wwPDB EM Validation Summary Report

Feb 24, 2025 – 12:00 PM EST

PDB ID	:	1FOQ
Title	:	PENTAMERIC MODEL OF THE BACTERIOPHAGE PHI29 PROHEAD RNA
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Deposited on	:	2000-08-28
Resolution	:	20.00 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB/EMDB 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 (i) 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 (i)) were used in the production of this report:

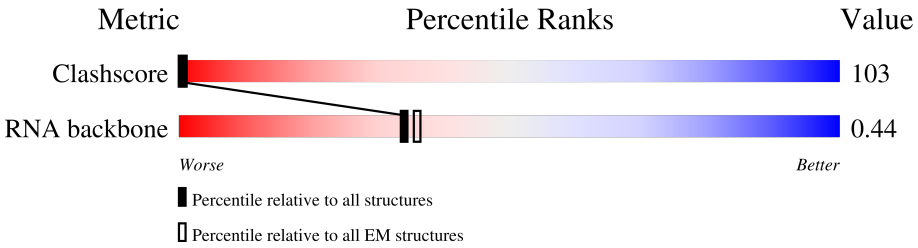
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

1 Overall quality at a glance (i)

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	210492	15764
RNA backbone	6643	2191

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 <=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 (i)

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.

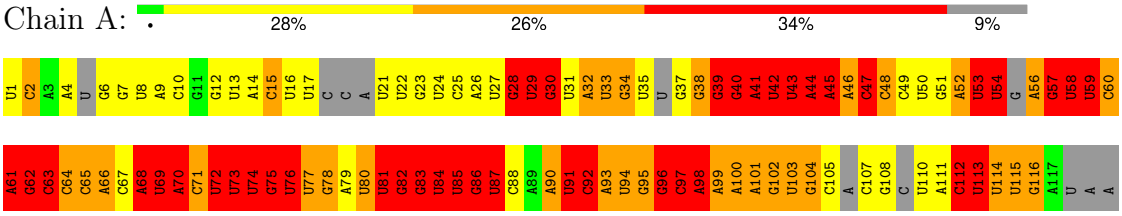
Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	109	Total	C	H	N	O	P	0	0
			2419	1033	109	393	775	109		
1	B	109	Total	C	H	N	O	P	0	0
			2419	1033	109	393	775	109		
1	C	109	Total	C	H	N	O	P	0	0
			2419	1033	109	393	775	109		
1	D	109	Total	C	H	N	O	P	0	0
			2419	1033	109	393	775	109		
1	E	109	Total	C	H	N	O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

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

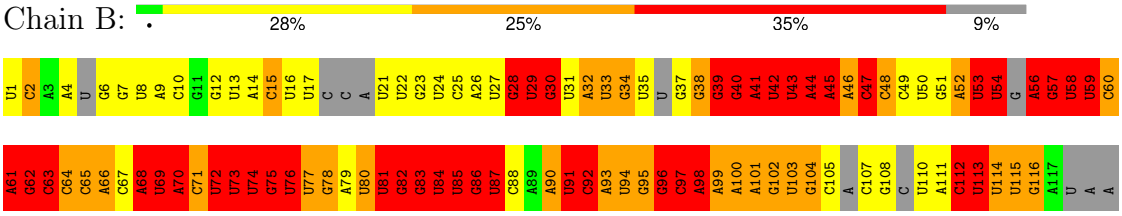
• Molecule 1: BACTERIOPHAGE PHI29 PROHEAD RNA

Chain A:



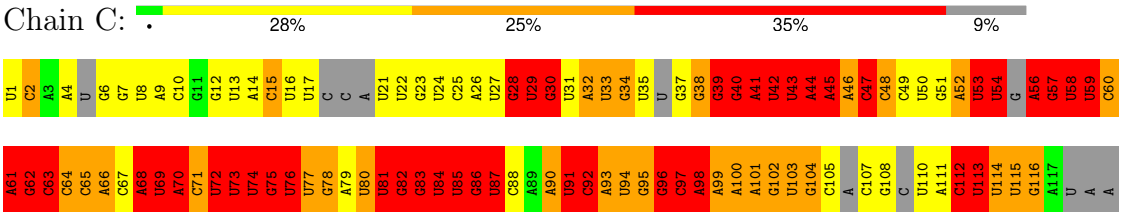
• Molecule 1: BACTERIOPHAGE PHI29 PROHEAD RNA

Chain B:



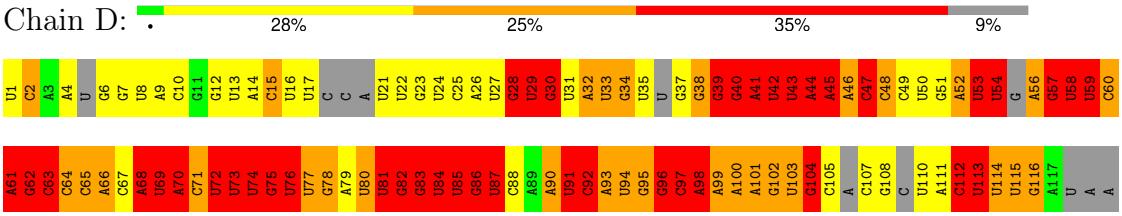
• Molecule 1: BACTERIOPHAGE PHI29 PROHEAD RNA

Chain C:



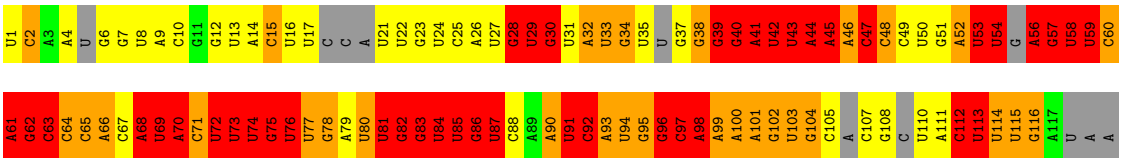
• Molecule 1: BACTERIOPHAGE PHI29 PROHEAD RNA

Chain D:



• Molecule 1: BACTERIOPHAGE PHI29 PROHEAD RNA

Chain E:


U1 C2 A3 A4 U G6 G7 U8 A9 C10 G11 G12 U13 A14 C15 U16 U17 C C A U21 U22 G23 U24 C25 A26 U27 G28 U29 G30 U31 A32 U33 G34 U35 U G37 G38 G39 G40 A41 U42 U43 A44 A45 A46 C47 C48 C49 U50 G51 A52 U53 U54 G A56 G57 U58 U59 C60
A61 G62 C63 C64 C65 A66 C67 A68 U69 A70 C71 U72 U73 U74 G75 U76 U77 G78 A79 U80 U81 G82 G83 U84 U85 G86 U87 C88 A89 A90 U91 C92 A93 U94 G95 G96 C97 A98 A99 A100 A101 G102 U103 G104 C105 A C107 G108 C U110 A111 C112 U113 U114 U115 G116 A117 U A A

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	1.00Å 1.00Å 1.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 20.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-20.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12095	wwPDB-VP
Average B, all atoms (Å^2)	0.0	wwPDB-VP

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	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
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(^{o})	Ideal(^{o})
1	B	29	U	P-O3'-C3'	-41.87	69.46	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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 (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	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: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:D:29:U:C6	1:D: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	D	112	C
1	E	103	U
1	E	39	G
1	E	72	U
1	B	84	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 oligosaccharides 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	53
1	B	53
1	C	53
1	D	53
1	E	53

The worst 5 of 265 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	51:G	O3'	52:A	P	3.32
1	B	51:G	O3'	52:A	P	3.32
1	C	51:G	O3'	52:A	P	3.32
1	D	51:G	O3'	52:A	P	3.32

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	51:G	O3'	52:A	P	3.32