



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 08:24 pm GMT

PDB ID : 2YF0
Title : Human Myotubularin related protein 6 (MTMR6)
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Deposited on : 2011-03-31
Resolution : 2.65 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
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

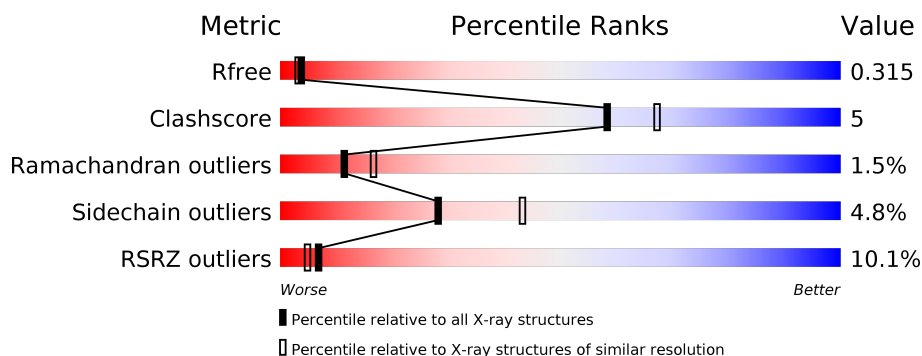
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 2.65 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}	111664	1112 (2.68-2.64)
Clashscore	122126	1151 (2.68-2.64)
Ramachandran outliers	120053	1133 (2.68-2.64)
Sidechain outliers	120020	1133 (2.68-2.64)
RSRZ outliers	108989	1098 (2.68-2.64)

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. 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	512	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3920 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 MYOTUBULARIN-RELATED PROTEIN 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	487	3913	2503	675	713	22	0	2	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	508	HIS	-	expression tag	UNP Q9Y217
A	509	HIS	-	expression tag	UNP Q9Y217
A	510	HIS	-	expression tag	UNP Q9Y217
A	511	HIS	-	expression tag	UNP Q9Y217
A	512	HIS	-	expression tag	UNP Q9Y217
A	319	VAL	ILE	cloning artifact	UNP Q9Y217

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

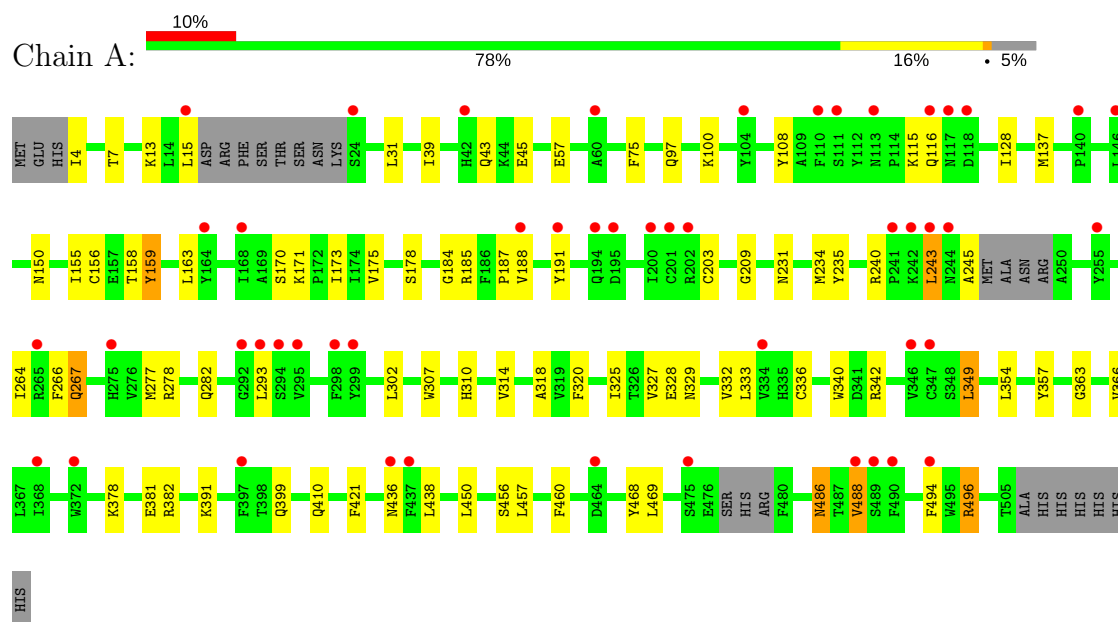
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	O	0	0
			2	2		

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: MYOTUBULARIN-RELATED PROTEIN 6



4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α , β , γ	85.73Å 85.73Å 448.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.77 – 2.65 29.77 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.77-2.65) 99.4 (29.77-2.65)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.15 (at 2.64Å)	Xtriage
Refinement program	BUSTER 2.11.1	Depositor
R, R_{free}	0.258 , 0.288 0.282 , 0.315	Depositor DCC
R_{free} test set	1503 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	59.8	Xtriage
Anisotropy	0.875	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 70.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3920	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.47	0/4011	0.65	0/5433

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

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	3913	0	3756	40	0
2	A	5	0	0	0	0
3	A	2	0	0	0	0
All	All	3920	0	3756	40	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 5.

All (40) 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:436:ASN:HD21	1:A:456:SER:HA	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:MET:SD	1:A:310:HIS:HD2	2.19	0.65
1:A:438:LEU:HB2	1:A:450:LEU:HD21	1.79	0.65
1:A:310:HIS:O	1:A:314:VAL:HG23	2.02	0.59
1:A:13:LYS:HE3	1:A:15:LEU:HB3	1.85	0.58
1:A:156:CYS:HB3	1:A:159:TYR:HB2	1.85	0.58
1:A:245:ALA:HB2	1:A:342:ARG:HH12	1.70	0.56
1:A:277:MET:SD	1:A:310:HIS:CD2	2.99	0.56
1:A:234:MET:HE2	1:A:333:LEU:HB2	1.88	0.56
1:A:421:PHE:HB2	1:A:468:TYR:HB3	1.89	0.55
1:A:410:GLN:HE22	1:A:486:ASN:HD22	1.55	0.54
1:A:163:LEU:HD22	1:A:188:VAL:HG21	1.90	0.53
1:A:128:ILE:HG23	1:A:366:VAL:HG12	1.89	0.53
1:A:235:TYR:HB2	1:A:332:VAL:HG22	1.91	0.52
1:A:378:LYS:HD3	1:A:382:ARG:HH21	1.74	0.51
1:A:240:ARG:HH12	1:A:266:PHE:HB3	1.77	0.50
1:A:39:ILE:HG12	1:A:45:GLU:HG2	1.93	0.50
1:A:170:SER:H	1:A:173:ILE:HD13	1.77	0.49
1:A:436:ASN:ND2	1:A:457:LEU:H	2.09	0.49
1:A:155:ILE:HD11	1:A:175:VAL:HG12	1.95	0.48
1:A:187:PRO:HA	1:A:203:CYS:HB3	1.96	0.48
1:A:318:ALA:HB2	1:A:349:LEU:HB3	1.94	0.48
1:A:307:TRP:CH2	1:A:399:GLN:HG3	2.50	0.47
1:A:278:ARG:O	1:A:282:GLN:HG2	2.17	0.45
1:A:325:ILE:HG21	1:A:354:LEU:HD22	1.99	0.45
1:A:234:MET:HB3	1:A:264:ILE:HD13	1.98	0.44
1:A:231:ASN:HB2	1:A:329:ASN:O	2.16	0.44
1:A:457:LEU:O	1:A:460:PHE:HB3	2.17	0.44
1:A:178:SER:O	1:A:184:GLY:HA2	2.18	0.43
1:A:4:ILE:HG23	1:A:31:LEU:HB3	2.01	0.43
1:A:496:ARG:H	1:A:496:ARG:HG2	1.53	0.42
1:A:158:THR:O	1:A:185:ARG:NH1	2.53	0.42
1:A:378:LYS:O	1:A:382:ARG:HG2	2.18	0.42
1:A:267:GLN:HG3	1:A:320:PHE:CE2	2.55	0.42
1:A:293:LEU:HG	1:A:293:LEU:H	1.77	0.41
1:A:378:LYS:HB3	1:A:381:GLU:HB2	2.02	0.41
1:A:278:ARG:NH2	1:A:391:LYS:O	2.53	0.41
1:A:357:TYR:O	1:A:363:GLY:HA3	2.21	0.41
1:A:191:TYR:CE2	1:A:354:LEU:HD11	2.56	0.41
1:A:97:GLN:HA	1:A:100:LYS:HE2	2.02	0.41

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	481/512 (94%)	433 (90%)	40 (8%)	8 (2%)	10	14

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	494	PHE
1	A	209	GLY
1	A	336[A]	CYS
1	A	336[B]	CYS
1	A	243	LEU
1	A	327	VAL
1	A	488	VAL

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	420/464 (90%)	400 (95%)	20 (5%)	28	43

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	57	GLU
1	A	75	PHE

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Mol	Chain	Res	Type
1	A	108	TYR
1	A	115	LYS
1	A	116	GLN
1	A	137	MET
1	A	150	ASN
1	A	159	TYR
1	A	171	LYS
1	A	243	LEU
1	A	267	GLN
1	A	302	LEU
1	A	328	GLU
1	A	340	TRP
1	A	349	LEU
1	A	469	LEU
1	A	486	ASN
1	A	488	VAL
1	A	496	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	310	HIS
1	A	335	HIS
1	A	426	HIS
1	A	436	ASN
1	A	486	ASN
1	A	491	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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
2	SO4	A	1506	-	4,4,4	0.35	0	6,6,6	0.64	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	1506	-	-	0/0/0/0	0/0/0/0

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.

No monomer is involved in short contacts.

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 ⓘ

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	487/512 (95%)	0.59	49 (10%) 7 5	57, 105, 145, 171	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	244	ASN	5.5
1	A	490	PHE	4.9
1	A	241	PRO	4.9
1	A	242	LYS	4.7
1	A	293	LEU	3.9
1	A	292	GLY	3.8
1	A	295	VAL	3.5
1	A	347	CYS	3.4
1	A	489	SER	3.3
1	A	188	VAL	3.1
1	A	243	LEU	3.1
1	A	201	CYS	3.1
1	A	294	SER	3.0
1	A	334	VAL	3.0
1	A	15	LEU	3.0
1	A	111	SER	2.9
1	A	164	TYR	2.9
1	A	200	ILE	2.9
1	A	117	ASN	2.9
1	A	191	TYR	2.6
1	A	299	TYR	2.6
1	A	118	ASP	2.6
1	A	265	ARG	2.6
1	A	494	PHE	2.5
1	A	202	ARG	2.5
1	A	436	ASN	2.5
1	A	368	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	488	VAL	2.5
1	A	437	PHE	2.4
1	A	116	GLN	2.4
1	A	346	VAL	2.3
1	A	397	PHE	2.3
1	A	60	ALA	2.3
1	A	104	TYR	2.3
1	A	168	ILE	2.3
1	A	298	PHE	2.3
1	A	146	LEU	2.2
1	A	195	ASP	2.2
1	A	464	ASP	2.2
1	A	194	GLN	2.2
1	A	42	HIS	2.2
1	A	372	TRP	2.1
1	A	113	ASN	2.1
1	A	475	SER	2.1
1	A	255	TYR	2.1
1	A	140	PRO	2.1
1	A	24	SER	2.0
1	A	275	HIS	2.0
1	A	110	PHE	2.0

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, 95th 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(\AA^2)	Q<0.9
2	SO4	A	1506	5/5	0.90	0.17	63,64,69,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.