



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jun 5, 2017 – 09:02 PM EDT

PDB ID : 5WVI
EMDB ID: : EMD-6693
Title : The resting state of yeast proteasome
Authors : Ding, Z.; Cong, Y.
Deposited on : 2016-12-25
Resolution : 6.30 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
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) : rb-20029077

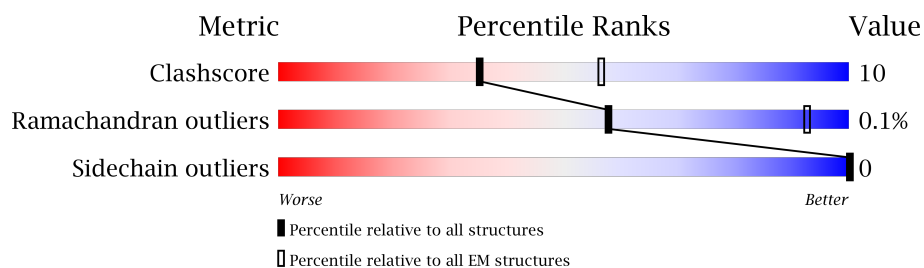
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.30 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.









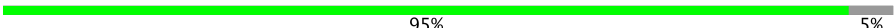















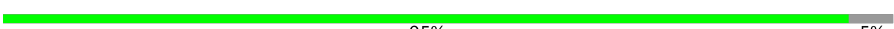


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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	I	437	58% 24% 17%
2	K	428	61% 28% 11%
3	2	261	68% 17% 15%
3	i	261	85% 15%
4	A	252	71% 26% .
4	c	252	96% .
5	3	205	71% 29%
5	h	205	99% .
6	G	288	65% 20% 15%


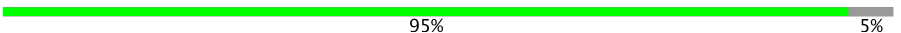

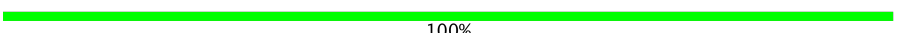






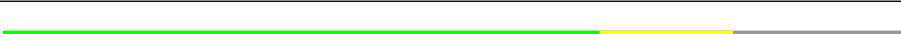


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Mol	Chain	Length	Quality of chain
6	k	288	
7	F	234	
7	l	234	
8	E	260	
8	m	260	
9	D	254	
9	n	254	
10	Y	89	
11	N	945	
12	S	523	
13	T	274	
14	R	429	
15	Q	434	
16	J	405	
17	L	437	
18	M	434	
19	U	338	
20	W	268	
21	O	393	
22	P	445	
23	H	467	
24	C	258	
24	d	258	
25	B	250	
25	j	250	

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Mol	Chain	Length	Quality of chain
26	1	215	
26	b	215	
27	4	198	
27	g	198	
28	5	287	
28	f	287	
29	6	241	
29	e	241	
30	7	266	
30	a	266	
31	X	156	
32	Z	993	
33	V	306	

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 105787 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 26S protease regulatory subunit 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	I	362	Total	C	N	O	S	0	0
			2822	1773	471	563	15		

- Molecule 2 is a protein called 26S protease regulatory subunit 6B homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	K	381	Total	C	N	O	S	0	0
			3019	1898	530	581	10		

- Molecule 3 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	i	222	Total	C	N	O	S	0	0
			1684	1061	293	323	7		
3	2	222	Total	C	N	O	S	0	0
			1684	1061	293	323	7		

- Molecule 4 is a protein called Proteasome subunit alpha type-1.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	h	204	Total	C	N	O	S	0	0
			1581	1010	258	305	8		
5	3	204	Total	C	N	O	S	0	0
			1581	1010	258	305	8		

- Molecule 6 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	k	245	Total	C	N	O	S	0	0
			1900	1207	331	358	4		
6	G	245	Total	C	N	O	S	0	0
			1900	1207	331	358	4		

- Molecule 7 is a protein called Proteasome subunit alpha type-6.

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

- Molecule 8 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	m	243	Total	C	N	O	S	0	0
			1867	1165	315	380	7		
8	E	243	Total	C	N	O	S	0	0
			1867	1165	315	380	7		

- Molecule 9 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	n	242	Total	C	N	O	S	0	0
			1899	1186	333	376	4		
9	D	242	Total	C	N	O	S	0	0
			1899	1186	333	376	4		

- Molecule 10 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	Y	27	Total	C	N	O	0	0
			236	143	39	54		

- Molecule 11 is a protein called 26S proteasome regulatory subunit RPN2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	849	Total	C	N	O	S	0	0
			6562	4174	1099	1261	28		

- Molecule 12 is a protein called 26S proteasome regulatory subunit RPN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	S	353	Total	C	N	O	S	0	0
			2893	1857	482	541	13		

- Molecule 13 is a protein called 26S proteasome regulatory subunit RPN12.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	T	272	Total	C	N	O	S	0	0
			2235	1432	355	441	7		

- Molecule 14 is a protein called 26S proteasome regulatory subunit RPN7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	R	400	Total	C	N	O	S	0	0
			3218	2051	527	630	10		

- Molecule 15 is a protein called 26S proteasome regulatory subunit RPN6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	431	Total	C	N	O	S	0	0
			3471	2205	574	676	16		

- Molecule 16 is a protein called 26S protease regulatory subunit 8 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	373	Total	C	N	O	S	0	0
			2928	1837	527	547	17		

- Molecule 17 is a protein called 26S protease subunit RPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	361	Total	C	N	O	S	0	0
			2853	1798	507	536	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	367	Total	C	N	O	S	0	0
			2866	1799	503	553	11		

- Molecule 19 is a protein called 26S proteasome regulatory subunit RPN8.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	282	Total	C	N	O	S	0	0
			2257	1429	387	435	6		

- Molecule 20 is a protein called 26S proteasome regulatory subunit RPN10.

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

- Molecule 21 is a protein called 26S proteasome regulatory subunit RPN9.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O	387	Total	C	N	O	S	0	0
			3182	2047	520	606	9		

- Molecule 22 is a protein called 26S proteasome regulatory subunit RPN5.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P	432	Total	C	N	O	S	0	0
			3545	2260	592	684	9		

- Molecule 23 is a protein called 26S protease regulatory subunit 7 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	H	370	Total	C	N	O	S	0	0
			2889	1815	515	543	16		

- Molecule 24 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	C	245	Total	C	N	O	S	0	0
			1913	1207	323	380	3		
24	d	245	Total	C	N	O	S	0	0
			1913	1207	323	380	3		

- Molecule 25 is a protein called Proteasome subunit alpha type-2.

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

- Molecule 26 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	1	205	Total	C	N	O	S	0	0
			1576	996	261	312	7		
26	b	205	Total	C	N	O	S	0	0
			1574	995	261	311	7		

- Molecule 27 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	4	198	Total	C	N	O	S	0	0
			1585	1005	269	305	6		
27	g	198	Total	C	N	O	S	0	0
			1585	1005	269	305	6		

- Molecule 28 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	5	212	Total	C	N	O	S	0	0
			1644	1045	280	312	7		
28	f	212	Total	C	N	O	S	0	0
			1644	1045	280	312	7		

- Molecule 29 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	6	222	Total	C	N	O	S	0	0
			1757	1115	303	335	4		
29	e	222	Total	C	N	O	S	0	0
			1757	1115	303	335	4		

- Molecule 30 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	7	233	Total	C	N	O	S	0	0
			1824	1154	312	351	7		
30	a	233	Total	C	N	O	S	0	0
			1824	1154	312	351	7		

- 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 regulatory subunit RPN1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Z	813	Total	C	N	O	S	0	0
			6289	3995	1029	1236	29		

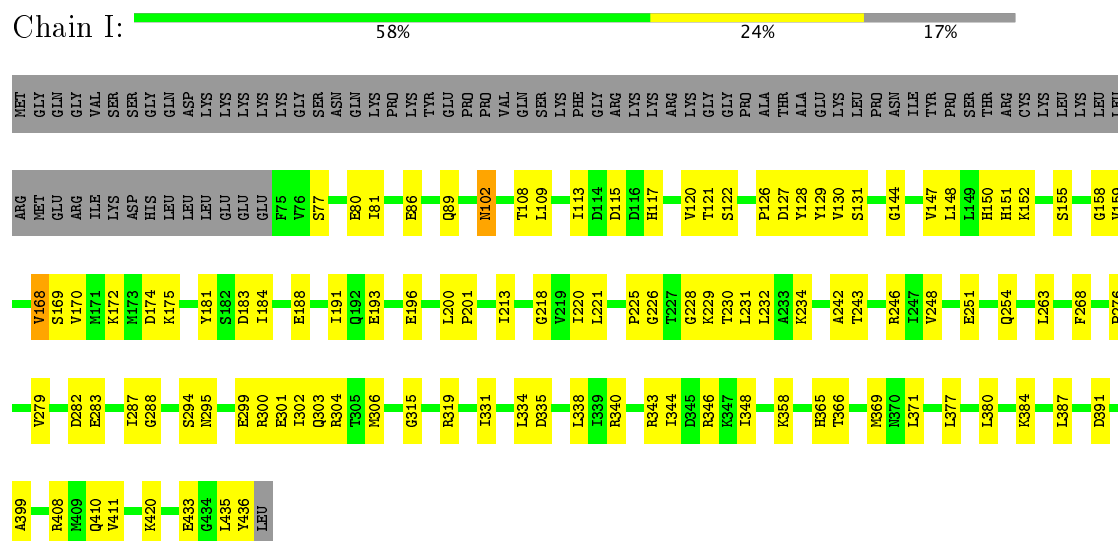
- Molecule 33 is a protein called Ubiquitin carboxyl-terminal hydrolase RPN11.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	V	284	Total	C	N	O	S	0	0
			2236	1405	381	436	14		

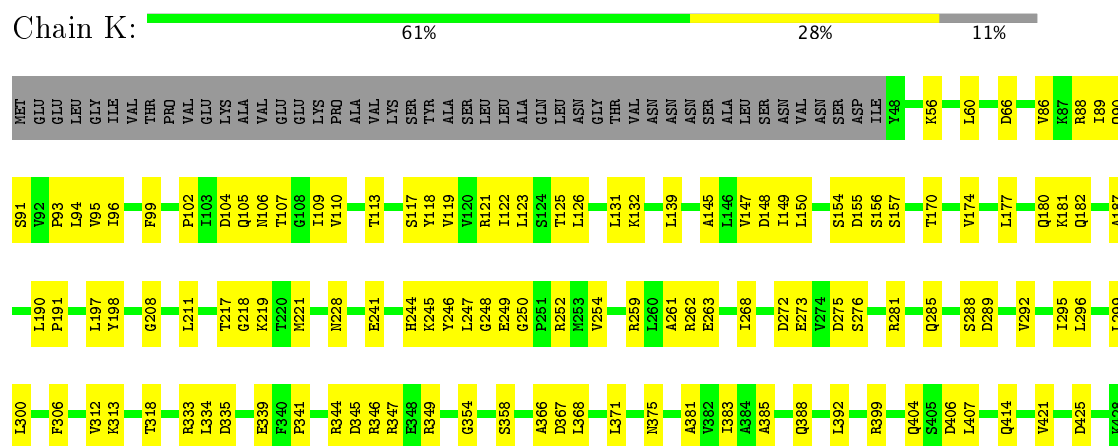
3 Residue-property plots

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.

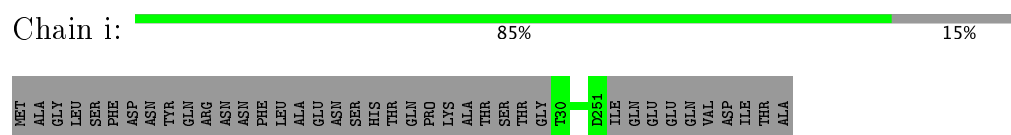
- Molecule 1: 26S protease regulatory subunit 4 homolog



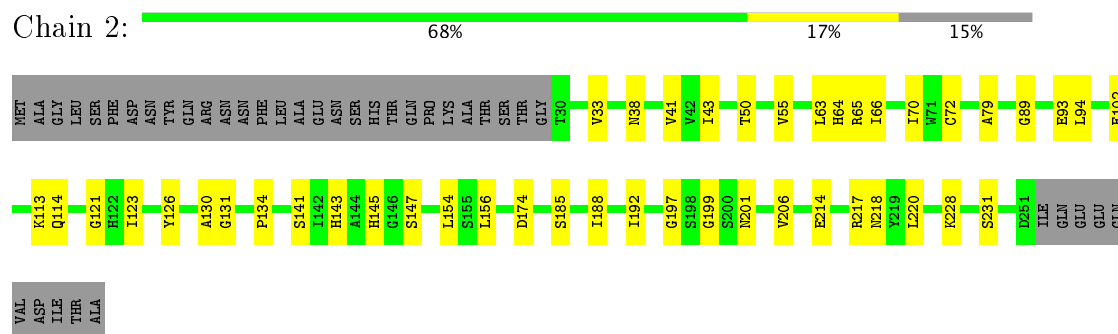
- Molecule 2: 26S protease regulatory subunit 6B homolog



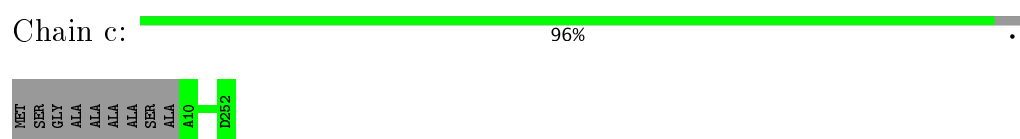
- Molecule 3: Proteasome subunit beta type-2



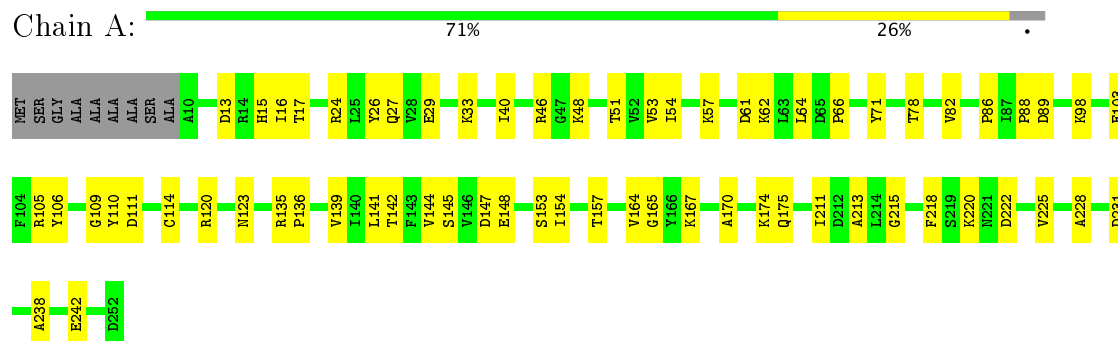
- Molecule 3: Proteasome subunit beta type-2



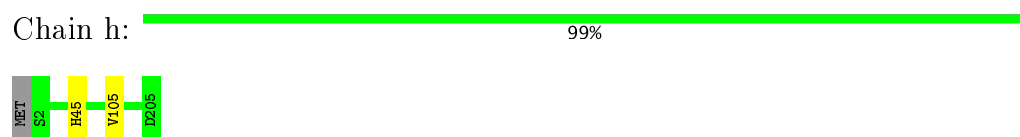
- Molecule 4: Proteasome subunit alpha type-1



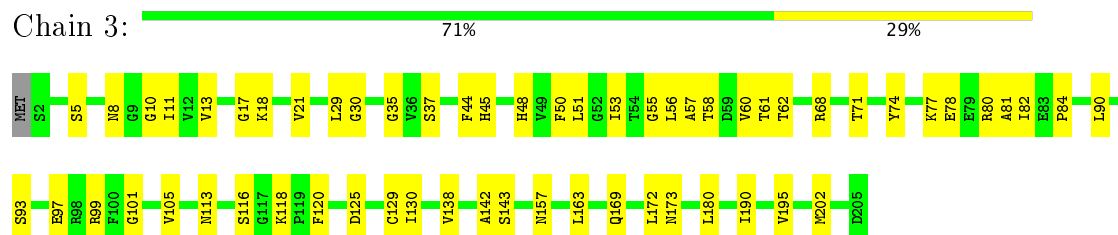
- Molecule 4: Proteasome subunit alpha type-1



- Molecule 5: Proteasome subunit beta type-3



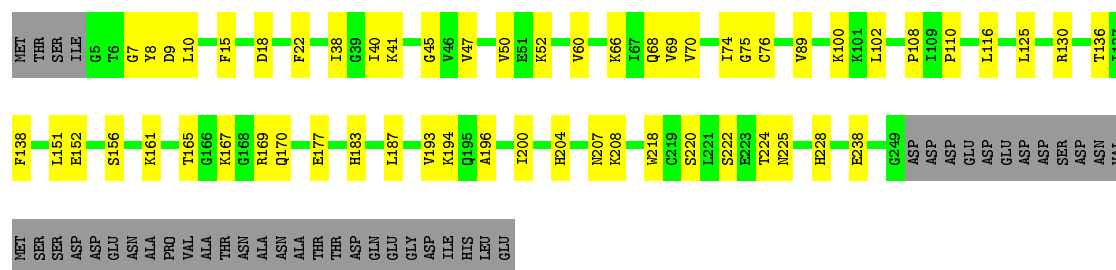
- Molecule 5: Proteasome subunit beta type-3



- Molecule 6: Probable proteasome subunit alpha type-7

MET	THR	SER	ILE	GLU	ASP	ASP	GLU	ASP	GLU	ASP	ASP	ASP	ASN	VAL	MET	SER	SER	ASP	ASP	GLU	ASN	PRO	VAL	THR	ASN	ASN	ALA	THR	THR	ASP	GLN	GLY	ASP	ILE	HIS	LEU	GLU
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

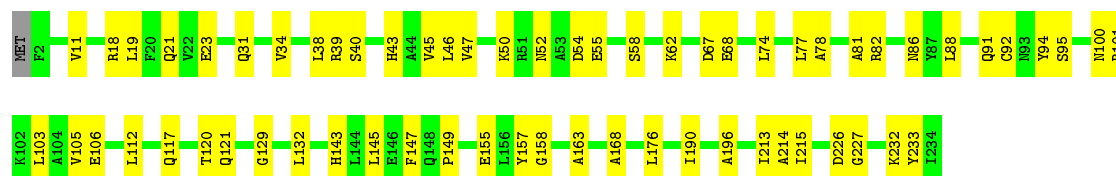
- Chain G: 65% 20% 15%



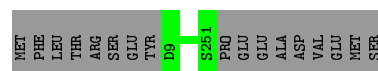
- Chain 1: 100%



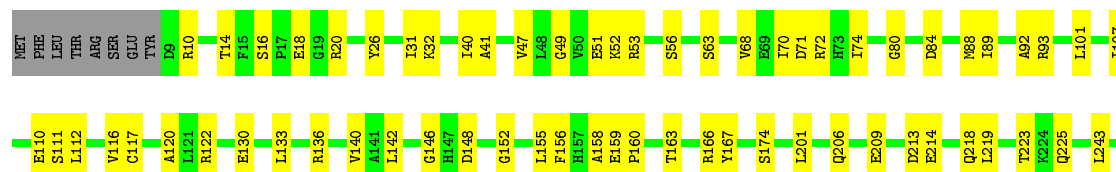
- Chain F: 73% 27%



- Chain m: 93% 7%



- Chain E:  69% 25% 7%



S251
PRO
GLU
GLU
GLU
ALA
ASP
VAL
GLU
MET
SER

- Molecule 9: Proteasome subunit alpha type-4

Chain n: 95% 5%

MET
SER
G3
Q244
GLU
GLN
ASP
LYS
LYS
LYS
LYS
LYS
ASN
HIS

- Molecule 9: Proteasome subunit alpha type-4

Chain D: 72% 24% 5%

MET
SER
G3
Y4
P13
I17
F18
Q19
V20
E21
E25
A26
K28
C32
A33
V34
K37
G38
K39
H40
C41
V42
G45
Q55
D66
T57
R58
I59
K63
V64
S65
K66
I67
D68
S69
V72
L73
S76
G77
L78
N79
R90
V106
T110
R111

G115
Y116
Q117
Y120
T121
Q122
S123
G124
G125
I135
F138
D139
D142
P145
K146
L147
Q149
Y156
S157
W158
W159
T163
I164
G165
S168
R172
A186
T187
E190
V215
I221
Q244
GLN
ASP
LYS
LYS
LYS
LYS
SER
ASN
HIS

- Molecule 10: 26S proteasome complex subunit SEM1

Chain Y: 28% 70%

MET
SER
THR
ASP
VAL
ALA
ALA
ALA
GLN
ALA
GLN
SER
LYS
ILE
ASP
LEU
THR
LYS
LYS
ASN
GLU
GLU
ILE
ASN
LYS
LYS
SER
LEU
GLU
GLU
ASP
ASP
PHE
PHE
GLU
ASP
PHE
PRO
ILE
ASP
THR
TRP
ALA
ASN
GLY
GLU
THR
ILE
LYS
SER
ASN
ALA
VAL
THR
GLN
THR
ASN
ILE
TRP

GLU
E62
D65
D66
V68
GLN

- Molecule 11: 26S proteasome regulatory subunit RPN2

Chain N: 70% 20% 10%

MET
SER
LEU
T4
T5
G6
A7
P8
L9
L13
S19
V20
K21
T22
T25
L25
L28
R29
D33
Q34
L35
K36
D45
Y50
F55
S56
D57
R58
E59
S66
R67
V68
N71
A78
R88
D120
E121
Q122
F123
Y124
F302
N306
E142
K307
L145
G312
N315
A153

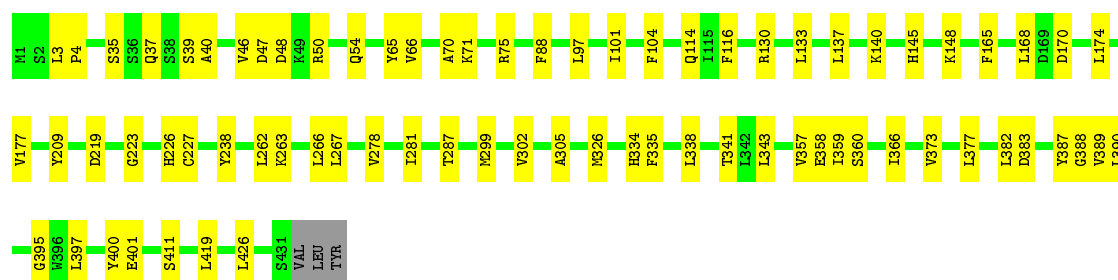
L158
L163
D164
I165
S168
Q176
ASP
S178
N182
L189
T196
R203
L206
L207
R208
V230
R231
N233
D234
D250
L253
A258
L261
S264
N288
I289
L290
L293
D297
Y298
Y299
F302
N306
E142
K307
L145
G312
N315
A153

K324
F325
T330
A331
G337
A341
N352
K355
Q360
T366
S370
L371
L374
R375
K376
G377
K378
K384
L390
F399
S400
K611
N614
A615
R616
V617
T621
A622
F623
A624
L625
G626
I627
A630
L634
Q635
S636
C488
N489
L490
T498
N512

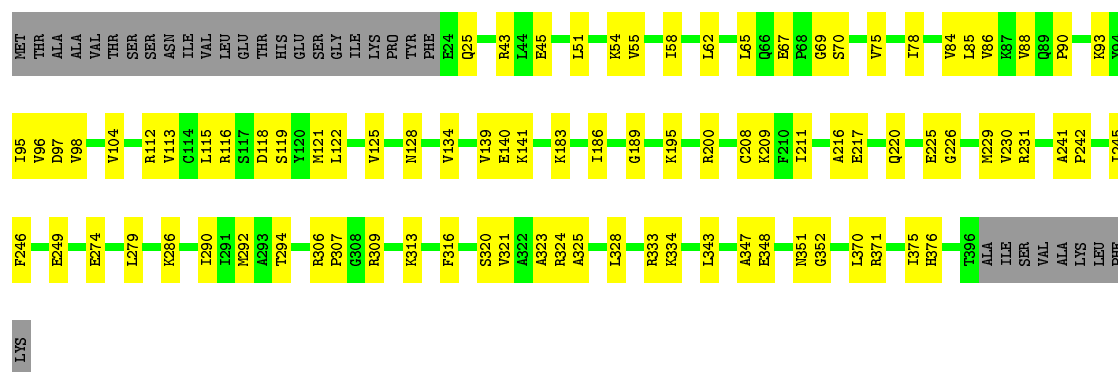
L521
Q529
L535
S545
R548
A558
H573
N580
D581
I582
V583
V588
L591
L595
L596
V602
Q607
L608
L609
S610
K611
N614
A615
R616
V617
T621
A622
F623
A624
L625
G626
I627
A630
L634
Q635
S636
C488
N489
L490
T498
N512

L663
Q666
T668
L671
V685
Q691
L694
F697
A702
G710
R711
H712
V713
A720
D721
T724
L725
D726
T727
K728
S729
L751
P755
R762
G763
S764
D765
Q766
A767
I768
P769
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K778
E779
D780
S783
Y784
L785
P785
M662

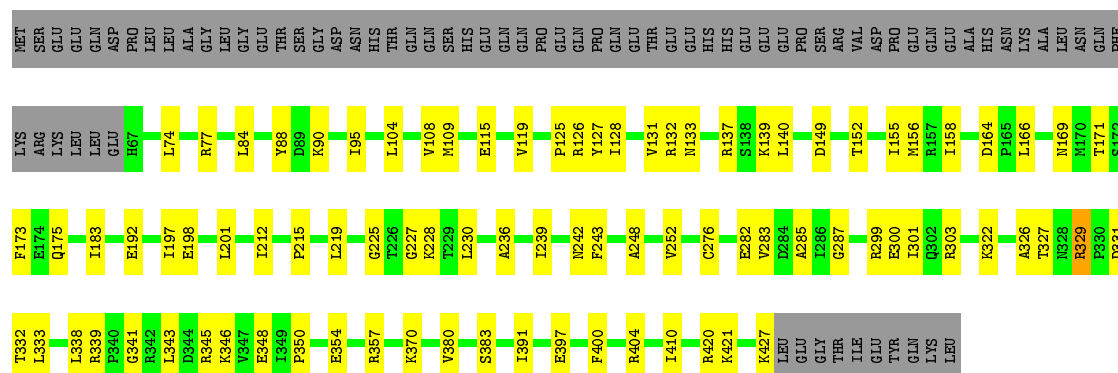
H787
TYR
GLU
GLU
ALA
SER
GLY
LYS
GLU
VAL
GLU
LYS
VAL
ALA
THR
VAL
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SER
THR
ALA
ARG
LYS
LYS
LYS
PRO
ASN
GLU
GLU
GLU
LYS
LYS
LYS
GLU
HIS
GLU
GLU
LYS
LYS
LYS
C775
Y776
K778
E779
D780
S783
Y784
L785
P785
M662



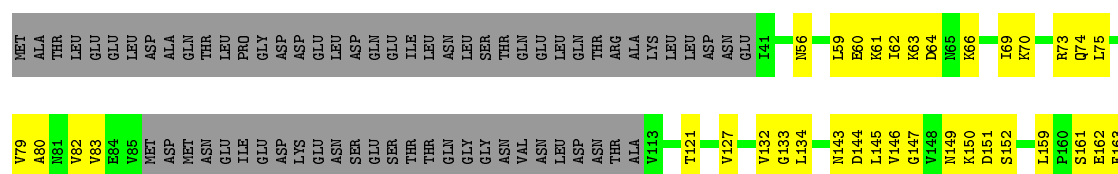
- Molecule 16: 26S protease regulatory subunit 8 homolog

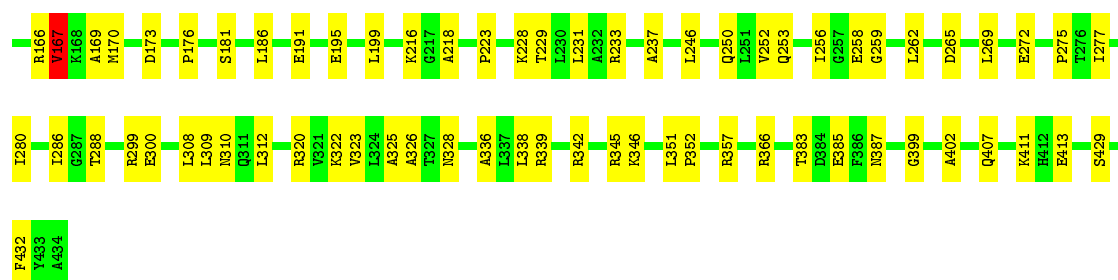


- Molecule 17: 26S protease subunit RPT4



- Molecule 18: 26S protease regulatory subunit 6A

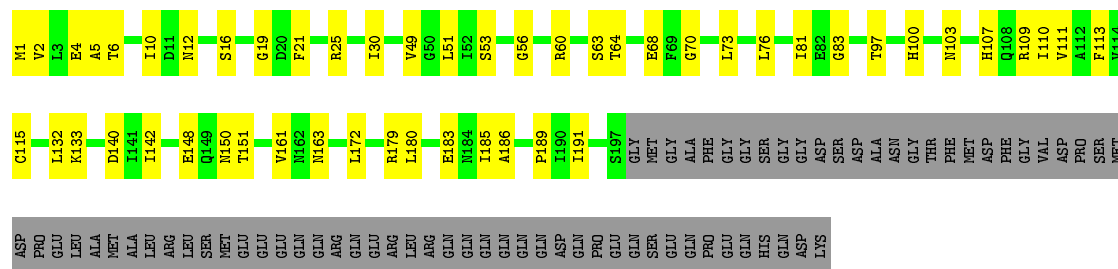




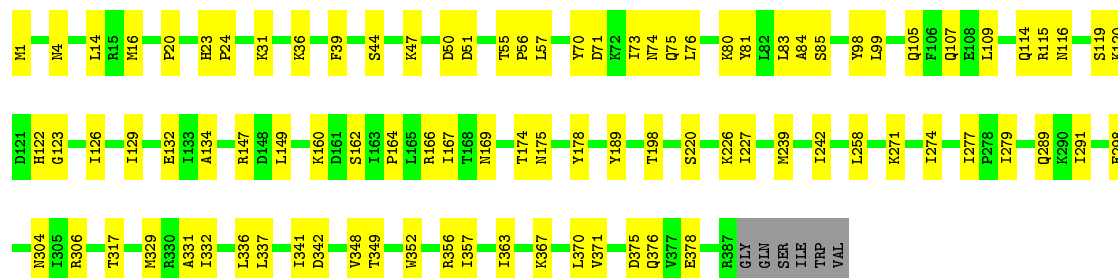
- Molecule 19: 26S proteasome regulatory subunit RPN8



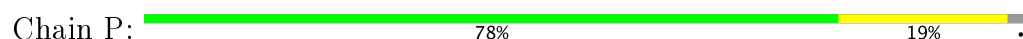
- Molecule 20: 26S proteasome regulatory subunit RPN10

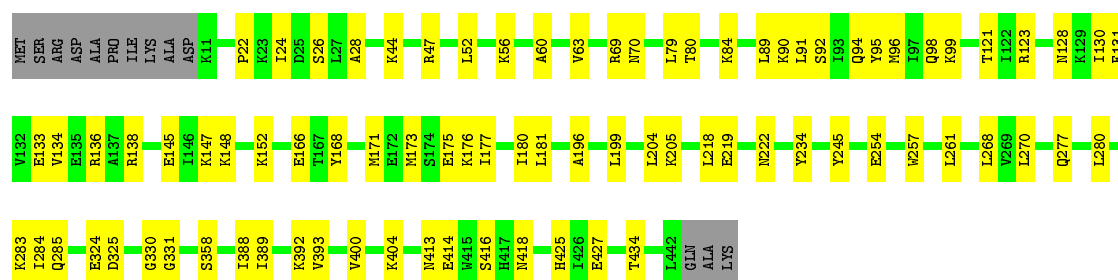


- Molecule 21: 26S proteasome regulatory subunit RPN9



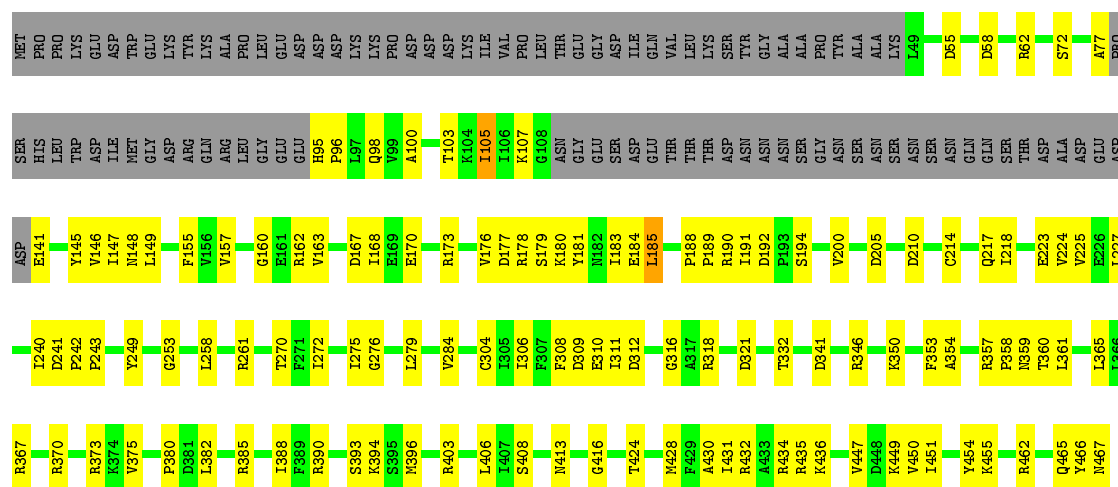
- Molecule 22: 26S proteasome regulatory subunit RPN5





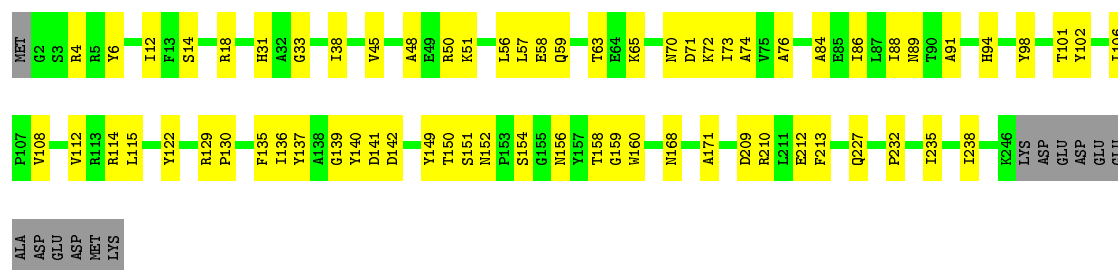
- Molecule 23: 26S protease regulatory subunit 7 homolog

Chain H: 53% 26% 21%



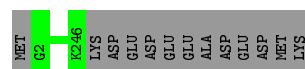
- Molecule 24: Proteasome subunit alpha type-3

Chain C: 69% 26% 5%



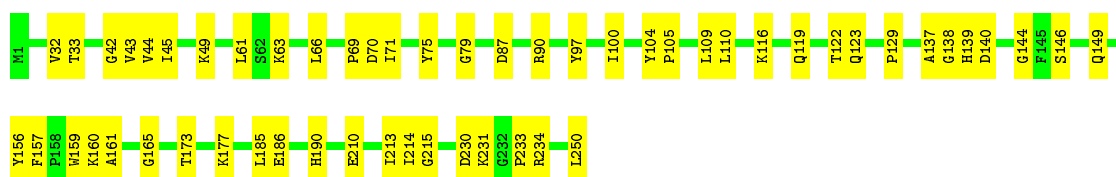
- Molecule 24: Proteasome subunit alpha type-3

Chain d: 95% 5%



- Molecule 25: Proteasome subunit alpha type-2

Chain B: 78% 22%



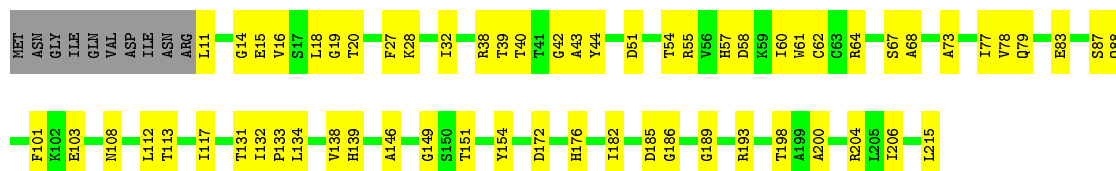
- Molecule 25: Proteasome subunit alpha type-2

Chain j: 100%

There are no outlier residues recorded for this chain.

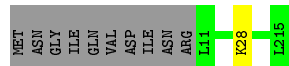
- Molecule 26: Proteasome subunit beta type-1

Chain 1: 67% 29% 5%



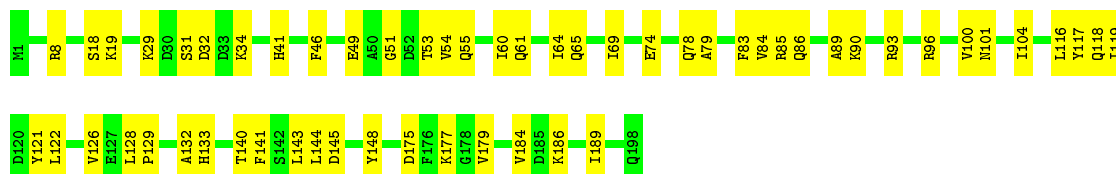
- Molecule 26: Proteasome subunit beta type-1

Chain b: 95% 5%



- Molecule 27: Proteasome subunit beta type-4

Chain 4: 72% 28%



- Molecule 27: Proteasome subunit beta type-4

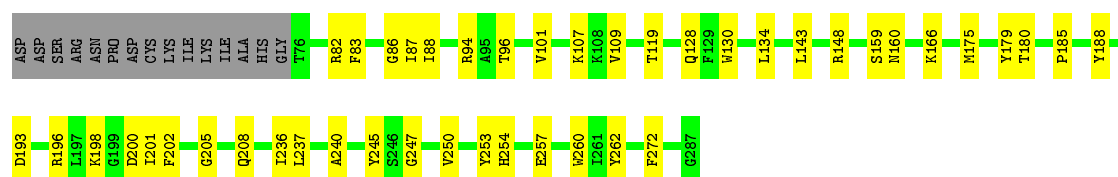
Chain g: 100%

There are no outlier residues recorded for this chain.

- Molecule 28: Proteasome subunit beta type-5

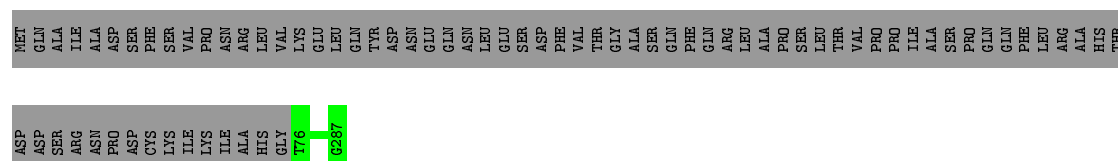
Chain 5: 59% 15% 26%





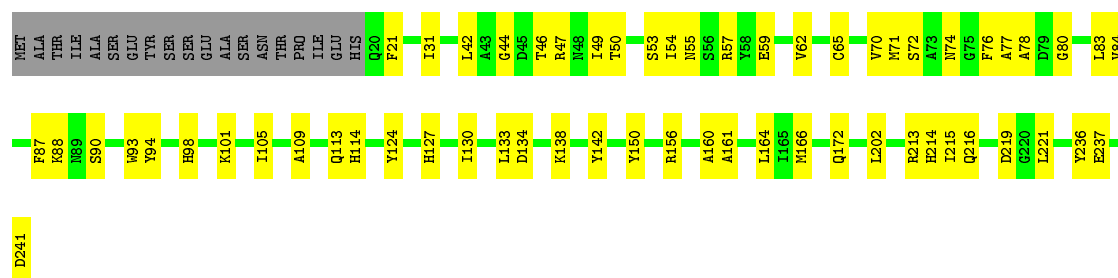
- Molecule 28: Proteasome subunit beta type-5

Chain f: 74% 26%



- Molecule 29: Proteasome subunit beta type-6

Chain 6: 67% 25% 8%



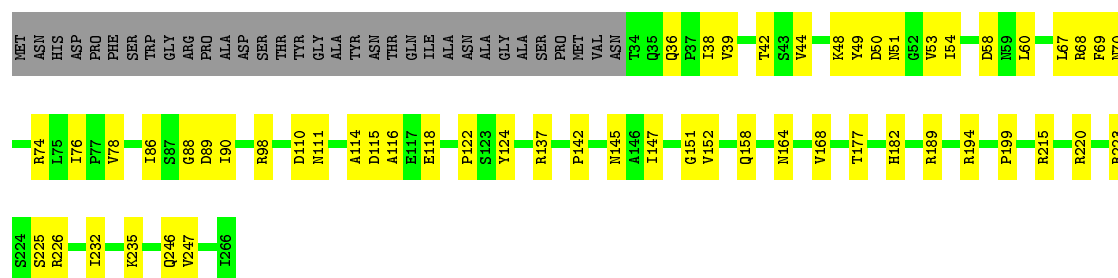
- Molecule 29: Proteasome subunit beta type-6

Chain e: 92% 8%




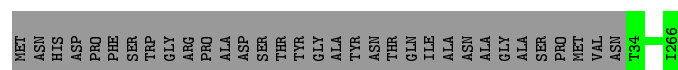
- Molecule 30: Proteasome subunit beta type-7

Chain 7: 67% 21% 12%



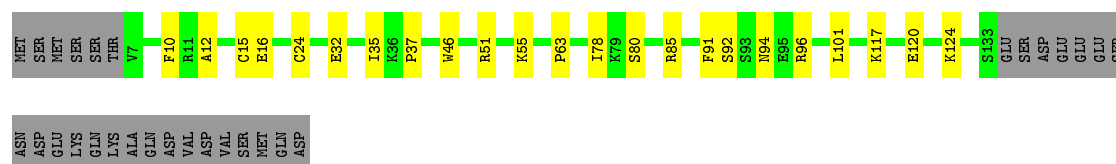
- Molecule 30: Proteasome subunit beta type-7

Chain a:  88% 12%



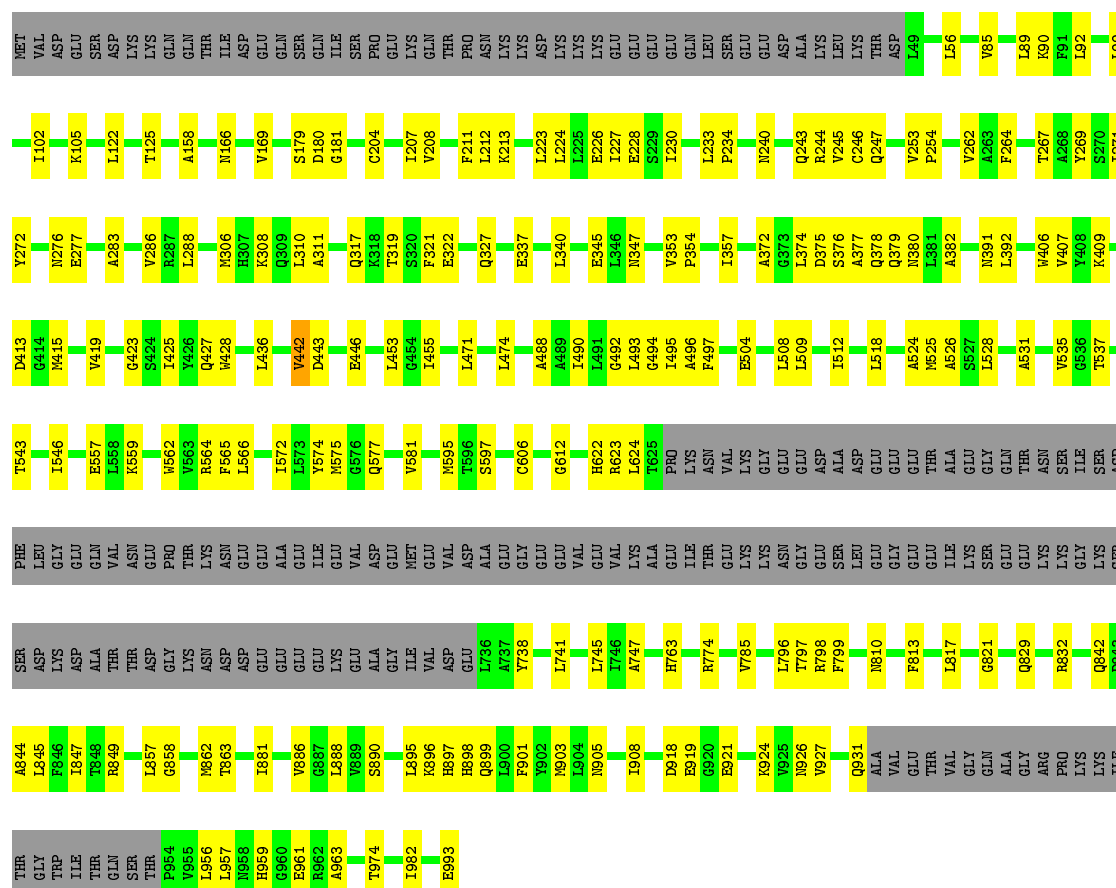
- Molecule 31: 26S proteasome regulatory subunit RPN13

Chain X: 67% 15% 19%



- Molecule 32: 26S proteasome regulatory subunit RPN1

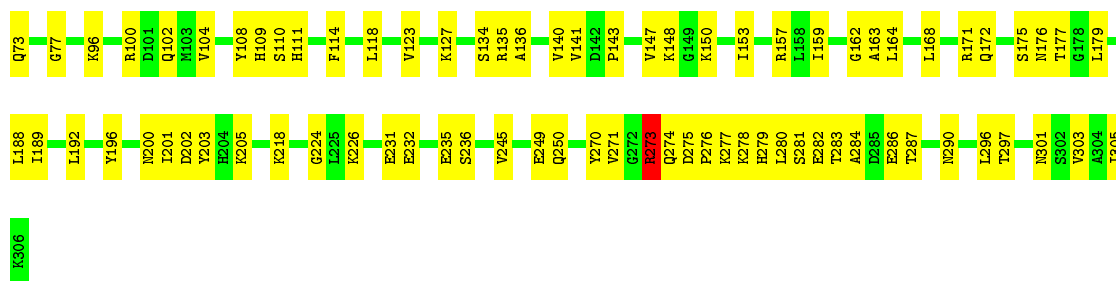
Chain Z: 63% 19% 18%



- Molecule 33: Ubiquitin carboxyl-terminal hydrolase RPN11

Chain V:  59% 33% 7%





4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	26000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	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 ⓘ

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	I	0.24	0/2860	0.44	0/3856
10	Y	0.21	0/239	0.32	0/322
11	N	0.24	0/6670	0.39	0/9023
12	S	0.23	0/2945	0.37	0/3976
13	T	0.23	0/2279	0.38	0/3077
14	R	0.23	0/3272	0.38	0/4412
15	Q	0.23	0/3527	0.37	0/4748
16	J	0.33	1/2964 (0.0%)	0.40	0/3981
17	L	0.28	1/2896 (0.0%)	0.40	0/3895
18	M	0.23	0/2903	0.41	0/3909
19	U	0.23	0/2287	0.40	0/3087
2	K	0.24	0/3062	0.42	0/4132
20	W	0.24	0/1557	0.40	0/2111
21	O	0.23	0/3243	0.38	0/4374
22	P	0.22	0/3599	0.38	0/4854
23	H	0.35	1/2931 (0.0%)	0.46	0/3941
24	C	0.23	0/1943	0.40	0/2629
24	d	0.23	0/1943	0.41	0/2629
25	B	0.24	0/1952	0.41	0/2642
25	j	0.24	0/1952	0.42	0/2642
26	l	0.23	0/1605	0.44	0/2171
26	b	0.23	0/1603	0.43	0/2168
27	4	0.23	0/1613	0.39	0/2173
27	g	0.23	0/1613	0.41	0/2173
28	5	0.24	0/1681	0.41	0/2274
28	f	0.23	0/1681	0.41	0/2274
29	6	0.24	0/1795	0.40	0/2420
29	e	0.24	0/1795	0.40	0/2420
3	2	0.23	0/1715	0.41	0/2326
3	i	0.23	0/1715	0.42	0/2326
30	7	0.24	0/1855	0.41	0/2514
30	a	0.24	0/1855	0.42	0/2514
31	X	0.23	0/1058	0.40	0/1432
32	Z	0.23	0/6403	0.41	0/8686

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
33	V	0.24	0/2271	0.47	0/3064
4	A	0.24	0/1959	0.39	0/2652
4	c	0.24	0/1959	0.39	0/2652
5	3	0.24	0/1611	0.41	0/2174
5	h	0.25	0/1611	0.42	0/2174
6	G	0.24	0/1940	0.38	0/2619
6	k	0.24	0/1940	0.39	0/2619
7	F	0.23	0/1823	0.42	0/2463
7	l	0.23	0/1823	0.41	0/2463
8	E	0.23	0/1892	0.40	0/2549
8	m	0.23	0/1892	0.40	0/2549
9	D	0.23	0/1928	0.41	0/2610
9	n	0.23	0/1928	0.40	0/2610
All	All	0.24	3/107588 (0.0%)	0.40	0/145309

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
1	I	0	1
18	M	0	1
26	1	0	1
33	V	0	2
5	h	0	1
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	H	185	LEU	C-N	12.79	1.58	1.34
16	J	241	ALA	C-N	12.54	1.58	1.34
17	L	329	ARG	C-N	8.34	1.50	1.34

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	1	42	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	I	102	ASN	Peptide
18	M	167	VAL	Peptide
33	V	162	GLY	Peptide
5	h	45	HIS	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	I	2822	0	2870	76	0
2	K	3019	0	3084	98	0
3	2	1684	0	1685	28	0
3	i	1684	0	1685	0	0
4	A	1921	0	1910	49	0
4	c	1921	0	1910	0	0
5	3	1581	0	1571	41	0
5	h	1581	0	1571	0	0
6	G	1900	0	1889	41	0
6	k	1900	0	1889	0	0
7	F	1795	0	1797	40	0
7	l	1795	0	1797	0	0
8	E	1867	0	1841	50	0
8	m	1867	0	1841	0	0
9	D	1899	0	1908	41	0
9	n	1899	0	1908	0	0
10	Y	236	0	203	2	0
11	N	6562	0	6625	125	0
12	S	2893	0	2937	55	0
13	T	2235	0	2207	36	0
14	R	3218	0	3216	58	0
15	Q	3471	0	3495	47	0
16	J	2928	0	3057	72	0
17	L	2853	0	2926	74	0
18	M	2866	0	2938	79	0
19	U	2257	0	2312	52	0
20	W	1534	0	1542	35	0
21	O	3182	0	3207	58	0
22	P	3545	0	3629	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	H	2889	0	2964	100	0
24	C	1913	0	1914	47	0
24	d	1913	0	1914	0	0
25	B	1915	0	1929	41	0
25	j	1915	0	1929	0	0
26	l	1576	0	1552	41	0
26	b	1574	0	1547	0	0
27	4	1585	0	1590	45	0
27	g	1585	0	1590	0	0
28	5	1644	0	1592	34	0
28	f	1644	0	1592	0	0
29	6	1757	0	1708	44	0
29	e	1757	0	1708	0	0
30	7	1824	0	1829	43	0
30	a	1824	0	1829	0	0
31	X	1032	0	1015	19	0
32	Z	6289	0	6236	123	0
33	V	2236	0	2242	81	0
All	All	105787	0	106130	1588	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 10.

The worst 5 of 1588 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)
11:N:25:LEU:HB3	11:N:29:ASN:HB2	1.63	0.80
18:M:162:GLU:HG2	18:M:166:ARG:HG2	1.64	0.80
9:D:63:LYS:HE2	9:D:76:SER:HB2	1.64	0.76
32:Z:233:LEU:HB3	32:Z:271:ILE:HD11	1.66	0.75
4:A:61:ASP:HB3	4:A:64:LEU:HG	1.68	0.75

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	I	360/437 (82%)	315 (88%)	44 (12%)	1 (0%)	44	81
2	K	379/428 (89%)	326 (86%)	53 (14%)	0	100	100
3	2	220/261 (84%)	210 (96%)	10 (4%)	0	100	100
3	i	220/261 (84%)	209 (95%)	11 (5%)	0	100	100
4	A	241/252 (96%)	228 (95%)	13 (5%)	0	100	100
4	c	241/252 (96%)	227 (94%)	14 (6%)	0	100	100
5	3	202/205 (98%)	190 (94%)	12 (6%)	0	100	100
5	h	202/205 (98%)	188 (93%)	13 (6%)	1 (0%)	32	74
6	G	243/288 (84%)	235 (97%)	8 (3%)	0	100	100
6	k	243/288 (84%)	233 (96%)	10 (4%)	0	100	100
7	F	231/234 (99%)	221 (96%)	10 (4%)	0	100	100
7	l	231/234 (99%)	221 (96%)	10 (4%)	0	100	100
8	E	241/260 (93%)	226 (94%)	15 (6%)	0	100	100
8	m	241/260 (93%)	227 (94%)	14 (6%)	0	100	100
9	D	240/254 (94%)	222 (92%)	18 (8%)	0	100	100
9	n	240/254 (94%)	226 (94%)	14 (6%)	0	100	100
10	Y	25/89 (28%)	23 (92%)	2 (8%)	0	100	100
11	N	843/945 (89%)	786 (93%)	57 (7%)	0	100	100
12	S	351/523 (67%)	313 (89%)	37 (10%)	1 (0%)	44	81
13	T	270/274 (98%)	231 (86%)	39 (14%)	0	100	100
14	R	398/429 (93%)	357 (90%)	40 (10%)	1 (0%)	44	81
15	Q	429/434 (99%)	393 (92%)	36 (8%)	0	100	100
16	J	371/405 (92%)	335 (90%)	35 (9%)	1 (0%)	44	81
17	L	359/437 (82%)	320 (89%)	38 (11%)	1 (0%)	44	81
18	M	363/434 (84%)	331 (91%)	31 (8%)	1 (0%)	44	81
19	U	278/338 (82%)	260 (94%)	18 (6%)	0	100	100
20	W	195/268 (73%)	182 (93%)	13 (7%)	0	100	100
21	O	385/393 (98%)	341 (89%)	43 (11%)	1 (0%)	44	81
22	P	430/445 (97%)	386 (90%)	44 (10%)	0	100	100
23	H	364/467 (78%)	311 (85%)	52 (14%)	1 (0%)	44	81

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	C	243/258 (94%)	228 (94%)	15 (6%)	0	100	100
24	d	243/258 (94%)	227 (93%)	16 (7%)	0	100	100
25	B	248/250 (99%)	234 (94%)	14 (6%)	0	100	100
25	j	248/250 (99%)	232 (94%)	16 (6%)	0	100	100
26	1	203/215 (94%)	185 (91%)	17 (8%)	1 (0%)	32	74
26	b	203/215 (94%)	184 (91%)	18 (9%)	1 (0%)	32	74
27	4	196/198 (99%)	186 (95%)	10 (5%)	0	100	100
27	g	196/198 (99%)	182 (93%)	14 (7%)	0	100	100
28	5	210/287 (73%)	200 (95%)	10 (5%)	0	100	100
28	f	210/287 (73%)	198 (94%)	12 (6%)	0	100	100
29	6	220/241 (91%)	204 (93%)	16 (7%)	0	100	100
29	e	220/241 (91%)	205 (93%)	15 (7%)	0	100	100
30	7	231/266 (87%)	215 (93%)	16 (7%)	0	100	100
30	a	231/266 (87%)	216 (94%)	15 (6%)	0	100	100
31	X	125/156 (80%)	113 (90%)	12 (10%)	0	100	100
32	Z	807/993 (81%)	716 (89%)	90 (11%)	1 (0%)	55	88
33	V	282/306 (92%)	234 (83%)	45 (16%)	3 (1%)	17	59
All	All	13352/15139 (88%)	12232 (92%)	1105 (8%)	15 (0%)	58	88

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	L	332	THR
5	h	105	VAL
14	R	241	ILE
33	V	305	ILE
16	J	134	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	I	319/385 (83%)	319 (100%)	0	100	100
2	K	334/374 (89%)	334 (100%)	0	100	100
3	2	181/214 (85%)	181 (100%)	0	100	100
3	i	181/214 (85%)	181 (100%)	0	100	100
4	A	207/210 (99%)	207 (100%)	0	100	100
4	c	207/210 (99%)	207 (100%)	0	100	100
5	3	172/173 (99%)	172 (100%)	0	100	100
5	h	172/173 (99%)	172 (100%)	0	100	100
6	G	201/239 (84%)	201 (100%)	0	100	100
6	k	201/239 (84%)	201 (100%)	0	100	100
7	F	192/193 (100%)	192 (100%)	0	100	100
7	l	192/193 (100%)	192 (100%)	0	100	100
8	E	199/215 (93%)	199 (100%)	0	100	100
8	m	199/215 (93%)	199 (100%)	0	100	100
9	D	214/226 (95%)	214 (100%)	0	100	100
9	n	214/226 (95%)	214 (100%)	0	100	100
10	Y	26/81 (32%)	26 (100%)	0	100	100
11	N	713/797 (90%)	713 (100%)	0	100	100
12	S	330/489 (68%)	330 (100%)	0	100	100
13	T	254/256 (99%)	254 (100%)	0	100	100
14	R	351/379 (93%)	351 (100%)	0	100	100
15	Q	388/391 (99%)	388 (100%)	0	100	100
16	J	325/352 (92%)	325 (100%)	0	100	100
17	L	308/377 (82%)	308 (100%)	0	100	100
18	M	315/375 (84%)	315 (100%)	0	100	100
19	U	256/308 (83%)	256 (100%)	0	100	100
20	W	171/230 (74%)	171 (100%)	0	100	100
21	O	363/368 (99%)	363 (100%)	0	100	100
22	P	405/415 (98%)	405 (100%)	0	100	100
23	H	314/399 (79%)	314 (100%)	0	100	100
24	C	204/216 (94%)	204 (100%)	0	100	100
24	d	204/216 (94%)	204 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	B	209/209 (100%)	209 (100%)	0	100	100
25	j	209/209 (100%)	209 (100%)	0	100	100
26	1	169/178 (95%)	169 (100%)	0	100	100
26	b	168/178 (94%)	168 (100%)	0	100	100
27	4	175/175 (100%)	175 (100%)	0	100	100
27	g	175/175 (100%)	175 (100%)	0	100	100
28	5	169/235 (72%)	169 (100%)	0	100	100
28	f	169/235 (72%)	169 (100%)	0	100	100
29	6	185/201 (92%)	185 (100%)	0	100	100
29	e	185/201 (92%)	185 (100%)	0	100	100
30	7	199/224 (89%)	199 (100%)	0	100	100
30	a	199/224 (89%)	199 (100%)	0	100	100
31	X	116/144 (81%)	116 (100%)	0	100	100
32	Z	692/850 (81%)	692 (100%)	0	100	100
33	V	249/268 (93%)	249 (100%)	0	100	100
All	All	11580/13054 (89%)	11580 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 129 such sidechains are listed below:

Mol	Chain	Res	Type
19	U	127	GLN
23	H	217	GLN
29	e	89	ASN
20	W	100	HIS
21	O	376	GLN

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 [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.