



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Jan 8, 2018 – 07:48 PM EST

PDB ID : 6AVB
EMDB ID: : EMD-7008
Title : CryoEM structure of Mical Oxidized Actin (Class 1)
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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.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

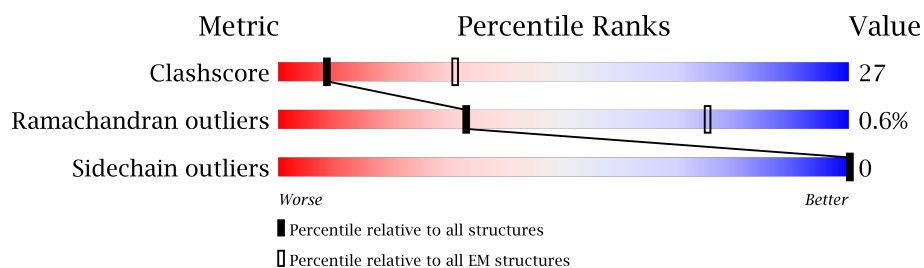
1 Overall quality at a glance

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	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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	377	
1	B	377	
1	C	377	

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: $C_{10}H_{15}N_5O_{10}P_2$).



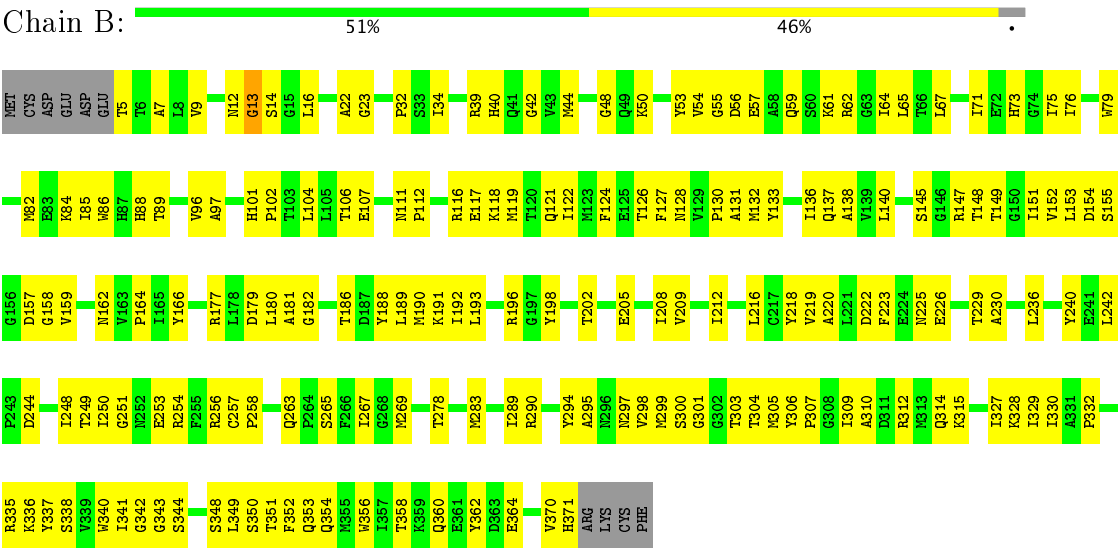
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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.

- [illegible]

- Chain A: 51% 46%

Position	Amino Acid	Conservation %
1	Met	51%
2	Cys	51%
3	Asp	51%
4	Glu	51%
5	Asp	51%
6	Glu	51%
7	T6	46%
8	A7	46%
9	L8	46%
10	V9	46%
11	N12	51%
12	G13	51%
13	S14	51%
14	G15	51%
15	L16	51%
16	V17	51%
17	K18	51%
18	R16	51%
19	E17	51%
20	K18	51%
21	M19	51%
22	T120	51%
23	Q121	51%
24	I122	51%
25	M123	51%
26	F124	51%
27	E125	51%
28	T126	51%
29	F127	51%
30	N128	51%
31	V129	51%
32	P130	51%
33	A131	51%
34	M132	51%
35	Y133	51%
36	I136	51%
37	Q137	51%
38	A138	51%
39	V139	51%
40	L140	51%
41	Y143	51%
42	A144	51%
43	S145	51%
44	G146	51%
45	R147	51%
46	T148	51%
47	T149	51%
48	G150	51%
49	T151	51%
50	V152	51%
51	L153	51%
52	D154	51%
53	S155	51%
54	G156	51%
55	D157	51%
56	G158	51%
57	V159	51%
58	N162	51%
59	V163	51%
60	P164	51%
61	I165	51%
62	V166	51%
63	A167	51%
64	G168	51%
65	Y169	51%
66	R177	51%
67	L178	51%
68	D179	51%
69	L180	51%
70	A181	51%
71	G182	51%
72	T186	51%
73	D187	51%
74	L188	51%
75	L189	51%
76	M190	51%
77	K191	51%
78	I192	51%
79	L193	51%
80	R196	51%
81	G197	51%
82	Y198	51%
83	T202	51%
84	E205	51%
85	I208	51%
86	V209	51%
87	I212	51%
88	L216	51%
89	G217	51%
90	Y218	51%
91	V219	51%
92	A220	51%
93	L221	51%
94	D222	51%
95	F223	51%
96	E224	51%
97	E226	51%
98	T229	51%
99	A230	51%
100	L236	51%
101	L242	51%
102	T248	51%
103	T278	51%
104	Y279	51%
105	N283	51%
106	T289	51%
107	R290	51%
108	L293	51%
109	V294	51%
110	A295	51%
111	N296	51%
112	T297	51%
113	V298	51%
114	N299	51%
115	S300	51%
116	G301	51%
117	G302	51%
118	T303	51%
119	T304	51%
120	R305	51%
121	V306	51%
122	F307	51%
123	G308	51%
124	A310	51%
125	R311	51%
126	R312	51%
127	R313	51%
128	Q314	51%
129	R315	51%
130	L320	51%
131	R327	51%
132	R328	51%
133	R329	51%
134	R330	51%
135	A331	51%
136	R332	51%

- 

4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-166.66°, rise=28.029 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 ($e^-/\text{\AA}^2$)	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

5.1 Standard geometry

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	0.45	0/2893	0.61	0/3919
1	B	0.45	0/2893	0.61	0/3919
1	C	0.45	0/2893	0.61	0/3919
All	All	0.45	0/8679	0.61	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

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	2831	155	0
1	B	2864	0	2831	153	0
1	C	2864	0	2831	148	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	8529	446	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 27.

The worst 5 of 446 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:242:LEU:HD23	1:B:248:ILE:HD11	1.52	0.92
1:C:242:LEU:HD23	1:C:248:ILE:HD11	1.52	0.92
1:A:242:LEU:HD23	1:A:248:ILE:HD11	1.52	0.91
1:A:216:LEU:HB2	1:A:254:ARG:HE	1.40	0.87
1:B:216:LEU:HB2	1:B:254:ARG:HE	1.40	0.87

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%)	313 (86%)	47 (13%)	2 (1%)	28	70
1	B	362/377 (96%)	313 (86%)	47 (13%)	2 (1%)	28	70
1	C	362/377 (96%)	313 (86%)	47 (13%)	2 (1%)	28	70
All	All	1086/1131 (96%)	939 (86%)	141 (13%)	6 (1%)	33	70

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	48	GLY
1	A	48	GLY
1	B	48	GLY
1	C	13	GLY
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%)	307 (100%)	0	100	100
1	B	307/317 (97%)	307 (100%)	0	100	100
1	C	307/317 (97%)	307 (100%)	0	100	100
All	All	921/951 (97%)	921 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	GLN
1	A	128	ASN
1	B	121	GLN
1	A	101	HIS
1	B	101	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	0.72	0
1	SME	A	47	1	8,8,9	1.01	0	6,9,11	1.32	1 (16%)
1	HIC	A	73	1	9,11,12	2.19	3 (33%)	7,14,16	1.21	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	SME	B	44	1	8,8,9	0.76	0	6,9,11	0.73	0
1	SME	B	47	1	8,8,9	1.01	0	6,9,11	1.31	1 (16%)
1	HIC	B	73	1	9,11,12	2.17	3 (33%)	7,14,16	1.20	1 (14%)
1	SME	C	44	1	8,8,9	0.77	0	6,9,11	0.72	0
1	SME	C	47	1	8,8,9	1.00	0	6,9,11	1.31	1 (16%)
1	HIC	C	73	1	9,11,12	2.17	3 (33%)	7,14,16	1.21	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	A	73	HIC	CD2-NE2	-4.19	1.32	1.38
1	B	73	HIC	CD2-NE2	-4.14	1.32	1.38
1	C	73	HIC	CD2-NE2	-4.11	1.32	1.38
1	C	73	HIC	CD2-CG	-3.44	1.31	1.36
1	A	73	HIC	CD2-CG	-3.44	1.31	1.36

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	SME	CB-CA-C	-3.08	106.58	111.65
1	C	47	SME	CB-CA-C	-3.07	106.59	111.65
1	B	47	SME	CB-CA-C	-3.07	106.59	111.65
1	C	73	HIC	CB-CA-C	-2.48	106.63	111.41
1	B	73	HIC	CB-CA-C	-2.48	106.63	111.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	73	HIC	2	0
1	B	44	SME	2	0
1	B	73	HIC	2	0
1	C	73	HIC	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	1.53	2 (8%)
2	ADP	B	801	-	25,29,29	0.95	1 (4%)	24,45,45	1.54	2 (8%)
2	ADP	C	801	-	25,29,29	0.95	1 (4%)	24,45,45	1.52	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	2.75	1.46	1.40
2	C	801	ADP	C5-C4	2.76	1.46	1.40
2	A	801	ADP	C5-C4	2.78	1.46	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	ADP	N3-C2-N1	-5.51	124.06	128.86
2	A	801	ADP	N3-C2-N1	-5.42	124.14	128.86
2	C	801	ADP	N3-C2-N1	-5.40	124.15	128.86
2	C	801	ADP	C4-C5-N7	-2.36	107.13	109.41
2	B	801	ADP	C4-C5-N7	-2.34	107.15	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.