



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:49 PM GMT

PDB ID : 1M7R
Title : Crystal Structure of Myotubularin-related Protein-2 (MTMR2) Complexed with Phosphate
Authors : Begley, M.J.; Taylor, G.S.; Kim, S.-A.; Veine, D.M.; Dixon, J.E.; Stuckey, J.A.
Deposited on : 2002-07-22
Resolution : 2.60 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
A user guide is available at
<http://wwpdb.org/validation/2016/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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

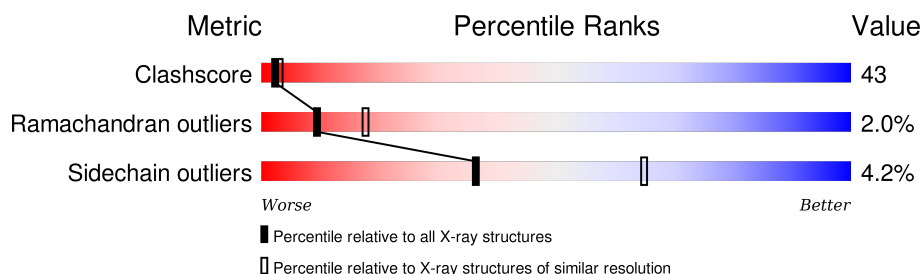
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)

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 ≥ 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	657	
1	B	657	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	656	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8632 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-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	513	Total	C	N	O	S	75	0	0
			4189	2679	729	764	17			
1	B	513	Total	C	N	O	S	114	0	0
			4189	2679	729	764	17			

There are 30 discrepancies between the modelled and reference sequences:

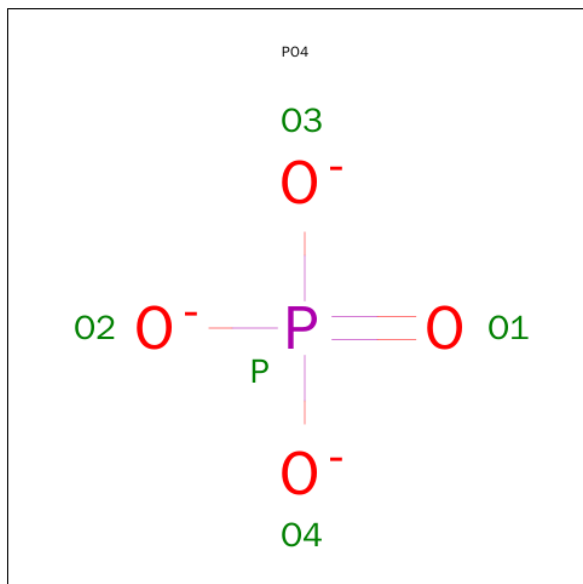
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	CLONING ARTIFACT	UNP Q13614
A	-1	ALA	-	CLONING ARTIFACT	UNP Q13614
A	0	SER	-	CLONING ARTIFACT	UNP Q13614
A	417	SER	CYS	ENGINEERED	UNP Q13614
A	644	ALA	-	EXPRESSION TAG	UNP Q13614
A	645	ALA	-	EXPRESSION TAG	UNP Q13614
A	646	ALA	-	EXPRESSION TAG	UNP Q13614
A	647	LEU	-	EXPRESSION TAG	UNP Q13614
A	648	GLU	-	EXPRESSION TAG	UNP Q13614
A	649	HIS	-	EXPRESSION TAG	UNP Q13614
A	650	HIS	-	EXPRESSION TAG	UNP Q13614
A	651	HIS	-	EXPRESSION TAG	UNP Q13614
A	652	HIS	-	EXPRESSION TAG	UNP Q13614
A	653	HIS	-	EXPRESSION TAG	UNP Q13614
A	654	HIS	-	EXPRESSION TAG	UNP Q13614
B	-2	MET	-	CLONING ARTIFACT	UNP Q13614
B	-1	ALA	-	CLONING ARTIFACT	UNP Q13614
B	0	SER	-	CLONING ARTIFACT	UNP Q13614
B	417	SER	CYS	ENGINEERED	UNP Q13614
B	644	ALA	-	EXPRESSION TAG	UNP Q13614
B	645	ALA	-	EXPRESSION TAG	UNP Q13614
B	646	ALA	-	EXPRESSION TAG	UNP Q13614
B	647	LEU	-	EXPRESSION TAG	UNP Q13614
B	648	GLU	-	EXPRESSION TAG	UNP Q13614
B	649	HIS	-	EXPRESSION TAG	UNP Q13614

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Chain	Residue	Modelled	Actual	Comment	Reference
B	650	HIS	-	EXPRESSION TAG	UNP Q13614
B	651	HIS	-	EXPRESSION TAG	UNP Q13614
B	652	HIS	-	EXPRESSION TAG	UNP Q13614
B	653	HIS	-	EXPRESSION TAG	UNP Q13614
B	654	HIS	-	EXPRESSION TAG	UNP Q13614

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	146	Total O 146 146	0	0
3	B	88	Total O 88 88	0	0



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	158.25Å 82.66Å 100.13Å 90.00° 117.93° 90.00°	Depositor
Resolution (Å)	8.00 – 2.60	Depositor
% Data completeness (in resolution range)	98.1 (8.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.207 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8632	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

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	0.73	13/4300 (0.3%)	0.80	8/5829 (0.1%)
1	B	0.77	13/4300 (0.3%)	0.81	8/5829 (0.1%)
All	All	0.75	26/8600 (0.3%)	0.80	16/11658 (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	7
1	B	0	2
All	All	0	9

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	554	PRO	N-CD	-18.06	1.22	1.47
1	A	220	ILE	CA-C	-6.00	1.37	1.52
1	B	323	PRO	N-CD	5.38	1.55	1.47
1	B	251	PRO	N-CD	5.37	1.55	1.47
1	B	585	PRO	N-CD	5.37	1.55	1.47

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	ILE	CB-CA-C	7.91	127.42	111.60
1	A	571	ARG	NE-CZ-NH2	6.81	123.70	120.30
1	A	459	ARG	NE-CZ-NH2	6.79	123.69	120.30
1	B	582	ARG	NE-CZ-NH2	6.68	123.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	459	ARG	NE-CZ-NH2	6.63	123.61	120.30

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	149	TYR	Mainchain
1	A	180	MET	Mainchain
1	A	220	ILE	Mainchain,Peptide
1	A	315	LYS	Mainchain
1	A	453	TRP	Mainchain

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	4189	0	4113	319	0
1	B	4189	0	4113	392	0
2	A	10	0	0	2	0
2	B	10	0	0	1	0
3	A	146	0	0	16	0
3	B	88	0	0	14	0
All	All	8632	0	8226	707	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 43.

The worst 5 of 707 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:317:PHE:CE1	1:A:405:LYS:HD2	1.60	1.36
1:A:454:LEU:HD13	3:A:1207:HOH:O	1.38	1.23
1:B:393:LYS:HG3	1:B:568:ALA:O	1.37	1.20
1:A:261:PHE:O	1:A:288:MET:HG2	1.42	1.16
1:B:370:VAL:CG1	1:B:581:ILE:HG12	1.75	1.14

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	511/657 (78%)	460 (90%)	44 (9%)	7 (1%)	14	28
1	B	511/657 (78%)	462 (90%)	36 (7%)	13 (2%)	7	12
All	All	1022/1314 (78%)	922 (90%)	80 (8%)	20 (2%)	9	18

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	221	PRO
1	A	223	GLU
1	A	559	TYR
1	B	344	GLN
1	B	548	LEU

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	A	456/584 (78%)	432 (95%)	24 (5%)	28	53
1	B	456/584 (78%)	442 (97%)	14 (3%)	47	76
All	All	912/1168 (78%)	874 (96%)	38 (4%)	36	65

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	423	ARG
1	A	552	THR
1	B	421	TRP
1	A	459	ARG
1	A	574	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	231	ASN
1	B	326	ASN
1	B	545	ASN
1	B	314	HIS
1	B	354	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](#)

4 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
2	PO4	A	655	-	4,4,4	1.22	0	6,6,6	0.27	0
2	PO4	A	656	-	4,4,4	1.23	0	6,6,6	0.27	0
2	PO4	B	655	-	4,4,4	1.23	0	6,6,6	0.27	0
2	PO4	B	656	-	4,4,4	1.23	0	6,6,6	0.27	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	PO4	A	655	-	-	0/0/0/0	0/0/0/0
2	PO4	A	656	-	-	0/0/0/0	0/0/0/0
2	PO4	B	655	-	-	0/0/0/0	0/0/0/0
2	PO4	B	656	-	-	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.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	656	PO4	2	0
2	B	656	PO4	1	0

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.