



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 21, 2017 – 07:18 PM EST

PDB ID : 5FM5  
Title : Crystal structure of the myomesin:obscurin-like-1 complex  
Authors : Pernigo, S.; Steiner, R.A.  
Deposited on : 2015-11-01  
Resolution : 3.10 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

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
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-20028442

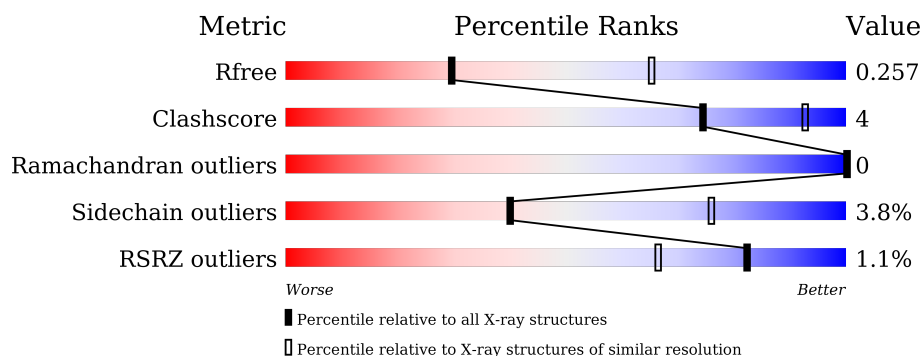
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
$R_{free}$	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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. 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	M	231	<div> <div>49%</div> <div>47%</div> </div>
1	N	231	<div> <div>48%</div> <div>47%</div> </div>
2	O	98	<div> <div>2%</div> <div>85%</div> <div>11%</div> <div>2%</div> </div>
2	P	98	<div> <div>3%</div> <div>82%</div> <div>16%</div> <div>1%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3566 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 MYOMESIN-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	M	123	Total	C	N	O	S	0	1	0
			955	612	162	177	4			
1	N	123	Total	C	N	O	S	0	0	0
			949	608	161	176	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	509	MET	-	EXPRESSION TAG	UNP P52179
N	509	MET	-	EXPRESSION TAG	UNP P52179

- Molecule 2 is a protein called OBSCURIN-LIKE-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	97	Total	C	N	O	S	0	0	0
			783	501	145	131	6			
2	P	98	Total	C	N	O	S	0	1	0
			795	511	146	132	6			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	242	GLY	-	EXPRESSION TAG	UNP O75147
O	243	PRO	-	EXPRESSION TAG	UNP O75147
O	244	LEU	-	EXPRESSION TAG	UNP O75147
O	245	GLY	-	EXPRESSION TAG	UNP O75147
O	246	SER	-	EXPRESSION TAG	UNP O75147
O	247	GLY	-	EXPRESSION TAG	UNP O75147
O	248	ILE	-	EXPRESSION TAG	UNP O75147
O	249	LEU	-	EXPRESSION TAG	UNP O75147
O	250	MET	-	EXPRESSION TAG	UNP O75147
P	242	GLY	-	EXPRESSION TAG	UNP O75147

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Chain	Residue	Modelled	Actual	Comment	Reference
P	243	PRO	-	EXPRESSION TAG	UNP O75147
P	244	LEU	-	EXPRESSION TAG	UNP O75147
P	245	GLY	-	EXPRESSION TAG	UNP O75147
P	246	SER	-	EXPRESSION TAG	UNP O75147
P	247	GLY	-	EXPRESSION TAG	UNP O75147
P	248	ILE	-	EXPRESSION TAG	UNP O75147
P	249	LEU	-	EXPRESSION TAG	UNP O75147
P	250	MET	-	EXPRESSION TAG	UNP O75147

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	M	37	Total O 37 37	0	0
3	N	24	Total O 24 24	0	0
3	O	14	Total O 14 14	0	0
3	P	9	Total O 9 9	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.18Å 134.38Å 68.39Å 90.00° 92.50° 90.00°	Depositor
Resolution (Å)	75.40 – 3.10 75.40 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.8 (75.40-3.10) 98.8 (75.40-3.10)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.02 (at 3.13Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.216 , 0.259 0.216 , 0.257	Depositor DCC
$R_{free}$ test set	747 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	72.3	Xtriage
Anisotropy	0.611	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 55.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.119 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3566	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.67% 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](#)

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	M	0.45	0/983	0.72	0/1338
1	N	0.47	0/974	0.67	0/1325
2	O	0.50	0/805	0.81	2/1085 (0.2%)
2	P	0.51	0/821	0.79	2/1107 (0.2%)
All	All	0.48	0/3583	0.74	4/4855 (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
2	O	0	1
2	P	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	P	314	ARG	NE-CZ-NH1	6.66	123.63	120.30
2	O	291	ARG	NE-CZ-NH1	6.00	123.30	120.30
2	P	266	ARG	NE-CZ-NH1	5.06	122.83	120.30
2	O	266	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	O	271	GLY	Peptide
2	P	271	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	M	955	0	959	8	1
1	N	949	0	951	10	1
2	O	783	0	787	6	0
2	P	795	0	798	9	0
3	M	37	0	0	0	0
3	N	24	0	0	0	0
3	O	14	0	0	0	0
3	P	9	0	0	0	0
All	All	3566	0	3495	28	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 4.

The worst 5 of 28 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:N:521:ALA:O	1:N:522:ASN:ND2	2.18	0.76
1:M:523:LYS:HD2	1:M:576:GLU:CD	2.20	0.60
1:M:523:LYS:HD2	1:M:576:GLU:OE1	2.07	0.54
2:P:262:HIS:HD2	2:P:308:TYR:H	1.57	0.52
2:P:298:ARG:O	2:P:299:ASP:HB2	2.10	0.52

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:M:568:ARG:NE	1:N:524:ASP:OD2[4_455]	2.18	0.02



## 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	M	122/231 (53%)	117 (96%)	5 (4%)	0	100	100
1	N	121/231 (52%)	115 (95%)	6 (5%)	0	100	100
2	O	95/98 (97%)	91 (96%)	4 (4%)	0	100	100
2	P	97/98 (99%)	92 (95%)	5 (5%)	0	100	100
All	All	435/658 (66%)	415 (95%)	20 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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 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	M	104/195 (53%)	101 (97%)	3 (3%)	50	81
1	N	103/195 (53%)	101 (98%)	2 (2%)	65	87
2	O	81/81 (100%)	76 (94%)	5 (6%)	23	59
2	P	82/81 (101%)	78 (95%)	4 (5%)	31	68
All	All	370/552 (67%)	356 (96%)	14 (4%)	40	76

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	O	306	VAL
2	O	307	LEU
2	P	306	VAL

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Mol	Chain	Res	Type
2	O	277	ILE
2	P	277	ILE

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

Mol	Chain	Res	Type
1	N	522	ASN
2	O	262	HIS
2	P	262	HIS

### 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 [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	M	123/231 (53%)	0.20	0 <span>100</span> <span>100</span>	57, 78, 118, 144	0
1	N	123/231 (53%)	0.23	0 <span>100</span> <span>100</span>	56, 80, 104, 114	0
2	O	97/98 (98%)	0.31	2 (2%) <span>67</span> <span>44</span>	61, 85, 113, 123	0
2	P	98/98 (100%)	0.44	3 (3%) <span>52</span> <span>28</span>	66, 91, 121, 139	0
All	All	441/658 (67%)	0.29	5 (1%) <span>82</span> <span>66</span>	56, 85, 115, 144	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	242	GLY	4.2
2	P	255[A]	PHE	2.3
2	P	299	ASP	2.2
2	O	339	PRO	2.2
2	O	243	PRO	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 ⓘ

There are no such residues in this entry.