

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	115D
Title	:	ORDERED WATER STRUCTURE IN AN A-DNA OCTAMER AT 1.7
		ANGSTROMS RESOLUTION
Authors	:	Kennard, O.; Cruse, W.B.T.; Nachman, J.; Prange, T.; Shakked, Z.; Rabi-
		novich, D.
Deposited on		
Resolution	:	1.70 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 (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
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.70 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	Percentil	le Ranks	Value
Clashscore			4
Worse	2		Better
Perc	centile relative to all X-ray structures		
Perc	centile relative to X-ray structures of simi	lar resolution	
	Whole archive	Sir	nilar resolution

Metric Clashscore	Whole archive	Similar resolution	
Metric	$(\# { m Entries})$	$(\# {\rm Entries}, {\rm resolution} {\rm range}({ m \AA}))$	
Clashscore	141614	4695 (1.70-1.70)	

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain				
1	А	8	88%	12%			
1	В	8	12% 75%	12%			



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2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 407 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 DNA chain called DNA (5'-D(*GP*GP*(BRU)P*AP*(BRU)P*AP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
1	Δ	8	Total	Br	С	Ν	0	Р	0	0	0
	A	0	161	2	76	30	46	7	0	0	0
1	р	0	Total	Br	С	Ν	Ο	Р	0	0	0
	D	0	161	2	76	30	46	7	0	0	0

• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	45	$\begin{array}{cc} \text{Total} & \text{O} \\ 45 & 45 \end{array}$	0	0
2	В	40	Total O 40 40	0	0



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.

Note EDS was not executed.

• Molecule 1: DNA (5'-D(*GP*GP*(BRU)P*AP*(BRU)P	'*AP*CP*C)-3')
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Chain A:	88%	12%
61 62 03 03 04 05 05 05 05 08 05 08 05 08 05 08 05 05 05 05 05 05 05 05 05 05 05 05 05		
• Molecule 1	: DNA (5'-D(*GP*GP*(BRU)P*AP*(BRU)P*AP*CP	» *С)-3')
Chain B:	2% 75%	12%
69 610 111 113 113 113 113 615 C15 C16		



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source	
Space group	P 61	Depositor	
Cell constants	45.08Å 45.08Å 41.72Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor	
Resolution (Å)	10.00 - 1.70	Depositor	
% Data completeness	(Not available) (10.00-1.70)	Depositor	
(in resolution range)	(100 available) (10.00 1.10)		
R_{merge}	(Not available)	Depositor	
R _{sym}	(Not available)	Depositor	
Refinement program	NUCLSQ	Depositor	
R, R_{free}	0.140 , (Not available)	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	407	wwPDB-VP	
Average B, all atoms $(Å^2)$	19.0	wwPDB-VP	



5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BRU

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	Bon	d lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	1.48	1/134~(0.7%)	2.41	11/200~(5.5%)	
1	В	1.79	2/134~(1.5%)	2.69	15/200~(7.5%)	
All	All	1.64	3/268~(1.1%)	2.55	26/400~(6.5%)	

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	В	16	DC	P-OP2	-6.46	1.38	1.49
1	А	4	DA	P-O5'	6.45	1.66	1.59
1	В	15	DC	P-O5'	5.49	1.65	1.59

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	16	DC	OP1-P-OP2	11.47	136.80	119.60
1	А	8	DC	O4'-C4'-C3'	-10.37	99.78	106.00
1	А	2	DG	O5'-P-OP1	-8.41	98.13	105.70
1	В	14	DA	O4'-C4'-C3'	-7.20	101.62	104.50
1	А	4	DA	O4'-C1'-N9	-7.06	103.06	108.00
1	А	4	DA	O4'-C4'-C3'	-6.64	101.84	104.50
1	В	12	DA	O5'-P-OP2	-6.53	99.82	105.70
1	А	1	DG	C5'-C4'-C3'	6.52	125.84	114.10
1	В	9	DG	C5-C6-N1	6.50	114.75	111.50
1	А	2	DG	OP1-P-OP2	6.46	129.29	119.60
1	А	6	DA	OP2-P-O3'	6.44	119.37	105.20
1	В	9	DG	C4'-C3'-C2'	-5.97	97.73	103.10
1	В	14	DA	O5'-P-OP2	5.87	117.74	110.70
1	А	4	DA	N1-C2-N3	-5.87	126.37	129.30
1	А	7	DC	N3-C4-N4	-5.76	113.97	118.00
1	А	8	DC	O5'-P-OP2	5.74	117.59	110.70

All (26) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^{o})$	$Ideal(^{o})$
1	А	7	DC	O4'-C4'-C3'	-5.67	102.23	104.50
1	В	15	DC	OP1-P-O3'	-5.48	93.14	105.20
1	В	9	DG	C5-C6-O6	-5.46	125.32	128.60
1	В	15	DC	C4'-C3'-C2'	-5.20	98.42	103.10
1	В	12	DA	C6-N1-C2	5.17	121.70	118.60
1	В	16	DC	C6-N1-C2	5.10	122.34	120.30
1	В	12	DA	O4'-C1'-N9	-5.09	104.44	108.00
1	В	14	DA	OP2-P-O3'	5.07	116.36	105.20
1	В	14	DA	C4'-C3'-C2'	-5.06	98.55	103.10
1	В	14	DA	N1-C2-N3	-5.04	126.78	129.30

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There are no chirality outliers.

There are no planarity outliers.

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	А	161	0	86	2	0
1	В	161	0	86	0	1
2	А	45	0	0	2	3
2	В	40	0	0	0	2
All	All	407	0	172	2	3

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 4.

All (2) 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:1:DG:H5'	2:A:79:HOH:O	1.18	1.33	
1:A:1:DG:C5'	2:A:79:HOH:O	1.94	0.73	

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)	
1:B:15:DC:OP1	2:A:83:HOH:O[6_655]	1.86	0.34	
2:A:35:HOH:O	2:B:88:HOH:O[3_664]	1.94	0.26	
2:A:35:HOH:O	2:B:26:HOH:O[5_564]	2.00	0.20	

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)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

4 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	Turne	Chain	Res	Link	Bo	ond leng	\mathbf{ths}	Bond angles		
WIOI	Type		nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
1	BRU	В	11	1	18,21,22	0.92	1 (5%)	26,30,33	0.94	1 (3%)
1	BRU	А	5	1	18,21,22	0.73	1 (5%)	26,30,33	1.50	5 (19%)
1	BRU	В	13	1	18,21,22	0.90	1 (5%)	26,30,33	1.26	4 (15%)
1	BRU	А	3	1	18,21,22	0.80	1 (5%)	26,30,33	1.22	3 (11%)

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.



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	BRU	В	11	1	-	0/7/21/22	0/2/2/2
1	BRU	А	5	1	-	0/7/21/22	0/2/2/2
1	BRU	В	13	1	-	0/7/21/22	0/2/2/2
1	BRU	А	3	1	-	0/7/21/22	0/2/2/2

'-' means no outliers of that kind were identified.

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	В	11	BRU	BR-C5	-3.15	1.81	1.88
1	В	13	BRU	BR-C5	-2.70	1.82	1.88
1	А	3	BRU	BR-C5	-2.36	1.83	1.88
1	А	5	BRU	BR-C5	-2.22	1.83	1.88

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	3	BRU	C6-C5-C4	-3.03	117.60	120.67
1	А	5	BRU	O2-C2-N1	-2.75	119.13	122.79
1	В	13	BRU	O4'-C4'-C3'	-2.71	99.34	105.67
1	А	3	BRU	C5-C4-N3	2.68	116.42	113.34
1	А	5	BRU	C6-N1-C2	-2.64	118.62	121.30
1	В	13	BRU	C5-C4-N3	2.43	116.14	113.34
1	А	5	BRU	O4'-C4'-C3'	-2.42	100.02	105.67
1	А	5	BRU	N3-C2-N1	2.36	118.03	114.89
1	В	13	BRU	C6-C5-C4	-2.29	118.35	120.67
1	А	5	BRU	C1'-N1-C6	2.18	124.53	120.77
1	А	3	BRU	BR-C5-C6	2.17	123.68	120.64
1	В	13	BRU	O4-C4-N3	-2.01	116.27	120.12
1	В	11	BRU	C5-C4-N3	2.00	115.65	113.34

There are no chirality outliers.

There are no torsion outliers.

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)

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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

