W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Mar 1, 2014 – 02:39 AM GMT

PDB ID : 1D89
Title : A DNA DODECAMER CONTAINING AN ADENINE TRACT CRYSTAL-
LIZES IN A UNIQUE LATTICE AND EXHIBITS A NEW BEND
Authors : DiGabriele, A.D.; Steitz, T.A.
Deposited on : 1992-07-17
Resolution : 2.30 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at http://wwpdb.org/ValidationPDFNotes.html

1 Overall quality at a glance (i)
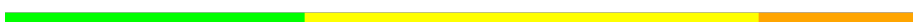
The reported resolution of this entry is 2.30 Å.

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	Percentile Ranks	Value
Clashscore		4
RSRZ outliers		25.0%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
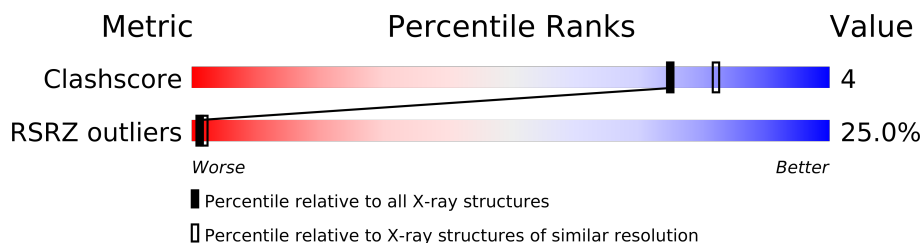
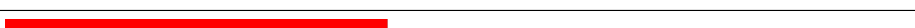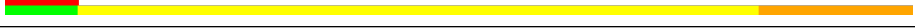| Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	3679 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	12	
1	C	12	
1	E	12	
2	B	12	
2	D	12	
2	F	12	

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 1513 atoms, of which 0 are hydrogen and 0 are deuterium.

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(*CP*GP*CP*GP*AP*AP*AP*AP*AP*AP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	12	Total 246	C 117	N 54	O 64	P 11	0	0	0
1	C	12	Total 246	C 117	N 54	O 64	P 11	0	0	0
1	E	12	Total 246	C 117	N 54	O 64	P 11	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	12	Total 240	C 117	N 36	O 76	P 11	0	0	0
2	D	12	Total 240	C 117	N 36	O 76	P 11	0	0	0
2	F	12	Total 240	C 117	N 36	O 76	P 11	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	21	Total 21	O 21	0	0
3	B	19	Total 19	O 19	0	0
3	C	4	Total 4	O 4	0	0
3	D	3	Total 3	O 3	0	0
3	E	3	Total 3	O 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	5	Total 5	O 5	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: DNA (5'-D(*CP*GP*CP*GP*AP*AP*AP*AP*AP*AP*CP*G)-3')

Chain A:
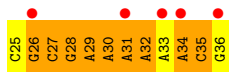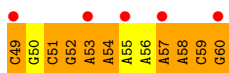

• Molecule 1: DNA (5'-D(*CP*GP*CP*GP*AP*AP*AP*AP*AP*AP*CP*G)-3')

Chain C:

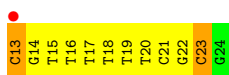• Molecule 1: DNA (5'-D(*CP*GP*CP*GP*AP*AP*AP*AP*AP*AP*CP*G)-3')

Chain E:

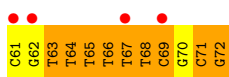• Molecule 2: DNA (5'-D(*CP*GP*TP*TP*TP*TP*TP*TP*CP*GP*CP*G)-3')

Chain B:

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

Chain D:

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

Chain F:

4   Data and refinement statistics   ⓘ

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	44.78Å 66.05Å 42.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.30 12.15 – 2.22	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-2.30) 84.1 (12.15-2.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.10 (at 2.21Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.232 , (Not available) 0.270 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	38.2	Xtriage
Anisotropy	0.785	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 74.2	EDS
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
L-test for twinning	$< |L| > = 0.52, < L^2 > = 0.36$	Xtriage
Outliers	4 of 5591 reflections (0.072%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	1513	wwPDB-VP
Average B, all atoms (Å^2)	46.0	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 44.63 % 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 1.4855e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.

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	1.45	1/278 (0.4%)	2.18	16/427 (3.7%)
1	C	1.00	0/278	2.00	15/427 (3.5%)
1	E	1.07	0/278	2.01	14/427 (3.3%)
2	B	1.49	2/266 (0.8%)	2.65	34/409 (8.3%)
2	D	1.16	2/266 (0.8%)	2.28	20/409 (4.9%)
2	F	1.11	0/266	2.31	24/409 (5.9%)
All	All	1.23	5/1632 (0.3%)	2.25	123/2508 (4.9%)

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
2	B	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	16	DT	C5-C7	8.25	1.54	1.50
2	D	39	DT	C5-C7	5.26	1.53	1.50
1	A	3	DC	C4'-C3'	-5.12	1.47	1.52
2	D	44	DT	C5-C7	5.06	1.53	1.50
2	B	16	DT	P-O5'	5.04	1.64	1.59

The worst 5 of 123 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	20	DT	C6-C5-C7	-10.77	116.44	122.90
1	A	3	DC	C4'-C3'-C2'	-9.65	94.42	103.10
1	A	9	DA	O4'-C1'-C2'	-9.45	98.34	105.90
2	B	16	DT	O4'-C1'-C2'	-9.22	98.52	105.90
1	E	54	DA	C1'-O4'-C4'	-8.81	101.29	110.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	23	DC	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	246	0	134	1	0
1	C	246	0	134	0	566
1	E	246	0	134	2	300
2	B	240	0	140	2	0
2	D	240	0	140	1	206
2	F	240	0	140	3	488
3	A	21	0	0	0	0
3	B	19	0	0	0	0
3	C	4	0	0	0	9
3	D	3	0	0	0	6
3	E	3	0	0	0	1
3	F	5	0	0	1	2
All	All	1513	0	822	9	789

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

The worst 5 of 9 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:62:DG:H4'	3:F:117:HOH:O	1.78	0.84
2:F:71:DC:H2"	2:F:72:DG:C8	2.38	0.58
1:A:3:DC:H2'	1:A:4:DG:C8	2.40	0.56
2:D:47:DC:H2"	2:D:48:DG:C8	2.43	0.53
2:B:13:DC:H2"	2:B:14:DG:H8	1.74	0.51

The worst 5 of 789 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	Distance(Å)	Clash(Å)
2:D:45:DC:N3	2:F:72:DG:C6[1_566]	0.22	1.98
1:C:32:DA:OP1	2:F:70:DG:OP1[1_566]	0.27	1.93
1:C:32:DA:C6	1:E:53:DA:N3[1_566]	0.43	1.77
1:C:35:DC:C2'	2:F:65:DT:C2[1_566]	0.43	1.77
1:C:33:DA:N7	1:E:54:DA:N3[1_566]	0.46	1.74

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

There are no protein chains in this entry.

5.3.2 Protein sidechains ⓘ

There are no protein chains in this entry.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95th 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(Å²)	Q<0.9
1	A	12/12 (100%)	0.25	0	100	100	26, 33, 35, 46	0
1	C	12/12 (100%)	1.86	5 (41%)	1	1	26, 45, 70, 112	12 (100%)
1	E	12/12 (100%)	1.78	5 (41%)	1	1	23, 37, 46, 62	12 (100%)
2	B	12/12 (100%)	0.71	1 (8%)	11	18	25, 31, 47, 191	0
2	D	12/12 (100%)	2.07	3 (25%)	1	2	32, 49, 64, 118	12 (100%)
2	F	12/12 (100%)	2.19	4 (33%)	1	1	24, 42, 70, 190	12 (100%)
All	All	72/72 (100%)	1.48	18 (25%)	1	2	23, 40, 70, 191	48 (66%)

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	61	DC	8.2
2	B	13	DC	7.9
2	D	48	DG	7.5
2	D	37	DC	4.8
2	F	62	DG	3.9

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.