



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:51 AM GMT

PDB ID : 3GBI  
Title : The Rational Design and Structural Analysis of a Self-Assembled Three-Dimensional DNA Crystal  
Authors : Birktoft, J.J.; Zheng, J.; Seeman, N.C.  
Deposited on : 2009-02-19  
Resolution : 4.02 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

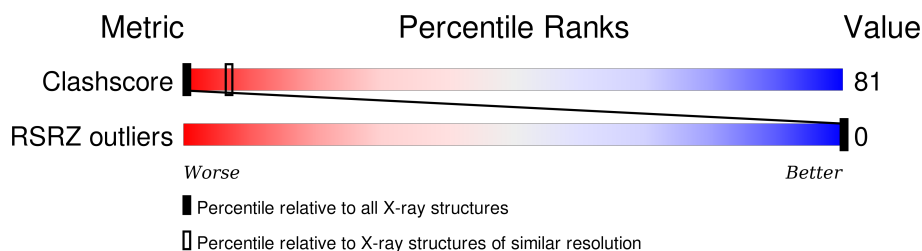
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.02 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))
Clashscore	102246	1054 (4.44-3.60)
RSRZ outliers	91569	1018 (4.48-3.56)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . 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	21	
2	B	7	
3	C	6	
4	D	8	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 855 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\*AP\*GP\*CP\*AP\*GP\*CP\*CP\*TP\*GP\*TP\*AP\*CP\*GP\*GP\*AP\*CP\*AP\*TP\*CP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	21	Total	C	N	O	P	0	0	0
			429	204	84	121	20			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	7	Total	C	N	O	P	0	0	0
			141	67	26	41	7			

- Molecule 3 is a DNA chain called DNA (5'-D(P\*GP\*GP\*CP\*TP\*GP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	6	Total	C	N	O	P	0	0	0
			124	58	23	37	6			

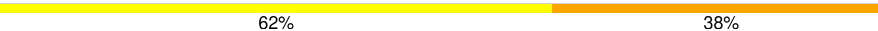
- Molecule 4 is a DNA chain called DNA (5'-D(\*TP\*CP\*TP\*GP\*AP\*TP\*GP\*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	8	Total	C	N	O	P	0	0	0
			161	79	26	49	7			

### 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(\*GP\*AP\*GP\*CP\*AP\*GP\*CP\*CP\*TP\*GP\*TP\*AP\*CP\*GP\*GP\*AP\*CP\*AP\*TP\*CP\*A)-3')

Chain A:  62% 38%


G101	A102	G103	C104	A105	G106	C107	C108	T109	G110	T111	A112	C113	G114	G115	A116	C117	A118	T119	C120	A121
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

- Molecule 2: DNA (5'-D(P\*CP\*CP\*GP\*TP\*AP\*CP\*A)-3')

Chain B:  86% 14%

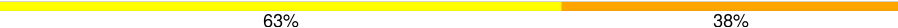
C119	C120	G121	T122	A123	C124	A125
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- Molecule 3: DNA (5'-D(P\*GP\*GP\*CP\*TP\*GP\*C)-3')

Chain C:  83% 17%

G209	G210	C211	T212	G213	C214
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- Molecule 4: DNA (5'-D(\*TP\*CP\*TP\*GP\*AP\*TP\*GP\*T)-3')

Chain D:  63% 38%

T101	C102	T103	G104	A105	T106	G107	T108
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## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.16 Å   107.16 Å   93.14 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	17.29 – 4.02 17.29 – 4.01	Depositor EDS
% Data completeness (in resolution range)	61.1 (17.29-4.02) 61.2 (17.29-4.01)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.92 (at 4.04 Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.240 ,      0.309 0.218 ,      (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	230.8	Xtriage
Anisotropy	0.555	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.03 , -10.0	EDS
Estimated twinning fraction	0.008 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.54$ , $\langle L^2 \rangle = 0.38$	Xtriage
Outliers	0 of 2775 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	855	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.20% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 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	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.51	0/482	1.47	12/742 (1.6%)
2	B	0.52	0/157	1.38	2/239 (0.8%)
3	C	0.51	0/138	1.38	2/211 (0.9%)
4	D	0.72	1/179 (0.6%)	1.60	4/275 (1.5%)
All	All	0.56	1/956 (0.1%)	1.47	20/1467 (1.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	106	DT	C5-C7	6.02	1.53	1.50

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	DA	O4'-C4'-C3'	-7.59	101.45	106.00
1	A	107	DC	O4'-C1'-N1	6.77	112.74	108.00
1	A	103	DG	O4'-C1'-N9	6.58	112.61	108.00
1	A	102	DA	O4'-C1'-N9	6.58	112.60	108.00
4	D	106	DT	C1'-O4'-C4'	-6.41	103.69	110.10
1	A	107	DC	C1'-O4'-C4'	-6.22	103.88	110.10
3	C	213	DG	C1'-O4'-C4'	-5.91	104.19	110.10
2	B	123	DA	C3'-C2'-C1'	-5.83	95.50	102.50
1	A	121	DA	C3'-C2'-C1'	-5.79	95.56	102.50
1	A	116	DA	O4'-C1'-N9	5.70	111.99	108.00
1	A	107	DC	O4'-C1'-C2'	-5.64	101.39	105.90
1	A	101	DG	P-O3'-C3'	5.47	126.26	119.70
1	A	103	DG	C1'-O4'-C4'	-5.46	104.64	110.10
4	D	103	DT	O4'-C1'-N1	5.40	111.78	108.00
1	A	115	DG	O4'-C4'-C3'	-5.34	102.36	104.50
2	B	123	DA	O4'-C1'-N9	5.34	111.74	108.00
4	D	103	DT	P-O3'-C3'	5.26	126.01	119.70
1	A	119	DT	C1'-O4'-C4'	-5.23	104.87	110.10
3	C	213	DG	O4'-C1'-N9	5.06	111.54	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	104	DG	C3'-C2'-C1'	-5.05	96.44	102.50

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	429	0	236	51	0
2	B	141	0	79	16	0
3	C	124	0	68	19	0
4	D	161	0	94	25	0
All	All	855	0	477	108	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 81.

All (108) 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:115:DG:H2'	1:A:116:DA:C8	1.95	1.00
1:A:114:DG:H2'	1:A:115:DG:C8	2.00	0.97
3:C:209:DG:H2'	3:C:210:DG:C8	2.06	0.90
4:D:104:DG:H1'	4:D:105:DA:H5'	1.59	0.85
2:B:120:DC:H2''	2:B:121:DG:N7	1.93	0.83
1:A:112:DA:H2'	1:A:113:DC:C6	2.16	0.81
2:B:120:DC:H2''	2:B:121:DG:C5	2.16	0.81
1:A:106:DG:H1	3:C:211:DC:H42	1.28	0.79
1:A:101:DG:N3	1:A:101:DG:H2'	1.98	0.77
1:A:110:DG:H3'	1:A:111:DT:C6	2.22	0.74
4:D:103:DT:H1'	4:D:104:DG:OP1	1.87	0.74
4:D:105:DA:H4'	4:D:106:DT:H5'	1.69	0.73
3:C:210:DG:H2''	3:C:211:DC:OP1	1.87	0.73
1:A:102:DA:H2''	1:A:103:DG:OP1	1.88	0.73
1:A:110:DG:H3'	1:A:111:DT:H6	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:DG:H2''	1:A:107:DC:O5'	1.90	0.72
1:A:115:DG:H2''	1:A:116:DA:OP1	1.88	0.71
2:B:119:DC:C6	4:D:108:DT:H2'	2.26	0.71
1:A:111:DT:H2''	1:A:112:DA:C8	2.25	0.70
1:A:112:DA:H2'	1:A:113:DC:H6	1.56	0.70
1:A:115:DG:OP2	1:A:115:DG:H8	1.74	0.69
1:A:109:DT:H3'	1:A:110:DG:O4'	1.93	0.68
1:A:102:DA:H1'	1:A:103:DG:OP2	1.93	0.68
2:B:124:DC:H2''	2:B:125:DA:H5'	1.75	0.68
3:C:211:DC:H2''	3:C:212:DT:O5'	1.92	0.68
4:D:101:DT:H2''	4:D:102:DC:OP1	1.94	0.68
1:A:111:DT:H2''	1:A:112:DA:H8	1.59	0.67
1:A:103:DG:H1'	1:A:104:DC:OP1	1.95	0.67
1:A:115:DG:H2'	1:A:116:DA:H8	1.58	0.66
4:D:105:DA:OP2	4:D:105:DA:H3'	1.95	0.66
1:A:109:DT:H2'	1:A:109:DT:O2	1.97	0.63
2:B:123:DA:H2''	2:B:124:DC:C5	2.32	0.63
4:D:104:DG:C1'	4:D:105:DA:H5'	2.27	0.63
2:B:121:DG:H2''	2:B:122:DT:O5'	2.00	0.62
1:A:119:DT:H2''	1:A:120:DC:O5'	1.99	0.61
1:A:112:DA:H8	1:A:112:DA:OP1	1.82	0.61
1:A:117:DC:H2''	1:A:118:DA:C8	2.36	0.60
1:A:113:DC:H2''	1:A:114:DG:N7	2.16	0.60
1:A:108:DC:H2'	1:A:109:DT:H6	1.67	0.60
1:A:112:DA:H2''	1:A:113:DC:O5'	2.01	0.60
2:B:125:DA:N3	3:C:209:DG:H1'	2.18	0.59
1:A:112:DA:O4'	1:A:112:DA:P	2.61	0.58
4:D:103:DT:H2''	4:D:104:DG:C8	2.38	0.58
2:B:119:DC:H2'	2:B:120:DC:C6	2.39	0.58
1:A:105:DA:C6	1:A:106:DG:C6	2.93	0.57
1:A:117:DC:H2''	1:A:118:DA:H8	1.69	0.56
4:D:105:DA:H1'	4:D:106:DT:O4'	2.06	0.55
4:D:104:DG:C6	4:D:105:DA:C6	2.95	0.55
4:D:105:DA:H1'	4:D:106:DT:C6	2.41	0.55
1:A:113:DC:H2''	1:A:114:DG:C8	2.42	0.53
4:D:107:DG:H2''	4:D:108:DT:O4'	2.09	0.53
4:D:101:DT:O2	4:D:101:DT:H2'	2.08	0.53
3:C:211:DC:OP1	3:C:211:DC:H6	1.91	0.53
3:C:210:DG:OP2	3:C:210:DG:C8	2.62	0.52
2:B:120:DC:H2''	2:B:121:DG:C8	2.45	0.51
3:C:210:DG:N2	3:C:211:DC:C2	2.78	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:210:DG:OP2	3:C:210:DG:H8	1.92	0.51
1:A:112:DA:H2'	1:A:113:DC:C5	2.46	0.51
4:D:107:DG:C4	4:D:108:DT:C6	2.98	0.51
1:A:110:DG:H2'	1:A:110:DG:N3	2.26	0.50
4:D:105:DA:P	4:D:105:DA:H3'	2.52	0.50
1:A:104:DC:H2'	1:A:105:DA:C8	2.47	0.50
3:C:212:DT:H2''	3:C:213:DG:OP1	2.11	0.50
3:C:211:DC:H1'	3:C:212:DT:OP1	2.11	0.50
1:A:112:DA:H8	1:A:112:DA:P	2.35	0.49
4:D:105:DA:C4'	4:D:106:DT:H5'	2.40	0.49
1:A:101:DG:H4'	1:A:102:DA:OP1	2.12	0.49
3:C:211:DC:OP1	3:C:211:DC:C6	2.66	0.49
4:D:104:DG:C2	4:D:105:DA:C4	3.01	0.49
2:B:124:DC:H2''	2:B:125:DA:H8	1.78	0.49
3:C:210:DG:C2'	3:C:211:DC:OP1	2.60	0.48
1:A:104:DC:C2'	1:A:105:DA:C8	2.97	0.47
3:C:212:DT:H3'	3:C:213:DG:C8	2.48	0.47
2:B:119:DC:H2'	2:B:120:DC:C5	2.49	0.47
3:C:209:DG:H2'	3:C:210:DG:H8	1.71	0.47
3:C:210:DG:H1'	3:C:211:DC:P	2.55	0.47
4:D:105:DA:H1'	4:D:106:DT:N1	2.30	0.47
4:D:103:DT:H2''	4:D:104:DG:N7	2.30	0.46
1:A:110:DG:C5	1:A:111:DT:C4	3.03	0.46
3:C:213:DG:H2''	3:C:214:DC:H5'	1.98	0.46
1:A:115:DG:C6	1:A:116:DA:C6	3.04	0.45
1:A:102:DA:H1'	1:A:103:DG:P	2.55	0.45
2:B:123:DA:H2''	2:B:124:DC:C6	2.52	0.45
4:D:104:DG:O3'	4:D:105:DA:H2'	2.17	0.45
1:A:112:DA:O4'	1:A:112:DA:OP2	2.33	0.45
4:D:104:DG:H4'	4:D:105:DA:OP1	2.15	0.45
1:A:112:DA:C8	1:A:112:DA:OP1	2.67	0.44
1:A:117:DC:H2''	1:A:118:DA:OP2	2.17	0.44
1:A:118:DA:H2''	1:A:119:DT:OP2	2.17	0.44
1:A:117:DC:C2	1:A:118:DA:N7	2.86	0.44
4:D:102:DC:H1'	4:D:103:DT:OP2	2.18	0.44
1:A:107:DC:H2''	1:A:108:DC:C5	2.52	0.44
2:B:124:DC:H2''	2:B:125:DA:C8	2.52	0.44
1:A:108:DC:H2''	1:A:109:DT:OP1	2.19	0.43
3:C:210:DG:H1'	3:C:211:DC:OP2	2.18	0.42
4:D:106:DT:C2	4:D:107:DG:N7	2.87	0.42
1:A:103:DG:H4'	1:A:104:DC:OP2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:104:DG:C5	4:D:105:DA:C5	3.08	0.42
1:A:110:DG:C8	1:A:111:DT:H72	2.55	0.42
1:A:113:DC:O3'	1:A:114:DG:C8	2.72	0.42
1:A:102:DA:H8	1:A:102:DA:OP2	2.03	0.41
1:A:118:DA:C2	1:A:119:DT:C2	3.09	0.41
4:D:107:DG:C5	4:D:108:DT:C5	3.08	0.41
2:B:121:DG:C2'	2:B:122:DT:O5'	2.68	0.41
3:C:209:DG:H2'	3:C:210:DG:N7	2.34	0.41
2:B:123:DA:C4	2:B:124:DC:C4	3.09	0.40
2:B:124:DC:C2'	2:B:125:DA:H8	2.35	0.40
1:A:119:DT:OP2	1:A:119:DT:H6	2.05	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 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 [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	21/21 (100%)	-0.93	0 100 100	80, 80, 80, 80	0
2	B	7/7 (100%)	-0.81	0 100 100	80, 80, 80, 80	0
3	C	6/6 (100%)	-0.90	0 100 100	80, 80, 80, 80	0
4	D	8/8 (100%)	-0.80	0 100 100	78, 80, 80, 80	0
All	All	42/42 (100%)	-0.88	0 100 100	78, 80, 80, 80	0

There are no RSRZ outliers to report.

### 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 carbohydrates 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.