Full wwPDB X-ray Structure Validation Report ⓘ

Feb 4, 2025 – 06:07 am GMT

PDB ID	:	9FF9
Title	:	Crystal structure of N-terminal acetylated tropomyosin Cdc8
Authors	:	Zahn, M.; Heiringhoff, R.S.; Fedorov, R.; Manstein, D.J.
Deposited on	:	2024-05-22
Resolution	:	2.19 Å(reported)

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

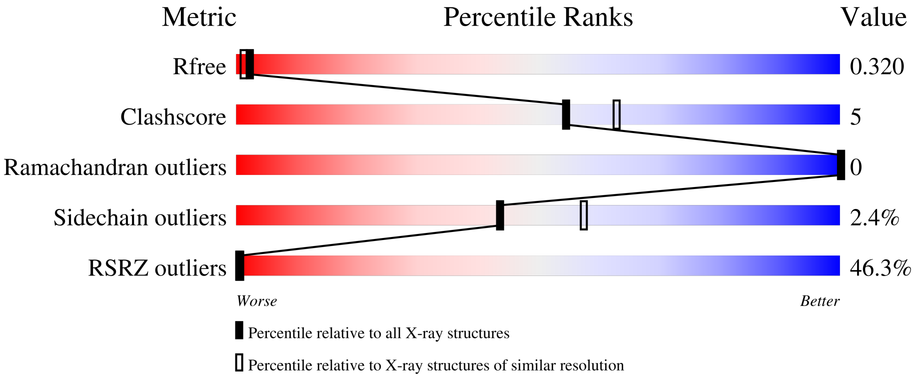
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance

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

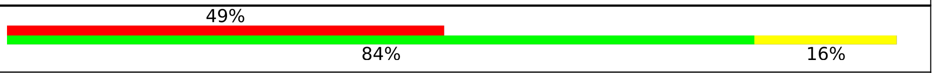
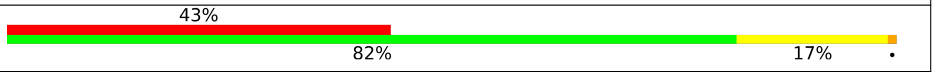
The reported resolution of this entry is 2.19 Å.

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}	164625	5791 (2.20-2.20)
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)
RSRZ outliers	164620	5791 (2.20-2.20)

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 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	162	
1	B	162	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2677 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 Tropomyosin.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	A	162	Total C N O S 1329 804 231 290 4	0	0	0
1	B	162	Total C N O S 1329 804 231 290 4	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ACE	-	acetylation	UNP Q02088
B	1	ACE	-	acetylation	UNP Q02088

- Molecule 2 is water.

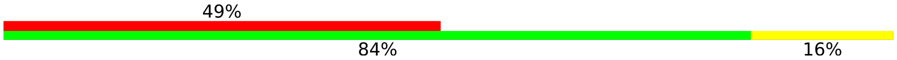
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	7	Total O 7 7	0	0
2	B	12	Total O 12 12	0	0

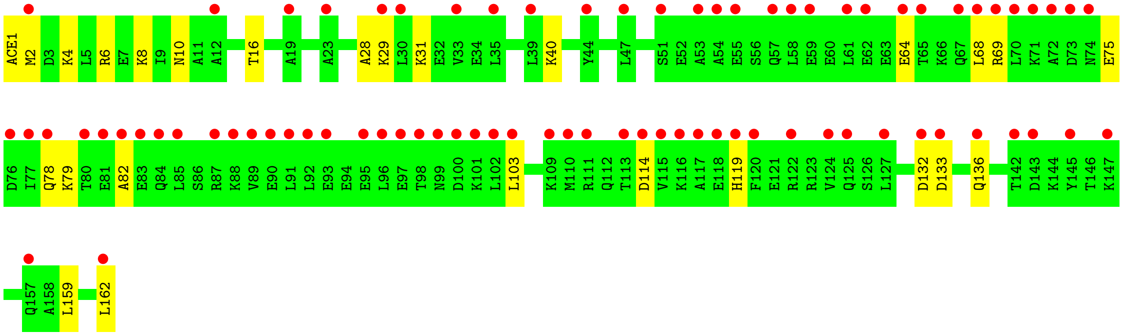
3 Residue-property plots

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: Tropomyosin

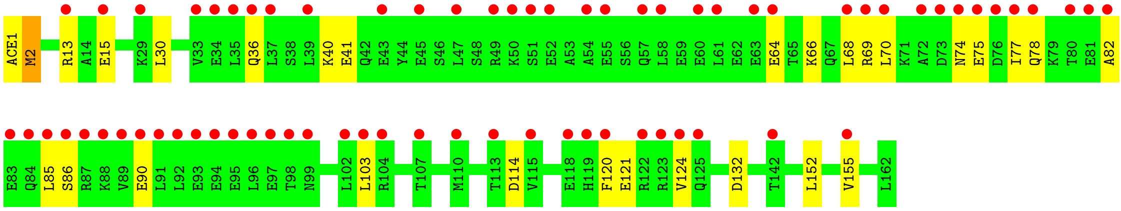
Chain A:





- Molecule 1: Tropomyosin

Chain B:



4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	25.40Å 38.32Å 97.54Å 97.71° 94.71° 101.50°	Depositor
Resolution (Å)	37.10 – 2.19 37.10 – 2.19	Depositor EDS
% Data completeness (in resolution range)	36.5 (37.10-2.19) 36.7 (37.10-2.19)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.67 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487:	Depositor
R, R_{free}	0.260 , 0.315 0.265 , 0.320	Depositor DCC
R_{free} test set	304 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å^2)	29.9	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 19.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,h+k+l	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	2677	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.11% 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: ACE

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	0.27	1/1331 (0.1%)	0.45	1/1775 (0.1%)
1	B	0.29	1/1331 (0.1%)	0.47	1/1775 (0.1%)
All	All	0.28	2/2662 (0.1%)	0.46	2/3550 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	ACE	C-N	5.04	1.45	1.34
1	B	1	ACE	C-N	5.01	1.45	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	2	MET	CG-SD-CE	5.70	109.32	100.20
1	A	2	MET	CG-SD-CE	5.46	108.94	100.20

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	1329	0	1315	17	0
1	B	1329	0	1315	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	7	0	0	0	0
2	B	12	0	0	1	0
All	All	2677	0	2630	25	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 5.

All (25) 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:68:LEU:HB3	1:B:68:LEU:HB3	1.84	0.60
1:B:13:ARG:NH1	2:B:202:HOH:O	2.36	0.58
1:A:6:ARG:O	1:A:10:ASN:ND2	2.29	0.57
1:A:69:ARG:NH2	1:B:64:GLU:OE2	2.36	0.57
1:A:29:LYS:HD2	1:B:30:LEU:HD21	1.90	0.53
1:A:78:GLN:O	1:B:78:GLN:NE2	2.41	0.53
1:B:74:ASN:O	1:B:77:ILE:HG13	2.09	0.53
1:A:75:GLU:HB3	1:B:75:GLU:HB3	1.92	0.51
1:A:82:ALA:HB2	1:B:82:ALA:HB2	1.95	0.49
1:A:28:ALA:HA	1:A:31:LYS:HE2	1.93	0.49
1:A:159:LEU:HA	1:A:162:LEU:HD23	1.94	0.47
1:B:86:SER:O	1:B:90:GLU:HG2	2.15	0.47
1:A:82:ALA:HB2	1:B:78:GLN:HE22	1.80	0.46
1:A:133:ASP:O	1:A:136:GLN:HG2	2.16	0.44
1:A:4:LYS:O	1:A:8:LYS:HG2	2.18	0.44
1:A:16:THR:HG21	1:B:15:GLU:HG2	2.00	0.44
1:B:152:LEU:HA	1:B:155:VAL:HG12	2.00	0.43
1:B:120:PHE:O	1:B:124:VAL:HG13	2.19	0.43
1:B:36:GLN:O	1:B:40:LYS:HD3	2.20	0.42
1:A:40:LYS:HE2	1:B:41:GLU:HG2	2.01	0.41
1:B:121:GLU:HA	1:B:124:VAL:HG22	2.01	0.41
1:A:103:LEU:HD13	1:B:103:LEU:HA	2.02	0.41
1:A:79:LYS:HA	1:B:78:GLN:CD	2.41	0.41
1:A:64:GLU:OE2	1:B:69:ARG:NH2	2.50	0.40
1:B:66:LYS:HD3	1:B:70:LEU:HD23	2.03	0.40

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	160/162 (99%)	160 (100%)	0	0	100	100
1	B	160/162 (99%)	160 (100%)	0	0	100	100
All	All	320/324 (99%)	320 (100%)	0	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	145/145 (100%)	142 (98%)	3 (2%)	48	63
1	B	145/145 (100%)	141 (97%)	4 (3%)	38	51
All	All	290/290 (100%)	283 (98%)	7 (2%)	44	57

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	ASP
1	A	119	HIS
1	A	132	ASP
1	B	2	MET
1	B	85	LEU
1	B	114	ASP
1	B	132	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	78	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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	161/162 (99%)	2.11	79 (49%)	0	0	14, 45, 85, 97	0
1	B	161/162 (99%)	2.02	70 (43%)	1	0	14, 42, 72, 92	0
All	All	322/324 (99%)	2.07	149 (46%)	1	0	14, 44, 78, 97	0

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	68	LEU	5.7
1	A	69	ARG	5.3
1	B	61	LEU	5.1
1	A	110	MET	4.9
1	A	96	LEU	4.8
1	A	72	ALA	4.8
1	A	77	ILE	4.7
1	B	85	LEU	4.7
1	B	102	LEU	4.7
1	B	96	LEU	4.6
1	A	80	THR	4.6
1	B	36	GLN	4.2
1	B	37	LEU	4.2
1	B	92	LEU	4.2
1	A	78	GLN	4.1
1	B	82	ALA	4.1
1	B	81	GLU	4.0
1	B	35	LEU	4.0
1	A	70	LEU	3.9
1	A	82	ALA	3.9
1	A	85	LEU	3.8
1	A	71	LYS	3.7
1	A	44	TYR	3.7
1	A	35	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	91	LEU	3.7
1	A	33	VAL	3.6
1	B	77	ILE	3.6
1	B	52	GLU	3.6
1	B	74	ASN	3.5
1	B	73	ASP	3.5
1	B	29	LYS	3.5
1	A	91	LEU	3.5
1	A	98	THR	3.5
1	B	99	ASN	3.5
1	B	84	GLN	3.4
1	B	63	GLU	3.4
1	B	57	GLN	3.4
1	A	92	LEU	3.4
1	B	113	THR	3.4
1	B	72	ALA	3.4
1	B	122	ARG	3.4
1	A	120	PHE	3.3
1	B	78	GLN	3.3
1	B	70	LEU	3.3
1	A	84	GLN	3.3
1	A	74	ASN	3.3
1	B	75	GLU	3.3
1	A	88	LYS	3.3
1	B	123	ARG	3.3
1	A	58	LEU	3.2
1	A	97	GLU	3.2
1	B	64	GLU	3.2
1	B	118	GLU	3.2
1	A	122	ARG	3.2
1	B	104	ARG	3.2
1	B	51	SER	3.1
1	A	76	ASP	3.1
1	B	33	VAL	3.1
1	A	73	ASP	3.1
1	B	115	VAL	3.1
1	A	61	LEU	3.1
1	A	119	HIS	3.0
1	A	111	ARG	3.0
1	A	81	GLU	3.0
1	A	19	ALA	3.0
1	A	90	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	102	LEU	2.9
1	A	157	GLN	2.9
1	B	87	ARG	2.9
1	A	95	GLU	2.9
1	A	133	ASP	2.9
1	B	58	LEU	2.9
1	A	100	ASP	2.9
1	A	99	ASN	2.9
1	A	89	VAL	2.8
1	B	89	VAL	2.8
1	A	51	SER	2.8
1	A	118	GLU	2.8
1	A	142	THR	2.8
1	A	103	LEU	2.8
1	A	127	LEU	2.8
1	B	76	ASP	2.8
1	B	95	GLU	2.8
1	A	109	LYS	2.8
1	B	68	LEU	2.8
1	A	116	LYS	2.8
1	A	23	ALA	2.7
1	B	54	ALA	2.7
1	B	124	VAL	2.7
1	A	87	ARG	2.7
1	B	142	THR	2.7
1	A	162	LEU	2.6
1	A	125	GLN	2.6
1	B	107	THR	2.6
1	A	117	ALA	2.6
1	A	59	GLU	2.6
1	B	83	GLU	2.6
1	B	94	GLU	2.6
1	A	57	GLN	2.5
1	A	62	GLU	2.5
1	B	90	GLU	2.5
1	B	60	GLU	2.5
1	B	86	SER	2.5
1	A	39	LEU	2.5
1	A	53	ALA	2.5
1	B	155	VAL	2.5
1	A	136	GLN	2.5
1	A	30	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	13	ARG	2.5
1	B	69	ARG	2.5
1	A	55	GLU	2.4
1	B	97	GLU	2.4
1	B	120	PHE	2.4
1	B	15	GLU	2.4
1	B	45	GLU	2.4
1	A	29	LYS	2.4
1	B	103	LEU	2.4
1	A	113	THR	2.4
1	B	119	HIS	2.4
1	A	2	MET	2.4
1	B	93	GLU	2.3
1	A	65	THR	2.3
1	B	125	GLN	2.3
1	B	47	LEU	2.3
1	A	115	VAL	2.3
1	A	132	ASP	2.3
1	B	39	LEU	2.3
1	A	54	ALA	2.3
1	B	98	THR	2.3
1	B	49	ARG	2.2
1	A	145	TYR	2.2
1	B	50	LYS	2.2
1	A	93	GLU	2.1
1	B	34	GLU	2.1
1	B	43	GLU	2.1
1	A	143	ASP	2.1
1	A	64	GLU	2.1
1	B	55	GLU	2.1
1	A	47	LEU	2.1
1	B	80	THR	2.1
1	A	67	GLN	2.1
1	A	83	GLU	2.1
1	A	101	LYS	2.1
1	B	110	MET	2.1
1	A	147	LYS	2.1
1	A	12	ALA	2.0
1	A	114	ASP	2.0
1	B	88	LYS	2.0
1	A	124	VAL	2.0

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 ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.