



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 12:01 pm GMT

PDB ID : 3JCP
Title : Structure of yeast 26S proteasome in M2 state derived from Titan dataset
Authors : Luan, B.; Huang, X.L.; Wu, J.P.; Shi, Y.G.; Wang, F.
Deposited on : 2016-01-06
Resolution : 4.60 Å (reported)
Based on PDB ID : 4CR2

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29047

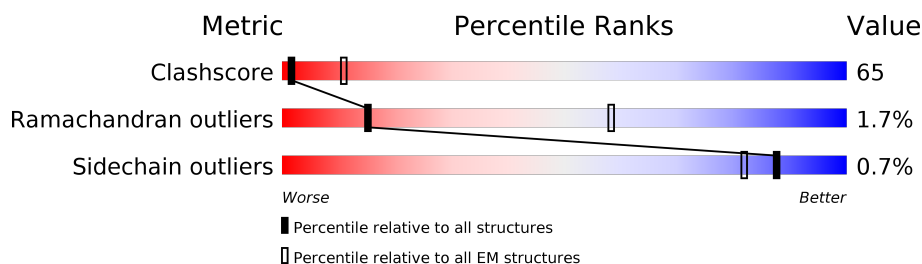
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.60 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.



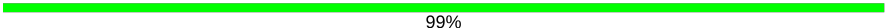


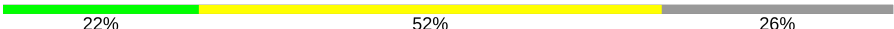

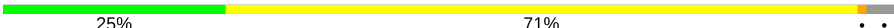
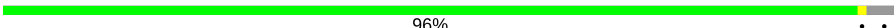

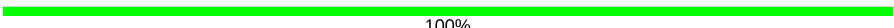
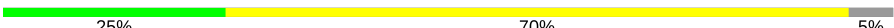

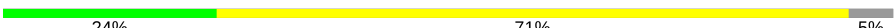
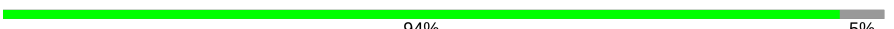




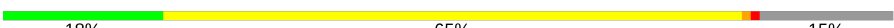

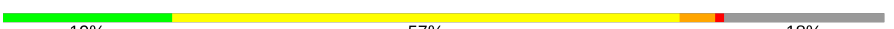
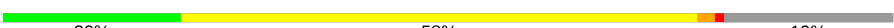

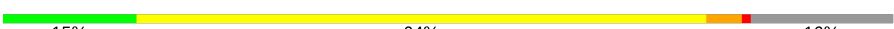


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	1	241	27% 66% 8%
1	8	241	27% 66% 8%
2	2	266	24% 63% 12%
2	9	266	26% 62% 12%
3	3	215	30% 65% 5%
3	h	215	94% • 5%
4	4	261	23% 62% 15%
4	i	261	85% 15%
5	5	205	26% 73%

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Mol	Chain	Length	Quality of chain
5	j	205	 99%
6	6	198	 22% 77%
6	k	198	 99%
7	7	287	 22% 52% 26%
7	l	287	 74% 26%
8	A	252	 25% 71%
8	a	252	 96%
9	B	250	 27% 73%
9	b	250	 100%
10	C	258	 25% 70% 5%
10	c	258	 95% 5%
11	D	254	 24% 71% 5%
11	d	254	 94% 5%
12	E	260	 28% 65% 7%
12	e	260	 93% 7%
13	F	234	 23% 77%
13	f	234	 100%
14	G	288	 18% 65% 15%
14	g	288	 84% 15%
15	H	467	 19% 57% 18%
16	I	437	 20% 58% 19%
17	J	405	 16% 74% 8%
18	K	428	 15% 64% 16%
19	L	437	 15% 63% 18%
20	M	434	 17% 64% 18%

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Mol	Chain	Length	Quality of chain
21	N	945	<div><div></div><div>17%71%10%</div></div>
22	O	393	<div><div></div><div>16%70%8%.</div></div>
23	P	445	<div><div></div><div>13%78%5%.</div></div>
24	Q	434	<div><div></div><div>18%73%7%..</div></div>
25	R	429	<div><div></div><div>9%76%8%7%</div></div>
26	S	523	<div><div></div><div>15%65%..16%</div></div>
27	T	274	<div><div></div><div>16%78%..</div></div>
28	U	338	<div><div></div><div>12%60%..25%</div></div>
29	V	306	<div><div></div><div>14%62%.20%</div></div>
30	W	268	<div><div></div><div>14%55%.26%</div></div>
31	X	156	<div><div></div><div>21%56%..19%</div></div>
32	Y	89	<div><div></div><div>10%26%.62%</div></div>
33	Z	993	<div><div></div><div>14%56%5%25%</div></div>

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 104170 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-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	222	Total	C	N	O	S	0	0
			1757	1115	303	335	4		
1	8	222	Total	C	N	O	S	0	0
			1757	1115	303	335	4		

- Molecule 2 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	233	Total	C	N	O	S	0	0
			1824	1154	312	351	7		
2	9	233	Total	C	N	O	S	0	0
			1824	1154	312	351	7		

- Molecule 3 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	205	Total	C	N	O	S	0	0
			1573	995	260	311	7		
3	h	205	Total	C	N	O	S	0	0
			1574	995	261	311	7		

- Molecule 4 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	222	Total	C	N	O	S	0	0
			1684	1061	293	323	7		
4	i	222	Total	C	N	O	S	0	0
			1684	1061	293	323	7		

- Molecule 5 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	204	Total	C	N	O	S	0	0
			1581	1010	258	305	8		
5	j	204	Total	C	N	O	S	0	0
			1578	1009	257	304	8		

- Molecule 6 is a protein called Proteasome subunit beta type-4.

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

- Molecule 7 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	212	Total	C	N	O	S	0	0
			1644	1045	280	312	7		
7	l	212	Total	C	N	O	S	0	0
			1644	1045	280	312	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	a	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	b	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	c	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	d	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	e	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	f	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	244	Total	C	N	O	S	0	0
			1896	1205	330	357	4		
14	g	244	Total	C	N	O	S	0	0
			1896	1205	330	357	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	381	Total	C	N	O	S	0	0
			2877	1806	519	537	15		

- Molecule 16 is a protein called 26S protease regulatory subunit 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	354	Total	C	N	O	S	0	0
			2652	1655	453	531	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	373	Total	C	N	O	S	0	0
			2914	1824	526	547	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	361	Total	C	N	O	S	0	0
			2835	1777	506	542	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	358	Total	C	N	O	S	0	0
			2829	1782	501	534	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	M	357	Total	C	N	O	S	0	0
			2754	1723	473	548	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	N	850	Total	C	N	O	S	0	0
			6570	4178	1100	1264	28		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	O	376	Total	C	N	O	S	0	0
			2912	1867	481	557	7		

- Molecule 23 is a protein called 26S proteasome regulatory subunit RPN5.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	P	431	Total	C	N	O	S	0	0
			3470	2210	585	667	8		

- 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
			3469	2203	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
			3187	2028	525	624	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	S	439	Total	C	N	O	S	0	0
			3384	2155	575	637	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	T	267	Total	C	N	O	S	0	0
			2201	1410	350	435	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	U	254	Total	C	N	O	S	0	0
			2049	1304	350	389	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	V	245	Total	C	N	O	S	0	0
			1912	1206	322	371	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	127	Total	C	N	O	S	0	0
			1032	664	169	195	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
32	Y	34	Total	C	N	O	0	0
			243	146	45	52		

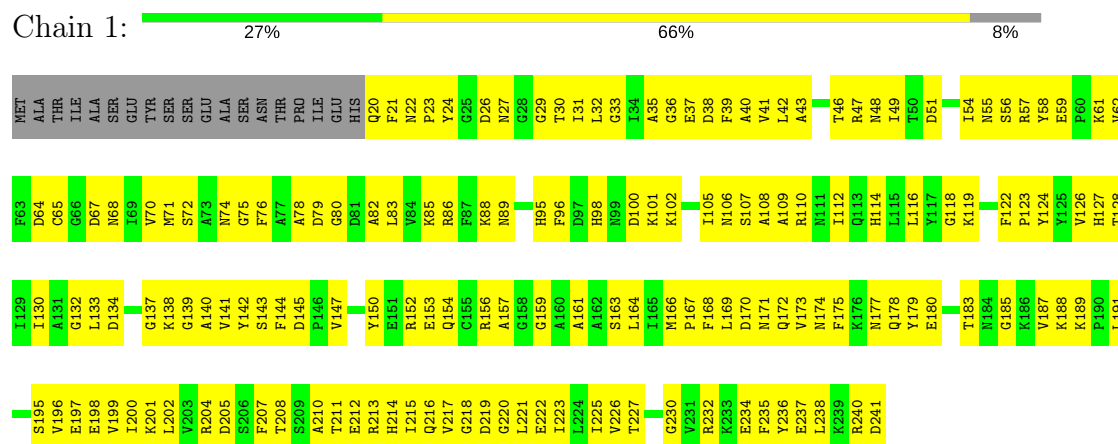
- Molecule 33 is a protein called 26S proteasome regulatory subunit RPN1.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Z	746	Total	C	N	O	S	0	0
			5688	3616	940	1106	26		

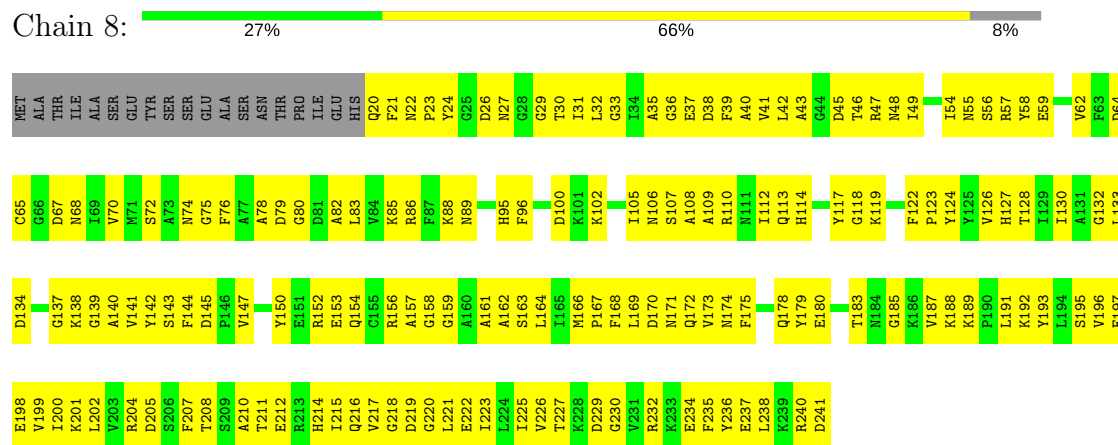
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

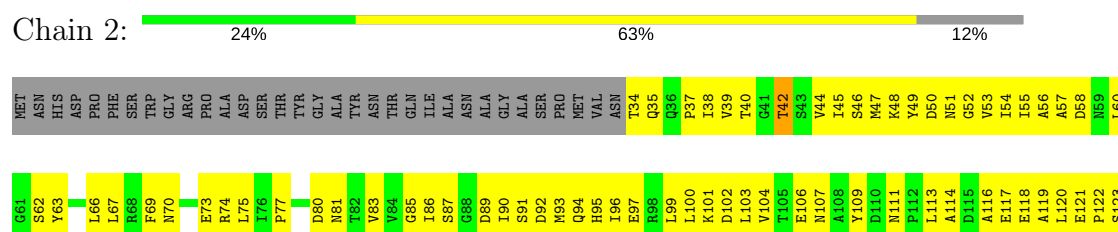
• Molecule 1: Proteasome subunit beta type-6

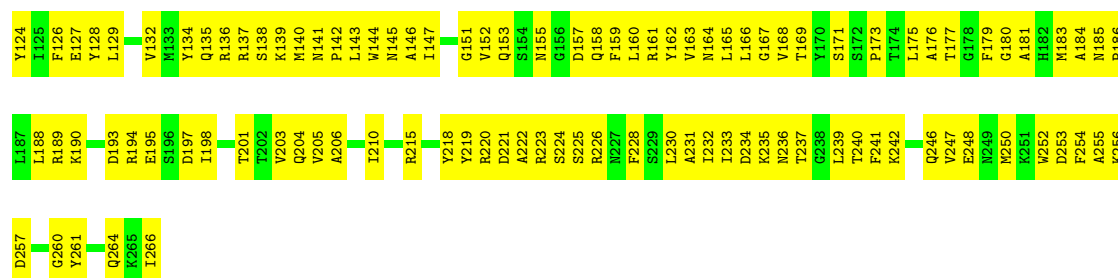


• Molecule 1: Proteasome subunit beta type-6

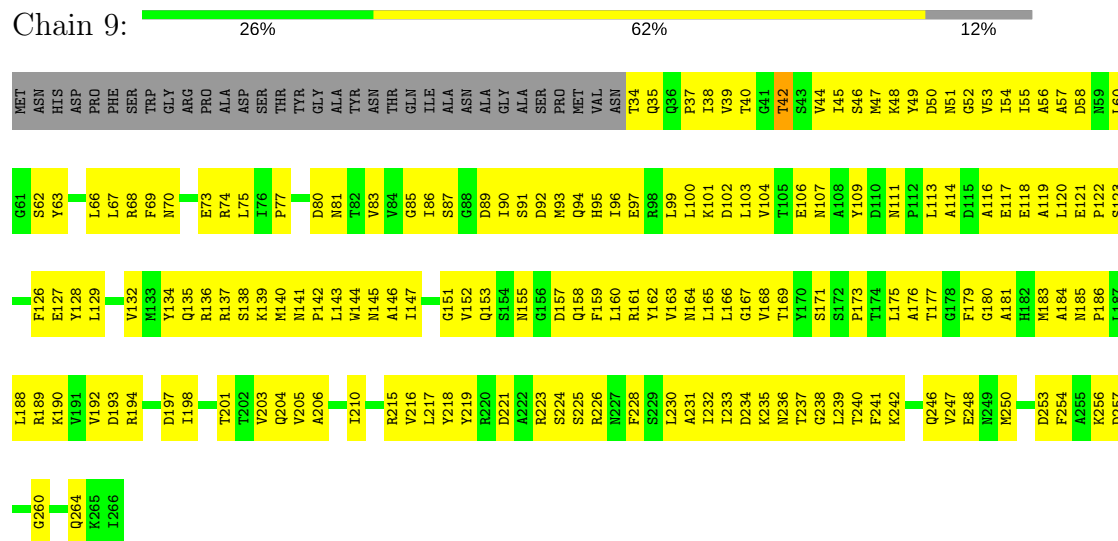


• Molecule 2: Proteasome subunit beta type-7

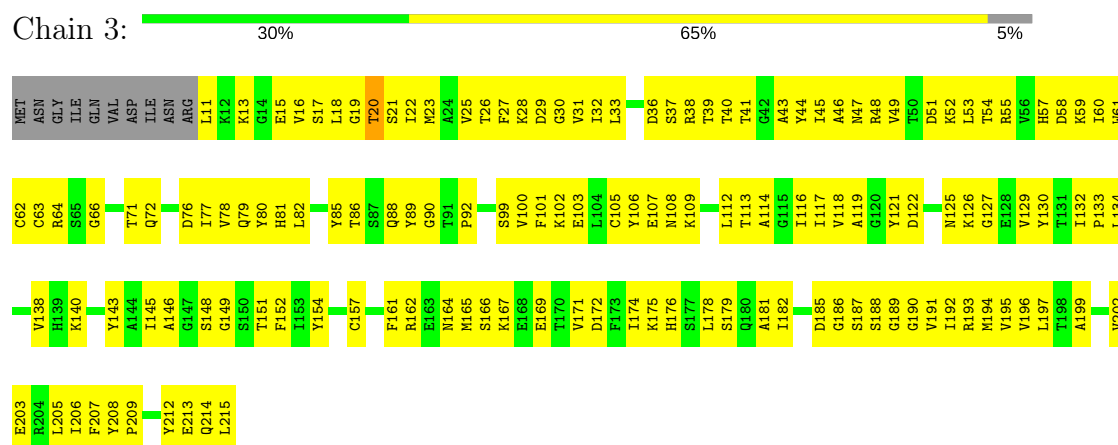




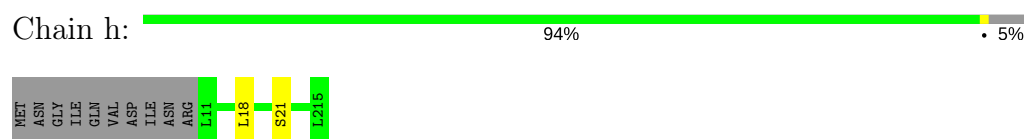
- Molecule 2: Proteasome subunit beta type-7



- Molecule 3: Proteasome subunit beta type-1

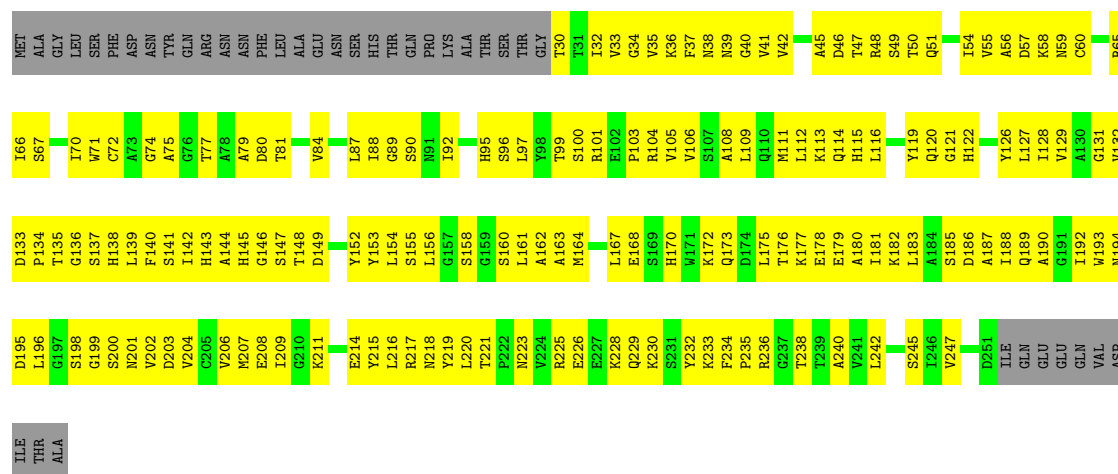


- Molecule 3: Proteasome subunit beta type-1




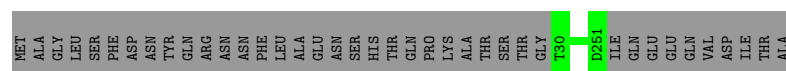
- Molecule 4: Proteasome subunit beta type-2

Chain 4:  23% 62% 15%



- Molecule 4: Proteasome subunit beta type-2

Chain i:  85% 15%



- Molecule 5: Proteasome subunit beta type-3

Chain 5:  26% 73%



- Molecule 5: Proteasome subunit beta type-3

Chain j:  99%



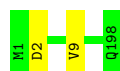
- Molecule 6: Proteasome subunit beta type-4

Chain 6:  22% 77%



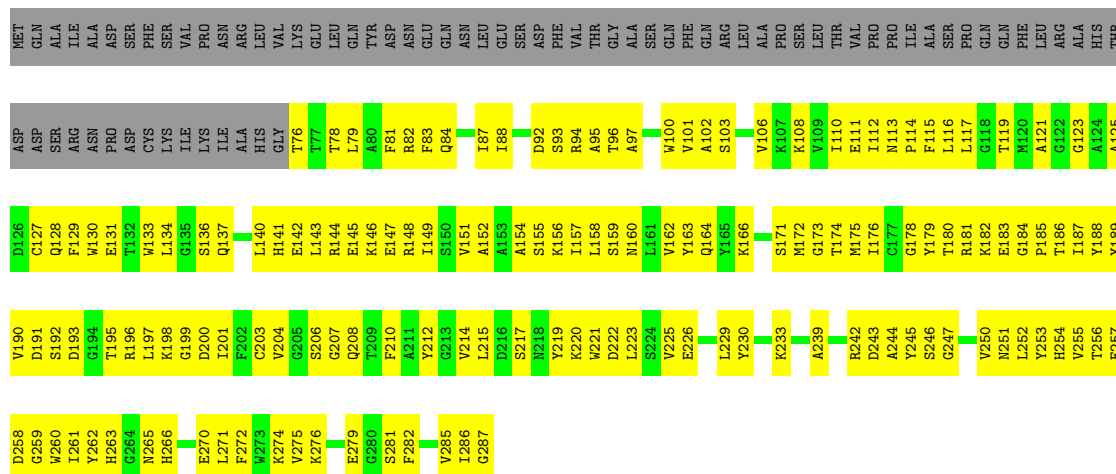
• Molecule 6: Proteasome subunit beta type-4

Chain k: 99%



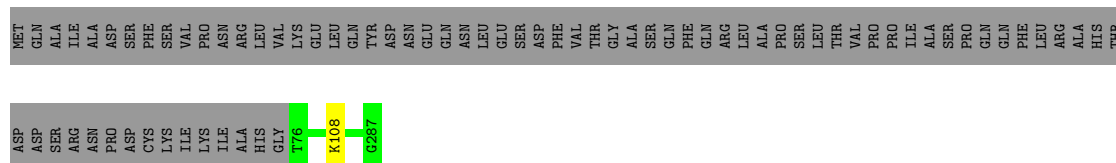
• Molecule 7: Proteasome subunit beta type-5

Chain 7: 22% 52% 26%



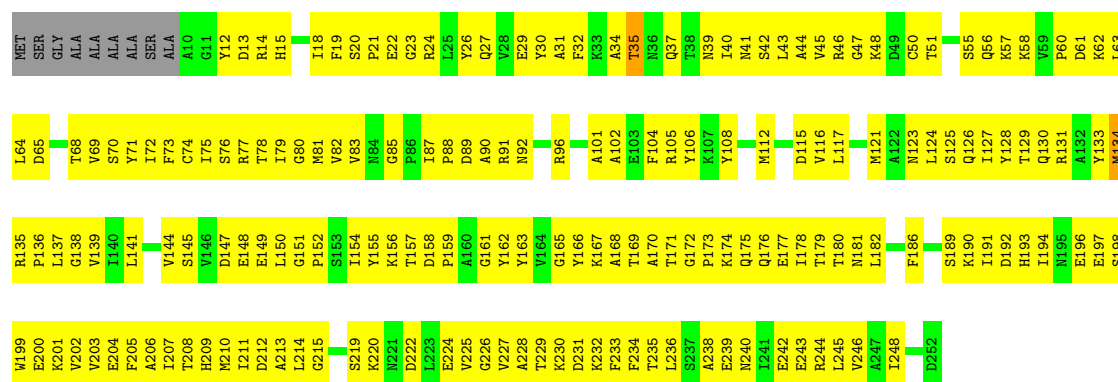
• Molecule 7: Proteasome subunit beta type-5

Chain l: 74% 26%



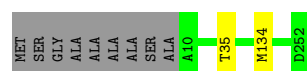
• Molecule 8: Proteasome subunit alpha type-1

Chain A: 25% 71%



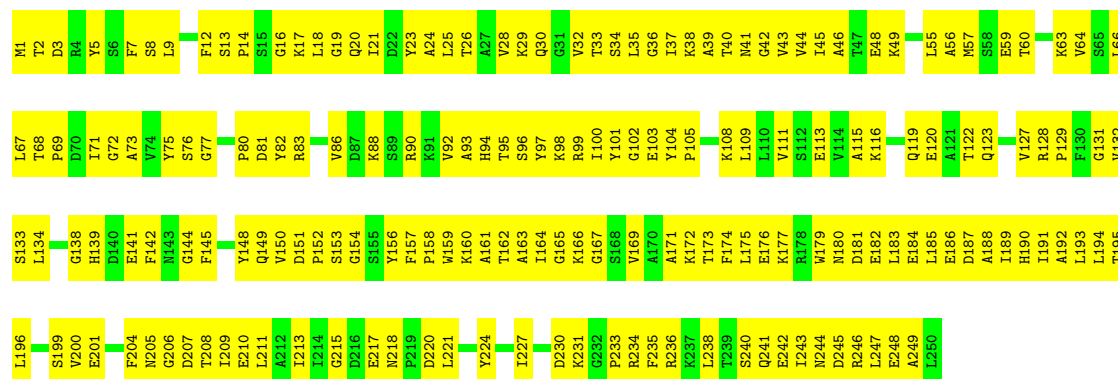
• Molecule 8: Proteasome subunit alpha type-1

Chain a: 96%



• Molecule 9: Proteasome subunit alpha type-2

Chain B: 27% 73%



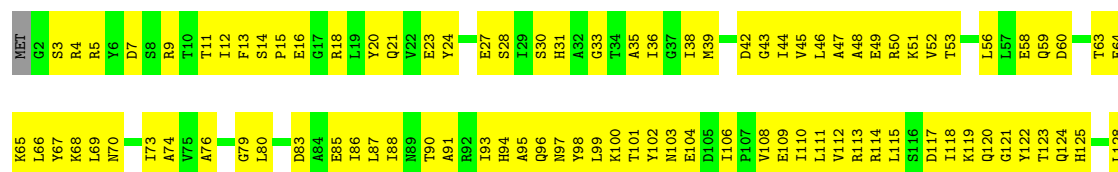
• Molecule 9: Proteasome subunit alpha type-2

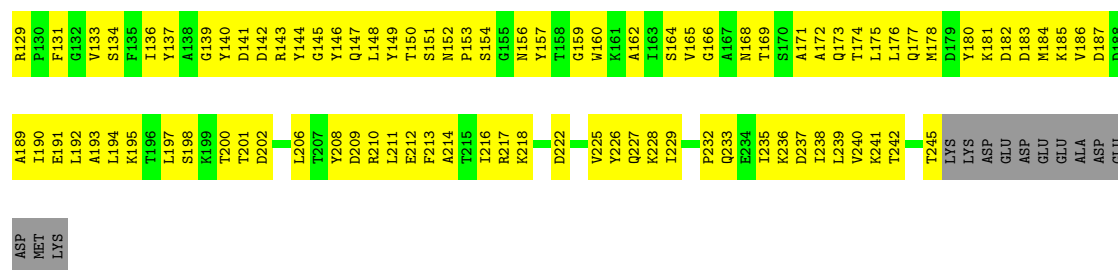
Chain b: 100%

There are no outlier residues recorded for this chain.

• Molecule 10: Proteasome subunit alpha type-3

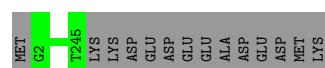
Chain C: 25% 70% 5%





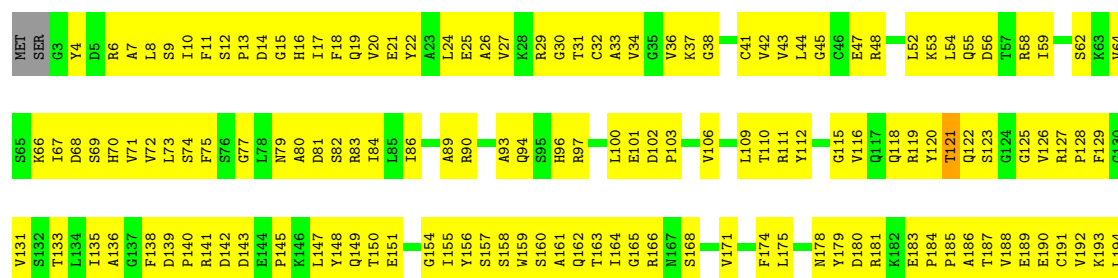
• Molecule 10: Proteasome subunit alpha type-3

Chain c: 95% 5%



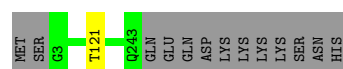
• Molecule 11: Proteasome subunit alpha type-4

Chain D: 24% 71% 5%



• Molecule 11: Proteasome subunit alpha type-4

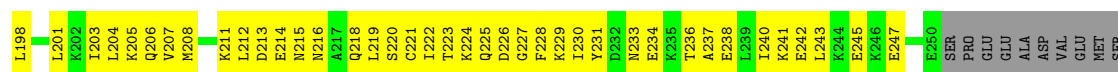
Chain d: 94% 5%



• Molecule 12: Proteasome subunit alpha type-5

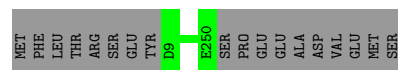
Chain E: 28% 65% 7%





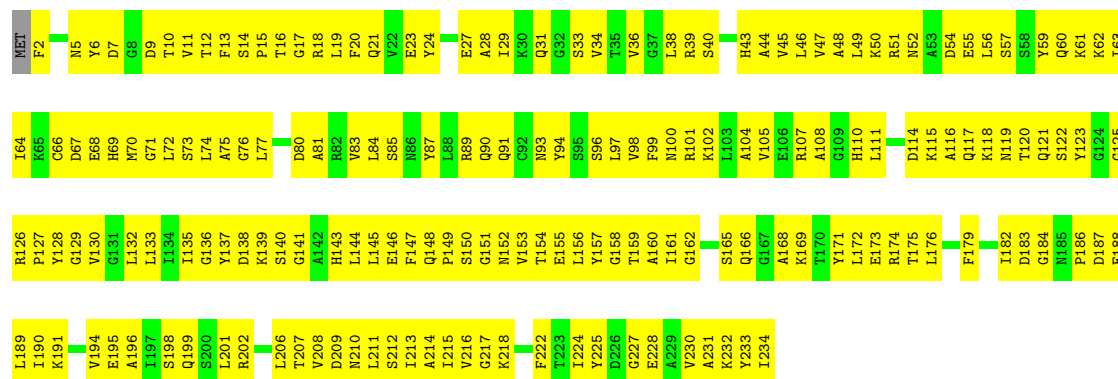
• Molecule 12: Proteasome subunit alpha type-5

Chain e: 93% 7%



• Molecule 13: Proteasome subunit alpha type-6

Chain F: 23% 77%



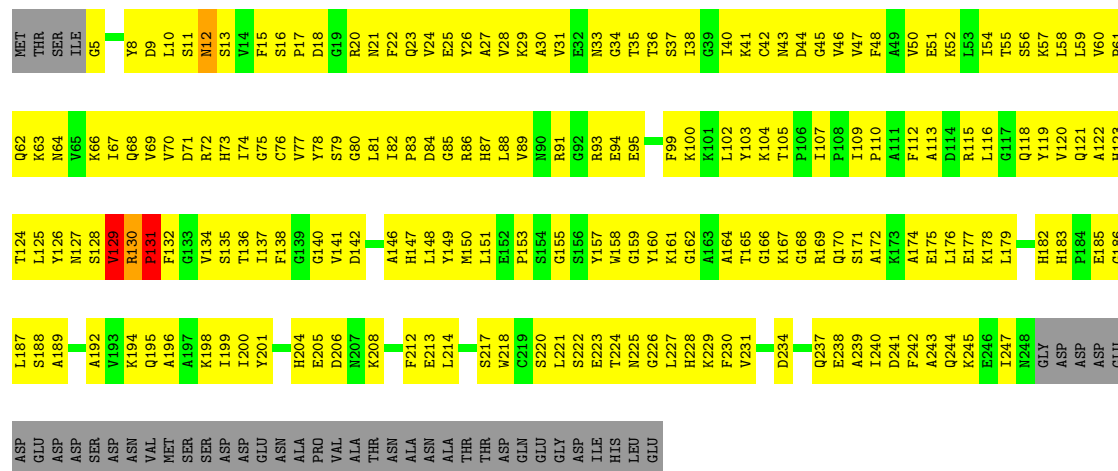
• Molecule 13: Proteasome subunit alpha type-6

Chain f: 100%

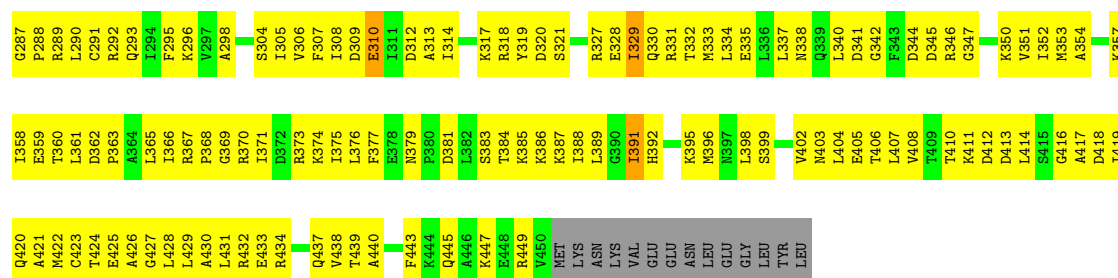


• Molecule 14: Probable proteasome subunit alpha type-7

Chain G: 18% 65% 15%

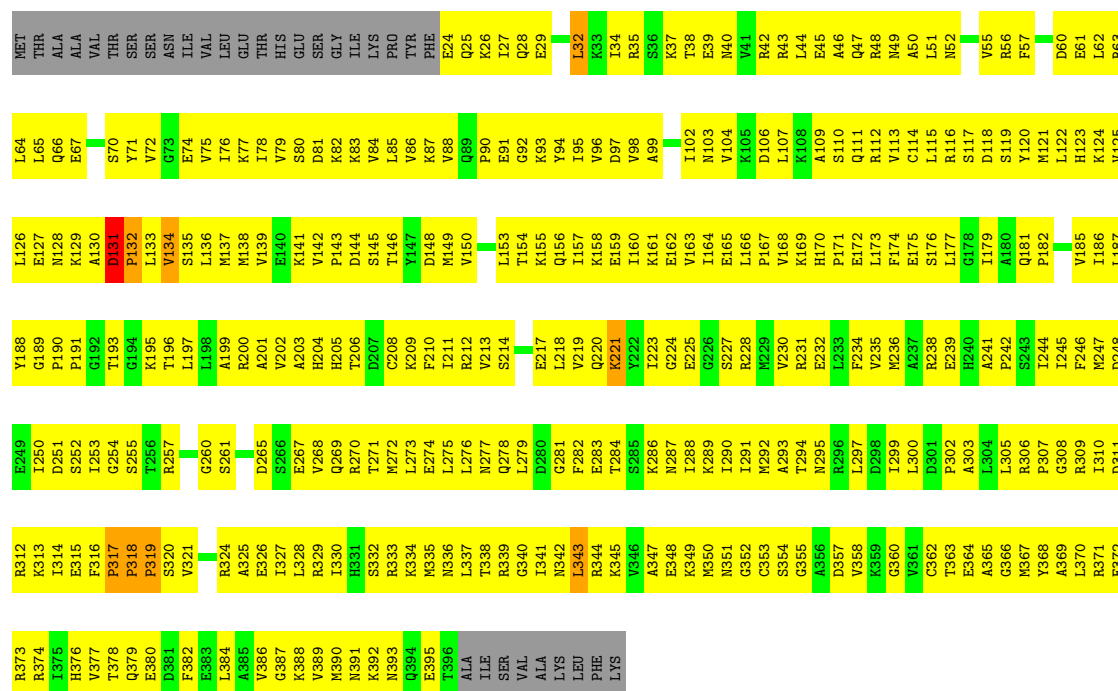


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|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| S224 | V225 | E226 | M228 | P228 | L229 | T230 | H231 | P232 | E236 | E237 | M238 | G239 | I1E | L1V5 | P242 | P243 | K244 | G245 | V246 | L247 | L248 | V249 | G250 | A251 | P252 | G253 | T254 | G255 | K256 | T257 | L258 | K261 | L262 | V263 | N265 | G266 | T267 | S268 | A269 | T270 | F271 | L272 | R273 | L274 | V275 | G276 | S277 | L278 | L279 | L280 | K281 | K282 | V283 | L284 | G285 | G286 | G287 | G288 | G289 | G290 | G291 | G292 | G293 | G294 | G295 | G296 | G297 | G298 | G299 | G300 | G301 | G302 | G303 | G304 | G305 | G306 | G307 | G308 | G309 | G310 | G311 | G312 | G313 | G314 | G315 | G316 | G317 | G318 | G319 | G320 | G321 | G322 | G323 | G324 | G325 | G326 | G327 | G328 | G329 | G330 | G331 | G332 | G333 | G334 | G335 | G336 | G337 | G338 | G339 | G340 | G341 | G342 | G343 | G344 | G345 | G346 | G347 | G348 | G349 | G350 | G351 | G352 | G353 | G354 | G355 | G356 | G357 | G358 | G359 | G360 | G361 | G362 | G363 | G364 | G365 | G366 | G367 | G368 | G369 | G370 | G371 | G372 | G373 | G374 | G375 | G376 | G377 | G378 | G379 | G380 | G381 | G382 | G383 | G384 | G385 | G386 | G387 | G388 | G389 | G390 | G391 | G392 | G393 | G394 | G395 | G396 | G397 | G398 | G399 | G400 | G401 | G402 | G403 | G404 | G405 | G406 | G407 | G408 | G409 | G410 | G411 | G412 | G413 | G414 | G415 | G416 | G417 | G418 | G419 | G420 | G421 | G422 | G423 | G424 | G425 | G426 | G427 | G428 | G429 | G430 | G431 | G432 | G433 | G434 | G435 | G436 | G437 | G438 | G439 | G440 | G441 | G442 | G443 | G444 | G445 | G446 | G447 | G448 | G449 | G450 | G451 | G452 | G453 | G454 | G455 | G456 | G457 | G458 | G459 | G460 | G461 | G462 | G463 | G464 | G465 | G466 | G467 | G468 | G469 | G470 | G471 | G472 | G473 | G474 | G475 | G476 | G477 | G478 | G479 | G480 | G481 | G482 | G483 | G484 | G485 | G486 | G487 | G488 | G489 | G490 | G491 | G492 | G493 | G494 | G495 | G496 | G497 | G498 | G499 | G500 | G501 | G502 | G503 | G504 | G505 | G506 | G507 | G508 | G509 | G510 | G511 | G512 | G513 | G514 | G515 | G516 | G517 | G518 | G519 | G520 | G521 | G522 | G523 | G524 | G525 | G526 | G527 | G528 | G529 | G530 | G531 | G532 | G533 | G534 | G535 | G536 | G537 | G538 | G539 | G540 | G541 | G542 | G543 | G544 | G545 | G546 | G547 | G548 | G549 | G550 | G551 | G552 | G553 | G554 | G555 | G556 | G557 | G558 | G559 | G560 | G561 | G562 | G563 | G564 | G565 | G566 | G567 | G568 | G569 | G570 | G571 | G572 | G573 | G574 | G575 | G576 | G577 | G578 | G579 | G580 | G581 | G582 | G583 | G584 | G585 | G586 | G587 | G588 | G589 | G590 | G591 | G592 | G593 | G594 | G595 | G596 | G597 | G598 | G599 | G600 | G601 | G602 | G603 | G604 | G605 | G606 | G607 | G608 | G609 | G610 | G611 | G612 | G613 | G614 | G615 | G616 | G617 | G618 | G619 | G620 | G621 | G622 | G623 | G624 | G625 | G626 | G627 | G628 | G629 | G630 | G631 | G632 | G633 | G634 | G635 | G636 | G637 | G638 | G639 | G640 | G641 | G642 | G643 | G644 | G645 | G646 | G647 | G648 | G649 | G650 | G651 | G652 | G653 | G654 | G655 | G656 | G657 | G658 | G659 | G660 | G661 | G662 | G663 | G664 | G665 | G666 | G667 | G668 | G669 | G670 | G671 | G672 | G673 | G674 | G675 | G676 | G677 | G678 | G679 | G680 | G681 | G682 | G683 | G684 | G685 | G686 | G687 | G688 | G689 | G690 | G691 | G692 | G693 | G694 | G695 | G696 | G697 | G698 | G699 | G700 | G701 | G702 | G703 | G704 | G705 | G706 | G707 | G708 | G709 | G710 | G711 | G712 | G713 | G714 | G715 | G716 | G717 | G718 | G719 | G720 | G721 | G722 | G723 | G724 | G725 | G726 | G727 | G728 | G729 | G730 | G731 | G732 | G733 | G734 | G735 | G736 | G737 | G738 | G739 | G740 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|



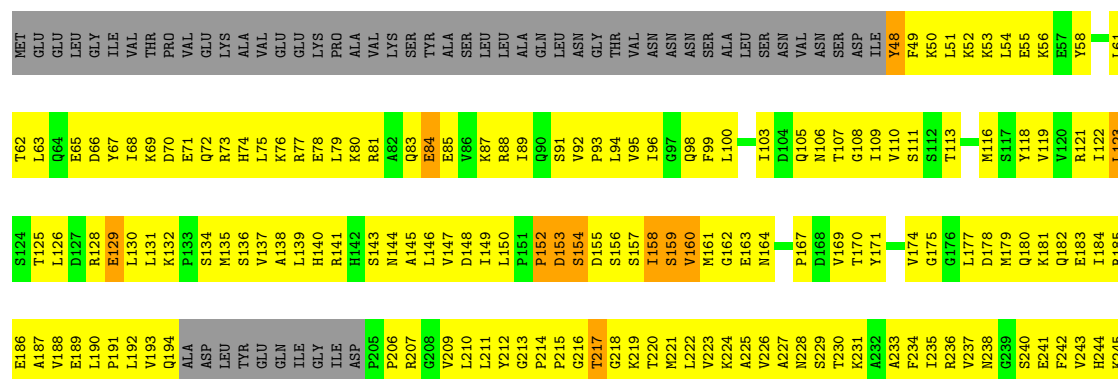
- Molecule 17: 26S protease regulatory subunit 8 homolog

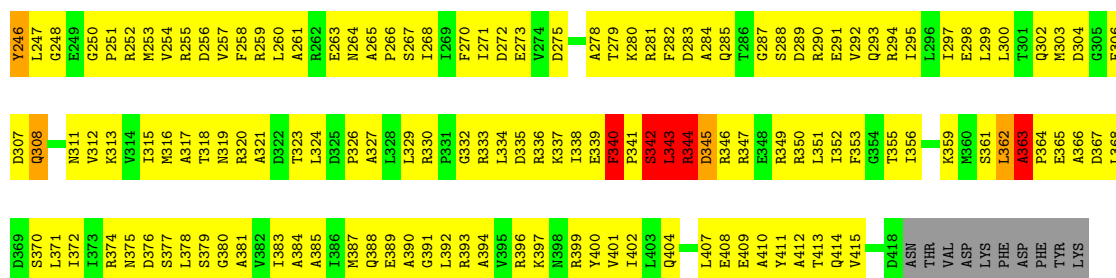
Chain J:  16% 74% 8%



- Molecule 18: 26S protease regulatory subunit 6B homolog

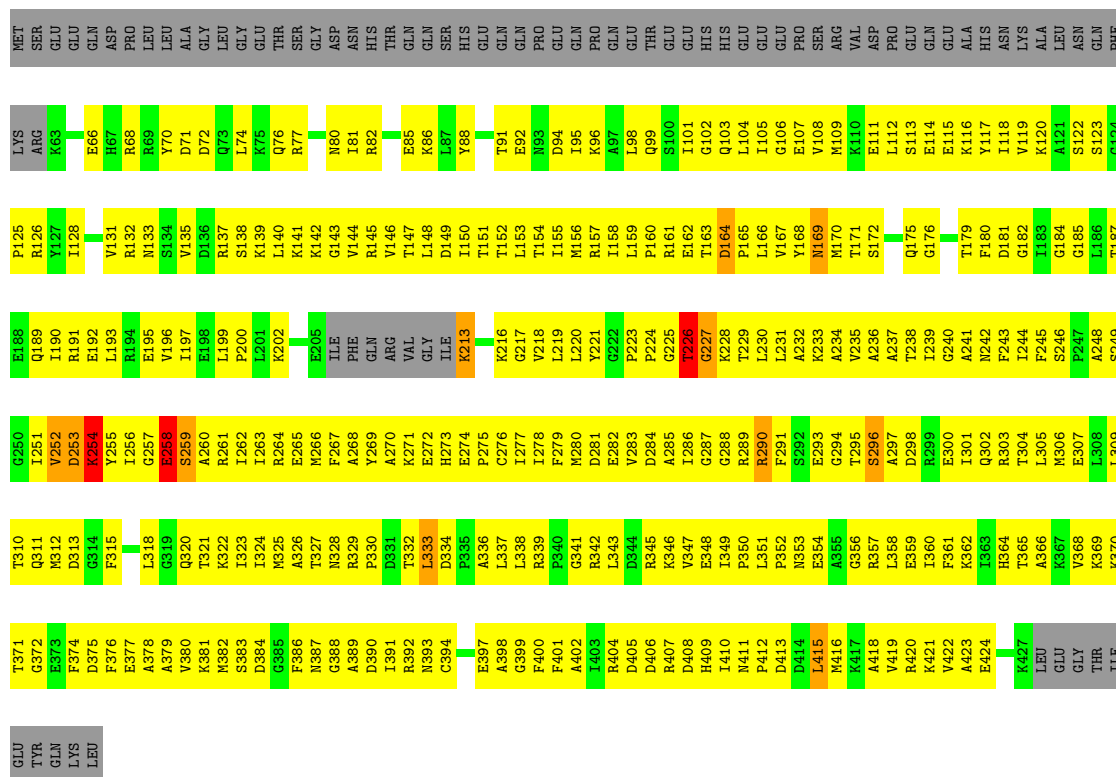
Chain K:  15% 64% . . 16%





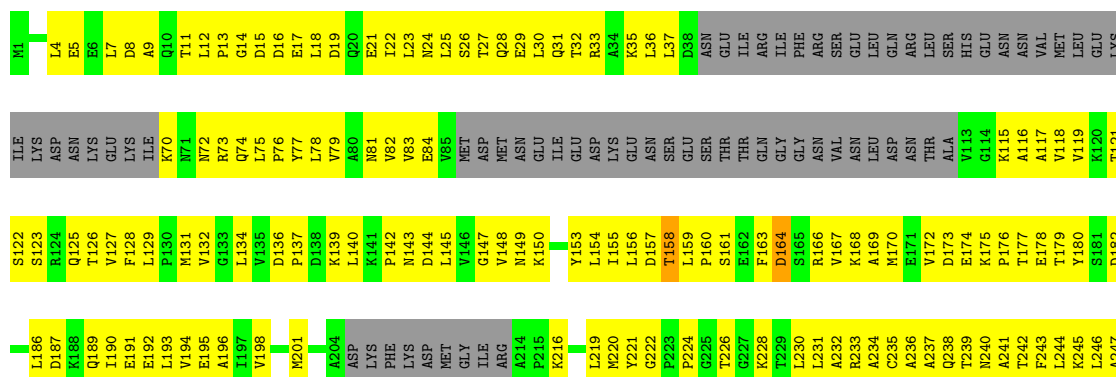
• Molecule 19: 26S protease subunit RPT4

Chain L: 15% 63% 18%



• Molecule 20: 26S protease regulatory subunit 6A

Chain M: 17% 64% 18%

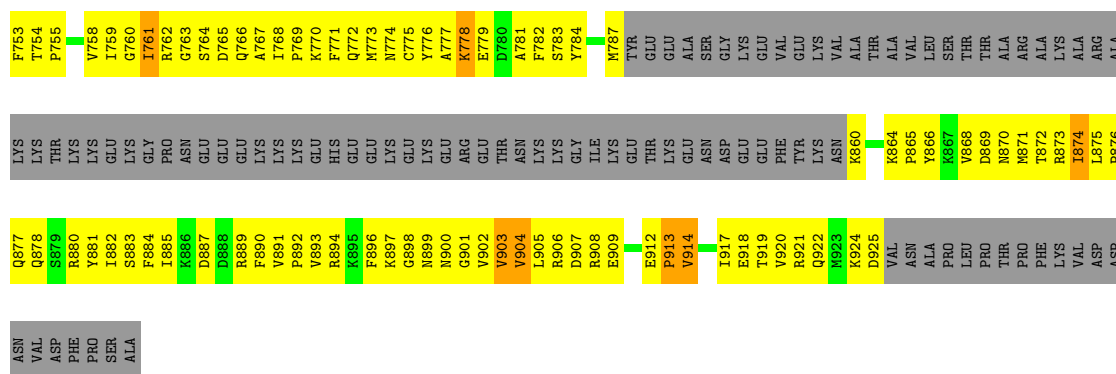


A248	L308	T370	SER
P249	L309	D371	PHE
Q250	N310	D372	TYR
L251	Q311	D373	ALA
V252	L312	L374	
Q253	D313	N375	
W254	G314	N376	
L255	F315	Q377	
L256	S316	E378	
G257	S317	L379	
E258	D318	A380	
G259	D319	L381	
A260	R320	L382	
K261	V321	T383	
L262	K322	D384	
V263	V323	E385	
R264	L324	F386	
D265	A325	N387	
A266	A326	G388	
F267	T327	A389	
A268	R328	Q390	
L269	R329	L391	
A270	V330	K392	
K271	D331	A393	
E272	V332	V394	
K273	L333	T395	
A274	D334	V396	
P275	P335	E397	
T276	A336	A398	
L277	L337	G399	
L278	L338	M400	
F279	R339	I401	
L280		A402	
D281	R342	L403	
E282	L343	R404	
L283	V36	N405	
D284	R344	G406	
A285	K346	Q407	
L286	L347	S408	
G287	E348	S409	
T288	F349	V410	
K289	P350	K411	
R290	L351	H412	
F291	P352	E413	
D292	S353	D414	
S293	E354	F415	
E294	D355	V416	
K295	S356	L49	
S296	R357	A48	
Q297	A358	Y50	
D298	Q359	D51	
R299	L360	D52	
E300	L361	Q423	
Q302	Q362	D53	
R303	L363	T54	
T304	H364	F55	
S365	H363	L117	
R366	S365	L118	
E307	T369	K119	
		L185	
		E121	
		I186	
		M60	

• Molecule 21: 26S proteasome regulatory subunit RPN2

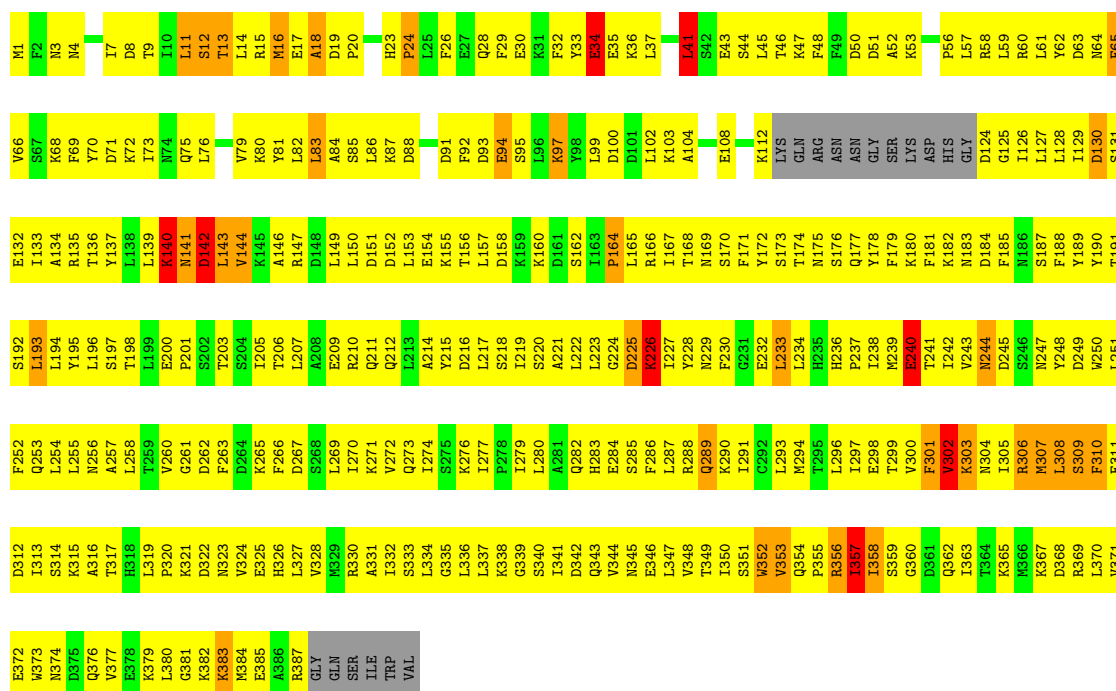
Chain N: 

MET	A61	F123	Y188	D250	L313	G377	V439	F502	T562	A622	N688
SER	A62	Y124	L189	E251	L314	N378	D440	T503	G563	F623	Q691
LEU	L63		L190	G252	N315	L379	V441	Y504	N564	A624	E692
T4	L64	P131	L191	L253	K316	L380	L442	S505	N565	L625	G693
T5	A65	L133	L192	S254	S317	E381	L443	Q506	G566	G626	L694
A6	S66	L133	A193	A255	K318	G382	H444	T508	A567	A628	G695
A7	K67	T134	L194	Q256	S319	K383	G445	Q509	V568	C629	K696
P8	V68	S135	T195	L257	S320	K384	A446	H510	K569	A630	F697
L9	L136	I336	T196	A258	L321	V385	S447	G511	R570	K632	G698
L10	V69	F137	V197	F259	G322	M386	L448	N512	L571	G633	
A11	M71	F137	T198	D260	G323	A387	G449	T513	H573	G634	V701
L12	L72	R381	N199	L261	K324	P388	L450	T514	A575	G635	A702
L13	G73	M140	S200	V262	F325	Y389	G451	R515	V576	S636	Q703
L14	E74	I141	K201	S263	S326	L390	L452	R516	S577	A637	G704
E15	Y75	E142	F202	S264	L327	P391	A453	L517	D578	L638	I705
N16		K143	R203		H329	S393	A454	A518	S579	L641	M706
V17		C144	S204		T330	R394	M455	V519	D580	D642	M707
D18	A78	L145	L207	Q267	A331	A395	M459	G520	D581		A708
N19	K80	K146	R208	L269	V332		E460	L521	E582	T645	G709
V20	Y81	A147	R209	L270	S333	R398	I461	A522	V583	K646	R710
K21	A82	S148	K209	E271	V334	F399	Y462	L523	R584		N711
T22	L83	E149	S210	L272	A335	I400	Y463	I524	N585	V649	V713
Y23	A84	L150	F211	L273	N336	K401	E464	N525	R586	D650	T714
A24	K85	K151	D212	V274	G337	G402	A465	Y526	A587	F651	I715
K25	K86	L152	F213	T275	F338	G403	L466	Q527	V588	V652	Q716
E26	D87	A153	L214	E276	H339	S404	K467	Q529	L589	R653	L717
S27	R88	L154	R215	L277	H340	L405	E468	E530	A590	A656	N718
P278	F89	G155	N216		A341	Y406	V469	L531	L591	M657	A720
N29	D90	I156	N217	Q280	G342	G407	L470	L532	A592	D658	D721
N30	I91	A157	N218	G281	G343	L408	Y471	L533	G593	L658	T722
V31	D92	L158	N219	V282	T344	G409	N472	D594	F594	A659	G723
V32	E93	E159	C220	D283	D345	L410	D473	L535	L595	L660	T724
D33	K94	Y161	Y222	P284	N346	I411	S474	I536	L596	S661	L725
Q34	S95	R162	L223	A285	G347	Y412	A475	T537	R597	M662	L726
L35	Q96	L163	L224	L286	F348	G413	S477	K538	D598	T663	T727
V36	F97	D163	T225	L287	I349	A414	G478	M539	Y599	L664	L728
S37	Y98	D164	N226	N288		F415	G478	L540	T600	Q666	S729
E38	E99	I165	N227	L289	N352	G416	E479	A541	T601	Q667	V730
L39	T100	I166	K227	L290	V355	T419	A481	S542	P602	T668	G732
I39	I101	E167	V228		L356	T420		D543	R604	E669	L733
S40	S409	S168	V229		A359	D421	G484	E544	L605	L671	S737
E42	M41	V102	N230	P294	Q360	L423	G485	S545	V606	M672	Q738
L43	E43	S103	N231	T295	N305	K424	G486	L546	Q607	P673	F739
P44	D45	K104	L43	C296	N306	N425	C488	L547	L608	Q674	W740
D45	I46	L170	L43	D297	G432	I426	N489	Y549	L609	V675	
A48	A48	K171	L43	T301	S370	I427	G491	G550	S610	A676	Y741
L49	L49	S172	N233	F302	S370	V428	G492	G551	K611	D677	W742
Y50	Y50	D177	N233	L303	S371	E429	T492	A552	S612		F743
D51	D51	A113	Q240	L304	A367	N430	G493	F553	H613	K680	T744
D52	D52	S114	L241	L304	T368	S431	K494	T554	A615	N681	L745
Q423	Q423	K115	F242	N305	A369	G432	P495	L585	G616	F682	A746
T54	T54	Q116	K243	N306	S370	T433	E496	A556	L617	L683	H747
F55	F55	Y117	K244	K307	S371	G435	I498	A558	R618	S684	F748
LYS	LYS	L118	L245	N308	L371	S434	A497	A559	C619	V685	L749
S56	S56	T118	K246	I309		G435	I498	Y559	G620	T686	S750
D57	D57	K184	E247	D310	T374	D436	A499	E560			
R58	R58	I185	E121	I311	H375	E437	M501				
E59	E59	I186			K376	D438					
M60	M60	N187	N249	G312							



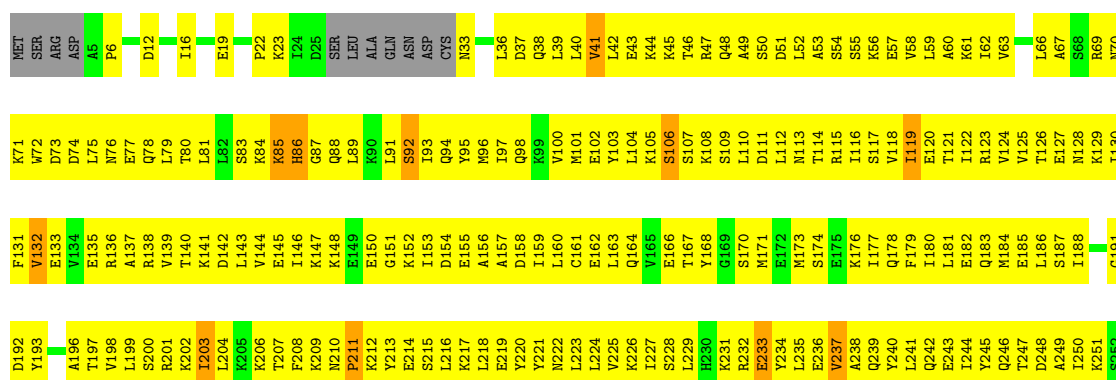
• Molecule 22: 26S proteasome regulatory subunit RPN9

Chain O: 16% 70% 8%



• Molecule 23: 26S proteasome regulatory subunit RPN5

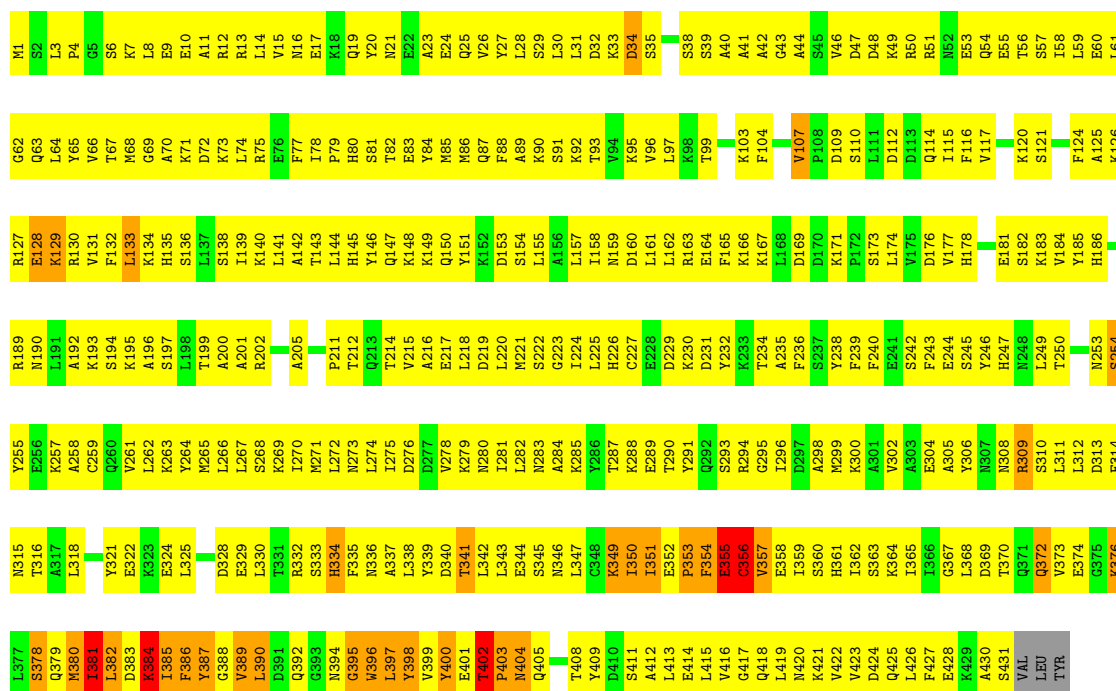
Chain P: 13% 78% 5%





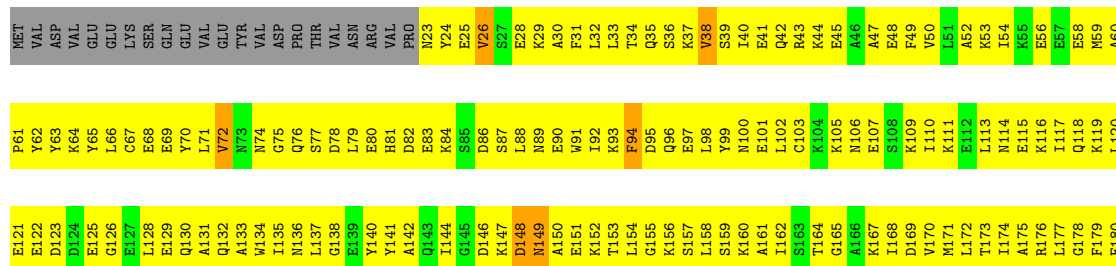
• Molecule 24: 26S proteasome regulatory subunit RPN6

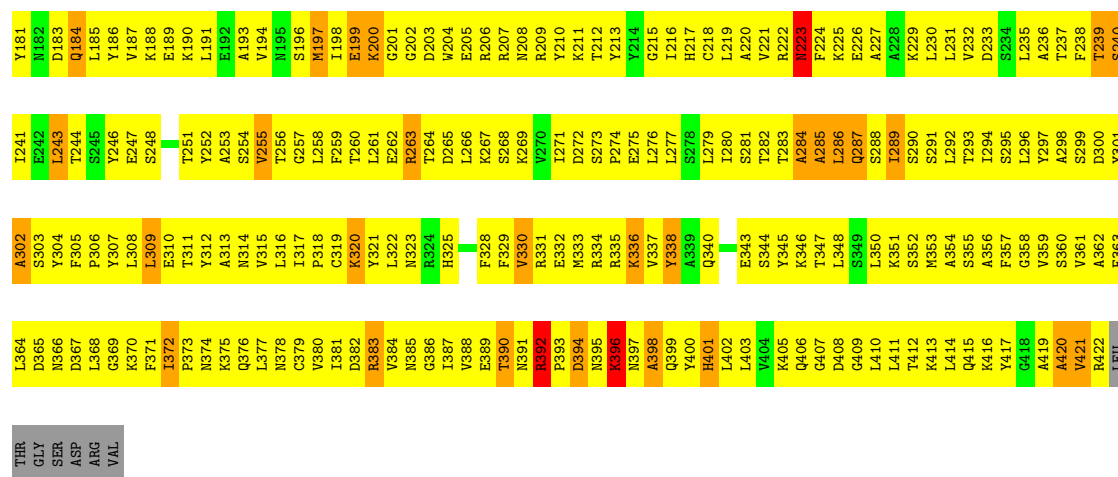
Chain Q: 18% 73% 7% ..



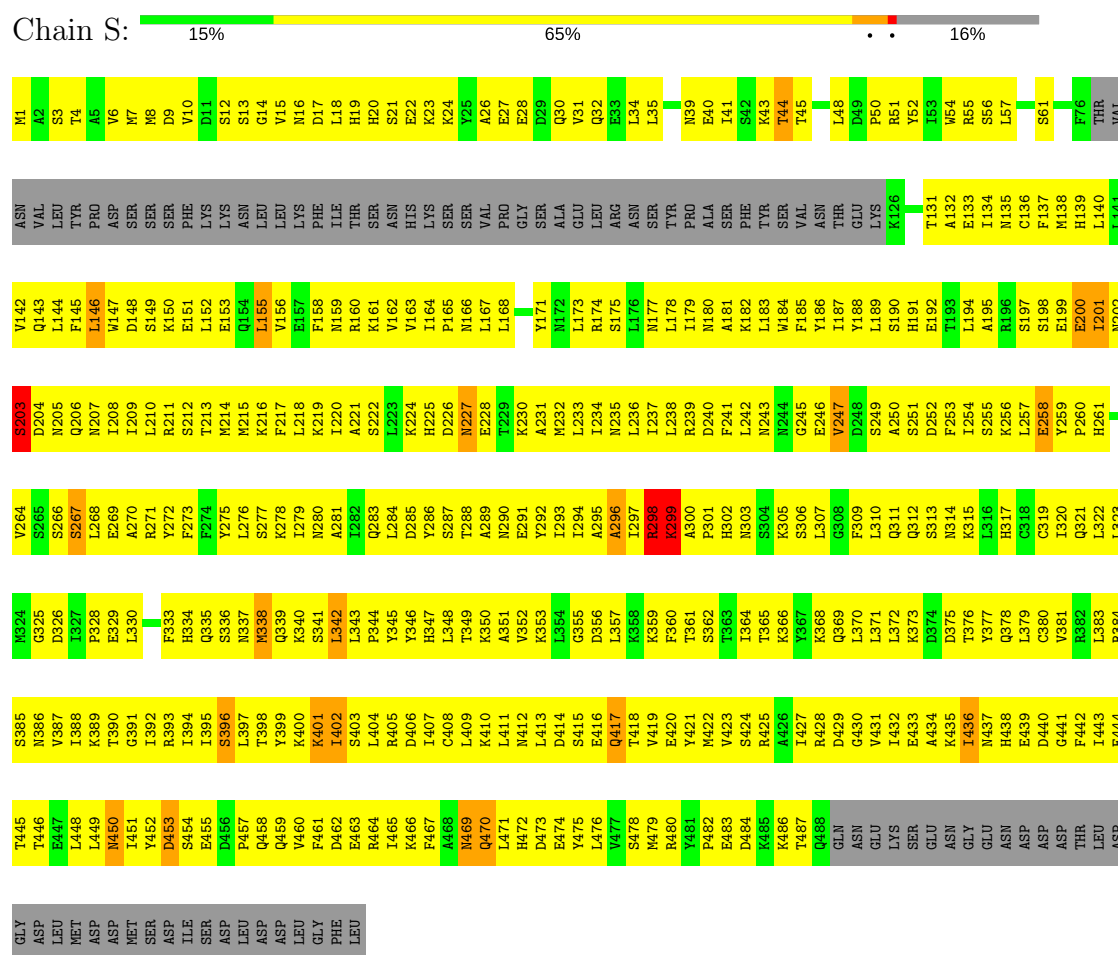
• Molecule 25: 26S proteasome regulatory subunit RPN7

Chain R: 9% 76% 8% 7%

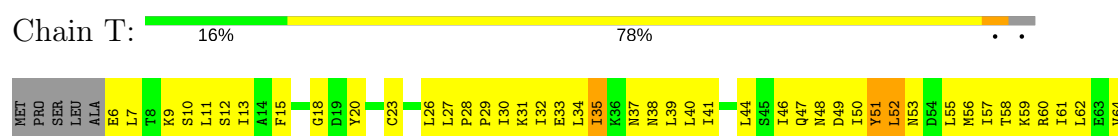


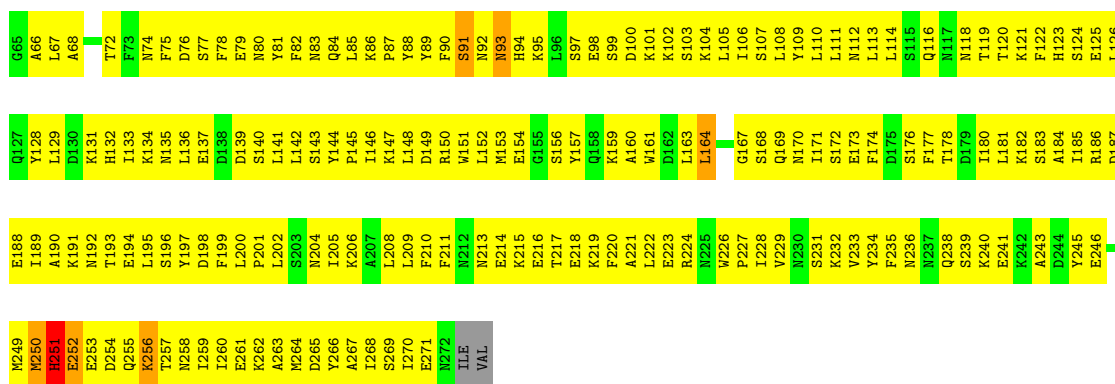


- Molecule 26: 26S proteasome regulatory subunit RPN3

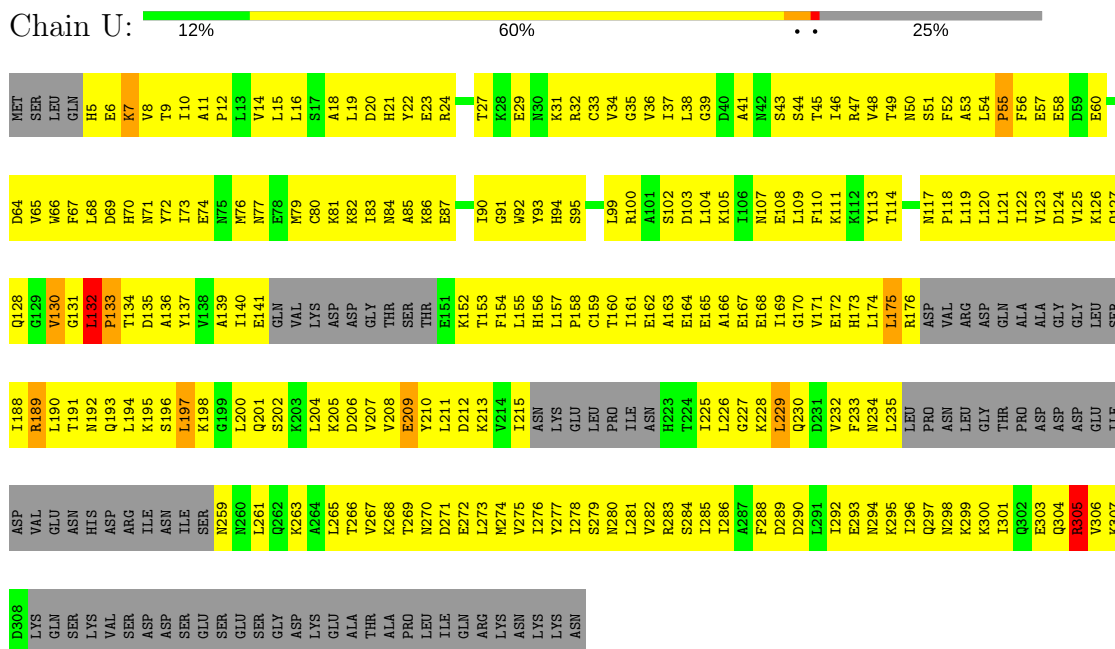


- Molecule 27: 26S proteasome regulatory subunit RPN12

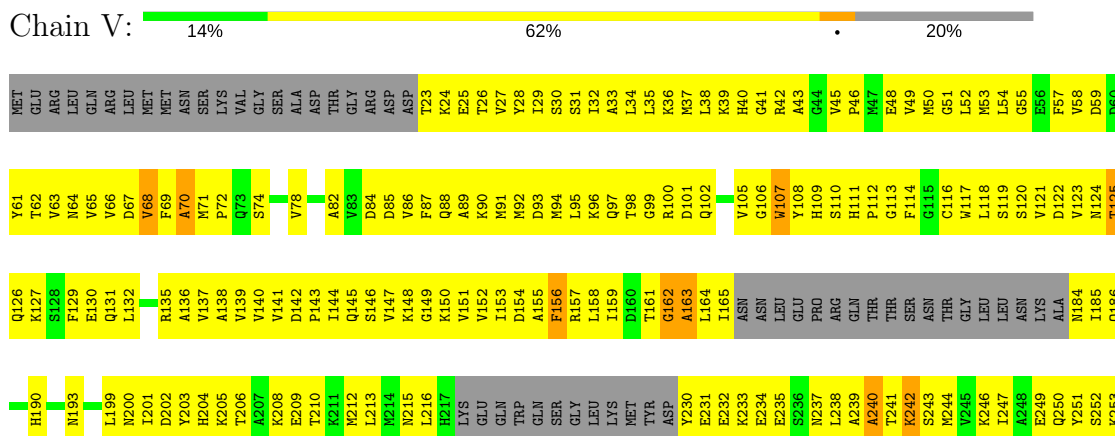


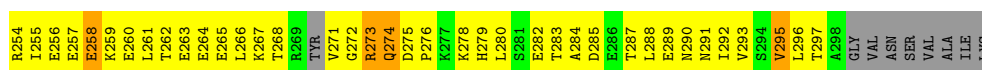


- Molecule 28: 26S proteasome regulatory subunit RPN8



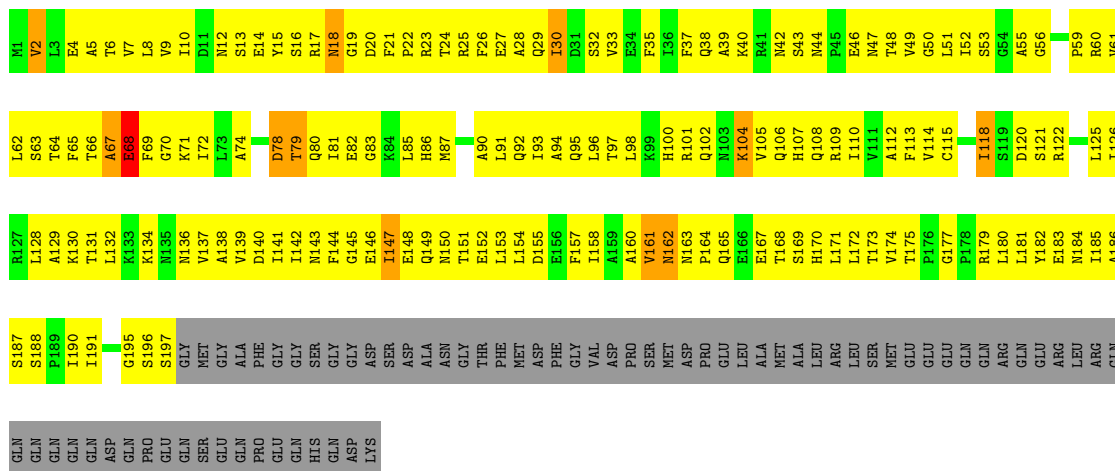
- Molecule 29: Ubiquitin carboxyl-terminal hydrolase RPN11





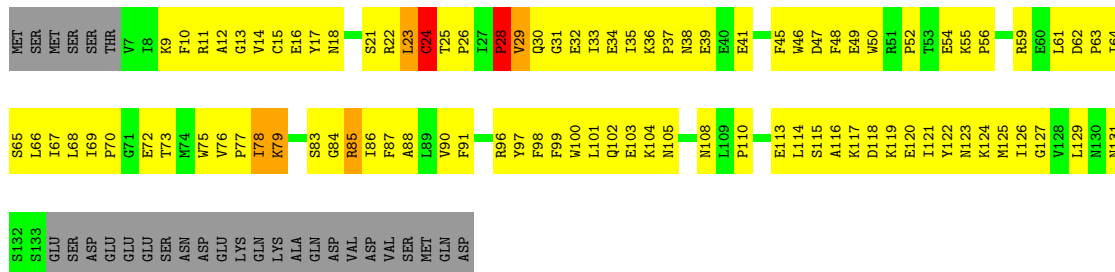
• Molecule 30: 26S proteasome regulatory subunit RPN10

Chain W: 14% 55% 26%



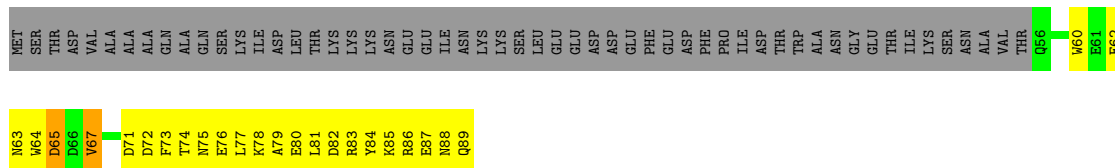
• Molecule 31: 26S proteasome regulatory subunit RPN13

Chain X: 21% 56% 19%



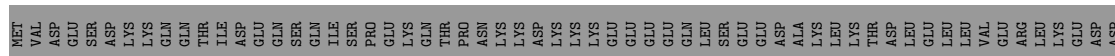
• Molecule 32: 26S proteasome complex subunit SEM1

Chain Y: 10% 26% 62%



• Molecule 33: 26S proteasome regulatory subunit RPN1

Chain Z: 14% 56% 5% 25%



LYS	T883	A820	S757	GLU	GLU	GLU	GLU	GLU	L509	V442	L381	G317	L256	PHE	T125	SER
LYS	T884	G821	L758	GLY	GLU	GLU	GLU	GLU	L510	D443	A382	K318	P257	GLU	Y126	SER
ILE	A885	T822	R759	GLU	GLU	GLU	GLU	GLU	P511	E444	S383	K318	P258	GLU	S127	LEU
THR	T886	T823	H760	THR	THR	THR	THR	THR	P512	E445	S384	F321	P259	GLU	E128	TYR
GLY	G887	N824	G761	ILE	GLU	GLU	GLU	GLU	A513	E446	F385	E322	E260	GLU	N129	GLU
TRP	L888	A825	E578	LYS	GLU	GLU	GLU	GLU	A514	V447	V386	Y323	D261	ALA	E198	ALA
ILE	T889	R826	H763	SER	GLY	GLY	GLY	GLY	S515	K448	N387	E324	V262	SER	K131	SER
THR	S890	L827	L764	GLU	GLU	GLU	GLU	GLU	T516	A449	G388	G325	A263	LEU	H132	LEU
GLN	P891	A828	M765	GLU	GLU	GLU	GLU	GLU	D517	G450	F389	G326	P264	ASN	L130	ASN
SER	S892	L829	H766	LYS	THR	THR	THR	THR	L518	A451	N391	Q327	L265	ALA	L136	ALA
THR	F893	L830	T767	LYS	ASN	ASN	ASN	ASN	L519	L452	L392	Q328	R202	LYS	R137	LYS
P964	M894	L831	G768	GLY	ILE	ILE	ILE	ILE	E521	L453	L393	T329	C204	GLY	Y137	GLY
V965	R895	R832	N769	LYS	SER	SER	SER	SER	T522	G454	G394	T330	C205	LYS	R138	LYS
L966	K896	Q833	E770	SER	ASP	ASP	ASP	ASP	A523	L455	Y394	G331	D206	SER	L139	SER
L957	H897	L834	H771	SER	PHE	PHE	PHE	PHE	A524	G456	C395	G332	L207	ILE	L140	ILE
N958	H898	L835	I772	ASP	LEU	LEU	LEU	LEU	M525	L457	N396	Q333	R203	LYS	S141	LYS
H959	R899	S836	R773	LYS	GLY	GLY	GLY	GLY	A526	S458	D397	K334	P209	ASN	D142	ASN
G960	L900	Y837	R774	ASP	GLU	GLU	GLU	GLU	S527	A459	K398	L335	V143	THR	S144	THR
E961	F901	V838	M775	ALA	GLN	GLN	GLN	GLN	L528	S460	L399	S336	G216	THR	G148	THR
R962	Y902	S839	V776	THR	VAL	VAL	VAL	VAL	A529	E466	I400	E337	L212	ALA	H151	ALA
A963	M903	R840	P777	THR	ASN	ASN	ASN	ASN	L530	L471	N405	L342	D219	PRO	E152	PRO
E964	L904	E841	M780	GLY	GLU	GLU	GLU	GLU	A531	L472	W406	A343	L282	LYS	Y153	LYS
L965	N905	D842	T596	GLY	GLU	GLU	GLU	GLU	H532	E467	D402	E344	A220	PRO	I154	PRO
E966	A906	D843	T597	LYS	THR	THR	THR	THR	V533	V467	N403	L340	E277	LEU	R155	LEU
T967	G907	A844	G781	ASN	LYS	LYS	LYS	LYS	V534	L473	D404	Y341	L278	LYS	H156	LYS
D968	L908	L845	V783	ASP	ASN	ASN	ASN	ASN	V535	L474	W407	A344	G217	PHE	L157	PHE
E969	R909	F846	S784	ASP	GLU	GLU	GLU	GLU	G536	L475	V401	E338	Q275	LEU	A158	LEU
Y970	P910	T847	V785	GLU	GLU	GLU	GLU	GLU	T537	L476	Y408	E345	A221	ARG	L159	ARG
L971	K911	T848	R786	GLU	ALA	ALA	ALA	ALA	C538	Q475	R409	L346	L222	THR	I161	THR
S972	F912	R849	D787	GLU	GLU	GLU	GLU	GLU	G539	Q476	T410	N347	L223	THR	G162	THR
Y973	I913	L850	V788	GLU	ILE	ILE	ILE	ILE	G540	Y477	K411	L348	L224	LEU	A160	LEU
T974	L914	A851	Q789	LYS	VAL	VAL	VAL	VAL	D541	Y478	G412	T349	L225	LEU	A161	LEU
S975	Q915	K852	M790	GLY	VAL	VAL	VAL	VAL	I542	T479	G413	K352	L288	ARG	L169	ARG
H976	L916	G853	K791	ALA	ASP	ASP	ASP	ASP	T543	M480	M415	V354	E289	THR	I161	THR
T977	N917	L854	V792	GLY	GLU	GLU	GLU	GLU	T544	T481	T416	P354	E290	THR	G162	THR
E978	D918	L855	F793	ILE	MET	MET	MET	MET	S545	T483	S417	K357	E291	THR	A173	THR
S979	E919	H856	D794	VAL	GLU	GLU	GLU	GLU	V546	K484	S417	K357	K232	PRO	A173	PRO
V980	G920	L857	T797	ASP	VAL	VAL	VAL	VAL	D548	L485	A418	K358	L233	ASP	Y165	ASP
N981	E921	G858	R798	GLU	ASP	ASP	ASP	ASP	N549	S486	V419	K359	L234	ASP	N106	ASP
L982	P922	K859	F799	ALA	ALA	ALA	ALA	ALA	F550	S487	A420	K359	Q235	ASP	E170	ASP
K983	I923	G860	S800	GLU	GLU	GLU	GLU	GLU	M551	A488	S421	S360	F236	ASP	Y103	ASP
K984	K924	T861	H801	GLY	GLY	GLY	GLY	GLY	R553	A489	I422	H361	V297	ASP	A173	ASP
K985	V925	N862	D802	GLY	GLY	GLY	GLY	GLY	T554	L490	G423	L362	F298	ASP	A173	ASP
N986	N926	T863	H802	VAL	VAL	VAL	VAL	VAL	A555	L491	S424	D363	D239	ASP	A173	ASP
P987	V927	H864	A803	VAL	VAL	VAL	VAL	VAL	L556	G492	I425	K364	A300	ASP	A173	ASP
S988	R928	D865	D804	GLU	GLU	GLU	GLU	GLU	E557	G493	Y426	K366	T301	ASP	A173	ASP
Y989	V929	V866	L805	VAL	VAL	VAL	VAL	VAL	H622	G494	W428	K366	F241	ASP	A173	ASP
R990	E906	F867	E806	LYS	LYS	LYS	LYS	LYS	T560	L495	W428	K366	Q243	ASP	A173	ASP
E991	Q931	N868	V807	ALA	ALA	ALA	ALA	ALA	B561	A496	N429	V368	Q244	ASP	A173	ASP
E992	ALA	ALA	P808	GLU	GLU	GLU	GLU	GLU	V562	F497	L430	F369	V245	ASP	A173	ASP
E993	VAL	L873	M809	ILE	ILE	ILE	ILE	ILE	V563	S500	L433	A372	C246	ASP	A173	ASP
	GLU	N874	N810	THR	THR	THR	THR	THR	A564	K501	Q434	K373	Q247	ASP	A173	ASP
	THR	K875	S811	GLU	GLU	GLU	GLU	GLU	F565	N502	Q435	L374	Q248	ASP	A173	ASP
	VAL	V876	E750	LYS	LYS	LYS	LYS	LYS	L566	D503	L436	D375	L310	ASP	A173	ASP
	GLY	T877	D751	LYS	GLY	GLY	GLY	GLY	A567	E504	D437	S376	A311	ASP	A173	ASP
	GLN	L878	M815	ASN	ASN	ASN	ASN	ASN	L568	E505	K438	A377	V250	ASP	A173	ASP
	ALA	A879	G816	GLY	GLY	GLY	GLY	GLY	A569	V505	K438	A377	C252	ASP	A173	ASP
	ALA	S880	L817	GLU	GLU	GLU	GLU	GLU	V572	G507	Y459	Q378	L314	ASP	A173	ASP
	GLY	T881	E755	GLU	GLU	GLU	GLU	GLU	L573	G507	Y459	Q378	L314	ASP	A173	ASP
	ARG	L882	G819	SER	SER	SER	SER	SER	L573	G507	Y459	Q378	L314	ASP	A173	ASP
	PRO	L882	G819	LEU	LEU	LEU	LEU	LEU	L573	G507	Y459	Q378	L314	ASP	A173	ASP

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	25151	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Each micrographs	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	1.5	Depositor
Maximum defocus (nm)	2.5	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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 > 2$	RMSZ	# $ Z > 2$
1	1	0.55	0/1795	0.60	0/2420
1	8	0.55	0/1795	0.60	0/2420
10	C	0.54	0/1934	0.60	0/2618
10	c	0.54	0/1934	0.60	0/2618
11	D	0.50	0/1919	0.58	0/2598
11	d	0.50	0/1919	0.58	0/2598
12	E	0.48	0/1886	0.59	0/2541
12	e	0.48	0/1886	0.59	0/2541
13	F	0.49	0/1823	0.58	0/2463
13	f	0.49	0/1823	0.58	0/2463
14	G	0.54	1/1936 (0.1%)	0.58	0/2614
14	g	0.55	1/1936 (0.1%)	0.59	1/2614 (0.0%)
15	H	0.53	1/2915 (0.0%)	0.74	7/3927 (0.2%)
16	I	0.46	0/2681	0.73	4/3620 (0.1%)
17	J	0.48	0/2945	0.67	2/3952 (0.1%)
18	K	0.52	0/2872	0.75	3/3874 (0.1%)
19	L	0.50	0/2870	0.70	4/3858 (0.1%)
2	2	0.55	0/1855	0.61	0/2514
2	9	0.55	0/1855	0.61	0/2514
20	M	0.48	0/2785	0.69	1/3763 (0.0%)
21	N	0.44	0/6679	0.62	2/9037 (0.0%)
22	O	0.50	1/2958 (0.0%)	0.78	5/4005 (0.1%)
23	P	0.53	0/3520	0.74	4/4752 (0.1%)
24	Q	0.48	0/3525	0.61	0/4745
25	R	0.59	1/3240 (0.0%)	0.95	8/4371 (0.2%)
26	S	0.46	0/3439	0.76	4/4657 (0.1%)
27	T	0.46	0/2244	0.65	1/3029 (0.0%)
28	U	0.48	0/2075	0.69	2/2795 (0.1%)
29	V	0.50	0/1939	0.77	2/2613 (0.1%)
3	3	0.59	0/1602	0.59	0/2166
3	h	0.59	0/1603	0.59	0/2168
30	W	0.41	0/1557	0.67	0/2111
31	X	0.41	0/1058	0.66	0/1432
32	Y	0.44	0/244	0.68	0/328

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
33	Z	0.41	0/5787	0.68	4/7857 (0.1%)
4	4	0.54	0/1715	0.61	0/2326
4	i	0.54	0/1715	0.61	0/2326
5	5	0.53	0/1611	0.61	1/2174 (0.0%)
5	j	0.53	0/1608	0.61	1/2170 (0.0%)
6	6	0.53	0/1613	0.60	0/2173
6	k	0.53	0/1613	0.60	0/2173
7	7	0.55	0/1681	0.60	0/2274
7	l	0.55	0/1681	0.60	0/2274
8	A	0.56	0/1959	0.61	1/2652 (0.0%)
8	a	0.56	0/1959	0.61	1/2652 (0.0%)
9	B	0.53	0/1952	0.59	0/2642
9	b	0.53	0/1952	0.59	0/2642
All	All	0.51	5/105893 (0.0%)	0.66	58/143074 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
15	H	0	11
16	I	0	4
17	J	0	1
18	K	0	7
19	L	0	5
20	M	0	4
21	N	0	6
22	O	0	17
23	P	0	11
24	Q	0	6
25	R	0	5
26	S	0	16
27	T	0	4
28	U	0	7
29	V	0	6
30	W	0	6
31	X	0	6
32	Y	0	2
33	Z	0	7
All	All	0	131

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	330	VAL	C-N	15.59	1.69	1.34
15	H	380	PRO	N-CD	5.39	1.55	1.47
14	G	131	PRO	N-CD	5.26	1.55	1.47
14	g	131	PRO	N-CD	5.26	1.55	1.47
22	O	34	GLU	C-N	5.07	1.45	1.34

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	R	330	VAL	O-C-N	27.20	166.22	122.70
25	R	330	VAL	CA-C-N	-21.39	70.15	117.20
25	R	330	VAL	C-N-CA	-19.67	72.53	121.70
25	R	338	TYR	CB-CA-C	11.26	132.92	110.40
21	N	152	LEU	CA-CB-CG	9.73	137.68	115.30

There are no chirality outliers.

5 of 131 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	H	102	CYS	Peptide
15	H	164	SER	Peptide
15	H	171	GLY	Peptide
15	H	173	ARG	Peptide
15	H	175	GLY	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1757	0	1708	210	0
1	8	1757	0	1708	186	0
2	2	1824	0	1829	220	0
2	9	1824	0	1829	203	0
3	3	1573	0	1546	169	0
3	h	1574	0	1547	0	0
4	4	1684	0	1685	188	0
4	i	1684	0	1685	0	0
5	5	1581	0	1571	173	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	j	1578	0	1567	0	0
6	6	1585	0	1590	181	0
6	k	1585	0	1590	0	0
7	7	1644	0	1592	183	0
7	l	1644	0	1592	0	0
8	A	1921	0	1910	235	0
8	a	1921	0	1910	0	0
9	B	1915	0	1929	230	0
9	b	1915	0	1929	0	0
10	C	1904	0	1901	228	0
10	c	1904	0	1901	0	0
11	D	1890	0	1900	236	0
11	d	1890	0	1900	0	0
12	E	1861	0	1836	207	0
12	e	1861	0	1836	0	0
13	F	1795	0	1797	261	0
13	f	1795	0	1797	0	0
14	G	1896	0	1886	325	0
14	g	1896	0	1886	0	0
15	H	2877	0	2891	573	0
16	I	2652	0	2610	516	0
17	J	2914	0	3016	524	0
18	K	2835	0	2909	528	0
19	L	2829	0	2902	532	0
20	M	2754	0	2799	457	0
21	N	6570	0	6630	926	0
22	O	2912	0	2817	606	0
23	P	3470	0	3500	690	0
24	Q	3469	0	3485	851	0
25	R	3187	0	3152	878	0
26	S	3384	0	3238	748	0
27	T	2201	0	2167	379	0
28	U	2049	0	2099	433	0
29	V	1912	0	1906	340	0
30	W	1534	0	1542	253	0
31	X	1032	0	1017	129	0
32	Y	243	0	183	33	0
33	Z	5688	0	5564	1168	0
All	All	104170	0	103784	12561	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 65.

The worst 5 of 12561 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Q:314:PHE:HE1	24:Q:335:PHE:CE2	1.02	1.70
24:Q:314:PHE:CE1	24:Q:335:PHE:CE2	1.80	1.67
25:R:384:VAL:CG2	26:S:406:ASP:HB2	1.31	1.59
24:Q:309:ARG:HB2	24:Q:349:LYS:CB	1.29	1.58
33:Z:605:SER:HB3	33:Z:878:LEU:CG	1.27	1.56

There are no symmetry-related clashes.

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	220/241 (91%)	207 (94%)	13 (6%)	0	100	100
1	8	220/241 (91%)	207 (94%)	13 (6%)	0	100	100
2	2	231/266 (87%)	222 (96%)	7 (3%)	2 (1%)	20	63
2	9	231/266 (87%)	222 (96%)	7 (3%)	2 (1%)	20	63
3	3	203/215 (94%)	189 (93%)	12 (6%)	2 (1%)	18	61
3	h	203/215 (94%)	188 (93%)	13 (6%)	2 (1%)	18	61
4	4	220/261 (84%)	211 (96%)	9 (4%)	0	100	100
4	i	220/261 (84%)	211 (96%)	9 (4%)	0	100	100
5	5	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
5	j	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
6	6	196/198 (99%)	186 (95%)	8 (4%)	2 (1%)	18	61
6	k	196/198 (99%)	186 (95%)	8 (4%)	2 (1%)	18	61
7	7	210/287 (73%)	203 (97%)	7 (3%)	0	100	100
7	l	210/287 (73%)	203 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	A	241/252 (96%)	227 (94%)	13 (5%)	1 (0%)	38	77
8	a	241/252 (96%)	227 (94%)	13 (5%)	1 (0%)	38	77
9	B	248/250 (99%)	235 (95%)	13 (5%)	0	100	100
9	b	248/250 (99%)	235 (95%)	13 (5%)	0	100	100
10	C	242/258 (94%)	232 (96%)	10 (4%)	0	100	100
10	c	242/258 (94%)	232 (96%)	10 (4%)	0	100	100
11	D	239/254 (94%)	224 (94%)	14 (6%)	1 (0%)	38	77
11	d	239/254 (94%)	224 (94%)	14 (6%)	1 (0%)	38	77
12	E	240/260 (92%)	228 (95%)	12 (5%)	0	100	100
12	e	240/260 (92%)	228 (95%)	12 (5%)	0	100	100
13	F	231/234 (99%)	221 (96%)	10 (4%)	0	100	100
13	f	231/234 (99%)	221 (96%)	10 (4%)	0	100	100
14	G	242/288 (84%)	224 (93%)	14 (6%)	4 (2%)	11	52
14	g	242/288 (84%)	226 (93%)	15 (6%)	1 (0%)	38	77
15	H	373/467 (80%)	301 (81%)	60 (16%)	12 (3%)	5	37
16	I	348/437 (80%)	297 (85%)	42 (12%)	9 (3%)	6	42
17	J	371/405 (92%)	325 (88%)	39 (10%)	7 (2%)	9	49
18	K	357/428 (83%)	300 (84%)	45 (13%)	12 (3%)	4	37
19	L	354/437 (81%)	291 (82%)	58 (16%)	5 (1%)	13	54
20	M	349/434 (80%)	310 (89%)	38 (11%)	1 (0%)	44	81
21	N	846/945 (90%)	665 (79%)	173 (20%)	8 (1%)	20	63
22	O	372/393 (95%)	263 (71%)	83 (22%)	26 (7%)	1	20
23	P	427/445 (96%)	315 (74%)	100 (23%)	12 (3%)	6	41
24	Q	429/434 (99%)	325 (76%)	92 (21%)	12 (3%)	6	41
25	R	398/429 (93%)	280 (70%)	95 (24%)	23 (6%)	2	25
26	S	435/523 (83%)	332 (76%)	89 (20%)	14 (3%)	5	37
27	T	265/274 (97%)	202 (76%)	60 (23%)	3 (1%)	17	60
28	U	244/338 (72%)	202 (83%)	37 (15%)	5 (2%)	9	48
29	V	237/306 (78%)	185 (78%)	44 (19%)	8 (3%)	4	37
30	W	195/268 (73%)	154 (79%)	33 (17%)	8 (4%)	3	32
31	X	125/156 (80%)	96 (77%)	24 (19%)	5 (4%)	3	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	Y	32/89 (36%)	21 (66%)	10 (31%)	1 (3%)	5	38
33	Z	738/993 (74%)	589 (80%)	119 (16%)	30 (4%)	3	32
All	All	13225/15139 (87%)	11460 (87%)	1543 (12%)	222 (2%)	15	52

5 of 222 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	G	130	ARG
14	G	131	PRO
15	H	377	PHE
15	H	378	SER
15	H	380	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	185/201 (92%)	185 (100%)	0	100	100
1	8	185/201 (92%)	185 (100%)	0	100	100
2	2	199/224 (89%)	199 (100%)	0	100	100
2	9	199/224 (89%)	199 (100%)	0	100	100
3	3	167/178 (94%)	167 (100%)	0	100	100
3	h	168/178 (94%)	168 (100%)	0	100	100
4	4	181/214 (85%)	181 (100%)	0	100	100
4	i	181/214 (85%)	181 (100%)	0	100	100
5	5	172/173 (99%)	172 (100%)	0	100	100
5	j	171/173 (99%)	171 (100%)	0	100	100
6	6	175/175 (100%)	175 (100%)	0	100	100
6	k	175/175 (100%)	175 (100%)	0	100	100
7	7	169/235 (72%)	169 (100%)	0	100	100
7	l	169/235 (72%)	168 (99%)	1 (1%)	89	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	A	207/210 (99%)	207 (100%)	0	100	100
8	a	207/210 (99%)	207 (100%)	0	100	100
9	B	209/209 (100%)	209 (100%)	0	100	100
9	b	209/209 (100%)	209 (100%)	0	100	100
10	C	203/216 (94%)	203 (100%)	0	100	100
10	c	203/216 (94%)	203 (100%)	0	100	100
11	D	213/226 (94%)	213 (100%)	0	100	100
11	d	213/226 (94%)	213 (100%)	0	100	100
12	E	198/215 (92%)	198 (100%)	0	100	100
12	e	198/215 (92%)	198 (100%)	0	100	100
13	F	192/193 (100%)	192 (100%)	0	100	100
13	f	192/193 (100%)	192 (100%)	0	100	100
14	G	201/239 (84%)	200 (100%)	1 (0%)	91	95
14	g	201/239 (84%)	201 (100%)	0	100	100
15	H	296/399 (74%)	292 (99%)	4 (1%)	71	86
16	I	282/385 (73%)	279 (99%)	3 (1%)	78	89
17	J	319/352 (91%)	318 (100%)	1 (0%)	94	96
18	K	313/374 (84%)	309 (99%)	4 (1%)	73	87
19	L	306/377 (81%)	303 (99%)	3 (1%)	80	90
20	M	303/375 (81%)	303 (100%)	0	100	100
21	N	714/797 (90%)	712 (100%)	2 (0%)	94	96
22	O	306/368 (83%)	300 (98%)	6 (2%)	60	82
23	P	384/415 (92%)	384 (100%)	0	100	100
24	Q	387/391 (99%)	362 (94%)	25 (6%)	20	54
25	R	342/379 (90%)	333 (97%)	9 (3%)	51	76
26	S	349/489 (71%)	349 (100%)	0	100	100
27	T	250/256 (98%)	247 (99%)	3 (1%)	75	88
28	U	232/308 (75%)	232 (100%)	0	100	100
29	V	211/268 (79%)	211 (100%)	0	100	100
30	W	171/230 (74%)	169 (99%)	2 (1%)	75	88
31	X	116/144 (81%)	116 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	Y	18/81 (22%)	18 (100%)	0	100	100
33	Z	606/850 (71%)	588 (97%)	18 (3%)	46	73
All	All	11247/13054 (86%)	11165 (99%)	82 (1%)	87	93

5 of 82 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
24	Q	381	ILE
24	Q	398	TYR
33	Z	758	LEU
24	Q	382	LEU
24	Q	386	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 238 such sidechains are listed below:

Mol	Chain	Res	Type
22	O	236	HIS
25	R	114	ASN
14	g	127	ASN
22	O	323	ASN
23	P	349	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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.