



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Nov 21, 2016 – 03:33 PM EST

PDB ID : 5T0G
EMDB ID: : EMD-8334
Title : Structural basis for dynamic regulation of the human 26S proteasome
Authors : Chen, S.; Wu, J.; Lu, Y.; Ma, Y.B.; Lee, B.H.; Yu, Z.; Ouyang, Q.; Finley, D.;
Kirschner, M.W.; Mao, Y.
Deposited on : 2016-08-16
Resolution : 4.40 Å(reported)

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
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
EM map analysis : **NOT EXECUTED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028320

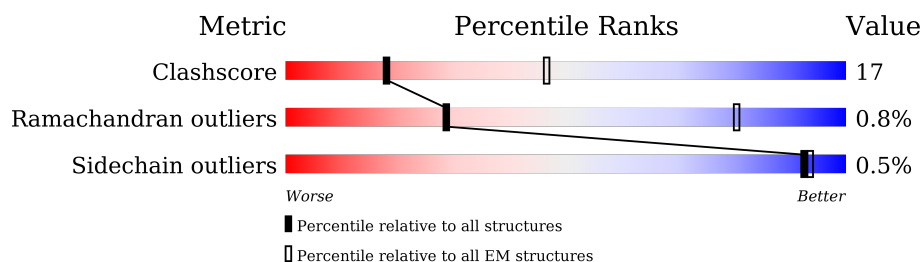
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	G	245	62% 35% ..
2	H	233	73% 27%
3	I	260	67% 29% .
4	J	247	67% 29% ..
5	K	240	64% 30% . 5%
6	L	268	56% 32% 11%
7	M	254	60% 34% 6%
8	N	238	64% 16% 20%
9	O	276	67% 13% 20%

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Mol	Chain	Length	Quality of chain
10	P	204	
11	Q	201	
12	R	262	
13	S	240	
14	T	263	
15	A	433	
16	B	440	
17	D	418	
18	E	403	
19	F	439	
20	C	398	
21	U	953	
22	V	533	
23	W	456	
24	X	422	
25	Y	389	
26	Z	324	
27	a	376	
28	b	377	
29	c	309	
30	d	349	
31	e	70	
32	f	749	

2 Entry composition [i](#)

There are 34 unique types of molecules in this entry. The entry contains 77800 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 alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	240	Total	C	N	O	S	0	0
			1826	1160	305	348	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	233	Total	C	N	O	S	0	0
			1713	1084	290	334	5		

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	250	Total	C	N	O	S	0	0
			1912	1204	329	371	8		

- Molecule 4 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	239	Total	C	N	O	S	0	0
			1704	1056	308	335	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	228	Total	C	N	O	S	0	0
			1722	1080	284	348	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	238	Total	C	N	O	S	0	0
			1850	1159	334	346	11		

- Molecule 7 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	240	Total	C	N	O	S	0	0
			1856	1178	314	353	11		

- Molecule 8 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	191	Total	C	N	O	S	0	0
			1430	893	245	280	12		

- Molecule 9 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	O	220	Total	C	N	O	S	0	0
			1643	1033	280	318	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	P	204	Total	C	N	O	S	0	0
			1585	1010	262	294	19		

- Molecule 11 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Q	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	R	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		

- Molecule 13 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	S	213	Total	C	N	O	S	0	0
			1641	1036	282	313	10		

- Molecule 14 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	A	361	Total	C	N	O	S	0	0
			2835	1788	501	528	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	B	341	Total	C	N	O	S	0	0
			2662	1671	453	526	12		

- Molecule 17 is a protein called 26S protease regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	D	380	Total	C	N	O	S	0	0
			3040	1923	524	580	13		

- Molecule 18 is a protein called 26S protease regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	E	353	Total	C	N	O	S	0	0
			2790	1755	494	525	16		

- Molecule 19 is a protein called 26S protease regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	F	366	Total	C	N	O	S	0	0
			2863	1802	496	549	16		

- Molecule 20 is a protein called 26S protease regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	C	384	Total	C	N	O	S	0	0
			3015	1894	540	564	17		

- Molecule 21 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	806	Total	C	N	O	S	0	0
			6287	3990	1075	1178	44		

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	480	Total	C	N	O	S	0	0
			3852	2444	684	710	14		

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	456	Total	C	N	O	S	0	0
			3703	2339	635	704	25		

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	380	Total	C	N	O	S	0	0
			3009	1918	509	570	12		

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	378	Total	C	N	O	S	0	0
			3115	1987	533	578	17		

- Molecule 26 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	286	Total	C	N	O	S	0	0
			2281	1457	392	427	5		

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	373	Total	C	N	O	S	0	0
			2995	1911	510	559	15		

- Molecule 28 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	191	Total	C	N	O	S	0	0
			1458	910	261	279	8		

- Molecule 29 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	287	Total	C	N	O	S	0	0
			2260	1430	389	422	19		

- Molecule 30 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	257	Total	C	N	O	S	0	0
			2116	1371	346	390	9		

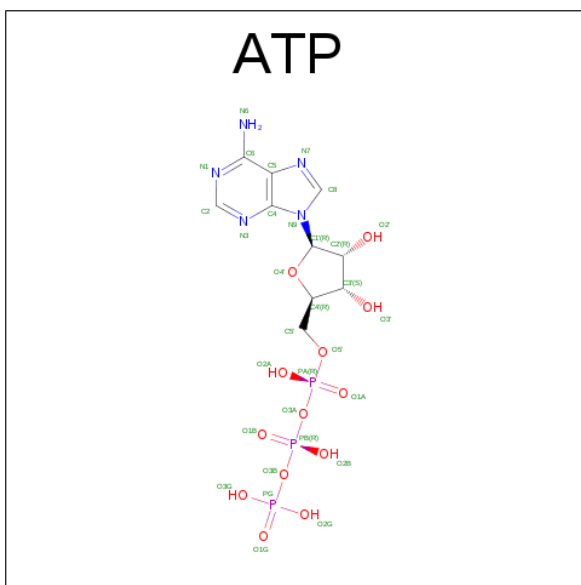
- Molecule 31 is a protein called 26S proteasome complex subunit DSS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	40	Total	C	N	O	S	0	0
			334	200	55	77	2		

- Molecule 32 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	694	Total	C	N	O	S	0	0
			5331	3364	899	1027	41		

- Molecule 33 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf
33	A	1	Total 31	C 10	N 5	O 13	P 3	0
33	B	1	Total 31	C 10	N 5	O 13	P 3	0
33	D	1	Total 31	C 10	N 5	O 13	P 3	0
33	E	1	Total 31	C 10	N 5	O 13	P 3	0
33	F	1	Total 31	C 10	N 5	O 13	P 3	0
33	C	1	Total 31	C 10	N 5	O 13	P 3	0

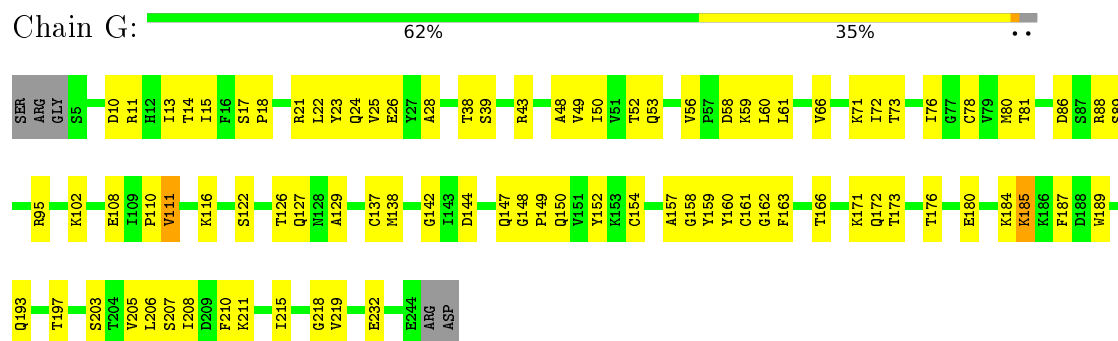
- Molecule 34 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
34	c	1	Total Zn 1 1	0

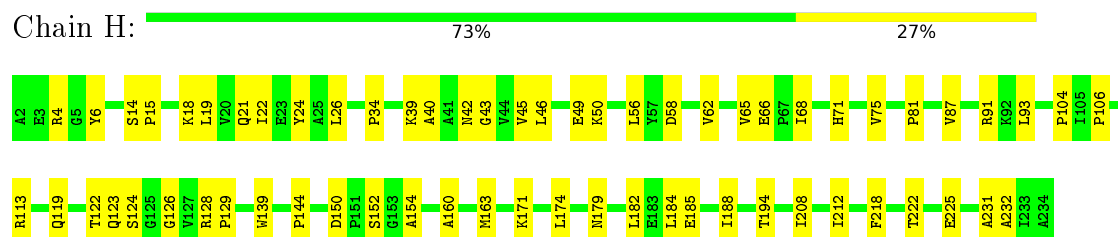
3 Residue-property plots

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.

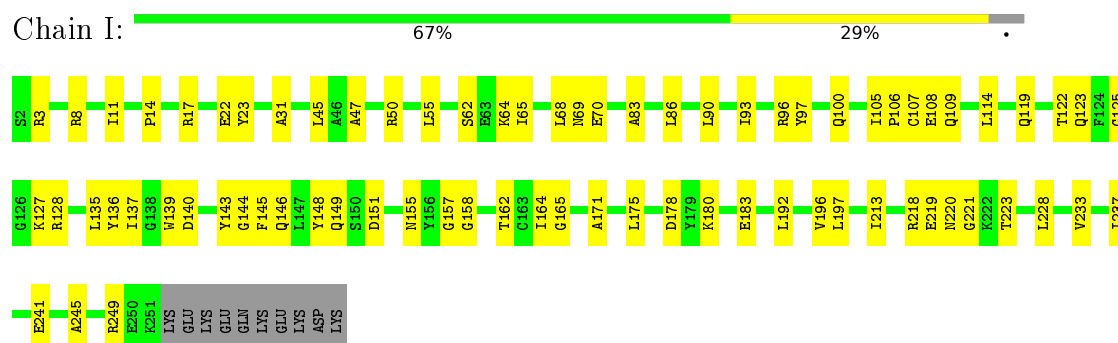
• Molecule 1: Proteasome subunit alpha type-6



• Molecule 2: Proteasome subunit alpha type-2

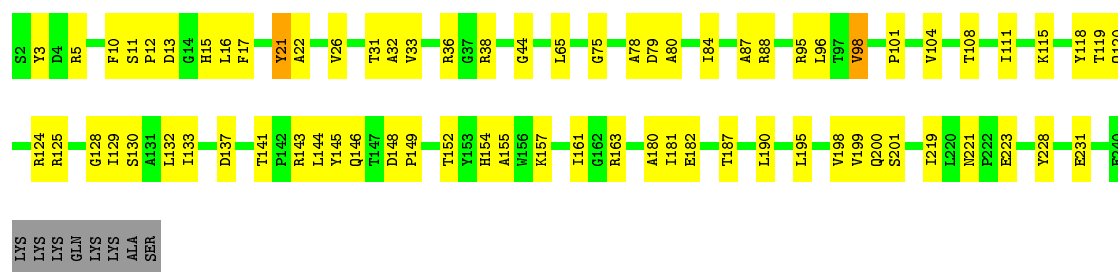


• Molecule 3: Proteasome subunit alpha type-4



• Molecule 4: Proteasome subunit alpha type-7





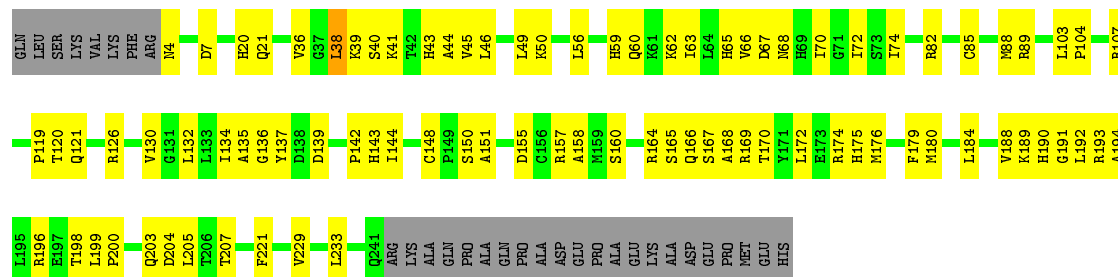
- Molecule 5: Proteasome subunit alpha type-5

Chain K: 64% 30% 5%



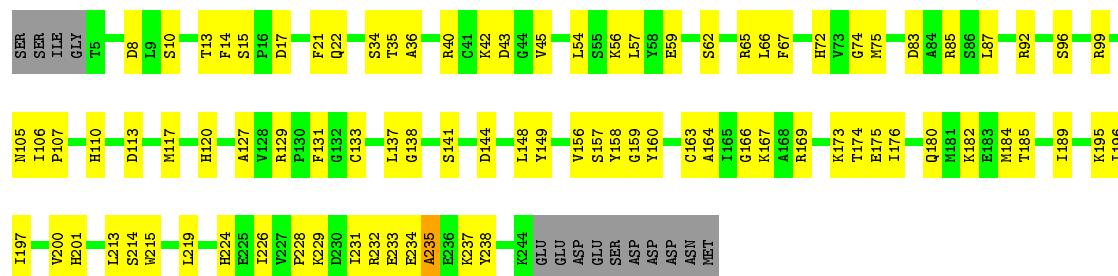
- Molecule 6: Proteasome subunit alpha type-1

Chain L:  56% 32% 11%



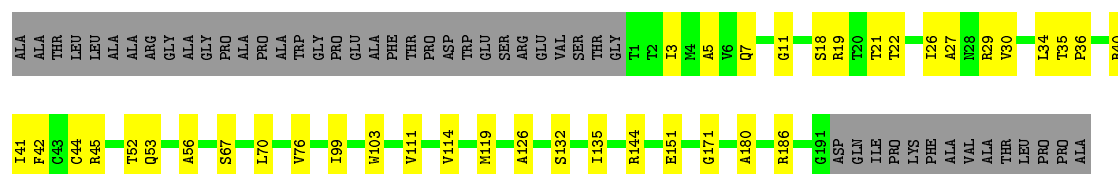
- Molecule 7: Proteasome subunit alpha type-3

Chain M: 60% 34% 6%



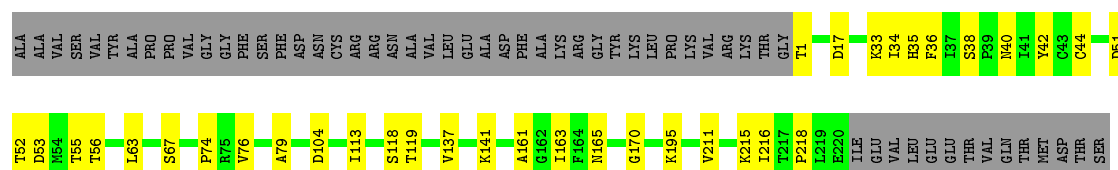
- Molecule 8: Proteasome subunit beta type-6

Chain N: 64% 16% 20%



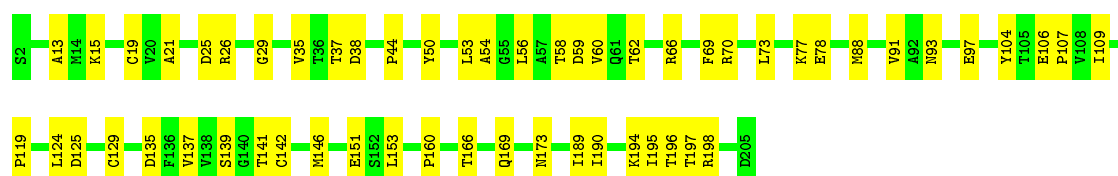
- Molecule 9: Proteasome subunit beta type-7

Chain O: 67% 13% 20%



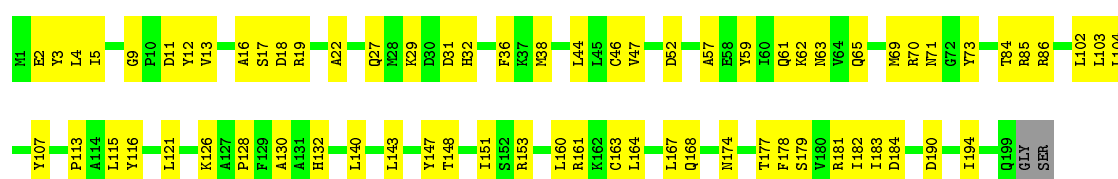
- Molecule 10: Proteasome subunit beta type-3

Chain P: 73% 27%



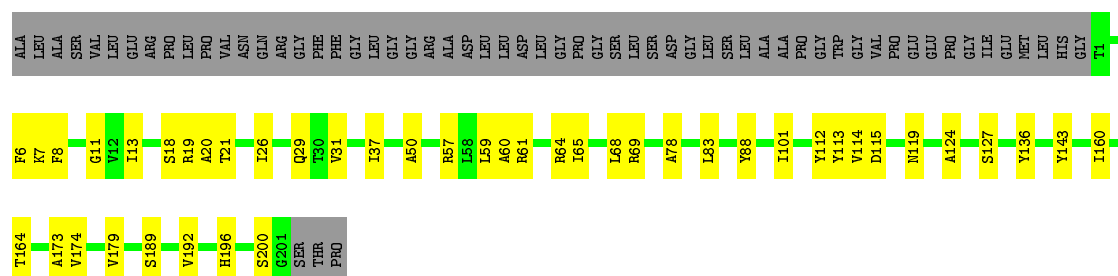
- Molecule 11: Proteasome subunit beta type-2

Chain Q: 64% 35%



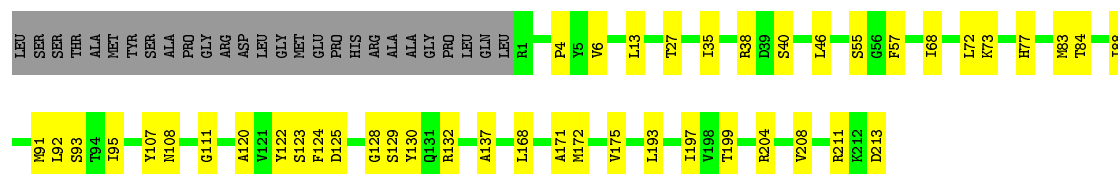
- Molecule 12: Proteasome subunit beta type-5

Chain R: 60% 17% 23%



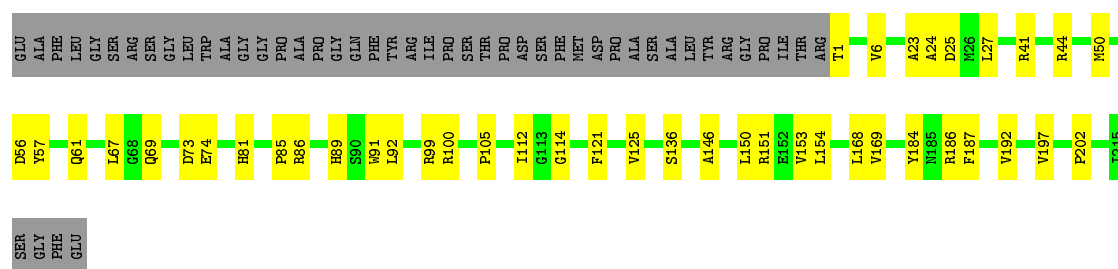
- Molecule 13: Proteasome subunit beta type-1

Chain S:  70% 19% 11%



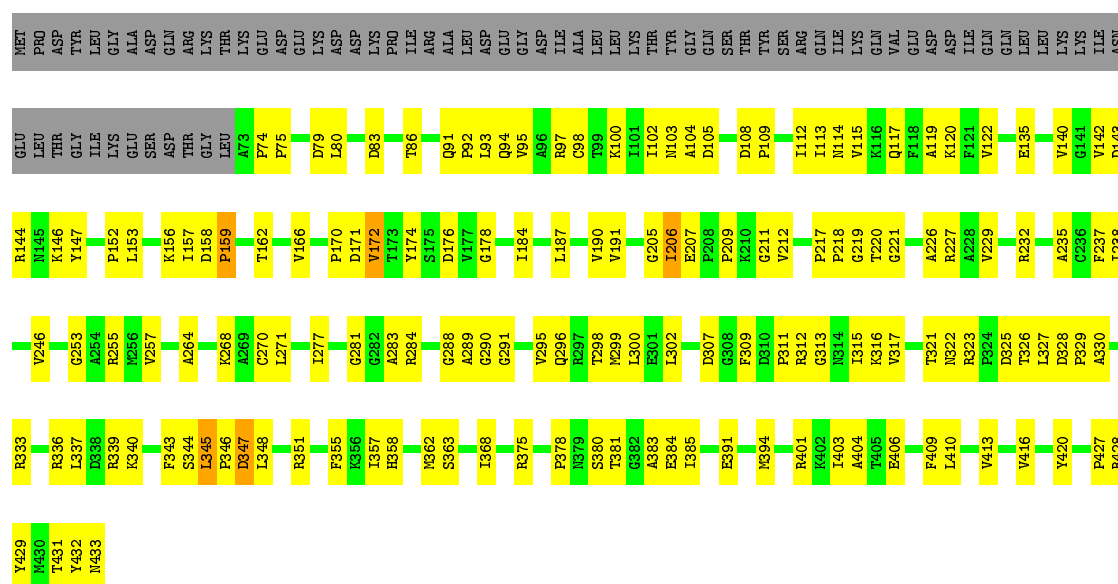
- Molecule 14: Proteasome subunit beta type-4

Chain T: 65% 16% 18%



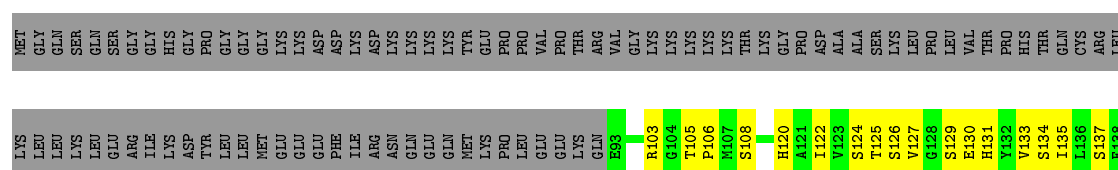
- Molecule 15: 26S protease regulatory subunit 7

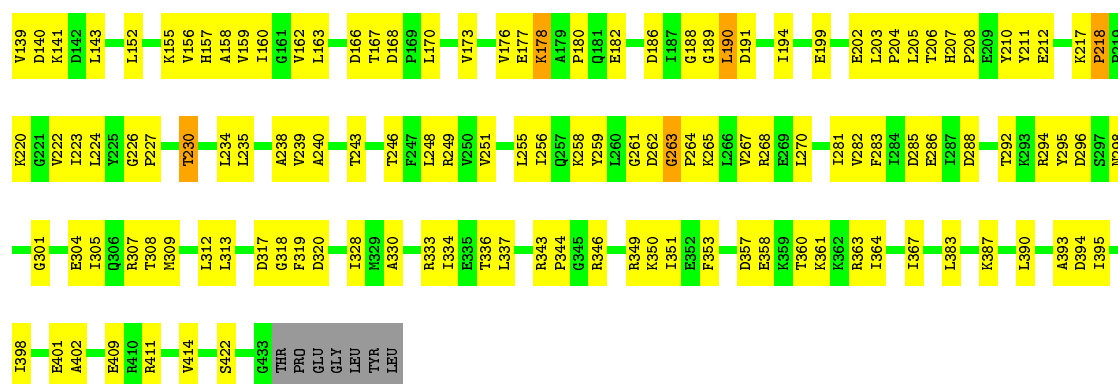
Chain A: 48% 34% • 17%



- Molecule 16: 26S protease regulatory subunit 4

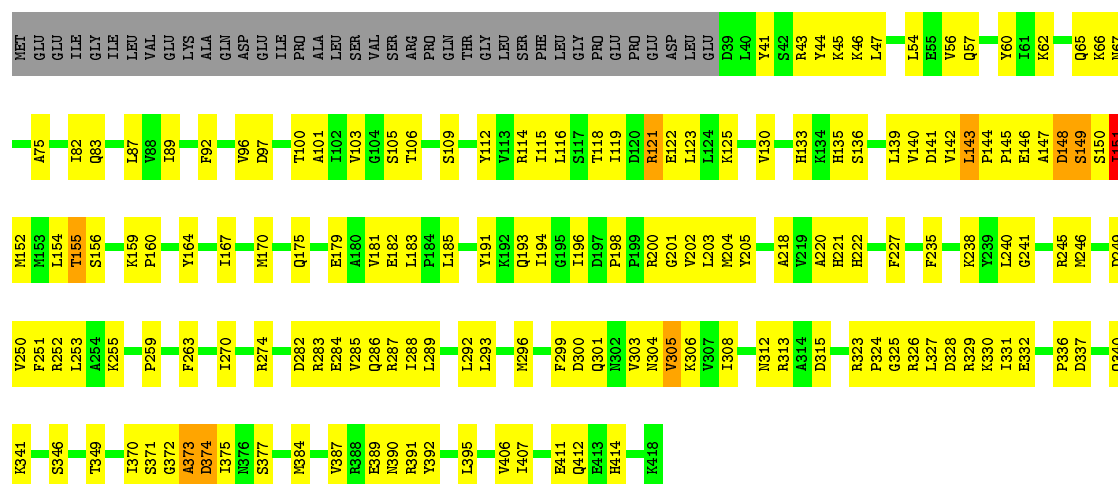
Chain B:  45% 32% • 23%





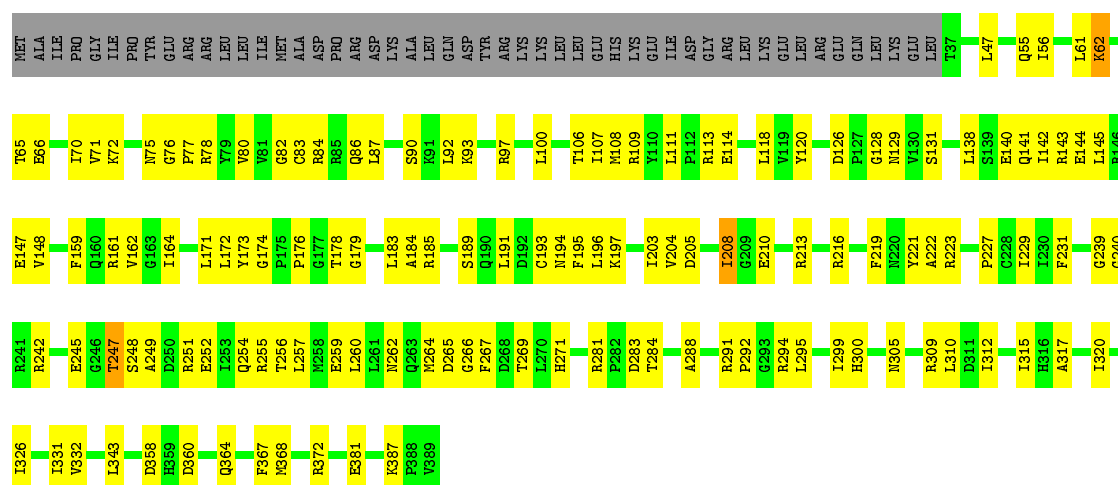
• Molecule 17: 26S protease regulatory subunit 6B

Chain D: 53% 36% 9%



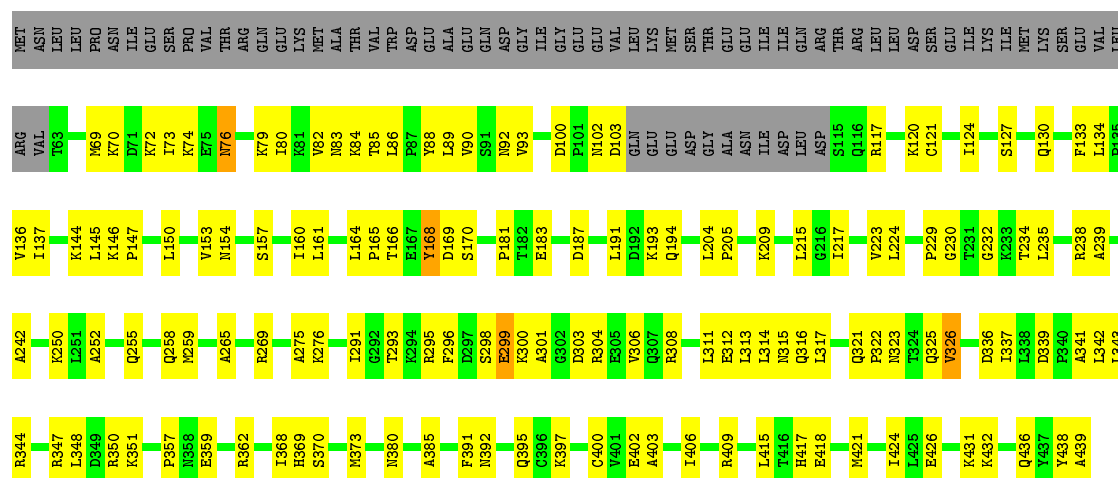
• Molecule 18: 26S protease regulatory subunit 10B

Chain E: 55% 32% 12%



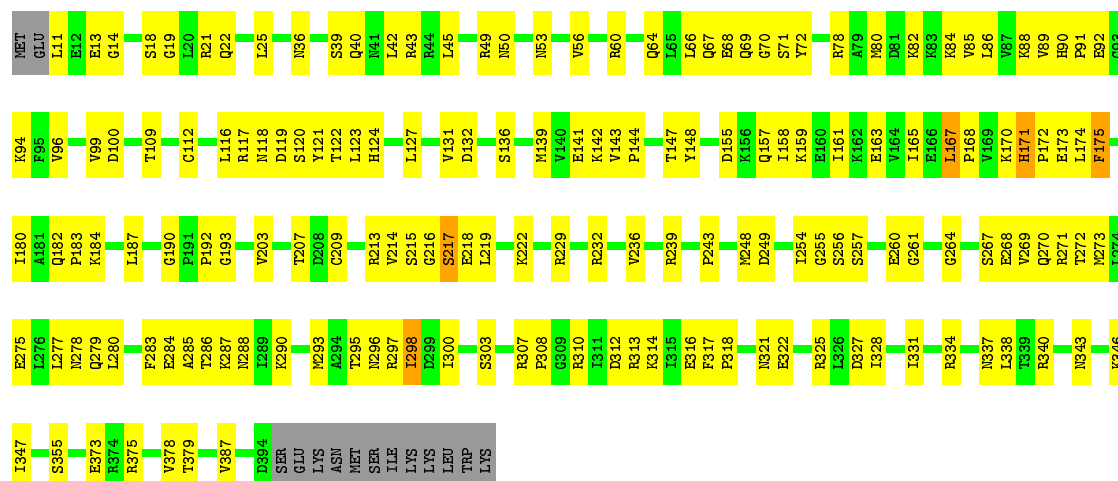
• Molecule 19: 26S protease regulatory subunit 6A

Chain F: 



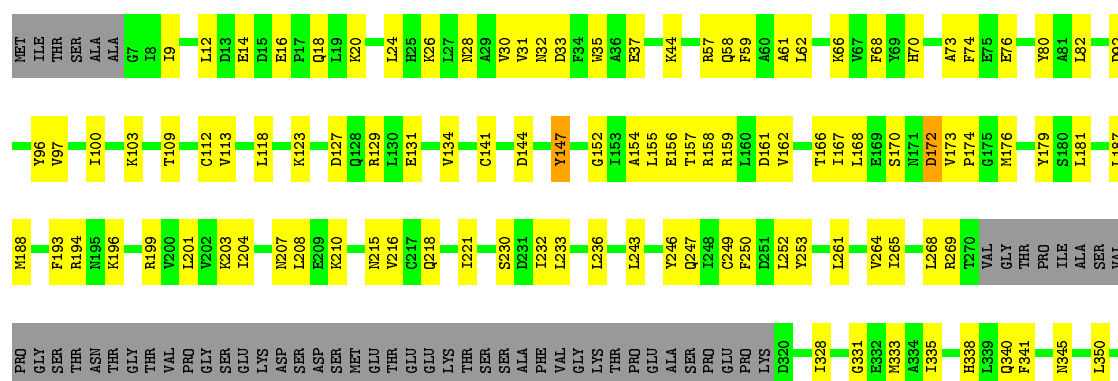
• Molecule 20: 26S protease regulatory subunit 8

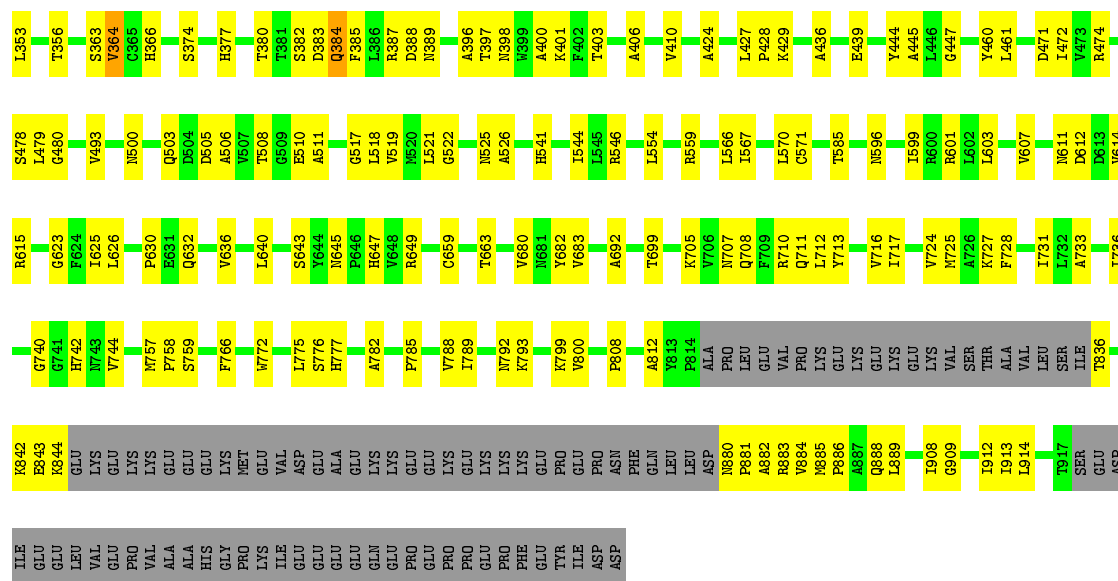
Chain C: 



• Molecule 21: 26S proteasome non-ATPase regulatory subunit 1

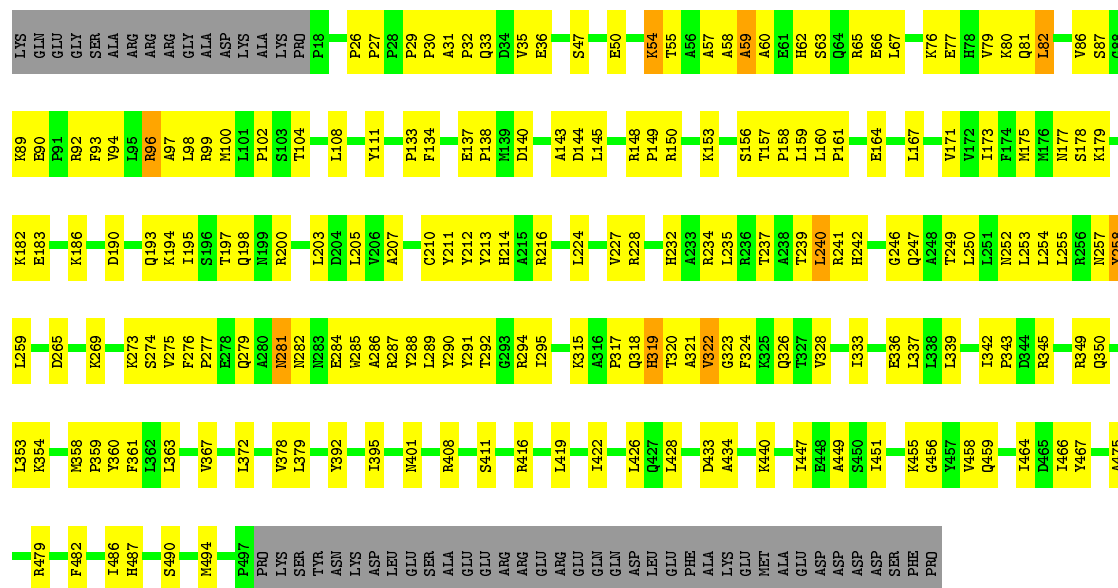
Chain U: 





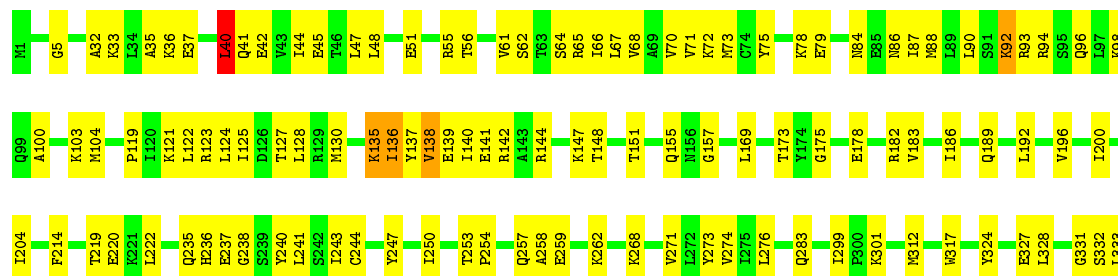
• Molecule 22: 26S proteasome non-ATPase regulatory subunit 3

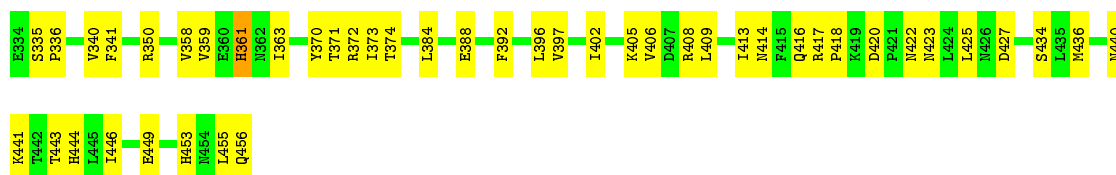
Chain V: 54% 35% 10%



• Molecule 23: 26S proteasome non-ATPase regulatory subunit 12

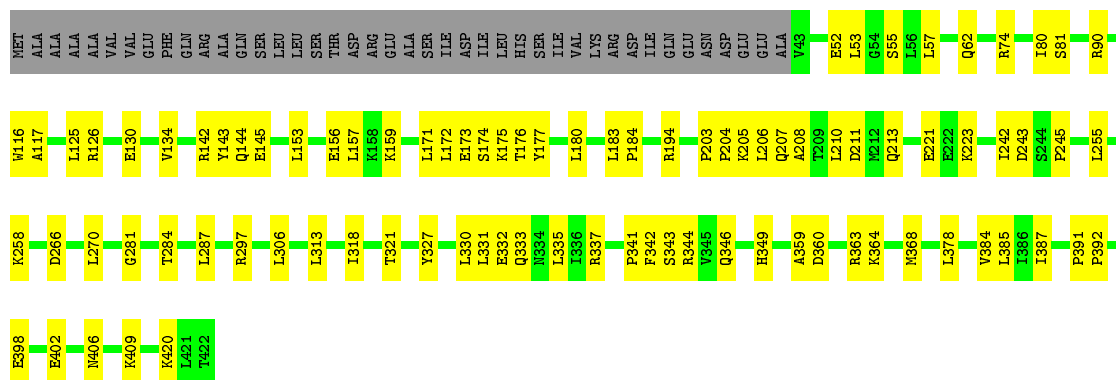
Chain W: 65% 34%





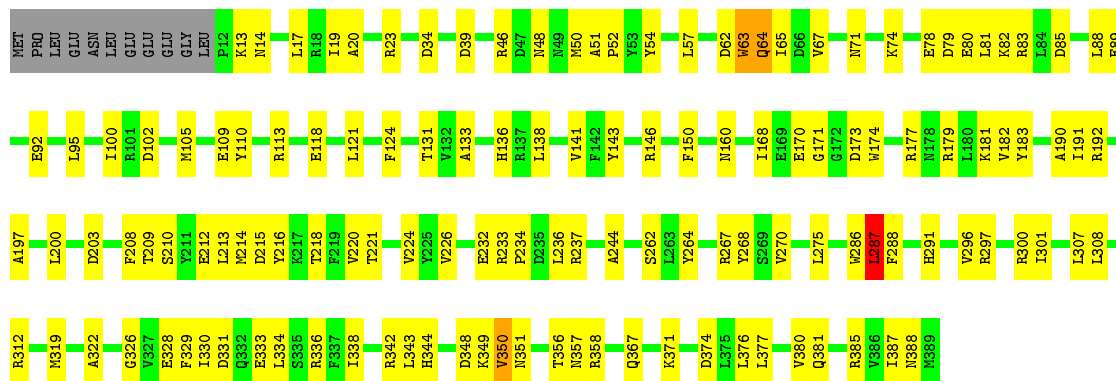
- Molecule 24: 26S proteasome non-ATPase regulatory subunit 11

Chain X: 69% 21% 10%



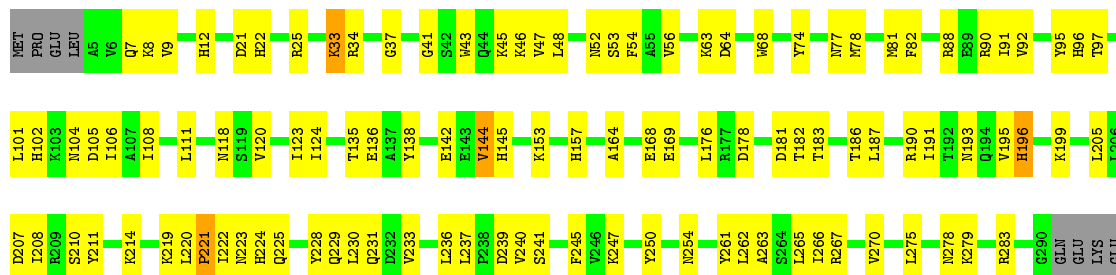
- Molecule 25: 26S proteasome non-ATPase regulatory subunit 6

Chain Y: 63% 33% 4%



- Molecule 26: 26S proteasome non-ATPase regulatory subunit 7

Chain Z: 55% 32% 12%



GLU
SER
LYS
LYS
ASP
ARG
LYS
GLU
ASP
LYS
GLU
LYS
LYS
LYS
ASP
LYS
LYS
GLU
LYS
SER
ASP
VAL
LYS
LYS
LYS
GLU
GLU
LYS
LYS
LYS
LYS

- Molecule 27: 26S proteasome non-ATPase regulatory subunit 13

Chain a:  98% ..

MET
LYS
ASP
V4
H69
L145
I166
D260
V336
V340
T376

- Molecule 28: 26S proteasome non-ATPase regulatory subunit 4

Chain b:  50% 49%


M1
T77
G191
GLU
GLY
GLY
MET
ALA
LEU
ASP
GLY
LEU
GLY
ALA
LYS
SER
ASP
PHE
GLU
PHE
GLY
VAL
ASP
PRO
SER
ALA
ALA
PRO
GLU
LEU
LEU
SER
LEU
LEU
SER
MET
GLU
GLN
ILE
ARG
ALA
ARG
GLN
GLU
GLU
SER
GLY
ALA
ARG
ALA
PHE
GLY
SER
ALA
ALA
GLU
SER
ALA

GLY
ILE
ALA
THR
THR
GLY
GLU
ASP
SER
SER
ASP
GLY
ALA
LEU
LEU
LYS
GLU
MET
THR
ILE
SER
PHE
PHE
GLY
ARG
THR
GLY
LEU
LEU
PRO
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SER
VAL
LEU
SER
ASP
GLY
ASP
MET
GLY
GLU
GLN
ILE
TYR
ALA
MET
MET
SER
GLY
LEU
GLY
GLY
MET
GLY
GLY
ALA
THR
ASP

ASP
ILE
ASP
ALA
SER
SER
ALA
MET
THR
THR
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GLU
PRO
ALA
ALA
LYS
GLU
GLU
MET
ASP
TYR
ASP
GLN
PHE
PRO
GLU
LEU
LEU
SER
VAL
LEU
SER
ASN
MET
THR
GLY
PRO
GLY
ASP
PRO
ASN
GLY
ALA
TLE
ARG
MET
SER
ALA
MET
GLY
GLY
SER
LEU
ALA
SER
GLN
ALA
THR
LYS
ASP

GLY
LYS
LYS
ASP
LYS
LYS
GLU
GLU
LYS

- Molecule 29: 26S proteasome non-ATPase regulatory subunit 14

Chain c:  90% 7%

ASP
ARG
LEU
LEU
ARG
GLY
GLY
MET
PRO
GLY
LEU
GLY
GLN
GLY
PRO
PRO
THR
ASP
ALA
ALA
A24
I38
P105
V151
V156
I157
I189
Y234
S243
V244
K310

- Molecule 30: 26S proteasome non-ATPase regulatory subunit 8

Chain d:  72% 26%

PHE
ILE
LYS
GLY
ARG
ALA
PRO
ARG
ALA
ASN
GLY
PRO
ALA
ARG
GLY
ARG
ARG
ARG
GLY
GLY
GLY
ARG
GLN
VAL
VAL
ALA
PRO
PRO
ALA
ARG
ALA
LEU
GLY
GLY
SER
THR
SER
GLY
ALA
ALA
THR
SER
GLY
ALA
VAL
VAL
LEU
GLN
ALA
ALA
ALA
GLY
M1
Y2
E3
P37
R213
G214
V257

ARG
LYS
MET
ALA
ALA
ALA
VAL
ASN
GLY
ALA
ALA
GLY
PHE
SER
SER
SER
GLY
PRO
ALA
ALA
THR
SER
GLY
ALA
VAL
VAL
LEU
ASP
ASP
ASP
ALA
HIS
VAL
TRP
E40
S70

- Molecule 31: 26S proteasome complex subunit DSS1

Chain e:  56% 43%

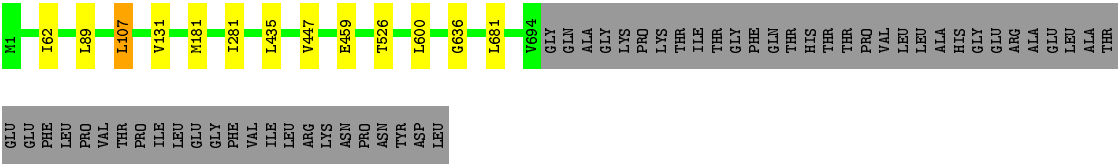
M1
K4
D9
LEU
GLY
LEU
GLU
GLU
ASP
ASP
GLU
PHE
GLU
PHE
PRO
ALA
ALA
ASP
TRP
ALA
GLY
LEU
ASP
ASP
ASP
ALA
HIS
VAL
TRP
E40
S70

- Molecule 32: 26S proteasome non-ATPase regulatory subunit 2

Chain f:

91%

• 7%



GLU
GLU
PHE
LEU
PRO
VAL
THR
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LEU
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GLY
PHE
VAL
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LEU
ARG
LYS
ASN
PRO
ASN
TYR
ASP
LEU

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	139236	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, ATP

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	G	0.30	0/1859	0.50	0/2523
10	P	0.28	0/1614	0.47	0/2177
11	Q	0.29	0/1603	0.49	0/2174
12	R	0.28	0/1579	0.45	0/2134
13	S	0.28	0/1671	0.47	0/2253
14	T	0.28	0/1700	0.46	0/2305
15	A	0.30	0/2886	0.53	0/3899
16	B	0.29	0/2700	0.51	0/3645
17	D	0.31	0/3090	0.59	2/4168 (0.0%)
18	E	0.30	0/2835	0.52	1/3821 (0.0%)
19	F	0.29	0/2903	0.51	1/3912 (0.0%)
2	H	0.30	0/1747	0.49	0/2376
20	C	0.29	0/3054	0.56	3/4107 (0.1%)
21	U	0.29	0/6396	0.49	0/8646
22	V	0.31	0/3929	0.57	0/5309
23	W	0.29	0/3751	0.54	3/5042 (0.1%)
24	X	0.27	0/3053	0.44	0/4115
25	Y	0.30	0/3173	0.53	2/4273 (0.0%)
26	Z	0.27	0/2324	0.55	0/3150
27	a	0.36	1/3053 (0.0%)	0.52	0/4133
28	b	0.27	0/1478	0.48	0/2001
29	c	0.33	0/2302	0.60	1/3110 (0.0%)
3	I	0.29	0/1942	0.51	0/2628
30	d	0.30	0/2162	0.57	0/2919
31	e	0.28	0/338	0.56	0/450
32	f	0.33	2/5413 (0.0%)	0.63	3/7317 (0.0%)
4	J	0.28	0/1728	0.48	0/2358
5	K	0.28	0/1747	0.48	0/2364
6	L	0.28	0/1885	0.48	0/2552
7	M	0.28	0/1891	0.46	0/2552
8	N	0.28	0/1454	0.48	0/1967
9	O	0.27	0/1670	0.49	0/2265

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
All	All	0.30	3/78930 (0.0%)	0.52	16/106645 (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
17	D	0	1
20	C	0	1
29	c	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	145	LEU	C-N	11.92	1.56	1.34
32	f	681	LEU	C-N	6.42	1.46	1.34
32	f	181	MET	C-N	-5.33	1.21	1.34

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	167	LEU	CB-CG-CD2	6.98	122.86	111.00
32	f	459	GLU	N-CA-C	6.02	127.25	111.00
20	C	217	SER	C-N-CA	5.95	136.58	121.70
17	D	151	ILE	C-N-CA	5.85	136.32	121.70
32	f	107	LEU	CA-CB-CG	5.62	128.22	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
20	C	171	HIS	Peptide
17	D	148	ASP	Peptide
29	c	243	SER	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	G	1826	0	1796	69	0
2	H	1713	0	1598	58	0
3	I	1912	0	1851	60	0
4	J	1704	0	1517	59	0
5	K	1722	0	1673	64	0
6	L	1850	0	1822	72	0
7	M	1856	0	1814	66	0
8	N	1430	0	1398	24	0
9	O	1643	0	1644	23	0
10	P	1585	0	1598	40	0
11	Q	1570	0	1547	51	0
12	R	1548	0	1499	30	0
13	S	1641	0	1618	30	0
14	T	1667	0	1628	31	0
15	A	2835	0	2879	133	0
16	B	2662	0	2702	134	0
17	D	3040	0	3076	158	0
18	E	2790	0	2846	113	0
19	F	2863	0	2931	110	0
20	C	3015	0	3125	160	0
21	U	6287	0	6338	169	0
22	V	3852	0	3893	155	0
23	W	3703	0	3822	127	0
24	X	3009	0	3113	63	0
25	Y	3115	0	3120	99	0
26	Z	2281	0	2312	99	0
27	a	2995	0	3012	0	0
28	b	1458	0	1505	0	0
29	c	2260	0	2276	0	0
30	d	2116	0	2146	0	0
31	e	334	0	294	0	0
32	f	5331	0	5343	0	0
33	A	31	0	12	2	0
33	B	31	0	12	3	0
33	C	31	0	12	1	0
33	D	31	0	12	3	0
33	E	31	0	12	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	F	31	0	12	3	0
34	c	1	0	0	0	0
All	All	77800	0	77808	1973	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 17.

The worst 5 of 1973 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)
26:Z:261:TYR:O	26:Z:265:LEU:HD13	1.20	1.35
26:Z:261:TYR:O	26:Z:265:LEU:CD1	1.86	1.24
20:C:217:SER:HB3	20:C:218:GLU:HB3	1.38	1.02
26:Z:261:TYR:C	26:Z:265:LEU:HD13	1.79	1.01
17:D:152:MET:CE	18:E:62:LYS:HG3	1.94	0.97

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	G	238/245 (97%)	223 (94%)	13 (6%)	2 (1%)	24	70
2	H	230/233 (99%)	216 (94%)	14 (6%)	0	100	100
3	I	248/260 (95%)	230 (93%)	17 (7%)	1 (0%)	39	80
4	J	237/247 (96%)	223 (94%)	12 (5%)	2 (1%)	24	70
5	K	224/240 (93%)	204 (91%)	16 (7%)	4 (2%)	11	55
6	L	236/268 (88%)	218 (92%)	18 (8%)	0	100	100
7	M	238/254 (94%)	219 (92%)	18 (8%)	1 (0%)	39	80
8	N	189/238 (79%)	182 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	O	218/276 (79%)	212 (97%)	6 (3%)	0	100	100
10	P	202/204 (99%)	192 (95%)	10 (5%)	0	100	100
11	Q	197/201 (98%)	185 (94%)	12 (6%)	0	100	100
12	R	199/262 (76%)	191 (96%)	8 (4%)	0	100	100
13	S	211/240 (88%)	203 (96%)	8 (4%)	0	100	100
14	T	213/263 (81%)	207 (97%)	6 (3%)	0	100	100
15	A	359/433 (83%)	317 (88%)	37 (10%)	5 (1%)	14	59
16	B	339/440 (77%)	308 (91%)	27 (8%)	4 (1%)	16	62
17	D	378/418 (90%)	339 (90%)	32 (8%)	7 (2%)	10	54
18	E	351/403 (87%)	321 (92%)	27 (8%)	3 (1%)	21	67
19	F	362/439 (82%)	326 (90%)	33 (9%)	3 (1%)	24	70
20	C	382/398 (96%)	337 (88%)	42 (11%)	3 (1%)	24	70
21	U	798/953 (84%)	762 (96%)	34 (4%)	2 (0%)	46	83
22	V	478/533 (90%)	431 (90%)	39 (8%)	8 (2%)	11	56
23	W	454/456 (100%)	412 (91%)	38 (8%)	4 (1%)	21	67
24	X	378/422 (90%)	363 (96%)	15 (4%)	0	100	100
25	Y	376/389 (97%)	341 (91%)	31 (8%)	4 (1%)	17	64
26	Z	284/324 (88%)	257 (90%)	23 (8%)	4 (1%)	14	59
27	a	371/376 (99%)	343 (92%)	23 (6%)	5 (1%)	15	61
28	b	189/377 (50%)	180 (95%)	8 (4%)	1 (0%)	34	77
29	c	285/309 (92%)	253 (89%)	26 (9%)	6 (2%)	9	52
30	d	255/349 (73%)	227 (89%)	25 (10%)	3 (1%)	16	62
31	e	36/70 (51%)	32 (89%)	3 (8%)	1 (3%)	6	46
32	f	686/749 (92%)	571 (83%)	110 (16%)	5 (1%)	26	71
All	All	9841/11269 (87%)	9025 (92%)	738 (8%)	78 (1%)	29	70

5 of 78 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	111	VAL
5	K	12	VAL
21	U	364	VAL
23	W	136	ILE
25	Y	350	VAL

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	G	193/209 (92%)	192 (100%)	1 (0%)	92	96
2	H	164/190 (86%)	164 (100%)	0	100	100
3	I	193/220 (88%)	193 (100%)	0	100	100
4	J	152/210 (72%)	151 (99%)	1 (1%)	88	94
5	K	186/202 (92%)	186 (100%)	0	100	100
6	L	198/229 (86%)	197 (100%)	1 (0%)	92	96
7	M	192/211 (91%)	191 (100%)	1 (0%)	92	96
8	N	148/180 (82%)	148 (100%)	0	100	100
9	O	177/227 (78%)	177 (100%)	0	100	100
10	P	172/173 (99%)	172 (100%)	0	100	100
11	Q	164/171 (96%)	164 (100%)	0	100	100
12	R	153/201 (76%)	153 (100%)	0	100	100
13	S	174/198 (88%)	174 (100%)	0	100	100
14	T	175/214 (82%)	175 (100%)	0	100	100
15	A	308/372 (83%)	306 (99%)	2 (1%)	90	95
16	B	298/385 (77%)	296 (99%)	2 (1%)	88	94
17	D	333/366 (91%)	331 (99%)	2 (1%)	90	95
18	E	308/353 (87%)	306 (99%)	2 (1%)	90	95
19	F	312/379 (82%)	307 (98%)	5 (2%)	70	88
20	C	332/346 (96%)	329 (99%)	3 (1%)	84	92
21	U	685/816 (84%)	681 (99%)	4 (1%)	90	95
22	V	414/459 (90%)	409 (99%)	5 (1%)	78	90
23	W	416/416 (100%)	413 (99%)	3 (1%)	88	94
24	X	327/362 (90%)	325 (99%)	2 (1%)	90	95
25	Y	334/344 (97%)	334 (100%)	0	100	100
26	Z	257/295 (87%)	256 (100%)	1 (0%)	93	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	a	333/336 (99%)	333 (100%)	0	100	100
28	b	167/312 (54%)	167 (100%)	0	100	100
29	c	252/267 (94%)	250 (99%)	2 (1%)	86	93
30	d	231/293 (79%)	230 (100%)	1 (0%)	93	96
31	e	38/63 (60%)	38 (100%)	0	100	100
32	f	582/628 (93%)	578 (99%)	4 (1%)	88	94
All	All	8368/9627 (87%)	8326 (100%)	42 (0%)	92	96

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	C	53	ASN
21	U	384	GLN
32	f	89	LEU
20	C	175	PHE
21	U	172	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
22	V	33	GLN
29	c	172	HIS
32	f	565	ASN
23	W	257	GLN
23	W	414	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

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
33	ATP	A	501	-	26,33,33	0.93	1 (3%)	26,52,52	1.82	4 (15%)
33	ATP	B	501	-	26,33,33	0.94	1 (3%)	26,52,52	1.75	3 (11%)
33	ATP	C	501	-	26,33,33	0.95	1 (3%)	26,52,52	1.74	3 (11%)
33	ATP	D	501	-	26,33,33	0.95	1 (3%)	26,52,52	1.76	2 (7%)
33	ATP	E	401	-	26,33,33	0.98	1 (3%)	26,52,52	1.78	2 (7%)
33	ATP	F	501	-	26,33,33	0.95	1 (3%)	26,52,52	1.70	3 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	ATP	A	501	-	-	0/18/38/38	0/3/3/3
33	ATP	B	501	-	-	0/18/38/38	0/3/3/3
33	ATP	C	501	-	-	0/18/38/38	0/3/3/3
33	ATP	D	501	-	-	0/18/38/38	0/3/3/3
33	ATP	E	401	-	-	0/18/38/38	0/3/3/3
33	ATP	F	501	-	-	0/18/38/38	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	A	501	ATP	C5-C4	2.97	1.47	1.40
33	B	501	ATP	C5-C4	2.98	1.47	1.40
33	F	501	ATP	C5-C4	2.99	1.47	1.40
33	D	501	ATP	C5-C4	3.00	1.47	1.40
33	C	501	ATP	C5-C4	3.05	1.47	1.40

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	A	501	ATP	N3-C2-N1	-7.19	123.22	128.87
33	E	401	ATP	N3-C2-N1	-6.93	123.42	128.87
33	B	501	ATP	N3-C2-N1	-6.87	123.48	128.87
33	C	501	ATP	N3-C2-N1	-6.70	123.61	128.87
33	D	501	ATP	N3-C2-N1	-6.70	123.61	128.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	A	501	ATP	2	0
33	B	501	ATP	3	0
33	C	501	ATP	1	0
33	D	501	ATP	3	0
33	E	401	ATP	4	0
33	F	501	ATP	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
32	f	3
2	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	f	110:ALA	C	111:LEU	N	9.72
1	f	79:ASN	C	80:TYR	N	7.23
1	f	348:ASP	C	349:SER	N	5.88
1	H	2:ALA	C	3:GLU	N	5.52