



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Dec 10, 2019 – 05:31 PM EST

PDB ID : 6ORB
EMDB ID: : EMD-9036
Title : Full-length S. pombe Mdn1 in the presence of ATP and Rbin-1
Authors : Chen, Z.; Suzuki, H.; Wang, A.C.; DiMaio, F.; Walz, T.; Kapoor, T.M.
Deposited on : 2019-04-29
Resolution : 7.70 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

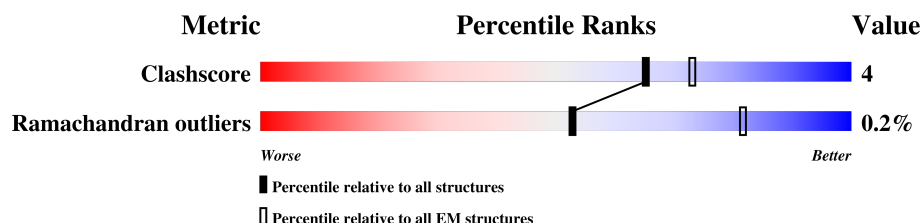
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	4717	 67% • 29%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 16655 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Midasin.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	A	3352	16655	9951	3352	3352	0	0

WORLDWIDE
PDB
PROTEIN DATA BANK

 **EMDataBank**
Unified Data Resource for 3DEM

LEU	GLU	SER
GLU	LYS	ILE
PRO	VAL	ASP
THR	PHE	ARG
LEU	LEU	ASP
ALA	LEU	GLU
THR	SER	SER
LYS	GLU	ALA
MET	ASP	ASN
GLN	GLU	ASN
GLY	ASP	ASN
ASP	ILE	PRO
PHE	GLU	ASP
ARG	ASP	SER
THR	GLU	MET
LYS	LEU	ASN
LYS	PRO	SER
ARG	ASP	THR
LEU	TYR	ASN
ASN	ASN	ILE
MET	VAL	ALA
LYS	VAL	GLU
ARG	ILE	ASP
ILE	THR	GLU
ILE	ASN	ALA
PRO	LEU	ASP
TYR	PRO	GLU
ILE	ALA	VAL
ALA	ALA	GLY
SER	MET	ASP
GLN	PRO	LYS
PHE	ILE	GLN
LYS	ASP	LEU
LYS	GLU	GLN
ASP	ALA	ASP
LYS	ARG	GLY
ILE	ASP	GLN
TRP	LEU	ASP
MET	TRP	ILE
ARG	ASN	SER
ARG	LYS	ASP
VAL	HIS	ILE
LYS	GLU	LYS
P4499	ASP	GLN
T4528	SER	THR
L4529	THR	GLY
F4577	LYS	GLU
E4578	GLN	ASP
D4619	LEU	THR
L4647	SER	LEU
V4650	ILE	PRO
Q4653	GLU	THR
S4656	GLY	PHE
	GLN	GLY
	LEU	SER
	ILE	ILE
	ARG	ASN
	LEU	GLN
	ILE	SER

Q4712	THR
GLN	
MET	
SER	
ASN	
THR	

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	54557	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	66.7	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	28000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	A	0.37	0/16570	0.51	0/22999

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	16655	0	7216	107	0
All	All	16655	0	7216	107	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (107) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:SER:CB	1:A:2122:PRO:HA	1.68	1.21
1:A:1229:ILE:O	1:A:1302:ALA:HB3	1.69	0.91
1:A:2059:VAL:O	1:A:2071:THR:HA	1.75	0.85
1:A:50:ALA:O	1:A:55:ARG:CB	2.26	0.83
1:A:1659:ALA:HA	1:A:1666:LYS:CB	2.10	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2222:PHE:O	1:A:2226:TYR:CB	2.28	0.80
1:A:4619:ASP:HA	1:A:4647:LEU:CB	2.14	0.78
1:A:3433:ILE:CB	1:A:3839:LYS:CB	2.64	0.76
1:A:2221:ARG:O	1:A:2225:ILE:CB	2.36	0.74
1:A:1659:ALA:C	1:A:1665:ASP:O	2.28	0.72
1:A:4619:ASP:HA	1:A:4647:LEU:H	1.57	0.69
1:A:4619:ASP:CB	1:A:4647:LEU:CB	2.72	0.67
1:A:4619:ASP:CA	1:A:4647:LEU:CB	2.74	0.65
1:A:3433:ILE:CB	1:A:3839:LYS:O	2.44	0.65
1:A:1311:ASP:O	1:A:1357:PHE:HA	1.97	0.65
1:A:1229:ILE:O	1:A:1302:ALA:CB	2.43	0.65
1:A:4619:ASP:HA	1:A:4647:LEU:N	2.12	0.64
1:A:1887:ARG:O	1:A:1891:ALA:HB2	1.98	0.62
1:A:1483:LEU:O	1:A:1487:ARG:N	2.34	0.61
1:A:1489:ARG:O	1:A:1492:ALA:HB3	2.01	0.61
1:A:81:SER:CB	1:A:2122:PRO:CA	2.63	0.60
1:A:1660:TYR:N	1:A:1665:ASP:O	2.36	0.59
1:A:2356:ILE:O	1:A:2360:THR:N	2.36	0.59
1:A:1482:SER:O	1:A:1485:ALA:HB3	2.04	0.58
1:A:2168:SER:O	1:A:2172:LEU:N	2.37	0.58
1:A:3736:GLU:O	1:A:3740:CYS:N	2.37	0.57
1:A:2918:LEU:O	1:A:2922:LEU:N	2.37	0.57
1:A:3106:VAL:O	1:A:3110:GLY:N	2.37	0.57
1:A:1658:GLU:O	1:A:1666:LYS:CB	2.53	0.56
1:A:3682:GLY:O	1:A:3686:SER:N	2.38	0.56
1:A:192:LYS:O	1:A:196:GLY:N	2.39	0.55
1:A:1228:ILE:HA	1:A:1231:ALA:O	2.05	0.55
1:A:3432:GLU:O	1:A:3436:LEU:N	2.39	0.55
1:A:3061:ASN:O	1:A:3065:SER:N	2.36	0.55
1:A:3532:ASN:O	1:A:3536:LEU:N	2.38	0.55
1:A:1862:VAL:O	1:A:1866:ILE:N	2.39	0.55
1:A:1377:ALA:O	1:A:1381:ARG:N	2.39	0.55
1:A:1112:MET:O	1:A:1116:GLU:N	2.37	0.54
1:A:1229:ILE:O	1:A:1302:ALA:N	2.41	0.54
1:A:1303:LEU:O	1:A:1307:MET:N	2.41	0.53
1:A:2536:THR:O	1:A:2539:PHE:CB	2.56	0.53
1:A:2221:ARG:O	1:A:2225:ILE:N	2.34	0.53
1:A:2210:ASP:O	1:A:2214:HIS:N	2.40	0.52
1:A:2951:ASP:O	1:A:2955:PHE:N	2.42	0.50
1:A:821:ASN:O	1:A:825:ARG:CB	2.60	0.50
1:A:1491:PHE:O	1:A:1495:ASN:N	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1590:ILE:N	1:A:1634:LEU:O	2.45	0.50
1:A:78:GLU:HA	1:A:2122:PRO:O	2.11	0.50
1:A:1488:GLN:O	1:A:1492:ALA:N	2.40	0.49
1:A:642:VAL:N	1:A:687:ARG:O	2.44	0.49
1:A:1588:VAL:O	1:A:1634:LEU:N	2.45	0.49
1:A:224:LEU:HA	1:A:266:PHE:O	2.12	0.49
1:A:2705:ILE:O	1:A:2709:ARG:N	2.41	0.49
1:A:2933:SER:O	1:A:2937:VAL:N	2.43	0.49
1:A:164:GLY:O	1:A:168:LEU:N	2.43	0.49
1:A:3:VAL:O	1:A:6:GLU:CB	2.61	0.48
1:A:3268:PHE:O	1:A:3272:ASN:N	2.45	0.48
1:A:3726:TYR:O	1:A:3730:LYS:N	2.46	0.48
1:A:1094:ARG:O	1:A:1098:ARG:CB	2.62	0.48
1:A:1709:LYS:O	1:A:1713:MET:N	2.45	0.47
1:A:1887:ARG:O	1:A:1891:ALA:CB	2.62	0.47
1:A:3303:SER:O	1:A:3307:ALA:HB2	2.15	0.47
1:A:3198:GLU:O	1:A:3202:LEU:CB	2.62	0.47
1:A:398:VAL:O	1:A:402:LEU:N	2.46	0.47
1:A:2240:GLN:O	1:A:2244:ASP:CB	2.62	0.47
1:A:2606:SER:O	1:A:2610:PHE:N	2.47	0.47
1:A:1949:PHE:O	1:A:1953:SER:N	2.45	0.46
1:A:2910:GLU:O	1:A:2914:ILE:N	2.43	0.46
1:A:1220:HIS:CB	1:A:1644:SER:CB	2.93	0.46
1:A:1487:ARG:O	1:A:1491:PHE:N	2.39	0.46
1:A:306:ILE:O	1:A:310:THR:N	2.44	0.46
1:A:4619:ASP:HA	1:A:4647:LEU:CA	2.44	0.46
1:A:634:LYS:O	1:A:638:SER:CB	2.63	0.46
1:A:1323:ASP:O	1:A:1327:GLU:N	2.48	0.46
1:A:1625:ALA:O	1:A:1629:ASN:N	2.45	0.46
1:A:1660:TYR:O	1:A:1665:ASP:O	2.34	0.45
1:A:3041:GLU:O	1:A:3045:GLU:N	2.46	0.45
1:A:487:LEU:O	1:A:492:GLY:N	2.50	0.45
1:A:1301:GLY:O	1:A:1305:THR:N	2.40	0.45
1:A:2223:MET:O	1:A:2227:GLU:CB	2.65	0.45
1:A:3691:LEU:O	1:A:3695:LYS:N	2.50	0.45
1:A:52:ASP:O	1:A:55:ARG:N	2.50	0.45
1:A:3679:GLN:O	1:A:3683:HIS:N	2.41	0.45
1:A:2588:LEU:O	1:A:2592:ALA:N	2.42	0.44
1:A:4653:GLN:O	1:A:4656:SER:N	2.51	0.44
1:A:1492:ALA:O	1:A:1496:GLU:N	2.41	0.44
1:A:1659:ALA:CA	1:A:1665:ASP:O	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4577:PHE:O	1:A:4578:GLU:C	2.55	0.44
1:A:2827:GLU:O	1:A:2831:LYS:CB	2.66	0.44
1:A:1572:LYS:O	1:A:1576:ILE:N	2.51	0.44
1:A:148:TYR:O	1:A:152:LYS:N	2.48	0.43
1:A:2417:ALA:O	1:A:2421:LYS:N	2.52	0.43
1:A:917:LYS:O	1:A:919:GLY:N	2.48	0.43
1:A:1565:GLU:N	1:A:1703:VAL:O	2.43	0.43
1:A:295:GLU:O	1:A:299:THR:N	2.52	0.42
1:A:3433:ILE:CB	1:A:3839:LYS:C	2.88	0.42
1:A:3723:LEU:O	1:A:3727:CYS:N	2.42	0.42
1:A:991:LEU:H	1:A:999:LEU:HA	1.85	0.41
1:A:3432:GLU:O	1:A:3436:LEU:CB	2.68	0.41
1:A:53:GLU:O	1:A:57:THR:CB	2.69	0.41
1:A:494:LYS:O	1:A:641:TRP:N	2.42	0.41
1:A:2591:ILE:O	1:A:2595:PHE:N	2.54	0.41
1:A:3803:ILE:O	1:A:3807:SER:N	2.47	0.41
1:A:1659:ALA:HA	1:A:1666:LYS:CA	2.51	0.41
1:A:832:ASN:O	1:A:836:GLN:N	2.46	0.40
1:A:1627:MET:O	1:A:1671:HIS:CB	2.69	0.40
1:A:4528:THR:O	1:A:4529:LEU:C	2.58	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	3182/4717 (68%)	2781 (87%)	396 (12%)	5 (0%)	49 85

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2073	LYS

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Mol	Chain	Res	Type
1	A	2232	LEU
1	A	1408	LYS
1	A	2075	HIS
1	A	4650	VAL

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.