



wwPDB EM Map/Model Validation Report ⓘ

Jun 28, 2016 – 12:30 PM EDT

PDB ID : 3JCO
EMDB ID: : EMD-6574
Title : Structure of yeast 26S proteasome in M1 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 : 4.80 Å(reported)
Based on PDB ID : PDB entry 4CR4

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027790

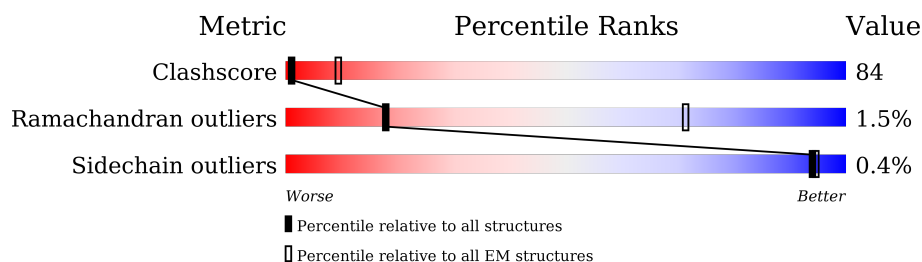
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.80 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.



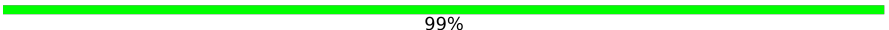

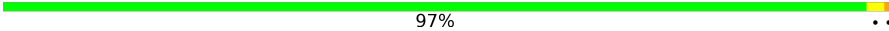



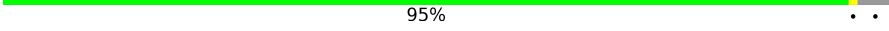

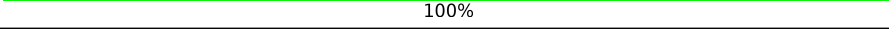
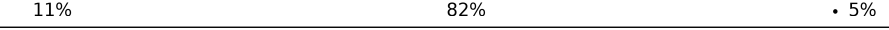
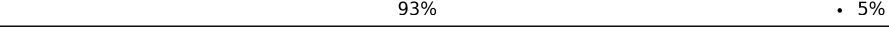
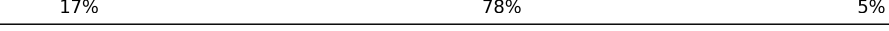
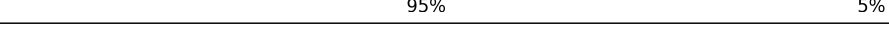

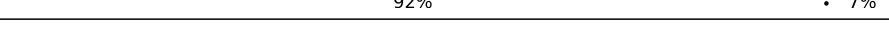

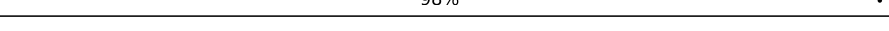


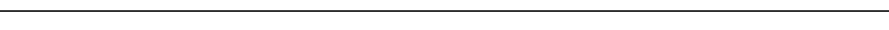

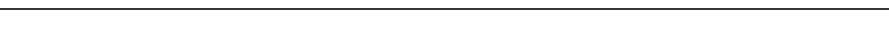
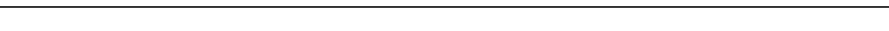


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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	13% 79% 8%
1	8	241	14% 78% 8%
2	2	266	13% 74% 12%
2	9	266	15% 72% 12%
3	3	215	14% 80% • 5%
3	h	215	95% 5%
4	4	261	13% 72% 15%
4	i	261	85% 15%
5	5	205	12% 87%

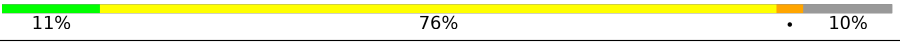
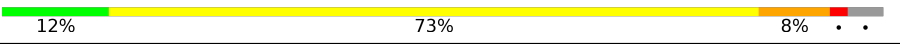
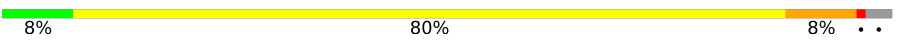
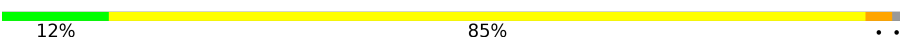

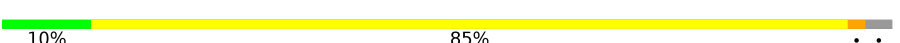
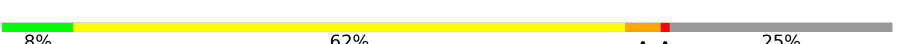
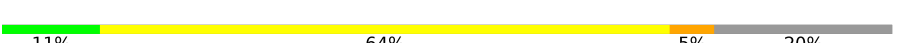
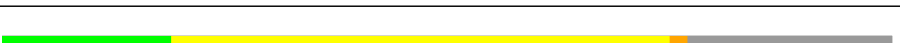
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Mol	Chain	Length	Quality of chain
5	j	205	 99%
6	6	198	 13% 85% .
6	k	198	 97% ..
7	7	287	 12% 61% . 26%
7	l	287	 73% . 26%
8	A	252	 12% 84% ..
8	a	252	 95% . .
9	B	250	 15% 84%
9	b	250	 100%
10	C	258	 11% 82% . 5%
10	c	258	 93% . 5%
11	D	254	 17% 78% 5%
11	d	254	 95% 5%
12	E	260	 17% 74% . 7%
12	e	260	 92% . 7%
13	F	234	 11% 88% .
13	f	234	 98% .
14	G	288	 7% 76% . 15%
14	g	288	 83% . 15%
15	H	467	 13% 60% . . 24%
16	I	437	 13% 60% . 26%
17	J	405	 19% 71% . . 8%
18	K	428	 15% 67% . 16%
19	L	437	 12% 68% . 18%
20	M	434	 15% 65% . 18%

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Mol	Chain	Length	Quality of chain
21	N	945	
22	O	393	
23	P	445	
24	Q	434	
25	R	429	
26	S	523	
27	T	274	
28	U	338	
29	V	306	
30	W	268	
31	X	156	
32	Y	89	
33	Z	993	

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 104317 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
			1574	995	261	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
			1581	1010	258	305	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	356	Total	C	N	O	S	0	0
			2771	1744	496	516	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	325	Total	C	N	O	S	0	0
			2513	1573	424	503	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
			2928	1837	527	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
			2849	1788	506	545	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	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	376	Total	C	N	O	S	0	0
			3083	1991	497	586	9		

- 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
			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	439	Total	C	N	O	S	0	0
			3357	2136	569	635	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
			2034	1291	350	387	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	763	Total	C	N	O	S	0	0
			5894	3744	966	1156	28		

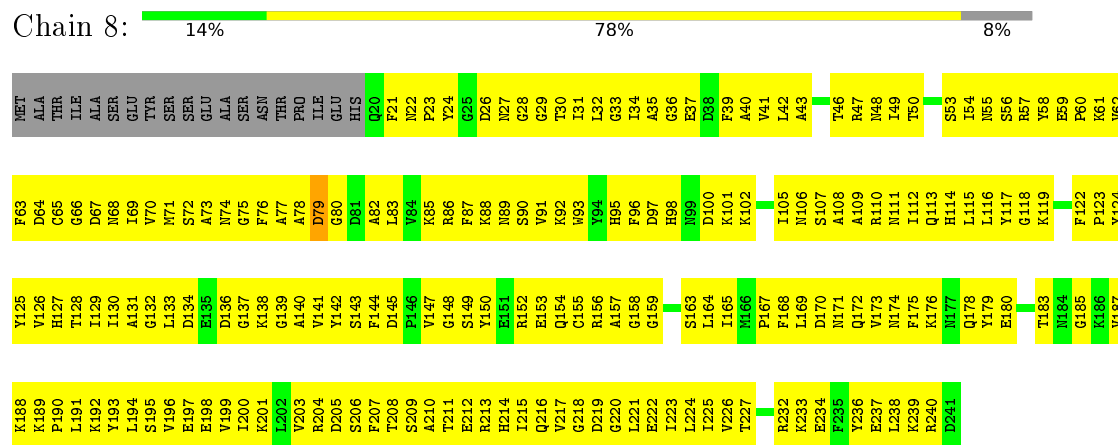
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

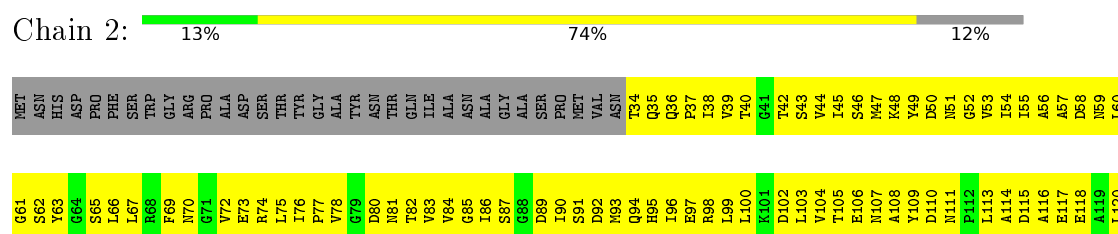
• Molecule 1: Proteasome subunit beta type-6

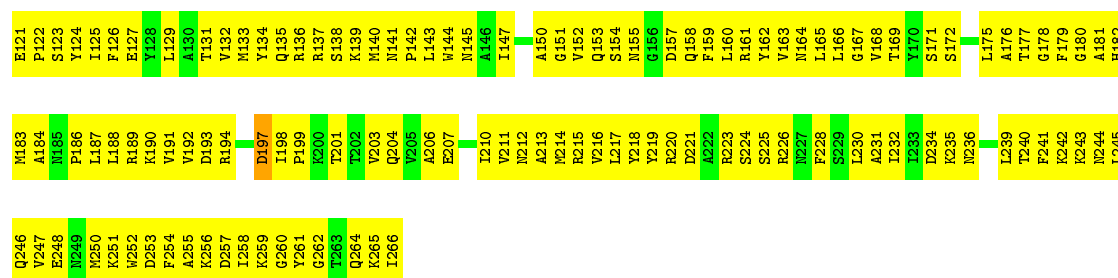


• Molecule 1: Proteasome subunit beta type-6



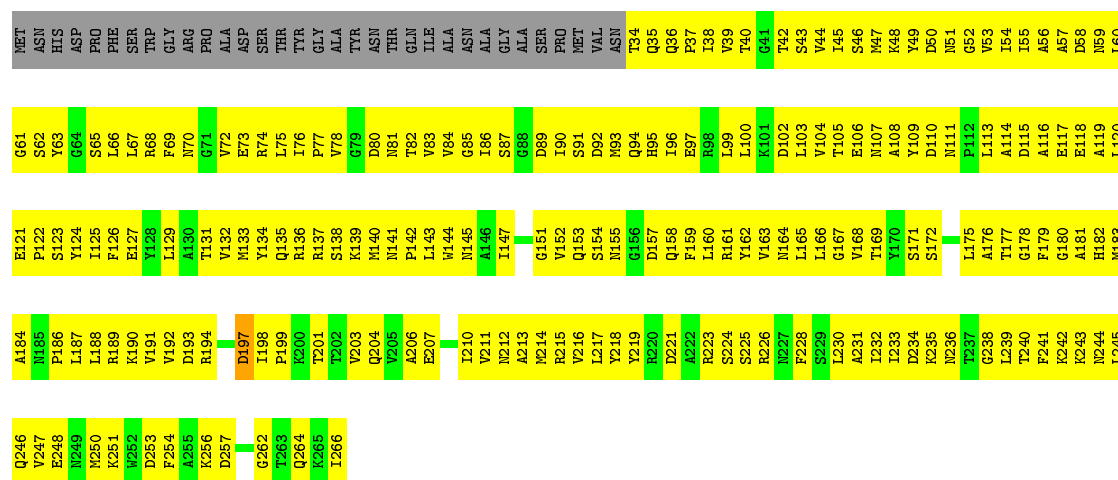
• Molecule 2: Proteasome subunit beta type-7





• Molecule 2: Proteasome subunit beta type-7

Chain 9: 15% 72% 12%



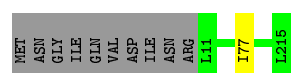
• Molecule 3: Proteasome subunit beta type-1

Chain 3: 14% 80% 5%



• Molecule 4: Proteasome subunit beta type-2

Chain h: 95% 5%



• Molecule 4: Proteasome subunit beta type-2



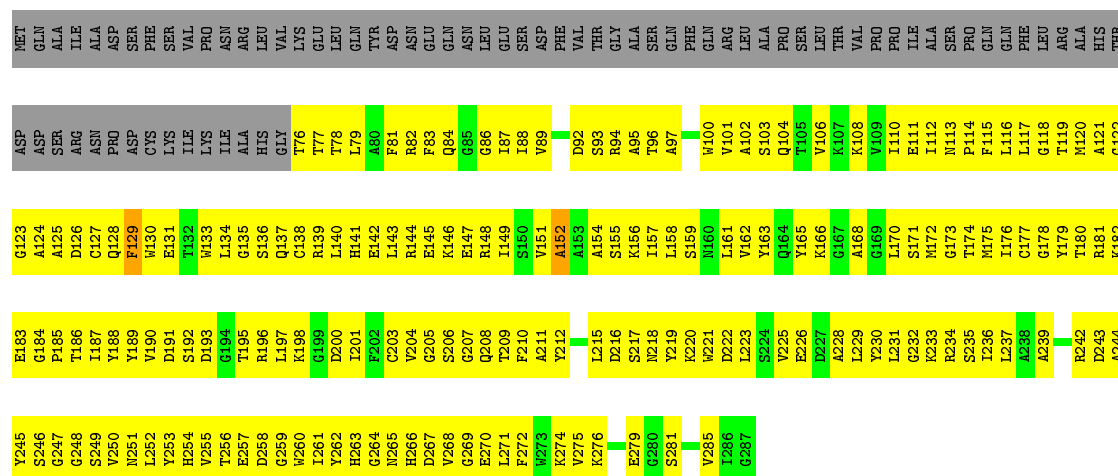
- Molecule 6: Proteasome subunit beta type-4

Chain k: 97%



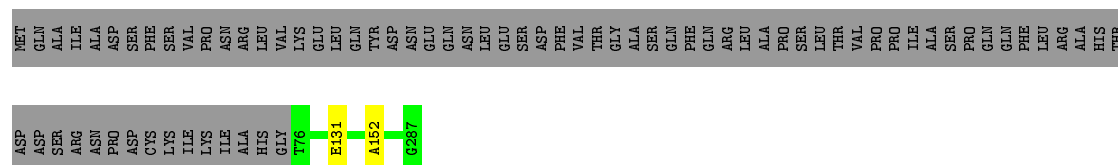
- Molecule 7: Proteasome subunit beta type-5

Chain 7: 12%



- Molecule 7: Proteasome subunit beta type-5

Chain l: 73%



- Molecule 8: Proteasome subunit alpha type-1

Chain A: 12%



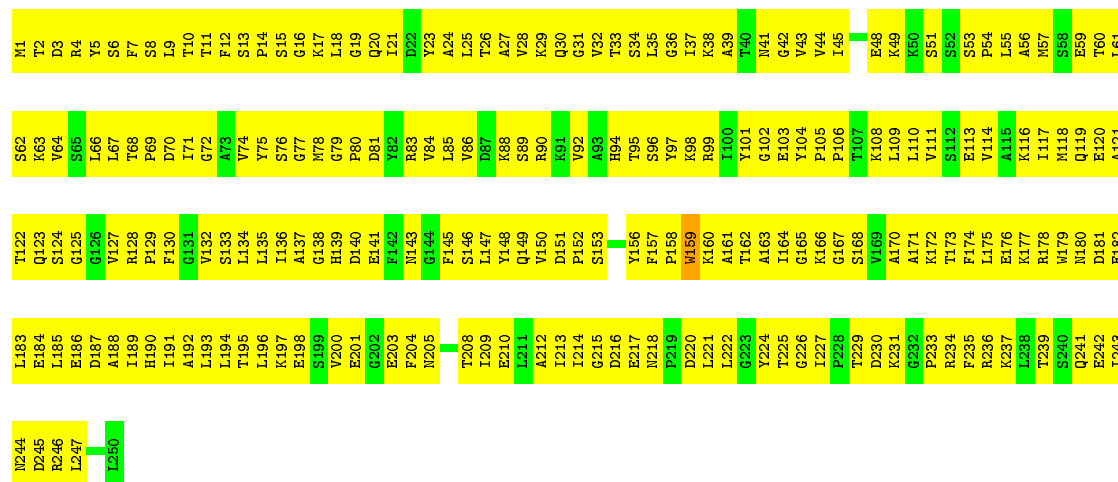
• Molecule 8: Proteasome subunit alpha type-1

Chain a: 95%



• Molecule 9: Proteasome subunit alpha type-2

Chain B: 15%



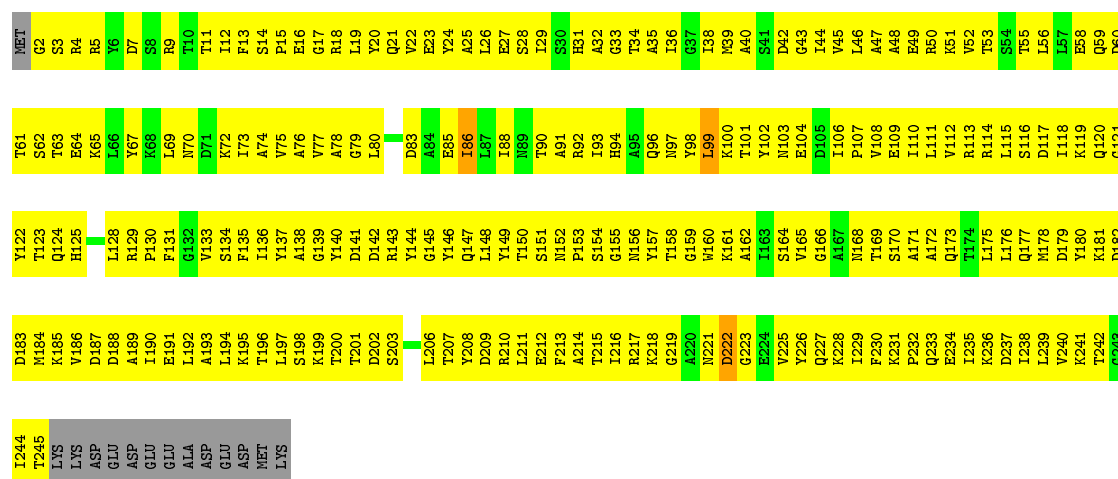
• Molecule 9: Proteasome subunit alpha type-2

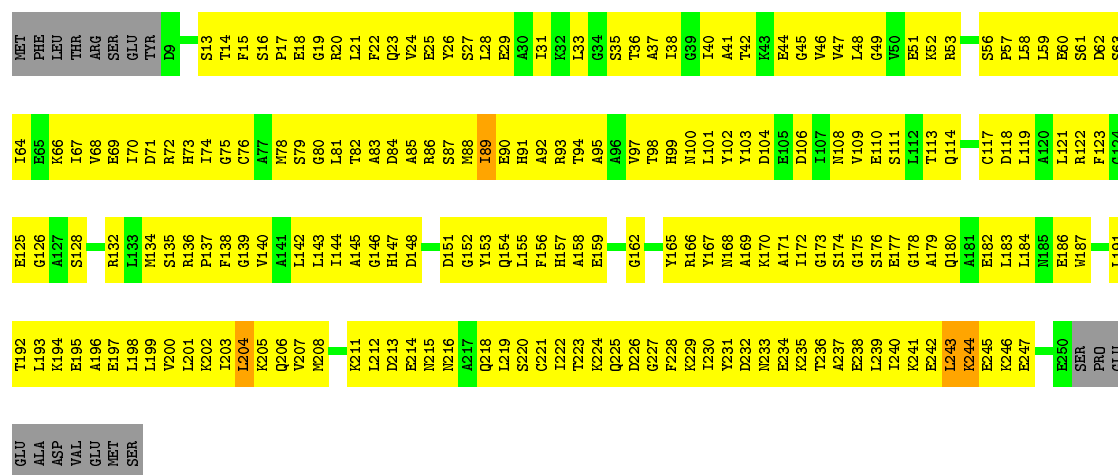
Chain b: 100%



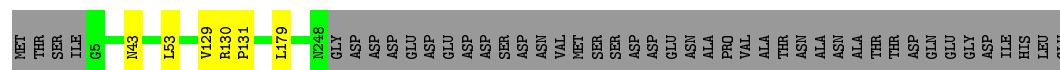
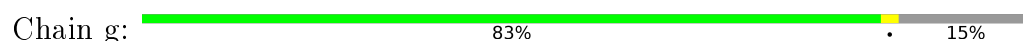
• Molecule 10: Proteasome subunit alpha type-3

Chain C: 11%

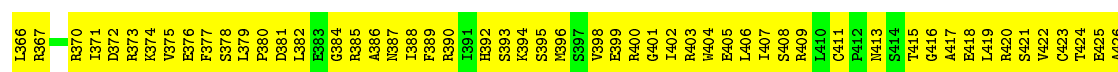
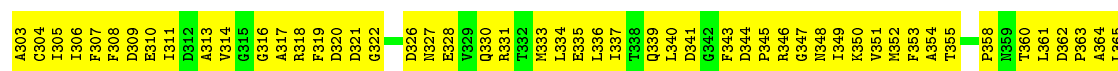
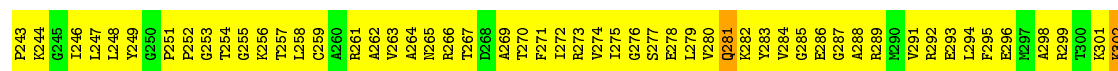
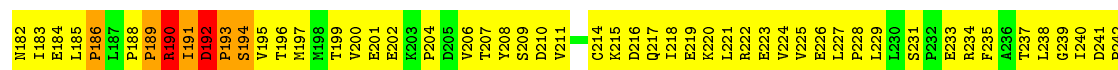
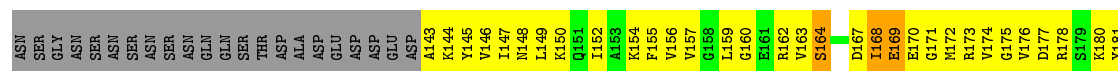
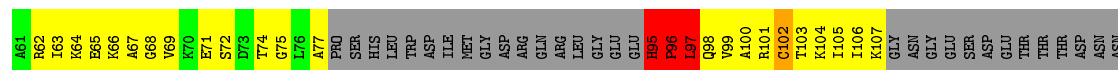
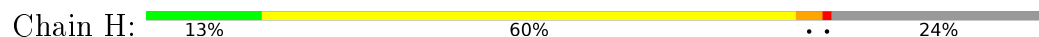




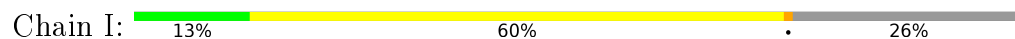
- Molecule 14: Probable proteasome subunit alpha type-7



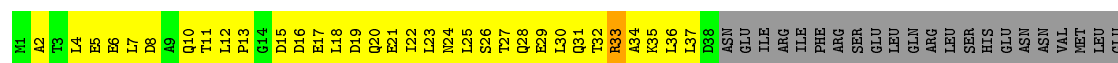
- Molecule 15: 26S protease regulatory subunit 7 homolog



- Molecule 16: 26S protease regulatory subunit 4 homolog







W376 Q377 L379 A380 R381 S382 T383 D384 A385 S386 R387 G388 A389 Q390 L391 K392 A393 V394 T395 S396 Q397 A398 G399 M400 L401 A402 L403 R404 M405 G406 Q407 S408 A409 V410 L411 H412 A413 D414 F415 V416 A417 L418 S419 A420 S421 V422 Q423 A424	F315 S316 D319 R320 V321 T322 L323 A324 S325 R326 T327 G328 A329 V330 L331 K332 A333 V334 T335 S336 Q337 L338 R339 S340 G341 A342 L343 D344 R345 K346 S347 A348 Q349 L350 P351 F352 S353 D354 F355 S356 R357 L358 A359 S420 S421 V422 Q423 A424	Q250 Q253 K254 T255 L256 Q257 E258 Q259 A260 K261 L262 R263 Q264 F267 A268 L269 D270 K271 E272 K273 A274 T275 T276 L278 D281 E282 L283 D284 A285 L286 Q287 T288 R289 Q290 T291 D292 S293 E294 D298 R299 A300 E301 Q302 R303 T304 K305 L308 L309 N310 Q311 L312 D313 E314 T315 R316 S317 L318 T319 V320 D321 Q322 R323 A324 E325 Q326 R327 S328 L329 A330 Q331 R332 T333 S334 L335 A336 Q337 R338 T339 S340 L341 K342 A343 V344 T345 S346 Q347 L348 R349 S350 T351 D352 A353 Q354 R355 L356 S357 A358 Q359 L360 S361 V362 Q363 R364 S365 R366 K367 L368 T369 V370 D371 R372 D373 T374 V375	L186 D187 I190 L193 V194 E195 A196 L197 M198 L199 P200 M201 K202 R203 A204 ASP L205 PHE L206 ASP MET GLY ILE ARG A214 P215 K216 L219 M220 Y221 D222 P223 P224 G225 T226 Q227 K228 T229 L230 L231 A232 R233 A234 C235 A236 Q237 Q238 T239 K240 A241 T242 F243 L244 K245 L246 P249	T121 S122 L123 R124 Q125 T126 V127 F128 L129 P130 M131 V132 G133 L134 V135 D136 P137 L140 L145 V146 G147 V148 M149 K150 D151 S152 V153 L154 L156 Y157 D158 T159 P160 S161 E162 F163 D164 V167 K168 A169 M170 E171 V172 D173 E174 K175 P176 T177 E178 T179 S180 L181 D182 V183 G184 C185 P200	LVS ILE LVS ASP ASN LVS GLU LVS ILE K70 N71 N72 R73 Q74 L75 P76 Y77 L78 V79 A80 N81 V82 V83 E84 V85 ASP MET MET ASN ASN GLU ILE LVS ASP LVS GLU ASN SER SER SER SER THR THR GLN GLY ASN ASN VAL ASN LEU LEU ASN THR THR ALA V113 G114 K115 A116 A117 V118 V119 V120
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• Molecule 21: 26S proteasome regulatory subunit RPN2

Chain N: 11% 76% 10%

L557	L497	E437	H375	L313	E247	L187	F123	L63
A558	L498	D438	H376	L314	E248	L188	F124	I64
H499	H499	G377	G377	L315	N249	L189	L125	A65
A560	A500	D440	N378	K316	D250	L190	K126	S66
M501	M501	V441	L379	S317		T191		K67
T562	F502	L442	L380	K318	L253	L192	T129	V68
G563	T503	L443	E381	S319	S254	A193	D130	Y69
H564	Y504	H444	G382	S320	A255	I194	F131	Y70
M565	S505	A445	K383	L321	Q256	K195	K132	N71
Q506	Q506	A446	K384	K322	L257	T196	L133	L72
E507	E507	S447	V385	G323	A258	V197	T134	G73
T508	T508	L448	H386	K324	P259	T198	S135	A11
Q509	Q509	G449	A387	F325	D260	N199	I136	L12
H510	H510	T450	P388	S326	L261	S200	F137	E74
L571	G511	L571	Y389	L327	V262	K201	E138	L13
N512	N512	L452	L390	F328	S263	F202	R139	L71
L513	L513	A453	P391	H329	S264	R203	M140	O17
T514	T514	A454	G392	T330		S204	T141	D18
R515	R515	M455	S393	A331	L269	S205	E142	Y81
A576	A576	G456		V332	L270	I206	K143	A82
L577	L577	S457	S397	F333	E271	L207	C144	L83
D578	D578	A458	K398	V334	L272	R208	L145	K21
S579	S579	N459	F399	A335	L273	K209	K146	T22
M580	G520	T460	I400	N336	V274	S210	A147	Y23
L521	L521	E461	K401	G337	T275	F211		A85
D582	D582	V462	G402	F338	E276	D212	L150	K86
L523	L523	G463	G403	N339	L277	F213	K151	D87
R584	R584	E464	S404	H340		L214	L152	R88
R585	N525	A465	L405	A341	Q280	M215	A153	F89
A586	Y526	L466	Y406	G342	G281	N216	L154	D90
H587	G527	G467	G407	T343	L282	M217	L155	I91
R588	R528	E468	L408	T344	D283	K218	I156	D92
H589	Q529	V469	G409	D345	E284	N219	A157	E93
Q530	Q530	L470	L410	N346	A285	G220	L158	K94
L531	L531	Y471	I411	S347	L286	D221	F159	S95
G592	A532	D472	Y412	F348	L287	Y222	G160	Q96
F593	F593	N473	A413	I349	N288	L223	Y161	F97
D594	D534	S474	F414	K350	L289	T225	L162	V98
L595	L535	A475	G415	A351	L290	K224	L163	E89
L596	L536	T476	G416	N352		K226	D164	T100
R597	T537	F477	R417		L293	K227	T165	I101
F598	K338	G478	D418	N355	P294	V228	I166	V102
H599	M539	E479	T419		T295	V229	E167	L43
T600	L540	A480	K358	K358	C296	V230	S168	S105
A541	A541	A481	D421	A359	D297	N231	A169	E107
V602	S542	A482	Y422	G360	Y298	L232	L170	M108
P603	P603	L483	L423	N361	N300	N233		Y109
R604	E544	G484	K424	K362	T301	D234	L174	V110
S545	S545	A485	K425	A363	F302	A235	D175	Q111
V606	L546	G486	I426	F363	F303	G236	K176	E112
Q607	L547	L487	I427	T365	L302	L237	ASP	A113
R608	R548	G488	V428	T366	L304	A238	S178	D53
L609	L609	V489	E429	G367	N305	L239	T179	T54
S610	G550	L490	N430	T368	N306	Q240	S180	K115
G611	G551	A491	S431	A369	K307	L241	E181	Q116
S612	A552	T492	G432	S370	N308	F242	I182	D57
H613	F553	K493	T433	K371	I309	K243	V183	N58
N614	T554	K494	S434	G372	D310	K244	K184	E59
A615	L555	P495	G435	V373	T311	L245	I185	N60
R616	A556	E506	D435	T374	C312	D246	T196	A61

VAL	ASN	T919	F739	1678	1617
K860	K860	V920	W740	M679	K618
Y861	Y861	Q921	W741	K880	K619
S862	S862	Q922	W742	K881	G620
K863	K863	K923	F743	F682	T621
K864	K864	K924	P744	L683	A622
P865	P865	D925	L745	S684	T623
Y866	Y866	VAL	A746	V685	A624
G867	G867	ASN	H747	V686	L625
V868	V868	ALA	H748	T887	L626
D869	D869	ALA	L749	N888	L627
N870	N870	LEU	S750	K689	A628
M871	M871	LEU	L751	C629	C629
T872	T872	THR	S752	Q691	A630
A873	A873	THR	A753	E631	E631
P874	P874	PHE	T754	G693	K632
L875	L875	VAL	P755	L694	G633
V876	V876	VAL	T756	A695	L634
Q877	Q877	ASP	T757	K696	O635
Q878	Q878	ASP	V758	F697	S636
S879	S879	ASN	L759	G698	A637
R880	R880	VAL	G760	A699	L638
Y881	Y881	ASP	I761	C700	D639
I882	I882	PHE	R762	V701	V640
S883	S883	PRO	G763	A702	L641
F884	F884	SER	S764	Q703	D642
I885	I885	ALA	D765	G704	T645
K886	K886	GLU	Q766	I705	K646
D887	D887	GLU	A767	M706	D647
N888	N888	LYS	L768	N707	P648
R889	R889	LYS	P769	A708	P648
F890	F890	LYS	K770	G709	V649
H891	H891	GLU	F771	G710	D650
P892	P892	HIS	Q772	R711	F651
V893	V893	GLU	M773	N712	V652
K894	K894	GLU	N774	K653	K653
L37	L37	LYS	G775	T714	O654
F895	F895	GLU	Y776	I715	A655
K896	K896	LYS	A777	Q716	A656
G898	G898	GLU	K778	L717	H657
N899	N899	ARG	E779	E718	L658
N900	N900	GLU	D780	T727	O666
G901	G901	THR	A781	N731	O667
V902	V902	ASN	F782	T728	T668
V903	V903	LYS	S783	S729	S729
V904	V904	LYS	Y784	V730	E669
L905	L905	LYS	P785	W731	K670
R906	R906	ILE	R786	L725	L664
D907	D907	LYS	N787	D726	L665
R908	R908	GLU	T788	T727	O666
E909	E909	THR	GLU	K728	O667
P910	P910	LYS	GLU	S729	T668
K911	K911	GLN	ALA	V730	E669
E912	E912	ASN	SER	W731	K670
P913	P913	ASP	GLY	G732	L671
V914	V914	ASN	LYS	L733	N672
A915	A915	GLU	GLU	P734	P673
L916	L916	PHE	VAL	M735	A674
I917	I917	LYS	TYR	F736	V675
E918	E918	LYS	LYS	S737	A676
				Q738	D677

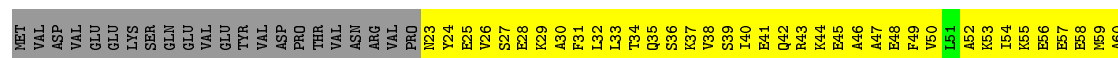
• Molecule 22: 26S proteasome regulatory subunit RPN9

Chain O: 

M1	Y62	H15	Y189	D249	F310	K373	MET	162
F2	D63	GLY	Y190	W250	E311	N374	SER	V63
N3	N64	D124	T191	L251	D312		ARG	D64
M4	F65	G125	S192	F252	I313	V377	ASP	L65
H5	V66	L126	L193	Q253	K314	K378	ALA	L66
E6	S67	L127	L194	L254	K315	K379	PRO	A67
I7	K68	L128	Y195	L255	A316	L380	ILE	S68
D8	F69	I129	L196	N256	L319	G381	LYS	R69
T9	Y70	D130	S197	A257	P320	K382	A5	N70
L11	K72	E131	T198	L258	K321	K383	D6	K71
S12	I73	L133	E200	V260	D322	E385	K7	D73
T13	N74	A134	P201	G261	N323	A386	S10	D74
L14	Q75	R135	S202	D262	V324	R387	Q11	L75
R15	L76	T136	T203	F263	E325		L12	M76
M16	S77	Y137	S204	D264	H326	GLN	L13	E77
L17	V78	L138	I205	K265	L327	SER	K14	Q78
A18	V79	L139	T206	F266	V328	ILE	K15	L79
D19	K80	L140	L207	D267	M329	TRP	E16	E80
P20	Y81		A208	S268	R330	VAL	F17	L81
S21	L82	R147	E209	L269	A331		P18	L82
L22	L83	D148	R210	K270	I332		K19	S83
H23	A84	L149	Q211	K271	S333		I20	K84
P24	S85	L150	Q212	V272	L334		D21	K85
L25	L86	D151	L213	Q273	G335		S22	H86
F26	K87	D152	A214	T274	L336		L23	G87
E27	D88	L153	D215	S275	K337		K24	Q88
Q28	S89	E154	T216	K276	K338		Q25	
F29	K90	L155	L217	I279	G339		ASN	L91
E30	D91	T156	K218	L280	S340		ASP	S92
K31	R92	L157	T219	A281	I341		CYS	I93
F32	D93	D158	S220	Q282	D342		H33	Q94
Y33	E94	K159	A221	Q283	Q343		S34	I95
E35	S95	K160	L222	E284	V344		A35	M96
K36	K97		G224	E285	N345		L36	I97
L37	Y98	L165	D225	F286	K346		D37	Q98
K38	L99	R166	K226	L287	L347		K38	K99
F39	D100	T167	I227	R288	V348		L39	V100
Q40	D101	T168	Y228	Q289	T349		L40	M101
L41	L102	N169	N229	K290	I350		V41	E102
S42	K103	S170	F230	I291	S351		L42	Y103
E43	A104	F171	G231	C292	V353		E43	L104
S44	Q105	Y172	E232	L293			K44	K105
L45	F106	S173	L233	M294			K45	S106
T46	Q107	T174	L234	T295			T46	S107
K47	E108	N175	H235	L296			R47	K108
F48	L109	S176	H236	I297			Q48	S109
F49	D110	Q177	P237	E298			A49	L110
D50	S111	Y178	T238	T299			S50	D111
D51	K112	F179	M239	V300			D51	L112
LYS	LYS	K180	E240	F301			L52	N113
GLN	K53	F181	T241	K302			A53	T114
ARG	ASN	K182	T242	K303			S54	R115
ASN	ASN	N183	V243	N304			S55	L116
ASN	ASN	D184	M244	L305			K56	S117
GLY	GLY	F185	D245	R306			V118	V118
SER	SER	T186	L246	K307			V58	V58
ASP	ASP	F188	M247	L308			L59	E120
			Y248				A60	T121
							LYS	L122

• Molecule 23: 26S proteasome regulatory subunit RPN5

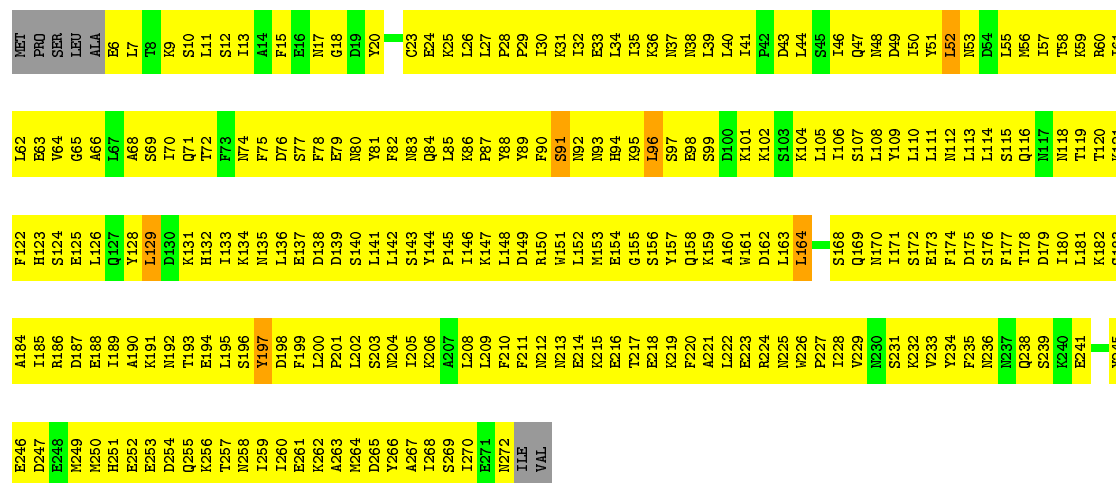
Chain P: 





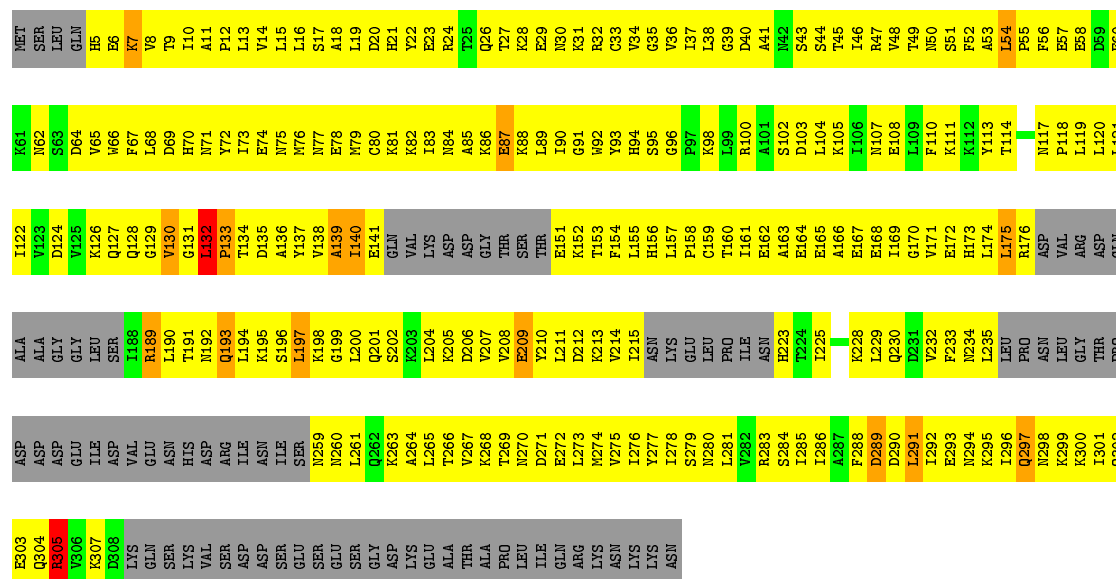

- Molecule 27: 26S proteasome regulatory subunit RPN12

Chain T:  10% 85% . .




- Molecule 28: 26S proteasome regulatory subunit RPN8

Chain U: 8% 62% .. 25%



- Molecule 29: Ubiquitin carboxyl-terminal hydrolase RPN11

Chain V:  11% 64% 5% 20%





4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	81782	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	each micrograph	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	0.62	0/1795	0.67	0/2420
1	8	0.61	0/1795	0.67	0/2420
10	C	0.56	0/1934	0.63	0/2618
10	c	0.56	0/1934	0.63	0/2618
11	D	0.57	0/1919	0.64	0/2598
11	d	0.57	0/1919	0.64	0/2598
12	E	0.57	0/1886	0.67	0/2541
12	e	0.58	0/1886	0.69	1/2541 (0.0%)
13	F	0.57	0/1823	0.68	0/2463
13	f	0.57	0/1823	0.68	0/2463
14	G	0.60	0/1936	0.67	3/2614 (0.1%)
14	g	0.60	1/1936 (0.1%)	0.67	3/2614 (0.1%)
15	H	0.51	1/2810 (0.0%)	0.70	2/3780 (0.1%)
16	I	0.41	0/2543	0.63	1/3429 (0.0%)
17	J	0.50	2/2964 (0.1%)	0.68	3/3981 (0.1%)
18	K	0.49	1/2887 (0.0%)	0.69	0/3894
19	L	0.48	0/2870	0.65	1/3858 (0.0%)
2	2	0.62	0/1855	0.67	0/2514
2	9	0.62	0/1855	0.67	0/2514
20	M	0.44	0/2785	0.66	2/3763 (0.1%)
21	N	0.55	1/6670 (0.0%)	0.69	4/9023 (0.0%)
22	O	0.63	0/3142	0.87	6/4241 (0.1%)
23	P	0.64	0/3520	0.82	6/4752 (0.1%)
24	Q	0.59	1/3527 (0.0%)	0.68	2/4748 (0.0%)
25	R	0.61	0/3272	0.75	2/4412 (0.0%)
26	S	0.54	0/3410	0.78	3/4621 (0.1%)
27	T	0.58	0/2244	0.73	2/3029 (0.1%)
28	U	0.56	0/2059	0.78	5/2774 (0.2%)
29	V	0.57	1/1939 (0.1%)	0.81	2/2613 (0.1%)
3	3	0.64	0/1603	0.66	0/2168
3	h	0.64	0/1603	0.67	0/2168
30	W	0.49	0/1557	0.72	0/2111
31	X	0.48	1/1058 (0.1%)	0.68	1/1432 (0.1%)
32	Y	0.62	0/244	0.82	0/328

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
33	Z	0.37	1/6001 (0.0%)	0.61	1/8141 (0.0%)
4	4	0.59	0/1715	0.67	0/2326
4	i	0.59	0/1715	0.67	0/2326
5	5	0.60	0/1611	0.64	0/2174
5	j	0.60	0/1611	0.64	0/2174
6	6	0.60	0/1613	0.69	1/2173 (0.0%)
6	k	0.60	0/1613	0.69	1/2173 (0.0%)
7	7	0.60	0/1681	0.67	0/2274
7	l	0.61	0/1681	0.67	0/2274
8	A	0.60	0/1959	0.69	1/2652 (0.0%)
8	a	0.61	0/1959	0.71	2/2652 (0.1%)
9	B	0.56	1/1952 (0.1%)	0.64	0/2642
9	b	0.56	1/1952 (0.1%)	0.64	0/2642
All	All	0.56	12/106066 (0.0%)	0.69	55/143284 (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
10	C	0	1
10	c	0	1
13	F	0	1
13	f	0	1
15	H	0	10
16	I	0	2
17	J	0	3
18	K	0	4
19	L	0	4
20	M	0	4
21	N	0	11
22	O	0	22
23	P	0	17
24	Q	0	8
25	R	0	8
26	S	0	16
27	T	0	4
28	U	0	8
29	V	0	6
30	W	0	8
31	X	0	6

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
32	Y	0	2
33	Z	0	5
6	6	0	1
6	k	0	1
8	A	0	1
8	a	0	1
All	All	0	156

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	V	107	TRP	CB-CG	-6.56	1.38	1.50
21	N	355	TRP	CB-CG	-5.89	1.39	1.50
24	Q	339	TYR	CE1-CZ	-5.77	1.31	1.38
9	B	159	TRP	CB-CG	-5.74	1.40	1.50
18	K	362	LEU	C-N	-5.73	1.20	1.34

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	S	155	LEU	CA-CB-CG	-10.11	92.05	115.30
25	R	309	LEU	CA-CB-CG	-9.51	93.44	115.30
23	P	412	LEU	CA-CB-CG	8.47	134.79	115.30
29	V	107	TRP	CB-CA-C	-8.08	94.25	110.40
29	V	70	ALA	C-N-CA	-7.60	102.71	121.70

There are no chirality outliers.

5 of 156 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	6	196	GLN	Peptide
8	A	64	LEU	Peptide
10	C	221	ASN	Peptide
13	F	175	THR	Peptide
15	H	97	LEU	Peptide

5.2 Too-close contacts

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	320	0
1	8	1757	0	1708	308	0
2	2	1824	0	1829	330	0
2	9	1824	0	1829	323	0
3	3	1574	0	1547	296	0
3	h	1574	0	1547	0	0
4	4	1684	0	1685	329	0
4	i	1684	0	1685	0	0
5	5	1581	0	1571	310	0
5	j	1581	0	1571	0	0
6	6	1585	0	1590	307	0
6	k	1585	0	1590	0	0
7	7	1644	0	1592	299	0
7	l	1644	0	1592	0	0
8	A	1921	0	1910	403	0
8	a	1921	0	1910	0	0
9	B	1915	0	1929	361	0
9	b	1915	0	1929	0	0
10	C	1904	0	1901	389	0
10	c	1904	0	1901	0	0
11	D	1890	0	1900	382	0
11	d	1890	0	1900	0	0
12	E	1861	0	1836	413	0
12	e	1861	0	1836	0	0
13	F	1795	0	1797	444	0
13	f	1795	0	1797	0	0
14	G	1896	0	1886	535	0
14	g	1896	0	1886	0	0
15	H	2771	0	2866	574	0
16	I	2513	0	2564	480	0
17	J	2928	0	3057	546	0
18	K	2849	0	2928	567	0
19	L	2829	0	2902	570	0
20	M	2754	0	2799	553	0
21	N	6562	0	6625	1318	0
22	O	3083	0	3099	843	0
23	P	3470	0	3500	924	0
24	Q	3471	0	3495	791	0
25	R	3218	0	3211	823	0
26	S	3357	0	3180	853	0
27	T	2201	0	2167	478	0
28	U	2034	0	2072	563	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	V	1912	0	1906	541	0
30	W	1534	0	1542	359	0
31	X	1032	0	1017	165	0
32	Y	243	0	182	47	0
33	Z	5894	0	5828	866	0
All	All	104317	0	104302	15935	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 84.

The worst 5 of 15935 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)
22:O:11:LEU:CD2	22:O:14:LEU:HD12	1.22	1.64
22:O:11:LEU:CD2	22:O:14:LEU:CD1	1.80	1.58
16:I:249:GLY:CA	16:I:252:LEU:HD11	1.08	1.55
24:Q:413:LEU:CD1	25:R:406:GLN:HG3	1.33	1.53
26:S:471:LEU:HD22	28:U:292:ILE:CD1	1.38	1.52

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%)	202 (92%)	17 (8%)	1 (0%)	34	77
1	8	220/241 (91%)	202 (92%)	17 (8%)	1 (0%)	34	77
2	2	231/266 (87%)	210 (91%)	21 (9%)	0	100	100
2	9	231/266 (87%)	210 (91%)	21 (9%)	0	100	100
3	3	203/215 (94%)	180 (89%)	22 (11%)	1 (0%)	34	77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	h	203/215 (94%)	179 (88%)	23 (11%)	1 (0%)	34	77
4	4	220/261 (84%)	206 (94%)	14 (6%)	0	100	100
4	i	220/261 (84%)	206 (94%)	14 (6%)	0	100	100
5	5	202/205 (98%)	185 (92%)	16 (8%)	1 (0%)	34	77
5	j	202/205 (98%)	185 (92%)	16 (8%)	1 (0%)	34	77
6	6	196/198 (99%)	175 (89%)	19 (10%)	2 (1%)	19	65
6	k	196/198 (99%)	174 (89%)	19 (10%)	3 (2%)	13	58
7	7	210/287 (73%)	188 (90%)	20 (10%)	2 (1%)	19	65
7	l	210/287 (73%)	190 (90%)	19 (9%)	1 (0%)	34	77
8	A	241/252 (96%)	220 (91%)	21 (9%)	0	100	100
8	a	241/252 (96%)	220 (91%)	21 (9%)	0	100	100
9	B	248/250 (99%)	225 (91%)	23 (9%)	0	100	100
9	b	248/250 (99%)	225 (91%)	23 (9%)	0	100	100
10	C	242/258 (94%)	220 (91%)	19 (8%)	3 (1%)	16	62
10	c	242/258 (94%)	220 (91%)	19 (8%)	3 (1%)	16	62
11	D	239/254 (94%)	215 (90%)	24 (10%)	0	100	100
11	d	239/254 (94%)	215 (90%)	24 (10%)	0	100	100
12	E	240/260 (92%)	215 (90%)	23 (10%)	2 (1%)	24	69
12	e	240/260 (92%)	215 (90%)	23 (10%)	2 (1%)	24	69
13	F	231/234 (99%)	210 (91%)	19 (8%)	2 (1%)	21	67
13	f	231/234 (99%)	210 (91%)	19 (8%)	2 (1%)	21	67
14	G	242/288 (84%)	216 (89%)	25 (10%)	1 (0%)	39	80
14	g	242/288 (84%)	216 (89%)	24 (10%)	2 (1%)	24	69
15	H	350/467 (75%)	286 (82%)	56 (16%)	8 (2%)	8	49
16	I	321/437 (74%)	286 (89%)	33 (10%)	2 (1%)	30	74
17	J	371/405 (92%)	332 (90%)	31 (8%)	8 (2%)	8	50
18	K	357/428 (83%)	306 (86%)	45 (13%)	6 (2%)	11	56
19	L	354/437 (81%)	302 (85%)	51 (14%)	1 (0%)	46	83
20	M	349/434 (80%)	306 (88%)	40 (12%)	3 (1%)	21	67
21	N	843/945 (89%)	656 (78%)	174 (21%)	13 (2%)	13	58
22	O	372/393 (95%)	250 (67%)	103 (28%)	19 (5%)	2	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	P	427/445 (96%)	305 (71%)	99 (23%)	23 (5%)	2	29
24	Q	429/434 (99%)	350 (82%)	76 (18%)	3 (1%)	26	71
25	R	398/429 (93%)	281 (71%)	94 (24%)	23 (6%)	2	27
26	S	435/523 (83%)	313 (72%)	103 (24%)	19 (4%)	3	34
27	T	265/274 (97%)	190 (72%)	74 (28%)	1 (0%)	39	80
28	U	244/338 (72%)	198 (81%)	39 (16%)	7 (3%)	6	44
29	V	237/306 (78%)	176 (74%)	53 (22%)	8 (3%)	5	41
30	W	195/268 (73%)	157 (80%)	30 (15%)	8 (4%)	3	35
31	X	125/156 (80%)	94 (75%)	26 (21%)	5 (4%)	4	36
32	Y	32/89 (36%)	21 (66%)	9 (28%)	2 (6%)	2	26
33	Z	757/993 (76%)	665 (88%)	80 (11%)	12 (2%)	12	57
All	All	13191/15139 (87%)	11208 (85%)	1781 (14%)	202 (2%)	18	58

5 of 202 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	I	253	ILE
17	J	321	VAL
18	K	342	SER
18	K	344	ARG
25	R	239	THR

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%)	198 (100%)	1 (0%)	92	96
2	9	199/224 (89%)	198 (100%)	1 (0%)	92	96
3	3	168/178 (94%)	167 (99%)	1 (1%)	90	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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	172/173 (99%)	172 (100%)	0	100	100
6	6	175/175 (100%)	174 (99%)	1 (1%)	90	95
6	k	175/175 (100%)	174 (99%)	1 (1%)	90	95
7	7	169/235 (72%)	169 (100%)	0	100	100
7	l	169/235 (72%)	168 (99%)	1 (1%)	90	95
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%)	196 (99%)	2 (1%)	82	92
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%)	201 (100%)	0	100	100
14	g	201/239 (84%)	201 (100%)	0	100	100
15	H	301/399 (75%)	300 (100%)	1 (0%)	94	96
16	I	284/385 (74%)	282 (99%)	2 (1%)	88	94
17	J	325/352 (92%)	324 (100%)	1 (0%)	94	96
18	K	316/374 (84%)	315 (100%)	1 (0%)	94	96
19	L	306/377 (81%)	306 (100%)	0	100	100
20	M	303/375 (81%)	303 (100%)	0	100	100
21	N	713/797 (90%)	713 (100%)	0	100	100
22	O	350/368 (95%)	347 (99%)	3 (1%)	84	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	P	384/415 (92%)	381 (99%)	3 (1%)	86	93
24	Q	388/391 (99%)	387 (100%)	1 (0%)	94	96
25	R	351/379 (93%)	348 (99%)	3 (1%)	84	93
26	S	342/489 (70%)	336 (98%)	6 (2%)	66	87
27	T	250/256 (98%)	250 (100%)	0	100	100
28	U	228/308 (74%)	225 (99%)	3 (1%)	76	90
29	V	211/268 (79%)	204 (97%)	7 (3%)	45	77
30	W	171/230 (74%)	171 (100%)	0	100	100
31	X	116/144 (81%)	116 (100%)	0	100	100
32	Y	18/81 (22%)	18 (100%)	0	100	100
33	Z	645/850 (76%)	643 (100%)	2 (0%)	94	96
All	All	11346/13054 (87%)	11305 (100%)	41 (0%)	94	96

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	R	148	ASP
26	S	179	ILE
33	Z	367	SER
25	R	406	GLN
25	R	417	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 275 such sidechains are listed below:

Mol	Chain	Res	Type
22	O	236	HIS
25	R	114	ASN
3	h	160	ASN
22	O	362	GLN
24	Q	19	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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.