wwPDB Validation Report

PDB ID: 4R6C
RCSB ID: RCSB086954
TITLE: X-ray diffraction in temporally and spatially resolved biomolecular science: the X-ray crystal structure of hen egg white lysozyme cocrystallized with Ta6Br12 and then a crystal soaked in K2PtBr6
AUTHOR(S): J.R.Helliwell

Summary of PDB Entry Validation

The results of the validation of this PDB entry are shown below. No major issues were raised during data processing.

Geometry Validation

1. **Atomic Clashes**

No issues found.

2. **Peptide Linkage**

No issues found.

3. **Covalent Geometry**

No issues found.

4. **Chirality Error**

No issues found.

5. **Phi/Psi Torsion Angles**

No issues found.

Individual Residue Outliers on Real Space R-value

No issues found.

Sequence Validation

The reported biological sequence shows no discrepancy with UniProt sequence (code P00698).

The reported biological sequence and the sequence given in the coordinates show no discrepancy.

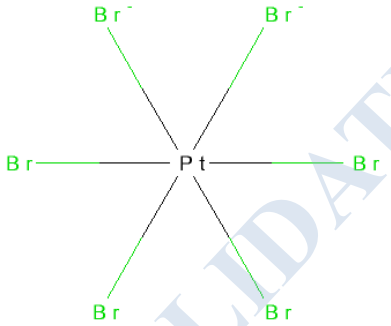
Biological Assembly

The biological assembly predicted by PISA is a monomer. This agrees with author's annotation.

Ligand Chemistry

Ligand chemistry has been checked against the Chemical Component Dictionary. The following is a summary.

Identifier: 6BP
Name: HEXABROMOPLATINATE(IV)
Formula: Br6 Pt



Type	Program	Version	Descriptor
SMILES CANONICAL	CACTVS	3.352	Br[Pt](Br)(Br)(Br)(Br)Br
SMILES	CACTVS	3.352	Br[Pt](Br)(Br)(Br)(Br)Br
SMILES CANONICAL	OpenEye OEToolkits	1.6.1	Br[Pt](Br)(Br)(Br)(Br)Br
SMILES	OpenEye OEToolkits	1.6.1	Br[Pt](Br)(Br)(Br)(Br)Br
InChI	InChI	1.03	InChI=1S/6BrH.Pt/h6*1H;/q;;;;;;+4/p-6
InChIKey	InChI	1.03	VOEHEFXBCNCSCK-UHFFFAOYSA-H

Identifier: BR
Name: BROMIDE ION
Formula: Br

Type	Program	Version	Descriptor
SMILES	ACDLabs	10.04	[Br-]
SMILES CANONICAL	CACTVS	3.341	[Br-]
SMILES	CACTVS	3.341	[Br-]
SMILES CANONICAL	OpenEye OEToolkits	1.5.0	[Br-]
SMILES	OpenEye OEToolkits	1.5.0	[Br-]
InChI	InChI	1.03	InChI=1S/BrH/h1H/p-1
InChIKey	InChI	1.03	CPELXLSAUQHCOX-UHFFFAOYSA-M

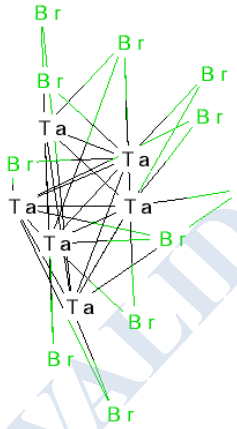
Identifier: CL
Name: CHLORIDE ION
Formula: Cl

Type	Program	Version	Descriptor
SMILES	ACDLabs	10.04	[Cl-]
SMILES CANONICAL	CACTVS	3.341	[Cl-]
SMILES	CACTVS	3.341	[Cl-]
SMILES CANONICAL	OpenEye OEToolkits	1.5.0	[Cl-]
SMILES	OpenEye OEToolkits	1.5.0	[Cl-]
InChI	InChI	1.03	InChI=1S/ClH/h1H/p-1
InChIKey	InChI	1.03	VEXZGXHMUGYJMC-UHFFFAOYSA-M

Identifier: NA
Name: SODIUM ION
Formula: Na

Type	Program	Version	Descriptor
SMILES	ACDLabs	10.04	[Na+]
SMILES CANONICAL	CACTVS	3.341	[Na+]
SMILES	CACTVS	3.341	[Na+]
SMILES CANONICAL	OpenEye OEToolkits	1.5.0	[Na+]
SMILES	OpenEye OEToolkits	1.5.0	[Na+]
InChI	InChI	1.03	InChI=1S/Na/q+1
InChIKey	InChI	1.03	FKNQFGJONOIPTF-UHFFFAOYSA-N

Identifier: TBR
Name: HEXATANTALUM DODECABROMIDE
Synonym: DODECABROMOHEXATANTALUM
Formula: Br12 Ta6



Type	Program	Version	Descriptor
InChI	InChI	1.02	InChI=1S/12BrH.6Ta/h12*1H;;;;;;/q;;;;;;;;;;;; ;;;;;+1/p-1
InChIKey	InChI	1.02	YWYIQTPPCOBSGN-UHFFFAOYSA-M
SMILES CANONICAL	CACTVS	3.370	Br|1[Ta]|2|3|4|5|Br[Ta]|6|7|89%10|2| Br[Ta]|%11|%12|%13|%14|1|3|6Br|[Ta]|%15| %16|%17|7|%11(Br|[Ta]|%18|4|%12|%15(Br|% 13)(Br|%14)|Br[Ta]|5|8|%16|%18(|Br9)(Br) Br|%17)|Br%10
SMILES	CACTVS	3.370	Br|1[Ta]|2|3|4|5|Br[Ta]|6|7|89%10|2| Br[Ta]|%11|%12|%13|%14|1|3|6Br|[Ta]|%15| %16|%17|7|%11(Br|[Ta]|%18|4|%12|%15(Br|% 13)(Br|%14)|Br[Ta]|5|8|%16|%18(|Br9)(Br) Br|%17)|Br%10
SMILES CANONICAL	OpenEye OEToolkits	1.7.0	Br[Ta]123456Br[Ta]17891%10[Ta]22%11(Br7) [Ta]337%12%13([Ta]484([Ta]923(Br%11) (Br1)(Br4)(Br7)Br%12)(Br5)(Br%10)Br%13) Br6
SMILES	OpenEye OEToolkits	1.7.0	Br[Ta]123456Br[Ta]17891%10[Ta]22%11(Br7) [Ta]337%12%13([Ta]484([Ta]923(Br%11) (Br1)(Br4)(Br7)Br%12)(Br5)(Br%10)Br%13) Br6

Summary of Structure Factor Validation

Structure quality	
Average Occupancy-weighted avg temperature factor	19.781

Resolution	
High Resolution (Author reported)	1.70
High Resolution (Calculated by REFMAC, V5.7.0029)	1.700
Low Resolution (Author reported)	25.02
Low Resolution (Calculated by REFMAC, V5.7.0029)	22.356

Crystal data	
Space group	P 43 21 2
Total number of reflections	12624
Number of reflections used	11933
Completeness of data	98.7

R-factors	
R-factor (Author reported)	0.179
R-factor (Calculated by REFMAC, V5.7.0029)	0.1921
Free R-factor (Author reported)	0.231
Free R-factor (Calculated by REFMAC, V5.7.0029)	0.2386

Wilson statistics (PHENIX, V1.8-1069)	
Wilson B-factor	14.50
Wilson Scale	0.69

Padilla-Yeates statistics for twin detection (PHENIX, V1.8-1069)	
Padilla-Yeates <|L|>	0.506
Padilla-Yeates <L*L>	0.342