



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 5HMO / pdb_00005hmo
Title : myosin X motor activity
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Deposited on : 2016-01-16
Resolution : 3.49 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
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

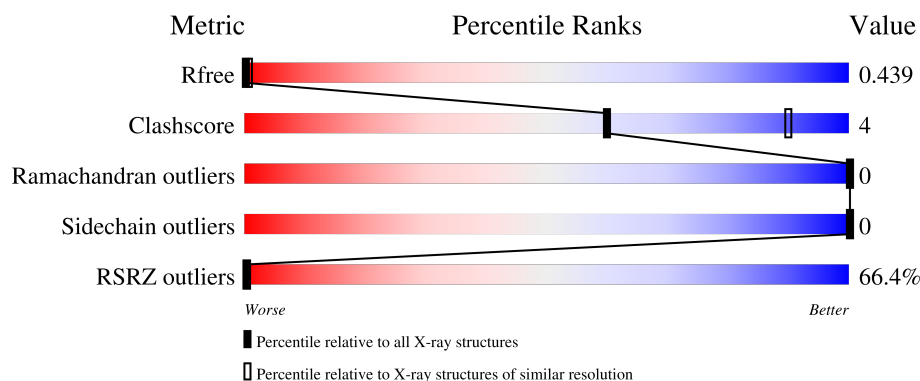
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.49 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	134	63% 84% 13% .
1	C	134	62% 80% 11% 9%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1946 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-X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	131	Total	C	N	O	S	0	0	0
			961	575	177	208	1			
1	C	122	Total	C	N	O	S	0	0	0
			985	590	189	205	1			

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	69.81Å 69.81Å 236.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.50 – 3.49 45.50 – 3.49	Depositor EDS
% Data completeness (in resolution range)	98.8 (45.50-3.49) 99.7 (45.50-3.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 3.48Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.391 , 0.437 0.391 , 0.439	Depositor DCC
R_{free} test set	401 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	126.1	Xtriage
Anisotropy	0.781	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 349.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	1946	wwPDB-VP
Average B, all atoms (Å ²)	193.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.27% 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

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	0.82	0/961	1.51	4/1289 (0.3%)
1	C	0.79	0/985	1.49	7/1307 (0.5%)
All	All	0.81	0/1946	1.50	11/2596 (0.4%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	876	SER	N-CA-C	-6.66	105.16	113.55
1	C	888	VAL	N-CA-C	-6.13	105.08	111.58
1	A	876	SER	N-CA-C	-6.04	105.94	113.55
1	C	885	ASN	CA-CB-CG	5.71	118.31	112.60
1	A	888	VAL	N-CA-C	-5.53	105.72	111.58
1	A	884	GLU	CA-C-N	5.47	127.56	120.44
1	A	884	GLU	C-N-CA	5.47	127.56	120.44
1	C	811	LEU	CA-C-N	5.08	130.03	122.82
1	C	811	LEU	C-N-CA	5.08	130.03	122.82
1	C	852	GLN	CA-C-N	5.04	127.04	120.28
1	C	852	GLN	C-N-CA	5.04	127.04	120.28

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	961	0	826	12	0
1	C	985	0	941	9	0
All	All	1946	0	1767	16	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 4.

All (16) 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:905:LYS:HB3	1:C:894:LEU:HD13	1.58	0.85
1:A:898:ILE:HD13	1:C:901:LEU:O	1.80	0.80
1:A:867:GLN:HE21	1:A:871:ARG:HH21	1.44	0.66
1:A:892:LEU:HD22	1:C:923:LEU:HD23	1.77	0.65
1:C:894:LEU:O	1:C:898:ILE:HG12	2.03	0.59
1:A:894:LEU:O	1:A:898:ILE:HG12	2.03	0.58
1:A:854:GLU:O	1:A:858:LYS:HB2	2.10	0.52
1:A:898:ILE:HG21	1:C:901:LEU:O	2.10	0.51
1:C:914:GLU:HG2	1:C:917:LEU:HD22	1.94	0.50
1:A:914:GLU:HG2	1:A:917:LEU:HD22	1.94	0.50
1:A:898:ILE:CD1	1:C:901:LEU:O	2.56	0.49
1:C:854:GLU:O	1:C:858:LYS:HB2	2.15	0.47
1:A:905:LYS:O	1:A:909:GLU:HG2	2.19	0.43
1:A:853:GLU:HG3	1:A:857:ARG:HH11	1.85	0.42
1:A:829:LYS:O	1:A:833:GLU:HG3	2.21	0.40
1:C:879:LEU:HD12	1:C:883:LYS:HB2	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 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	129/134 (96%)	119 (92%)	10 (8%)	0	100	100
1	C	120/134 (90%)	112 (93%)	8 (7%)	0	100	100
All	All	249/268 (93%)	231 (93%)	18 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	80/122 (66%)	80 (100%)	0	100	100
1	C	95/122 (78%)	95 (100%)	0	100	100
All	All	175/244 (72%)	175 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	852	GLN
1	A	867	GLN
1	A	870	GLN
1	A	882	GLN
1	A	908	GLN
1	C	852	GLN
1	C	870	GLN
1	C	882	GLN
1	C	908	GLN

5.3.3 RNA ⓘ

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.

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	131/134 (97%)	3.21	85 (64%) 0 0	148, 194, 222, 233	0
1	C	122/134 (91%)	3.72	83 (68%) 0 0	143, 195, 220, 232	0
All	All	253/268 (94%)	3.45	168 (66%) 0 0	143, 195, 222, 233	0

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	835	GLU	12.9
1	C	847	GLU	12.4
1	C	854	GLU	12.1
1	A	803	ILE	11.8
1	C	815	LYS	11.3
1	A	859	GLN	11.2
1	C	908	GLN	10.4
1	C	858	LYS	9.7
1	A	920	LEU	9.6
1	A	909	GLU	8.7
1	C	842	GLU	8.6
1	A	840	GLU	8.4
1	C	861	GLU	8.1
1	A	867	GLN	7.9
1	A	892	LEU	7.8
1	A	862	LEU	7.6
1	A	888	VAL	7.6
1	C	891	ILE	7.5
1	C	905	LYS	7.4
1	C	878	GLU	7.3
1	A	887	GLN	7.3
1	C	887	GLN	6.9
1	C	924	ARG	6.8
1	C	893	ARG	6.7

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Mol	Chain	Res	Type	RSRZ
1	C	827	GLU	6.7
1	C	888	VAL	6.7
1	A	802	GLN	6.6
1	A	808	TYR	6.6
1	A	848	LEU	6.5
1	C	863	GLU	6.5
1	C	811	LEU	6.4
1	A	868	GLU	6.4
1	A	910	LEU	6.4
1	C	892	LEU	6.3
1	A	880	GLU	6.3
1	C	866	GLN	6.3
1	C	875	LEU	6.2
1	A	901	LEU	6.2
1	A	863	GLU	6.1
1	C	895	GLU	6.1
1	C	883	LYS	6.1
1	A	923	LEU	6.0
1	C	882	GLN	6.0
1	A	893	ARG	6.0
1	A	833	GLU	5.9
1	C	904	MET	5.8
1	C	920	LEU	5.8
1	C	843	ARG	5.8
1	C	845	GLU	5.8
1	C	859	GLN	5.7
1	C	889	GLU	5.6
1	A	908	GLN	5.5
1	C	831	LYS	5.5
1	A	814	GLU	5.5
1	C	876	SER	5.3
1	C	897	GLU	5.1
1	A	904	MET	5.1
1	A	861	GLU	5.1
1	C	870	GLN	5.0
1	A	845	GLU	5.0
1	C	901	LEU	4.9
1	C	894	LEU	4.9
1	A	894	LEU	4.9
1	A	897	GLU	4.9
1	C	851	GLN	4.8
1	C	820	GLU	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	898	ILE	4.6
1	C	898	ILE	4.6
1	C	862	LEU	4.5
1	C	855	ALA	4.5
1	A	883	LYS	4.5
1	A	877	ARG	4.4
1	C	871	ARG	4.4
1	A	799	LEU	4.4
1	C	909	GLU	4.4
1	A	899	GLU	4.3
1	A	896	LYS	4.2
1	A	869	SER	4.2
1	C	917	LEU	4.1
1	A	902	GLN	4.0
1	C	919	LYS	4.0
1	A	864	ALA	4.0
1	A	872	ALA	4.0
1	C	864	ALA	3.9
1	A	828	GLU	3.9
1	A	806	ARG	3.8
1	C	838	GLU	3.8
1	A	807	VAL	3.7
1	C	890	GLU	3.7
1	C	916	SER	3.7
1	C	910	LEU	3.7
1	C	828	GLU	3.7
1	A	922	GLN	3.7
1	C	867	GLN	3.7
1	C	836	GLU	3.6
1	A	827	GLU	3.5
1	C	834	GLU	3.4
1	A	832	ARG	3.4
1	A	903	ARG	3.3
1	A	921	GLN	3.3
1	C	879	LEU	3.3
1	C	874	GLU	3.3
1	A	916	SER	3.3
1	C	869	SER	3.3
1	C	860	ARG	3.3
1	A	870	GLN	3.2
1	C	915	ALA	3.2
1	A	810	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	905	LYS	3.1
1	C	886	LYS	3.1
1	C	865	LEU	3.1
1	A	825	GLU	3.0
1	A	842	GLU	3.0
1	C	852	GLN	3.0
1	C	880	GLU	2.9
1	A	876	SER	2.9
1	C	899	GLU	2.9
1	A	820	GLU	2.9
1	A	891	ILE	2.9
1	A	858	LYS	2.9
1	C	872	ALA	2.9
1	C	841	ARG	2.9
1	A	906	GLU	2.9
1	A	900	ASP	2.8
1	C	833	GLU	2.8
1	A	911	SER	2.8
1	C	823	LYS	2.8
1	A	912	LEU	2.8
1	C	885	ASN	2.7
1	A	854	GLU	2.7
1	A	895	GLU	2.7
1	A	856	ALA	2.7
1	A	836	GLU	2.7
1	C	906	GLU	2.7
1	A	834	GLU	2.6
1	A	875	LEU	2.6
1	A	822	ARG	2.6
1	A	865	LEU	2.5
1	A	852	GLN	2.5
1	A	826	GLU	2.5
1	C	913	THR	2.5
1	A	917	LEU	2.5
1	A	913	THR	2.5
1	A	835	GLU	2.4
1	A	855	ALA	2.4
1	C	817	ALA	2.4
1	C	825	GLU	2.3
1	C	857	ARG	2.3
1	A	866	GLN	2.3
1	A	829	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	926	GLU	2.3
1	C	850	ALA	2.3
1	C	812	LEU	2.3
1	A	907	ARG	2.3
1	C	923	LEU	2.2
1	A	857	ARG	2.2
1	A	871	ARG	2.2
1	C	900	ASP	2.2
1	C	819	GLU	2.2
1	A	915	ALA	2.2
1	C	928	LEU	2.2
1	A	851	GLN	2.2
1	A	831	LYS	2.1
1	A	823	LYS	2.1
1	A	885	ASN	2.1
1	C	822	ARG	2.1
1	C	848	LEU	2.1
1	A	847	GLU	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.