



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 09:34 pm BST

PDB ID : 5YK7  
Title : Crystal Structure of Mdm12-Mmm1 complex  
Authors : Jeong, H.; Park, J.; Lee, C.  
Deposited on : 2017-10-12  
Resolution : 3.80 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](mailto: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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
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

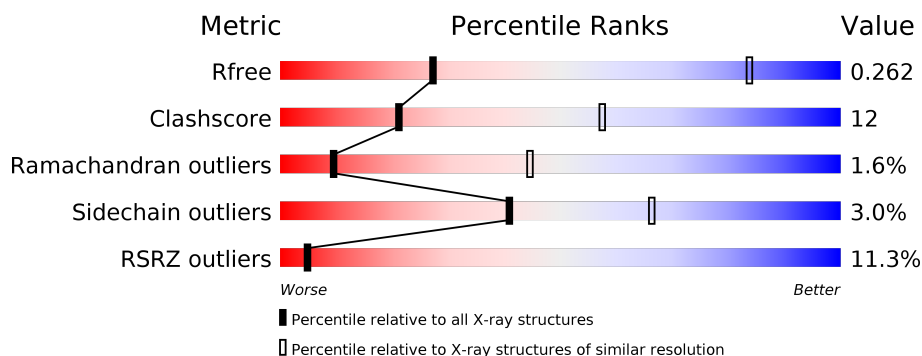
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.80 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	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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  $\geq 3$ , 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	255	<div> <div>6%</div> <div> <div></div> <div>58%</div> <div>27%</div> <div>•</div> <div>13%</div> </div> </div>
1	C	255	<div> <div>5%</div> <div> <div></div> <div>60%</div> <div>25%</div> <div>•</div> <div>14%</div> </div> </div>
2	B	208	<div> <div>17%</div> <div> <div></div> <div>68%</div> <div>25%</div> <div>•</div> <div>5%</div> </div> </div>
2	D	208	<div> <div>15%</div> <div> <div></div> <div>65%</div> <div>29%</div> <div>6%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	B	301	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6817 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 Maintenance of mitochondrial morphology protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1817	1168	307	337	5			
1	C	220	Total	C	N	O	S	0	0	0
			1810	1164	306	335	5			

- Molecule 2 is a protein called Mitochondrial distribution and morphology protein 12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	197	Total	C	N	O	S	0	0	0
			1583	1021	252	304	6			
2	D	196	Total	C	N	O	S	0	0	0
			1577	1018	251	302	6			

There are 14 discrepancies between the modelled and reference sequences:

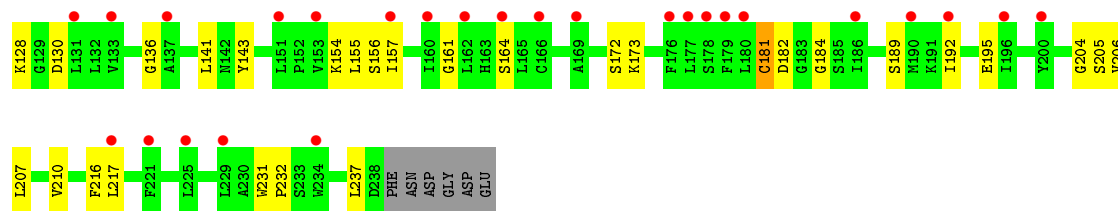
Chain	Residue	Modelled	Actual	Comment	Reference
B	110	GLY	-	linker	UNP Q92328
B	111	GLY	-	linker	UNP Q92328
B	112	SER	-	linker	UNP Q92328
B	113	GLY	-	linker	UNP Q92328
B	114	GLY	-	linker	UNP Q92328
B	183	GLY	-	linker	UNP Q92328
B	184	GLY	-	linker	UNP Q92328
D	110	GLY	-	linker	UNP Q92328
D	111	GLY	-	linker	UNP Q92328
D	112	SER	-	linker	UNP Q92328
D	113	GLY	-	linker	UNP Q92328
D	114	GLY	-	linker	UNP Q92328
D	183	GLY	-	linker	UNP Q92328
D	184	GLY	-	linker	UNP Q92328

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).

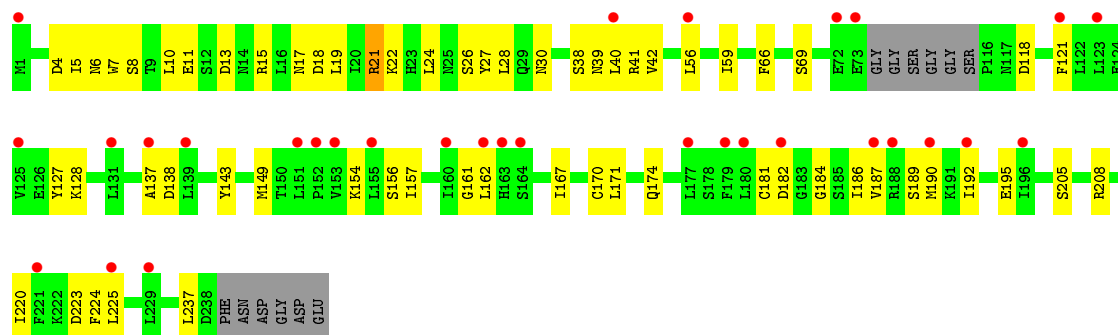


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		





● Molecule 2: Mitochondrial distribution and morphology protein 12



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.56 Å 87.56 Å 436.88 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.14 – 3.80 39.14 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (39.14-3.80) 99.6 (39.14-3.80)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.56 (at 3.76 Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, $R_{free}$	0.238 , 0.262 0.238 , 0.262	Depositor DCC
$R_{free}$ test set	916 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	170.4	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 172.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.448 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6817	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	240.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.26	0/1856	0.49	0/2513
1	C	0.27	0/1849	0.49	0/2503
2	B	0.27	0/1613	0.48	0/2184
2	D	0.26	0/1607	0.47	0/2175
All	All	0.26	0/6925	0.48	0/9375

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	1817	0	1820	57	0
1	C	1810	0	1813	55	0
2	B	1583	0	1585	35	0
2	D	1577	0	1581	41	0
3	A	10	0	0	1	0
3	B	5	0	0	0	0
3	C	10	0	0	1	0
3	D	5	0	0	0	0
All	All	6817	0	6799	165	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 12.

The worst 5 of 165 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)
2:B:21:ARG:O	2:B:25:ASN:HB2	1.69	0.93
2:D:18:ASP:O	2:D:22:LYS:HB2	1.77	0.84
1:A:431:PRO:HB3	1:C:422:GLN:HE22	1.48	0.78
1:A:343:THR:O	1:A:372:PHE:HA	1.87	0.74
2:D:24:LEU:HB3	2:D:42:VAL:HG21	1.69	0.73

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 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	215/255 (84%)	195 (91%)	15 (7%)	5 (2%)	6	38
1	C	214/255 (84%)	198 (92%)	12 (6%)	4 (2%)	8	42
2	B	193/208 (93%)	174 (90%)	17 (9%)	2 (1%)	15	52
2	D	192/208 (92%)	173 (90%)	17 (9%)	2 (1%)	15	52
All	All	814/926 (88%)	740 (91%)	61 (8%)	13 (2%)	9	44

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	396	ASN
1	A	389	GLY
2	B	62	PRO
2	D	184	GLY
2	D	237	LEU

### 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	204/235 (87%)	198 (97%)	6 (3%)	42	67
1	C	203/235 (86%)	197 (97%)	6 (3%)	41	66
2	B	182/188 (97%)	176 (97%)	6 (3%)	38	65
2	D	181/188 (96%)	176 (97%)	5 (3%)	43	68
All	All	770/846 (91%)	747 (97%)	23 (3%)	41	66

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	127	TYR
1	C	222	PHE
2	D	149	MET
2	B	181	CYS
1	C	294	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	422	GLN
1	C	422	GLN
2	D	30	ASN

### 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](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	PO4	A	502	-	4,4,4	0.93	0	6,6,6	0.42	0
3	PO4	C	502	-	4,4,4	0.92	0	6,6,6	0.42	0
3	PO4	D	301	-	4,4,4	0.92	0	6,6,6	0.43	0
3	PO4	A	501	-	4,4,4	0.92	0	6,6,6	0.43	0
3	PO4	B	301	-	4,4,4	0.92	0	6,6,6	0.44	0
3	PO4	C	501	-	4,4,4	0.96	0	6,6,6	0.41	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	PO4	1	0
3	C	501	PO4	1	0

## 5.7 Other polymers [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	221/255 (86%)	0.19	16 (7%) 15 12	157, 234, 326, 394	0
1	C	220/255 (86%)	0.18	12 (5%) 25 21	158, 237, 335, 461	0
2	B	197/208 (94%)	0.59	35 (17%) 1 1	166, 227, 345, 448	0
2	D	196/208 (94%)	0.54	31 (15%) 2 2	154, 219, 332, 432	0
All	All	834/926 (90%)	0.36	94 (11%) 5 5	154, 230, 333, 461	0

The worst 5 of 94 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	345	SER	7.5
2	B	192	ILE	4.6
1	A	346	LEU	4.2
2	D	180	LEU	4.0
1	C	346	LEU	4.0

### 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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PO4	C	501	5/5	0.55	0.15	225,230,249,284	0
3	PO4	B	301	5/5	0.60	0.40	260,267,269,275	0
3	PO4	C	502	5/5	0.64	0.20	267,288,291,293	0
3	PO4	A	501	5/5	0.71	0.27	270,275,281,281	0
3	PO4	D	301	5/5	0.72	0.35	247,262,277,293	0
3	PO4	A	502	5/5	0.78	0.18	228,232,256,267	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.