



Full wwPDB Integrative Structure Validation Report

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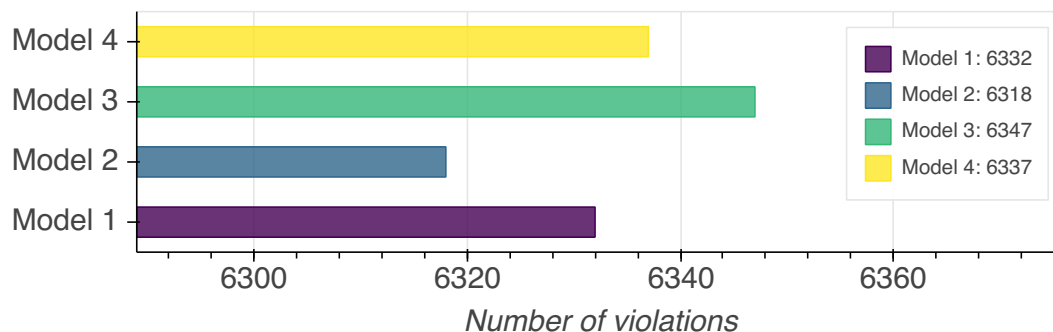
The following software were used in the production of this report:

Integrative Modeling Validation Package : Version 1.0

PDB ID	PDBDEV_00000003
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 RD

Overall quality

Model quality: Excluded Volume Analysis



Ensemble information

This entry consists of 4 distinct ensembles.

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

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Total residues
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

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Total residues
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
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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

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Total residues
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

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

Data quality

Model quality

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	6332.0
2	99.83	6318.0
3	99.83	6347.0
4	99.83	6337.0

Fit of model to data used for modeling

Fit of model to data not used for modeling

Uncertainty of data and model