



wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 10:58 PM GMT

PDB ID : 2EC6
Title : Placopecten Striated Muscle Myosin II
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Deposited on : 2007-02-10
Resolution : 3.25 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

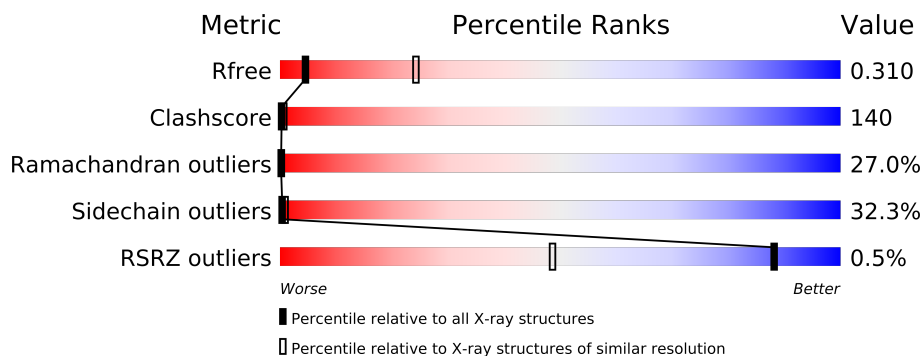
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance


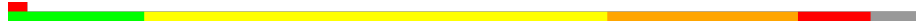

The reported resolution of this entry is 3.25 Å.

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}	66092	1085 (3.32-3.20)
Clashscore	79885	1374 (3.32-3.20)
Ramachandran outliers	78287	1348 (3.32-3.20)
Sidechain outliers	78261	1346 (3.32-3.20)
RSRZ outliers	66119	1086 (3.32-3.20)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	838	
2	B	133	
3	C	156	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8577 atoms, of which 0 are hydrogen and 0 are deuterium.

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 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	802	Total	C	N	O	S	0	0	0
			6338	4031	1084	1186	37			

- Molecule 2 is a protein called Myosin regulatory light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	126	Total	C	N	O	S	0	0	0
			979	624	154	191	10			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	49	GLU	MET	CONFLICT	UNP Q26069
B	105	ASP	LEU	CONFLICT	UNP Q26069
B	106	ALA	ASP	CONFLICT	UNP Q26069

- Molecule 3 is a protein called Myosin essential light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	155	Total	C	N	O	S	0	0	0
			1228	776	195	250	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	14	ASP	GLU	CONFLICT	UNP Q26066
C	34	LEU	ILE	CONFLICT	UNP Q26066
C	84	PHE	TYR	ENGINEERED	UNP Q26066
C	151	ALA	THR	ENGINEERED	UNP Q26066

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total 1	Ca 1	0	0

- Molecule 5 is water.

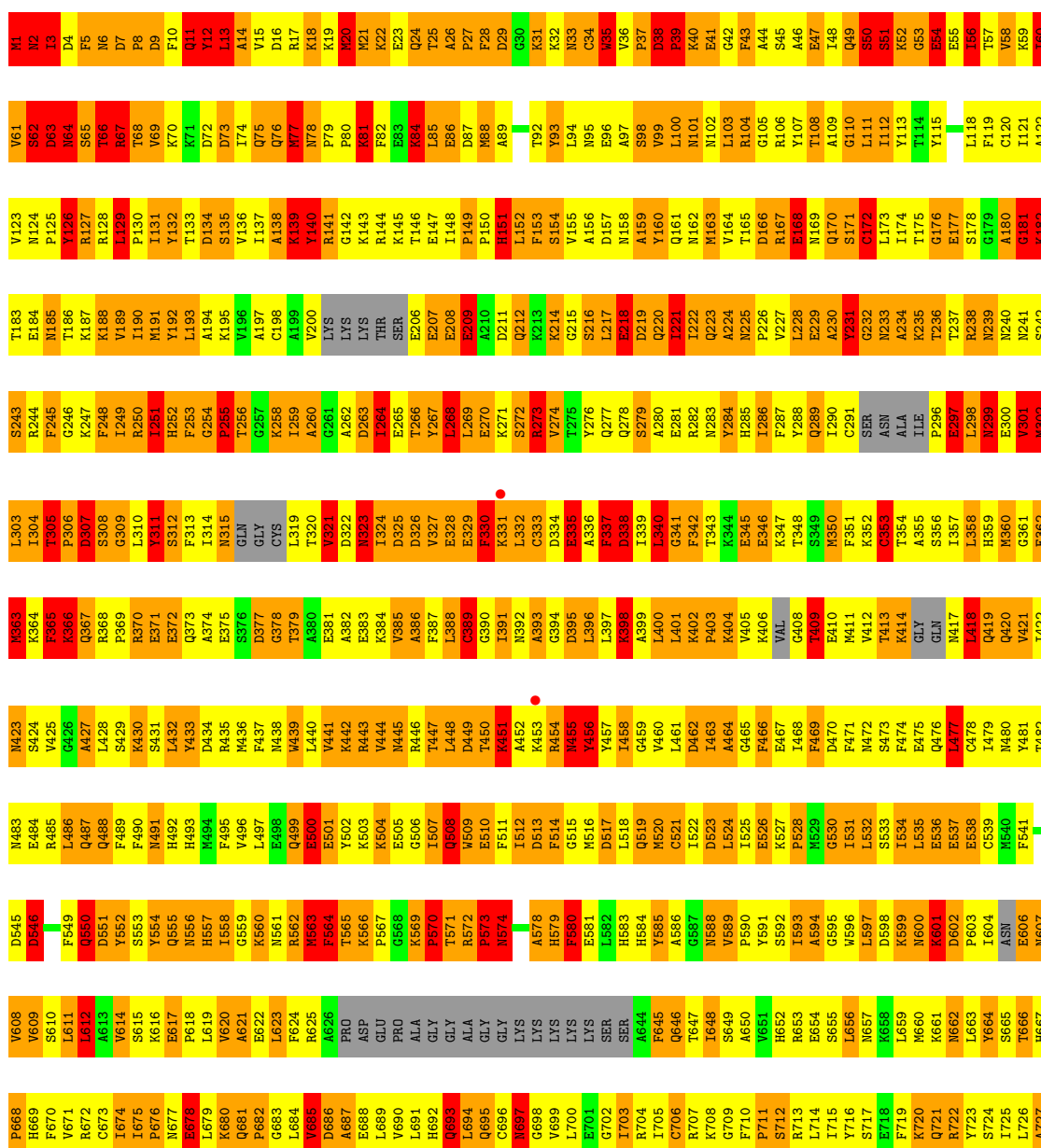
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	16	Total 16	O 16	0	0
5	B	3	Total 3	O 3	0	0
5	C	12	Total 12	O 12	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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: Myosin heavy chain

Chain A:



Q728 N729 A790 A730 I731 P732 Q733 GLY PHE VAL D737 G738 K739 A800 Y801 T740 K802 S742 E743 K744 I745 L746 T747 G749 M751 D752 P753 S754 E755 Y756 R757 L758 G759 T760 I761 K762 V763 L764 F765 F766 A767 V769 L770 G771 N772 L773 E774 K775 M776 R777 D778 E779 R780 L781 S782 K783 I784 I785 S786 M787 F788

Q789 A790 H791 I792 R793 Q794 Y795 L796 L797 K798 R799 A800 Y801 K802 K803 L804 E805 D806 Q807 R808 I809 S810 L811 S812 V813 I814 Q815 R816 N817 I818 L819 K820 W821 L822 V823 ASP L824 F825 N826 W827 Q828 W829 L830 K831 N832 Y833 A834 K835 V836 K837 P838

• Molecule 2: Myosin regulatory light chain

Chain B: 

M23 Q24 E25 M26 K27 E28 A29 F30 T31 M32 I33 D34 A35 N36 A37 D38 M39 F40 G41 I42 D43 T44 K45 L46 K47 E48 E49 S52 Y53 I54 G55 R56 T57 P58 ASP M59 LYS L62 L63 T63 A64 M65 L66 K67 E68 A69 P70 M71 G72 L73 N74 T75 T76 M77 S80 T81 P82 S83 Y84

K85 L86 T89 D90 S91 E92 E93 T94 I95 R96 N97 A98 F99 G100 M101 D102 F103 D104 I105 A106 T107 K108 L109 K110 L111 I112 E113 Y114 I115 L116 D117 L118 L119 M121 M122 G123 D124 M125 F126 M127 K128 D129 E130 M131 M132 M133 T134 F135 K136 E137 E141 K144 F145 D146 Y147 V148

R149 F150 V151 A152 M153 I154 K155

• Molecule 3: Myosin essential light chain

Chain C: 

F2 K3 L4 S5 Q6 D7 E8 I9 D10 D11 L12 K13 K14 V15 F16 E17 L18 F19 D20 F21 W22 R25 A28 V29 D30 A31 F32 K33 L34 C35 D36 V37 G38 R39 C40 L41 G42 I43 N44 P45 R46 M47 E48 D49 V50 F51 A52 V53 G54 G55 T56 H57 K58 M59 G60 E61 L64

P65 F66 E67 E68 F69 L70 P71 A72 Y73 L76 M77 D78 C79 E80 Q81 G82 T83 F84 A85 D86 Y87 E88 E89 F91 K92 T93 F94 D95 R96 E97 G98 Q99 G100 F101 I102 S103 G104 A105 E106 L107 R108 H109 V110 L111 L114 G115 E116 R117 L118 S119 D120 E121 E122 V123 D124 I125 I126

I127 M128 L129 T130 D131 L132 Q133 E134 D135 L136 E137 G138 M139 V140 K141 Y142 E143 K144 F145 V146 K147 K148 V149 P153 Y154 P155 D156 LYS

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.27Å 50.37Å 156.77Å 90.00° 101.04° 90.00°	Depositor
Resolution (Å)	20.00 – 3.25 19.94 – 3.25	Depositor EDS
% Data completeness (in resolution range)	89.4 (20.00-3.25) 89.4 (19.94-3.25)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 3.22Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.279 , 0.300 0.289 , 0.310	Depositor DCC
R_{free} test set	1851 reflections (10.90%)	DCC
Wilson B-factor (Å ²)	72.6	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 14.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 19945 reflections	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	8577	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.65	13/6463 (0.2%)	1.10	55/8722 (0.6%)
2	B	0.91	4/993 (0.4%)	1.09	8/1326 (0.6%)
3	C	0.53	0/1253	0.81	0/1686
All	All	0.67	17/8709 (0.2%)	1.06	63/11734 (0.5%)

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	24
2	B	0	1
3	C	0	1
All	All	0	26

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	456	TYR	CE1-CZ	-15.72	1.18	1.38
1	A	63	ASP	CB-CG	-11.48	1.27	1.51
2	B	105	ASP	C-N	11.45	1.60	1.34
1	A	456	TYR	CD1-CE1	-11.26	1.22	1.39
1	A	67	ARG	C-N	10.33	1.57	1.34

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	564	PHE	N-CA-C	11.40	141.79	111.00
1	A	127	ARG	N-CA-C	-11.03	81.22	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	340	LEU	CA-CB-CG	9.88	138.01	115.30
1	A	66	THR	N-CA-C	-9.72	84.75	111.00
1	A	794	GLY	N-CA-C	-8.77	91.19	113.10

There are no chirality outliers.

5 of 26 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	MET	Peptide
1	A	11	GLN	Peptide
1	A	12	TYR	Peptide
1	A	2	ASN	Peptide
1	A	8	PRO	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6338	0	6173	1960	0
2	B	979	0	936	192	0
3	C	1228	0	1149	249	0
4	C	1	0	0	0	0
5	A	16	0	0	0	0
5	B	3	0	0	0	0
5	C	12	0	0	1	0
All	All	8577	0	8258	2347	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 140.

The worst 5 of 2347 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:53:GLY:CA	1:A:54:GLU:HB2	1.39	1.43
1:A:231:TYR:HB2	1:A:437:PHE:CE1	1.56	1.40
1:A:56:ILE:HD12	1:A:57:THR:CA	1.53	1.36

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:230:ALA:N	1:A:232:GLY:HA3	1.35	1.35
1:A:103:LEU:HD23	1:A:104:ARG:N	1.43	1.31

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	784/838 (94%)	329 (42%)	224 (29%)	231 (30%)	0	0
2	B	120/133 (90%)	69 (58%)	31 (26%)	20 (17%)	0	1
3	C	153/156 (98%)	77 (50%)	42 (28%)	34 (22%)	0	0
All	All	1057/1127 (94%)	475 (45%)	297 (28%)	285 (27%)	0	0

5 of 285 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	5	PHE
1	A	7	ASP
1	A	9	ASP
1	A	11	GLN

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	671/734 (91%)	443 (66%)	228 (34%)	0	1
2	B	102/118 (86%)	76 (74%)	26 (26%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	131/132 (99%)	93 (71%)	38 (29%)	0	2
All	All	904/984 (92%)	612 (68%)	292 (32%)	0	1

5 of 292 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	447	THR
1	A	550	GLN
3	C	66	PHE
1	A	451	LYS
1	A	511	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	472	ASN
1	A	519	GLN
2	B	111	ASN
1	A	480	ASN
1	A	483	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	802/838 (95%)	-0.01	2 (0%) 93 67	0, 45, 83, 97	0
2	B	126/133 (94%)	0.06	3 (2%) 56 14	0, 19, 87, 100	0
3	C	155/156 (99%)	-0.23	0 100 100	0, 16, 38, 48	0
All	All	1083/1127 (96%)	-0.04	5 (0%) 88 48	0, 38, 84, 100	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	34	ASP	2.8
2	B	32	MET	2.3
1	A	453	LYS	2.2
2	B	71	GLY	2.1
1	A	331	LYS	2.1

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	CA	C	1	1/1	0.31	1.49	23,23,23,23	0

6.5 Other polymers ⓘ

There are no such residues in this entry.