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wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 11:29 am GMT

PDB ID	:	3J47
EMDB ID:	:	EMD-2165
Title	:	Formation of an intricate helical bundle dictates the assembly of the 26S proteasome lid
Authors	:	Estrin, E.; Lopez-Blanco, J.R.; Chacon, P.; Martin, A.
Deposited on	:	2013-06-27
Resolution	:	unknown (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
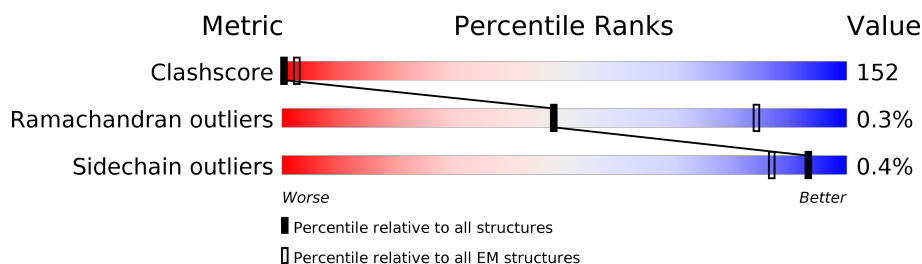with specific help available everywhere you see the ⓘ symbol.

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 unknown.

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	Percentile Ranks	Value
Clashscore		152
Ramachandran outliers		0.3%
Sidechain outliers		0.4%

Worse ... *Better*

▮ Percentile relative to all structures
▯ Percentile relative to all EM structures

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 <=5%

Mol	Chain	Length	Quality of chain
1	V	69	33% 55% • 9%
2	U	121	37% 38% 25%
3	O	28	64% 36%
4	P	34	62% 38%
5	Q	25	28% 72%
6	R	26	58% 42%
7	S	24	29% 67% •
8	T	17	71% 29%

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 2498 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 RPN11.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	V	63	Total	C	N	O	S	0	0
			509	313	83	112	1		

- Molecule 2 is a protein called 26S proteasome regulatory subunit RPN8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	U	91	Total	C	N	O	S	0	0
			742	474	129	138	1		

- Molecule 3 is a protein called 26S proteasome regulatory subunit RPN9.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	O	28	Total	C	N	O	S	0	0
			232	143	43	44	2		

- Molecule 4 is a protein called 26S proteasome regulatory subunit RPN5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	34	Total	C	N	O	S	0	0
			279	176	47	55	1		

- Molecule 5 is a protein called 26S proteasome regulatory subunit RPN6.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	Q	25	Total	C	N	O	0	0
			192	122	30	40		

- Molecule 6 is a protein called 26S proteasome regulatory subunit RPN7.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	R	26	Total	C	N	O	0	0
			203	130	38	35		

• Molecule 7 is a protein called 26S proteasome regulatory subunit RPN3.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	S	24	Total 206	C 130	N 34	O 42	0	0

• Molecule 8 is a protein called 26S proteasome regulatory subunit RPN12.

| Mol	Chain	Residues	Atoms					AltConf	Trace
8	T	17	Total 135	C 85	N 21	O 28	S 1	0	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 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.
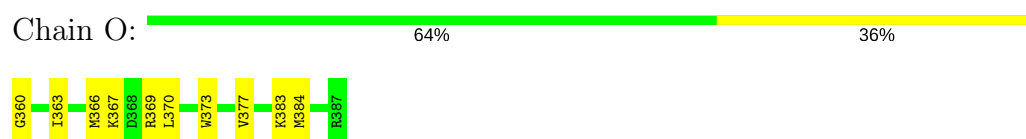
• Molecule 1: 26S proteasome regulatory subunit RPN11

Chain V:
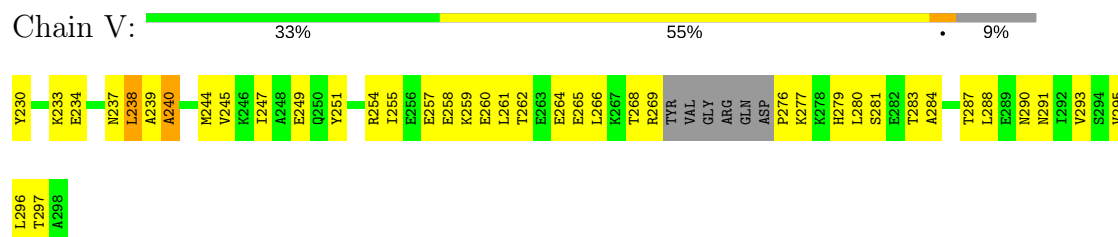
• Molecule 2: 26S proteasome regulatory subunit RPN8
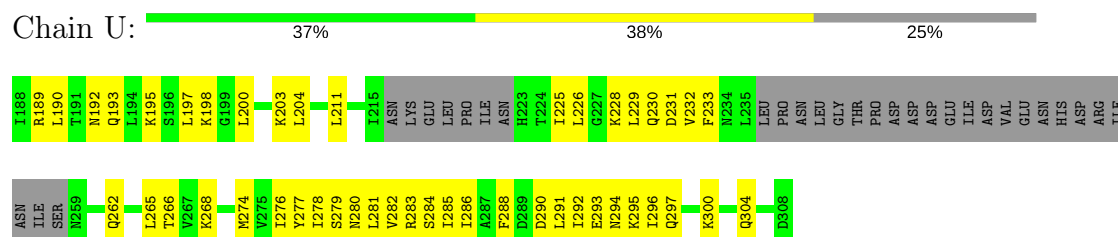
Chain U:

• Molecule 3: 26S proteasome regulatory subunit RPN9

Chain O:

• Molecule 4: 26S proteasome regulatory subunit RPN5

Chain P:

• Molecule 5: 26S proteasome regulatory subunit RPN6
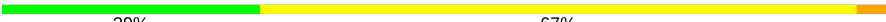
Chain Q:

• Molecule 6: 26S proteasome regulatory subunit RPN7

Chain R:

58%   42%

N397 Y400 H401 L402 L403 V404 K405 Q406 L410 L411 T412 K413 L414 Y417 R422

• Molecule 7: 26S proteasome regulatory subunit RPN3

Chain S:

29%   67%   .

E455 D456 P457 V460 F461 D462 E463 R464 I465 K466 F467 A468 N469 Q470 L471 E474 Y475 L476 V477 S478
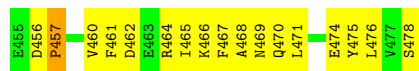
• Molecule 8: 26S proteasome regulatory subunit RPN12

Chain T:

71%   29%

K256 T257 I260 E261 K262 Y266 I270 E271 N272

4 Experimental information ⓘ

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	Not provided	Depositor
Voltage (kV)	Not provided	Depositor
Electron dose $(e^-/\text{Å}^2)$	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	V	1.06	3/511 (0.6%)	1.09	2/682 (0.3%)
2	U	0.46	0/744	0.90	0/995
3	O	0.76	1/233 (0.4%)	1.06	1/307 (0.3%)
4	P	0.53	0/284	0.92	0/384
5	Q	0.86	1/193 (0.5%)	0.90	0/260
6	R	0.48	0/205	0.90	0/274
7	S	1.29	1/210 (0.5%)	0.96	0/283
8	T	0.50	0/135	0.84	0/180
All	All	0.78	6/2515 (0.2%)	0.96	3/3365 (0.1%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	S	457	PRO	N-CD	15.78	1.70	1.47
1	V	239	ALA	N-CA	-14.14	1.18	1.46
1	V	276	PRO	N-CD	11.48	1.64	1.47
5	Q	407	ALA	N-CA	-7.42	1.31	1.46
1	V	238	LEU	C-N	7.04	1.50	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	238	LEU	O-C-N	-5.45	113.98	122.70
1	V	240	ALA	CB-CA-C	5.17	117.85	110.10
3	O	373	TRP	CG-CD2-CE3	-5.09	129.32	133.90

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	V	509	0	499	244	0
2	U	742	0	787	488	0
3	O	232	0	236	126	0
4	P	279	0	266	130	0
5	Q	192	0	187	142	0
6	R	203	0	211	84	0
7	S	206	0	185	179	0
8	T	135	0	137	56	0
All	All	2498	0	2508	762	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 152.

The worst 5 of 762 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:R:422:ARG:HH21	7:S:474:GLU:CG	1.02	1.66
2:U:288:PHE:CD1	7:S:471:LEU:HG	1.23	1.65
1:V:264:GLU:CB	1:V:280:LEU:HB2	1.23	1.61
2:U:288:PHE:CZ	7:S:471:LEU:HD11	1.27	1.61
2:U:233:PHE:CG	3:O:369:ARG:HD2	1.08	1.60

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	V	59/69 (86%)	57 (97%)	1 (2%)	1 (2%)	11	11
2	U	85/121 (70%)	83 (98%)	2 (2%)	0	100	100
3	O	26/28 (93%)	26 (100%)	0	0	100	100
4	P	32/34 (94%)	32 (100%)	0	0	100	100
5	Q	23/25 (92%)	23 (100%)	0	0	100	100
6	R	24/26 (92%)	24 (100%)	0	0	100	100
7	S	22/24 (92%)	22 (100%)	0	0	100	100
8	T	15/17 (88%)	15 (100%)	0	0	100	100
All	All	286/344 (83%)	282 (99%)	3 (1%)	1 (0%)	48	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	V	247	ILE

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	V	58/63 (92%)	57 (98%)	1 (2%)	66	66
2	U	87/116 (75%)	87 (100%)	0	100	100
3	O	25/25 (100%)	25 (100%)	0	100	100
4	P	32/32 (100%)	32 (100%)	0	100	100
5	Q	21/21 (100%)	21 (100%)	0	100	100
6	R	20/20 (100%)	20 (100%)	0	100	100
7	S	23/23 (100%)	23 (100%)	0	100	100
8	T	15/15 (100%)	15 (100%)	0	100	100
All	All	281/315 (89%)	280 (100%)	1 (0%)	93	93

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	V	249	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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.