



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 11:40 am GMT

PDB ID : 3JB5  
EMDB ID: : EMD-6398  
Title : Capsid Structure of the Propionibacterium acnes Bacteriophage ATCC\_Clear  
Authors : Chiou, J.; Zhang, X.; Marinelli, L.J.; Modlin, R.L.; Zhou, Z.H.  
Deposited on : 2015-07-23  
Resolution : 3.70 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](mailto: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.

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MolProbity : 4.02b-467  
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) : recalc29047

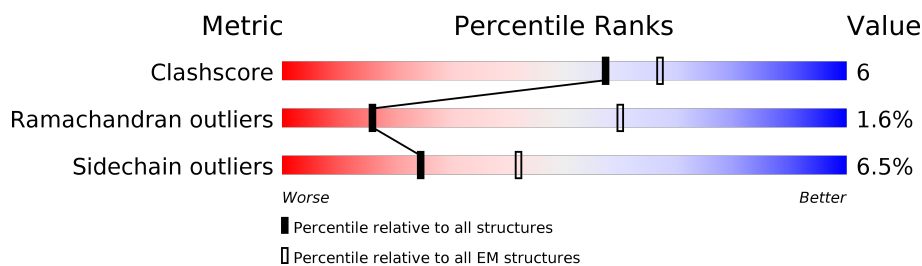
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.70 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  $\geq 3$ , 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	315	81% 13% • 5%
1	B	315	78% 15% • 5%
1	C	315	70% 23% • 5%
1	D	315	78% 15% • 5%
1	E	315	78% 15% • 5%
1	F	315	78% 15% • 5%
1	G	315	70% 17% • 12%

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 15232 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 major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	300	Total	C	N	O	S	0	0
			2200	1398	374	423	5		
1	B	300	Total	C	N	O	S	0	0
			2200	1398	374	423	5		
1	C	300	Total	C	N	O	S	0	0
			2200	1398	374	423	5		
1	D	300	Total	C	N	O	S	0	0
			2200	1398	374	423	5		
1	E	300	Total	C	N	O	S	0	0
			2200	1398	374	423	5		
1	F	300	Total	C	N	O	S	0	0
			2200	1398	374	423	5		
1	G	276	Total	C	N	O	S	0	0
			2032	1289	348	391	4		

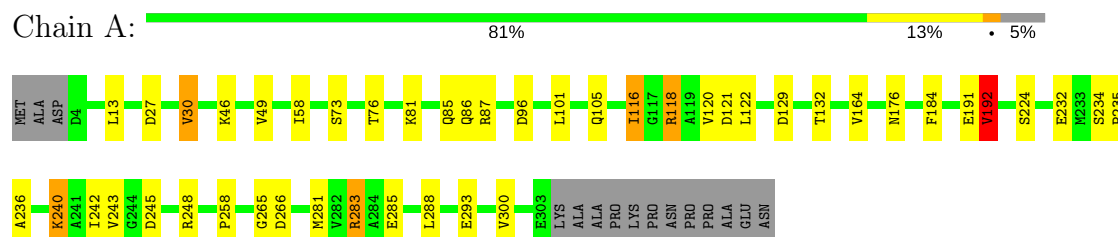
There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	VAL	ALA	CONFLICT	UNP A4K473
B	8	VAL	ALA	CONFLICT	UNP A4K473
C	8	VAL	ALA	CONFLICT	UNP A4K473
D	8	VAL	ALA	CONFLICT	UNP A4K473
E	8	VAL	ALA	CONFLICT	UNP A4K473
F	8	VAL	ALA	CONFLICT	UNP A4K473
G	8	VAL	ALA	CONFLICT	UNP A4K473

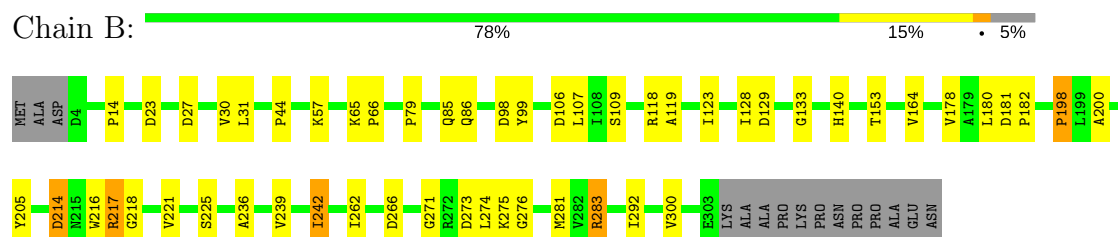
### 3 Residue-property plots

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.

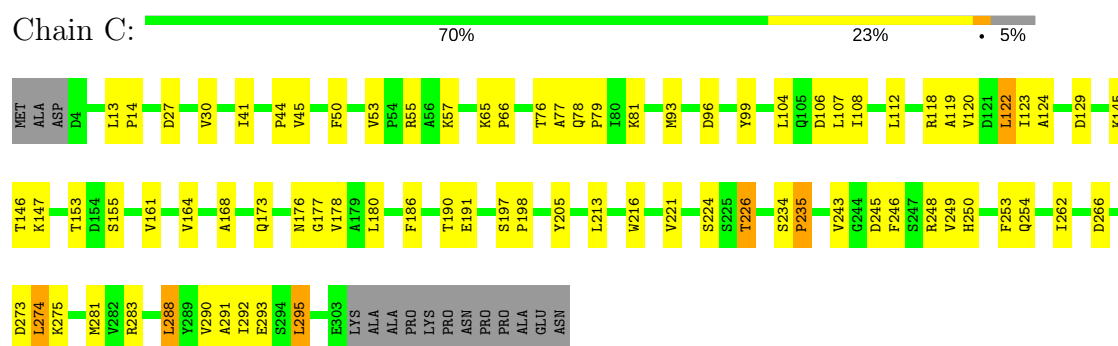
- Molecule 1: major capsid protein



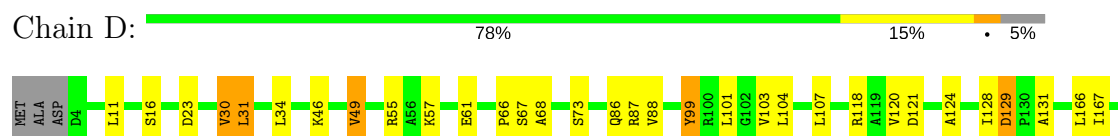
- Molecule 1: major capsid protein

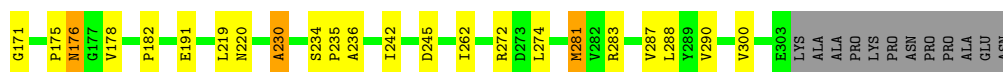


- Molecule 1: major capsid protein



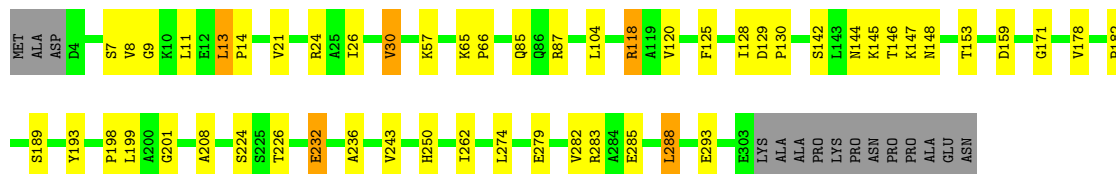
- Molecule 1: major capsid protein





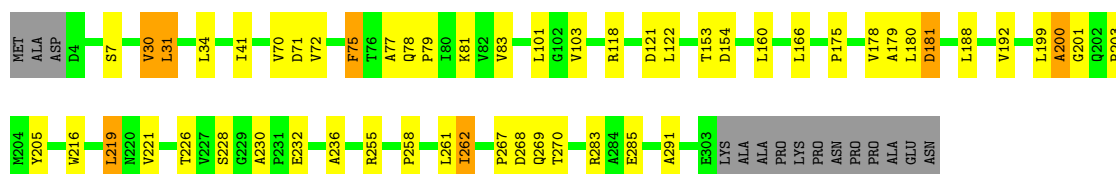
- Molecule 1: major capsid protein

Chain E: 78% 15% • 5%



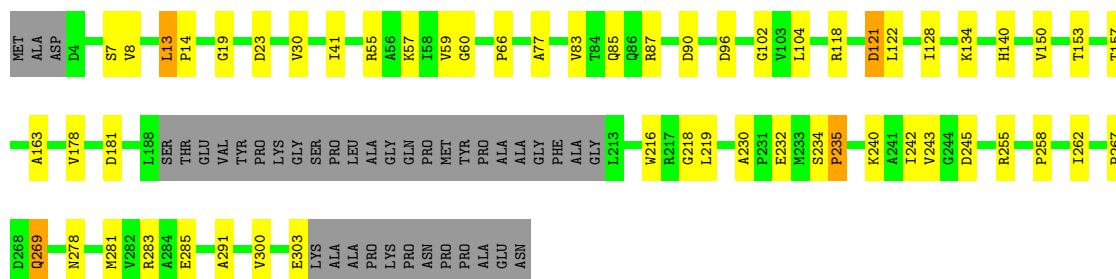
- Molecule 1: major capsid protein

Chain F: 78% 15% • 5%



- Molecule 1: major capsid protein

Chain G: 70% 17% • 12%



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	27504	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	25	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2270	Depositor
Magnification	38462	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.21	0/2246	0.40	0/3057
1	B	0.21	0/2246	0.39	0/3057
1	C	0.21	0/2246	0.41	0/3057
1	D	0.21	0/2246	0.38	0/3057
1	E	0.21	0/2246	0.40	0/3057
1	F	0.21	0/2246	0.39	0/3057
1	G	0.21	0/2070	0.39	0/2814
All	All	0.21	0/15546	0.40	0/21156

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	2200	0	2199	21	0
1	B	2200	0	2199	27	0
1	C	2200	0	2199	44	0
1	D	2200	0	2199	29	0
1	E	2200	0	2199	27	0
1	F	2200	0	2199	24	0
1	G	2032	0	2038	25	0
All	All	15232	0	15232	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 6.

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:F:181:ASP:HB2	1:F:228:SER:HB3	1.70	0.72
1:B:271:GLY:O	1:G:269:GLN:NE2	2.24	0.71
1:C:77:ALA:HB2	1:C:291:ALA:HB2	1.76	0.67
1:B:65:LYS:HD3	1:C:283:ARG:HH12	1.58	0.67
1:E:57:LYS:HD3	1:E:66:PRO:HG3	1.77	0.67

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	298/315 (95%)	266 (89%)	28 (9%)	4 (1%)	14	57
1	B	298/315 (95%)	272 (91%)	21 (7%)	5 (2%)	11	53
1	C	298/315 (95%)	274 (92%)	20 (7%)	4 (1%)	14	57
1	D	298/315 (95%)	272 (91%)	21 (7%)	5 (2%)	11	53
1	E	298/315 (95%)	278 (93%)	17 (6%)	3 (1%)	18	62
1	F	298/315 (95%)	275 (92%)	17 (6%)	6 (2%)	9	50
1	G	272/315 (86%)	251 (92%)	15 (6%)	6 (2%)	8	48
All	All	2060/2205 (93%)	1888 (92%)	139 (7%)	33 (2%)	16	54

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	192	VAL
1	A	258	PRO

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Mol	Chain	Res	Type
1	B	198	PRO
1	C	107	LEU
1	F	30	VAL

### 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	230/241 (95%)	215 (94%)	15 (6%)	20	59
1	B	230/241 (95%)	215 (94%)	15 (6%)	20	59
1	C	230/241 (95%)	212 (92%)	18 (8%)	15	52
1	D	230/241 (95%)	215 (94%)	15 (6%)	20	59
1	E	230/241 (95%)	217 (94%)	13 (6%)	24	63
1	F	230/241 (95%)	216 (94%)	14 (6%)	22	61
1	G	214/241 (89%)	201 (94%)	13 (6%)	22	61
All	All	1594/1687 (94%)	1491 (94%)	103 (6%)	24	59

5 of 103 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	288	LEU
1	D	128	ILE
1	G	122	LEU
1	C	295	LEU
1	D	49	VAL

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

Mol	Chain	Res	Type
1	D	176	ASN
1	G	85	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 carbohydrates 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.