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Data Article

# Analysis of the conformations of the HIV-1 protease from a large crystallographic data set

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ABSTRACT

The HIV-1 protease performs essential roles in viral maturation by processing specific cleavage sites in the Gag and Gag-Pol precursor polyproteins to release their mature forms. Here the analysis of a large HIV-1 protease data set (containing 552 dimer structures) are reported. These data are related to article entitled “Conformations of the HIV-1 protease: a crystal structure data set analysis” (Palese, 2017) [1].

## Specifications Table

| | |
|---|---|
| Subject area | *Chemistry, Biology.* |
| More specific subject area | *Biochemistry, HIV-1 protease structure.* |
| Type of data | *Table (csv files), text file, figure, animated figures.* |
| How data was acquired | *Input data for analysis were obtained as pdb files from public database.* |
| Data format | *Raw: pdb files (as text files). Analyzed: table (csv files), text file, graph, animated GIF.* |
| Experimental factors | *Raw pdb files were checked for quality.* |

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| | |
|---|---|
| Experimental features | *The pdb files included in the database were analyzed by different computational protocols.* |
| Data source location | *Not applicable.* |
| Data accessibility | *Analyzed data are within this article.* |

## Value of the data

- The described data set includes a very large number of the public available structures of the HIV-1 protease.
- The database can be useful in the drug design and analysis studies.
- The evidence that preferential conformations are adopted by different sequences could represent an interesting benchmark for the computational prediction and fine tuning of protein structures.

## 1. Data

### 1.1. Data sets

The large HIV-1 protease data set used in the analysis is reported in csv format (file name HIV-1_dataset.csv). Data in this file are arranged in columns (headers in the first row): the first column reports the PDB id of each entry; the second column refers to the internal sequence id; the last two columns report the calculated first and second principal component projections, respectively (calculated by the truncated SVD method [1]). The high quality structures are listed in the file HIV-1_HQ_dataset.csv. In the file are reported the PDB id, the available quality data (R observed, R all, R work, R free, refinement resolution, and the R difference); last column reports the sequence cluster id.

The full set of fluctuations (see [1]) is reported in the file fluctuations.csv. Each row in this file represents an eigenvector (297 eigenvector describe the monomer), and each amino acid is reported as a column (99 amino acid compose the monomer).

The first and second principal modes calculated for the monomer data set are reported as animated GIF image (see [1] for details). Some relevant modes are reported as nmd file [1–3].

Supplementary material related to this article can be found online at: doi:10.1016/j.dib.2017.09.076.

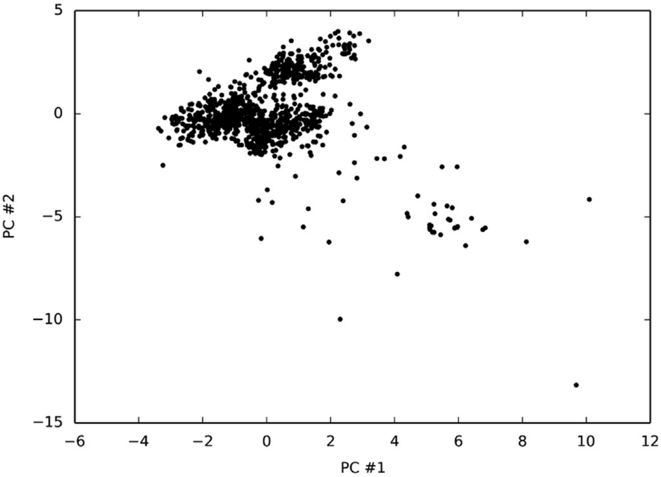


**Fig. 1.** The PCA of the monomer structures calculated by the covariance matrix method.

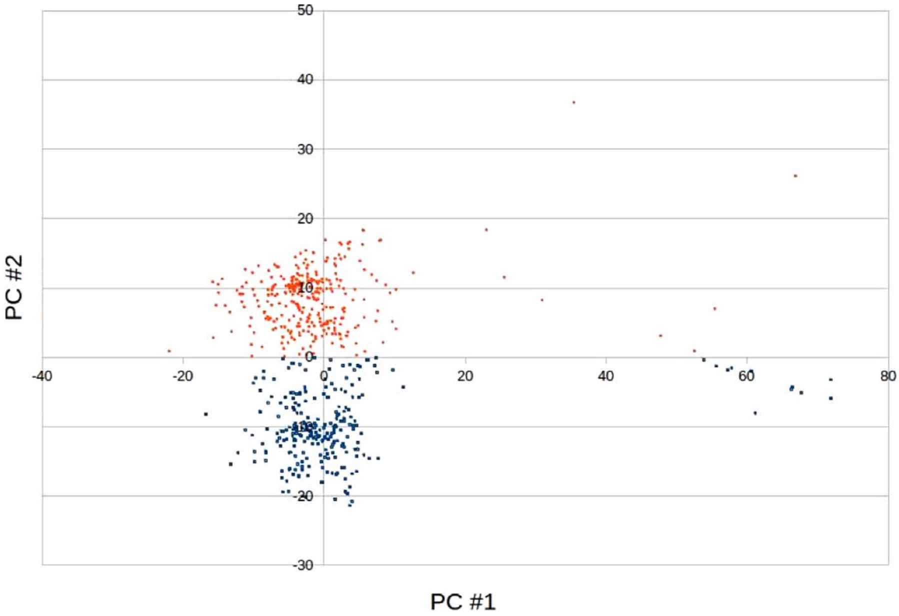


**Fig. 2.** PCA projection of the dimer data set. The entries are colored in blue if their second PC was negative, in red if positive.

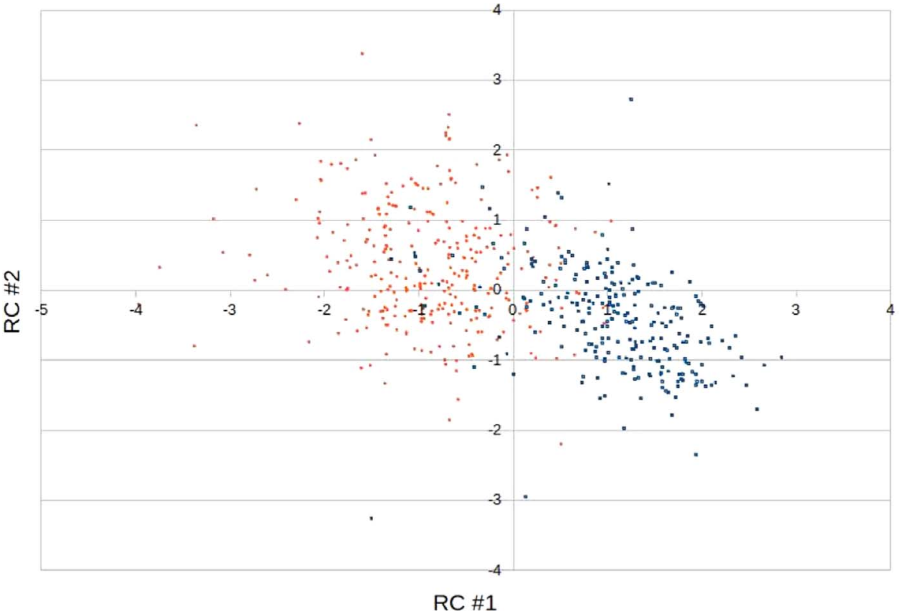


**Fig. 3.** Random projection of the dimer data set. Color code for each entry is the same as in Fig. 2.

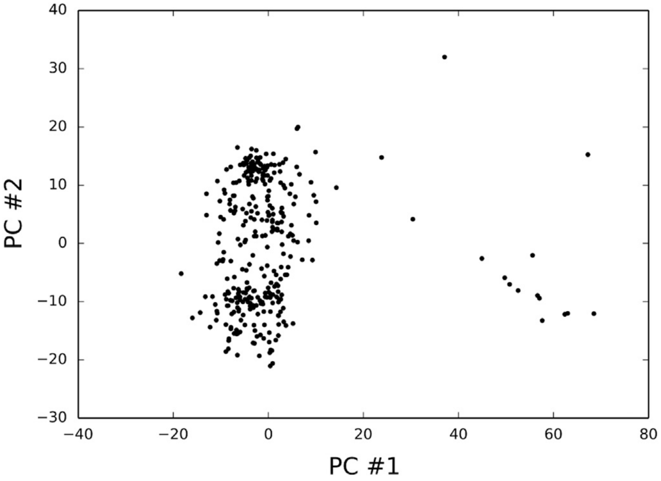
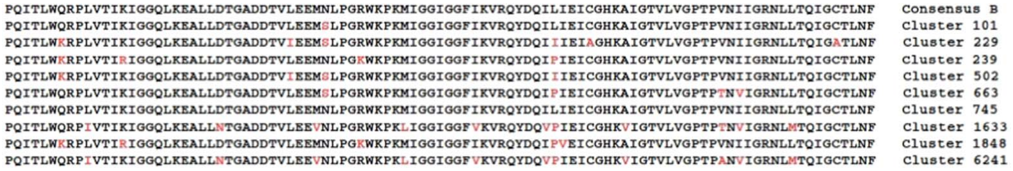


**Fig. 4.** PCA of the HQ dimer data set (truncated SVD method).



```
PQITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMNLPGRWKPKMIGGIGGFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNF   Consensus B
PQITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWKPKMIGGIGGFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNF   Cluster 101
PQITLWKRPLVTIKIGGQLKEALLDTGADDTVIEEMSLPGRWKPKMIGGIGGFIKVRQYDQIIIEIAGHKAIGTVLVGPTPVNIIGRNLLTQIGATLNF   Cluster 229
PQITLWKRPLVTIRIGGQLKEALLDTGADDTVLEEMNLPGKWKPKMIGGIGGFIKVRQYDQIPIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNF   Cluster 239
PQITLWKRPLVTIKIGGQLKEALLDTGADDTVIEEMSLPGRWKPKMIGGIGGFIKVRQYDQIIIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNF   Cluster 502
PQITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWKPKMIGGIGGFIKVRQYDQIPIEICGHKAIGTVLVGPTPTNVIGRNLLTQIGCTLNF   Cluster 663
PQITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMNLPGRWKPKMIGGIGGFIKVRQYDQILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNF   Cluster 745
PQITLWQRPIVTIKIGGQLKEALLNTGADDTVLEEVNLPGRWKPKLIGGIGGFVKVRQYDQVPIEICGHKVIGTVLVGPTPTNVIGRNLMTQIGCTLNF   Cluster 1633
PQITLWKRPLVTIRIGGQLKEALLDTGADDTVLEEMNLPGKWKPKMIGGIGGFIKVRQYDQIPVEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNF   Cluster 1848
PQITLWQRPIVTIKIGGQLKEALLNTGADDTVLEEVNLPGRWKPKLIGGIGGFVKVRQYDQVPIEICGHKVIGTVLVGPTPANVIGRNLMTQIGCTLNF   Cluster 6241
```

**Fig. 5.** Some sequence groups of the HIV-1 protease data set (see [1]).

Some results of the analysis reported in [1] on the above described data set are reported as Figs. 1–4. The reader could refers to [1] for full details.

## 2. Relevant sequence clusters in the data set

Some of the sequence clusters of the HIV-1 protease data set discussed in [1] are reported in Fig. 5; differences respect to the Consensus B sequence (Stanford HIV database) [2–5] are in red.

## 3. Experimental design, materials and methods

The structures sharing the 90% identity with the Consensus B sequence (Stanford HIV database) [4–7] were initially considered. The X-ray structures of the HIV-1 protease were obtained from the PDB [8–10]. A total number of 581 structures in the PDB met this criterion. The structures obtained by X-ray, of dimeric form, classified with an E.C. number 3.4.23.16 (HIV-1 retropepsin), and with a refinement resolution better of at least 3.1 Å were further selected. The number of alpha-carbon atoms in the downloaded pdb files was checked by the bash *grep* function after deleting the multiple conformations by the bash *sed* command. Few structures requested a further manual editing step. Finally 552 HIV-1 protease structures, as dimer, were included in the data set.

The structures contained in a data set were aligned to a common reference by Tcl (www.tcl.tk) scripting in VMD [3]. The new atomic coordinates were stored in a pdb file. For the analysis, the Cartesian coordinates of alpha-carbon atoms of the superposed structures of the data set were extracted and arranged in a matrix form by a Tcl script in VMD. Bracket in the obtained text file were removed in vi (www.vim.org). The result was that the coarse grained data conformations were arranged in a matrix such that each row represented a sample, and each column a degree of freedom. This data matrix was analyzed by methods described in [11–25], as reported in [1].

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## Transparency document. Supplementary material

Transparency data associated with this article can be found in the online version at http://dx.doi.org/10.1016/j.dib.2017.09.076.

## Appendix A. Supporting information

Supplementary data associated with this article can be found in the online version at http://dx.doi.org/10.1016/j.dib.2017.09.076.

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