WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Feb 17, 2024 – 03:53 PM EST

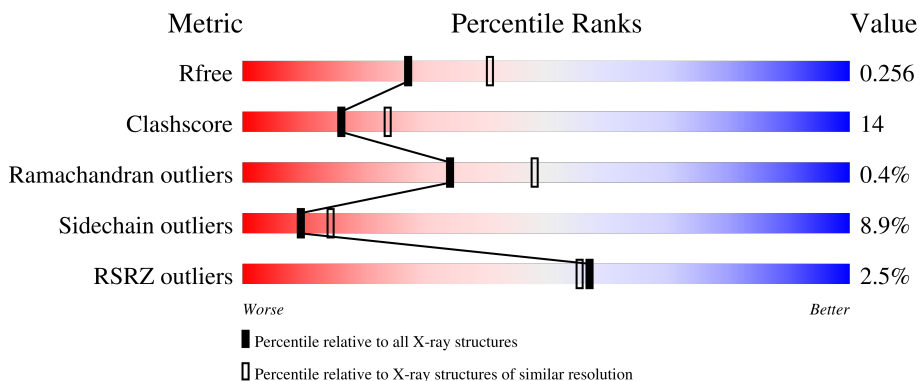|		
PDB ID	:	3TS5
Title	:	Crystal Structure of a Light Chain Domain of Scallop Smooth Muscle Myosin
Authors	:	Kumar, V.S.S.; O'Neall-Hennessey, E.; Reshetnikova, L.; Brown, J.H.; Robinson, H.; Szent-Gyorgyi, A.G.; Cohen, C.
Deposited on	:	2011-09-12
Resolution	:	2.39 Å(reported)

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 2.39 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.
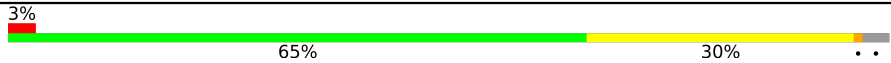
Metric	Percentile Ranks	Value
Rfree		0.256
Clashscore		14
Ramachandran outliers		0.4%
Sidechain outliers		8.9%
RSRZ outliers		2.5%

Worse — *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 <=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	69	70% 25% · ·
1	D	69	75% 22% ·
2	B	161	% 66% 18% · · 12%
2	E	161	7% 60% 25% 5% · 9%
3	C	156	74% 22% · ·

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Mol	Chain	Length	Quality of chain
3	F	156	

3%

65%　　　　　　　　　　　30%

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 6145 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 Myosin heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	68	Total 598	C 392	N 113	O 91	S 2	0	0	0
1	D	69	Total 606	C 396	N 115	O 93	S 2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	142	Total 1140	C 721	N 184	O 224	S 11	0	0	0
2	E	146	Total 1172	C 742	N 189	O 230	S 11	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	152	Total 1210	C 764	N 192	O 247	S 7	0	0	0
3	F	151	Total 1198	C 755	N 191	O 245	S 7	0	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Mg 1	0	0
4	E	1	Total 1	Mg 1	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total 1	Ca 1	0	0
5	F	1	Total 1	Ca 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	24	Total 24	O 24	0	0
6	B	58	Total 58	O 58	0	0
6	C	65	Total 65	O 65	0	0
6	D	16	Total 16	O 16	0	0
6	E	20	Total 20	O 20	0	0
6	F	34	Total 34	O 34	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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 (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.
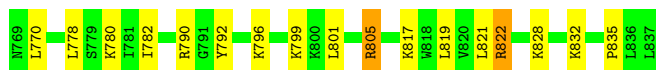
- Molecule 1: Myosin heavy chain

Chain A:

- Molecule 1: Myosin heavy chain

Chain D:

- Molecule 2: Myosin regulatory light chain

Chain B:
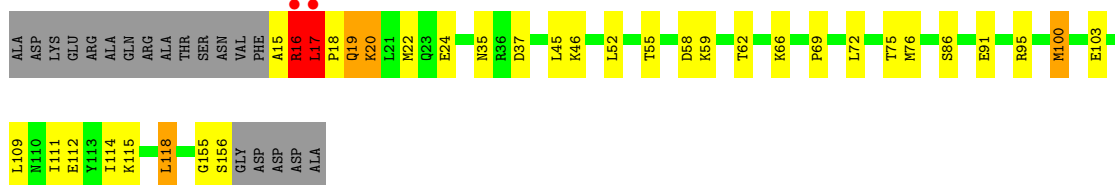
- Molecule 2: Myosin regulatory light chain

Chain E:
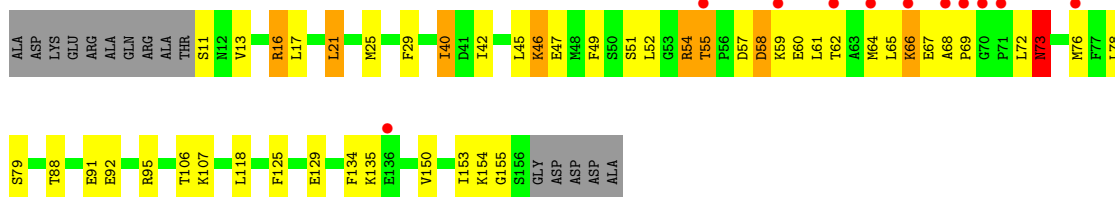
- Molecule 3: Myosin essential light chain

Chain C:

PRO K2 L3 S4 Q5 D6 E7 I8 K12 E16 D25 R38 R45 D48 K57 E60 K61 S62 L63 L69 P70 E73 M76 D77 Q80 E88 A89 F90 K91 F100 I101 S102 E105 Q132 E133 G137 K140 K146 T150

Y153 PRO ASP LYS

• Molecule 3: Myosin essential light chain

Chain F:

3%
65% 30%

PRO K2 L3 S4 Q5 D6 E7 I8 E16 D19 F20 W21 R24 D25 I33 V36 C37 I42 V49 K57 K61 S62 L63 E67 F68 L69 P70 E73 M76 M87 F93 D94 R95 E96 G97 Q98 G99 F100 I101 S102 G103 A104 E105 L106 V109

L113 G114 E115 L128 T129 D130 L131 Q132 E133 D134 L135 E136 G137 N138 V139 K140 G151 P152 TYR PRO ASP LYS

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	50.81Å 68.78Å 79.42Å 77.33° 85.99° 73.65°	Depositor
Resolution (Å)	48.75 – 2.39 48.75 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.75-2.39) 94.6 (48.75-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.59 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.191 , 0.241 0.202 , 0.256	Depositor DCC
R_{free} test set	2000 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	45.2	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 45.2	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6145	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.67% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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 ⓘ

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

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	0.50	0/611	0.58	0/818
1	D	0.39	0/619	0.51	0/829
2	B	0.48	0/1158	0.62	1/1547 (0.1%)
2	E	0.45	1/1191 (0.1%)	0.54	0/1592
3	C	0.53	0/1233	0.60	0/1658
3	F	0.47	0/1220	0.58	0/1640
All	All	0.47	1/6032 (0.0%)	0.58	1/8084 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	73	ASN	C-N	-5.59	1.21	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	17	LEU	N-CA-C	-5.43	96.35	111.00

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.

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	598	0	643	23	0
1	D	606	0	649	14	0
2	B	1140	0	1123	37	0
2	E	1172	0	1152	46	0
3	C	1210	0	1134	28	0
3	F	1198	0	1125	40	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
5	C	1	0	0	0	0
5	F	1	0	0	0	0
6	A	24	0	0	5	0
6	B	58	0	0	1	0
6	C	65	0	0	2	0
6	D	16	0	0	1	0
6	E	20	0	0	2	0
6	F	34	0	0	0	0
All	All	6145	0	5826	169	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 14.

The worst 5 of 169 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)
2:B:16:ARG:CB	2:B:17:LEU:HA	1.74	1.17
2:B:16:ARG:HG2	2:B:18:PRO:HD3	1.30	1.13
2:B:16:ARG:HB3	2:B:17:LEU:HA	1.05	1.03
2:E:61:LEU:O	2:E:65:LEU:HD23	1.59	1.00
2:B:16:ARG:HB3	2:B:17:LEU:CA	1.92	0.97

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	66/69 (96%)	66 (100%)	0	0	100	100
1	D	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
2	B	140/161 (87%)	135 (96%)	4 (3%)	1 (1%)	22	32
2	E	144/161 (89%)	138 (96%)	5 (4%)	1 (1%)	22	32
3	C	150/156 (96%)	147 (98%)	3 (2%)	0	100	100
3	F	149/156 (96%)	141 (95%)	7 (5%)	1 (1%)	22	32
All	All	716/772 (93%)	692 (97%)	21 (3%)	3 (0%)	34	48

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	16	ARG
3	F	102	SER
2	E	69	PRO

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	63/64 (98%)	58 (92%)	5 (8%)	12	19
1	D	64/64 (100%)	57 (89%)	7 (11%)	6	8
2	B	126/140 (90%)	112 (89%)	14 (11%)	6	8
2	E	130/140 (93%)	115 (88%)	15 (12%)	5	7
3	C	129/133 (97%)	120 (93%)	9 (7%)	15	24
3	F	128/133 (96%)	121 (94%)	7 (6%)	21	35
All	All	640/674 (95%)	583 (91%)	57 (9%)	9	14

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	770	LEU
3	F	95	ARG

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Mol	Chain	Res	Type
2	E	13	VAL
3	F	62	SER
2	E	135	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	19	GLN
2	E	73	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are 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.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

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	68/69 (98%)	0.03	0	100	100	32, 42, 66, 76	0
1	D	69/69 (100%)	0.05	0	100	100	39, 49, 88, 94	0
2	B	142/161 (88%)	0.08	2 (1%)	75	73	20, 46, 69, 87	0
2	E	146/161 (90%)	0.32	11 (7%)	14	13	25, 60, 88, 103	0
3	C	152/156 (97%)	0.01	0	100	100	32, 46, 65, 75	0
3	F	151/156 (96%)	0.07	5 (3%)	46	45	37, 56, 96, 107	0
All	All	728/772 (94%)	0.11	18 (2%)	57	55	20, 50, 85, 107	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	69	PRO	7.0
2	B	16	ARG	5.2
2	B	17	LEU	4.6
2	E	66	LYS	3.5
3	F	135	LEU	3.0

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 monosaccharides 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. 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($Å^2$)	Q<0.9
4	MG	E	162	1/1	0.94	0.12	71,71,71,71	0
5	CA	C	157	1/1	0.95	0.12	43,43,43,43	0
4	MG	B	162	1/1	0.98	0.34	42,42,42,42	0
5	CA	F	157	1/1	0.99	0.14	44,44,44,44	0

6.5 Other polymers ⓘ

There are no such residues in this entry.