Integrative Structure Validation Report ?

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

Python-IHM Version 1.3
Integrative Modeling Validation Version 1.2

PDB ID	8ZZ3
PDB-Dev ID	PDBDEV_00000003
Structure Title	Molecular architecture of the yeast Mediator complex
Structure Authors	Robinson PJ; Trnka MJ; Pellarin R; Greenberg CH; Bushnell DA; Davis R; Burlingame AL; Sali A; Kornberg RD

Overall quality ?

This validation report contains model quality assessments for all structures, data quality assessment for SAS datasets and fit to model assessments for SAS datasets. Data quality and fit to model assessments for other datasets and model uncertainty are under development. Number of plots is limited to 256.

Model Quality: Excluded Volume Analysis

Model 1 — [bar] Model 1: 6332(99.83 %)

6320   6340

Number of violations
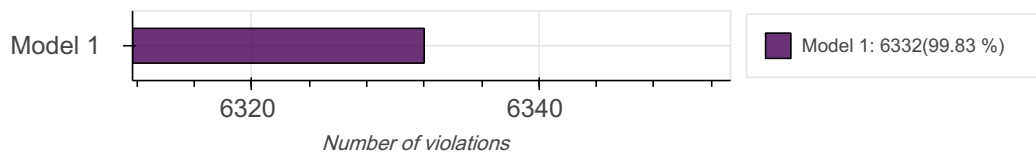
Ensemble information ⓘ

This entry consists of 4 distinct ensemble(s).

Summary ⓘ

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

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	Chain ID [auth]	Total residues
1	1	1	med6	A	A	295
1	2	2	med8	B	B	223
1	3	3	med11	C	C	115
1	4	4	med17	D	D	687
1	5	5	med18	E	E	307
1	6	6	med20	F	F	210
1	7	7	med22	G	G	121

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

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

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

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
4	13	13	med10	M	M	157
4	14	14	med1	N	N	566
4	15	15	med14	O	O	1082
4	16	16	med19	P	P	220
4	17	17	med2	Q	Q	436
4	18	18	med3	R	R	401
4	19	19	med5	S	S	1146
4	20	20	med15	T	T	1094
4	21	21	med16	U	U	986

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	File	10.1093/nar/gkt704
3	Comparative model	File	10.5281/zenodo.802915
4	Experimental model	PDB	3FBI
5	Experimental model	File	10.5281/zenodo.802915
6	Experimental model	PDB	1YKH
7	Experimental model	File	10.5281/zenodo.802915
8	Experimental model	PDB	4BZK
9	Comparative model	File	10.5281/zenodo.802915
10	Mass Spectrometry data	MASSIVE	MSV000079237

ID	Dataset type	Database name	Data access code
11	Crosslinking-MS data	File	10.5281/zenodo.802915
12	3DEM volume	EMDB	EMD-2634
13	3DEM volume	File	10.5281/zenodo.802915
14	3DEM volume	File	10.5281/zenodo.802915
15	3DEM volume	File	10.5281/zenodo.802915
16	3DEM volume	File	10.5281/zenodo.802915

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	1-36, 128-284
I	12-84, 112-206	1-11, 85-111, 207-222
J	65-149	1-64
K	19-110	1-18, 111-127
L	2-128	1-1, 129-140

Chain ID	Rigid bodies	Non-rigid segments
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, 94-150, 165-174, 231-406, 437-476, 503-538	50-93, 151-164, 175-230, 407-436, 477-502, 539-986

Methodology and software ?

This entry is a result of 1 distinct protocol(s).

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
1	1	Replica exchange monte carlo	Sampling	None	20000	False	True

There are 5 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	Integrative Modeling Platform (IMP)	develop-0a5706e202	integrative model building	https://integrativemodeling.org
2	IMP PMI module	67456c0	integrative model building	https://integrativemodeling.org
3	Protein Prospector	5.13.1	mass spectrometry	http://prospector.ucsf.edu/

ID	Software name	Software version	Software classification	Software location
4	Situs	2.7	density map fitting	http://situs.biomachina.org/
5	Phyre2	2.0	protein homology modeling	http://www.sbg.bio.ic.ac.uk/~phyre2/

Data quality ?

Crosslinking-MS

Validation for this section is under development.

Mass Spectrometry

Validation for this section is under development.

3DEM volume

Validation for this section is under development.

Model quality ?

For models with atomic structures, molprobity analysis is performed. For models with coarse-grained or multi-scale structures, excluded volume analysis is performed.

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 ?

Crosslinking-MS

Validation for this section is under development.

IM Structure Validation Report

Mass Spectrometry

Validation for this section is under development.

3DEM volume

Validation for this section is under development.

Fit of model to data used for validation ❓

Validation for this section is under development.