



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:35 PM BST

PDB ID : 1FOQ
EMDB ID: : unknown
Title : PENTAMERIC MODEL OF THE BACTERIOPHAGE PHI29 PROHEAD
RNA
Authors : Simpson, A.A.; Tao, Y.; Leiman, P.G.; Badasso, M.O.; He, Y.; Jardine, P.J.;
Olson, N.H.; Morais, M.C.; Grimes, S.; Anderson, D.L.; Baker, T.S.; Ross-
mann, M.G.
Deposited on : 2000-08-28
Resolution : 20.00 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 : 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

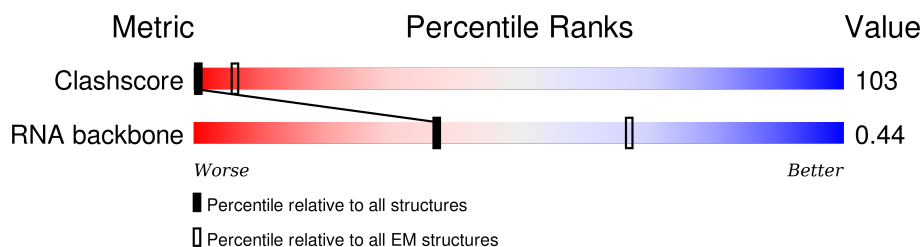
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY






The reported resolution of this entry is 20.00 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	114402	924
RNA backbone	3027	244

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	120	 28% 26% 34% 9%
1	B	120	 28% 25% 35% 9%
1	C	120	 28% 25% 35% 9%
1	D	120	 28% 25% 35% 9%
1	E	120	 28% 25% 35% 9%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12095 atoms, of which 545 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.

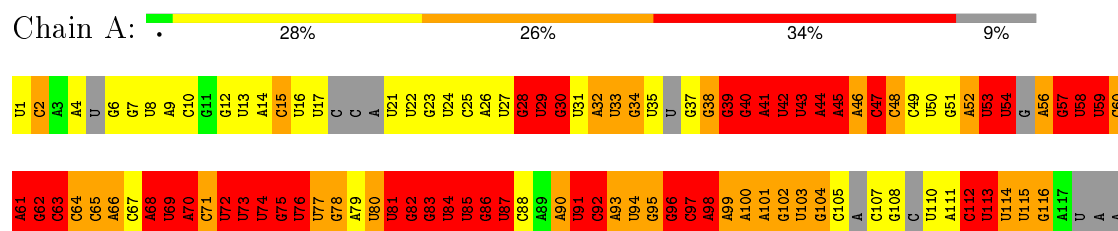
- Molecule 1 is a RNA chain called BACTERIOPHAGE PHI29 PROHEAD RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	109	Total	C	H	N	O	P	0	0
			2419	1033	109	393	775	109		
1	B	109	Total	C	H	N	O	P	0	0
			2419	1033	109	393	775	109		
1	C	109	Total	C	H	N	O	P	0	0
			2419	1033	109	393	775	109		
1	D	109	Total	C	H	N	O	P	0	0
			2419	1033	109	393	775	109		
1	E	109	Total	C	H	N	O	P	0	0
			2419	1033	109	393	775	109		

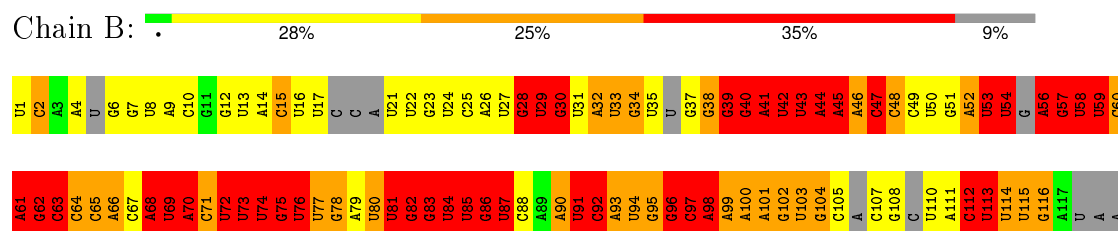
3 Residue-property plots

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.

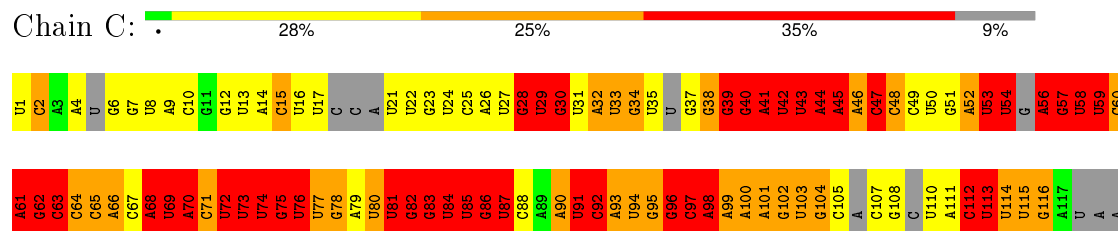
- Molecule 1: BACTERIOPHAGE PHI29 PROHEAD RNA



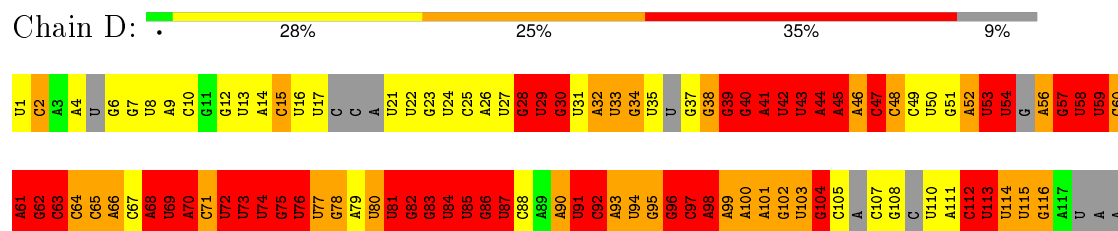
- Molecule 1: BACTERIOPHAGE PHI29 PROHEAD RNA



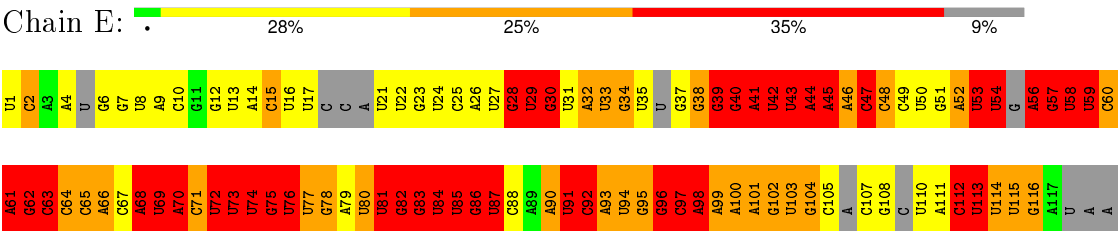
- Molecule 1: BACTERIOPHAGE PHI29 PROHEAD RNA



- Molecule 1: BACTERIOPHAGE PHI29 PROHEAD RNA



- Molecule 1: BACTERIOPHAGE PHI29 PROHEAD RNA



4 Experimental information

Property	Value	Source
Reconstruction method	Not provided	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	Not provided	Depositor
Voltage (kV)	Not provided	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	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	4.36	77/2567 (3.0%)	3.81	261/3966 (6.6%)
1	B	4.36	77/2567 (3.0%)	3.81	264/3966 (6.7%)
1	C	4.36	77/2567 (3.0%)	3.81	262/3966 (6.6%)
1	D	4.36	76/2567 (3.0%)	3.81	261/3966 (6.6%)
1	E	4.36	76/2567 (3.0%)	3.81	261/3966 (6.6%)
All	All	4.36	383/12835 (3.0%)	3.81	1309/19830 (6.6%)

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	1	1
1	B	1	1
1	C	1	1
1	D	1	1
1	E	1	1
All	All	5	5

The worst 5 of 383 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	44	A	O3'-P	49.39	2.20	1.61
1	C	44	A	O3'-P	49.38	2.20	1.61
1	A	44	A	O3'-P	49.36	2.20	1.61
1	E	44	A	O3'-P	49.35	2.20	1.61
1	D	44	A	O3'-P	49.31	2.20	1.61

The worst 5 of 1309 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	29	U	P-O3'-C3'	-41.87	69.46	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	29	U	P-O3'-C3'	-41.83	69.51	119.70
1	A	29	U	P-O3'-C3'	-41.82	69.51	119.70
1	E	29	U	P-O3'-C3'	-41.82	69.52	119.70
1	D	29	U	P-O3'-C3'	-41.80	69.54	119.70

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	40	G	C3'
1	B	40	G	C3'
1	C	40	G	C3'
1	D	40	G	C3'
1	E	40	G	C3'

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	87	U	Sidechain
1	B	87	U	Sidechain
1	C	87	U	Sidechain
1	D	87	U	Sidechain
1	E	87	U	Sidechain

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	2310	109	1181	368	0
1	B	2310	109	1183	370	0
1	C	2310	109	1182	367	0
1	D	2310	109	1182	367	0
1	E	2310	109	1181	369	0
All	All	11550	545	5909	1788	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 103.

The worst 5 of 1788 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:D:29:U:C6	1:D:30:G:H4'	1.31	1.66
1:A:29:U:C6	1:A:30:G:H4'	1.31	1.66
1:B:29:U:C6	1:B:30:G:H4'	1.31	1.66
1:C:29:U:C6	1:C:30:G:H4'	1.31	1.65
1:C:28:G:H4'	1:C:29:U:C5'	1.22	1.62

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	96/120 (80%)	49 (51%)	14 (14%)
1	B	97/120 (80%)	49 (50%)	15 (15%)
1	C	97/120 (80%)	49 (50%)	15 (15%)
1	D	96/120 (80%)	49 (51%)	14 (14%)
1	E	97/120 (80%)	49 (50%)	15 (15%)
All	All	483/600 (80%)	245 (50%)	73 (15%)

5 of 245 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	C
1	A	29	U
1	A	30	G
1	A	40	G
1	A	41	A

5 of 73 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C	56	A
1	C	86	G
1	E	83	G
1	C	73	U
1	C	103	U

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](#)

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.