1. Abstract

Protein Structure Alignment is one of the major areas in Structure biology. Many techniques and algorithms proposed by various authors do exist. For example: DALI, MaxSub, Combinatorial Extension, TM align, TMscore. But, none of them is perfect. One technique take one feature into account and other technique takes other features into account based on the understanding of the authors. For example some compare the distance matrices of both the proteins and give some similarity measure based on the similarity of the values and then they do some scoring. Some are based on the defining equivalences and doing superposition and calculating the number of C-alpha atoms whose distances are below the threshold. Others calculate the secondary state structure of each and every residue and then proceed further for the alignment procedure. Here, I have done studies of the various existing algorithms and I have proposed a new idea for the protein-protein structure alignment. My implementation of algorithm idea for protein structure alignment is exciting and studying this new algorithm provides new insights in the field of protein protein structure alignment. My algorithm studies are based on the modification of existing TM-score .My algorithm takes into account contribution from each and every atom constituting the structure. Earlier algorithm only takes one atom as representation of the protein residue and ignores every other atom. Here, I have developed the weightage scheme which will allow us to take the contribution from every atom. Allowing taking contribution from each and every atom is helpful to us to have real picture of the alignment, which was not clear to us when we blindly take only one atom as the representation of the whole residue. Also, I have compared the results of the new algorithm with the existing one.

Keywords: Protein Structure Alignment, DALI, Maxsub, TM align, TMscore, Centre of Mass.

2. Introduction

Protein structural alignment is a valuable tool for protein folds and function classification. The success of the structural genomics initiative, which aims to experimentally determine 3D structures of thousands of representative proteins, critically depends on our ability to develop accurate tools for comparison of protein structures [1]. However, despite its utmost importance, the problem still lacks a fast and accurate solution. While some structural similarity scoring functions can be approximated, there has been no procedure to optimize any commonly used structural alignment measure [1,2]. In their review article on progress in the field of structure comparison, Taylor and coworkers write: 'In structure comparison, we do not even have an algorithm that guarantees an optimal answer for pairs of structures'.

There are several different, but related definitions of an optimal alignment of two proteins. Some methods define an optimal superposition as a superposition that minimizes the distances between the aligned atoms [3, 4]. Other methods attempt to minimize the difference between the intra-atomic distances.[5]

Several methods for improved matching of protein structures have recently been introduced, including the methods based on the *phenotypic plasticity* and the method for flexible alignments by a sequence of local transformations [1].

Perhaps the most intuitive and most widely used measure of similarity of two proteins is the largest number of atoms (such as alpha-carbons, *CA*) in two structures that can be superimposed under a specified distance of each other. From now on, we will denote this metric by "$CA \leq \sigma$", where $\sigma > 0$ denotes the distance threshold in angstroms. Many structural alignment measures build upon $CA \leq \sigma$, including GDT, AL0 [1], *MaxSub* [3], *CA*-atoms <3Å, Q-*score* and TM-*Score* [2]. The TM-Score is routinely used to evaluate the quality of models in the CASP experiment [5].

One of the main measures of model quality in Live Bench is '*CA*-atoms <3 Å' [1] (in notation *CA*<3). Due to the difficulty in optimizing the scoring function itself, Live Bench approximates *CA*<3 using *3deval*, a program that attempts to maximize another metric, namely 3D-*score* [1].

CAFASP benchmark of structure prediction servers uses *MaxSub* to assess the quality of servers' predictions. [3] *MaxSub* is defined as the fraction of the residues in the model falling within 3.5Å of the aligned residues in the experimental structure [3].

In the TMscore distances between the corresponding residues and following function is evaluated.

d_0=1.24*(nseqB-15) ** (1.0/3.0)-1.8

With respect to this function all the corresponding distances are normalized and scoring function is evaluated as follows for all the residues.

score_sum=score_sum+1/(1+(dis/d_0)**2)

Finally, Score =score_sum/float (nseqB), is given as TMscore.

Irrespective of the scoring system used, in all the above methods C-alpha is used as representative of the residue and every other atom is ignored.
Here, in this we propose a method in which we take into account the weighted contribution of each and every atom that compose the residue. Now instead of just using c-alpha as representation, we use the weighted contribution taken from each and every atom that constitutes the residue and that weight is centre of mass of every atom that is used for analyses.

3. Definitions [6]:

3.1 Units of Structure Descriptions

Briefly, we can say that a protein structure consists of *elements:* atoms, residues, fragments or secondary structure elements (SSEs). A fragment is the structure of a sequence segment. A structure description can consist of *architecture, topology* and *properties.*

Architecture is the position of the elements, coordinates or relative positions. When the elements are atoms or residues, the architecture is sometimes called *geometry.*

Topology is the elements' order along the backbone. Usually, by the topology of a structure one means the architecture and the order of the elements.

Properties of the elements, e.g. physio-chemical properties of the residues and types or exposure of the SSEs.The most common description is *element based,* meaning that the description has reference to each element. Further, a description can be on fine *(low)* level or a *coarse (high)* level.

Fine: the elements are atoms or residues.

Coarse: the elements are fragments or SSEs.

Several descriptions exist for specifying the architecture and topology of proteins. For the fine level it is done by specifying coordinates, distances or torsion angles.

Coordinates: The fundamental three-dimensional (3D) structure description consists of the specification of the coordinates of each atom, as given in the PDB file. The coordinates are determined by either X-ray crystallography or by nuclear magnetic resonance (NMR). Structures are 'vibrating', and that there might also be uncertainty in the determinations. In structure comparison it is common to let one or two atoms represent each residue, often the C_{alpha} atom. The coordinates of C_{beta} are sometimes used, in order to include some information on the orientation of the side chains. The side chain is alternatively represented by a 'mean' side chain atom.

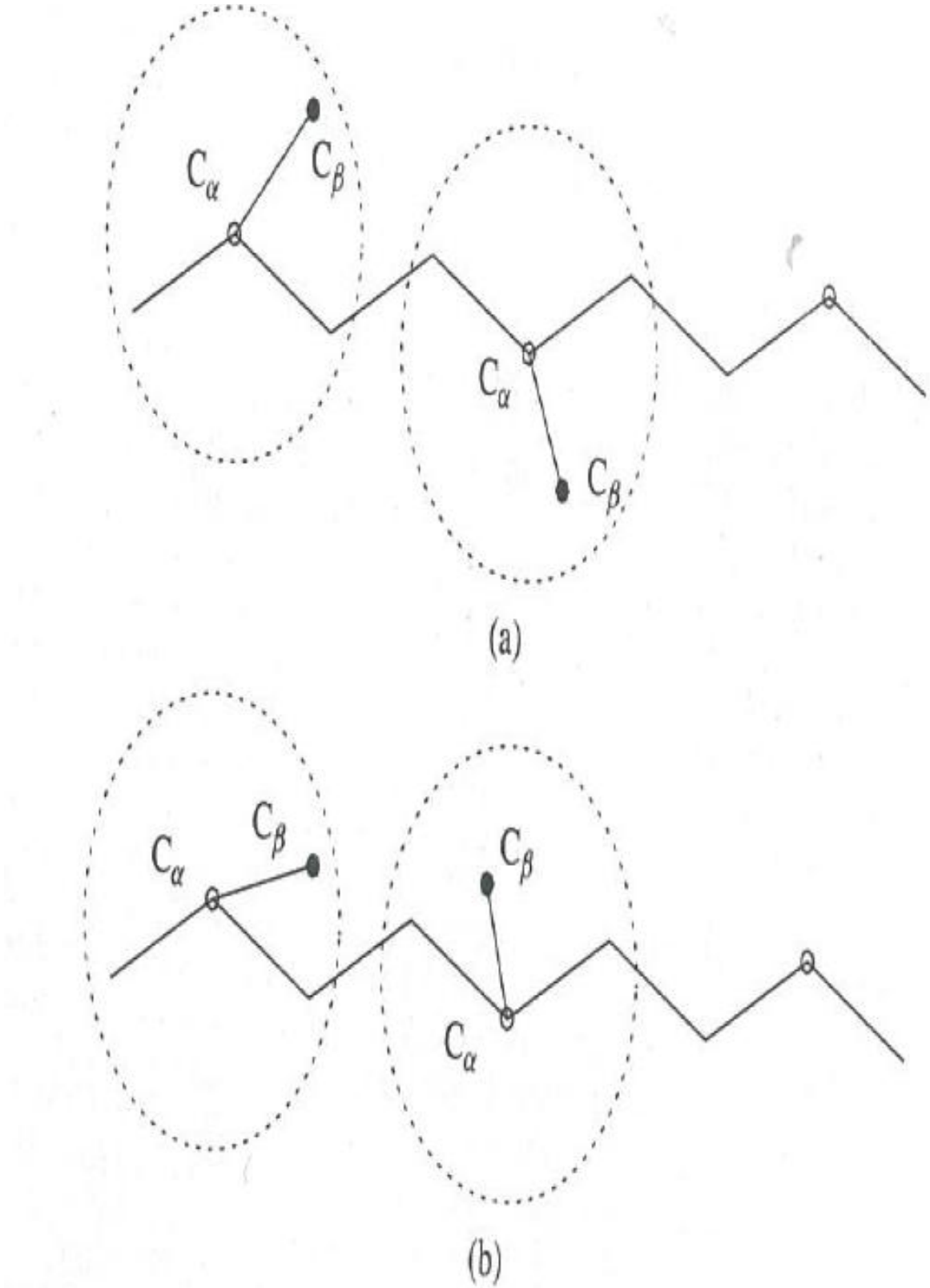
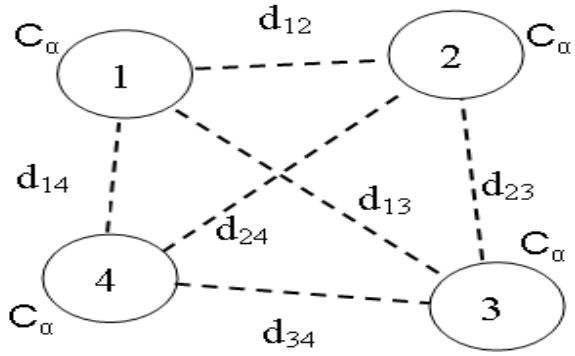


Figure1: Shows differences when c-alpha and c-beta are taken for representation [6].

3.2 Distance Matrices

A distance matrix for a structure shows the pairwise distances between elements. In this way it is a 2D representation of the 3D structure. Following Figure shows a distance matrix, where the distances between the C_{alpha} atoms are used. The distances are in angstroms and rounded to integers, and distances larger than nine are represented by a dot.
A distance matrix contains more than enough information to reconstruct the 3D structure, except for *handedness* or *chirality* (mirror images) Figure3 shows the difference.



0	**d_{12}**	**d_{13}**	**d_{14}**
d_{12}	**0**	**d_{23}**	**d_{24}**
d_{13}	**d_{23}**	**0**	**d_{34}**
d_{14}	**d_{24}**	**d_{34}**	**0**

Figure2 Distance Matrix[6].

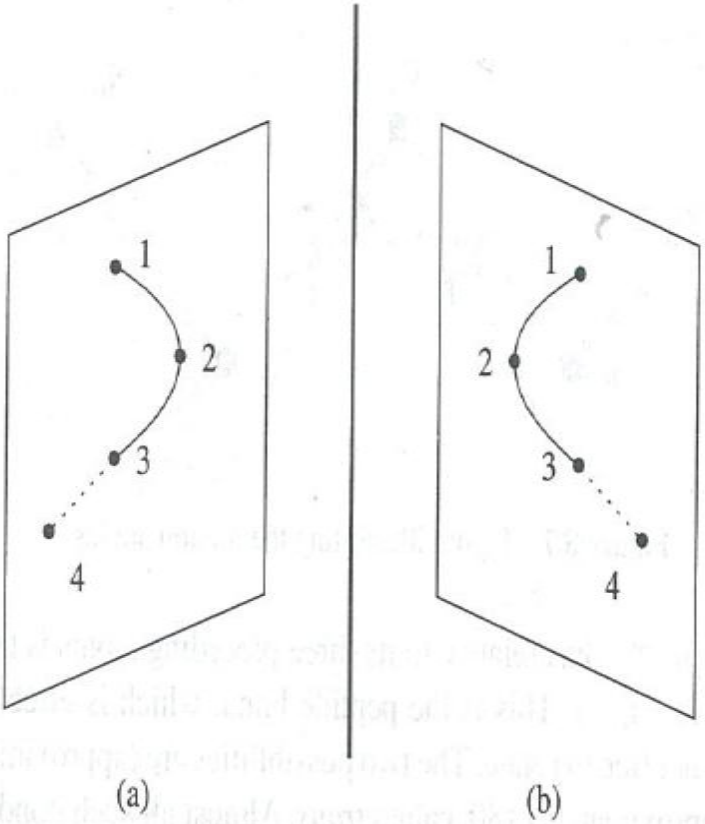


Figure 3 A structure A and its minor image B. They will get equal distance matrices, but trying to superpose B onto A will fail. Assume the plane drawn goes through points 1, 2, 3. Placing points 1, 2, 3 from B onto those from A will result in the two residues 4 being on opposite sides of the plane[6].

3.3 Torsion Angles

Geometrically, the backbone chain of a protein is a succession of points (atoms) in space:,

$$\bullet\bullet\ C_{i-1} = N_i — C_i^{alpha} — C_i = N_{i+1} — C_{i+1}^{alpha} — C_{i+1}, \bullet\bullet$$

where `—' means a single bond and '= ' a double bond……

The distance between the successive atoms on the backbone is approximately contant. They are specified by Schulz and Schirmer (1979) as 1.47 for $N—C^{alpha}$, 1.53 for $C^{alpha}—C$ and 1.32 for C—N (in angstroms). The angles between the two bonds of each atom are also approximately equal. The only freedom the proteins have in folding is to rotate around the bonds (in the backbone and side chains). Generally, three points define a plane, and due to the constant values the position of the fourth can be defined an angle relative to this plane. This angle is the rotational angle between the second and third of the three points. Consider atom C_i in Figure 8.7. The angle δ and the distance $C_i^{alpha}—C_i$ are constants, hence the only freedom C_i, has relative to the plane of three points (C_{i-1}, N_1, C_i^{α}) is the angle ϕ_i 'around' the bond (N_i, C_i^{α}) (the angle of $C_i^{alpha}—C_i$ to the plane of (C_{i-1}, N_i , C_i^{α})).

Positive values of the angles are defined to be in the clockwise direction.

The only freedom C_i has to be placed relative to the plane of (C_{i-1}, N_i, C_i^{alpha}) is to rotate 'around' the bond (N_i, C_i^{alpha}). This angle is denoted ϕ_i •

- The freedom N_{i+1} has relative its three preceding atoms is to rotate around the bond (C_i^{alpha}, C_i). This angle is denoted ψ_i.

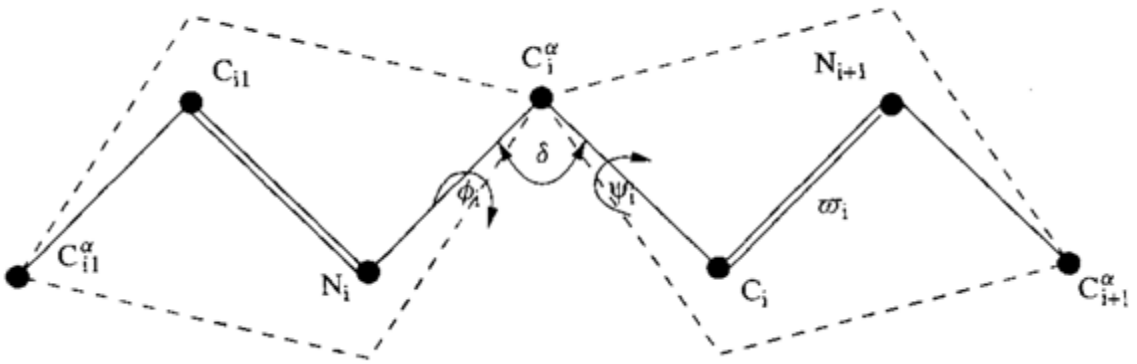


Figure 4.Description of ϕ_i and ψ_i [6].

- The freedom C_{i+1}^{alpha} has relative to its three preceding atoms is to rotate around the bond (C_i , N_{i+1}). This is the peptide bond, which is effectively a double bound and not free to rotate. The two possibilities are (approximately) 0, called *cis* and (approximately) 180, called *trans.*

- We can calculate the coordinates of the backbone chain by using these angles. The 3D structure of a protein is therefore completely specified by the torsion angles and the rotational angles of all the side chains. We can 'go in the opposite direction' : the torsion angles can be calculated from the coordinates.

The rotation around the single bonds is only restricted by possible steric collisions in the conformation. A Ramachandran plot (named after the Indian biophysicist, G. N. Ramachandran) is a plot where the angles ψ_i and ϕ_i are plotted. The preferred rotational angles for the side chains are called *rotamers*.

3.4 Helices

The main SSEs, helices and strands, are formed by hydrogen bonds. Let Hbond (i, *j)* mean that there is a hydrogen bond between the C=0 group of residue *i* and the N—H group of residue *j*. Hbond is thus a logical function which is *true* when there is an H-bond between the residues given as its parameters.

Helices are formed by hydrogen bonds between residues in the same helix. Three different types of helices exist.

α-helix is made by successive hydrogen bonds:Hbond (i, i+ 4), Hbond (i + 1, *i* + 5),

The average length is 10 residues. This is by far the most common helix.

3_{10}-helix is made by successive hydrogen bonds: Hbond(i, i + 3), Hbond(i + 1, i + 4), ...

π-helix is made by successive hydrogen bonds: Hbond(i, i + 5), Hbond(i + 1, *i*+ 6), They are very rare in proteins.

The bonds forming helices restrict the torsion angles, and the idealized angles for 'geometrically correct' α-helix are Φ = —57.8 and ψ = —47.0. However, the real angles usually deviate from these.

3.5 Strands and sheets

Strands and sheets are formed by successive hydrogen bonds between residues which can be far apart in sequence. The backbone hydrogen-bonding groups (N—H and 0=C) are in the plane of the sheet, with the bonding groups from successive residues pointing in opposite directions. Let residue *i* be in one strand, and residue *j* in another. Then the bonding of the two strands can be either parallel or antiparallel.

- Parallel bonding is formed by each residue forming hydrogen bonds to two residues on the other strand, separated by a residue in the sequence. This means successive hydrogen bonds:

  [Hbond((i, *j),*Hbond*((* j , i+2)], [Hbond((i+2, j+2), Hbond ((j+2, *i+4)],*……..

- Antiparallel bonding is formed by each residue forming two hydrogen bonds with a single residue on the other strand. This means successive hydrogen bonds:

[Hbond((j, *i),* Hbond((i, j)], [Hbond((j-2, *i* +2), Hbond((i + 2, *j — 2)],*……..

Sheets can be parallel, antiparallel or mixed (with both parallel and antiparallel bondings). The idealized strand satisfying these constraints can be thought of as a helix with two residues per turn, with torsion angles of approximately $\Phi = —120$ and $\psi = +120$.

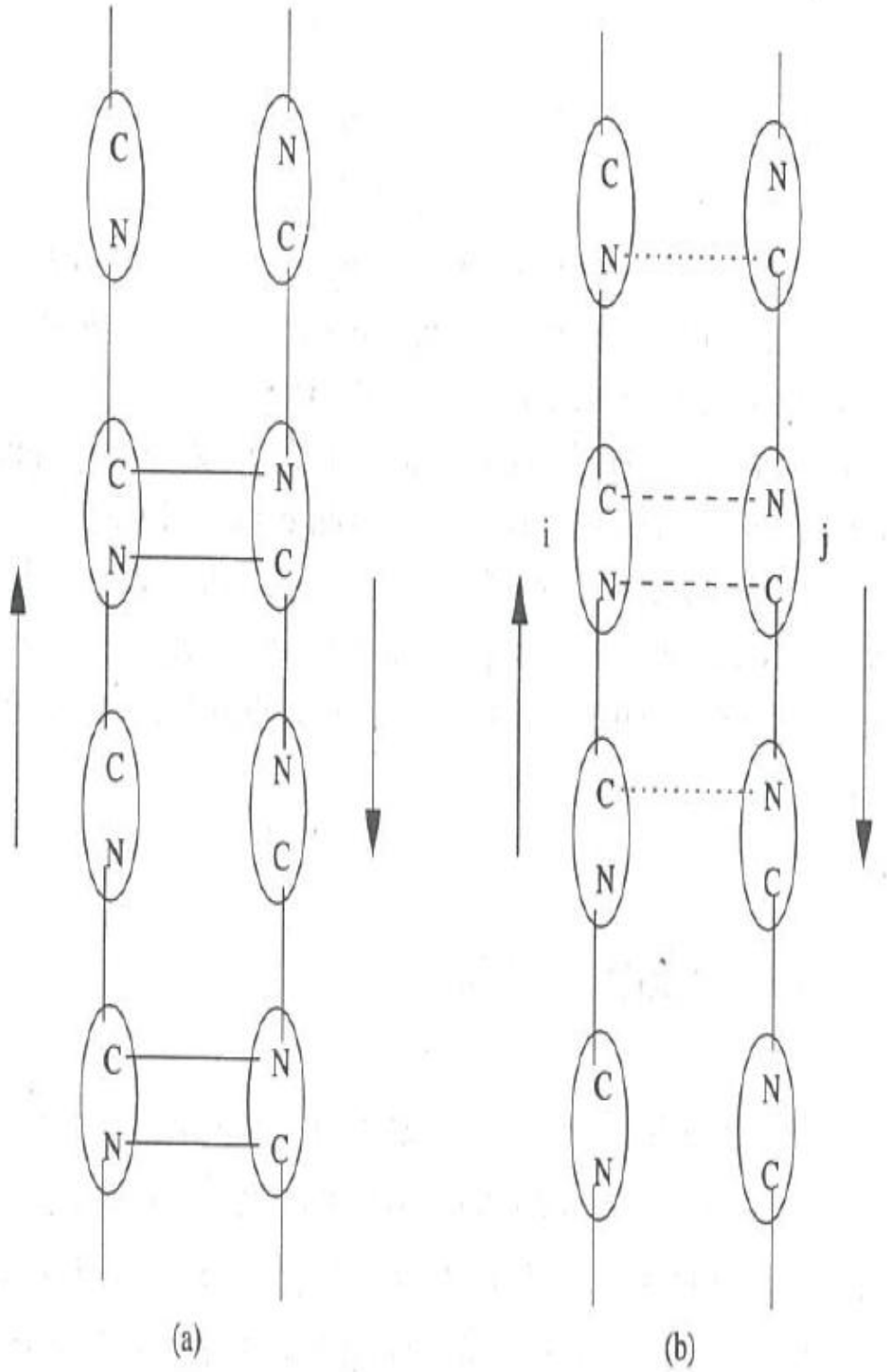


Figure 5: Antiparallel and Parallel Bridge[6].

3.6 Identifying the SSEs

There does not exist a precise universal definition for SSEs. Some automatic methods for identification of SSE do exist. Three different tools are mainly used: angle plots, distance matrices and hydrogen bonds. Plots of the torsion angles are least used, mostly because the helices and strands can have angles that differ considerably from the typical values.

Use of distance matrices

Distance matrices can be useful, either manually or automatically, to indicate where there can be SSEs. For idealized α-helices, the distances between the C_α, atoms from the start of the helix can be roughly calculated to be 3.8, 5.4, 5.1, 6.3, 8.7, 9.9, 10.6, 12.5, ... These distances are found by using an idealized angle pair for a-helices and the distances between the backbone atoms. Real helices usually deviates from these due to irregularities, as shown in following table.

Some distances in the helix (residues 31-38) of PDB entry lchc.

	31	32	33	34	35	36	37
31	0.0	3.9	5.5	5.1	7.1	9.3	10.4
32	3.9	0.0	3.8	5.5	5.8	7.0	9.4
33	5.5	3.8	0.0	3.8	5.3	4.8	6.3
34	5.1	5.5	3.8	0.0	3.8	5.4	5.4

Figure6: Distance Matrix for alpha helix. [6]

For an idealized β-strand the successive distances from a residue *i* can be calculated to be 3.8, 6.6, 10.3, 13.5, 16.9, . . Again, real strands deviate from these, as following figure.

(b)

	18	19	20	21	22
18	0.0	3.8	6.2	9.5	12.2
19	3.8	0.0	3.8	6.3	9.2
20	6.2	3.8	0.0	3.8	6.1
21	9.5	6.3	3.8	0.0	3.8
22	12.2	9.2	6.1	3.8	0.0

Figure7: Distance matrix for β-strand. [6]

It is sometimes possible to recognize adjacent strands by looking around the diagonal of a distance matrix, but as the distances grow, the strand interactions appear further away from the diagonal in the distance matrix. However, it is often possible to detect the connections between the strands in a sheet. These occur as areas of small distances around local subdiagonals and anti-subdiagonals. Parallel sheets appear as areas around subdiagonals, antiparallel as areas around anti-subdiagonals.

Define Secondary Structure of Proteins (DSSP)

The most commonly used program to identify (define) SSEs from structures is probably Define Secondary Structure of Proteins (DSSP) by Kabsch and Sander (1983), which is mainly based on H-bonding patterns [25].
DSSP identifies both the SSEs and solvent exposure of proteins.

Defining SSEs

A minimal helix of length *n (n* = 3, 4, 5) from residue *i* to residue i+n-1 is defined by Hbond (i - 1, i +n -1) and Hbond (i, i + n*)*. Longer helices are defined by overlaps of minimal helices.

To determine the strands the concept of the *bridge* is defined:

Parallel_bridge (i, j) = [Hbond (i-1, *j)* and Hbond (j, *i* + 1)] or [Hbond (j-1, *i)* and Hbond(i, j + 1*)*]

Antiparallel_bridge (i, j) = [Hbond (i, j) and Hbond (j, *i)*] or [Hbond (i-1, *j* + 1) and Hbond(j-1, i +1)].

3.7 Protein Domains

A domain is part of a polypeptide chain of a protein or the whole chain. They are compact, local and semi-independent units, but there is no general agreement as to the exact definition of what a domain is. One definition is that it is part of the chain that can independently fold into a stable structure, and that it is also a unit of function (different domains of a protein are often associated with different functions). This implies that a domain should contain a hydrophobic core and should therefore be larger than, roughly, 40 residues (the rule is that a domain consists of one hydrophobic core, but in rare cases it might consist of two). The number of domains in proteins can be from one up to several dozens, and also a domain does not need to comprise a sequential region of the polypeptide chain.

Figure8: The PDB entry 3grs with three domains.

Since different classification methods generally use different methods for domain identification, the domains will not always correspond. Several approaches have been used when developing methods for domain identification. Some of the concepts used are the following.

- Local compactness, which means that a domain will make more intra-domain contacts than contacts to the residues in the remainder of the structure. Almost all methods use this, but can in addition use some of the other points.
- Domains must contain at least one hydrophobic core.
- Minimizing the number of chain-breaks needed to separate domains while also measuring the degree of association (number of contacts) between the separating units. This implies a trade-off in trying to both minimize the number of chain-breaks and the number of contacts.
- Solvent area calculation. Let D_1 and D2 be two potential domains. If the solvent area calculated when the potential domains are split is almost equal to the one calculated when not split, then it indicates two domains.
- Secondary structures (including β-sheets) should rarely cross between different domains.

Domain Classes

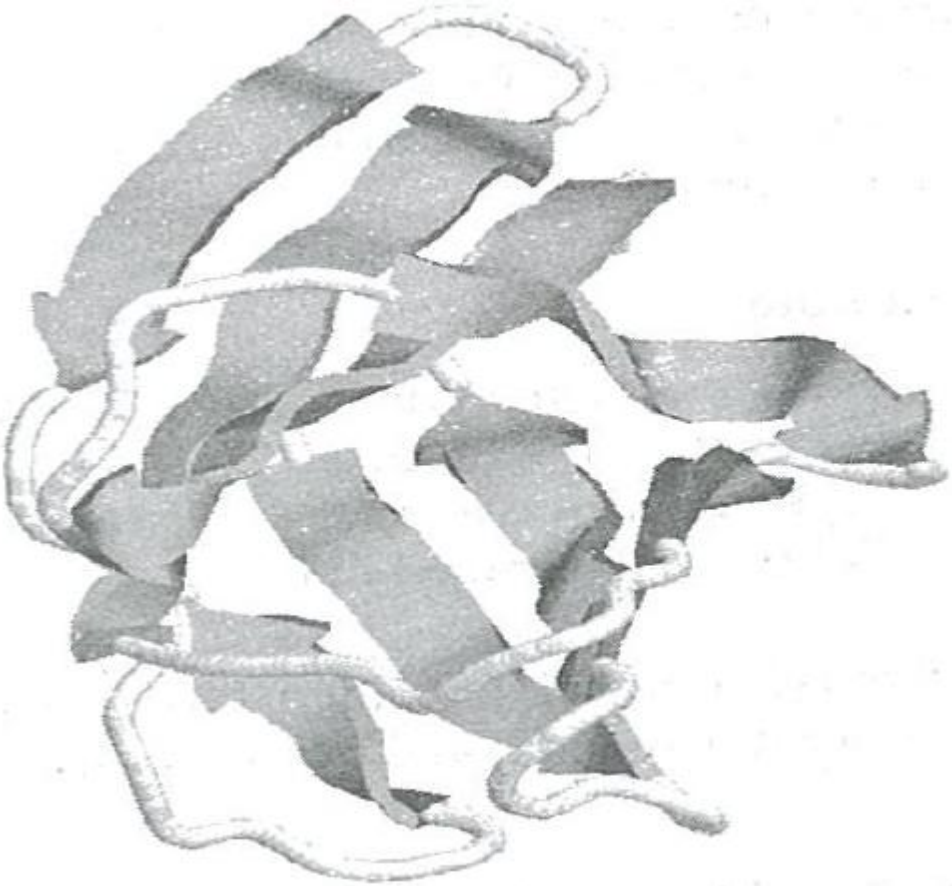
The core of the proteins is made by packing of the secondary structure elements. Since

there are only two types of SSE taking part in the packing, there are only three types of pairwise combinations:

1. α with α
2. β with β
3. α with β

Many domains contain almost exclusively one of the combinations, and these lead to the definition of three (main) classes of domains: mainly- α, mainly- β and α with β.

Mainly-α



Mainly-β

α/β

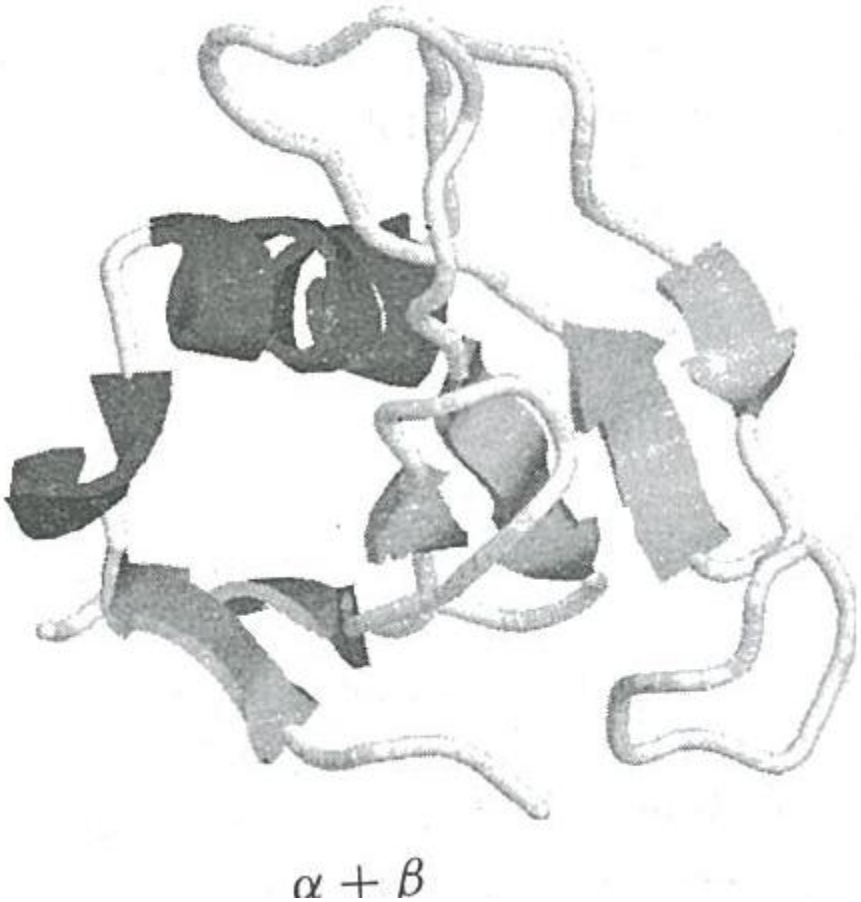


Figure 9 Examples of the four classes, mainly-α, mainly-β, α/ β, α +β .[6]

3.8 Folds

The way the secondary structure elements are packed, together with how the chain 'runs' through the secondary structures, is referred to as the fold of the chain.

It is assumed that there is a relatively small number of different folds. That only some of the possible packing and topological arrangements are observed probably comes from the physical and chemical constraints on the chain. Several people have tried to predict the number of different folds, with results ranging from some hundreds to a few thousands. Most groups seem to agree that among the currently known structures (in 2002) there are around 800 different folds.

Proteins having the same fold are assumed to have a greater probability of having a common ancestor (being homologous), but they might also have the same fold due to convergence to the same fold from different ancestors (being analogous).

3.9 Structure Comparison

Structures are compared for the same reasons as sequences are compared: to find homologous proteins and for the discovery of motifs .Comparing structures can reveal relations that are not possible to identify using sequences alone. Comparing structures is a more complicated problem than comparing sequences, and a larger variety of methods exist.

The different steps involve the following.

Feature extraction. In this the features to be used in the comparison of the structures or in the pattern discovery method are extracted. This might include comprehensive computing, e.g. assigning secondary structures to the residues.

Comparison This takes as input a pair of structure descriptions (or a pair of description/pattern) and finds (local or global) similarities between the two, optimizing a similarity measure and outputting a score. The similarity may also be represented as a pattern.

Discovery Patterns matching many or all of the input structures are found. The patterns are chosen from a solution space so that their fitness with respect to the input structures is as high as possible.

Matcher This takes as input one pattern and one structure and evaluates the match between the two; the output is 'yes' or 'no' if the pattern is deterministic or a score if the pattern is probabilistic.

Structure descriptions for comparison

When performing structure comparison one must first decide on which structure level similarities are sought (e.g. atom group, residue, secondary structures). Also, one needs to decide whether the similarities should require sequence order to be preserved, a reasonable requirement if we assume that the proteins are evolutionarily related. The structure description to be used as input to the comparison or pattern discovery algorithms should contain only the features which we would like to compare and/or to describe as patterns.

In the framework used, patterns are to be found from structure descriptions so that they represent features common to a set of such structure descriptions. Patterns will therefore be generalizations of structure descriptions, and are limited to features included in these.

In order to provide the comparison (pattern discovery) algorithms with a good starting point, the structure descriptions should ideally satisfy the following properties.

1. *invariant to trivial changes,* such as translation and rotation.
2. *Robust—the* description should not change drastically due to minor changes in the structure. This is important, since the determination of structures can contain errors. Small errors should result in similar structure descriptions, for example, the SSEs found at the same positions.
3. *Similar* structures should get similar descriptions. This point is important for classification.
4. *Different* structures should get different descriptions.

A natural way to describe a complex object like a protein structure is to break it into pieces (units) and to describe each unit separately and (most often) the relationship between the units. As already noted, the natural structure of elements such as *atoms, residues, fragments, SSEs* are used as the basic units. These descriptions make use of the *element class, property* and *relation.*

Element class The level of the description varies: atom (group), residue, backbone fragment and secondary structure element.

Property This is used for specifying the properties of each element, such as three-dimensional coordinates physico-chemical properties, amino acid type, secondary structure type, curvature and torsion.

Relation. This is used for describing the relation between the elements. In practice, the relations are binary, such as geometrical distances, difference in orientation and bonding.

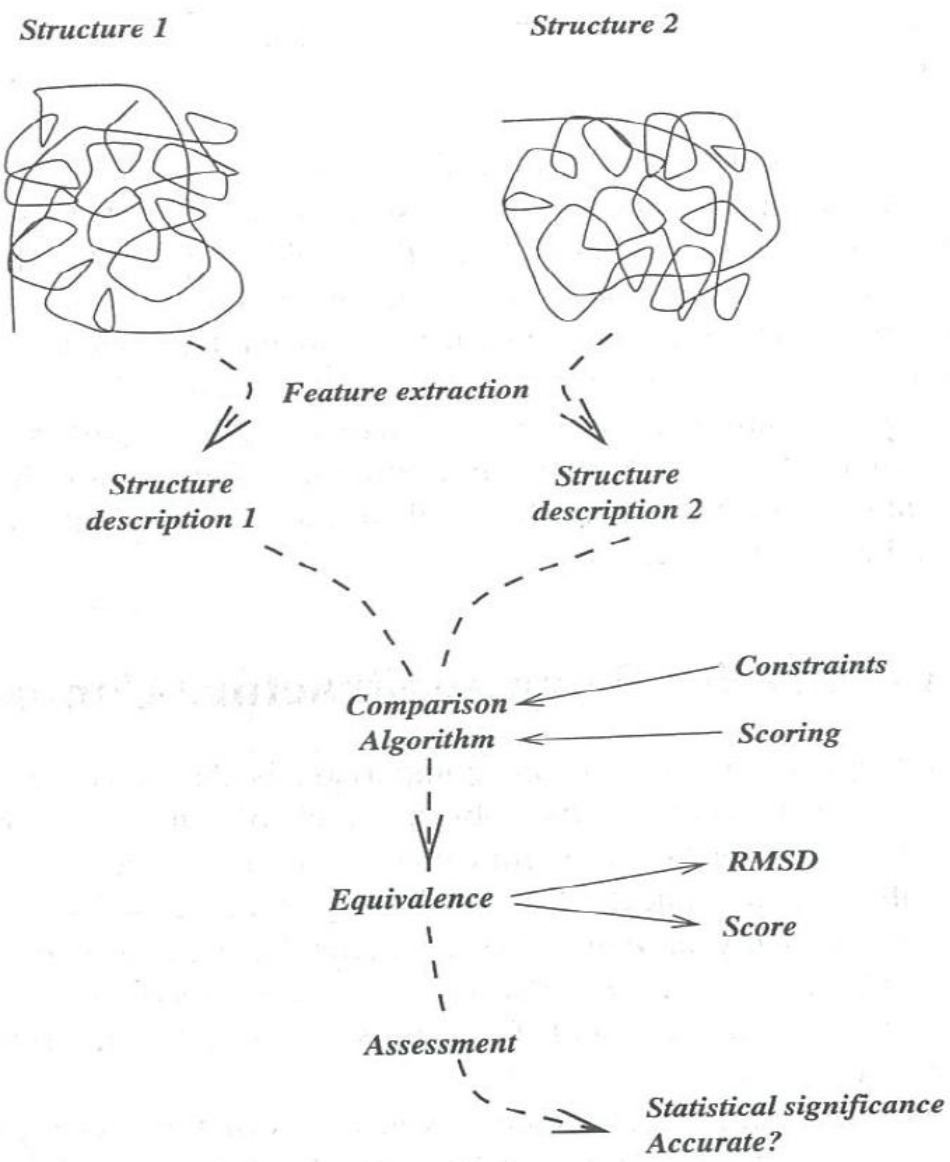


Figure10: General Algorithm Description [6].

3.10 Superposition and Dynamic Programming

Superposition

Superposition can be used to find and score equivalences, by measuring how close the equivalent pairs can come together. One way of thinking of it is to put, the structures on top of each other so that the equivalence elements from the two structures lie as close as possible. If the geometry of the structures is not changed in this process, it is referred to as rigid-body superposition. The score can then be a function of the distances between the elements of each equivalent pair in the equivalence. Commonly, the root of the mean of the squares of the distances is used, and is called the *root mean square deviation* (RMSD). Low

RMSD values are best, zero indicates exact equality.

Note that superposition can be used to measure (score) equivalences, not necessarily alignments directly. Two different measures are mainly used.

a) Coordinate RMSD

Superposition can be done by a *transformation* of structure A over *B* such that the equivalent pairs come as close as possible.

Let $(\alpha_1,\beta_1)\ldots\ldots\ (\alpha_r,\beta_r)$ be the coordinate sets of the equivalenced elements of the equivalence *E* (α_i from A and β_i from *B*, for three dimensions a coordinate set consisting of three values). The problem is then to find a transformation *T* for A which minimizes the *coordinate* root mean square deviation, that is,

$$\mathbf{RMSD_C(E) = minT}\sqrt{\sum_{i=1}^{r} \boldsymbol{wi}(\boldsymbol{T\alpha i - \beta i})\ **\ \mathbf{2}/\sum_{i=1}^{r} \boldsymbol{wi}}$$

A transformation can be performed as a *translation* (three distances), and a *rotation* (three angles, around each of the x , *y* and z-axes). The rotation can also be performed in one operation around a line, the direction of the line has to be calculated for each rotation: cf. Euler's theorem.

It has been shown that a transformation for the minimum RMSD can be found by first shifting the centroids (geometrical centres) of each structure to the origin of a common coordinate system, and then finding the rotation of A which minimizes the $RMSD_c$.

A rotation around the origin can be described by an *orthogonal* matrix $R_{3,3}$ (3D space) with determinant equal to 1. A matrix is orthogonal if the scalar product of any two different columns is 0 and the result of taking the scalar product of any column with itself is 1. The matrix must be orthogonal to assure that the distances between the points of the same structure are not changed (cf. rigid-body superposition).

The formula can therefore be described by a rotation matrix *R* and a translation vector *t*, and we search for a pair (R, t) which minimizes the expression (assuming wi = 1 for all *i):*

$$\sum_{i=1}^{r} (R\alpha i + t - \beta i)\ **\ 2$$

b) Distance RMSD

The distance score method *Distance RMSD* ($RMSD_D$) alleviates the need for finding a translation and rotation of one of the structures and is given by

$$RMSD_D(E) = \left(\sqrt{\sum_{i=1}^{r} \sum_{j=1}^{r} \left(\delta A(ij) - \delta B(ij) \right) ** 2} \right) / r$$

where δA(ij) is the spatial distance between the elements of A in pairs *i* and *j* of the equivalence. Since there is no need to calculate a transformation, it is a faster calculation. However, it has a (sometimes serious) weakness: it is invariant under reflection. This means that if structure *B* is the mirror image of structure A, then $RMSD_D$(A,B*)* = 0 and $RMSD_D$(C, A) = RMSDD(C, *B)* for all structures C.

Using RMSD as scoring of structure similarities

The problem of pairwise structure comparison is often the problem of finding equivalences with low RMSD value(s). However, several quite different equivalences with similar scores might be found and which of these equivalences represent the 'correct' solution is not an easy task to decide. However, one always needs to consider how many elements were equivalenced, since for random comparisons the expected RMSD value seems to be proportional to the square root of the number of equivalenced residues. When taking this into consideration, different measures can be used for evaluating how well two structures can be superposed.

1. Find the equivalence that minimizes the RMSD divided by the square root of the length of the equivalence: $\min_E$ RMSD(E(A,B))/$\sqrt{n_E}$ where n_E is the number of pairs in the equivalence *E*.
2. Define a threshold *L*. Find the maximum number of elements that can be superposed such that RMSD is less than or equal to *L*.
3. Define a threshold l. Find the maximum number of elements that can be superposed such that the distance between each equivalenced element is less than or equal to l.

The two last methods are mostly used to improve detection of regions of similar topology, excluding structurally unrelated regions.

3.11 Protein Structure Classification The number of proteins with known 3D structure has grown to several thousands, and to be accessible this large number of structures needs to be organized and classified. Like any Natural history collection a classification or taxonomy of the objects is especially helpful for the understanding of their evolution. In addition, when taxonomy exists, new protein structures can be placed into this, helping to understand the function of the protein. If it is discovered that there exists only a fixed number of structure classes, structure prediction will be easier.

Since the evolution of protein structure is not fully understood, there is no definitive taxonomy that can be used to derive a classification and, as a result, several systems have been developed. The most widely used classification systems are CATH, SCOP, Dali-FSSP and Dali-DD. They are all hierarchical, and most use the *protein domain* as classification unit. Their databases are all accessible via the World Wide Web.

3.12 Databases for Structure Classification

The three most popular databases for structure classifications are (all accessible via, the web) the following.

FSSP-Dali DD. FSSP is a fold classification based on structure-structure alignment of proteins (or protein chains). FSSP classification is done fully automatically, by use of the pairwise structure alignment program, DALI. The pairwise alignments of a representative subset of PDB are scored by the Z values, and a hierarchical classification is done based on the Z values. A Z value of 2 is used to divide into different folds.

weblink- http://www2.ebi.ac.ukklali/fssp/

Dali Domain Dictionary classifies domains fully automatically. It has five levels: class, fold, functional family, sequence family and PDB entry of representative domain.

weblink- http:/www2.ebi.ac.uk/dali/domain

CATH: Class, Architecture, Topology, Homologous superfamily

CATH classification is done by using both automated and manual approaches. It has six levels: class, architecture, topology, homologous superfamily,sequence family.

weblink- http://www.biochem.ucl.ac.u1c/bsmicath_new/

SCOP: A Structural Classification of Proteins Database[6,8,9]. •

SCOP classification is essentially done manually, and has seven levels: class, fold, superfamily, family, protein domain, species and PDB entry. It has become the gold standard for assessing sequence and structure comparison methods.

Weblink: http://scop.mrc-lmb.cana.ac.uk/scop/.

Since the methods used for classification are different, the resulting classifications are different. A systematic comparison of the results of these three classifications has been made which fortunately shows a high degree of agreement. Most of the discrepancies arise from different domain definitions.

4. Literature survey:

The comparison of protein structures has played an important role in developing our current understanding of protein structure and function [27]. Through this approach, many duplicated domains and structural similarities have been identified, even between proteins with no apparent sequence identity. Comparison of more closely related structures has also proved useful in understanding how proteins accommodate slight alterations in amino acid sequence and the analysis of such changes provides a vital guide to the introduction of genetically engineered changes in sequence [26]. Structures have been compared by finding the superposition that will produce the closest approach between equivalent atoms and the technique of least-squares has generally been employed to find a best solution (Matthews & Rossmann, 1985).

In the many years that structure comparison has been practised, no wholly satisfactory solution has been found to either problem.

Mainly two types of assessment methods are there known as ‘sequence- independent’ and ‘sequence-dependent’. In the former, the structural similarity of the predicted model and the experimental structure is measured, without requiring that each model residue be structurally matched to its corresponding residue in the experimental structure. The displacement of a model residue from its corresponding residue in the experimental structure, as measured from the best structural alignment, is referred to as a ‘shift’[3,11].

In the latter (sequence-dependent assessment), only corresponding residues are compared (Hubbard, 1999; Zemla et al., 1999). Thus, this is a stricter assessment criterion.In the method developed by Sippl and colleagues which is a sequence-independent method and is based on the structural superposition of the model over the experimental structure[3]. From structural superposition, a set of numbers is generated, which include the number of equivalent residues of the optimum match and the number of residues aligned at shifts zero, one, five, and above five, plus the average over the shifts. A similar method based on structural superposition that measures both the shift error and ‘contact specificity’ was developed by Bryant and colleagues [12].

These sequence-independent methods award credit to fold-recognition predictions that resemble the correct fold, but in which, due to errors in the alignment methods, some fragments may have been displaced (i.e. inaccurate alignments). Being based on structural superposition, these methods suffer from some of the limitations inherent in structural superposition programs, such as the need of a similarity score definition or the need of predefined thresholds, among others[3].

Another set of approaches is based on the sequence- dependent alignment, where each predicted residue is compared to its corresponding residue in the experimental structure.[14,15,16]. Sequence-dependent approaches are stricter in their evaluation criteria simpler and more straightforward measure of similarity between a model and an experimental structure[3].

Hubbard's RMS/Coverage graphs (Hubbard, 1999) is a sequence-dependent method that samples the best RMSD from a large number of structural super positions, each having a different number of equivalent residues. The graphs plot the best RMSD values against the number of equivalent residues [13]. A related method named GDT was developed by Adam Zemla as part of the evaluation (Zemla et al., 1999). GDT is aimed at identifying any accurately, not necessarily contiguous, predicted substructures. GDT attempts to find the maximum number of predicted residues that can be superimposed over the experimental structure within a given threshold[3]. Because each model residue lies at a distance below the given threshold, the resulting RMSD of the superimposed residues is always smaller than the given threshold. GDT's approach corresponds to the notion of identifying the largest 'well-predicted' subset in the model based on given constraints [12].

In other measure called MaxSub, which is based on similar principles as GDT. MaxSub computes a single scalar in the range of 0 to 1, which measures the similarity of a model to its corresponding experimental structure (0 for a completely wrong model, 1 for a perfect model). The scalar is a normalization of the size of the largest 'well-predicted' subset and is computed using a variation of a formula suggested by Levitt and Gerstein (1999)[3].

4.1 DALI[17,18]

Dali is for optimal pairwise alignment of protein structure. In this, C-alpha-C-alpha distances were calculated and were used to build distance matrix. The three-dimensional co-ordinates of each protein are used to calculate residue—residue (C_α--C_α) distance matrices. **A distance matrix is a 2D representation of 3D) structure. The matrix is independent of the co-ordinate frame and contains more than enough information to build up the structure.** The distance matrices are first decomposed into elementary contact patterns, e.g. hexapeptide—hexapeptide sub matrices. Then, similar contact patterns in the two matrices are paired and combined into larger consistent sets of pairs. A Monte Carlo procedure is used to optimize a similarity score defined in terms of equivalent intramolecular distances. Several alignments are optimized in parallel, leading to simultaneous detection of the best, second-best and so on solutions. The method is fully automatic and identifies structural resemblances and common structural cores accurately and sensitively, even in the presence of geometrical distortions.

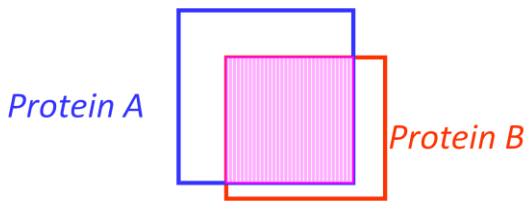


Figure 11: Distance matrix for two proteins[18].

Algorithm Description

Two proteins labeled A and B. The match of 2 substructures is evaluated using an additive similarity score S of the form.

$$\mathbf{S} = \sum_{i=1}^{L} \sum_{J=1}^{L} \boldsymbol{\phi}(\boldsymbol{i}, \boldsymbol{j})$$

Where i and j label pairs of equivalent (matched residues).

L is the number of such pairs.

And ϕ is the similarity measure.

Unmatched residues don't contribute to overall score.

For a given functional largest form of ϕ(i,j),the largest value of S corresponds to optimal set of residue equivalences.

Where:

$$\phi^{E}(i,j) = \begin{cases} \left(\theta^{E} - \dfrac{|d_{ij}^{A} - d_{ij}^{B}|}{d_{ij}^{*}}\right) w(d_{ij}^{*}), & i \neq j \\ \theta^{E}, & i = j \end{cases}$$

In this d^*_{ij} is the average of d^A_{ij} $d^B_{ij,}$

Θ^E is the measure of similarity threshold and w is envelope function.

Value of Θ^E is 0.20.

$w(r) = \exp(-r^2/\alpha^2)$, where $\alpha = 20$ angstrom

The first step is the systematic comparision of all elementary contact patterns in the 2 distance matrices..they use hexapeptide –hexapeptide contact patterns(i_A…….i_A+5,j_A……..j_A+5)in protein A paired with(i_B……i_B+5,j_B ……..j_B+5)in protein B, where the hexapeptide i_A…….i_A+5 is equivalence with i_B……i_B+5 and the hexapeptide ,j_A……..j_A+5 is equivalence with ,j_B ……..j_B+5.Similar contact patterns are stored in a non-exclusive list of pairs('pair list').This acts as a raw material for structural alignment.The goal of 2nd step is to assemble pairs of contact patterns into larger consistent sets of pairs, maximizing the similarity score. A montecarlo algorithm is used to deal with combinatorial complexity of building up alignments from contact patterns.

Step 1: Decomposition of distance matrix:

1) By restricting number of hexapeptide –hexapeptide contact patterns in each protein. Successive hexapeptide fragments that repeat a strongly similar contact pattern along the main diagonal are merged into longer segments.
2) By restricting the number of pairs of such patterns.

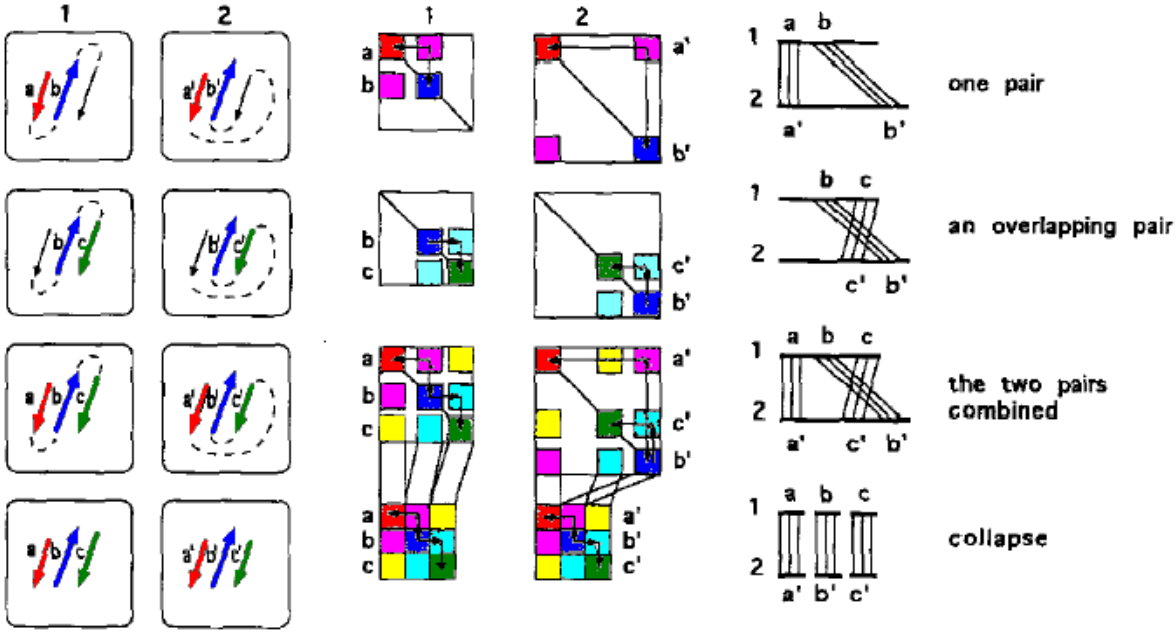
   Pair list is closed when

   a) Mean intra –pattern distance reaches 25 angstrom
   b) 80,000 pairs with a positive similarity score have been recorded.

Step 2: Assembly of alignments:

i Monte Carlo Optimization: It is an iterative improvement by a random walk exploration of search space.A move is a randomly chosen change in the configuration of system. Probability p of accepting a move is $p = \exp(\beta*(S'-S))$,where S' is the new score and S is old score and β is a parameter. β is inversely proportional to temperature of the system.

Moves that improve the score are always accepted .Sets of residue pair equivalences is called trajectory. The alignment with the highest score along each trajectory is remembered. The optimization starts from a seed alignment. The Monte Carlo algorithm has two basic modes of operation. In the expansion mode, an alignment is incremented using contact patterns that overlap with it. One expansion cycle corresponds to testing all prospective candidates in the pair list in random order. The trimming mode removes from the alignment fragments that give a net negative contribution to total similarity score.



3D (Spatial) **2D (Distance Matrix)** **1D (Sequence)**

Figure12:DALI Algorithm[18].

Selection protocol:

To cover a broad range of potential optima, several trajectories are optimized in parallel. The range of alignments is narrowed onto the highest scoring one(s) in 3 stages.

Each stage consists of 1or more expansion/trimming cycles.

In stage 1, a large number of seed alignments are generated. The pair list is screened for all triplets of non-overlapping hexapeptides.

In stage 2 optimization is continued in parallel until all alignments have settled in an optimum.

The 3rd stage consists of refining the best alignment.

4.2 MaxSub[3]: Aim is at identifying the largest subset of C-alpha atoms of a model that superimposes well with the experimental structure .It produces a single normalized score that represents the quality of the model.

Consider two ordered set of points:

A = {a1,a2,a3……an}

B = {b1,b2,b3……bn}

A match is an optimal transformation T (rotation and translation) that superimposes the points of B over A , T minimizes

$$\mathbf{RMS} = \sqrt{\sum ||\mathbf{a_i - T(b_i)}||^2 / |\mathbf{M}|}$$

Algorithm is:

for i =1 to n-L+1

let M ={(a(i) , b(i)),(a(i+1),b(i+1)),.....(a(i+L-1),b(i+L-1)}

M = extend (M,A,B,d)

if $|M| > s_{max}$ then $s_{max} = |M|$

* s_{max} =0; it holds the size of largest subset found so far.....

Extend (M , A ,B ,d)

for j =1 to k (Extends M in k = 4 iterations)

1.1 compute the transformation T that optimally superimposes the residues in M.

1.2 N = { }

1.3 for i =1 to n do

i. If the distance between a(i) and T(b(i)) is below the threshold j*d/k then N= N U {(a(i),b(i)}

1.4 M = N

2. using the last M recompute the transformation T that optimally superimposes B onto A. if for some (a(i),b(i)) Ɛ M , the distance is above threshold remove (a(i),b(i)) from M.

return M.

Result is presented as structural similarity score, which is $S= \Sigma 1/1+(di/d)^2/q$.

where q is the number of C-alpha atoms in the experimental structure.

4.3 RMS/Coverage Graphs [13]: The other way to compare pairs of three dimensional protein structures has long been root mean square distance (RMS) superposition. A large number of super positions are used to sample the best RMS for each number of equivalent residues (not necessarily contiguous). The graphical representation is a line for each prediction relating these best RMS values to number of equivalent residues. The result is the RMS/Coverage graph, which appears to represent the best prediction as the lowest line on the graph.

A structural superposition results from the unique transformation, which minimizes the RMS between two lists of atomic coordinates. Different super positions therefore result from different lists. In this algorithm the lists are generated by iterating from all possible starting points of three consecutive results.

Iteration consists of building a new list from the result of the previous superposition, followed by a new superposition etc. The new list is constructed by measuring the distance between equivalent residues. Any pair for which the distance is less than six Angstroms is included in the new list. In this experiment, three iterations are carried from each starting point. For many prediction/target pairs, after three iterations many of these super positions and their corresponding residue pair lists will be very similar, i.e., the iteration converges.

Coverage is defined here as the fraction of the target being predicted for the number of residues being considered. Coverage as defined here is non-consecutive. The minimum RMS for each coverage value out of all the super positions sampled can be determined by measuring the distance between each equivalent residue pair; sorting this list and then calculating the RMS for the first two residue pairs in the list, the first three pairs, etc. The minimum RMS for each coverage value for the entire prediction/target comparison is the set of lowest RMSs for each coverage value, across all the different super positions. It is this minimum RMS that is plotted against coverage as a line on an RMS/Coverage graph.

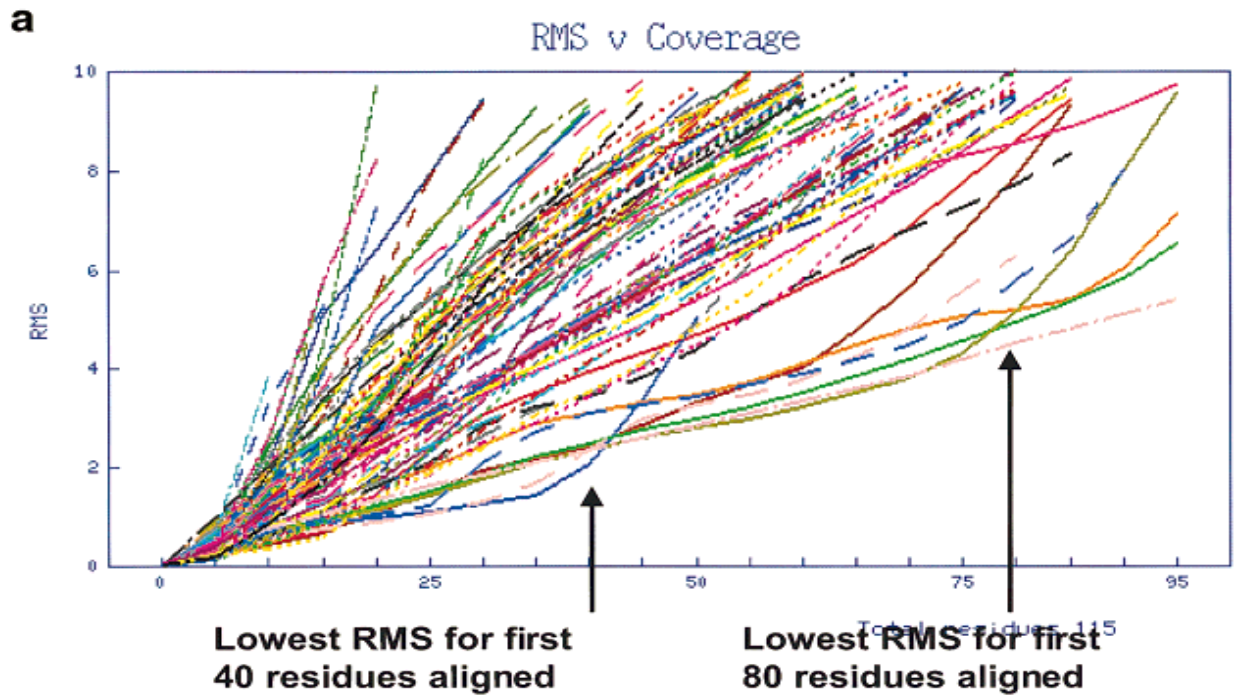


Figure 13 :RMS vs. Coverage[13].

4.4 Protein structure alignment by combinatorial extension (CE)[4]:

The alignment between two protein structures A and B of length nA and nB, respectively, is considered the longest continuous path P of AFPs of size m in a similarity matrix S, of size (nA – m)·(nB – m) representing all possible AFPs that conform to the criteria for structure similarity. One of the following three conditions should be satisfied for every two consecutive AFPs i and i+1 in the alignment path:

$p_{i+1}^{A} = p_i^{A} + m$ and $p_{i+1}^{B} = p_i^{B} + m$ 1

$p_{i+1}^{A} > p_i^{A} + m$ and $p_{i+1}^{B} = p_i^{B} + m$.....2

$p_{i+1}^{A} = p_i^{A} + m$ and $p_{i+1}^{B} > p_i^{B} + m$.....3

Where p^{A}_{i} is the AFP's is the starting residue position in protein A at the ith position in the alignment path; similarly for $p^{B}i$.

The alignment path is constructed from AFPs of fixed size m.That is, one fragment of length m from the first protein and another fragment from the second protein form a pair if they satisfy a similarity criterion described below. The first AFP starting the path can be selected at any position within the similarity matrix S, consecutive AFPs are added such that conditions (1–3) are satisfied.

We study the following three distance measures:

(i) distance Dij calculated using an 'independent' set of inter- residue distances, where each residue participates once and only once in the selected distance set:

$$Dij = 1/m(|d^{A}_{pi\,pi}{}^{A} - d^{B}_{pi\,pi}{}^{B}| + |d^{A}_{pi+m-1,pj}{}^{A}{}_{+m-1} - d^{B}_{pi+m-1,pj}{}^{B}{}_{+m-1}| + \sum_{k=1}^{m-2}(d^{A}_{pi+k,pj}{}^{A}{}_{+m-l-k} - d^{B}$$

$_{pi}{}^{B}{}_{+k,pj}{}^{B}{}_{+m-l-k}$))

……..1

(ii) distance Dij calculated using a full set of inter-residue distances, where all possible distances except those for neighboring residues are evaluated:
$|d^{A}{}_{p}{}^{A}{}_{i+k}, p_{j+l}{}^{A} - d^{B}{}_{p}{}^{B}{}_{i+k}, p_{j+l}{}^{B})|$

$$Dij = 1/m^2(\sum_{k=0}^{m-1} \sum_{l=0}^{m-1} / d^{A}{}_{p}{}^{A}{}_{i+k}, p_{j+l}{}^{A} - d^{B}{}_{p}{}^{B}{}_{i+k}, p_{j+l}{}^{B} |) \quad \text{……..2}$$

(iii) r.m.s.d obtained from structures optimally superimposed as rigid bodies using least square minimization. 3

Distance measure 1 is used to evaluate the combination of two AFPs, one already in the alignment path and one to be added.
Distance measure 2 is used to evaluate a single AFP .
3 is used as last step in selecting few best alignments and for optimizing gaps..

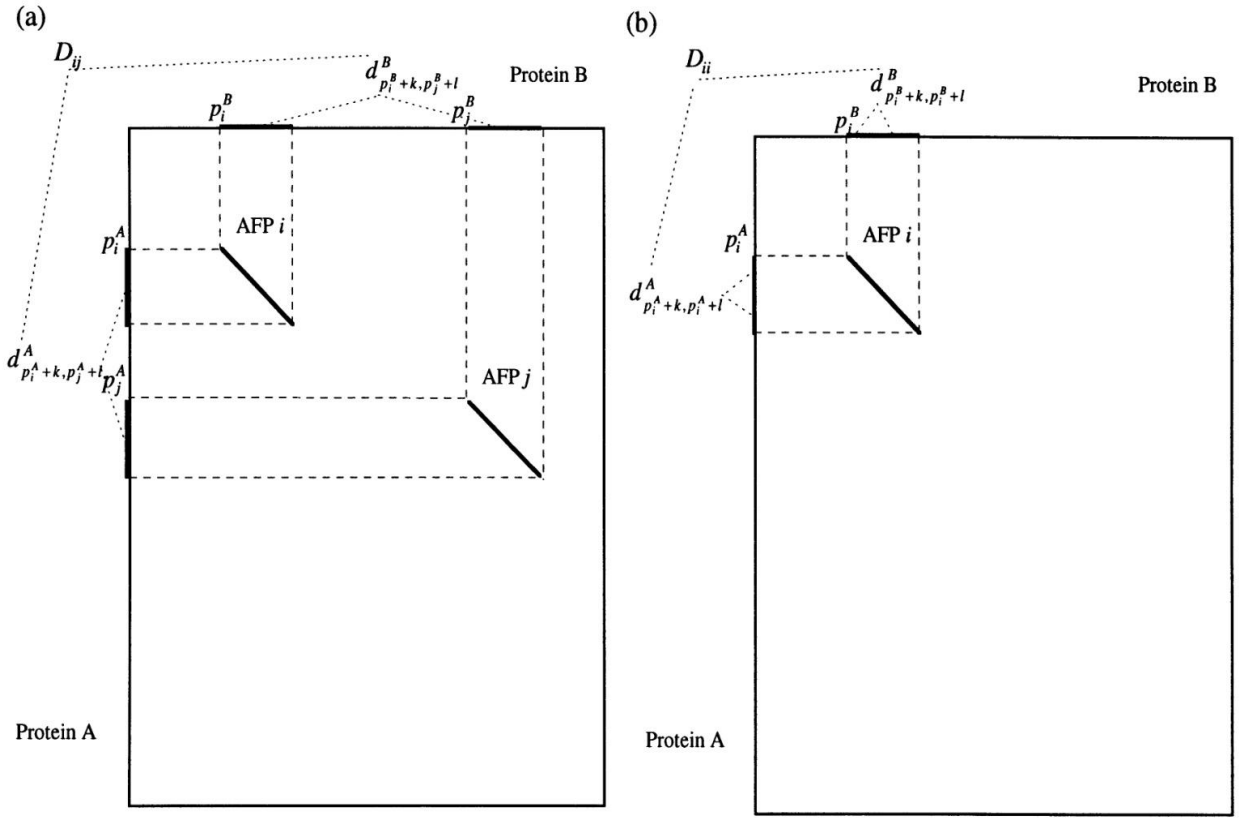


Figure14:Combinatorial Extension Algorithm[4].

Path extension strategy....

1. We can consider all possible AFPs that extend the path and satisfy similarity criteria.
2. consider only the best AFP..
3. use some intermediate strategy

Heuristics used for the extension of the path....
Decisions are made at three levels:

i) single AFP
ii) AFP against the path
iii) whole path

This result in following three conditions:

- Dnn < Do ……4
- 1/n-1 (Σ(i=0 to n-1))Din<D1.....5
- 1/n2 Σ(i=0 to n) Σ(j=0 to n)Dij<D1.....6

  Dij is the distance between aligned fragments defined by the AFPs i and j in the alignment path and n is the next AFP to be considered for addition to the alignment path of n-1 AFPs in length
  D_o = 3 angtrom
  D_1 = 4 angstrom

- All candidate AFP are selected on condition 4
- Best is chosen based on condition 5
- Decision to extend or terminate the path is made on condition 6.

4.5 TMalign[2]: TM-align, an algorithm to identify the structural alignment between protein pairs that combines the TM-score rotation matrix and Dynamic Programming.

- TM-align employs the backbone C-alpha coordinates of the given protein structures.
- Three kinds of quickly identified initial alignments are exploited. The first type of initial alignment is obtained by aligning the secondary structures (SSs) of two proteins using dynamic programming.
- For a given residue, an SS state (alpha, beta or coil) is assigned based on the C-alpha coordinates of five neighboring residues, i.e. ith residue is assigned as alpha(beta) when
  $|d_{j, j+k} - \lambda_k{}^{\alpha(\beta)}| < \delta^{\alpha(\beta)}$ (j=i-2,i-1 : k=2,3,4,)
  is satisfied for all $d_{j, j+k}$
  Otherwise it is assigned to be a coil.
- The second type of initial alignment is based on the gapless matching of two structures..
- The third initial alignment is also obtained by DP using a gap-opening penalty of 1, but the score matrix is a half/half combination of the SS score matrix and the distance score matrix selected in the second initial alignment.
- The above-obtained initial alignments are submitted to a heuristic iterative algorithm.
- In this procedure, we first rotate the structures by the TMscore rotation matrix based on the aligned residues in the initial alignments.
  The score similarity matrix is defined as
- $S(i, j) = 1/1+d^2_{ij}/d_o(Lmin)^2$
- Where dij is the distance of the ith residue in structure 1 and the jth residue in structure 2 under the TM-score superposition.
- $d_o(Lmin) = 1.24 * cuberoot(Lmin-15)-1.8$
- Lmin is the length of smaller protein.
- A new alignment can be obtained by implementing DP on the matrix S(i, j) with an

optimal gap opening penalty of 0.6.

- We then again superimpose the structures by the TM-score rotation matrix according to the new alignment and obtain a newer alignment by implementing DP with the new score matrix.
- The procedure is repeated until the alignment becomes stable and the alignment with the Highest TM-score is returned.
- To have a single scoring function that can reasonably assess the alignment quality and balance the coverage and accuracy,we use the TM-score, which is defined as

$$\text{TM-score} = \text{Max}\left[\frac{1}{L_{\text{Target}}}\sum_{i}^{L_{\text{ali}}}\frac{1}{1+\left(\frac{d_i}{d_0\left(L_{\text{Target}}\right)}\right)^2}\right].$$

- L_{Target} is the length of target protein.
- L_{ali} is the number of aligned residues.
- d_i is the distance between the ith pair of aligned residues.
- $d_o(L_{target})$= 1.24 * cuberoot(L_{target}-15)-1.8
- that normalizes the distance so that the average TM-score is not dependent on the protein size for random structure pairs.

5 Methodology:

5.1 Idea behind TMscore[5,]: TM-score use an iterative search algorithm to find the spatially optimal superposition of the template and the native structure. Starting with an initial fragment of the template that consists of L_{int} *neighboring aligned residues, we superposed* the fragment to the corresponding residues of the native structure according to rotation matrix. Then, we collected all of the residues of the template with distance to native of less than *d0 and* superposed this set of residues onto the native structure again. The process was repeated till the rotation matrix converged. Since the converged superposition is usually sensitive to the initial selection of the fragment L_{int}, *we ran an* iterative process with *n_ali, n_ali /2, n_ali /4… 4, respectively*. With L_{int}, *we ran all the iterations with the* location of initial fragments shifting continuously from the N- to the C-terminus. The rotation matrix with the highest TM-score was selected.

Step by step description:

- We have pdb file of protein 1 and x, y, and z coordinates and residue sequence number of all the residues from protein 1.
- Likewise, We have pdb file of protein 2 and x,y, and z coordinates and residue sequence number of all the residues from protein 2 i.e.target protein.
- Picking the aligned residues say n_ali.
- Calculation of parameters: d_0,d0_search
- d_0=1.24*(nseqB-15)**(1.0/3.0)-1.8
- if(d_0.lt.0.5)d_0=0.5
- d0_search=d0 if(d0_search.gt.8)d0_search=8 if(d0_search.lt.4.5)d0_search=4.5
- Formation of a list L_ini whose elements are [n_ali, n_ali/2, n_ali/4, n_ali/8, n_ali/16….4].
- Now pick one by one element of the list and do the following calculations.
- Say first element n_ali
- Store the coordinates in the lists for protein structure 1 and 2.
- Perform rotation.
- Output will be a rotation matrix and translation vector for the optimal superposition.
- Apply that rotation matrix to all of c-alpha of protein 1.
- Do scoring
  for all 1,n_ali:
- Calculate distance between the corresponding c-alpha atoms in two structures.
- Count the residues and store the residues position for which distance is less than threshold.
- And calculate
  score_sum=score_sum+1/(1+(dis/d_0)**2)
- If the counts of atoms for which the distance is less than 3(i.e. n_cut<3) but n_ali>3:
  increase the threshold value of the distance with .5 and repeat the procedure till n_cut>3

- Calculate: score=score_sum/float(nseqB)
  This is actually TM-score value.
- Store the value of maximum score and corresponding residue position.
- Next for 20 number of iterations:
  for those residues position for which distance was less than the threshold retrieve their coordinates and perform rotation.

- Apply the result of rotation matrix to all the c-alpha atom positions:
- Now for rotated structure 1 and other structure 2:
- Call the scoring function: Calculate the no: of residues for which the distance is less than the threshold(say n_cut)
  for every residue 1,n_ali calculate scoring:
- score_sum=score_sum+1/(1+(dis/d_0)**2)
- Now if n_cut<3 but n_ali>3:
  increase the distance threshold with .5 and again perform the above scoring .repeat the procedure until I get n_cut>3.
  And calculate:
  score =score_sum/float(nseqB) which is TMscore…
- Best iteration which gives maximum TMscore is stored….
- Whole above procedure is repeated for the rest of elements of the list:
  [n_ali, n_ali/2, n_ali/4, n_ali/8, n_ali/16….4]
  and with their correspoding shifts as well ..
  and the one that gives me value of maximum TMscore is finally printed out.

5.2 Modification of TM-score:

- In scoring function we are calculating the distances between the corresponding c-alpha and c-alpha positions.
- So, I calculated the centre of masses for each residue position in both the proteins.
- After i get the rotation matrix[21,22], i apply that to all the atoms and get the new coordinates for each and every atom.
- Next,i multiply respective positions with their respective masses in a single residue and divide that with sum of all the masses of atoms[19].

  center_of _mass_x = $\sum x_i * m_i / \sum m_i$

  And calculated the distances between their centres of masses and used those distances in the scoring function instead of C-alpha C-alpha distances…

  score_sum=score_sum+1/(1+(dis/d0)**2)
- I ran this on 602 protein structure alignments and compare the results with the original TMscore.
- Idea behind this was to take the weight age from each and every atom present in the residue.

5.3 Source Code:

```
import math
import sys
import time
tt = time.time()
print(tt)
def rotation(w,x,y,n,mode):
    xc=[None]*3
    yc=[None]*3
    wc=0.0
    rr=[None]*6
    ss=[None]*6
    e=[None]*3
    sqrt3 = 1.73205080756888
    tol = .01
#value of 1.0d-2 is tol value

    ip=[0,1,3,1,2,4,3,4,5]
    ip2312 = [1,2,0,1]
    rms=0.0
    e0=0.0
    t=[None]*3
    s1x = 0.0
    s1y = 0.0
    s1z = 0.0
    s2x = 0.0
    s2y = 0.0
    s2z = 0.0
    sxx = 0.0
    sxy = 0.0
    sxz = 0.0
    syx = 0.0
    syy = 0.0
    syz = 0.0
    szx = 0.0
    szy = 0.0
    szz = 0.0
    u= [[None]*3 for i in range(3)]
    r= [[None]*3 for i in range(3)]
    a= [[None]*3 for i in range(3)]
    b= [[None]*3 for i in range(3)]
    for i in range(0,3,1):
        xc[i] = 0.0
        yc[i] = 0.0
        t[i] =  0.0
        for j in range(0,3,1):
```

```
            r[j][i]=0.0
            u[j][i]=0.0
            a[j][i]=0.0
            if i == j:
               u[j][i]=1.0
               a[j][i]=1.0

    #print("u",u,"a",a,"r",r)
    #print("xc",xc,"yc",yc, "t",t)
    ier = -1
    if n < 1:
       return("no rotation possible")

    ier = -2

    for m in range(0,n,1):
           c1x = x[m][0]
        c1y = x[m][1]
        c1z = x[m][2]

        c2x = y[m][0]
        c2y = y[m][1]
        c2z = y[m][2]

        s1x = s1x + c1x
        s1y = s1y + c1y
        s1z = s1z + c1z

        s2x = s2x + c2x
        s2y = s2y + c2y
        s2z = s2z + c2z

        sxx = sxx + c1x*c2x
        sxy = sxy + c1x*c2y
        sxz = sxz + c1x*c2z

        syx = syx + c1y*c2x
        syy = syy + c1y*c2y
        syz = syz + c1y*c2z

        szx = szx + c1z*c2x
        szy = szy + c1z*c2y
        szz = szz + c1z*c2z
#         out.write('sxx')
#         out.write('%f \n' %(sxx))
#         out.write('sxy')
```

```
#         out.write('%f \n' %(sxy))
#         out.write('sxz')
#         out.write('%f \n' %(sxz))
#         out.write('syx')
#         out.write('%f \n' %(syx))
#         out.write('syy')
#         out.write("%f \n" %(syy))
#         out.write('syz')
#         out.write("%f \n" %(syz))
#         out.write('szx')
#         out.write('%f \n' %(szx))
#         out.write('szy')
#         out.write("%f \n" %(szy))
#         out.write('szz')
#         out.write("%f \n" %(szz))

    xc[0] = s1x/n
    xc[1] = s1y/n
    xc[2] = s1z/n

    yc[0] = s2x/n
    yc[1] = s2y/n
    yc[2] = s2z/n
#    out.write('xc[0]')
#    out.write('%f \n' %(xc[0]))
#    out.write('xc[1]')
#    out.write('%f \n' %(xc[1]))
#    out.write('xc[2]')
#    out.write('%f \n' %(xc[2]))
#    out.write('yc[0]')
#    out.write('%f \n' %(yc[0]))
#    out.write('yc[1]')
#    out.write('%f \n' %(yc[1]))
#    out.write('yc[2]')
#    out.write('%f \n' %(yc[2]))
    for m in range(0,n,1):
        for i in range(0,3,1):
            e0 = e0+ pow((x[m][i]-xc[i]),2)+(pow((y[m][i]-yc[i]),2))
#         out.write('x[m][i]')
#         out.write('%f  \n' %(x[m][i]))
#         out.write('y[m][i]')
#         out.write('%f \n' %(y[m][i]))
#         out.write('xc[i]')
#         out.write('%f \n' %(xc[i]))
#         out.write('yc[i]')
#         out.write('%f \n' %(yc[i]))
```

```
#    out.write('e0')
#    out.write('%f \n' %(e0))

    r[0][0] = sxx-s1x*s2x/n
    r[0][1] = sxy-s1x*s2y/n
    r[0][2] = sxz-s1x*s2z/n
    r[1][0] = syx-s1y*s2x/n
    r[1][1] = syy-s1y*s2y/n
    r[1][2] = syz-s1y*s2z/n
    r[2][0] = szx-s1z*s2x/n
    r[2][1] = szy-s1z*s2y/n
    r[2][2] = szz-s1z*s2z/n



#    out.write('r[0][0] r[0][1] r[0][2] r[1][0] r[1][1] r[1][2] r[2][0] r[2][1] r[2][2]')
    print('r[0][0] r[0][1] r[0][2] r[1][0] r[1][1] r[1][2] r[2][0] r[2][1] r[2][2]')
    print(r[0][0], r[0][1], r[0][2], r[1][0], r[1][1], r[1][2], r[2][0], r[2][1], r[2][2])
#    out.write('%f \n' %(r[0][0]))
#    out.write('%f \n' %(r[0][1]))
#    out.write('%f \n' %(r[0][2]))
#    out.write('%f \n' %(r[1][0]))
#    out.write('%f \n' %(r[1][1]))
#    out.write('%f \n' %(r[1][2]))
#    out.write('%f \n' %(r[2][0]))
#    out.write('%f \n' %(r[2][1]))
#     out.write('%f \n' %(r[2][2]))
    #print("r",r)

    det                =                (r[0][0]*(r[1][1]*r[2][2]-r[2][1]*r[1][2]))-(r[1][0]*(r[0][1]*r[2][2]-
r[2][1]*r[0][2]))+r[2][0]*(r[0][1]*r[1][2]-r[1][1]*r[0][2])
#    out.write('det')
#    out.write('%f \n'%(det))
    sigma=det


    m = 0
    for j in range(0,3,1):
        for i in range(0,j+1,1):
            rr[m] = (r[i][0]*r[j][0]+r[i][1]*r[j][1]+r[i][2]*r[j][2])
            m=m+1
    #print('rr',rr)
#    out.write('rr')
#    out.write('%f %f %f %f %f %f' %(rr[0],rr[1],rr[2],rr[3],rr[4],rr[5]))

    spur = (rr[0]+rr[2]+rr[5])/3.0
```

```
#    out.write('spur')
#    out.write('%f \n' %(spur))

    cof = (((((rr[2]*rr[5]-rr[4]*rr[4])+rr[0]*rr[5])-rr[3]*rr[3])+rr[0]*rr[2])-rr[1]*rr[1])/3.0
    det=det*det
#    out.write('cof')
#    out.write('%f \n' %(cof))
#    out.write('det')
#    out.write('%f \n' %(det))
    #print('spur',spur)
    #print('cof',cof)
    #print('det_new',det)
    for i in range(0,3,1):
        e[i]=spur
#    out.write('e')
#    out.write('%f \t %f \t  %f \n'%(e[0],e[1],e[2]))
    #print('e',e)

    if spur<=0.0:
        for i in range(0,3,1):
            t[i]= ((yc[i]-u[0][i]*xc[0])-u[1][i]*xc[1])-u[2][i]*xc[2]

        for i in range(0,3,1):
            if e[i]<0.0:
                e[i]=0.0
            e[i]=math.sqrt(e[i])
        #print('e',e)
        ier = 0
        if e[1]<=(e[0]*.00001):
            ier = -1
        d = e[2]
        #print('ier',ier)
        #print('d',d)
        if sigma<0.0:
            d = -d
            if(e[1]-e[2])<=(e[0]*.00001):
                ier=-1
        d = d +e[1]+e[0]
#          out.write('d')
#          out.write('%f' %(d))
        #print('final_d','e1','e0',d,e[1],e[0])
        #print('e0',e0)
        #print('e0-d)',e0-d)
        rms = (e0-d)-d
        #print('rms',rms)
        if rms<0.0:
```

```
                rms = 0.0
                return(rms,u,t,ier)
#           out.write('rms')
#           out.write('%f' %(rms))

                #print('rms',rms)


    d = spur*spur
    h = d-cof
    g = (spur*cof-det)/2.0 - spur*h
#    out.write('d')
#    out.write('%f \n' %(d))
#    out.write('h')
#    out.write('%f \n' %(h))
#    out.write('g')
#    out.write('%f \n' %(g))
    #print('d','h','g',d,h,g)

    if h<=0.0:
        if mode==0:
            for i in range(0,3,1):
                if e[i]<0.0:
                    e[i]=0
                e[i]=math.sqrt(e[i])
            ier = 0
            if e[1]<=(e[0]*.00001):
                ier = -1
            d = e[2]
            #print('e0,e1,e2',e[0],e[1],e[2])
            #print('d latest',d)
            if sigma<0.0:
                d = -d
                ('d more latest',d)
                if(e[1]-e[2])<=(e[0]*.00001):
                    ier=-1
            d = d +e[1]+e[0]
#              out.write('d')
#              out.write('%f' %(d))
            #print('d more more latest',d)
            rms = (e0-d)-d
            #print('rms ',rms)
            if rms<0.0:
                rms = 0.0
                return(rms,u,t,ier)
```

```
                #print("rms",rms)

#               out.write('rms')
#               out.write('%f' %(rms))
        else:
            for l in range(0,2,1):
                d = 0.0
                for i in range(0,3,1):
                    b[l][i]=r[0][i]*a[l][0]+r[1][i]*a[l][1]+r[2][i]*a[l][2]
                    #print('l','i',l,i)
                    #print('b',b)
                    d =  d+pow(b[l][i],2)

                if d >0.0:
                    d = 1/math.sqrt(d)
                #print("one more d",d)
                for i in range(0,3,1):
                    b[l][i]=b[l][i]*d

            d = b[0][0]*b[1][0]+b[0][1]*b[1][1]+b[0][2]*b[1][2]
#               out.write('d')
#               out.write('%f \n' %(p))
            #print('end d',d)
            p = 0.0
            for i in range(0,3,1):
                b[1][i]=b[1][i]-d*b[0][i]

                p = p+pow(b[1][i],2)
#               out.write('p')
#               out.write('%f \n' %(p))

                #print('p_nw',p)
            if p<=tol:
                p = 1.0
                for i in range(0,3,1):

                    if p <math.fabs(b[0][i]):
                        break
                    p = math.fabs(b[0][i])

                    j = i

                k = ip2312[j]
                #print('k',k)
                l = ip2312[j+1]
                #print('l',l)
```

```
            p = math.sqrt(pow(b[0][k],2)+pow(b[0][l],2))

            if p <= .01:
                for i in range(0,3,1):
                    t[i]=((yc[i]-u[0][i]*xc[0])-u[1][i]*xc[1])-u[2][i]*xc[2]
#                     out.write('t[i]')
#                     out.write('%f \n' %(t[i]))
                for i in range(0,3,1):
                    if e[i]<0.0:
                        e[i]=0.0
                    e[i]=math.sqrt(e[i])
                ier = 0

                if e[1]<=(e[0]*.00001):
                    ier = -1
                d = e[2]
                if sigma<0.0:
                    d = -d
                    if(e[1]-e[2])<=(e[0]*.00001):
                        ier=-1
                d = d+e[1]+e[0]
                #print('d',d)
                rms = (e0-d)-d
                print('rms',rms)
                if rms<0.0:
                    rms=0.0
#                     out.write('rms')
#                     out.write('%f \n' %(rms))
                    print("rms,u,t,ier",rms,u,t,ier)
                return(rms,u,t,ier)




            b[1][j]=0.0
            b[1][k]= -b[0][l]/p
            b[1][l]= b[0][k]/p
#             out.write("b[1][j],b[1][k],b[1][l]",b[1][j],b[1][k],b[1][l])
#             out.write("%f %f %f "%(b[1][j],b[1][k],b[1][l]))
        else:
            p = 1.0/math.sqrt(p)
            #print("p at last and b",p,b)
            for i in range(0,3,1):
                b[1][i]=b[1][i]*p
#                 out.write('b[1][i]')
#                 out.write('%f' %(b[1][i]))
```

```
            b[2][0] = b[0][1]*b[1][2]-b[1][1]*b[0][2]
            b[2][1] = b[0][2]*b[1][0]-b[1][2]*b[0][0]
            b[2][2] = b[0][0]*b[1][1]-b[1][0]*b[0][1]
#             out.write("b[2][0],b[2][1],b[2][2]")
#             out.write("%f %f %f " (b[2][0],b[2][1],b[2][2]))



            for j in range(0,3,1):
                for i in range(0,3,1):
                    u[i][j]= b[0][j]*a[0][i]+b[1][j]*a[1][i]+b[2][j]*a[2][i]
#                     out.write('i j')
#                     out.write('%d %d'%(i,j))
#                     out.write('u[i][j]')
#                     out.write('%f' %(u[i][j]))
            for i in range(0,3,1):
                t[i]=((yc[i]-u[0][i]*xc[0])-u[1][i]*xc[1])-u[2][i]*xc[2]
#                 out.write('t[i]')
#                 out.write('%f' %(t[i]))
            #print("t",t)

            for i in range(0,3,1):
                if e[i]<0.0:
                    e[i]=0.0
                e[i]=math.sqrt(e[i])
            ier = 0
            if e[1]<=(e[0]*.00001):
                ier = -1
            d = e[2]
            if sigma<0:
                d = -d
                if(e[1]-e[2])<=(e[0]*.00001):
                    ier=-1
            d = d +e[1]+e[0]
            rms = (e0-d)-d

            if rms<0.0:
                rms = 0.0
#             out.write('rms')
#             out.write('%f' %(rms))
            return(rms,u,t,ier)


    sqrth = math.sqrt(h)
    d = h*h*h-g*g
#   out.write('sqrth')
```

```
#    out.write('%f' %(sqrth))
#    out.write('d')
#    out.write('%f' %(d))
    if d<0.0:
        d = 0.0
    d1 = math.sqrt(d)
    d = (math.atan2(d1,-g))/3.0
#    out.write('other d')
#    out.write('%f \n' %(d))

    cth = sqrth*math.cos(d)
    sth = sqrth*sqrt3*math.sin(d)
#    out.write('cth')
#    out.write('%f \n' %(cth))
#    out.write('sth')
#    out.write('%f \n' %(sth))

    e[0]=(spur+cth)+cth
    e[1]=(spur-cth)+sth
    e[2]=(spur-cth)-sth

#    out.write('e[0]')
#    out.write('%f \n' %(e[0]))
#    out.write('e[1]')
#    out.write('%f \n' %(e[1]))
#    out.write('e[2]')
#    out.write('%f \n' %(e[2]))


    if mode==0:
        for i in range(0,3,1):
            if e[i]<0.0:
                e[i]=0.0
            e[i]=math.sqrt(e[i])
        ier = 0
        if e[1]<=(e[0]*.00001):
            ier = -1
        d = e[2]
        if sigma<0.0:
            d = -d
            if(e[1]-e[2])<=(e[0]*.00001):
                ier=-1
        d = d +e[1]+e[0]
        rms = (e0-d)-d

        if rms<0.0:
```

```
            rms = 0.0
        return(rms,u,t,ier)

            #print('rms',rms)
#         out.write('rms')
#         out.write('%f' %(rms))
        #print('rms_old',rms)


   for l in range(0,3,2):
        d = e[l]
#         out.write('e[l]')
#         out.write('%f' %(d))
        ss[0]= (d-rr[2])*(d-rr[5])-rr[4]*rr[4]
        ss[1]= (d-rr[5])*rr[1]+rr[3]*rr[4]
        ss[2]= (d-rr[0])*(d-rr[5])-rr[3]*rr[3]
        ss[3]= (d-rr[2])*rr[3]+rr[1]*rr[4]
        ss[4]= (d-rr[0])*rr[4]+rr[1]*rr[3]
        ss[5]= (d-rr[0])*(d-rr[2])-rr[1]*rr[1]
#         #print("ss",ss)
#         out.write('ss[0] ss[1] ss[2] ss[3] ss[4] ss[5]')
#         out.write('%f \n' %(ss[0]))
#         out.write('%f \n' %(ss[1]))
#         out.write('%f \n' %(ss[2]))
#         out.write('%f \n' %(ss[3]))
#         out.write('%f \n' %(ss[4]))
#         out.write('%f \n' %(ss[5]))

        if math.fabs(ss[0])>=math.fabs(ss[2]):
            j = 1
            if math.fabs(ss[0])<math.fabs(ss[5]):
                j = 3
        elif math.fabs(ss[2])>=math.fabs(ss[5]):
            j = 2

        else:
            j = 3
        #print('j_old',j)
#         out.write('math.fabs(ss[0])')
#         out.write('%f \n' %(math.fabs(ss[0])))
#         out.write('math.fabs(ss[2])')
#         out.write('%f \n' %(math.fabs(ss[2])))
 #         out.write('math.fabs(ss[5])')
 ##          out.write('%f \n' %(math.fabs(ss[0])))
  #         out.write('above j')
  #         out.write('%d \n' %(j))
```

```
        d = 0.0
        j = 3*(j-1)
#         out.write('j')
#         out.write('%d \n' %(j))
        #print("j",j)

        for i in range(0,3,1):
            k = ip[i+j]
            #print("value of k ,l,i",k,l,i)
            a[l][i]=ss[k]
            d = d+ ss[k]*ss[k]
#             out.write('k')
#             out.write('%d \n'%(k))
#             out.write('a[l][i]')
#             out.write('%f \n' %(a[l][i]))
#             out.write('d')
#             out.write('%d \n' %(d))
        #print('d',d)
        if d>0.0:
            d = 1.0/math.sqrt(d)
#             out.write('d after sqroot')
#             out.write('%f \n' %(d))
        for i in range(0,3,1):
            a[l][i]=a[l][i]*d
#             out.write('new a(i,l)')
#             out.write('%f \n' %(a[l][i]))
            #print('a[l][i]',a[l][i])
    d = a[0][0]*a[2][0]+a[0][1]*a[2][1]+a[0][2]*a[2][2]
#   out.write('last d')
#   out.write('%f \n' %(d))
    #print('at last d',d)
    if (e[0]-e[1])>(e[1]-e[2]):
        m1=2
        m =0
    else:
        m1=0
        m=2
#   out.write('m1')
#   out.write('%d \n' %(m1))
#   out.write('m')
#   out.write('%d \n' %(m))
    p = 0.0
    #print('m1,m',m1,m)
    for i in range(0,3,1):
        a[m1][i]=a[m1][i]-d*a[m][i]
#         out.write('other a[m1][i]')
```

```
#           out.write('%f' %(a[m1][i]))
          #print('a[m1][i]',a[m1][i])
          p = p+pow(a[m1][i],2)
#           out.write('p')
#           out.write('%f' %(p))
    if p<=tol:
          p = 1.0
#           out.write('other p')
#           out.write('%f' %(p))
          for i in range(0,3,1):
                if p<math.fabs(a[m][i]):
                      break
                p = math.fabs(a[m][i])
                j = i
          k = ip2312[j]
          l = ip2312[j+1]
          #print('j k l',j,k,l)
          p = math.sqrt(pow(a[m][k],2)+pow(a[m][l],2))

          #print("nw_p",p)
          if p <=tol:
                for i in range(0,3,1):
                      t[i]=((yc[i]-u[0][i]*xc[0])-u[1][i]*xc[1])-u[2][i]*xc[2]
#                       out.write('t[i]')
#                       out.write('%f' %(t[i]))
                #print('t',t)
                for i in range(0,3,1):
                      if e[i]<0.0:
                            e[i]=0.0
                      e[i]=math.sqrt(e[i])
                ier = 0
                if e[1]<=(e[0]*.00001):
                      ier = -1
                d = e[2]
                if sigma<0.0:
                      d = -d
                      if(e[1]-e[2])<=(e[0]*.00001):
                            ier=-1
                d = d +e[1]+e[0]
                rms = (e0-d)-d

                if rms<0.0:
                      rms=0.0
#                 out.write('rms')
#                 out.write('%f \n' %(rms))
                return(rms,u,t,ier)
```

```
            a[m1][j]=0.0
            a[m1][k]=-a[m][l]/p
            a[m1][l]=a[m][k]/p
            #print("a[m1][j],a[m1][k],a[m1][l]",a[m1][j],a[m1][k],a[m1][l])
      else:
            p = 1.0/math.sqrt(p)
            for i in range(0,3,1):
                  a[m1][i]=a[m1][i]*p
#                   out.write('a[m1][i]')
#                   out.write("%f" %(a[m1][i]))
      a[1][0]=a[2][1]*a[0][2]-a[0][1]*a[2][2]
      a[1][1]=a[2][2]*a[0][0]-a[0][2]*a[2][0]
      a[1][2]=a[2][0]*a[0][1]-a[0][0]*a[2][1]
#     out.write('a[1][0]')
#     out.write("%f" %(a[1][0]))
#     out.write('a[1][1]')
#     out.write("%f" %(a[1][1]))
#     out.write('a[1][2]')
#     out.write("%f" %(a[1][2]))
      #print("a",a)
      for l in range(0,2,1):
            d = 0.0
            for i in range(0,3,1):
                  b[l][i]=r[0][i]*a[l][0]+r[1][i]*a[l][1]+r[2][i]*a[l][2]
#                   out.write('b[l][i]')
#                   out.write('%f \n' %(b[l][i]))

                  d =  d+pow(b[l][i],2)
#                   out.write('d')
#                   out.write('%f \n' %(d))
            if d >0.0:
                  d = 1/math.sqrt(d)
            for i in range(0,3,1):
                  b[l][i]=b[l][i]*d
#                   out.write('one more b(l,i)')
#                   out.write('%f' %(b[l][i]))
      d = b[0][0]*b[1][0]+b[0][1]*b[1][1]+b[0][2]*b[1][2]
#     out.write('one more d')
#     out.write('%f' %(d))
      p = 0.0
      for i in range(0,3,1):
            b[1][i]=b[1][i]-d*b[0][i]
```

```
        p = p+pow(b[1][i],2)
#         out.write('b[1][i]')
#         out.write('%f' %(b[1][i]))
#         out.write('p')
#         out.write('%f' %(p))
    if p<=tol:
        p = 1.0
        for i in range(0,3,1):
            if p <math.fabs(b[0][i]):
                continue
            p = math.fabs(b[0][i])
            j = i
        k = ip2312[j]
        l = ip2312[j+1]
        p = math.sqrt(pow(b[0][k],2)+pow(b[0][l],2))
        if p<= tol:
            for i in range(0,3,1):
                t[i]=((yc[i]-u[0][i]*xc[0])-u[1][i]*xc[1])-u[2][i]*xc[2]
            for i in range(0,3,1):
                if e[i]<0.0:
                    e[i]=0.0
                e[i]=math.sqrt(e[i])
            ier = 0

            if e[1]<=(e[0]*.00001):
                ier = -1
            d = e[2]
            if sigma<0.0:
                d = -d
                if(e[1]-e[2])<=(e[0]*.00001):
                    ier=-1
            d = d+e[1]+e[0]
            rms = (e0-d)-d
            if rms<0.0:
                rms=0.0
#             out.write('rms')
#             out.write('%f \n' %(rms))
            return(rms,u,t,ier)



        #print('p',p)
        b[1][j]=0.0

        b[1][k]=-b[0][l]/p
        b[1][l]= b[0][k]/p
```

```
    else:
            p = 1.0/math.sqrt(p)
            for i in range(0,3,1):
                    b[1][i]=b[1][i]*p
#                     out.write('b[1][i]')
#                     out.write('%f \n' %(b[1][i]))
    b[2][0] = b[0][1]*b[1][2]-b[1][1]*b[0][2]
    b[2][1] = b[0][2]*b[1][0]-b[1][2]*b[0][0]
    b[2][2] = b[0][0]*b[1][1]-b[1][0]*b[0][1]
#    out.write('b[2][0]')
#    out.write('%f \n' %(b[2][0]))
#    out.write('b[2][1]')
#    out.write('%f \n' %(b[2][1]))
 #   out.write('b[2][2]')
 #   out.write('%f \n' %(b[2][2]))

    for j in range(0,3,1):
            for i in range(0,3,1):
                    u[i][j]=b[0][j]*a[0][i]+b[1][j]*a[1][i]+b[2][j]*a[2][i]
#                     out.write('i j')
#                     out.write('%d %d' %(i,j))
 #                    out.write('u[j][i]')
#                     out.write('%f \n' %(u[j][i]))
    #print('u',u)

#            out.write('u[0][0]')
#            out.write('%f \n' %(u[0][0]))
#            out.write('u[1][0]')
#            out.write('%f \n' %(u[1][0]))
#            out.write('u[2][0]')
#            out.write('%f \n' %(u[2][0]))
#            out.write('u[0][1]')
#            out.write('%f \n' %(u[0][1]))
#            out.write('u[1][1]')
#            out.write('%f \n' %(u[1][1]))
#            out.write('u[2][1]')
 #           out.write('%f \n' %(u[2][1]))
 #           out.write('u[0][2]')
#            out.write('%f \n' %(u[0][2]))
#            out.write('u[1][2]')
#            out.write('%f \n' %(u[1][2]))
#            out.write('u[2][2]')
#            out.write('%f \n' %(u[2][2]))
    for i in range(0,3,1):
#            out.write('yc[i]')
#            out.write('%f \n' %(yc[i]))
```

```
#           out.write('xc[0]')
#           out.write('%f \n' %(xc[0]))
#           out.write('xc[1]')
#           out.write('%f \n' %(xc[1]))
#           out.write('xc[2]')
#           out.write('%f \n' %(xc[2]))
#           out.write('xc[2]')
#           out.write('%f \n' %(xc[2]))
#           out.write('u[0][i]')
#           out.write('%f \n' %(u[0][i]))
#           out.write('u[1][i]')
#           out.write('%f \n' %(u[1][i]))
#           out.write('u[2][i]')
#           out.write('%f \n' %(u[2][i]))
          t[i]=((yc[i]-u[0][i]*xc[0])-u[1][i]*xc[1])-u[2][i]*xc[2]
#           out.write('t[i]')
#           out.write('%f \n' %(t[i]))
#   out.write('e[0]')
#   out.write('%f \n' %(e[0]))
#   out.write('e[1]')
#   out.write('%f \n' %(e[1]))
#   out.write('e[2]')
 #   out.write('%f \n' %(e[2]))

   for i in range(0,3,1):
          if e[i]<0.0:
                e[i]=0.0
          e[i]=math.sqrt(e[i])
#           out.write('e[i]')
#           out.write('%f \n' %(e[i]))
   ier = 0
   if e[1]<=(e[0]*.00001):
          ier = -1
#   out.write('ier')
#   out.write('%f \n' %(ier))
   d = e[2]
   if sigma<0.0:
          d = -d
          if(e[1]-e[2])<=(e[0]*.00001):
                ier=-1
#           out.write('d')
#           out.write('%f \n' %(d))
#           out.write('ier')
#           out.write('%f \n' %(ier))

   d = d +e[1]+e[0]
```

```
#    out.write('d')
#    out.write('%f \n' %(d))
#    out.write('e0')
#    out.write('%f \n' %(e0))
    rms = (e0-d)-d
#    out.write('rms')
#    out.write('%f \n' %(rms))
    if rms<0.0:
            rms = 0.0
#    out.write('new rms')
#    out.write('%f \n' %(rms))

    if mode==0:
        return(rms)
    else:
        return(rms,u,t,ier)

def score_fun():
    d_tmp = d
#    out.write('d_tmp')
#    out.write('%f' %(d_tmp))
    n_cut =0
    score_sum=0
    i_ali=[None]*3000
    for k in range(0,n_ali):
        i = iA[k]
        j = iB[k]
#        out.write('i')
#        out.write('%d' %(i))
#        out.write('j')
#        out.write('%d' %(j))
#        out.write('xa[i]')
#        out.write('%f \n' %(i))
#        out.write('xb[j]')
#        out.write('%f \n' %(j))
#        out.write('ya[i]')
#        out.write('%f \n' %(i))
#        out.write('yb[j]')
#        out.write('%f \n' %(j))
#        out.write('za[i]')
#        out.write('%f \n' %(i))
#        out.write('zb[j]')
#        out.write('%f \n' %(j))
#        print('xt2[i]')
#        print(xt2[i])
#        print('yt2[i]')
```

```
#       print(yt2[i])
#       print('zt2')
#       print(zt2[i])
      dis=      math.sqrt(pow((xt2[i]-      x2_final[j]),2)+pow((yt2[i]-y2_final[j]),2)+pow((zt2[i]-
z2_final[j]),2))
      out.write('distance inside score')
      out.write('%f \n' %(dis))
      if dis<d_tmp:

         i_ali[n_cut]=k
         n_cut=n_cut+1

      score_sum = score_sum+1/(1+(dis/d0)**2)
   score = score_sum/float(nseqB)
#   out.write('scores')
#   out.write('%f' %(score))
#   print('score')
#   print('%f' %(score))
#   out.write('n_cut')
#   out.write('%d' %(n_cut))

   while n_cut<3 and n_ali>3:
      d_tmp= d_tmp+.5
      n_cut =0
      score_sum=0
      for k in range(0,n_ali):
         i = iA[k]
         j = iB[k]
#          out.write('xa[i]')
#          out.write('%f \n' %(i))
#          out.write('xb[j]')
#          out.write('%f \n' %(j))
#          out.write('ya[i]')
#          out.write('%f \n' %(i))
#          out.write('yb[j]')
#          out.write('%f \n' %(j))
#          out.write('za[i]')
#          out.write('%f \n' %(i))
#          out.write('zb[j]')
#          out.write('%f \n' %(j))
#          print('i')
#          print(i)
#          print('j')
#          print(j)
#          print('xt2[i]')
#          print(xt2[i])
```

```
#           print('yt2')
#           print(yt2[i])
#           print('zt2')
#           print(zt2[i])
#           print("x2_final[j]")
#           print(x2_final[j])
#           print('y2_final[j]')
#           print(y2_final[j])
#           print('z2_final[j]')
#           print(z2_final[j])

          dis=          math.sqrt(pow((xt2[i]-x2_final[j]),2)+pow((yt2[i]-y2_final[j]),2)+pow((zt2[i]-
z2_final[j]),2))
          out.write('distance inside score')
          out.write('%f \n' %(dis))
          if dis<d_tmp:
             print('ncut inside inside score',n_cut)
             i_ali[n_cut]=k
             n_cut=n_cut+1
          score_sum = score_sum+1/(1+(dis/d0)**2)
       score = score_sum/float(nseqB)
#    out.write('scoreinside')
#    out.write('%f \n' %(score))
    print('score')
    print('%f \n' %(score))
    return(score,n_cut,i_ali)
p1 =open(sys.argv[1],'r')
p2 =open(sys.argv[2],'r')
#p1 = open(input('enter the pdb file/1'),'r')
#p2 = open(input('enter the pdb file/2'),'r')
out = open('result_python_TMscore.txt','w')
line1 = p1.readline()
line2 = p2.readline()
count1 = 0
count2 = 0
x1=[]
y1=[]
z1=[]
x2=[]
y2=[]
z2=[]
xa=[]
ya=[]
za=[]
xb=[]
yb=[]
```

```
zb=[]
nresA=[]
nresB=[]
res_seq1=[]
res_seq2=[]
iA=[]
iB=[]
w=[]
L_ini=[]
k_ali=[None]*3000
k_ali0=[None]*3000
xt = [None]*3000
yt = [None]*3000
zt = [None]*3000
r_1 = [[None]*3 for i in range(3000)]
r_2 = [[None]*3 for i in range(3000)]
r_3 = [[None]*3 for i in range(3000)]
t = [None]*3
u = [[None]*3 for i in range (3)]
x1_atoms =[]
y1_atoms =[]
z1_atoms =[]
atom_name_1 =[]
x2_atoms =[]
y2_atoms =[]
z2_atoms =[]
atom_name_2 =[]
xt2=[None]*3000
yt2=[None]*3000
zt2=[None]*3000
x2_final=[]
y2_final=[]
z2_final=[]
x_rotated_1 =[None]*40000
y_rotated_1 =[None]*40000
z_rotated_1 =[None]*40000


order = ['H', 'C', 'O', 'N', 'P', 'S']
masses = [1.6738e-24,1.994e-23,2.65e-23,2.32e-23,5.14e-23,5.31e-23]
serial_number1=[]
serial_number2=[]
res_seq11=[]
for line1 in p1:
    if 'ATOM' in line1[:6] and 'CA' in line1[13:17]:
        x1.append(float(line1[31:39]))
```

```
        y1.append(float(line1[39:47]))
        z1.append(float(line1[47:55]))
        res_seq1.append(int(line1[23:27]))
#         out.write('%f %f %f %d' %(x1[count1], y1[count1], z1[count1],res_seq1[count1]))
        count1= count1+1
        line1 = p1.readline()
p1.close()
p1 =open(sys.argv[1],'r')
while 1:
    line1 = p1.readline()
    if 'ATOM' in line1[:6]and('C' in line1[77:78] or'N' in line1[77:78]or 'H' in line1[77:78]or'O' in
line1[77:78] or'S' in line1[77:78]) :
        atom_name_1.append(line1[77:78])
        serial_number1.append(int(line1[7:12]))
        x1_atoms.append(float(line1[31:39]))
        y1_atoms.append(float(line1[39:47]))
        z1_atoms.append(float(line1[47:55]))
        res_seq11.append(int(line1[23:27]))
    if not line1:
        break
print('serial_number1')
print(serial_number1)
print('x1_atoms')
print(x1_atoms)

#print(x1,y1,z1)
#print('res_sequence',res_seq1)
#print('count/1',count1)
#print('serial_number1')
#print(serial_number1)
for line2 in p2:
    if 'ATOM' in line2[:6] and 'CA' in line2[13:17]:

        x2.append(float(line2[31:39]))
        y2.append(float(line2[39:47]))
        z2.append(float(line2[47:55]))
        res_seq2.append(int(line2[23:27]))
        line2= p2.readline()
        count2 = count2+1
p2.close()
res_seq33=[]
p2 =open(sys.argv[2],'r')
while 1:
    line2 = p2.readline()
    if'ATOM' in line2[:6] and('C' in line2[77:78] or'N' in line2[77:78]or 'H' in line2[77:78]or'O' in
line2[77:78] or'S' in line2[77:78]):
```

```
        atom_name_2.append(line2[77:78])
        serial_number2.append(int(line2[7:12]))
        x2_atoms.append(float(line2[31:39]))
        y2_atoms.append(float(line2[39:47]))
        z2_atoms.append(float(line2[47:55]))
        res_seq33.append(int(line2[23:27]))
    if not line2:
        break
print('x2_atoms')
print(x2_atoms)
print(len(x2))
print(len(x2_atoms))

x2_atoms_inter =0
y2_atoms_inter=0
z2_atoms_inter=0
tot_mass2=0

j=0
#print('x2_atoms')
#print(x2_atoms)
#print('res_seq33')
#print(res_seq33)
p = len(serial_number2)
for i in range(0,len(serial_number2),1):
    zz = order.index(atom_name_2[i])
    x2_atoms_inter = x2_atoms_inter+x2_atoms[i]*masses[zz]
    y2_atoms_inter = y2_atoms_inter+y2_atoms[i]*masses[zz]
    z2_atoms_inter = z2_atoms_inter+z2_atoms[i]*masses[zz]
    tot_mass2 = tot_mass2+masses[zz]
    if i!=(p-1) and res_seq33[i]!=res_seq33[i+1]:
        x2_final.append(x2_atoms_inter/tot_mass2)
        y2_final.append(y2_atoms_inter/tot_mass2)
        z2_final.append( z2_atoms_inter/tot_mass2)
        tot_mass2 = 0
        x2_atoms_inter =0
        y2_atoms_inter=0
        z2_atoms_inter=0

        j = j+1
    if i == p-1:
        x2_final.append(x2_atoms_inter/tot_mass2)
        y2_final.append(y2_atoms_inter/tot_mass2)
        z2_final.append(z2_atoms_inter/tot_mass2)
print('len_x2_final')
print(len(x2_final))
```

```
print('count2')
print(count2)


#       out.write('x2_final \n')
#       out.write(x2_final[j])
#       out.write('y2_final \n')
#       out.write(y2_final[j])
#       out.write('z2_final \n')
#       out.write(z2_final[j])

#print('p')
#print(p)

print('x2_final \n')
print(x2_final)
print('y2_final \n')
print(y2_final)
print('z2_final \n')
print(z2_final)
print('j')
print(j)
print('p')
print(p)
print('len-of_x2')
print(len(x2_final))
print('len_of_x2')
print(len(x2))

xa= list(x1)
ya= list(y1)
za= list(z1)
xb= list(x2)
yb= list(y2)
zb= list(z2)
x1_atoms_inter =0
#print('count1')
#print(count1)
for m in range(0,count1,1):
   w.append(float(1.0))
for i in range(0,count1,1):
   nresA.append(i)
#print('nresA',nresA)
for i in range(0,count2,1):
   nresB.append(i)
#print('nresB',nresB)
```

```
k =0
for i in range(0,count1,1):
    for j in range(0,count2,1):
        if nresA[i]== nresB[j]:
            print('nresA[i]')
            print(nresA[i])
            iA.append(i)
            iB.append(j)
            out.write('iA iB')
            out.write('%d %d'%(iA[k], iB[k]))
            k = k+1
            break
n_ali=k
#print('n_ali')
#print(n_ali)

Lcomm = n_ali
nseqA = count1
nseqB = count2
if n_ali<1:
    TM=0
    Rcomm=0
    print('TM','Rcomm',TM,Rcomm)
    sys.exit()
d0=1.24*(nseqB-15)**(1.0/3.0)-1.8
if d0<0.5:
    d0=0.5
d0_search = d0

if d0_search>8:
    d0_search = 8

if d0_search<4.5:
    d0_search = 4.5
n_it = 20
d_output=5
n_init_max=6
n_init =0
L_ini_min=4
if n_ali<4:
    L_ini_min = n_ali

for i in range(0,n_init_max):
    L_ini.append(int(n_ali/2**(n_init)))
    if L_ini[n_init]<=L_ini_min:
```

```
        L_ini[n_init]=L_ini_min
        break
    n_init = n_init+1
#out.write('L_ini total')
#out.write('%d %d %d %d %d' %(L_ini[0],L_ini[1],L_ini[2],L_ini[3],L_ini[4]))
if len(L_ini)==6 and  L_ini[5]>4:
    L_ini.append(L_ini_min)
#    out.write('L_ini total')
#    out.write('%d %d %d %d %d %d' %(L_ini[0],L_ini[1],L_ini[2],L_ini[3],L_ini[4],L_ini[5]))
#print("L_ini",L_ini)
score_max = -1
for i_init in range(0,n_init):
    L_init = int(L_ini[i_init])
    iL_max = int(n_ali-L_init+1)
#    out.write('L_init iL_max')
#    out.write('%d  %d'%(L_init, iL_max))

#    print('r_1',r_1)
#    print('r_2',r_2)
    for iL in range(0,iL_max):
        LL=0
        ka=0
        print('L_init',L_init)
        for i in range(0,int(L_init)):
            k = iL+i
            p = iA[k]
            q = iB[k]
#            out.write('k')
#            out.write('%d' %(k))
#           out.write('p')
#            out.write('%d' %(p))
#            out.write('%d' %(q))

            r_1[i][0]=xa[p]
            r_1[i][1]=ya[p]
            r_1[i][2]=za[p]
            r_2[i][0]=xb[q]
            r_2[i][1]=yb[q]
            r_2[i][2]=zb[q]
            LL=LL+1
#            out.write('k')
#            out.write('%d \n' %(k))
#            out.write('r_1[i][0]')
#            out.write('%f \n' %(r_1[i][0]))
#             out.write('r_1[i][1]')
 #           out.write('%f \n' %(r_1[i][1]))
```

```
#           out.write('r_1[i][2]')
#           out.write('%f \n' %(r_1[i][2]))
#           out.write('r_2[i][0]')
#           out.write('%f \n' %(r_2[i][0]))
#           out.write('r_2[i][1]')
 #          out.write('%f \n' %(r_2[i][1]))
 ##           out.write('r_2[i][2]')
#           out.write('%f \n' %(r_2[i][2]))
          k_ali[ka]=k
          ka = ka+1
#           out.write('ka')
#           out.write('%d' %(ka))
      #print('p',p)
      #print('q',q)
      #print('xa[p]',xa[p])
      #print('ya[p]',ya[p])
      #print('za[p]',za[p])
      rms,u,t,ier = rotation(w,r_1,r_2,LL,1)
#       out.write('rms u t ier')
#       out.write('%g %g %g %g %g %g %g %g %g %g %g %g %g %g %d' %(rms,u[0][0],\
#       u[0][1],u[0][2],u[1][0],u[1][1],u[1][2],u[2][0],u[2][1],u[2][2],t[0],\
#       t[1],t[2],ier))
      print('rms,u,t,ier')
      print(rms,u,t,ier)
      if i_init==0:
         armsd = math.sqrt(rms/LL)
         rmsd_ali = armsd
#           out.write('rms of superposed region')
#           out.write('%f' %(rms))
#           out.write('LL')
#           out.write('%d' %(LL))

      for j in range(0,nseqA):
         xt[j]=t[0]+u[0][0]*xa[j]+u[1][0]*ya[j]+u[2][0]*za[j]
         yt[j]=t[1]+u[0][1]*xa[j]+u[1][1]*ya[j]+u[2][1]*za[j]
         zt[j]=t[2]+u[0][2]*xa[j]+u[1][2]*ya[j]+u[2][2]*za[j]



      for j in range(0,len(serial_number1),1):
         x_rotated_1[j] = t[0]+u[0][0]*x1_atoms[j]+u[1][0]*y1_atoms[j]+u[2][0]*z1_atoms[j]
         y_rotated_1[j] = t[1]+u[0][1]*x1_atoms[j]+u[1][1]*y1_atoms[j]+u[2][1]*z1_atoms[j]
         z_rotated_1[j] = t[2]+u[0][2]*x1_atoms[j]+u[1][2]*y1_atoms[j]+u[2][2]*z1_atoms[j]

      x1_atoms_inter =0
      y1_atoms_inter=0
```

```
        z1_atoms_inter=0
        tot_mass1=0

        j =0
        m = len(serial_number1)
        xt2=[]
        yt2=[]
        zt2=[]
        for i in range(0,len(serial_number1),1):
            zz = order.index(atom_name_1[i])
            x1_atoms_inter = x1_atoms_inter+x_rotated_1[i]*masses[zz]
            y1_atoms_inter = y1_atoms_inter+y_rotated_1[i]*masses[zz]
            z1_atoms_inter = z1_atoms_inter+z_rotated_1[i]*masses[zz]
            tot_mass1 = tot_mass1+masses[zz]
            if i!=(m-1) and res_seq11[i]!=res_seq11[i+1]:
                xt2.append( x1_atoms_inter/tot_mass1)
                yt2.append( y1_atoms_inter/tot_mass1)
                zt2.append( z1_atoms_inter/tot_mass1)
                j = j+1
                tot_mass1 =0
                x1_atoms_inter =0
                y1_atoms_inter=0
                z1_atoms_inter=0

            if i== m-1:
                xt2.append(x1_atoms_inter/tot_mass1)
                yt2.append(y1_atoms_inter/tot_mass1)
                zt2.append(z1_atoms_inter/tot_mass1)

#       print('xt2')
#       print(xt2)
#       print('yt2')
#       print(yt2)
#       print('zt2')
#       print(zt2)
        print('xt2')
        print(len(xt2))
        print('yt2')
        print(len(yt2))
        print('zt2')
        print(len(zt2))
        print('count1')
        print(count1)


#       out.write('x2_final \n')
```

```
#       out.write(x2_final[j])
#       out.write('y2_final \n')
#       out.write(y2_final[j])
#       out.write('z2_final \n')
#       out.write(z2_final[j])


        d = d0_search-1
 #       out.write('d')
 #       out.write('%f \n'%(d))
        score,n_cut,i_ali = score_fun()
        print('score')
        print(score)
 #       out.write('score outside')
 #       out.write('%f \n' %(score))

        if score_max<score:
            score_max=score
            ka0 = ka
#             out.write('score_max')
#             out.write('%f \n' %(score_max))
#             out.write('ka0')
#             out.write('%f \n' %(ka0))
            for i in range(0,ka0):
                k_ali0[i]=k_ali[i]
#                 out.write('k_ali0[i]')
#                 out.write('%f \n' %(k_ali0[i]))
#             print('k_ali0000')
#             print(k_ali0)

        d = d0_search+1
        for it in range(1,n_it):
            LL=0
            ka=0
            for i in range(0,n_cut):
#                 print('i',i)
                m=i_ali[i]
#                 print('m',m)
#                 print('iA[m]',iA[m])
                r_1[i][0]=xa[iA[m]]
                r_1[i][1]=ya[iA[m]]
                r_1[i][2]=za[iA[m]]
                r_2[i][0]=xb[iB[m]]
                r_2[i][1]=yb[iB[m]]
                r_2[i][2]=zb[iB[m]]
#                 out.write('r_1[i][0]')
```

```
#              out.write('%f \n' %(r_1[i][0]))
#              out.write('r_1[i][1]')
#              out.write('%f \n' %(r_1[i][1]))
#              out.write('r_1[i][2]')
#              out.write('%f \n' %(r_1[i][2]))
#              out.write('r_2[i][0]')
#              out.write('%f \n' %(r_2[i][0]))
#              out.write('r_2[i][1]')
 #             out.write('%f \n' %(r_2[i][1]))
 #             out.write('r_2[i][2]')
 ##              out.write('%f \n' %(r_2[i][2]))
              LL=LL+1
#              print('ka')
#              print(ka)
              k_ali[ka]=m
#              print('k_ali[ka]')
#              print(k_ali[ka])
              ka = ka+1
#           print('r_1[i][0]r_1[i][1]r_1[i][2]r_2[i][0]r_2[i][1]r_2[i][2]')
#           print(r_1[i][0],r_1[i][1],r_1[i][2],r_2[i][0],r_2[i][1],r_2[i][2])
#           out.write('r_1[i][0]r_1[i][1]r_1[i][2]r_2[i][0]r_2[i][1]r_2[i][2]')
          rms,u,t,ier=rotation(w,r_1,r_2,LL,1)
#           print('rms,u,t,ier',rms,u,t,ier)
#           out.write('rms u t ier')
#           out.write('%g %g %g %g %g %g %g %g %g %g %g %g %g %d' %(rms,u[0][0],\
#           u[0][1],u[0][2],u[1][0],u[1][1],u[1][2],u[2][0],u[2][1],u[2][2],t[0],\
#           t[1],t[2],ier))
          for j in range(0,nseqA):
             xt[j]=t[0]+u[0][0]*xa[j]+u[1][0]*ya[j]+u[2][0]*za[j]
             yt[j]=t[1]+u[0][1]*xa[j]+u[1][1]*ya[j]+u[2][1]*za[j]
             zt[j]=t[2]+u[0][2]*xa[j]+u[1][2]*ya[j]+u[2][2]*za[j]
#              out.write('xt')
#              out.write('%f' %(xt[j]))
#              out.write('yt')
#              out.write('%f' %(yt[j]))
#              out.write('zt')
#              out.write('%f' %(zt[j]))

          for j in range(0,len(serial_number1),1):
             x_rotated_1[j] = t[0]+u[0][0]*x1_atoms[j]+u[1][0]*y1_atoms[j]+u[2][0]*z1_atoms[j]
             y_rotated_1[j] = t[1]+u[0][1]*x1_atoms[j]+u[1][1]*y1_atoms[j]+u[2][1]*z1_atoms[j]
             z_rotated_1[j] = t[2]+u[0][2]*x1_atoms[j]+u[1][2]*y1_atoms[j]+u[2][2]*z1_atoms[j]


          x1_atoms_inter =0
          y1_atoms_inter=0
```

```
        z1_atoms_inter=0
        tot_mass1=0
        xt2=[]
        yt2=[]
        zt2=[]

        j =0
        m = len(serial_number1)
        for i in range(0,len(serial_number1),1):
            zz = order.index(atom_name_1[i])
            x1_atoms_inter = x1_atoms_inter+x_rotated_1[i]*masses[zz]
            y1_atoms_inter = y1_atoms_inter+y_rotated_1[i]*masses[zz]
            z1_atoms_inter = z1_atoms_inter+z_rotated_1[i]*masses[zz]
            tot_mass1 = tot_mass1+masses[zz]
            if i!=(m-1) and res_seq11[i]!=res_seq11[i+1]:
                xt2.append(x1_atoms_inter/tot_mass1)
                yt2.append(y1_atoms_inter/tot_mass1)
                zt2.append(z1_atoms_inter/tot_mass1)
                j = j+1
                tot_mass1 =0
                x1_atoms_inter =0
                y1_atoms_inter=0
                z1_atoms_inter=0
            if i==m-1:
                xt2.append(x1_atoms_inter/tot_mass1)
                yt2.append(y1_atoms_inter/tot_mass1)
                zt2.append( z1_atoms_inter/tot_mass1)

        print('xt2')
        print(len(xt2))
        print('yt2')
        print(len(yt2))
        print('zt2')
        print(len(zt2))
        score,n_cut,i_ali = score_fun()
        #print('score,n_cut,i_ali',score,n_cut,i_ali)

        if score_max<score:
            score_max=score
#             out.write('score_max')
#             out.write('%f' %(score_max))
            ka0=ka
            for i in range(0,ka):
                k_ali0[i]=k_ali[i]
#                 out.write('k_ali0[i]')
#                 out.write('%f' %(k_ali0[i]))
```

```
            print('k_ali0[i]')
#               print(k_ali0)
        if it==n:
            break
        if n_cut==ka:
            neq=0
            for i in range(0,n_cut):
                if i_ali[i]==k_ali[i]:
                    neq=neq+1
            if n_cut==neq:
                break

#out.write('number of residues in common')
#out.write('%d' %(n_ali))
#out.write('rmsd of common residues')
#out.write('%f' %(rmsd_ali))
#out.write('TMscore   d0')
#out.write('%f %f' %(score_max,d0))
print('number of residues in common %d' %(n_ali))
print('rmsd of common residues %f' %(rmsd_ali))
print('TMscore   d0')
print('%f %f' %(score_max,d0))
cov = n_ali/count2
print('coverage')
print(cov)

TMfinal = score_max
print('TMfinal',TMfinal)
ttt = time.time()
tb = ttt-tt
print('time_taken')
print(tb)
out.close()
```

6. Results and Discussion:

6.1 Original TMscore

- Minimum coverage 0.10412
- maximum coverage 1.00000
- Average coverage0.798685
- min_aligned_length 53
- max_aligned_length 456
- min_rmsd 8.718909
- max_rmsd 25.813628
- min_tm_score 0.034275
- max_tm_score 0.230733
- Avg time taken 34.112822s
- average no: of residue in common144.990033
- Average rmsd of common residue 17.772953
- average TMscore 0.145405
- no of alignments between 0 and .17 477
- no of alignments between .4 and1 0

6.2 Modified TMscore

- Minimum coverage 0.10412
- maximum coverage 1.00000
- Average coverage0.798685
- min_aligned_length 53
- max_aligned_length 456
- min_rmsd 8.718909
- max_rmsd 25.813628
- min_tm_score 0.032508
- max_tm_score 0.225588
- avg time taken33.87848s
- average no: of residue in common 144.598006
- Average rmsd of common residue 17.7202
- Average Tmscore 0.136190
- no of alignments between 0 and .17 534
- no of alignments between .4 and1 0

6.3 Discussion, Conclusion and Future Work:

As, we can see there is no difference in the coverage value between the two algorithms. Average coverage value of the two algorithms and minimum and maximum coverage is the same in both cases, which is true, because as long as we don't change the dataset, they will remain same for the same proteins taken into consideration. As coverage is number of aligned residues divided by the target length [2]. The same explanation is for the aligned length as well in both the cases. It will remain same as long as we don't change the dataset. RMSD value also remains same. As long as we don't take centre of masses into account in the calculation of RMSD value, it will remain same. There is lower shift in case of TM-score evaluation in modified algorithm. When we take centre of masses into account, value of TMscore gets lower. In modified one, average time taken is lower than original. Average numbers of residues in common are same in both cases. In, case of original TMscore, if we calculate the number of random alignments, they are lower and their number gets higher in case of modified one.

The center of mass of a protein is an artificial point useful for detecting important and simple features of proteins structure, shape and association [19]. The center of mass of a protein is used for defining constraints useful to predict protein tertiary models, to assess the global shape of proteins in protein-protein complexes and to measure their distance. One explanation is that when we take centre of masses into account so it happens that in a particular residue position in protein A there is a residue which is compact and light weight but the corresponding residue in the protein B may be very wide and heavier so that there is a great shift in the centre of mass positions, hence high distances between them and finally low TMscore, as TMscore calculations are inversely proportional to the distance. But when we are comparing two model structures of the same protein, centre of mass can give us useful findings, because in that case we have same residue correspondence. In that case, taking centre of mass into consideration becomes a true evaluation criteria.

Suggestions for future work:

(1) Comparision of the center of mass of a protein chain of one protein with the center of mass of a protein chain of other protein, and take the distance between the two in scoring function.

(2) The center of mass of two proteins chains and takes their distance in scoring function;

(3) For multi-chains complexes the centers of mass and the distance for each pair of chains and take their distance in scoring function.

(4) The distance to the center of mass for specific protein amino acid(s); for example first calculating surface residues and core residues and then doing all distance calculations and take their distance in scoring function.

(5) The average distance to the center of mass for a list of protein residues and take that distance in the calculation of coring function.

(6) Evaluation of RMSD value with centre of masses in all the above cases.

(7) Redefine the d0 value when we are taking centre of masses into account

d0=1.24*(nseqB-15) ** (1.0/3.0)-1.8.

It shud have some high value.

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8Appendix

8.1 Results with original code:

```
time1340798447.825823

pdb_35/1amm_.pdb pdb_35/1amuA.pdb

number of residues in common174

rmsd of common residues19.737357

coverage0.341840

TMfinal0.097811

pdb_35/1amm_.pdb pdb_35/1amx_.pdb

number of residues in common150

rmsd of common residues19.891091

coverage1.000000

TMfinal0.143090

pdb_35/1amm_.pdb pdb_35/1an8_.pdb

number of residues in common174

rmsd of common residues17.630455

coverage0.844660

TMfinal0.169118

pdb_35/1amm_.pdb pdb_35/1an9A.pdb

number of residues in common174

rmsd of common residues18.921813

coverage0.511760

TMfinal0.115626

pdb_35/1amm_.pdb pdb_35/1aoa_.pdb

number of residues in common174
```

rmsd of common residues19.904385

coverage0.704450

TMfinal0.131195

pdb_35/1amm_.pdb pdb_35/1aocA.pdb

number of residues in common174

rmsd of common residues21.627235

coverage0.994280

TMfinal0.143718

pdb_35/1amm_.pdb pdb_35/1aoeA.pdb

number of residues in common174

rmsd of common residues19.318845

coverage0.906250

TMfinal0.145482

pdb_35/1amm_.pdb pdb_35/1aohA.pdb

number of residues in common143

rmsd of common residues19.966991

coverage1.000000

TMfinal0.161979

pdb_35/1amm_.pdb pdb_35/1aol_.pdb

number of residues in common174

rmsd of common residues18.983933

coverage0.763150

TMfinal0.145265

pdb_35/1amm_.pdb pdb_35/1aop_.pdb

number of residues in common174

rmsd of common residues17.459590

coverage0.381570

TMfinal0.096609

pdb_35/1amm_.pdb pdb_35/1aoy_.pdb

number of residues in common78

rmsd of common residues13.658349

coverage1.000000

TMfinal0.195342

pdb_35/1amm_.pdb pdb_35/1ap8_.pdb

number of residues in common174

rmsd of common residues19.524679

coverage0.816900

TMfinal0.145132

pdb_35/1amm_.pdb pdb_35/1apj_.pdb

number of residues in common74

rmsd of common residues12.787075

coverage1.000000

TMfinal0.164220

pdb_35/1amm_.pdb pdb_35/1apq_.pdb

number of residues in common53

rmsd of common residues11.308121

coverage1.000000

TMfinal0.178753

pdb_35/1amm_.pdb pdb_35/1aq0A.pdb

number of residues in common174

rmsd of common residues17.671342

coverage0.568620

TMfinal0.135122

pdb_35/1amm_.pdb pdb_35/1aqb_.pdb

number of residues in common174

rmsd of common residues20.675146

coverage0.994280

TMfinal0.197550

pdb_35/1amm_.pdb pdb_35/1aqcA.pdb

number of residues in common121

rmsd of common residues18.712583

coverage1.000000

TMfinal0.157286

pdb_35/1amm_.pdb pdb_35/1aqe_.pdb

number of residues in common110

rmsd of common residues16.502564

coverage1.000000

TMfinal0.143345

pdb_35/1amm_.pdb pdb_35/1aqt_.pdb

number of residues in common135

rmsd of common residues14.431519

coverage1.000000

TMfinal0.187136

pdb_35/1amm_.pdb pdb_35/1aquA.pdb

number of residues in common174

rmsd of common residues19.426155

coverage0.619210

TMfinal0.135132

pdb_35/1amm_.pdb pdb_35/1aqzA.pdb

number of residues in common142

rmsd of common residues19.681408

coverage1.000000

TMfinal0.153145

pdb_35/1amm_.pdb pdb_35/1at0_.pdb

number of residues in common142

rmsd of common residues18.693595

coverage1.000000

TMfinal0.161249

pdb_35/1amm_.pdb pdb_35/1at3A.pdb

number of residues in common174

rmsd of common residues18.870589

coverage0.801840

TMfinal0.163825

pdb_35/1amm_.pdb pdb_35/1atb_.pdb

pdb_35/1amm_.pdb pdb_35/1atg_.pdb

number of residues in common174

rmsd of common residues14.385261

coverage0.753240

TMfinal0.161386

pdb_35/1amuA.pdb pdb_35/1amm_.pdb

number of residues in common174

rmsd of common residues19.737357

coverage1.000000

TMfinal0.190308

pdb_35/1amuA.pdb pdb_35/1amp_.pdb

pdb_35/1amuA.pdb pdb_35/1amx_.pdb

number of residues in common150

rmsd of common residues22.218321

coverage1.000000

TMfinal0.155664

pdb_35/1amuA.pdb pdb_35/1an8_.pdb

number of residues in common206

rmsd of common residues21.721178

coverage1.000000

TMfinal0.163495

pdb_35/1amuA.pdb pdb_35/1an9A.pdb

number of residues in common340

rmsd of common residues21.114435

coverage1.000000

TMfinal0.193054

pdb_35/1amuA.pdb pdb_35/1aoa_.pdb

number of residues in common247

rmsd of common residues22.287718

coverage1.000000

TMfinal0.172720

pdb_35/1amuA.pdb pdb_35/1aocA.pdb

number of residues in common175

rmsd of common residues19.275388

coverage1.000000

TMfinal0.190400

pdb_35/1amuA.pdb pdb_35/1aoeA.pdb

number of residues in common192

rmsd of common residues22.245406

coverage1.000000

TMfinal0.163386

pdb_35/1amuA.pdb pdb_35/1aohA.pdb

number of residues in common143

rmsd of common residues21.324346

coverage1.000000

TMfinal0.161966

pdb_35/1amuA.pdb pdb_35/1aol_.pdb

number of residues in common228

rmsd of common residues19.585450

coverage1.000000

TMfinal0.194559

pdb_35/1amuA.pdb pdb_35/1aop_.pdb

number of residues in common456

rmsd of common residues21.696198

coverage1.000000

TMfinal0.230134

pdb_35/1amuA.pdb pdb_35/1aorA.pdb

pdb_35/1amuA.pdb pdb_35/1aoy_.pdb

number of residues in common78

rmsd of common residues15.107924

coverage1.000000

TMfinal0.181411

pdb_35/1amuA.pdb pdb_35/1aozA.pdb

pdb_35/1amuA.pdb pdb_35/1ap8_.pdb

number of residues in common213

rmsd of common residues20.312366

coverage1.000000

TMfinal0.169134

pdb_35/1amuA.pdb pdb_35/1apj_.pdb

number of residues in common74

rmsd of common residues18.672592

coverage1.000000

TMfinal0.178974

pdb_35/1amuA.pdb pdb_35/1apmE.pdb

pdb_35/1amuA.pdb pdb_35/1apq_.pdb

number of residues in common53

rmsd of common residues16.304880

coverage1.000000

TMfinal0.139662

pdb_35/1amuA.pdb pdb_35/1apxA.pdb

pdb_35/1amuA.pdb pdb_35/1aq0A.pdb

number of residues in common306

rmsd of common residues20.759635

coverage1.000000

TMfinal0.194609

pdb_35/1amuA.pdb pdb_35/1aqb_.pdb

number of residues in common175

rmsd of common residues21.475181

coverage1.000000

TMfinal0.155102

pdb_35/1amuA.pdb pdb_35/1aqcA.pdb

number of residues in common121

rmsd of common residues19.874976

coverage1.000000

TMfinal0.153017

pdb_35/1amuA.pdb pdb_35/1aqe_.pdb

number of residues in common110

rmsd of common residues17.688878

coverage1.000000

TMfinal0.212389

pdb_35/1amuA.pdb pdb_35/1aqt_.pdb

number of residues in common135

rmsd of common residues18.986028

coverage1.000000

TMfinal0.170840

pdb_35/1amuA.pdb pdb_35/1aquA.pdb

number of residues in common281

rmsd of common residues24.078919

coverage1.000000

TMfinal0.164127

pdb_35/1amuA.pdb pdb_35/1aqzA.pdb

number of residues in common142

rmsd of common residues19.554735

coverage1.000000

TMfinal0.157966

pdb_35/1amuA.pdb pdb_35/1at0_.pdb

number of residues in common142

rmsd of common residues20.442807

coverage1.000000

TMfinal0.135844

pdb_35/1amuA.pdb pdb_35/1at3A.pdb

number of residues in common217

rmsd of common residues22.425179

coverage1.000000

TMfinal0.164875

pdb_35/1amuA.pdb pdb_35/1atb_.pdb

pdb_35/1amuA.pdb pdb_35/1atg_.pdb

number of residues in common231

rmsd of common residues19.793872

coverage1.000000

TMfinal0.169708

pdb_35/1amx_.pdb pdb_35/1amm_.pdb

number of residues in common150

rmsd of common residues19.891091

coverage0.862060

TMfinal0.134778

pdb_35/1amx_.pdb pdb_35/1amp_.pdb

pdb_35/1amx_.pdb pdb_35/1amuA.pdb

number of residues in common150

rmsd of common residues22.218321

coverage0.294690

TMfinal0.079140

pdb_35/1amx_.pdb pdb_35/1an8_.pdb

number of residues in common150

rmsd of common residues19.393080

coverage0.728150

TMfinal0.122303

pdb_35/1amx_.pdb pdb_35/1an9A.pdb

number of residues in common150

rmsd of common residues20.638173

coverage0.441170

TMfinal0.115788

pdb_35/1amx_.pdb pdb_35/1aoa_.pdb

number of residues in common150

rmsd of common residues18.519452

coverage0.607280

TMfinal0.138593

pdb_35/1amx_.pdb pdb_35/1aocA.pdb

number of residues in common150

rmsd of common residues18.197335

coverage0.857140

TMfinal0.157869

pdb_35/1amx_.pdb pdb_35/1aoeA.pdb

number of residues in common150

rmsd of common residues17.193091

coverage0.781250

TMfinal0.171791

pdb_35/1amx_.pdb pdb_35/1aohA.pdb

number of residues in common143

rmsd of common residues17.186102

coverage1.000000

TMfinal0.178064

pdb_35/1amx_.pdb pdb_35/1aol_.pdb

number of residues in common150

rmsd of common residues18.837804

coverage0.657890

TMfinal0.120383

pdb_35/1amx_.pdb pdb_35/1aop_.pdb

number of residues in common150

rmsd of common residues19.634690

coverage0.328940

TMfinal0.088180

pdb_35/1amx_.pdb pdb_35/1aorA.pdb

pdb_35/1amx_.pdb pdb_35/1aoy_.pdb

number of residues in common78

rmsd of common residues14.528715

coverage1.000000

TMfinal0.179442

pdb_35/1amx_.pdb pdb_35/1aozA.pdb

pdb_35/1amx_.pdb pdb_35/1ap8_.pdb

number of residues in common150

rmsd of common residues22.776661

coverage0.704220

TMfinal0.121070

pdb_35/1amx_.pdb pdb_35/1apj_.pdb

number of residues in common74

rmsd of common residues11.751448

coverage1.000000

TMfinal0.198923

pdb_35/1amx_.pdb pdb_35/1apmE.pdb

pdb_35/1amx_.pdb pdb_35/1apq_.pdb

number of residues in common53

rmsd of common residues9.855834

coverage1.000000

TMfinal0.186915

pdb_35/1amx_.pdb pdb_35/1apxA.pdb

pdb_35/1amx_.pdb pdb_35/1aq0A.pdb

number of residues in common150

rmsd of common residues18.045554

coverage0.490190

TMfinal0.114406

pdb_35/1amx_.pdb pdb_35/1aqb_.pdb

number of residues in common150

rmsd of common residues16.281107

coverage0.857140

TMfinal0.175415

pdb_35/1amx_.pdb pdb_35/1aqcA.pdb

number of residues in common121

rmsd of common residues16.714081

coverage1.000000

TMfinal0.180817

pdb_35/1amx_.pdb pdb_35/1aqe_.pdb

number of residues in common110

rmsd of common residues15.002468

coverage1.000000

TMfinal0.200535

pdb_35/1amx_.pdb pdb_35/1aqt_.pdb

number of residues in common135

rmsd of common residues19.973741

coverage1.000000

TMfinal0.144835

pdb_35/1amx_.pdb pdb_35/1aquA.pdb

number of residues in common150

rmsd of common residues16.372136

coverage0.533800

TMfinal0.128734

pdb_35/1amx_.pdb pdb_35/1aqzA.pdb

number of residues in common142

rmsd of common residues17.044477

coverage1.000000

TMfinal0.156258

pdb_35/1amx_.pdb pdb_35/1at0_.pdb

number of residues in common142

rmsd of common residues15.354356

coverage1.000000

TMfinal0.166039

pdb_35/1amx_.pdb pdb_35/1at3A.pdb

number of residues in common150

rmsd of common residues18.043908

coverage0.691240

TMfinal0.150309

pdb_35/1amx_.pdb pdb_35/1atb_.pdb

pdb_35/1amx_.pdb pdb_35/1atg_.pdb

number of residues in common150

rmsd of common residues19.733939

coverage0.649350

TMfinal0.137481

pdb_35/1an8_.pdb pdb_35/1amm_.pdb

number of residues in common174

rmsd of common residues17.630455

coverage1.000000

TMfinal0.184803

pdb_35/1an8_.pdb pdb_35/1amp_.pdb

pdb_35/1an8_.pdb pdb_35/1amuA.pdb

number of residues in common206

rmsd of common residues21.721178

coverage0.404710

TMfinal0.100995

pdb_35/1an8_.pdb pdb_35/1amx_.pdb

number of residues in common150

rmsd of common residues19.393080

coverage1.000000

TMfinal0.142865

pdb_35/1an8_.pdb pdb_35/1an9A.pdb

number of residues in common206

rmsd of common residues22.110851

coverage0.605880

TMfinal0.111643

pdb_35/1an8_.pdb pdb_35/1aoa_.pdb

number of residues in common206

rmsd of common residues19.866652

coverage0.834000

TMfinal0.135950

pdb_35/1an8_.pdb pdb_35/1aocA.pdb

number of residues in common175

rmsd of common residues20.898762

coverage1.000000

TMfinal0.134125

pdb_35/1an8_.pdb pdb_35/1aoeA.pdb

number of residues in common192

rmsd of common residues18.545583

coverage1.000000

TMfinal0.187190

pdb_35/1an8_.pdb pdb_35/1aohA.pdb

number of residues in common143

rmsd of common residues16.850978

coverage1.000000

TMfinal0.175772

pdb_35/1an8_.pdb pdb_35/1aol_.pdb

number of residues in common206

rmsd of common residues20.349374

coverage0.903500

TMfinal0.149221

pdb_35/1an8_.pdb pdb_35/1aop_.pdb

number of residues in common206

rmsd of common residues19.277687

coverage0.451750

TMfinal0.107538

pdb_35/1an8_.pdb pdb_35/1aorA.pdb

pdb_35/1an8_.pdb pdb_35/1aoy_.pdb

number of residues in common78

rmsd of common residues12.626557

coverage1.000000

TMfinal0.175910

pdb_35/1an8_.pdb pdb_35/1aozA.pdb

pdb_35/1an8_.pdb pdb_35/1ap8_.pdb

number of residues in common206

rmsd of common residues20.841873

coverage0.967130

TMfinal0.169690

pdb_35/1an8_.pdb pdb_35/1apj_.pdb

number of residues in common74

rmsd of common residues14.370451

coverage1.000000

TMfinal0.164993

pdb_35/1an8_.pdb pdb_35/1apmE.pdb

pdb_35/1an8_.pdb pdb_35/1apq_.pdb

number of residues in common53

rmsd of common residues11.416533

coverage1.000000

TMfinal0.183252

pdb_35/1an8_.pdb pdb_35/1apxA.pdb

pdb_35/1an8_.pdb pdb_35/1aq0A.pdb

number of residues in common206

rmsd of common residues19.755022

coverage0.673200

TMfinal0.131333

pdb_35/1an8_.pdb pdb_35/1aqb_.pdb

number of residues in common175

rmsd of common residues17.852260

coverage1.000000

TMfinal0.162187

pdb_35/1an8_.pdb pdb_35/1aqcA.pdb

number of residues in common121

rmsd of common residues18.575698

coverage1.000000

TMfinal0.150636

pdb_35/1an8_.pdb pdb_35/1aqe_.pdb

number of residues in common110

rmsd of common residues16.580280

coverage1.000000

TMfinal0.157469

pdb_35/1an8_.pdb pdb_35/1aqt_.pdb

number of residues in common135

rmsd of common residues16.211305

coverage1.000000

TMfinal0.170834

pdb_35/1an8_.pdb pdb_35/1aquA.pdb

number of residues in common206

rmsd of common residues19.156693

coverage0.733090

TMfinal0.141976

pdb_35/1an8_.pdb pdb_35/1aqzA.pdb

number of residues in common142

rmsd of common residues17.080092

coverage1.000000

TMfinal0.180772

pdb_35/1an8_.pdb pdb_35/1at0_.pdb

number of residues in common142

rmsd of common residues19.193526

coverage1.000000

TMfinal0.157238

pdb_35/1an8_.pdb pdb_35/1at3A.pdb

number of residues in common206

rmsd of common residues20.984940

coverage0.949300

TMfinal0.153513

pdb_35/1an8_.pdb pdb_35/1atb_.pdb

pdb_35/1an8_.pdb pdb_35/1atg_.pdb

number of residues in common206

rmsd of common residues20.044364

coverage0.891770

TMfinal0.150510

pdb_35/1an9A.pdb pdb_35/1amm_.pdb

number of residues in common174

rmsd of common residues18.921813

coverage1.000000

TMfinal0.157156

pdb_35/1an9A.pdb pdb_35/1amp_.pdb

pdb_35/1an9A.pdb pdb_35/1amuA.pdb

number of residues in common340

rmsd of common residues21.114435

coverage0.667970

TMfinal0.157067

pdb_35/1an9A.pdb pdb_35/1amx_.pdb

number of residues in common150

rmsd of common residues20.638173

coverage1.000000

TMfinal0.176075

pdb_35/1an9A.pdb pdb_35/1an8_.pdb

number of residues in common206

rmsd of common residues22.110851

coverage1.000000

TMfinal0.142325

pdb_35/1an9A.pdb pdb_35/1aoa_.pdb

number of residues in common247

rmsd of common residues23.744534

coverage1.000000

TMfinal0.154496

pdb_35/1an9A.pdb pdb_35/1aocA.pdb

number of residues in common175

rmsd of common residues24.106042

coverage1.000000

TMfinal0.137275

pdb_35/1an9A.pdb pdb_35/1aoeA.pdb

number of residues in common192

rmsd of common residues20.100994

coverage1.000000

TMfinal0.170426

pdb_35/1an9A.pdb pdb_35/1aohA.pdb

number of residues in common143

rmsd of common residues22.315467

coverage1.000000

TMfinal0.148027

pdb_35/1an9A.pdb pdb_35/1aol_.pdb

number of residues in common228

rmsd of common residues22.570624

coverage1.000000

TMfinal0.162402

pdb_35/1an9A.pdb pdb_35/1aop_.pdb

number of residues in common340

rmsd of common residues25.813628

coverage0.745610

TMfinal0.130852

pdb_35/1an9A.pdb pdb_35/1aorA.pdb

pdb_35/1an9A.pdb pdb_35/1aoy_.pdb

number of residues in common78

rmsd of common residues14.169116

coverage1.000000

TMfinal0.192271

pdb_35/1an9A.pdb pdb_35/1aozA.pdb

pdb_35/1an9A.pdb pdb_35/1ap8_.pdb

number of residues in common213

rmsd of common residues23.593618

coverage1.000000

TMfinal0.147005

pdb_35/1an9A.pdb pdb_35/1apj_.pdb

number of residues in common74

rmsd of common residues12.764772

coverage1.000000

TMfinal0.160768

pdb_35/1an9A.pdb pdb_35/1apmE.pdb

pdb_35/1an9A.pdb pdb_35/1apq_.pdb

number of residues in common53

rmsd of common residues12.228052

coverage1.000000

TMfinal0.145656

pdb_35/1an9A.pdb pdb_35/1apxA.pdb

pdb_35/1an9A.pdb pdb_35/1aq0A.pdb

number of residues in common306

rmsd of common residues20.967718

coverage1.000000

TMfinal0.211753

pdb_35/1an9A.pdb pdb_35/1aqb_.pdb

number of residues in common175

rmsd of common residues21.244033

coverage1.000000

TMfinal0.139198

pdb_35/1an9A.pdb pdb_35/1aqcA.pdb

number of residues in common121

rmsd of common residues17.849008

coverage1.000000

TMfinal0.173408

pdb_35/1an9A.pdb pdb_35/1aqe_.pdb

number of residues in common110

rmsd of common residues17.093370

coverage1.000000

TMfinal0.171655

pdb_35/1an9A.pdb pdb_35/1aqt_.pdb

number of residues in common135

rmsd of common residues17.850258

coverage1.000000

TMfinal0.147447

pdb_35/1an9A.pdb pdb_35/1aquA.pdb

number of residues in common281

rmsd of common residues20.629246

coverage1.000000

TMfinal0.204471

pdb_35/1an9A.pdb pdb_35/1aqzA.pdb

number of residues in common142

rmsd of common residues21.376947

coverage1.000000

TMfinal0.160483

pdb_35/1an9A.pdb pdb_35/1at0_.pdb

number of residues in common142

rmsd of common residues19.934466

coverage1.000000

TMfinal0.142337

pdb_35/1an9A.pdb pdb_35/1at3A.pdb

number of residues in common217

rmsd of common residues21.600447

coverage1.000000

TMfinal0.155963

pdb_35/1an9A.pdb pdb_35/1atb_.pdb

pdb_35/1an9A.pdb pdb_35/1atg_.pdb

number of residues in common231

rmsd of common residues22.707749

coverage1.000000

TMfinal0.165446

pdb_35/1aoa_.pdb pdb_35/1amm_.pdb

number of residues in common174

rmsd of common residues19.904385

coverage1.000000

TMfinal0.154465

pdb_35/1aoa_.pdb pdb_35/1amp_.pdb

pdb_35/1aoa_.pdb pdb_35/1amuA.pdb

number of residues in common247

rmsd of common residues22.287718

coverage0.485260

TMfinal0.114788

pdb_35/1aoa_.pdb pdb_35/1amx_.pdb

number of residues in common150

rmsd of common residues18.519452

coverage1.000000

TMfinal0.179600

pdb_35/1aoa_.pdb pdb_35/1an8_.pdb

number of residues in common206

rmsd of common residues19.866652

coverage1.000000

TMfinal0.147074

pdb_35/1aoa_.pdb pdb_35/1an9A.pdb

number of residues in common247

rmsd of common residues23.744534

coverage0.726470

TMfinal0.133157

pdb_35/1aoa_.pdb pdb_35/1aocA.pdb

number of residues in common175

rmsd of common residues20.324616

coverage1.000000

TMfinal0.147082

pdb_35/1aoa_.pdb pdb_35/1aoeA.pdb

number of residues in common192

rmsd of common residues18.732762

coverage1.000000

TMfinal0.183886

pdb_35/1aoa_.pdb pdb_35/1aohA.pdb

number of residues in common143

rmsd of common residues17.853984

coverage1.000000

TMfinal0.160040

pdb_35/1aoa_.pdb pdb_35/1aol_.pdb

number of residues in common228

rmsd of common residues18.748010

coverage1.000000

TMfinal0.194825

pdb_35/1aoa_.pdb pdb_35/1aop_.pdb

number of residues in common247

rmsd of common residues20.653704

coverage0.541660

TMfinal0.130976

pdb_35/1aoa_.pdb pdb_35/1aorA.pdb

pdb_35/1aoa_.pdb pdb_35/1aoy_.pdb

number of residues in common78

rmsd of common residues11.218511

coverage1.000000

TMfinal0.230733

pdb_35/1aoa_.pdb pdb_35/1aozA.pdb

pdb_35/1aoa_.pdb pdb_35/1ap8_.pdb

number of residues in common213

rmsd of common residues22.275435

coverage1.000000

TMfinal0.176820

pdb_35/1aoa_.pdb pdb_35/1apj_.pdb

number of residues in common74

rmsd of common residues10.959227

coverage1.000000

TMfinal0.147874

pdb_35/1aoa_.pdb pdb_35/1apmE.pdb

pdb_35/1aoa_.pdb pdb_35/1apq_.pdb

number of residues in common53

rmsd of common residues8.718909

coverage1.000000

TMfinal0.167607

pdb_35/1aoa_.pdb pdb_35/1apxA.pdb

pdb_35/1aoa_.pdb pdb_35/1aq0A.pdb

number of residues in common247

rmsd of common residues17.877404

coverage0.807190

TMfinal0.185028

pdb_35/1aoa_.pdb pdb_35/1aqb_.pdb

number of residues in common175

rmsd of common residues19.626528

coverage1.000000

TMfinal0.148759

pdb_35/1aoa_.pdb pdb_35/1aqcA.pdb

number of residues in common121

rmsd of common residues15.433222

coverage1.000000

TMfinal0.186639

pdb_35/1aoa_.pdb pdb_35/1aqe_.pdb

number of residues in common110

rmsd of common residues12.482603

coverage1.000000

TMfinal0.196602

pdb_35/1aoa_.pdb pdb_35/1aqt_.pdb

number of residues in common135

rmsd of common residues17.687686

coverage1.000000

TMfinal0.172289

pdb_35/1aoa_.pdb pdb_35/1aquA.pdb

number of residues in common247

rmsd of common residues20.849604

coverage0.879000

TMfinal0.163272

pdb_35/1aoa_.pdb pdb_35/1aqzA.pdb

number of residues in common142

rmsd of common residues17.292341

coverage1.000000

TMfinal0.166220

pdb_35/1aoa_.pdb pdb_35/1at0_.pdb

number of residues in common142

rmsd of common residues17.197258

coverage1.000000

TMfinal0.176152

pdb_35/1aoa_.pdb pdb_35/1at3A.pdb

number of residues in common217

rmsd of common residues22.004300

coverage1.000000

TMfinal0.162685

pdb_35/1aoa_.pdb pdb_35/1atb_.pdb

pdb_35/1aoa_.pdb pdb_35/1atg_.pdb

number of residues in common231

rmsd of common residues20.104588

coverage1.000000

TMfinal0.214900

pdb_35/1aocA.pdb pdb_35/1amm_.pdb

number of residues in common174

rmsd of common residues21.627235

coverage1.000000

TMfinal0.144158

pdb_35/1aocA.pdb pdb_35/1amp_.pdb

pdb_35/1aocA.pdb pdb_35/1amuA.pdb

number of residues in common175

rmsd of common residues19.275388

coverage0.343810

TMfinal0.106930

pdb_35/1aocA.pdb pdb_35/1amx_.pdb

number of residues in common150

rmsd of common residues18.197335

coverage1.000000

TMfinal0.168430

pdb_35/1aocA.pdb pdb_35/1an8_.pdb

number of residues in common175

rmsd of common residues20.898762

coverage0.849510

TMfinal0.124236

pdb_35/1aocA.pdb pdb_35/1an9A.pdb

number of residues in common175

rmsd of common residues24.106042

coverage0.514700

TMfinal0.099422

pdb_35/1aocA.pdb pdb_35/1aoa_.pdb

number of residues in common175

rmsd of common residues20.324616

coverage0.708500

TMfinal0.124166

pdb_35/1aocA.pdb pdb_35/1aoeA.pdb

number of residues in common175

rmsd of common residues21.138997

coverage0.911450

TMfinal0.143963

pdb_35/1aocA.pdb pdb_35/1aohA.pdb

number of residues in common143

rmsd of common residues20.124257

coverage1.000000

TMfinal0.136864

pdb_35/1aocA.pdb pdb_35/1aol_.pdb

number of residues in common175

rmsd of common residues21.127731

coverage0.767540

TMfinal0.136826

pdb_35/1aocA.pdb pdb_35/1aop_.pdb

number of residues in common175

rmsd of common residues19.158489

coverage0.383770

TMfinal0.088759

pdb_35/1aocA.pdb pdb_35/1aorA.pdb

pdb_35/1aocA.pdb pdb_35/1aoy_.pdb

number of residues in common78

rmsd of common residues14.047876

coverage1.000000

TMfinal0.178581

pdb_35/1aocA.pdb pdb_35/1aozA.pdb

pdb_35/1aocA.pdb pdb_35/1ap8_.pdb

number of residues in common175

rmsd of common residues22.046566

coverage0.821590

TMfinal0.153637

pdb_35/1aocA.pdb pdb_35/1apj_.pdb

number of residues in common74

rmsd of common residues15.423336

coverage1.000000

TMfinal0.175206

pdb_35/1aocA.pdb pdb_35/1apmE.pdb

pdb_35/1aocA.pdb pdb_35/1apq_.pdb

number of residues in common53

rmsd of common residues12.779239

coverage1.000000

TMfinal0.158412

pdb_35/1aocA.pdb pdb_35/1apxA.pdb

pdb_35/1aocA.pdb pdb_35/1aq0A.pdb

number of residues in common175

rmsd of common residues18.924453

coverage0.571890

TMfinal0.121015

pdb_35/1aocA.pdb pdb_35/1aqb_.pdb

number of residues in common175

rmsd of common residues20.782697

coverage1.000000

TMfinal0.140680

pdb_35/1aocA.pdb pdb_35/1aqcA.pdb

number of residues in common121

rmsd of common residues20.300408

coverage1.000000

TMfinal0.140776

pdb_35/1aocA.pdb pdb_35/1aqe_.pdb

number of residues in common110

rmsd of common residues16.803439

coverage1.000000

TMfinal0.150510

pdb_35/1aocA.pdb pdb_35/1aqt_.pdb

number of residues in common135

rmsd of common residues20.246087

coverage1.000000

TMfinal0.149078

pdb_35/1aocA.pdb pdb_35/1aquA.pdb

number of residues in common175

rmsd of common residues19.468265

coverage0.622770

TMfinal0.142695

pdb_35/1aocA.pdb pdb_35/1aqzA.pdb

number of residues in common142

rmsd of common residues16.778563

coverage1.000000

TMfinal0.175465

pdb_35/1aocA.pdb pdb_35/1at0_.pdb

number of residues in common142

rmsd of common residues19.185779

coverage1.000000

TMfinal0.152799

pdb_35/1aocA.pdb pdb_35/1at3A.pdb

number of residues in common175

rmsd of common residues17.933026

coverage0.806450

TMfinal0.166659

pdb_35/1aocA.pdb pdb_35/1atb_.pdb

pdb_35/1aocA.pdb pdb_35/1atg_.pdb

number of residues in common175

rmsd of common residues19.326012

coverage0.757570

TMfinal0.145858

pdb_35/1aoeA.pdb pdb_35/1amm_.pdb

number of residues in common174

rmsd of common residues19.318845

coverage1.000000

TMfinal0.152715

pdb_35/1aoeA.pdb pdb_35/1amp_.pdb

pdb_35/1aoeA.pdb pdb_35/1amuA.pdb

number of residues in common192

rmsd of common residues22.245406

coverage0.377210

TMfinal0.098444

pdb_35/1aoeA.pdb pdb_35/1amx_.pdb

number of residues in common150

rmsd of common residues17.193091

coverage1.000000

TMfinal0.194077

pdb_35/1aoeA.pdb pdb_35/1an8_.pdb

number of residues in common192

rmsd of common residues18.545583

coverage0.932030

TMfinal0.181874

pdb_35/1aoeA.pdb pdb_35/1an9A.pdb

number of residues in common192

rmsd of common residues20.100994

coverage0.564700

TMfinal0.130492

pdb_35/1aoeA.pdb pdb_35/1aoa_.pdb

number of residues in common192

rmsd of common residues18.732762

coverage0.777320

TMfinal0.164287

pdb_35/1aoeA.pdb pdb_35/1aocA.pdb

number of residues in common175

rmsd of common residues21.138997

coverage1.000000

TMfinal0.150440

pdb_35/1aoeA.pdb pdb_35/1aohA.pdb

number of residues in common143

rmsd of common residues18.103426

coverage1.000000

TMfinal0.175352

pdb_35/1aoeA.pdb pdb_35/1aol_.pdb

number of residues in common192

rmsd of common residues18.684735

coverage0.842100

TMfinal0.165600

pdb_35/1aoeA.pdb pdb_35/1aop_.pdb

number of residues in common192

rmsd of common residues20.957986

coverage0.421050

TMfinal0.096092

pdb_35/1aoeA.pdb pdb_35/1aorA.pdb

pdb_35/1aoeA.pdb pdb_35/1aoy_.pdb

number of residues in common78

rmsd of common residues11.248152

coverage1.000000

TMfinal0.169833

pdb_35/1aoeA.pdb pdb_35/1aozA.pdb

pdb_35/1aoeA.pdb pdb_35/1ap8_.pdb

number of residues in common192

rmsd of common residues22.072761

coverage0.901400

TMfinal0.134864

pdb_35/1aoeA.pdb pdb_35/1apj_.pdb

number of residues in common74

rmsd of common residues14.267161

coverage1.000000

TMfinal0.153151

pdb_35/1aoeA.pdb pdb_35/1apmE.pdb

pdb_35/1aoeA.pdb pdb_35/1apq_.pdb

number of residues in common53

rmsd of common residues14.741566

coverage1.000000

TMfinal0.139589

pdb_35/1aoeA.pdb pdb_35/1apxA.pdb

pdb_35/1aoeA.pdb pdb_35/1aq0A.pdb

number of residues in common192

rmsd of common residues18.390247

coverage0.627450

TMfinal0.141971

pdb_35/1aoeA.pdb pdb_35/1aqb_.pdb

number of residues in common175

rmsd of common residues15.254669

coverage1.000000

TMfinal0.192672

pdb_35/1aoeA.pdb pdb_35/1aqcA.pdb

number of residues in common121

rmsd of common residues17.246834

coverage1.000000

TMfinal0.169209

pdb_35/1aoeA.pdb pdb_35/1aqe_.pdb

number of residues in common110

rmsd of common residues14.018807

coverage1.000000

TMfinal0.180458

pdb_35/1aoeA.pdb pdb_35/1aqt_.pdb

number of residues in common135

rmsd of common residues17.706268

coverage1.000000

TMfinal0.138424

pdb_35/1aoeA.pdb pdb_35/1aquA.pdb

number of residues in common192

rmsd of common residues17.393857

coverage0.683270

TMfinal0.158273

pdb_35/1aoeA.pdb pdb_35/1aqzA.pdb

number of residues in common142

rmsd of common residues17.493066

coverage1.000000

TMfinal0.162716

pdb_35/1aoeA.pdb pdb_35/1at0_.pdb

number of residues in common142

rmsd of common residues17.441553

coverage1.000000

TMfinal0.157740

pdb_35/1aoeA.pdb pdb_35/1at3A.pdb

number of residues in common192

rmsd of common residues18.553312

coverage0.884790

TMfinal0.185974

pdb_35/1aoeA.pdb pdb_35/1atb_.pdb

pdb_35/1aoeA.pdb pdb_35/1atg_.pdb

number of residues in common192

rmsd of common residues21.126670

coverage0.831160

TMfinal0.175189

pdb_35/1aohA.pdb pdb_35/1amm_.pdb

number of residues in common143

rmsd of common residues19.966991

coverage0.821830

TMfinal0.145079

pdb_35/1aohA.pdb pdb_35/1amp_.pdb

pdb_35/1aohA.pdb pdb_35/1amuA.pdb

number of residues in common143

rmsd of common residues21.324346

coverage0.280940

TMfinal0.082795

pdb_35/1aohA.pdb pdb_35/1amx_.pdb

number of residues in common143

rmsd of common residues17.186102

coverage0.953330

TMfinal0.173910

pdb_35/1aohA.pdb pdb_35/1an8_.pdb

number of residues in common143

rmsd of common residues16.850978

coverage0.694170

TMfinal0.147139

pdb_35/1aohA.pdb pdb_35/1an9A.pdb

number of residues in common143

rmsd of common residues22.315467

coverage0.420580

TMfinal0.095027

pdb_35/1aohA.pdb pdb_35/1aoa_.pdb

number of residues in common143

rmsd of common residues17.853984

coverage0.578940

TMfinal0.123646

pdb_35/1aohA.pdb pdb_35/1aocA.pdb

number of residues in common143

rmsd of common residues20.124257

coverage0.817140

TMfinal0.127217

pdb_35/1aohA.pdb pdb_35/1aoeA.pdb

number of residues in common143

rmsd of common residues18.103426

coverage0.744790

TMfinal0.154153

pdb_35/1aohA.pdb pdb_35/1aol_.pdb

number of residues in common143

rmsd of common residues19.790503

coverage0.627190

TMfinal0.111714

pdb_35/1aohA.pdb pdb_35/1aop_.pdb

number of residues in common143

rmsd of common residues18.896587

coverage0.313590

TMfinal0.079641

pdb_35/1aohA.pdb pdb_35/1aorA.pdb

pdb_35/1aohA.pdb pdb_35/1aoy_.pdb

number of residues in common78

rmsd of common residues14.524921

coverage1.000000

TMfinal0.162597

pdb_35/1aohA.pdb pdb_35/1aozA.pdb

pdb_35/1aohA.pdb pdb_35/1ap8_.pdb

number of residues in common143

rmsd of common residues22.050241

coverage0.671360

TMfinal0.147381

pdb_35/1aohA.pdb pdb_35/1apj_.pdb

number of residues in common74

rmsd of common residues11.138078

coverage1.000000

TMfinal0.166709

pdb_35/1aohA.pdb pdb_35/1apmE.pdb

pdb_35/1aohA.pdb pdb_35/1apq_.pdb

number of residues in common53

rmsd of common residues11.826628

coverage1.000000

TMfinal0.155543

pdb_35/1aohA.pdb pdb_35/1apxA.pdb

pdb_35/1aohA.pdb pdb_35/1aq0A.pdb

number of residues in common143

rmsd of common residues19.607984

coverage0.467320

TMfinal0.103414

pdb_35/1aohA.pdb pdb_35/1aqb_.pdb

number of residues in common143

rmsd of common residues16.627085

coverage0.817140

TMfinal0.164562

pdb_35/1aohA.pdb pdb_35/1aqcA.pdb

number of residues in common121

rmsd of common residues17.298634

coverage1.000000

TMfinal0.133226

pdb_35/1aohA.pdb pdb_35/1aqe_.pdb

number of residues in common110

rmsd of common residues16.882596

coverage1.000000

TMfinal0.147321

pdb_35/1aohA.pdb pdb_35/1aqt_.pdb

number of residues in common135

rmsd of common residues17.757580

coverage1.000000

TMfinal0.162565

pdb_35/1aohA.pdb pdb_35/1aquA.pdb

number of residues in common143

rmsd of common residues17.325502

coverage0.508890

TMfinal0.119889

pdb_35/1aohA.pdb pdb_35/1aqzA.pdb

number of residues in common142

rmsd of common residues16.309530

coverage1.000000

TMfinal0.155927

pdb_35/1aohA.pdb pdb_35/1at0_.pdb

number of residues in common142

rmsd of common residues18.057295

coverage1.000000

TMfinal0.146988

pdb_35/1aohA.pdb pdb_35/1at3A.pdb

number of residues in common143

rmsd of common residues18.281737

coverage0.658980

TMfinal0.163189

pdb_35/1aohA.pdb pdb_35/1atb_.pdb

pdb_35/1aohA.pdb pdb_35/1atg_.pdb

number of residues in common143

rmsd of common residues20.037547

coverage0.619040

TMfinal0.115423

pdb_35/1aol_.pdb pdb_35/1amm_.pdb

number of residues in common174

rmsd of common residues18.983933

coverage1.000000

TMfinal0.166776

pdb_35/1aol_.pdb pdb_35/1amp_.pdb

pdb_35/1aol_.pdb pdb_35/1amuA.pdb

number of residues in common228

rmsd of common residues19.585450

coverage0.447930

TMfinal0.127419

pdb_35/1aol_.pdb pdb_35/1amx_.pdb

number of residues in common150

rmsd of common residues18.837804

coverage1.000000

TMfinal0.145124

pdb_35/1aol_.pdb pdb_35/1an8_.pdb

number of residues in common206

rmsd of common residues20.349374

coverage1.000000

TMfinal0.156870

pdb_35/1aol_.pdb pdb_35/1an9A.pdb

number of residues in common228

rmsd of common residues22.570624

coverage0.670580

TMfinal0.132708

pdb_35/1aol_.pdb pdb_35/1aoa_.pdb

number of residues in common228

rmsd of common residues18.748010

coverage0.923070

TMfinal0.187577

pdb_35/1aol_.pdb pdb_35/1aocA.pdb

number of residues in common175

rmsd of common residues21.127731

coverage1.000000

TMfinal0.155918

pdb_35/1aol_.pdb pdb_35/1aoeA.pdb

number of residues in common192

rmsd of common residues18.684735

coverage1.000000

TMfinal0.179937

pdb_35/1aol_.pdb pdb_35/1aohA.pdb

number of residues in common143

rmsd of common residues19.790503

coverage1.000000

TMfinal0.154099

pdb_35/1aol_.pdb pdb_35/1aop_.pdb

number of residues in common228

rmsd of common residues20.740942

coverage0.500000

TMfinal0.123125

pdb_35/1aol_.pdb pdb_35/1aorA.pdb

pdb_35/1aol_.pdb pdb_35/1aoy_.pdb

number of residues in common78

rmsd of common residues17.136313

coverage1.000000

TMfinal0.129204

pdb_35/1aol_.pdb pdb_35/1aozA.pdb

pdb_35/1aol_.pdb pdb_35/1ap8_.pdb

number of residues in common213

rmsd of common residues21.205976

coverage1.000000

TMfinal0.159137

pdb_35/1aol_.pdb pdb_35/1apj_.pdb

number of residues in common74

rmsd of common residues14.400698

coverage1.000000

TMfinal0.139505

pdb_35/1aol_.pdb pdb_35/1apmE.pdb

pdb_35/1aol_.pdb pdb_35/1apq_.pdb

number of residues in common53

rmsd of common residues11.581109

coverage1.000000

TMfinal0.143496

pdb_35/1aol_.pdb pdb_35/1apxA.pdb

pdb_35/1aol_.pdb pdb_35/1aq0A.pdb

number of residues in common228

rmsd of common residues20.697081

coverage0.745090

TMfinal0.142709

pdb_35/1aol_.pdb pdb_35/1aqb_.pdb

number of residues in common175

rmsd of common residues18.058771

coverage1.000000

TMfinal0.170716

pdb_35/1aol_.pdb pdb_35/1aqcA.pdb

number of residues in common121

rmsd of common residues18.788377

coverage1.000000

TMfinal0.158582

pdb_35/1aol_.pdb pdb_35/1aqe_.pdb

number of residues in common110

rmsd of common residues14.661004

coverage1.000000

TMfinal0.154988

pdb_35/1aol_.pdb pdb_35/1aqt_.pdb

number of residues in common135

rmsd of common residues19.204563

coverage1.000000

TMfinal0.156105

pdb_35/1aol_.pdb pdb_35/1aquA.pdb

number of residues in common228

rmsd of common residues20.406063

coverage0.811380

TMfinal0.174805

pdb_35/1aol_.pdb pdb_35/1aqzA.pdb

number of residues in common142

rmsd of common residues19.879900

coverage1.000000

TMfinal0.136552

pdb_35/1aol_.pdb pdb_35/1at0_.pdb

number of residues in common142

rmsd of common residues17.754407

coverage1.000000

TMfinal0.130177

pdb_35/1aol_.pdb pdb_35/1at3A.pdb

number of residues in common217

rmsd of common residues18.952376

coverage1.000000

TMfinal0.191524

pdb_35/1aol_.pdb pdb_35/1atb_.pdb

pdb_35/1aol_.pdb pdb_35/1atg_.pdb

number of residues in common228

rmsd of common residues21.435441

coverage0.987010

TMfinal0.170492

pdb_35/1aop_.pdb pdb_35/1amm_.pdb

number of residues in common174

rmsd of common residues17.459590

coverage1.000000

TMfinal0.157173

pdb_35/1aop_.pdb pdb_35/1amp_.pdb

pdb_35/1aop_.pdb pdb_35/1amuA.pdb

number of residues in common456

rmsd of common residues21.696198

coverage0.895870

TMfinal0.217158

pdb_35/1aop_.pdb pdb_35/1amx_.pdb

number of residues in common150

rmsd of common residues19.634690

coverage1.000000

TMfinal0.158127

pdb_35/1aop_.pdb pdb_35/1an8_.pdb

number of residues in common206

rmsd of common residues19.277687

coverage1.000000

TMfinal0.162554

pdb_35/1aop_.pdb pdb_35/1an9A.pdb

number of residues in common340

rmsd of common residues25.813628

coverage1.000000

TMfinal0.147070

pdb_35/1aop_.pdb pdb_35/1aoa_.pdb

number of residues in common247

rmsd of common residues20.653704

coverage1.000000

TMfinal0.183098

pdb_35/1aop_.pdb pdb_35/1aocA.pdb

number of residues in common175

rmsd of common residues19.158489

coverage1.000000

TMfinal0.142231

pdb_35/1aop_.pdb pdb_35/1aoeA.pdb

number of residues in common192

rmsd of common residues20.957986

coverage1.000000

TMfinal0.148942

pdb_35/1aop_.pdb pdb_35/1aohA.pdb

number of residues in common143

rmsd of common residues18.896587

coverage1.000000

TMfinal0.156286

pdb_35/1aop_.pdb pdb_35/1aol_.pdb

number of residues in common228

rmsd of common residues20.740942

coverage1.000000

TMfinal0.173656

pdb_35/1aop_.pdb pdb_35/1aorA.pdb

pdb_35/1aop_.pdb pdb_35/1aoy_.pdb

number of residues in common78

rmsd of common residues14.198814

coverage1.000000

TMfinal0.169275

pdb_35/1aop_.pdb pdb_35/1aozA.pdb

pdb_35/1aop_.pdb pdb_35/1ap8_.pdb

number of residues in common213

rmsd of common residues21.839926

coverage1.000000

TMfinal0.156520

pdb_35/1aop_.pdb pdb_35/1apj_.pdb

number of residues in common74

rmsd of common residues12.548253

coverage1.000000

TMfinal0.159369

pdb_35/1aop_.pdb pdb_35/1apmE.pdb

pdb_35/1aop_.pdb pdb_35/1apq_.pdb

number of residues in common53

rmsd of common residues12.347238

coverage1.000000

TMfinal0.162781

pdb_35/1aop_.pdb pdb_35/1apxA.pdb

pdb_35/1aop_.pdb pdb_35/1aq0A.pdb

number of residues in common306

rmsd of common residues21.444117

coverage1.000000

TMfinal0.188088

pdb_35/1aop_.pdb pdb_35/1aqb_.pdb

number of residues in common175

rmsd of common residues20.440615

coverage1.000000

TMfinal0.153963

pdb_35/1aop_.pdb pdb_35/1aqcA.pdb

number of residues in common121

rmsd of common residues16.571488

coverage1.000000

TMfinal0.134705

pdb_35/1aop_.pdb pdb_35/1aqe_.pdb

number of residues in common110

rmsd of common residues16.339511

coverage1.000000

TMfinal0.165353

pdb_35/1aop_.pdb pdb_35/1aqt_.pdb

number of residues in common135

rmsd of common residues15.418265

coverage1.000000

TMfinal0.180106

pdb_35/1aop_.pdb pdb_35/1aquA.pdb

number of residues in common281

rmsd of common residues21.554555

coverage1.000000

TMfinal0.169653

pdb_35/1aop_.pdb pdb_35/1aqzA.pdb

number of residues in common142

rmsd of common residues19.457345

coverage1.000000

TMfinal0.130526

pdb_35/1aop_.pdb pdb_35/1at0_.pdb

number of residues in common142

rmsd of common residues17.148450

coverage1.000000

TMfinal0.156789

pdb_35/1aop_.pdb pdb_35/1at3A.pdb

number of residues in common217

rmsd of common residues21.027798

coverage1.000000

TMfinal0.173091

pdb_35/1aop_.pdb pdb_35/1atb_.pdb

pdb_35/1aop_.pdb pdb_35/1atg_.pdb

number of residues in common231

rmsd of common residues22.069328

coverage1.000000

TMfinal0.179866

pdb_35/1aoy_.pdb pdb_35/1amm_.pdb

number of residues in common78

rmsd of common residues13.658349

coverage0.448270

TMfinal0.127370

pdb_35/1aoy_.pdb pdb_35/1amp_.pdb

pdb_35/1aoy_.pdb pdb_35/1amuA.pdb

number of residues in common78

rmsd of common residues15.107924

coverage0.153240

TMfinal0.051697

pdb_35/1aoy_.pdb pdb_35/1amx_.pdb

number of residues in common78

rmsd of common residues14.528715

coverage0.520000

TMfinal0.130657

pdb_35/1aoy_.pdb pdb_35/1an8_.pdb

number of residues in common78

rmsd of common residues12.626557

coverage0.378640

TMfinal0.113603

pdb_35/1aoy_.pdb pdb_35/1an9A.pdb

number of residues in common78

rmsd of common residues14.169116

coverage0.229410

TMfinal0.084484

pdb_35/1aoy_.pdb pdb_35/1aoa_.pdb

number of residues in common78

rmsd of common residues11.218511

coverage0.315780

TMfinal0.110120

pdb_35/1aoy_.pdb pdb_35/1aocA.pdb

number of residues in common78

rmsd of common residues14.047876

coverage0.445710

TMfinal0.108353

pdb_35/1aoy_.pdb pdb_35/1aoeA.pdb

number of residues in common78

rmsd of common residues11.248152

coverage0.406250

TMfinal0.117689

pdb_35/1aoy_.pdb pdb_35/1aohA.pdb

number of residues in common78

rmsd of common residues14.524921

coverage0.545450

TMfinal0.114991

pdb_35/1aoy_.pdb pdb_35/1aol_.pdb

number of residues in common78

rmsd of common residues17.136313

coverage0.342100

TMfinal0.079761

pdb_35/1aoy_.pdb pdb_35/1aop_.pdb

number of residues in common78

rmsd of common residues14.198814

coverage0.171050

TMfinal0.065144

pdb_35/1aoy_.pdb pdb_35/1ap8_.pdb

number of residues in common78

rmsd of common residues21.607494

coverage0.366190

TMfinal0.071489

pdb_35/1aoy_.pdb pdb_35/1apj_.pdb

number of residues in common74

rmsd of common residues14.152012

coverage1.000000

TMfinal0.178917

pdb_35/1aoy_.pdb pdb_35/1apq_.pdb

number of residues in common53

rmsd of common residues11.183607

coverage1.000000

TMfinal0.155871

pdb_35/1aoy_.pdb pdb_35/1aq0A.pdb

number of residues in common78

rmsd of common residues14.927847

coverage0.254900

TMfinal0.076209

pdb_35/1aoy_.pdb pdb_35/1aqb_.pdb

number of residues in common78

rmsd of common residues14.177464

coverage0.445710

TMfinal0.108791

pdb_35/1aoy_.pdb pdb_35/1aqcA.pdb

number of residues in common78

rmsd of common residues15.312153

coverage0.644620

TMfinal0.131275

pdb_35/1aoy_.pdb pdb_35/1aqe_.pdb

number of residues in common78

rmsd of common residues13.566144

coverage0.709090

TMfinal0.136303

pdb_35/1aoy_.pdb pdb_35/1aqt_.pdb

number of residues in common78

rmsd of common residues13.323101

coverage0.577770

TMfinal0.124300

pdb_35/1aoy_.pdb pdb_35/1aquA.pdb

number of residues in common78

rmsd of common residues14.805076

coverage0.277580

TMfinal0.075269

pdb_35/1aoy_.pdb pdb_35/1aqzA.pdb

number of residues in common78

rmsd of common residues14.238004

coverage0.549290

TMfinal0.123548

pdb_35/1aoy_.pdb pdb_35/1at0_.pdb

number of residues in common78

rmsd of common residues15.061864

coverage0.549290

TMfinal0.106387

pdb_35/1aoy_.pdb pdb_35/1at3A.pdb

number of residues in common78

rmsd of common residues13.522765

coverage0.359440

TMfinal0.112384

pdb_35/1aoy_.pdb pdb_35/1atg_.pdb

number of residues in common78

rmsd of common residues14.675436

coverage0.337660

TMfinal0.099039

pdb_35/1ap8_.pdb pdb_35/1amm_.pdb

number of residues in common174

rmsd of common residues19.524679

coverage1.000000

TMfinal0.159663

pdb_35/1ap8_.pdb pdb_35/1amuA.pdb

number of residues in common213

rmsd of common residues20.312366

coverage0.418460

TMfinal0.109252

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number of residues in common150

rmsd of common residues22.776661

coverage1.000000

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number of residues in common206

rmsd of common residues20.841873

coverage1.000000

TMfinal0.173004

pdb_35/1ap8_.pdb pdb_35/1an9A.pdb

number of residues in common213

rmsd of common residues23.593618

coverage0.626470

TMfinal0.116231

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number of residues in common213

rmsd of common residues22.275435

coverage0.862340

TMfinal0.164650

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number of residues in common175

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coverage1.000000

TMfinal0.167700

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number of residues in common192

rmsd of common residues22.072761

coverage1.000000

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number of residues in common143

rmsd of common residues22.050241

coverage1.000000

TMfinal0.172940

pdb_35/1ap8_.pdb pdb_35/1aol_.pdb

number of residues in common213

rmsd of common residues21.205976

coverage0.934210

TMfinal0.154896

pdb_35/1ap8_.pdb pdb_35/1aop_.pdb

number of residues in common213

rmsd of common residues21.839926

coverage0.467100

TMfinal0.118062

pdb_35/1ap8_.pdb pdb_35/1aoy_.pdb

number of residues in common78

rmsd of common residues21.607494

coverage1.000000

TMfinal0.124728

pdb_35/1ap8_.pdb pdb_35/1apj_.pdb

number of residues in common74

rmsd of common residues21.302682

coverage1.000000

TMfinal0.140132

pdb_35/1ap8_.pdb pdb_35/1apq_.pdb

number of residues in common53

rmsd of common residues18.071859

coverage1.000000

TMfinal0.129546

pdb_35/1ap8_.pdb pdb_35/1aq0A.pdb

number of residues in common213

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coverage0.696070

TMfinal0.125361

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number of residues in common175

rmsd of common residues23.392765

coverage1.000000

TMfinal0.149003

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number of residues in common121

rmsd of common residues23.997634

coverage1.000000

TMfinal0.141114

pdb_35/1ap8_.pdb pdb_35/1aqe_.pdb

number of residues in common110

rmsd of common residues21.923635

coverage1.000000

TMfinal0.137721

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number of residues in common135

rmsd of common residues22.071688

coverage1.000000

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coverage0.758000

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number of residues in common142

rmsd of common residues20.735017

coverage1.000000

TMfinal0.169376

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number of residues in common142

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coverage1.000000

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coverage0.981560

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coverage0.922070

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number of residues in common74

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coverage0.425280

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pdb_35/1apj_.pdb pdb_35/1amuA.pdb

number of residues in common74

rmsd of common residues18.672592

coverage0.145380

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pdb_35/1apj_.pdb pdb_35/1amx_.pdb

number of residues in common74

rmsd of common residues11.751448

coverage0.493330

TMfinal0.140716

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number of residues in common74

rmsd of common residues14.370451

coverage0.359220

TMfinal0.105214

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number of residues in common74

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coverage0.217640

TMfinal0.075502

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number of residues in common74

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coverage0.299590

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number of residues in common74

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coverage0.422850

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number of residues in common74

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coverage0.385410

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number of residues in common74

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coverage0.517480

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number of residues in common74

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coverage0.324560

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number of residues in common74

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coverage0.162280

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number of residues in common74

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coverage0.948710

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number of residues in common74

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coverage0.347410

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number of residues in common53

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coverage1.000000

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number of residues in common74

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coverage0.241830

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number of residues in common74

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coverage0.422850

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number of residues in common74

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coverage0.611570

TMfinal0.125625

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number of residues in common74

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coverage0.672720

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number of residues in common74

rmsd of common residues13.100471

coverage0.548140

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number of residues in common74

rmsd of common residues13.929327

coverage0.263340

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number of residues in common74

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coverage0.521120

TMfinal0.112988

pdb_35/1apj_.pdb pdb_35/1at0_.pdb

number of residues in common74

rmsd of common residues11.498072

coverage0.521120

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number of residues in common74

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coverage0.341010

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number of residues in common74

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coverage0.320340

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number of residues in common53

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coverage0.304590

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number of residues in common53

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coverage0.104120

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number of residues in common53

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coverage0.353330

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number of residues in common53

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coverage0.257280

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number of residues in common53

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number of residues in common53

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coverage0.302850

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number of residues in common53

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coverage0.276040

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number of residues in common53

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coverage0.370620

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number of residues in common53

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coverage0.116220

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number of residues in common53

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number of residues in common53

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number of residues in common53

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number of residues in common53

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coverage0.173200

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number of residues in common53

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coverage0.302850

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number of residues in common53

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coverage0.438010

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number of residues in common53

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coverage0.481810

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number of residues in common53

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coverage0.373230

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number of residues in common53

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coverage0.373230

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coverage0.244240

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coverage1.000000

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coverage0.601170

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number of residues in common150

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coverage1.000000

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number of residues in common206

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coverage1.000000

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number of residues in common306

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coverage0.900000

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number of residues in common247

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coverage1.000000

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coverage1.000000

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number of residues in common192

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coverage1.000000

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coverage1.000000

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number of residues in common228

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coverage1.000000

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number of residues in common306

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number of residues in common78

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coverage1.000000

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coverage1.000000

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number of residues in common74

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coverage1.000000

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number of residues in common53

rmsd of common residues10.515152

coverage1.000000

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number of residues in common175

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coverage1.000000

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number of residues in common121

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coverage1.000000

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number of residues in common110

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coverage1.000000

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number of residues in common135

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coverage1.000000

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number of residues in common281

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coverage1.000000

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number of residues in common142

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coverage1.000000

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number of residues in common142

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coverage1.000000

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number of residues in common217

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number of residues in common231

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coverage1.000000

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number of residues in common174

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coverage1.000000

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number of residues in common175

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number of residues in common150

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coverage1.000000

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number of residues in common175

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number of residues in common175

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coverage1.000000

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number of residues in common175

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coverage0.911450

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number of residues in common143

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coverage1.000000

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number of residues in common175

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coverage0.767540

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number of residues in common175

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coverage0.383770

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number of residues in common78

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coverage1.000000

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number of residues in common175

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coverage0.821590

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number of residues in common74

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coverage1.000000

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number of residues in common53

rmsd of common residues10.186784

coverage1.000000

TMfinal0.158138

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number of residues in common175

rmsd of common residues19.261487

coverage0.571890

TMfinal0.129859

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number of residues in common121

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coverage1.000000

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number of residues in common110

rmsd of common residues15.937471

coverage1.000000

TMfinal0.179705

pdb_35/1aqb_.pdb pdb_35/1aqt_.pdb

number of residues in common135

rmsd of common residues20.236544

coverage1.000000

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number of residues in common175

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coverage0.622770

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number of residues in common142

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coverage1.000000

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number of residues in common142

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coverage1.000000

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coverage0.806450

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number of residues in common175

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coverage0.757570

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number of residues in common121

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coverage0.695400

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number of residues in common121

rmsd of common residues19.874976

coverage0.237720

TMfinal0.071098

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number of residues in common121

rmsd of common residues16.714081

coverage0.806660

TMfinal0.163911

pdb_35/1aqcA.pdb pdb_35/1an8_.pdb

number of residues in common121

rmsd of common residues18.575698

coverage0.587370

TMfinal0.117360

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number of residues in common121

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coverage0.355880

TMfinal0.101225

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number of residues in common121

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coverage0.489870

TMfinal0.128234

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number of residues in common121

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coverage0.691420

TMfinal0.118544

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number of residues in common121

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coverage0.630200

TMfinal0.133372

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number of residues in common121

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coverage0.846150

TMfinal0.122605

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number of residues in common121

rmsd of common residues18.788377

coverage0.530700

TMfinal0.124647

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number of residues in common121

rmsd of common residues16.571488

coverage0.265350

TMfinal0.075027

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pdb_35/1aqcA.pdb pdb_35/1aoy_.pdb

number of residues in common78

rmsd of common residues15.312153

coverage1.000000

TMfinal0.155855

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pdb_35/1aqcA.pdb pdb_35/1ap8_.pdb

number of residues in common121

rmsd of common residues23.997634

coverage0.568070

TMfinal0.106084

pdb_35/1aqcA.pdb pdb_35/1apj_.pdb

number of residues in common74

rmsd of common residues14.364467

coverage1.000000

TMfinal0.160468

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number of residues in common53

rmsd of common residues14.731629

coverage1.000000

TMfinal0.133338

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pdb_35/1aqcA.pdb pdb_35/1aq0A.pdb

number of residues in common121

rmsd of common residues15.852089

coverage0.395420

TMfinal0.123520

pdb_35/1aqcA.pdb pdb_35/1aqb_.pdb

number of residues in common121

rmsd of common residues17.333204

coverage0.691420

TMfinal0.123164

pdb_35/1aqcA.pdb pdb_35/1aqe_.pdb

number of residues in common110

rmsd of common residues15.169231

coverage1.000000

TMfinal0.190924

pdb_35/1aqcA.pdb pdb_35/1aqt_.pdb

number of residues in common121

rmsd of common residues19.089246

coverage0.896290

TMfinal0.148004

pdb_35/1aqcA.pdb pdb_35/1aquA.pdb

number of residues in common121

rmsd of common residues17.608923

coverage0.430600

TMfinal0.111281

pdb_35/1aqcA.pdb pdb_35/1aqzA.pdb

number of residues in common121

rmsd of common residues16.278623

coverage0.852110

TMfinal0.157612

pdb_35/1aqcA.pdb pdb_35/1at0_.pdb

number of residues in common121

rmsd of common residues15.460685

coverage0.852110

TMfinal0.158807

pdb_35/1aqcA.pdb pdb_35/1at3A.pdb

number of residues in common121

rmsd of common residues18.710968

coverage0.557600

TMfinal0.121326

pdb_35/1aqcA.pdb pdb_35/1atg_.pdb

number of residues in common121

rmsd of common residues19.120635

coverage0.523810

TMfinal0.099074

pdb_35/1aqe_.pdb pdb_35/1amm_.pdb

number of residues in common110

rmsd of common residues16.502564

coverage0.632180

TMfinal0.118010

pdb_35/1aqe_.pdb pdb_35/1amuA.pdb

number of residues in common110

rmsd of common residues17.688878

coverage0.216110

TMfinal0.084419

pdb_35/1aqe_.pdb pdb_35/1amx_.pdb

number of residues in common110

rmsd of common residues15.002468

coverage0.733330

TMfinal0.175664

pdb_35/1aqe_.pdb pdb_35/1an8_.pdb

number of residues in common110

rmsd of common residues16.580280

coverage0.533980

TMfinal0.110983

pdb_35/1aqe_.pdb pdb_35/1an9A.pdb

number of residues in common110

rmsd of common residues17.093370

coverage0.323520

TMfinal0.091449

pdb_35/1aqe_.pdb pdb_35/1aoa_.pdb

number of residues in common110

rmsd of common residues12.482603

coverage0.445340

TMfinal0.135173

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number of residues in common110

rmsd of common residues16.803439

coverage0.628570

TMfinal0.121746

pdb_35/1aqe_.pdb pdb_35/1aoeA.pdb

number of residues in common110

rmsd of common residues14.018807

coverage0.572910

TMfinal0.142437

pdb_35/1aqe_.pdb pdb_35/1aohA.pdb

number of residues in common110

rmsd of common residues16.882596

coverage0.769230

TMfinal0.131036

pdb_35/1aqe_.pdb pdb_35/1aol_.pdb

number of residues in common110

rmsd of common residues14.661004

coverage0.482450

TMfinal0.112319

pdb_35/1aqe_.pdb pdb_35/1aop_.pdb

number of residues in common110

rmsd of common residues16.339511

coverage0.241220

TMfinal0.067674

pdb_35/1aqe_.pdb pdb_35/1aoy_.pdb

number of residues in common78

rmsd of common residues13.566144

coverage1.000000

TMfinal0.157340

pdb_35/1aqe_.pdb pdb_35/1ap8_.pdb

number of residues in common110

rmsd of common residues21.923635

coverage0.516430

TMfinal0.097937

pdb_35/1aqe_.pdb pdb_35/1apj_.pdb

number of residues in common74

rmsd of common residues12.675291

coverage1.000000

TMfinal0.200019

pdb_35/1aqe_.pdb pdb_35/1apq_.pdb

number of residues in common53

rmsd of common residues10.476801

coverage1.000000

TMfinal0.172039

pdb_35/1aqe_.pdb pdb_35/1aq0A.pdb

number of residues in common110

rmsd of common residues14.908206

coverage0.359470

TMfinal0.118435

pdb_35/1aqe_.pdb pdb_35/1aqb_.pdb

number of residues in common110

rmsd of common residues15.937471

coverage0.628570

TMfinal0.145437

pdb_35/1aqe_.pdb pdb_35/1aqcA.pdb

number of residues in common110

rmsd of common residues15.169231

coverage0.909090

TMfinal0.182579

pdb_35/1aqe_.pdb pdb_35/1aqt_.pdb

number of residues in common110

rmsd of common residues16.409157

coverage0.814810

TMfinal0.144499

pdb_35/1aqe_.pdb pdb_35/1aquA.pdb

number of residues in common110

rmsd of common residues14.137646

coverage0.391450

TMfinal0.123103

pdb_35/1aqe_.pdb pdb_35/1aqzA.pdb

number of residues in common110

rmsd of common residues15.375237

coverage0.774640

TMfinal0.151175

pdb_35/1aqe_.pdb pdb_35/1at0_.pdb

number of residues in common110

rmsd of common residues13.685743

coverage0.774640

TMfinal0.136641

pdb_35/1aqe_.pdb pdb_35/1at3A.pdb

number of residues in common110

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coverage0.506910

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number of residues in common110

rmsd of common residues17.077941

coverage0.476190

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number of residues in common135

rmsd of common residues14.431519

coverage0.775860

TMfinal0.165875

pdb_35/1aqt_.pdb pdb_35/1amuA.pdb

number of residues in common135

rmsd of common residues18.986028

coverage0.265220

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pdb_35/1aqt_.pdb pdb_35/1amx_.pdb

number of residues in common135

rmsd of common residues19.973741

coverage0.900000

TMfinal0.137935

pdb_35/1aqt_.pdb pdb_35/1an8_.pdb

number of residues in common135

rmsd of common residues16.211305

coverage0.655340

TMfinal0.141835

pdb_35/1aqt_.pdb pdb_35/1an9A.pdb

number of residues in common135

rmsd of common residues17.850258

coverage0.397050

TMfinal0.098665

pdb_35/1aqt_.pdb pdb_35/1aoa_.pdb

number of residues in common135

rmsd of common residues17.687686

coverage0.546550

TMfinal0.119054

pdb_35/1aqt_.pdb pdb_35/1aocA.pdb

number of residues in common135

rmsd of common residues20.246087

coverage0.771420

TMfinal0.131237

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number of residues in common135

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coverage0.703120

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number of residues in common135

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coverage0.944050

TMfinal0.157727

pdb_35/1aqt_.pdb pdb_35/1aol_.pdb

number of residues in common135

rmsd of common residues19.204563

coverage0.592100

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pdb_35/1aqt_.pdb pdb_35/1aop_.pdb

number of residues in common135

rmsd of common residues15.418265

coverage0.296050

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number of residues in common78

rmsd of common residues13.323101

coverage1.000000

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number of residues in common135

rmsd of common residues22.071688

coverage0.633800

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number of residues in common74

rmsd of common residues13.100471

coverage1.000000

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number of residues in common53

rmsd of common residues12.659478

coverage1.000000

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number of residues in common135

rmsd of common residues14.500546

coverage0.441170

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number of residues in common135

rmsd of common residues20.236544

coverage0.771420

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number of residues in common121

rmsd of common residues19.089246

coverage1.000000

TMfinal0.156267

pdb_35/1aqt_.pdb pdb_35/1aqe_.pdb

number of residues in common110

rmsd of common residues16.409157

coverage1.000000

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pdb_35/1aqt_.pdb pdb_35/1aquA.pdb

number of residues in common135

rmsd of common residues17.954278

coverage0.480420

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number of residues in common135

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coverage0.950700

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number of residues in common135

rmsd of common residues18.643341

coverage0.950700

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number of residues in common135

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coverage0.622120

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number of residues in common135

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coverage0.584410

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number of residues in common174

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coverage1.000000

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number of residues in common281

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coverage0.552060

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number of residues in common150

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coverage1.000000

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number of residues in common206

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coverage1.000000

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number of residues in common281

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coverage0.826470

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number of residues in common247

rmsd of common residues20.849604

coverage1.000000

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number of residues in common175

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coverage1.000000

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number of residues in common192

rmsd of common residues17.393857

coverage1.000000

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number of residues in common143

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coverage1.000000

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number of residues in common228

rmsd of common residues20.406063

coverage1.000000

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number of residues in common281

rmsd of common residues21.554555

coverage0.616220

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number of residues in common78

rmsd of common residues14.805076

coverage1.000000

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number of residues in common213

rmsd of common residues21.121397

coverage1.000000

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number of residues in common74

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coverage1.000000

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number of residues in common53

rmsd of common residues13.441735

coverage1.000000

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number of residues in common281

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number of residues in common175

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coverage1.000000

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number of residues in common121

rmsd of common residues17.608923

coverage1.000000

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number of residues in common110

rmsd of common residues14.137646

coverage1.000000

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number of residues in common135

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coverage1.000000

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number of residues in common142

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coverage1.000000

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coverage1.000000

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coverage1.000000

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number of residues in common231

rmsd of common residues20.955674

coverage1.000000

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number of residues in common142

rmsd of common residues19.681408

coverage0.816090

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number of residues in common142

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coverage0.278970

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number of residues in common142

rmsd of common residues17.044477

coverage0.946660

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number of residues in common142

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coverage0.689320

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number of residues in common142

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coverage0.417640

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number of residues in common142

rmsd of common residues17.292341

coverage0.574890

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number of residues in common142

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coverage0.811420

TMfinal0.160218

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number of residues in common142

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coverage0.739580

TMfinal0.142405

pdb_35/1aqzA.pdb pdb_35/1aohA.pdb

number of residues in common142

rmsd of common residues16.309530

coverage0.993000

TMfinal0.155409

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number of residues in common142

rmsd of common residues19.879900

coverage0.622800

TMfinal0.110775

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number of residues in common142

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coverage0.311400

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pdb_35/1aqzA.pdb pdb_35/1aoy_.pdb

number of residues in common78

rmsd of common residues14.238004

coverage1.000000

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number of residues in common142

rmsd of common residues20.735017

coverage0.666660

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number of residues in common74

rmsd of common residues13.794999

coverage1.000000

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number of residues in common53

rmsd of common residues12.542869

coverage1.000000

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number of residues in common142

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coverage0.464050

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number of residues in common142

rmsd of common residues17.787576

coverage0.811420

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number of residues in common121

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coverage1.000000

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number of residues in common110

rmsd of common residues15.375237

coverage1.000000

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number of residues in common135

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coverage1.000000

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number of residues in common142

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coverage0.505330

TMfinal0.122051

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number of residues in common142

rmsd of common residues14.476397

coverage1.000000

TMfinal0.209702

pdb_35/1aqzA.pdb pdb_35/1at3A.pdb

number of residues in common142

rmsd of common residues17.762094

coverage0.654370

TMfinal0.129077

pdb_35/1aqzA.pdb pdb_35/1atg_.pdb

number of residues in common142

rmsd of common residues18.261920

coverage0.614710

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number of residues in common142

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coverage0.816090

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number of residues in common142

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coverage0.278970

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number of residues in common142

rmsd of common residues15.354356

coverage0.946660

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number of residues in common142

rmsd of common residues19.193526

coverage0.689320

TMfinal0.130893

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number of residues in common142

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coverage0.417640

TMfinal0.094108

pdb_35/1at0_.pdb pdb_35/1aoa_.pdb

number of residues in common142

rmsd of common residues17.197258

coverage0.574890

TMfinal0.132441

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number of residues in common142

rmsd of common residues19.185779

coverage0.811420

TMfinal0.138130

pdb_35/1at0_.pdb pdb_35/1aoeA.pdb

number of residues in common142

rmsd of common residues17.441553

coverage0.739580

TMfinal0.139025

pdb_35/1at0_.pdb pdb_35/1aohA.pdb

number of residues in common142

rmsd of common residues18.057295

coverage0.993000

TMfinal0.146578

pdb_35/1at0_.pdb pdb_35/1aol_.pdb

number of residues in common142

rmsd of common residues17.754407

coverage0.622800

TMfinal0.106243

pdb_35/1at0_.pdb pdb_35/1aop_.pdb

number of residues in common142

rmsd of common residues17.148450

coverage0.311400

TMfinal0.088730

pdb_35/1at0_.pdb pdb_35/1aoy_.pdb

number of residues in common78

rmsd of common residues15.061864

coverage1.000000

TMfinal0.138173

pdb_35/1at0_.pdb pdb_35/1ap8_.pdb

number of residues in common142

rmsd of common residues19.702157

coverage0.666660

TMfinal0.120293

pdb_35/1at0_.pdb pdb_35/1apj_.pdb

number of residues in common74

rmsd of common residues11.498072

coverage1.000000

TMfinal0.157725

pdb_35/1at0_.pdb pdb_35/1apq_.pdb

number of residues in common53

rmsd of common residues13.276603

coverage1.000000

TMfinal0.147954

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number of residues in common142

rmsd of common residues15.976193

coverage0.464050

TMfinal0.117468

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number of residues in common142

rmsd of common residues17.859761

coverage0.811420

TMfinal0.141098

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number of residues in common121

rmsd of common residues15.460685

coverage1.000000

TMfinal0.168705

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number of residues in common110

rmsd of common residues13.685743

coverage1.000000

TMfinal0.150167

pdb_35/1at0_.pdb pdb_35/1aqt_.pdb

number of residues in common135

rmsd of common residues18.643341

coverage1.000000

TMfinal0.140258

pdb_35/1at0_.pdb pdb_35/1aquA.pdb

number of residues in common142

rmsd of common residues16.369786

coverage0.505330

TMfinal0.109780

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number of residues in common142

rmsd of common residues14.476397

coverage1.000000

TMfinal0.209702

pdb_35/1at0_.pdb pdb_35/1at3A.pdb

number of residues in common142

rmsd of common residues16.345438

coverage0.654370

TMfinal0.149183

pdb_35/1at0_.pdb pdb_35/1atg_.pdb

number of residues in common142

rmsd of common residues18.843293

coverage0.614710

TMfinal0.111522

pdb_35/1at3A.pdb pdb_35/1amm_.pdb

number of residues in common174

rmsd of common residues18.870589

coverage1.000000

TMfinal0.182586

pdb_35/1at3A.pdb pdb_35/1amuA.pdb

number of residues in common217

rmsd of common residues22.425179

coverage0.426320

TMfinal0.103186

pdb_35/1at3A.pdb pdb_35/1amx_.pdb

number of residues in common150

rmsd of common residues18.043908

coverage1.000000

TMfinal0.185543

pdb_35/1at3A.pdb pdb_35/1an8_.pdb

number of residues in common206

rmsd of common residues20.984940

coverage1.000000

TMfinal0.157094

pdb_35/1at3A.pdb pdb_35/1an9A.pdb

number of residues in common217

rmsd of common residues21.600447

coverage0.638230

TMfinal0.125239

pdb_35/1at3A.pdb pdb_35/1aoa_.pdb

number of residues in common217

rmsd of common residues22.004300

coverage0.878540

TMfinal0.152396

pdb_35/1at3A.pdb pdb_35/1aocA.pdb

number of residues in common175

rmsd of common residues17.933026

coverage1.000000

TMfinal0.184017

pdb_35/1at3A.pdb pdb_35/1aoeA.pdb

number of residues in common192

rmsd of common residues18.553312

coverage1.000000

TMfinal0.196385

pdb_35/1at3A.pdb pdb_35/1aohA.pdb

number of residues in common143

rmsd of common residues18.281737

coverage1.000000

TMfinal0.203890

pdb_35/1at3A.pdb pdb_35/1aol_.pdb

number of residues in common217

rmsd of common residues18.952376

coverage0.951750

TMfinal0.186978

pdb_35/1at3A.pdb pdb_35/1aop_.pdb

number of residues in common217

rmsd of common residues21.027798

coverage0.475870

TMfinal0.115656

pdb_35/1at3A.pdb pdb_35/1aoy_.pdb

number of residues in common78

rmsd of common residues13.522765

coverage1.000000

TMfinal0.196443

pdb_35/1at3A.pdb pdb_35/1ap8_.pdb

number of residues in common213

rmsd of common residues23.238933

coverage1.000000

TMfinal0.166210

pdb_35/1at3A.pdb pdb_35/1apj_.pdb

number of residues in common74

rmsd of common residues14.551395

coverage1.000000

TMfinal0.149367

pdb_35/1at3A.pdb pdb_35/1apq_.pdb

number of residues in common53

rmsd of common residues13.283036

coverage1.000000

TMfinal0.155797

pdb_35/1at3A.pdb pdb_35/1aq0A.pdb

number of residues in common217

rmsd of common residues20.472847

coverage0.709150

TMfinal0.133195

pdb_35/1at3A.pdb pdb_35/1aqb_.pdb

number of residues in common175

rmsd of common residues18.892587

coverage1.000000

TMfinal0.164164

pdb_35/1at3A.pdb pdb_35/1aqcA.pdb

number of residues in common121

rmsd of common residues18.710968

coverage1.000000

TMfinal0.163939

pdb_35/1at3A.pdb pdb_35/1aqe_.pdb

number of residues in common110

rmsd of common residues15.709912

coverage1.000000

TMfinal0.162176

pdb_35/1at3A.pdb pdb_35/1aqt_.pdb

number of residues in common135

rmsd of common residues17.854322

coverage1.000000

TMfinal0.145023

pdb_35/1at3A.pdb pdb_35/1aquA.pdb

number of residues in common217

rmsd of common residues20.662016

coverage0.772240

TMfinal0.145698

pdb_35/1at3A.pdb pdb_35/1aqzA.pdb

number of residues in common142

rmsd of common residues17.762094

coverage1.000000

TMfinal0.158802

pdb_35/1at3A.pdb pdb_35/1at0_.pdb

number of residues in common142

rmsd of common residues16.345438

coverage1.000000

TMfinal0.183309

pdb_35/1at3A.pdb pdb_35/1atg_.pdb

number of residues in common217

rmsd of common residues20.356250

coverage0.939390

TMfinal0.152118

pdb_35/1atg_.pdb pdb_35/1amm_.pdb

number of residues in common174

rmsd of common residues14.385261

coverage1.000000

TMfinal0.180425

pdb_35/1atg_.pdb pdb_35/1amuA.pdb

number of residues in common231

rmsd of common residues19.793872

coverage0.453830

TMfinal0.115163

pdb_35/1atg_.pdb pdb_35/1amx_.pdb

number of residues in common150

rmsd of common residues19.733939

coverage1.000000

TMfinal0.168855

pdb_35/1atg_.pdb pdb_35/1an8_.pdb

number of residues in common206

rmsd of common residues20.044364

coverage1.000000

TMfinal0.157360

pdb_35/1atg_.pdb pdb_35/1an9A.pdb

number of residues in common231

rmsd of common residues22.707749

coverage0.679410

TMfinal0.138267

pdb_35/1atg_.pdb pdb_35/1aoa_.pdb

number of residues in common231

rmsd of common residues20.104588

coverage0.935220

TMfinal0.208214

pdb_35/1atg_.pdb pdb_35/1aocA.pdb

number of residues in common175

rmsd of common residues19.326012

coverage1.000000

TMfinal0.160966

pdb_35/1atg_.pdb pdb_35/1aoeA.pdb

number of residues in common192

rmsd of common residues21.126670

coverage1.000000

TMfinal0.191743

pdb_35/1atg_.pdb pdb_35/1aohA.pdb

number of residues in common143

rmsd of common residues20.037547

coverage1.000000

TMfinal0.147234

pdb_35/1atg_.pdb pdb_35/1aol_.pdb

number of residues in common228

rmsd of common residues21.435441

coverage1.000000

TMfinal0.170989

pdb_35/1atg_.pdb pdb_35/1aop_.pdb

number of residues in common231

rmsd of common residues22.069328

coverage0.506570

TMfinal0.125362

pdb_35/1atg_.pdb pdb_35/1aoy_.pdb

number of residues in common78

rmsd of common residues14.675436

coverage1.000000

TMfinal0.194408

pdb_35/1atg_.pdb pdb_35/1ap8_.pdb

number of residues in common213

rmsd of common residues22.062598

coverage1.000000

TMfinal0.152622

pdb_35/1atg_.pdb pdb_35/1apj_.pdb

number of residues in common74

rmsd of common residues11.748913

coverage1.000000

TMfinal0.163717

pdb_35/1atg_.pdb pdb_35/1apq_.pdb

number of residues in common53

rmsd of common residues12.436005

coverage1.000000

TMfinal0.168471

pdb_35/1atg_.pdb pdb_35/1aq0A.pdb

number of residues in common231

rmsd of common residues21.313044

coverage0.754900

TMfinal0.145918

pdb_35/1atg_.pdb pdb_35/1aqb_.pdb

number of residues in common175

rmsd of common residues20.474842

coverage1.000000

TMfinal0.160696

pdb_35/1atg_.pdb pdb_35/1aqcA.pdb

number of residues in common121

rmsd of common residues19.120635

coverage1.000000

TMfinal0.135661

pdb_35/1atg_.pdb pdb_35/1aqe_.pdb

number of residues in common110

rmsd of common residues17.077941

coverage1.000000

TMfinal0.155732

pdb_35/1atg_.pdb pdb_35/1aqt_.pdb

number of residues in common135

rmsd of common residues15.547058

coverage1.000000

TMfinal0.179758

pdb_35/1atg_.pdb pdb_35/1aquA.pdb

number of residues in common231

rmsd of common residues20.955674

coverage0.822060

TMfinal0.155682

pdb_35/1atg_.pdb pdb_35/1aqzA.pdb

number of residues in common142

rmsd of common residues18.261920

coverage1.000000

TMfinal0.131204

pdb_35/1atg_.pdb pdb_35/1at0_.pdb

number of residues in common142

rmsd of common residues18.843293

coverage1.000000

TMfinal0.141919

pdb_35/1atg_.pdb pdb_35/1at3A.pdb

number of residues in common217

rmsd of common residues20.356250

coverage1.000000

TMfinal0.156107

pdb_35/1atg_.pdb pdb_35/1atb_.pdb

number of residues in common62

rmsd of common residues12.595425

coverage1.000000

TMfinal0.172354

minimum coverage0.104120maximum coverage1.000000average coverage0.798685min_aligned_length53

min_rmsd8.718909

min_tm_score0.034275

max_aligned_length456

max_rmsd25.813628

max_tm_score0.230733

time1340818983.744571

count602

sum_of_residues87284

sum_rmsd10699.317573

sum_tm87.533815

avg time taken34.112822

average no: of residue in common144.990033

rmsd of common residue17.772953

average TMscore0.145405

no of alignments between 0 and .17 477

no of alignments between .4 and1 0

8.2 Results with modified code:

time1340701429.184738

pdb_35/1amm_.pdb pdb_35/1amuA.pdb

number of residues in common174

rmsd of common residues19.737357

TMfinal0.094839

pdb_35/1amm_.pdb pdb_35/1amx_.pdb

number of residues in common150

rmsd of common residues19.891091

TMfinal0.140656

pdb_35/1amm_.pdb pdb_35/1an8_.pdb

number of residues in common174

rmsd of common residues17.630455

TMfinal0.157357

pdb_35/1amm_.pdb pdb_35/1an9A.pdb

number of residues in common174

rmsd of common residues18.921813

TMfinal0.110498

pdb_35/1amm_.pdb pdb_35/1aoa_.pdb

number of residues in common174

rmsd of common residues19.904385

TMfinal0.127709

pdb_35/1amm_.pdb pdb_35/1aocA.pdb

number of residues in common174

rmsd of common residues21.627235

TMfinal0.136207

pdb_35/1amm_.pdb pdb_35/1aoeA.pdb

number of residues in common174

rmsd of common residues19.318845

TMfinal0.134164

pdb_35/1amm_.pdb pdb_35/1aohA.pdb

number of residues in common143

rmsd of common residues19.966991

TMfinal0.143871

pdb_35/1amm_.pdb pdb_35/1aol_.pdb

number of residues in common174

rmsd of common residues18.983933

TMfinal0.134245

pdb_35/1amm_.pdb pdb_35/1aop_.pdb

number of residues in common174

rmsd of common residues17.459590

TMfinal0.095709

pdb_35/1amm_.pdb pdb_35/1aoy_.pdb

number of residues in common78

rmsd of common residues13.658349

TMfinal0.166353

pdb_35/1amm_.pdb pdb_35/1ap8_.pdb

number of residues in common174

rmsd of common residues19.524679

TMfinal0.133849

pdb_35/1amm_.pdb pdb_35/1apj_.pdb

number of residues in common74

rmsd of common residues12.787075

TMfinal0.151982

pdb_35/1amm_.pdb pdb_35/1apq_.pdb

number of residues in common53

rmsd of common residues11.308121

TMfinal0.146990

pdb_35/1amm_.pdb pdb_35/1aq0A.pdb

number of residues in common174

rmsd of common residues17.671342

TMfinal0.131028

pdb_35/1amm_.pdb pdb_35/1aqb_.pdb

number of residues in common174

rmsd of common residues20.675146

TMfinal0.183476

pdb_35/1amm_.pdb pdb_35/1aqcA.pdb

number of residues in common121

rmsd of common residues18.712583

TMfinal0.138406

pdb_35/1amm_.pdb pdb_35/1aqe_.pdb

number of residues in common110

rmsd of common residues16.502564

TMfinal0.130552

pdb_35/1amm_.pdb pdb_35/1aqt_.pdb

number of residues in common135

rmsd of common residues14.431519

TMfinal0.170718

pdb_35/1amm_.pdb pdb_35/1aquA.pdb

number of residues in common174

rmsd of common residues19.426155

TMfinal0.126871

pdb_35/1amm_.pdb pdb_35/1aqzA.pdb

number of residues in common142

rmsd of common residues19.681408

TMfinal0.140459

pdb_35/1amm_.pdb pdb_35/1at0_.pdb

number of residues in common142

rmsd of common residues18.693595

TMfinal0.151839

pdb_35/1amm_.pdb pdb_35/1at3A.pdb

number of residues in common174

rmsd of common residues18.870589

TMfinal0.158666

pdb_35/1amm_.pdb pdb_35/1atb_.pdb

pdb_35/1amm_.pdb pdb_35/1atg_.pdb

number of residues in common174

rmsd of common residues14.385261

TMfinal0.151885

pdb_35/1amuA.pdb pdb_35/1amm_.pdb

number of residues in common174

rmsd of common residues19.737357

TMfinal0.178762

pdb_35/1amuA.pdb pdb_35/1amp_.pdb

pdb_35/1amuA.pdb pdb_35/1amx_.pdb

number of residues in common150

rmsd of common residues22.218321

TMfinal0.152109

pdb_35/1amuA.pdb pdb_35/1an8_.pdb

number of residues in common206

rmsd of common residues21.721178

TMfinal0.151786

pdb_35/1amuA.pdb pdb_35/1an9A.pdb

number of residues in common340

rmsd of common residues21.114435

TMfinal0.185736

pdb_35/1amuA.pdb pdb_35/1aoa_.pdb

number of residues in common247

rmsd of common residues22.287718

TMfinal0.164765

pdb_35/1amuA.pdb pdb_35/1aocA.pdb

number of residues in common175

rmsd of common residues19.275388

TMfinal0.179213

pdb_35/1amuA.pdb pdb_35/1aoeA.pdb

number of residues in common192

rmsd of common residues22.245406

TMfinal0.154361

pdb_35/1amuA.pdb pdb_35/1aohA.pdb

number of residues in common143

rmsd of common residues21.324346

TMfinal0.151576

pdb_35/1amuA.pdb pdb_35/1aol_.pdb

number of residues in common228

rmsd of common residues19.585450

TMfinal0.183552

pdb_35/1amuA.pdb pdb_35/1aop_.pdb

number of residues in common456

rmsd of common residues21.696198

TMfinal0.225588

pdb_35/1amuA.pdb pdb_35/1aorA.pdb

pdb_35/1amuA.pdb pdb_35/1aoy_.pdb

number of residues in common78

rmsd of common residues15.107924

TMfinal0.160068

pdb_35/1amuA.pdb pdb_35/1aozA.pdb

pdb_35/1amuA.pdb pdb_35/1ap8_.pdb

number of residues in common213

rmsd of common residues20.312366

TMfinal0.164190

pdb_35/1amuA.pdb pdb_35/1apj_.pdb

number of residues in common74

rmsd of common residues18.672592

TMfinal0.164747

pdb_35/1amuA.pdb pdb_35/1apmE.pdb

pdb_35/1amuA.pdb pdb_35/1apq_.pdb

number of residues in common53

rmsd of common residues16.304880

TMfinal0.120777

pdb_35/1amuA.pdb pdb_35/1apxA.pdb

pdb_35/1amuA.pdb pdb_35/1aq0A.pdb

number of residues in common306

rmsd of common residues20.759635

TMfinal0.186949

pdb_35/1amuA.pdb pdb_35/1aqb_.pdb

number of residues in common175

rmsd of common residues21.475181

TMfinal0.144483

pdb_35/1amuA.pdb pdb_35/1aqcA.pdb

number of residues in common121

rmsd of common residues19.874976

TMfinal0.142873

pdb_35/1amuA.pdb pdb_35/1aqe_.pdb

number of residues in common110

rmsd of common residues17.688878

TMfinal0.194184

pdb_35/1amuA.pdb pdb_35/1aqt_.pdb

number of residues in common135

rmsd of common residues18.986028

TMfinal0.156731

pdb_35/1amuA.pdb pdb_35/1aquA.pdb

number of residues in common281

rmsd of common residues24.078919

TMfinal0.155094

pdb_35/1amuA.pdb pdb_35/1aqzA.pdb

number of residues in common142

rmsd of common residues19.554735

TMfinal0.156711

pdb_35/1amuA.pdb pdb_35/1at0_.pdb

number of residues in common142

rmsd of common residues20.442807

TMfinal0.126381

pdb_35/1amuA.pdb pdb_35/1at3A.pdb

number of residues in common217

rmsd of common residues22.425179

TMfinal0.160743

pdb_35/1amuA.pdb pdb_35/1atb_.pdb

pdb_35/1amuA.pdb pdb_35/1atg_.pdb

number of residues in common231

rmsd of common residues19.793872

TMfinal0.160422

pdb_35/1amx_.pdb pdb_35/1amm_.pdb

number of residues in common150

rmsd of common residues19.891091

TMfinal0.134356

pdb_35/1amx_.pdb pdb_35/1amp_.pdb

pdb_35/1amx_.pdb pdb_35/1amuA.pdb

number of residues in common150

rmsd of common residues22.218321

TMfinal0.078363

pdb_35/1amx_.pdb pdb_35/1an8_.pdb

number of residues in common150

rmsd of common residues19.393080

TMfinal0.115382

pdb_35/1amx_.pdb pdb_35/1an9A.pdb

number of residues in common150

rmsd of common residues20.638173

TMfinal0.109490

pdb_35/1amx_.pdb pdb_35/1aoa_.pdb

number of residues in common150

rmsd of common residues18.519452

TMfinal0.131219

pdb_35/1amx_.pdb pdb_35/1aocA.pdb

number of residues in common150

rmsd of common residues18.197335

TMfinal0.151929

pdb_35/1amx_.pdb pdb_35/1aoeA.pdb

number of residues in common150

rmsd of common residues17.193091

TMfinal0.163931

pdb_35/1amx_.pdb pdb_35/1aohA.pdb

number of residues in common143

rmsd of common residues17.186102

TMfinal0.167027

pdb_35/1amx_.pdb pdb_35/1aol_.pdb

number of residues in common150

rmsd of common residues18.837804

TMfinal0.116202

pdb_35/1amx_.pdb pdb_35/1aop_.pdb

number of residues in common150

rmsd of common residues19.634690

TMfinal0.084268

pdb_35/1amx_.pdb pdb_35/1aorA.pdb

pdb_35/1amx_.pdb pdb_35/1aoy_.pdb

number of residues in common78

rmsd of common residues14.528715

TMfinal0.160286

pdb_35/1amx_.pdb pdb_35/1aozA.pdb

pdb_35/1amx_.pdb pdb_35/1ap8_.pdb

number of residues in common150

rmsd of common residues22.776661

TMfinal0.111031

pdb_35/1amx_.pdb pdb_35/1apj_.pdb

number of residues in common74

rmsd of common residues11.751448

TMfinal0.170089

pdb_35/1amx_.pdb pdb_35/1apmE.pdb

pdb_35/1amx_.pdb pdb_35/1apq_.pdb

number of residues in common53

rmsd of common residues9.855834

TMfinal0.168297

pdb_35/1amx_.pdb pdb_35/1apxA.pdb

pdb_35/1amx_.pdb pdb_35/1aq0A.pdb

number of residues in common150

rmsd of common residues18.045554

TMfinal0.112079

pdb_35/1amx_.pdb pdb_35/1aqb_.pdb

number of residues in common150

rmsd of common residues16.281107

TMfinal0.164135

pdb_35/1amx_.pdb pdb_35/1aqcA.pdb

number of residues in common121

rmsd of common residues16.714081

TMfinal0.167762

pdb_35/1amx_.pdb pdb_35/1aqe_.pdb

number of residues in common110

rmsd of common residues15.002468

TMfinal0.180535

pdb_35/1amx_.pdb pdb_35/1aqt_.pdb

number of residues in common135

rmsd of common residues19.973741

TMfinal0.143834

pdb_35/1amx_.pdb pdb_35/1aquA.pdb

number of residues in common150

rmsd of common residues16.372136

TMfinal0.123739

pdb_35/1amx_.pdb pdb_35/1aqzA.pdb

number of residues in common142

rmsd of common residues17.044477

TMfinal0.149622

pdb_35/1amx_.pdb pdb_35/1at0_.pdb

number of residues in common142

rmsd of common residues15.354356

TMfinal0.155694

pdb_35/1amx_.pdb pdb_35/1at3A.pdb

number of residues in common150

rmsd of common residues18.043908

TMfinal0.142398

pdb_35/1amx_.pdb pdb_35/1atb_.pdb

pdb_35/1amx_.pdb pdb_35/1atg_.pdb

number of residues in common150

rmsd of common residues19.733939

TMfinal0.134619

pdb_35/1an8_.pdb pdb_35/1amm_.pdb

number of residues in common174

rmsd of common residues17.630455

TMfinal0.169908

pdb_35/1an8_.pdb pdb_35/1amp_.pdb

pdb_35/1an8_.pdb pdb_35/1amuA.pdb

number of residues in common206

rmsd of common residues21.721178

TMfinal0.097757

pdb_35/1an8_.pdb pdb_35/1amx_.pdb

number of residues in common150

rmsd of common residues19.393080

TMfinal0.135357

pdb_35/1an8_.pdb pdb_35/1an9A.pdb

number of residues in common206

rmsd of common residues22.110851

TMfinal0.108194

pdb_35/1an8_.pdb pdb_35/1aoa_.pdb

number of residues in common206

rmsd of common residues19.866652

TMfinal0.132701

pdb_35/1an8_.pdb pdb_35/1aocA.pdb

number of residues in common175

rmsd of common residues20.898762

TMfinal0.127711

pdb_35/1an8_.pdb pdb_35/1aoeA.pdb

number of residues in common192

rmsd of common residues18.545583

TMfinal0.179802

pdb_35/1an8_.pdb pdb_35/1aohA.pdb

number of residues in common143

rmsd of common residues16.850978

TMfinal0.162367

pdb_35/1an8_.pdb pdb_35/1aol_.pdb

number of residues in common206

rmsd of common residues20.349374

TMfinal0.139570

pdb_35/1an8_.pdb pdb_35/1aop_.pdb

number of residues in common206

rmsd of common residues19.277687

TMfinal0.105241

pdb_35/1an8_.pdb pdb_35/1aorA.pdb

pdb_35/1an8_.pdb pdb_35/1aoy_.pdb

number of residues in common78

rmsd of common residues12.626557

TMfinal0.160846

pdb_35/1an8_.pdb pdb_35/1aozA.pdb

pdb_35/1an8_.pdb pdb_35/1ap8_.pdb

number of residues in common206

rmsd of common residues20.841873

TMfinal0.161543

pdb_35/1an8_.pdb pdb_35/1apj_.pdb

number of residues in common74

rmsd of common residues14.370451

TMfinal0.169772

pdb_35/1an8_.pdb pdb_35/1apmE.pdb

pdb_35/1an8_.pdb pdb_35/1apq_.pdb

number of residues in common53

rmsd of common residues11.416533

TMfinal0.148762

pdb_35/1an8_.pdb pdb_35/1apxA.pdb

pdb_35/1an8_.pdb pdb_35/1aq0A.pdb

number of residues in common206

rmsd of common residues19.755022

TMfinal0.123448

pdb_35/1an8_.pdb pdb_35/1aqb_.pdb

number of residues in common175

rmsd of common residues17.852260

TMfinal0.152628

pdb_35/1an8_.pdb pdb_35/1aqcA.pdb

number of residues in common121

rmsd of common residues18.575698

TMfinal0.135236

pdb_35/1an8_.pdb pdb_35/1aqe_.pdb

number of residues in common110

rmsd of common residues16.580280

TMfinal0.135724

pdb_35/1an8_.pdb pdb_35/1aqt_.pdb

number of residues in common135

rmsd of common residues16.211305

TMfinal0.164501

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number of residues in common206

rmsd of common residues19.156693

TMfinal0.134270

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number of residues in common142

rmsd of common residues17.080092

TMfinal0.164291

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number of residues in common142

rmsd of common residues19.193526

TMfinal0.144022

pdb_35/1an8_.pdb pdb_35/1at3A.pdb

number of residues in common206

rmsd of common residues20.984940

TMfinal0.147365

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pdb_35/1an8_.pdb pdb_35/1atg_.pdb

number of residues in common206

rmsd of common residues20.044364

TMfinal0.146079

pdb_35/1an9A.pdb pdb_35/1amm_.pdb

number of residues in common174

rmsd of common residues18.921813

TMfinal0.151440

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pdb_35/1an9A.pdb pdb_35/1amuA.pdb

number of residues in common340

rmsd of common residues21.114435

TMfinal0.152329

pdb_35/1an9A.pdb pdb_35/1amx_.pdb

number of residues in common150

rmsd of common residues20.638173

TMfinal0.162479

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number of residues in common206

rmsd of common residues22.110851

TMfinal0.139465

pdb_35/1an9A.pdb pdb_35/1aoa_.pdb

number of residues in common247

rmsd of common residues23.744534

TMfinal0.150888

pdb_35/1an9A.pdb pdb_35/1aocA.pdb

number of residues in common175

rmsd of common residues24.106042

TMfinal0.131959

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number of residues in common192

rmsd of common residues20.100994

TMfinal0.162218

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number of residues in common143

rmsd of common residues22.315467

TMfinal0.136762

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number of residues in common228

rmsd of common residues22.570624

TMfinal0.150748

pdb_35/1an9A.pdb pdb_35/1aop_.pdb

number of residues in common340

rmsd of common residues25.813628

TMfinal0.122780

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pdb_35/1an9A.pdb pdb_35/1aoy_.pdb

number of residues in common78

rmsd of common residues14.169116

TMfinal0.165110

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pdb_35/1an9A.pdb pdb_35/1ap8_.pdb

number of residues in common213

rmsd of common residues23.593618

TMfinal0.140409

pdb_35/1an9A.pdb pdb_35/1apj_.pdb

number of residues in common74

rmsd of common residues12.764772

TMfinal0.156396

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number of residues in common53

rmsd of common residues12.228052

TMfinal0.133966

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number of residues in common306

rmsd of common residues20.967718

TMfinal0.201873

pdb_35/1an9A.pdb pdb_35/1aqb_.pdb

number of residues in common175

rmsd of common residues21.244033

TMfinal0.131431

pdb_35/1an9A.pdb pdb_35/1aqcA.pdb

number of residues in common121

rmsd of common residues17.849008

TMfinal0.162171

pdb_35/1an9A.pdb pdb_35/1aqe_.pdb

number of residues in common110

rmsd of common residues17.093370

TMfinal0.163279

pdb_35/1an9A.pdb pdb_35/1aqt_.pdb

number of residues in common135

rmsd of common residues17.850258

TMfinal0.140207

pdb_35/1an9A.pdb pdb_35/1aquA.pdb

number of residues in common281

rmsd of common residues20.629246

TMfinal0.194689

pdb_35/1an9A.pdb pdb_35/1aqzA.pdb

number of residues in common142

rmsd of common residues21.376947

TMfinal0.155096

pdb_35/1an9A.pdb pdb_35/1at0_.pdb

number of residues in common142

rmsd of common residues19.934466

TMfinal0.137079

pdb_35/1an9A.pdb pdb_35/1at3A.pdb

number of residues in common217

rmsd of common residues21.600447

TMfinal0.152705

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number of residues in common231

rmsd of common residues22.707749

TMfinal0.157278

pdb_35/1aoa_.pdb pdb_35/1amm_.pdb

number of residues in common174

rmsd of common residues19.904385

TMfinal0.148037

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pdb_35/1aoa_.pdb pdb_35/1amuA.pdb

number of residues in common247

rmsd of common residues22.287718

TMfinal0.111327

pdb_35/1aoa_.pdb pdb_35/1amx_.pdb

number of residues in common150

rmsd of common residues18.519452

TMfinal0.165625

pdb_35/1aoa_.pdb pdb_35/1an8_.pdb

number of residues in common206

rmsd of common residues19.866652

TMfinal0.142935

pdb_35/1aoa_.pdb pdb_35/1an9A.pdb

number of residues in common247

rmsd of common residues23.744534

TMfinal0.129051

pdb_35/1aoa_.pdb pdb_35/1aocA.pdb

number of residues in common175

rmsd of common residues20.324616

TMfinal0.141776

pdb_35/1aoa_.pdb pdb_35/1aoeA.pdb

number of residues in common192

rmsd of common residues18.732762

TMfinal0.175320

pdb_35/1aoa_.pdb pdb_35/1aohA.pdb

number of residues in common143

rmsd of common residues17.853984

TMfinal0.153733

pdb_35/1aoa_.pdb pdb_35/1aol_.pdb

number of residues in common228

rmsd of common residues18.748010

TMfinal0.187439

pdb_35/1aoa_.pdb pdb_35/1aop_.pdb

number of residues in common247

rmsd of common residues20.653704

TMfinal0.124700

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number of residues in common78

rmsd of common residues11.218511

TMfinal0.214820

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number of residues in common213

rmsd of common residues22.275435

TMfinal0.163506

pdb_35/1aoa_.pdb pdb_35/1apj_.pdb

number of residues in common74

rmsd of common residues10.959227

TMfinal0.145230

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pdb_35/1aoa_.pdb pdb_35/1apq_.pdb

number of residues in common53

rmsd of common residues8.718909

TMfinal0.150205

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pdb_35/1aoa_.pdb pdb_35/1aq0A.pdb

number of residues in common247

rmsd of common residues17.877404

TMfinal0.179926

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number of residues in common175

rmsd of common residues19.626528

TMfinal0.158111

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number of residues in common121

rmsd of common residues15.433222

TMfinal0.168182

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number of residues in common110

rmsd of common residues12.482603

TMfinal0.181093

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number of residues in common135

rmsd of common residues17.687686

TMfinal0.163358

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number of residues in common247

rmsd of common residues20.849604

TMfinal0.156419

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number of residues in common142

rmsd of common residues17.292341

TMfinal0.156859

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number of residues in common142

rmsd of common residues17.197258

TMfinal0.162574

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number of residues in common217

rmsd of common residues22.004300

TMfinal0.155651

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pdb_35/1aoa_.pdb pdb_35/1atg_.pdb

number of residues in common231

rmsd of common residues20.104588

TMfinal0.205769

pdb_35/1aocA.pdb pdb_35/1amm_.pdb

number of residues in common174

rmsd of common residues21.627235

TMfinal0.136616

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pdb_35/1aocA.pdb pdb_35/1amuA.pdb

number of residues in common175

rmsd of common residues19.275388

TMfinal0.101922

pdb_35/1aocA.pdb pdb_35/1amx_.pdb

number of residues in common150

rmsd of common residues18.197335

TMfinal0.161311

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number of residues in common175

rmsd of common residues20.898762

TMfinal0.119389

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number of residues in common175

rmsd of common residues24.106042

TMfinal0.095709

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number of residues in common175

rmsd of common residues20.324616

TMfinal0.122002

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number of residues in common175

rmsd of common residues21.138997

TMfinal0.137296

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number of residues in common143

rmsd of common residues20.124257

TMfinal0.134387

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number of residues in common175

rmsd of common residues21.127731

TMfinal0.134875

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number of residues in common175

rmsd of common residues19.158489

TMfinal0.085881

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number of residues in common78

rmsd of common residues14.047876

TMfinal0.155755

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number of residues in common175

rmsd of common residues22.046566

TMfinal0.141854

pdb_35/1aocA.pdb pdb_35/1apj_.pdb

number of residues in common74

rmsd of common residues15.423336

TMfinal0.145177

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number of residues in common53

rmsd of common residues12.779239

TMfinal0.140882

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number of residues in common175

rmsd of common residues18.924453

TMfinal0.117860

pdb_35/1aocA.pdb pdb_35/1aqb_.pdb

number of residues in common175

rmsd of common residues20.782697

TMfinal0.132198

pdb_35/1aocA.pdb pdb_35/1aqcA.pdb

number of residues in common121

rmsd of common residues20.300408

TMfinal0.129975

pdb_35/1aocA.pdb pdb_35/1aqe_.pdb

number of residues in common110

rmsd of common residues16.803439

TMfinal0.147835

pdb_35/1aocA.pdb pdb_35/1aqt_.pdb

number of residues in common135

rmsd of common residues20.246087

TMfinal0.140502

pdb_35/1aocA.pdb pdb_35/1aquA.pdb

number of residues in common175

rmsd of common residues19.468265

TMfinal0.137057

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number of residues in common142

rmsd of common residues16.778563

TMfinal0.163949

pdb_35/1aocA.pdb pdb_35/1at0_.pdb

number of residues in common142

rmsd of common residues19.185779

TMfinal0.145226

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number of residues in common175

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TMfinal0.159827

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number of residues in common175

rmsd of common residues19.326012

TMfinal0.139013

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number of residues in common174

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TMfinal0.138664

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number of residues in common192

rmsd of common residues22.245406

TMfinal0.095782

pdb_35/1aoeA.pdb pdb_35/1amx_.pdb

number of residues in common150

rmsd of common residues17.193091

TMfinal0.183622

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number of residues in common192

rmsd of common residues18.545583

TMfinal0.174155

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number of residues in common192

rmsd of common residues20.100994

TMfinal0.124126

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number of residues in common192

rmsd of common residues18.732762

TMfinal0.158472

pdb_35/1aoeA.pdb pdb_35/1aocA.pdb

number of residues in common175

rmsd of common residues21.138997

TMfinal0.143096

pdb_35/1aoeA.pdb pdb_35/1aohA.pdb

number of residues in common143

rmsd of common residues18.103426

TMfinal0.163503

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number of residues in common192

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TMfinal0.158616

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number of residues in common192

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TMfinal0.093152

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number of residues in common78

rmsd of common residues11.248152

TMfinal0.150428

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number of residues in common192

rmsd of common residues22.072761

TMfinal0.131596

pdb_35/1aoeA.pdb pdb_35/1apj_.pdb

number of residues in common74

rmsd of common residues14.267161

TMfinal0.144422

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number of residues in common53

rmsd of common residues14.741566

TMfinal0.114849

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number of residues in common192

rmsd of common residues18.390247

TMfinal0.139382

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number of residues in common175

rmsd of common residues15.254669

TMfinal0.186902

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number of residues in common121

rmsd of common residues17.246834

TMfinal0.157255

pdb_35/1aoeA.pdb pdb_35/1aqe_.pdb

number of residues in common110

rmsd of common residues14.018807

TMfinal0.168637

pdb_35/1aoeA.pdb pdb_35/1aqt_.pdb

number of residues in common135

rmsd of common residues17.706268

TMfinal0.138304

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number of residues in common192

rmsd of common residues17.393857

TMfinal0.147373

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number of residues in common142

rmsd of common residues17.493066

TMfinal0.150184

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number of residues in common142

rmsd of common residues17.441553

TMfinal0.153090

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number of residues in common192

rmsd of common residues18.553312

TMfinal0.176931

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number of residues in common192

rmsd of common residues21.126670

TMfinal0.167764

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number of residues in common143

rmsd of common residues19.966991

TMfinal0.131004

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number of residues in common143

rmsd of common residues21.324346

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number of residues in common143

rmsd of common residues17.186102

TMfinal0.163617

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number of residues in common143

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TMfinal0.137183

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number of residues in common143

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TMfinal0.091176

pdb_35/1aohA.pdb pdb_35/1aoa_.pdb

number of residues in common143

rmsd of common residues17.853984

TMfinal0.118563

pdb_35/1aohA.pdb pdb_35/1aocA.pdb

number of residues in common143

rmsd of common residues20.124257

TMfinal0.124081

pdb_35/1aohA.pdb pdb_35/1aoeA.pdb

number of residues in common143

rmsd of common residues18.103426

TMfinal0.144762

pdb_35/1aohA.pdb pdb_35/1aol_.pdb

number of residues in common143

rmsd of common residues19.790503

TMfinal0.107893

pdb_35/1aohA.pdb pdb_35/1aop_.pdb

number of residues in common143

rmsd of common residues18.896587

TMfinal0.079215

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pdb_35/1aohA.pdb pdb_35/1aoy_.pdb

number of residues in common78

rmsd of common residues14.524921

TMfinal0.142753

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pdb_35/1aohA.pdb pdb_35/1ap8_.pdb

number of residues in common143

rmsd of common residues22.050241

TMfinal0.144004

pdb_35/1aohA.pdb pdb_35/1apj_.pdb

number of residues in common74

rmsd of common residues11.138078

TMfinal0.149003

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pdb_35/1aohA.pdb pdb_35/1apq_.pdb

number of residues in common53

rmsd of common residues11.826628

TMfinal0.132517

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number of residues in common143

rmsd of common residues19.607984

TMfinal0.100958

pdb_35/1aohA.pdb pdb_35/1aqb_.pdb

number of residues in common143

rmsd of common residues16.627085

TMfinal0.160111

pdb_35/1aohA.pdb pdb_35/1aqcA.pdb

number of residues in common121

rmsd of common residues17.298634

TMfinal0.124695

pdb_35/1aohA.pdb pdb_35/1aqe_.pdb

number of residues in common110

rmsd of common residues16.882596

TMfinal0.134564

pdb_35/1aohA.pdb pdb_35/1aqt_.pdb

number of residues in common135

rmsd of common residues17.757580

TMfinal0.157517

pdb_35/1aohA.pdb pdb_35/1aquA.pdb

number of residues in common143

rmsd of common residues17.325502

TMfinal0.114310

pdb_35/1aohA.pdb pdb_35/1aqzA.pdb

number of residues in common142

rmsd of common residues16.309530

TMfinal0.155614

pdb_35/1aohA.pdb pdb_35/1at0_.pdb

number of residues in common142

rmsd of common residues18.057295

TMfinal0.135015

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number of residues in common143

rmsd of common residues18.281737

TMfinal0.149946

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pdb_35/1aohA.pdb pdb_35/1atg_.pdb

number of residues in common143

rmsd of common residues20.037547

TMfinal0.112593

pdb_35/1aol_.pdb pdb_35/1amm_.pdb

number of residues in common174

rmsd of common residues18.983933

TMfinal0.152646

pdb_35/1aol_.pdb pdb_35/1amp_.pdb

pdb_35/1aol_.pdb pdb_35/1amuA.pdb

number of residues in common228

rmsd of common residues19.585450

TMfinal0.122120

pdb_35/1aol_.pdb pdb_35/1amx_.pdb

number of residues in common150

rmsd of common residues18.837804

TMfinal0.139739

pdb_35/1aol_.pdb pdb_35/1an8_.pdb

number of residues in common206

rmsd of common residues20.349374

TMfinal0.145626

pdb_35/1aol_.pdb pdb_35/1an9A.pdb

number of residues in common228

rmsd of common residues22.570624

TMfinal0.122944

pdb_35/1aol_.pdb pdb_35/1aoa_.pdb

number of residues in common228

rmsd of common residues18.748010

TMfinal0.182092

pdb_35/1aol_.pdb pdb_35/1aocA.pdb

number of residues in common175

rmsd of common residues21.127731

TMfinal0.152514

pdb_35/1aol_.pdb pdb_35/1aoeA.pdb

number of residues in common192

rmsd of common residues18.684735

TMfinal0.171425

pdb_35/1aol_.pdb pdb_35/1aohA.pdb

number of residues in common143

rmsd of common residues19.790503

TMfinal0.142346

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number of residues in common228

rmsd of common residues20.740942

TMfinal0.121171

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number of residues in common78

rmsd of common residues17.136313

TMfinal0.118656

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number of residues in common213

rmsd of common residues21.205976

TMfinal0.154695

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number of residues in common74

rmsd of common residues14.400698

TMfinal0.126726

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number of residues in common53

rmsd of common residues11.581109

TMfinal0.126739

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number of residues in common228

rmsd of common residues20.697081

TMfinal0.139645

pdb_35/1aol_.pdb pdb_35/1aqb_.pdb

number of residues in common175

rmsd of common residues18.058771

TMfinal0.170363

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number of residues in common121

rmsd of common residues18.788377

TMfinal0.150545

pdb_35/1aol_.pdb pdb_35/1aqe_.pdb

number of residues in common110

rmsd of common residues14.661004

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pdb_35/1aol_.pdb pdb_35/1aqt_.pdb

number of residues in common135

rmsd of common residues19.204563

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number of residues in common228

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number of residues in common142

rmsd of common residues19.879900

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number of residues in common142

rmsd of common residues17.754407

TMfinal0.128560

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number of residues in common217

rmsd of common residues18.952376

TMfinal0.187623

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pdb_35/1aol_.pdb pdb_35/1atg_.pdb

number of residues in common228

rmsd of common residues21.435441

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number of residues in common174

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number of residues in common456

rmsd of common residues21.696198

TMfinal0.213198

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number of residues in common150

rmsd of common residues19.634690

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number of residues in common206

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number of residues in common340

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number of residues in common247

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number of residues in common175

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number of residues in common192

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number of residues in common143

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number of residues in common228

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number of residues in common78

rmsd of common residues14.198814

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number of residues in common213

rmsd of common residues21.839926

TMfinal0.147115

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number of residues in common74

rmsd of common residues12.548253

TMfinal0.151382

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number of residues in common53

rmsd of common residues12.347238

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number of residues in common306

rmsd of common residues21.444117

TMfinal0.181909

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number of residues in common175

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TMfinal0.143573

pdb_35/1aop_.pdb pdb_35/1aqcA.pdb

number of residues in common121

rmsd of common residues16.571488

TMfinal0.126805

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number of residues in common110

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TMfinal0.148296

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number of residues in common135

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number of residues in common281

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number of residues in common142

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number of residues in common142

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number of residues in common217

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pdb_35/1aop_.pdb pdb_35/1atg_.pdb

number of residues in common231

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number of residues in common78

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TMfinal0.115326

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number of residues in common78

rmsd of common residues15.107924

TMfinal0.049578

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number of residues in common78

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TMfinal0.119348

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number of residues in common78

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number of residues in common78

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number of residues in common78

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number of residues in common78

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number of residues in common74

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number of residues in common53

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number of residues in common78

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number of residues in common78

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number of residues in common78

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number of residues in common78

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number of residues in common174

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number of residues in common150

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number of residues in common206

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number of residues in common213

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number of residues in common213

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number of residues in common175

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number of residues in common192

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number of residues in common213

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number of residues in common213

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number of residues in common78

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number of residues in common74

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number of residues in common53

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number of residues in common175

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number of residues in common74

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number of residues in common74

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number of residues in common74

rmsd of common residues14.152012

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number of residues in common53

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number of residues in common74

rmsd of common residues12.278370

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number of residues in common74

rmsd of common residues14.499716

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number of residues in common74

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number of residues in common74

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number of residues in common74

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number of residues in common74

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number of residues in common53

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number of residues in common53

rmsd of common residues12.779239

TMfinal0.079813

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number of residues in common53

rmsd of common residues14.741566

TMfinal0.070689

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number of residues in common53

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number of residues in common53

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number of residues in common53

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number of residues in common53

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number of residues in common53

rmsd of common residues12.659478

TMfinal0.099276

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number of residues in common53

rmsd of common residues13.441735

TMfinal0.057068

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number of residues in common53

rmsd of common residues12.542869

TMfinal0.083942

pdb_35/1apq_.pdb pdb_35/1at0_.pdb

number of residues in common53

rmsd of common residues13.276603

TMfinal0.088339

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number of residues in common53

rmsd of common residues13.283036

TMfinal0.061061

pdb_35/1apq_.pdb pdb_35/1atg_.pdb

number of residues in common53

rmsd of common residues12.436005

TMfinal0.070289

pdb_35/1aq0A.pdb pdb_35/1amm_.pdb

number of residues in common174

rmsd of common residues17.671342

TMfinal0.167674

pdb_35/1aq0A.pdb pdb_35/1amuA.pdb

number of residues in common306

rmsd of common residues20.759635

TMfinal0.143337

pdb_35/1aq0A.pdb pdb_35/1amx_.pdb

number of residues in common150

rmsd of common residues18.045554

TMfinal0.158721

pdb_35/1aq0A.pdb pdb_35/1an8_.pdb

number of residues in common206

rmsd of common residues19.755022

TMfinal0.148035

pdb_35/1aq0A.pdb pdb_35/1an9A.pdb

number of residues in common306

rmsd of common residues20.967718

TMfinal0.191672

pdb_35/1aq0A.pdb pdb_35/1aoa_.pdb

number of residues in common247

rmsd of common residues17.877404

TMfinal0.200399

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number of residues in common175

rmsd of common residues18.924453

TMfinal0.155206

pdb_35/1aq0A.pdb pdb_35/1aoeA.pdb

number of residues in common192

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TMfinal0.182975

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number of residues in common78

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number of residues in common213

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number of residues in common53

rmsd of common residues10.515152

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number of residues in common175

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number of residues in common121

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rmsd of common residues15.937471

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number of residues in common78

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number of residues in common121

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number of residues in common74

rmsd of common residues14.364467

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number of residues in common53

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number of residues in common121

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number of residues in common110

rmsd of common residues15.169231

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number of residues in common121

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number of residues in common110

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number of residues in common228

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number of residues in common281

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number of residues in common213

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number of residues in common74

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number of residues in common53

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number of residues in common281

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number of residues in common175

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number of residues in common121

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number of residues in common110

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number of residues in common135

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number of residues in common231

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number of residues in common142

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number of residues in common142

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number of residues in common142

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number of residues in common142

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number of residues in common142

rmsd of common residues19.879900

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number of residues in common142

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number of residues in common78

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number of residues in common142

rmsd of common residues20.735017

TMfinal0.128528

pdb_35/1aqzA.pdb pdb_35/1apj_.pdb

number of residues in common74

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number of residues in common53

rmsd of common residues12.542869

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number of residues in common142

rmsd of common residues18.083662

TMfinal0.114267

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number of residues in common142

rmsd of common residues17.787576

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number of residues in common121

rmsd of common residues16.278623

TMfinal0.161367

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number of residues in common110

rmsd of common residues15.375237

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number of residues in common135

rmsd of common residues17.811805

TMfinal0.156526

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number of residues in common142

rmsd of common residues15.862749

TMfinal0.119497

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number of residues in common142

rmsd of common residues14.476397

TMfinal0.203586

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number of residues in common142

rmsd of common residues17.762094

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number of residues in common142

rmsd of common residues18.261920

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number of residues in common142

rmsd of common residues18.693595

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number of residues in common142

rmsd of common residues20.442807

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number of residues in common142

rmsd of common residues15.354356

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number of residues in common142

rmsd of common residues19.193526

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rmsd of common residues19.934466

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number of residues in common142

rmsd of common residues17.197258

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rmsd of common residues19.185779

TMfinal0.132861

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rmsd of common residues17.441553

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rmsd of common residues18.057295

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number of residues in common78

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number of residues in common142

rmsd of common residues19.702157

TMfinal0.113419

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number of residues in common74

rmsd of common residues11.498072

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number of residues in common53

rmsd of common residues13.276603

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number of residues in common142

rmsd of common residues15.976193

TMfinal0.114382

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number of residues in common142

rmsd of common residues17.859761

TMfinal0.132803

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number of residues in common121

rmsd of common residues15.460685

TMfinal0.160100

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number of residues in common110

rmsd of common residues13.685743

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number of residues in common135

rmsd of common residues18.643341

TMfinal0.125468

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number of residues in common142

rmsd of common residues16.369786

TMfinal0.107323

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number of residues in common142

rmsd of common residues14.476397

TMfinal0.203586

pdb_35/1at0_.pdb pdb_35/1at3A.pdb

number of residues in common142

rmsd of common residues16.345438

TMfinal0.141333

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number of residues in common142

rmsd of common residues18.843293

TMfinal0.110120

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number of residues in common174

rmsd of common residues18.870589

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number of residues in common217

rmsd of common residues22.425179

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number of residues in common150

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number of residues in common206

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number of residues in common217

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TMfinal0.123261

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number of residues in common217

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TMfinal0.146342

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number of residues in common175

rmsd of common residues17.933026

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number of residues in common192

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TMfinal0.187121

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number of residues in common143

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number of residues in common121

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number of residues in common135

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number of residues in common142

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number of residues in common231

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number of residues in common150

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number of residues in common192

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number of residues in common78

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number of residues in common213

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number of residues in common74

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number of residues in common175

rmsd of common residues20.474842

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number of residues in common110

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number of residues in common135

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number of residues in common231

rmsd of common residues20.955674

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number of residues in common142

rmsd of common residues18.261920

TMfinal0.128873

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number of residues in common142

rmsd of common residues18.843293

TMfinal0.139284

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number of residues in common217

rmsd of common residues20.356250

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min_rmsd8.718909

min_tm_score0.032508

max_aligned_length456

max_rmsd25.813628

max_tm_score0.225588

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sum_tm81.986449

avg time taken33.87138529

average no: of residue in common144.59580

rmsd of common residue17.7202

average TMscore0.136190

no of alignments between 0 and .17 534