



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 03:42 pm BST

PDB ID : 5VKZ
Title : Crystal structure of Mdm12 and combinatorial reconstitution of Mdm12/Mmm1 ERMES complexes for structural studies
Authors : Egea, P.F.; AhYoung, A.P.; Lu, B.; Tan, H.R.; Cascio, D.
Deposited on : 2017-04-24
Resolution : 4.10 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

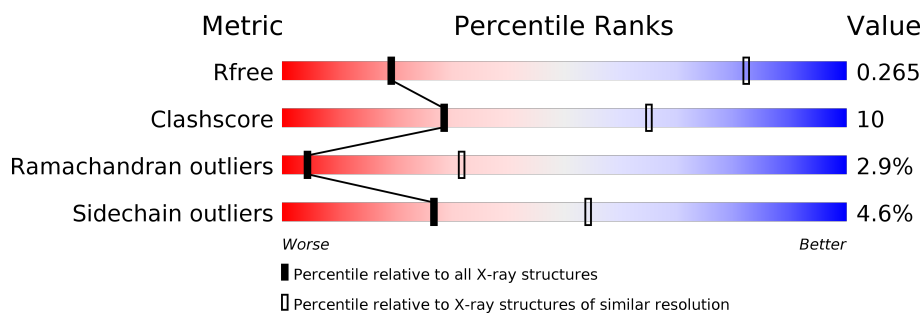
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.10 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	1193 (4.50-3.70)
Clashscore	141614	1003 (4.44-3.76)
Ramachandran outliers	138981	1005 (4.48-3.72)
Sidechain outliers	138945	1199 (4.50-3.70)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	275	
1	B	275	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3424 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 Mitochondrial distribution and morphology protein 12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1730	1120	277	327	6			
1	B	212	Total	C	N	O	S	0	0	0
			1694	1096	271	322	5			

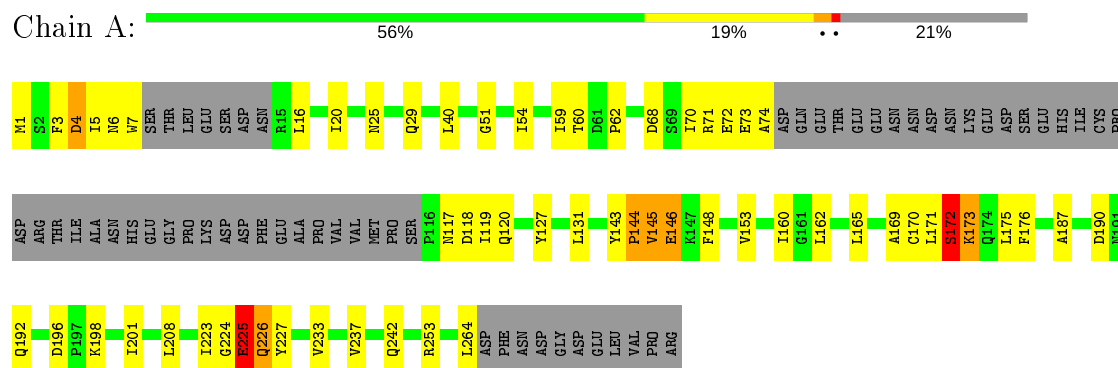
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	272	LEU	-	expression tag	UNP B5VRP4
A	273	VAL	-	expression tag	UNP B5VRP4
A	274	PRO	-	expression tag	UNP B5VRP4
A	275	ARG	-	expression tag	UNP B5VRP4
B	272	LEU	-	expression tag	UNP B5VRP4
B	273	VAL	-	expression tag	UNP B5VRP4
B	274	PRO	-	expression tag	UNP B5VRP4
B	275	ARG	-	expression tag	UNP B5VRP4

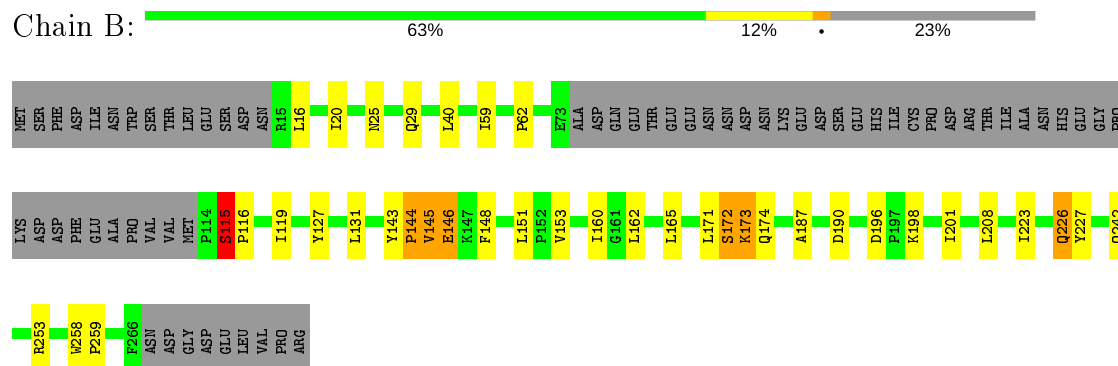
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-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 outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Mitochondrial distribution and morphology protein 12



- Molecule 1: Mitochondrial distribution and morphology protein 12



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	116.02Å 116.02Å 161.66Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	85.34 – 4.10 85.34 – 4.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (85.34-4.10) 99.5 (85.34-4.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.92 (at 4.15Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.242 , 0.254 0.248 , 0.265	Depositor DCC
R_{free} test set	1027 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å ²)	136.8	Xtriage
Anisotropy	0.926	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 188.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.079 for -h,-k,l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	3424	wwPDB-VP
Average B, all atoms (Å ²)	263.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% 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	0.62	1/1763 (0.1%)	0.81	2/2390 (0.1%)
1	B	0.52	0/1727	0.77	1/2343 (0.0%)
All	All	0.58	1/3490 (0.0%)	0.79	3/4733 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3	PHE	CB-CG	6.45	1.62	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	GLU	CA-CB-CG	6.36	127.39	113.40
1	A	3	PHE	CB-CG-CD1	5.36	124.55	120.80
1	B	115	SER	CB-CA-C	5.22	120.02	110.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	224	GLY	Peptide

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	1730	0	1755	37	1
1	B	1694	0	1719	33	0
All	All	3424	0	3474	67	1

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 10.

All (67) 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:5:ILE:HD13	1:A:54:ILE:HD12	1.40	1.04
1:A:59:ILE:HD11	1:A:119:ILE:HD11	1.46	0.94
1:B:59:ILE:HD11	1:B:119:ILE:HD11	1.50	0.93
1:B:144:PRO:O	1:B:145:VAL:HG12	1.69	0.92
1:A:144:PRO:O	1:A:145:VAL:HG12	1.70	0.92
1:B:115:SER:HB3	1:B:172:SER:HB3	1.50	0.92
1:B:143:TYR:HB3	1:B:144:PRO:HD3	1.55	0.87
1:A:143:TYR:HB3	1:A:144:PRO:HD3	1.58	0.83
1:A:4:ASP:O	1:A:5:ILE:HD12	1.92	0.69
1:B:115:SER:HB3	1:B:172:SER:CB	2.23	0.66
1:B:143:TYR:HB3	1:B:144:PRO:CD	2.25	0.66
1:A:143:TYR:HB3	1:A:144:PRO:CD	2.29	0.62
1:B:171:LEU:O	1:B:174:GLN:N	2.31	0.61
1:A:118:ASP:HB3	1:A:170:CYS:O	2.00	0.60
1:B:131:LEU:HD22	1:B:160:ILE:HD12	1.85	0.57
1:B:62:PRO:HB3	1:B:171:LEU:HD11	1.85	0.57
1:A:208:LEU:HG	1:B:242:GLN:HA	1.87	0.56
1:A:145:VAL:HG12	1:A:148:PHE:HB2	1.87	0.56
1:A:144:PRO:O	1:A:148:PHE:HB2	2.04	0.56
1:B:144:PRO:O	1:B:148:PHE:HB2	2.06	0.56
1:A:143:TYR:CB	1:A:144:PRO:HD3	2.32	0.55
1:A:62:PRO:HB3	1:A:171:LEU:HD11	1.89	0.55
1:A:70:ILE:HA	1:A:74:ALA:HB3	1.87	0.55
1:B:143:TYR:CB	1:B:144:PRO:HD3	2.32	0.55
1:A:131:LEU:HD22	1:A:160:ILE:HD12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:LEU:O	1:A:20:ILE:HG12	2.08	0.53
1:B:145:VAL:HG12	1:B:148:PHE:HB2	1.89	0.53
1:A:242:GLN:HA	1:B:208:LEU:HG	1.90	0.53
1:B:153:VAL:CG2	1:B:223:ILE:HG22	2.40	0.52
1:B:29:GLN:NE2	1:B:40:LEU:O	2.42	0.52
1:B:25:ASN:O	1:B:29:GLN:HG2	2.10	0.51
1:B:116:PRO:HB2	1:B:173:LYS:NZ	2.25	0.51
1:A:25:ASN:O	1:A:29:GLN:HG2	2.10	0.50
1:B:127:TYR:HB3	1:B:162:LEU:HB3	1.92	0.50
1:A:6:ASN:ND2	1:A:51:GLY:H	2.09	0.50
1:A:227:TYR:HB3	1:A:233:VAL:HG11	1.95	0.49
1:B:153:VAL:HG22	1:B:223:ILE:HG22	1.93	0.48
1:A:29:GLN:NE2	1:A:40:LEU:O	2.42	0.48
1:B:116:PRO:HB2	1:B:173:LYS:HZ1	1.78	0.48
1:B:16:LEU:O	1:B:20:ILE:HG12	2.12	0.48
1:A:144:PRO:O	1:A:145:VAL:CG1	2.53	0.48
1:A:172:SER:HA	1:A:173:LYS:HA	1.60	0.48
1:A:6:ASN:HD22	1:A:51:GLY:H	1.64	0.46
1:A:242:GLN:NE2	1:B:208:LEU:HA	2.31	0.45
1:B:59:ILE:O	1:B:59:ILE:HG23	2.16	0.45
1:A:127:TYR:HB3	1:A:162:LEU:HB3	1.99	0.45
1:A:187:ALA:HB3	1:A:201:ILE:HD11	1.99	0.44
1:B:145:VAL:HG22	1:B:146:GLU:H	1.81	0.44
1:B:196:ASP:OD1	1:B:198:LYS:HG2	2.18	0.44
1:A:196:ASP:OD1	1:A:198:LYS:HG2	2.17	0.44
1:A:145:VAL:HG22	1:A:146:GLU:H	1.83	0.43
1:B:151:LEU:HD22	1:B:227:TYR:CZ	2.54	0.43
1:A:68:ASP:O	1:A:72:GLU:OE1	2.36	0.43
1:B:172:SER:HA	1:B:173:LYS:HA	1.51	0.43
1:B:226:GLN:H	1:B:226:GLN:HG3	1.40	0.43
1:A:226:GLN:H	1:A:226:GLN:HG3	1.42	0.42
1:B:258:TRP:CG	1:B:259:PRO:HA	2.54	0.42
1:A:169:ALA:HB3	1:A:176:PHE:HB2	2.02	0.42
1:B:144:PRO:O	1:B:145:VAL:CG1	2.53	0.41
1:B:187:ALA:HB3	1:B:201:ILE:HD11	2.01	0.41
1:A:153:VAL:CG2	1:A:223:ILE:HG22	2.50	0.41
1:A:59:ILE:HG23	1:A:59:ILE:O	2.18	0.41
1:A:153:VAL:HG22	1:A:223:ILE:HG22	2.03	0.41
1:B:62:PRO:CB	1:B:171:LEU:HD11	2.50	0.41
1:A:119:ILE:HG12	1:A:120:GLN:N	2.36	0.41
1:A:175:LEU:HD23	1:A:264:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:VAL:O	1:A:237:VAL:HG23	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:GLU:CB	1:A:225:GLU:CB[5_555]	1.98	0.22

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 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	210/275 (76%)	194 (92%)	9 (4%)	7 (3%)	4	29
1	B	208/275 (76%)	195 (94%)	8 (4%)	5 (2%)	6	35
All	All	418/550 (76%)	389 (93%)	17 (4%)	12 (3%)	4	32

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	145	VAL
1	A	225	GLU
1	B	115	SER
1	B	145	VAL
1	A	172	SER
1	B	190	ASP
1	A	117	ASN
1	A	190	ASP
1	B	172	SER
1	B	144	PRO
1	A	144	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	198/253 (78%)	185 (93%)	13 (7%)	16	44
1	B	195/253 (77%)	190 (97%)	5 (3%)	46	67
All	All	393/506 (78%)	375 (95%)	18 (5%)	27	54

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	7	TRP
1	A	60	THR
1	A	71	ARG
1	A	73	GLU
1	A	146	GLU
1	A	165	LEU
1	A	172	SER
1	A	173	LYS
1	A	192	GLN
1	A	225	GLU
1	A	226	GLN
1	A	253	ARG
1	B	146	GLU
1	B	165	LEU
1	B	173	LYS
1	B	226	GLN
1	B	253	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	192	GLN

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.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.