Integrative Structure Validation Report ?

July 22, 2024 - 04:15 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	9A0T
PDB-Dev ID	PDBDEV_00000065
Structure Title	Molecular architecture of the endocytic TPLATE/TSET complex
Structure Authors	Yperman K; Wang J; Eeckhout D; Winkler J; Vu LD; Vandorpe M; Grones P; Mylle E; Kraus M; Merceron R; Nolf J; Mor E; De Bruyn P; Loris R; Potocky M; Savvides SN; De Rybel B; De Jager G; Van Damme D; Pleskot R

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*

A user guide is available at 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

Model 1: 11105(99.89 %)

Number of violations
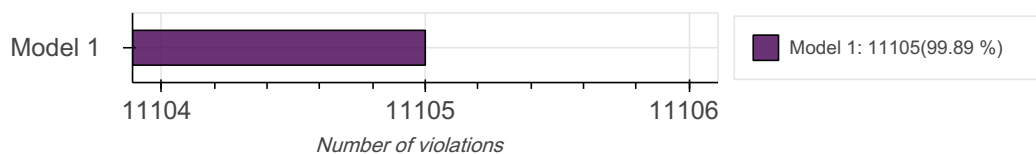
Ensemble information ⊙

This entry consists of 1 distinct ensemble(s).

Summary ⊙

This entry consists of 1 unique models, with 8 subunits in each model. A total of 28 datasets or restraints were used to build this entry. Each model is represented by 26 rigid bodies and 24 flexible or non-rigid units.

Entry composition⊙

There is 1 unique type of models in this entry. This model is titled Cluster 0 in state State_0/None.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	lol	A	A	147
1	2	2	tash3	B	B	1198
1	3	3	tplate	C	C	1176
1	4	4	tml	D	D	646
1	5	5	wd1	E	E	1592
1	6	6	wd2	F	F	1376
1	7	7	eh1	G	G	1019
1	8	8	eh2	H	H	1218

Datasets used for modeling ⊙

There are 28 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.3979550

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ID	Dataset type	Database name	Data access code
2	Comparative model	File	10.5281/zenodo.3979550
3	Comparative model	File	10.5281/zenodo.3979550
4	Comparative model	File	10.5281/zenodo.3979550
5	Comparative model	File	10.5281/zenodo.3979550
6	Comparative model	File	10.5281/zenodo.3979550
7	Comparative model	File	10.5281/zenodo.3979550
8	Comparative model	File	10.5281/zenodo.3979550
9	Comparative model	File	10.5281/zenodo.3979550
10	Comparative model	File	10.5281/zenodo.3979550
11	Comparative model	File	10.5281/zenodo.3979550
12	Comparative model	File	10.5281/zenodo.3979550
13	Comparative model	File	10.5281/zenodo.3979550
14	Comparative model	File	10.5281/zenodo.3979550
15	Crosslinking-MS data	PRIDE	PXD023051
16	Experimental model	PDB	5NZR
17	Experimental model	PDB	5MU7
18	Experimental model	PDB	6OWT
19	Experimental model	PDB	2KYM
20	Experimental model	PDB	2JKR
21	Experimental model	PDB	5JP2
22	Experimental model	PDB	5AWS
23	Experimental model	PDB	3G9H
24	Experimental model	PDB	3MKQ

ID	Dataset type	Database name	Data access code
25	Experimental model	PDB	3MKR
26	Experimental model	PDB	2YNP
27	Experimental model	PDB	6YEU
28	Experimental model	PDB	6YET

Representation ?

This entry has only one representation and includes 26 rigid bodies and 24 flexible units

Chain ID	Rigid bodies	Non-rigid segments
A	1-147	-
B	104-171, 205-258, 281-419, 464-499, 551-686, 716-734, 766-812, 1131-1198	1-103, 172-204, 259-280, 420-463, 500-550, 687-715, 735-765, 813-1130
C	1-467, 771-1045	468-770, 1046-1176
D	1-40, 96-191, 407-646	41-95, 192-406
E	18-349, 450-1002, 1303-1592	1-17, 350-449, 1003-1302
F	1-52, 125-534, 676-752, 771-974, 1012-1167	53-124, 535-675, 753-770, 975-1011, 1168-1376
G	1-110, 346-449	111-345, 450-1019
H	1-112, 400-512	113-399, 513-1218

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

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	1000000	False	True

There are 2 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	IMP PMI module	2.12.0	integrative model building	https://integrativemodeling.org
2	Integrative Modeling Platform (IMP)	2.12.0	integrative model building	https://integrativemodeling.org

Data quality ?

Crosslinking-MS

Validation for this section is under development.

Model quality ?

For models with atomic structures, molprobity 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	99.89	11105.0

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.