



## Full wwPDB EM Validation Report ⓘ

Oct 7, 2024 – 02:12 PM JST

PDB ID : 8JGA  
EMDB ID : EMD-36228  
Title : Cryo-EM structure of Mi3 fused with FKBP  
Authors : Zhang, H.W.; Kang, W.; Xue, C.  
Deposited on : 2023-05-20  
Resolution : 3.68 Å(reported)

This is a Full wwPDB EM 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

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : **FAILED**  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

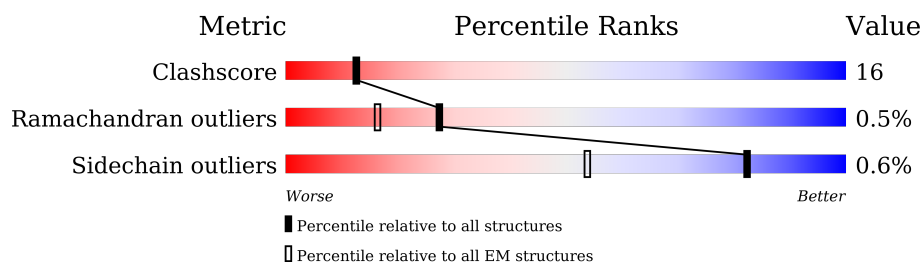
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.68 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	344	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1516 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Peptidyl-prolyl cis-trans isomerase FKBP1A,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	202	Total	C	N	O	S	0	0
			1516	987	249	273	7		

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-131	MET	-	initiating methionine	UNP P62942
A	-130	GLY	-	expression tag	UNP P62942
A	-129	SER	-	expression tag	UNP P62942
A	-128	SER	-	expression tag	UNP P62942
A	-127	HIS	-	expression tag	UNP P62942
A	-126	HIS	-	expression tag	UNP P62942
A	-125	HIS	-	expression tag	UNP P62942
A	-124	HIS	-	expression tag	UNP P62942
A	-123	HIS	-	expression tag	UNP P62942
A	-122	HIS	-	expression tag	UNP P62942
A	-121	GLY	-	expression tag	UNP P62942
A	-120	GLY	-	expression tag	UNP P62942
A	-119	SER	-	expression tag	UNP P62942
A	-11	GLY	-	linker	UNP P62942
A	-10	GLY	-	linker	UNP P62942
A	-9	SER	-	linker	UNP P62942
A	-8	GLY	-	linker	UNP P62942
A	-7	GLY	-	linker	UNP P62942
A	-6	SER	-	linker	UNP P62942
A	-5	GLY	-	linker	UNP P62942
A	-4	GLY	-	linker	UNP P62942
A	-3	SER	-	linker	UNP P62942
A	-2	GLY	-	linker	UNP P62942
A	-1	GLY	-	linker	UNP P62942
A	0	SER	-	linker	UNP P62942
A	26	LYS	GLU	conflict	UNP Q9WXS1
A	33	LEU	GLU	conflict	UNP Q9WXS1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	61	MET	LYS	conflict	UNP Q9WXS1
A	76	ALA	CYS	conflict	UNP Q9WXS1
A	100	ALA	CYS	conflict	UNP Q9WXS1
A	187	VAL	ASP	conflict	UNP Q9WXS1
A	190	ALA	ARG	conflict	UNP Q9WXS1
A	206	GLY	-	expression tag	UNP Q9WXS1
A	207	SER	-	expression tag	UNP Q9WXS1
A	208	GLY	-	expression tag	UNP Q9WXS1
A	209	GLU	-	expression tag	UNP Q9WXS1
A	210	PRO	-	expression tag	UNP Q9WXS1
A	211	GLU	-	expression tag	UNP Q9WXS1
A	212	ALA	-	expression tag	UNP Q9WXS1



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	33473	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50.0	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

## 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	0.31	0/1545	0.51	0/2084

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	1516	0	1580	51	0
All	All	1516	0	1580	51	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 16.

All (51) 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:183:LYS:HB3	1:A:183:LYS:NZ	2.00	0.77
1:A:183:LYS:HB3	1:A:183:LYS:HZ3	1.53	0.73
1:A:16:LEU:HD23	1:A:182:VAL:HG21	1.74	0.68
1:A:181:LEU:O	1:A:181:LEU:HG	1.98	0.63
1:A:111:VAL:HG21	1:A:128:LEU:HD13	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:LEU:HD23	1:A:182:VAL:CG2	2.29	0.62
1:A:58:LEU:HB3	1:A:63:ALA:HB3	1.81	0.62
1:A:52:ILE:HG23	1:A:65:ILE:HD12	1.84	0.59
1:A:97:SER:OG	1:A:125:HIS:NE2	2.27	0.59
1:A:165:CYS:HA	1:A:168:PHE:HB2	1.83	0.59
1:A:181:LEU:CD1	1:A:193:ALA:HA	2.37	0.55
1:A:49:ASP:O	1:A:82:SER:OG	2.23	0.54
1:A:16:LEU:CD2	1:A:182:VAL:CG2	2.86	0.53
1:A:185:THR:HG23	1:A:187:VAL:HG12	1.91	0.53
1:A:126:THR:OG1	1:A:150:ASN:O	2.26	0.53
1:A:181:LEU:HD11	1:A:193:ALA:HA	1.90	0.53
1:A:106:PHE:HZ	1:A:127:ILE:HD13	1.74	0.52
1:A:80:VAL:HG23	1:A:87:ILE:HD11	1.92	0.52
1:A:156:THR:HG22	1:A:176:GLY:HA3	1.92	0.52
1:A:164:VAL:HG23	1:A:175:VAL:HG11	1.92	0.51
1:A:183:LYS:NZ	1:A:183:LYS:CB	2.73	0.51
1:A:28:ALA:HB3	1:A:55:LEU:HD11	1.92	0.51
1:A:93:ASP:HB3	1:A:96:ILE:HB	1.93	0.51
1:A:6:LEU:HD23	1:A:64:ILE:HD13	1.93	0.50
1:A:177:VAL:HG11	1:A:196:PHE:CE2	2.48	0.48
1:A:192:LYS:O	1:A:196:PHE:HB2	2.13	0.48
1:A:154:VAL:HG13	1:A:174:ALA:O	2.14	0.48
1:A:163:ASN:O	1:A:167:TRP:HD1	1.97	0.47
1:A:12:ILE:HG23	1:A:36:VAL:HG13	1.96	0.46
1:A:21:VAL:HG22	1:A:51:VAL:HG23	1.97	0.45
1:A:29:LEU:O	1:A:33:LEU:HG	2.17	0.44
1:A:92:LEU:HD21	1:A:123:LEU:HD12	1.99	0.44
1:A:132:PRO:O	1:A:136:VAL:HG22	2.18	0.43
1:A:109:PRO:HD2	1:A:128:LEU:HD23	2.00	0.43
1:A:55:LEU:HD23	1:A:55:LEU:O	2.18	0.43
1:A:6:LEU:HD23	1:A:64:ILE:CD1	2.48	0.43
1:A:18:ALA:O	1:A:45:VAL:HG12	2.18	0.43
1:A:29:LEU:HD23	1:A:58:LEU:HD11	2.00	0.42
1:A:70:VAL:HG21	1:A:87:ILE:HG23	2.01	0.42
1:A:168:PHE:HE2	1:A:200:ILE:HG12	1.84	0.42
1:A:15:VAL:CG2	1:A:178:GLY:HA3	2.50	0.41
1:A:106:PHE:CZ	1:A:127:ILE:HD13	2.54	0.41
1:A:119:LYS:HB2	1:A:119:LYS:HE2	1.90	0.41
1:A:16:LEU:HA	1:A:182:VAL:HG21	2.02	0.41
1:A:27:LYS:HD3	1:A:182:VAL:O	2.20	0.41
1:A:15:VAL:HG12	1:A:40:GLU:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:LYS:NZ	1:A:184:GLY:O	2.38	0.41
1:A:55:LEU:HD21	1:A:58:LEU:HD12	2.02	0.40
1:A:42:THR:O	1:A:45:VAL:HG22	2.21	0.40
1:A:77:ARG:NH1	1:A:99:PHE:CD2	2.90	0.40
1:A:99:PHE:HA	1:A:102:GLU:HG2	2.03	0.40

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 PDB entries followed by that with respect to all EM 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	200/344 (58%)	185 (92%)	14 (7%)	1 (0%)	25 57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	182	VAL

### 5.3.2 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 EM 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	161/273 (59%)	160 (99%)	1 (1%)	84 90

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	183	LYS

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

### 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 oligosaccharides 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.