Supplementary Material

Main Title: Investigation of the probable homo-dimer model of the *Xeroderma pigmentosum* complementation group A (XPA) protein to represent the DNA binding core

Running Title: Determining the factors stabilizing the dimerization of *Xeroderma pigmentosum* complementation group A (XPA)

Supplementary Tables

**Table S1.** Intermolecular Hydrogen bond occupancy of XPA98-210/239 homo-dimer.

**Table S1A.** Intermolecular Hydrogen bond occupancy of XPA98-210 homo-dimer.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | Donor atom | Acceptor atom | Fractions | Bond  distance (Å) | Bond  angle |
| XPA98-210 monomer 1 as Donor:  XPA98-210 monomer 2 as Acceptor | ASN\_210@ND2 | ASP\_177@OD1 | 0.8212 | 2.8243 | 159.7947 |
| LYS\_198@NZ | ASN\_210@O | 0.8145 | 2.7952 | 157.6399 |
| LYS\_198@NZ | ASN\_210@OXT | 0.6459 | 2.7913 | 156.2205 |
| LYS\_198@NZ | ASN\_210@O | 0.6343 | 2.7928 | 155.2498 |
| LYS\_198@NZ | ASN\_210@O | 0.6341 | 2.8073 | 154.9492 |
| LYS\_198@NZ | GLU\_209@O | 0.0326 | 2.8275 | 156.4583 |
| LYS\_280@NZ | ASN\_210@OD1 | 0.5314 | 2.8066 | 155.6701 |
| LYS\_280@NZ | ASN\_210@OXT | 0.5308 | 2.7979 | 157.2485 |
| LYS\_280@NZ | ASN\_210@OD1 | 0.4228 | 2.8143 | 153.9806 |
| LYS\_198@NZ | ASN\_210@OXT | 0.3272 | 2.7872 | 155.3173 |
| LYS\_198@NZ | GLU\_209@O | 0.3269 | 2.8198 | 156.7902 |
| LYS\_280@NZ | ASN\_210@OXT | 0.2261 | 2.7912 | 153.6551 |
| ASN\_210@ND2 | ASP\_177@OD1 | 0.2216 | 2.8387 | 161.3973 |
| LYS\_198@NZ | ASN\_210@OD1 | 0.2189 | 2.8194 | 152.8281 |
| LYS\_280@NZ | ASN\_210@OD1 | 0.2176 | 2.814 | 152.9007 |
| LYS\_198@NZ | GLU\_209@O | 0.2175 | 2.8198 | 156.0743 |
| ASN\_210@ND2 | HIE\_172@O | 0.2172 | 2.8707 | 159.367 |
| LYS\_280@NZ | ASN\_210@O | 0.2104 | 2.7917 | 155.2914 |
| XPA98-210 monomer 2 as Donor:  XPA98-210 monomer 1 as Acceptor | ASN\_210@ND2 | TYR\_148@OH | 0.739 | 2.8922 | 141.5984 |
| THR\_142@OG1 | GLU\_209@OE1 | 0.645 | 2.7021 | 163.7317 |
| HIE\_171@NE2 | ASN\_210@O | 0.627 | 2.8304 | 160.2596 |
| LYS\_141@NZ | ASN\_210@O | 0.58 | 2.7879 | 155.6725 |
| LYS\_145@NZ | GLU\_209@OE1 | 0.556 | 2.8005 | 154.9723 |
| THR\_142@OG1 | GLU\_209@OE2 | 0.552 | 2.7029 | 146.8115 |
| SER\_157@OG | GLU\_209@OE2 | 0.547 | 2.6609 | 164.4769 |
| LYS\_145@NZ | GLU\_209@OE2 | 0.148 | 2.7993 | 155.0495 |
| LYS\_145@NZ | GLU\_209@OE2 | 0.1476 | 2.8026 | 154.8315 |
| LYS\_141@NZ | ASN\_210@OXT | 0.44 | 2.7882 | 156.1439 |
| LYS\_141@NZ | ASN\_210@O | 0.433 | 2.7792 | 153.1475 |
| LYS\_151@NZ | GLU\_147@OE1 | 0.24 | 2.788 | 154.5639 |
| LYS\_145@NZ | GLU\_209@OE2 | 0.24 | 2.803 | 154.8673 |
| LYS\_145@NZ | GLU\_209@OE1 | 0.1388 | 2.8066 | 154.0318 |
| HIE\_172@NE2 | ASN\_210@O | 0.134 | 2.83143 | 142.6013 |

**Table S1B.** Intermolecular Hydrogen bond occupancy of XPA98-239 homo-dimer.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | Donor atom | Acceptor atom | Fractions | Bond  distance (Å) | Bond  angle |
| XPA98-239 monomer 1 as Donor:  XPA98-239 monomer 2 as Acceptor | LEU\_138@N | ASP\_133@OD1 | 0.913 | 2.8631 | 163.0901 |
| GLN\_208@NE2 | GLN\_208@OE1 | 0.903 | 2.8567 | 159.877 |
| ARG\_227@NH2 | ASP\_220@OD1 | 0.8181 | 2.8025 | 159.8594 |
| LYS\_218@NZ | ASP\_131@OD1 | 0.7811 | 2.8012 | 156.4888 |
| LYS\_218@NZ | GLU\_202@OE2 | 0.6424 | 2.7985 | 157.118 |
| LYS\_222@NZ | GLU\_205@OE2 | 0.6415 | 2.7873 | 156.6412 |
| LYS\_222@NZ | GLU\_202@OE1 | 0.6409 | 2.7955 | 158.3446 |
| LYS\_222@NZ | GLU\_205@OE2 | 0.5421 | 2.7919 | 157.5471 |
| LYS\_218@NZ | GLU\_202@OE2 | 0.5403 | 2.806 | 157.2897 |
| LYS\_215@NZ | GLU\_198@OE2 | 0.5389 | 2.7927 | 156.4132 |
| LYS\_218@NZ | GLU\_202@OE2 | 0.5381 | 2.8053 | 155.4826 |
| LYS\_215@NZ | GLU\_198@OE1 | 0.5365 | 2.7937 | 155.6763 |
| LYS\_215@NZ | GLU\_198@OE2 | 0.5351 | 2.792 | 156.3356 |
| LYS\_215@NZ | GLU\_198@OE2 | 0.3512 | 2.7805 | 157.1491 |
| ARG\_227@NH2 | ASP\_220@OD1 | 0.3381 | 2.7845 | 155.581 |
| LYS\_222@NZ | GLU\_205@OE1 | 0.3293 | 2.796 | 157.4168 |
| LYS\_215@NZ | GLU\_198@OE1 | 0.3245 | 2.7973 | 156.5131 |
| LYS\_218@NZ | GLU\_202@OE1 | 0.3236 | 2.8036 | 154.1143 |
| XPA98-239 monomer 2 as Donor:  XPA98-239 monomer 2 as Acceptor | LYS\_222@NZ | GLU\_202@OE1 | 0.9038 | 2.7896 | 158.2899 |
| LYS\_222@NZ | GLU\_205@OE1 | 0.9015 | 2.7922 | 156.3216 |
| ARG\_227@NH2 | ASP\_220@OD2 | 0.9013 | 2.8099 | 158.3146 |
| LYS\_222@NZ | GLU\_205@OE1 | 0.892 | 2.7857 | 157.7273 |
| LYS\_222@NZ | GLU\_205@OE1 | 0.8651 | 2.7854 | 155.8971 |
| ARG\_227@NH1 | ASP\_220@OD1 | 0.8315 | 2.8019 | 158.104 |
| LYS\_222@NZ | GLU\_205@OE2 | 0.8232 | 2.7898 | 156.9231 |
| LYS\_222@NZ | GLU\_202@OE1 | 0.756 | 2.7912 | 158.6096 |
| LYS\_222@NZ | GLU\_205@OE2 | 0.7278 | 2.8098 | 155.1849 |
| ARG\_211@NH2 | GLU\_201@OE2 | 0.6649 | 2.8046 | 158.4043 |
| LYS\_222@NZ | GLU\_205@OE2 | 0.6568 | 2.7887 | 157.168 |
| ARG\_227@NH2 | ASP\_220@OD1 | 0.6011 | 2.8247 | 156.3326 |
| ARG\_227@NH1 | ASP\_220@OD2 | 0.5772 | 2.8075 | 155.8179 |
| GLN\_208@NE2 | GLN\_208@OE1 | 0.5413 | 2.8557 | 160.5261 |
| LYS\_222@NZ | GLU\_202@OE1 | 0.5342 | 2.7876 | 157.8085 |
| ARG\_211@NH1 | GLU\_201@OE2 | 0.5019 | 2.8077 | 157.4414 |
| LYS\_167@NZ | ASP\_133@OD2 | 0.4280 | 2.7749 | 157.3798 |
| LYS\_222@NZ | GLU\_202@OE2 | 0.4257 | 2.7892 | 157.54 |

**Table S2.** Intermolecular interactions across monomer-monomer interface of XPA98-210 homo-dimer

**Table S2A:** Intermolecular Hydrogen Bond formation.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Sl. No. | Monomer 1 | | | Monomer 2 | | | Hydrogen Bond Distance (Å) |
| Atom Name | Residues |  | | Atom Name | Residues |
| 1.  2.  3.  4.  5. | OE1  NZ  OE2  ND2  OXT | GLU143  LYS183  GLU209  ASN210  ASN210 | <-->  <-->  <-->  <-->  <--> | | NZ  O  NZ  OD2  NZ | LYS151  ASN210  LYS145  ASP177  LYS141 | 2.76  2.63  2.69  3.30  2.90 |

**Table S2B:** Intermolecular Salt Bridge formation.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Sl. No. | Monomer 1 | | | Monomer 2 | | | Salt Bridge Distance (Å) |
| Atom Name | Residues |  | | Atom Name | Residues |
| 1.  2.  3. | OE1  OE2  OE2 | GLU143  GLU147  GLU209 | <-->  <-->  <--> | | NZ  NZ  NZ | LYS151  LYS151  LYS145 | 2.76  2.85  2.69 |

**Table S2C:** Intermolecular Non-Bonded Contacts.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Sl. No. | Monomer 1 | | | Monomer 2 | | | Non-bonded Contacts Distance (Å) |
| Atom Name | Residues |  | | Atom Name | Residues |
| 1.  2.  3.  4.  5.  6.  7.  8.  9.  10.  11.  12.  13.  14.  15.  16.  17.  18.  19.  20.  21.  22.  23.  24.  25.  26.  27.  28.  29.  30.  31.  32.  33.  34.  35.  36.  37.  38.  39. | O  O  CD  OE1  OE1  OE2  OE2  CB  CD  OE1  OE1  OE1  OE1  CD  OE1  OE1  OE1  OE2  OE2  C  CE  NZ  NZ  NZ  CA  O  O  CB  CG  O  CD  OE2  OE2  C  CG  OD1  ND2  OXT  OXT | LEU138  LEU138  GLU143  GLU143  GLU143  GLU143  GLU143  GLN146  GLN146  GLN146  GLN146  GLN146  GLN146  GLU147  GLU147  GLU147  GLU147  GLU147  GLU147  LYS183  LYS183  LYS183  LYS183  LYS183  GLN208  GLN208  GLN208  GLN208  GLN208  GLU209  GLU209  GLU209  GLU209  ASN210  ASN210  ASN210  ASN210  ASN210  ASN210 | <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <--> | | OD1  ND2  NZ  CE  NZ  NZ  OE1  CB  CB  CE  C  O  CB  NZ  CD  CE  NZ  NZ  OE1  O  OD1  C  O  OD1  OD2  CB  CG  OD2  OD2  CE  NZ  CE  NZ  NZ  OD2  OD2  OD2  CE  NZ | ASN210  ASN210  LYS151  LYS151  LYS151  LYS151  GLU209  CYS153  CYS153  LYS151  CYS153  CYS153  CYS153  LYS151  LYS151  LYS151  LYS151  LYS151  GLU209  ASN210  ASN210  ASN210  ASN210  ASN210  ASP152  ASP152  ASP152  ASP152  ASP152  LYS141  LYS145  LYS145  LYS145  LYS141  ASP177  ASP177  ASP177  LYS141  LYS141 | 3.25  3.45  3.26  3.60  2.76  3.10  3.72  3.73  3.55  3.51  3.84  3.87  3.32  3.13  3.57  3.48  3.00  2.85  3.83  3.71  3.23  3.80  2.63  3.41  3.60  3.30  3.85  3.83  3.86  3.24  3.83  3.65  2.69  3.87  3.87  3.75  3.30  3.77  2.90 |

**Table S3.** Intermolecular interactions across monomer-monomer interface of XPA98-239 homo-dimer

**Table S3A:** Intermolecular Hydrogen bond formation.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Sl. No. | Chain A | | | Chain B | | | Hydrogen Bond Distance (Å) |
| Atom Name | Residues |  | | Atom Name | Residues |
| 1.  2.  3.  4.  5.  6.  7.  8.  9. | OE1  OE1  O  O  OE1  NE2  NZ  NZ  NZ | GLU198  GLU201  ARG207  GLN208  GLN208  GLN208  LYS215  LYS215  LYS222 | <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <--> | | NZ  NZ  NH2  NH2  N  O  OE1  OE2  OE1 | LYS236  LYS218  ARG211  ARG211  LYS218  MET214  GLU198  GLU201  GLU205 | 2.79  2.96  2.87  3.01  2.95  3.15  2.73  2.77  2.9 |

**Table S3B:** Intermolecular Salt Bridge formation.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Sl. No. | Chain A | | | Chain B | | | Salt Bridge Distance (Å) |
| Atom Name | Residues |  | | Atom Name | Residues |
| 1.  2.  3.  4.  5.  6. | OE2  OE2  OE2  NZ  NZ  NZ | GLU198  GLU201  GLU205  LYS215  LYS215  LYS222 | <-->  <-->  <-->  <-->  <-->  <--> | | NZ  NZ  NZ  OE1  OE1  OE1 | LYS236  LYS218  LYS222  GLU198  GLU201  GLU205 | 2.79  2.96  2.69  2.73  2.77  2.96 |

**Table S3C:** Intermolecular Non-Bonded Contacts.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Sl. No. | Chain A | | | Chain B | | Non-bonded Contacts Distance (Å) |
| Atom Name | Residues |  | Atom Name | Residues |
| 1.  2.  3.  4.  5.  6.  7.  8.  9.  10.  11.  12.  13.  14.  15.  16.  17.  18.  19.  20.  21.  22.  23.  24.  25.  26.  27.  28.  29.  30.  31.  32.  33.  34.  35.  36.  37.  38.  39.  40.  41.  42.  43.  44.  45.  46.  47.  48.  49.  50.  51.  52.  53.  54.  55.  56.  57.  58.  59.  60.  61.  62.  63.  64.  65. | CD  OE1  OE1  OE1  OE1  OE1  CD  OE1  OE2  OE2  OE2  C  O  O  O  CA  CA  C  C  O  O  O  O  O  CD  CD  CD  OE1  OE1  OE1  OE1  OE1  OE1  OE1  OE1  OE1  OE1  OE1  NE2  NE2  NE2  NE2  NE2  C  O  N  N  CA  CB  CB  CB  CG  OD1  ND2  ND2  CD  CE  CE  NZ  NZ  NZ  NZ  CD  CE  NZ | GLU198  GLU198  GLU198  GLU201  GLU201  GLU201  GLU205  GLU205  GLU205  GLU205  GLU205  ARG207  ARG207  ARG207  ARG207  GLN208  GLN208  GLN208  GLN208  GLN208  GLN208  GLN208  GLN208  GLN208  GLN208  GLN208  GLN208  GLN208  GLN208  GLN208  GLN208  GLN208  GLN208  GLN208  GLN208  GLN208  GLN208  GLN208  GLN208  GLN208  GLN208  GLN208  GLN208  GLU209  GLU209  ASN210  ASN210  ASN210  ASN210  ASN210  ASN210  ASN210  ASN210  ASN210  ASN210  LYS215  LYS215  LYS215  LYS215  LYS215  LYS215  LYS215  LYS222  LYS222  LYS222 | <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <-->  <--> | NZ  CE  NZ  CD  CE  NZ  NZ  NZ  CD  CE  NZ  NH2  CZ  NH1  NH2  NH2  O  NH2  O  NH2  O  CA  CD  OE1  C  O  N  N  CA  C  O  N  C  N  CA  CB  CG  N  O  CA  C  O  N  NH2  NH2  NH2  OE1  NH2  ND2  NE  OE1  ND2  CD  OD2  ND2  OE2  OE1  OE2  CD  OE1  CD  OE2  OE1  OE1  OE1 | LYS236  LYS236  LYS236  LYS218  LYS218  LYS218  LYS222  LYS222  LYS222  LYS222  LYS222  ARG211  ARG211  ARG211  ARG211  ARG211  LYS215  ARG211  LYS215  ARG211  LYS215  GLN216  GLN216  GLN216  LYS215  LYS215  GLN216  GLN216  GLN216  GLN216  GLN216  LYS217  LYS217  LYS218  LYS218  LYS218  LYS218  PHE219  MET214  LYS215  LYS215  LYS215  GLN216  ARG211  ARG211  ARG211  GLN216  ARG211  ASN210  ARG211  GLN216  ASN210  ARG211  ASN210  ASN210  GLU201  GLU198  GLU201  GLU198  GLU198  GLU201  GLU201  GLU205  GLU205  GLU205 | 3.79  3.59  2.79  3.36  3.53  2.96  3.30  3.13  3.30  3.58  2.69  3.89  3.60  3.59  2.87  3.88  3.51  3.42  3.84  3.01  3.31  3.56  3.51  2.93  3.73  3.79  3.77  3.67  3.71  3.13  3.04  3.52  3.88  2.95  3.48  3.27  3.59  3.37  3.15  3.41  3.16  3.38  3.52  3.48  3.43  3.64  3.89  3.78  3.82  3.84  3.53  3.83  3.78  3.83  3.47  3.71  3.73  3.59  3.78  2.73  3.65  2.77  3.81  3.84  2.96 |

Supplementary Figures

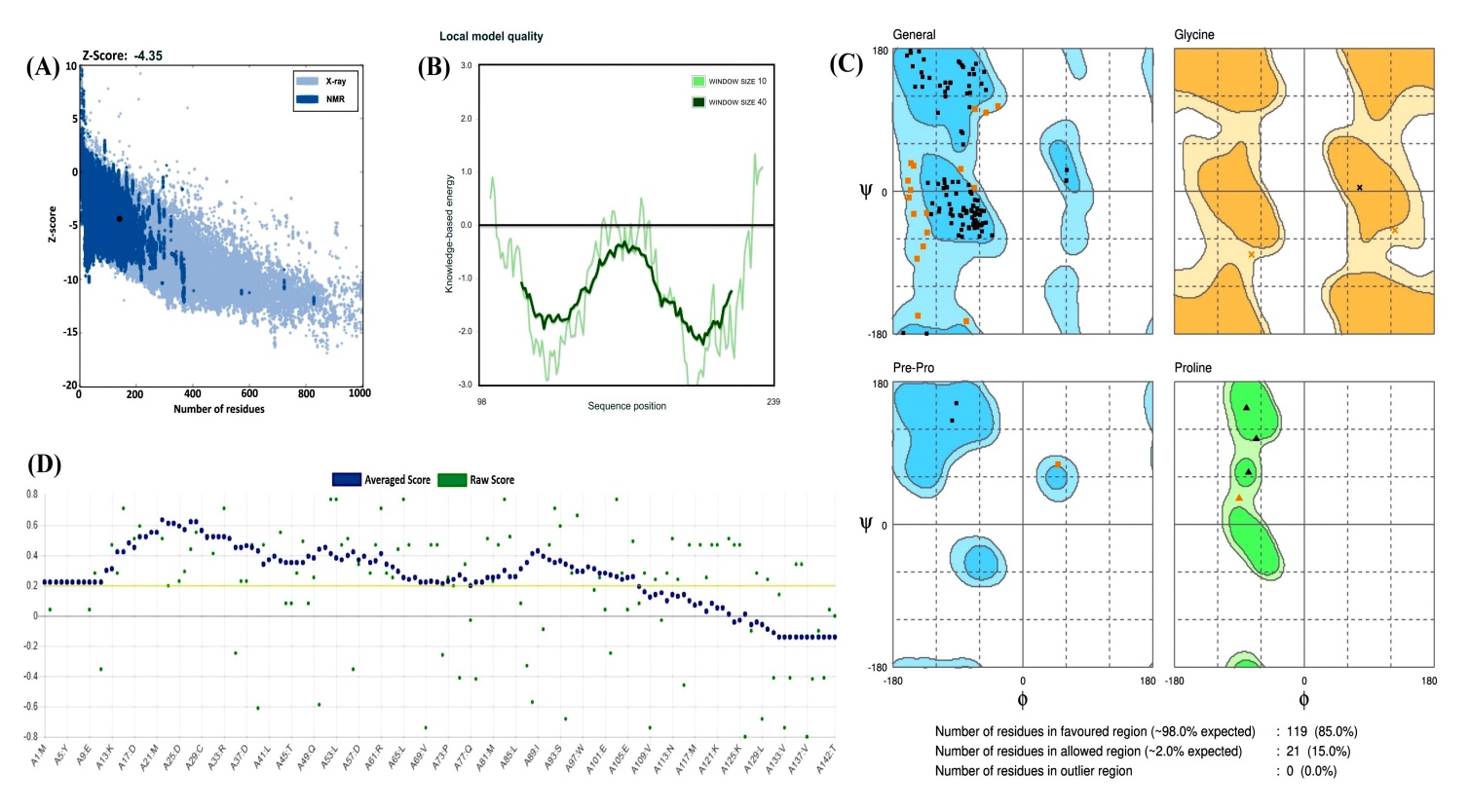
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**Figure S1.** (A) Temperature plot and (B) Energy plot for XPA98-210 homo-dimer.

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**Figure S2.** (A) Temperature plot and (B) Energy plot for XPA98-210 homo-dimer.

The following graphs were revised:



**Figure S3.** Structure validation of the modeled XPA98-239 monomer: (A) z-Score plot and (B) energy plot obtained using ProsA server, (C) Ramachandran plot, and (D) Verify 3D plot for the modeled XPA98-239 monomer.

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**Figure S4.** Docked structures of XPA98-210 homo-dimer.

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**Figure S5**. Docked structures of XPA98-239 homo-dimer.

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**Figure S6.** Distance between the monomeric units of (A) XPA98-210 homo-dimer and (B) XPA98-239 homo-dimer as a function of time.