Full wwPDB Integrative Structure Validation Report

July 06, 2020 -- 10:19 PM

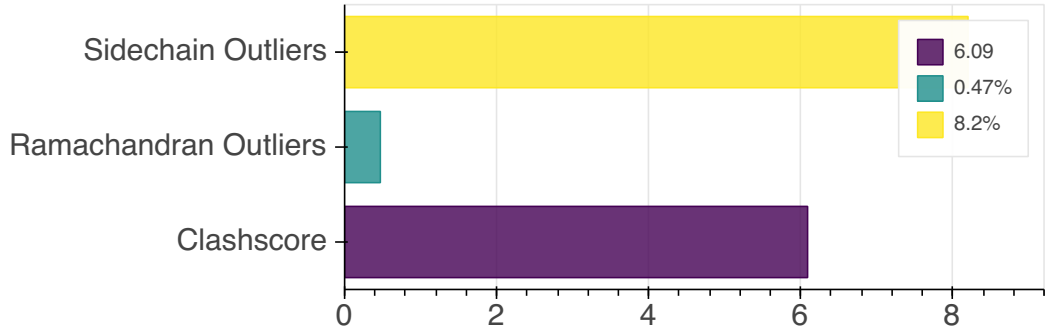
The following software were used in the production of this report:

Molprobity : Version 4.4
Integrative Modeling Validation Package : Version 1.0

PDB ID	PDBDEV_00000043
Molecule Name	Integrative Modeling of a Sin3/HDAC Complex Sub-structure
Title	Integrative Modeling of a Sin3/HDAC Complex Sub-structure
Authors	Banks CAS;Zhang Y;Miah S;Hao Y;Adams MK;Wen Z;Thornton JL;Florens L;Washburn MP

Overall quality

Model Quality: Molprobity Analysis



Ensemble information

This entry consists of 0 distinct ensemble.

Summary

This entry consists of 1 unique models, with 4 subunits in each model. A total of 10 datasets or restraints was used to build this entry. Each model is represented by 4 rigid bodies and 0 flexible or non-rigid units.

Entry composition

There is 1 unique type of model in this entry.This model is titled None/Best scoring model in cluster 1 respectively.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Total residues
1	1	1	SAP30L C terminal	A	90
1	2	2	SAP30L N terminal	B	68
1	3	3	SIN3A	C	122
1	4	4	HDAC1	D	369

Methodology and software

Step number	Protocol ID	Method name	Method type	Number of computed models	Multi state modeling	Multi scale modeling
1	1	comparative modeling	?	?	False	False
2	1	docking	?	200	False	False

Data quality

Model quality

Standard geometry

There are 1260 bond outliers in this entry.

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NZ--HZ3	1.037	0.89	52
NZ--HZ1	1.037	0.89	52
NZ--HZ2	1.036	0.89	52
NH1--HH12	0.998	0.86	43
NH2--HH21	1.001	0.86	43
NH1--HH11	0.999	0.86	43
NH2--HH22	1.0	0.86	43
OH--HH	0.961	0.84	37
OG--HG	0.959	0.84	36
OG1--HG1	0.961	0.84	26
ND1--HD1	0.984	0.86	4
NE2--HE2	0.979	0.86	15
NE--HE	0.983	0.86	43
SG--HG	1.326	1.2	12
ND2--HD22	0.978	0.86	32
N--H	0.976	0.86	622
ND2--HD21	0.978	0.86	32
NE2--HE22	0.978	0.86	25
NE2--HE21	0.977	0.86	25
NE1--HE1	0.979	0.86	3

There are 0 angle outliers in this entry.

Too-close contacts

The following all-atom clashscore is based on a MolProbity analysis. All-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The table below contains clashscores for all the models in this entry.

Model ID	Clash score	Number of clashes
Model 1	6.09	64

All 64 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Torsion angles: Protein backbone

In the following table, Ramachandran outliers are listed. The Analysed column shows the number of residues for which the backbone conformation was analysed.

Model ID	Analyzed	Favored	Allowed	Outliers
1	641	599	39	3

Detailed list of outliers are tabulated below.

Model ID	Chain and res ID	Residue type
1	A:106	ILE
1	A:177	GLU
1	C:614	ASP

Torsion angles: Protein sidechains

In the following table, sidechain outliers are listed. The Analysed column shows the number of residues for which the sidechain conformation was analysed.

Model ID	Analyzed	Favored	Allowed	Outliers
1	573	474	52	47

Detailed list of outliers are tabulated below.

Model ID	Chain and res ID	Residue type
1	A:92	THR
1	A:95	ASP

Model ID	Chain and res ID	Residue type
1	A:103	ASP
1	A:104	THR
1	A:105	ASP
1	A:130	THR
1	A:171	ARG
1	A:173	ASP
1	A:176	SER
1	B:28	SER
1	B:37	ARG
1	B:58	LYS
1	B:64	ILE
1	B:67	SER
1	B:77	HIS
1	B:87	LYS
1	B:89	LYS
1	C:612	CYS
1	C:613	GLU
1	C:623	LEU
1	C:638	LYS
1	C:656	THR
1	C:660	THR
1	C:661	SER
1	C:679	ASP

Model ID	Chain and res ID	Residue type
1	C:728	SER
1	D:21	ASN
1	D:45	TYR
1	D:85	SER
1	D:88	SER
1	D:98	GLU
1	D:124	LEU
1	D:141	HIS
1	D:185	GLU
1	D:189	THR
1	D:195	THR
1	D:204	TYR
1	D:208	THR
1	D:233	ASP
1	D:245	MET
1	D:255	SER
1	D:263	SER
1	D:265	SER
1	D:321	ASP
1	D:346	SER
1	D:351	THR
1	D:355	THR

Fit of model to data used for modeling

Fit of model to data not used for modeling

Uncertainty of data and model