

Summary of integrative structure determination of The proteasome-interacting Ecm29 protein disassembles the 26S proteasome in response to oxidative stress (PDB ID: 8ZZQ, PDB-Dev ID: PDBDEV_00000026)

1. Model Composition	
<i>Entry composition</i>	<ul style="list-style-type: none"> - Rpn11: Chain I (310 residues) - ecm29: Chain S (1845 residues) - Rpn8: Chain Q (324 residues) - Rpn12: Chain G (350 residues) - Rpt4: Chain B (389 residues) - Rpt2: Chain D (440 residues) - Rpn10: Chain H (377 residues) - Rpn5: Chain N (456 residues) - Rpn7: Chain P (389 residues) - Rpn6: Chain O (422 residues) - Rpn2: Chain L (953 residues) - Rpt1: Chain F (433 residues) - Rpn15: Chain J (70 residues) - Rpn9: Chain R (376 residues) - Rpn1: Chain K (908 residues) - Rpt3: Chain E (418 residues) - Rpt6: Chain A (406 residues) - Rpn3: Chain M (534 residues) - Rpt5: Chain C (439 residues)
<i>Datasets used for modeling</i>	<ul style="list-style-type: none"> - Experimental model, PDB ID: 5GJR - Experimental model, PDB ID: Not available - Experimental model, PDB ID: 1U6G - Comparative model, template PDB ID: Not available - Experimental model, PDB ID: 3W3W - Comparative model, template PDB ID: Not available - Crosslinking-MS data, Linker name and number of cross-links: DSSO, 63 cross-links
2. Representation	
<i>Resolution</i>	Coarse-grained: 1, 2, 3, 4, 5, 6, 7, 9, 11, 19, 36 residue(s) per bead
<i>Number of rigid bodies, flexible units</i>	7, 101

<i>Rigid bodies</i>	<ul style="list-style-type: none"> - A: - - B: - - C: - - D: - - E: - - F: - - G: - - H: - - I: - - J: - - K: - - L: - - M: - - N: - - O: - - P: - - Q: - - R: - - S: 352-504, 686-760, 788-911, 934-1035, 1062-1306, 1331-1666, 1689-1738
<i>Flexible units</i>	<ul style="list-style-type: none"> - A: 1-23, 24-250, 251-266, 267-397, 398-406 - B: 1-14, 15-389 - C: 1-43, 44-99, 100-119, 120-439 - D: 1-64, 65-84, 85-90, 91-429, 430-440 - E: 1-38, 39-418 - F: 1-46, 47-72, 73-79, 80-433 - G: 1-88, 89-130, 131-134, 135-350 - H: 1-193, 194-377 - I: 1-27, 28-163, 164-189, 190-310 - J: 1-2, 3-27, 28-34, 35-68, 69-70 - K: 1-105, 106-170, 171-178, 179-301, 302-308, 309-618, 619-652, 653-848, 849-870, 871-908 - L: 1-2, 3-272, 273-320, 321-750, 751-752, 753-816, 817-877, 878-917, 918-922, 923-939, 940-953 - M: 1-56, 57-101, 102-103, 104-116, 117-159, 160-496, 497-499, 500-525, 526-534 - N: 1-4, 5-24, 25-39, 40-94, 95-98, 99-112, 113-116, 117-132, 133-138, 139-332, 333-340, 341-454, 455-456 - O: 1-1, 2-422 - P: 1-13, 14-389 - Q: 1-3, 4-142, 143-151, 152-295, 296-324 - R: 1-2, 3-54, 55-56, 57-376 - S: 1-351, 505-685, 761-787, 912-933, 1036-1061, 1307-1330, 1667-1688, 1739-1845
<u>Structural coverage (rigid bodies)</u>	11%
3. Restraints	
<u>Physical principles</u>	Information about physical principles was not provided
<u>Experimental data</u>	- 1 unique CrossLinkRestraint: DSSO, 63 cross-links
4. Validation	
<u>Number of ensembles</u>	2

<u>Number of models in ensembles</u>	11980, 6261
<u>Number of deposited models</u>	2
<u>Model precision (uncertainty of models)</u>	60.0, Å, 60.0, Å
<u>Data quality</u>	Data quality has not been assessed
<u>Model quality: assessment of excluded volume</u>	Satisfaction: 99.93-99.93%
<u>Fit to data used for modeling</u>	Fit of model to information used to compute it has not been determined
<u>Fit to data used for validation</u>	Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
<u>1. Method</u>	Sampling
<u>Name</u>	Replica exchange monte carlo
<u>Number of computed models</u>	3750000
<u>Software</u>	<ul style="list-style-type: none"> - IMP PMI module (version develop-7c7c0f4348) - Integrative Modeling Platform (IMP) (version develop-0a5706e202) - MODELLER (version 9.17)