

# Integrative Structure Validation Report ?

July 22, 2024 - 04:05 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	9A0D
PDB-Dev ID	PDBDEV_00000049
Structure Title	In-cell architecture of an actively transcribing-translating expressome from <i>M. pneumoniae</i>
Structure Authors	O'Reilly FJ; Xue L; Graziadei A; Sinn L; Lenz S; Tegunov D; Bloetz C; Singh N; Hagen WJH; Cramer P; Stuelke J; Mahamid J; Rappsilber J

*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)*

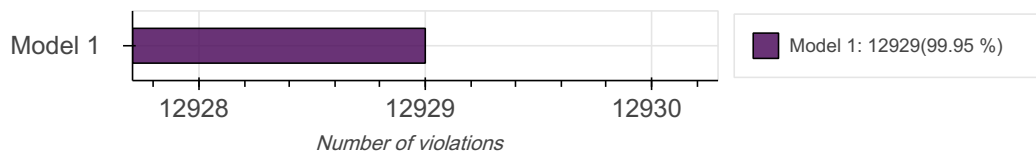
*A user guide is available at [https://pdb-dev.wwpdb.org/validation\\_help.html](https://pdb-dev.wwpdb.org/validation_help.html) with specific help available everywhere you see the ? symbol.*

*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 1 distinct ensemble(s).*

## Summary

*This entry consists of 1 unique models, with 32 subunits in each model. A total of 27 datasets or restraints were used to build this entry. Each model is represented by 39 rigid bodies and 47 flexible or non-rigid units.*

## Entry composition

*There is 1 unique type of models in this entry. This model is titled Cluster 0/None.*

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	P75591	A	A	540
1	2	2	Q50295	B	B	327
1	3	2	Q50295	C	C	327
1	4	3	P78013	D	D	1391
1	5	4	P75271	E	E	1290
1	6	5	P75049	F	F	320
1	7	6	Q50301	G	G	219
1	8	7	P75560	H	H	294
1	9	8	P75581	I	I	108
1	10	9	P41205	J	J	273
1	11	10	P46775	K	K	205
1	12	11	Q50304	L	L	142
1	13	12	P75179	M	M	132
1	14	13	DNA1N	N	N	39

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	15	14	longRNAR1	O	O	46
1	16	14	longRNAR1	P	P	46
1	17	15	DNA1T	Q	Q	39
1	18	16	P75090	R	R	144
1	19	17	30SsubunitE	S	S	92
1	20	18	30SsubunitF	T	T	153
1	21	19	30SsubunitJ	U	U	118
1	22	20	30SsubunitK	V	V	135
1	23	21	30SsubunitL	W	W	119
1	24	22	30SsubunitM	X	X	60
1	25	23	30SsubunitN	Y	Y	84
1	26	24	30SsubunitO	Z	Z	80
1	27	25	30SsubunitP	AA	AA	83
1	28	26	30SsubunitQ	AB	AB	71
1	29	27	30SsubunitR	AC	AC	83
1	30	28	30SsubunitT	AD	AD	1544
1	31	29	30Ssubunitj	AE	AE	77
1	32	30	30SsubunitZ	AF	AF	77

### Datasets used for modeling

There are 27 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Comparative model	File	10.5281/zenodo.3837625

<b>ID</b>	<b>Dataset type</b>	<b>Database name</b>	<b>Data access code</b>
2	Experimental model	PDB	6flq
3	Comparative model	File	10.5281/zenodo.3837625
4	Comparative model	File	10.5281/zenodo.3837625
5	Comparative model	File	10.5281/zenodo.3837625
6	Comparative model	File	10.5281/zenodo.3837625
7	Experimental model	PDB	3j9w
8	Comparative model	File	10.5281/zenodo.3837625
9	Comparative model	File	10.5281/zenodo.3837625
10	Comparative model	File	10.5281/zenodo.3837625
11	Comparative model	File	10.5281/zenodo.3837625
12	Comparative model	File	10.5281/zenodo.3837625
13	Comparative model	File	10.5281/zenodo.3837625
14	Comparative model	File	10.5281/zenodo.3837625
15	Comparative model	File	10.5281/zenodo.3837625
16	Comparative model	File	10.5281/zenodo.3837625
17	Comparative model	File	10.5281/zenodo.3837625
18	Comparative model	File	10.5281/zenodo.3837625
19	Comparative model	File	10.5281/zenodo.3837625
20	Comparative model	File	10.5281/zenodo.3837625
21	Crosslinking-MS data	PRIDE	PXD017695
22	Crosslinking-MS data	PRIDE	PXD017711
23	3DEM volume	EMDB	EMD-10680
24	3DEM volume	File	10.5281/zenodo.3837625

ID	Dataset type	Database name	Data access code
25	Experimental model	PDB	6FLQ
26	Experimental model	PDB	6C6U
27	Experimental model	PDB	3J9W

## Representation ?

*This entry has only one representation and includes 39 rigid bodies and 47 flexible units*

Chain ID	Rigid bodies	Non-rigid segments
A	12-141, 145-212, 216-364	1-11, 142-144, 213-215, 365-540
B	29-233, 234-239, 266-325	1-28, 240-265, 326-327
C	29-233, 234-325	1-28, 240-265, 326-327
D	14-980, 990-998, 1006-1356	1-13, 225-342, 398-498, 981-989, 999-1005, 1357-1391
E	14-1280	1-13, 137-237, 266-272, 658-690, 836-848, 1027-1047, 1056-1056, 1064-1068, 1117-1120, 1281-1290
F	7-146	1-6, 48-91, 147-150
G	70-212	1-69, 213-219
H	20-241	1-19, 242-294
I	12-107	1-11, 108-108
J	2-206	1-1, 207-273
K	2-202	1-1, 203-205
L	10-142	1-9
M	6-132	1-5
N	1-38	16-24, 39-39

Chain ID	Rigid bodies	Non-rigid segments
O	1-9	10-11
P	37-46	-
Q	2-39	1-1
R	9-74	1-8, 75-85
S	1-92	-
T	1-153	-
U	1-118	-
V	1-135	-
W	1-119	-
X	1-60	-
Y	1-84	-
Z	1-80	-
AA	1-83	-
AB	1-71	-
AC	1-83	-
AD	1-1544	-
AE	1-77	-
AF	1-77	-

### 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
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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	14400000	False	True

There are 6 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	<a href="#">IMP PMI module</a>	2.12.0	integrative model building	<a href="https://integrativemodeling.org">https://integrativemodeling.org</a>
2	<a href="#">Integrative Modeling Platform (IMP)</a>	2.12.0	integrative model building	<a href="https://integrativemodeling.org">https://integrativemodeling.org</a>
3	<a href="#">SWISS-MODEL</a>	2019-11-21	comparative modeling	<a href="https://swissmodel.expasy.org/">https://swissmodel.expasy.org/</a>
4	<a href="#">MODELLER</a>	9.21	comparative modeling	<a href="https://salilab.org/modeller/">https://salilab.org/modeller/</a>
5	<a href="#">SWISS-MODEL</a>	2.0.0	protein homology modeling	<a href="https://swissmodel.expasy.org/">https://swissmodel.expasy.org/</a>
6	<a href="#">SWISS-MODEL</a>	1.3.0	protein homology modeling	<a href="https://swissmodel.expasy.org/">https://swissmodel.expasy.org/</a>

### Data quality ?

#### 3DEM volume

Validation for this section is under development.

#### Crosslinking-MS

Validation for this section is under development.

### Model quality ?

For models with atomic structures, molprobtity 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	99.95	12929.0

### Fit of model to data used for modeling ?

#### 3DEM volume

Validation for this section is under development.

#### 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.*