

REFERENCES - S.W. PROVENCHER (1982) COMPUT. PHYS. COMMUN., VOL. 27, PAGES 213-227, 229-242.
 (1984) EMBL TECHNICAL REPORT DA07 (EUROPEAN MOLECULAR BIOLOGY
 LABORATORY, HEIDELBERG, F.R. OF GERMANY)

INPUT DATA FOR CHANGES TO COMMON VARIABLES

```
IFORMY      0      0.00000E+00
(7F9.0)

LAST         0      1.00000E+00

IWT          0      5.00000E+00

IUSER        14      3.10000E+01

IUSER        15     -1.00000E+00

RUSER        14      1.00000E+00

RUSER        15      3.00000E-02

RUSER        16      5.00000E+02

END           0      0.00000E+00
NSTEND       51      2.40000E+02      1.90000E+02
```

FINAL VALUES OF CONTROL VARIABLES

```
DFMIN  = 3.00000E+00
SRMIN  = 1.00000E-02
ALPST  = 0.00000E+00 0.00000E+00
GMNMX  = 1.00000E+00 1.60000E+01
PLEVEL = 5.00000E-01 5.00000E-01 5.00000E-01 5.00000E-01
RSVMNX = 1.00000E+00 1.00000E+00 0.00000E+00 0.00000E+00
RUSER  = 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 1.00000E+00 3.00000E-02 5.00000E+02
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
IGRID  = 1
IQUAD  = 1
IUNIT  = -1
IWT     = 5
LINEPG = 60
MIOERR = 5
MPKMOM = 0
MQPITR = 35
NEQ     = 0
NERFIT  = 0
NG      = 16
NINTT   = 1
NLINF   = 0
```

[illegible]

Widy-oPOE.txt
OPRECIS = 1.49E-15 SRANGE = 1.00E+35 RANGE = 1.00E+35

GRID POINT	MIN IN MATRIX A	AT T =	MAX IN MATRIX A	AT T =	SCALE FACTOR
1.0000E+00	-2.4876E+04	2.22E+02	5.5079E+04	1.92E+02	2.078E-06
2.0000E+00	-1.3387E+04	2.08E+02	1.7434E+04	1.92E+02	2.078E-06
3.0000E+00	-1.1109E+04	2.11E+02	1.6667E+04	0.00E+00	2.078E-06
4.0000E+00	-1.2593E+04	2.09E+02	1.6667E+04	0.00E+00	2.078E-06
5.0000E+00	-1.3227E+04	2.22E+02	2.4142E+04	1.93E+02	2.078E-06
6.0000E+00	-9.7762E+03	2.03E+02	1.6667E+04	0.00E+00	2.078E-06
7.0000E+00	-6.6914E+03	2.24E+02	1.6667E+04	0.00E+00	2.078E-06
8.0000E+00	-1.2254E+04	2.23E+02	1.6667E+04	0.00E+00	2.078E-06
9.0000E+00	-1.2473E+04	1.99E+02	1.6667E+04	0.00E+00	2.078E-06
1.0000E+01	-1.1208E+04	2.09E+02	1.6667E+04	0.00E+00	2.078E-06
1.1000E+01	-1.3714E+04	2.09E+02	2.5943E+04	1.96E+02	2.078E-06
1.2000E+01	-1.4514E+04	2.22E+02	1.9732E+04	1.95E+02	2.078E-06
1.3000E+01	-9.9252E+03	2.12E+02	1.6667E+04	0.00E+00	2.078E-06
1.4000E+01	-1.8628E+04	2.03E+02	1.6667E+04	0.00E+00	2.078E-06
1.5000E+01	-1.4012E+04	2.10E+02	2.8231E+04	1.92E+02	2.078E-06
1.6000E+01	-1.1083E+04	2.11E+02	1.6667E+04	0.00E+00	2.078E-06

OSCALE FACTOR FOR ALPHA = 7.700E+06

0 UNREGULARIZED VARIABLES

SINGULAR VALUES

4.036E-02	1.461E-02	6.268E-03	3.163E-03	1.902E-03	1.817E-03	1.383E-03
5.122E-04	4.872E-04	3.099E-04				
2.796E-04	1.190E-04	8.184E-05	6.539E-05	2.937E-05	2.580E-05	

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TEST DATA SET 1 - FOR CD PACKAGE
PRELIMINARY UNWEIGHTED ANALYSIS

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM
PROB1 TO REJECT	PROB2 TO REJECT				
* 6.01E-17	1.49E-15	1.09006E+06	1.09006E+06	1.740E+02	16.000
0.000	1.000				

FRACTION	HELIX	BETA-SHEET	REMAINDER	SCALE FACTOR
	0.09	0.67	0.24	0.999
STANDARD ERROR	4.5E-02	4.4E-02	7.7E-02	
0 (FOR ALPHA/S(1) = 1.49E-15)	PRUNS = 0.7619		PUNCOR = 0.0770	0.0002 0.0127 0.3671
0.0103				

TEST DATA SET 1 - FOR CD PACKAGE
PRELIMINARY UNWEIGHTED ANALYSIS

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM
PROB1 TO REJECT	PROB2 TO REJECT				
* 4.41E-14	1.09E-12	1.09006E+06	1.09006E+06	1.740E+02	16.000
0.000	1.000				

FRACTION	HELIX	BETA-SHEET	REMAINDER	SCALE FACTOR
	0.09	0.67	0.24	0.999
STANDARD ERROR	4.5E-02	4.4E-02	7.7E-02	
0 (FOR ALPHA/S(1) = 1.09E-12)	PRUNS = 0.7619		PUNCOR = 0.0770	0.0002 0.0127 0.3671
0.0103				

TEST DATA SET 1 - FOR CD PACKAGE
PRELIMINARY UNWEIGHTED ANALYSIS

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM
PROB1 TO REJECT	PROB2 TO REJECT				
* 3.23E-11	8.02E-10	1.09006E+06	1.09006E+06	1.740E+02	16.000
0.000	1.000				

FRACTION	HELIX	BETA-SHEET	REMAINDER	SCALE FACTOR
	0.09	0.67	0.24	0.999
STANDARD ERROR	4.5E-02	4.4E-02	7.7E-02	

0 (FOR ALPHA/S(1) = 8.02E-10) PRUNS = 0.7619 PUNCOR = 0.0770 0.0002 0.0127 0.3671
0.0103

TEST DATA SET 1 - FOR CD PACKAGE
PRELIMINARY UNWEIGHTED ANALYSIS

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM
PROB1 TO REJECT	PROB2 TO REJECT				
2.37E-08	5.88E-07	1.09006E+06	1.09006E+06	1.740E+02	16.000
0.000	1.000				

FRACTION	HELIX	BETA-SHEET	REMAINDER	SCALE FACTOR
	0.09	0.67	0.24	0.999
STANDARD ERROR	4.5E-02	4.4E-02	7.7E-02	

0 (FOR ALPHA/S(1) = 5.88E-07) PRUNS = 0.7619 PUNCOR = 0.0770 0.0002 0.0127 0.3671
0.0103

TEST DATA SET 1 - FOR CD PACKAGE
PRELIMINARY UNWEIGHTED ANALYSIS

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM
PROB1 TO REJECT	PROB2 TO REJECT				
1.74E-05	4.31E-04	1.25607E+06	1.11035E+06	1.739E+02	15.288
0.000	0.694				

FRACTION	HELIX	BETA-SHEET	REMAINDER	SCALE FACTOR
	0.10	0.68	0.22	0.999
STANDARD ERROR	3.7E-02	3.6E-02	6.4E-02	

0 (FOR ALPHA/S(1) = 4.31E-04) PRUNS = 0.5598 PUNCOR = 0.2030 0.0005 0.0336 0.3862
0.0034

TEST DATA SET 1 - FOR CD PACKAGE
PRELIMINARY UNWEIGHTED ANALYSIS

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM
PROB1 TO REJECT	PROB2 TO REJECT				
1.28E-02	3.16E-01	2.66881E+08	1.24425E+08	1.574E+03	1.786
1.000	1.000				

FRACTION	HELIX	BETA-SHEET	REMAINDER	SCALE FACTOR
	0.27	0.29	0.44	0.569
STANDARD ERROR	1.3E-02	1.1E-02	1.7E-02	

0 (FOR ALPHA/S(1) = 3.16E-01) PRUNS = -1.0000 PUNCOR = 0.0000 0.0004 0.0005 0.0030
0.3683

TEST DATA SET 1 - FOR CD PACKAGE
PRELIMINARY UNWEIGHTED ANALYSIS

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM
PROB1 TO REJECT	PROB2 TO REJECT				
4.47E-05	1.11E-03	1.82837E+06	1.31197E+06	1.854E+02	13.818
0.048	0.958				

FRACTION	HELIX	BETA-SHEET	REMAINDER	SCALE FACTOR
	0.11	0.67	0.23	0.997
STANDARD ERROR	2.4E-02	2.6E-02	4.5E-02	

0 (FOR ALPHA/S(1) = 1.11E-03) PRUNS = 0.1854 PUNCOR = 0.8350 0.0068 0.3893 0.6244
0.0008

TEST DATA SET 1 - FOR CD PACKAGE
PRELIMINARY UNWEIGHTED ANALYSIS

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM
PROB1 TO REJECT	PROB2 TO REJECT				
1.15E-04	2.84E-03	3.45961E+06	2.11532E+06	2.295E+02	11.832
0.969	1.000				
	HELIX	BETA-SHEET	REMAINDER		SCALE FACTOR
FRACTION	0.08	0.61	0.31		0.991
STANDARD ERROR	1.4E-02	2.0E-02	2.5E-02		
0 (FOR ALPHA/S(1) = 2.84E-03) PRUNS = 0.0055			PUNCOR =	0.0523	0.1009 0.5092 0.8426
0.0015					

TEST DATA SET 1 - FOR CD PACKAGE
PRELIMINARY UNWEIGHTED ANALYSIS

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM
PROB1 TO REJECT	PROB2 TO REJECT				
2.94E-04	7.29E-03	8.06379E+06	3.99736E+06	3.073E+02	9.659
1.000	1.000				
	HELIX	BETA-SHEET	REMAINDER		SCALE FACTOR
FRACTION	0.05	0.58	0.37		0.972
STANDARD ERROR	9.2E-03	2.1E-02	1.8E-02		
0 (FOR ALPHA/S(1) = 7.29E-03) PRUNS = 0.0590			PUNCOR =	0.0029	0.9377 0.8773 0.7843
0.0002					

TEST DATA SET 1 - FOR CD PACKAGE
PRELIMINARY UNWEIGHTED ANALYSIS

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM
PROB1 TO REJECT	PROB2 TO REJECT				
7.55E-04	1.87E-02	2.30797E+07	9.07446E+06	4.507E+02	7.336
1.000	1.000				
	HELIX	BETA-SHEET	REMAINDER		SCALE FACTOR
FRACTION	0.04	0.55	0.41		0.906
STANDARD ERROR	8.5E-03	2.2E-02	1.7E-02		
0 (FOR ALPHA/S(1) = 1.87E-02) PRUNS = 0.0095			PUNCOR =	0.0065	0.1880 0.2021 0.3313
0.0062					

TEST DATA SET 1 - FOR CD PACKAGE
PRELIMINARY UNWEIGHTED ANALYSIS

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM
PROB1 TO REJECT	PROB2 TO REJECT				
1.94E-03	4.80E-02	6.61764E+07	3.65367E+07	8.826E+02	5.094
1.000	1.000				
	HELIX	BETA-SHEET	REMAINDER		SCALE FACTOR
FRACTION	0.11	0.47	0.43		0.719
STANDARD ERROR	1.2E-02	2.9E-02	2.7E-02		
0 (FOR ALPHA/S(1) = 4.80E-02) PRUNS = -1.0000			PUNCOR =	0.0231	0.0166 0.0008 0.0004
0.9751					

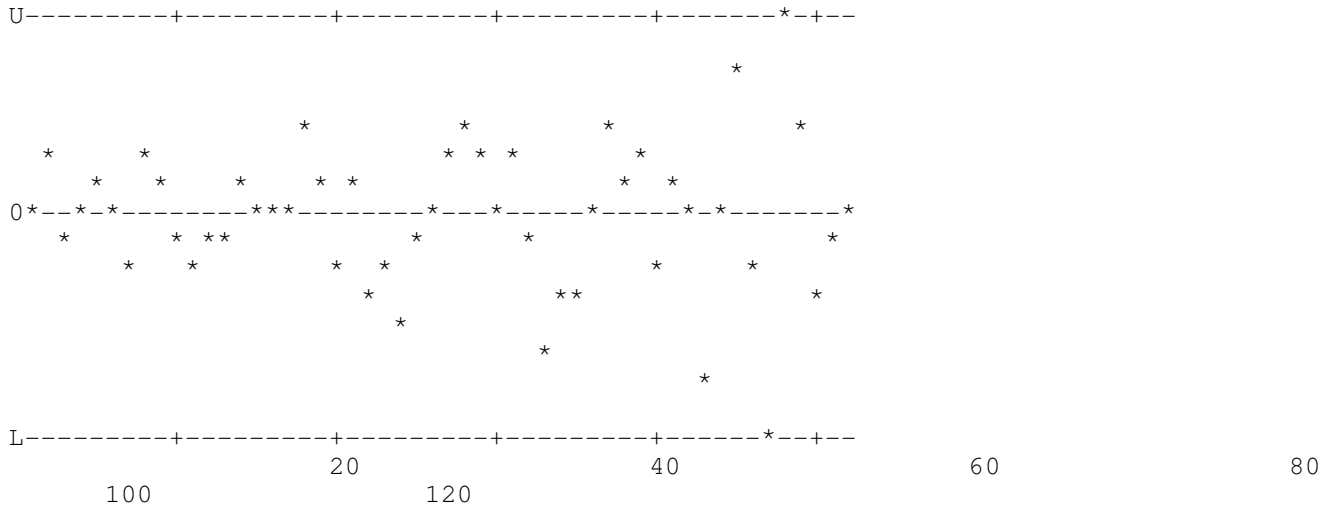
TEST DATA SET 1 - FOR CD PACKAGE
PRELIMINARY UNWEIGHTED ANALYSIS

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM
PROB1 TO REJECT	PROB2 TO REJECT				
4.97E-03	1.23E-01	1.25233E+08	8.80614E+07	1.342E+03	3.128
1.000	1.000				
	HELIX	BETA-SHEET	REMAINDER		SCALE FACTOR
FRACTION	0.22	0.34	0.44		0.558
STANDARD ERROR	1.4E-02	2.2E-02	2.9E-02		

0(FOR ALPHA/S(1) = 1.23E-01) PRUNS =-1.0000 PUNCOR = 0.0003 0.0011 0.0002 0.0008
0.6419

1CONTIN 2DP (MAR 84) (CD-1) TEST DATA SET 1 - FOR CD PACKAGE
CHOSEN SOLUTION

WEIGHTED RESIDUALS (ALPHA/S(1)= 1.11E-03) MAX=U= 4.6E+02 MIN=L=-4.8E+02 (PRUNS= 0.1854)
PUNCOR= 0.8350 0.0068 0.3893 0.6244 0.0008



0PLOT OF DATA (O) AND FIT TO DATA (X). ORDINATES LISTED ARE FIT VALUES.

ORDINATE	ABSCISSA	
-4.605E+01	2.40E+02	XO
-6.096E+01	2.39E+02	XO
-1.401E+02	2.38E+02	*
-2.651E+02	2.37E+02	*
-4.138E+02	2.36E+02	*
-5.730E+02	2.35E+02	*
-7.487E+02	2.34E+02	OX
-9.423E+02	2.33E+02	XO
-1.150E+03	2.32E+02	XO
-1.378E+03	2.31E+02	OX
-1.637E+03	2.30E+02	OX
-1.920E+03	2.29E+02	OX
-2.189E+03	2.28E+02	*
-2.460E+03	2.27E+02	XO
-2.696E+03	2.26E+02	*
-2.908E+03	2.25E+02	*
-3.101E+03	2.24E+02	*
-3.235E+03	2.23E+02	X O
-3.357E+03	2.22E+02	XO
-3.480E+03	2.21E+02	OX

-3.558E+03	2.20E+02	XO							
-3.601E+03	2.19E+02	OX							
-3.588E+03	2.18E+02	OX							
-3.549E+03	2.17E+02	O X							
-3.595E+03	2.16E+02	OX							
-3.724E+03	2.15E+02	XO							
-3.858E+03	2.14E+02	X O							
-4.024E+03	2.13E+02	X O							
-4.101E+03	2.12E+02	X O							
-4.089E+03	2.11E+02	*							
-4.054E+03	2.10E+02	XO							
-4.010E+03	2.09E+02	*							
-3.871E+03	2.08E+02	O X							
-3.742E+03	2.07E+02	O X							
-3.567E+03	2.06E+02	O X							
-3.394E+03	2.05E+02	*							
-2.989E+03	2.04E+02	X O							
-2.332E+03	2.03E+02	XO							
-1.442E+03	2.02E+02	XO							
-4.427E+02	2.01E+02	OX							
4.166E+02	2.00E+02	XO							
1.088E+03	1.99E+02	*							
1.995E+03	1.98E+02	O X							
3.048E+03	1.97E+02	XO							
4.025E+03	1.96E+02	X O							
4.914E+03	1.95E+02	OX							
5.565E+03	1.94E+02	O X							
5.869E+03	1.93E+02	X O							
6.093E+03	1.92E+02	X O							
6.055E+03	1.91E+02	O X							
5.682E+03	1.90E+02	OX							
9.970E-01	0.00E+00	*							

RMS RESIDUAL FOR PTS. 1 TO 31 = 1.03E+02
RMS RESIDUAL FOR REMAINING PTS. = 2.21E+02

ERRFIT = 0.00E+00

SQUARE ROOTS OF LEAST SQUARES WEIGHTS

Widy-oPOE.txt

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9.6692E-03 9.6692E-03 9.6692E-03 9.6692E-03 9.6692E-03 9.6692E-03 9.6692E-03
9.6692E-03 9.6692E-03 9.6692E-03
9.6692E-03 9.6692E-03 9.6692E-03 9.6692E-03 9.6692E-03 9.6692E-03 9.6692E-03
9.6692E-03 9.6692E-03 9.6692E-03
9.6692E-03 9.6692E-03 9.6692E-03 9.6692E-03 9.6692E-03 9.6692E-03 9.6692E-03
9.6692E-03 9.6692E-03 9.6692E-03
9.6692E-03 4.5225E-03 4.5225E-03 4.5225E-03 4.5225E-03 4.5225E-03 4.5225E-03
4.5225E-03 4.5225E-03 4.5225E-03
4.5225E-03 4.5225E-03 4.5225E-03 4.5225E-03 4.5225E-03 4.5225E-03 4.5225E-03
4.5225E-03 4.5225E-03 4.5225E-03
4.5225E-03 3.3333E+01

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GRID POINT      MIN IN MATRIX A      AT T =      MAX IN MATRIX A      AT T =      SCALE FACTOR
1.0000E+00      -2.4053E+02  2.22E+02      2.4909E+02  1.92E+02      2.958E-04
2.0000E+00      -1.2449E+02  2.10E+02      7.8843E+01  1.92E+02      2.958E-04
3.0000E+00      -1.0741E+02  2.11E+02      3.3333E+01  0.00E+00      2.958E-04
4.0000E+00      -1.2171E+02  2.10E+02      6.6936E+01  1.90E+02      2.958E-04
5.0000E+00      -1.2789E+02  2.22E+02      1.0918E+02  1.93E+02      2.958E-04
6.0000E+00      -7.0295E+01  2.10E+02      3.3333E+01  0.00E+00      2.958E-04
7.0000E+00      -6.4701E+01  2.24E+02      5.4248E+01  1.97E+02      2.958E-04
8.0000E+00      -1.1848E+02  2.23E+02      5.8613E+01  1.96E+02      2.958E-04
9.0000E+00      -6.9503E+01  2.10E+02      3.3333E+01  0.00E+00      2.958E-04
1.0000E+01      -1.0708E+02  2.10E+02      5.6035E+01  1.90E+02      2.958E-04
1.1000E+01      -1.3127E+02  2.10E+02      1.1733E+02  1.96E+02      2.958E-04
1.2000E+01      -1.4034E+02  2.22E+02      8.9235E+01  1.95E+02      2.958E-04
1.3000E+01      -9.5969E+01  2.12E+02      6.6382E+01  1.98E+02      2.958E-04
1.4000E+01      -1.2146E+02  2.10E+02      3.3333E+01  0.00E+00      2.958E-04
1.5000E+01      -1.3548E+02  2.10E+02      1.2767E+02  1.92E+02      2.958E-04
1.6000E+01      -1.0717E+02  2.11E+02      3.3333E+01  0.00E+00      2.958E-04
OSCALE FACTOR FOR ALPHA = 5.409E+04

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0 UNREGULARIZED VARIABLES

SINGULAR VALUES

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4.130E-02 1.018E-02 4.116E-03 3.097E-03 1.954E-03 1.507E-03 7.028E-04
5.202E-04 4.293E-04 2.744E-04
2.246E-04 1.180E-04 7.509E-05 4.513E-05 3.248E-05 2.414E-05

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1

TEST DATA SET 1 - FOR CD PACKAGE

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ALPHA      ALPHA/S(1)      OBJ. FCTN.      VARIANCE      STD. DEV.      DEG FREEDOM
PROB1 TO REJECT      PROB2 TO REJECT
* 6.15E-17      1.49E-15      3.66052E+01      3.66052E+01      1.008E+00      16.000
0.000      1.000

ORDINATE      ERROR      ABSCISSA
1.026E+00      2.1E-01      1.00E+00
.....X.....
-2.561E-01      2.4E-01      2.00E+00      .....X.....
6.680E-01      5.2E-01      3.00E+00
.....X.....
-4.400E-01      8.5E-02      4.00E+00      ..X...
-1.422E+00      4.8E-01      5.00E+00X.....
4.343E-01      1.4E-01      6.00E+00      ....X....
7.491E-01      1.4E-01      7.00E+00
.....X.....
3.895E-01      1.5E-01      8.00E+00      .....X....
1.866E+00      1.9E-01      9.00E+00      .....X
-1.406E+00      3.6E-01      1.00E+01X.....
-3.643E-01      7.6E-02      1.10E+01      ...X..
3.460E-01      1.4E-01      1.20E+01      ....X.....
8.212E-02      1.2E-01      1.30E+01      ...X....

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-1.666E-01  1.3E-01  1.40E+01          ....X....
 3.764E-01  1.6E-01  1.50E+01          .....X.....
-8.879E-01  5.3E-01  1.60E+01.....X.....

```

	HELIX	BETA-SHEET	REMAINDER	SCALE FACTOR			
FRACTION	0.08	0.66	0.26	0.995			
STANDARD ERROR	4.1E-02	4.7E-02	7.4E-02				
0 (FOR ALPHA/S(1) = 1.49E-15) PRUNS = 0.7727				PUNCOR =	0.1428	0.0014	0.2139 0.4502
0.0716							

TEST DATA SET 1 - FOR CD PACKAGE

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM
PROB1 TO REJECT	PROB2 TO REJECT				
* 4.51E-14	1.09E-12	3.66052E+01	3.66052E+01	1.008E+00	16.000
0.000	1.000				

ORDINATE	ERROR	ABSCISSA	
1.026E+00	2.1E-01	1.00E+00	
.....X.....			
-2.561E-01	2.4E-01	2.00E+00	X.....
6.680E-01	5.2E-01	3.00E+00	
.....X.....			
-4.400E-01	8.5E-02	4.00E+00	..X...
-1.422E+00	4.8E-01	5.00E+00	X.....
4.343E-01	1.4E-01	6.00E+00	X.....
7.491E-01	1.4E-01	7.00E+00	
.....X.....			
3.895E-01	1.5E-01	8.00E+00	X.....
1.866E+00	1.9E-01	9.00E+00	
.....X			
-1.406E+00	3.6E-01	1.00E+01	X.....
-3.643E-01	7.6E-02	1.10E+01	...X..
3.460E-01	1.4E-01	1.20E+01	X.....
8.212E-02	1.2E-01	1.30E+01	...X....
-1.666E-01	1.3E-01	1.40E+01	X.....
3.764E-01	1.6E-01	1.50E+01	X.....
-8.879E-01	5.3E-01	1.60E+01	X.....

	HELIX	BETA-SHEET	REMAINDER	SCALE FACTOR			
FRACTION	0.08	0.66	0.26	0.995			
STANDARD ERROR	4.1E-02	4.7E-02	7.4E-02				
0 (FOR ALPHA/S(1) = 1.09E-12) PRUNS = 0.7727				PUNCOR =	0.1428	0.0014	0.2139 0.4502
0.0716							

TEST DATA SET 1 - FOR CD PACKAGE

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM
PROB1 TO REJECT	PROB2 TO REJECT				
* 3.31E-11	8.02E-10	3.66052E+01	3.66052E+01	1.008E+00	16.000
0.000	1.000				

ORDINATE	ERROR	ABSCISSA	
1.026E+00	2.1E-01	1.00E+00	
.....X.....			
-2.561E-01	2.4E-01	2.00E+00	X.....
6.680E-01	5.2E-01	3.00E+00	
.....X.....			
-4.400E-01	8.5E-02	4.00E+00	..X...
-1.422E+00	4.8E-01	5.00E+00	X.....
4.343E-01	1.4E-01	6.00E+00	X....
7.491E-01	1.4E-01	7.00E+00	
.....X.....			
3.895E-01	1.5E-01	8.00E+00	X....
1.866E+00	1.9E-01	9.00E+00	
.....X.....			
-1.406E+00	3.6E-01	1.00E+01	X.....
-3.643E-01	7.6E-02	1.10E+01	...X..
3.460E-01	1.4E-01	1.20E+01	X....
8.212E-02	1.2E-01	1.30E+01	...X....
-1.666E-01	1.3E-01	1.40E+01	X....
3.764E-01	1.6E-01	1.50E+01	X....
-8.879E-01	5.3E-01	1.60E+01	X.....

FRACTION	HELIX	BETA-SHEET	REMAINDER	SCALE FACTOR
	0.08	0.66	0.26	0.995
STANDARD ERROR	4.1E-02	4.7E-02	7.4E-02	
0(FOR ALPHA/S(1) = 8.02E-10)	PRUNS = 0.7727	PUNCOR = 0.1428	0.0014	0.2139 0.4502
0.0716				

TEST DATA SET 1 - FOR CD PACKAGE

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM
PROB1 TO REJECT	PROB2 TO REJECT				
* 2.43E-08	5.88E-07	3.66053E+01	3.66052E+01	1.008E+00	16.000
0.000	1.000				

ORDINATE	ERROR	ABSCISSA	
1.026E+00	2.1E-01	1.00E+00	
.....X.....			
-2.561E-01	2.4E-01	2.00E+00	X.....
6.680E-01	5.2E-01	3.00E+00	
.....X.....			
-4.400E-01	8.5E-02	4.00E+00	..X...
-1.422E+00	4.8E-01	5.00E+00	X.....
4.343E-01	1.4E-01	6.00E+00	X....
7.491E-01	1.4E-01	7.00E+00	
.....X.....			
3.895E-01	1.5E-01	8.00E+00	X....
1.866E+00	1.9E-01	9.00E+00	
.....X.....			
-1.406E+00	3.6E-01	1.00E+01	X.....
-3.643E-01	7.6E-02	1.10E+01	...X..

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3.460E-01  1.4E-01  1.20E+01          ....X.....
8.212E-02  1.2E-01  1.30E+01          ...X....
-1.666E-01  1.3E-01  1.40E+01          ....X....
3.764E-01  1.6E-01  1.50E+01          .....X.....
-8.879E-01  5.3E-01  1.60E+01.....X.....

```

	HELIX	BETA-SHEET	REMAINDER	SCALE FACTOR			
FRACTION	0.08	0.66	0.26	0.995			
STANDARD ERROR	4.1E-02	4.7E-02	7.4E-02				
0 (FOR ALPHA/S(1) = 5.88E-07) PRUNS = 0.7727 PUNCOR = 0.1429 0.0014 0.2139 0.4502							
0.0716							

TEST DATA SET 1 - FOR CD PACKAGE

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM
PROB1 TO REJECT	PROB2 TO REJECT				
1.78E-05	4.31E-04	4.51068E+01	3.80763E+01	1.017E+00	15.192
0.000	0.813				
ORDINATE	ERROR	ABSCISSA			
8.141E-01	1.7E-01	1.00E+00			
.....X.....					
-7.659E-02	2.0E-01	2.00E+00		X.....	
4.069E-01	3.4E-01	3.00E+00			
.....X.....					
-3.895E-01	7.1E-02	4.00E+00	...X..		
-1.077E+00	3.8E-01	5.00E+00	X.....		
3.318E-01	1.1E-01	6.00E+00			X....
6.630E-01	1.1E-01	7.00E+00			
...X....					
3.806E-01	1.3E-01	8.00E+00			X....
1.670E+00	1.6E-01	9.00E+00	X		
-1.205E+00	3.1E-01	1.00E+01	X.....		
-3.004E-01	6.7E-02	1.10E+01		..X..	
2.199E-01	1.1E-01	1.20E+01			X....
-3.319E-02	9.5E-02	1.30E+01		...X....	
-2.219E-01	1.2E-01	1.40E+01		X....	
3.226E-01	1.5E-01	1.50E+01			X.....
-5.168E-01	3.5E-01	1.60E+01	X.....		

	HELIX	BETA-SHEET	REMAINDER	SCALE FACTOR			
FRACTION	0.08	0.66	0.26	0.989			
STANDARD ERROR	3.5E-02	4.1E-02	6.4E-02				
0 (FOR ALPHA/S(1) = 4.31E-04) PRUNS = 0.5598 PUNCOR = 0.3632 0.0049 0.3407 0.5021							
0.0142							

TEST DATA SET 1 - FOR CD PACKAGE

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM
PROB1 TO REJECT	PROB2 TO REJECT				

1.31E-02	3.16E-01	1.19287E+04	2.54701E+03	7.100E+00	1.472
1.000	1.000				

ORDINATE	ERROR	ABSCISSA			
-2.160E-03	2.7E-03	1.00E+00X.....			
3.012E-02	1.1E-03	2.00E+00			
..X..					
3.642E-02	1.6E-03	3.00E+00			
....X....					
2.414E-02	2.2E-03	4.00E+00		X.....	
2.498E-02	1.1E-03	5.00E+00		..X..	
4.397E-02	1.6E-03	6.00E+00			
4.729E-02	1.7E-03	7.00E+00			
....X....					
2.702E-02	1.3E-03	8.00E+00		X....	
4.943E-02	2.1E-03	9.00E+00			
2.984E-02	1.0E-03	1.00E+01	X		
..X.					
2.907E-02	1.5E-03	1.10E+01			
...X...					
1.681E-02	1.6E-03	1.20E+01		X....	
3.485E-02	1.7E-03	1.30E+01			
....X....					
3.243E-02	2.8E-03	1.40E+01			
.....X.....					
2.551E-02	1.3E-03	1.50E+01		..X...	
3.605E-02	1.6E-03	1.60E+01			
....X....					

FRACTION	HELIX	BETA-SHEET	REMAINDER	SCALE FACTOR
	0.27	0.29	0.44	0.486
STANDARD ERROR	9.4E-03	7.0E-03	1.1E-02	
0 (FOR ALPHA/S(1) = 3.16E-01)	PRUNS = -1.0000	PUNCOR =	0.0000	0.0000 0.0000 0.0000 0.0000
0.0023				

TEST DATA SET 1 - FOR CD PACKAGE

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM
PROB1 TO REJECT	PROB2 TO REJECT				
4.57E-05	1.11E-03	6.86016E+01	4.98373E+01	1.139E+00	13.555
0.337	0.994				

ORDINATE	ERROR	ABSCISSA		
3.694E-01	9.7E-02	1.00E+00		X.....
1.988E-01	1.5E-01	2.00E+00		X.....
1.755E-01	1.4E-01	3.00E+00		X.....
-2.890E-01	5.8E-02	4.00E+00	...X...	
-4.332E-01	1.9E-01	5.00E+00	X.....	
1.690E-01	8.5E-02	6.00E+00		X.....
4.800E-01	6.8E-02	7.00E+00		
...X....				
3.021E-01	9.7E-02	8.00E+00		X.....
1.233E+00	1.2E-01	9.00E+00		
-6.979E-01	2.0E-01	1.00E+01X.....	X	

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-1.621E-01  5.8E-02  1.10E+01          ...X...
  1.260E-02  7.9E-02  1.20E+01          ....X....
-2.487E-01  6.3E-02  1.30E+01          ...X...
-3.452E-01  9.8E-02  1.40E+01        .....X.....
  2.837E-01  1.3E-01  1.50E+01          .....X.....
-7.827E-02  1.4E-01  1.60E+01        .....X.....

```

	HELIX	BETA-SHEET	REMAINDER	SCALE FACTOR			
FRACTION	0.07	0.63	0.30				0.970
STANDARD ERROR	2.3E-02	3.4E-02	4.5E-02				
0(FOR ALPHA/S(1) = 1.11E-03) PRUNS = 0.1730			PUNCOR =	0.5192	0.0607	0.9145	0.9857
0.0008							

TEST DATA SET 1 - FOR CD PACKAGE

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM
PROB1 TO REJECT	PROB2 TO REJECT				
1.17E-04	2.84E-03	1.25390E+02	7.86924E+01	1.394E+00	11.509
0.991	1.000				

ORDINATE	ERROR	ABSCISSA	
2.041E-02	4.3E-02	1.00E+00	X....
2.867E-01	7.6E-02	2.00E+00	
.....X.....			
1.390E-01	4.3E-02	3.00E+00	X....
-1.638E-01	4.7E-02	4.00E+00	X.....
-6.371E-02	5.4E-02	5.00E+00	X.....
8.861E-02	5.8E-02	6.00E+00	X.....
3.666E-01	4.1E-02	7.00E+00	
....X....			
1.305E-01	6.3E-02	8.00E+00	X.....
7.240E-01	7.6E-02	9.00E+00	
		X	
-2.189E-01	7.4E-02	1.00E+01	X.....
8.923E-03	4.9E-02	1.10E+01	X....
-1.422E-01	5.2E-02	1.20E+01	X.....
-3.307E-01	4.3E-02	1.30E+01	X....
-3.263E-01	6.6E-02	1.40E+01	X.....
3.277E-01	7.9E-02	1.50E+01	
.....X.....			
6.791E-02	4.2E-02	1.60E+01	X....

	HELIX	BETA-SHEET	REMAINDER	SCALE FACTOR			
FRACTION	0.06	0.58	0.36				0.915
STANDARD ERROR	1.3E-02	3.3E-02	2.9E-02				
0(FOR ALPHA/S(1) = 2.84E-03) PRUNS = 0.1637			PUNCOR =	0.1216	0.3579	0.6599	0.8271
0.0001							

TEST DATA SET 1 - FOR CD PACKAGE

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM
PROB1 TO REJECT	PROB2 TO REJECT				
3.01E-04	7.29E-03	2.66412E+02	1.58732E+02	1.926E+00	9.230
1.000	1.000				

ORDINATE	ERROR	ABSCISSA	
-2.517E-02	2.1E-02	1.00E+00	X....
1.622E-01	3.5E-02	2.00E+00	X.....
1.217E-01	2.0E-02	3.00E+00	X.....
-1.014E-01	3.5E-02	4.00E+00	X.....
1.518E-02	2.2E-02	5.00E+00	X.....
1.199E-01	4.4E-02	6.00E+00	X.....
2.943E-01	3.4E-02	7.00E+00	X.....
1.813E-02	4.3E-02	8.00E+00	X.....
3.292E-01	4.1E-02	9.00E+00	X.....
-5.113E-02	2.8E-02	1.00E+01	X.....
9.867E-02	4.1E-02	1.10E+01	X.....
-2.197E-01	3.5E-02	1.20E+01	X.....
-1.903E-01	3.0E-02	1.30E+01	X.....
-1.264E-01	3.4E-02	1.40E+01	X.....
2.418E-01	4.2E-02	1.50E+01	X.....
8.151E-02	2.0E-02	1.60E+01	X.....

FRACTION	HELIX	BETA-SHEET	REMAINDER	SCALE FACTOR
STANDARD ERROR	0.06	0.55	0.38	0.768
0(FOR ALPHA/S(1) = 7.29E-03)	PRUNS = 0.0626	PUNCOR = 0.1980	0.9172	0.5711
0.0003			0.5398	

TEST DATA SET 1 - FOR CD PACKAGE

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM
PROB1 TO REJECT	PROB2 TO REJECT				
7.73E-04	1.87E-02	5.45864E+02	3.53090E+02	2.795E+00	6.787
1.000	1.000				

ORDINATE	ERROR	ABSCISSA	
2.783E-02	1.0E-02	1.00E+00	X....
5.828E-02	1.6E-02	2.00E+00	X.....
9.876E-02	1.3E-02	3.00E+00	X.....
-6.463E-02	2.2E-02	4.00E+00	X.....
2.817E-02	1.2E-02	5.00E+00	X.....
8.571E-02	2.4E-02	6.00E+00	X.....
1.461E-01	2.5E-02	7.00E+00	X.....
-2.297E-02	2.1E-02	8.00E+00	X.....

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1.261E-01  1.8E-02  9.00E+00
          .....X.....
5.568E-03  9.7E-03  1.00E+01
                                     ...X....
6.218E-02  2.4E-02  1.10E+01
.....X.....
-1.523E-01  2.2E-02  1.20E+01X.....
-5.856E-02  2.2E-02  1.30E+01
                                     .....X.....
-7.016E-03  1.7E-02  1.40E+01
                                     .....X.....
1.120E-01  1.6E-02  1.50E+01
          .....X.....
8.111E-02  1.3E-02  1.60E+01
          .....X.....

```

	HELIX	BETA-SHEET	REMAINDER	SCALE FACTOR			
FRACTION	0.13	0.50	0.37				
STANDARD ERROR	1.4E-02	4.4E-02	3.4E-02				
0 (FOR ALPHA/S(1) = 1.87E-02) PRUNS = 0.1733				PUNCOR =	0.6202	0.6363	0.0635 0.0123
0.0847							

TEST DATA SET 1 - FOR CD PACKAGE

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM
PROB1 TO REJECT	PROB2 TO REJECT				
1.98E-03	4.80E-02	1.10337E+03	6.24608E+02	3.630E+00	4.599
1.000	1.000				

```

ORDINATE  ERROR  ABSCISSA
3.837E-02  7.9E-03  1.00E+00
          .....X.....
3.081E-02  7.9E-03  2.00E+00
          .....X.....
6.470E-02  9.6E-03  3.00E+00
          .....X.....
-2.081E-02  1.1E-02  4.00E+00
                                     .....X.....
2.158E-02  4.5E-03  5.00E+00
...X....
3.702E-02  8.9E-03  6.00E+00
          .....X.....
4.259E-02  1.1E-02  7.00E+00
          .....X.....
-1.413E-02  8.7E-03  8.00E+00
                                     .....X.....
5.907E-02  5.8E-03  9.00E+00
          .....X.....
1.519E-02  3.3E-03  1.00E+01
...X....
3.676E-02  1.1E-02  1.10E+01
          .....X.....
-6.086E-02  1.1E-02  1.20E+01X.....
-6.592E-03  1.3E-02  1.30E+01
                                     .....X.....
2.292E-02  7.5E-03  1.40E+01
...X....
5.862E-02  6.1E-03  1.50E+01
          .....X.....
5.787E-02  9.5E-03  1.60E+01
          .....X.....

```

	HELIX	BETA-SHEET	REMAINDER	SCALE FACTOR			
FRACTION	0.26	0.38	0.36				
STANDARD ERROR	1.3E-02	2.5E-02	2.9E-02				
0 (FOR ALPHA/S(1) = 4.80E-02) PRUNS = 0.0002				PUNCOR =	0.0071	0.0111	0.0004 0.0001
0.6062							

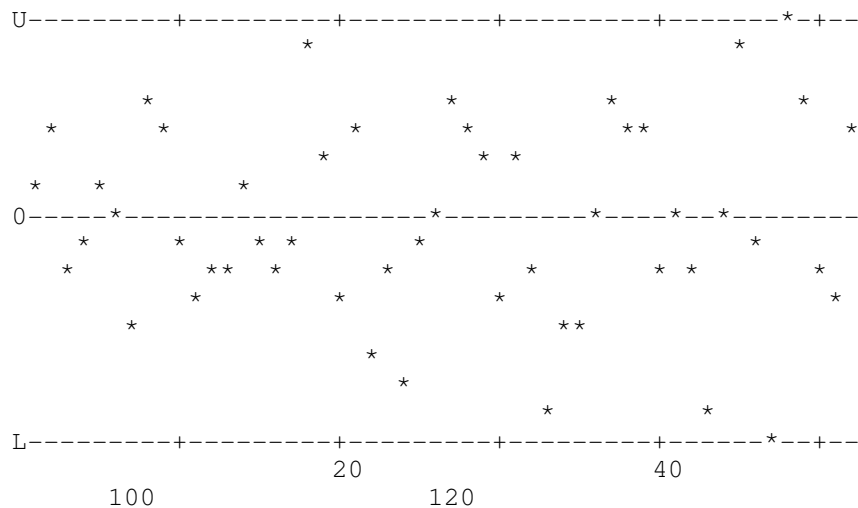
TEST DATA SET 1 - FOR CD PACKAGE

ALPHA PROB1 TO REJECT	ALPHA/S(1) PROB2 TO REJECT	OBJ. FCTN. 3.01445E+03	VARIANCE 1.09215E+03	STD. DEV. 4.707E+00	DEG FREEDOM 2.702
5.09E-03	1.23E-01				
1.000	1.000				
ORDINATE	ERROR	ABSCISSA			
1.422E-02	5.0E-03	1.00E+00		X.....	
2.886E-02	2.9E-03	2.00E+00			
.....X.....					
3.850E-02	4.2E-03	3.00E+00			
	X.....				
6.271E-03	4.9E-03	4.00E+00	X.....		
2.274E-02	1.8E-03	5.00E+00			X...
3.651E-02	3.3E-03	6.00E+00			
	X.....				
3.771E-02	4.8E-03	7.00E+00			
	X.....				
9.832E-03	3.8E-03	8.00E+00		X.....	
4.531E-02	3.2E-03	9.00E+00			
	X				
2.187E-02	1.6E-03	1.00E+01			...X...
3.016E-02	4.2E-03	1.10E+01			
.....X.....					
-7.566E-03	4.4E-03	1.20E+01	X.....		
2.062E-02	5.1E-03	1.30E+01			
.....X.....					
2.502E-02	4.4E-03	1.40E+01			
.....X.....					
3.432E-02	2.4E-03	1.50E+01			
	X.....				
3.645E-02	4.3E-03	1.60E+01			
	X.....				

FRACTION	HELIX	BETA-SHEET	REMAINDER	SCALE FACTOR
	0.28	0.31	0.41	0.401
STANDARD ERROR	9.1E-03	1.3E-02	1.8E-02	
0 (FOR ALPHA/S(1) = 1.23E-01)	PRUNS = 0.0000	PUNCOR = 0.0000	0.0000	0.0000
0.0145				

1CONTIN 2DP (MAR 84) (CD-1) TEST DATA SET 1 - FOR CD PACKAGE
CHOSEN SOLUTION

WEIGHTED RESIDUALS (ALPHA/S(1)= 1.11E-03) MAX=U= 2.2E+00 MIN=L=-2.2E+00 (PRUNS= 0.1730)
PUNCOR= 0.5192 0.0607 0.9145 0.9857 0.0008



OPLOT OF DATA (O) AND FIT TO DATA (X). ORDINATES LISTED ARE FIT VALUES.

ORDINATE	ABSCISSA	
-4.289E+01	2.40E+02	XO
-4.677E+01	2.39E+02	XO
-1.157E+02	2.38E+02	OX
-2.328E+02	2.37E+02	*
-3.772E+02	2.36E+02	*
-5.391E+02	2.35E+02	*
-7.264E+02	2.34E+02	OX
-9.377E+02	2.33E+02	XO
-1.171E+03	2.32E+02	XO
-1.412E+03	2.31E+02	*
-1.667E+03	2.30E+02	OX
-1.934E+03	2.29E+02	OX
-2.178E+03	2.28E+02	*
-2.426E+03	2.27E+02	*
-2.652E+03	2.26E+02	*
-2.867E+03	2.25E+02	*
-3.071E+03	2.24E+02	*
-3.226E+03	2.23E+02	X O
-3.364E+03	2.22E+02	XO
-3.496E+03	2.21E+02	OX
-3.587E+03	2.20E+02	XO
-3.644E+03	2.19E+02	OX
-3.633E+03	2.18E+02	*
-3.589E+03	2.17E+02	O X
-3.611E+03	2.16E+02	*
-3.704E+03	2.15E+02	XO
-3.812E+03	2.14E+02	X O
-3.950E+03	2.13E+02	XO
-4.015E+03	2.12E+02	XO
-4.005E+03	2.11E+02	OX
-3.978E+03	2.10E+02	*
-3.925E+03	2.09E+02	OX
-3.770E+03	2.08E+02	O X

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-3.631E+03  2.07E+02  O  X
-3.470E+03  2.06E+02      O  X
-3.388E+03  2.05E+02      *
-3.047E+03  2.04E+02      X  O
-2.437E+03  2.03E+02      X  O
-1.551E+03  2.02E+02      X  O
-4.806E+02  2.01E+02      OX
 4.874E+02  2.00E+02      *
 1.177E+03  1.99E+02      OX
 2.068E+03  1.98E+02      O  X
 3.048E+03  1.97E+02
XO
 3.972E+03  1.96E+02
X  O
 4.881E+03  1.95E+02
*
 5.568E+03  1.94E+02      O  X
 5.852E+03  1.93E+02      X  O
 6.023E+03  1.92E+02      X  O
 6.000E+03  1.91E+02      OX
 5.780E+03  1.90E+02      O  X
 9.700E-01  0.00E+00      *

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1CONTIN VERSION 2DP (MAR 1984) (CD-1 PACKAGE) ++++++ CHOSEN
 SOLUTION ++++++

TEST DATA SET 1 - FOR CD PACKAGE

ALPHA PROB1 TO REJECT	ALPHA/S(1) PROB2 TO REJECT	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM
4.57E-05	1.11E-03	6.86016E+01	4.98373E+01	1.139E+00	13.555
0.337	0.994				
ORDINATE	ERROR	ABSCISSA			
3.694E-01	9.7E-02	1.00E+00			X.....
1.988E-01	1.5E-01	2.00E+00			X.....
1.755E-01	1.4E-01	3.00E+00			X.....
-2.890E-01	5.8E-02	4.00E+00	...X...		
-4.332E-01	1.9E-01	5.00E+00	X.....		
1.690E-01	8.5E-02	6.00E+00			X.....
4.800E-01	6.8E-02	7.00E+00			
...X.....					
3.021E-01	9.7E-02	8.00E+00			X.....
1.233E+00	1.2E-01	9.00E+00	X		
-6.979E-01	2.0E-01	1.00E+01	X.....		
-1.621E-01	5.8E-02	1.10E+01	...X...		
1.260E-02	7.9E-02	1.20E+01			X.....

-2.487E-01	6.3E-02	1.30E+01	...	X...
-3.452E-01	9.8E-02	1.40E+01		X.....
2.837E-01	1.3E-01	1.50E+01		X.....
-7.827E-02	1.4E-01	1.60E+01		X.....

	HELIX	BETA-SHEET	REMAINDER	SCALE FACTOR
FRACTION	0.07	0.63	0.30	0.970
STANDARD ERROR	2.3E-02	3.4E-02	4.5E-02	