

Full wwPDB Integrative Structure Validation Report

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PDB ID	PDBDEV00000003
Molecule Name	Molecular architecture of the yeast Mediator complex
Title	Molecular architecture of the yeast Mediator complex.
Authors	Robinson PJ;Trnka MJ;Pellarin R;Greenberg CH;Bushnell DA;Davis R;Burlingame AL;Sali A;Kornberg

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

Integrative Modeling Package : Version XX
Molprobit : Version XX
Phenix : Version XX
Integrative Modeling Validation Package : Version XX

1. Overall quality at a glance

2. Entry composition

There are 1 unique types of models in this entry. The entry contains 37 chains.

Molecule ID	Molecule Name	Chain ID	Total Residues
1	med6	A	295
1	med8	B	223
1	med11	C	115
1	med17	D	687
1	med18	E	307
1	med20	F	210
1	med22	G	121
1	med4	H	284
1	med7	I	222
1	med9	J	149
1	med31	K	127
1	med21	I	140

ID	Model ID	Label	Count
1	med10	M	157
1	med1	N	566
1	med14	O	1082
1	med19	P	220
1	med2	Q	436
1	med3	R	401
1	med5	S	1146
1	med15	T	1094
1	med16	U	986

There are 5 software packages reported in this entry.

ID	Software Name	Software Version	Software Classification
1	Integrative Modeling Platform (IMP)	develop-0a5706e202	integrative model building
2	IMP PMI module	67456c0	integrative model building
3	Protein Prospector	5.13.1	mass spectrometry
4	Situs	2.7	density map fitting
5	Phyre2	2.0	protein homology modeling

There are 16 unique datasets used to build the model(s) in this entry.

ID	Dataset Type	Database Name	Data Access Code
1	Experimental model	PDB	4GWP
2	Comparative model	Not Listed	None
3	Comparative model	Not Listed	None
4	Experimental model	PDB	3FBI
5	Experimental model	Not Listed	None
6	Experimental model	PDB	1YKH
7	Experimental model	Not Listed	None
8	Experimental model	PDB	4BZK
9	Comparative model	Not Listed	None
10	Mass Spectrometry data	MASSIVE	MSV000079237

11	CX-MS data	Not Listed	None
12	3DEM volume	EMDB	EMD-2634
13	3DEM volume	Not Listed	None
14	3DEM volume	Not Listed	None
15	3DEM volume	Not Listed	None
16	3DEM volume	Not Listed	None

3. Data quality

4. Model quality

4.1 Too-close contacts

4.2 Torsion angles

4.2.1 Protein backbone

4.2.2 Protein sidechains

5. Fit of model and data

6. Uncertainty of model
