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TITLE : The crystal structure of rat angiogenin−heparin complex
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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
B	O	HOH	341	− B	O	HOH	404	(1, 5, 5, 5)	Dist = 2.04
B	O	HOH	353	− B	O	HOH	411	(1, 5, 5, 5)	Dist = 2.08
B	O	HOH	357	− B	O	HOH	405	(1, 5, 5, 5)	Dist = 2.09
B	O	HOH	377	− B	O	HOH	379	(1, 5, 5, 5)	Dist = 2.10
B	OE1	GLN	72	− B	O	HOH	357	(1, 5, 5, 5)	Dist = 2.10
A	O	HOH	379	− A	O	HOH	390	(1, 5, 5, 5)	Dist = 2.10
A	O	HOH	330	− A	O	HOH	365	(1, 5, 5, 5)	Dist = 2.12
B	O	HOH	349	− B	O	HOH	382	(1, 5, 5, 5)	Dist = 2.13
A	OE1	GLU	41	− A	O	HOH	370	(1, 5, 5, 5)	Dist = 2.13
B	O	HOH	347	− B	O	HOH	368	(1, 5, 5, 5)	Dist = 2.13
A	O	HOH	371	− A	O	HOH	372	(1, 5, 5, 5)	Dist = 2.13
A	O	GLY	84	− A	O	HOH	385	(1, 5, 5, 5)	Dist = 2.13
B	O	HOH	318	− B	O	HOH	332	(1, 5, 5, 5)	Dist = 2.14
A	O	HOH	323	− A	O	HOH	410	(1, 5, 5, 5)	Dist = 2.16
A	O	HOH	394	− A	O	HOH	411	(1, 5, 5, 5)	Dist = 2.16
B	O	HOH	362	− B	O	HOH	385	(1, 5, 5, 5)	Dist = 2.16
A	O	HOH	331	− A	O	HOH	369	(1, 5, 5, 5)	Dist = 2.18
B	O	HOH	347	− B	O	HOH	371	(1, 5, 5, 5)	Dist = 2.18

==> 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 0.009 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 1.1 degrees.

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

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
GLU	A	66	−76.35	−75.03
PRO	A	87	47.47	−85.02
PRO	A	89	150.22	−48.55
PRO	B	87	48.41	−73.96
PHE	B	118	152.76	−49.28

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 1938  O   HOH A 394      −6.903  15.800   3.781  1.00 42.59      DIST =   3.93 A
HETATM 1943  O   HOH A 399     −15.629 −14.469  −0.653  1.00 39.28      DIST =   4.57 A
HETATM 1949  O   HOH A 405     −15.800 −13.963  −2.793  1.00 36.99      DIST =   4.84 A
HETATM 1955  O   HOH A 411      −5.003  15.629   2.773  1.00 29.85      DIST =   5.83 A
HETATM 2015  O   HOH B 353     −34.108   5.276  33.320  1.00 40.97      DIST =   5.73 A
HETATM 2073  O   HOH B 411     −36.038   6.027  33.525  1.00 31.39      DIST =   7.10 A
```

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 RESIDUES

==> The following residues are missing:
(Note: The SEQ number starts from 1 for each chain according to SEQRES sequence record.)

RES	MOD	#C	SEQ
GLY(		A	−4)
SER(		A	−3)
HIS(		A	−2)
MET(		A	−1)
ALA(		A	0)
GLN(		A	1)
ASP(		A	2)
ILE(		A	119)

```
  SER(    A 120 )
  LEU(    A 121 )
  GLY(    B  -4 )
  SER(    B  -3 )
  HIS(    B  -2 )
  MET(    B  -1 )
  ALA(    B   0 )
  GLN(    B   1 )
  ASP(    B   2 )
  SER(    B 120 )
  LEU(    B 121 )


PDB Chain_ID: A

        1                                                       15
SEQRES: GLY SER HIS MET ALA GLN ASP ASP PRO ARG TYR THR LYS PHE LEU
COORDS:   ?   ?   ?   ?   ?   ?   ? ASP PRO ARG TYR THR LYS PHE LEU
                                    3                           10

        16                                                      30
SEQRES: THR GLN HIS TYR ASP ALA LYS PRO LYS GLY ARG ASP ALA ARG TYR
COORDS: THR GLN HIS TYR ASP ALA LYS PRO LYS GLY ARG ASP ALA ARG TYR
        11                                                      25

        31                                                      45
SEQRES: CYS GLU SER MET MET ARG ARG ARG GLY LEU THR SER PRO CYS LYS
COORDS: CYS GLU SER MET MET ARG ARG ARG GLY LEU THR SER PRO CYS LYS
        26                                                      40

        46                                                      60
SEQRES: GLU VAL ASN THR PHE ILE HIS GLY ASN LYS GLY SER ILE LYS ALA
COORDS: GLU VAL ASN THR PHE ILE HIS GLY ASN LYS GLY SER ILE LYS ALA
        41                                                      55

        61                                                      75
SEQRES: ILE CYS GLY ALA ASN GLY SER PRO TYR GLY GLU ASN LEU ARG ILE
COORDS: ILE CYS GLY ALA ASN GLY SER PRO TYR GLY GLU ASN LEU ARG ILE
        56                                                      70

        76                                                      90
SEQRES: SER GLN SER PRO PHE GLN ILE THR THR CYS LYS HIS THR GLY GLY
COORDS: SER GLN SER PRO PHE GLN ILE THR THR CYS LYS HIS THR GLY GLY
        71                                                      85

        91                                                     105
SEQRES: SER PRO ARG PRO PRO CYS ARG TYR ARG ALA SER ALA GLY PHE ARG
COORDS: SER PRO ARG PRO PRO CYS ARG TYR ARG ALA SER ALA GLY PHE ARG
        86                                                     100

        106                                                    120
SEQRES: HIS VAL VAL ILE ALA CYS GLU ASN GLY LEU PRO VAL HIS PHE ASP
COORDS: HIS VAL VAL ILE ALA CYS GLU ASN GLY LEU PRO VAL HIS PHE ASP
        101                                                    115

        121                 126
SEQRES: GLU SER PHE ILE SER LEU
COORDS: GLU SER PHE   ?   ?   ?
        116     118


PDB Chain_ID: B

        1                                                       15
SEQRES: GLY SER HIS MET ALA GLN ASP ASP PRO ARG TYR THR LYS PHE LEU
COORDS:   ?   ?   ?   ?   ?   ?   ? ASP PRO ARG TYR THR LYS PHE LEU
                                    3                           10

        16                                                      30
SEQRES: THR GLN HIS TYR ASP ALA LYS PRO LYS GLY ARG ASP ALA ARG TYR
COORDS: THR GLN HIS TYR ASP ALA LYS PRO LYS GLY ARG ASP ALA ARG TYR
        11                                                      25

        31                                                      45
SEQRES: CYS GLU SER MET MET ARG ARG ARG GLY LEU THR SER PRO CYS LYS
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COORDS: CYS GLU SER MET MET ARG ARG ARG GLY LEU THR SER PRO CYS LYS
        26                                                      40

        46                                                      60
SEQRES: GLU VAL ASN THR PHE ILE HIS GLY ASN LYS GLY SER ILE LYS ALA
COORDS: GLU VAL ASN THR PHE ILE HIS GLY ASN LYS GLY SER ILE LYS ALA
        41                                                      55

        61                                                      75
SEQRES: ILE CYS GLY ALA ASN GLY SER PRO TYR GLY GLU ASN LEU ARG ILE
COORDS: ILE CYS GLY ALA ASN GLY SER PRO TYR GLY GLU ASN LEU ARG ILE
        56                                                      70

        76                                                      90
SEQRES: SER GLN SER PRO PHE GLN ILE THR THR CYS LYS HIS THR GLY GLY
COORDS: SER GLN SER PRO PHE GLN ILE THR THR CYS LYS HIS THR GLY GLY
        71                                                      85

        91                                                     105
SEQRES: SER PRO ARG PRO PRO CYS ARG TYR ARG ALA SER ALA GLY PHE ARG
COORDS: SER PRO ARG PRO PRO CYS ARG TYR ARG ALA SER ALA GLY PHE ARG
        86                                                     100

        106                                                    120
SEQRES: HIS VAL VAL ILE ALA CYS GLU ASN GLY LEU PRO VAL HIS PHE ASP
COORDS: HIS VAL VAL ILE ALA CYS GLU ASN GLY LEU PRO VAL HIS PHE ASP
        101                                                    115

        121                 126
SEQRES: GLU SER PHE ILE SER LEU
COORDS: GLU SER PHE ILE   ?   ?
        116         119
```