



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 10:07 am BST

PDB ID : 6IM9
Title : MDM2 bound CueO-PM2 sensor
Authors : Wongsantichon, J.; Robinson, R.; Ghadessy, F.
Deposited on : 2018-10-22
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/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) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

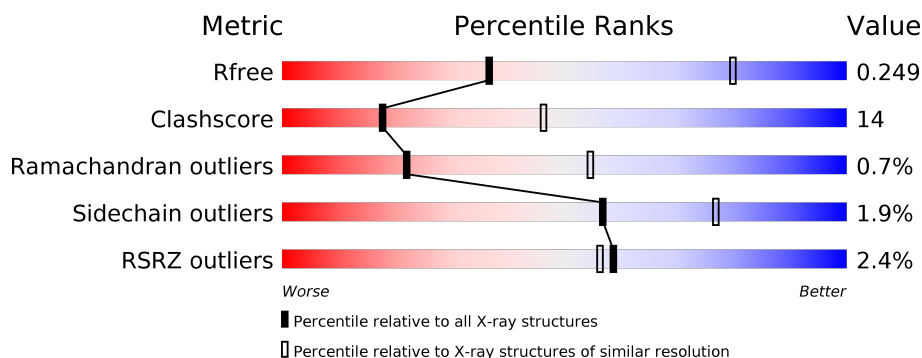
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 respectively. 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	509	<div> <div>3%</div> <div>68%</div> <div>27%</div> <div>• •</div> </div>
2	B	122	<div> <div>47%</div> <div>24%</div> <div>•</div> <div>29%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4493 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 Blue copper oxidase CueO,PM2 peptide,Blue copper oxidase CueO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total	C	N	O	S	0	0	0
			3773	2398	656	692	27			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	358	ILE	MET	engineered mutation	UNP P36649
A	517	LYS	-	expression tag	UNP P36649
A	518	ASP	-	expression tag	UNP P36649
A	519	PRO	-	expression tag	UNP P36649
A	520	ASN	-	expression tag	UNP P36649
A	521	SER	-	expression tag	UNP P36649
A	522	SER	-	expression tag	UNP P36649
A	523	SER	-	expression tag	UNP P36649
A	524	VAL	-	expression tag	UNP P36649
A	525	ASP	-	expression tag	UNP P36649
A	526	LYS	-	expression tag	UNP P36649
A	527	LEU	-	expression tag	UNP P36649
A	528	ALA	-	expression tag	UNP P36649
A	529	ALA	-	expression tag	UNP P36649
A	530	ALA	-	expression tag	UNP P36649
A	531	LEU	-	expression tag	UNP P36649
A	532	GLU	-	expression tag	UNP P36649
A	533	HIS	-	expression tag	UNP P36649
A	534	HIS	-	expression tag	UNP P36649
A	535	HIS	-	expression tag	UNP P36649
A	536	HIS	-	expression tag	UNP P36649
A	537	HIS	-	expression tag	UNP P36649

- Molecule 2 is a protein called E3 ubiquitin-protein ligase Mdm2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	87	Total	C	N	O	S	0	0	0
			720	471	119	126	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	4	GLY	-	expression tag	UNP Q00987
B	5	PRO	-	expression tag	UNP Q00987

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	83.64Å 83.64Å 240.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.92 – 3.30 28.92 – 3.30	Depositor EDS
% Data completeness (in resolution range)	92.1 (28.92-3.30) 92.1 (28.92-3.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.21 (at 3.31Å)	Xtriage
Refinement program	PHENIX 1.13_2998, PHENIX 1.13_2998	Depositor
R, R_{free}	0.177 , 0.249 0.176 , 0.249	Depositor DCC
R_{free} test set	707 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	66.8	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.031 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4493	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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 [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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.51	0/3870	0.69	1/5259 (0.0%)
2	B	0.53	0/734	0.69	0/989
All	All	0.51	0/4604	0.69	1/6248 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	466	ARG	NE-CZ-NH1	-5.12	117.74	120.30

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	3773	0	3734	104	0
2	B	720	0	755	24	0
All	All	4493	0	4489	122	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 14.

All (122) 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:93:GLN:N	1:A:93:GLN:OE1	2.08	0.87
1:A:322:ILE:HG13	1:A:324:ILE:HG13	1.66	0.77
2:B:61:ILE:HG23	2:B:66:LEU:HB2	1.67	0.76
1:A:348:VAL:HG22	1:A:431:ARG:HB2	1.70	0.73
1:A:99:THR:HG22	1:A:100:LEU:H	1.56	0.70
1:A:221:TYR:OH	1:A:294:ASP:OD2	2.04	0.70
2:B:60:TYR:OH	2:B:80:ASP:OD2	2.12	0.68
1:A:117:GLY:O	1:A:125:ARG:NH1	2.27	0.67
1:A:74:LEU:HD22	1:A:157:ALA:HB3	1.75	0.67
1:A:408:ASN:HB3	1:A:510:MET:HB2	1.77	0.67
1:A:56:GLN:O	1:A:72:ASN:ND2	2.28	0.66
1:A:442:LEU:HG	1:A:444:PRO:HD3	1.76	0.66
1:A:350:LYS:HE3	1:A:352:GLN:HB2	1.79	0.65
1:A:202:VAL:HG12	1:A:404:PHE:CD2	2.33	0.63
1:A:47:ARG:NH1	1:A:89:ASP:OD2	2.31	0.63
1:A:368:MET:HE1	1:A:376:MET:HB3	1.80	0.63
1:A:62:LYS:NZ	1:A:192:ALA:O	2.31	0.63
1:A:82:ARG:HA	1:A:131:VAL:HB	1.82	0.61
1:A:45:ARG:O	1:A:47:ARG:N	2.33	0.61
1:A:265:PRO:HD3	1:A:337:LEU:HD12	1.83	0.61
1:A:102:TRP:HB3	1:A:105:LEU:HD22	1.84	0.59
2:B:45:LYS:NZ	2:B:52:GLU:OE1	2.31	0.59
1:A:69:TYR:O	1:A:75:GLY:HA2	2.03	0.58
1:A:454:ILE:HG21	1:A:457:GLU:HB2	1.83	0.58
1:A:376:MET:HG3	1:A:380:ASP:HB2	1.86	0.57
1:A:357:PRO:HB2	1:A:393:LEU:HD21	1.87	0.56
1:A:473:VAL:HG21	1:A:482:VAL:HG11	1.88	0.55
1:A:42:THR:HG21	1:A:86:VAL:HG11	1.89	0.55
1:A:111:VAL:HG21	1:A:129:LEU:HD21	1.88	0.55
2:B:60:TYR:CE1	2:B:64:LYS:HD2	2.42	0.55
1:A:107:VAL:HB	1:A:111:VAL:HG11	1.88	0.55
1:A:64:ALA:HB2	1:A:194:GLY:O	2.07	0.55
1:A:167:ILE:O	1:A:170:LEU:HB2	2.07	0.54
1:A:166:GLU:OE2	1:A:335:SER:HB2	2.06	0.54
2:B:73:HIS:H	2:B:73:HIS:CD2	2.25	0.54
1:A:69:TYR:CE1	1:A:156:LEU:HD22	2.43	0.54
1:A:103:HIS:O	1:A:138:CYS:HB3	2.08	0.54
1:A:148:THR:OG1	1:A:507:ASP:OD1	2.25	0.54
1:A:108:PRO:O	1:A:111:VAL:HG12	2.09	0.53
1:A:142:PRO:HD3	1:A:156:LEU:HB3	1.91	0.53
1:A:80:LEU:HB3	1:A:131:VAL:HG21	1.90	0.53
1:A:260:ASP:HB2	1:A:470:LYS:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:LYS:HB3	1:A:371:TYR:CD1	2.44	0.53
2:B:73:HIS:ND1	2:B:94:LYS:HD2	2.24	0.53
1:A:179:ASP:OD2	1:A:327:SER:HB3	2.10	0.52
2:B:60:TYR:CZ	2:B:64:LYS:HD2	2.45	0.52
1:A:355:MET:HG2	1:A:408:ASN:OD1	2.09	0.52
1:A:408:ASN:HD22	1:A:505:HIS:HA	1.74	0.52
1:A:165:ASP:O	1:A:169:LYS:HG3	2.09	0.52
1:A:410:ILE:HG21	1:A:512:LEU:HD23	1.91	0.51
2:B:58:GLY:O	2:B:62:MET:HG3	2.10	0.51
1:A:91:TYR:CE1	1:A:124:LYS:HG3	2.46	0.51
1:A:202:VAL:HG12	1:A:404:PHE:CE2	2.45	0.51
1:A:143:HIS:HA	1:A:148:THR:CG2	2.41	0.51
1:A:89:ASP:OD1	1:A:126:SER:OG	2.29	0.51
1:A:337:LEU:HD23	1:A:338:PRO:HD2	1.93	0.50
2:B:68:ASP:HB2	2:B:76:TYR:CE2	2.46	0.50
1:A:398:HIS:CD2	2:B:50:MET:HG2	2.46	0.50
1:A:368:MET:CE	1:A:376:MET:HB3	2.42	0.50
1:A:356:ASP:HB3	1:A:407:ALA:HB1	1.94	0.49
1:A:113:GLY:HA3	1:A:117:GLY:HA3	1.94	0.48
1:A:111:VAL:HG21	1:A:129:LEU:CD2	2.43	0.48
1:A:308:ALA:HA	1:A:311:ASP:OD1	2.14	0.48
1:A:517:LYS:HG3	1:A:518:ASP:OD1	2.13	0.48
1:A:245:ASN:HA	1:A:274:PRO:HA	1.96	0.48
1:A:228:ARG:NH2	1:A:290:ASN:OD1	2.44	0.48
1:A:341:PRO:HG3	1:A:429:TYR:CD2	2.48	0.47
1:A:518:ASP:N	1:A:518:ASP:OD1	2.46	0.47
1:A:67:TRP:O	1:A:73:LEU:HA	2.14	0.47
1:A:230:TRP:HD1	1:A:329:ALA:HA	1.80	0.47
1:A:390:TYR:CE2	2:B:73:HIS:HB3	2.50	0.47
2:B:73:HIS:H	2:B:73:HIS:HD2	1.63	0.47
1:A:329:ALA:O	1:A:331:PRO:HD3	2.15	0.47
1:A:398:HIS:HA	2:B:100:TYR:CE2	2.49	0.47
1:A:387:PHE:HE2	2:B:93:VAL:HG21	1.81	0.46
1:A:418:ASN:OD1	1:A:419:LYS:N	2.48	0.46
1:A:92:ASN:C	1:A:93:GLN:OE1	2.53	0.46
1:A:42:THR:HG21	1:A:86:VAL:CG1	2.45	0.46
1:A:413:GLN:HG3	1:A:414:ALA:O	2.16	0.46
1:A:42:THR:HB	1:A:46:ASN:HA	1.98	0.46
1:A:165:ASP:OD1	1:A:165:ASP:N	2.41	0.46
1:A:499:HIS:HB2	1:A:506:GLU:HG3	1.98	0.45
1:A:170:LEU:O	1:A:171:MET:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:80:ASP:OD2	2:B:81:LEU:N	2.50	0.45
1:A:387:PHE:CE2	2:B:93:VAL:HG21	2.51	0.45
1:A:150:ARG:HG3	1:A:198:TYR:CD1	2.52	0.45
2:B:31:LYS:HD2	2:B:106:ASN:HA	1.98	0.45
1:A:105:LEU:HA	1:A:133:GLN:HE22	1.82	0.45
1:A:99:THR:HB	1:A:143:HIS:H	1.80	0.45
1:A:142:PRO:O	1:A:148:THR:HG22	2.17	0.45
1:A:455:LEU:HD12	1:A:481:GLU:HG2	1.98	0.44
1:A:135:ALA:HB2	1:A:164:ASP:H	1.82	0.44
2:B:50:MET:HE1	2:B:104:TYR:HE1	1.81	0.44
1:A:304:GLY:HA2	1:A:307:ILE:HD11	2.00	0.44
1:A:94:LEU:O	1:A:121:PRO:HB3	2.17	0.44
1:A:358:ILE:O	1:A:362:MET:HG3	2.18	0.44
2:B:99:ILE:HA	2:B:102:MET:HE3	2.00	0.44
1:A:228:ARG:HG2	1:A:228:ARG:H	1.59	0.44
2:B:38:LEU:HD23	2:B:38:LEU:HA	1.69	0.44
1:A:143:HIS:HA	1:A:148:THR:HG22	1.99	0.44
1:A:355:MET:HE2	1:A:360:ASP:HB2	2.00	0.44
1:A:69:TYR:HE2	1:A:100:LEU:HD12	1.83	0.44
1:A:390:TYR:CD2	2:B:73:HIS:HB3	2.52	0.43
1:A:215:LEU:HA	1:A:219:ALA:O	2.19	0.43
2:B:49:THR:O	2:B:53:VAL:HG23	2.18	0.43
1:A:384:MET:HG2	1:A:385:THR:H	1.84	0.43
1:A:370:LYS:HB3	1:A:371:TYR:CE1	2.54	0.43
2:B:62:MET:HE3	2:B:62:MET:HB3	1.64	0.42
1:A:69:TYR:OH	1:A:156:LEU:HD13	2.19	0.42
1:A:99:THR:HG22	1:A:100:LEU:N	2.30	0.42
1:A:190:PHE:CE1	1:A:196:ILE:HG12	2.55	0.42
1:A:74:LEU:HD21	1:A:186:GLN:HE22	1.84	0.42
1:A:279:GLU:OE2	1:A:466:ARG:NH2	2.51	0.42
1:A:322:ILE:HD13	1:A:322:ILE:HG21	1.82	0.42
1:A:56:GLN:HG3	1:A:64:ALA:O	2.19	0.42
1:A:230:TRP:CD1	1:A:329:ALA:HA	2.55	0.42
1:A:431:ARG:NE	1:A:481:GLU:OE2	2.44	0.41
1:A:500:CYS:O	1:A:506:GLU:HB2	2.20	0.41
2:B:28:VAL:HA	2:B:110:VAL:HG23	2.02	0.41
1:A:255:TYR:CD2	1:A:330:LEU:HD21	2.55	0.40
1:A:353:LEU:CD2	1:A:410:ILE:HG12	2.51	0.40
1:A:47:ARG:HA	1:A:87:THR:O	2.22	0.40

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	488/509 (96%)	451 (92%)	34 (7%)	3 (1%)	25	57
2	B	85/122 (70%)	77 (91%)	7 (8%)	1 (1%)	13	42
All	All	573/631 (91%)	528 (92%)	41 (7%)	4 (1%)	22	54

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	76	PRO
1	A	381	HIS
2	B	89	PRO

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	404/419 (96%)	398 (98%)	6 (2%)	65	81
2	B	82/112 (73%)	79 (96%)	3 (4%)	34	63
All	All	486/531 (92%)	477 (98%)	9 (2%)	57	77

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ARG
1	A	199	GLN

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Mol	Chain	Res	Type
1	A	228	ARG
1	A	280	ARG
1	A	350	LYS
1	A	383	GLN
2	B	65	ARG
2	B	70	LYS
2	B	73	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	490/509 (96%)	-0.11	14 (2%) 51 50	36, 65, 116, 168	0
2	B	87/122 (71%)	-0.25	0 100 100	46, 69, 100, 120	0
All	All	577/631 (91%)	-0.13	14 (2%) 59 56	36, 66, 115, 168	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	382	SER	4.9
1	A	383	GLN	4.1
1	A	520	ASN	3.9
1	A	380	ASP	3.6
1	A	61	GLY	2.9
1	A	402	PHE	2.8
1	A	44	ALA	2.8
1	A	413	GLN	2.7
1	A	374	GLN	2.7
1	A	403	ASP	2.6
1	A	116	GLN	2.6
1	A	378	GLY	2.3
1	A	381	HIS	2.2
1	A	400	GLY	2.2

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.