Some output from X-ray file-geometry computing with Seqelf18 (AG-April-2010)

```
> Minimal and maximal distance for atomic interactions  2.70  4.00

                Sigma { VDW } factor  1.000 (Seqelf18)

              Codes for 1M63.pdb (CnA/CnB/hCyPA/CsA complex)

CnA ==== A ****  CnB ==== B **** CyP-A ==== C ***** CsA ==== D

                  This is step * * *   1 * * *

          * * * The PDB coordinates /users/andrzej/musca/cypx/1M63.pdb
          Chain identifier (sequence) >>> |D|
          Number of residues in IDRES(*)    11
          Starting from the index IDRES   1
          Number of effective XYZ-coordinates    84

          * * * The PDB coordinates /users/andrzej/musca/cypx/1M63.pdb
          Chain identifier (sequence) >>> |B|
          Number of residues in IDRES(*)   158
          Starting from the index IDRES  12
          Number of effective XYZ-coordinates  1262

  Number of used coordinates   84 1262

   1   3.86       1-BMT   CE    122-ASN   ND2
   2   3.71       1-BMT   CZ    122-ASN   CB
   3   3.45       1-BMT   CZ    122-ASN   ND2
   4   3.96       1-BMT   CH    122-ASN   CB
   5   4.00       1-BMT   CH    122-ASN   CG
   6   3.10       1-BMT   CH    122-ASN   ND2
   7   3.91       4-MLE   CD1   118-MET   CB
   8   3.78       4-MLE   CD1   119-VAL   N
   9   3.91       4-MLE   CD1   119-VAL   CA
  10   3.88       4-MLE   CD1   119-VAL   CB
  11   3.40       6-MLE   CD1   122-ASN   O
  12   3.90       6-MLE   CD2   123-LEU   CG
  13   3.79       6-MLE   CD2   123-LEU   CD1

   <.......> Number of potential hydrogen bonds    0

              AA-residue-###     Contacts
               BMT-----  1         5
               MLE-----  4         5
               MLE-----  6         4

>>>> Inter-molecular distances  13 Below 4-A  13
>>> Hydrophobic    6 Hydrophilic    0 Mixed    7
>> Main-chain/Main-chain    0 Side-chain/Side-chain    7 Mixed    6

                  This is step * * *   2 * * *

          * * * The PDB coordinates /users/andrzej/musca/cypx/1M63.pdb
          Chain identifier (sequence) >>> |D|
          Number of residues in IDRES(*)    11
          Starting from the index IDRES   1
          Number of effective XYZ-coordinates    84

          * * * The PDB coordinates /users/andrzej/musca/cypx/1M63.pdb
          Chain identifier (sequence) >>> |A|
          Number of residues in IDRES(*)   372
          Starting from the index IDRES   1
```

```
         Number of effective XYZ-coordinates  3013

  Number of used coordinates   84 3013

   1   3.78        2-ABA   O      356-PHE   CE1
   2   3.46        3-SAR   CA     356-PHE   CD1
   3   3.85        3-SAR   CA     356-PHE   CE1
   4   3.94        3-SAR   C      356-PHE   CD1
   5   3.76        4-MLE   CA     352-TRP   NE1
   6   3.80        4-MLE   CB     352-TRP   NE1
   7   3.92        4-MLE   CB     352-TRP   CE2
   8   3.90        4-MLE   CB     352-TRP   CZ2
   9   3.97        4-MLE   CG     356-PHE   CD2
  10   3.99        4-MLE   CD1    352-TRP   CZ2
  11   3.26        4-MLE   CD2    352-TRP   O
  12   3.98        4-MLE   CD2    352-TRP   CD2
  13   3.87        4-MLE   CD2    352-TRP   CE2
  14   3.95        4-MLE   CD2    353-SER   CA
  15   3.91        4-MLE   CD2    356-PHE   CB
  16   3.66        4-MLE   C      352-TRP   NE1
  17   3.60        5-VAL   N      352-TRP   NE1
  18   3.76        5-VAL   C      352-TRP   NE1
  19   3.71        5-VAL   O      344-PRO   CG
  20   3.73        5-VAL   O      344-PRO   CD
  21   3.37        5-VAL   O      352-TRP   CD1
  22   2.84 *      5-VAL   O      352-TRP   NE1
  23   3.92        6-MLE   CA     341-TYR   OH
  24   3.36        6-MLE   CB     341-TYR   OH
  25   3.59        6-MLE   CD2    352-TRP   CZ2
  26   3.90        6-MLE   C      341-TYR   OH
  27   3.67        6-MLE   C      344-PRO   CD
  28   3.68        6-MLE   O      344-PRO   CG
  29   3.70        6-MLE   O      344-PRO   CD
  30   3.86        7-ALA   N      341-TYR   CZ
  31   2.99        7-ALA   N      341-TYR   OH
  32   3.85        7-ALA   N      344-PRO   CD
  33   3.80        7-ALA   CA     341-TYR   OH
  34   3.71        7-ALA   CB     341-TYR   CZ
  35   3.61        7-ALA   CB     341-TYR   OH
  36   3.50        7-ALA   CB     342-TRP   O
  37   3.99        8-DAL   CA     312-LEU   O
  38   3.56        8-DAL   CB     312-LEU   O
  39   3.75        9-MLE   CN     312-LEU   O
  40   3.95        9-MLE   CD1    312-LEU   CD2

   <.......> Number of potential hydrogen bonds    1

              AA-residue-###     Contacts
               ABA-----  2         1
               SAR-----  3         3
               MLE-----  4        13
               VAL-----  5         7
               MLE-----  6         8
               ALA-----  7         8
               DAL-----  8         3
               MLE-----  9         3

>>>> Inter-molecular distances  40 Below 4-A  40
>>> Hydrophobic   15 Hydrophilic    3 Mixed   22
>> Main-chain/Main-chain    1 Side-chain/Side-chain   13 Mixed   26

                  This is step * * *   3 * * *
```

```
        * * * The PDB coordinates /users/andrzej/musca/cypx/1M63.pdb
        Chain identifier (sequence) >>> |D|
        Number of residues in IDRES(*)    11
        Starting from the index IDRES   1
        Number of effective XYZ-coordinates    84

        * * * The PDB coordinates /users/andrzej/musca/cypx/1M63.pdb
        Chain identifier (sequence) >>> |C|
        Number of residues in IDRES(*)   165
        Starting from the index IDRES   1
        Number of effective XYZ-coordinates  1265

Number of used coordinates   84 1265

 1   3.86       1-BMT   CN     55-ARG   CZ
 2   3.65       1-BMT   CN     55-ARG   NH2
 3   3.91       1-BMT   CN     63-GLN   NE2
 4   3.13       1-BMT   CA    102-ASN   O
 5   3.36       1-BMT   C     102-ASN   O
 6   3.67       1-BMT   O      63-GLN   OE1
 7   3.65       1-BMT   O      63-GLN   NE2
 8   3.51       1-BMT   CB    102-ASN   O
 9   3.51       1-BMT   CD1   102-ASN   O
10   3.45       1-BMT   CD1   102-ASN   OD1
11   3.86       2-ABA   N     102-ASN   C
12   2.78 *     2-ABA   N     102-ASN   O
13   3.30       2-ABA   CA     72-GLY   O
14   3.77       2-ABA   CA    102-ASN   O
15   3.20       2-ABA   C      72-GLY   O
16   3.67       2-ABA   O      72-GLY   O
17   3.57       2-ABA   CB     72-GLY   O
18   3.62       2-ABA   CB    102-ASN   O
19   3.93       2-ABA   CB    111-GLN   CD
20   3.34       2-ABA   CB    111-GLN   NE2
21   3.71       2-ABA   CG    101-ALA   C
22   3.66       2-ABA   CG    101-ALA   O
23   3.75       2-ABA   CG    101-ALA   CB
24   3.85       2-ABA   CG    102-ASN   N
25   3.87       2-ABA   CG    102-ASN   C
26   3.41       2-ABA   CG    102-ASN   O
27   3.89       2-ABA   CG    111-GLN   CB
28   3.62       2-ABA   CG    111-GLN   CD
29   3.80       2-ABA   CG    111-GLN   OE1
30   3.49       2-ABA   CG    111-GLN   NE2
31   3.39       3-SAR   N      72-GLY   O
32   3.72       3-SAR   CN     72-GLY   C
33   3.35       3-SAR   CN     72-GLY   O
34   3.80       5-VAL   CG1    55-ARG   NH1
35   3.28       8-DAL   O     148-ARG   NH2
36   3.96       9-MLE   CB    121-TRP   NE1
37   3.49       9-MLE   CD1   148-ARG   NH2
38   3.53       9-MLE   CD2   121-TRP   CZ2
39   3.84       9-MLE   C      60-PHE   CE2
40   3.58       9-MLE   C      60-PHE   CZ
41   3.80       9-MLE   O      60-PHE   CE1
42   3.96       9-MLE   O      60-PHE   CE2
43   3.25       9-MLE   O      60-PHE   CZ
44   3.79       9-MLE   O     121-TRP   CD1
45   3.15 *     9-MLE   O     121-TRP   NE1
46   3.61      10-MLE   CN     55-ARG   NH1
47   3.36      10-MLE   O      55-ARG   CZ
48   2.81      10-MLE   O      55-ARG   NH1
49   3.10 *    10-MLE   O      55-ARG   NH2
```

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  50   3.79       10-MLE   O       60-PHE   CE2
  51   3.70       11-MVA   CN     122-LEU   CD2
  52   3.65       11-MVA   CN     126-HIS   CE1
  53   3.26       11-MVA   CN     126-HIS   NE2
  54   3.92       11-MVA   CA      55-ARG   NH2
  55   3.88       11-MVA   CA      63-GLN   NE2
  56   3.95       11-MVA   CB      63-GLN   NE2
  57   3.86       11-MVA   CB     113-PHE   CD1
  58   3.95       11-MVA   CG1     63-GLN   CD
  59   2.92       11-MVA   CG1     63-GLN   NE2
  60   3.75       11-MVA   CG1    101-ALA   CB
  61   3.89       11-MVA   CG1    113-PHE   CB
  62   3.79       11-MVA   CG1    113-PHE   CG
  63   3.41       11-MVA   CG1    113-PHE   CD1
  64   3.68       11-MVA   CG2     60-PHE   CZ
  65   3.78       11-MVA   CG2    113-PHE   CG
  66   3.86       11-MVA   CG2    113-PHE   CD1
  67   3.89       11-MVA   CG2    113-PHE   CD2
  68   3.98       11-MVA   C       63-GLN   NE2

   <.......> Number of potential hydrogen bonds    3

              AA-residue-###     Contacts
               BMT-----  1         9
               ABA-----  2        21
               SAR-----  3         4
               VAL-----  5         2
               DAL-----  8         2
               MLE-----  9        11
               MLE----- 10         6
               MVA----- 11        19

>>>> Inter-molecular distances  68 Below 4-A  68
>>> Hydrophobic   19 Hydrophilic    9 Mixed   40
>> Main-chain/Main-chain    9 Side-chain/Side-chain   24 Mixed   35

            This is step * * *   4 * * *

          * * * The PDB coordinates /users/andrzej/musca/cypx/1M63.pdb
          Chain identifier (sequence) >>> |C|
          Number of residues in IDRES(*)   165
          Starting from the index IDRES   1
          Number of effective XYZ-coordinates  1265

          * * * The PDB coordinates /users/andrzej/musca/cypx/1M63.pdb
          Chain identifier (sequence) >>> |D|
          Number of residues in IDRES(*)    11
          Starting from the index IDRES   1
          Number of effective XYZ-coordinates    84

  Number of used coordinates 1265   84

   1   3.86       55-ARG   CZ       1-BMT   CN
   2   3.36       55-ARG   CZ      10-MLE   O
   3   3.80       55-ARG   NH1      5-VAL   CG1
   4   3.61       55-ARG   NH1     10-MLE   CN
   5   2.81       55-ARG   NH1     10-MLE   O
   6   3.65       55-ARG   NH2      1-BMT   CN
   7   3.10 *     55-ARG   NH2     10-MLE   O
   8   3.92       55-ARG   NH2     11-MVA   CA
   9   3.80       60-PHE   CE1      9-MLE   O
  10   3.84       60-PHE   CE2      9-MLE   C
  11   3.96       60-PHE   CE2      9-MLE   O
```

12	3.79		60-PHE	CE2	10-MLE	O
13	3.58		60-PHE	CZ	9-MLE	C
14	3.25		60-PHE	CZ	9-MLE	O
15	3.68		60-PHE	CZ	11-MVA	CG2
16	3.95		63-GLN	CD	11-MVA	CG1
17	3.67		63-GLN	OE1	1-BMT	O
18	3.91		63-GLN	NE2	1-BMT	CN
19	3.65		63-GLN	NE2	1-BMT	O
20	3.88		63-GLN	NE2	11-MVA	CA
21	3.95		63-GLN	NE2	11-MVA	CB
22	2.92		63-GLN	NE2	11-MVA	CG1
23	3.98		63-GLN	NE2	11-MVA	C
24	3.72		72-GLY	C	3-SAR	CN
25	3.30		72-GLY	O	2-ABA	CA
26	3.20		72-GLY	O	2-ABA	C
27	3.67		72-GLY	O	2-ABA	O
28	3.57		72-GLY	O	2-ABA	CB
29	3.39		72-GLY	O	3-SAR	N
30	3.35		72-GLY	O	3-SAR	CN
31	3.71		101-ALA	C	2-ABA	CG
32	3.66		101-ALA	O	2-ABA	CG
33	3.75		101-ALA	CB	2-ABA	CG
34	3.75		101-ALA	CB	11-MVA	CG1
35	3.85		102-ASN	N	2-ABA	CG
36	3.86		102-ASN	C	2-ABA	N
37	3.87		102-ASN	C	2-ABA	CG
38	3.13		102-ASN	O	1-BMT	CA
39	3.36		102-ASN	O	1-BMT	C
40	3.51		102-ASN	O	1-BMT	CB
41	3.51		102-ASN	O	1-BMT	CD1
42	2.78	*	102-ASN	O	2-ABA	N
43	3.77		102-ASN	O	2-ABA	CA
44	3.62		102-ASN	O	2-ABA	CB
45	3.41		102-ASN	O	2-ABA	CG
46	3.45		102-ASN	OD1	1-BMT	CD1
47	3.89		111-GLN	CB	2-ABA	CG
48	3.93		111-GLN	CD	2-ABA	CB
49	3.62		111-GLN	CD	2-ABA	CG
50	3.80		111-GLN	OE1	2-ABA	CG
51	3.34		111-GLN	NE2	2-ABA	CB
52	3.49		111-GLN	NE2	2-ABA	CG
53	3.89		113-PHE	CB	11-MVA	CG1
54	3.79		113-PHE	CG	11-MVA	CG1
55	3.78		113-PHE	CG	11-MVA	CG2
56	3.86		113-PHE	CD1	11-MVA	CB
57	3.41		113-PHE	CD1	11-MVA	CG1
58	3.86		113-PHE	CD1	11-MVA	CG2
59	3.89		113-PHE	CD2	11-MVA	CG2
60	3.79		121-TRP	CD1	9-MLE	O
61	3.96		121-TRP	NE1	9-MLE	CB
62	3.15	*	121-TRP	NE1	9-MLE	O
63	3.53		121-TRP	CZ2	9-MLE	CD2
64	3.70		122-LEU	CD2	11-MVA	CN
65	3.65		126-HIS	CE1	11-MVA	CN
66	3.26		126-HIS	NE2	11-MVA	CN
67	3.28		148-ARG	NH2	8-DAL	O
68	3.49		148-ARG	NH2	9-MLE	CD1

<.......> Number of potential hydrogen bonds 3

AA-residue-###	Contacts
ARG----- 55	7
PHE----- 60	8

```
                GLN----- 63         9
                GLY----- 72         8
                ALA-----101         5
                ASN-----102        13
                GLN-----111         7
                PHE-----113         8
                TRP-----121         5
                LEU-----122         2
                HIS-----126         3
                ARG-----148         3

>>>> Inter-molecular distances  68 Below 4-A  68
>>> Hydrophobic   19 Hydrophilic    9 Mixed   40
>> Main-chain/Main-chain    9 Side-chain/Side-chain   24 Mixed   35

                  This is step * * *   5 * * *

          * * * The PDB coordinates /users/andrzej/musca/cypx/1M63.pdb
          Chain identifier (sequence) >>> |A|
          Number of residues in IDRES(*)   372
          Starting from the index IDRES   1
          Number of effective XYZ-coordinates  3013

          * * * The PDB coordinates /users/andrzej/musca/cypx/1M63.pdb
          Chain identifier (sequence) >>> |D|
          Number of residues in IDRES(*)    11
          Starting from the index IDRES   1
          Number of effective XYZ-coordinates    84

  Number of used coordinates 3013   84

   1   3.99      312-LEU   O       8-DAL   CA
   2   3.56      312-LEU   O       8-DAL   CB
   3   3.75      312-LEU   O       9-MLE   CN
   4   3.95      312-LEU   CD2     9-MLE   CD1
   5   3.86      341-TYR   CZ      7-ALA   N
   6   3.71      341-TYR   CZ      7-ALA   CB
   7   3.92      341-TYR   OH      6-MLE   CA
   8   3.36      341-TYR   OH      6-MLE   CB
   9   3.90      341-TYR   OH      6-MLE   C
  10   2.99      341-TYR   OH      7-ALA   N
  11   3.80      341-TYR   OH      7-ALA   CA
  12   3.61      341-TYR   OH      7-ALA   CB
  13   3.50      342-TRP   O       7-ALA   CB
  14   3.71      344-PRO   CG      5-VAL   O
  15   3.68      344-PRO   CG      6-MLE   O
  16   3.73      344-PRO   CD      5-VAL   O
  17   3.67      344-PRO   CD      6-MLE   C
  18   3.70      344-PRO   CD      6-MLE   O
  19   3.85      344-PRO   CD      7-ALA   N
  20   3.26      352-TRP   O       4-MLE   CD2
  21   3.37      352-TRP   CD1     5-VAL   O
  22   3.98      352-TRP   CD2     4-MLE   CD2
  23   3.76      352-TRP   NE1     4-MLE   CA
  24   3.80      352-TRP   NE1     4-MLE   CB
  25   3.66      352-TRP   NE1     4-MLE   C
  26   3.60      352-TRP   NE1     5-VAL   N
  27   3.76      352-TRP   NE1     5-VAL   C
  28   2.84 *    352-TRP   NE1     5-VAL   O
  29   3.92      352-TRP   CE2     4-MLE   CB
  30   3.87      352-TRP   CE2     4-MLE   CD2
  31   3.90      352-TRP   CZ2     4-MLE   CB
  32   3.99      352-TRP   CZ2     4-MLE   CD1
```

```
  33   3.59     352-TRP   CZ2     6-MLE   CD2
  34   3.95     353-SER   CA      4-MLE   CD2
  35   3.91     356-PHE   CB      4-MLE   CD2
  36   3.46     356-PHE   CD1     3-SAR   CA
  37   3.94     356-PHE   CD1     3-SAR   C
  38   3.97     356-PHE   CD2     4-MLE   CG
  39   3.78     356-PHE   CE1     2-ABA   O
  40   3.85     356-PHE   CE1     3-SAR   CA

   <.......> Number of potential hydrogen bonds    1

              AA-residue-###     Contacts
               LEU-----312         3
               TYR-----341         9
               TRP-----342         2
               PRO-----344         7
               TRP-----352        15
               SER-----353         2
               PHE-----356         7

>>>> Inter-molecular distances  40 Below 4-A  40
>>> Hydrophobic   15 Hydrophilic    3 Mixed   22
>> Main-chain/Main-chain    1 Side-chain/Side-chain   13 Mixed   26

                This is step * * *   7 * * *

> Minimal and maximal distance for atomic interactions  2.70  4.00

                    Sigma { VDW } factor     1.000


          * * * The PDB coordinates /users/andrzej/musca/cypx/1M63.pdb
          Chain identifier (sequence) >>> |B|
          Number of residues in IDRES(*)   158
          Starting from the index IDRES  12
          Number of effective XYZ-coordinates  1262

          * * * The PDB coordinates /users/andrzej/musca/cypx/1M63.pdb
          Chain identifier (sequence) >>> |D|
          Number of residues in IDRES(*)    11
          Starting from the index IDRES   1
          Number of effective XYZ-coordinates    84

  Number of used coordinates 1262   84

   1   3.91     118-MET   CB      4-MLE   CD1
   2   3.78     119-VAL   N       4-MLE   CD1
   3   3.91     119-VAL   CA      4-MLE   CD1
   4   3.88     119-VAL   CB      4-MLE   CD1
   5   3.40     122-ASN   O       6-MLE   CD1
   6   3.71     122-ASN   CB      1-BMT   CZ
   7   3.96     122-ASN   CB      1-BMT   CH
   8   4.00     122-ASN   CG      1-BMT   CH
   9   3.86     122-ASN   ND2     1-BMT   CE
  10   3.45     122-ASN   ND2     1-BMT   CZ
  11   3.10     122-ASN   ND2     1-BMT   CH
  12   3.90     123-LEU   CG      6-MLE   CD2
  13   3.79     123-LEU   CD1     6-MLE   CD2

   <.......> Number of potential hydrogen bonds    0

              AA-residue-###     Contacts
               MET-----118         1
```

```
                VAL-----119         3
                ASN-----122         8
                LEU-----123         3

>>>> Inter-molecular distances  13 Below 4-A  13
>>> Hydrophobic    6 Hydrophilic    0 Mixed    7
>> Main-chain/Main-chain    0 Side-chain/Side-chain    7 Mixed    6

                  This is step * * *   8 * * *

          * * * The PDB coordinates /users/andrzej/musca/cypx/1M63.pdb
          Chain identifier (sequence) >>> |A|
          Number of residues in IDRES(*)   372
          Starting from the index IDRES   1
          Number of effective XYZ-coordinates  3013

          * * * The PDB coordinates /users/andrzej/musca/cypx/1M63.pdb
          Chain identifier (sequence) >>> |C|
          Number of residues in IDRES(*)   165
          Starting from the index IDRES   1
          Number of effective XYZ-coordinates  1265

  Number of used coordinates 3013 1265

   1   3.82     159-TYR   O     148-ARG   CB
   2   3.93     159-TYR   CE1   148-ARG   CB
   3   3.91     159-TYR   CZ    147-SER   C
   4   3.66     159-TYR   CZ    148-ARG   N
   5   3.87     159-TYR   OH     58-PRO   CG
   6   3.64     159-TYR   OH     58-PRO   CD
   7   3.56     159-TYR   OH    147-SER   CA
   8   3.25     159-TYR   OH    147-SER   C
   9   3.62     159-TYR   OH    147-SER   O
  10   3.40     159-TYR   OH    148-ARG   N
  11   4.00     159-TYR   OH    148-ARG   CA
  12   3.99     160-PHE   CD1   148-ARG   CD
  13   3.85     314-VAL   CG1   121-TRP   CG
  14   3.55     314-VAL   CG1   121-TRP   CD2
  15   3.75     314-VAL   CG1   121-TRP   CE2
  16   3.85     314-VAL   CG1   121-TRP   CE3
  17   3.45     314-VAL   CG2   121-TRP   CB
  18   3.45     314-VAL   CG2   121-TRP   CG
  19   3.70     314-VAL   CG2   121-TRP   CD1
  20   3.88     315-TYR   CE1   121-TRP   CZ3
  21   3.82     315-TYR   CE1   121-TRP   CH2
  22   3.68     355-PRO   C      73-THR   CG2
  23   3.53     355-PRO   O      73-THR   CG2
  24   3.87     355-PRO   CB     73-THR   CG2
  25   3.97     356-PHE   N      73-THR   CG2
  26   3.73     359-GLU   CG     73-THR   O
  27   3.02     359-GLU   OE2    69-ARG   CG
  28   3.79     359-GLU   OE2    69-ARG   CD
  29   3.41     359-GLU   OE2    69-ARG   NE
  30   3.90     362-THR   CB     69-ARG   NH1
  31   3.31     362-THR   CG2    69-ARG   NH1

   <.......> Number of potential hydrogen bonds    0

              AA-residue-###     Contacts
               TYR-----159        10
               PHE-----160         2
               VAL-----314         8
               TYR-----315         3
```

```
                PRO-----355         4
                PHE-----356         2
                GLU-----359         5
                THR-----362         3

>>>> Inter-molecular distances  31 Below 4-A  31
>>> Hydrophobic   14 Hydrophilic    3 Mixed   14
>> Main-chain/Main-chain    0 Side-chain/Side-chain   19 Mixed   12

                  This is step * * *   9 * * *

          * * * The PDB coordinates /users/andrzej/musca/cypx/1M63.pdb
          Chain identifier (sequence) >>> |C|
          Number of residues in IDRES(*)   165
          Starting from the index IDRES   1
          Number of effective XYZ-coordinates  1265

          * * * The PDB coordinates /users/andrzej/musca/cypx/1M63.pdb
          Chain identifier (sequence) >>> |A|
          Number of residues in IDRES(*)   372
          Starting from the index IDRES   1
          Number of effective XYZ-coordinates  3013

  Number of used coordinates 1265 3013

   1   3.87      58-PRO   CG    159-TYR   OH
   2   3.64      58-PRO   CD    159-TYR   OH
   3   3.02      69-ARG   CG    359-GLU   OE2
   4   3.79      69-ARG   CD    359-GLU   OE2
   5   3.41      69-ARG   NE    359-GLU   OE2
   6   3.90      69-ARG   NH1   362-THR   CB
   7   3.31      69-ARG   NH1   362-THR   CG2
   8   3.73      73-THR   O     359-GLU   CG
   9   3.68      73-THR   CG2   355-PRO   C
  10   3.53      73-THR   CG2   355-PRO   O
  11   3.87      73-THR   CG2   355-PRO   CB
  12   3.97      73-THR   CG2   356-PHE   N
  13   3.45     121-TRP   CB    314-VAL   CG2
  14   3.85     121-TRP   CG    314-VAL   CG1
  15   3.45     121-TRP   CG    314-VAL   CG2
  16   3.70     121-TRP   CD1   314-VAL   CG2
  17   3.55     121-TRP   CD2   314-VAL   CG1
  18   3.75     121-TRP   CE2   314-VAL   CG1
  19   3.85     121-TRP   CE3   314-VAL   CG1
  20   3.88     121-TRP   CZ3   315-TYR   CE1
  21   3.82     121-TRP   CH2   315-TYR   CE1
  22   3.56     147-SER   CA    159-TYR   OH
  23   3.91     147-SER   C     159-TYR   CZ
  24   3.25     147-SER   C     159-TYR   OH
  25   3.62     147-SER   O     159-TYR   OH
  26   3.66     148-ARG   N     159-TYR   CZ
  27   3.40     148-ARG   N     159-TYR   OH
  28   4.00     148-ARG   CA    159-TYR   OH
  29   3.82     148-ARG   CB    159-TYR   O
  30   3.93     148-ARG   CB    159-TYR   CE1
  31   3.99     148-ARG   CD    160-PHE   CD1

   <.......> Number of potential hydrogen bonds    0

              AA-residue-###     Contacts
               PRO----- 58         1
               ARG----- 69         6
               THR----- 73         6
```

```
                TRP-----121        10
                SER-----147         5
                ARG-----148         7

>>>> Inter-molecular distances  31 Below 4-A  31
>>> Hydrophobic   14 Hydrophilic    3 Mixed   14
>> Main-chain/Main-chain    0 Side-chain/Side-chain   19 Mixed   12

             This is step * * *   10 * * *

          * * * The PDB coordinates file-name /users/andrzej/musca/cypx/1M63.pdb
          Chain identifier (sequence) >>> |C|
          Number of residues in IDRES(*)   165
          Starting from the index IDRES   1
          Number of effective XYZ-coordinates  1265

          * * * The PDB coordinates file-name /users/andrzej/musca/cypx/1M63.pdb
          Chain identifier (sequence) >>> |B|
          Number of residues in IDRES(*)   158
          Starting from the index IDRES  12
          Number of effective XYZ-coordinates  1262

  Number of used coordinates 1265 1262

   1   3.85       69-ARG   CZ    164-LYS   O
   2   3.51       69-ARG   NH1   164-LYS   O
   3   3.73       69-ARG   NH2   164-LYS   CA
   4   3.39       69-ARG   NH2   164-LYS   O
   5   3.44       69-ARG   NH2   164-LYS   CB
   6   3.66       69-ARG   NH2   164-LYS   CG
   7   3.96       71-ASN   CG    164-LYS   NZ
   8   3.56       71-ASN   ND2   164-LYS   CE
   9   2.79       71-ASN   ND2   164-LYS   NZ
  10   3.41      103-ALA   C     122-ASN   ND2
  11   3.06 *    103-ALA   O     122-ASN   ND2
  12   3.51      104-GLY   N     122-ASN   ND2
  13   3.88      104-GLY   CA    122-ASN   CG
  14   3.91      104-GLY   CA    122-ASN   OD1
  15   3.25      104-GLY   CA    122-ASN   ND2
  16   3.86      105-PRO   CD    122-ASN   OD1

   <.......> Number of potential hydrogen bonds    1

              AA-residue-###     Contacts
               ARG----- 69         5
               ASN----- 71         4
               ALA-----103         3
               GLY-----104         5
               PRO-----105         2

>>>> Inter-molecular distances  16 Below 4-A  16
>>> Hydrophobic    1 Hydrophilic    5 Mixed   10
>> Main-chain/Main-chain    0 Side-chain/Side-chain    6 Mixed   10

                This is step * * *   11 * * *

          * * * The PDB coordinates file-name /users/andrzej/musca/cypx/1CWA.pdb
          Chain identifier (sequence) >>> |C|
          Number of residues in IDRES(*)    11
          Starting from the index IDRES   1
          Number of effective XYZ-coordinates    84

          * * * The PDB coordinates file-name /users/andrzej/musca/cypx/1CWA.pdb
```

```
        Chain identifier (sequence) >>> |A|
        Number of residues in IDRES(*)   165
        Starting from the index IDRES   1
        Number of effective XYZ-coordinates  1265

Number of used coordinates   84 1265

 1   3.63       1-BMT   CN     55-ARG   NH1
 2   3.05       1-BMT   CA    102-ASN   O
 3   3.41       1-BMT   C     102-ASN   O
 4   3.15 *     1-BMT   O      63-GLN   NE2
 5   3.39       1-BMT   CB    102-ASN   O
 6   3.41       1-BMT   CD1   102-ASN   O
 7   3.95       1-BMT   CD1   102-ASN   ND2
 8   3.64       1-BMT   CH    103-ALA   O
 9   3.86       2-ABA   N     102-ASN   C
10   2.92 *     2-ABA   N     102-ASN   O
11   3.27       2-ABA   CA     72-GLY   O
12   3.16       2-ABA   C      72-GLY   O
13   3.82       2-ABA   O      72-GLY   O
14   3.94       2-ABA   O     103-ALA   CB
15   3.55       2-ABA   CB     72-GLY   O
16   3.94       2-ABA   CB    102-ASN   O
17   3.64       2-ABA   CB    111-GLN   NE2
18   3.80       2-ABA   CG    101-ALA   C
19   3.72       2-ABA   CG    101-ALA   CB
20   3.58       2-ABA   CG    102-ASN   N
21   3.78       2-ABA   CG    102-ASN   CA
22   3.86       2-ABA   CG    102-ASN   C
23   3.64       2-ABA   CG    102-ASN   O
24   3.87       2-ABA   CG    111-GLN   CB
25   3.72       2-ABA   CG    111-GLN   CD
26   3.81       2-ABA   CG    111-GLN   OE1
27   3.78       2-ABA   CG    111-GLN   NE2
28   3.98       3-SAR   N      72-GLY   C
29   3.16 *     3-SAR   N      72-GLY   O
30   3.99       3-SAR   CA     72-GLY   O
31   3.88       3-SAR   CN     72-GLY   C
32   3.32       3-SAR   CN     72-GLY   O
33   3.81       5-VAL   CG1    55-ARG   NE
34   3.77       5-VAL   CG1    55-ARG   NH2
35   3.93       9-MLE   CB     60-PHE   CE2
36   3.81       9-MLE   CB    121-TRP   NE1
37   3.70       9-MLE   CB    121-TRP   CZ2
38   3.50       9-MLE   CD1   121-TRP   CZ2
39   3.94       9-MLE   CD1   121-TRP   CH2
40   3.89       9-MLE   CD2    60-PHE   CD2
41   3.68       9-MLE   C      60-PHE   CE2
42   3.60       9-MLE   C      60-PHE   CZ
43   3.96       9-MLE   C     121-TRP   NE1
44   3.89       9-MLE   O      60-PHE   CE1
45   3.73       9-MLE   O      60-PHE   CE2
46   3.19       9-MLE   O      60-PHE   CZ
47   3.74       9-MLE   O     121-TRP   CD1
48   2.90 *     9-MLE   O     121-TRP   NE1
49   3.88       9-MLE   O     121-TRP   CE2
50   3.32      10-MLE   CN     55-ARG   NH2
51   3.92      10-MLE   C      55-ARG   NH1
52   3.25      10-MLE   O      55-ARG   CZ
53   2.77      10-MLE   O      55-ARG   NH1
54   2.85 *    10-MLE   O      55-ARG   NH2
55   3.70      10-MLE   O      60-PHE   CE2
56   3.63      11-MVA   CN    122-LEU   CD2
```

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  57   3.40       11-MVA   CN    126-HIS   CE1
  58   3.23       11-MVA   CN    126-HIS   NE2
  59   3.80       11-MVA   CA     55-ARG   NH1
  60   3.85       11-MVA   CB    113-PHE   CD1
  61   3.96       11-MVA   CB    113-PHE   CE1
  62   3.93       11-MVA   CG1    63-GLN   CG
  63   3.54       11-MVA   CG1    63-GLN   CD
  64   3.50       11-MVA   CG1    63-GLN   OE1
  65   3.99       11-MVA   CG1    63-GLN   NE2
  66   3.74       11-MVA   CG1   101-ALA   CB
  67   3.88       11-MVA   CG1   113-PHE   CB
  68   3.74       11-MVA   CG1   113-PHE   CG
  69   3.49       11-MVA   CG1   113-PHE   CD1
  70   3.50       11-MVA   CG2    60-PHE   CZ
  71   3.89       11-MVA   CG2    61-MET   CG
  72   3.90       11-MVA   CG2   113-PHE   CG
  73   3.88       11-MVA   CG2   113-PHE   CD2
  74   3.95       11-MVA   CG2   113-PHE   CE2

   <.......> Number of potential hydrogen bonds    5

              AA-residue-###     Contacts

               BMT-----  1         7
               ABA-----  2        20
               SAR-----  3         6
               VAL-----  5         3
               MLE-----  9        16
               MLE----- 10         7
               MVA----- 11        20

>>>> Inter-molecular distances  74 Below 4-A  74

>>> Hydrophobic   26 Hydrophilic    7 Mixed   41

>> Main-chain/Main-chain   10 Side-chain/Side-chain   30 Mixed   34

                 This is step * * *   12 * * *

* * * The PDB coordinates file-name /users/andrzej/musca/cypx/1CWA.pdb
          Chain identifier (sequence) >>> |A|
          Number of residues in IDRES(*)   165
          Starting from the index IDRES   1
          Number of effective XYZ-coordinates  1265

          * * * The PDB coordinates file-name /users/andrzej/musca/cypx/1CWA.pdb
          Chain identifier (sequence) >>> |C|
          Number of residues in IDRES(*)    11
          Starting from the index IDRES   1
          Number of effective XYZ-coordinates    84

  Number of used coordinates 1265   84

   1   3.81       55-ARG   NE      5-VAL   CG1
   2   3.25       55-ARG   CZ     10-MLE   O
   3   3.63       55-ARG   NH1     1-BMT   CN
   4   3.92       55-ARG   NH1    10-MLE   C
   5   2.77       55-ARG   NH1    10-MLE   O
   6   3.80       55-ARG   NH1    11-MVA   CA
   7   3.77       55-ARG   NH2     5-VAL   CG1
   8   3.32       55-ARG   NH2    10-MLE   CN
   9   2.85 *     55-ARG   NH2    10-MLE   O
  10   3.89       60-PHE   CD2     9-MLE   CD2
```

11	3.89		60-PHE	CE1	9-MLE	O
12	3.93		60-PHE	CE2	9-MLE	CB
13	3.68		60-PHE	CE2	9-MLE	C
14	3.73		60-PHE	CE2	9-MLE	O
15	3.70		60-PHE	CE2	10-MLE	O
16	3.60		60-PHE	CZ	9-MLE	C
17	3.19		60-PHE	CZ	9-MLE	O
18	3.50		60-PHE	CZ	11-MVA	CG2
19	3.89		61-MET	CG	11-MVA	CG2
20	3.93		63-GLN	CG	11-MVA	CG1
21	3.54		63-GLN	CD	11-MVA	CG1
22	3.50		63-GLN	OE1	11-MVA	CG1
23	3.15	*	63-GLN	NE2	1-BMT	O
24	3.99		63-GLN	NE2	11-MVA	CG1
25	3.98		72-GLY	C	3-SAR	N
26	3.88		72-GLY	C	3-SAR	CN
27	3.27		72-GLY	O	2-ABA	CA
28	3.16		72-GLY	O	2-ABA	C
29	3.82		72-GLY	O	2-ABA	O
30	3.55		72-GLY	O	2-ABA	CB
31	3.16	*	72-GLY	O	3-SAR	N
32	3.99		72-GLY	O	3-SAR	CA
33	3.32		72-GLY	O	3-SAR	CN
34	3.80		101-ALA	C	2-ABA	CG
35	3.72		101-ALA	CB	2-ABA	CG
36	3.74		101-ALA	CB	11-MVA	CG1
37	3.58		102-ASN	N	2-ABA	CG
38	3.78		102-ASN	CA	2-ABA	CG
39	3.86		102-ASN	C	2-ABA	N
40	3.86		102-ASN	C	2-ABA	CG
41	3.05		102-ASN	O	1-BMT	CA
42	3.41		102-ASN	O	1-BMT	C
43	3.39		102-ASN	O	1-BMT	CB
44	3.41		102-ASN	O	1-BMT	CD1
45	2.92	*	102-ASN	O	2-ABA	N
46	3.94		102-ASN	O	2-ABA	CB
47	3.64		102-ASN	O	2-ABA	CG
48	3.95		102-ASN	ND2	1-BMT	CD1
49	3.64		103-ALA	O	1-BMT	CH
50	3.94		103-ALA	CB	2-ABA	O
51	3.87		111-GLN	CB	2-ABA	CG
52	3.72		111-GLN	CD	2-ABA	CG
53	3.81		111-GLN	OE1	2-ABA	CG
54	3.64		111-GLN	NE2	2-ABA	CB
55	3.78		111-GLN	NE2	2-ABA	CG
56	3.88		113-PHE	CB	11-MVA	CG1
57	3.74		113-PHE	CG	11-MVA	CG1
58	3.90		113-PHE	CG	11-MVA	CG2
59	3.85		113-PHE	CD1	11-MVA	CB
60	3.49		113-PHE	CD1	11-MVA	CG1
61	3.88		113-PHE	CD2	11-MVA	CG2
62	3.96		113-PHE	CE1	11-MVA	CB
63	3.95		113-PHE	CE2	11-MVA	CG2
64	3.74		121-TRP	CD1	9-MLE	O
65	3.81		121-TRP	NE1	9-MLE	CB
66	3.96		121-TRP	NE1	9-MLE	C
67	2.90	*	121-TRP	NE1	9-MLE	O
68	3.88		121-TRP	CE2	9-MLE	O
69	3.70		121-TRP	CZ2	9-MLE	CB
70	3.50		121-TRP	CZ2	9-MLE	CD1
71	3.94		121-TRP	CH2	9-MLE	CD1
72	3.63		122-LEU	CD2	11-MVA	CN
73	3.40		126-HIS	CE1	11-MVA	CN

```
  74   3.23     126-HIS   NE2    11-MVA   CN

   <.......> Number of potential hydrogen bonds    5

               AA-residue-###     Contacts

                ARG----- 55         8
                PHE----- 60        10
                MET----- 61         2
                GLN----- 63         6
                GLY----- 72        10
                ALA-----101         4
                ASN-----102        13
                ALA-----103         3
                GLN-----111         6
                PHE-----113         9
                TRP-----121         9
                LEU-----122         2
                HIS-----126         3

>>>> Inter-molecular distances  74 Below 4-A  74

>>> Hydrophobic   26 Hydrophilic    7 Mixed   41

>> Main-chain/Main-chain   10 Side-chain/Side-chain   30 Mixed   34

                  This is step * * *   13 * * *

          * * * The PDB coordinates file-name /users/andrzej/musca/cypx/1ZKF.pdb
          Chain identifier (sequence) >>> |A|
          Number of residues in IDRES(*)   165
          Starting from the index IDRES   1
          Number of effective XYZ-coordinates  1265

          * * * The PDB coordinates file-name /users/andrzej/musca/cypx/1ZKF.pdb
          Chain identifier (sequence) >>> |C|
          Number of residues in IDRES(*)     6
          Starting from the index IDRES   1
          Number of effective XYZ-coordinates    43

  Number of used coordinates 1265   43

   1   3.40       55-ARG   CZ      4-PRO   O
   2   3.92       55-ARG   NH1     2-ALA   O
   3   3.62       55-ARG   NH1     3-GLY   C
   4   3.77       55-ARG   NH1     3-GLY   O
   5   3.70       55-ARG   NH1     4-PRO   N
   6   3.94       55-ARG   NH1     4-PRO   C
   7   2.95       55-ARG   NH1     4-PRO   O
   8   3.85       55-ARG   NH1     4-PRO   CD
   9   2.98 *     55-ARG   NH2     4-PRO   O
  10   3.69       57-ILE   CG2     6-NIT   ON1
  11   3.97       57-ILE   CD1     6-NIT   C5
  12   3.81       60-PHE   CD2     6-NIT   C4
  13   3.70       60-PHE   CD2     6-NIT   C5
  14   3.65       60-PHE   CE2     6-NIT   C1
  15   3.86       60-PHE   CE2     6-NIT   C2
  16   3.89       60-PHE   CE2     6-NIT   C5
  17   3.75       60-PHE   CZ      4-PRO   CG
  18   3.88       60-PHE   CZ      5-PHE   O
  19   3.99       63-GLN   CD      2-ALA   O
  20   3.45       63-GLN   CD      3-GLY   O
  21   3.77       63-GLN   OE1     2-ALA   O
```

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  22    3.91       63-GLN    OE1      3-GLY    C
  23    3.16       63-GLN    OE1      3-GLY    O
  24    3.83       63-GLN    OE1      4-PRO    CD
  25    3.35       63-GLN    NE2      2-ALA    O
  26    3.34       63-GLN    NE2      3-GLY    O
  27    3.56       72-GLY    O        1-SIN    C3
  28    3.82       72-GLY    O        1-SIN    C4
  29    3.11 *     72-GLY    O        2-ALA    N
  30    3.93       72-GLY    O        2-ALA    CB
  31    3.78       73-THR    CG2      1-SIN    C1
  32    3.80       73-THR    CG2      1-SIN    O1
  33    3.77       73-THR    CG2      1-SIN    O2
  34    3.47      101-ALA    CB       3-GLY    O
  35    3.89      102-ASN    N        2-ALA    CB
  36    3.97      102-ASN    C        2-ALA    CA
  37    3.82      102-ASN    C        2-ALA    CB
  38    3.76      102-ASN    C        3-GLY    N
  39    3.52      102-ASN    O        2-ALA    CA
  40    3.52      102-ASN    O        2-ALA    C
  41    3.71      102-ASN    O        2-ALA    CB
  42    2.69 *    102-ASN    O        3-GLY    N
  43    3.57      102-ASN    O        3-GLY    CA
  44    3.86      111-GLN    OE1      2-ALA    CB
  45    3.66      113-PHE    CD1      4-PRO    CD
  46    3.77      113-PHE    CE1      4-PRO    CD
  47    3.99      113-PHE    CZ       4-PRO    CG
  48    3.33      121-TRP    NE1      5-PHE    O
  49    3.84      121-TRP    CZ2      6-NIT    C2
  50    3.67      121-TRP    CZ2      6-NIT    C3
  51    3.76      122-LEU    CD1      4-PRO    CB
  52    3.50      122-LEU    CD2      4-PRO    CB
  53    3.84      126-HIS    CE1      4-PRO    N
  54    3.73      126-HIS    CE1      4-PRO    CA
  55    3.97      126-HIS    CE1      4-PRO    CB
  56    3.58      126-HIS    NE2      4-PRO    CA
  57    3.62      126-HIS    NE2      4-PRO    CB

   <.......> Number of potential hydrogen bonds    3

              AA-residue-###     Contacts

               ARG----- 55         8
               ILE----- 57         3
               PHE----- 60         8
               GLN----- 63         9
               GLY----- 72         5
               THR----- 73         4
               ALA-----101         2
               ASN-----102        10
               GLN-----111         2
               PHE-----113         4
               TRP-----121         4
               LEU-----122         3
               HIS-----126         6

>>>> Inter-molecular distances  57 Below 4-A  57

>>> Hydrophobic   10 Hydrophilic   12 Mixed   35

                  This is step * * *   14 * * *

          * * * The PDB coordinates file-name /users/andrzej/musca/cypx/1YND.pdb
          Chain identifier (sequence) >>> |A|
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        Number of residues in IDRES(*)   164
        Starting from the index IDRES   2
        Number of effective XYZ-coordinates  1257

        * * * The PDB coordinates file-name /users/andrzej/musca/cypx/1YND.pdb
        Chain identifier (sequence) >>> | |
        Number of residues in IDRES(*)     2
        Starting from the index IDRES 401
        Number of effective XYZ-coordinates   155

Number of used coordinates 1257  155

 1   3.20      55-ARG   CD    401-SFA   O66
 2   4.00      55-ARG   CZ    401-SFA   C19
 3   3.91      55-ARG   NH1   401-SFA   C17
 4   3.68      55-ARG   NH1   401-SFA   O72
 5   3.21      55-ARG   NH2   401-SFA   O69
 6   3.71      55-ARG   NH2   401-SFA   N65
 7   3.71      55-ARG   NH2   401-SFA   O66
 8   3.75      57-ILE   CG2   401-SFA   C45
 9   3.51      59-GLY   O     401-SFA   C35
10   3.56      59-GLY   O     401-SFA   C34
11   3.74      59-GLY   O     401-SFA   C47
12   3.98      60-PHE   CD1   401-SFA   C45
13   3.93      60-PHE   CD2   401-SFA   C32
14   3.94      60-PHE   CE1   401-SFA   C26
15   3.60      60-PHE   CE1   401-SFA   C25
16   3.61      60-PHE   CE1   401-SFA   C24
17   3.98      60-PHE   CE1   401-SFA   O65
18   3.97      60-PHE   CE1   401-SFA   C3
19   3.94      60-PHE   CE2   401-SFA   C48
20   3.85      60-PHE   CZ    401-SFA   C3
21   3.57      61-MET   CE    401-SFA   O66
22   3.98      63-GLN   CD    401-SFA   N6
23   3.97      63-GLN   CD    401-SFA   N65
24   3.39      63-GLN   OE1   401-SFA   N6
25   3.06      63-GLN   OE1   401-SFA   N65
26   3.65      63-GLN   OE1   401-SFA   C5
27   3.87      63-GLN   OE1   401-SFA   O66
28   3.88      63-GLN   NE2   401-SFA   C10
29   3.03      63-GLN   NE2   401-SFA   O69
30   3.98      72-GLY   O     401-SFA   C55
31   3.74      73-THR   O     401-SFA   C54
32   3.92      73-THR   CB    401-SFA   C53
33   3.44      73-THR   CB    401-SFA   O71
34   3.41      73-THR   CG2   401-SFA   O71
35   3.30     101-ALA   CA    401-SFA   O67
36   3.62     101-ALA   C     401-SFA   O67
37   3.86     101-ALA   CB    401-SFA   C57
38   3.93     101-ALA   CB    401-SFA   C7
39   3.35     101-ALA   CB    401-SFA   O67
40   3.98     101-ALA   CB    401-SFA   C5
41   3.90     102-ASN   N     401-SFA   C57
42   2.99     102-ASN   N     401-SFA   O67
43   3.88     102-ASN   C     401-SFA   N9
44   3.65     102-ASN   O     401-SFA   C11
45   3.68     102-ASN   O     401-SFA   C10
46   2.80     102-ASN   O     401-SFA   N9
47   3.59     102-ASN   O     401-SFA   C8
48   3.50     102-ASN   O     401-SFA   C58
49   3.87     102-ASN   O     401-SFA   C7
50   3.26     102-ASN   O     401-SFA   O67
51   3.74     103-ALA   CA    401-SFA   O70
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52	3.49	103-ALA	C	402-SFA	O73
53	3.79	103-ALA	O	402-SFA	O73
54	3.83	103-ALA	O	402-SFA	C15
55	3.98	103-ALA	O	402-SFA	C51
56	3.27	103-ALA	CB	401-SFA	O70
57	3.40	104-GLY	N	402-SFA	O73
58	3.73	104-GLY	CA	402-SFA	O73
59	3.89	111-GLN	CB	401-SFA	C57
60	3.79	111-GLN	CD	401-SFA	C55
61	3.57	111-GLN	CD	401-SFA	C57
62	3.71	111-GLN	OE1	401-SFA	C55
63	3.55	111-GLN	OE1	401-SFA	C57
64	3.64	111-GLN	NE2	401-SFA	C55
65	3.72	111-GLN	NE2	401-SFA	C56
66	3.84	111-GLN	NE2	401-SFA	C57
67	3.54	113-PHE	CD1	401-SFA	C5
68	3.96	113-PHE	CD1	401-SFA	C4
69	3.69	113-PHE	CE1	401-SFA	C5
70	3.83	113-PHE	CE1	401-SFA	C4
71	3.99	118-LYS	O	401-SFA	C47
72	3.75	119-THR	CB	401-SFA	C48
73	3.87	121-TRP	CB	401-SFA	C29
74	3.89	121-TRP	CZ2	402-SFA	C49
75	3.72	121-TRP	CZ3	401-SFA	O68
76	3.90	121-TRP	CZ3	402-SFA	C22
77	3.97	121-TRP	CH2	402-SFA	C49
78	3.51	121-TRP	CH2	402-SFA	C22
79	3.32	122-LEU	CD2	401-SFA	O68
80	3.92	126-HIS	ND1	401-SFA	O67
81	3.59	126-HIS	CD2	401-SFA	O68
82	3.65	126-HIS	CE1	401-SFA	C60
83	3.72	126-HIS	CE1	401-SFA	O68
84	4.00	126-HIS	CE1	401-SFA	C7
85	3.17	126-HIS	CE1	401-SFA	O67
86	3.45	126-HIS	NE2	401-SFA	C60
87	3.49	126-HIS	NE2	401-SFA	C61
88	2.71	126-HIS	NE2	401-SFA	O68

<.......> Number of potential hydrogen bonds 0

AA-residue-###	Contacts
ARG----- 55	6
ILE----- 57	2
GLY----- 59	4
PHE----- 60	10
MET----- 61	2
GLN----- 63	9
GLY----- 72	2
THR----- 73	5
ALA-----101	7
ASN-----102	11
ALA-----103	7
GLY-----104	3
GLN-----111	9
PHE-----113	5
LYS-----118	2
THR-----119	2
TRP-----121	7
LEU-----122	2
HIS-----126	10

>>>> Inter-molecular distances 88 Below 4-A 88

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>>> Hydrophobic    0 Hydrophilic    0 Mixed   88

>> Main-chain/Main-chain    0 Side-chain/Side-chain    0 Mixed   88

                  This is step * * *   15 * * *

          * * * The PDB coordinates file-name /users/andrzej/musca/cypx/1YND.pdb
          Chain identifier (sequence) >>> | |
          Number of residues in IDRES(*)     2
          Starting from the index IDRES 401
          Number of effective XYZ-coordinates   155

          * * * The PDB coordinates file-name /users/andrzej/musca/cypx/1YND.pdb
          Chain identifier (sequence) >>> |B|
          Number of residues in IDRES(*)   164
          Starting from the index IDRES   2
          Number of effective XYZ-coordinates  1257

  Number of used coordinates  155 1257

   1   3.88     401-SFA   C43   121-TRP   CG
   2   3.45     401-SFA   C43   121-TRP   CD2
   3   3.95     401-SFA   C43   121-TRP   CE2
   4   3.40     401-SFA   C43   121-TRP   CE3
   5   3.87     401-SFA   C43   121-TRP   CZ3
   6   3.86     401-SFA   C44   121-TRP   CE3
   7   3.84     401-SFA   C38   121-TRP   CZ2
   8   3.73     401-SFA   C45   121-TRP   CZ2
   9   3.81     401-SFA   C20   125-LYS   CE
  10   3.99     401-SFA   C19   125-LYS   CE
  11   3.77     401-SFA   C19   125-LYS   NZ
  12   3.81     401-SFA   C18   125-LYS   NZ
  13   3.84     401-SFA   O73   103-ALA   CA
  14   3.36     401-SFA   O73   103-ALA   C
  15   3.80     401-SFA   O73   103-ALA   O
  16   3.19     401-SFA   O73   104-GLY   N
  17   3.60     401-SFA   O73   104-GLY   CA
  18   3.85     401-SFA   O73   125-LYS   NZ
  19   3.75     401-SFA   C15   103-ALA   O
  20   3.82     401-SFA   C51   103-ALA   O
  21   3.75     402-SFA   C45    57-ILE   CG2
  22   3.90     402-SFA   C45    60-PHE   CD1
  23   3.60     402-SFA   C35    59-GLY   O
  24   3.55     402-SFA   C34    59-GLY   O
  25   3.53     402-SFA   C47    59-GLY   O
  26   3.81     402-SFA   C32    60-PHE   CD2
  27   3.89     402-SFA   C32    60-PHE   CE2
  28   3.95     402-SFA   C30    60-PHE   CE2
  29   3.91     402-SFA   C30    60-PHE   CZ
  30   3.84     402-SFA   C48    60-PHE   CE2
  31   3.77     402-SFA   C48   119-THR   CB
  32   3.94     402-SFA   C26    60-PHE   CE1
  33   3.65     402-SFA   C25    60-PHE   CE1
  34   3.66     402-SFA   C24    60-PHE   CE1
  35   3.98     402-SFA   C19    55-ARG   NH1
  36   3.95     402-SFA   C17    55-ARG   NH1
  37   3.67     402-SFA   O72    55-ARG   NH1
  38   3.75     402-SFA   C54    73-THR   O
  39   3.64     402-SFA   O71    73-THR   CB
  40   3.75     402-SFA   O71    73-THR   CG2
  41   3.84     402-SFA   O70   103-ALA   CA
  42   3.40     402-SFA   O70   103-ALA   CB
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43	3.72	402-SFA	C11	102-ASN	O
44	3.86	402-SFA	C55	72-GLY	O
45	3.83	402-SFA	C55	111-GLN	CD
46	3.73	402-SFA	C55	111-GLN	OE1
47	3.61	402-SFA	C55	111-GLN	NE2
48	3.88	402-SFA	C56	72-GLY	O
49	3.66	402-SFA	C56	111-GLN	NE2
50	3.84	402-SFA	C57	101-ALA	CB
51	3.88	402-SFA	C57	102-ASN	N
52	3.94	402-SFA	C57	111-GLN	CB
53	3.57	402-SFA	C57	111-GLN	CD
54	3.53	402-SFA	C57	111-GLN	OE1
55	3.77	402-SFA	C57	111-GLN	NE2
56	3.86	402-SFA	C10	63-GLN	NE2
57	3.74	402-SFA	C10	102-ASN	O
58	3.19	402-SFA	O69	55-ARG	NH2
59	3.03	402-SFA	O69	63-GLN	NE2
60	3.90	402-SFA	N9	102-ASN	C
61	2.85	402-SFA	N9	102-ASN	O
62	3.65	402-SFA	C8	102-ASN	O
63	3.57	402-SFA	C58	102-ASN	O
64	3.91	402-SFA	C60	125-LYS	CE
65	3.68	402-SFA	C60	126-HIS	CE1
66	3.48	402-SFA	C60	126-HIS	NE2
67	3.83	402-SFA	C61	125-LYS	CE
68	3.55	402-SFA	C61	126-HIS	NE2
69	3.46	402-SFA	O68	122-LEU	CD2
70	3.61	402-SFA	O68	125-LYS	CD
71	3.37	402-SFA	O68	125-LYS	CE
72	3.62	402-SFA	O68	126-HIS	CD2
73	3.72	402-SFA	O68	126-HIS	CE1
74	2.73	402-SFA	O68	126-HIS	NE2
75	3.92	402-SFA	C7	101-ALA	CB
76	3.97	402-SFA	C7	102-ASN	O
77	3.26	402-SFA	O67	101-ALA	CA
78	3.58	402-SFA	O67	101-ALA	C
79	3.31	402-SFA	O67	101-ALA	CB
80	2.96	402-SFA	O67	102-ASN	N
81	3.36	402-SFA	O67	102-ASN	O
82	3.98	402-SFA	O67	126-HIS	ND1
83	3.24	402-SFA	O67	126-HIS	CE1
84	3.99	402-SFA	N6	63-GLN	CD
85	3.44	402-SFA	N6	63-GLN	OE1
86	3.69	402-SFA	N65	55-ARG	NH2
87	3.99	402-SFA	N65	63-GLN	CD
88	3.10	402-SFA	N65	63-GLN	OE1
89	3.72	402-SFA	C5	63-GLN	OE1
90	3.98	402-SFA	C5	101-ALA	CB
91	3.52	402-SFA	C5	113-PHE	CD1
92	3.69	402-SFA	C5	113-PHE	CE1
93	3.86	402-SFA	C4	113-PHE	CD1
94	3.74	402-SFA	C4	113-PHE	CE1
95	3.96	402-SFA	C4	113-PHE	CZ

<.......> Number of potential hydrogen bonds 0

AA-residue-###	Contacts
SFA-----401	19
SFA-----402	76

>>>> Inter-molecular distances 95 Below 4-A 95

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>>> Hydrophobic    0 Hydrophilic    0 Mixed   95

>> Main-chain/Main-chain    0 Side-chain/Side-chain    0 Mixed   95

                This is step * * *   16 * * *

          * * * The PDB coordinates file-name /users/andrzej/musca/cypx/1C5F.pdb
          Chain identifier (sequence) >>> |B|
          Number of residues in IDRES(*)    11
          Starting from the index IDRES   1
          Number of effective XYZ-coordinates    84

          * * * The PDB coordinates file-name /users/andrzej/musca/cypx/1C5F.pdb
          Chain identifier (sequence) >>> |A|
          Number of residues in IDRES(*)   177
          Starting from the index IDRES   1
          Number of effective XYZ-coordinates  1364

  Number of used coordinates   84 1364

    1   3.95        1-BMT   CN      66-ARG   CZ
    2   3.70        1-BMT   CN      66-ARG   NH1
    3   2.88        1-BMT   CA     113-ASN   O
    4   3.30        1-BMT   C      113-ASN   O
    5   3.24        1-BMT   O       74-GLN   NE2
    6   3.29        1-BMT   CB     113-ASN   O
    7   3.74        1-BMT   CG2    113-ASN   O
    8   3.86        1-BMT   CD1    113-ASN   C
    9   2.98        1-BMT   CD1    113-ASN   O
   10   3.91        1-BMT   CD1    113-ASN   OD1
   11   3.99        1-BMT   CD1    137-HIS   CE1
   12   3.74        2-ABA   N      113-ASN   C
   13   2.90 *      2-ABA   N      113-ASN   O
   14   3.09        2-ABA   CA      83-GLY   O
   15   3.08        2-ABA   C       83-GLY   O
   16   3.74        2-ABA   O       83-GLY   O
   17   3.74        2-ABA   O      114-LYS   CB
   18   3.58        2-ABA   O      114-LYS   CD
   19   3.48        2-ABA   CB      83-GLY   O
   20   3.96        2-ABA   CB     122-GLN   CD
   21   3.40        2-ABA   CB     122-GLN   NE2
   22   3.74        2-ABA   CG     112-ALA   C
   23   3.91        2-ABA   CG     112-ALA   O
   24   3.92        2-ABA   CG     112-ALA   CB
   25   3.61        2-ABA   CG     113-ASN   N
   26   3.65        2-ABA   CG     113-ASN   CA
   27   3.75        2-ABA   CG     113-ASN   C
   28   3.61        2-ABA   CG     113-ASN   O
   29   3.79        2-ABA   CG     122-GLN   CD
   30   3.97        2-ABA   CG     122-GLN   OE1
   31   3.71        2-ABA   CG     122-GLN   NE2
   32   3.13 *      3-SAR   N       83-GLY   O
   33   4.00        3-SAR   CA      83-GLY   O
   34   3.26        3-SAR   CN      83-GLY   O
   35   3.90        5-VAL   CG1     66-ARG   NE
   36   3.67        9-MLE   CA      71-PHE   CE2
   37   3.96        9-MLE   CB      71-PHE   CD2
   38   3.74        9-MLE   CB      71-PHE   CE2
   39   3.89        9-MLE   CB      71-PHE   CZ
   40   3.79        9-MLE   CB     132-HIS   NE2
   41   3.90        9-MLE   CD2     68-ILE   CG2
   42   3.96        9-MLE   CD2     71-PHE   CG
   43   3.79        9-MLE   CD2     71-PHE   CD2
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  44   3.49        9-MLE   C       71-PHE   CE2
  45   3.61        9-MLE   C       71-PHE   CZ
  46   3.86        9-MLE   C      132-HIS   NE2
  47   3.62        9-MLE   O       71-PHE   CE2
  48   3.26        9-MLE   O       71-PHE   CZ
  49   3.58        9-MLE   O      132-HIS   CD2
  50   3.75        9-MLE   O      132-HIS   CE1
  51   2.73 *      9-MLE   O      132-HIS   NE2
  52   3.94       10-MLE   N       71-PHE   CE2
  53   3.41       10-MLE   CN      66-ARG   NH2
  54   3.96       10-MLE   C       66-ARG   NH1
  55   3.85       10-MLE   C       66-ARG   NH2
  56   3.15       10-MLE   O       66-ARG   CZ
  57   2.87       10-MLE   O       66-ARG   NH1
  58   2.66 *     10-MLE   O       66-ARG   NH2
  59   3.82       11-MVA   CN     133-LEU   CD2
  60   3.86       11-MVA   CN     137-HIS   CE1
  61   3.27       11-MVA   CN     137-HIS   NE2
  62   3.77       11-MVA   CA      66-ARG   NH1
  63   3.96       11-MVA   CB     124-PHE   CD1
  64   3.36       11-MVA   CG1     74-GLN   CD
  65   3.46       11-MVA   CG1     74-GLN   OE1
  66   3.36       11-MVA   CG1     74-GLN   NE2
  67   3.54       11-MVA   CG1    112-ALA   CB
  68   3.84       11-MVA   CG1    124-PHE   CB
  69   3.78       11-MVA   CG1    124-PHE   CG
  70   3.60       11-MVA   CG1    124-PHE   CD1
  71   3.80       11-MVA   CG2     71-PHE   CZ
  72   3.77       11-MVA   CG2     72-MET   CG
  73   3.76       11-MVA   CG2     72-MET   SD
  74   3.89       11-MVA   CG2    124-PHE   CG
  75   3.83       11-MVA   CG2    124-PHE   CD2

   <.......> Number of potential hydrogen bonds    4

              AA-residue-###     Contacts

               BMT-----  1        10
               ABA-----  2        21
               SAR-----  3         4
               VAL-----  5         2
               MLE-----  9        17
               MLE----- 10         8
               MVA----- 11        18

>>>> Inter-molecular distances  75 Below 4-A  75

>>> Hydrophobic   28 Hydrophilic    7 Mixed   40

>> Main-chain/Main-chain    9 Side-chain/Side-chain   29 Mixed   37

                This is step * * *   17 * * *

          * * * The PDB coordinates file-name /users/andrzej/musca/cypx/2Z6W.pdb
          Chain identifier (sequence) >>> |M|
          Number of residues in IDRES(*)    11
          Starting from the index IDRES   1
          Number of effective XYZ-coordinates    84

          * * * The PDB coordinates file-name /users/andrzej/musca/cypx/2Z6W.pdb
          Chain identifier (sequence) >>> |A|
          Number of residues in IDRES(*)   164
          Starting from the index IDRES   2
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Number of effective XYZ-coordinates 1239

Number of used coordinates 84 1239

1	3.59		1-BMT	CN	55-ARG	NH1
2	2.95		1-BMT	CA	102-ASN	O
3	3.36		1-BMT	C	102-ASN	O
4	3.12	*	1-BMT	O	63-GLN	NE2
5	3.30		1-BMT	CB	102-ASN	O
6	3.91		1-BMT	CG2	102-ASN	O
7	3.31		1-BMT	CD1	102-ASN	O
8	3.64		1-BMT	CD1	102-ASN	OD1
9	3.85		1-BMT	CH	103-ALA	C
10	3.66		1-BMT	CH	103-ALA	O
11	3.92		2-ABA	N	102-ASN	C
12	2.93	*	2-ABA	N	102-ASN	O
13	3.13		2-ABA	CA	72-GLY	O
14	3.90		2-ABA	CA	102-ASN	O
15	3.00		2-ABA	C	72-GLY	O
16	3.62		2-ABA	O	72-GLY	O
17	3.82		2-ABA	O	103-ALA	CB
18	3.69		2-ABA	CB	72-GLY	O
19	3.71		2-ABA	CB	102-ASN	O
20	3.57		2-ABA	CB	111-GLN	NE2
21	3.93		2-ABA	CG	101-ALA	C
22	3.59		2-ABA	CG	101-ALA	CB
23	3.68		2-ABA	CG	102-ASN	N
24	3.92		2-ABA	CG	102-ASN	CA
25	3.90		2-ABA	CG	102-ASN	C
26	3.59		2-ABA	CG	102-ASN	O
27	3.89		2-ABA	CG	111-GLN	CB
28	3.62		2-ABA	CG	111-GLN	CD
29	3.74		2-ABA	CG	111-GLN	OE1
30	3.56		2-ABA	CG	111-GLN	NE2
31	3.07	*	3-SAR	N	72-GLY	O
32	3.82		3-SAR	CA	72-GLY	O
33	3.98		3-SAR	CN	72-GLY	C
34	3.21		3-SAR	CN	72-GLY	O
35	3.84		5-VAL	CG1	55-ARG	NE
36	3.78		5-VAL	CG1	55-ARG	NH2
37	3.76		9-MLE	CA	60-PHE	CE2
38	3.91		9-MLE	CA	60-PHE	CZ
39	3.85		9-MLE	CB	60-PHE	CE2
40	3.83		9-MLE	CB	60-PHE	CZ
41	3.99		9-MLE	CB	121-TRP	NE1
42	3.84		9-MLE	CB	121-TRP	CZ2
43	3.92		9-MLE	CD1	121-TRP	CZ2
44	3.83		9-MLE	CD2	60-PHE	CD2
45	3.53		9-MLE	C	60-PHE	CE2
46	3.30		9-MLE	C	60-PHE	CZ
47	3.70		9-MLE	O	60-PHE	CE1
48	3.83		9-MLE	O	60-PHE	CE2
49	3.13		9-MLE	O	60-PHE	CZ
50	3.78		9-MLE	O	121-TRP	CD1
51	2.87	*	9-MLE	O	121-TRP	NE1
52	3.87		9-MLE	O	121-TRP	CE2
53	3.81		10-MLE	N	60-PHE	CE2
54	3.75		10-MLE	N	60-PHE	CZ
55	3.59		10-MLE	CN	55-ARG	NH2
56	3.88		10-MLE	C	60-PHE	CZ
57	3.39		10-MLE	O	55-ARG	CZ
58	2.93		10-MLE	O	55-ARG	NH1
59	2.95	*	10-MLE	O	55-ARG	NH2

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  60   3.49      10-MLE   O      60-PHE   CE2
  61   3.67      10-MLE   O      60-PHE   CZ
  62   3.83      11-MVA   CN    122-LEU   CD2
  63   3.46      11-MVA   CN    126-HIS   CE1
  64   3.27      11-MVA   CN    126-HIS   NE2
  65   3.83      11-MVA   CA     55-ARG   NH1
  66   3.80      11-MVA   CB    113-PHE   CD1
  67   3.90      11-MVA   CB    113-PHE   CE1
  68   3.91      11-MVA   CG1    63-GLN   CG
  69   3.45      11-MVA   CG1    63-GLN   CD
  70   3.37      11-MVA   CG1    63-GLN   OE1
  71   3.82      11-MVA   CG1    63-GLN   NE2
  72   3.78      11-MVA   CG1   101-ALA   CB
  73   3.88      11-MVA   CG1   113-PHE   CG
  74   3.55      11-MVA   CG1   113-PHE   CD1
  75   3.67      11-MVA   CG2    60-PHE   CZ
  76   3.87      11-MVA   CG2    61-MET   CG
  77   3.87      11-MVA   CG2   113-PHE   CG
  78   3.86      11-MVA   CG2   113-PHE   CD1
  79   3.90      11-MVA   CG2   113-PHE   CD2
  80   3.90      11-MVA   CG2   113-PHE   CE1
  81   3.92      11-MVA   CG2   113-PHE   CE2
  82   3.91      11-MVA   CG2   113-PHE   CZ

   <.......> Number of potential hydrogen bonds    5

              AA-residue-###     Contacts

               BMT-----  1         9
               ABA-----  2        21
               SAR-----  3         5
               VAL-----  5         3
               MLE-----  9        17
               MLE----- 10        10
               MVA----- 11        22

>>>> Inter-molecular distances  82 Below 4-A  82

>>> Hydrophobic   31 Hydrophilic    7 Mixed   44

>> Main-chain/Main-chain   10 Side-chain/Side-chain   32 Mixed   40

                  This is step * * *   18 * * *

          * * * The PDB coordinates file-name /users/andrzej/musca/cypx/1M9C.pdb
          Chain identifier (sequence) >>> |A|
          Number of residues in IDRES(*)   165
          Starting from the index IDRES   1
          Number of effective XYZ-coordinates  1265

          * * * The PDB coordinates file-name /users/andrzej/musca/cypx/1M9C.pdb
          Chain identifier (sequence) >>> |D|
          Number of residues in IDRES(*)   136
          Starting from the index IDRES  11
          Number of effective XYZ-coordinates  1058

  Number of used coordinates 1265 1058

   1   3.21      55-ARG   CZ     90-PRO   O
   2   3.97      55-ARG   NH1    89-GLY   CA
   3   3.93      55-ARG   NH1    89-GLY   C
   4   3.73      55-ARG   NH1    90-PRO   N
   5   3.81      55-ARG   NH1    90-PRO   C
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6	2.69		55-ARG	NH1	90-PRO	O
7	3.50		55-ARG	NH1	90-PRO	CD
8	2.89	*	55-ARG	NH2	90-PRO	O
9	3.69		55-ARG	NH2	95-GLN	CD
10	2.94	*	55-ARG	NH2	95-GLN	OE1
11	3.88		55-ARG	NH2	95-GLN	NE2
12	3.82		60-PHE	CD2	92-ALA	CA
13	3.28		60-PHE	CD2	92-ALA	CB
14	3.90		60-PHE	CE2	90-PRO	O
15	3.79		60-PHE	CE2	91-ILE	C
16	3.80		60-PHE	CE2	91-ILE	O
17	3.61		60-PHE	CE2	92-ALA	N
18	3.35		60-PHE	CE2	92-ALA	CA
19	3.30		60-PHE	CE2	92-ALA	CB
20	3.93		60-PHE	CZ	90-PRO	CB
21	3.87		60-PHE	CZ	90-PRO	CG
22	3.70		60-PHE	CZ	91-ILE	C
23	3.30		60-PHE	CZ	91-ILE	O
24	3.92		60-PHE	CZ	92-ALA	N
25	3.66		60-PHE	CZ	92-ALA	CA
26	3.99		61-MET	SD	90-PRO	CG
27	3.92		63-GLN	CD	88-ALA	O
28	3.83		63-GLN	CD	89-GLY	CA
29	3.41		63-GLN	OE1	89-GLY	CA
30	3.58		63-GLN	OE1	90-PRO	CD
31	3.53		63-GLN	NE2	88-ALA	C
32	2.97	*	63-GLN	NE2	88-ALA	O
33	3.86		63-GLN	NE2	89-GLY	N
34	3.69		63-GLN	NE2	89-GLY	CA
35	3.48		71-ASN	O	87-HIS	ND1
36	3.75		72-GLY	C	88-ALA	N
37	3.70		72-GLY	O	87-HIS	CA
38	3.68		72-GLY	O	87-HIS	C
39	2.76	*	72-GLY	O	88-ALA	N
40	3.69		72-GLY	O	88-ALA	CA
41	3.51		72-GLY	O	88-ALA	CB
42	3.98		73-THR	CG2	86-VAL	O
43	3.61		73-THR	CG2	87-HIS	ND1
44	3.57		73-THR	CG2	87-HIS	CE1
45	3.93		101-ALA	CB	89-GLY	CA
46	3.79		102-ASN	C	88-ALA	CB
47	3.46		102-ASN	O	88-ALA	CA
48	3.74		102-ASN	O	88-ALA	C
49	3.64		102-ASN	O	88-ALA	CB
50	3.01	*	102-ASN	O	89-GLY	N
51	3.88		102-ASN	O	89-GLY	CA
52	3.92		102-ASN	O	89-GLY	O
53	3.67		103-ALA	CB	86-VAL	CG1
54	3.83		111-GLN	CD	88-ALA	CB
55	3.88		111-GLN	OE1	88-ALA	CB
56	3.61		111-GLN	NE2	88-ALA	CB
57	3.91		113-PHE	CD1	90-PRO	CG
58	3.77		113-PHE	CD1	90-PRO	CD
59	3.97		113-PHE	CD2	90-PRO	CG
60	3.80		113-PHE	CE1	90-PRO	CG
61	3.91		113-PHE	CE1	90-PRO	CD
62	3.96		113-PHE	CE2	90-PRO	CG
63	3.95		113-PHE	CZ	90-PRO	CB
64	3.80		113-PHE	CZ	90-PRO	CG
65	3.56		121-TRP	NE1	91-ILE	O
66	3.95		121-TRP	NE1	93-PRO	CD
67	3.89		121-TRP	CE2	93-PRO	CG
68	3.82		121-TRP	CE2	93-PRO	CD

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  69   3.35     121-TRP   CZ2    93-PRO   CG
  70   3.29     121-TRP   CZ2    93-PRO   CD
  71   3.78     121-TRP   CH2    93-PRO   CG
  72   3.64     122-LEU   CD1    90-PRO   CB
  73   3.82     122-LEU   CD2    90-PRO   CB
  74   3.86     126-HIS   CE1    90-PRO   N
  75   3.73     126-HIS   CE1    90-PRO   CA
  76   3.82     126-HIS   CE1    90-PRO   CB
  77   3.82     126-HIS   NE2    90-PRO   CA
  78   3.76     126-HIS   NE2    90-PRO   CB

   <.......> Number of potential hydrogen bonds    5

               AA-residue-###     Contacts

                ARG----- 55        10
                PHE----- 60        15
                MET----- 61         2
                GLN----- 63         9
                ASN----- 71         2
                GLY----- 72         7
                THR----- 73         4
                ALA-----101         2
                ASN-----102         8
                ALA-----103         2
                GLN-----111         4
                PHE-----113         9
                TRP-----121         8
                LEU-----122         3
                HIS-----126         6

>>>> Inter-molecular distances  78 Below 4-A  78

>>> Hydrophobic   33 Hydrophilic   12 Mixed   33

>> Main-chain/Main-chain   10 Side-chain/Side-chain   34 Mixed   34
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