



# Full wwPDB Integrative Structure Validation Report

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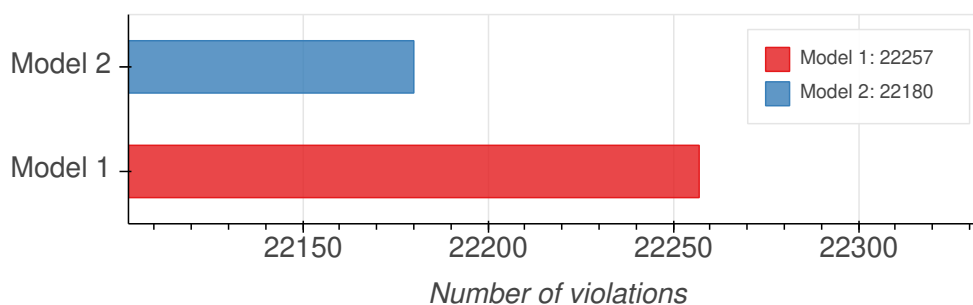
PDB ID	PDBDEV00000026
Molecule Name	The proteasome-interacting Ecm29 protein disassembles the 26S proteasome in response to oxidative stress
Title	The proteasome-interacting Ecm29 protein disassembles the 26S proteasome in response to oxidative stress.
Authors	Wang X;Chemmama IE;Yu C;Huszagh A;Xu Y;Viner R;Block SA;Cimermancic P;Rychnovsky SD;Ye Y;Sali A;Huang L

The following software were used in the production of this report:

*Integrative Modeling Validation Package : Version 1.0*

## 1. Overall quality at a glance

Model quality: Excluded Volume Analysis



## 2. Ensemble information

This entry consists of 2 distinct ensembles.

Ensemble number	Ensemble name	Model ID	Number of models	Clustering method	Clustering feature	Cluster precision
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1	Cluster 0 in state State_0	1	11980	None	dRMSD	60.0
2	Cluster 1 in state State_0	2	6261	None	dRMSD	60.0

### 3. Model composition

#### 3.1 Summary

*This entry consists of 2 unique models, with 19 subunits in each model. A total of 7 datasets or restraints was used to build this entry. Each model is represented by 7 rigid bodies and 101 flexible or non-rigid units.*

#### 3.2 Entry composition

*There are 2 unique types of models in this entry. These models are titled Cluster 0 in state State\_0/None, Cluster 1 in state State\_0/None respectively.*

<b>Model ID</b>	<b>Subunit number</b>	<b>Subunit ID</b>	<b>Subunit name</b>	<b>Chain ID</b>	<b>Total residues</b>
1	1	1	Rpt6	A	406
1	2	2	Rpt4	B	389
1	3	3	Rpt5	C	439
1	4	4	Rpt2	D	440
1	5	5	Rpt3	E	418
1	6	6	Rpt1	F	433
1	7	7	Rpn12	G	350
1	8	8	Rpn10	H	377
1	9	9	Rpn11	I	310
1	10	10	Rpn15	J	70
1	11	11	Rpn1	K	908
1	12	12	Rpn2	L	953
1	13	13	Rpn3	M	534
1	14	14	Rpn5	N	456
1	15	15	Rpn6	O	422
1	16	16	Rpn7	P	389
1	17	17	Rpn8	Q	324

1	18	18	Rpn9	R	376
1	19	19	ecm29	S	1845
2	1	1	Rpt6	A	406
2	2	2	Rpt4	B	389
2	3	3	Rpt5	C	439
2	4	4	Rpt2	D	440
2	5	5	Rpt3	E	418
2	6	6	Rpt1	F	433
2	7	7	Rpn12	G	350
2	8	8	Rpn10	H	377
2	9	9	Rpn11	I	310
2	10	10	Rpn15	J	70
2	11	11	Rpn1	K	908
2	12	12	Rpn2	L	953
2	13	13	Rpn3	M	534
2	14	14	Rpn5	N	456
2	15	15	Rpn6	O	422
2	16	16	Rpn7	P	389
2	17	17	Rpn8	Q	324
2	18	18	Rpn9	R	376
2	19	19	ecm29	S	1845

### 3.3 Datasets used for modeling

*There are 7 unique datasets used to build the models in this entry.*

<i>ID</i>	<i>Dataset type</i>	<i>Database name</i>	<i>Data access code</i>
1	Experimental model	PDB	5GJR
2	Experimental model	Not listed	None
3	Experimental model	PDB	1U6G
4	Comparative model	Not listed	None

5	Experimental model	PDB	3W3W
6	Comparative model	Not listed	None
7	CX-MS data	Not listed	None

## 4. Representation

*This entry has only one representation and includes 7 rigid bodies and 101 flexible units.*

<b>Chain ID</b>	<b>Rigid bodies</b>	<b>Non-rigid segments</b>
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	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.	1-351, 505-685, 761-787, 912-933, 1036-1061, 1307-1330, 1667-1688, 1739-1845.

## 5. Methodology and software

<i>Step number</i>	<i>Protocol ID</i>	<i>Method name</i>	<i>Method type</i>	<i>Number of computed models</i>	<i>Multi state modeling</i>	<i>Multi scale modeling</i>
1	1	Replica exchange monte carlo	Sampling	3750000	False	True

*There are 3 software packages reported in this entry.*

<i>ID</i>	<i>Software name</i>	<i>Software version</i>	<i>Software classification</i>	<i>Software location</i>
1	IMP PMI module	develop-7c7c0f4348	integrative model building	<a href="https://integrativemodeling">https://integrativemodeling</a>
2	Integrative Modeling Platform (IMP)	develop-0a5706e202	integrative model building	<a href="https://integrativemodeling">https://integrativemodeling</a>
3	MODELLER	9.17	comparative modeling	<a href="https://salilab.org/modeller">https://salilab.org/modeller</a>

## 6. Data quality

## 7. Model quality

### 7.1 Excluded volume satisfaction

*Excluded volume satisfaction for the models in the entry are listed below.*

<i>Models</i>	<i>Excluded Volume Satisfaction</i>	<i>Number of violations</i>
1	99.93	22257
2	99.93	22180

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## 8. Fit of model to data used for modeling

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## 9. Fit of model to data not used for modeling

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## 10. Uncertainty of model

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