11gs
Evolutionary trace report by report_maker
August 1, 2010

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1 INTRODUCTION
From the original Protein Data Bank entry (PDB id 11gs):
Title: Glutathione s-transferase complexed with ethacrynic acid-glutathione conjugate (form ii)
Compound: Mol id: 1; molecule: glutathione s-transferase; chain: a, b; synonym: gst; ec: 2.5.1.18; engineered: yes
Organism, scientific name: Homo Sapiens;
11gs contains a single unique chain 11gsA (208 residues long) and its homologue 11gsB.

2 CHAIN 11GSA
2.1 Q5TZY3 overview
From SwissProt, id Q5TZY3, 100% identical to 11gsA:
Description: Glutathione S-transferase pi (GSTP1 protein).
Organism, scientific name: Homo sapiens (Human).
Taxonomy: Eukaryota; Metazoa; Chordata; Craniata; Vertebrata; Euteleostomi; Mammalia; Eutheria; Euarchontoglires; Primates; Catarrhini; Hominidae; Homo.
Catalytic activity: RX + glutathione = HX + R-S-glutathione.
Similarity: Belongs to the GST superfamily.

2.2 Multiple sequence alignment for 11gsA
For the chain 11gsA, the alignment 11gsA.msf (attached) with 179 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 11gsA.msf. Its statistics, from the alstat program are the following:
Format: MSF
Number of sequences: 179
Total number of residues: 35220
Smallest: 156
Largest: 208
Average length: 196.8
Alignment length: 208
Average identity: 34%
Most related pair: 99%
Most unrelated pair: 12%
Most distant seq: 31%

Furthermore, <1% of residues show as conserved in this alignment.

The alignment consists of 55% eukaryotic (40% vertebrata, 2% arthropoda, <1% plantae), and <1% 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 11gsA.descr.

2.3 Residue ranking in 11gsA
The 11gsA sequence is shown in Figs. 1–2, with each residue colored according to its estimated importance. The full listing of residues in 11gsA can be found in the file called 11gsA.ranks_sorted in the attachment.

2.4 Top ranking residues in 11gsA 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 11gsA 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.

Furthermore, <1% of residues show as conserved in this alignment.

The alignment consists of 55% eukaryotic (40% vertebrata, 2% arthropoda, <1% plantae), and <1% 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 11gsA.descr.

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.

Fig. 1. Residues 2-105 in 11gsA colored by their relative importance. (See Appendix, Fig.10, for the coloring scheme.)

Fig. 2. Residues 106-209 in 11gsA colored by their relative importance. (See Appendix, Fig.10, for the coloring scheme.)

Fig. 3. Residues in 11gsA, colored by their relative importance. Clockwise: front, back, top and bottom views.

Fig. 4. Residues in 11gsA, 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.
Table 1. Clusters of top ranking residues in 11gsA.

<table>
<thead>
<tr>
<th>cluster color</th>
<th>size</th>
<th>member residues</th>
</tr>
</thead>
<tbody>
<tr>
<td>red</td>
<td>48</td>
<td>5, 7, 8, 12, 18, 21, 30, 49, 50, 51</td>
</tr>
<tr>
<td></td>
<td></td>
<td>52, 53, 55, 57, 58, 59, 64, 65, 67</td>
</tr>
<tr>
<td></td>
<td></td>
<td>68, 69, 70, 71, 72, 73, 74, 78, 80</td>
</tr>
<tr>
<td></td>
<td></td>
<td>85, 90, 91, 94, 98, 122, 126, 130</td>
</tr>
<tr>
<td></td>
<td></td>
<td>133, 145, 149, 151, 152, 153, 157</td>
</tr>
<tr>
<td></td>
<td></td>
<td>159, 170, 174, 176, 192</td>
</tr>
<tr>
<td>blue</td>
<td>2</td>
<td>186, 187</td>
</tr>
</tbody>
</table>

Table 1. Clusters of top ranking residues in 11gsA.

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.

Glutathione binding site. Table 2 lists the top 25% of residues at the interface with 11gsAGTT1 (glutathione). 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/ dist</th>
</tr>
</thead>
<tbody>
<tr>
<td>53</td>
<td>P</td>
<td>P(98)V. L</td>
<td>0.01</td>
<td>10/4 3.48</td>
</tr>
<tr>
<td>64</td>
<td>Q</td>
<td>Q(96) E(2) .</td>
<td>0.01</td>
<td>33/11 2.49</td>
</tr>
<tr>
<td>51</td>
<td>Q</td>
<td>Q(62) N(34) K(1) S(1) E</td>
<td>0.03</td>
<td>61/9 2.95</td>
</tr>
<tr>
<td>65</td>
<td>S</td>
<td>T(24) S(73) GC . A</td>
<td>0.03</td>
<td>15/8 2.73</td>
</tr>
<tr>
<td>7</td>
<td>Y</td>
<td>Y(91) (7) PHV . A</td>
<td>0.09</td>
<td>6/0 3.08</td>
</tr>
<tr>
<td>50</td>
<td>G</td>
<td>Q(14) P(35) G(40) R(2) H E(1) N D(3) FA</td>
<td>0.14</td>
<td>5/5 3.81</td>
</tr>
<tr>
<td>8</td>
<td>F</td>
<td>AF(53) W(34) .(6) YV P(1) L(1) TS</td>
<td>0.18</td>
<td>13/0 3.73</td>
</tr>
<tr>
<td>52</td>
<td>L</td>
<td>V(27) L(59) A(1) I(7) M(1)</td>
<td>0.20</td>
<td>30/28 2.69</td>
</tr>
</tbody>
</table>

continued in next column
Table 2. The top 25% of residues in 11gsA at the interface with glutathione. (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. List of disruptive mutations for the top 25% of residues in 11gsA, that are at the interface with glutathione.

Table 4. The top 25% of residues in 11gsA at the interface with ethacrynic acid. (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 5. List of disruptive mutations for the top 25% of residues in 11gsA, that are at the interface with ethacrynic acid.

Table 6. The top 25% of residues in 11gsA at the interface with glutathione. (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.)

Fig. 5. Residues in 11gsA, at the interface with glutathione, colored by their relative importance. The ligand (glutathione) 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 11gsA.)

Figure 5 shows residues in 11gsA colored by their importance, at the interface with 11gsAGTT1.

Ethacrynic acid binding site. Table 4 lists the top 25% of residues at the interface with 11gsAEAA2 (ethacrynic acid). The following table (Table 5) suggests possible disruptive replacements for these residues (see Section 3.6).

Glutathione binding site. Table 6 lists the top 25% of residues at the interface with 11gsBGGT1 (glutathione). The following table (Table 7) suggests possible disruptive replacements for these residues (see Section 3.6).
Fig. 6. Residues in 11gsA, at the interface with ethacrynic acid, colored by their relative importance. The ligand (ethacrynic acid) 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 11gsA.)

Table 7. List of disruptive mutations for the top 25% of residues in 11gsA, that are at the interface with glutathione.

<table>
<thead>
<tr>
<th>res</th>
<th>type</th>
<th>disruptive mutations</th>
</tr>
</thead>
<tbody>
<tr>
<td>98</td>
<td>D</td>
<td>(R) (H) (FW) (Y)</td>
</tr>
</tbody>
</table>

Figure 7 shows residues in 11gsA colored by their importance, at the interface with 11gsBGTT1.

**MES binding site.** Table 8 lists the top 25% of residues at the interface with 11gsAMES3 (mes). The following table (Table 9) suggests possible disruptive replacements for these residues (see Section 3.6).

Table 8. The top 25% of residues in 11gsA at the interface with MES. (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>
</tr>
</thead>
<tbody>
<tr>
<td>30</td>
<td>E</td>
<td>E (65) D (27) F (1) N Y (1) LV (1) A F (33) Y (50) V (2) A (1)</td>
<td>0.23</td>
<td>13/4</td>
<td>3.28</td>
</tr>
<tr>
<td>192</td>
<td>F</td>
<td>E (65) D (27) F (1) N Y (1) LV (1) A F (33) Y (50) V (2) A (1)</td>
<td>0.24</td>
<td>5/1</td>
<td>4.44</td>
</tr>
</tbody>
</table>

Table 8. continued

<table>
<thead>
<tr>
<th>res</th>
<th>type</th>
<th>subst's (%</th>
<th>cvg</th>
<th>noc/ bb</th>
<th>dist (Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>R (1) L (3) W (2) H (1) G A (1) T</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 9. List of disruptive mutations for the top 25% of residues in 11gsA, that are at the interface with MES.

<table>
<thead>
<tr>
<th>res</th>
<th>type</th>
<th>disruptive mutations</th>
</tr>
</thead>
<tbody>
<tr>
<td>30</td>
<td>E</td>
<td>(H) (R) (FW) (Y)</td>
</tr>
<tr>
<td>192</td>
<td>F</td>
<td>(E) (K) (QD) (T)</td>
</tr>
</tbody>
</table>

Figure 8 shows residues in 11gsA colored by their importance, at the interface with 11gsAMES3.
Fig. 8. Residues in 11gsA, at the interface with MES, colored by their relative importance. The ligand (MES) 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 11gsA.)

**Interface with 11gsB.** Table 10 lists the top 25% of residues at the interface with 11gsB. The following table (Table 11) suggests possible disruptive replacements for these residues (see Section 3.6).

<table>
<thead>
<tr>
<th>res</th>
<th>type</th>
<th>subst's (%)</th>
<th>cvg</th>
<th>noc/bb</th>
<th>dist (Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>64</td>
<td>Q</td>
<td>Q(96)</td>
<td>0.01</td>
<td>52/3</td>
<td>3.07</td>
</tr>
<tr>
<td></td>
<td></td>
<td>E(2)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>H(2)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>S(1)L</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>N</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>98</td>
<td>D</td>
<td>D(92)</td>
<td>0.02</td>
<td>11/0</td>
<td>3.07</td>
</tr>
<tr>
<td></td>
<td></td>
<td>E(1)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>H(2)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>S(1)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>N</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>51</td>
<td>Q</td>
<td>Q(62)</td>
<td>0.03</td>
<td>1/0</td>
<td>4.84</td>
</tr>
<tr>
<td></td>
<td></td>
<td>N(34)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>K(1)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>S(1)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>90</td>
<td>D</td>
<td>D(84)</td>
<td>0.06</td>
<td>39/6</td>
<td>3.12</td>
</tr>
<tr>
<td></td>
<td></td>
<td>T(1)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>S(4)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>H(1)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>A(1)Y</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>E(2)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>N(2)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>49</td>
<td>Y</td>
<td>F(84)</td>
<td>0.09</td>
<td>60/4</td>
<td>2.93</td>
</tr>
</tbody>
</table>

*Table 10. The top 25% of residues in 11gsA at the interface with 11gsB. (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; cvg: number of contacts realized through backbone atoms given 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 11. List of disruptive mutations for the top 25% of residues in 11gsA, that are at the interface with 11gsB.

<table>
<thead>
<tr>
<th>res</th>
<th>type</th>
<th>disruptive mutations</th>
</tr>
</thead>
<tbody>
<tr>
<td>64</td>
<td>Q</td>
<td>(Y) (FWH) (T) (VCAG)</td>
</tr>
<tr>
<td>98</td>
<td>D</td>
<td>(R) (H) (FW) (Y)</td>
</tr>
<tr>
<td>51</td>
<td>Q</td>
<td>(Y) (FW) (H) (T)</td>
</tr>
<tr>
<td>90</td>
<td>D</td>
<td>(R) (H) (FW) (K)</td>
</tr>
<tr>
<td>49</td>
<td>Y</td>
<td>(K) (R) (Q) (E)</td>
</tr>
<tr>
<td>71</td>
<td>H</td>
<td>(E) (Q) (FMW) (D)</td>
</tr>
<tr>
<td>67</td>
<td>T</td>
<td>(KR) (QH) (FMW) (NE)</td>
</tr>
<tr>
<td>70</td>
<td>R</td>
<td>(T) (Y) (D) (E)</td>
</tr>
<tr>
<td>91</td>
<td>M</td>
<td>(Y) (H) (R) (T)</td>
</tr>
<tr>
<td>74</td>
<td>R</td>
<td>(Y) (T) (D) (FW)</td>
</tr>
<tr>
<td>94</td>
<td>D</td>
<td>(R) (H) (FW) (Y)</td>
</tr>
</tbody>
</table>

Figure 9. Residues in 11gsA, at the interface with 11gsB, colored by their relative importance. 11gsB is shown in backbone representation (See Appendix for the coloring scheme for the protein chain 11gsA.)

Figure 9 shows residues in 11gsA colored by their importance, at the interface with 11gsB.

### 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 10Å², 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 5Å 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 5Å.

### 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 (disulfide bond forming residue), hb (hydrogen bond forming residue), jb (james bond forming residue), and sb (for 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 [LPNQDEMIK], large [WFYHR], hydrophobic [LPVAMWFI], polar [GTCY]; positively [KHR], or negatively [DE] charged, aromatic [WFYH], long aliphatic chain [EKQRM], OH-group possession [SDETY], and NH2 group possession [NQKR]. The suggestions are listed

...
Fig. 10. Coloring scheme used to color residues by their relative importance.

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 researchers will choose, however, the straightforward alanine mutations, especially in the beginning stages of their investigation.

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, BlanchedAlmond.

The colors used to distinguish the residues by the estimated evolutionary pressure they experience can be seen in Fig. 10.

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 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 into 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].

4.3.4 HSSP  

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

4.3.6 Muscle  

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


4.6 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.

4.7 Attachments

The following files should accompany this report:

- 11gsA.complex.pdb - coordinates of 11gsA with all of its interacting partners
- 11gsA.etvx - ET viewer input file for 11gsA
- 11gsA.cluster_report.summary - Cluster report summary for 11gsA
- 11gsA.ranks - Ranks file in sequence order for 11gsA
- 11gsA.clusters - Cluster descriptions for 11gsA
- 11gsA.msF - the multiple sequence alignment used for the chain 11gsA
- 11gsA.descr - description of sequences used in 11gsA msF
- 11gsA.ranks_sorted - full listing of residues and their ranking for 11gsA
- 11gsA.11gsAGTT1.if.pml - Pymol script for Figure 5
- 11gsA.cbcvg - used by other 11gsA – related pymol scripts
- 11gsA.11gsAEAA2.if.pml - Pymol script for Figure 6
- 11gsA.11gsBGTT1.if.pml - Pymol script for Figure 7
- 11gsA.11gsAMES3.if.pml - Pymol script for Figure 8
- 11gsA.11gsB.if.pml - Pymol script for Figure 9