



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 29, 2017 – 11:32 AM EDT

PDB ID : 1GO4
Title : Crystal structure of Mad1-Mad2 reveals a conserved Mad2 binding motif in Mad1 and Cdc20.
Authors : Sironi, L.; Mapelli, M.; Jeang, K.T.; Musacchio, A.
Deposited on : 2001-10-17
Resolution : 2.05 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029077
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029077

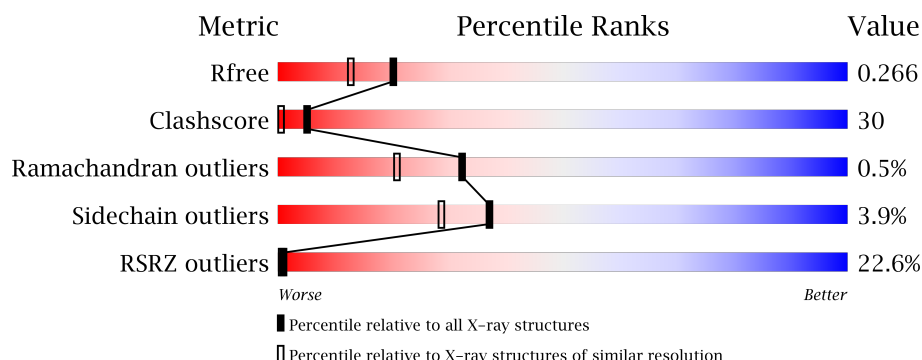
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1316 (2.04-2.04)
Clashscore	112137	1394 (2.04-2.04)
Ramachandran outliers	110173	1383 (2.04-2.04)
Sidechain outliers	110143	1383 (2.04-2.04)
RSRZ outliers	101464	1319 (2.04-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	205	<div> <div>12%</div> <div>61%</div> <div>32%</div> <div>• •</div> </div>
1	B	205	<div> <div>9%</div> <div>71%</div> <div>21%</div> <div>• 5%</div> </div>
1	C	205	<div> <div>8%</div> <div>76%</div> <div>17%</div> <div>• • 5%</div> </div>
1	D	205	<div> <div>57%</div> <div>30%</div> <div>60%</div> <div>• • 6%</div> </div>
2	E	100	<div> <div>13%</div> <div>51%</div> <div>34%</div> <div>• • 13%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	100	<div><div></div><div>20%</div><div>57%</div><div>26%</div><div>•</div><div>13%</div></div>
2	G	100	<div><div></div><div>20%</div><div>51%</div><div>42%</div><div></div><div>6%</div><div>•</div></div>
2	H	100	<div><div></div><div>30%</div><div>42%</div><div>47%</div><div></div><div>•</div><div>•</div><div>7%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9928 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 MITOTIC SPINDLE ASSEMBLY CHECKPOINT PROTEIN MAD2A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	196	Total	C	N	O	S	0	0	0
			1578	1014	254	306	4			
1	B	195	Total	C	N	O	S	0	0	0
			1568	1008	253	303	4			
1	C	195	Total	C	N	O	S	0	0	0
			1568	1008	253	303	4			
1	D	193	Total	C	N	O	S	0	0	0
			1556	1002	250	300	4			

There are 4 discrepancies between the modelled and reference sequences:

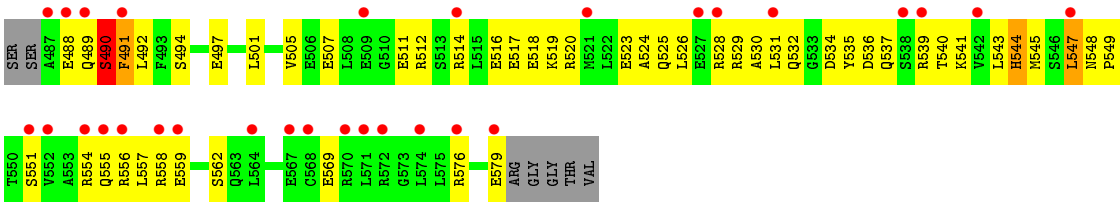
Chain	Residue	Modelled	Actual	Comment	Reference
A	133	ALA	ARG	engineered mutation	UNP Q13257
B	133	ALA	ARG	engineered mutation	UNP Q13257
C	133	ALA	ARG	engineered mutation	UNP Q13257
D	133	ALA	ARG	engineered mutation	UNP Q13257

- Molecule 2 is a protein called MAD1 (MITOTIC ARREST DEFICIENT)-LIKE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	87	Total	C	N	O	S	0	0	0
			722	433	143	142	4			
2	F	87	Total	C	N	O	S	0	0	0
			722	433	143	142	4			
2	G	100	Total	C	N	O	S	0	0	0
			816	489	160	163	4			
2	H	93	Total	C	N	O	S	0	0	0
			770	464	150	152	4			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	88	Total 88	O 88	0	0
3	B	124	Total 124	O 124	0	0
3	C	225	Total 225	O 225	0	0
3	D	45	Total 45	O 45	0	0
3	E	56	Total 56	O 56	0	0
3	F	35	Total 35	O 35	0	0
3	G	24	Total 24	O 24	0	0
3	H	31	Total 31	O 31	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	111.04Å 63.02Å 139.51Å 90.00° 111.65° 90.00°	Depositor
Resolution (Å)	24.50 – 2.05 24.50 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.6 (24.50-2.05) 99.8 (24.50-2.05)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.04Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.240 , 0.268 0.238 , 0.266	Depositor DCC
R_{free} test set	5665 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	41.5	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 59.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9928	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.85	3/1606 (0.2%)	0.83	2/2179 (0.1%)
1	B	0.66	0/1596	0.81	3/2166 (0.1%)
1	C	0.86	0/1596	0.99	7/2166 (0.3%)
1	D	0.42	0/1584	1.05	9/2150 (0.4%)
2	E	0.61	0/726	0.94	7/966 (0.7%)
2	F	0.46	0/726	0.62	0/966
2	G	0.48	0/821	0.83	3/1092 (0.3%)
2	H	0.39	0/775	0.77	2/1032 (0.2%)
All	All	0.65	3/9430 (0.0%)	0.89	33/12717 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	10	GLY	N-CA	21.90	1.78	1.46
1	A	8	GLU	CG-CD	-8.78	1.38	1.51
1	A	9	GLN	CG-CD	-6.40	1.36	1.51

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	195	SER	N-CA-CB	-28.89	67.16	110.50
1	C	203	VAL	CA-C-N	-15.38	83.37	117.20
1	A	9	GLN	C-N-CA	-13.24	94.50	122.30
1	D	59	LEU	N-CA-CB	-12.80	84.80	110.40
1	C	203	VAL	O-C-N	11.13	140.51	122.70

There are no chirality outliers.

There are no planarity outliers.

5.2 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 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	1578	0	1596	73	0
1	B	1568	0	1588	46	0
1	C	1568	0	1587	38	0
1	D	1556	0	1579	202	0
2	E	722	0	720	58	0
2	F	722	0	722	40	0
2	G	816	0	811	61	0
2	H	770	0	766	79	0
3	A	88	0	0	12	0
3	B	124	0	0	17	0
3	C	225	0	0	18	0
3	D	45	0	0	69	0
3	E	56	0	0	13	0
3	F	35	0	0	4	0
3	G	24	0	0	7	0
3	H	31	0	0	24	0
All	All	9928	0	9369	553	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 30.

The worst 5 of 553 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:D:141:PHE:HE2	1:D:199:TYR:CE2	1.30	1.47
1:A:10:GLY:N	1:A:10:GLY:CA	1.78	1.46
2:E:529:ARG:CZ	3:E:2018:HOH:O	1.81	1.26
1:D:141:PHE:CE2	1:D:199:TYR:CE2	2.22	1.25
1:D:152:ASP:OD2	3:D:2030:HOH:O	1.57	1.16

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	194/205 (95%)	185 (95%)	8 (4%)	1 (0%)	32	21
1	B	193/205 (94%)	187 (97%)	5 (3%)	1 (0%)	32	21
1	C	193/205 (94%)	190 (98%)	3 (2%)	0	100	100
1	D	191/205 (93%)	167 (87%)	22 (12%)	2 (1%)	18	8
2	E	85/100 (85%)	82 (96%)	3 (4%)	0	100	100
2	F	85/100 (85%)	80 (94%)	5 (6%)	0	100	100
2	G	98/100 (98%)	95 (97%)	2 (2%)	1 (1%)	18	8
2	H	91/100 (91%)	84 (92%)	6 (7%)	1 (1%)	17	6
All	All	1130/1220 (93%)	1070 (95%)	54 (5%)	6 (0%)	32	21

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	GLY
1	D	41	GLU
1	D	114	SER
2	G	582	GLY
2	H	490	SER

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	181/189 (96%)	178 (98%)	3 (2%)	66	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	180/189 (95%)	174 (97%)	6 (3%)	43	36
1	C	180/189 (95%)	174 (97%)	6 (3%)	43	36
1	D	179/189 (95%)	175 (98%)	4 (2%)	57	51
2	E	78/88 (89%)	72 (92%)	6 (8%)	15	7
2	F	78/88 (89%)	72 (92%)	6 (8%)	15	7
2	G	88/88 (100%)	82 (93%)	6 (7%)	18	10
2	H	83/88 (94%)	79 (95%)	4 (5%)	30	21
All	All	1047/1108 (94%)	1006 (96%)	41 (4%)	37	29

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	194	ASN
2	E	561	HIS
2	H	490	SER
2	E	509	GLU
2	E	531	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	71	GLN
1	D	125	GLN
2	G	525	GLN
1	D	66	ASN
2	G	561	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	196/205 (95%)	0.65	25 (12%) 4 3	34, 53, 80, 95	0
1	B	195/205 (95%)	0.54	19 (9%) 8 9	29, 45, 69, 86	0
1	C	195/205 (95%)	0.40	16 (8%) 12 13	21, 33, 61, 87	0
1	D	193/205 (94%)	3.18	116 (60%) 0 0	80, 98, 103, 105	0
2	E	87/100 (87%)	0.92	13 (14%) 3 2	27, 68, 94, 100	0
2	F	87/100 (87%)	1.09	20 (22%) 1 0	30, 69, 100, 104	0
2	G	100/100 (100%)	1.26	20 (20%) 1 1	49, 78, 92, 95	0
2	H	93/100 (93%)	1.58	30 (32%) 0 0	52, 82, 95, 101	0
All	All	1146/1220 (93%)	1.20	259 (22%) 1 1	21, 62, 100, 105	0

The worst 5 of 259 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	114	SER	16.5
1	D	190	ILE	12.8
1	D	120	SER	9.5
1	D	123	ALA	9.2
1	D	203	VAL	8.7

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.