

wwPDB X-ray Structure Validation Summary Report (i)

Oct 14, 2020 - 11:03 PM BST

PDB ID	:	6Z7T
Title	:	Nucleotide-free Myosin-II motor domain
Authors	:	Ewert, W.; Preller, M.
Deposited on	:	2020-06-01
Resolution	:	1.88 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 https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 24654 atoms, of which 11696 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 Myosin-2 heavy chain.

Mol	Chain	Residues			Aton	ns	ZeroOcc	AltConf	Trace		
1	Λ	796	Total	С	Η	Ν	Ο	S	0	8	0
		120	11523	3695	5711	995	1105	17	0		
1	В	730	Total	С	Η	Ν	Ο	S	0	4	0
	В 730		11613	3719	5763	1001	1113	17	0	±	0

Chain	Residue	Modelled	Actual	$\mathbf{Comment}$	Reference
A	-10	MET	-	initiating methionine	UNP P08799
A	-9	HIS	-	expression tag	UNP P08799
A	-8	HIS	-	expression tag	UNP P08799
A	-7	HIS	-	expression tag	UNP P08799
A	-6	HIS	-	expression tag	UNP P08799
A	-5	HIS	-	expression tag	UNP P08799
A	-4	HIS	-	expression tag	UNP P08799
A	-3	HIS	-	expression tag	UNP P08799
A	-2	ASP	-	expression tag	UNP P08799
A	-1	GLY	-	expression tag	UNP P08799
А	0	THR	-	expression tag	UNP P08799
A	1	GLU	-	expression tag	UNP P08799
A	762	LEU	-	expression tag	UNP P08799
A	763	GLU	-	expression tag	UNP P08799
A	764	SER	-	expression tag	UNP P08799
A	765	ASN	-	expression tag	UNP P08799
A	766	GLU	-	expression tag	UNP P08799
A	767	PRO	-	expression tag	UNP P08799
A	768	PRO	-	expression tag	UNP P08799
A	769	MET	-	expression tag	UNP P08799
A	770	ASP	-	expression tag	UNP P08799
A	771	PHE	-	expression tag	UNP P08799
A	772	ASP	-	expression tag	UNP P08799
A	773	ASP	-	expression tag	UNP P08799
А	774	ASP	-	expression tag	UNP P08799

There are 56 discrepancies between the modelled and reference sequences:

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Chain	Residue	Modelled	Actual	Comment	Reference
А	775	ILE	-	expression tag	UNP P08799
А	776	PRO	-	expression tag	UNP P08799
А	777	PHE	-	expression tag	UNP P08799
В	-10	MET	-	initiating methionine	UNP P08799
В	-9	HIS	-	expression tag	UNP P08799
В	-8	HIS	-	expression tag	UNP P08799
В	-7	HIS	-	expression tag	UNP P08799
В	-6	HIS	-	expression tag	UNP P08799
В	-5	HIS	-	expression tag	UNP P08799
В	-4	HIS	-	expression tag	UNP P08799
В	-3	HIS	-	expression tag	UNP P08799
В	-2	ASP	-	expression tag	UNP P08799
В	-1	GLY	-	expression tag	UNP P08799
В	0	THR	-	expression tag	UNP P08799
В	1	GLU	-	expression tag	UNP P08799
В	762	LEU	-	expression tag	UNP P08799
В	763	GLU	-	expression tag	UNP P08799
В	764	SER	-	expression tag	UNP P08799
В	765	ASN	-	expression tag	UNP P08799
В	766	GLU	-	expression tag	UNP P08799
В	767	PRO	-	expression tag	UNP P08799
В	768	PRO	-	expression tag	UNP P08799
В	769	MET	-	expression tag	UNP P08799
В	770	ASP	-	expression tag	UNP P08799
В	771	PHE	-	expression tag	UNP P08799
В	772	ASP	-	expression tag	UNP P08799
В	773	ASP	-	expression tag	UNP P08799
В	774	ASP	-	expression tag	UNP P08799
В	775	ILE	-	expression tag	UNP P08799
В	776	PRO	-	expression tag	UNP P08799
В	777	PHE	-	expression tag	UNP P08799

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• Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	2	Total Mg 2 2	0	0
2	А	2	Total Mg 2 2	0	0

• Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).





Mol	Chain	Residues	A	ton	ns		ZeroOcc	AltConf
2	Δ	1	Total	С	Η	Ο	0	0
3	A	1	10	2	6	2	0	0
2	Λ	1	Total	С	Η	Ο	0	0
3	A		10	2	6	2	0	0
9	Λ	1	Total	С	Η	Ο	0	0
	A		10	2	6	2	0	0
2	Δ	1	Total	С	Η	Ο	0	0
	A	L	10	2	6	2	0	0
2	Λ	1	Total	С	Η	Ο	0	0
J J	A	L	10	2	6	2	0	0
2	Δ	1	Total	С	Η	Ο	0 0	0
J J	A	L	10	2	6	2		0
2	Δ	1	Total	С	Η	Ο	0	0
J J	A	L	10	2	6	2	0	0
2	Δ	1	Total	С	Η	Ο	0	0
J J	A	L	10	2	6	2	0	
2	Δ	1	Total	С	Η	Ο	0	0
J J	A	L	10	2	6	2	0	0
9	Λ	1	Total	С	Η	Ο	0	0
3	A	L	10	2	6	2	0	0
9	D	1	Total	С	Η	Ο	0	0
3	D	L	10	2	6	2	0	0
9	D	1	Total	С	Η	Ο	0	0
3	D	L	10	2	6	2	U	0
3	В	1	Total	С	Η	Ο	0	0
³	D		10	2	6	2	0	U
2	В	1	Total	С	Η	Ο	0	0
O	D		10	2	6	2	U	U

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Mol	Chain	Residues	A	ton	ns		ZeroOcc	AltConf	
2	В	1	Total	С	Η	Ο	0	0	
J	5 В	L	10	2	6	2	0	0	
2	В	1	Total	С	Η	Ο	0	0	
0	D	L	10	2	6	2	0	0	
2	В	1	Total	С	Η	Ο	Ο	0	
0	o D	L	10	2	6	2	0	0	
2	В	1	Total	С	Η	Ο	0	0	
J	D		10	2	6	2	0		
3	В	1	Total	С	Η	Ο	0	0	
5	D	T	10	2	6	2	0	0	
3	В	1	Total	С	Η	O	0	0	
0			10	2	6	2			

• Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
4	Δ	1	Total C H O	0	0	
4 11	L	14 3 8 3	0	0		
1	Δ	1	Total C H O	0	0	
	11	I	14 3 8 3	0	0	
4	Δ	Λ	1	Total C H O	0	0
4	Л	T	13 3 7 3		0	
4	Λ	1	Total C H O	0	0	
4 7	T	14 3 8 3	0			
4	4 A	1	Total C H O	0	0	
4		1	14 3 8 3	0	0	

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Mol	Chain	Residues	A	ton	ns		ZeroOcc	AltConf
4	В	1	Total	С	Η	Ο	0	0
4	D	L	14	3	8	3	0	0
4	В	1	Total	С	Η	Ο	0	0
4	D	L	14	3	8	3	0	
4	В	1	Total	С	Η	Ο	0	0
4	D	L	13	3	7	3		
4	В	1	Total	С	Η	Ο	0	0
4	D	T	14	3	8	3	0	0
4	4 D	1	Total	С	Η	Ο	0	0
1 4			14	3	8	3		0

• Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	В	1	Total	С	Η	Ο	0	0
0	D	T	24	6	14	4	0	0

• Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	В	1	Total	С	Η	Ο	0	0
0	D	L	17	4	10	3	0	0

• Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	555	Total O 555 555	0	0
7	В	580	Total O 580 580	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.



3 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 1 21 1	Depositor	
Cell constants	$56.68 \mathrm{\AA}$ 174.40 $\mathrm{\AA}$ 100.25 $\mathrm{\AA}$	Depositor	
a, b, c, α , β , γ	90.00° 106.38° 90.00°	Depositor	
Resolution (Å)	46.36 - 1.88	Depositor	
% Data completeness	98 5 (46 36-1 88)	Depositor	
(in resolution range)	30.0 (40.00-1.00)	Depositor	
R _{merge}	(Not available)	Depositor	
R _{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	$0.80 (at 1.88 \text{\AA})$	Xtriage	
Refinement program	PHENIX 1.17.1_3660	Depositor	
R, R_{free}	0.191 , 0.217	Depositor	
Wilson B-factor $(Å^2)$	23.0	Xtriage	
Anisotropy	0.571	Xtriage	
L-test for twinning ²	$< L > = 0.47, < L^2 > = 0.29$	Xtriage	
Estimated twinning fraction	0.249 for h,-k,-h-l	Xtriage	
Total number of atoms	24654	wwPDB-VP	
Average B, all atoms $(Å^2)$	43.0	wwPDB-VP	

EDS failed to run properly - this section is therefore incomplete.

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 9.53% of the height of the origin peak. No significant pseudotranslation is detected.

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.



 $^{^1 \}mathrm{Intensities}$ estimated from amplitudes.

4 Model quality (i)

4.1 Standard geometry (i)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts (i)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

Of 36 ligands modelled in this entry, 4 are monoatomic - leaving 32 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



					Bond lengths			Bond angles			
Mol	Type	Chain	Res	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
3	EDO	A	805	-	3,3,3	0.38	0	2,2,2	0.55	0	
3	EDO	A	812	-	3,3,3	0.45	0	2,2,2	0.15	0	
3	EDO	В	812	-	3,3,3	0.35	0	2,2,2	0.62	0	
3	EDO	В	808	-	3,3,3	0.47	0	2,2,2	0.35	0	
4	GOL	А	813	-	5, 5, 5	0.77	0	$5,\!5,\!5$	1.49	1 (20%)	
4	GOL	А	817	-	5, 5, 5	0.76	0	$5,\!5,\!5$	0.53	0	
3	EDO	В	803	-	3, 3, 3	0.52	0	2,2,2	0.14	0	
3	EDO	А	811	-	3,3,3	0.68	0	2,2,2	0.18	0	
5	PGE	В	818	-	9,9,9	0.26	0	8,8,8	0.70	0	
3	EDO	В	805	-	3,3,3	0.47	0	2,2,2	0.35	0	
4	GOL	В	815	-	5, 5, 5	1.10	0	$5,\!5,\!5$	1.26	1 (20%)	
4	GOL	А	815	-	5, 5, 5	1.21	0	$5,\!5,\!5$	1.06	0	
3	EDO	В	811	-	3,3,3	0.61	0	$2,\!2,\!2$	0.57	0	
3	EDO	В	810	-	3,3,3	0.42	0	2,2,2	0.52	0	
4	GOL	А	814	-	5, 5, 5	1.62	1 (20%)	$5,\!5,\!5$	2.54	2(40%)	
4	GOL	В	816	-	5, 5, 5	1.17	0	$5,\!5,\!5$	1.42	1 (20%)	
4	GOL	А	816	-	5, 5, 5	1.93	3 (60%)	$5,\!5,\!5$	1.97	1 (20%)	
4	GOL	В	813	-	5, 5, 5	1.14	1 (20%)	$5,\!5,\!5$	1.10	0	
4	GOL	В	814	-	5, 5, 5	0.59	0	$5,\!5,\!5$	0.96	0	
3	EDO	А	810	-	3,3,3	0.49	0	2,2,2	0.30	0	
3	EDO	В	804	-	3,3,3	0.50	0	2,2,2	0.41	0	
3	EDO	A	806	-	3,3,3	0.50	0	2,2,2	0.27	0	
3	EDO	В	809	-	3,3,3	0.49	0	2,2,2	0.41	0	
3	EDO	А	804	-	3,3,3	0.46	0	2,2,2	0.40	0	
3	EDO	В	806	-	3,3,3	0.53	0	2,2,2	0.70	0	
3	EDO	В	807	_	3,3,3	0.63	0	2,2,2	0.36	0	
3	EDO	A	809		3,3,3	0.44	0	2,2,2	0.36	0	
3	EDO	A	803	-	3,3,3	0.33	0	2,2,2	0.48	0	
3	EDO	A	807	-	3,3,3	0.62	0	2,2,2	0.11	0	
3	EDO	A	808	-	3,3,3	0.70	0	2,2,2	0.55	0	
4	GOL	В	817	-	5,5,5	0.82	0	$5,\!5,\!5$	1.15	0	
6	PEG	B	819	-	6,6,6	0.50	0	$5,\!5,\!5$	0.27	0	

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).

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	\mathbf{Res}	Link	Chirals	Torsions	Rings
3	EDO	А	805	-	-	1/1/1/1	-
3	EDO	А	812	-	-	1/1/1/1	-
3	EDO	В	812	-	-	1/1/1/1	-
3	EDO	В	808	-	-	1/1/1/1	-
4	GOL	А	813	-	-	4/4/4/4	-
4	GOL	А	817	-	-	2/4/4/4	-
3	EDO	В	803	-	-	0/1/1/1	-
3	EDO	А	811	-	-	0/1/1/1	-
5	PGE	В	818	-	-	4/7/7/7	-
3	EDO	В	805	-	_	0/1/1/1	-
4	GOL	В	815	-	-	0/4/4/4	-
4	GOL	А	815	-	-	4/4/4/4	-
3	EDO	В	811	-	-	1/1/1/1	-
3	EDO	В	810	-	-	1/1/1/1	-
4	GOL	А	814	-	-	0/4/4/4	-
4	GOL	В	816	-	-	0/4/4/4	-
4	GOL	А	816	-	-	0/4/4/4	-
4	GOL	В	813	-	-	0/4/4/4	-
4	GOL	В	814	-	-	0/4/4/4	-
3	EDO	А	810	-	-	0/1/1/1	-
3	EDO	В	804	-	-	1/1/1/1	-
3	EDO	А	806	-	-	0/1/1/1	-
3	EDO	В	809	-	-	1/1/1/1	-
3	EDO	A	804	_	-	1/1/1/1	-
3	EDO	В	806	_	_	1/1/1/1	-
3	EDO	В	807	-	-	1/1/1/1	-
3	EDO	A	809	-	-	1/1/1/1	-
3	EDO	A	803	-	-	0/1/1/1	-
3	EDO	A	807	-	-	1/1/1/1	-
3	EDO	A	808	-	-	1/1/1/1	-
4	GOL	В	817	-	-	2/4/4/4	-
6	PEG	В	819	-	-	1/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(\text{\AA})$	Ideal(Å)
4	А	814	GOL	O2-C2	-2.80	1.35	1.43
4	А	816	GOL	C1-C2	2.74	1.63	1.51
4	А	816	GOL	O2-C2	-2.59	1.35	1.43
4	В	813	GOL	O2-C2	-2.43	1.36	1.43
4	А	816	GOL	C3-C2	2.02	1.60	1.51



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	А	814	GOL	C3-C2-C1	-4.73	93.31	111.70
4	А	816	GOL	C3-C2-C1	-3.79	96.96	111.70
4	В	816	GOL	C3-C2-C1	-2.84	100.67	111.70
4	А	813	GOL	O1-C1-C2	-2.69	97.31	110.20
4	А	814	GOL	O2-C2-C3	2.27	119.14	109.12

The worst 5 of 6 bond angle outliers are listed below:

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	А	813	GOL	O1-C1-C2-C3
4	А	813	GOL	C1-C2-C3-O3
4	А	815	GOL	O1-C1-C2-C3
4	А	815	GOL	C1-C2-C3-O3
4	В	817	GOL	O1-C1-C2-C3

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



5 Fit of model and data (i)

5.1 Protein, DNA and RNA chains (i)

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

5.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.

