

# Integrative Structure Validation Report ?

July 22, 2024 - 03:49 PM PDT

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

*Python-IHM Version 1.3*  
*Integrative Modeling Validation Version 1.2*

PDB ID	8ZZQ
PDB-Dev ID	PDBDEV_00000026
Structure Title	The proteasome-interacting Ecm29 protein disassembles the 26S proteasome in response to oxidative stress
Structure 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

*This is a PDB-Dev IM Structure Validation Report for a publicly released PDB-Dev entry.*

*We welcome your comments at [pdb-dev@mail.wwpdb.org](mailto:pdb-dev@mail.wwpdb.org)*

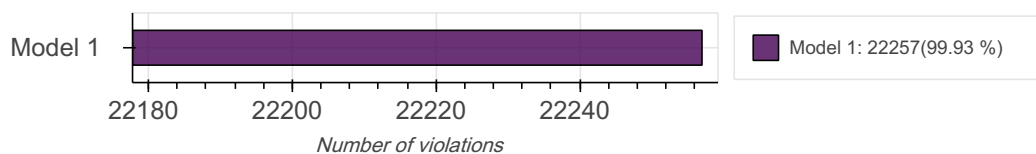
*A user guide is available at [https://pdb-dev.wwpdb.org/validation\\_help.html](https://pdb-dev.wwpdb.org/validation_help.html) with specific help available everywhere you see the ? symbol.*

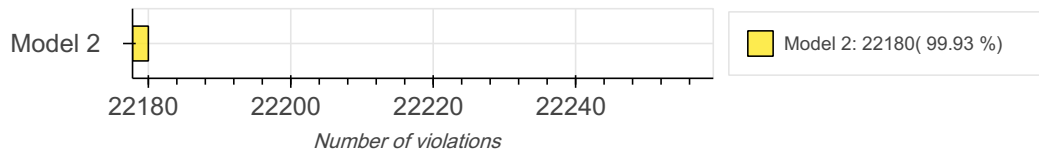
*List of references used to build this report is available [here](#).*

## Overall quality ?

*This validation report contains model quality assessments for all structures, data quality assessment for SAS datasets and fit to model assessments for SAS datasets. Data quality and fit to model assessments for other datasets and model uncertainty are under development. Number of plots is limited to 256.*

### Model Quality: Excluded Volume Analysis





## Ensemble information ?

*This entry consists of 2 distinct ensemble(s).*

## Summary ?

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

## 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.*

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	Rpt6	A	A	406
1	2	2	Rpt4	B	B	389
1	3	3	Rpt5	C	C	439
1	4	4	Rpt2	D	D	440
1	5	5	Rpt3	E	E	418
1	6	6	Rpt1	F	F	433
1	7	7	Rpn12	G	G	350
1	8	8	Rpn10	H	H	377
1	9	9	Rpn11	I	I	310
1	10	10	Rpn15	J	J	70
1	11	11	Rpn1	K	K	908

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

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
2	16	16	Rpn7	P	P	389
2	17	17	Rpn8	Q	Q	324
2	18	18	Rpn9	R	R	376
2	19	19	ecm29	S	S	1845

### Datasets used for modeling ?

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

ID	Dataset type	Database name	Data access code
1	Experimental model	PDB	5GJR
2	Experimental model	File	10.5281/zenodo.1445841
3	Experimental model	PDB	1U6G
4	Comparative model	File	10.5281/zenodo.1445841
5	Experimental model	PDB	3W3W
6	Comparative model	File	10.5281/zenodo.1445841
7	Crosslinking-MS data	File	10.5281/zenodo.1445841

### Representation ?

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

Chain ID	Rigid bodies	Non-rigid segments
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

Chain ID	Rigid bodies	Non-rigid segments
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, 686-760, 788-911, 934-1035, 1062-1306, 1331-1666, 1689-1738	1-351, 505-685, 761-787, 912-933, 1036-1061, 1307-1330, 1667-1688, 1739-1845

## Methodology and software

*This entry is a result of 1 distinct protocol(s).*

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
1	1	Replica exchange monte carlo	Sampling	None	3750000	False	True

There are 3 software packages reported in this entry.

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

## Data quality

### Crosslinking-MS

Validation for this section is under development.

## Model quality

For models with atomic structures, molprobit analysis is performed. For models with coarse-grained or multi-scale structures, excluded volume analysis is performed.

### Excluded volume satisfaction

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

Models	Excluded Volume Satisfaction (%)	Number of violations
1	99.93	22257.0
2	99.93	22180.0

## Fit of model to data used for modeling ?

### Crosslinking-MS

Validation for this section is under development.

## Fit of model to data used for validation ?

Validation for this section is under development.

### *Acknowledgements*

*Development of integrative model validation metrics, implementation of a model validation pipeline, and creation of a validation report for integrative structures, are funded by NSF ABI awards (DBI-1756248, DBI-2112966, DBI-2112967, DBI-2112968, and DBI-1756250). The [PDB-Dev team](#) and members of [Sali lab](#) contributed model validation metrics and software packages.*

*Implementation of validation methods for SAS data and SAS-based models are funded by [RCSB PDB](#) (grant number DBI-1832184). Dr. Stephen Burley, Dr. John Westbrook, and Dr. Jasmine Young from [RCSB PDB](#), Dr. Jill Trehwella, Dr. Dina Schneidman, and members of the [SASBDB](#) repository are acknowledged for their advice and support in implementing SAS validation methods.*

*Members of the [wwPDB Integrative/Hybrid Methods Task Force](#) provided recommendations and community support for the project.*