



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:11 PM BST

PDB ID : 5AEY
EMDB ID: : EMD-2850
Title : actin-like ParM protein bound to AMPPNP
Authors : Bharat, T.A.M.; Murshudov, G.N.; Sachse, C.; Lowe, J.
Deposited on : 2015-01-12
Resolution : 4.30 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

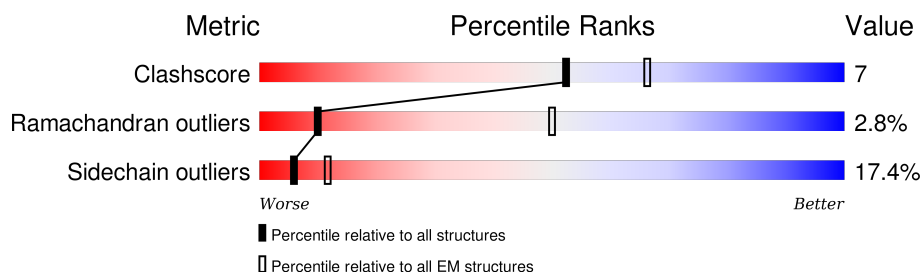
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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	318	67% 28% 5% .
1	B	318	69% 25% 6%
1	C	318	68% 26% 6%
1	D	318	69% 26% 5%
1	E	318	69% 25% 6%

2 Entry composition i

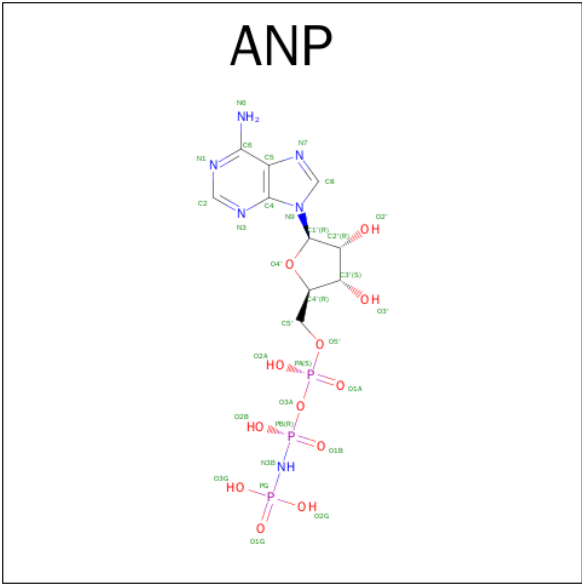
There are 2 unique types of molecules in this entry. The entry contains 12675 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PLASMID SEGREGATION PROTEIN PARM.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	318	Total	C	N	O	S	0	0
			2504	1580	422	494	8		
1	B	318	Total	C	N	O	S	0	0
			2504	1580	422	494	8		
1	C	318	Total	C	N	O	S	0	0
			2504	1580	422	494	8		
1	D	318	Total	C	N	O	S	0	0
			2504	1580	422	494	8		
1	E	318	Total	C	N	O	S	0	0
			2504	1580	422	494	8		

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



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Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	N	O	P	0
			31	10	6	12	3	
2	C	1	Total	C	N	O	P	0
			31	10	6	12	3	
2	D	1	Total	C	N	O	P	0
			31	10	6	12	3	
2	E	1	Total	C	N	O	P	0
			31	10	6	12	3	

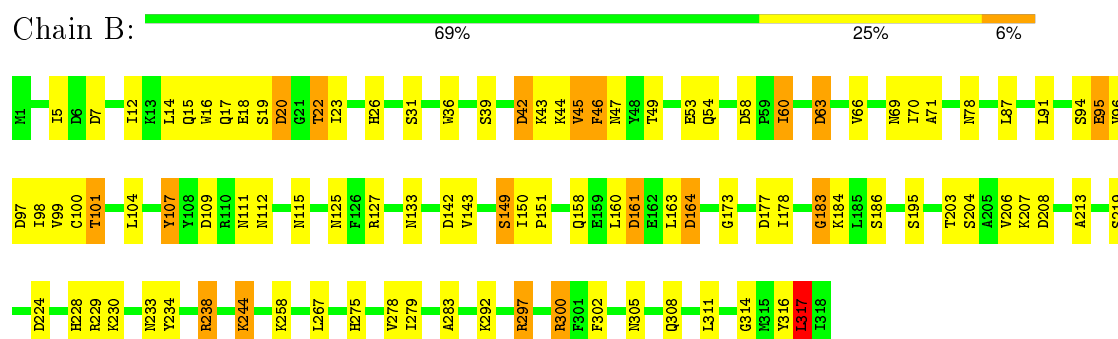
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

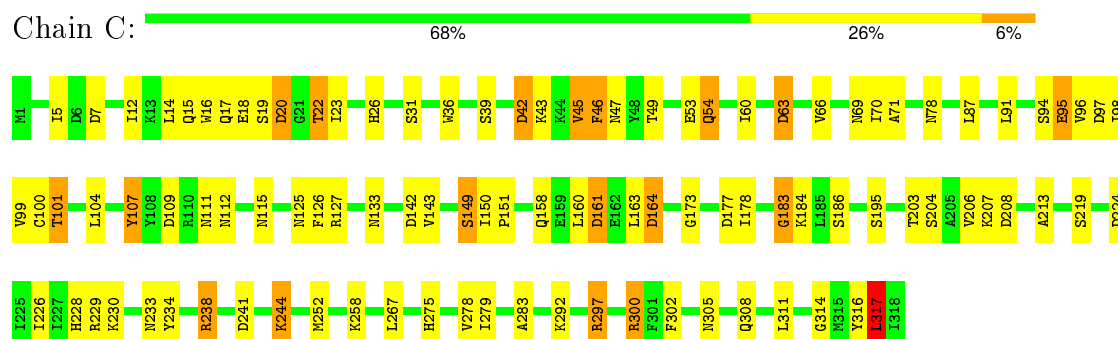
• Molecule 1: PLASMID SEGREGATION PROTEIN PARM



• Molecule 1: PLASMID SEGREGATION PROTEIN PARM

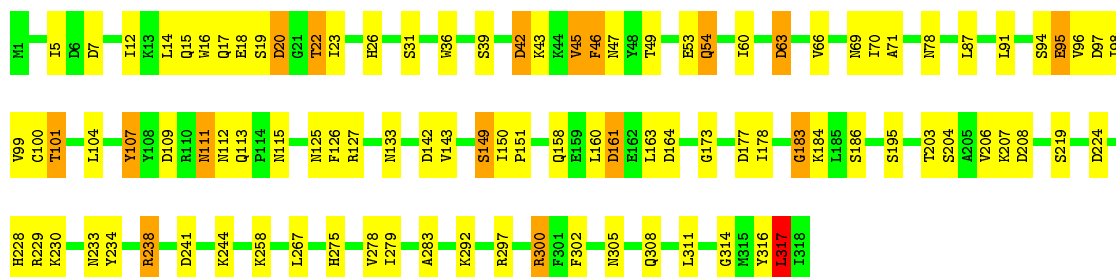


• Molecule 1: PLASMID SEGREGATION PROTEIN PARM



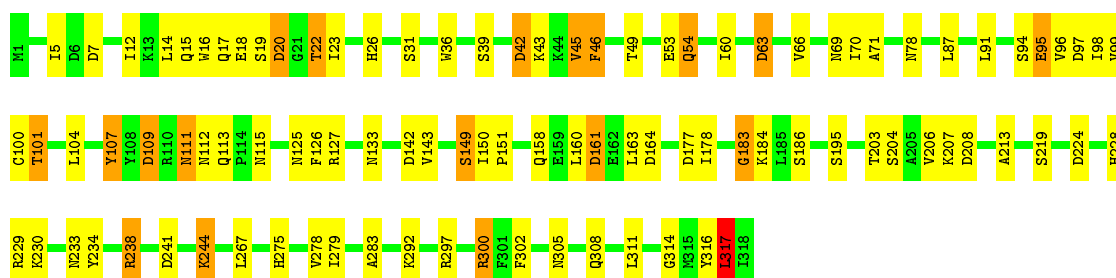
• Molecule 1: PLASMID SEGREGATION PROTEIN PARM

Chain D:  69% 26% 5%



• Molecule 1: PLASMID SEGREGATION PROTEIN PARM

Chain E:  69% 25% 6%



4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	28	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON II (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: ANP

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	0.57	0/2545	0.84	1/3447 (0.0%)
1	B	0.56	0/2545	0.83	0/3447
1	C	0.53	0/2545	0.83	0/3447
1	D	0.53	0/2545	0.82	0/3447
1	E	0.54	0/2545	0.83	0/3447
All	All	0.55	0/12725	0.83	1/17235 (0.0%)

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	5
1	B	0	6
1	C	0	5
1	D	0	5
1	E	0	5
All	All	0	26

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	107	TYR	CB-CA-C	-5.01	100.37	110.40

There are no chirality outliers.

5 of 26 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	THR	Peptide
1	A	244	LYS	Peptide
1	A	317	LEU	Peptide
1	A	39	SER	Peptide
1	A	63	ASP	Peptide

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	2504	0	2501	37	0
1	B	2504	0	2501	33	0
1	C	2504	0	2501	37	0
1	D	2504	0	2501	35	0
1	E	2504	0	2501	35	0
2	A	31	0	13	2	0
2	B	31	0	13	1	0
2	C	31	0	13	1	0
2	D	31	0	13	1	0
2	E	31	0	13	0	0
All	All	12675	0	12570	174	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 7.

The worst 5 of 174 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:297:ARG:N	1:C:241:ASP:OD2	2.20	0.74
1:C:297:ARG:N	1:E:241:ASP:OD2	2.22	0.72
1:B:297:ARG:N	1:D:241:ASP:OD2	2.22	0.72
1:E:164:ASP:O	1:E:183:GLY:N	2.30	0.65
1:A:17:GLN:HA	1:A:22:THR:O	1.96	0.64

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 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	316/318 (99%)	278 (88%)	29 (9%)	9 (3%)	6	46
1	B	316/318 (99%)	279 (88%)	28 (9%)	9 (3%)	6	46
1	C	316/318 (99%)	281 (89%)	26 (8%)	9 (3%)	6	46
1	D	316/318 (99%)	280 (89%)	27 (8%)	9 (3%)	6	46
1	E	316/318 (99%)	280 (89%)	27 (8%)	9 (3%)	6	46
All	All	1580/1590 (99%)	1398 (88%)	137 (9%)	45 (3%)	10	46

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	ASP
1	A	46	PHE
1	A	70	ILE
1	A	112	ASN
1	A	133	ASN

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 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	283/283 (100%)	234 (83%)	49 (17%)	2	18
1	B	283/283 (100%)	233 (82%)	50 (18%)	2	17
1	C	283/283 (100%)	233 (82%)	50 (18%)	2	17
1	D	283/283 (100%)	234 (83%)	49 (17%)	2	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	283/283 (100%)	235 (83%)	48 (17%)	2	19
All	All	1415/1415 (100%)	1169 (83%)	246 (17%)	6	18

5 of 246 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	78	ASN
1	C	238	ARG
1	E	195	SER
1	C	96	VAL
1	C	149	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	308	GLN
1	C	78	ASN
1	D	118	ASN
1	B	111	ASN
1	B	118	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](#)

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](#)

5 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	ANP	A	500	-	29,33,33	1.64	3 (10%)	26,52,52	1.32	2 (7%)
2	ANP	B	500	-	29,33,33	1.67	3 (10%)	26,52,52	1.25	1 (3%)
2	ANP	C	500	-	29,33,33	1.67	3 (10%)	26,52,52	1.25	2 (7%)
2	ANP	D	500	-	29,33,33	1.66	3 (10%)	26,52,52	1.23	1 (3%)
2	ANP	E	500	-	29,33,33	1.67	3 (10%)	26,52,52	1.23	2 (7%)

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	ANP	A	500	-	-	0/13/38/38	0/3/3/3
2	ANP	B	500	-	-	0/13/38/38	0/3/3/3
2	ANP	C	500	-	-	0/13/38/38	0/3/3/3
2	ANP	D	500	-	-	0/13/38/38	0/3/3/3
2	ANP	E	500	-	-	0/13/38/38	0/3/3/3

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	500	ANP	PB-O2B	-2.65	1.49	1.56
2	C	500	ANP	PB-O2B	-2.64	1.49	1.56
2	D	500	ANP	PB-O2B	-2.63	1.49	1.56
2	B	500	ANP	PB-O2B	-2.62	1.49	1.56
2	A	500	ANP	PB-O2B	-2.60	1.49	1.56

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	ANP	O2G-PG-O1G	-2.53	106.92	113.58
2	E	500	ANP	O2G-PG-O1G	-2.19	107.82	113.58
2	C	500	ANP	O2G-PG-O1G	-2.00	108.31	113.58
2	E	500	ANP	O2B-PB-O1B	4.30	118.49	110.02
2	C	500	ANP	O2B-PB-O1B	4.33	118.54	110.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	ANP	2	0
2	B	500	ANP	1	0
2	C	500	ANP	1	0
2	D	500	ANP	1	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.