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
AUTHORS : J.R.Helliwell

The following geometrical and stereochemical features have been calculated
for your structure.

CLOSE CONTACTS

==> Close contacts in same asymmetric unit. Distances smaller than 2.2
    Angstroms are considered as close contacts.

Chain	Atom	Res	Seq		Chain	Atom	Res	Seq		Symm_Code				Distance
A	TA3	TBR	201	-	A	BR	BR	207	(	1,	5,	5,	5)	Dist = 2.01
A	OD2	ASP	18	-	A	TA4	TBR	201	(	1,	5,	5,	5)	Dist = 2.03

==> Close contacts based on crystal symmetry. Distances smaller than 2.2
    Angstroms are considered as close contacts.

      none

BOND DISTANCES AND ANGLES

    Bond and angle checks are performed by first computing the average rms
    error for all bonds and angles relative to standard values for nucleotide
    units [L. Clowney et al., Geometric Parameters in Nucleic Acids: Nitrogenous
    Bases, J.Am.Chem.Soc. 1996, 118, 509-518; A. Gelbin et al., Geometric
    Parameters in Nucleic Acids: Sugar and Phosphate Constituents, J.Am.Chem.Soc.
    1996, 118, 519-529] and amino acid units [R.A. Engh and R. Huber, Structure
    quality and target parameters, International Tables for Crystallography,
    Volume F, 2001, 382-392]. Any bond or angle which deviates from the
    dictionary values by more than six times this computed rms error is
    identified as an outlier.

==> Covalent Bond Lengths:

    The overall RMS deviation for covalent bonds relative to the standard
    dictionary is   0.019 Angstroms

    All covalent bonds lie within a 6.0*RMSD range about the
    standard dictionary values.

==> Covalent Angle Values:

    The overall RMS deviation for covalent angles relative to the standard
    dictionary is   1.9 degrees.

    The following table contains a list of the covalent bond angles
    greater than 6 times standard deviation.

Deviation	Residue Name	Chain ID	Sequence Number	AT1	-	AT2	-	AT3	Bond Angle	Dictionary Value	Standard Deviation
6.4	ASP	A	18	CB	-	CG	-	OD1	124.7	118.3	0.9

    1 out of total 1379 bond angles (0.073%) have greater than 6 times
    standard deviation.

TORSION ANGLES

The torsion angle distributions have been checked. To view these reports, please refer to the ADIT Validation Server at http://deposit.pdb.org/validate.

==> The following table contains a list of torsion angles outside the expected Ramachandran regions [GJ. Kleywegt and TA. Jones, PHI/PSI-chology: Ramachandran Revisited, Structure 1996, 4, 1395 - 1400].

Residue	Chain	Sequence	PSI	PHI
ASN	A	19	18.06	58.67

CHIRALITY

The chirality has been checked. O1P, O2P, and hydrogen atoms which do not follow the convention defined in the IUBMB (Liebecq, C. Compendium of Biochemical Nomenclature and Related Documents, 2nd ed.; Portland Press: London and Chapel Hill, 1992) and IUPAC nomenclature (J.L. Markley, A. Bax, Y. Arata, C.W. Hilbers, R. Kaptein, B.D. Sykes, P.E. Wright and K. Wuthrich, Recommendations for the Presentation of NMR Structures of Proteins and Nucleic Acids, Pure & Appl. Chem., Vol. 70, pp. 117-142, 1998) have been standardized. Any other stereochemical violations are listed below.

none

SOLVENT

The following solvent molecules are further than 3.5 Angstroms away from macromolecule atoms in the asymmetric unit that are available for hydrogen bonding. Solvent molecules in extended hydration shells separated by 3.5 Angstroms or less are not listed.

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HETATM 1125  O   HOH A 363      98.584  61.382  23.240  1.00 26.36      DIST =   3.63 A
HETATM 1141  O   HOH A 379     101.054  57.505  25.705  1.00 14.78      DIST =   4.33 A
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We have replaced the coordinates for solvent molecules which could be translated back into the asymmetric unit. Please review all solvent molecules in your file and contact us if you have any serious objections.

MISSING ATOMS

==> The following residues have missing atoms:

RES	MOD#C	SEQ	ATOMS
TBR(	A	202)	TA4 TA5 BR1 BR3 BR6 BR7 BR8 BR9 BRA BRB
6BP(	A	203)	BR4
6BP(	A	204)	BR4 BR5