Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2023 – 03:20 pm GMT

PDB ID	:	7OOO
Title	:	The crystal structure of a DNA:RNA hybrid duplex sequence CTTTTCTTTG containing an LNA-Amide-LNA modification
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Deposited on	:	2021-05-28
Resolution	:	2.57 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 ⓘ 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 ⓘ) were used in the production of this report:

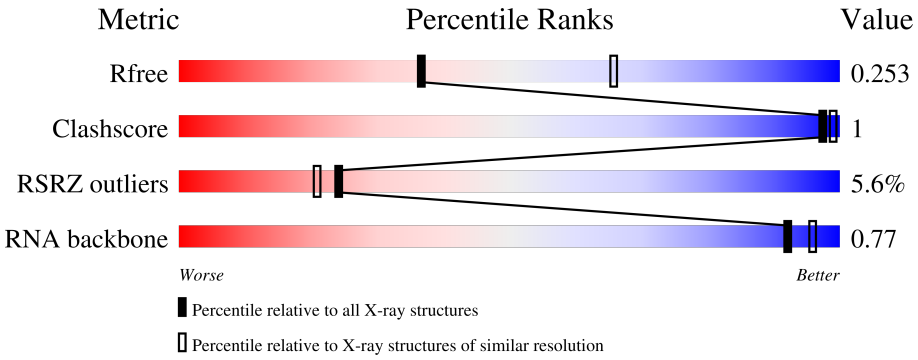
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

1 Overall quality at a glance

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

The reported resolution of this entry is 2.57 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	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)
RNA backbone	3102	1075 (2.90-2.26)

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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	10	90% 10%
1	D	10	90% 10%
2	B	9	22% 89% 11%
2	E	9	67% 33%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 837 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(*CP*AP*AP*AP*GP*AP*AP*AP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	10	Total	C	N	O	P	0	0	0
			217	99	48	61	9			
1	D	10	Total	C	N	O	P	0	0	0
			217	99	48	61	9			

- Molecule 2 is a DNA chain called DNA (5'-D(*CP*TP*(05A)P*TP*CP*TP*TP*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	9	Total	C	N	O	P	0	0	0
			200	102	26	64	8			
2	E	9	Total	C	N	O	P	0	0	0
			200	102	26	64	8			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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(*CP*AP*AP*AP*GP*AP*AP*AP*AP*G)-3')

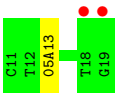
Chain A:

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

Chain D:

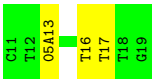
• Molecule 2: DNA (5'-D(*CP*TP*(05A)P*TP*CP*TP*TP*TP*G)-3')

Chain B:



• Molecule 2: DNA (5'-D(*CP*TP*(05A)P*TP*CP*TP*TP*TP*G)-3')

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	49.15Å 49.15Å 90.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.08 – 2.57 31.08 – 2.57	Depositor EDS
% Data completeness (in resolution range)	99.0 (31.08-2.57) 99.3 (31.08-2.57)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.14 (at 2.57Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.233 , 0.251 0.226 , 0.253	Depositor DCC
R_{free} test set	210 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å^2)	95.1	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 67.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	837	wwPDB-VP
Average B, all atoms (Å^2)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.46 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5220e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

Bond lengths and bond angles in the following residue types are not validated in this section: 05A, MG

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	0.51	0/245	0.89	0/381
1	D	0.50	0/245	0.98	0/381
2	B	0.73	0/172	1.04	0/261
2	E	0.77	0/172	1.04	0/261
All	All	0.62	0/834	0.98	0/1284

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

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	217	0	112	0	0
1	D	217	0	112	0	0
2	B	200	0	95	0	0
2	E	200	0	95	1	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	E	1	0	0	0	0
All	All	837	0	414	1	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 1.

All (1) 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)
2:E:16:DT:H2'	2:E:17:DT:C6	2.49	0.48

There are no symmetry-related clashes.

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	9/10 (90%)	1 (11%)	0
1	D	9/10 (90%)	1 (11%)	0
All	All	18/20 (90%)	2 (11%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	A
1	D	6	A

There are no RNA pucker outliers to report.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	05A	E	13	2	44,48,49	1.55	13 (29%)	60,75,78	2.04	15 (25%)
2	05A	B	13	3,2	44,48,49	1.59	12 (27%)	60,75,78	2.08	17 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	05A	E	13	2	-	5/22/74/75	0/8/6/6
2	05A	B	13	3,2	-	2/22/74/75	0/8/6/6

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	13	05A	C4'-C3'	-4.06	1.48	1.53
2	E	13	05A	C4'-C3'	-3.44	1.49	1.53
2	B	13	05A	C8-N3	-3.20	1.32	1.38
2	E	13	05A	C41-N31	-3.17	1.32	1.38
2	B	13	05A	C41-N31	-3.12	1.33	1.38
2	E	13	05A	C8-N3	-3.12	1.33	1.38
2	B	13	05A	C2-N3	-2.55	1.33	1.38
2	B	13	05A	C21-N31	-2.52	1.33	1.38
2	E	13	05A	C21-N31	-2.49	1.33	1.38
2	B	13	05A	C61-N11	-2.44	1.33	1.38
2	B	13	05A	C4'1-C3'1	-2.39	1.49	1.54
2	E	13	05A	C61-N11	-2.38	1.34	1.38
2	E	13	05A	C2-N3	-2.37	1.33	1.38
2	B	13	05A	C6-N1	-2.33	1.34	1.38
2	E	13	05A	C4'1-C3'1	-2.31	1.49	1.54
2	E	13	05A	O4'1-C4'1	-2.31	1.42	1.45
2	E	13	05A	C6-C5	2.29	1.38	1.34
2	E	13	05A	C6-N1	-2.27	1.34	1.38
2	B	13	05A	C6-C5	2.26	1.38	1.34
2	B	13	05A	O4'1-C4'1	-2.25	1.42	1.45
2	E	13	05A	C61-C51	2.18	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	13	05A	O4'-C4'	-2.17	1.42	1.45
2	B	13	05A	C61-C51	2.07	1.38	1.34
2	E	13	05A	O4'-C4'	-2.04	1.42	1.45
2	E	13	05A	C2-N1	2.01	1.41	1.38

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	13	05A	N31-C21-N11	4.98	121.50	114.89
2	B	13	05A	C41-N31-C21	-4.90	121.01	127.35
2	E	13	05A	N31-C21-N11	4.89	121.38	114.89
2	E	13	05A	N3-C2-N1	4.83	121.30	114.89
2	B	13	05A	N3-C2-N1	4.77	121.22	114.89
2	E	13	05A	C41-N31-C21	-4.73	121.23	127.35
2	E	13	05A	C8-N3-C2	-4.64	121.35	127.35
2	B	13	05A	C8-N3-C2	-4.32	121.77	127.35
2	E	13	05A	C51-C41-N31	4.13	118.84	115.31
2	B	13	05A	C51-C41-N31	4.12	118.82	115.31
2	E	13	05A	C5-C8-N3	4.09	118.81	115.31
2	B	13	05A	O4'-C4'-C5'	3.74	115.60	108.97
2	B	13	05A	C5-C8-N3	3.74	118.50	115.31
2	E	13	05A	O41-C41-C51	-3.70	120.62	124.90
2	B	13	05A	O41-C41-C51	-3.62	120.70	124.90
2	E	13	05A	O4-C8-C5	-3.55	120.78	124.90
2	B	13	05A	O4-C8-C5	-3.42	120.94	124.90
2	B	13	05A	C51-C61-N11	-3.40	119.84	123.34
2	E	13	05A	O4'-C4'-C5'	3.22	114.67	108.97
2	E	13	05A	C51-C61-N11	-3.19	120.06	123.34
2	E	13	05A	C5-C6-N1	-3.11	120.14	123.34
2	B	13	05A	C5-C6-N1	-2.89	120.37	123.34
2	E	13	05A	O2'-C2'1-C3'1	-2.80	100.63	103.67
2	B	13	05A	C3'1-C11-C1	-2.62	107.46	113.98
2	B	13	05A	C1'-N1-C2	2.56	122.21	117.57
2	B	13	05A	O2-C2-N3	-2.31	117.19	121.50
2	B	13	05A	O2'-C2'1-C3'1	-2.29	101.19	103.67
2	B	13	05A	C5A-C51-C41	2.19	121.17	118.77
2	E	13	05A	O2-C2-N3	-2.14	117.52	121.50
2	E	13	05A	C1'-N1-C2	2.08	121.34	117.57
2	B	13	05A	O21-C21-N11	-2.03	120.08	122.79
2	E	13	05A	C5A-C51-C41	2.01	120.98	118.77

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	13	05A	C1-C11-C3'1-C4'1
2	E	13	05A	C1-C11-C3'1-C4'1
2	E	13	05A	C7-C4'-C5'-N5'
2	E	13	05A	C3'-C4'-C5'-N5'
2	E	13	05A	O4'-C4'-C5'-N5'
2	B	13	05A	C1-C11-C3'1-C2'1
2	E	13	05A	C1-C11-C3'1-C2'1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	10/10 (100%)	0.58	0 100 100	80, 89, 97, 98	0
1	D	10/10 (100%)	0.38	0 100 100	82, 92, 100, 102	0
2	B	8/9 (88%)	0.79	2 (25%) 0 0	77, 82, 94, 98	0
2	E	8/9 (88%)	0.67	0 100 100	77, 86, 92, 94	0
All	All	36/38 (94%)	0.59	2 (5%) 24 21	77, 89, 98, 102	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	19	DG	2.2
2	B	18	DT	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	05A	E	13	43/44	0.90	0.17	79,88,97,103	0
2	05A	B	13	43/44	0.94	0.18	75,82,94,113	0

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	D	101	1/1	0.82	0.33	98,98,98,98	0
3	MG	B	101	1/1	0.93	0.33	85,85,85,85	1

6.5 Other polymers

There are no such residues in this entry.