



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jul 24, 2017 – 02:01 PM EDT

PDB ID : 5MPD  
EMDB ID: : EMD-3534  
Title : 26S proteasome in presence of ATP (s1)  
Authors : Wehmer, M.; Rudack, T.; Beck, F.; Aufderheide, A.; Pfeifer, G.; Plitzko, J.M.;  
Foerster, F.; Schulten, K.; Baumeister, W.; Sakata, E.  
Deposited on : unknown  
Resolution : 4.10 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](mailto: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.

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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-20029824

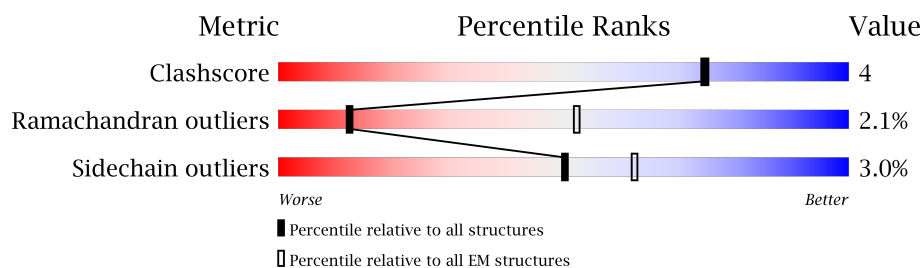
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.10 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  $\geq 3$ , 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	W	268	
2	V	306	
3	T	274	
4	X	156	
5	Y	89	
6	Z	993	
7	N	945	
8	S	523	
9	P	445	

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Mol	Chain	Length	Quality of chain
10	Q	434	<div><div></div><div>76%</div><div>20%</div><div>.</div></div>
11	R	429	<div><div></div><div>67%</div><div>18%</div><div>.</div><div>11%</div></div>
12	U	338	<div><div></div><div>74%</div><div>13%</div><div>.</div><div>12%</div></div>
13	O	393	<div><div></div><div>74%</div><div>21%</div><div>.</div><div>..</div></div>

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 40974 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 proteasome regulatory subunit RPN10.

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

- Molecule 2 is a protein called Ubiquitin carboxyl-terminal hydrolase RPN11.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	V	289	Total	C	N	O	S	0	0
			2274	1425	389	446	14		

- Molecule 3 is a protein called 26S proteasome regulatory subunit RPN12.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	T	266	Total	C	N	O	S	0	0
			2192	1405	349	432	6		

- Molecule 4 is a protein called 26S proteasome regulatory subunit RPN13.

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

- Molecule 5 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	Y	51	Total	C	N	O	0	0
			435	264	69	102		

- Molecule 6 is a protein called 26S proteasome regulatory subunit RPN1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Z	906	Total	C	N	O	S	0	0
			7005	4416	1150	1409	30		

- Molecule 7 is a protein called 26S proteasome regulatory subunit RPN2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	890	Total	C	N	O	S	0	0
			6882	4373	1156	1325	28		

- Molecule 8 is a protein called 26S proteasome regulatory subunit RPN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	S	475	Total	C	N	O	S	0	0
			3894	2488	653	738	15		

- Molecule 9 is a protein called 26S proteasome regulatory subunit RPN5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	P	440	Total	C	N	O	S	0	0
			3608	2297	604	697	10		

- Molecule 10 is a protein called 26S proteasome regulatory subunit RPN6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Q	434	Total	C	N	O	S	0	0
			3499	2225	577	681	16		

- Molecule 11 is a protein called 26S proteasome regulatory subunit RPN7.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	R	381	Total	C	N	O	S	0	0
			3060	1955	502	593	10		

- Molecule 12 is a protein called 26S proteasome regulatory subunit RPN8.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	U	298	Total	C	N	O	S	0	0
			2373	1496	404	466	7		

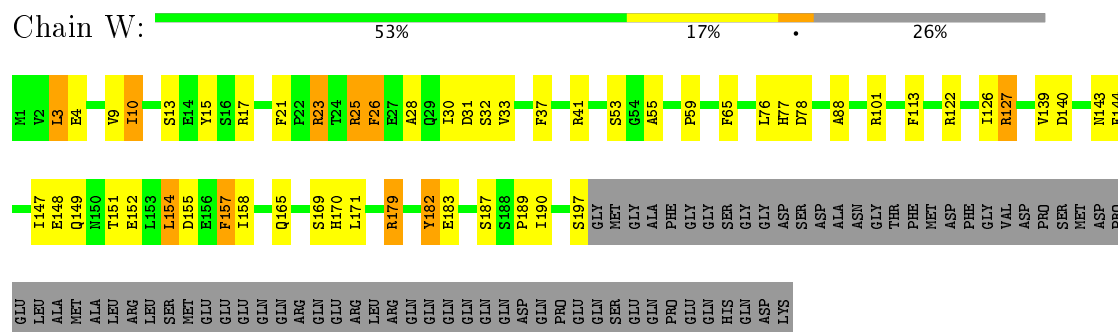
- Molecule 13 is a protein called 26S proteasome regulatory subunit RPN9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	388	Total	C	N	O	S	0	0
			3186	2051	519	608	8		

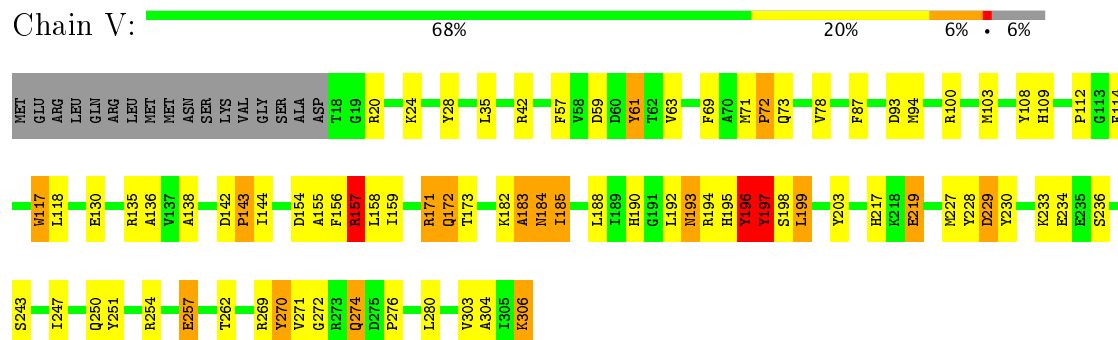
### 3 Residue-property plots

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.

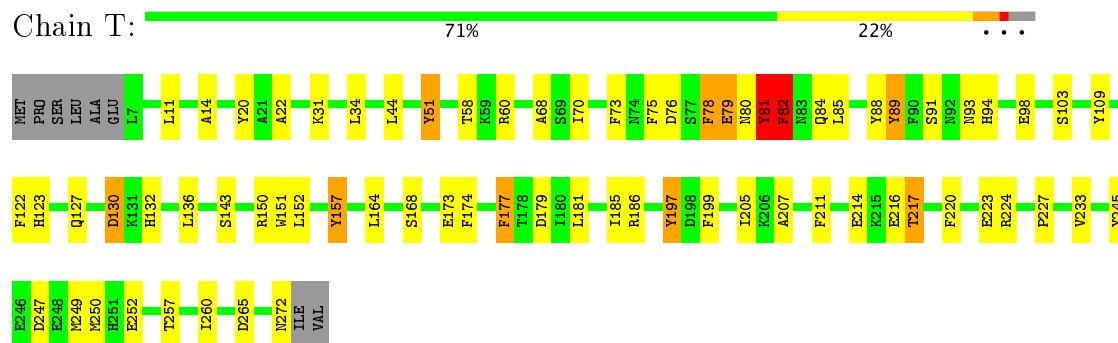
- Molecule 1: 26S proteasome regulatory subunit RPN10



- Molecule 2: Ubiquitin carboxyl-terminal hydrolase RPN11

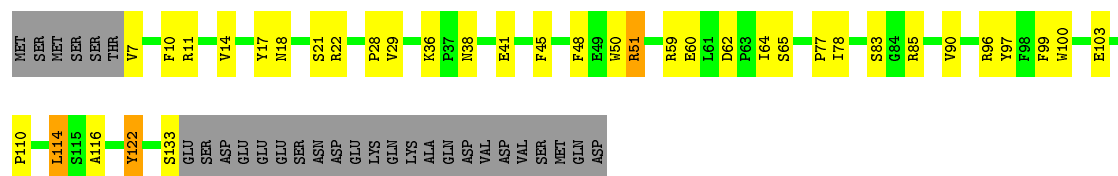


- Molecule 3: 26S proteasome regulatory subunit RPN12



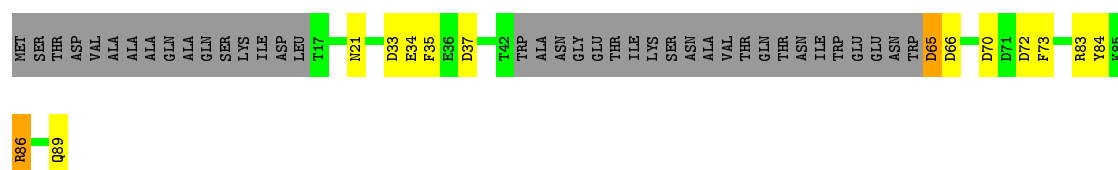
- Molecule 4: 26S proteasome regulatory subunit RPN13

Chain X: 



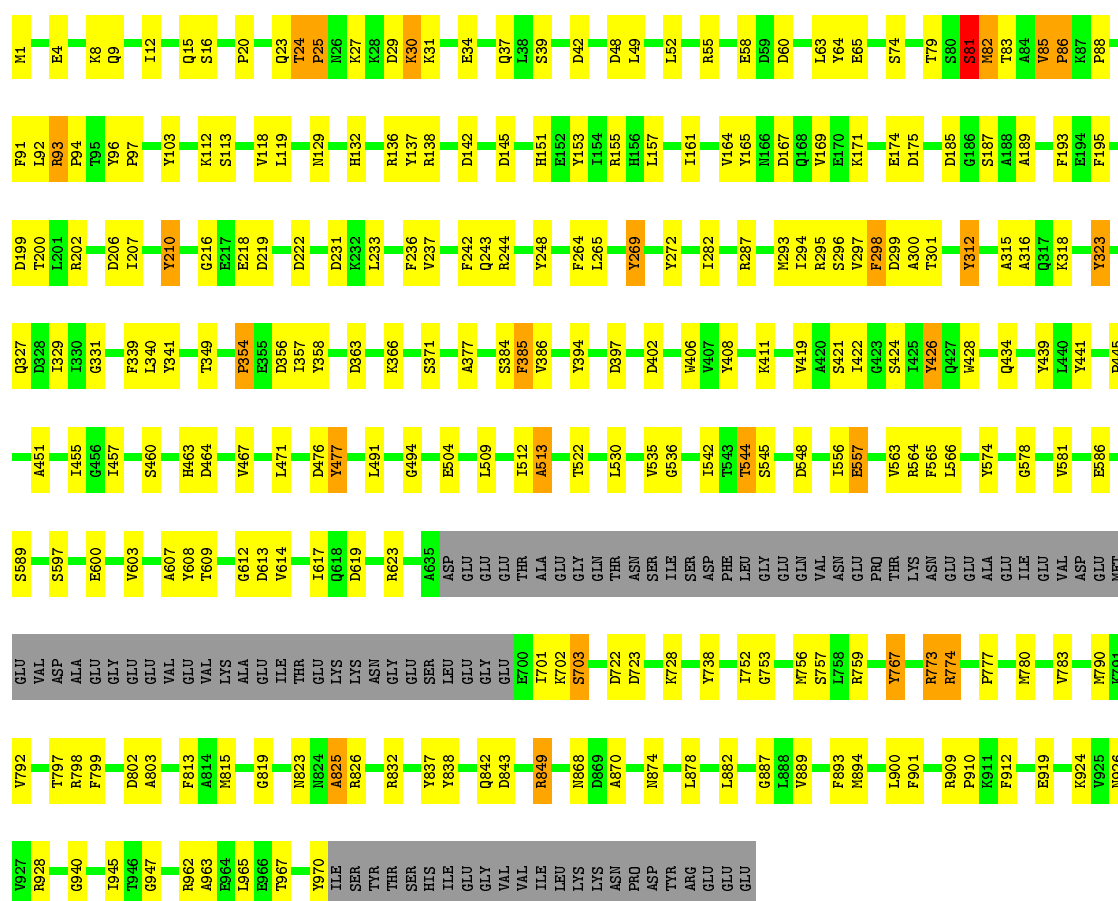
- Molecule 5: 26S proteasome complex subunit SEM1

Chain Y: 



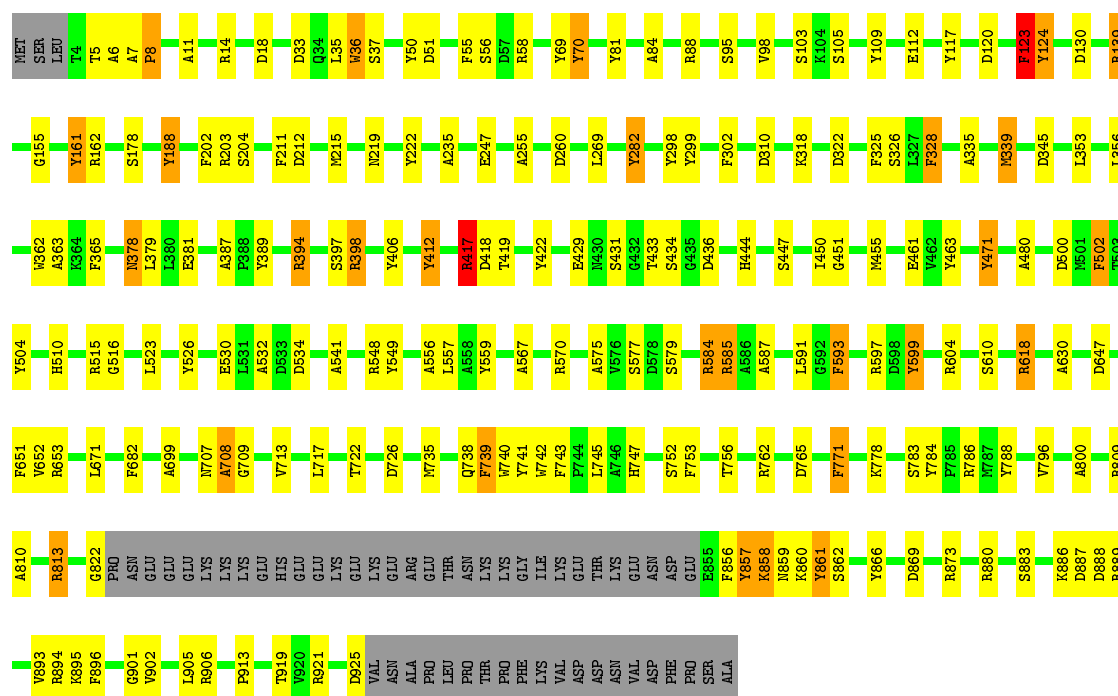
- Molecule 6: 26S proteasome regulatory subunit RPN1

Chain Z: 



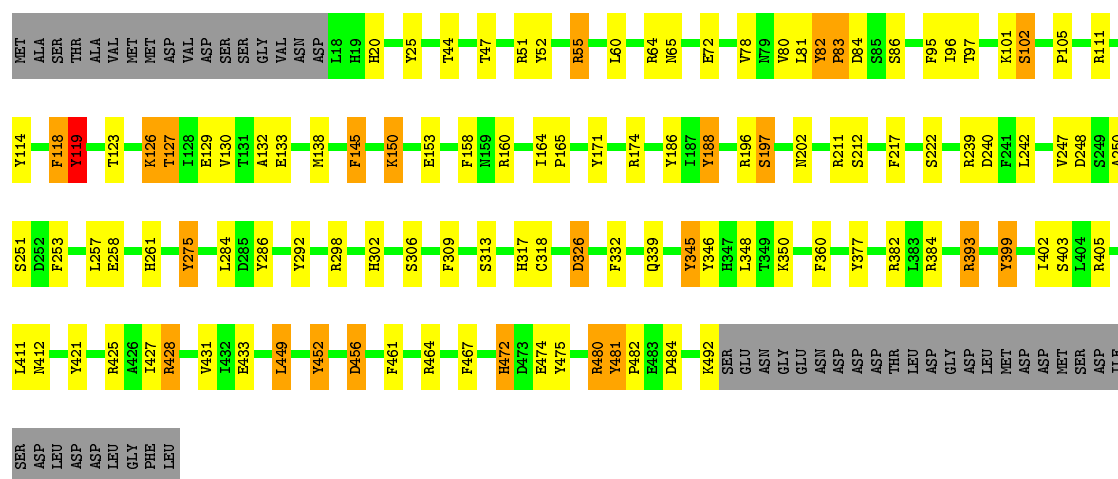
- Molecule 7: 26S proteasome regulatory subunit RPN2

Chain N: 



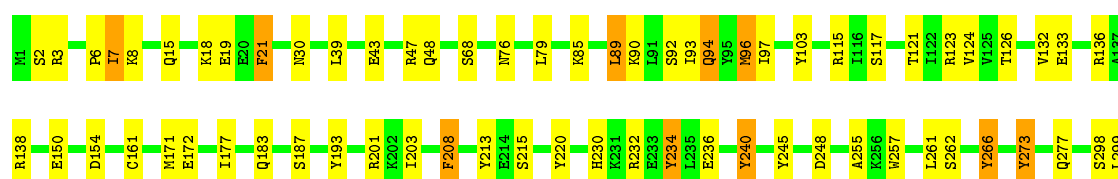
- Molecule 8: 26S proteasome regulatory subunit RPN3

Chain S: 



- Molecule 9: 26S proteasome regulatory subunit RPN5

Chain P: 

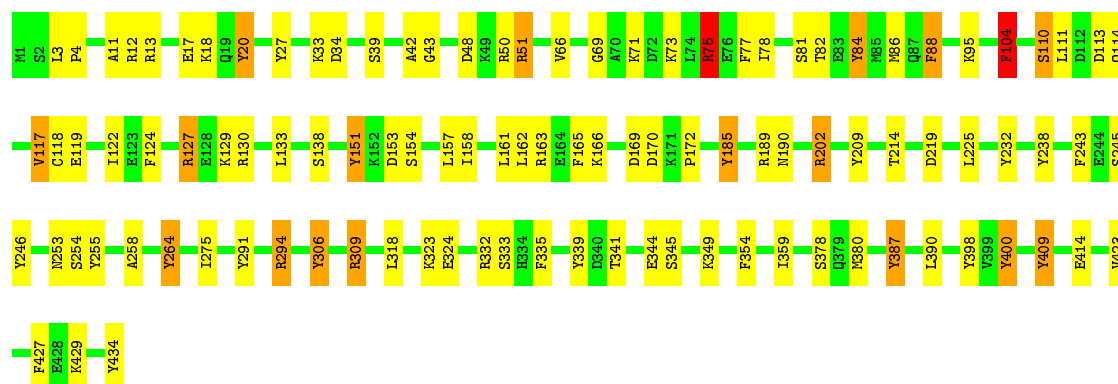






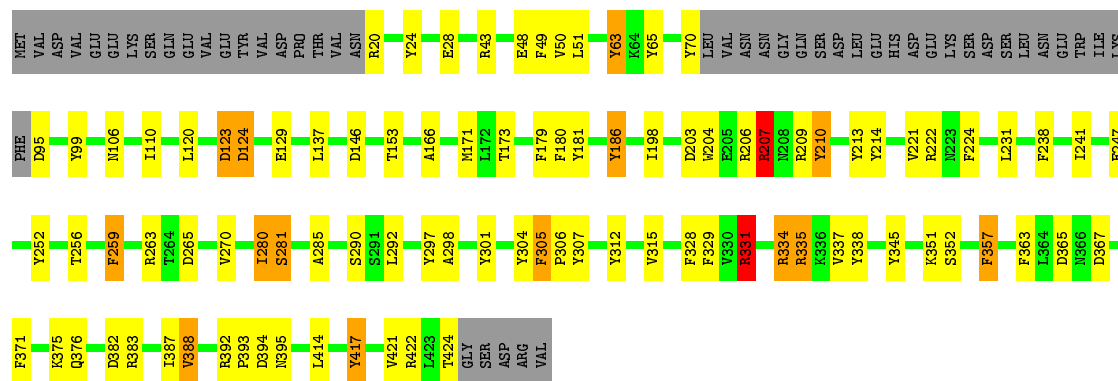
- Molecule 10: 26S proteasome regulatory subunit RPN6

Chain Q: 76% 20%



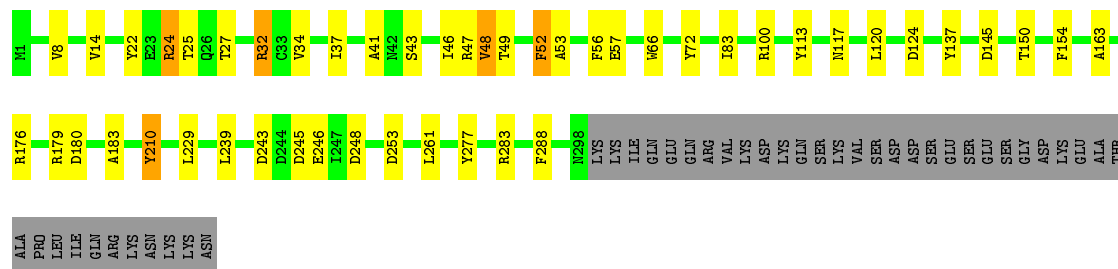
- Molecule 11: 26S proteasome regulatory subunit RPN7

Chain R: 67% 18% 11%



- Molecule 12: 26S proteasome regulatory subunit RPN8

Chain U: 74% 13% 12%



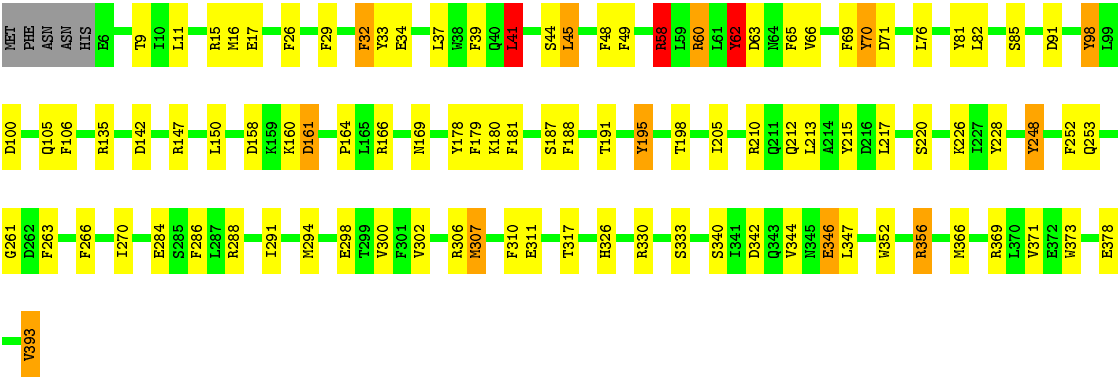
- Molecule 13: 26S proteasome regulatory subunit RPN9

Chain O: 

74%

21%

• • •



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	286500	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	45	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 QUANTUM (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	W	1.70	14/1557 (0.9%)	1.79	29/2111 (1.4%)
10	Q	1.68	28/3556 (0.8%)	1.89	77/4787 (1.6%)
11	R	1.73	31/3110 (1.0%)	1.95	83/4193 (2.0%)
12	U	1.58	11/2407 (0.5%)	1.76	41/3258 (1.3%)
13	O	1.68	36/3247 (1.1%)	1.93	86/4380 (2.0%)
2	V	1.74	22/2309 (1.0%)	2.02	64/3115 (2.1%)
3	T	1.71	27/2235 (1.2%)	1.82	45/3017 (1.5%)
4	X	1.75	12/1058 (1.1%)	1.90	24/1432 (1.7%)
5	Y	1.90	7/438 (1.6%)	1.92	10/583 (1.7%)
6	Z	1.66	59/7122 (0.8%)	1.88	169/9645 (1.8%)
7	N	1.74	61/6994 (0.9%)	1.84	142/9455 (1.5%)
8	S	1.68	33/3966 (0.8%)	1.84	98/5355 (1.8%)
9	P	1.67	29/3663 (0.8%)	1.77	60/4940 (1.2%)
All	All	1.69	370/41662 (0.9%)	1.86	928/56271 (1.6%)

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	W	0	6
10	Q	0	19
11	R	0	12
12	U	0	4
13	O	0	11
2	V	0	5
3	T	0	6
4	X	0	2
5	Y	0	1
6	Z	0	12
7	N	0	23
8	S	0	14

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Mol	Chain	#Chirality outliers	#Planarity outliers
9	P	0	8
All	All	0	123

The worst 5 of 370 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	N	8	PRO	CA-CB	32.16	2.17	1.53
5	Y	89	GLN	C-OXT	-12.08	1.00	1.23
9	P	440	HIS	C-O	-12.08	1.00	1.23
3	T	272	ASN	C-O	-12.07	1.00	1.23
13	O	393	VAL	C-O	-12.07	1.00	1.23

The worst 5 of 928 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	8	PRO	N-CA-CB	-29.24	68.21	103.30
2	V	196	TYR	CB-CA-C	-25.02	60.37	110.40
2	V	157	ARG	NE-CZ-NH1	16.47	128.53	120.30
13	O	330	ARG	NE-CZ-NH1	16.47	128.53	120.30
10	Q	409	TYR	CB-CG-CD2	-16.00	111.40	121.00

There are no chirality outliers.

5 of 123 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	W	122	ARG	Sidechain
1	W	127	ARG	Sidechain
1	W	23	ARG	Sidechain
1	W	25	ARG	Sidechain
1	W	77	HIS	Sidechain

## 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	W	1534	0	1542	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	V	2274	0	2272	51	0
3	T	2192	0	2157	12	0
4	X	1032	0	1017	5	0
5	Y	435	0	394	17	0
6	Z	7005	0	6932	85	0
7	N	6882	0	6959	42	0
8	S	3894	0	3937	32	0
9	P	3608	0	3694	15	0
10	Q	3499	0	3524	18	0
11	R	3060	0	3083	12	0
12	U	2373	0	2403	6	0
13	O	3186	0	3213	11	0
All	All	40974	0	41127	301	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 4.

The worst 5 of 301 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)
8:S:127:THR:CB	8:S:127:THR:CA	1.80	1.58
6:Z:30:LYS:CG	6:Z:37:GLN:HB3	1.22	1.55
6:Z:24:THR:HB	6:Z:25:PRO:CD	1.36	1.51
2:V:118:LEU:HB2	2:V:195:HIS:CD2	1.47	1.49
2:V:118:LEU:CB	2:V:195:HIS:NE2	1.80	1.44

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	W	195/268 (73%)	175 (90%)	13 (7%)	7 (4%)	4	36
2	V	287/306 (94%)	262 (91%)	15 (5%)	10 (4%)	4	36
3	T	264/274 (96%)	240 (91%)	20 (8%)	4 (2%)	12	53
4	X	125/156 (80%)	105 (84%)	19 (15%)	1 (1%)	22	65
5	Y	47/89 (53%)	39 (83%)	6 (13%)	2 (4%)	3	31
6	Z	902/993 (91%)	813 (90%)	66 (7%)	23 (2%)	6	43
7	N	886/945 (94%)	842 (95%)	31 (4%)	13 (2%)	12	53
8	S	473/523 (90%)	441 (93%)	17 (4%)	15 (3%)	5	38
9	P	438/445 (98%)	405 (92%)	22 (5%)	11 (2%)	6	43
10	Q	432/434 (100%)	392 (91%)	32 (7%)	8 (2%)	9	49
11	R	377/429 (88%)	353 (94%)	16 (4%)	8 (2%)	8	47
12	U	296/338 (88%)	282 (95%)	12 (4%)	2 (1%)	25	67
13	O	386/393 (98%)	366 (95%)	17 (4%)	3 (1%)	22	65
All	All	5108/5593 (91%)	4715 (92%)	286 (6%)	107 (2%)	12	47

5 of 107 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	V	184	ASN
2	V	197	TYR
2	V	274	GLN
4	X	116	ALA
6	Z	24	THR

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	W	171/230 (74%)	165 (96%)	6 (4%)	41	72
2	V	253/268 (94%)	242 (96%)	11 (4%)	33	68
3	T	249/256 (97%)	239 (96%)	10 (4%)	36	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	X	116/144 (81%)	112 (97%)	4 (3%)	42	73
5	Y	50/81 (62%)	48 (96%)	2 (4%)	36	69
6	Z	773/850 (91%)	745 (96%)	28 (4%)	40	72
7	N	745/797 (94%)	724 (97%)	21 (3%)	49	76
8	S	447/489 (91%)	436 (98%)	11 (2%)	53	78
9	P	412/415 (99%)	402 (98%)	10 (2%)	54	79
10	Q	391/391 (100%)	382 (98%)	9 (2%)	56	80
11	R	333/379 (88%)	325 (98%)	8 (2%)	54	79
12	U	271/308 (88%)	269 (99%)	2 (1%)	87	94
13	O	363/368 (99%)	349 (96%)	14 (4%)	37	70
All	All	4574/4976 (92%)	4438 (97%)	136 (3%)	50	74

5 of 136 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	N	105	SER
7	N	717	LEU
13	O	58	ARG
7	N	219	ASN
7	N	412	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
7	N	703	GLN
8	S	172	ASN
12	U	156	HIS
7	N	747	HIS
8	S	112	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.