

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

#### Sep 26, 2022 – 04:05 PM EDT

PDB ID : 7SE1

Title : [iU:Hg2+:mC] Metal-mediated DNA base pair in a self-assembling rhombohe-

dral lattice

Authors: Lu, B.; Vecchioni, S.; Seeman, N.C.; Sha, R.; Ohayon, Y.P.

Deposited on : 2021-09-29

Resolution : 4.19 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) : 1.13

EDS : 2.31.2

buster-report : 1.1.7 (2018)

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)

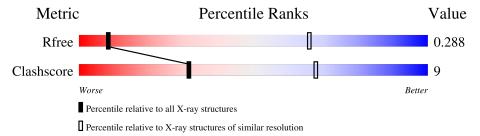
Validation Pipeline (wwPDB-VP) : 2.31.2

## 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 4.19 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 $(\# \mathrm{Entries})$	$egin{aligned}  ext{Similar resolution} \ (\# ext{Entries, resolution range}(\mathring{ ext{A}})) \end{aligned}$				
$R_{free}$	130704	1005 (4.62-3.78)				
Clashscore	141614	1044 (4.60-3.80)				

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	48%	48%	5%			
2	В	7	71%	29%				
3	С	7	86%		14%			
4	D	7	57%	43%				



## 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 859 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\*(5IU)P\*TP\*GP\*AP\*CP\*AP\*TP\*CP\*A)-3').

N	/Iol	Chain	Residues	${f Atoms}$			ZeroOcc	AltConf	Trace			
	1	A	21	Total 429	C 204	I 1	N 80	O 124	P 20	0	0	0

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	В	7	Total 140	C 67	N 27	O 39	P 7	0	0	0

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	C	7	Total	С	N	О	Р	0	0	0
3		1	144	68	25	44	7		U	U

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
4	D	7	Total 145	C 69	N 24	O 45	P 7	0	0	0

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

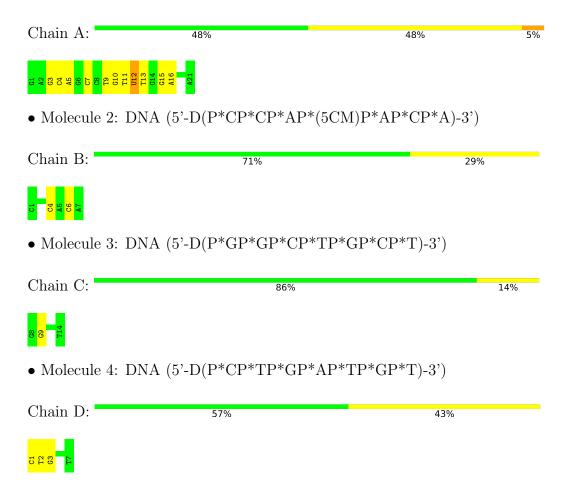
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	В	1	Total Hg 1 1	0	0



## 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\*TP\*GP\*TP\*(5IU)P\*TP\*GP\*GP\*AP\*CP\*AP\*TP\*CP\*A)-3')





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants	107.08Å 107.08Å 86.81Å	Donositon
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
Resolution (Å)	32.50 - 4.19	Depositor
Resolution (A)	63.38 - 4.19	EDS
% Data completeness	56.3 (32.50-4.19)	Depositor
(in resolution range)	56.3 (63.38-4.19)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.37 (at 4.14Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
D.D.	0.184 , 0.290	Depositor
$R, R_{free}$	0.184 , $0.288$	DCC
$R_{free}$ test set	76 reflections $(4.93\%)$	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	287.9	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.14 , 196.7	EDS
L-test for twinning <sup>2</sup>	$< L > = 0.42, < L^2> = 0.24$	Xtriage
Estimated twinning fraction	0.117 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.77	EDS
Total number of atoms	859	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	319.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.13% 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: 5IU, HG, 5CM

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	nd lengths	Bond angles		
IVIOI		RMSZ	# Z  > 5	RMSZ	# Z >5	
1	A	0.56	0/458	0.88	0/703	
2	В	0.45	0/133	0.72	0/199	
3	С	0.47	0/160	0.90	0/245	
4	D	1.00	1/161 (0.6%)	1.00	0/245	
All	All	0.63	1/912 (0.1%)	0.89	0/1392	

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	Observed(A)	$Ideal(\AA)$
4	D	1	DC	OP3-P	-10.63	1.48	1.61

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	429	0	235	9	0
2	В	140	0	76	1	0
3	С	144	0	80	1	0
4	D	145	0	81	1	0
5	В	1	0	0	0	0
All	All	859	0	472	10	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 9.

All (10) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:A:7:DC:O2	3:C:9:DG:N2	2.24	0.71
1:A:10:DG:N2	2:B:6:DC:N3	2.42	0.67
1:A:3:DG:H2"	1:A:4:DC:O5'	2.05	0.57
1:A:4:DC:H2'	1:A:5:DA:C8	2.44	0.53
1:A:12:5IU:H2"	1:A:13:DT:O5'	2.11	0.51
1:A:9:DT:H3'	1:A:10:DG:C8	2.51	0.45
1:A:15:DG:H4'	1:A:16:DA:OP1	2.16	0.45
4:D:2:DT:H2"	4:D:3:DG:O5'	2.18	0.43
1:A:11:DT:H2"	1:A:12:5IU:OP1	2.20	0.41
1:A:12:5IU:OP1	1:A:12:5IU:H6	2.20	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)

2 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	Trmo	Chain	Dag	Link	B	Bond lengths		Bond angles		
MIOI	Type	Chain	Res	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	5CM	В	4	2,5,1	17,21,22	4.41	11 (64%)	24,30,33	1.73	5 (20%)
1	5IU	A	12	2,1	18,21,22	4.00	12 (66%)	26,30,33	2.15	6 (23%)

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

Mol	Type	Chain				Torsions	Rings
2	5CM	В	4	2,5,1	-	0/7/21/22	0/2/2/2
1	5IU	A	12	2,1	-	3/7/21/22	0/2/2/2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(A)
2	В	4	5CM	C2'-C3'	-11.24	1.23	1.52
1	A	12	5IU	O4-C4	8.92	1.40	1.23
1	A	12	5IU	O4'-C4'	7.87	1.62	1.45
2	В	4	5CM	O4'-C4'	-7.70	1.27	1.45
1	A	12	5IU	C3'-C4'	-6.24	1.35	1.53
1	A	12	5IU	O4'-C1'	-5.48	1.30	1.42
2	В	4	5CM	C1'-N1	-5.03	1.35	1.48
2	В	4	5CM	C4-N4	4.94	1.46	1.34
2	В	4	5CM	C3'-C4'	4.84	1.66	1.53
1	A	12	5IU	C2-N1	-3.67	1.32	1.38
2	В	4	5CM	O4'-C1'	3.62	1.50	1.42
2	В	4	5CM	C2-N1	-3.42	1.32	1.40
1	A	12	5IU	C4-N3	-3.36	1.32	1.38
1	A	12	5IU	O3'-C3'	3.33	1.50	1.43
2	В	4	5CM	O3'-C3'	3.20	1.50	1.43
2	В	4	5CM	C6-C5	3.13	1.39	1.34
1	A	12	5IU	C2-N3	-3.10	1.32	1.38
2	В	4	5CM	C6-N1	-3.07	1.32	1.38
1	A	12	5IU	C6-N1	-3.05	1.32	1.38
1	A	12	5IU	C4-C5	-2.85	1.39	1.45
2	В	4	5CM	O2-C2	-2.55	1.19	1.23
1	A	12	5IU	O2-C2	-2.18	1.19	1.23
1	A	12	5IU	C2'-C1'	2.08	1.58	1.52



All (11) bond angle outliers are listed below:
--

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$Ideal(^{o})$
1	A	12	5IU	N3-C2-N1	6.04	122.91	114.89
1	A	12	5IU	C4-N3-C2	-5.24	120.57	127.35
2	В	4	5CM	C5-C6-N1	-4.56	118.64	123.34
2	В	4	5CM	C5-C4-N3	-3.58	117.82	121.67
1	A	12	5IU	O2-C2-N1	-3.07	118.71	122.79
1	A	12	5IU	C5-C4-N3	2.89	118.68	113.86
1	A	12	5IU	O4-C4-C5	-2.84	120.63	125.69
2	В	4	5CM	C4'-O4'-C1'	-2.72	102.87	109.45
2	В	4	5CM	O4'-C1'-N1	2.61	112.53	107.86
2	В	4	5CM	O4'-C1'-C2'	-2.14	102.20	106.25
1	A	12	5IU	C2'-C3'-C4'	2.12	107.17	102.76

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	12	5IU	C4'-C5'-O5'-P
1	A	12	5IU	C3'-C4'-C5'-O5'
1	A	12	5IU	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	12	5IU	3	0

### 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)

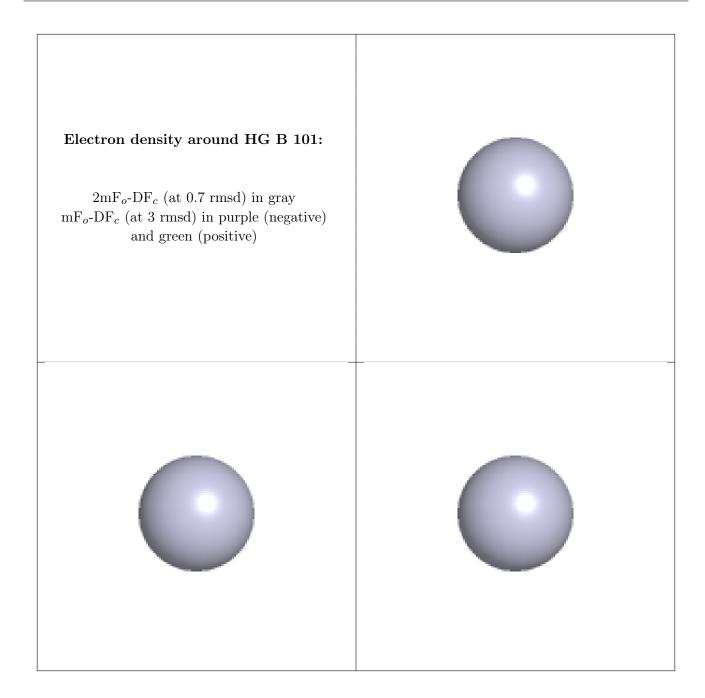
Unable to reproduce the depositors R factor - this section is therefore empty.

#### 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.

