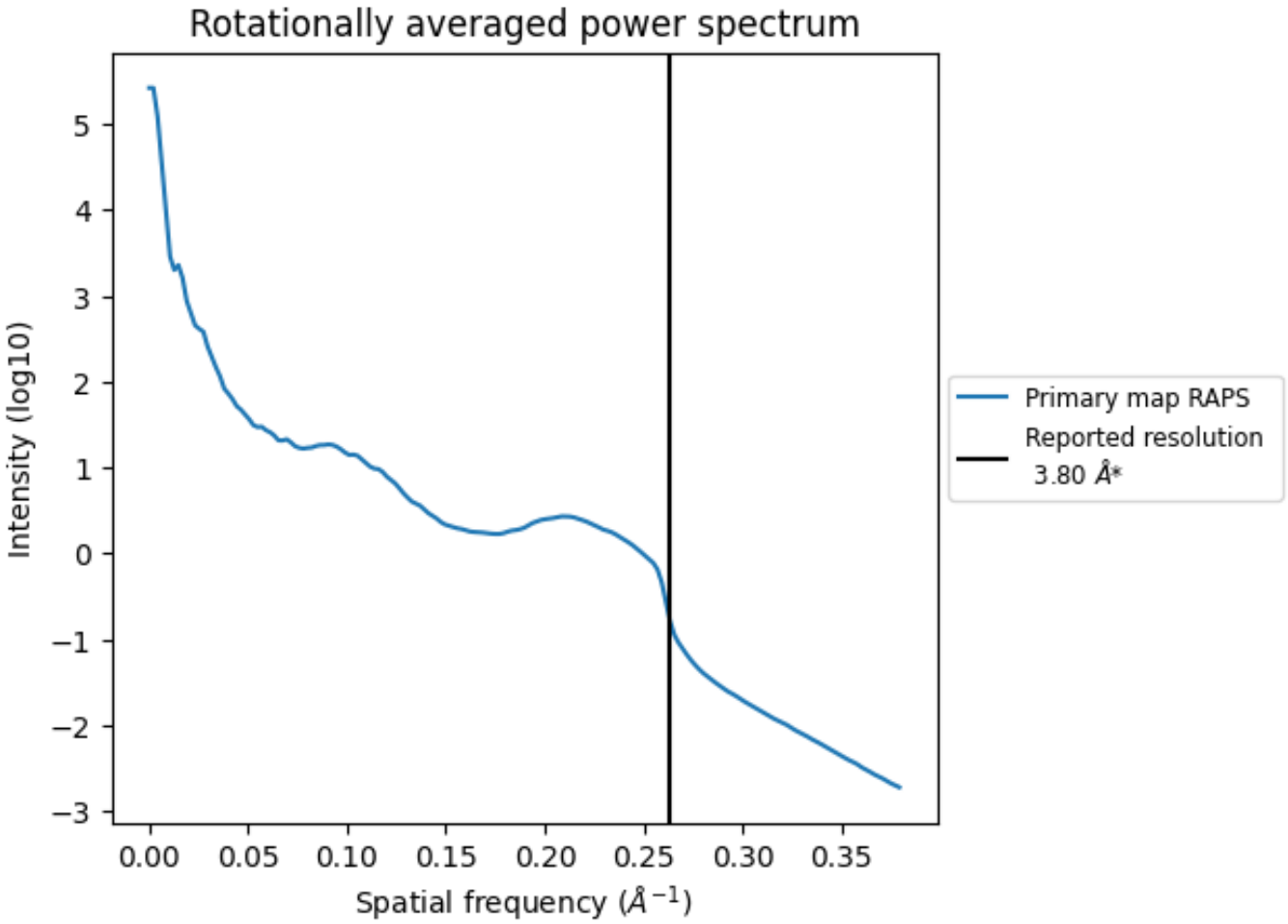
7.2 Volume estimate (i)



The volume at the recommended contour level is 639 nm^3; this corresponds to an approximate mass of 578 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 0.263 Å^{-1}

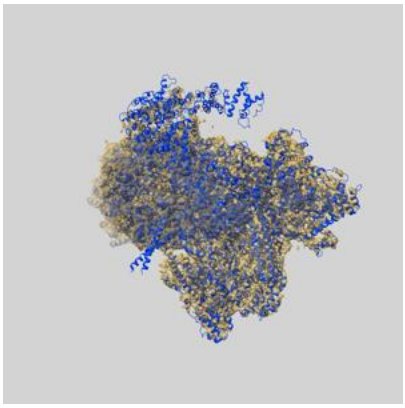
8 Fourier-Shell correlation (i)

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

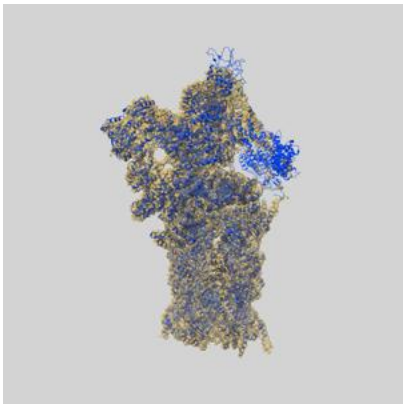
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9772 and PDB model 6J2X. Per-residue inclusion information can be found in section 3 on page 11.

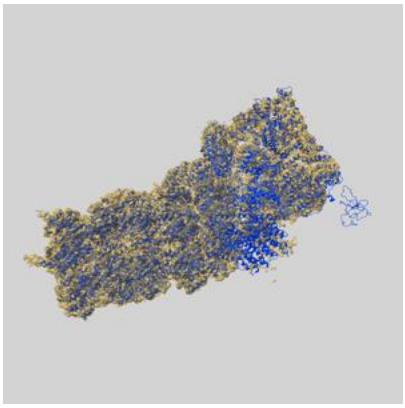
9.1 Map-model overlay



X



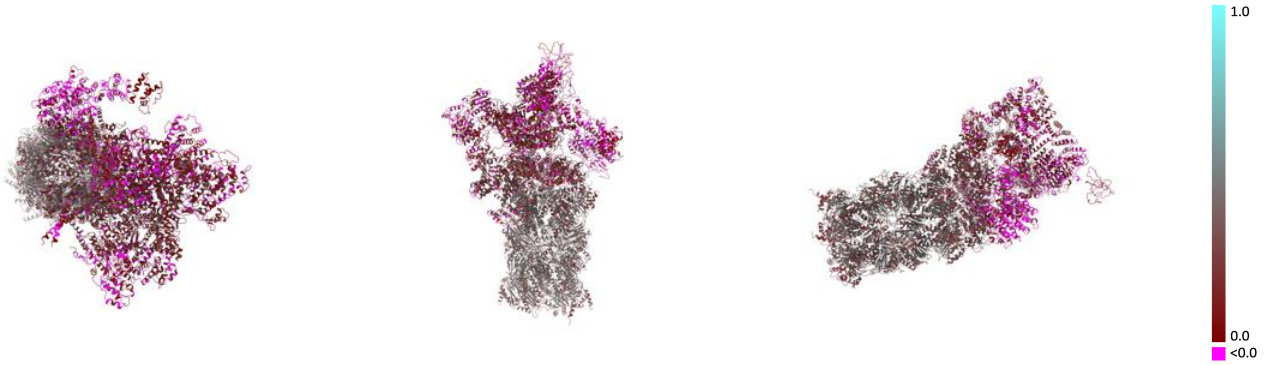
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.704 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.

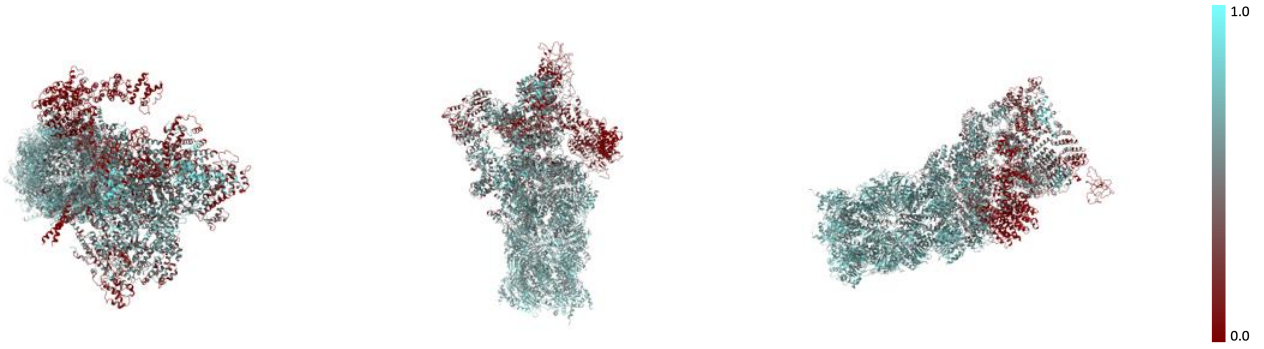
9.2 Q-score mapped to coordinate model



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.

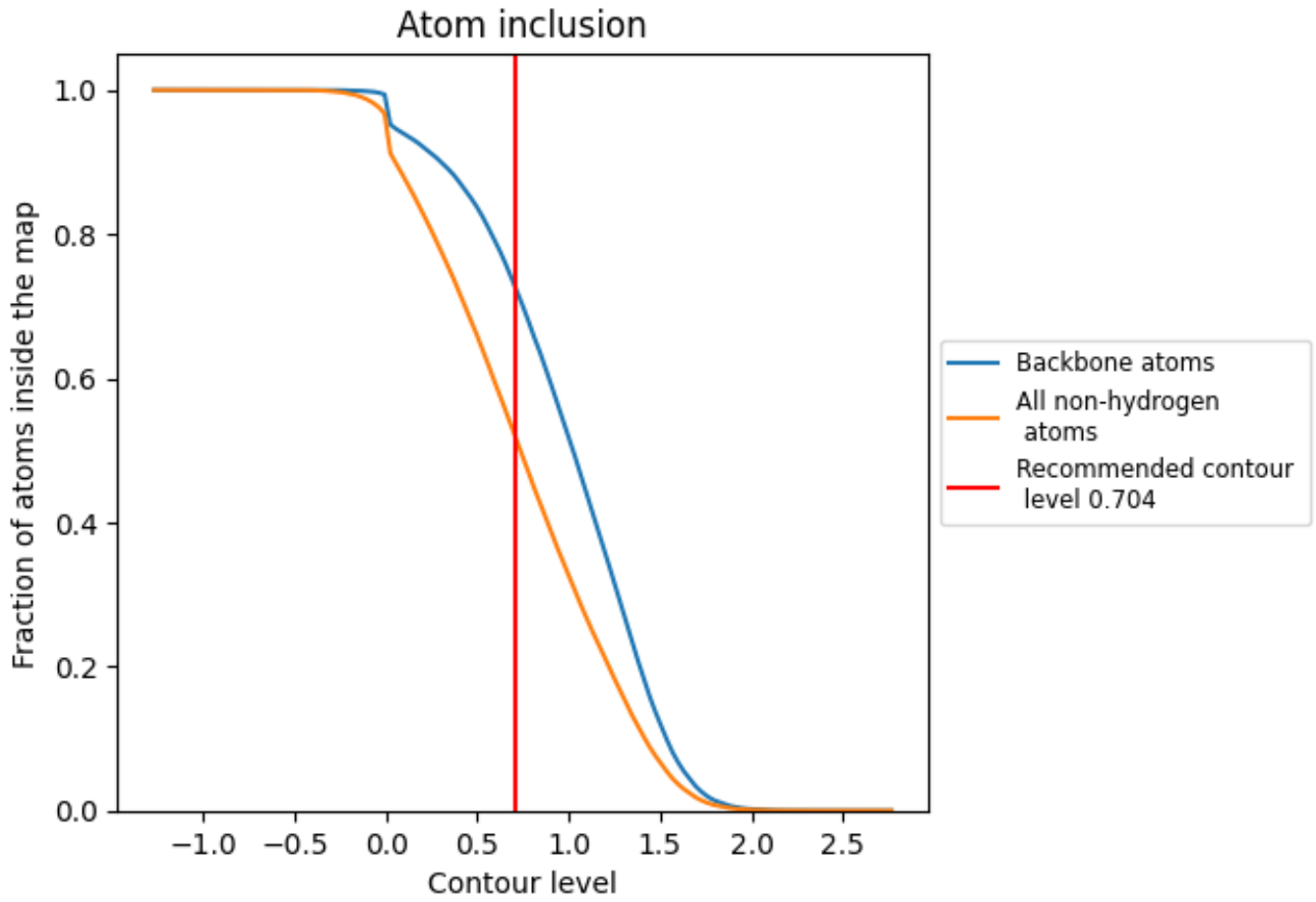
9.3 Atom inclusion mapped to coordinate model



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 (0.704).

9.4 Atom inclusion (i)



At the recommended contour level, 73% of all backbone atoms, 52% 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 (0.704) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5214	0.2420
1	0.6253	0.3670
2	0.6594	0.3730
3	0.6452	0.3700
4	0.6115	0.3420
5	0.6613	0.3550
6	0.6365	0.3430
7	0.6435	0.3790
A	0.6175	0.3540
B	0.6095	0.3600
C	0.6237	0.3390
D	0.6423	0.3390
E	0.6268	0.3330
F	0.6271	0.3530
G	0.6292	0.3590
H	0.5433	0.2570
I	0.5287	0.2360
J	0.5019	0.1970
K	0.5237	0.2320
L	0.5209	0.2460
M	0.5187	0.2360
N	0.4398	0.1000
O	0.3485	0.1030
P	0.5192	0.1610
Q	0.5561	0.2120
R	0.5127	0.1640
S	0.3778	0.1010
T	0.2564	0.0860
U	0.5285	0.1690
V	0.5043	0.1680
W	0.3062	0.0750
X	0.0011	-0.0020
Y	0.4522	0.0930
Z	0.0293	-0.0050
a	0.6564	0.3740

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Chain	Atom inclusion	Q-score
b	0.6234	0.3560
c	0.6631	0.3260
d	0.6769	0.3360
e	0.6510	0.3580
f	0.6644	0.3700
g	0.6173	0.3470
h	0.6510	0.3720
i	0.6600	0.3770
j	0.6658	0.3450
k	0.6570	0.3410
l	0.6634	0.3390
m	0.6416	0.3340
n	0.6791	0.3320