



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

Aug 14, 2017 – 05:48 PM EDT

PDB ID : 5VHF  
EMDB ID: : EMD-8674  
Title : Conformational Landscape of the p28-Bound Human Proteasome Regulatory Particle  
Authors : Lu, Y.; Wu, J.; Dong, Y.; Chen, S.; Sun, S.; Ma, Y.B.; Ouyang, Q.; Finley, D.; Kirschner, M.W.; Mao, Y.  
Deposited on : unknown  
Resolution : 5.70 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

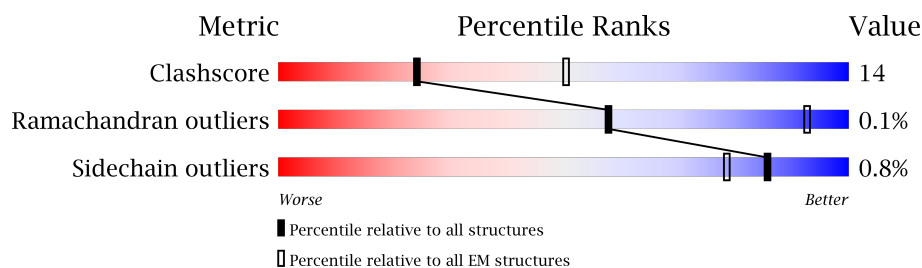
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 5.70 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.







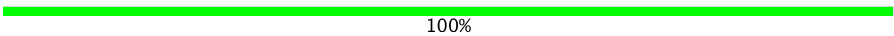
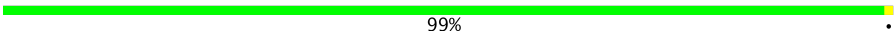
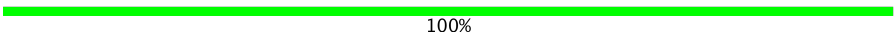

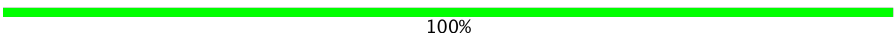

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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	G	223	
2	A	352	
3	B	340	
4	C	385	
5	D	368	
6	E	379	
7	F	380	
8	U	841	
9	V	183	

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Mol	Chain	Length	Quality of chain
10	W	456	 73%26%
11	X	385	 82%18%
12	Y	378	 70%30%
13	Z	286	 75%25%
14	a	374	 100%
15	b	191	 99%.
16	c	287	 100%
17	d	136	 99%.
18	e	70	 100%
19	f	848	 79%.19%

## 2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 51096 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 non-ATPase regulatory subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	219	Total	C	N	O	S	0	0
			1662	1036	294	323	9		

- Molecule 2 is a protein called 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	341	Total	C	N	O	S	0	0
			2677	1690	473	497	17		

- Molecule 3 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	330	Total	C	N	O	S	0	0
			2579	1624	437	506	12		

- Molecule 4 is a protein called 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	342	Total	C	N	O	S	0	0
			2709	1701	493	501	14		

- Molecule 5 is a protein called 26S proteasome regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	344	Total	C	N	O	S	0	0
			2751	1744	480	517	10		

- Molecule 6 is a protein called 26S proteasome regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	345	Total	C	N	O	S	0	0
			2736	1715	490	515	16		

- Molecule 7 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	359	Total	C	N	O	S	0	0
			2808	1772	488	531	17		

- Molecule 8 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	U	751	Total	C	N	O	S	0	0
			5829	3696	1001	1088	44		

- Molecule 9 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	V	183	Total	C	N	O	S	0	0
			1480	949	260	265	6		

- Molecule 10 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	X	385	Total	C	N	O	S	0	0
			3048	1939	515	582	12		

- Molecule 12 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

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

- Molecule 13 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

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

- Molecule 14 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	a	374	Total	C	N	O	S	0	0
			3003	1915	511	562	15		

- Molecule 15 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

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

- Molecule 16 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

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

- Molecule 17 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	d	136	Total	C	N	O	S	0	0
			1109	720	176	209	4		

- Molecule 18 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	e	70	Total	C	N	O	S	0	0
			583	357	89	135	2		

- Molecule 19 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	f	686	Total	C	N	O	S	0	0
			5304	3335	901	1033	35		

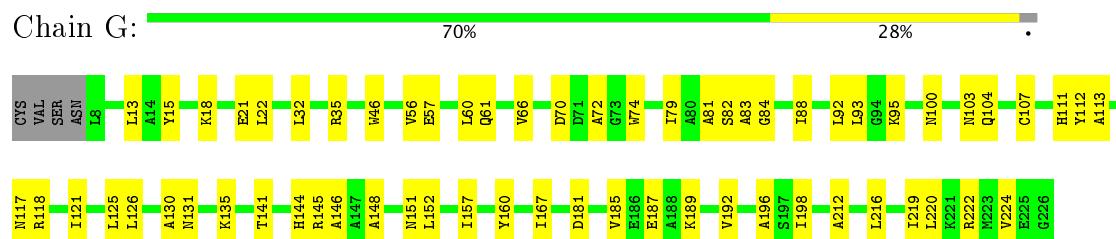
- Molecule 20 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

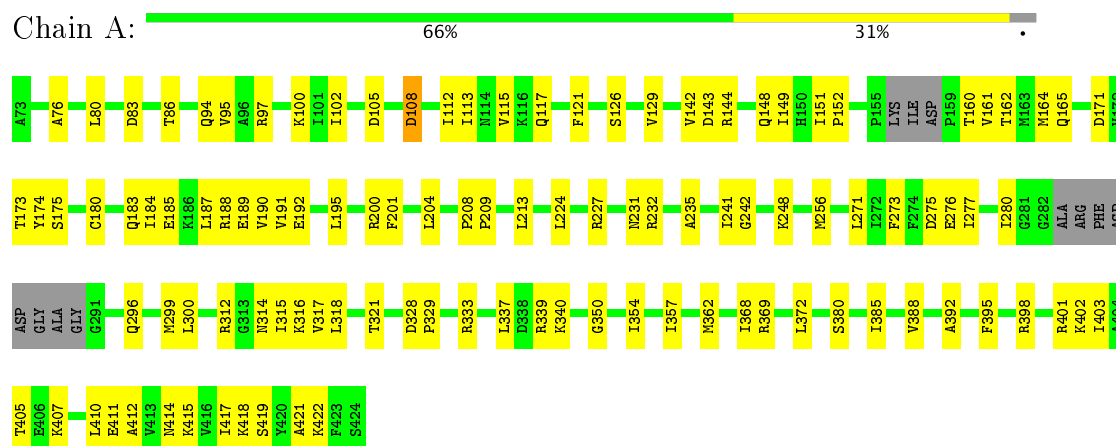
### 3 Residue-property plots

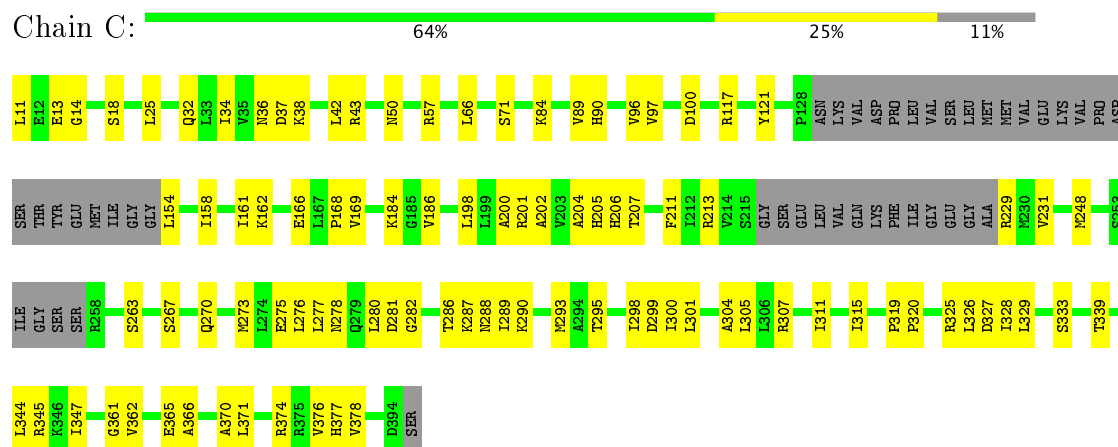
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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 non-ATPase regulatory subunit 10

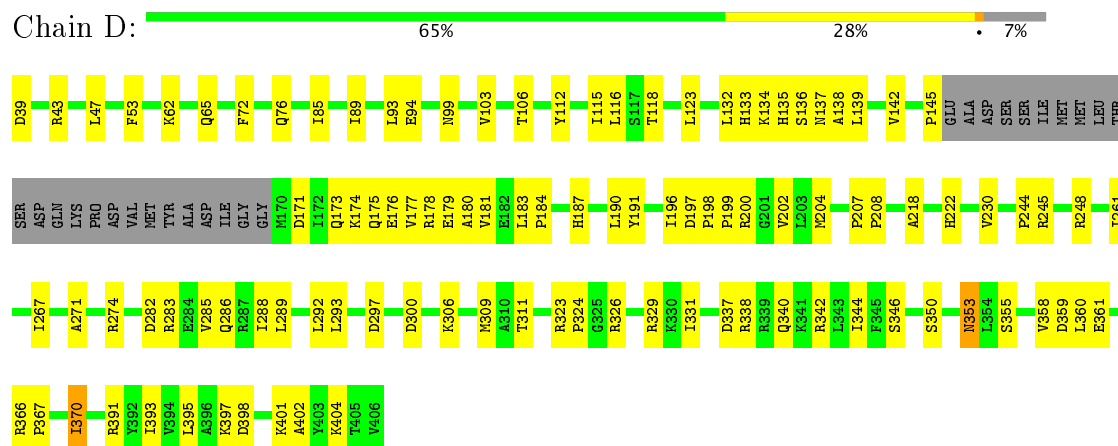


- Molecule 2: 26S proteasome regulatory subunit 7

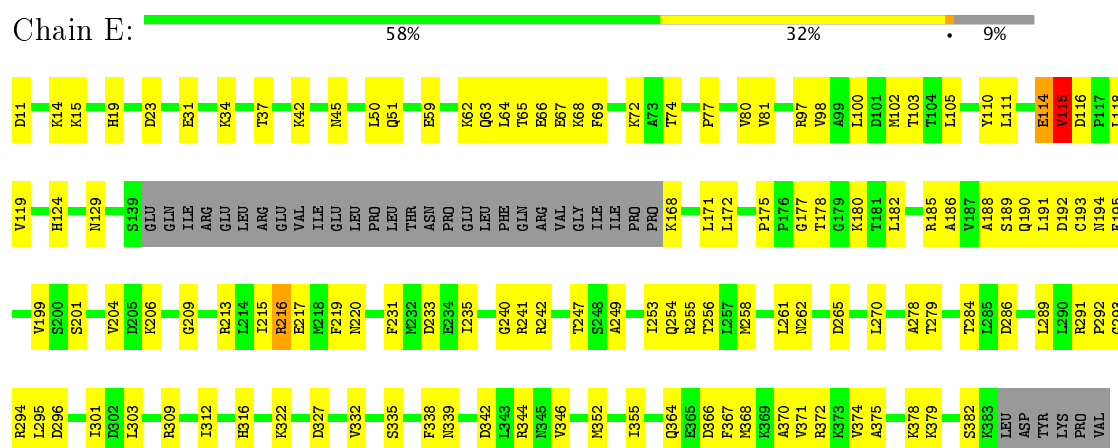




- Molecule 5: 26S proteasome regulatory subunit 6B



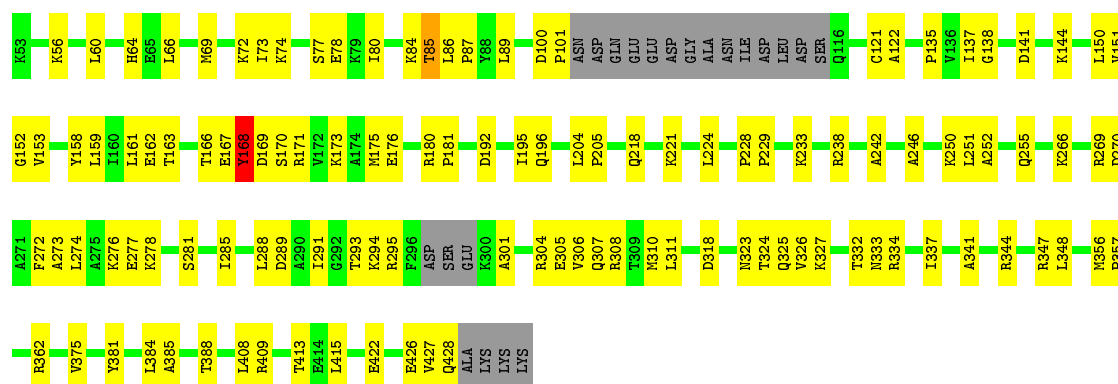
- Molecule 6: 26S proteasome regulatory subunit 10B



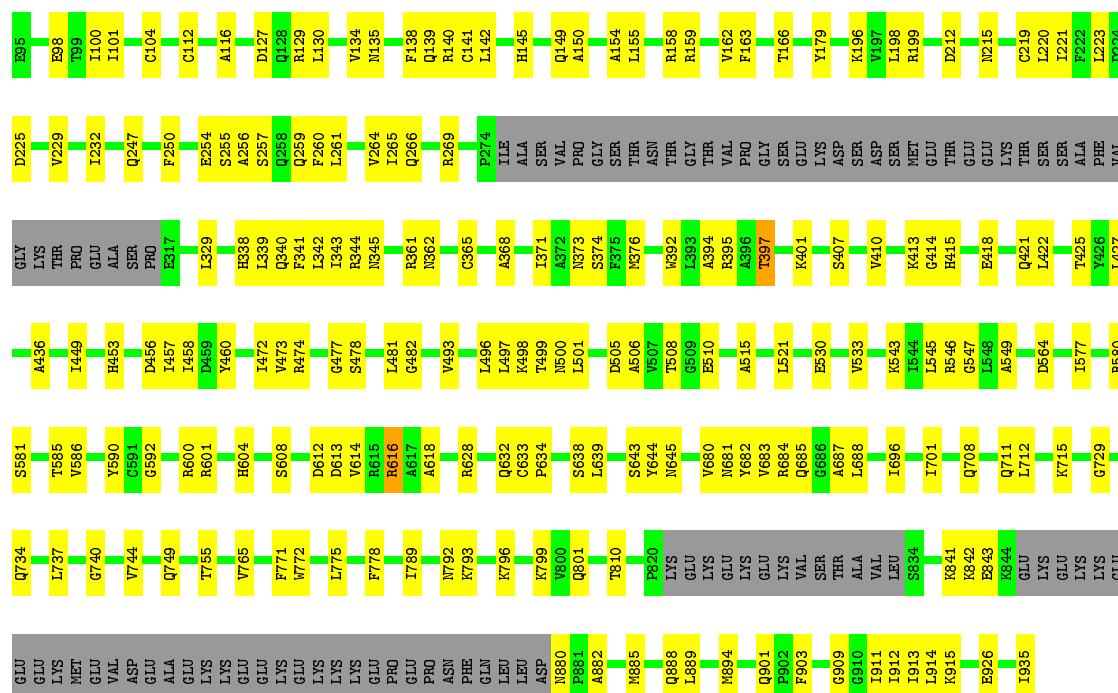
- Molecule 7: 26S proteasome regulatory subunit 6A



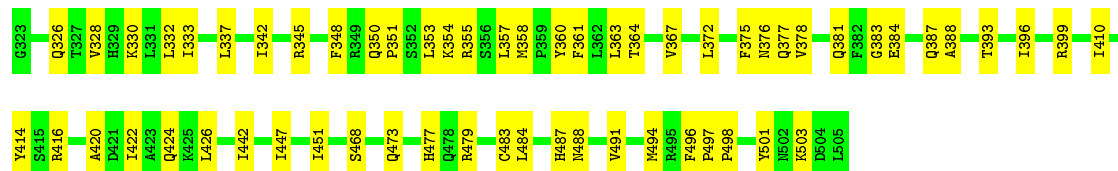




- Molecule 8: 26S proteasome non-ATPase regulatory subunit 1

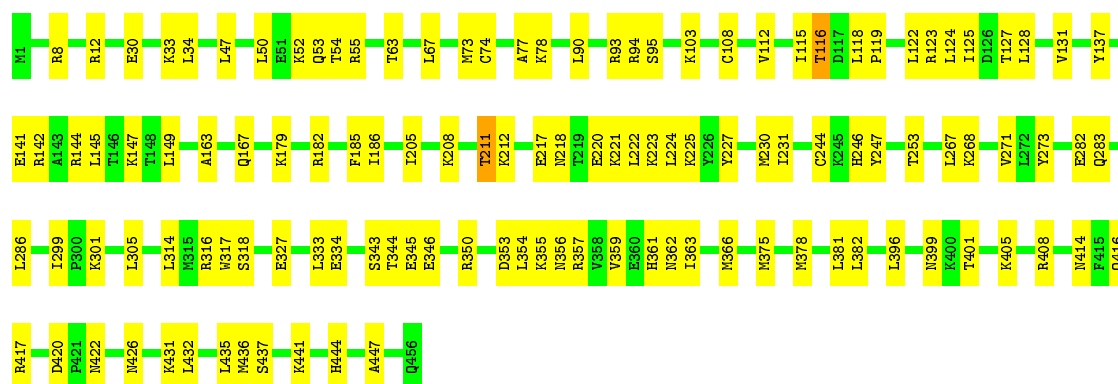


- Molecule 9: 26S proteasome non-ATPase regulatory subunit 3

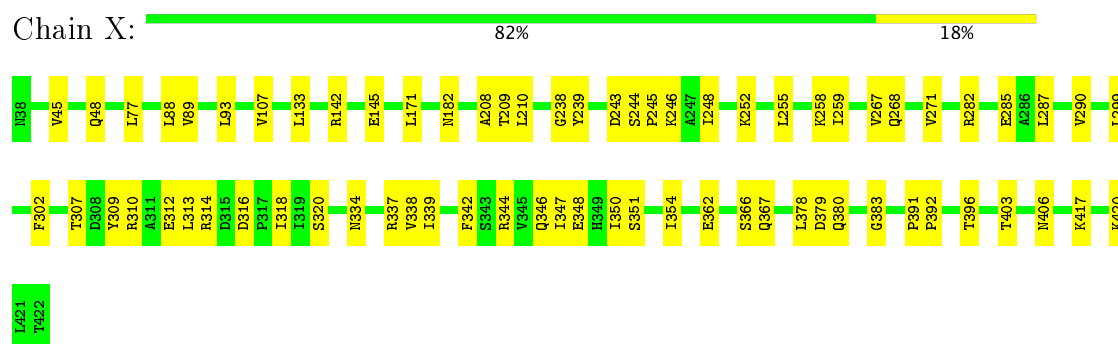


- Molecule 10: 26S proteasome non-ATPase regulatory subunit 12

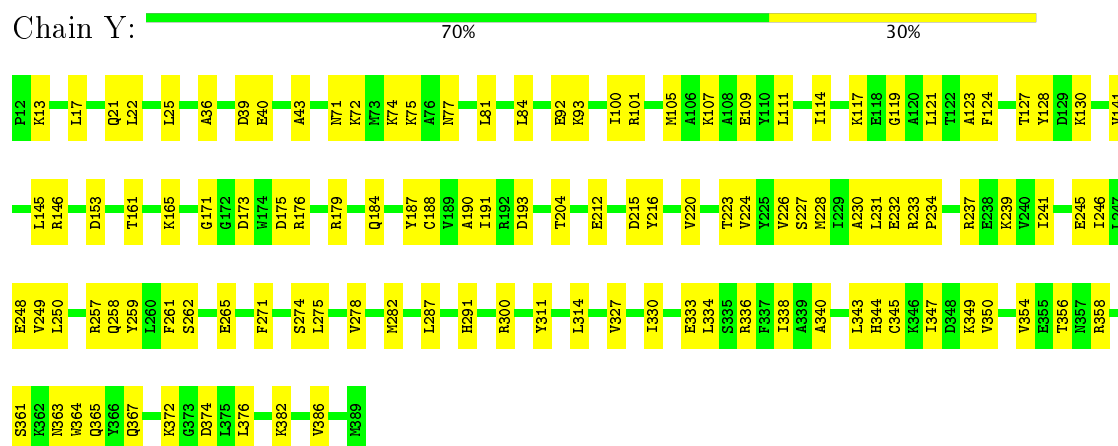




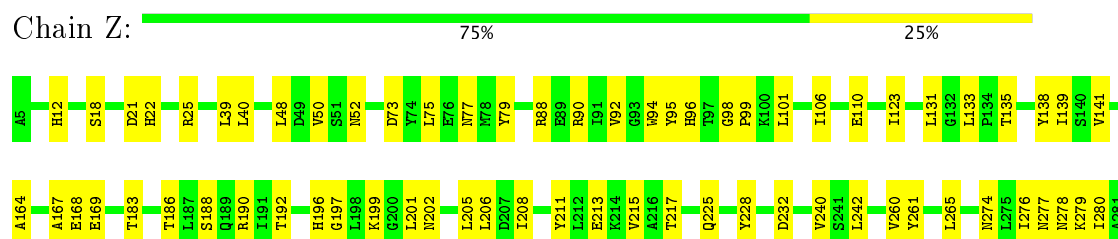
- Molecule 11: 26S proteasome non-ATPase regulatory subunit 11



- Molecule 12: 26S proteasome non-ATPase regulatory subunit 6



- Molecule 13: 26S proteasome non-ATPase regulatory subunit 7





- Molecule 14: 26S proteasome non-ATPase regulatory subunit 13

Chain a: 100%

There are no outlier residues recorded for this chain.

- Molecule 15: 26S proteasome non-ATPase regulatory subunit 4

Chain b: 99%



- Molecule 16: 26S proteasome non-ATPase regulatory subunit 14

Chain c: 100%



- Molecule 17: 26S proteasome non-ATPase regulatory subunit 8

Chain d: 99%



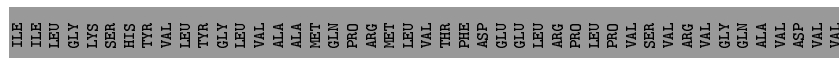
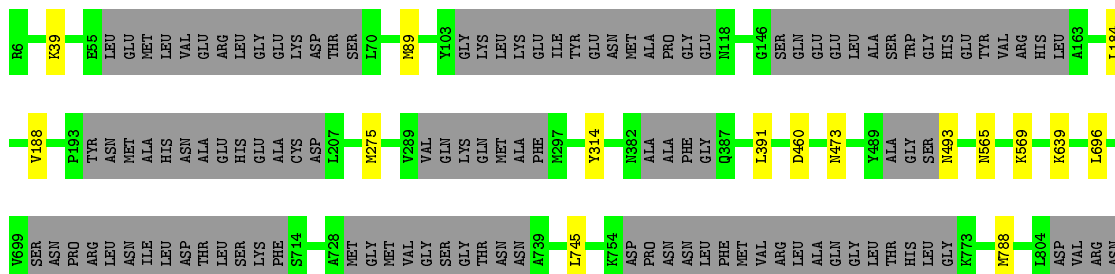
- Molecule 18: 26S proteasome complex subunit SEM1

Chain e: 100%

There are no outlier residues recorded for this chain.

- Molecule 19: 26S proteasome non-ATPase regulatory subunit 2

Chain f: 79% 19%



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	39520	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.23	0/1687	0.37	0/2279
10	W	0.23	0/3750	0.39	0/5039
11	X	0.23	0/3091	0.36	0/4165
12	Y	0.23	0/3173	0.37	0/4273
13	Z	0.23	0/2324	0.39	0/3150
14	a	0.23	0/3061	0.38	0/4144
15	b	0.23	0/1478	0.40	0/2001
16	c	0.23	0/2302	0.38	0/3110
17	d	0.24	0/1134	0.39	0/1534
18	e	0.23	0/596	0.40	0/805
19	f	0.24	0/5377	0.42	0/7248
2	A	0.23	0/2722	0.42	0/3673
3	B	0.23	0/2615	0.44	0/3530
4	C	0.23	0/2741	0.39	0/3681
5	D	0.24	0/2795	0.42	0/3773
6	E	0.32	2/2775 (0.1%)	0.47	3/3727 (0.1%)
7	F	0.24	0/2845	0.42	0/3832
8	U	0.23	0/5930	0.40	0/8021
9	V	0.24	0/1507	0.39	0/2029
All	All	0.24	2/51903 (0.0%)	0.40	3/70014 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	115	VAL	N-CA	8.47	1.63	1.46
6	E	115	VAL	CA-C	5.87	1.68	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	115	VAL	C-N-CA	-8.17	101.28	121.70
6	E	115	VAL	CA-C-N	7.58	133.87	117.20
6	E	115	VAL	O-C-N	-5.00	114.69	122.70

There are no chirality outliers.

There are no planarity outliers.

## 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	1662	0	1667	40	0
2	A	2677	0	2732	86	0
3	B	2579	0	2628	61	0
4	C	2709	0	2812	69	0
5	D	2751	0	2804	77	0
6	E	2736	0	2794	115	0
7	F	2808	0	2902	121	0
8	U	5829	0	5920	134	0
9	V	1480	0	1527	44	0
10	W	3703	0	3821	90	0
11	X	3048	0	3139	47	0
12	Y	3115	0	3120	79	0
13	Z	2281	0	2312	49	0
14	a	3003	0	3016	0	0
15	b	1458	0	1505	0	0
16	c	2260	0	2276	0	0
17	d	1109	0	1114	0	0
18	e	583	0	493	0	0
19	f	5304	0	5315	0	0
20	c	1	0	0	0	0
All	All	51096	0	51897	944	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 14.

The worst 5 of 944 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)
6:E:115:VAL:CG1	6:E:118:LEU:HB2	1.72	1.19
6:E:124:HIS:CD2	6:E:195:PHE:CE2	2.31	1.19
7:F:150:LEU:CB	7:F:166:THR:OG1	2.00	1.09
7:F:150:LEU:HB2	7:F:166:THR:OG1	1.52	1.08
6:E:124:HIS:CD2	6:E:195:PHE:CZ	2.43	1.05

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	217/223 (97%)	214 (99%)	3 (1%)	0	100	100
2	A	335/352 (95%)	301 (90%)	34 (10%)	0	100	100
3	B	326/340 (96%)	294 (90%)	30 (9%)	2 (1%)	28	70
4	C	334/385 (87%)	313 (94%)	21 (6%)	0	100	100
5	D	340/368 (92%)	317 (93%)	23 (7%)	0	100	100
6	E	341/379 (90%)	311 (91%)	28 (8%)	2 (1%)	28	70
7	F	353/380 (93%)	329 (93%)	23 (6%)	1 (0%)	44	81
8	U	743/841 (88%)	714 (96%)	29 (4%)	0	100	100
9	V	181/183 (99%)	170 (94%)	11 (6%)	0	100	100
10	W	452/456 (99%)	414 (92%)	38 (8%)	0	100	100
11	X	381/385 (99%)	375 (98%)	6 (2%)	0	100	100
12	Y	376/378 (100%)	357 (95%)	19 (5%)	0	100	100
13	Z	284/286 (99%)	267 (94%)	17 (6%)	0	100	100
14	a	372/374 (100%)	351 (94%)	21 (6%)	0	100	100
15	b	189/191 (99%)	174 (92%)	15 (8%)	0	100	100
16	c	285/287 (99%)	271 (95%)	14 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	d	134/136 (98%)	123 (92%)	11 (8%)	0	100	100
18	e	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
19	f	664/848 (78%)	597 (90%)	67 (10%)	0	100	100
All	All	6375/6862 (93%)	5956 (93%)	414 (6%)	5 (0%)	58	88

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	169	PRO
3	B	168	ASP
7	F	168	TYR
6	E	114	GLU
6	E	115	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	174/178 (98%)	173 (99%)	1 (1%)	89	94
2	A	293/300 (98%)	292 (100%)	1 (0%)	94	96
3	B	289/298 (97%)	286 (99%)	3 (1%)	80	90
4	C	297/333 (89%)	292 (98%)	5 (2%)	66	84
5	D	301/321 (94%)	298 (99%)	3 (1%)	80	90
6	E	300/333 (90%)	297 (99%)	3 (1%)	80	90
7	F	308/326 (94%)	304 (99%)	4 (1%)	73	87
8	U	639/720 (89%)	636 (100%)	3 (0%)	91	95
9	V	164/164 (100%)	164 (100%)	0	100	100
10	W	416/416 (100%)	413 (99%)	3 (1%)	87	93
11	X	331/331 (100%)	331 (100%)	0	100	100
12	Y	334/334 (100%)	333 (100%)	1 (0%)	94	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	Z	257/257 (100%)	256 (100%)	1 (0%)	93	95
14	a	334/334 (100%)	334 (100%)	0	100	100
15	b	167/167 (100%)	166 (99%)	1 (1%)	89	94
16	c	252/252 (100%)	251 (100%)	1 (0%)	93	95
17	d	121/121 (100%)	120 (99%)	1 (1%)	85	92
18	e	63/63 (100%)	63 (100%)	0	100	100
19	f	579/714 (81%)	563 (97%)	16 (3%)	49	74
All	All	5619/5962 (94%)	5572 (99%)	47 (1%)	86	92

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	U	427	LEU
12	Y	343	LEU
19	f	639	LYS
10	W	33	LYS
13	Z	90	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
8	U	754	HIS
11	X	406	ASN
19	f	327	ASN
8	U	801	GLN
10	W	86	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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
11	X	1
10	W	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	W	205:ILE	C	206:SER	N	3.19
1	X	311:ALA	C	312:GLU	N	3.16