



wwPDB EM Validation Summary Report ⓘ

Dec 25, 2023 – 04:07 PM JST

PDB ID : 8JWX
EMDB ID : EMD-35794
Title : bottom segment of the bacteriophage M13 mini variant
Authors : Xiang, Y.; Jia, Q.
Deposited on : 2023-06-29
Resolution : 3.30 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : **FAILED**
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

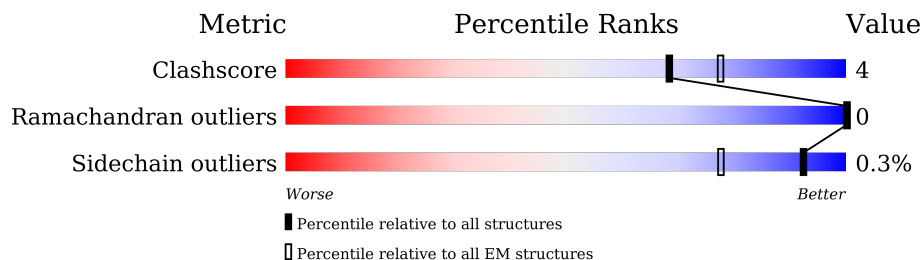
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	406	
1	F	406	
1	K	406	
1	R	406	
1	T	406	
2	B	50	
2	C	50	
2	D	50	
2	G	50	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	50	 84% 8% 8%
2	I	50	 76% 12% 12%
2	L	50	 82% 10% 8%
2	M	50	 86% 6% 8%
2	N	50	 76% 12% 12%
2	P	50	 82% 10% 8%
2	Q	50	 86% 6% 8%
2	S	50	 76% 12% 12%
2	V	50	 78% 14% 8%
2	W	50	 86% 6% 8%
2	X	50	 76% 12% 12%
3	E	112	 88% 9% .
3	J	112	 88% 9% .
3	O	112	 89% 8% .
3	Y	112	 89% 8% .
3	Z	112	 88% 9% .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 14790 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 Attachment protein G3P.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	R	145	1091	685	182	217	7	0	0
1	A	145	1091	685	182	217	7	0	0
1	F	145	1091	685	182	217	7	0	0
1	K	145	1091	685	182	217	7	0	0
1	T	145	1091	685	182	217	7	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	360	GLY	SER	conflict	UNP P69168
A	360	GLY	SER	conflict	UNP P69168
F	360	GLY	SER	conflict	UNP P69168
K	360	GLY	SER	conflict	UNP P69168
T	360	GLY	SER	conflict	UNP P69168

- Molecule 2 is a protein called Capsid protein G8P.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	P	46	344	227	54	62	1	0	0
2	Q	46	344	227	54	62	1	0	0
2	S	44	329	218	52	58	1	0	0
2	B	46	344	227	54	62	1	0	0
2	C	46	344	227	54	62	1	0	0

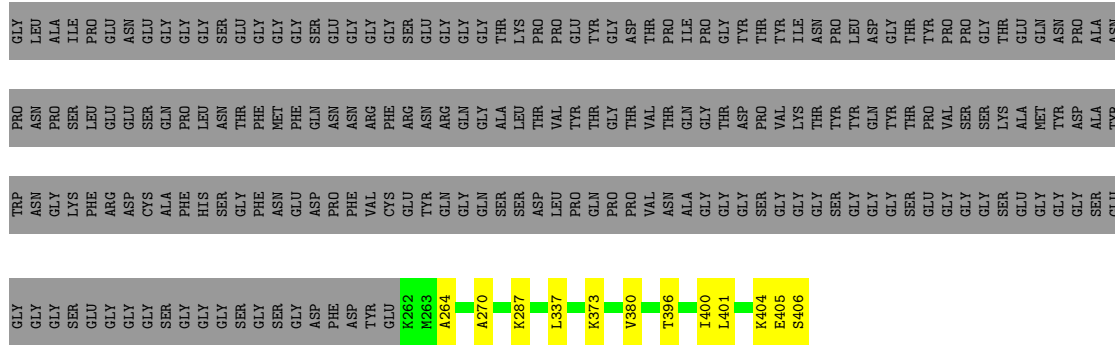
Continued on next page...

Continued from previous page...

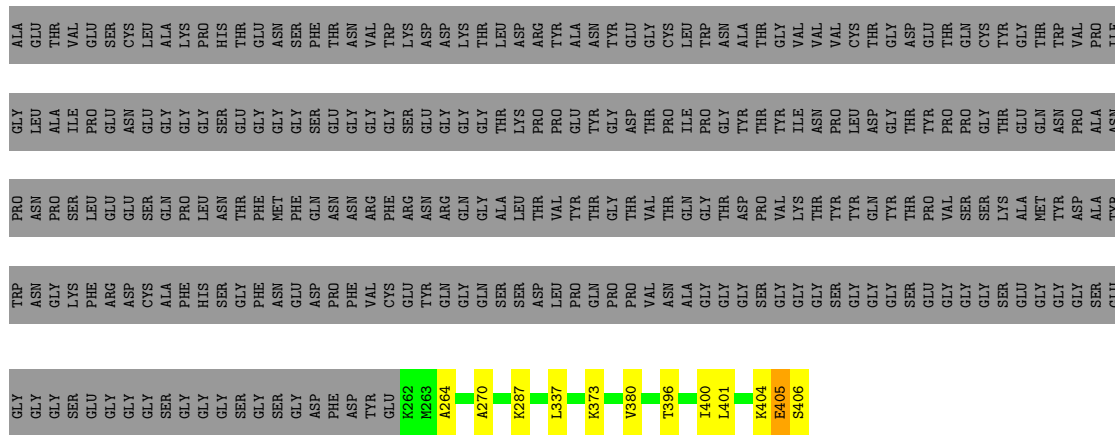
Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	44	Total	C	N	O	S	0	0
			329	218	52	58	1		
2	G	46	Total	C	N	O	S	0	0
			344	227	54	62	1		
2	H	46	Total	C	N	O	S	0	0
			344	227	54	62	1		
2	I	44	Total	C	N	O	S	0	0
			329	218	52	58	1		
2	L	46	Total	C	N	O	S	0	0
			344	227	54	62	1		
2	M	46	Total	C	N	O	S	0	0
			344	227	54	62	1		
2	N	44	Total	C	N	O	S	0	0
			329	218	52	58	1		
2	V	46	Total	C	N	O	S	0	0
			344	227	54	62	1		
2	W	46	Total	C	N	O	S	0	0
			344	227	54	62	1		
2	X	44	Total	C	N	O	S	0	0
			329	218	52	58	1		

- Molecule 3 is a protein called Head virion protein G6P.

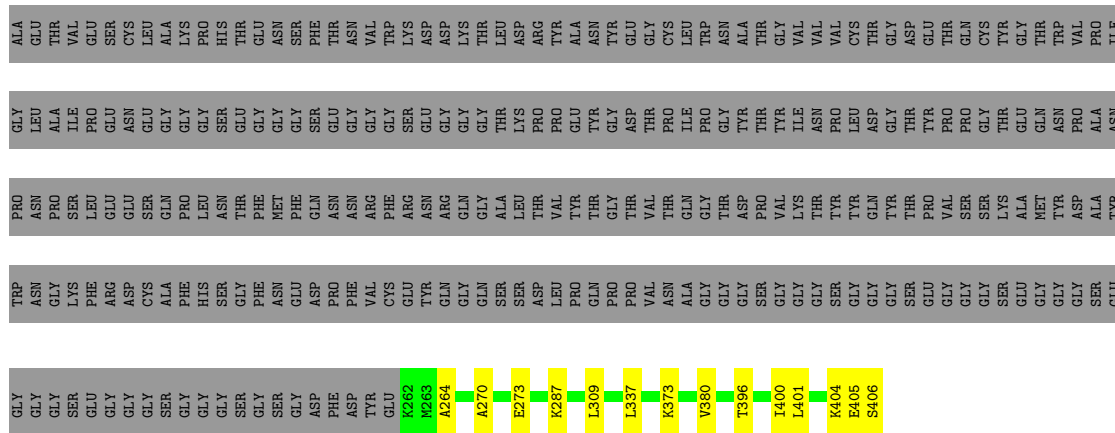
Mol	Chain	Residues	Atoms					AltConf	Trace
3	Z	109	Total	C	N	O	S	0	0
			850	587	125	137	1		
3	E	109	Total	C	N	O	S	0	0
			850	587	125	137	1		
3	J	109	Total	C	N	O	S	0	0
			850	587	125	137	1		
3	O	109	Total	C	N	O	S	0	0
			850	587	125	137	1		
3	Y	109	Total	C	N	O	S	0	0
			850	587	125	137	1		



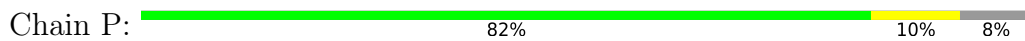
• Molecule 1: Attachment protein G3P



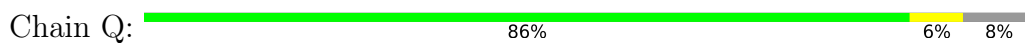
• Molecule 1: Attachment protein G3P



• Molecule 2: Capsid protein G8P



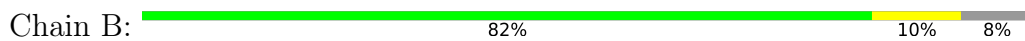
● Molecule 2: Capsid protein G8P



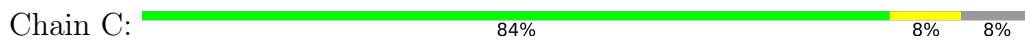
● Molecule 2: Capsid protein G8P



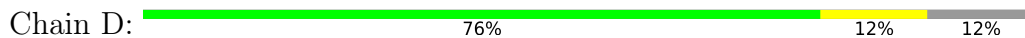
● Molecule 2: Capsid protein G8P



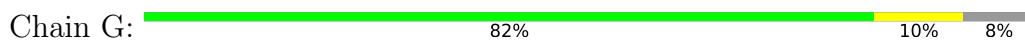
● Molecule 2: Capsid protein G8P



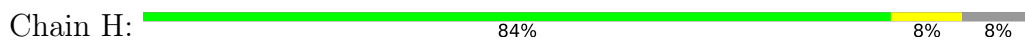
● Molecule 2: Capsid protein G8P



● Molecule 2: Capsid protein G8P



● Molecule 2: Capsid protein G8P




● Molecule 2: Capsid protein G8P

Chain I:  76% 12% 12%




● Molecule 2: Capsid protein G8P

Chain L:  82% 10% 8%



● Molecule 2: Capsid protein G8P

Chain M:  86% 6% 8%




● Molecule 2: Capsid protein G8P

Chain N:  76% 12% 12%




● Molecule 2: Capsid protein G8P

Chain V:  78% 14% 8%




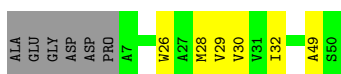
● Molecule 2: Capsid protein G8P

Chain W:  86% 6% 8%




● Molecule 2: Capsid protein G8P

Chain X:  76% 12% 12%




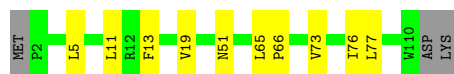
● Molecule 3: Head virion protein G6P

Chain Z:  88% 9%




• Molecule 3: Head virion protein G6P

Chain E:  88% 9%




• Molecule 3: Head virion protein G6P

Chain J:  88% 9%




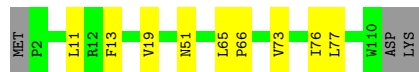
• Molecule 3: Head virion protein G6P

Chain O:  89% 8%



• Molecule 3: Head virion protein G6P

Chain Y:  89% 8%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45177	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k 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 >5	RMSZ	# Z >5
1	A	0.36	0/1112	0.46	0/1499
1	F	0.36	0/1112	0.46	0/1499
1	K	0.36	0/1112	0.46	0/1499
1	R	0.36	0/1112	0.46	0/1499
1	T	0.36	0/1112	0.46	0/1499
2	B	0.38	0/351	0.47	0/473
2	C	0.28	0/351	0.38	0/473
2	D	0.36	0/335	0.40	0/450
2	G	0.38	0/351	0.47	0/473
2	H	0.28	0/351	0.38	0/473
2	I	0.36	0/335	0.40	0/450
2	L	0.38	0/351	0.47	0/473
2	M	0.28	0/351	0.38	0/473
2	N	0.36	0/335	0.40	0/450
2	P	0.38	0/351	0.47	0/473
2	Q	0.28	0/351	0.38	0/473
2	S	0.36	0/335	0.40	0/450
2	V	0.38	0/351	0.47	0/473
2	W	0.28	0/351	0.38	0/473
2	X	0.36	0/335	0.40	0/450
3	E	0.31	0/870	0.45	0/1183
3	J	0.31	0/870	0.45	0/1183
3	O	0.31	0/870	0.45	0/1183
3	Y	0.31	0/870	0.45	0/1183
3	Z	0.31	0/870	0.45	0/1183
All	All	0.34	0/15095	0.44	0/20390

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	1091	0	1034	16	0
1	F	1091	0	1034	15	0
1	K	1091	0	1034	15	0
1	R	1091	0	1034	17	0
1	T	1091	0	1034	17	0
2	B	344	0	356	6	0
2	C	344	0	356	3	0
2	D	329	0	345	4	0
2	G	344	0	356	5	0
2	H	344	0	356	3	0
2	I	329	0	345	5	0
2	L	344	0	356	6	0
2	M	344	0	356	2	0
2	N	329	0	345	4	0
2	P	344	0	356	6	0
2	Q	344	0	356	2	0
2	S	329	0	345	5	0
2	V	344	0	356	6	0
2	W	344	0	356	2	0
2	X	329	0	345	5	0
3	E	850	0	928	8	0
3	J	850	0	928	8	0
3	O	850	0	928	7	0
3	Y	850	0	928	7	0
3	Z	850	0	928	8	0
All	All	14790	0	15095	114	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 4.

The worst 5 of 114 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)
2:P:33:VAL:HG13	2:Q:46:THR:HG21	1.68	0.76
2:V:33:VAL:HG13	2:W:46:THR:HG21	1.68	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:33:VAL:HG13	2:C:46:THR:HG21	1.68	0.75
2:L:33:VAL:HG13	2:M:46:THR:HG21	1.68	0.74
2:G:33:VAL:HG13	2:H:46:THR:HG21	1.68	0.74

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	143/406 (35%)	136 (95%)	7 (5%)	0	100	100
1	F	143/406 (35%)	136 (95%)	7 (5%)	0	100	100
1	K	143/406 (35%)	136 (95%)	7 (5%)	0	100	100
1	R	143/406 (35%)	136 (95%)	7 (5%)	0	100	100
1	T	143/406 (35%)	136 (95%)	7 (5%)	0	100	100
2	B	44/50 (88%)	43 (98%)	1 (2%)	0	100	100
2	C	44/50 (88%)	44 (100%)	0	0	100	100
2	D	42/50 (84%)	42 (100%)	0	0	100	100
2	G	44/50 (88%)	43 (98%)	1 (2%)	0	100	100
2	H	44/50 (88%)	44 (100%)	0	0	100	100
2	I	42/50 (84%)	42 (100%)	0	0	100	100
2	L	44/50 (88%)	43 (98%)	1 (2%)	0	100	100
2	M	44/50 (88%)	44 (100%)	0	0	100	100
2	N	42/50 (84%)	42 (100%)	0	0	100	100
2	P	44/50 (88%)	43 (98%)	1 (2%)	0	100	100
2	Q	44/50 (88%)	44 (100%)	0	0	100	100
2	S	42/50 (84%)	42 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	V	44/50 (88%)	43 (98%)	1 (2%)	0	100	100
2	W	44/50 (88%)	44 (100%)	0	0	100	100
2	X	42/50 (84%)	42 (100%)	0	0	100	100
3	E	107/112 (96%)	104 (97%)	3 (3%)	0	100	100
3	J	107/112 (96%)	104 (97%)	3 (3%)	0	100	100
3	O	107/112 (96%)	104 (97%)	3 (3%)	0	100	100
3	Y	107/112 (96%)	104 (97%)	3 (3%)	0	100	100
3	Z	107/112 (96%)	104 (97%)	3 (3%)	0	100	100
All	All	1900/3340 (57%)	1845 (97%)	55 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	113/310 (36%)	112 (99%)	1 (1%)	78	87
1	F	113/310 (36%)	112 (99%)	1 (1%)	78	87
1	K	113/310 (36%)	112 (99%)	1 (1%)	78	87
1	R	113/310 (36%)	112 (99%)	1 (1%)	78	87
1	T	113/310 (36%)	112 (99%)	1 (1%)	78	87
2	B	34/36 (94%)	34 (100%)	0	100	100
2	C	34/36 (94%)	34 (100%)	0	100	100
2	D	32/36 (89%)	32 (100%)	0	100	100
2	G	34/36 (94%)	34 (100%)	0	100	100
2	H	34/36 (94%)	34 (100%)	0	100	100
2	I	32/36 (89%)	32 (100%)	0	100	100
2	L	34/36 (94%)	34 (100%)	0	100	100
2	M	34/36 (94%)	34 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	N	32/36 (89%)	32 (100%)	0	100	100
2	P	34/36 (94%)	34 (100%)	0	100	100
2	Q	34/36 (94%)	34 (100%)	0	100	100
2	S	32/36 (89%)	32 (100%)	0	100	100
2	V	34/36 (94%)	34 (100%)	0	100	100
2	W	34/36 (94%)	34 (100%)	0	100	100
2	X	32/36 (89%)	32 (100%)	0	100	100
3	E	94/97 (97%)	94 (100%)	0	100	100
3	J	94/97 (97%)	94 (100%)	0	100	100
3	O	94/97 (97%)	94 (100%)	0	100	100
3	Y	94/97 (97%)	94 (100%)	0	100	100
3	Z	94/97 (97%)	94 (100%)	0	100	100
All	All	1535/2575 (60%)	1530 (100%)	5 (0%)	92	96

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	405	GLU
1	A	405	GLU
1	F	405	GLU
1	K	405	GLU
1	T	405	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
3	Y	74	GLN
3	Y	51	ASN
3	J	74	GLN
3	J	51	ASN
3	O	51	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.