



## wwPDB EM Map/Model Validation Report ⓘ

Jun 28, 2016 – 01:50 PM EDT

PDB ID : 3JCP  
EMDB ID: : EMD-6575  
Title : Structure of yeast 26S proteasome in M2 state derived from Titan dataset  
Authors : Luan, B.; Huang, X.L.; Wu, J.P.; Shi, Y.G.; Wang, F.  
Deposited on : 2016-01-06  
Resolution : 4.60 Å(reported)  
Based on PDB ID : 4CR2

This is a wwPDB 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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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

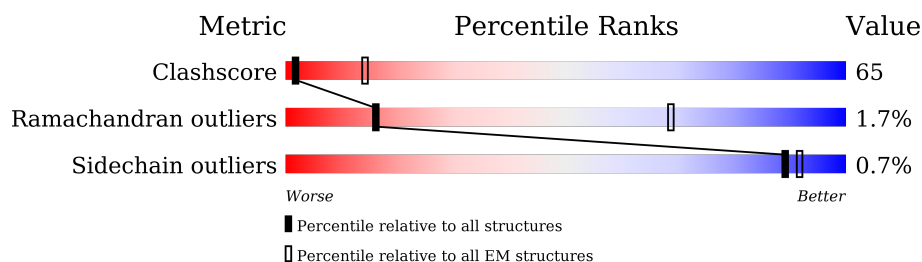
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.60 Å.

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



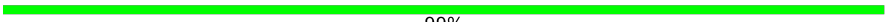
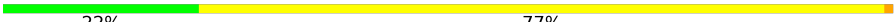
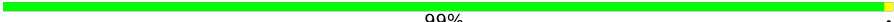
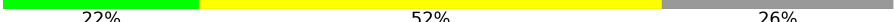


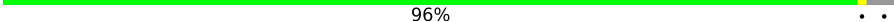

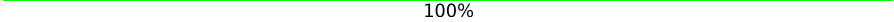

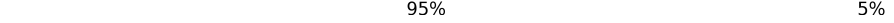

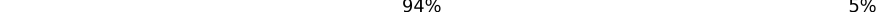



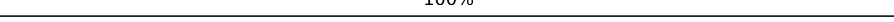
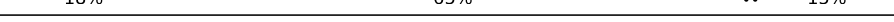







Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

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

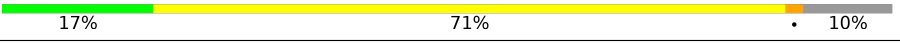
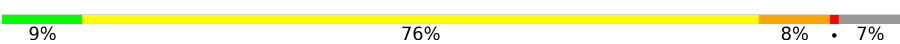
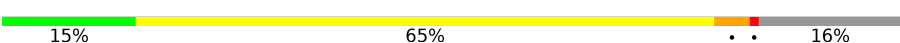
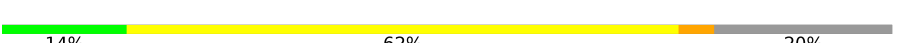
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Mol	Chain	Length	Quality of chain
5	j	205	 99%
6	6	198	 22% 77%
6	k	198	 99%
7	7	287	 22% 52% 26%
7	l	287	 74% 26%
8	A	252	 25% 71% ..
8	a	252	 96% ..
9	B	250	 27% 73%
9	b	250	 100%
10	C	258	 25% 70% 5%
10	c	258	 95% 5%
11	D	254	 24% 71% 5%
11	d	254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

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Mol	Chain	Length	Quality of chain
21	N	945	
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 104170 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Proteasome subunit beta type-6.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	244	Total	C	N	O	S	0	0
			1896	1205	330	357	4		
14	g	244	Total	C	N	O	S	0	0
			1896	1205	330	357	4		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Q	431	Total	C	N	O	S	0	0
			3469	2203	574	676	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	R	400	Total	C	N	O	S	0	0
			3187	2028	525	624	10		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	V	245	Total	C	N	O	S	0	0
			1912	1206	322	371	13		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	X	127	Total	C	N	O	S	0	0
			1032	664	169	195	4		

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

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

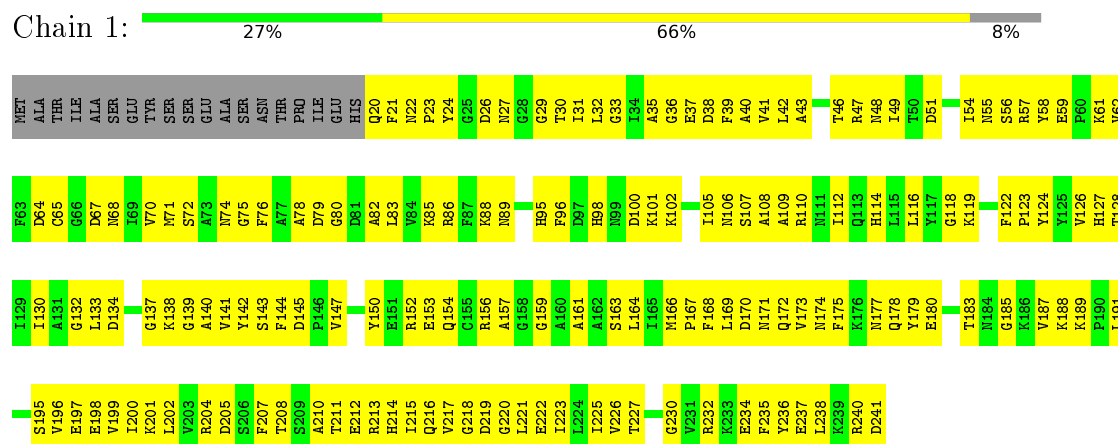
- Molecule 33 is a protein called 26S proteasome regulatory subunit RPN1.

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

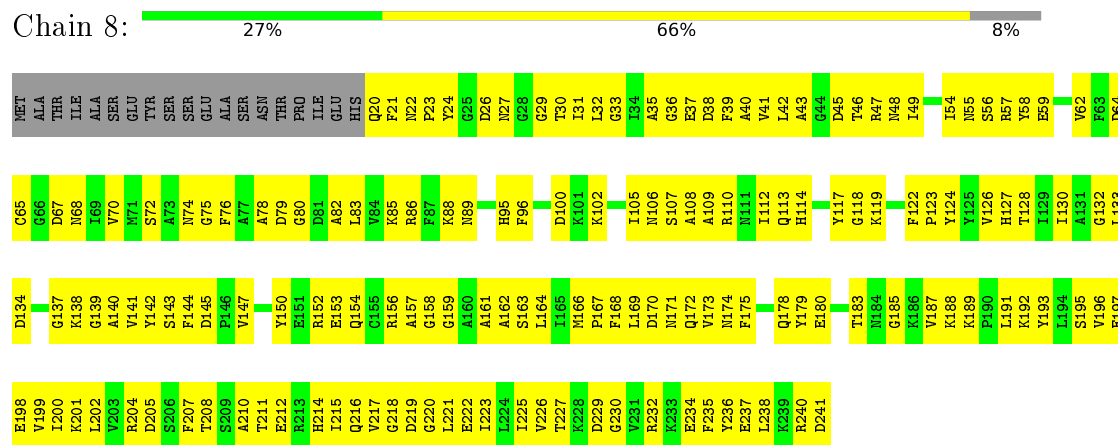
### 3 Residue-property plots

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

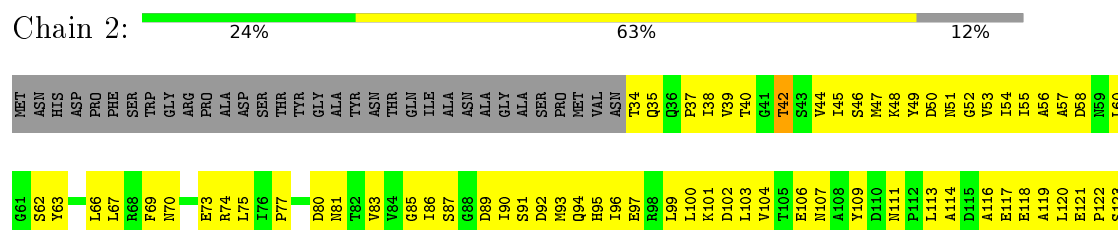
#### • Molecule 1: Proteasome subunit beta type-6



#### • Molecule 1: Proteasome subunit beta type-6



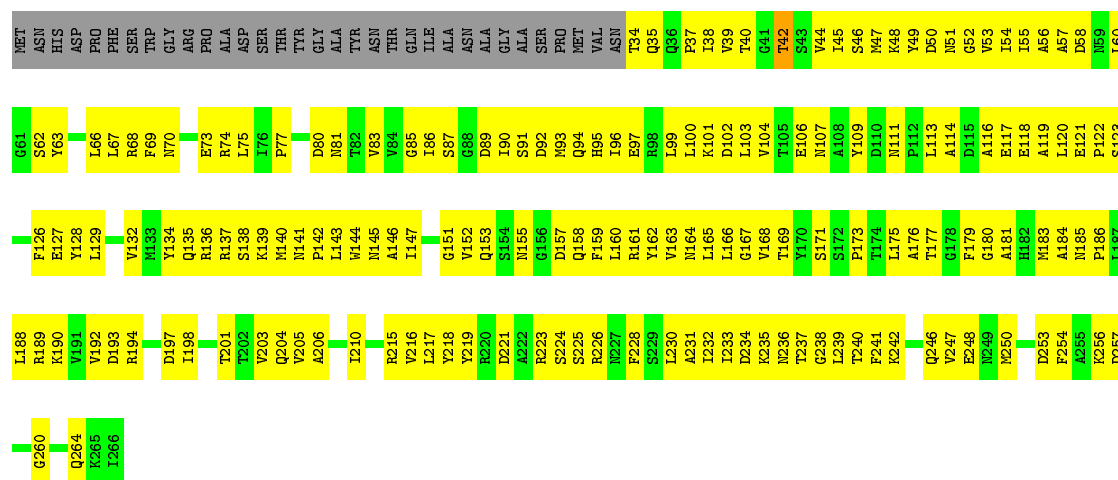
#### • Molecule 2: Proteasome subunit beta type-7





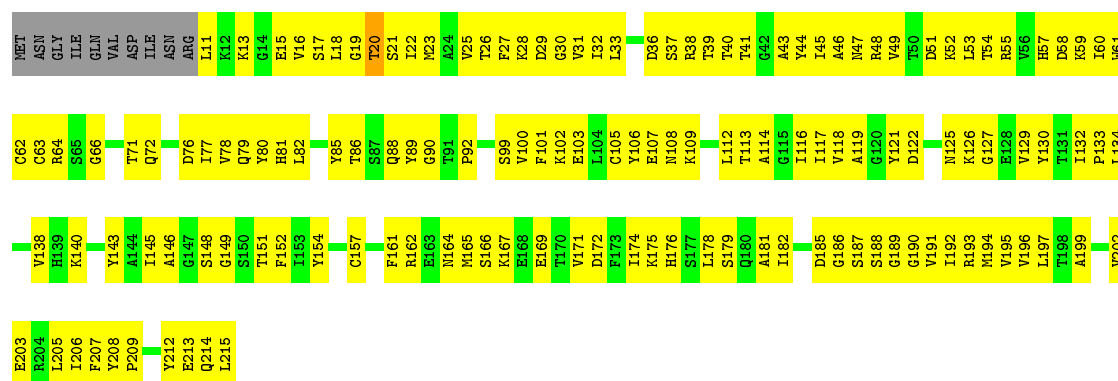
• Molecule 2: Proteasome subunit beta type-7

Chain 9: 26% 62% 12%



• Molecule 3: Proteasome subunit beta type-1

Chain 3: 30% 65% 5%



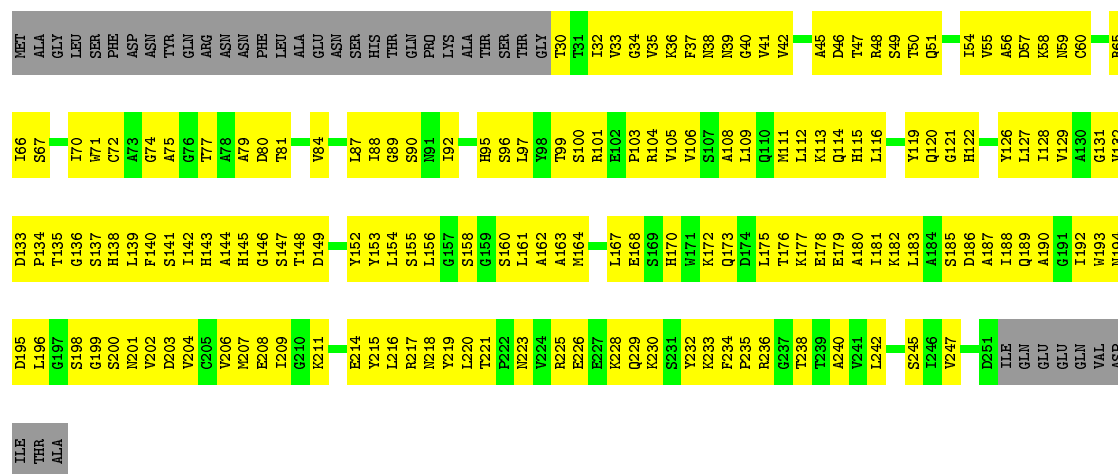
• Molecule 3: Proteasome subunit beta type-1

Chain h: 94% 5%




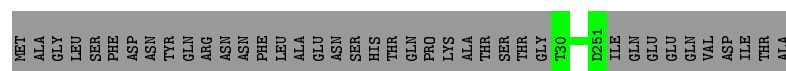
• Molecule 4: Proteasome subunit beta type-2

Chain 4:  23% 62% 15%



• Molecule 4: Proteasome subunit beta type-2

Chain i:  85% 15%



• Molecule 5: Proteasome subunit beta type-3

Chain 5:  26% 73%



• Molecule 5: Proteasome subunit beta type-3

Chain j:  99%



• Molecule 6: Proteasome subunit beta type-4

Chain 6:  22% 77%



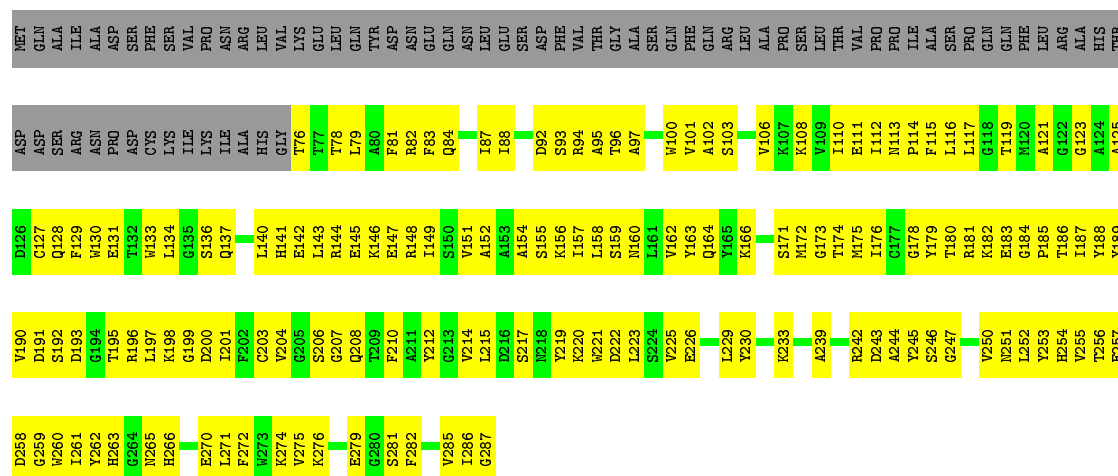
• Molecule 6: Proteasome subunit beta type-4

Chain k:  99%



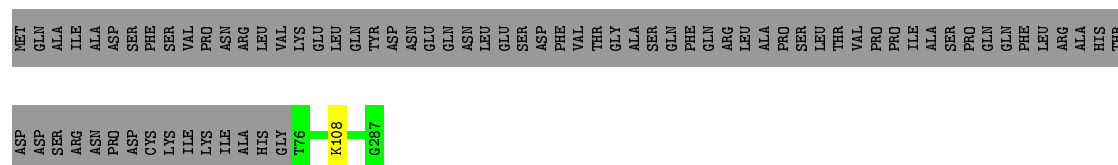
• Molecule 7: Proteasome subunit beta type-5

Chain 7:  52%



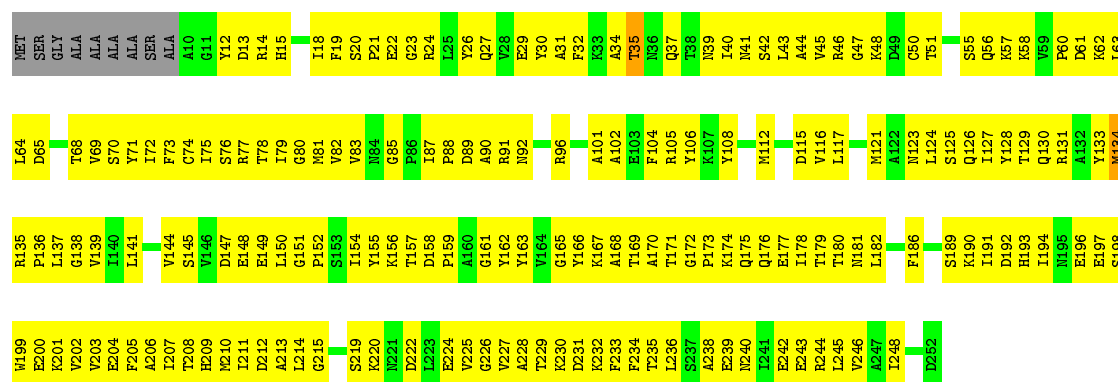
• Molecule 7: Proteasome subunit beta type-5

Chain l:  74%



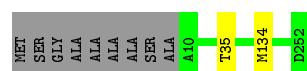
• Molecule 8: Proteasome subunit alpha type-1

Chain A:  71%



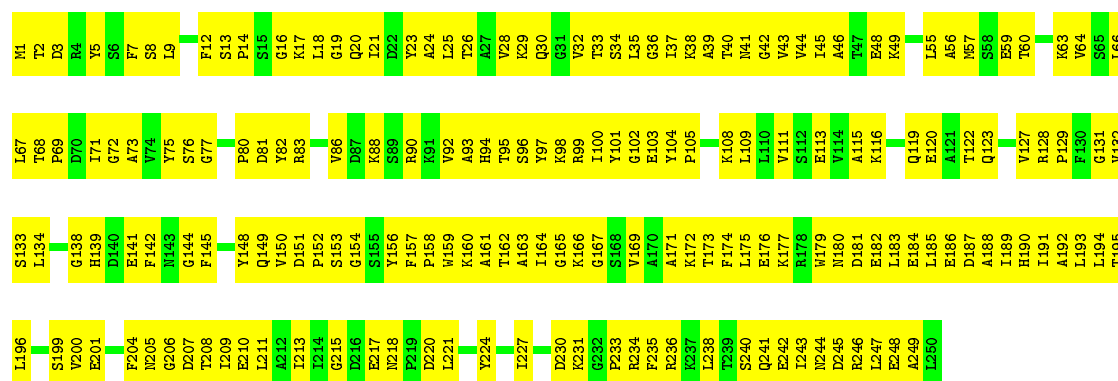
- Molecule 8: Proteasome subunit alpha type-1

Chain a: 96%



- Molecule 9: Proteasome subunit alpha type-2

Chain B: 27% 73%



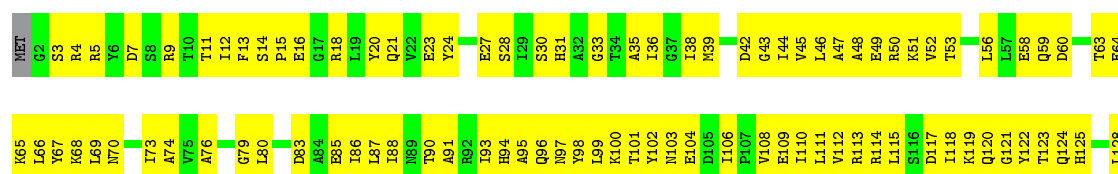
- Molecule 9: Proteasome subunit alpha type-2

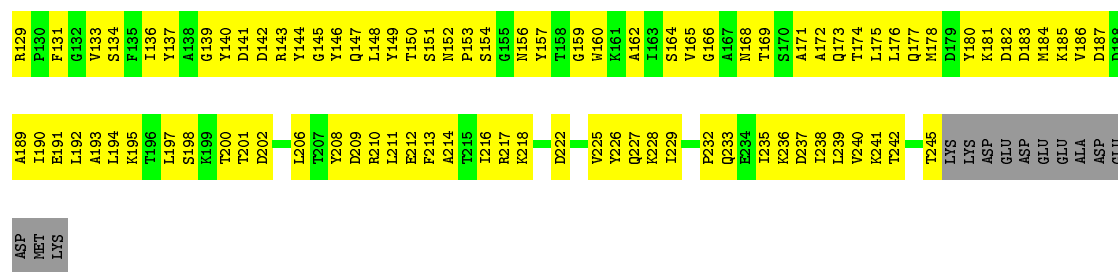
Chain b: 100%

There are no outlier residues recorded for this chain.

- Molecule 10: Proteasome subunit alpha type-3

Chain C: 25% 70% 5%





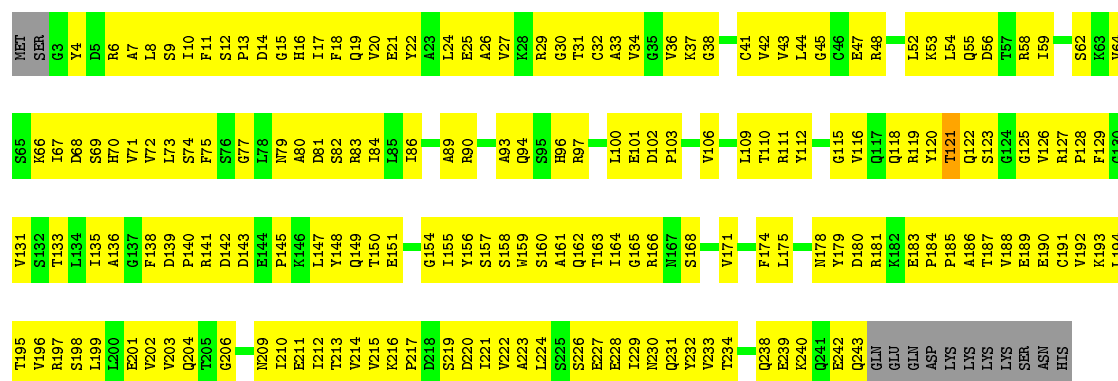
• Molecule 10: Proteasome subunit alpha type-3

Chain c: 95%



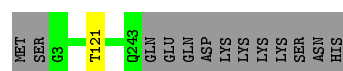
• Molecule 11: Proteasome subunit alpha type-4

Chain D: 24% 71% 5%



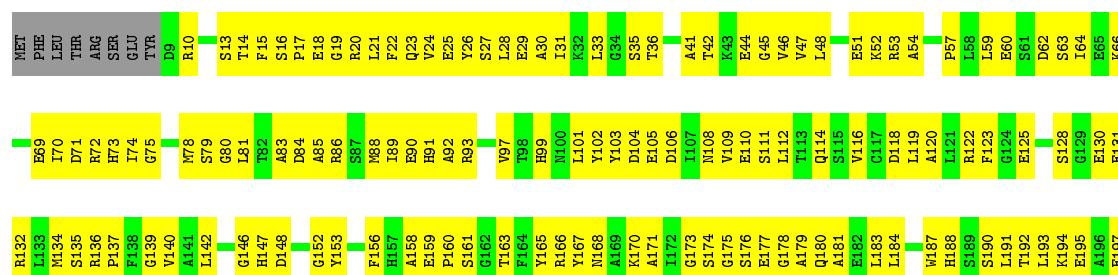
• Molecule 11: Proteasome subunit alpha type-4

Chain d: 94% 5%

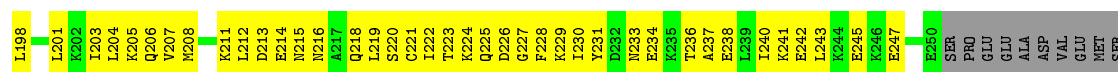


• Molecule 12: Proteasome subunit alpha type-5

Chain E: 28% 65% 7%







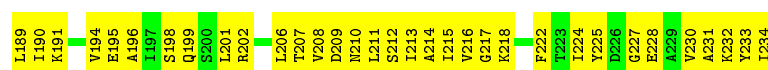
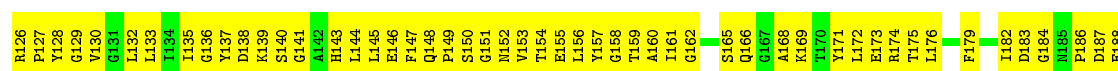
- Molecule 12: Proteasome subunit alpha type-5

Chain e:  93% 7%



- Molecule 13: Proteasome subunit alpha type-6

Chain F:  23% 77%



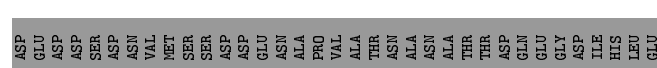
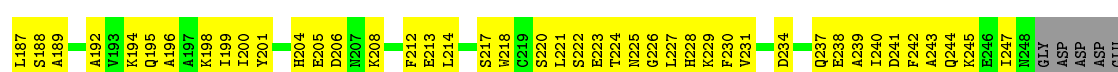
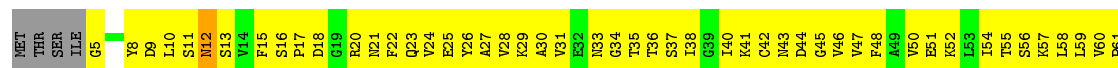
- Molecule 13: Proteasome subunit alpha type-6

Chain f:  100%

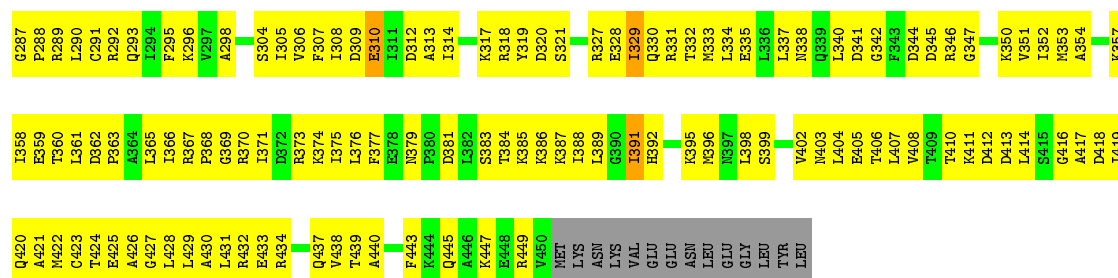


- Molecule 14: Probable proteasome subunit alpha type-7

Chain G:  18% 65% .. 15%

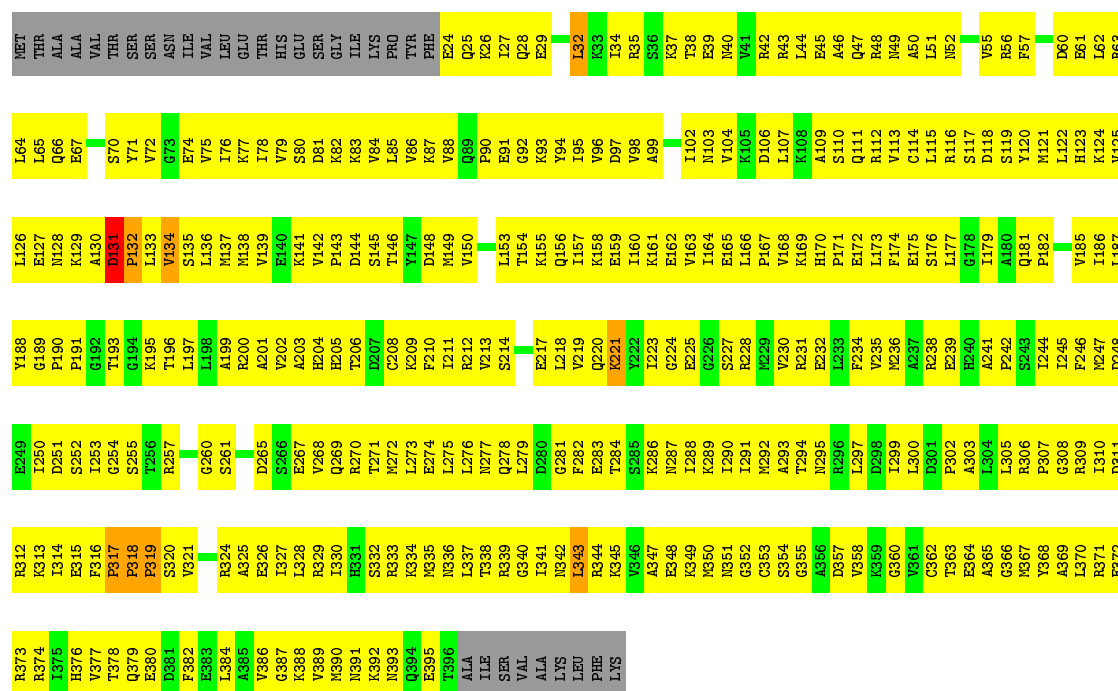






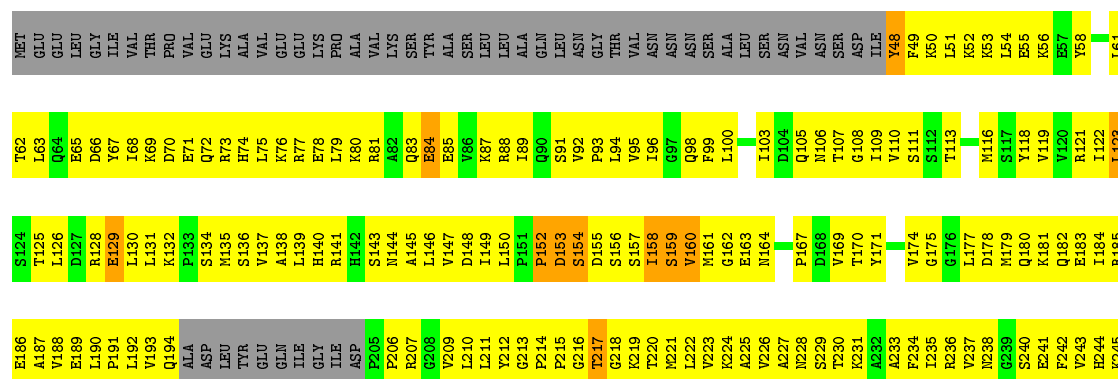
• Molecule 17: 26S protease regulatory subunit 8 homolog

Chain J: 16% 74% 8%

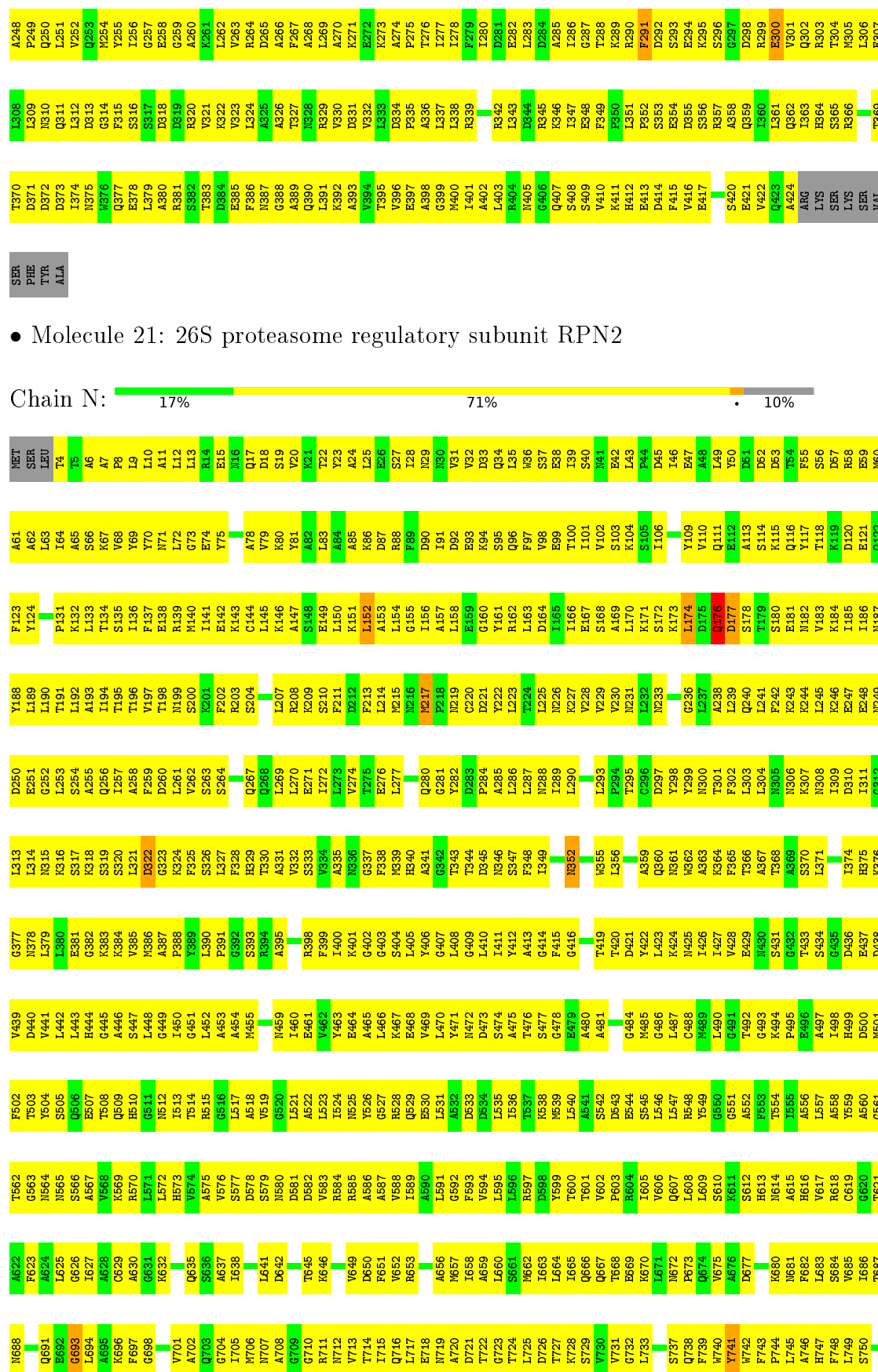


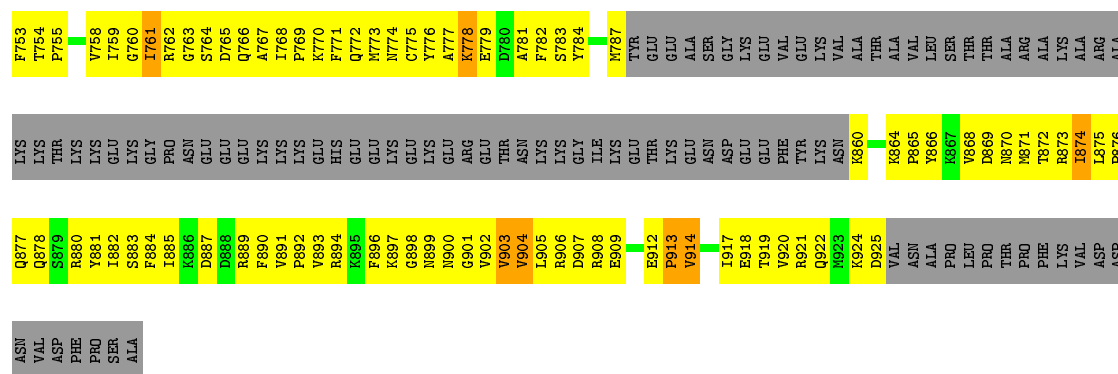
• Molecule 18: 26S protease regulatory subunit 6B homolog

Chain K: 15% 64% 16%



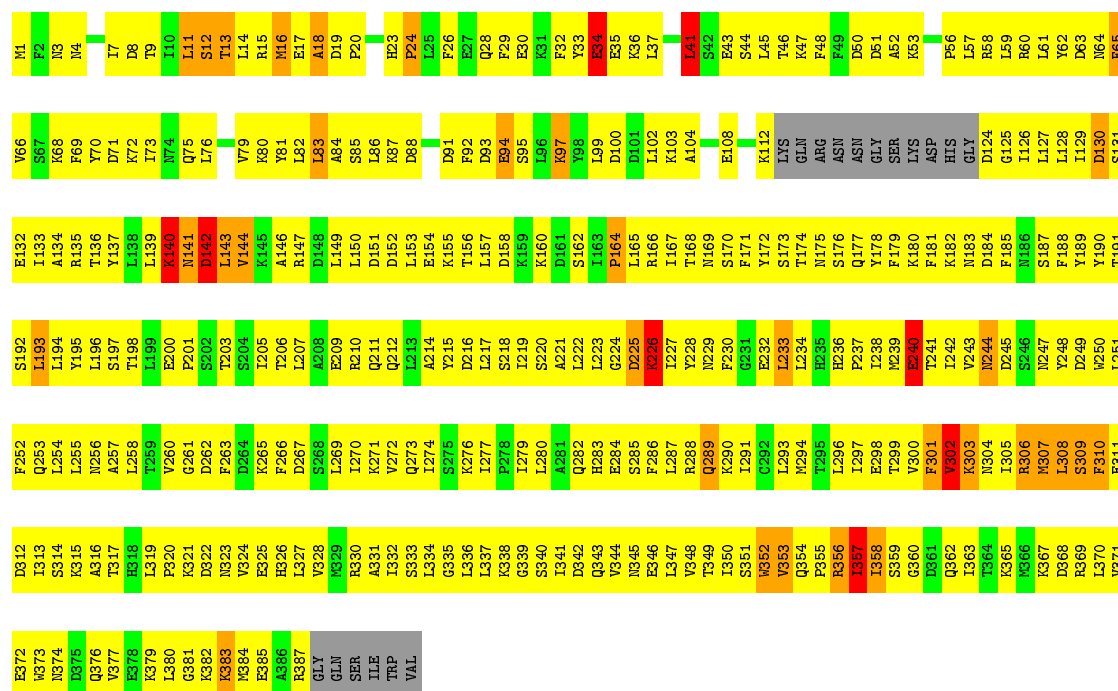






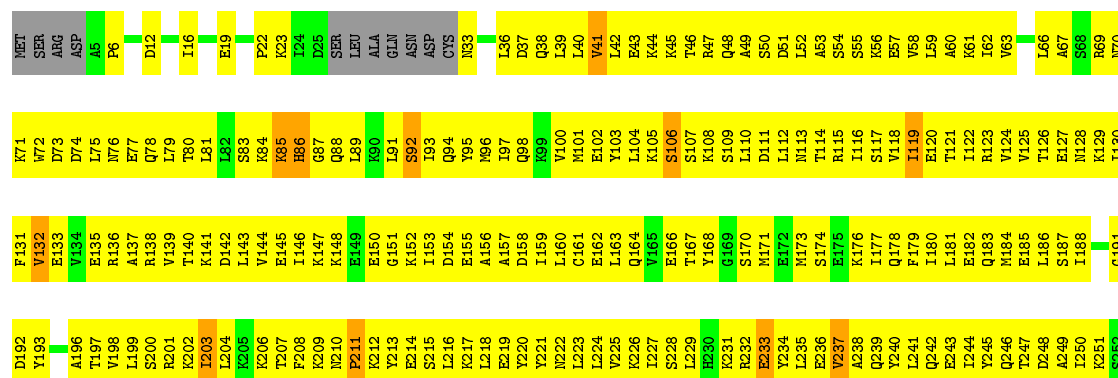
• Molecule 22: 26S proteasome regulatory subunit RPN9

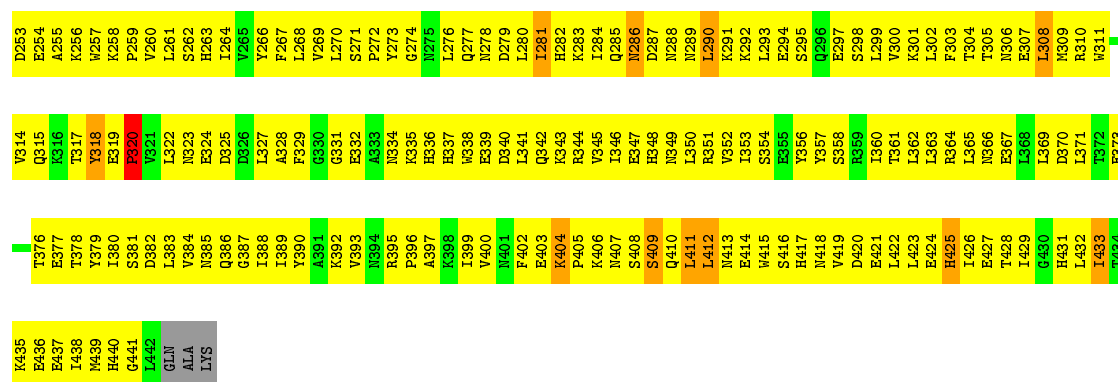
Chain O: 16% 70% 8%



• Molecule 23: 26S proteasome regulatory subunit RPN5

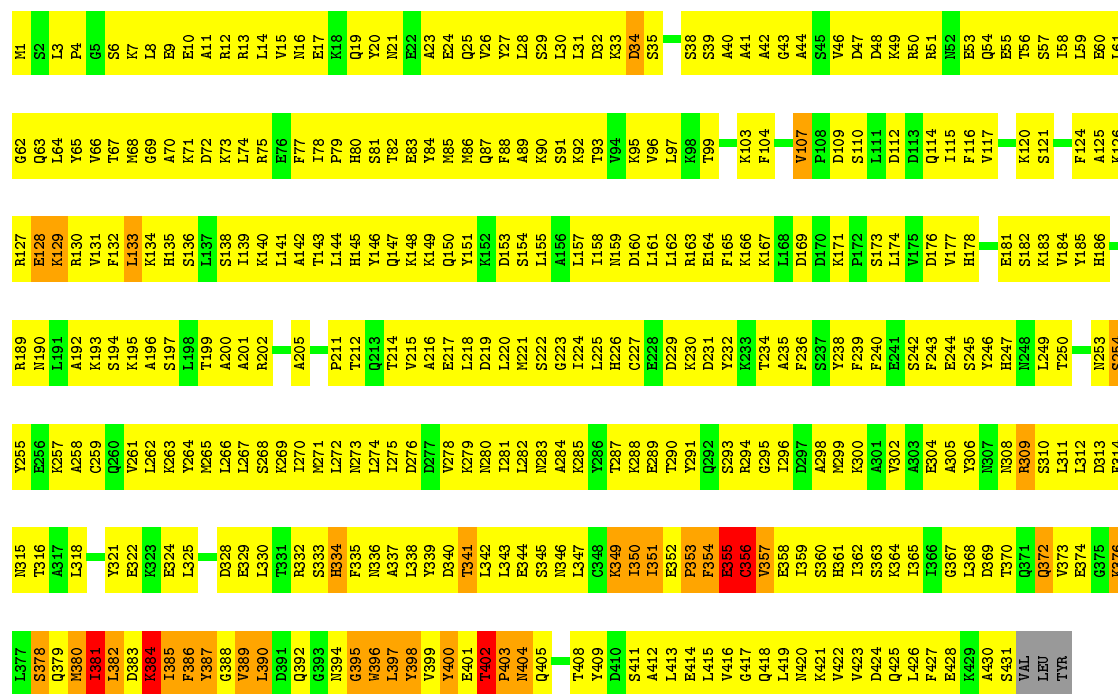
Chain P: 13% 78% 5%





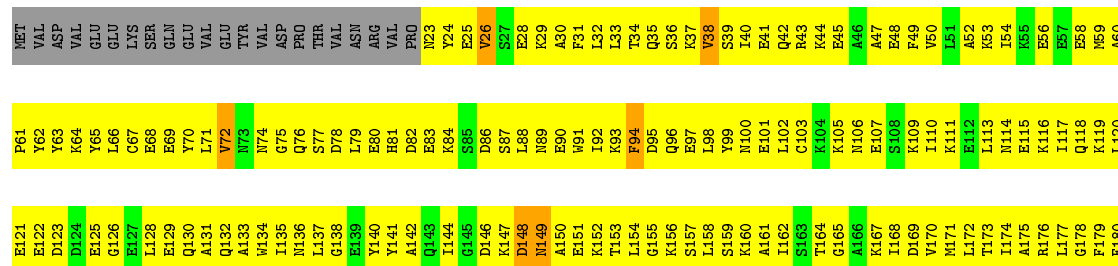
• Molecule 24: 26S proteasome regulatory subunit RPN6

Chain Q: 18% 73% 7% ..



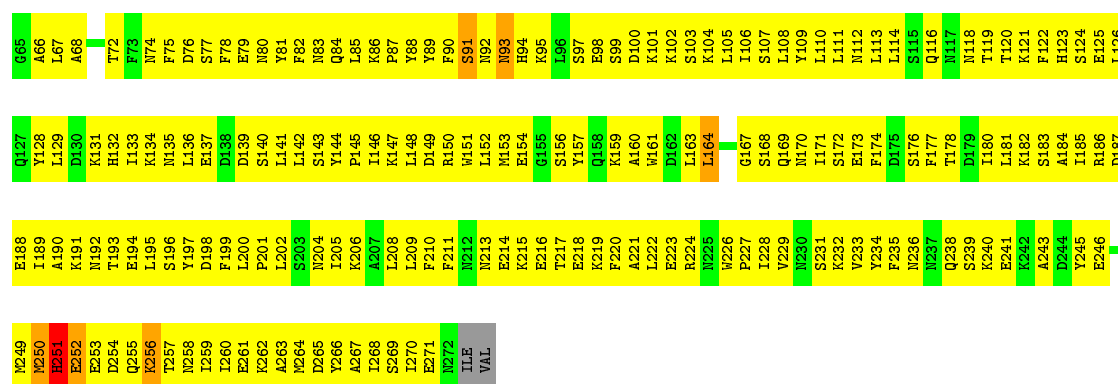
• Molecule 25: 26S proteasome regulatory subunit RPN7

Chain R: 9% 76% 8% 7%



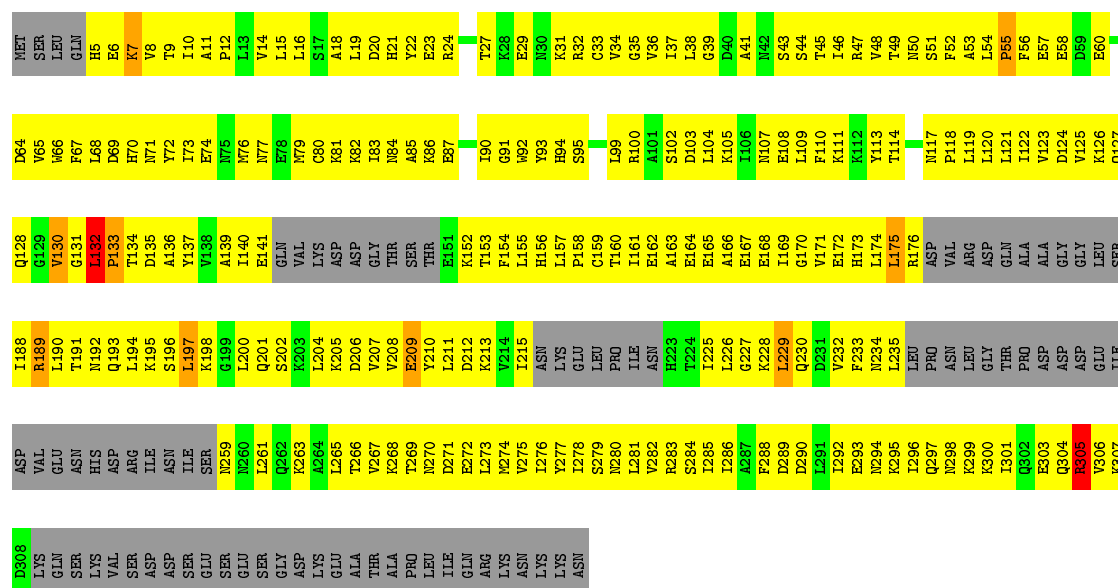






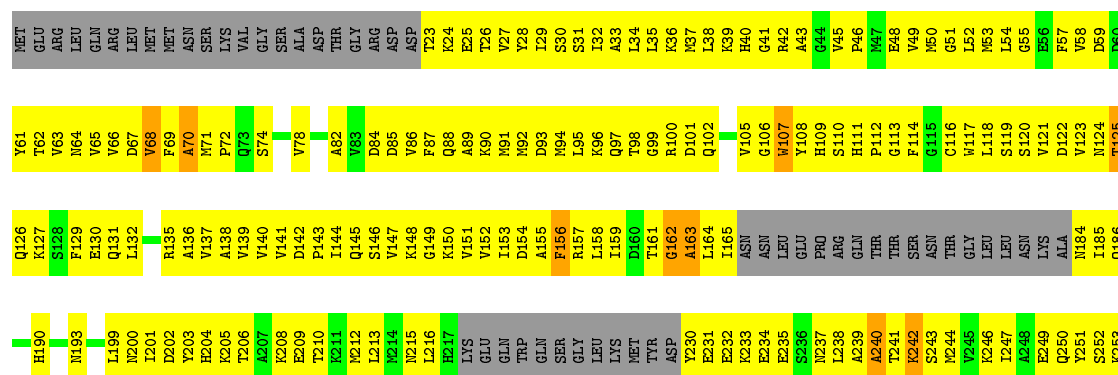
• Molecule 28: 26S proteasome regulatory subunit RPN8

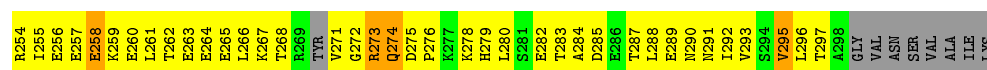
Chain U: 12% 60% 25%



• Molecule 29: Ubiquitin carboxyl-terminal hydrolase RPN11

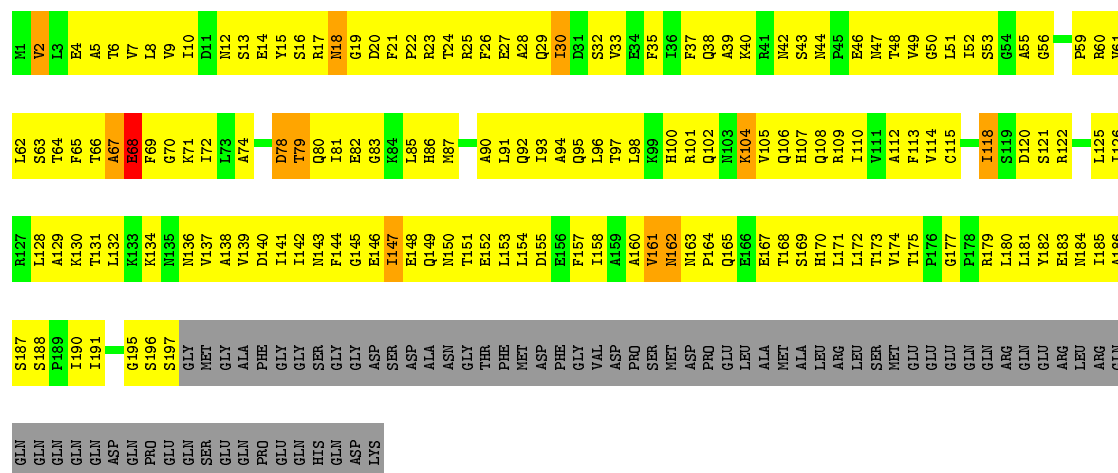
Chain V: 14% 62% 20%





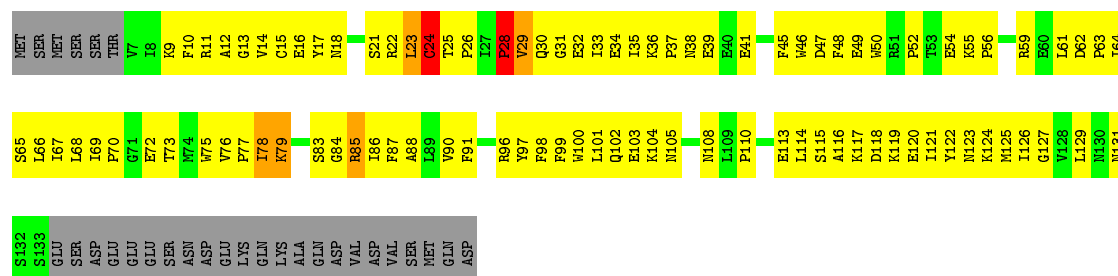
• Molecule 30: 26S proteasome regulatory subunit RPN10

Chain W: 14% 55% 26%



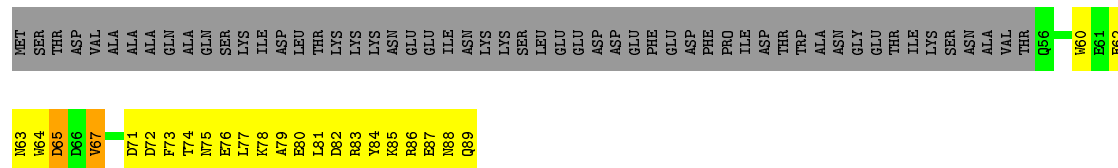
• Molecule 31: 26S proteasome regulatory subunit RPN13

Chain X: 21% 56% 19%



• Molecule 32: 26S proteasome complex subunit SEM1

Chain Y: 10% 26% 62%



• Molecule 33: 26S proteasome regulatory subunit RPN1

Chain Z: 14% 56% 5% 25%



LYS	T883	GLU	GLU	GLU	L509	V442	L381	GLU	L256	PHE	T125	SER
LYS	T884	GLY	GLU	GLU	L510	D443	A382	K318	P257	GLU	Y126	SER
ILE	T885	GLU	THR	P511	P512	E444	S383	K321	P258	F195	S127	LEU
THR	T886	THR	THR	P513	P514	E445	S384	F321	P259	E196	E128	TTR
GLY	T887	ILE	ALA	A513	A514	E446	F385	E322	E260	K197	N129	GLU
TRP	T888	LYS	GLU	A515	A516	E447	F386	E323	D261	E198	G130	ALA
ILE	T889	SER	GLY	S515	S516	K448	N387	E324	V262	D199	K131	SER
THR	T890	GLN	GLN	T516	T517	K449	G388	G325	A263	T200	H132	LEU
GLN	T891	THR	THR	D517	D518	G450	F389	G326	F264	L201	L135	ASN
SER	T892	ASN	ASN	L518	L519	A451	L390	Q327	L265	R203	L136	ALA
THR	T893	LYS	LYS	V584	V585	L452	N391	Q328	K266	L204	Y137	LEU
PHE	T894	GLY	GLY	L585	L586	L453	L392	E329	T267	C204	R138	LYS
ASP	T895	LYS	ASP	E586	E587	G454	G393	G330	A268	L205	L139	GLU
SER	T896	SER	ASP	T587	T588	L455	Y394	G331	Y269	D206	L140	SER
THR	T897	SER	PHE	A524	A525	G456	C395	G332	S270	L207	L141	ILE
ASP	T898	THR	LEU	M525	M526	L457	N396	G333	I271	V208	S141	LYS
LYS	T899	GLY	GLY	E526	E527	S458	D397	K334	K272	P209	D142	ASN
ASP	T900	GLY	GLY	S527	S528	A459	K398	L335	L273	P210	V143	THR
ALA	T901	GLN	GLN	L528	L529	S460	L399	S336	S274	P211	S144	SER
THR	T902	VAL	VAL	E529	E530	E466	I400	E337	Q275	L212	D145	THR
ASN	T903	ASN	ASN	L530	L531	V467	V401	E338	T276	K213	F146	SER
ASP	T904	GLU	GLU	A531	A532	E468	N402	F339	E277	K214	E147	SER
GLY	T905	GLY	GLY	H532	H533	L471	N403	L340	L278	G216	G148	THR
LYS	T906	THR	THR	V533	V534	L472	D404	Y341	T279	E217	ALA	ALA
ASN	T907	LYS	LYS	F534	F535	L473	N405	L342	D280	E218	H151	VAL
ASP	T908	ASN	ASN	V535	V536	L474	N406	K343	A281	D219	E152	PRO
ASP	T909	GLU	GLU	E536	E537	L475	V407	K344	I282	K215	Y153	LYS
GLU	T910	GLU	GLU	G536	G537	L476	N408	E345	A283	V221	I154	PRO
GLU	T911	ALA	ALA	H538	H539	Q475	K409	L346	L284	D223	R155	LEU
GLU	T912	GLU	GLU	V603	V604	D476	T410	L347	A285	L224	H156	LYS
ILE	T913	ILE	ILE	G540	G541	Y477	K411	L348	V286	L225	L157	PHE
LYS	T914	GLU	GLU	S605	S606	Y478	D412	T349	K287	L226	A158	LEU
GLY	T915	VAL	VAL	C606	C607	T479	G413	K352	L288	E226	L159	ARG
ALA	T916	ASP	ASP	A607	A608	N480	N414	V353	G289	I227	E160	PRO
ILE	T917	ILE	ILE	V608	V609	N481	N415	P354	E290	E228	I161	THR
VAL	T918	VAL	VAL	T609	T610	K483	T416	K354	E291	K232	G162	TTR
ASP	T919	ASP	ASP	V614	V615	K484	S417	L357	D292	L233	Y165	PRO
GLU	T920	GLU	GLU	L615	L616	L485	A418	K358	M293	L234	M166	ASP
THR	T921	THR	THR	F550	F551	S486	V419	K359	P234	Q235	E170	L99
GLY	T922	GLY	GLY	R553	R554	A488	S420	S360	F236	F237	Y103	Y103
GLY	T923	GLY	GLY	T553	T554	A489	I422	H361	V297	D238	A173	H106
GLY	T924	GLY	GLY	L554	L555	L490	G423	L362	F298	E239	T177	H106
GLY	T925	VAL	VAL	E555	E556	L491	S424	K363	D299	N240	SER	L110
GLY	T926	VAL	VAL	L556	L557	G492	I425	K364	A300	T241	GLY	L111
GLY	T927	VAL	VAL	T557	T558	G493	Q427	S365	F242	Q243	ASP	L112
GLY	T928	LYS	LYS	H623	H624	G494	W428	S367	F243	Q244	GLY	S113
GLY	T929	ALA	ALA	L624	L625	L495	N429	V368	R244	V245	SER	L114
GLY	T930	GLY	GLY	T625	T626	A496	L430	F369	M306	C246	LYS	L115
GLY	T931	THR	THR	V562	V563	F497	L431	K372	H307	Q247	SER	L116
GLY	T932	ILE	ILE	V564	V565	S500	L432	K373	K308	Q248	GLY	D117
GLY	T933	VAL	VAL	F565	F566	K501	Q434	L374	Q309	Y249	ASP	V118
GLY	T934	LYS	LYS	L566	L567	N502	Q435	D375	L310	M249	SER	L119
GLY	T935	GLY	GLY	A567	A568	D503	L436	E376	A311	V250	ALA	S120
GLY	T936	ASN	ASN	L568	L569	E504	D437	K376	Y312	C252	ALA	L121
GLY	T937	GLY	GLY	A569	A570	V505	K438	K377	I313	P253	THR	L122
GLY	T938	GLY	GLY	L572	L573	G507	Y439	Q378	L314	V254	SER	L123
ASP	T939	ASP	ASP	V572	V573	L506	Y440	K379	L315	P255	GLY	M124
ASP	T940	ASP	ASP	L574	L575	L508	Y441	N380	A316	L255	GLY	M124

## 4 Experimental information

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

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

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

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

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

All (5) bond length outliers are listed below:

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

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

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

There are no chirality outliers.

5 of 131 planarity outliers are listed below:

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

## 5.2 Too-close contacts [i](#)

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

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

*Continued on next page...*

*Continued from previous page...*

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

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



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

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

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	220/241 (91%)	207 (94%)	13 (6%)	0	100	100
1	8	220/241 (91%)	207 (94%)	13 (6%)	0	100	100
2	2	231/266 (87%)	222 (96%)	7 (3%)	2 (1%)	21	67
2	9	231/266 (87%)	222 (96%)	7 (3%)	2 (1%)	21	67
3	3	203/215 (94%)	189 (93%)	12 (6%)	2 (1%)	19	65
3	h	203/215 (94%)	188 (93%)	13 (6%)	2 (1%)	19	65
4	4	220/261 (84%)	211 (96%)	9 (4%)	0	100	100
4	i	220/261 (84%)	211 (96%)	9 (4%)	0	100	100
5	5	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
5	j	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
6	6	196/198 (99%)	186 (95%)	8 (4%)	2 (1%)	19	65
6	k	196/198 (99%)	186 (95%)	8 (4%)	2 (1%)	19	65
7	7	210/287 (73%)	203 (97%)	7 (3%)	0	100	100
7	l	210/287 (73%)	203 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	A	241/252 (96%)	227 (94%)	13 (5%)	1 (0%)	39	80
8	a	241/252 (96%)	227 (94%)	13 (5%)	1 (0%)	39	80
9	B	248/250 (99%)	235 (95%)	13 (5%)	0	100	100
9	b	248/250 (99%)	235 (95%)	13 (5%)	0	100	100
10	C	242/258 (94%)	232 (96%)	10 (4%)	0	100	100
10	c	242/258 (94%)	232 (96%)	10 (4%)	0	100	100
11	D	239/254 (94%)	224 (94%)	14 (6%)	1 (0%)	39	80
11	d	239/254 (94%)	224 (94%)	14 (6%)	1 (0%)	39	80
12	E	240/260 (92%)	228 (95%)	12 (5%)	0	100	100
12	e	240/260 (92%)	228 (95%)	12 (5%)	0	100	100
13	F	231/234 (99%)	221 (96%)	10 (4%)	0	100	100
13	f	231/234 (99%)	221 (96%)	10 (4%)	0	100	100
14	G	242/288 (84%)	224 (93%)	14 (6%)	4 (2%)	11	56
14	g	242/288 (84%)	226 (93%)	15 (6%)	1 (0%)	39	80
15	H	373/467 (80%)	301 (81%)	60 (16%)	12 (3%)	5	43
16	I	348/437 (80%)	297 (85%)	42 (12%)	9 (3%)	7	47
17	J	371/405 (92%)	325 (88%)	39 (10%)	7 (2%)	10	53
18	K	357/428 (83%)	300 (84%)	45 (13%)	12 (3%)	5	42
19	L	354/437 (81%)	291 (82%)	58 (16%)	5 (1%)	14	59
20	M	349/434 (80%)	310 (89%)	38 (11%)	1 (0%)	46	83
21	N	846/945 (90%)	665 (79%)	173 (20%)	8 (1%)	21	67
22	O	372/393 (95%)	263 (71%)	83 (22%)	26 (7%)	1	23
23	P	427/445 (96%)	315 (74%)	100 (23%)	12 (3%)	6	46
24	Q	429/434 (99%)	325 (76%)	92 (21%)	12 (3%)	6	46
25	R	398/429 (93%)	280 (70%)	95 (24%)	23 (6%)	2	27
26	S	435/523 (83%)	332 (76%)	89 (20%)	14 (3%)	5	43
27	T	265/274 (97%)	202 (76%)	60 (23%)	3 (1%)	17	64
28	U	244/338 (72%)	202 (83%)	37 (15%)	5 (2%)	9	53
29	V	237/306 (78%)	185 (78%)	44 (19%)	8 (3%)	5	42
30	W	195/268 (73%)	154 (79%)	33 (17%)	8 (4%)	3	36
31	X	125/156 (80%)	96 (77%)	24 (19%)	5 (4%)	4	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	Y	32/89 (36%)	21 (66%)	10 (31%)	1 (3%)	5	44
33	Z	738/993 (74%)	589 (80%)	119 (16%)	30 (4%)	3	36
All	All	13225/15139 (87%)	11460 (87%)	1543 (12%)	222 (2%)	16	56

5 of 222 Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	185/201 (92%)	185 (100%)	0	100	100
1	8	185/201 (92%)	185 (100%)	0	100	100
2	2	199/224 (89%)	199 (100%)	0	100	100
2	9	199/224 (89%)	199 (100%)	0	100	100
3	3	167/178 (94%)	167 (100%)	0	100	100
3	h	168/178 (94%)	168 (100%)	0	100	100
4	4	181/214 (85%)	181 (100%)	0	100	100
4	i	181/214 (85%)	181 (100%)	0	100	100
5	5	172/173 (99%)	172 (100%)	0	100	100
5	j	171/173 (99%)	171 (100%)	0	100	100
6	6	175/175 (100%)	175 (100%)	0	100	100
6	k	175/175 (100%)	175 (100%)	0	100	100
7	7	169/235 (72%)	169 (100%)	0	100	100
7	l	169/235 (72%)	168 (99%)	1 (1%)	90	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	A	207/210 (99%)	207 (100%)	0	100	100
8	a	207/210 (99%)	207 (100%)	0	100	100
9	B	209/209 (100%)	209 (100%)	0	100	100
9	b	209/209 (100%)	209 (100%)	0	100	100
10	C	203/216 (94%)	203 (100%)	0	100	100
10	c	203/216 (94%)	203 (100%)	0	100	100
11	D	213/226 (94%)	213 (100%)	0	100	100
11	d	213/226 (94%)	213 (100%)	0	100	100
12	E	198/215 (92%)	198 (100%)	0	100	100
12	e	198/215 (92%)	198 (100%)	0	100	100
13	F	192/193 (100%)	192 (100%)	0	100	100
13	f	192/193 (100%)	192 (100%)	0	100	100
14	G	201/239 (84%)	200 (100%)	1 (0%)	92	96
14	g	201/239 (84%)	201 (100%)	0	100	100
15	H	296/399 (74%)	292 (99%)	4 (1%)	74	89
16	I	282/385 (73%)	279 (99%)	3 (1%)	80	91
17	J	319/352 (91%)	318 (100%)	1 (0%)	94	96
18	K	313/374 (84%)	309 (99%)	4 (1%)	76	89
19	L	306/377 (81%)	303 (99%)	3 (1%)	82	92
20	M	303/375 (81%)	303 (100%)	0	100	100
21	N	714/797 (90%)	712 (100%)	2 (0%)	94	96
22	O	306/368 (83%)	300 (98%)	6 (2%)	63	86
23	P	384/415 (92%)	384 (100%)	0	100	100
24	Q	387/391 (99%)	362 (94%)	25 (6%)	21	60
25	R	342/379 (90%)	333 (97%)	9 (3%)	54	81
26	S	349/489 (71%)	349 (100%)	0	100	100
27	T	250/256 (98%)	247 (99%)	3 (1%)	78	90
28	U	232/308 (75%)	232 (100%)	0	100	100
29	V	211/268 (79%)	211 (100%)	0	100	100
30	W	171/230 (74%)	169 (99%)	2 (1%)	78	90
31	X	116/144 (81%)	116 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	Y	18/81 (22%)	18 (100%)	0	100	100
33	Z	606/850 (71%)	588 (97%)	18 (3%)	48	78
All	All	11247/13054 (86%)	11165 (99%)	82 (1%)	89	94

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

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

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

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.