



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:49 AM UTC

PDB ID : 5MV8 / pdb_00005mv8
Title : Structure of human Myosin 7b C-terminal MyTH4-FERM domain in complex with harmonin-a PDZ3 domain
Authors : Yu, I.; Sourigues, Y.; Titus, M.A.; Houdusse, A.
Deposited on : 2017-01-16
Resolution : 1.88 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 types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

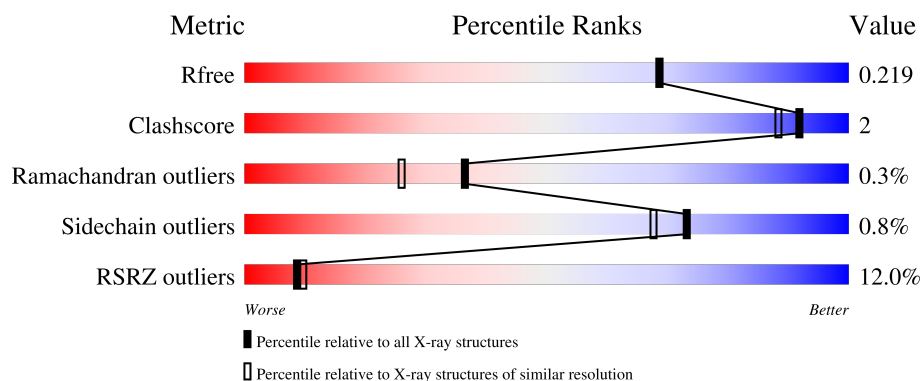
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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}	180053	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	527	9% 87% 9%
2	B	130	19% 85% 8% 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5206 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 Unconventional myosin-VIIb.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	479	3897	2523	662	691	21	0	13	0

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	initiating methionine	UNP Q6PIF6
A	-4	GLY	-	expression tag	UNP Q6PIF6
A	-3	SER	-	expression tag	UNP Q6PIF6
A	-2	SER	-	expression tag	UNP Q6PIF6
A	-1	HIS	-	expression tag	UNP Q6PIF6
A	0	HIS	-	expression tag	UNP Q6PIF6
A	1	HIS	-	expression tag	UNP Q6PIF6
A	2	HIS	-	expression tag	UNP Q6PIF6
A	3	HIS	-	expression tag	UNP Q6PIF6
A	4	HIS	-	expression tag	UNP Q6PIF6
A	5	HIS	-	expression tag	UNP Q6PIF6
A	6	SER	-	expression tag	UNP Q6PIF6
A	7	SER	-	expression tag	UNP Q6PIF6
A	8	HIS	-	expression tag	UNP Q6PIF6
A	9	HIS	-	expression tag	UNP Q6PIF6
A	1605	LYS	-	expression tag	UNP Q6PIF6
A	1606	GLU	-	expression tag	UNP Q6PIF6
A	1607	LYS	-	expression tag	UNP Q6PIF6
A	1608	LEU	-	expression tag	UNP Q6PIF6
A	1660	ASP	ASN	conflict	UNP Q6PIF6
A	1665	ASN	ASP	conflict	UNP Q6PIF6
A	1669	GLU	GLN	conflict	UNP Q6PIF6
A	1786	GLU	GLN	conflict	UNP Q6PIF6

- Molecule 2 is a protein called cDNA FLJ51329, highly similar to Harmonin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	120	Total	C	N	O	S	0	3	0
			892	575	140	173	4			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	423	GLY	-	expression tag	UNP B4DV53
B	424	ALA	-	expression tag	UNP B4DV53
B	425	MET	-	expression tag	UNP B4DV53
B	426	GLY	-	expression tag	UNP B4DV53
B	427	SER	-	expression tag	UNP B4DV53

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Mg 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	306	Total 306	O 306	0	0
5	B	74	Total 74	O 74	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.62Å 42.56Å 118.17Å 90.00° 98.02° 90.00°	Depositor
Resolution (Å)	35.33 – 1.88 35.33 – 1.88	Depositor EDS
% Data completeness (in resolution range)	94.9 (35.33-1.88) 95.5 (35.33-1.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 1.88Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.190 , 0.219 (Not available) , 0.219	Depositor DCC
R_{free} test set	2676 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	32.7	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5206	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.46% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.83	0/4041	1.16	3/5486 (0.1%)
2	B	0.81	0/918	1.15	5/1250 (0.4%)
All	All	0.82	0/4959	1.16	8/6736 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1619	PHE	CA-CB-CG	5.38	119.18	113.80
1	A	1685	GLN	CA-C-N	5.36	131.78	121.54
1	A	1685	GLN	C-N-CA	5.36	131.78	121.54
2	B	473	ASP	CA-CB-CG	5.31	117.91	112.60
2	B	488	GLY	CA-C-N	5.19	131.46	121.54
2	B	488	GLY	C-N-CA	5.19	131.46	121.54
2	B	472	VAL	CA-C-N	5.01	129.91	121.14
2	B	472	VAL	C-N-CA	5.01	129.91	121.14

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	3897	0	3826	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	892	0	852	5	0
3	A	30	0	40	2	0
3	B	6	0	8	0	0
4	A	1	0	0	0	0
5	A	306	0	0	2	0
5	B	74	0	0	0	0
All	All	5206	0	4726	15	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 2.

All (15) 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:1964:ASN:HB2	3:A:2205:GOL:H31	1.68	0.76
1:A:1964:ASN:HD22	3:A:2205:GOL:H12	1.56	0.70
2:B:465:ASP:HB3	2:B:485:TYR:HB2	1.86	0.56
1:A:1943:PHE:CE2	1:A:1956:ILE:HD11	2.41	0.56
1:A:1875:PRO:HG2	2:B:485:TYR:HA	1.89	0.53
1:A:1928:ARG:HD2	1:A:1969[A]:MET:HE3	1.93	0.51
1:A:1819:THR:HB	5:A:2408:HOH:O	2.13	0.48
1:A:2029:ALA:HB3	1:A:2036:LEU:HB2	1.97	0.46
2:B:501:GLU:HB3	2:B:538:ALA:HB3	1.98	0.45
1:A:1872:LYS:O	2:B:485:TYR:HE1	2.00	0.45
1:A:1740:LEU:HD11	1:A:1784:PRO:HD3	1.99	0.44
1:A:1980[A]:LEU:HG	5:A:2406:HOH:O	2.18	0.42
1:A:1932:ILE:HD11	1:A:1969[B]:MET:HE1	2.02	0.41
1:A:2002:CYS:HA	1:A:2007:PHE:CG	2.55	0.41
2:B:504:ALA:HB3	2:B:536:VAL:HB	2.02	0.41

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	484/527 (92%)	472 (98%)	11 (2%)	1 (0%)	43	34
2	B	122/130 (94%)	117 (96%)	4 (3%)	1 (1%)	16	5
All	All	606/657 (92%)	589 (97%)	15 (2%)	2 (0%)	36	26

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1686	ALA
2	B	526	TRP

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	324/471 (69%)	321 (99%)	3 (1%)	70	63
2	B	75/103 (73%)	75 (100%)	0	100	100
All	All	399/574 (70%)	396 (99%)	3 (1%)	73	68

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1950	LEU
1	A	2000	TRP
1	A	2046	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	4	HIS
1	A	1795	ASN

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Mol	Chain	Res	Type
1	A	1944	ASN
1	A	1964	ASN
1	A	2033	HIS
2	B	493	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 for Mogul analysis.

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	GOL	A	2204	-	5,5,5	0.10	0	5,5,5	0.18	0
3	GOL	A	2203	-	5,5,5	0.11	0	5,5,5	0.17	0
3	GOL	A	2201	-	5,5,5	0.05	0	5,5,5	0.12	0
3	GOL	B	601	-	5,5,5	0.08	0	5,5,5	0.17	0
3	GOL	A	2202	-	5,5,5	0.07	0	5,5,5	0.13	0
3	GOL	A	2205	-	5,5,5	0.08	0	5,5,5	0.28	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
3	GOL	A	2204	-	-	0/4/4/4	-
3	GOL	A	2203	-	-	2/4/4/4	-
3	GOL	A	2201	-	-	0/4/4/4	-
3	GOL	B	601	-	-	0/4/4/4	-
3	GOL	A	2202	-	-	0/4/4/4	-
3	GOL	A	2205	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2203	GOL	C1-C2-C3-O3
3	A	2203	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2205	GOL	2	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

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	479/527 (90%)	0.60	47 (9%) 13 15	18, 38, 77, 110	13 (2%)
2	B	120/130 (92%)	0.99	25 (20%) 2 2	15, 44, 85, 100	3 (2%)
All	All	599/657 (91%)	0.68	72 (12%) 9 10	15, 40, 79, 110	16 (2%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1875	PRO	5.3
1	A	1	HIS	5.0
1	A	2099	LEU	4.9
1	A	1682	PRO	4.9
1	A	1683	SER	4.9
1	A	1686	ALA	4.6
1	A	2100	SER	4.6
2	B	526	TRP	4.3
1	A	2068	LEU	4.2
1	A	1661	VAL	4.1
1	A	1681	TYR	4.0
1	A	1687	TRP	3.9
1	A	1663	LEU	3.9
1	A	2098	LEU	3.6
2	B	494	GLY	3.6
1	A	1882	VAL	3.5
2	B	525	ALA	3.5
1	A	0	HIS	3.4
1	A	2	HIS	3.4
1	A	1872	LYS	3.4
1	A	1623	GLU	3.3
2	B	433	TYR	3.2
1	A	1873	ASN	3.2
1	A	1656	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	435	GLU	3.1
2	B	532	TRP	3.1
1	A	1667	ALA	3.0
2	B	458	ILE	3.0
2	B	491	GLU	2.9
1	A	1955	LYS	2.9
1	A	1953	VAL	2.9
2	B	462	GLY	2.9
1	A	2075	SER	2.8
1	A	1871	LYS	2.8
2	B	436	GLY	2.6
1	A	1950	LEU	2.6
2	B	464	LEU	2.6
1	A	1619	PHE	2.6
2	B	489	ALA	2.6
1	A	1664	TRP	2.5
1	A	1954	PRO	2.5
2	B	473	ASP	2.5
1	A	1649	LEU	2.5
2	B	529	GLY	2.5
1	A	1870	VAL	2.5
2	B	531	ASP	2.5
1	A	1666	ILE	2.5
2	B	527	ASN	2.4
1	A	1874	LYS	2.4
1	A	1951	ALA	2.4
2	B	535	LEU	2.4
1	A	2054	ILE	2.4
1	A	1622	PRO	2.4
2	B	490	ALA	2.3
1	A	1869	TRP	2.3
1	A	2055	SER	2.2
1	A	1712	CYS	2.2
1	A	1883	THR	2.2
1	A	1848	ASP	2.2
2	B	533	ILE	2.2
1	A	1684	ARG	2.2
2	B	459	LYS	2.1
1	A	1650	ARG	2.1
2	B	530	GLY	2.1
1	A	1660	ASP	2.1
1	A	2049	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	2045	LEU	2.1
1	A	3	HIS	2.0
2	B	495	GLY	2.0
2	B	523	GLN	2.0
2	B	456	LEU	2.0
2	B	457	ARG	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	GOL	A	2205	6/6	0.57	0.25	82,83,84,85	0
3	GOL	A	2201	6/6	0.63	0.28	107,107,107,108	0
3	GOL	A	2202	6/6	0.67	0.18	69,72,74,76	0
3	GOL	B	601	6/6	0.81	0.24	64,67,70,73	0
3	GOL	A	2204	6/6	0.83	0.11	57,63,66,69	0
4	MG	A	2206	1/1	0.85	0.14	73,73,73,73	0
3	GOL	A	2203	6/6	0.86	0.11	50,56,56,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.