



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:39 PM BST

PDB ID : 1GW8  
EMDB ID: : EMD-1012  
Title : quasi-atomic resolution model of bacteriophage PRD1 sus607 mutant, obtained by combined cryo-EM and X-ray crystallography.  
Authors : San Martin, C.; Huiskonen, J.; Bamford, J.K.H.; Butcher, S.J.; Fuller, S.D.; Bamford, D.H.; Burnett, R.M.  
Deposited on : 2002-03-08  
Resolution : 13.30 Å(reported)  
Based on PDB ID : 1HX6

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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : unknown  
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

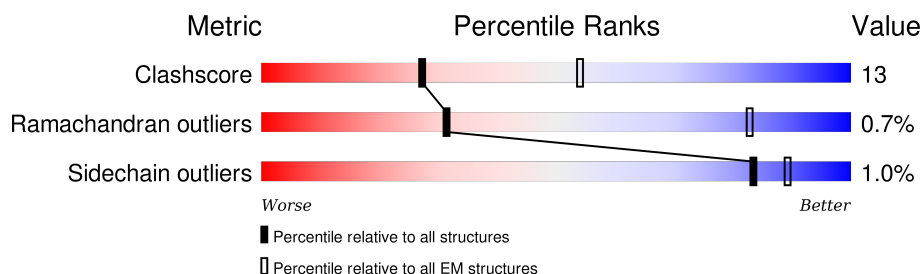
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 13.30 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  $\geq 3$ , 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	79% 14% • 6%
1	B	394	78% 15% • 5%
1	C	394	82% 11% • 6%
1	D	394	76% 17% • 6%
1	E	394	80% 14% • 5%
1	F	394	83% 10% • 6%
1	G	394	79% 14% • 6%
1	H	394	84% 10% • 5%
1	I	394	79% 14% • 6%

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Mol	Chain	Length	Quality of chain
1	J	394	<div><div></div><div>81%13%• 6%</div></div>
1	K	394	<div><div></div><div>81%13%• 5%</div></div>
1	L	394	<div><div></div><div>83%10%• 6%</div></div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 34170 atoms, of which 0 are hydrogens and 0 are deuteriums.

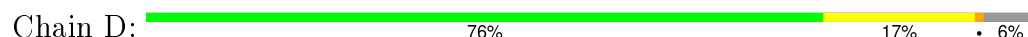
In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

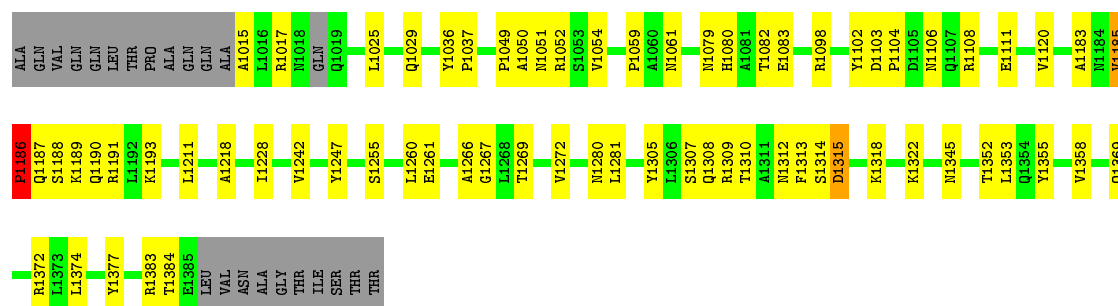
- Molecule 1 is a protein called MAJOR CAPSID PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	371	Total	C	N	O	S	0	1
			2837	1803	479	548	7		
1	B	373	Total	C	N	O	S	0	1
			2847	1804	485	551	7		
1	C	372	Total	C	N	O	S	0	1
			2861	1817	484	553	7		
1	D	371	Total	C	N	O	S	0	1
			2827	1795	478	547	7		
1	E	373	Total	C	N	O	S	0	1
			2847	1804	485	551	7		
1	F	372	Total	C	N	O	S	0	1
			2861	1817	484	553	7		
1	G	371	Total	C	N	O	S	0	1
			2837	1803	479	548	7		
1	H	373	Total	C	N	O	S	0	1
			2847	1804	485	551	7		
1	I	372	Total	C	N	O	S	0	1
			2861	1817	484	553	7		
1	J	371	Total	C	N	O	S	0	1
			2837	1803	479	548	7		
1	K	373	Total	C	N	O	S	0	1
			2847	1804	485	551	7		
1	L	372	Total	C	N	O	S	0	1
			2861	1817	484	553	7		



- Molecule 1: MAJOR CAPSID PROTEIN





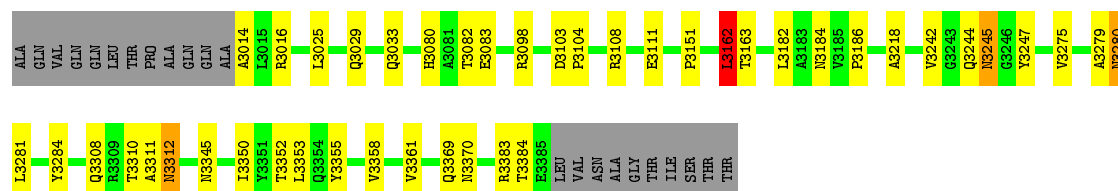
• Molecule 1: MAJOR CAPSID PROTEIN

Chain E: 80% 14% • 5%



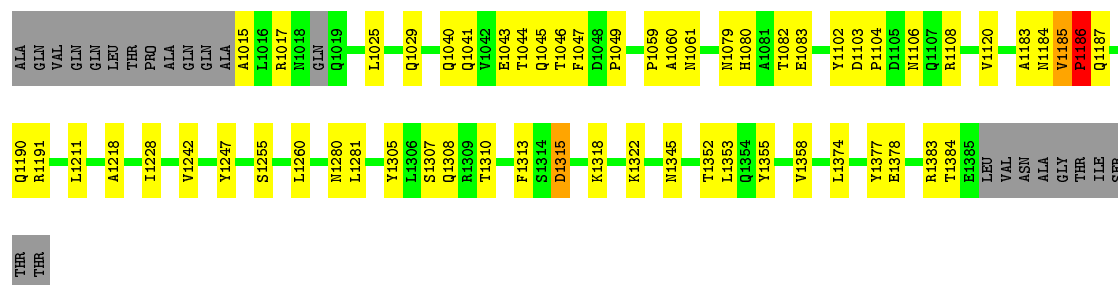
• Molecule 1: MAJOR CAPSID PROTEIN

Chain F: 83% 10% • 6%



• Molecule 1: MAJOR CAPSID PROTEIN

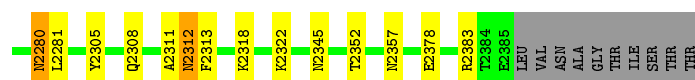
Chain G: 79% 14% • 6%



• Molecule 1: MAJOR CAPSID PROTEIN

Chain H: 84% 10% • 5%





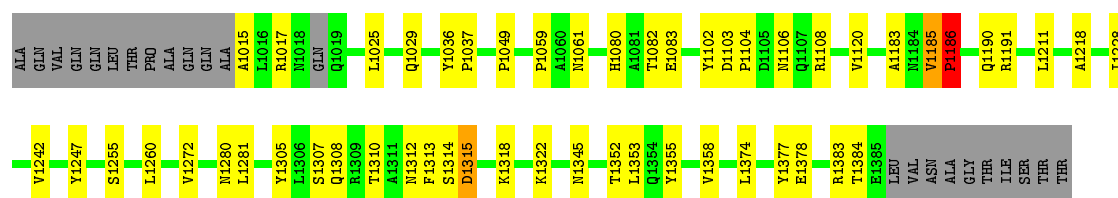
• Molecule 1: MAJOR CAPSID PROTEIN

Chain I: 79% 14% 6%



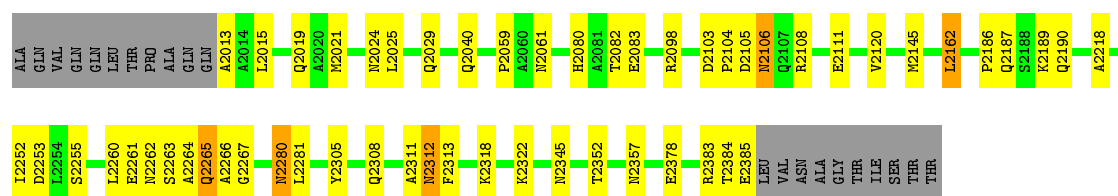
• Molecule 1: MAJOR CAPSID PROTEIN

Chain J: 81% 13% 6%



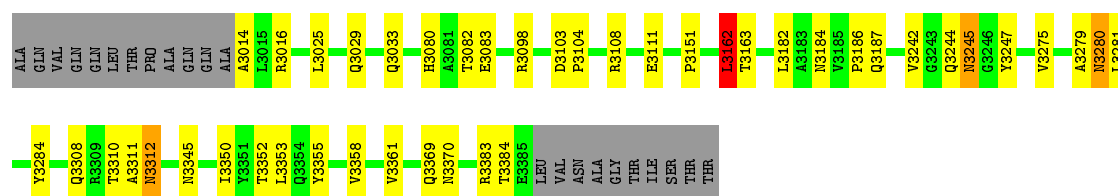
• Molecule 1: MAJOR CAPSID PROTEIN

Chain K: 81% 13% 5%



• Molecule 1: MAJOR CAPSID PROTEIN

Chain L: 83% 10% 6%



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	PHASE RESTORATION BY CTF- MULTIPLICATION OF IMAGES; AMPLITUDE RESTORATION BY COMPARISON WITH QUASI- ATOMIC MODEL	Depositor
Microscope	FEI CM200 FEG	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	4100	Depositor
Magnification	50000	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	0.44	0/2902	0.72	0/3971
1	B	0.45	0/2910	0.73	1/3982 (0.0%)
1	C	0.44	0/2926	0.72	1/4003 (0.0%)
1	D	0.44	0/2888	0.72	0/3948
1	E	0.45	0/2910	0.73	1/3982 (0.0%)
1	F	0.43	0/2926	0.72	1/4003 (0.0%)
1	G	0.44	0/2902	0.72	0/3971
1	H	0.46	0/2910	0.73	1/3982 (0.0%)
1	I	0.43	0/2926	0.72	1/4003 (0.0%)
1	J	0.44	0/2902	0.72	0/3971
1	K	0.46	0/2910	0.73	1/3982 (0.0%)
1	L	0.44	0/2926	0.73	1/4003 (0.0%)
All	All	0.44	0/34938	0.72	8/47801 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	2162	LEU	CA-CB-CG	6.46	130.16	115.30
1	H	2162	LEU	CA-CB-CG	6.44	130.10	115.30
1	B	2162	LEU	CA-CB-CG	6.43	130.09	115.30
1	K	2162	LEU	CA-CB-CG	6.42	130.07	115.30
1	L	3162	LEU	CA-CB-CG	5.99	129.08	115.30

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	2837	0	2713	110	0
1	B	2847	0	2723	225	0
1	C	2861	0	2751	60	0
1	D	2827	0	2697	206	0
1	E	2847	0	2721	162	0
1	F	2861	0	2752	35	0
1	G	2837	0	2713	117	0
1	H	2847	0	2729	34	0
1	I	2861	0	2742	158	0
1	J	2837	0	2714	57	0
1	K	2847	0	2728	130	0
1	L	2861	0	2752	34	0
All	All	34170	0	32735	863	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 13.

The worst 5 of 863 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:2264:ALA:CB	1:D:1272:VAL:HG11	1.22	1.62
1:B:2189:LYS:CD	1:E:2061:ASN:H	1.15	1.60
1:B:2108:ARG:CD	1:D:1314:SER:HB2	1.19	1.58
1:B:2108:ARG:HD3	1:D:1314:SER:CB	1.12	1.58
1:B:2269:THR:CG2	1:I:3372:ARG:HD3	1.13	1.57

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	369/394 (94%)	349 (95%)	16 (4%)	4 (1%)	17	63
1	B	371/394 (94%)	349 (94%)	21 (6%)	1 (0%)	46	83
1	C	370/394 (94%)	348 (94%)	19 (5%)	3 (1%)	24	69
1	D	367/394 (93%)	347 (95%)	16 (4%)	4 (1%)	17	63
1	E	371/394 (94%)	349 (94%)	21 (6%)	1 (0%)	46	83
1	F	370/394 (94%)	348 (94%)	19 (5%)	3 (1%)	24	69
1	G	369/394 (94%)	349 (95%)	16 (4%)	4 (1%)	17	63
1	H	371/394 (94%)	349 (94%)	21 (6%)	1 (0%)	46	83
1	I	370/394 (94%)	348 (94%)	19 (5%)	3 (1%)	24	69
1	J	369/394 (94%)	349 (95%)	16 (4%)	4 (1%)	17	63
1	K	371/394 (94%)	349 (94%)	21 (6%)	1 (0%)	46	83
1	L	370/394 (94%)	348 (94%)	19 (5%)	3 (1%)	24	69
All	All	4438/4728 (94%)	4182 (94%)	224 (5%)	32 (1%)	31	71

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1185	VAL
1	C	3245	ASN
1	C	3280	ASN
1	C	3312	ASN
1	D	1185	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	292/325 (90%)	290 (99%)	2 (1%)	88	94
1	B	294/325 (90%)	289 (98%)	5 (2%)	68	87
1	C	298/325 (92%)	296 (99%)	2 (1%)	88	94
1	D	291/325 (90%)	289 (99%)	2 (1%)	88	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	294/325 (90%)	289 (98%)	5 (2%)	68	87
1	F	298/325 (92%)	296 (99%)	2 (1%)	88	94
1	G	292/325 (90%)	290 (99%)	2 (1%)	88	94
1	H	294/325 (90%)	289 (98%)	5 (2%)	68	87
1	I	298/325 (92%)	296 (99%)	2 (1%)	88	94
1	J	292/325 (90%)	290 (99%)	2 (1%)	88	94
1	K	294/325 (90%)	289 (98%)	5 (2%)	68	87
1	L	298/325 (92%)	296 (99%)	2 (1%)	88	94
All	All	3535/3900 (91%)	3499 (99%)	36 (1%)	83	92

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	3162	LEU
1	H	2106	ASN
1	K	2357	ASN
1	G	1186	PRO
1	H	2162	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 111 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	3041	GLN
1	G	1200	ASN
1	K	2200	ASN
1	F	3080	HIS
1	G	1041	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 [i](#)

There are no carbohydrates 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.