



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 11:57 am GMT

PDB ID : 3JCO
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/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

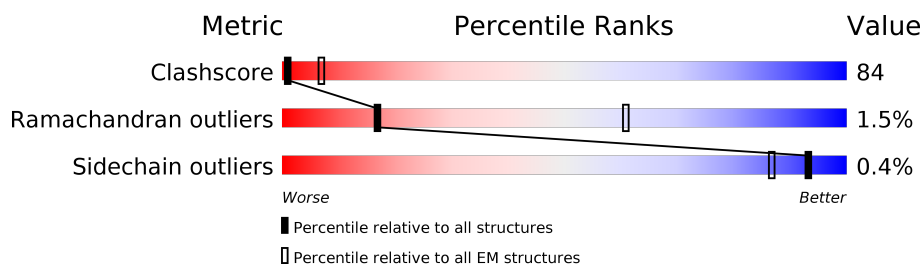
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.80 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.



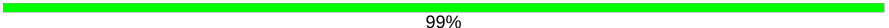




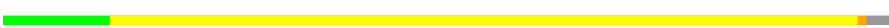











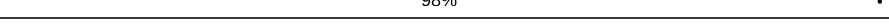





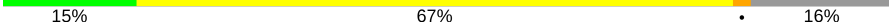

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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	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%

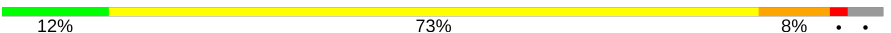
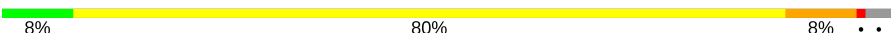


Continued on next page...

Continued from previous page...

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%

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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		

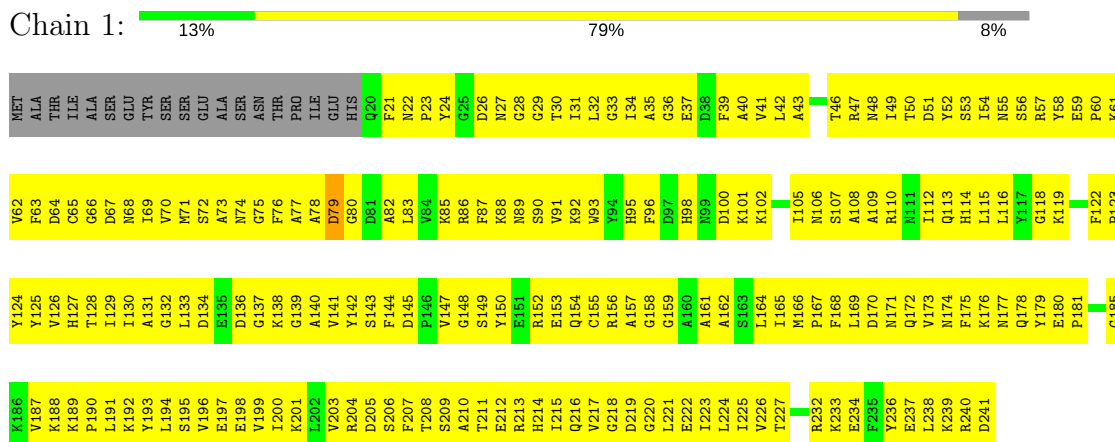
- Molecule 33 is a protein called 26S proteasome regulatory subunit RPN1.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Z	763	Total	C	N	O	S	0	0
			5894	3744	966	1156	28		

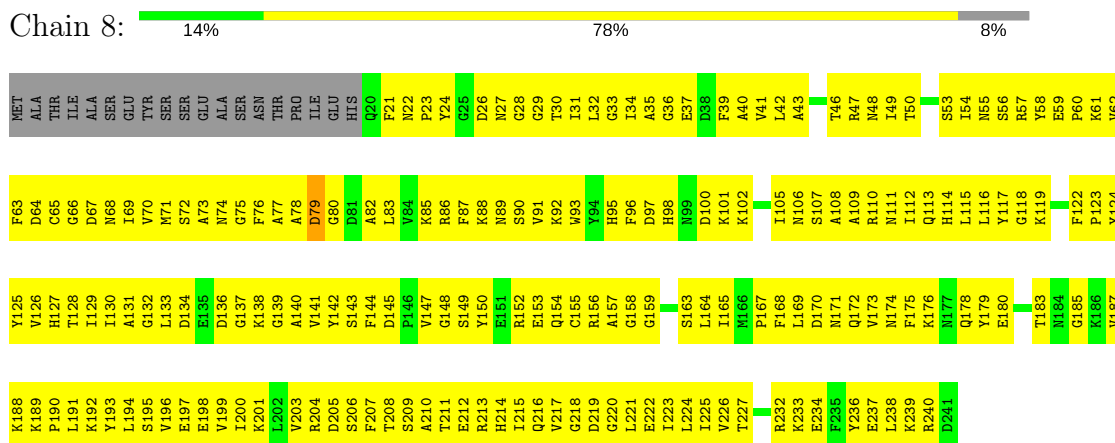
3 Residue-property plots

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

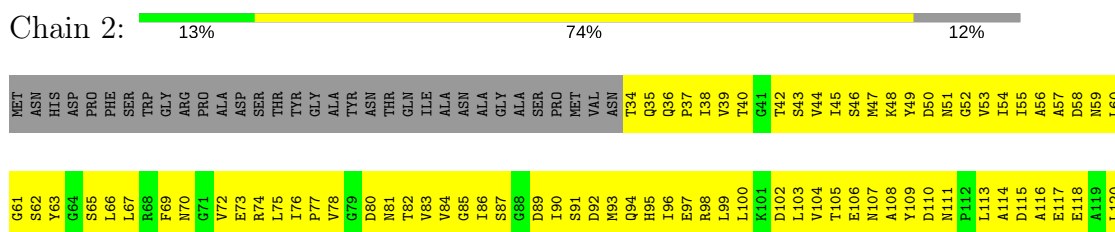
- Molecule 1: Proteasome subunit beta type-6

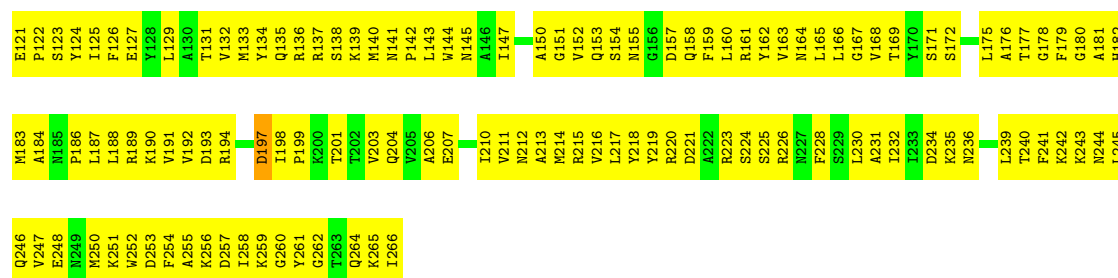


- Molecule 1: Proteasome subunit beta type-6



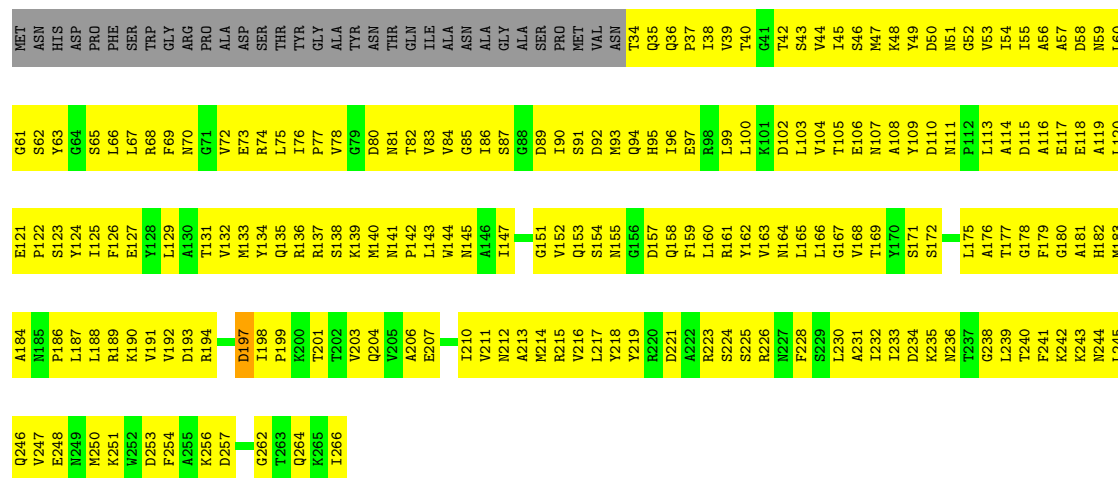
- Molecule 2: Proteasome subunit beta type-7





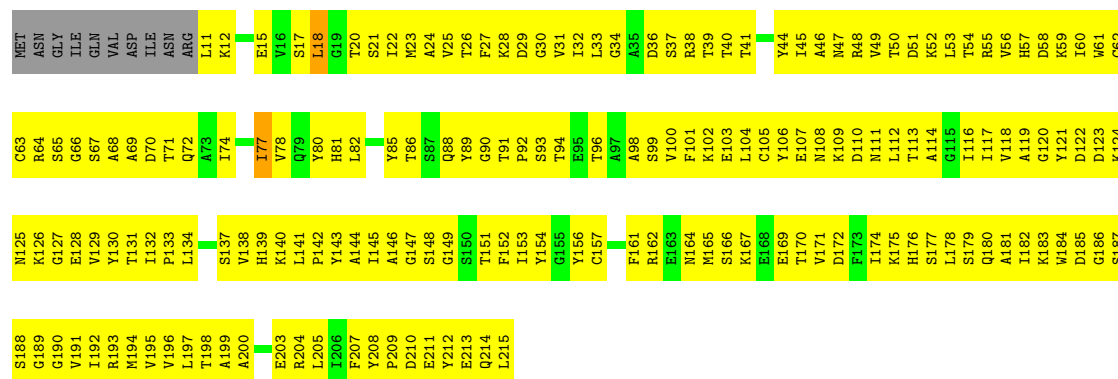
• Molecule 2: Proteasome subunit beta type-7

Chain 9: 15% 72% 12%



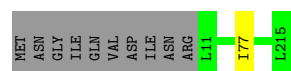
• Molecule 3: Proteasome subunit beta type-1

Chain 3: 14% 80% 5%



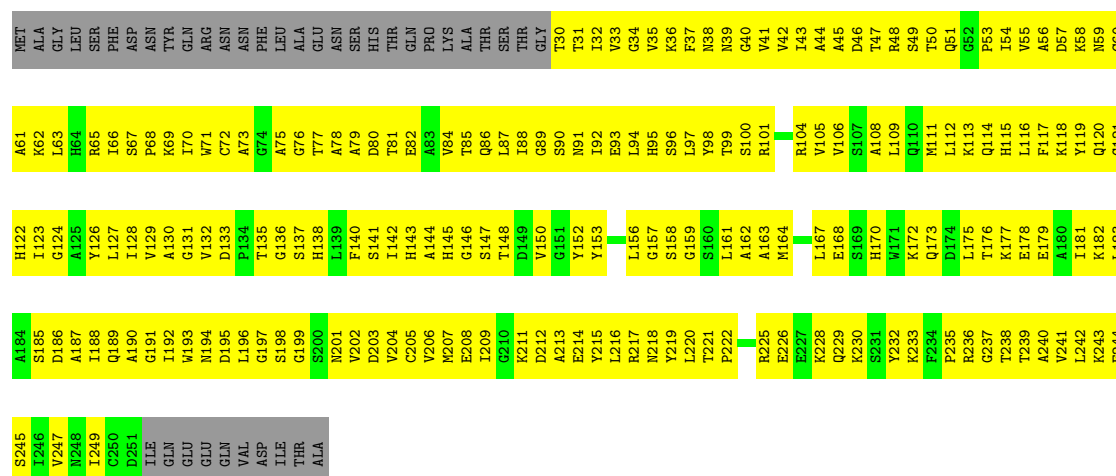
• Molecule 3: Proteasome subunit beta type-1

Chain h: 95% 5%




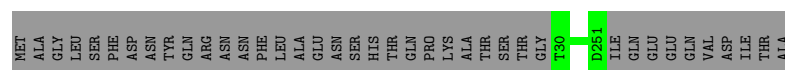
• Molecule 4: Proteasome subunit beta type-2

Chain 4: 13% 72% 15%



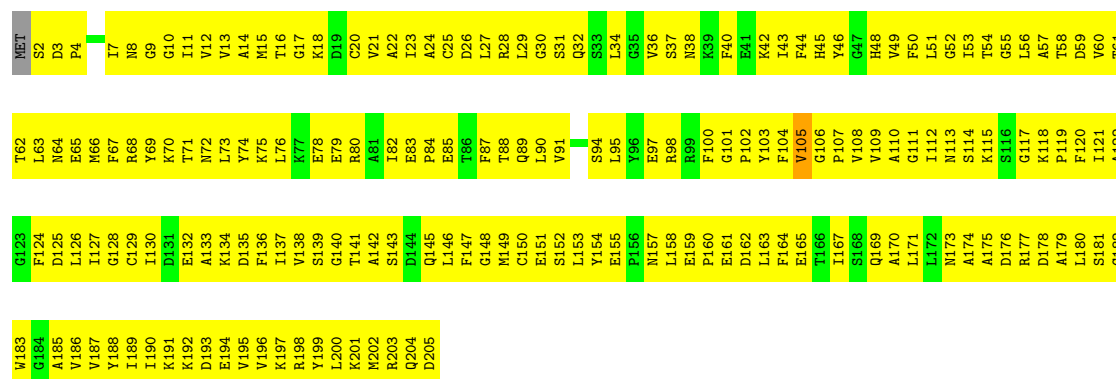
- Molecule 4: Proteasome subunit beta type-2

Chain i:  85% 15%



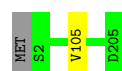
- Molecule 5: Proteasome subunit beta type-3

Chain 5:  12% 87%

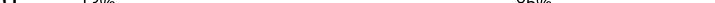


- Molecule 5: Proteasome subunit beta type-3

Chain j:



- Molecule 6: Proteasome subunit beta type-4

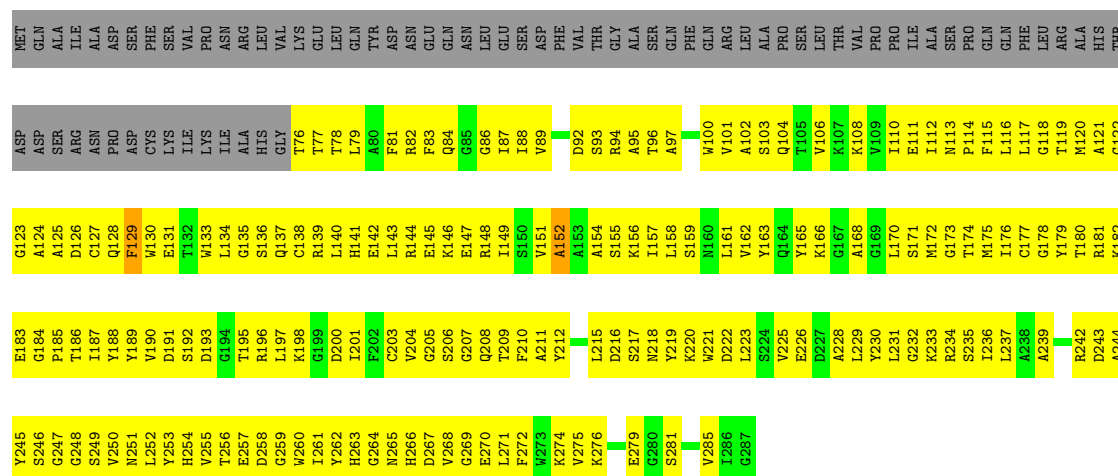
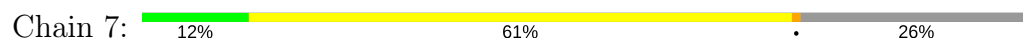
Chain 6:  13% 85%



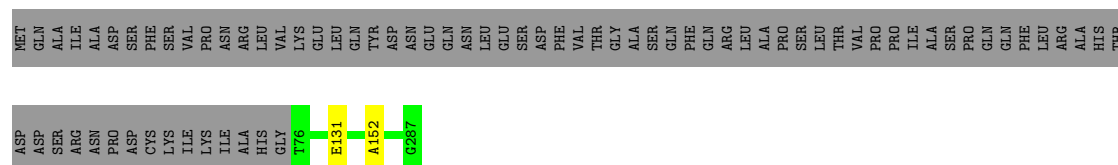
- Molecule 6: Proteasome subunit beta type-4



- Molecule 7: Proteasome subunit beta type-5

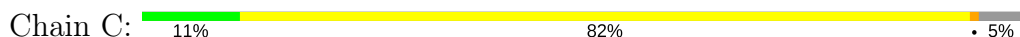


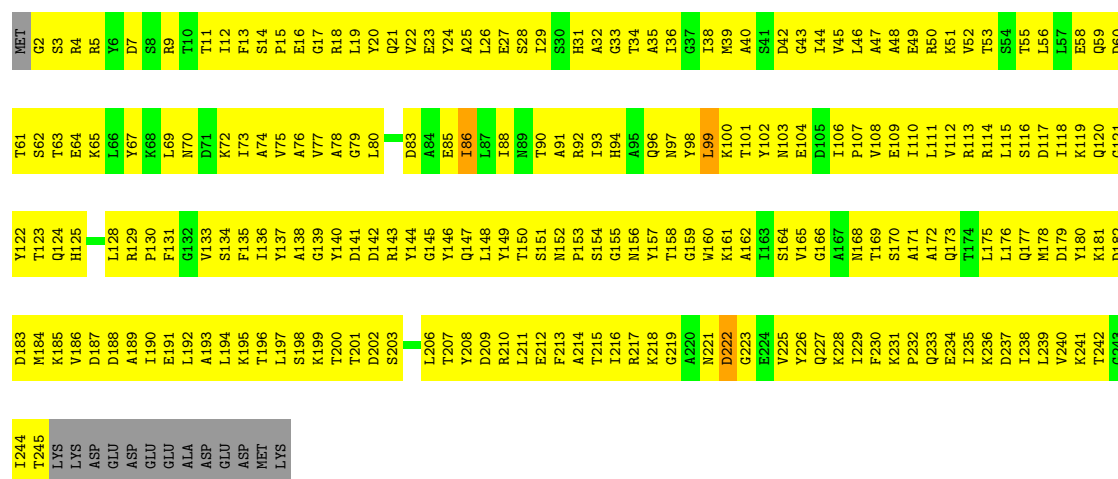
- Molecule 7: Proteasome subunit beta type-5



- Molecule 8: Proteasome subunit alpha type-1







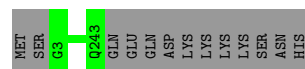
- Molecule 10: Proteasome subunit alpha type-3



- Molecule 11: Proteasome subunit alpha type-4

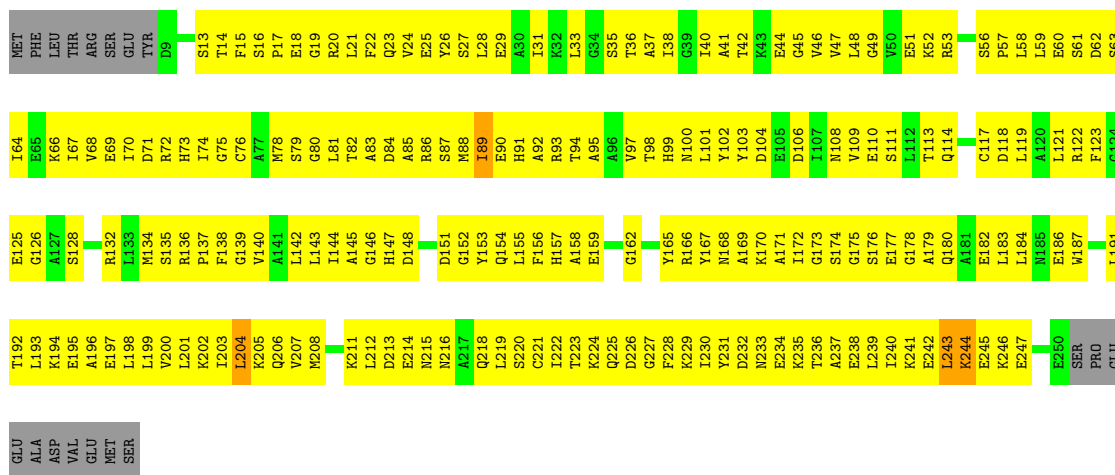


- Molecule 11: Proteasome subunit alpha type-4



- Molecule 12: Proteasome subunit alpha type-5





• Molecule 12: Proteasome subunit alpha type-5

Chain e: 92% 7%



• Molecule 13: Proteasome subunit alpha type-6

Chain F: 11% 88%



• Molecule 13: Proteasome subunit alpha type-6

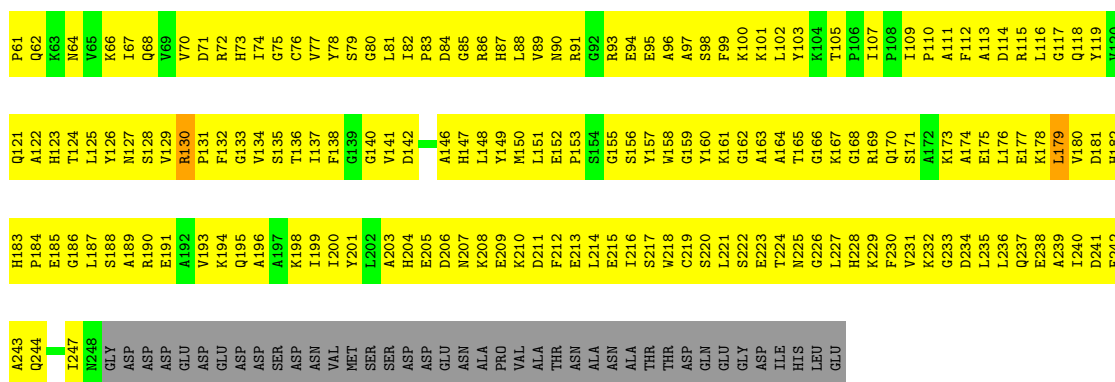
Chain f: 98%



• Molecule 14: Probable proteasome subunit alpha type-7

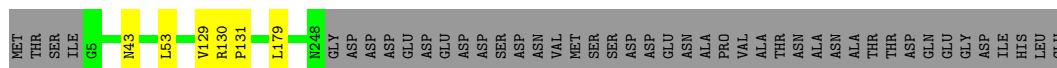
Chain G: 7% 76% 15%






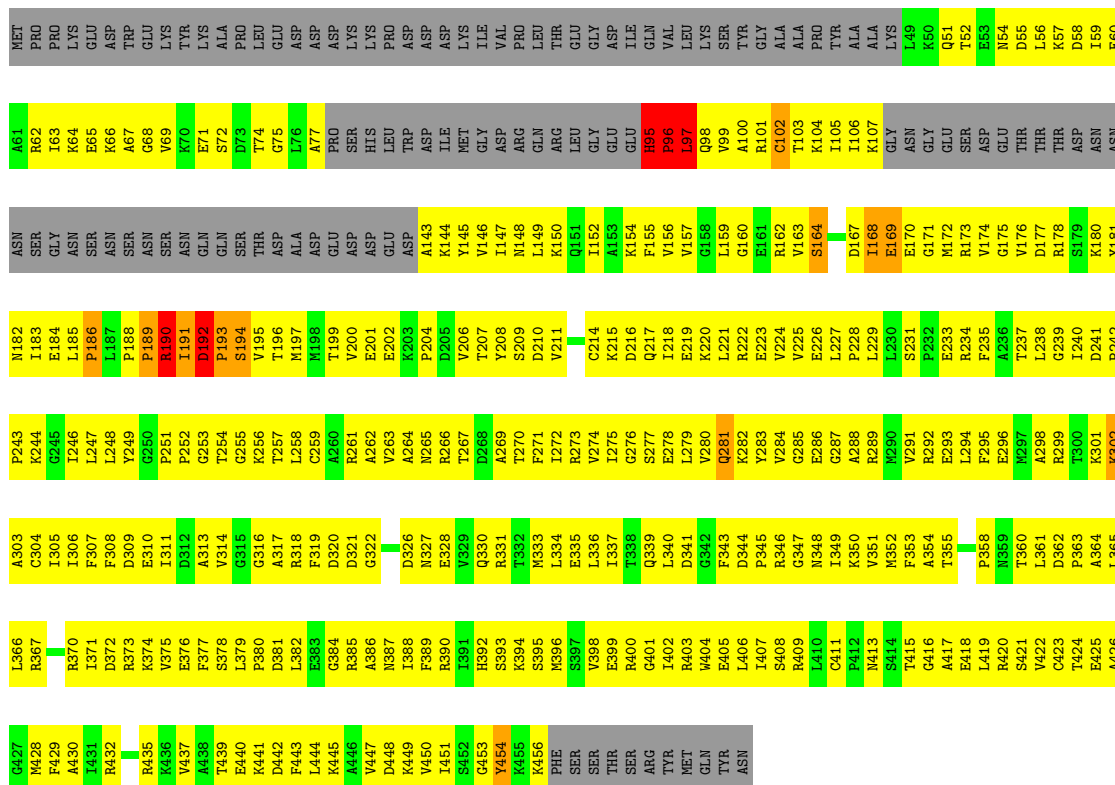
- Molecule 14: Probable proteasome subunit alpha type-7

Chain g: 83% • 15%



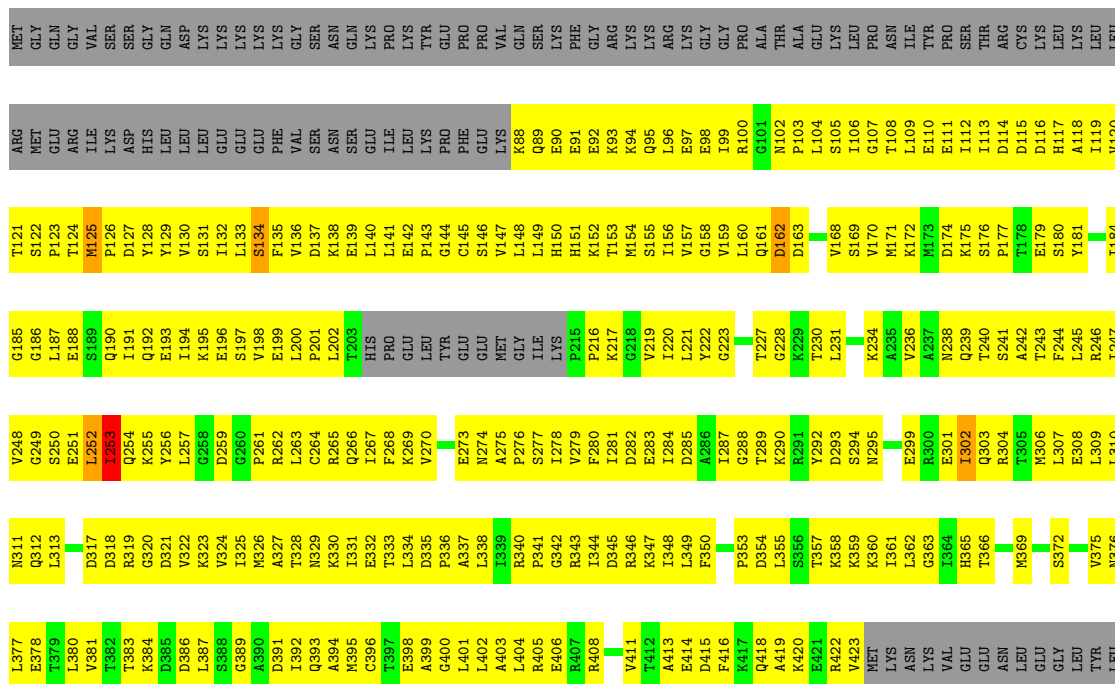
- Molecule 15: 26S protease regulatory subunit 7 homolog

Chain H:  13% 60% 24%



- Molecule 16: 26S protease regulatory subunit 4 homolog

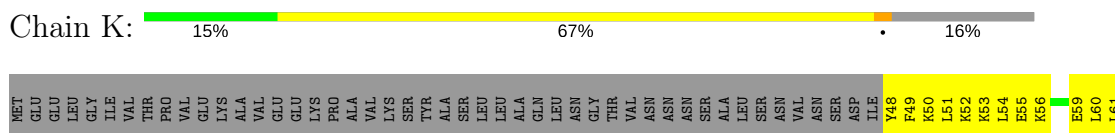
Chain I: 13% 60% . 26%



- Molecule 17: 26S protease regulatory subunit 8 homolog



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



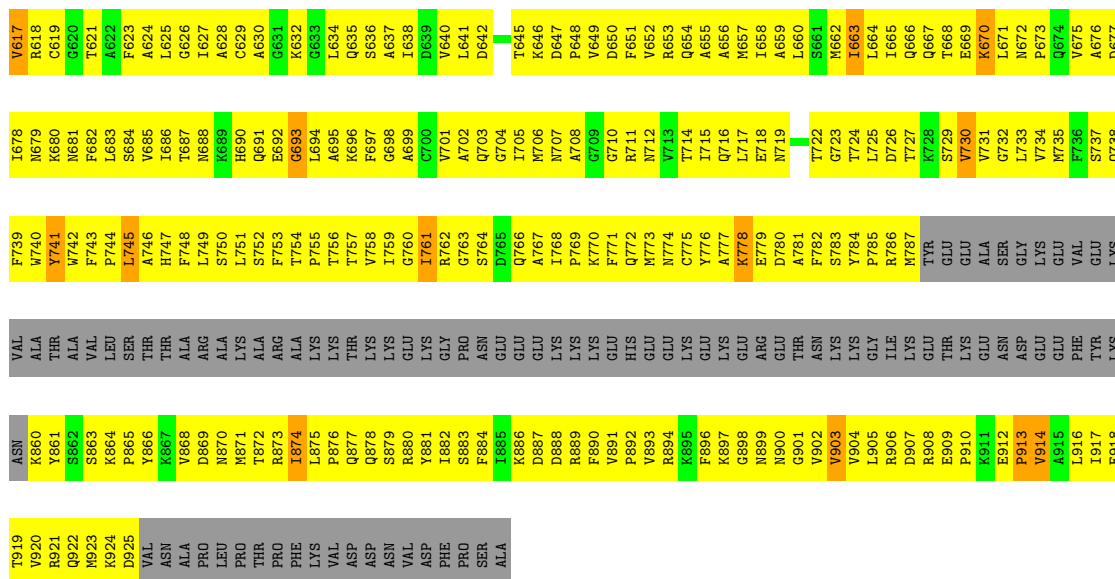
T62	T125	E189	R252	V314	R374	T62	T125	E189	R252	V314	R374
L63	L126	L190	M253	L315	N375	L63	L126	L190	M253	L315	N375
Q64	D127	P191	V254	M316	D376	Q64	D127	P191	V254	M316	D376
E65	R128		R255	A317	S377	E65	R128		R255	A317	S377
D66	E129		D256	L318	L378	D66	E129		D256	L318	L378
Y67	L130		V257	N319	S379	Y67	L130		V257	N319	S379
T68	L131		F258	R320	G380	T68	L131		F258	R320	G380
K69	K132		R259	A321	A381	K69	K132		R259	A321	A381
D70			L260	D322	V382	D70			L260	D322	V382
E71	M135		A261	L323	L383	E71	M135		A261	L323	L383
Q72	L136		R262	L324	A384	Q72	L136		R262	L324	A384
R73	S136		E263	D325	A385	R73	S136		E263	D325	A385
H74	V137		N264	P326	I386	H74	V137		N264	P326	I386
L75	A138		A265	A327	M387	L75	A138		A265	A327	M387
	L139		P266	L328	Q388		L139		P266	L328	Q388
	H140		S267	L329	R389		H140		S267	L329	R389
	R141		I268	R330	A390		R141		I268	R330	A390
	H142		I269	P331	G391		H142		I269	P331	G391
	L143		G208	G332	L392		L143		G208	G332	L392
	N144		I271	R333	R393		N144		I271	R333	R393
	A145		D272	L334	A394		A145		D272	L334	A394
	L146		E273	D335	V395		L146		E273	D335	V395
	E84		V274	R336	R396		E84		V274	R336	R396
	I149		D275	K337	K397		I149		D275	K337	K397
	E85		S276	I338	N398		E85		S276	I338	N398
	V86		I277	E339	R399		V86		I277	E339	R399
	K87		A278	F340	Y400		K87		A278	F340	Y400
	R88		T279	P341	V401		R88		T279	P341	V401
	L89		K280	L342	I402		L89		K280	L342	I402
			R281	S343	L403				R281	S343	L403
			G282	R344	Q404				G282	R344	Q404
			D283	D345	S405				D283	D345	S405
			A284	R346	D406				A284	R346	D406
			Q285	R347	L407				Q285	R347	L407
				E348	E408					E348	E408
				A409	E409					A409	E409
			D289	R350	A410				D289	R350	A410
			E291	L351	Y411				E291	L351	Y411
			V292	I352	A412				V292	I352	A412
			Q293	F353					Q293	F353	
			R294	G354	V415				R294	G354	V415
			I295	T355					I295	T355	
			L296	I356	D418				L296	I356	D418
			I297	A357	ASN				I297	A357	ASN
			E298	S358	THR				E298	S358	THR
			L299	K359	VAL				L299	K359	VAL
			L300	K360	ASP				L300	K360	ASP
			T301	S361	LYS				T301	S361	LYS
			Q302	L362	PHE				Q302	L362	PHE
			M303	A363	ASP				M303	A363	ASP
			D304	F364	TYR				D304	F364	TYR
			G305	E365	LYS				G305	E365	LYS
			F306	A366					F306	A366	
			D307	D367					D307	D367	
			Q308	L368					Q308	L368	
			S309	D369					S309	D369	
			T310	S370					T310	S370	
			N311	E371					N311	E371	
			V312	L372					V312	L372	
			K313	I373					K313	I373	

• Molecule 19: 26S protease subunit RPT4

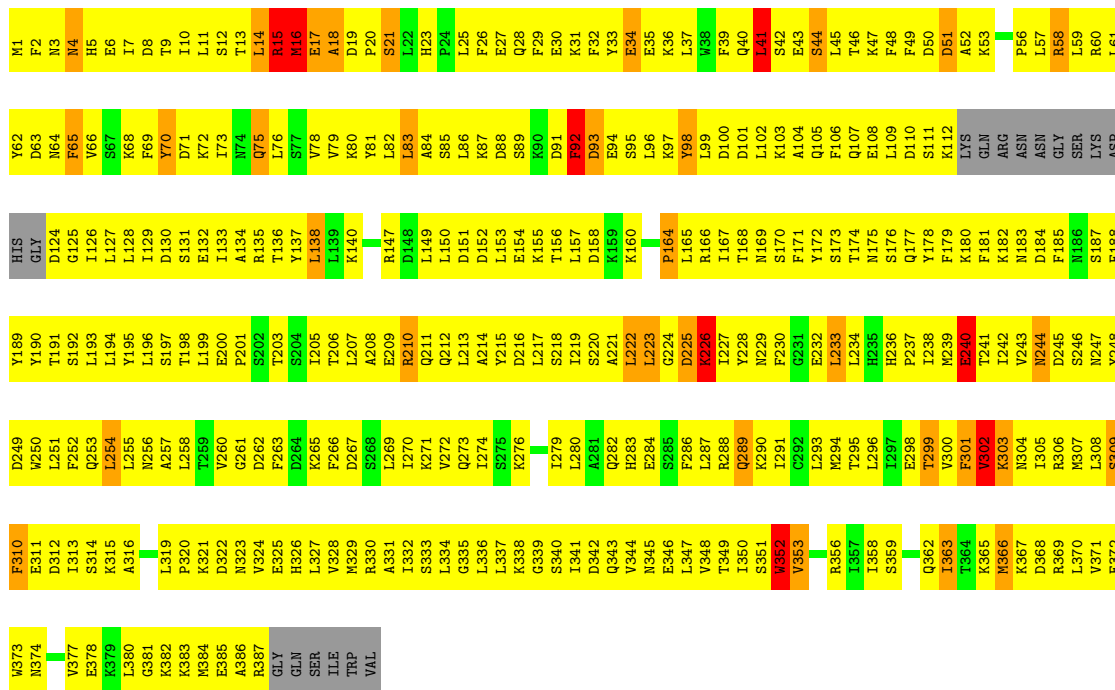
Chain L: 12% 68% 18%

LEU	V368	M306	F245	I183	S122	LVS	MET
GLU	K369	E307	S246	G184	G123	ARG	SER
GLY	K370	L308	P247	T187	G124	K63	GLU
THR	T371	L309	A248	Q189	P125	L64	GLN
ILE	K372	T310	S249	Q188	P126	L65	GLN
GLU	E373	Q311	G250	Q189	Y127	E66	ASP
TYR	F374	K312	T251	R190	I128	H67	PRO
GLN	D313	D313	V252	R191	I129	R68	LEU
LYS	F376	G314	D253	E192	G130	R69	LEU
LEU	E377	F315	K254	L193	V131	Y70	ALA
	A378	D316	V255	R194	R132	D71	GLY
	A379	K317	T256	E195	N133	D72	LEU
	V380	L318	G257	V196	S134	Q73	GLY
	K381	G319	E258	E197	V135	L74	GLU
	M382	Q320	S259	E198	D136	K75	THR
	S383	T321	A260	L199	R137	Q76	SER
	D384	K322	R261	P200	S138	R77	GLY
	G385	I323	T262	L201	K139	R78	ASP
	F386	I324	T263	K202	L140	Q79	ASN
	K387	M325	R264	N203	K141	N80	HIS
	G388	A326	E265	E204	K142	I81	THR
	M389	T327	M266	E205	G143	R82	GLN
	D390	K328	F267	ILE	V144	D83	GLN
	I391	K329	A268	PHE	R145	L84	SER
	R392	P330	V269	GLN	V146	E85	HIS
	K393	L333	A270	ARG	T147	K86	GLU
	C394	L334	K271	VAL	L148	L87	GLN
	A395	D334	E272	GLY	D149	Y88	GLN
	T396	F335	H273	ILE	I150	D89	PRO
	E397	A336	E274	K213	T151	K90	GLU
	A398	L337	T275	P214	T152	T91	GLN
	G399	L338	C276	P215	L153	E92	PRO
	F400	R339	T277	T216	T154	N93	GLN
	A401	P340	T278	G217	I155	D94	GLU
	A402	G341	F279	V218	M156	I95	THR
	I403	R342	M280	L219	R157	K96	GLU
	A404	L343	D281	L220	I158	A97	GLU
	D405	D344	E282	Y221	L159	L98	HIS
	D406	R345	V283	G222	P160	Q99	HIS
	R407	K346	D284	P223	R161		GLU
	D408	V347	A285	P224	E162	G102	GLU
	H409	E348	T286	G225	T163	Q103	GLU
	I410	I349	G287	T226	D164	T104	PRO
	N411		G288	G227	P165	I105	SER
	P412		R289	K228	L166	G106	ARG
	D413	K352	R290	T229	V167	E107	VAL
	D414	N353	E354	L230	Y168	V108	ASP
	L415	A355	F291	L231	M169	M109	PRO
	M416	G356	G294		M170	K110	GLU
	K417	R357	T295	A234	T171	E111	GLN
	A418	L358	S296	D235	S172	L112	GLU
	V419	E359	A297	A236	F173	S113	ALA
	R420	V420	D298	A237	E174	E114	HIS
	K421	F361	R299	T338	Q175	E115	ASN
	V422	K362	E300	L239		K116	LYS
	A423	I363	T301	G240	I178	Y117	ALA
	E424	K364	Q302	N241	T179	I118	LEU
	V425	T365	R303	N242	F180	V119	ASN
	K426	A366	T304	F243	D181	K120	GLN
	M427	V367	T305	T244	G182	A121	THR

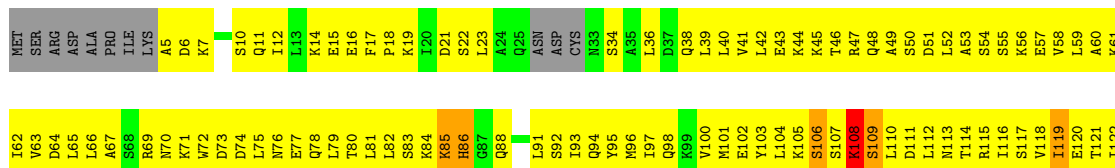
L557	L558	A497	E437	H375	L313	E247	N187	F123	L63	MET
A558	A559	L498	D438	K376	L314	E248	Y188	Y124	I64	SER
A560	D500	H499	V439	G377	N315	N249	L189	T125	A65	LEU
A561	G561	M501	V441	L379	K316	D250	L190	K126	S66	T4
T562	G563	F502	L442	L380	S317	L253	L192	I129	K67	T5
G564	G565	T503	L443	E381	S319	S254	A193	D130	V68	A6
N565	N566	S505	H444	G382	S320	A255	A194	P131	Y69	A7
S567	S568	G506	A445	K383	L321	K256	L195	K132	T70	P8
E567	T508	E507	S447	K384	D322	T257	L196	L133	L72	L9
V568	O509	T509	L448	M386	G323	A258	G73	T134	G73	L10
K569	K570	H510	G449	A387	K324	P259	L198	S135	E74	L12
R570	L571	L511	T450	P388	S326	L261	S200	F137	Y75	L13
L572	L573	N512	G451	Y389	L327	V262	K201	E138	E76	R14
H573	T514	L452	A453	L390	F328	S263	F202	E139	S77	E15
V574	R515	G392	A454	P391	H329	S264	R203	N16	A78	N16
A575	M455	S393	M455	S393	T330	L269	S204	D18	V79	K17
V576	G458	S397	G458	S397	V332	L270	S205	E142	Y81	S19
S577	A458	R398	A458	R398	S333	L271	T206	K143	A82	V20
D578	V519	P399	M459	P399	V334	L272	R208	C144	L83	K21
S579	G520	K400	I460	K401	A335	L273	K209	L145	A84	T22
N580	L521	K401	E461	G337	N336	V274	S210	K146	A85	Y23
D582	L522	G402	V462	G402	G337	T275	F211	A147	K86	A24
H583	L523	G403	V463	G403	F338	E276	D212	L180	R88	L25
S584	T524	H404	E464	S404	H340	L277	F213	K151	F89	I28
R585	N525	L405	A465	L405	A341	Q280	M215	L152	D90	N29
A586	Y526	L466	V466	L466	G342	G281	N216	A153	I91	D32
G587	G527	K467	G407	G407	T343	Y282	M217	I154	D92	V32
V588	R528	L408	E468	L408	T344	D283	P218	G155	E93	D33
S589	Q529	L409	V469	L409	D345	E284	N219	A157	S95	Q34
A590	E530	L410	L470	L410	N346	A285	C220	E159	Q96	W36
L591	L531	Y411	Y471	Y412	S347	L286	D221	G160	F97	S37
G592	D533	A413	D473	A413	F348	L287	L223	Y161	E98	E38
F593	F594	S474	S474	G414	K350	L288	T224	R162	E99	I39
L595	L536	T476	A475	F415	A351	L289	L225	L163	T100	S40
R597	T537	G416	T477	R417	N352	L290	N226	D164	I101	M41
G598	K538	D418	G478	T419	N355	L293	N227	I165	S103	E42
V599	L540	T420	A480	T420	K358	T295	V228	I166	K104	P44
T601	A541	D421	A481	D421	A359	C296	V230	E167	S105	D45
V602	S542	L423	A482	L423	Q360	D297	N231	A169	E107	I46
P603	D543	K424	L483	K424	N361	Y298	L232	L170	M108	E48
R604	E544	M485	G484	M485	N362	N300	D234	Y109	Y110	L49
I605	S545	L426	G486	L426	A363	T301	A235	D175	Q111	Y50
V606	L547	L427	L487	L427	K364	F302	G236	Q176	E112	D52
Q607	L547	R548	L487	R548	F365	L303	L237	ASP	A113	D53
L608	R549	M489	M489	M489	T366	L304	A238	S178	S114	T54
S610	O550	G491	L490	G491	N305	N306	Q240	T179	K115	F55
K611	S551	G492	L491	G492	T368	K307	L241	S180	Q116	S56
S612	A552	T493	G493	T493	S370	N308	F242	E181	Y117	D57
H613	T554	F553	G494	S434	L371	I309	K243	N182	T118	R58
N614	A615	T555	P495	S435	G372	D310	L244	K184	E121	M60
A615	A616	V118	V119	V118	V373	I311	K245	L246	PHE	E59
H616	K120	G185	G185	ALA	I374	Q122	A62	I186	Q122	A62
L121	S122	L186	D187	Q250	F315	W376	Q377	W376	Q377	Q377
S123	R124	M254	T190	Q253	D319	L378	E378	L378	E378	L378
ASN	ASN	L193	V194	M254	R320	A380	A380	A380	A380	A380
LVS	T126	L193	V194	Q255	R321	R381	R381	R381	R381	R381
GLU	T127	L193	V194	Q256	R322	S382	S382	S382	S382	S382
LVS	F128	L193	V194	Q257	R323	T383	T383	T383	T383	T383
LVS	L129	L193	V194	Q258	R324	D384	D384	D384	D384	D384
LVS	L130	L193	V194	Q259	R325	E385	E385	E385	E385	E385
LVS	L131	L193	V194	Q260	R326	F386	F386	F386	F386	F386
LVS	L132	L193	V194	Q261	R327	N387	N387	N387	N387	N387
LVS	L133	L193	V194	Q262	R328	G388	G388	G388	G388	G388
LVS	L134	L193	V194	Q263	R329	A389	A389	A389	A389	A389
LVS	L135	L193	V194	Q264	R330	Q390	Q390	Q390	Q390	Q390
LVS	L136	L193	V194	Q265	R331	L391	L391	L391	L391	L391
LVS	L137	L193	V194	Q266	R332	K392	K392	K392	K392	K392
LVS	L138	L193	V194	Q267	R333	A393	A393	A393	A393	A393
LVS	L139	L193	V194	Q268	R334	L394	L394	L394	L394	L394
LVS	L140	L193	V194	Q269	R335	T395	T395	T395	T395	T395
LVS	L141	L193	V194	Q270	R336	V396	V396	V396	V396	V396
LVS	L142	L193	V194	Q271	R337	E397	E397	E397	E397	E397
LVS	L143	L193	V194	Q272	R338	A398	A398	A398	A398	A398
LVS	L144	L193	V194	Q273	R339	G399	G399	G399	G399	G399
LVS	L145	L193	V194	Q274	R340	M400	M400	M400	M400	M400
LVS	L146	L193	V194	Q275	R341	I401	I401	I401	I401	I401
LVS	L147	L193	V194	Q276	R342	A402	A402	A402	A402	A402
LVS	L148	L193	V194	Q277	R343	L403	L403	L403	L403	L403
LVS	L149	L193	V194	Q278	R344	R404	R404	R404	R404	R404
LVS	L150	L193	V194	Q279	R345	N405	N405	N405	N405	N405
LVS	L151	L193	V194	Q280	R346	G406	G406	G406	G406	G406
LVS	L152	L193	V194	Q281	R347	Q407	Q407	Q407	Q407	Q407
LVS	L153	L193	V194	Q282	R348	S408	S408	S408	S408	S408
LVS	L154	L193	V194	Q283	R349	S409	S409	S409	S409	S409
LVS	L155	L193	V194	Q284	R350	V410	V410	V410	V410	V410
LVS	L156	L193	V194	Q285	R351	L351	L351	L351	L351	L351
LVS	L157	L193	V194	Q286	R352	K411	K411	K411	K411	K411
LVS	L158	L193	V194	Q287	R353	H412	H412	H412	H412	H412
LVS	L159	L193	V194	Q288	R354	E413	E413	E413	E413	E413
LVS	L160	L193	V194	Q289	R355	D414	D414	D414	D414	D414
LVS	L161	L193	V194	Q290	R356	F415	F415	F415	F415	F415
LVS	L162	L193	V194	Q291	R357	V416	V416	V416	V416	V416
LVS	L163	L193	V194	Q292	R358	E417	E417	E417	E417	E417
LVS	L164	L193	V194	Q293	R359	L418	L418	L418	L418	L418
LVS	L165	L193	V194	Q294	R360	Q419	Q419	Q419	Q419	Q419
LVS	L166	L193	V194	Q295	R361	S420	S420	S420	S420	S420
LVS	L167	L193	V194	Q296	R362	E421	E421	E421	E421	E421
LVS	L168	L193	V194	Q297	R363	L419	L419	L419	L419	L419
LVS	L169	L193	V194	Q298	R364	I418	I418	I418	I418	I418
LVS	L170	L193	V194	Q299	R365	E422	E422	E422	E422	E422
LVS	L171	L193	V194	Q300	R366	V423	V423	V423	V423	V423
LVS	L172	L193	V194	Q301	R367	Q424	Q424	Q424	Q424	Q424
LVS	L173	L193	V194	Q302	R368	H364	H364	H364	H364	H364
LVS	L174	L193	V194	Q303	R369	S365	S365	S365	S365	S365
LVS	L175	L193	V194	Q304	R370	T366	T366	T366	T366	T366
LVS	L176	L193	V194	Q305	R371	L367	L367	L367	L367	L367
LVS	L177	L193	V194	Q306	R372	Q368	Q368	Q368	Q368	Q368
LVS	L178	L193	V194	Q307	R373	T369	T369	T369	T369	T369
LVS	L179	L193	V194	Q308	R374	S370	S370	S370	S370	S370
LVS	L180	L193	V194	Q309	R375	N371	N371	N371	N371	N371
LVS	L181	L193	V194	Q310	R376	V372	V372	V372	V372	V372
LVS	L182	L193	V194	Q311	R377	I373	I373	I373	I373	I373
LVS	L183	L193	V194	Q312	R378	D374	D374	D374	D374	D374
LVS	L184	L193	V194	Q313	R379	E375	E375	E375	E375	E375
LVS	L185	L193	V194	Q314	R380	L375	L375	L375	L375	L375
LVS	L186	L193	V194	Q315	R381	T376	T376	T376	T376	T376
LVS	L187	L193	V194	Q316	R382	Q377	Q377	Q377	Q377	Q377
LVS	L188	L193	V194	Q317	R383	S378	S378	S378	S378	S378
LVS	L189	L193	V194	Q318	R384	T379	T379	T379	T379	T379
LVS	L190	L193	V194	Q319	R385	N380	N380	N380	N380	N380
LVS	L191	L193	V194	Q320	R386	L381	L381	L381	L381	L381
LVS	L192	L193	V194	Q321	R387	E382	E382	E382	E382	E382
LVS	L193	L193	V194	Q322	R388	S383	S383	S383	S383	S383
LVS	L194	L193	V194	Q323	R389	T384	T384	T384	T384	T384
LVS	L195	L193	V194	Q324	R390	V385	V385	V385	V385	V385
LVS	L196	L193	V194	Q325	R391	A386	A386	A386	A386	A386
LVS	L197	L193	V194	Q326	R392	M387	M387	M387	M387	M387
LVS	L198	L193	V194	Q327	R393	L388	L388	L388	L388	L388
LVS	L199	L193	V194	Q328	R394	E389	E389	E389	E389	E389
LVS	L200	L193	V194	Q329	R395	T390	T390	T390	T390	T390
LVS	L201	L193	V194	Q330	R396	V391	V391	V391	V391	V391
LVS	L202	L193	V194	Q331	R39					



- Molecule 22: 26S proteasome regulatory subunit RPN9



- Molecule 23: 26S proteasome regulatory subunit RPN5



L423	E243	F303	L363	L423	R123
E424	E245	T304	R364	E425	V124
H425	Y245	T305	L365	H426	V125
L426	Y246	N306	L366	E427	T126
E427	E247	E307	E367	T428	S127
T428	D248	L308	L368	T429	N128
L309	D249	M309	L369	G430	K129
L310	L250	W311	D370	H431	K130
L311	K251	F312	L371	G432	F131
F312	S252	I313	T372	L433	V132
I313	D253	A111	E373	L434	E133
A111	E254	R112	S374	T434	V134
R112	E255	R113	Q375	K435	E135
R113	Q256	Q315	T376	E436	R136
Q315	K256	K316	E377	E437	A196
K316	W257	T317	T378	I438	T197
T317	K258	F318	T379	M439	R198
F318	P259	R320	V380	H440	L199
R320	V260	V321	S381	G441	P199
V321	L261	L322	D382	L442	R201
L261	S262	N323	L383	GLN	K202
N323	H263	E324	V384	ALA	L143
E324	L264	D325	N385	LYS	L144
D325	V265	D326	Q386		E145
D326	Y266	L327	Q387		K206
L327	F267	A328	T388		T207
A328	L268	F329	I389		F208
F329	Y269	G330	L270		K209
G330	N210	G331	Y390		E149
G331	E151	E332	A391		N210
E332	K212	L332	K392		G151
L332	K152	V393	L393		P212
V393	I153	K394	K395		Y213
K394	D154	K396	P396		E214
K396	E155	S397	A397		S215
S397	A157	W398	K398		L216
W398	D158	L399	T399		K217
L399	E159	Q400	I399		L218
Q400	L160	M401	Q400		E219
M401	C161	F402	F402		Y220
F402	L162	E403	E403		Y221
E403	L163	A404	A404		N222
A404	Q164	F405	F405		L223
F405	V165	K406	K406		L224
K406	E166	M407	M407		V225
M407	T167	S408	S408		K226
S408	Y168	D409	D409		D287
D409	G169	L110	L110		S228
L110	L169	P172	P172		L229
P172	K230	D112	D112		L230
D112	S170	D113	D113		H231
D113	M171	Q114	Q114		K291
Q114	E172	I115	I115		R292
I115	M173	F116	F116		L293
F116	S174	L117	L117		E294
L117	E175	L180	L180		S295
L180	K176	E181	E181		E296
E181	V237	K120	K120		E297
K120	I177	S182	S182		Y297
S182	I178	K183	K183		A238
K183	F179	N248	N248		Q239
N248	L180	L249	L249		Y240
L249	L281	E123	E123		K301
E123	E182				L302

• Molecule 24: 26S proteasome regulatory subunit RPN6

Chain Q:  12% 85%

M1	L61	A125	K187	T251	L311	Q372	VAL
S2	G62	K126	L188	H252	L312	V373	LEU
L3	Q63	R127	R189	N253	D313	E374	TYR
P4	L64	E128	M190	S254	F314	G375	
G5	Y65	K129	L191	Y255	N315	K376	
S6	V66	R130	A192	E256	T316	L377	GLU
K7	T67	V131	K193	K257	A317	S378	LYS
L8	M68	F132	S194	A258	L318	Q379	SRR
E9	G69	L133	K195	C259		M380	
E10	A70	K134	A196	Q260	Y321	L381	GLN
A11	R71	H135	K197	V261	E322	L382	GLU
R12	D72	L136	L198	L262	K323	D383	GLU
R13	K73	S137	T199	K263	E324	K384	TVR
L14	L74	S138	A200	Y264	L325	I385	VAL
V15	R75	I139	A201	M265	M326	F386	ASP
N16	E76	K140	E202	L266	G327	F387	PRO
E17	F77	L141	A205	L267	D328	G388	THR
K18	I78	A142		S268	E329	V389	VAL
Q19	P79	T143	T208	K269	L330	L390	ASN
Y20	H80	L144		L270	T331	D391	ARG
N21	S81	H145		M271	R332	L392	VAL
E22	T82	Y146	T212	L272	S333	G393	PRO
A23	E83	Q147	Q213	N273	H334	N394	N23
E24	Y84	K148	T214	L274	F335	G395	Y24
Q25	M85	K149	V215	L275	N336	W396	E25
V26	M86	Q150	A216	D276	A337	L397	V26
Y27	Q87	Y151	E217	D277	L338	F398	S27
L28	F88	S154	L218	V278	Y339	V399	E28
S29	A89	L155	D219	K279	D340	Y400	K29
K90	K90	L156	L220	N280	T341	E401	A30
L31	T93	L157	M221	L221	L342	T402	F31
D32		L158	S222	G223	L343	F403	L32
K33		I158	S223	L283	E344	M404	L33
D34		L97	L224	A284	S345	Q405	T34
S35		K98	L225	K285	N346	D406	Q35
S36		T99	H226	Y286	L347	A407	S36
Q37		L161	C227	T287	G348	T408	K37
S38		L162	L162	K288	K349	Y409	V38
S39		E102	E228	E289	I350	D410	S39
A40		K103	D229	E290	L351	S411	T40
A41		F104	K230	T290	E352	A412	E41
E403		E105	D231	Y291	P353	L413	Q42
A42		Q106	D232	Y292	F354	E414	R43
G43		V107	Y232	S293	R294	L415	K44
A44		P108	K233	K294	C355	V416	E45
S45		D109	T234	R295	G356	G417	A46
V46		S110	A235	G295	V357	Q418	A47
D47		P172	F236	L296	I359	L419	E48
D48		S173	S237	A298	S360	M299	F49
R50		L174	Y238	M299	K300	K421	V50
K49		D113	F239	E241	A301	V422	L51
R51		Q114	E242	E241	V302	V423	A52
N52		F116	S242	E242	K364	D424	K53
E53		L117	F243	F243	L365	Q425	I54
Q54		C118	E244	E244	L366	L426	K55
E55		E119	S245	S245	G367	F427	E56
T56		K120	Y246	Y246	L368	S428	E57
S57		S121	K183	H247	D369	K429	E58
L58		I122	V184	N248	A309	T370	M59
E60		E123	Y185	L249	S431		A60
		F124	H186				

• Molecule 25: 26S proteasome regulatory subunit RPN7

Chain R:  6% 79% 8% 7%

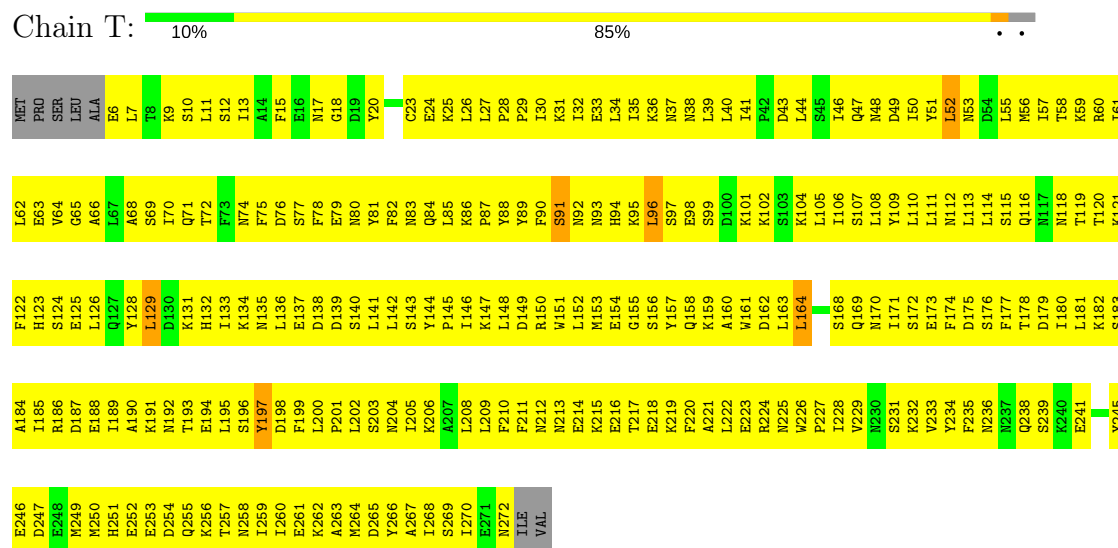
MET	N23	F31	L32	L33	Q35	S36	K37	V38	S39	T40	E41	Q42	R43	K44	E45	A46	A47	E48	F49	V50	L51	A52	K53	I54	K55	E56	E57	E58	M59	A60
ASP	Y24																													
VAL	V26																													
GLU	S27																													
GLU	E28																													
LYS	K29																													
SER	A30																													
GLN	F31																													
GLU	L32																													
VAL	L33																													
GLU	T34																													
VAL	Q35																													
GLU	S36																													
VAL	K37																													
TYR	V38																													
ASP	S39																													
VAL	T40																													
PRO	E41																													
THR	Q42																													
VAL	R43																													
ASN	K44																													
ARG	E45																													
VAL	A46																													
PRO	A47																													
VAL	E48																													

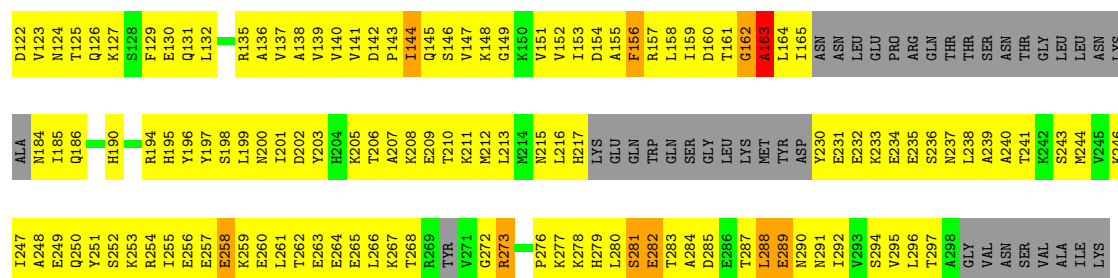
THR	D440	C380	I320	K256	H196	I134	T73	R422	A362	A302	E242	N182	E122	P61
LEU	G441	V381	Q321	L257	S197	N136	L74	LEU	F363	S303	L243	D183	D123	Y62
ASP	F442	R382	L322	E258	S198	C136	C75	THR	L364	F304	T244	D184	D124	X64
GLY	I443	L383	L323	Y259	E199	F137	F76	GLY	F305	P306	S245	L185	K185	K64
ASP	E444	R384	M324	E260	E200	H138	THR	SER	N366	P307	Y246	Y186	E127	Y65
LEU	T445	S385	G325	H261	I201	H139	VAL	ASP	D367	Y307	S248	V187	E128	L66
MET	T446	N386	D326	H262	N202	L140	ASN	ARG	L368	L308	S249	K188	E129	C67
ASP	E447	V387	I327	Y264	S203	L141	VAL	VAL	C369	L309	I250	E189	E129	E68
ASP			P328	S265	D204	Y142	LEU	V10	K370	E310	A259	K190	Q130	E69
MET	I451	K388	E329	S266	N205	Q143	TYR	D11	F371	T311	I251	L191	A131	Y70
SER	Y452	K389	L330	S267	Q206	L144	PRO	S12	I372	Y252	Y252	E192	Q132	L71
ASP	D453	T390	S331	L268	N207	F145	ASP	S13	P373	A313	A253	A193	A133	V72
ILE	S454	I392	F332	E269	I208	L146	SER	G14	N374	N314	S254	V194	W134	N73
SER	E455	R393	F383	A270	I209	W147	SER	V15	K375	V315	V255	N195	I135	N74
ASP	D456	I394	H334	R271	L210	D148	SER	N16	Q376	L316	T256	S196	N136	G75
LEU	P457	I395	Q335	Y272	R211	S149	PHE	D17	L377	T317	G257	M197	L137	G76
ASP	Q458	S396	S336	F273	L212	K150	LYS	L18	N378	P318	F259	I198	G138	S77
ASP	Q459	S397	N337	F274	T213	E151	LYS	H19	C379	C319	L258	E199	E139	D78
LEU	V460	T398	M338	Y275	M214	L152	ASN	H20	V380	K320	T260	K200	Y140	L79
GLY	F461	Y399	Q339	L276	M215	E153	LEU	S21	I381	Y321	L261	G201	Y141	E80
PHE	D462	K401	K340	S277	K216	Q154	LEU	E22	D382	L322	E262	G202	A142	H81
LEU	E463	L342	S341	K278	F217	L155	LYS	K23	R383	R263	D263	D203	Q143	D82
ASP	R464	I402	L342	I279	L218	V156	PHE	K24	V384	R324	T264	W204	I144	E83
LEU	I465	S403	L343	N280	K219	E157	ILE	Y25	N385	H325	D265	E205	G145	X84
	K466	L404	P344	A281	T220	F158	THR	A26	G386	A326	L266	R206	D146	
	F467	R405	Y345	I282	A221	N159	SER	E27	I387	D327	K267	R207	K147	S87
	A468	D406	Y346	Q283	S222	R160	ASN		V388	F328	S268	N208	D148	L88
	N469	I407	H347	L284	L223	K161	HIS		F329	F329	K269	R209	N149	N89
	Q470	C408	L348	D285	K224	V162	LYS		Y330	V330	V270	Y210	A150	E90
	L471	L409	T349	Y286	H225	V163	SER		N391	R331	T271	K211	E151	W91
	H472	K410	K350	S287	D226	I164	SER		R392	E332	D272	T212	K152	I92
	D473	L411	A351	T288	N227	P165	VAL		P393	K333	S273	Y213	T153	K93
	E474	M412	V352	A289	E228	L166	PRO		D394	R334	T274	Y214	L154	F94
	L476	D414	K353	N290	T229	L167	GLY		N395	R335	E275	G215	K155	D95
	V477	S415	G355	Y292	K230	L167	SER		K396	R336	L276	T216	K156	Q96
	S478	F416	D356	I293	A231	Y170	ALA		N397	V337	L277	H217	E157	E97
	Q479	T418	D357	I294	M232	Y171	GLU		A398	Y338	S278	C218	L158	L98
	Y480	V419	L357	I294	L233	Y171	LEU		Q399	A339	L279	L219	S159	Y99
	P482	E420	K358	A296	I234	R174	ARG		Y400	Q340	I280	A220	K160	N100
	E483	Y421	P360	A296	N235	S175	ASN		H401	L341	S281	Y221	A161	E101
	D484	M422	T361	I297	L236	L176	SER		L402	E342	T282	R222	I162	L102
	K485	V423	S362	P301	L238	N177	TYR		L403	E343	T283	N223	S163	C103
	K486	S424	T363		R239	L178	PRO		V404	S344	T47	F224	T164	K104
	Q488	S424	I364		R239	I179	ALA		K405	Y345	A284	K225	G165	K105
ASN	GLN	R428	T365	K305	D240	N180	SER		Q406	K346	L286	E226	A166	N106
GLU	GLU	D429	L370	S306	F241	A181	PHE		G407	T347	Q287	A227	K167	E107
LYS	SER	G430	L310	S307	N243	L183	TYR		D408	L348	S288	A228	I168	S108
GLU	GLU	V431	Q311	L307	N244	L184	SER		G409	S349	I289	K229	D169	K109
ASN	GLU	D429	L310	G308	G245	W184	VAL		L410	L350	S290	L230	V170	I110
LYS	SER	G430	L310	F185	E246	F185	THR		L411	K351	S291	L231	M171	K111
GLU	GLU	V431	Q311	Y186	V247	I187	GLU		T412	S352	L292	V232	L172	E112
ASN	GLU	T432	Q312	D248	D248	L188	LYS		K353	R353	T293	D233	L173	E113
ASN	GLU	E433	S313	S249	L189	L57	LYS		L414	A354	I294	S234	I174	N114
GLY	GLU	A434	D374	A250	S249	L189	LYS		Q415	S355	S295	L235	A175	E115
GLY	GLU	K435	D375	S251	N244	S190	K416		K416	A356	L296	A236	R176	K116
ASN	ASN	I436	K315	D252	G245	H191	Y417		Y417	F357	Y297	T237	L177	I117
ASP	ASP	N437	L316	D252	E246	E192	E129		G418	G358	A298	F238	G178	Q118
ASP	ASP	H438	H317	F253	E246	I193	V130		A419	V359	S299	T239	F179	K119
ASP	ASP	L379	Q378	L254	E246	L194	T131		A420	S360	D300	S240	F180	L120
				S255		A195	E133		V421	V361	Y301	I241	Y181	E121

• Molecule 26: 26S proteasome regulatory subunit RPN3

Chain S: 13% 64% 7% 16%

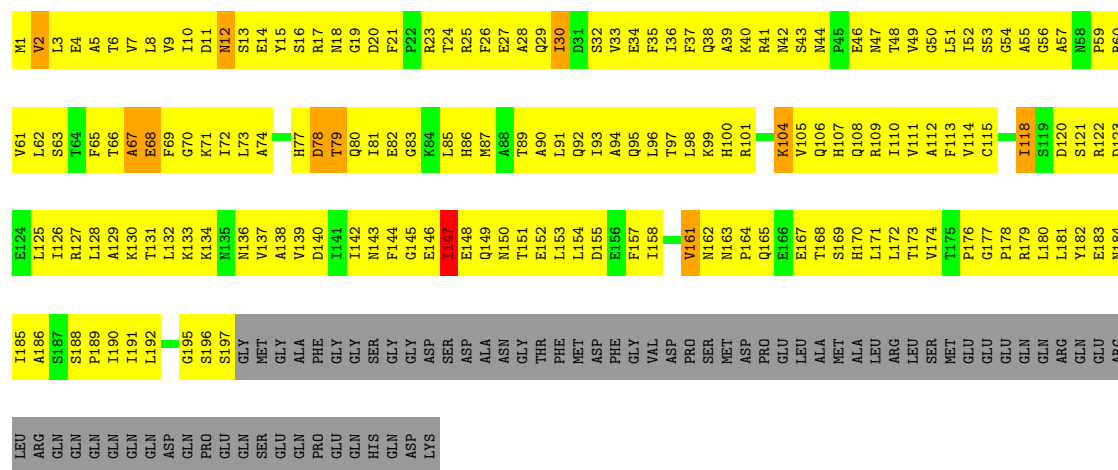
• Molecule 27: 26S proteasome regulatory subunit RPN12





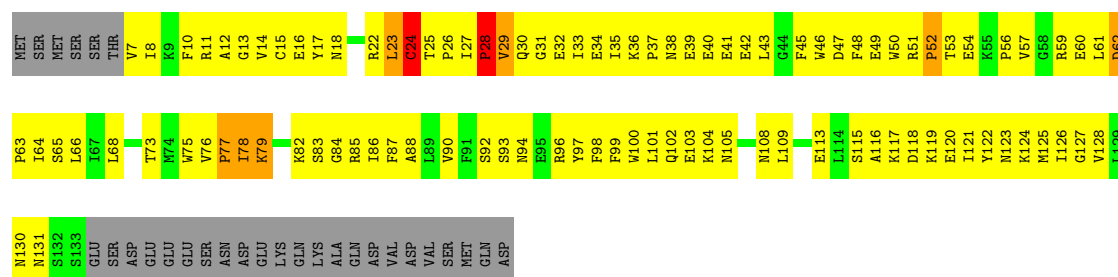
• Molecule 30: 26S proteasome regulatory subunit RPN10

Chain W: 9% 60% 26%



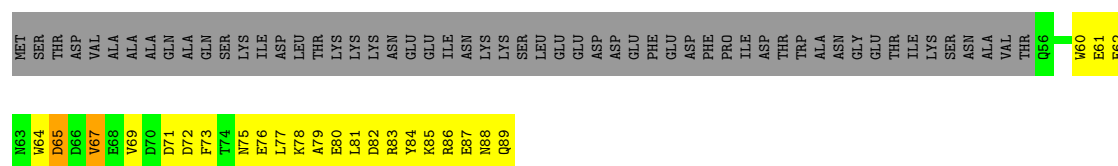
• Molecule 31: 26S proteasome regulatory subunit RPN13

Chain X: 17% 58% 19%



• Molecule 32: 26S proteasome complex subunit SEM1

Chain Y: 10% 26% 62%



• Molecule 33: 26S proteasome regulatory subunit RPN1

Response	Percentage
No	19%
Yes	56%
Don't know	23%




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

Continued on next page...

Continued from previous page...

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%)	32	74
1	8	220/241 (91%)	202 (92%)	17 (8%)	1 (0%)	32	74
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%)	32	74

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	h	203/215 (94%)	179 (88%)	23 (11%)	1 (0%)	32	74
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%)	32	74
5	j	202/205 (98%)	185 (92%)	16 (8%)	1 (0%)	32	74
6	6	196/198 (99%)	175 (89%)	19 (10%)	2 (1%)	18	61
6	k	196/198 (99%)	174 (89%)	19 (10%)	3 (2%)	12	53
7	7	210/287 (73%)	188 (90%)	20 (10%)	2 (1%)	18	61
7	l	210/287 (73%)	190 (90%)	19 (9%)	1 (0%)	32	74
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%)	15	58
10	c	242/258 (94%)	220 (91%)	19 (8%)	3 (1%)	15	58
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%)	22	66
12	e	240/260 (92%)	215 (90%)	23 (10%)	2 (1%)	22	66
13	F	231/234 (99%)	210 (91%)	19 (8%)	2 (1%)	20	63
13	f	231/234 (99%)	210 (91%)	19 (8%)	2 (1%)	20	63
14	G	242/288 (84%)	216 (89%)	25 (10%)	1 (0%)	38	77
14	g	242/288 (84%)	216 (89%)	24 (10%)	2 (1%)	22	66
15	H	350/467 (75%)	286 (82%)	56 (16%)	8 (2%)	7	44
16	I	321/437 (74%)	286 (89%)	33 (10%)	2 (1%)	28	70
17	J	371/405 (92%)	332 (90%)	31 (8%)	8 (2%)	8	45
18	K	357/428 (83%)	306 (86%)	45 (13%)	6 (2%)	11	51
19	L	354/437 (81%)	302 (85%)	51 (14%)	1 (0%)	44	81
20	M	349/434 (80%)	306 (88%)	40 (12%)	3 (1%)	20	63
21	N	843/945 (89%)	656 (78%)	174 (21%)	13 (2%)	12	53
22	O	372/393 (95%)	250 (67%)	103 (28%)	19 (5%)	2	27

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	P	427/445 (96%)	305 (71%)	99 (23%)	23 (5%)	2	26
24	Q	429/434 (99%)	350 (82%)	76 (18%)	3 (1%)	25	68
25	R	398/429 (93%)	281 (71%)	94 (24%)	23 (6%)	2	24
26	S	435/523 (83%)	313 (72%)	103 (24%)	19 (4%)	3	30
27	T	265/274 (97%)	190 (72%)	74 (28%)	1 (0%)	38	77
28	U	244/338 (72%)	198 (81%)	39 (16%)	7 (3%)	5	39
29	V	237/306 (78%)	176 (74%)	53 (22%)	8 (3%)	4	36
30	W	195/268 (73%)	157 (80%)	30 (15%)	8 (4%)	3	31
31	X	125/156 (80%)	94 (75%)	26 (21%)	5 (4%)	3	32
32	Y	32/89 (36%)	21 (66%)	9 (28%)	2 (6%)	1	23
33	Z	757/993 (76%)	665 (88%)	80 (11%)	12 (2%)	11	52
All	All	13191/15139 (87%)	11208 (85%)	1781 (14%)	202 (2%)	17	53

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%)	91	95
2	9	199/224 (89%)	198 (100%)	1 (0%)	91	95
3	3	168/178 (94%)	167 (99%)	1 (1%)	89	94

Continued on next page...

Continued from previous page...

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%)	89	94
6	k	175/175 (100%)	174 (99%)	1 (1%)	89	94
7	7	169/235 (72%)	169 (100%)	0	100	100
7	l	169/235 (72%)	168 (99%)	1 (1%)	89	94
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%)	80	90
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%)	87	93
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%)	82	91

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	P	384/415 (92%)	381 (99%)	3 (1%)	85	92
24	Q	388/391 (99%)	387 (100%)	1 (0%)	94	96
25	R	351/379 (93%)	348 (99%)	3 (1%)	82	91
26	S	342/489 (70%)	336 (98%)	6 (2%)	64	84
27	T	250/256 (98%)	250 (100%)	0	100	100
28	U	228/308 (74%)	225 (99%)	3 (1%)	73	87
29	V	211/268 (79%)	204 (97%)	7 (3%)	43	71
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%)	93	95

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.