Full wwPDB Integrative Structure Validation Report

December 11, 2019 -- 11:33 PM

PDB ID	*PDBDEV00000009*
Molecule Name	Structure of the human Rev7 dimer
Title	Rev7 dimerization is important for assembly and function of the Rev1/Pol translesion synthesis complex
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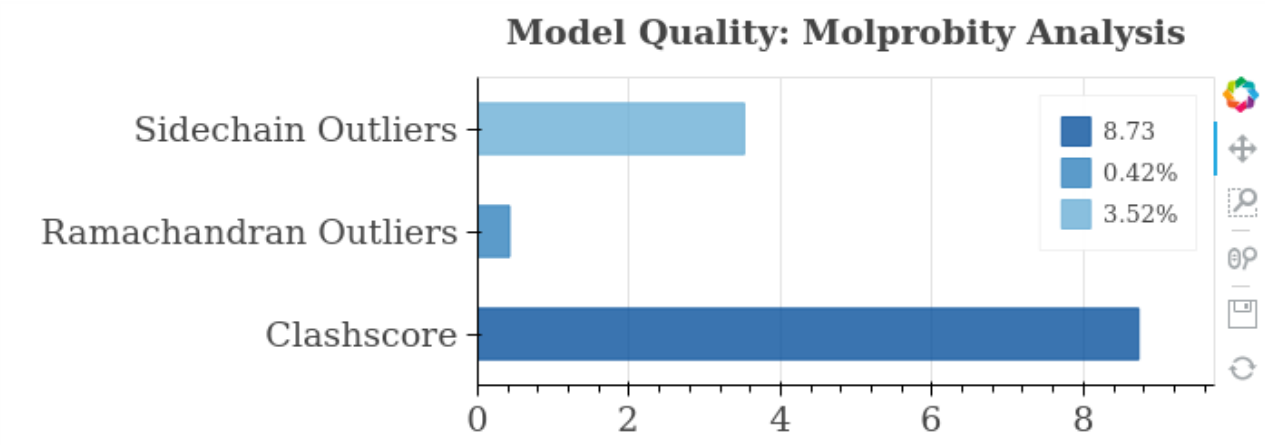
The following software were used in the production of this report:

Molprobity : Version 4.4
Integrative Modeling Validation Package : Version 1.0

1. Overall quality at a glance



2. Ensemble information

This entry consists of 0 distinct ensemble.

3. Model composition

3.1 Summary

This entry consists of 1 unique models, with 4 subunits in each model. A total of 3 datasets or restraints was used to build this entry. Each model is represented by 0 rigid bodies and 4 flexible or non-rigid units.

3.2 Entry composition

There is 1 unique type of model in this entry.This model is titled None/Best scoring model, N/C-termini built respectively.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Total residues
1	1	1	Rev7-monomer	A	212
1	2	1	Rev7-monomer	C	212
1	3	2	Rev3-RBM2	B	28
1	4	2	Rev3-RBM2	D	28

3.3 Datasets used for modeling

There are 3 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	SAS data	SASBDB	SASDC29
2	Experimental model	PDB	6BC8
3	Mutagenesis data	Not listed	None

4. Representation

This entry has only one representation and includes 0 rigid bodies and 4 flexible units.

Chain ID	Rigid bodies	Non-rigid segments
A	-	1-212.
B	-	1-28.
C	-	1-212.

D	-	1-28.

5. Methodology and software

Step number	Protocol ID	Method name	Method type	Number of computed models	Multi state modeling	Multi scale modeling
1	1	None	None	None	False	False

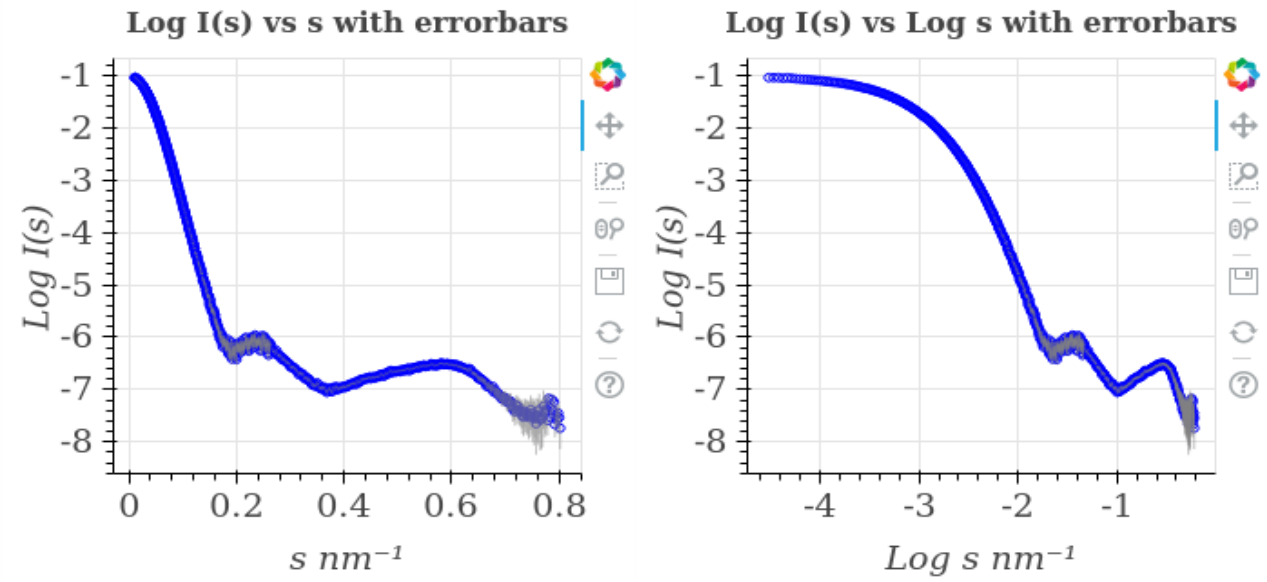
Software packages used for modeling were either not reported or not used.

6. Data quality

6.1 Analysis of SAXS data used in this entry

6.1.1 Intensity plots

SAXS data was obtained from deposited SASBDB entry: SASDC29. Below are plots of intentisities, for further information, refer to entry on SASBDB.



6.1.2. Key experimental estimates

Molecular weight (MW) estimates from experiments and analysis.

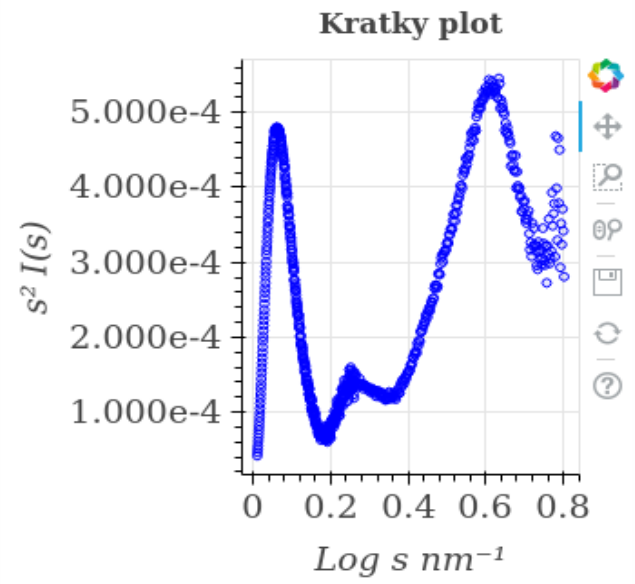
Molecule MW	Experimental MW	Porod MW	Guinier MW
48.782	53.400	63.800	53.400

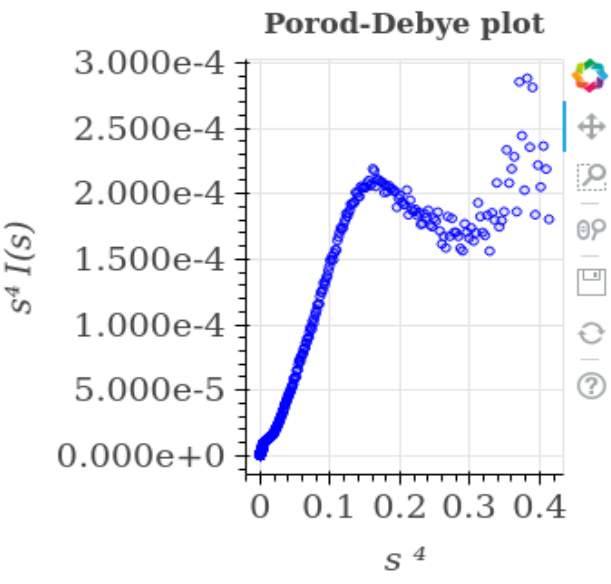
Volume estimates from experiments and analysis.

Estimated volume	Estimated volume method	Porod volume
None	None	108.40 nmÂ³

6.1.3. Flexibility analysis

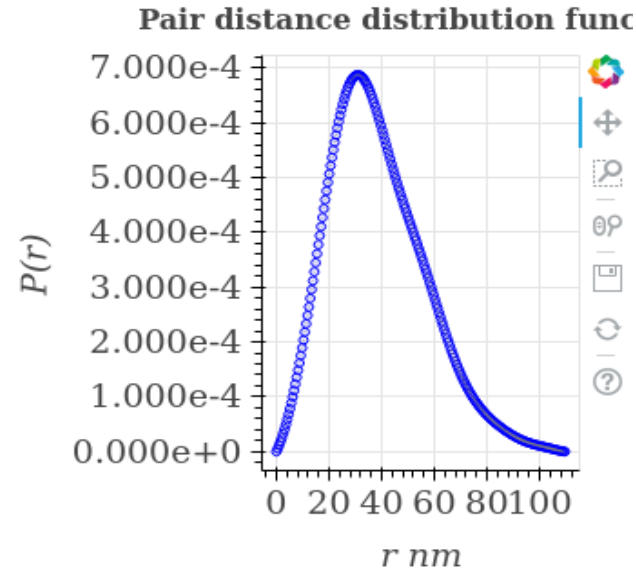
Flexibility is assessed by Kratky and Porod-Debye plots. For details, refer to Rambo and Tainer,2011.





6.1.4. Pair-distance distribution analysis

Pair-distance distribution was evaluated using ATSAS software. The analysis resulted in a D_{max} of 11nm and a radius of gyration of 3.01nm



7. Model quality

7.1 Standard geometry

There are 123 bond outliers in this entry.

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
N--H	1.079	0.86	13
NE2--HE2	1.03	0.86	1
CD2--HD2	1.086	0.93	1
CE1--HE1	1.082	0.93	1
CB--HB	1.111	0.97	1
CE--HE3	1.102	0.97	5
CB--HB2	1.106	0.97	11
CB--HB3	1.106	0.97	11
CE--HE2	1.104	0.97	5
CD--HD2	1.109	0.97	1
CG--HG2	1.102	0.97	7
NZ--HZ1	1.027	0.89	1
CA--HA2	1.105	0.97	3
CD--HD3	1.106	0.97	1
CA--HA	1.102	0.97	13
CG2--HG23	1.106	0.97	1
CG--HG3	1.102	0.97	7
CG2--HG21	1.106	0.97	1
CE--HE1	1.105	0.97	3
CG2--HG22	1.105	0.97	1
NZ--HZ2	1.025	0.89	1
N--H1	1.08	0.96	3
OG--HG	0.961	0.84	1
OG1--HG1	0.96	0.84	1
NZ--HZ3	1.009	0.89	1
CA--HA3	1.05	0.97	2

There are 14 angle outliers in this entry.

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-N-H	126.774	114.0	13

7.2 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	8.73	69

All 69 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

7.3 Torsion angles

7.3.1 Protein backbone

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

Model ID	Analyzed	Favored	Allowed	Outliers
1	482	472	8	2

Detailed list of outliers are tabulated below.

Model ID	Chain and res ID	Residue type
1	A:110	ILE
1	C:110	ILE

7.3.2 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	454	416	22	16

Detailed list of outliers are tabulated below.

Model ID	Chain and res ID	Residue type
1	A:3	THR
1	A:110	ILE
1	A:120	GLU
1	A:158	ARG
1	A:168	ASP
1	A:208	HIS
1	B1990	LYS
1	B2011	GLN
1	C:3	THR
1	C:110	ILE
1	C:120	GLU
1	C:158	ARG
1	C:168	ASP
1	C:208	HIS
1	D1990	LYS
1	D2011	GLN

8. Fit of model to data used for modeling

8.1 Fit of model to SAS data

This entry has 1 distinct model fits.

9. Fit of model to data not used for modeling

10. Uncertainty of model