wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jan 10, 2018 – 02:07 PM EST

PDB ID	:	6AV9
EMDB ID:	:	EMD-7007
Title	:	CryoEM structure of Mical Oxidized Actin (Class 1)
Authors	:	Grintsevich, E.E.; Ge, P.; Sawaya, M.R.; Yesilyurt, H.G.; Terman, J.R.; Zhou, Z.H.; Reisler, E.
Deposited on	:	2017-09-01
Resolution	:	3.90 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp
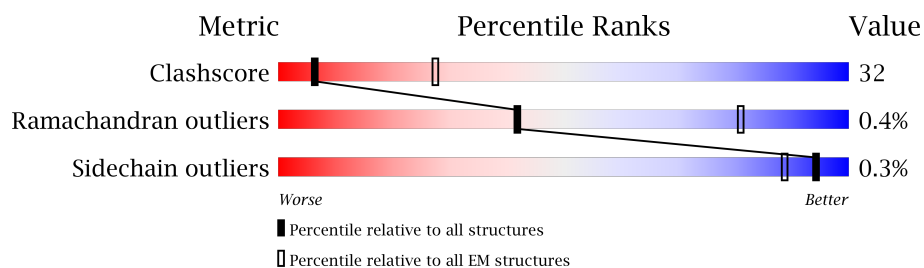with specific help available everywhere you see the ⓘ symbol.

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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
Clashscore		32
Ramachandran outliers		0.4%
Sidechain outliers		0.3%

Worse   *Better*

▌ Percentile relative to all structures
▯ Percentile relative to all EM structures

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 <=5%

| Mol	Chain	Length	Quality of chain
1	A	377	50% 47% •
1	B	377	49% 49% •
1	C	377	50% 47% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8673 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	367	Total	C	N	O	S	0	0
			2864	1813	481	550	20		
1	A	367	Total	C	N	O	S	0	0
			2864	1813	481	550	20		
1	B	367	Total	C	N	O	S	0	0
			2864	1813	481	550	20		

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).
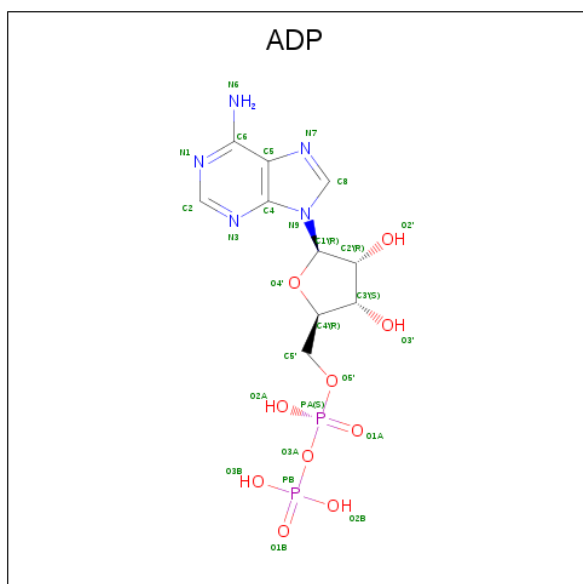
Mol	Chain	Residues	Atoms					AltConf
2	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	B	1	Total	C	N	O	P	0
			27	10	5	10	2	

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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.
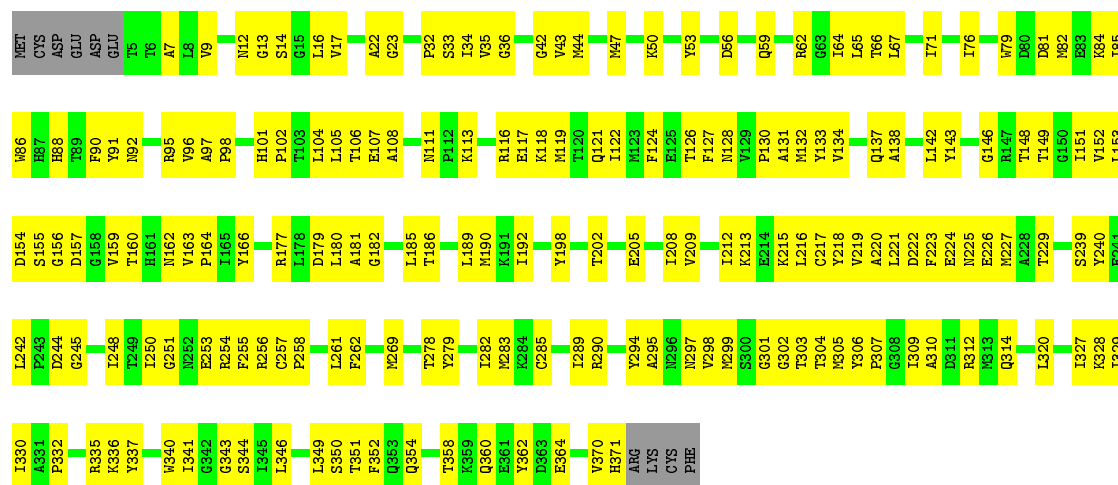
- Molecule 1: Actin, alpha skeletal muscle
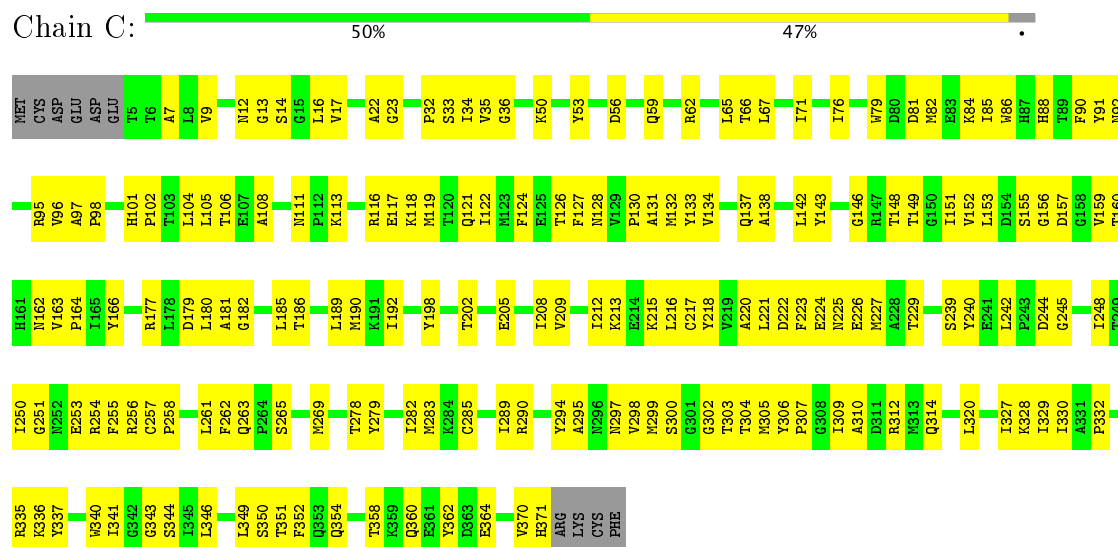
Chain C:

- Molecule 1: Actin, alpha skeletal muscle
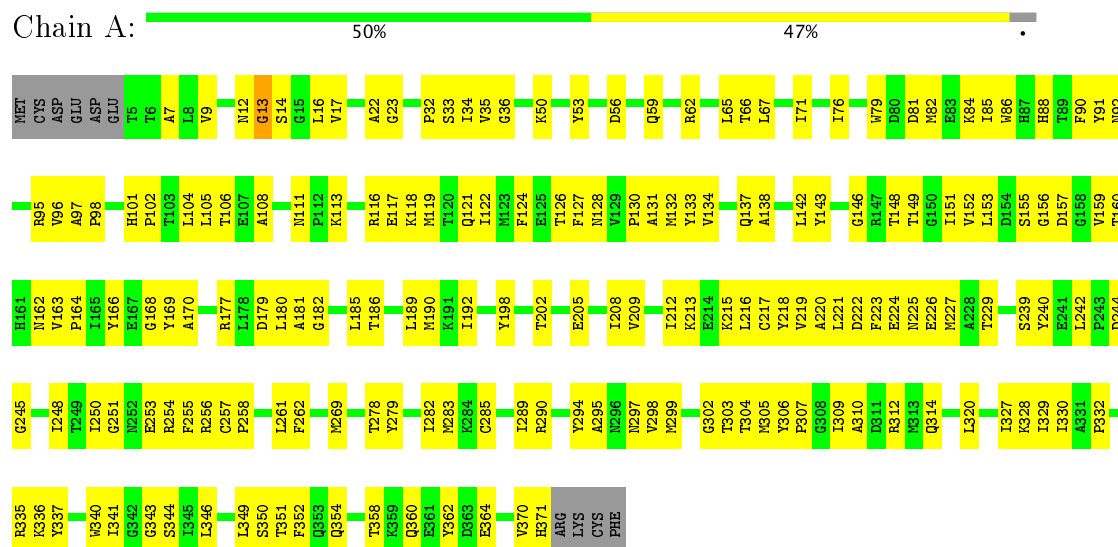
Chain A:

- Molecule 1: Actin, alpha skeletal muscle

Chain B:

49%   49%

4 Experimental information (i)

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-166.64°, rise=28.042 Å, axial sym=C1	Depositor
Number of segments used	102700	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	30	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SME, HIC, ADP

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	#$|Z|$>2	RMSZ	#$|Z|$>2
1	A	0.42	0/2893	0.58	0/3919
1	B	0.41	0/2893	0.58	0/3919
1	C	0.41	0/2893	0.58	0/3919
All	All	0.41	0/8679	0.58	0/11757

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2864	0	2832	183	0
1	B	2864	0	2832	184	0
1	C	2864	0	2832	171	0
2	A	27	0	12	3	0
2	B	27	0	12	3	0
2	C	27	0	12	3	0
All	All	8673	0	8532	525	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 32.

The worst 5 of 525 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:C:220:ALA:CB	1:C:223:PHE:HB3	1.61	1.30
1:A:220:ALA:CB	1:A:223:PHE:HB3	1.61	1.29
1:B:220:ALA:CB	1:B:223:PHE:HB3	1.61	1.28
1:A:113:LYS:NZ	1:A:116:ARG:NH2	1.92	1.18
1:B:113:LYS:NZ	1:B:116:ARG:NH2	1.92	1.17

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	362/377 (96%)	312 (86%)	48 (13%)	2 (1%)	28	70
1	B	362/377 (96%)	312 (86%)	49 (14%)	1 (0%)	44	80
1	C	362/377 (96%)	312 (86%)	49 (14%)	1 (0%)	44	80
All	All	1086/1131 (96%)	936 (86%)	146 (13%)	4 (0%)	42	76

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	117	GLU
1	A	117	GLU
1	B	117	GLU
1	A	13	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	307/317 (97%)	306 (100%)	1 (0%)	94	97
1	B	307/317 (97%)	306 (100%)	1 (0%)	94	97
1	C	307/317 (97%)	306 (100%)	1 (0%)	94	97
All	All	921/951 (97%)	918 (100%)	3 (0%)	94	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	224	GLU
1	A	224	GLU
1	B	224	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	GLN
1	A	314	GLN
1	B	314	GLN
1	A	128	ASN
1	A	296	ASN

5.3.3   RNA (i)

There are no RNA molecules in this entry.

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

9 non-standard protein/DNA/RNA residues are modelled in this entry.

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 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
1	SME	A	44	1	8,8,9	0.77	0	6,9,11	1.86	1 (16%)
1	SME	A	47	1	8,8,9	0.83	0	6,9,11	1.39	1 (16%)
1	HIC	A	73	1	9,11,12	2.18	3 (33%)	7,14,16	1.06	1 (14%)
1	SME	B	44	1	8,8,9	0.76	0	6,9,11	1.86	1 (16%)
1	SME	B	47	1	8,8,9	0.82	0	6,9,11	1.39	1 (16%)
1	HIC	B	73	1	9,11,12	2.16	3 (33%)	7,14,16	1.07	1 (14%)
1	SME	C	44	1	8,8,9	0.77	0	6,9,11	1.87	1 (16%)
1	SME	C	47	1	8,8,9	0.82	0	6,9,11	1.39	1 (16%)
1	HIC	C	73	1	9,11,12	2.16	3 (33%)	7,14,16	1.07	1 (14%)

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	Res	Link	Chirals	Torsions	Rings
1	SME	A	44	1	-	0/5/7/9	0/0/0/0
1	SME	A	47	1	-	0/5/7/9	0/0/0/0
1	HIC	A	73	1	-	0/4/6/8	0/1/1/1
1	SME	B	44	1	-	0/5/7/9	0/0/0/0
1	SME	B	47	1	-	0/5/7/9	0/0/0/0
1	HIC	B	73	1	-	0/4/6/8	0/1/1/1
1	SME	C	44	1	-	0/5/7/9	0/0/0/0
1	SME	C	47	1	-	0/5/7/9	0/0/0/0
1	HIC	C	73	1	-	0/4/6/8	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	73	HIC	CD2-NE2	-4.09	1.32	1.38
1	A	73	HIC	CD2-NE2	-4.08	1.32	1.38
1	B	73	HIC	CD2-NE2	-4.08	1.32	1.38
1	A	73	HIC	CD2-CG	-3.54	1.31	1.36
1	C	73	HIC	CD2-CG	-3.46	1.31	1.36

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	44	SME	CB-CA-C	-4.47	104.28	111.65
1	A	44	SME	CB-CA-C	-4.47	104.29	111.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	44	SME	CB-CA-C	-4.45	104.31	111.65
1	A	47	SME	CB-CA-C	-3.17	106.42	111.65
1	C	47	SME	CB-CA-C	-3.17	106.43	111.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	44	SME	3	0
1	B	47	SME	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

3 ligands are modelled in this entry.

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 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	ADP	A	801	-	25,29,29	0.96	1 (4%)	24,45,45	1.55	2 (8%)
2	ADP	B	801	-	25,29,29	0.95	1 (4%)	24,45,45	1.56	2 (8%)
2	ADP	C	801	-	25,29,29	0.96	1 (4%)	24,45,45	1.55	2 (8%)

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	Res	Link	Chirals	Torsions	Rings
2	ADP	A	801	-	-	0/12/32/32	0/3/3/3
2	ADP	B	801	-	-	0/12/32/32	0/3/3/3
2	ADP	C	801	-	-	0/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	ADP	C5-C4	2.84	1.46	1.40
2	C	801	ADP	C5-C4	2.88	1.47	1.40
2	A	801	ADP	C5-C4	2.88	1.47	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	801	ADP	N3-C2-N1	-5.73	123.87	128.86
2	C	801	ADP	N3-C2-N1	-5.68	123.91	128.86
2	A	801	ADP	N3-C2-N1	-5.67	123.92	128.86
2	A	801	ADP	C4-C5-N7	-2.44	107.05	109.41
2	B	801	ADP	C4-C5-N7	-2.38	107.11	109.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	ADP	3	0
2	B	801	ADP	3	0
2	C	801	ADP	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.