Summary of integrative structure determination of the proteasome-interacting ecm29 protein disassembles the 26s proteasome in response to oxidative stress (PDBDEV00000026)

1. Model Composition	
Entry composition	- Rpn15: Chain J (70 residues) - Rpn6: Chain O (422 residues) - Rpn9: Chain R (376 residues) - Rpt3: Chain E (418 residues) - Rpn8: Chain Q (324 residues) - Rpn11: Chain I (310 residues) - Rpt1: Chain F (433 residues) - Rpn5: Chain N (456 residues) - Rpn12: Chain G (350 residues) - ecm29: Chain S (1845 residues) - Rpt6: Chain A (406 residues) - Rpt5: Chain C (439 residues) - Rpn7: Chain P (389 residues) - Rpn1: Chain K (908 residues) - Rpt4: Chain B (389 residues) - Rpn3: Chain M (534 residues) - Rpt2: Chain D (440 residues) - Rpn2: Chain L (953 residues) - Rpn10: Chain H (377 residues)
Datasets used for modeling	- Experimental model, PDB ID: 5GJR - Experimental model, PDB ID: Not listed - Experimental model, PDB ID: 1U6G - Comparative model, template PDB ID: Not listed - Experimental model, PDB ID: 3W3W - Comparative model, template PDB ID: Not listed - CX-MS data, Linker name and number of cross-links: DSSO, 63 cross-links
2. Representation	
Atomic structural coverage	11%
Number of rigid bodies, flexible units	7, 101

Rigid bodies	- A: - - B: - - C: - - D: - - E: - - F: - - G: - - H: - - I: - - J: - - K: - - L: - - M: - - N: - - O: - - P: - - Q: - - R: - - S: 352-504:Comparative model/None, 686-760:Comparative model/None, 788-911:Comparative model/None, 934-1035:Comparative model/None, 1062-1306:Comparative model/None, 1331-1666:Comparative model/None, 1689-1738:Comparative model/None.
Flexible units	- 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.
Resolution	- Rigid bodies: 1 residue per bead. - Flexible regions: N/A
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 1 unique CrossLinkRestraint: DSSO, 63 cross-links
4. Validation	
Sampling validation	- Information related to sampling validation has not been provided

Clustering algorithm ,*clustering feature*	Distance threshold-based clustering used if ensembles are deposited, dRMSD
Number of ensembles	2
Number of models in ensembles	11980, 6261
Model precision (uncertainty of models)	60.0Å, 60.0Å
Quality of data	- Quality of input data has not be assessed
Model quality: assessment of atomic segments	Not applicable
Model quality: assessment of excluded volume	- Model-1: Number of violations-22257.0 - Model-2: Number of violations-22180.0
Fit of the model to information used to compute it	- Fit of model to information used to compute it has not been determined
Fit of the model to information not used to compute it	- Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
Method	Sampling
Name	Replica exchange Monte Carlo
Details	- Method details unspecified
Software	- IMP PMI module (version develop-7c7c0f4348) - Integrative Modeling Platform (IMP) (version develop-0a5706e202) - MODELLER (version 9.17) - No location specified