

# Full wwPDB X-ray Structure Validation Report (i)

#### Sep 26, 2022 – 04:06 PM EDT

PDB ID : 7SD7

Title: [C:Hg2+:T] Metal-mediated DNA base pair in a self-assembling rhombohedral

lattice

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Deposited on : 2021-09-29

Resolution : 3.68 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:

 $\begin{array}{ccc} & Mol Probity & : & 4.02b\text{-}467 \\ Xtriage \left(Phenix\right) & : & 1.13 \end{array}$ 

EDS : 2.31.2buster-report : 1.1.7 (2018)

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

Refmac : 5.8.0158

CCP4 : 7.0.044 (Gargrove) roteins) : Engh & Huber (2001)

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

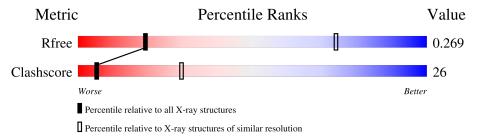
Validation Pipeline (wwPDB-VP) : 2.31.2

# 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 3.68 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 $(\# \mathrm{Entries})$	Similar resolution $(\#\text{Entries, resolution range}(\mathring{A}))$			
$R_{free}$	130704	1013 (3.84-3.52)			
Clashscore	141614	1070 (3.84-3.52)			

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%

Mol	Chain	Length	Quality of chain					
1	A	21	38%	57%	5%			
2	В	7	29%	71%	_			
3	С	6		100%				
4	D	8		75%	25%			



# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 854 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\*TP\*GP\*TP\*GP\*TP\*GP\*AP\*TP\*CP\*A)-3').

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	21	Total 428	C 204	N 81	O 123	P 20	0	0	0

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	R	7	Total	С	N	О	Р	0	0	0
	ט	1	140	67	26	40	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		
2	C	6	Total	С	N	О	Р	0	0	0
3		0	124	58	23	37	6	0	U	U

• 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 161	C 79	N 26	O 49	P 7	0	0	0

• Molecule 5 is MERCURY (II) ION (three-letter code: HG) (formula: Hg) (labeled as "Ligand of Interest" by depositor).

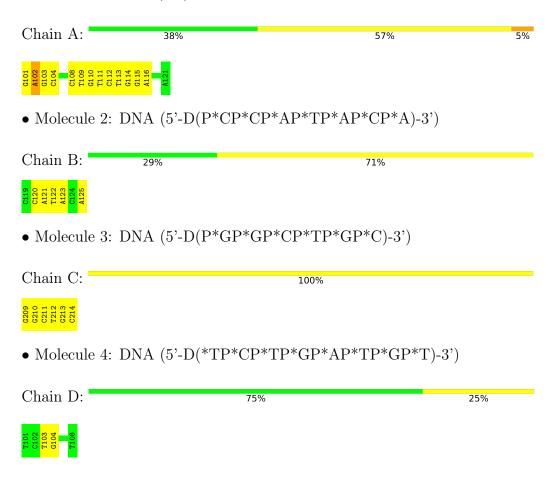
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	В	1	Total Hg 1 1	0	0



## 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.

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





# 4 Data and refinement statistics (i)

Property	Value	Source	
Space group	Н 3	Depositor	
Cell constants	105.59Å 105.59Å 89.08Å	Depositor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor	
Resolution (Å)	32.22 - 3.68	Depositor	
Resolution (A)	63.81 - 3.68	EDS	
% Data completeness	71.3 (32.22-3.68)	Depositor	
(in resolution range)	64.1 (63.81-3.68)	EDS	
$R_{merge}$	(Not available)	Depositor	
$R_{sym}$	(Not available)	Depositor	
$< I/\sigma(I) > 1$	0.21  (at  3.67Å)	Xtriage	
Refinement program	PHENIX 1.18.2_3874	Depositor	
D.D.	0.223 , $0.275$	Depositor	
$R, R_{free}$	0.220 , $0.269$	DCC	
$R_{free}$ test set	129 reflections $(4.48\%)$	wwPDB-VP	
Wilson B-factor (Å <sup>2</sup> )	230.2	Xtriage	
Anisotropy	0.191	Xtriage	
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.17 , 176.8	EDS	
L-test for twinning <sup>2</sup>	$< L > = 0.47, < L^2> = 0.30$	Xtriage	
Estimated twinning fraction	0.054 for h,-h-k,-l	Xtriage	
$F_o, F_c$ correlation	0.84	EDS	
Total number of atoms	854	wwPDB-VP	
Average B, all atoms (Å <sup>2</sup> )	301.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.78% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

## 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: HG

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		
IVIOI		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	0.78	0/480	1.14	1/739 (0.1%)	
2	В	0.60	0/156	0.91	0/237	
3	С	0.65	0/138	0.97	0/211	
4	D	0.65	0/179	1.18	0/275	
All	All	0.71	0/953	1.09	1/1462 (0.1%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	102	DA	O4'-C1'-N9	6.82	112.78	108.00

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	428	0	237	21	0
2	В	140	0	78	5	0
3	С	124	0	68	10	0
4	D	161	0	94	1	0
5	В	1	0	0	0	0
All	All	854	0	477	34	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 26.

All (34) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
		distance (Å)	overlap (Å)
1:A:109:DT:H3'	1:A:110:DG:H8	1.51	0.76
1:A:103:DG:H2"	1:A:104:DC:H5"	1.68	0.76
1:A:110:DG:H2'	1:A:111:DT:C6	2.26	0.70
1:A:111:DT:H2"	1:A:112:DC:H5"	1.73	0.69
1:A:109:DT:H3'	1:A:110:DG:C8	2.26	0.68
2:B:122:DT:H2"	2:B:123:DA:C8	2.32	0.65
1:A:114:DG:H2"	1:A:115:DG:N7	2.12	0.64
1:A:112:DC:H2"	1:A:113:DT:H5'	1.81	0.61
1:A:115:DG:H2"	1:A:116:DA:H8	1.67	0.59
3:C:212:DT:H2'	3:C:213:DG:C8	2.36	0.59
1:A:101:DG:N3	1:A:101:DG:H2'	2.20	0.57
1:A:115:DG:H4'	1:A:116:DA:OP1	2.06	0.56
4:D:103:DT:H2"	4:D:104:DG:C8	2.43	0.54
2:B:120:DC:H2'	2:B:121:DA:C8	2.44	0.52
1:A:102:DA:H1'	1:A:103:DG:OP2	2.10	0.51
1:A:114:DG:H2"	1:A:115:DG:C8	2.45	0.51
1:A:113:DT:H1'	1:A:114:DG:N7	2.25	0.50
1:A:112:DC:H3'	1:A:113:DT:H72	1.95	0.48
2:B:125:DA:OP2	2:B:125:DA:H3'	2.14	0.47
3:C:209:DG:H2'	3:C:209:DG:N3	2.28	0.47
1:A:108:DC:N3	3:C:210:DG:N2	2.63	0.47
1:A:111:DT:H2"	1:A:112:DC:C5'	2.42	0.47
1:A:102:DA:C8	1:A:102:DA:OP2	2.69	0.46
3:C:212:DT:H2"	3:C:213:DG:OP1	2.16	0.45
3:C:209:DG:C6	3:C:210:DG:C6	3.05	0.44
3:C:211:DC:H2'	3:C:212:DT:H6	1.82	0.44
2:B:125:DA:C6	3:C:209:DG:C5	3.06	0.44
3:C:213:DG:H2"	3:C:214:DC:H5'	2.01	0.43
1:A:102:DA:H8	1:A:102:DA:P	2.43	0.42
1:A:113:DT:C4	2:B:120:DC:N4	2.86	0.42
1:A:108:DC:H2'	1:A:109:DT:O4'	2.20	0.42
3:C:211:DC:H2'	3:C:212:DT:C6	2.54	0.42
3:C:212:DT:C2	3:C:213:DG:N7	2.88	0.42
1:A:113:DT:O3'	1:A:114:DG:C8	2.74	0.41

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)

Of 1 ligands modelled in this entry, 1 is 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 (i)

#### 6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates (i)

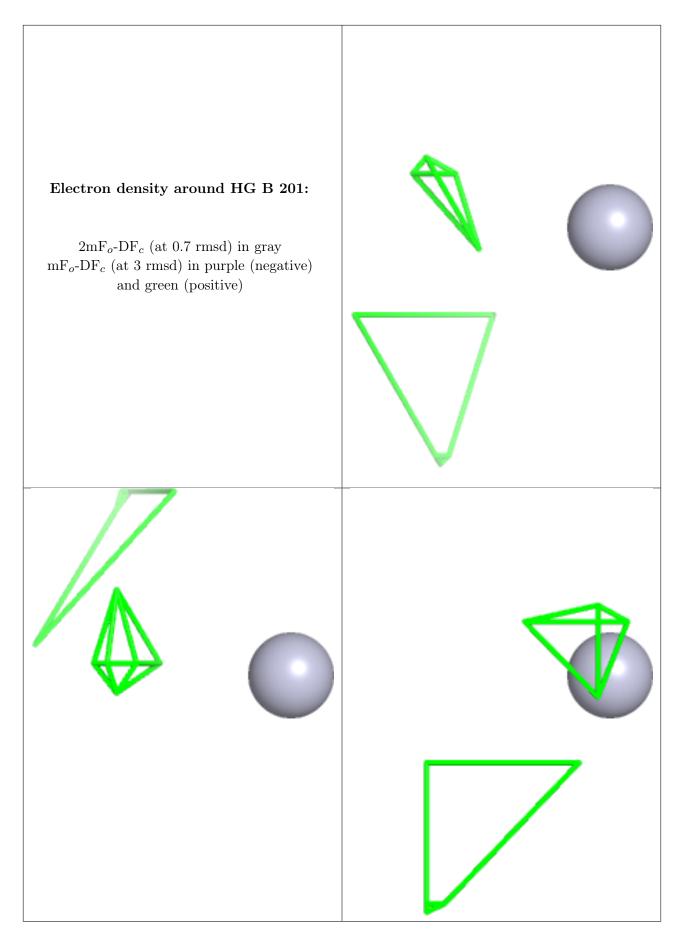
Unable to reproduce the depositors R factor - this section is therefore empty.

#### 6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.







# 6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

