



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

Jan 22, 2018 – 06:02 PM EST

PDB ID : 1HB5  
EMDB ID: : EMD-1014  
Title : quasi-atomic resolution model of bacteriophage PRD1 P3-shell, obtained by combined cryo-EM and X-ray crystallography.  
Authors : San Martin, C.; Burnett, R.M.; De Haas, F.; Heinkel, R.; Rutten, T.; Fuller, S.D.; Butcher, S.J.; Bamford, D.H.  
Deposited on : 2001-04-11  
Resolution : 12.00 Å(reported)  
Based on PDB ID : 1HX6

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) : rb-20030736

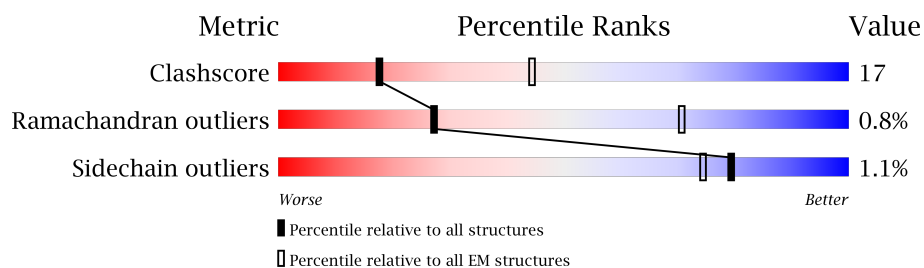
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 12.00 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	394	
1	B	394	
1	C	394	
1	D	394	
1	E	394	
1	F	394	
1	G	394	
1	H	394	
1	I	394	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 27273 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.

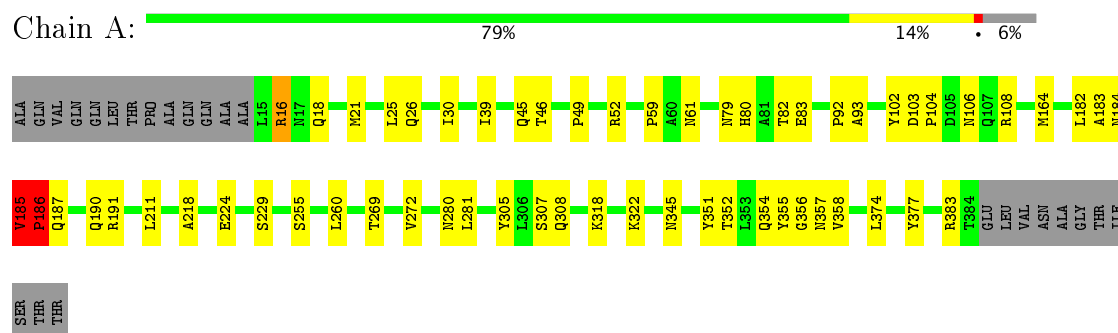
- Molecule 1 is a protein called BACTERIOPHAGE PRD1 P3-SHELL.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	370	Total	C	N	O	S	24	0
			3047	1924	520	595	8		
1	B	374	Total	C	N	O	S	22	0
			3056	1932	518	598	8		
1	C	371	Total	C	N	O	S	15	0
			2988	1892	504	584	8		
1	D	370	Total	C	N	O	S	24	0
			3047	1924	520	595	8		
1	E	374	Total	C	N	O	S	22	0
			3056	1932	518	598	8		
1	F	371	Total	C	N	O	S	15	0
			2988	1892	504	584	8		
1	G	370	Total	C	N	O	S	24	0
			3047	1924	520	595	8		
1	H	374	Total	C	N	O	S	22	0
			3056	1932	518	598	8		
1	I	371	Total	C	N	O	S	15	0
			2988	1892	504	584	8		

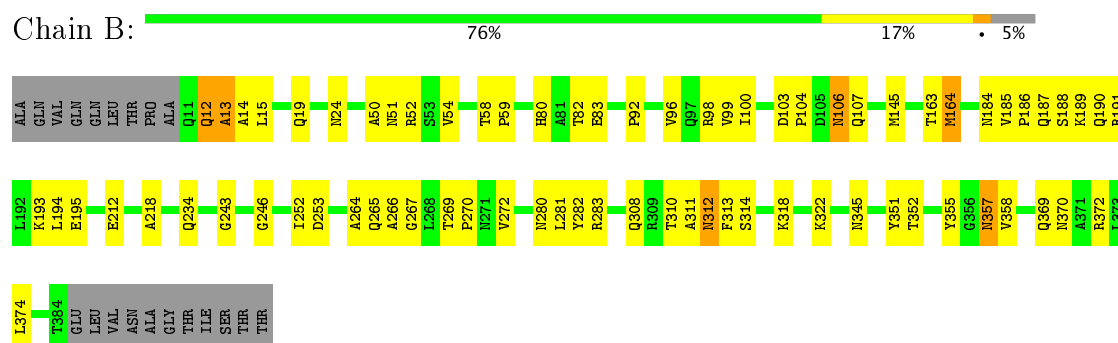
### 3 Residue-property plots

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.

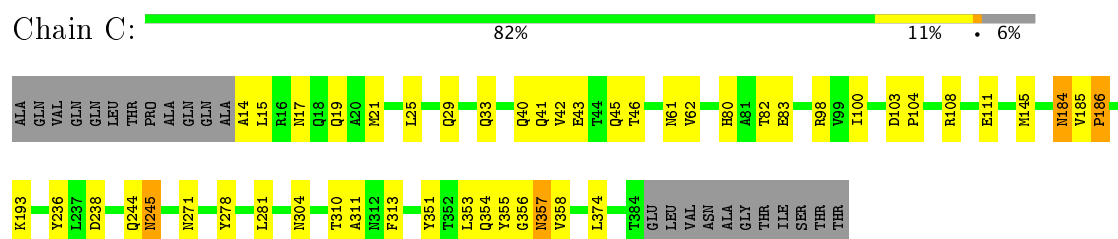
#### • Molecule 1: BACTERIOPHAGE PRD1 P3-SHELL



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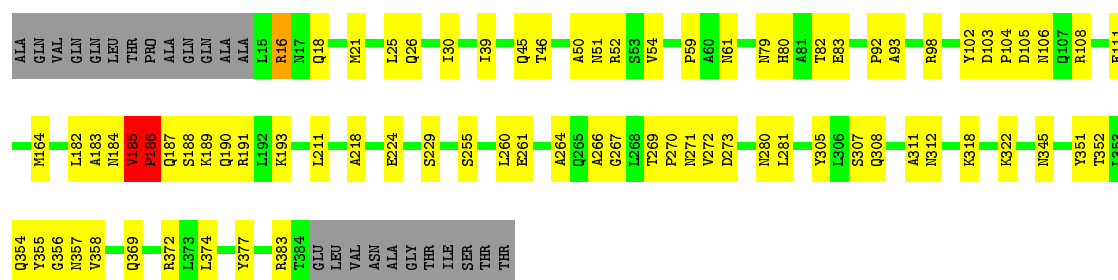


#### • Molecule 1: BACTERIOPHAGE PRD1 P3-SHELL



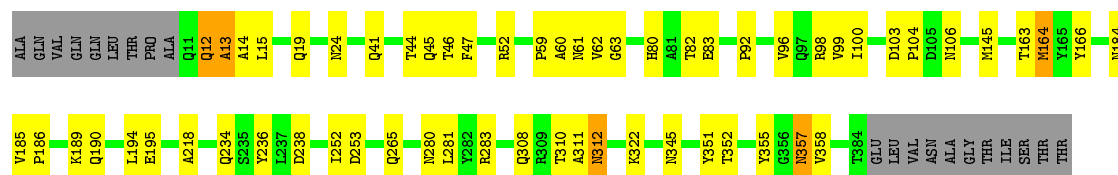
#### • Molecule 1: BACTERIOPHAGE PRD1 P3-SHELL





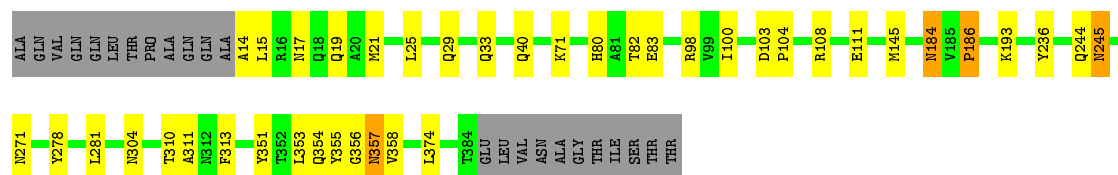
• Molecule 1: BACTERIOPHAGE PRD1 P3-SHELL

Chain E: 80% 14% 5%



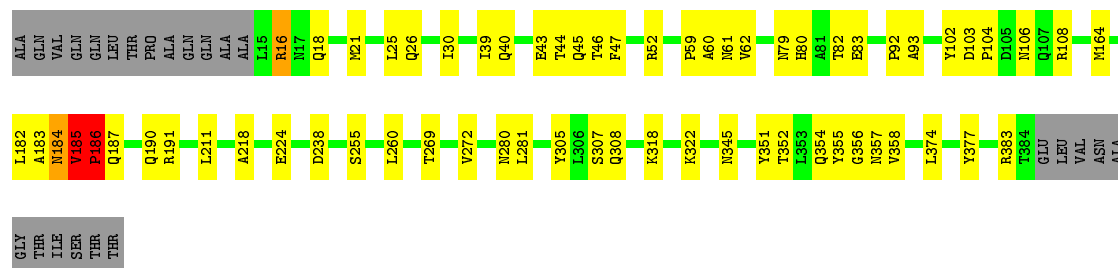
• Molecule 1: BACTERIOPHAGE PRD1 P3-SHELL

Chain F: 84% 9% 6%



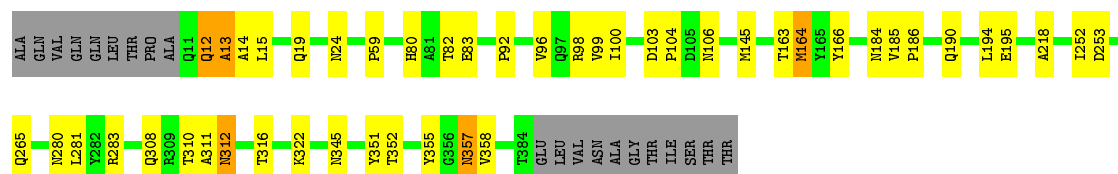
• Molecule 1: BACTERIOPHAGE PRD1 P3-SHELL

Chain G: 78% 15% 6%

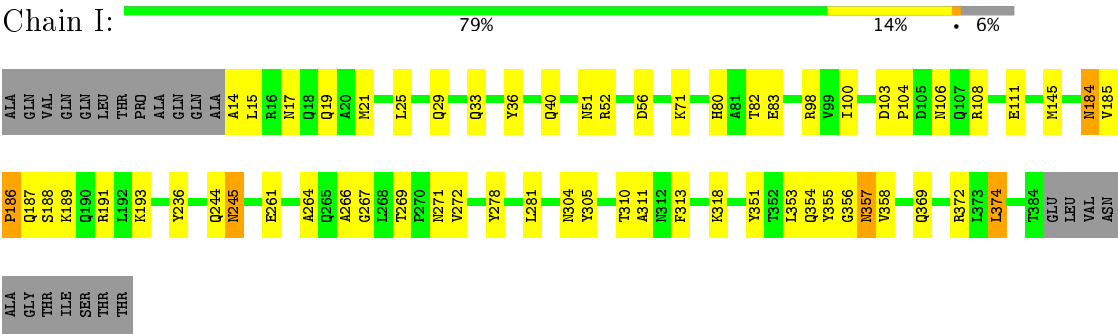


• Molecule 1: BACTERIOPHAGE PRD1 P3-SHELL

Chain H: 83% 11% 5%



● Molecule 1: BACTERIOPHAGE PRD1 P3-SHELL



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	471	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI/PHILIPS CM200FEG	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	10	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	4100	Depositor
Magnification	36000	Depositor
Image detector	KODAK SO-163 FILM	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	0.47	0/3113	0.71	0/4255
1	B	0.48	1/3121 (0.0%)	0.74	1/4265 (0.0%)
1	C	0.44	0/3053	0.73	1/4173 (0.0%)
1	D	0.47	0/3113	0.71	0/4255
1	E	0.48	1/3121 (0.0%)	0.74	1/4265 (0.0%)
1	F	0.44	0/3053	0.73	1/4173 (0.0%)
1	G	0.47	0/3113	0.71	0/4255
1	H	0.48	1/3121 (0.0%)	0.74	1/4265 (0.0%)
1	I	0.44	0/3053	0.73	1/4173 (0.0%)
All	All	0.46	3/27861 (0.0%)	0.73	6/38079 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	164	MET	CB-CG	7.50	1.75	1.51
1	H	164	MET	CB-CG	7.49	1.75	1.51
1	E	164	MET	CB-CG	7.49	1.75	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	164	MET	CB-CG-SD	-11.60	77.60	112.40
1	H	164	MET	CB-CG-SD	-11.59	77.62	112.40
1	E	164	MET	CB-CG-SD	-11.59	77.63	112.40
1	I	278	TYR	N-CA-C	-5.46	96.26	111.00
1	F	278	TYR	N-CA-C	-5.45	96.28	111.00

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	3047	0	2910	55	0
1	B	3056	0	2913	330	0
1	C	2988	0	2863	89	0
1	D	3047	0	2897	292	0
1	E	3056	0	2918	169	0
1	F	2988	0	2863	34	0
1	G	3047	0	2909	178	0
1	H	3056	0	2923	51	0
1	I	2988	0	2855	229	0
All	All	27273	0	26051	908	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 17.

The worst 5 of 908 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:164:MET:CG	1:B:164:MET:CB	1.75	1.64
1:D:52[A]:ARG:CZ	1:G:43:GLU:HG3	1.16	1.60
1:B:269[B]:THR:HG21	1:I:372:ARG:CD	1.24	1.59
1:B:266:ALA:HB3	1:D:267:GLY:CA	1.34	1.57
1:H:164:MET:CB	1:H:164:MET:CG	1.75	1.56

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	392/394 (100%)	365 (93%)	24 (6%)	3 (1%)	22	67
1	B	394/394 (100%)	371 (94%)	20 (5%)	3 (1%)	22	67
1	C	384/394 (98%)	367 (96%)	14 (4%)	3 (1%)	22	67
1	D	392/394 (100%)	365 (93%)	24 (6%)	3 (1%)	22	67
1	E	394/394 (100%)	371 (94%)	20 (5%)	3 (1%)	22	67
1	F	384/394 (98%)	367 (96%)	14 (4%)	3 (1%)	22	67
1	G	392/394 (100%)	365 (93%)	24 (6%)	3 (1%)	22	67
1	H	394/394 (100%)	371 (94%)	20 (5%)	3 (1%)	22	67
1	I	384/394 (98%)	367 (96%)	14 (4%)	3 (1%)	22	67
All	All	3510/3546 (99%)	3309 (94%)	174 (5%)	27 (1%)	27	67

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	PRO
1	B	12	GLN
1	B	312	ASN
1	C	245	ASN
1	D	186	PRO

### 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	321/325 (99%)	318 (99%)	3 (1%)	82	91
1	B	321/325 (99%)	317 (99%)	4 (1%)	75	88
1	C	315/325 (97%)	311 (99%)	4 (1%)	73	87
1	D	321/325 (99%)	318 (99%)	3 (1%)	82	91
1	E	321/325 (99%)	317 (99%)	4 (1%)	75	88
1	F	315/325 (97%)	311 (99%)	4 (1%)	73	87
1	G	321/325 (99%)	318 (99%)	3 (1%)	82	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	321/325 (99%)	317 (99%)	4 (1%)	75	88
1	I	315/325 (97%)	311 (99%)	4 (1%)	73	87
All	All	2871/2925 (98%)	2838 (99%)	33 (1%)	79	89

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	106[A]	ASN
1	F	184	ASN
1	I	355	TYR
1	E	106[B]	ASN
1	E	265	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 91 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	17	ASN
1	E	354	GLN
1	I	41	GLN
1	E	24	ASN
1	E	80	HIS

### 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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.