Full wwPDB Integrative Structure Validation Report

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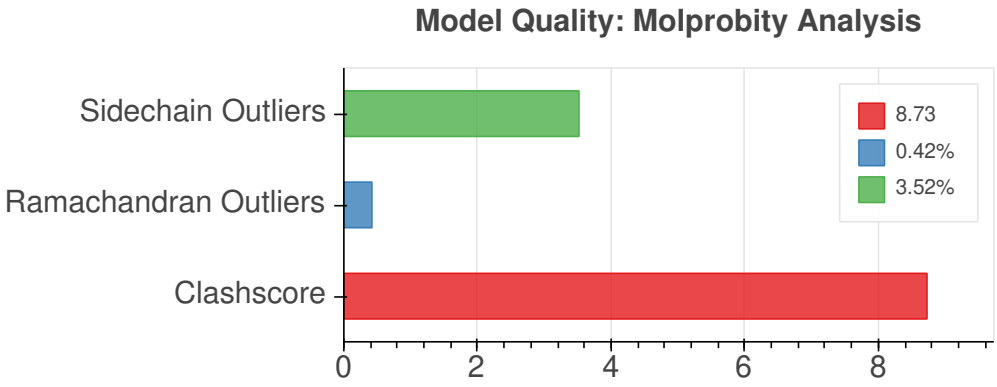
The following software were used in the production of this report:

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

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

6. Data quality

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	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

9. Fit of model to data not used for modeling

10. Uncertainty of model