

wwPDB X-ray Structure Validation Summary Report (i)

Sep 26, 2022 – 03:38 PM EDT

PDB ID	:	7SE4
Title	:	[iU:Hg2+:C] Metal-mediated DNA base pair in a self-assembling rhombohedral
		lattice
Authors	:	Lu, B.; Vecchioni, S.; Seeman, N.C.; Sha, R.; Ohayon, Y.P.
Deposited on	:	2021-09-29
Resolution	:	4.65 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

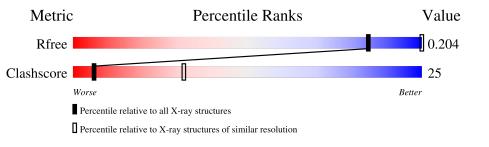
Xtriage (Phenix) EDS buster-report Percentile statistics Refmac CCP4 Ideal geometry (proteins) Ideal geometry (DNA, RNA)	: : : : :	20191225.v01 (using entries in the PDB archive December 25th 2019) 5.8.0158 7.0.044 (Gargrove) Engh & Huber (2001)
Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)		Parkinson et al. (1996) 2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 4.65 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	1083 (5.52-3.80)
Clashscore	141614	1156 (5.52-3.80)

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	А	21	14%	71%	14%			
2	В	7	57%		43%			
3	С	7	43%	57%				
4	D	7	29%	71%				

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	5IU	А	12	-	-	Х	-



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 858 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*(5IU)P*TP*GP*GP*AP*CP*AP*TP*CP*A)-3').

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace			
1	А	21	Total 429	C 204	I 1	N 80	0 124	Р 20	0	0	0

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	В	7	Total 139	C 66	N 27	O 39	Р 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		
3	С	7	Total 144	C 68	N 25	0 44	Р 7	0	0	0

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

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
4	D	7	Total 145	C 69	N 24	0 45	Р 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	Ator	ns	ZeroOcc	AltConf
5	В	1	Total 1	Hg 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*(5IU)P*TP*GP*GP*AP*CP*AP*TP*CP*A)-3')

Chain A:	14%	71%	14%
6 42 43 45 45 45 45 45 45 45 45 45 45 45 45 45	10 112 112 113 113 113 113 113 113 113 113		
• Molecule	2: DNA (5'-D(F	P*CP*CP*AP*CP*AP*CP*A	A)-3')
Chain B:	5	57%	43%
C1 C2 A3 A7			
• Molecule	3: DNA (5'-D(F	P*GP*GP*CP*TP*GP*CP*7	Г)-З')
Chain C:	43%	57	7%
68 69 111 612 114 114			
• Molecule	4: DNA (5'-D(F	P*CP*TP*GP*AP*TP*GP*T	Г)-3')
Chain D:	29%	71%	
C1 T2 G3 G6 T7			



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants	106.20Å 106.20Å 92.31Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	32.58 - 4.65	Depositor
Resolution (A)	65.15 - 4.65	EDS
% Data completeness	74.2 (32.58-4.65)	Depositor
(in resolution range)	74.5(65.15-4.65)	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.41 (at 4.65 Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
D D	0.188 , 0.201	Depositor
R, R_{free}	0.189 , 0.204	DCC
R_{free} test set	71 reflections (4.53%)	wwPDB-VP
Wilson B-factor $(Å^2)$	367.4	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.34, 476.8	EDS
L-test for twinning ²	$< L > = 0.40, < L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.114 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	858	wwPDB-VP
Average B, all atoms $(Å^2)$	436.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.52% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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)

Bond lengths and bond angles in the following residue types are not validated in this section: HG, $5\mathrm{IU}$

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	d lengths	Bo	nd angles
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.71	0/458	1.09	2/703~(0.3%)
2	В	0.79	0/155	0.90	0/235
3	С	0.64	0/160	0.99	0/245
4	D	1.02	1/161~(0.6%)	1.15	0/245
All	All	0.77	1/934~(0.1%)	1.05	2/1428~(0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1	DC	OP3-P	-10.40	1.48	1.61

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	А	11	DT	O4'-C1'-N1	7.16	113.01	108.00
1	А	2	DA	O4'-C1'-N9	6.64	112.65	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	А	429	0	235	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	В	139	0	77	4	0
3	С	144	0	80	3	0
4	D	145	0	81	5	0
5	В	1	0	0	0	0
All	All	858	0	473	33	0

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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 25.

The worst 5 of 33 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:9:DT:H2'	1:A:10:DG:C8	2.21	0.75
1:A:4:DC:H2'	1:A:5:DA:C8	2.32	0.63
2:B:2:DC:H2"	2:B:3:DA:N7	2.13	0.62
1:A:9:DT:H2'	1:A:10:DG:H8	1.63	0.62
4:D:2:DT:H2'	4:D:3:DG:C8	2.36	0.60

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)

1 non-standard protein/DNA/RNA residue is 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	Type	Chain	Res	Link	Bo	ond leng	\mathbf{ths}	В	ond ang	les
	WIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
	1	$5\mathrm{IU}$	А	12	5,1	18,21,22	1.63	1 (5%)	26,30,33	0.75	0

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	Res	Link	Chirals	Torsions	Rings
1	5IU	А	12	5,1	-	3/7/21/22	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	12	5IU	C5-I5	-6.50	1.88	2.08

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	А	12	5IU	7	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)

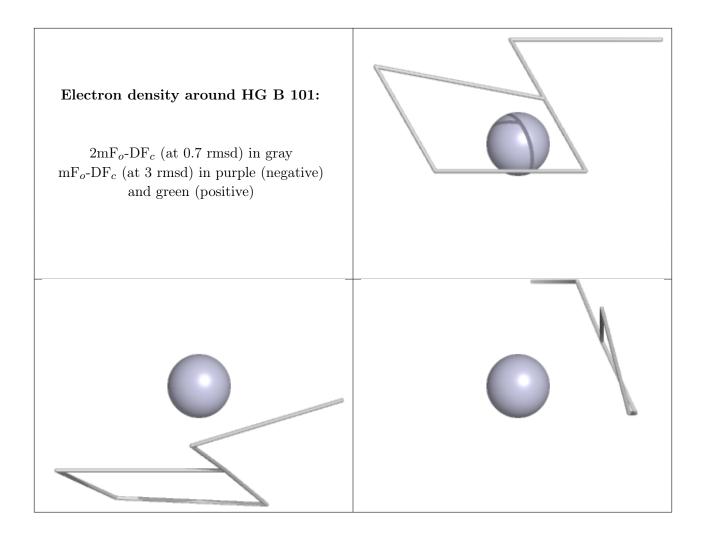
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

