

RESI E2B -1.00

GROUP

ATOM N NH1 -0.47 ! |

ATOM HN H 0.31 ! HN-N

ATOM CA CT1 0.07 ! | HB1 HG1 OE1

ATOM HA HB 0.09 ! | | | //

GROUP ! HA-CA--CB--CG--CD

ATOM CB CT2 -0.18 ! | | | \

ATOM HB1 HA 0.09 ! | HB2 HG2 OE2(-)

ATOM HB2 HA 0.09 ! O=C

GROUP ! |

ATOM CGA CT2 -0.28

ATOM HG1A HA 0.09

ATOM HG2A HA 0.09

ATOM CDA CC 0.62

ATOM OE1A OC -0.76

ATOM OE2A OC -0.76

GROUP ! via acetic acid, use in a patch statement

ATOM CGB CT2 -0.21 !

ATOM HG1B HA 0.09 ! HG1 OE1

ATOM HG2B HA 0.09 ! | //

ATOM CDB CD 0.75 ! -CG--CD

ATOM OE1B OB -0.55 ! | \

ATOM OE2B OH1 -0.61 ! HG2 OE2-HE2

ATOM HE2B H 0.44 !

GROUP

ATOM C C 0.51

ATOM O O -0.51

BOND CB CA CGA CB CDA CGA OE2A CDA

BOND CB CA CGB CB CDB CGB OE2B CDB

BOND N HN N CA C CA

BOND C +N CA HA CB HB1 CB HB2 CGA HG1A

BOND C +N CA HA CB HB1 CB HB2 CGB HG1B

BOND CGA HG2A

BOND CGB HG2B

BOND OE2B HE2B

ANGLE HE2B OE2B CDB

DIHE HE2B OE2B CDB OE1B HE2B OE2B CDB CGB

DOUBLE O C CDA OE1A

DOUBLE O C CDB OE1B

IMPR N -C CA HN C CA +N O

!IMPR OE1A CGA OE2A CDA

!IMPR OE1B CGB OE2B CDB

IMPR CDA CGA OE2A OE1A

IMPR CDB CGB OE2B OE1B

DONOR HN N

DONOR HE2B OE2B

ACCEPTOR OE1A CDA

ACCEPTOR OE1B CDB

ACCEPTOR OE2A CDA

ACCEPTOR O C

IC -C CA *N HN 1.3471 124.4500 180.0000 113.9900 0.9961

IC -C N CA C 1.3471 124.4500 180.0000 107.2700 1.5216

IC N CA C +N 1.4512 107.2700 180.0000 117.2500 1.3501

IC +N CA *C O 1.3501 117.2500 180.0000 121.0700 1.2306
IC CA C +N +CA 1.5216 117.2500 180.0000 124.3000 1.4530
IC N C *CA CB 1.4512 107.2700 121.9000 111.7100 1.5516
IC N C *CA HA 1.4512 107.2700 -118.0600 107.2600 1.0828
IC N CA CB CGA 1.4512 111.0400 180.0000 115.6900 1.5557
IC N CA CB CGB 1.4512 111.0400 180.0000 115.6900 1.5557
IC CGA CA *CB HB1 1.5557 115.6900 121.2200 108.1600 1.1145
IC CGB CA *CB HB1 1.5557 115.6900 121.2200 108.1600 1.1145
IC CGA CA *CB HB2 1.5557 115.6900 -123.6500 109.8100 1.1131
IC CGB CA *CB HB2 1.5557 115.6900 -123.6500 109.8100 1.1131
IC CA CB CGA CDA 1.5516 115.6900 180.0000 115.7300 1.5307
IC CA CB CGB CDB 1.5516 115.6900 180.0000 115.7300 1.5307
IC CDA CB *CGA HG1A 1.5307 115.7300 117.3800 109.5000 1.1053
IC CDB CB *CGB HG1B 1.5307 115.7300 117.3800 109.5000 1.1053
IC CDA CB *CGA HG2A 1.5307 115.7300 -121.9600 111.0000 1.1081
IC CDB CB *CGB HG2B 1.5307 115.7300 -121.9600 111.0000 1.1081
IC CB CGA CDA OE1A 1.5557 115.7300 180.0000 114.9900 1.2590
IC CB CGB CDB OE1B 1.5557 115.7300 180.0000 114.9900 1.2590
IC OE1A CGA *CDA OE2A 1.2590 114.9900 -179.1000 120.0800 1.2532
IC OE1B CGB *CDB OE2B 1.2590 114.9900 -179.1000 120.0800 1.2532
IC HE2B OE2B CDB OE1B 0.0000 0.0000 0.0000 0.0000 0.0000