

Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 06:28 AM EDT

PDB ID : 4J2I

Title : Multiple crystal structures of an all-AT DNA dodecamer stabilized by weak

interactions

Authors: Acosta-Reyes, F.J.; Subirana, J.A.; Pous, J.; Sanchez, R.; Condom, N.; Bal-

dini, R.; Malinina, L.; Campos, J.L.

Deposited on : 2013-02-04

Resolution : 2.98 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:

 $\begin{array}{ccc} & Mol Probity & : & 4.02b\text{-}467 \\ Xtriage & (Phenix) & : & 1.20.1 \end{array}$

EDS : 2.36.2

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

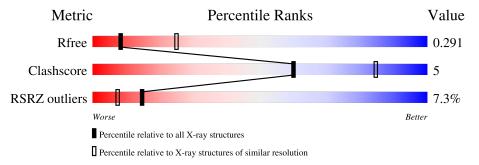
Validation Pipeline (wwPDB-VP) : 2.36.2

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 2.98 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	Similar resolution		
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$		
R_{free}	130704	2754 (3.00-2.96)		
Clashscore	141614	3103 (3.00-2.96)		
RSRZ outliers	127900	2644 (3.00-2.96)		

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	12	83%	17%			
1	В	12	92%	8%			
1	С	12	25% 75%	25%			
1	D	12	75%	25%			
1	Е	12	25% 83%	17%			
1	F	12	100%				
1	G	12	83%	17%			

Continued on next page...



Continued from previous page...

Mol	Chain	Length	Quality of chain	
		10	8%	
1	Н	12	83%	17%



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1961 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 5'-D(*AP*AP*TP*AP*AP*AP*TP*TP*TP*TP*T)-3'.

Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf	Trace
1	1 Λ	12	Total	С	N	О	Р	0	0	0
1	A	12	243	120	42	70	11	U	0	0
1	В	12	Total	С	N	О	Р	0	0	0
1	Б	12	243	120	42	70	11	0	U	U
1	С	12	Total	С	N	О	Р	0	0	0
1		12	243	120	42	70	11	0	0	0
1	D	12	Total	С	N	О	Р	0	0	0
1	D	12	243	120	42	70	11	U		
1	E	12	Total	С	N	О	Р	0	0	0
1	E	12	243	120	42	70	11	U		
1	F	12	Total	С	N	О	Р	0	0	0
1	Г	12	243	120	42	70	11	0	U	U
1	G	19	Total	С	N	О	Р	0	0	0
1	G	12	243	120	42	70	11	U	U	U
1	1 Н	12	Total	С	N	О	Р	0	0	0
1		12	243	120	42	70	11	0	U	U

• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O 1 1	0	0
2	В	2	Total O 2 2	0	0
2	С	1	Total O 1 1	0	0
2	D	5	Total O 5 5	0	0
2	E	1	Total O 1 1	0	0
2	G	4	Total O 4 4	0	0

Continued on next page...



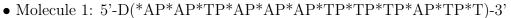
Continued from previous page...

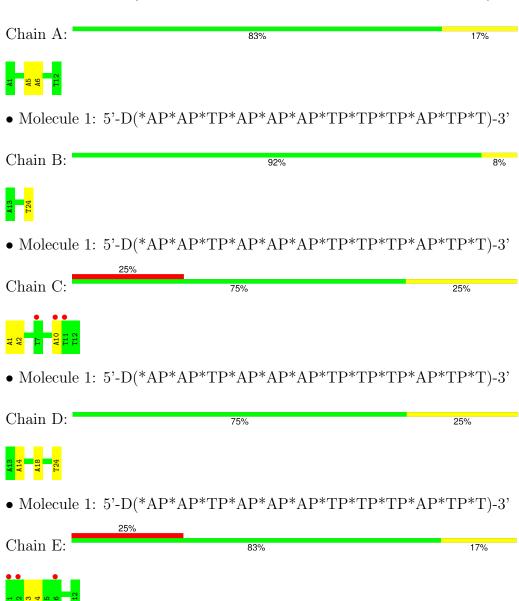
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	Н	3	Total O 3 3	0	0



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 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: 5'-D(*AP*AP*TP*AP*AP*AP*TP*TP*TP*AP*TP*T)-3'



Chain F:	100%					
There are no outlier residues recorded for this chain.						
• Molecule 1: 5'-	-D(*AP*AP*TP*AP*AP*AP*TP*TP*AP*	'TP*T)-3'				
Chain G:	83%	17%				
A1 A5 A5 T12						
• Molecule 1: 5'-	-D(*AP*AP*TP*AP*AP*AP*TP*TP*AP*	'TP*T)-3'				
8%						
Chain H:	83%	17%				
A13 T21 A22 T28 T24						



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	72.40Å 27.95Å 159.72Å	Donositon
a, b, c, α , β , γ	90.00° 103.10° 90.00°	Depositor
Resolution (Å)	26.50 - 2.98	Depositor
Resolution (A)	26.50 - 2.98	EDS
% Data completeness	99.0 (26.50-2.98)	Depositor
(in resolution range)	99.6 (26.50-2.98)	EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.75 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.8.0024	Depositor
D.D.	0.270 , 0.287	Depositor
R, R_{free}	0.273 , 0.291	DCC
R_{free} test set	293 reflections (4.39%)	wwPDB-VP
Wilson B-factor (Å ²)	45.2	Xtriage
Anisotropy	1.036	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.16 , 96.7	EDS
L-test for twinning ²	$< L > = 0.40, < L^2> = 0.23$	Xtriage
Estimated twinning fraction	0.071 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.502 for H, K, L	Depositor
Reported twinning fraction	$0.498 ext{ for -H, -K, H+L}$	Depositor
Outliers	0 of 6668 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	1961	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 17.91% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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	Mol Chain		lengths	Bond angles	
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	0.74	0/272	0.98	0/418
1	В	0.70	0/272	0.96	0/418
1	С	0.70	0/272	0.95	0/418
1	D	0.70	0/272	0.98	0/418
1	Е	0.71	0/272	0.90	0/418
1	F	0.68	0/272	0.93	0/418
1	G	0.75	0/272	0.86	0/418
1	Н	0.75	0/272	0.95	0/418
All	All	0.71	0/2176	0.94	0/3344

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 (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	243	0	140	1	0
1	В	243	0	140	1	0
1	С	243	0	140	3	0
1	D	243	0	140	4	0
1	Е	243	0	140	2	0
1	F	243	0	140	0	0
1	G	243	0	140	2	0
1	Н	243	0	140	3	0

Continued on next page...



Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	В	2	0	0	1	0
2	С	1	0	0	0	0
2	D	5	0	0	2	0
2	Е	1	0	0	1	0
2	G	4	0	0	0	0
2	Н	3	0	0	0	0
All	All	1961	0	1120	13	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 5.

All (13) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${\rm distance} \ ({\rm \AA})$	overlap (Å)
1:D:18:DA:H5"	2:D:104:HOH:O	1.83	0.77
1:E:4:DA:H5"	2:E:101:HOH:O	2.01	0.59
1:C:10:DA:N6	1:D:14:DA:N6	2.61	0.49
1:D:18:DA:C5'	2:D:104:HOH:O	2.51	0.48
1:E:3:DT:H1'	1:E:4:DA:H5'	1.95	0.47
1:C:1:DA:H61	1:D:24:DT:H3	1.62	0.47
1:G:4:DA:C2	1:G:5:DA:C4	3.04	0.46
1:H:21:DT:H2"	1:H:22:DA:H8	1.83	0.44
1:H:21:DT:H2"	1:H:22:DA:C8	2.54	0.43
1:B:24:DT:OP1	2:B:101:HOH:O	2.20	0.43
1:G:4:DA:C2	1:H:22:DA:C2	3.08	0.41
1:A:5:DA:C6	1:A:6:DA:C6	3.08	0.41
1:C:1:DA:C6	1:C:2:DA:C6	3.09	0.40

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)

There are no RNA molecules in this entry.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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>	# RSRZ > 2	$OWAB(Å^2)$	Q < 0.9
1	A	12/12 (100%)	-0.23	0 100 100	15, 31, 46, 51	0
1	В	12/12 (100%)	-0.21	0 100 100	26, 33, 49, 60	0
1	С	12/12 (100%)	0.82	3 (25%) 0 0	44, 72, 93, 104	0
1	D	12/12 (100%)	0.39	0 100 100	44, 66, 95, 101	0
1	E	12/12 (100%)	0.69	3 (25%) 0 0	54, 70, 113, 113	0
1	F	12/12 (100%)	0.53	0 100 100	57, 75, 104, 108	0
1	G	12/12 (100%)	-0.33	0 100 100	29, 32, 50, 51	0
1	Н	12/12 (100%)	-0.05	1 (8%) 11 5	26, 30, 40, 75	0
All	All	96/96 (100%)	0.20	7 (7%) 15 7	15, 51, 104, 113	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Е	1	DA	4.0
1	С	10	DA	3.3
1	Н	13	DA	3.3
1	Е	2	DA	2.6
1	Е	6	DA	2.5
1	С	11	DT	2.1
1	С	7	DT	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.



6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.

