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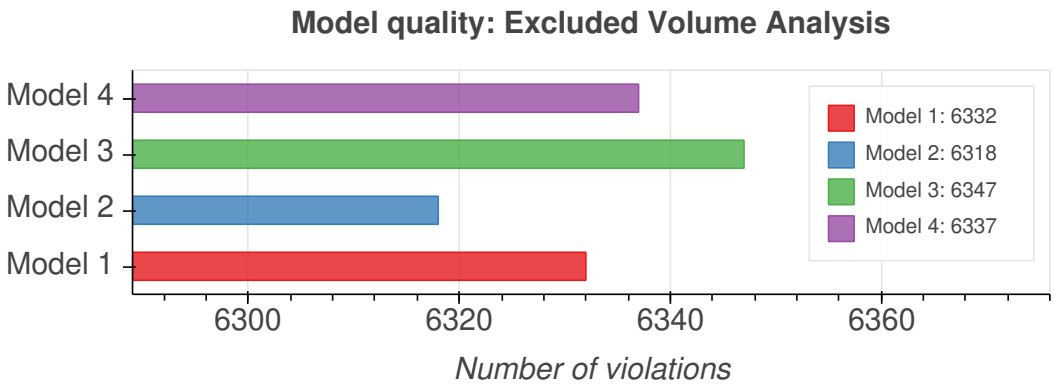
The following software were used in the production of this report:

Integrative Modeling Validation Package : Version 1.0

1. Overall quality at a glance



2. Ensemble information

This entry consists of 4 distinct ensembles.

Ensemble number	*Ensemble name*	*Model ID*	*Number of models*	*Clustering method*	*Clustering feature*	*Cluster precision*

1	Cluster 1	1	142	None	RMSD	19.519
2	Cluster 2	2	192	None	RMSD	21.833
3	Cluster 3	3	39	None	RMSD	25.289
4	Cluster 4	4	126	None	RMSD	21.061

3. Model composition

3.1 Summary

This entry consists of 4 unique models, with 21 subunits in each model. A total of 16 datasets or restraints was used to build this entry. Each model is represented by 12 rigid bodies and 50 flexible or non-rigid units.

3.2 Entry composition

There are 4 unique types of models in this entry.These models are titled Cluster 1/Best scoring model, Cluster 2/Best scoring model, Cluster 3/Best scoring model, Cluster 4/Best scoring model respectively.

Model ID	***Subunit number***	***Subunit ID***	***Subunit name***	***Chain ID***	***Total residues***
1	1	1	med6	A	295
1	2	2	med8	B	223
1	3	3	med11	C	115
1	4	4	med17	D	687
1	5	5	med18	E	307
1	6	6	med20	F	210
1	7	7	med22	G	121
1	8	8	med4	H	284
1	9	9	med7	I	222
1	10	10	med9	J	149
1	11	11	med31	K	127
1	12	12	med21	L	140
1	13	13	med10	M	157
1	14	14	med1	N	566
1	15	15	med14	O	1082

1	16	16	med19	P	220
1	17	17	med2	Q	436
1	18	18	med3	R	401
1	19	19	med5	S	1146
1	20	20	med15	T	1094
1	21	21	med16	U	986
2	1	1	med6	A	295
2	2	2	med8	B	223
2	3	3	med11	C	115
2	4	4	med17	D	687
2	5	5	med18	E	307
2	6	6	med20	F	210
2	7	7	med22	G	121
2	8	8	med4	H	284
2	9	9	med7	I	222
2	10	10	med9	J	149
2	11	11	med31	K	127
2	12	12	med21	L	140
2	13	13	med10	M	157
2	14	14	med1	N	566
2	15	15	med14	O	1082
2	16	16	med19	P	220
2	17	17	med2	Q	436
2	18	18	med3	R	401
2	19	19	med5	S	1146
2	20	20	med15	T	1094
2	21	21	med16	U	986

3	1	1	med6	A	295
3	2	2	med8	B	223
3	3	3	med11	C	115
3	4	4	med17	D	687
3	5	5	med18	E	307
3	6	6	med20	F	210
3	7	7	med22	G	121
3	8	8	med4	H	284
3	9	9	med7	I	222
3	10	10	med9	J	149
3	11	11	med31	K	127
3	12	12	med21	L	140
3	13	13	med10	M	157
3	14	14	med1	N	566
3	15	15	med14	O	1082
3	16	16	med19	P	220
3	17	17	med2	Q	436
3	18	18	med3	R	401
3	19	19	med5	S	1146
3	20	20	med15	T	1094
3	21	21	med16	U	986
4	1	1	med6	A	295
4	2	2	med8	B	223
4	3	3	med11	C	115
4	4	4	med17	D	687
4	5	5	med18	E	307
4	6	6	med20	F	210

4	7	7	med22	G	121
4	8	8	med4	H	284
4	9	9	med7	I	222
4	10	10	med9	J	149
4	11	11	med31	K	127
4	12	12	med21	L	140
4	13	13	med10	M	157
4	14	14	med1	N	566
4	15	15	med14	O	1082
4	16	16	med19	P	220
4	17	17	med2	Q	436
4	18	18	med3	R	401
4	19	19	med5	S	1146
4	20	20	med15	T	1094
4	21	21	med16	U	986

3.3 Datasets used for modeling

There are 16 unique datasets used to build the models 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

4. Representation

This entry has only one representation and includes 12 rigid bodies and 50 flexible units.

Chain ID	***Rigid bodies***	***Non-rigid segments***
A	-	1-60, 61-82, 83-192, 193-295.
B	-	1-22, 23-173, 174-181, 182-214, 215-223.
C	-	1-3, 4-115.
D	-	123-181, 182-371, 372-377, 378-661, 662-669, 670-687, 1-122.
E	-	1-1, 2-110, 111-157, 158-301, 302-307.
F	-	1-1, 2-210.
G	-	1-121.
H	37-127:Comparative model/None.	1-36, 128-284.
I	12-84:Experimental model/None, 112-206:Experimental model/None.	1-11, 85-111, 207-222.
J	65-149:Comparative model/None.	1-64.
K	19-110:Experimental model/None.	1-18, 111-127.

L	2-128:Experimental model/None.	1-1, 129-140.
M	-	1-157.
N	-	1-566.
O	-	1-1082.
P	-	1-220.
Q	-	1-436.
R	-	1-401.
S	-	1-1146.
T	-	1-1094.
U	8-49:Comparative model/None, 94-150:Comparative model/None, 165-174:Comparative model/None, 231-406:Comparative model/None, 437-476:Comparative model/None, 503-538:Comparative model/None.	50-93, 151-164, 175-230, 407-436, 477-502, 539-986.

5. Methodology and software

Step number	*Protocol ID*	*Method name*	*Method type*	*Number of computed models*	*Multi state modeling*	*Multi scale modeling*
1	1	Replica exchange monte carlo	Sampling	20000	False	True

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

6. Data quality

7. Model quality

7.1 Excluded volume satisfaction

Excluded volume satisfaction for the models in the entry are listed below.

Models	***Excluded Volume Satisfaction***	***Number of violations***
1	99.83	6332
2	99.83	6318
3	99.83	6347
4	99.83	6337

8. Fit of model to data used for modeling

9. Fit of model to data not used for modeling

10. Uncertainty of model