1 INTRODUCTION

From the original Protein Data Bank entry (PDB id 1a9p):
Title: Bovine purine nucleoside phosphorylase complexed with 9-deazainosine and phosphate
Compound: Mol id: 1; molecule: purine nucleoside phosphorylase; chain: a; ec: 2.4.2.1
Organism, scientific name: Bos Taurus;
1a9p contains a single unique chain 1a9pA (289 residues long).

2 CHAIN 1A9PA

2.1 P55859 overview
From SwissProt, id P55859, 99% identical to 1a9pA:
Description: Purine nucleoside phosphorylase (EC 2.4.2.1) (Inosine
phosphorylase) (PNP).
Organism, scientific name: Bos taurus (Bovine).
Taxonomy:
Eukaryota; Metazoa; Chordata; Vertebrata; Euteleostomi; Mammalia; Eutheria; Laurasiatheria; Cetartiodactyla;
Ruminantia; Pecora; Bovidae; Bovinae; Bos.
Catalytic activity: Purine nucleoside + phosphate = purine + alpha-
D-ribose 1-phosphate.
Subunit: Homotrimer.
Similarity: Belongs to the PNP/MTAP phosphorylase 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.

2.2 Multiple sequence alignment for 1a9pA
For the chain 1a9pA, the alignment 1a9pA.msf (attached) with 32
sequences was used. The alignment was assembled through combi-
nation of BLAST searching on the UniProt database and alignment
using Muscle program. It can be found in the attachment to this
report, under the name of 1a9pA.msf. Its statistics, from the alistat
program are the following:

CONTENTS
1 Introduction
2 Chain 1a9pA
3 Notes on using trace results
4 Appendix

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using Muscle program. It can be found in the attachment to this
report, under the name of 1a9pA.msf. Its statistics, from the alistat
program are the following:
2.3 Residue ranking in 1a9pA

The 1a9pA sequence is shown in Figs. 1–2, with each residue colored according to its estimated importance. The full listing of residues in 1a9pA can be found in the file called 1a9pA.ranks.sorted in the attachment.

2.4 Top ranking residues in 1a9pA and their position on the structure

In the following we consider residues ranking among top 25% of residues in the protein. Figure 3 shows residues in 1a9pA 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 25% coverage. Fig. 4 shows the top 25% of all residues, this time colored according to clusters they belong to. The clusters in Fig.4 are composed of the residues listed in Table 1.
### Table 1.

<table>
<thead>
<tr>
<th>cluster color</th>
<th>size</th>
<th>member residues</th>
</tr>
</thead>
</table>

**Table 1.** Clusters of top ranking residues in 1a9pA.

#### 2.4.2 Overlap with known functional surfaces at 25% coverage.

The name of the ligand is composed of the source PDB identifier and the heteroatom name used in that file.

**Interface with 1a9pA2.** Table 2 lists the top 25% of residues at the interface with 1a9pA2. The following table (Table 3) suggests possible disruptive replacements for these residues (see Section 3.6).

### Table 2.

<table>
<thead>
<tr>
<th>res</th>
<th>type</th>
<th>subst’s (%)</th>
<th>cvg</th>
<th>noc/bb</th>
<th>dist (Å)</th>
<th>antn</th>
</tr>
</thead>
<tbody>
<tr>
<td>197</td>
<td>G</td>
<td>G(100)</td>
<td>0.04</td>
<td>15/15</td>
<td>3.16</td>
<td></td>
</tr>
<tr>
<td>198</td>
<td>P</td>
<td>P(100)</td>
<td>0.04</td>
<td>53/24</td>
<td>3.19</td>
<td></td>
</tr>
<tr>
<td>205</td>
<td>E</td>
<td>E(100)</td>
<td>0.04</td>
<td>55/6</td>
<td>2.59</td>
<td></td>
</tr>
<tr>
<td>219</td>
<td>M</td>
<td>M(100)</td>
<td>0.04</td>
<td>4/0</td>
<td>4.47</td>
<td>site</td>
</tr>
<tr>
<td>89</td>
<td>E</td>
<td>E(90)</td>
<td>0.07</td>
<td>24/23</td>
<td>3.18</td>
<td></td>
</tr>
<tr>
<td>90</td>
<td>G</td>
<td>G(90)</td>
<td>0.07</td>
<td>24/24</td>
<td>3.60</td>
<td></td>
</tr>
<tr>
<td>201</td>
<td>E</td>
<td>E(93)</td>
<td>0.09</td>
<td>10/10</td>
<td>3.98</td>
<td>site</td>
</tr>
<tr>
<td>257</td>
<td>H</td>
<td>H(93)</td>
<td>0.09</td>
<td>24/3</td>
<td>3.39</td>
<td>site</td>
</tr>
<tr>
<td>204</td>
<td>A</td>
<td>A(96)</td>
<td>0.10</td>
<td>25/13</td>
<td>3.05</td>
<td></td>
</tr>
<tr>
<td>88</td>
<td>Y</td>
<td>Y(90)</td>
<td>0.11</td>
<td>60/35</td>
<td>3.04</td>
<td>site</td>
</tr>
<tr>
<td>200</td>
<td>F</td>
<td>F(40)</td>
<td>0.16</td>
<td>47/20</td>
<td>3.12</td>
<td></td>
</tr>
<tr>
<td>202</td>
<td>T</td>
<td>T(15)</td>
<td>0.19</td>
<td>54/16</td>
<td>2.69</td>
<td></td>
</tr>
<tr>
<td>61</td>
<td>V</td>
<td>V(68)</td>
<td>0.25</td>
<td>3/0</td>
<td>4.07</td>
<td></td>
</tr>
</tbody>
</table>

**Table 2.** The top 25% of residues in 1a9pA at the interface with 1a9pA2. (Field names: res: residue number in the PDB entry; type: amino acid type; subst’s: 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 3.

<table>
<thead>
<tr>
<th>res</th>
<th>type</th>
<th>disruptive mutations</th>
</tr>
</thead>
<tbody>
<tr>
<td>197</td>
<td>G</td>
<td>(KER) (FQMWHD) (NYLPI) (SVA)</td>
</tr>
<tr>
<td>198</td>
<td>P</td>
<td>(YR) (TH) (SKECG) (FQWD)</td>
</tr>
<tr>
<td>205</td>
<td>E</td>
<td>(FWH) (YVCARG) (T) (SNKLPI)</td>
</tr>
<tr>
<td>219</td>
<td>M</td>
<td>(Y) (TH) (SCRG) (FWD)</td>
</tr>
<tr>
<td>89</td>
<td>E</td>
<td>(FYWR) (CG) (TVA)</td>
</tr>
<tr>
<td>90</td>
<td>G</td>
<td>(R) (KE) (H) (FYQWD)</td>
</tr>
<tr>
<td>201</td>
<td>E</td>
<td>(FWH) (R) (Y) (VCAG)</td>
</tr>
<tr>
<td>257</td>
<td>H</td>
<td>(E) (QD) (TKM) (N)</td>
</tr>
<tr>
<td>204</td>
<td>A</td>
<td>(KR) (E) (YQH) (D)</td>
</tr>
<tr>
<td>88</td>
<td>Y</td>
<td>(K) (Q) (E) (R)</td>
</tr>
<tr>
<td>200</td>
<td>F</td>
<td>(K) (E) (Q) (D)</td>
</tr>
<tr>
<td>202</td>
<td>T</td>
<td>(KR) (FQMW) (NELPI) (D)</td>
</tr>
<tr>
<td>61</td>
<td>V</td>
<td>(R) (Y) (KE) (H)</td>
</tr>
</tbody>
</table>

**Table 3.** List of disruptive mutations for the top 25% of residues in 1a9pA2, that are at the interface with 1a9pA2.

Figure 5 shows residues in 1a9pA colored by their importance, at the interface with 1a9pA2.

**Interface with 1a9pA1.** Table 4 lists the top 25% of residues at the interface with 1a9pA1. The following table (Table 5) suggests possible disruptive replacements for these residues (see Section 3.6).

---

**Fig. 5.** Residues in 1a9pA, at the interface with 1a9pA2, colored by their relative importance. 1a9pA2 is shown in backbone representation (See Appendix for the coloring scheme for the protein chain 1a9pA.)

Figure 5 shows residues in 1a9pA colored by their importance, at the interface with 1a9pA2.

**Interface with 1a9pA1.** Table 4 lists the top 25% of residues at the interface with 1a9pA1. The following table (Table 5) suggests possible disruptive replacements for these residues (see Section 3.6).
Table 4. The top 25% of residues in 1a9pA at the interface with 1a9pA1. (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 5. List of disruptive mutations for the top 25% of residues in 1a9pA, that are at the interface with 1a9pA1.

Table 6. The top 25% of residues in 1a9pA at the interface with phosphate ion. (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 7. List of disruptive mutations for the top 25% of residues in 1a9pA, that are at the interface with phosphate ion.

<table>
<thead>
<tr>
<th>res</th>
<th>type</th>
<th>disruptive mutations</th>
</tr>
</thead>
<tbody>
<tr>
<td>86</td>
<td>H</td>
<td>(E) (TQMD) (SNKVCLAPIG) (YR)</td>
</tr>
<tr>
<td>192</td>
<td>Y</td>
<td>(K) (QM) (NEVLAPIR) (D)</td>
</tr>
<tr>
<td>219</td>
<td>M</td>
<td>(Y) (TH) (SCRG) (FWD)</td>
</tr>
<tr>
<td>64</td>
<td>H</td>
<td>(E) (TQMD) (SNVCLAPIG) (K)</td>
</tr>
<tr>
<td>115</td>
<td>N</td>
<td>(FYWH) (R) (E) (TVMA)</td>
</tr>
<tr>
<td>220</td>
<td>S</td>
<td>(KR) (FQMH) (NELPI) (Y)</td>
</tr>
<tr>
<td>84</td>
<td>R</td>
<td>(TYD) (E) (SCG) (FVLAWPI)</td>
</tr>
<tr>
<td>88</td>
<td>Y</td>
<td>(K) (Q) (E) (R)</td>
</tr>
<tr>
<td>32</td>
<td>G</td>
<td>(KER) (FQMWHD) (NLPI) (Y)</td>
</tr>
<tr>
<td>116</td>
<td>A</td>
<td>(KER) (Y) (QHD) (N)</td>
</tr>
<tr>
<td>33</td>
<td>S</td>
<td>(KR) (FWH) (QM) (LPI)</td>
</tr>
<tr>
<td>114</td>
<td>T</td>
<td>(R) (K) (H) (Q)</td>
</tr>
</tbody>
</table>

Fig. 7. Residues in 1a9pA, at the interface with phosphate ion, colored by their relative importance. The ligand (phosphate ion) 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 1a9pA.)

Figure 7 shows residues in 1a9pA colored by their importance, at the interface with 1a9pPO4291.

9-deazainosine binding site. Table 8 lists the top 25% of residues at the interface with 1a9p9D1290 (9-deazainosine). The following table (Table 9) suggests possible disruptive replacements for these residues (see Section 3.6).

Table 8. The top 25% of residues in 1a9pA at the interface with 9-deazainosine. (Field names: res: residue number in the PDB entry; type: amino acid type; subst’s: 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>
<thead>
<tr>
<th>res</th>
<th>type</th>
<th>subst’s</th>
<th>cvg</th>
<th>noc/bb</th>
<th>dist (Å)</th>
<th>antn</th>
</tr>
</thead>
<tbody>
<tr>
<td>86</td>
<td>H</td>
<td>H(100)</td>
<td>0.04</td>
<td>8/0</td>
<td>3.40</td>
<td></td>
</tr>
<tr>
<td>118</td>
<td>G</td>
<td>G(100)</td>
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<td>14/14</td>
<td>3.31</td>
<td></td>
</tr>
<tr>
<td>192</td>
<td>Y</td>
<td>Y(100)</td>
<td>0.04</td>
<td>1/0</td>
<td>4.83</td>
<td></td>
</tr>
<tr>
<td>218</td>
<td>G</td>
<td>G(100)</td>
<td>0.04</td>
<td>17/17</td>
<td>3.77</td>
<td></td>
</tr>
<tr>
<td>219</td>
<td>M</td>
<td>M(100)</td>
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<td>34/9</td>
<td>2.80</td>
<td>site</td>
</tr>
<tr>
<td>220</td>
<td>S</td>
<td>S(90)</td>
<td>0.07</td>
<td>3/1</td>
<td>4.36</td>
<td>site</td>
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<tr>
<td>201</td>
<td>E</td>
<td>E(93)</td>
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<td>12/0</td>
<td>3.00</td>
<td>site</td>
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<tr>
<td>243</td>
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<td>N(93)</td>
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<td>13/0</td>
<td>2.92</td>
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<tr>
<td>257</td>
<td>H</td>
<td>H(93)</td>
<td>0.09</td>
<td>16/3</td>
<td>2.80</td>
<td>site</td>
</tr>
<tr>
<td>88</td>
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<td>Y(90)</td>
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<td>11/0</td>
<td>2.79</td>
<td>site</td>
</tr>
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<td>2/0</td>
<td>3.68</td>
<td></td>
</tr>
<tr>
<td>217</td>
<td>V</td>
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<td>0.15</td>
<td>21/14</td>
<td>3.78</td>
<td></td>
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<td>S(93)</td>
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<td>8/0</td>
<td>3.73</td>
<td>site</td>
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<tr>
<td>117</td>
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<td>A(84)</td>
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<td>20/16</td>
<td>3.24</td>
<td>site</td>
</tr>
<tr>
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<td>F</td>
<td>F(40)</td>
<td>0.16</td>
<td>27/0</td>
<td>3.67</td>
<td></td>
</tr>
<tr>
<td>259</td>
<td>E</td>
<td>E(90)</td>
<td>0.20</td>
<td>23/0</td>
<td>3.12</td>
<td>site</td>
</tr>
</tbody>
</table>

Table 9. Possible disruptive replacements for residues at the interface with 9-deazainosine.

<table>
<thead>
<tr>
<th>res</th>
<th>type</th>
<th>disruptive mutations</th>
</tr>
</thead>
<tbody>
<tr>
<td>86</td>
<td>H</td>
<td>(E) (TQMD) (SNKVCLAPIG) (YR)</td>
</tr>
<tr>
<td>118</td>
<td>G</td>
<td>(KER) (FQMWHD) (NYLPI) (SVA)</td>
</tr>
<tr>
<td>192</td>
<td>Y</td>
<td>(K) (QM) (NEVLAPIR) (D)</td>
</tr>
<tr>
<td>218</td>
<td>G</td>
<td>(KER) (FQMWHD) (NYLPI) (SVA)</td>
</tr>
<tr>
<td>219</td>
<td>M</td>
<td>(Y) (TH) (SCRG) (FWD)</td>
</tr>
<tr>
<td>220</td>
<td>S</td>
<td>(KR) (FQMH) (NELPI) (Y)</td>
</tr>
<tr>
<td>201</td>
<td>E</td>
<td>(FWH) (R) (Y) (VCAG)</td>
</tr>
</tbody>
</table>

continued in next column
3.1 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.

3.2 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%.

3.3 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 Å², 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 Å 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.)

3.4 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 Å.

3.5 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 (disulde bond forming residue), hb (hydrogen bond forming residue), jb (james bond forming residue), and sb (salt bridge forming residue).

3.6 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 [LPNQDEMlk], large [W FY HR], hydrophilic [LPV AM W FT], polar [GT CY]; positively [KH r], or negatively [DE] charged, aromatic [W FY H], long aliphatic chain [EK RQM], OH-group possession [SD E TY],
4 APPENDIX

4.1 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
  2. their type
- rho 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 rho or smaller
- gaps percentage of gaps in this column

4.2 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, BlanchenedAlmond.

The colors used to distinguish the residues by the estimated evolutionary pressure they experience can be seen in Fig. 9.

4.3 Credits

4.3.1 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 (idents / MIN(len1, 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.

4.3.2 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.

4.3.3 DSSP In this work a residue is considered solvent accessible if the DSSP program finds it exposed to water by at least 10Å², 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.


4.3.5 LaTeX The text for this report was processed using LATEX; Leslie Lamport, “LaTeX: A Document Preparation System Addison-Wesley,” Reading, Mass. (1986).


4.3.7 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.)

4.4 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.

4.5 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 Evolu-
tionary Trace Method Defines Binding Surfaces Common to Protein

report maker itself is described in Mihalek I., I. Res and O.
of service for comparative analysis of proteins." Bioinformatics

4.6 About report maker
report maker was written in 2006 by Ivana Mihalek. The 1D ran-
k ing visualization program was written by Ivica Reš. report maker
is copyrighted by Lichtarge Lab, Baylor College of Medicine,
Houston.

4.7 Attachments
The following files should accompany this report:
- 1a9pA.complex.pdb - coordinates of 1a9pA with all of its
  interacting partners
- 1a9pA.etvx - ET viewer input file for 1a9pA
- 1a9pA.cluster_report.summary - Cluster report summary for
  1a9pA
- 1a9pA.ranks - Ranks file in sequence order for 1a9pA
- 1a9pA.clusters - Cluster descriptions for 1a9pA
- 1a9pA.msf - the multiple sequence alignment used for the chain
  1a9pA
- 1a9pA.descr - description of sequences used in 1a9pA msf
- 1a9pA.ranks_sorted - full listing of residues and their ranking
  for 1a9pA
- 1a9pA.1a9pA2.if.pml - Pymol script for Figure 5
- 1a9pA.cbcvg - used by other 1a9pA – related pymol scripts
- 1a9pA.1a9pA1.if.pml - Pymol script for Figure 6
- 1a9pA.1a9pPO4291.if.pml - Pymol script for Figure 7
- 1a9pA.1a9p9DI290.if.pml - Pymol script for Figure 8