



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 04:28 PM BST

PDB ID : 1S2H  
Title : The Mad2 spindle checkpoint protein possesses two distinct natively folded states  
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Deposited on : 2004-01-08

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : rb-20027457  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027457

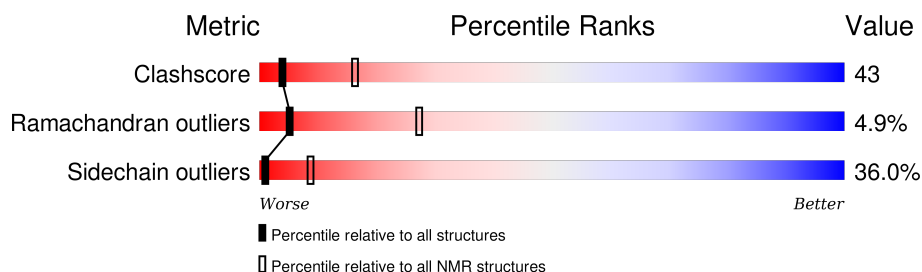
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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	206	<div> <div>36%</div> <div>40%</div> <div>23%</div> </div>

## 2 Ensemble composition and analysis ⓘ

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3320 atoms, of which 1670 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Mitotic spindle assembly checkpoint protein MAD2A.

Mol	Chain	Residues	Atoms						Trace
1	A	205	Total	C	H	N	O	S	0
			3320	1056	1670	268	321	5	

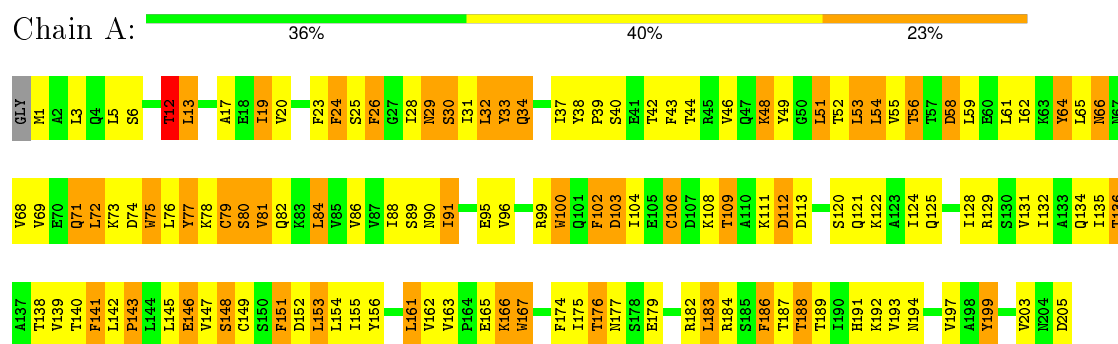
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	CLONING ARTIFACT	UNP Q13257
A	133	ALA	ARG	ENGINEERED	UNP Q13257

## 4 Residue-property plots

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Mitotic spindle assembly checkpoint protein MAD2A



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 500 calculated structures, 1 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CNS	refinement	1.0

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality ⓘ

### 6.1 Standard geometry ⓘ

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1650	1670	1671	143
All	All	1650	1670	1671	143

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 43.

All clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:124:ILE:O	1:A:128:ILE:HG22	0.91	1.66
1:A:17:ALA:HB2	1:A:77:TYR:CE2	0.84	2.08
1:A:142:LEU:HD21	1:A:199:TYR:CD2	0.81	2.10
1:A:17:ALA:HB2	1:A:77:TYR:CZ	0.81	2.11
1:A:33:TYR:CD2	1:A:43:PHE:CE2	0.80	2.70
1:A:26:PHE:CE1	1:A:53:LEU:HD12	0.79	2.12
1:A:32:LEU:HD11	1:A:61:LEU:CD1	0.79	2.06
1:A:135:ILE:O	1:A:139:VAL:HG23	0.77	1.77
1:A:51:LEU:HD13	1:A:53:LEU:HD21	0.76	1.56
1:A:32:LEU:HD11	1:A:61:LEU:HD13	0.73	1.61
1:A:103:ASP:C	1:A:104:ILE:HD12	0.72	2.05
1:A:64:TYR:O	1:A:68:VAL:HG23	0.71	1.85
1:A:72:LEU:HG	1:A:76:LEU:HD12	0.69	1.64
1:A:76:LEU:HD22	1:A:81:VAL:HA	0.68	1.66
1:A:65:LEU:O	1:A:69:VAL:HG23	0.68	1.88

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:71:GLN:O	1:A:75:TRP:N	0.66	2.28
1:A:134:GLN:OE1	1:A:183:LEU:HD13	0.66	1.89
1:A:90:ASN:ND2	1:A:147:VAL:HG11	0.66	2.05
1:A:175:ILE:HG22	1:A:176:THR:HG22	0.66	1.65
1:A:76:LEU:HD13	1:A:81:VAL:HG13	0.65	1.68
1:A:53:LEU:HB3	1:A:132:ILE:HD13	0.65	1.67
1:A:91:ILE:HB	1:A:148:SER:O	0.64	1.92
1:A:76:LEU:HB3	1:A:81:VAL:HG22	0.64	1.70
1:A:53:LEU:HD13	1:A:132:ILE:CD1	0.63	2.23
1:A:26:PHE:CD1	1:A:53:LEU:HD12	0.62	2.30
1:A:24:PHE:CE2	1:A:28:ILE:CD1	0.62	2.83
1:A:20:VAL:HG21	1:A:106:CYS:SG	0.61	2.36
1:A:24:PHE:CE2	1:A:28:ILE:HD11	0.61	2.30
1:A:104:ILE:HD12	1:A:104:ILE:N	0.60	2.11
1:A:100:TRP:CZ2	1:A:135:ILE:HG12	0.60	2.31
1:A:147:VAL:HG23	1:A:149:CYS:SG	0.60	2.37
1:A:51:LEU:H	1:A:51:LEU:HD12	0.59	1.57
1:A:64:TYR:OH	1:A:153:LEU:HD21	0.59	1.96
1:A:51:LEU:HD12	1:A:51:LEU:N	0.59	2.13
1:A:52:THR:C	1:A:53:LEU:HD23	0.58	2.19
1:A:31:ILE:HG12	1:A:135:ILE:HG21	0.58	1.74
1:A:33:TYR:CE2	1:A:43:PHE:CE2	0.58	2.90
1:A:75:TRP:C	1:A:75:TRP:CD1	0.58	2.78
1:A:30:SER:OG	1:A:132:ILE:HG23	0.57	1.98
1:A:43:PHE:HB3	1:A:54:LEU:HD23	0.57	1.76
1:A:33:TYR:CD2	1:A:54:LEU:HD22	0.56	2.34
1:A:33:TYR:CG	1:A:43:PHE:CE2	0.56	2.94
1:A:43:PHE:HB3	1:A:54:LEU:CD2	0.56	2.31
1:A:33:TYR:CD1	1:A:33:TYR:C	0.55	2.80
1:A:53:LEU:HD13	1:A:132:ILE:HD11	0.54	1.77
1:A:24:PHE:CD1	1:A:25:SER:N	0.54	2.75
1:A:79:CYS:O	1:A:80:SER:CB	0.54	2.56
1:A:38:TYR:HB2	1:A:39:PRO:HD2	0.53	1.79
1:A:86:VAL:HG23	1:A:102:PHE:CE1	0.53	2.38
1:A:132:ILE:HA	1:A:135:ILE:HD12	0.53	1.80
1:A:131:VAL:O	1:A:135:ILE:HG13	0.53	2.04
1:A:32:LEU:HD11	1:A:61:LEU:HD11	0.53	1.79
1:A:34:GLN:HG3	1:A:136:THR:HA	0.52	1.80
1:A:32:LEU:CD1	1:A:61:LEU:HD13	0.52	2.32
1:A:19:ILE:HG22	1:A:20:VAL:N	0.52	2.20
1:A:64:TYR:CE1	1:A:65:LEU:HD23	0.52	2.40
1:A:64:TYR:CD1	1:A:64:TYR:C	0.52	2.83

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:51:LEU:N	1:A:51:LEU:CD1	0.51	2.73
1:A:40:SER:HA	1:A:43:PHE:CE1	0.51	2.39
1:A:76:LEU:HD11	1:A:155:ILE:HG23	0.51	1.83
1:A:64:TYR:CZ	1:A:65:LEU:CD2	0.51	2.93
1:A:12:THR:HG22	1:A:109:THR:CG2	0.51	2.36
1:A:64:TYR:CE1	1:A:153:LEU:HD13	0.51	2.41
1:A:131:VAL:O	1:A:134:GLN:HG2	0.51	2.06
1:A:48:LYS:O	1:A:51:LEU:CD1	0.51	2.59
1:A:103:ASP:O	1:A:193:VAL:HG13	0.50	2.07
1:A:121:GLN:O	1:A:124:ILE:HB	0.50	2.06
1:A:156:TYR:CE1	1:A:167:TRP:CD1	0.50	2.99
1:A:33:TYR:HD1	1:A:33:TYR:C	0.50	2.09
1:A:33:TYR:CG	1:A:43:PHE:CZ	0.49	3.00
1:A:73:LYS:O	1:A:77:TYR:CB	0.49	2.61
1:A:64:TYR:CZ	1:A:65:LEU:HD21	0.49	2.43
1:A:19:ILE:O	1:A:23:PHE:HB2	0.49	2.07
1:A:33:TYR:CE2	1:A:54:LEU:HD22	0.49	2.43
1:A:183:LEU:HD11	1:A:197:VAL:HG12	0.49	1.84
1:A:5:LEU:HD23	1:A:6:SER:N	0.49	2.23
1:A:162:VAL:O	1:A:162:VAL:HG12	0.49	2.07
1:A:73:LYS:O	1:A:77:TYR:HB2	0.48	2.07
1:A:34:GLN:CB	1:A:135:ILE:HG22	0.48	2.38
1:A:86:VAL:HG23	1:A:102:PHE:CZ	0.48	2.43
1:A:142:LEU:HD21	1:A:199:TYR:CE2	0.48	2.42
1:A:24:PHE:CZ	1:A:65:LEU:HD22	0.48	2.43
1:A:13:LEU:HD23	1:A:108:LYS:HA	0.47	1.87
1:A:68:VAL:HG12	1:A:72:LEU:HD13	0.47	1.86
1:A:86:VAL:HA	1:A:152:ASP:O	0.47	2.10
1:A:38:TYR:CE2	1:A:42:THR:OG1	0.47	2.65
1:A:43:PHE:CD2	1:A:54:LEU:HD22	0.47	2.45
1:A:44:THR:HG23	1:A:55:VAL:HB	0.47	1.85
1:A:31:ILE:CD1	1:A:100:TRP:CD2	0.46	2.98
1:A:34:GLN:CB	1:A:139:VAL:HG21	0.46	2.40
1:A:48:LYS:HB3	1:A:49:TYR:CD1	0.46	2.46
1:A:51:LEU:H	1:A:51:LEU:CD1	0.46	2.24
1:A:32:LEU:HD12	1:A:38:TYR:HE1	0.46	1.71
1:A:186:PHE:HE1	1:A:193:VAL:HG23	0.46	1.71
1:A:24:PHE:CE1	1:A:65:LEU:HD22	0.46	2.46
1:A:71:GLN:O	1:A:75:TRP:HB3	0.46	2.11
1:A:102:PHE:N	1:A:102:PHE:CD1	0.46	2.83
1:A:32:LEU:HD21	1:A:151:PHE:CZ	0.46	2.45
1:A:51:LEU:HD21	1:A:129:ARG:HA	0.45	1.88

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:26:PHE:CZ	1:A:53:LEU:HD12	0.45	2.46
1:A:174:PHE:CD1	1:A:174:PHE:N	0.45	2.83
1:A:29:ASN:OD1	1:A:55:VAL:HG12	0.45	2.11
1:A:38:TYR:CE2	1:A:58:ASP:OD1	0.45	2.70
1:A:43:PHE:CD2	1:A:54:LEU:CD2	0.45	2.99
1:A:104:ILE:CD1	1:A:104:ILE:N	0.45	2.79
1:A:187:THR:HG23	1:A:192:LYS:HG3	0.45	1.88
1:A:100:TRP:CH2	1:A:135:ILE:HG12	0.45	2.47
1:A:51:LEU:HD13	1:A:53:LEU:CD2	0.45	2.38
1:A:62:ILE:O	1:A:66:ASN:HB2	0.45	2.11
1:A:199:TYR:N	1:A:199:TYR:CD1	0.44	2.83
1:A:19:ILE:HD12	1:A:124:ILE:HG21	0.44	1.88
1:A:64:TYR:CE1	1:A:65:LEU:CD2	0.44	3.00
1:A:38:TYR:OH	1:A:56:THR:CG2	0.44	2.66
1:A:186:PHE:CZ	1:A:188:THR:OG1	0.44	2.71
1:A:132:ILE:O	1:A:136:THR:OG1	0.43	2.36
1:A:96:VAL:HB	1:A:175:ILE:HG23	0.43	1.88
1:A:138:THR:O	1:A:142:LEU:N	0.43	2.52
1:A:33:TYR:O	1:A:33:TYR:HD1	0.42	1.96
1:A:58:ASP:O	1:A:62:ILE:CG1	0.42	2.67
1:A:145:LEU:HG	1:A:146:GLU:N	0.42	2.29
1:A:58:ASP:O	1:A:62:ILE:HD12	0.42	2.14
1:A:40:SER:CB	1:A:43:PHE:CZ	0.42	3.03
1:A:128:ILE:HD11	1:A:132:ILE:HD11	0.42	1.91
1:A:72:LEU:O	1:A:76:LEU:CB	0.42	2.67
1:A:31:ILE:HD11	1:A:100:TRP:CE3	0.42	2.50
1:A:32:LEU:HD21	1:A:151:PHE:CE2	0.42	2.50
1:A:44:THR:N	1:A:55:VAL:O	0.42	2.52
1:A:43:PHE:HA	1:A:55:VAL:O	0.42	2.15
1:A:24:PHE:CD1	1:A:24:PHE:C	0.42	2.93
1:A:141:PHE:HE2	1:A:199:TYR:CE2	0.41	2.32
1:A:82:GLN:O	1:A:104:ILE:N	0.41	2.49
1:A:89:SER:O	1:A:149:CYS:HB3	0.41	2.15
1:A:64:TYR:CE1	1:A:153:LEU:CD1	0.41	3.03
1:A:100:TRP:NE1	1:A:197:VAL:HG21	0.40	2.32
1:A:68:VAL:O	1:A:72:LEU:HB2	0.40	2.17
1:A:125:GLN:HA	1:A:128:ILE:CG2	0.40	2.47
1:A:19:ILE:CG2	1:A:20:VAL:N	0.40	2.83
1:A:186:PHE:CE2	1:A:188:THR:OG1	0.40	2.74
1:A:75:TRP:CZ2	1:A:155:ILE:HG13	0.40	2.51
1:A:88:ILE:CG2	1:A:149:CYS:CB	0.40	2.99
1:A:84:LEU:HB2	1:A:104:ILE:HD13	0.40	1.93

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:142:LEU:HB3	1:A:143:PRO:HD2	0.40	1.93
1:A:72:LEU:O	1:A:76:LEU:HB2	0.40	2.16

## 6.3 Torsion angles [i](#)

### 6.3.1 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 NMR 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	203/206 (99%)	172 (85%)	21 (10%)	10 (5%)	5	27
All	All	203/206 (99%)	172 (85%)	21 (10%)	10 (5%)	5	27

All 10 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	203	VAL
1	A	166	LYS
1	A	161	LEU
1	A	176	THR
1	A	143	PRO
1	A	81	VAL
1	A	163	VAL
1	A	12	THR
1	A	80	SER
1	A	112	ASP

### 6.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	189/189 (100%)	121 (64%)	68 (36%)	1	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	189/189 (100%)	121 (64%)	68 (36%)	<b>1</b> <b>9</b>

All 68 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	74	ASP
1	A	34	GLN
1	A	1	MET
1	A	141	PHE
1	A	99	ARG
1	A	37	ILE
1	A	120	SER
1	A	199	TYR
1	A	19	ILE
1	A	33	TYR
1	A	77	TYR
1	A	30	SER
1	A	51	LEU
1	A	122	LYS
1	A	182	ARG
1	A	46	VAL
1	A	66	ASN
1	A	58	ASP
1	A	112	ASP
1	A	100	TRP
1	A	109	THR
1	A	166	LYS
1	A	161	LEU
1	A	140	THR
1	A	95	GLU
1	A	183	LEU
1	A	194	ASN
1	A	111	LYS
1	A	191	HIS
1	A	71	GLN
1	A	84	LEU
1	A	136	THR
1	A	32	LEU
1	A	154	LEU
1	A	79	CYS
1	A	91	ILE

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Mol	Chain	Res	Type
1	A	167	TRP
1	A	48	LYS
1	A	113	ASP
1	A	26	PHE
1	A	59	LEU
1	A	179	GLU
1	A	106	CYS
1	A	3	LEU
1	A	188	THR
1	A	78	LYS
1	A	53	LEU
1	A	151	PHE
1	A	186	PHE
1	A	56	THR
1	A	13	LEU
1	A	29	ASN
1	A	103	ASP
1	A	177	ASN
1	A	148	SER
1	A	189	THR
1	A	165	GLU
1	A	146	GLU
1	A	72	LEU
1	A	205	ASP
1	A	12	THR
1	A	102	PHE
1	A	54	LEU
1	A	24	PHE
1	A	75	TRP
1	A	64	TYR
1	A	153	LEU
1	A	184	ARG

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided