wwPDB X-ray Structure Validation Summary Report (i)

Nov 14, 2022 – 03:26 pm GMT

PDB ID	:	8AMK
Title	:	Crystal structure of AUGUGGCAU duplex crystallized in the presence of calcium ions
Authors	:	Kiliszek, A.; Rypniewski, W.
Deposited on	:	2022-08-03
Resolution	:	2.85 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp
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 (1)) were used in the production of this report:

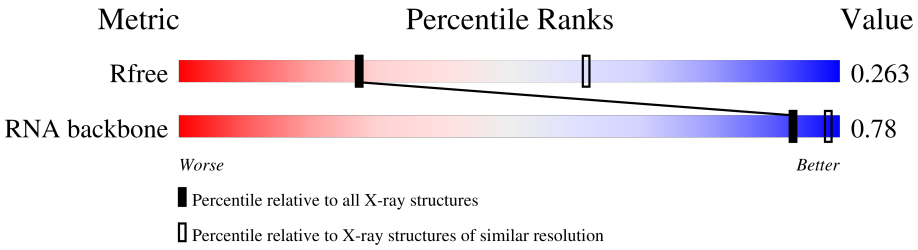
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3168 (2.90-2.82)
RNA backbone	3102	1088 (3.12-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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	9	100%
1	B	9	100%
1	C	9	89% 11%
1	D	9	100%
1	E	9	89% 11%
1	F	9	100%
1	G	9	89% 11%
1	H	9	100%
1	I	9	100%
1	J	9	100%

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Mol	Chain	Length	Quality of chain
1	K	9	100%
1	L	9	100%
1	M	9	89% 11%
1	N	9	100%
1	O	9	89% 11%
1	P	9	89% 11%
1	Q	9	89% 11%
1	R	9	100%
1	S	9	89% 11%
1	T	9	78% 22%
1	U	9	100%
1	V	9	100%
1	Y	9	100%
1	Z	9	89% 11%
1	a	9	100%
1	b	9	100%
1	c	9	100%
1	d	9	100%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5323 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 RNA (5'-R(*AP*UP*GP*UP*GP*GP*CP*AP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	9	Total	C	N	O	P	0	0	0
			190	86	34	62	8			
1	B	9	Total	C	N	O	P	0	0	0
			190	86	34	62	8			
1	C	9	Total	C	N	O	P	0	0	0
			190	86	34	62	8			
1	D	9	Total	C	N	O	P	0	0	0
			190	86	34	62	8			
1	E	9	Total	C	N	O	P	0	0	0
			190	86	34	62	8			
1	F	9	Total	C	N	O	P	0	0	0
			190	86	34	62	8			
1	G	9	Total	C	N	O	P	0	0	0
			190	86	34	62	8			
1	H	9	Total	C	N	O	P	0	0	0
			190	86	34	62	8			
1	I	9	Total	C	N	O	P	0	0	0
			190	86	34	62	8			
1	J	9	Total	C	N	O	P	0	0	0
			190	86	34	62	8			
1	K	9	Total	C	N	O	P	0	0	0
			190	86	34	62	8			
1	L	9	Total	C	N	O	P	0	0	0
			190	86	34	62	8			
1	M	9	Total	C	N	O	P	0	0	0
			190	86	34	62	8			
1	N	9	Total	C	N	O	P	0	0	0
			190	86	34	62	8			
1	O	9	Total	C	N	O	P	0	0	0
			190	86	34	62	8			
1	P	9	Total	C	N	O	P	0	0	0
			190	86	34	62	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	9	Total	C	N	O	P	0	0	0
			190	86	34	62	8			
1	R	9	Total	C	N	O	P	0	0	0
			190	86	34	62	8			
1	S	9	Total	C	N	O	P	0	0	0
			190	86	34	62	8			
1	T	9	Total	C	N	O	P	0	0	0
			190	86	34	62	8			
1	U	9	Total	C	N	O	P	0	0	0
			190	86	34	62	8			
1	V	9	Total	C	N	O	P	0	0	0
			190	86	34	62	8			
1	Y	9	Total	C	N	O	P	0	0	0
			190	86	34	62	8			
1	Z	9	Total	C	N	O	P	0	0	0
			190	86	34	62	8			
1	a	9	Total	C	N	O	P	0	0	0
			190	86	34	62	8			
1	b	9	Total	C	N	O	P	0	0	0
			190	86	34	62	8			
1	c	9	Total	C	N	O	P	0	0	0
			190	86	34	62	8			
1	d	9	Total	C	N	O	P	0	0	0
			190	86	34	62	8			

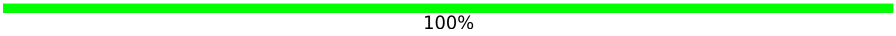
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	O	0	0
			1	1		
2	D	1	Total	O	0	0
			1	1		
2	N	1	Total	O	0	0
			1	1		

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: RNA (5'-R(*AP*UP*GP*UP*GP*GP*CP*AP*U)-3')

Chain A: 

There are no outlier residues recorded for this chain.

• Molecule 1: RNA (5'-R(*AP*UP*GP*UP*GP*GP*CP*AP*U)-3')

Chain B: 

There are no outlier residues recorded for this chain.

• Molecule 1: RNA (5'-R(*AP*UP*GP*UP*GP*GP*CP*AP*U)-3')

Chain C: 

• Molecule 1: RNA (5'-R(*AP*UP*GP*UP*GP*GP*CP*AP*U)-3')

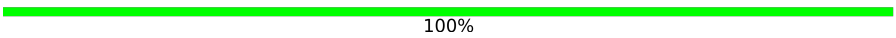
Chain D: 

There are no outlier residues recorded for this chain.

• Molecule 1: RNA (5'-R(*AP*UP*GP*UP*GP*GP*CP*AP*U)-3')

Chain E: 

• Molecule 1: RNA (5'-R(*AP*UP*GP*UP*GP*GP*CP*AP*U)-3')

Chain F: 

There are no outlier residues recorded for this chain.

• Molecule 1: RNA (5'-R(*AP*UP*GP*UP*GP*GP*CP*AP*U)-3')

Chain G: 

• Molecule 1: RNA (5'-R(*AP*UP*GP*UP*GP*GP*CP*AP*U)-3')

Chain H: 100%

There are no outlier residues recorded for this chain.

• Molecule 1: RNA (5'-R(*AP*UP*GP*UP*GP*GP*CP*AP*U)-3')

Chain I: 100%

There are no outlier residues recorded for this chain.

• Molecule 1: RNA (5'-R(*AP*UP*GP*UP*GP*GP*CP*AP*U)-3')

Chain J: 100%

There are no outlier residues recorded for this chain.

• Molecule 1: RNA (5'-R(*AP*UP*GP*UP*GP*GP*CP*AP*U)-3')

Chain K: 100%

There are no outlier residues recorded for this chain.

• Molecule 1: RNA (5'-R(*AP*UP*GP*UP*GP*GP*CP*AP*U)-3')

Chain L: 100%

There are no outlier residues recorded for this chain.

• Molecule 1: RNA (5'-R(*AP*UP*GP*UP*GP*GP*CP*AP*U)-3')

Chain M: 89% 11%

• Molecule 1: RNA (5'-R(*AP*UP*GP*UP*GP*GP*CP*AP*U)-3')

Chain N: 100%

There are no outlier residues recorded for this chain.

• Molecule 1: RNA (5'-R(*AP*UP*GP*UP*GP*GP*CP*AP*U)-3')

Chain O: 89% 11%

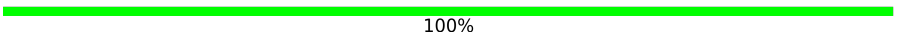
• Molecule 1: RNA (5'-R(*AP*UP*GP*UP*GP*GP*CP*AP*U)-3')

Chain P: 

• Molecule 1: RNA (5'-R(*AP*UP*GP*UP*GP*GP*CP*AP*U)-3')

Chain Q: 

• Molecule 1: RNA (5'-R(*AP*UP*GP*UP*GP*GP*CP*AP*U)-3')

Chain R: 

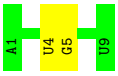
There are no outlier residues recorded for this chain.

• Molecule 1: RNA (5'-R(*AP*UP*GP*UP*GP*GP*CP*AP*U)-3')

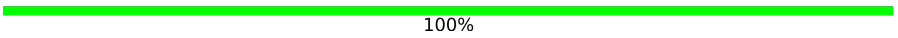
Chain S: 

• Molecule 1: RNA (5'-R(*AP*UP*GP*UP*GP*GP*CP*AP*U)-3')

Chain T: 

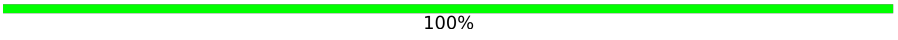


• Molecule 1: RNA (5'-R(*AP*UP*GP*UP*GP*GP*CP*AP*U)-3')

Chain U: 

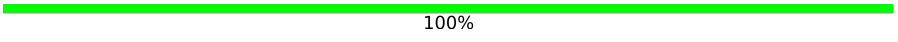
There are no outlier residues recorded for this chain.

• Molecule 1: RNA (5'-R(*AP*UP*GP*UP*GP*GP*CP*AP*U)-3')

Chain V: 

There are no outlier residues recorded for this chain.

• Molecule 1: RNA (5'-R(*AP*UP*GP*UP*GP*GP*CP*AP*U)-3')

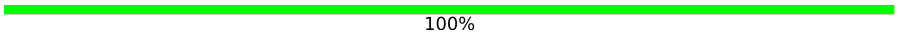
Chain Y: 

There are no outlier residues recorded for this chain.

• Molecule 1: RNA (5'-R(*AP*UP*GP*UP*GP*GP*CP*AP*U)-3')

Chain Z: 

• Molecule 1: RNA (5'-R(*AP*UP*GP*UP*GP*GP*CP*AP*U)-3')

Chain a: 

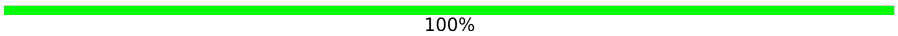
There are no outlier residues recorded for this chain.

• Molecule 1: RNA (5'-R(*AP*UP*GP*UP*GP*GP*CP*AP*U)-3')

Chain b: 

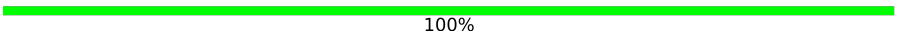
There are no outlier residues recorded for this chain.

• Molecule 1: RNA (5'-R(*AP*UP*GP*UP*GP*GP*CP*AP*U)-3')

Chain c: 

There are no outlier residues recorded for this chain.

• Molecule 1: RNA (5'-R(*AP*UP*GP*UP*GP*GP*CP*AP*U)-3')

Chain d: 

There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	28.07Å 90.16Å 137.95Å 90.00° 91.38° 90.00°	Depositor
Resolution (Å)	45.97 – 2.85 45.97 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.3 (45.97-2.85) 99.5 (45.97-2.85)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.69 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.208 , 0.266 0.205 , 0.263	Depositor DCC
R_{free} test set	969 reflections (6.00%)	wwPDB-VP
Wilson B-factor (Å^2)	80.8	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.054 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5323	wwPDB-VP
Average B, all atoms (Å^2)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.61% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.25	0/212	0.92	0/329
1	B	0.24	0/212	0.82	0/329
1	C	0.18	0/212	0.70	0/329
1	D	0.19	0/212	0.75	0/329
1	E	0.18	0/212	0.71	0/329
1	F	0.18	0/212	0.77	0/329
1	G	0.19	0/212	0.70	0/329
1	H	0.16	0/212	0.67	0/329
1	I	0.25	0/212	0.93	0/329
1	J	0.20	0/212	0.77	0/329
1	K	0.22	0/212	0.81	0/329
1	L	0.19	0/212	0.75	0/329
1	M	0.18	0/212	0.71	0/329
1	N	0.18	0/212	0.69	0/329
1	O	0.15	0/212	0.72	0/329
1	P	0.15	0/212	0.68	0/329
1	Q	0.19	0/212	0.76	0/329
1	R	0.17	0/212	0.74	0/329
1	S	0.23	0/212	0.88	0/329
1	T	0.17	0/212	0.67	0/329
1	U	0.17	0/212	0.72	0/329
1	V	0.19	0/212	0.80	0/329
1	Y	0.19	0/212	0.74	0/329
1	Z	0.19	0/212	0.77	0/329
1	a	0.18	0/212	0.75	0/329
1	b	0.21	0/212	0.87	0/329
1	c	0.15	0/212	0.73	0/329
1	d	0.21	0/212	0.86	0/329
All	All	0.19	0/5936	0.77	0/9212

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

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles

5.3.1 Protein backbone

There are no protein molecules in this entry.

5.3.2 Protein sidechains

There are no protein molecules in this entry.

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	8/9 (88%)	0	0
1	B	8/9 (88%)	0	0
1	C	8/9 (88%)	1 (12%)	0
1	D	8/9 (88%)	0	0
1	E	8/9 (88%)	1 (12%)	0
1	F	8/9 (88%)	0	0
1	G	8/9 (88%)	1 (12%)	0
1	H	8/9 (88%)	0	0
1	I	8/9 (88%)	0	0
1	J	8/9 (88%)	0	0
1	K	8/9 (88%)	0	0
1	L	8/9 (88%)	0	0
1	M	8/9 (88%)	1 (12%)	0
1	N	8/9 (88%)	0	0
1	O	8/9 (88%)	1 (12%)	0
1	P	8/9 (88%)	1 (12%)	0
1	Q	8/9 (88%)	1 (12%)	0
1	R	8/9 (88%)	0	0
1	S	8/9 (88%)	1 (12%)	0
1	T	8/9 (88%)	2 (25%)	0
1	U	8/9 (88%)	0	0
1	V	8/9 (88%)	0	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	Y	8/9 (88%)	0	0
1	Z	8/9 (88%)	1 (12%)	0
1	a	8/9 (88%)	0	0
1	b	8/9 (88%)	0	0
1	c	8/9 (88%)	0	0
1	d	8/9 (88%)	0	0
All	All	224/252 (88%)	11 (4%)	0

5 of 11 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	5	G
1	E	5	G
1	G	5	G
1	M	5	G
1	O	5	G

There are no RNA pucker outliers to report.

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.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.