



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2018 – 10:55 am GMT

PDB ID : 2B9C
Title : Structure of tropomyosin's mid-region: bending and binding sites for actin
Authors : Brown, J.H.; Zhou, Z.; Reshetnikova, L.; Robinson, H.; Yammani, R.D.; Tobacman, L.S.; Cohen, C.
Deposited on : 2005-10-11
Resolution : 2.30 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

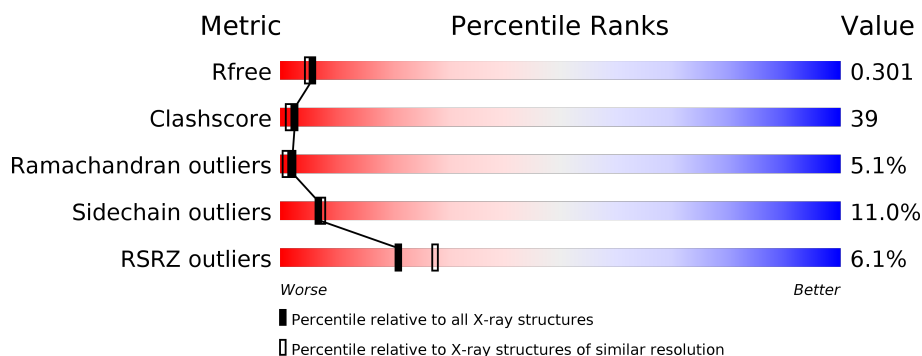
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	111664	4477 (2.30-2.30)
Clashscore	122126	5072 (2.30-2.30)
Ramachandran outliers	120053	5022 (2.30-2.30)
Sidechain outliers	120020	5021 (2.30-2.30)
RSRZ outliers	108989	4374 (2.30-2.30)

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. 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	147	<div> <div>9%</div> <div>25% 41% 24% 7%</div> </div>
1	B	147	<div> <div>3%</div> <div>25% 44% 23%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2650 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 striated-muscle alpha tropomyosin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	136	Total	C	N	O	S	0	8	0
			1151	701	211	236	3			
1	B	142	Total	C	N	O	S	0	3	0
			1150	700	199	248	3			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	88	MET	-	INITIATING MET	UNP P04692
A	209	ASP	-	GCN4 TAG	UNP P04692
A	210	LYS	-	GCN4 TAG	UNP P04692
A	211	VAL	-	GCN4 TAG	UNP P04692
A	212	GLU	-	GCN4 TAG	UNP P04692
A	213	GLU	-	GCN4 TAG	UNP P04692
A	214	LEU	-	GCN4 TAG	UNP P04692
A	215	LEU	-	GCN4 TAG	UNP P04692
A	216	SER	-	GCN4 TAG	UNP P04692
A	217	LYS	-	GCN4 TAG	UNP P04692
A	218	ASN	-	GCN4 TAG	UNP P04692
A	219	TYR	-	GCN4 TAG	UNP P04692
A	220	HIS	-	GCN4 TAG	UNP P04692
A	221	LEU	-	GCN4 TAG	UNP P04692
A	222	GLU	-	GCN4 TAG	UNP P04692
A	223	ASN	-	GCN4 TAG	UNP P04692
A	224	GLU	-	GCN4 TAG	UNP P04692
A	225	VAL	-	GCN4 TAG	UNP P04692
A	226	ALA	-	GCN4 TAG	UNP P04692
A	227	ARG	-	GCN4 TAG	UNP P04692
A	228	LEU	-	GCN4 TAG	UNP P04692
A	229	LYS	-	GCN4 TAG	UNP P04692
A	230	LYS	-	GCN4 TAG	UNP P04692
A	231	LEU	-	GCN4 TAG	UNP P04692
A	232	VAL	-	GCN4 TAG	UNP P04692

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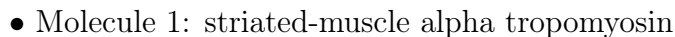
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Chain	Residue	Modelled	Actual	Comment	Reference
A	233	GLY	-	GCN4 TAG	UNP P04692
A	234	GLU	-	GCN4 TAG	UNP P04692
B	1088	MET	-	INITIATING MET	UNP P04692
B	1209	ASP	-	GCN4 TAG	UNP P04692
B	1210	LYS	-	GCN4 TAG	UNP P04692
B	1211	VAL	-	GCN4 TAG	UNP P04692
B	1212	GLU	-	GCN4 TAG	UNP P04692
B	1213	GLU	-	GCN4 TAG	UNP P04692
B	1214	LEU	-	GCN4 TAG	UNP P04692
B	1215	LEU	-	GCN4 TAG	UNP P04692
B	1216	SER	-	GCN4 TAG	UNP P04692
B	1217	LYS	-	GCN4 TAG	UNP P04692
B	1218	ASN	-	GCN4 TAG	UNP P04692
B	1219	TYR	-	GCN4 TAG	UNP P04692
B	1220	HIS	-	GCN4 TAG	UNP P04692
B	1221	LEU	-	GCN4 TAG	UNP P04692
B	1222	GLU	-	GCN4 TAG	UNP P04692
B	1223	ASN	-	GCN4 TAG	UNP P04692
B	1224	GLU	-	GCN4 TAG	UNP P04692
B	1225	VAL	-	GCN4 TAG	UNP P04692
B	1226	ALA	-	GCN4 TAG	UNP P04692
B	1227	ARG	-	GCN4 TAG	UNP P04692
B	1228	LEU	-	GCN4 TAG	UNP P04692
B	1229	LYS	-	GCN4 TAG	UNP P04692
B	1230	LYS	-	GCN4 TAG	UNP P04692
B	1231	LEU	-	GCN4 TAG	UNP P04692
B	1232	VAL	-	GCN4 TAG	UNP P04692
B	1233	GLY	-	GCN4 TAG	UNP P04692
B	1234	GLU	-	GCN4 TAG	UNP P04692

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	156	Total O 156 156	0	0
2	B	193	Total O 193 193	0	0

- Molecule 1: striated-muscle alpha tropomyosin



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	80.52Å 80.52Å 112.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.30 19.63 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.8 (20.00-2.30) 96.8 (19.63-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 2.30Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.256 , 0.296 0.267 , 0.301	Depositor DCC
R_{free} test set	706 reflections (3.98%)	wwPDB-VP
Wilson B-factor (Å ²)	44.3	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 101.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.052 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2650	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.86% 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	2.48	63/1156 (5.4%)	2.06	38/1543 (2.5%)
1	B	2.52	58/1153 (5.0%)	2.13	46/1539 (3.0%)
All	All	2.50	121/2309 (5.2%)	2.10	84/3082 (2.7%)

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	4
1	B	0	4
All	All	0	8

The worst 5 of 121 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	162	TYR	CD1-CE1	13.60	1.59	1.39
1	A	181	GLU	CG-CD	13.37	1.72	1.51
1	A	162	TYR	CD2-CE2	13.11	1.59	1.39
1	A	162	TYR	CE2-CZ	-12.40	1.22	1.38
1	B	1162	TYR	CZ-OH	11.91	1.58	1.37

The worst 5 of 84 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	178	ARG	NE-CZ-NH2	-24.50	108.05	120.30
1	B	1182	ARG	NE-CZ-NH1	-20.30	110.15	120.30
1	A	178	ARG	NE-CZ-NH1	15.52	128.06	120.30
1	A	182	ARG	NE-CZ-NH1	15.08	127.84	120.30
1	B	1175	ASP	CB-CG-OD2	14.46	131.31	118.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	169	LEU	Mainchain
1	A	171	ILE	Mainchain
1	A	180	GLU	Mainchain
1	A	219	TYR	Sidechain
1	B	1162	TYR	Sidechain

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	1151	0	1130	103	0
1	B	1150	0	1119	105	0
2	A	156	0	0	11	0
2	B	193	0	0	11	0
All	All	2650	0	2249	178	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 39.

The worst 5 of 178 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:B:1171:ILE:CB	1:B:1171:ILE:CG2	1.75	1.60
1:B:1169:LEU:CD2	1:B:1169:LEU:CG	1.74	1.59
1:A:171:ILE:CG1	1:A:171:ILE:CD1	1.78	1.59
1:A:122[A]:GLU:OE1	1:A:122[A]:GLU:HA	1.51	1.11
1:B:1169:LEU:CD2	1:B:1169:LEU:CD1	2.36	1.02

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	142/147 (97%)	119 (84%)	15 (11%)	8 (6%)	2	1
1	B	143/147 (97%)	122 (85%)	15 (10%)	6 (4%)	3	1
All	All	285/294 (97%)	241 (85%)	30 (10%)	14 (5%)	2	1

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	ALA
1	A	103	GLN
1	A	210	LYS
1	A	231	LEU
1	B	1094	LEU

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	119/129 (92%)	107 (90%)	12 (10%)	8	10
1	B	120/129 (93%)	106 (88%)	14 (12%)	6	6
All	All	239/258 (93%)	213 (89%)	26 (11%)	7	8

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	232	VAL

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Mol	Chain	Res	Type
1	B	1100	ASP
1	B	1192	GLU
1	B	1093	GLN
1	B	1099	LEU

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

Mol	Chain	Res	Type
1	A	144	GLN
1	B	1093	GLN

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 carbohydrates 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1166:ALA	C	1167:ARG	N	1.20

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	136/147 (92%)	0.51	13 (9%) 8 11	15, 71, 93, 101	0
1	B	142/147 (96%)	0.31	4 (2%) 53 60	15, 66, 87, 98	0
All	All	278/294 (94%)	0.41	17 (6%) 21 27	15, 68, 91, 101	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	232	VAL	4.9
1	B	1094	LEU	4.4
1	B	1093	GLN	4.0
1	A	231	LEU	3.9
1	A	109	ALA	3.8

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 carbohydrates 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.