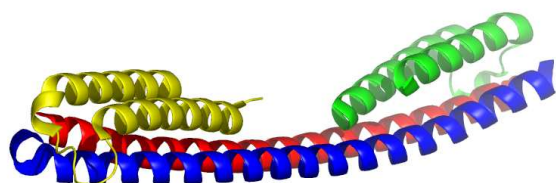


3h6p

Evolutionary trace report by `report_maker`

October 6, 2009



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1 INTRODUCTION

From the original Protein Data Bank entry (PDB id 3h6p):

Title: Crystal structure of rv3019c-rv3020c from mycobacterium tuberculosis

Compound: Mol id: 1; molecule: esat-6 like protein exs; chain: a, b; engineered: yes; mol id: 2; molecule: esat-6-like protein esxr; chain: c, d; engineered: yes

Organism, scientific name: Mycobacterium Tuberculosis; 3h6p contains unique chains 3h6pB (67 residues) and 3h6pC (56 residues) 3h6pA is a homologue of chain 3h6pB. 3h6pD is a homologue of chain 3h6pC.

2 CHAIN 3H6PB

2.1 Q7TXF7 overview

From SwissProt, id Q7TXF7, 76% identical to 3h6pB:

Description: PE FAMILY PROTEIN.

Organism, scientific name: Mycobacterium bovis.

Taxonomy: Bacteria; Actinobacteria; Actinobacteridae; Actinomycetales; Corynebacterineae; Mycobacteriaceae; Mycobacterium; Mycobacterium tuberculosis complex.

2.2 Multiple sequence alignment for 3h6pB

For the chain 3h6pB, the alignment 3h6pB.msf (attached) with 15 sequences was used. The alignment was downloaded from the HSSP database, and fragments shorter than 75% of the query as well as duplicate sequences were removed. It can be found in the attachment to this report, under the name of 3h6pB.msf. Its statistics, from the *alistat* program are the following:



Fig. 1. Residues 14-80 in 3h6pB colored by their relative importance. (See Appendix, Fig.11, for the coloring scheme.)

```

Format:                MSF
Number of sequences:  15
Total number of residues: 992
Smallest:             63
Largest:              67
Average length:       66.1
Alignment length:     67
Average identity:     75%
Most related pair:    98%
Most unrelated pair:  52%
Most distant seq:     61%

```

Furthermore, 34% of residues show as conserved in this alignment. The alignment consists of 6% prokaryotic sequences. (Descriptions of some sequences were not readily available.) The file containing the sequence descriptions can be found in the attachment, under the name 3h6pB.descr.

2.3 Residue ranking in 3h6pB

The 3h6pB sequence is shown in Fig. 1, with each residue colored according to its estimated importance. The full listing of residues in 3h6pB can be found in the file called 3h6pB.ranks_sorted in the attachment.

2.4 Top ranking residues in 3h6pB and their position on the structure

In the following we consider residues ranking among top 34% of residues in the protein (the closest this analysis allows us to get to 25%). Figure 2 shows residues in 3h6pB colored by their importance: bright red and yellow indicate more conserved/important residues (see Appendix for the coloring scheme). A Pymol script for producing this figure can be found in the attachment.

2.4.1 Clustering of residues at 34% coverage. Fig. 3 shows the top 34% of all residues, this time colored according to clusters they belong to. The clusters in Fig.3 are composed of the residues listed in Table 1.

Table 1.		
cluster color	size	member residues
red	9	32, 33, 36, 40, 41, 42, 43, 45, 46
blue	6	51, 52, 54, 55, 56, 58
yellow	5	66, 68, 69, 70, 72

Table 1. Clusters of top ranking residues in 3h6pB.

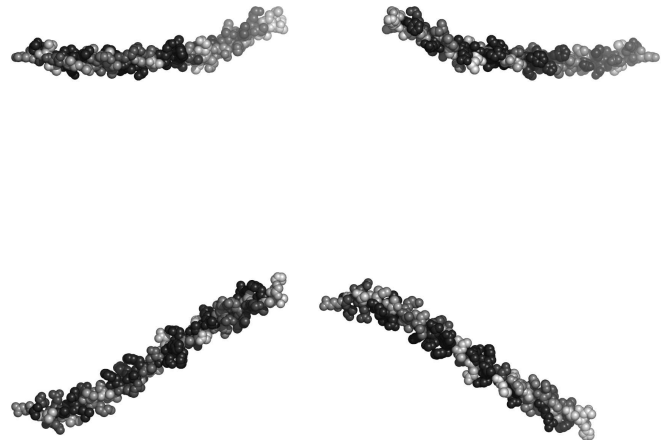


Fig. 2. Residues in 3h6pB, colored by their relative importance. Clockwise: front, back, top and bottom views.

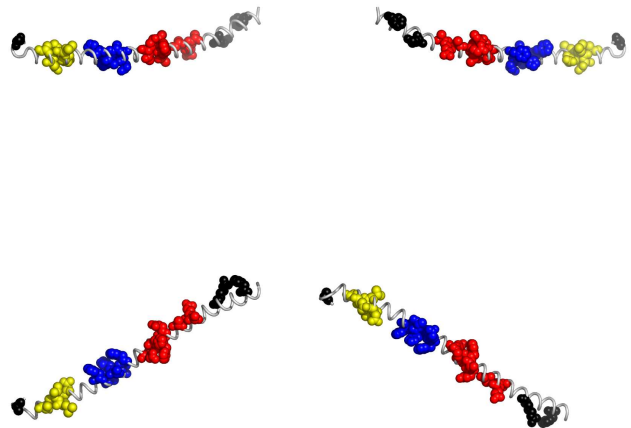


Fig. 3. Residues in 3h6pB, colored according to the cluster they belong to: red, followed by blue and yellow are the largest clusters (see Appendix for the coloring scheme). Clockwise: front, back, top and bottom views. The corresponding Pymol script is attached.

3 CHAIN 3H6PC

3.1 P64093 overview

From SwissProt, id P64093, 100% identical to 3h6pC:

Description: ESAT-6-like protein esxR.

Organism, scientific name: Mycobacterium tuberculosis.

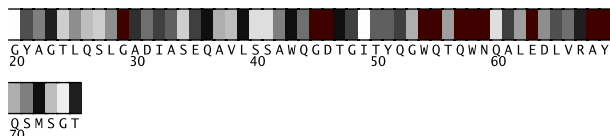


Fig. 4. Residues 20-75 in 3h6pC colored by their relative importance. (See Appendix, Fig.11, for the coloring scheme.)

Taxonomy: Bacteria; Actinobacteria; Actinobacteridae; Actinomycetales; Corynebacterineae; Mycobacteriaceae; Mycobacterium; Mycobacterium tuberculosis complex.

Similarity: Belongs to the ESAT-6 (esx) family.

About: This Swiss-Prot entry is copyright. It is produced through a collaboration between the Swiss Institute of Bioinformatics and the EMBL outstation - the European Bioinformatics Institute. There are no restrictions on its use as long as its content is in no way modified and this statement is not removed.

3.2 Multiple sequence alignment for 3h6pC

For the chain 3h6pC, the alignment 3h6pC.msf (attached) with 14 sequences was used. The alignment was downloaded from the HSSP database, and fragments shorter than 75% of the query as well as duplicate sequences were removed. It can be found in the attachment to this report, under the name of 3h6pC.msf. Its statistics, from the *alistat* program are the following:

```

Format:                MSF
Number of sequences:   14
Total number of residues: 772
Smallest:              54
Largest:               56
Average length:       55.1
Alignment length:     56
Average identity:     67%
Most related pair:    98%
Most unrelated pair:  43%
Most distant seq:     63%

```

Furthermore, 19% of residues show as conserved in this alignment.

The alignment consists of 7% prokaryotic sequences. (Descriptions of some sequences were not readily available.) The file containing the sequence descriptions can be found in the attachment, under the name 3h6pC.descr.

3.3 Residue ranking in 3h6pC

The 3h6pC sequence is shown in Fig. 4, with each residue colored according to its estimated importance. The full listing of residues in 3h6pC can be found in the file called 3h6pC.ranks_sorted in the attachment.

3.4 Top ranking residues in 3h6pC and their position on the structure

In the following we consider residues ranking among top 28% of residues in the protein (the closest this analysis allows us to get to 25%). Figure 5 shows residues in 3h6pC colored by their importance: bright red and yellow indicate more conserved/important residues (see

Appendix for the coloring scheme). A Pymol script for producing this figure can be found in the attachment.

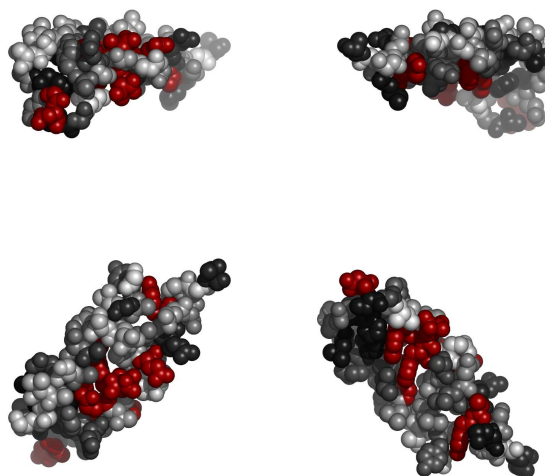


Fig. 5. Residues in 3h6pC, colored by their relative importance. Clockwise: front, back, top and bottom views.

3.4.1 Clustering of residues at 28% coverage. Fig. 6 shows the top 28% of all residues, this time colored according to clusters they belong to. The clusters in Fig.6 are composed of the residues listed in Table 2.

cluster color	size	member residues
red	13	29, 36, 39, 43, 45, 46, 47, 54, 55, 57, 58, 59, 63
blue	3	68, 69, 72

Table 2. Clusters of top ranking residues in 3h6pC.

3.4.2 Overlap with known functional surfaces at 28% coverage. The name of the ligand is composed of the source PDB identifier and the heteroatom name used in that file.

Glycerol binding site. By analogy with 3h6pD – 3h6pDGOL501 interface. Table 3 lists the top 28% of residues at the interface with 3h6pDGOL501 (glycerol). The following table (Table 4) suggests possible disruptive replacements for these residues (see Section 4.6).

res	type	subst's (%)	cvg	noc/bb	dist (Å)
57	Q	Q(100)	0.20	6/0	3.60

Table 3. The top 28% of residues in 3h6pC at the interface with glycerol. (Field names: res: residue number in the PDB entry; type: amino acid

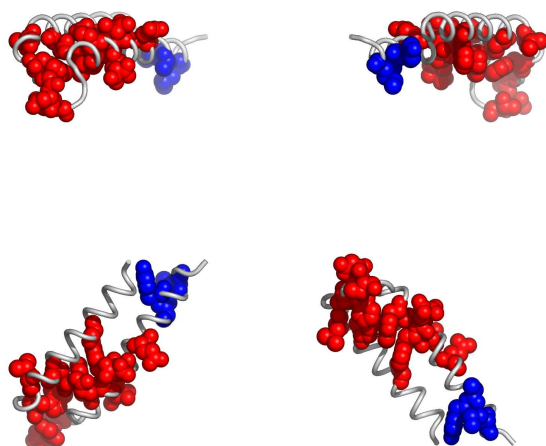


Fig. 6. Residues in 3h6pC, colored according to the cluster they belong to: red, followed by blue and yellow are the largest clusters (see Appendix for the coloring scheme). Clockwise: front, back, top and bottom views. The corresponding Pymol script is attached.

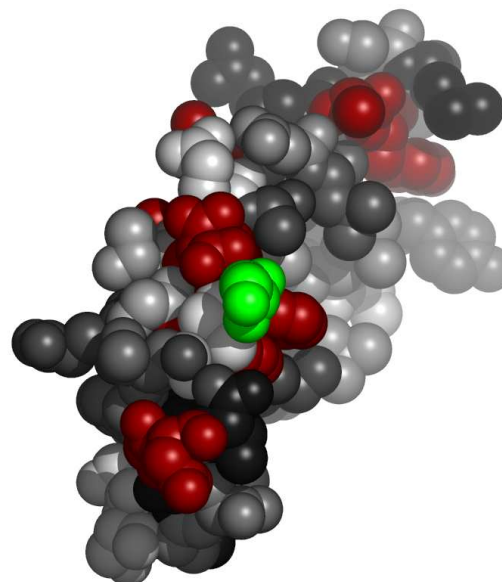


Fig. 7. Residues in 3h6pC, at the interface with glycerol, colored by their relative importance. The ligand (glycerol) is colored green. Atoms further than 30 Å away from the geometric center of the ligand, as well as on the line of sight to the ligand were removed. (See Appendix for the coloring scheme for the protein chain 3h6pC.)

type; subst: substitutions seen in the alignment; with the percentage of each type in the bracket; noc/bb: number of contacts with the ligand, with the number of contacts realized through backbone atoms given in the bracket; dist: distance of closest approach to the ligand.)

Table 4.		
res	type	disruptive mutations
57	Q	(Y) (FTWH) (SVCAG) (D)

Table 4. List of disruptive mutations for the top 28% of residues in 3h6pC, that are at the interface with glycerol.

Figure 7 shows residues in 3h6pC colored by their importance, at the interface with 3h6pDGOL501.

Interface with 3h6pA. Table 5 lists the top 28% of residues at the interface with 3h6pA. The following table (Table 6) suggests possible disruptive replacements for these residues (see Section 4.6).

Table 5.					
res	type	subst's (%)	cvg	noc/bb	dist (Å)
29	G	G(100)	0.20	2/2	3.42
54	W	W(100)	0.20	3/0	4.71
58	W	W(100)	0.20	3/0	4.28
69	Y	Y(100)	0.20	25/0	2.21

Table 5. The top 28% of residues in 3h6pC at the interface with 3h6pA. (Field names: res: residue number in the PDB entry; type: amino acid type; substs: substitutions seen in the alignment; with the percentage of each type

in the bracket; noc/bb: number of contacts with the ligand, with the number of contacts realized through backbone atoms given in the bracket; dist: distance of closest approach to the ligand.)

Table 6.		
res	type	disruptive mutations
29	G	(KER) (FQMWH) (NYLPI) (SVA)
54	W	(KE) (TQD) (SNCRG) (M)
58	W	(KE) (TQD) (SNCRG) (M)
69	Y	(K) (QM) (NEVLAPIR) (D)

Table 6. List of disruptive mutations for the top 28% of residues in 3h6pC, that are at the interface with 3h6pA.

Figure 8 shows residues in 3h6pC colored by their importance, at the interface with 3h6pA.

Interface with 3h6pB. Table 7 lists the top 28% of residues at the interface with 3h6pB. The following table (Table 8) suggests possible disruptive replacements for these residues (see Section 4.6).

Table 7.					
res	type	subst's (%)	cvg	noc/bb	dist (Å)
54	W	W(100)	0.20	47/2	2.88
57	Q	Q(100)	0.20	14/5	3.63
58	W	W(100)	0.20	43/6	3.60

continued in next column

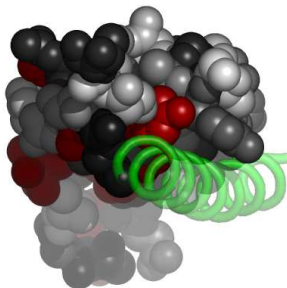


Fig. 8. Residues in 3h6pC, at the interface with 3h6pA, colored by their relative importance. 3h6pA is shown in backbone representation (See Appendix for the coloring scheme for the protein chain 3h6pC.)

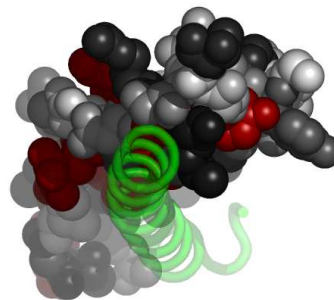


Fig. 9. Residues in 3h6pC, at the interface with 3h6pB, colored by their relative importance. 3h6pB is shown in backbone representation (See Appendix for the coloring scheme for the protein chain 3h6pC.)

Table 7. continued

res	type	subst's (%)	cvg	noc/ bb	dist (Å)
68	A	A(100)	0.20	29/16	3.41
69	Y	Y(100)	0.20	14/7	3.87

Table 7. The top 28% of residues in 3h6pC at the interface with 3h6pB. (Field names: res: residue number in the PDB entry; type: amino acid type; substs: substitutions seen in the alignment; with the percentage of each type in the bracket; noc/bb: number of contacts with the ligand, with the number of contacts realized through backbone atoms given in the bracket; dist: distance of closest approach to the ligand.)

substantially larger than) other functional sites and interfaces recognizable in PDB entry 3h6p. It is shown in Fig. 10. The right panel shows (in blue) the rest of the larger cluster this surface belongs to.

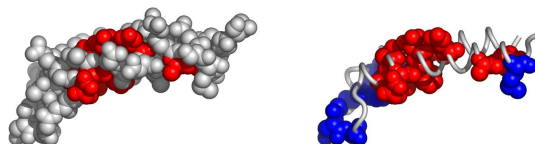


Fig. 10. A possible active surface on the chain 3h6pC. The larger cluster it belongs to is shown in blue.

Table 8.

res	type	disruptive mutations
54	W	(KE)(TQD)(SNCRG)(M)
57	Q	(Y)(FTWH)(SVCAG)(D)
58	W	(KE)(TQD)(SNCRG)(M)
68	A	(KYER)(QHD)(N)(FTMW)
69	Y	(K)(QM)(NEVLAPIR)(D)

Table 8. List of disruptive mutations for the top 28% of residues in 3h6pC, that are at the interface with 3h6pB.

Figure 9 shows residues in 3h6pC colored by their importance, at the interface with 3h6pB.

3.4.3 Possible novel functional surfaces at 28% coverage. One group of residues is conserved on the 3h6pC surface, away from (or

The residues belonging to this surface "patch" are listed in Table 9, while Table 10 suggests possible disruptive replacements for these residues (see Section 4.6).

Table 9.

res	type	substitutions(%)	cvg
29	G	G(100)	0.20
54	W	W(100)	0.20
55	Q	Q(100)	0.20
57	Q	Q(100)	0.20

continued in next column

Table 9. continued			
res	type	substitutions(%)	cvg
58	W	W(100)	0.20
59	N	N(100)	0.20
63	E	E(100)	0.20
68	A	A(100)	0.20
69	Y	Y(100)	0.20

Table 9. Residues forming surface "patch" in 3h6pC.

Table 10.		
res	type	disruptive mutations
29	G	(KER) (FQMWHD) (NYLPI) (SVA)
54	W	(KE) (TQD) (SNCRG) (M)
55	Q	(Y) (FTWH) (SVCAG) (D)
57	Q	(Y) (FTWH) (SVCAG) (D)
58	W	(KE) (TQD) (SNCRG) (M)
59	N	(Y) (FTWH) (SEVCARG) (MD)
63	E	(FWH) (YVCARG) (T) (SNKLPPI)
68	A	(KYER) (QHD) (N) (FTMW)
69	Y	(K) (QM) (NEVLAPIR) (D)

Table 10. Disruptive mutations for the surface patch in 3h6pC.

4 NOTES ON USING TRACE RESULTS

4.1 Coverage

Trace results are commonly expressed in terms of coverage: the residue is important if its "coverage" is small - that is if it belongs to some small top percentage of residues [100% is all of the residues in a chain], according to trace. The ET results are presented in the form of a table, usually limited to top 25% percent of residues (or to some nearby percentage), sorted by the strength of the presumed evolutionary pressure. (I.e., the smaller the coverage, the stronger the pressure on the residue.) Starting from the top of that list, mutating a couple of residues should affect the protein somehow, with the exact effects to be determined experimentally.

4.2 Known substitutions

One of the table columns is "substitutions" - other amino acid types seen at the same position in the alignment. These amino acid types may be interchangeable at that position in the protein, so if one wants to affect the protein by a point mutation, they should be avoided. For example if the substitutions are "RVK" and the original protein has an R at that position, it is advisable to try anything, but RVK. Conversely, when looking for substitutions which will *not* affect the protein, one may try replacing, R with K, or (perhaps more surprisingly), with V. The percentage of times the substitution appears in the alignment is given in the immediately following bracket. No percentage is given in the cases when it is smaller than 1%. This is meant to be a rough guide - due to rounding errors these percentages often do not add up to 100%.

4.3 Surface

To detect candidates for novel functional interfaces, first we look for residues that are solvent accessible (according to DSSP program) by

at least 10\AA^2 , which is roughly the area needed for one water molecule to come in the contact with the residue. Furthermore, we require that these residues form a "cluster" of residues which have neighbor within 5\AA from any of their heavy atoms.

Note, however, that, if our picture of protein evolution is correct, the neighboring residues which *are not* surface accessible might be equally important in maintaining the interaction specificity - they should not be automatically dropped from consideration when choosing the set for mutagenesis. (Especially if they form a cluster with the surface residues.)

4.4 Number of contacts

Another column worth noting is denoted "noc/bb"; it tells the number of contacts heavy atoms of the residue in question make across the interface, as well as how many of them are realized through the backbone atoms (if all or most contacts are through the backbone, mutation presumably won't have strong impact). Two heavy atoms are considered to be "in contact" if their centers are closer than 5\AA .

4.5 Annotation

If the residue annotation is available (either from the pdb file or from other sources), another column, with the header "annotation" appears. Annotations carried over from PDB are the following: site (indicating existence of related site record in PDB), S-S (disulfide bond forming residue), hb (hydrogen bond forming residue), jb (james bond forming residue), and sb (for salt bridge forming residue).

4.6 Mutation suggestions

Mutation suggestions are completely heuristic and based on complementarity with the substitutions found in the alignment. Note that they are meant to be **disruptive** to the interaction of the protein with its ligand. The attempt is made to complement the following properties: small [AVGSTC], medium [LPNQDEMILK], large [WFYHR], hydrophobic [LPVAMWFI], polar [GTCY]; positively [KHR], or negatively [DE] charged, aromatic [WFYH], long aliphatic chain [EKRRQM], OH-group possession [SDETY], and NH2 group possession [NQRK]. The suggestions are listed according to how different they appear to be from the original amino acid, and they are grouped in round brackets if they appear equally disruptive. From left to right, each bracketed group of amino acid types resembles more strongly the original (i.e. is, presumably, less disruptive) These suggestions are tentative - they might prove disruptive to the fold rather than to the interaction. Many researcher will choose, however, the straightforward alanine mutations, especially in the beginning stages of their investigation.

5 APPENDIX

5.1 File formats

Files with extension "ranks_sorted" are the actual trace results. The fields in the table in this file:

- `alignment#` number of the position in the alignment
- `residue#` residue number in the PDB file
- `type` amino acid type
- `rank` rank of the position according to older version of ET
- `variability` has two subfields:
 1. number of different amino acids appearing in in this column of the alignment

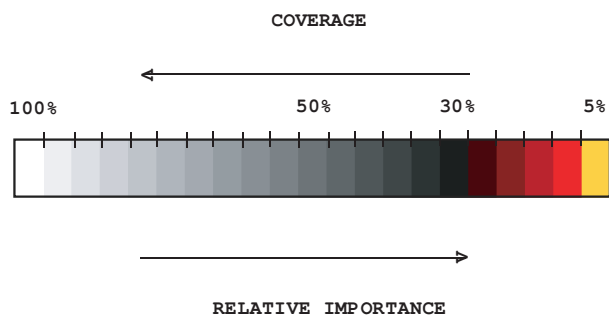


Fig. 11. Coloring scheme used to color residues by their relative importance.

2. their type

- ρ ET score - the smaller this value, the lesser variability of this position across the branches of the tree (and, presumably, the greater the importance for the protein)
- cvg coverage - percentage of the residues on the structure which have this ρ or smaller
- gaps percentage of gaps in this column

5.2 Color schemes used

The following color scheme is used in figures with residues colored by cluster size: black is a single-residue cluster; clusters composed of more than one residue colored according to this hierarchy (ordered by descending size): red, blue, yellow, green, purple, azure, turquoise, brown, coral, magenta, LightSalmon, SkyBlue, violet, gold, bisque, LightSlateBlue, orchid, RosyBrown, MediumAquamarine, DarkOliveGreen, CornflowerBlue, grey55, burlywood, LimeGreen, tan, DarkOrange, DeepPink, maroon, BlanchedAlmond.

The colors used to distinguish the residues by the estimated evolutionary pressure they experience can be seen in Fig. 11.

5.3 Credits

5.3.1 Alistat *alistat* reads a multiple sequence alignment from the file and shows a number of simple statistics about it. These statistics include the format, the number of sequences, the total number of residues, the average and range of the sequence lengths, and the alignment length (e.g. including gap characters). Also shown are some percent identities. A percent pairwise alignment identity is defined as $(\text{idents} / \text{MIN}(\text{len1}, \text{len2}))$ where *idents* is the number of exact identities and *len1*, *len2* are the unaligned lengths of the two sequences. The "average percent identity", "most related pair", and "most unrelated pair" of the alignment are the average, maximum, and minimum of all $(N)(N-1)/2$ pairs, respectively. The "most distant seq" is calculated by finding the maximum pairwise identity (best relative) for all *N* sequences, then finding the minimum of these *N* numbers (hence, the most outlying sequence). *alistat* is copyrighted by HHMI/Washington University School of Medicine, 1992-2001, and freely distributed under the GNU General Public License.

5.3.2 CE To map ligand binding sites from different source structures, *report_maker* uses the CE program: <http://cl.sdsc.edu/>. Shindyalov IN, Bourne PE (1998) "Protein structure alignment by incremental combinatorial extension (CE) of the optimal path". *Protein Engineering* 11(9) 739-747.

5.3.3 DSSP In this work a residue is considered solvent accessible if the DSSP program finds it exposed to water by at least 10\AA^2 , which is roughly the area needed for one water molecule to come in the contact with the residue. DSSP is copyrighted by W. Kabsch, C. Sander and MPI-MF, 1983, 1985, 1988, 1994 1995, CMBI version by Elmar.Krieger@cmbi.kun.nl November 18,2002,

<http://www.cmbi.kun.nl/gv/dssp/descrip.html>.

5.3.4 HSSP Whenever available, *report_maker* uses HSSP alignment as a starting point for the analysis (sequences shorter than 75% of the query are taken out, however); R. Schneider, A. de Daruvar, and C. Sander. "The HSSP database of protein structure-sequence alignments." *Nucleic Acids Res.*, 25:226-230, 1997.

<http://swift.cmbi.kun.nl/swift/hssp/>

5.3.5 LaTeX The text for this report was processed using \LaTeX ; Leslie Lamport, "LaTeX: A Document Preparation System Addison-Wesley," Reading, Mass. (1986).

5.3.6 Muscle When making alignments "from scratch", *report_maker* uses Muscle alignment program: Edgar, Robert C. (2004), "MUSCLE: multiple sequence alignment with high accuracy and high throughput." *Nucleic Acids Research* 32(5), 1792-97.

<http://www.drive5.com/muscle/>

5.3.7 Pymol The figures in this report were produced using Pymol. The scripts can be found in the attachment. Pymol is an open-source application copyrighted by DeLano Scientific LLC (2005). For more information about Pymol see <http://pymol.sourceforge.net/>. (Note for Windows users: the attached package needs to be unzipped for Pymol to read the scripts and launch the viewer.)

5.4 Note about ET Viewer

Dan Morgan from the Lichtarge lab has developed a visualization tool specifically for viewing trace results. If you are interested, please visit:

<http://mammoth.bcm.tmc.edu/traceview/>

The viewer is self-unpacking and self-installing. Input files to be used with ETV (extension .etvx) can be found in the attachment to the main report.

5.5 Citing this work

The method used to rank residues and make predictions in this report can be found in Mihalek, I., I. Reš, O. Lichtarge. (2004). "A Family of Evolution-Entropy Hybrid Methods for Ranking of Protein Residues by Importance" *J. Mol. Bio.* **336**: 1265-82. For the original version of ET see O. Lichtarge, H.Bourne and F. Cohen (1996). "An Evolutionary Trace Method Defines Binding Surfaces Common to Protein Families" *J. Mol. Bio.* **257**: 342-358.

report_maker itself is described in Mihalek I., I. Res and O. Lichtarge (2006). "Evolutionary Trace Report Maker: a new type

of service for comparative analysis of proteins." Bioinformatics 22:1656-7.

5.6 About report_maker

report_maker was written in 2006 by Ivana Mihalek. The 1D ranking visualization program was written by Ivica Reš. **report_maker** is copyrighted by Lichtarge Lab, Baylor College of Medicine, Houston.

5.7 Attachments

The following files should accompany this report:

- 3h6pB.complex.pdb - coordinates of 3h6pB with all of its interacting partners
- 3h6pB.etvx - ET viewer input file for 3h6pB
- 3h6pB.cluster_report.summary - Cluster report summary for 3h6pB
- 3h6pB.ranks - Ranks file in sequence order for 3h6pB
- 3h6pB.clusters - Cluster descriptions for 3h6pB
- 3h6pB.msf - the multiple sequence alignment used for the chain 3h6pB
- 3h6pB.descr - description of sequences used in 3h6pB msf
- 3h6pB.ranks_sorted - full listing of residues and their ranking for 3h6pB
- 3h6pC.complex.pdb - coordinates of 3h6pC with all of its interacting partners
- 3h6pC.etvx - ET viewer input file for 3h6pC
- 3h6pC.cluster_report.summary - Cluster report summary for 3h6pC
- 3h6pC.ranks - Ranks file in sequence order for 3h6pC
- 3h6pC.clusters - Cluster descriptions for 3h6pC
- 3h6pC.msf - the multiple sequence alignment used for the chain 3h6pC
- 3h6pC.descr - description of sequences used in 3h6pC msf
- 3h6pC.ranks_sorted - full listing of residues and their ranking for 3h6pC
- 3h6pC.3h6pDGOL501.if.pml - Pymol script for Figure 7
- 3h6pC.cbvcg - used by other 3h6pC – related pymol scripts
- 3h6pC.3h6pA.if.pml - Pymol script for Figure 8
- 3h6pC.3h6pB.if.pml - Pymol script for Figure 9