New guidelines for deposition of nucleic acid structures

Joel L Sussman and Helen M Berman: From January 1, 1996, data for crystal structures of oligonucleotides should be deposited directly with the Nucleic Acid Database (NDB). Once the data are processed they will be forwarded to the Protein Data Bank (PDB) for deposit in the central single archive. This will simplify current procedures and make the data on nucleic acids available more quickly. Protein–nucleic acid complexes and all NMR structures should continue to be deposited at the PDB. All crystal structure data for DNA and RNA will continue to be available from both the NDB and the PDB.

To deposit the data, submit the coordinates, structure factors and current PDB deposition form to:

deposit@ndbserver.rutgers.edu.

A preprint of the related manuscript should be mailed or faxed to:

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CORRIGENDUM

2 Å crystal structure of an extracellular fragment of human CD40 ligand

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In the sequence alignment of TNF-like domains (Fig. 4), the correspondence of some residues was not entirely optimal because not enough weight was assigned to structural considerations (such as Cα–Cα distance homology). The following alignment takes into account structural homology more than sequence homology.

```
              ---A--                    -A"-    -B'-   --B-
      116      125       135        145       155
TNFα:  RTPSDKPVAHVVANPQAEGQ  LQWLNRRANALLANG VELRD NQLVVP
LTα:     TLKPAAHLIGDPSKQNS  LLWRANTDRAFLQDG FSLSN NSLLVP
CD40L: GDQNPQIAAHVISEASSKTTSVLQWAEKG YYTMSNNLVTLENGKQLTVK
(1)                *  ** *       ********
(2)    .......-..-.--.+...+....-..--.-.........-.........


  -----C-------             ----D----       -----E--
165       175           185       195        205
SEGLYLIYSQVLFKGQGCP    STHVLLTHTISRIAVSYQTKVNLLSAIKSPCQR
TSGIYFVYSQVVFSGKAYSPKATSSPLYLAHEVQLFSSQYPFHVPLLSSQKMVY
RQGLYYIYAQVTFCSNREA    SSQAPFIASLCLKSPG RFERILLRAANTHS S
             ***        ** *          ***** *     * *
..............+.........................++........-....


         -----F--------    --G---                ---H---
215              225       235       245        255
ETPEGAEAKPWYEPIYLGGVFQLEKGDRLSAEINRPDYLLFAESGQVYFGIIAL
  PGLQE  PWLHSMYHGAAFQLTQGDQLSTHTDGIPHLVLSP STVFFGAFAL
AKP      CGQQSIHLGGVFELQPGASVFVNVTDPSQVSHGT GFTSFGLLKL
     *   * *                      * *  ***** *
.................-.......-....+..+..................
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Fig. 4. Sequence alignment of the TNF-like domains of TNFα, LTα and CD40L based on structural considerations. The secondary structure assignment and numbering at the top of the figure correspond to CD40L. Asterisks in line 1 indicate residues of the LTα sequence that are involved in contacts with the TNF receptor. In line 2, CD40L residues for which mutations affect CD40 binding are indicated with a minus (–) sign, while those at which mutations have a minimal effect or no effect on CD40 binding are indicated by a plus (+) sign.