

## **Supporting Information for**

### **The Active Site of Melanopsin: The Biological Clock Photoreceptor**

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## I. Full sequence alignment of squid rhodopsin and mouse melanopsin.

FASTA sequences of squid rhodopsin (P31356) and mouse melanopsin (Q9QXZ9) were aligned using CLUSTALW2 (ref-1) as shown below. Alignments of the transmembrane portions of squid rhodopsin (2Z73 at 2.8 Å), and that of melanopsin, according to the TMHMM prediction (ref-2) using the TMHMM v2 server, were performed using CLUSTALW2 and are displayed below. The transmembrane region alignments were found to be in agreement with the full FASTA sequence alignment with only one exception in Helix II. In GPCRs, the extracellular domain, intracellular domain, and interhelical loops are structures that are directly responsible for the function of the protein; consequently, these regions will have great diversity in their primary sequence and may not show strong sequence alignments to other GPCRs. On the other hand, the transmembrane domain serves mostly the same function in GPCRs, which is to span and stabilize the protein in the cell membrane. In order to maintain the functionality of these regions, the hydrophobicity and overall dipole moment of the helix must be preserved, so it is expected that the transmembrane helices between GPCRs will show greater conservation than the other regions. Since the alignment for Helix II contained no gaps, it was adopted into the main sequence alignment. The modified alignment used for determining correspondence between rhodopsin and melanopsin residues is shown below. Residues marked in blue indicate the 163 out of 373 residues in squid rhodopsin mutated to make the mouse melanopsin homology model. The following mutations resulted in the loss of negative (D27V, D194T, E231G, E233A, E245R, E290H, D340S, D341G) and positive (K109E, K145G, R193F, K239E, K244L) charge. Similarly, the following mutations resulted in the gain of negative (Q28D, F105E, K109E, N229E, A235E, K239E) and positive charge (K61R, K63R, Q66R, K146R, H149K, M225R, S228R, K232R, E245R, K248R, G252R, R258K). The residues at 94, 240, and 241 in squid rhodopsin were used to fill the corresponding positions in the homology model. Within the 4.5Å of the active site, marked by the red boxes in the alignment, 18 out of 38 residues were mutated. Although this alignment contains some large gaps, they occur before and after the seven transmembrane regions, indicating that the gaps are found only in the extracellular domain and intracellular domain respectively. Since these domains are outside of the 4.5Å radius of retinal, residues in these regions are not expected to impact

the calculations. For the homology model, residues 1-25 and 342-373 of squid rhodopsin were used for the extracellular and intracellular domain respectively.

>Squid Rhodopsin (P31356) FASTA Sequence from www.uniprot.org  
MGRDLRDNETWWYNPSIVVHPHWREFDQVPDAVYYSLGIFIGICGIHCGGNGIVIYLFTKTKSLQ  
TPANMFIINLAFSDFTFSLVNGFPLMTISCFLKKWIFGFAACKVYGFIFGIFGMSIMTMAMISIDRY  
NVIGRPMMAASKKMSHRRAFIMIIIFVWLWSVLWAIGPIFGWGAYTLEGVLCNCSFDYISRSTTRSN  
ILCMFILGFFGPIIIFFCYFNIVMSVSNHEKEMAAMAKRLNAKELRKAQAGANAEMRLAKISIVIV  
SQFLLSWSPYAVVALLAQFGPLEWVTPYAAQLPVMFAKASAIHNPMIYSVSHPKFREAISQTFPWV  
LTCCQFDDKETEDDKDAETEIPAGESSDAAPSADAAQMKEMMAMMQMQQQAAYPPQGYAP  
PPQGYPPQGYPPQGYPPQGYPPQGYPPPPQGAPPQGAAPPAAPPQGVNDQAYQA

> Mouse Melanopsin (Q9QXZ9) FASTA Sequence from www.uniprot.org  
MDSPSGPRVLSLSTQDPSFTTSPALQGIWNGTQNVSVRAQLLSVSPTTSAHQAAA WVPFPTVDVDP  
HAHYTLGTVILLVGLTGMLGNLTVIYTFRCNRGLRTPANMFIINLAVSDFLMSVTQAPVFFASSLY  
KKWLFGETGCEFYAFCGAVFGITSMITLTAIAMDRYL VITRPLATIGRSGKRRTALVLLGVWLYAL  
AWSLPPFFGWSAYVPEGLLTSCSWDYMTFTQVRA YTMLLFCVFFLPLIIIFCYIFIFRAIRETGR  
ACEGCGESPLRQRRQWQRLQSEWKMAKVALIVILLFVLSWAPYSTVALVAFAGYSHILTPYMSSV  
PAVIAKASAIHNPIIYAITHPKYRVAIAQHL PCLGVLLGVSGQRSHPSLSYRSTHRSTLSSQSSDLSWI  
SGRKRQESLGSESEVGWTD TETTAAWGAAQQASGQSFCSQNLEDGELKASSSPQVQRSKTPKVP  
PSTCRPMKGQGARPS SLRGDQKGR LAVCTGLSECPHPTSQFPLAFLEDDVTLRHL

**Full alignment between Rhodopsin and Melanopsin**

|       |   |     |
|-------|---|-----|
| Squid | --MGRDLRDNETWWYNPSIVVHPHWR-----E                              | 25  |
| Mouse | MDSPSGPRVLSLSTQDPSFTTSPALQGIWNGTQNVSVRAQLLSVSPTTSAHQAAA WVPFP | 60  |
| Squid | FDQVPDAVYYSLGIFIGICGIHCGGNGIVIYLFTKTKSLQTPANMFIINLAFSDFTFSL   | 85  |
| Mouse | TVDVDPHAHYTLGTVILLVGLTGMLGNLTVIYTFRCNRGLRTPANMFIINLAVSDFLMSV  | 120 |
| Squid | VNGFPLMTISCFLKKWIFGFAACKVYGFIFGIFGMSIMTMAMISIDRYNVIGRPMMAASK  | 145 |
| Mouse | T-QAPVFFASSLYKKWLFGETGCEFYAFCGAVFGITSMITLTAIAMDRYL VITRPLATIG | 179 |
| Squid | KMSHRRAFIMIIIFVWLWSVLWAIGPIFGWGAYTLEGVLCNCSFDYISRSTTRSNILCMF  | 205 |
| Mouse | RGSKRRTALVLLGVWLYALAWSLPPFFGWSAYVPEGLLTSCSWDYMTFTQVRA YTMLLF  | 239 |
| Squid | ILGFFGPIIIFFCYFNIVMSVSNHEKEMAAMAKRLNAKELRKAQAGANAEMRLAKISIV   | 265 |
| Mouse | CFVFFLPLIIIFCYIFIFRAIRETGRACEGCGE--SPLRQRRQWQRLQSEWKMAKVALI   | 297 |
| Squid | IVSQFLLSWSPYAVVALLAQFGPLEWVTPYAAQLPVMFAKASAIHNPMIYSVSHPKFREA  | 325 |
| Mouse | VILLFVLSWAPYSTVALVAFAGYSHILTPYMSSVPAVIAKASAIHNPIIYAITHPKYRVA  | 357 |
| Squid | ISQTFPWVLTCCQFDD-----KETEDDKDAETEIPA                          | 356 |
| Mouse | IAQHL PCLGVLLGVSGQRSHPSLSYRSTHRSTLSSQSSDLSWISGRKRQESLGSESEVGW | 417 |
| Squid | GESSDAAPSADAAQMKEMMAMMQMQQ---QQAAYPPQGYAPPQGYPPQGYPPQGYPPQ    | 413 |
| Mouse | TDTETTAAWGAAQQASGQSFCSQNLEDGELKASSSPQVQRSKTPKVPGPSTCRP--MKGQ  | 475 |
| Squid | GYPQGYPPPPQGAPPQGAAPPAAPPQGVNDQAYQA-----                      | 448 |
| Mouse | GARPSSLRGDQKGR LAVCTGLSECPHPTSQFPLAFLEDDVTLRHL                | 521 |

## Alignment within the transmembrane regions

|       |     |                                   |                |      |           |        |       |       |         |    |           |
|-------|-----|-----------------------------------|----------------|------|-----------|--------|-------|-------|---------|----|-----------|
| Squid | TM1 | PDAVYYSLGIFIGICGIICGGNGIIVIYLF    | TKT            | 33   | (30-62)   |        |       |       |         |    |           |
| Mouse | TM1 | -----LGTVILLVGLTGMLGNLTVIYTF      |                | 23   | (72-94)   |        |       |       |         |    |           |
| Squid | TM2 | ANMFIINLAFSDFTFSLVNGFPLMTISCF     | L              | 30   | (69-98)   |        |       |       |         |    |           |
| Mouse | TM2 | --MFIINLAVSDFLMSVTQAPVFFA-----    |                | 23   | (106-128) |        |       |       |         |    |           |
| Squid | TM3 | FGFAACKVYGFIFGGIFGFMSIMTMAMIS     | IDRYNVI        | 35   | (103-137) |        |       |       |         |    |           |
| Mouse | TM3 | -----EFYAFCGAVFGITSMITLTAIAM----- |                | 23   | (143-165) |        |       |       |         |    |           |
| Squid | TM4 | SHRRAFIMIIFVWLSVWLAIGPIFG-        |                | 26   | (148-173) |        |       |       |         |    |           |
| Mouse | TM4 | ----TALVLLGVWLYALAWSLPFFGW        |                | 23   | (186-208) |        |       |       |         |    |           |
| Squid | TM5 | DSTTRSNI                          | LCMFI          | LGFF | GPILII    | FFCYFN | IVMSV | SNHEK | EMAAMAK | 46 | (194-239) |
| Mouse | TM5 | -----TMLLFCFVFFLPLIIIFCYIFI-----  |                |      |           |        |       |       |         | 23 | (235-257) |
| Squid | TM6 | ELRKAQAGANAEMRLAKISIVIVSQFLLS     | WSPYAVVALLAQFG | 43   | (245-287) |        |       |       |         |    |           |
| Mouse | TM6 | -----LIVILLFVLSWAPYSTVALVAFA-     |                | 23   | (296-318) |        |       |       |         |    |           |
| Squid | TM7 | --TPYAAQLPVMFAKASAIHNPMIYSVSH     |                | 27   | (293-319) |        |       |       |         |    |           |
| Mouse | TM7 | ILTPYMSSVPAVIAKASAIHNPIIYAIT-     |                | 28   | (319-521) |        |       |       |         |    |           |

## Modified alignment (Helix II alignment incorporated)

|       |  |  |   |                       |                  |            |       |  |  |  |  |   |    |     |
|-------|--|--|---|-----------------------|------------------|------------|-------|--|--|--|--|---|----|-----|
| Squid |  | --MGRDLRDNETWYWNPSIVVHPHR-----                               |   |                       |                  |            |       |  |  |  |  | E | 25 |     |
| Mouse |  | MDSPSGPRVLSLTDPSFTTSPALQGIWNGTQNVSVRAQLLSVSPTTSAHQAAA        |   |                       |                  |            |       |  |  |  |  |   | V  | 60  |
| Squid |  | FDQVPDAVYYS  | LGIFIGICGIICGGNGIIVIYLF                                 | TKTKSLQ               | TPANMFIINLAFSDFT | FSL        |       |  |  |  |  |   |    | 85  |
| Mouse |  | TVDVPDHAHYTLGTV  | ILLVGLTGMLGNLTVIYTF                                     | CRNRGLR               | TPANMFIINLAVSDFI | MSV        |       |  |  |  |  |   |    | 120 |
| Squid |  | VNGFPLMTISCF   | LKKWIFGFAACKVYGFIFGGIFGFMSIMTMAMIS                      | IDRYN                 | VIGR             | MAASK      |       |  |  |  |  |   |    | 145 |
| Mouse |  | TQAPVFFA   | ISSLYKKWLFGETGCE  | YAFCGAVFGITSMITLTAIAM | DRYL             | VITRPLATIG |       |  |  |  |  |   |    | 179 |
| Squid |  | KMSHRRAFIMIIFVWLSVWLAIGPIFGW                                 | CAYTLEGVLCNCSFDY  | ISR                   | DSTTRSNI         | L          | CMF   |  |  |  |  |   |    | 205 |
| Mouse |  | RGSKRRRTALVLLGVWLYALAWSLPFFGW                                | SAYVPEGLL   | SCSWDY                | MTFT             | PQVRA      | TMLLF |  |  |  |  |   |    | 239 |
| Squid |  | ILGFF  | GPILIIFFCYFNIVMSVSNHEKEMAAMAKRLNAKELRKAQAGANAEMRLAKISIV |                       |                  |            |       |  |  |  |  |   |    | 265 |
| Mouse |  | CFVFF  | LPLIIIFCYIFIFRAIRETGRACEGGERLSPLRQRQWQRLQSEWKMAKVALI    |                       |                  |            |       |  |  |  |  |   |    | 297 |
| Squid |  | IVSQFLLS   | WSPYAVVALLAQFGPLEWVTPYAAQLPVMFAKASAIHNPMIYSVSHPKFREA    |                       |                  |            |       |  |  |  |  |   |    | 325 |
| Mouse |  | VILLFVLSWAPYSTVALVAFAGYSHILTPYMSVPAVIAKASAIHNPIIYAITHPKYRVA  |   |                       |                  |            |       |  |  |  |  |   |    | 357 |
| Squid |  | ISQTFPWVLTCCQFDD-----  |   |                       |                  |            |       |  |  |  |  |   |    | 356 |
| Mouse |  | IAQHLPCLGVLLGVSGQRSHPSLSYRSTHRSTLSSQSSDLSWISGRKRQESLGSESEVGV |   |                       |                  |            |       |  |  |  |  |   |    | 417 |
| Squid |  | GESSDAAPSADAAQMKEMMAMMQMQQ---                                | QAAYPPQGYAPPPQGYPPQGYPPQGYPPQ                           |                       |                  |            |       |  |  |  |  |   |    | 413 |
| Mouse |  | TDTETTAAWGAAQQASGQSFCSQNL                                    | EDGELKASSPQVQRSKTPKVPGPSTCRP--                          |                       |                  |            |       |  |  |  |  |   |    | 475 |
| Squid |  | GYPYPQGYPPPPQGAPPQGAPPAAPPQGV                                | DNQAYQA-----  |                       |                  |            |       |  |  |  |  |   |    | 448 |
| Mouse |  | GARPSSLRGDQKRLAVCTGLSECPHPTSQFPLAFLEDDVTLRHL                 |   |                       |                  |            |       |  |  |  |  |   |    | 521 |

**II. Distance of the Schiff-base nitrogen to key amino acid residues in the squid rhodopsin and mouse rhodopsin.**

**Table S1:** Comparison of distances from the PSB nitrogen atom to side chain oxygen atom of N87, Y111 and E180 residues in squid rhodopsin and Q87, Y111 and E180 residues in mouse melanopsin.

| Distance (Å)          | Squid Rhodopsin | Mouse Melanopsin |
|-----------------------|-----------------|------------------|
| OH (Y111)...N (PSBR)  | 3.41            | 3.08             |
| OD1 (N87Q)...N (PSBR) | 3.93            | 4.71             |
| OE2 (E180)...N (PSBR) | 4.29            | 4.12             |

**III. Bond lengths, angles and dihedral angles along the retinal polyene chain of the PSB11 chromophore in squid rhodopsin and mouse melanopsin.1.3595**

**BOND LENGTH (Å)**

| Bond                  | Squid Rhodopsin | Mouse Melanopsin |
|-----------------------|-----------------|------------------|
| C5=C6                 | 1.361           | 1.358            |
| C6-C7                 | 1.469           | 1.472            |
| C7=C8                 | 1.357           | 1.355            |
| C8-C9                 | 1.444           | 1.448            |
| C9=C10                | 1.377           | 1.373            |
| C10-C11               | 1.421           | 1.430            |
| C11=C12               | 1.379           | 1.371            |
| C12-C13               | 1.431           | 1.435            |
| C13=C14               | 1.391           | 1.385            |
| C14-C15               | 1.397           | 1.400            |
| C15=N                 | 1.324           | 1.315            |
| BLA (Å)               | 0.068           | 0.078            |
| $\lambda_{\max}$ (nm) | 490             | 447              |

**Note:** Increase in BLA contributes to the decrease in  $\lambda_{\max}$ .

**BOND ANGLE (deg)**

| Bond       | Squid Rhodopsin | Mouse Melanopsin |
|------------|-----------------|------------------|
| C5=C6-C7   | 121.748         | 123.105          |
| C6-C7=C8   | 122.567         | 124.644          |
| C7=C8-C9   | 127.903         | 127.113          |
| C8-C9=C10  | 115.826         | 116.648          |
| C9=C10-C11 | 128.475         | 128.095          |

|             |         |         |
|-------------|---------|---------|
| C10-C11=C12 | 126.459 | 126.314 |
| C11=C12-C13 | 129.361 | 128.297 |
| C12-C13=C14 | 117.101 | 117.475 |
| C13=C14-C15 | 123.500 | 122.806 |
| C14-C15=N   | 123.102 | 122.929 |

#### DIHEDRAL ANGLE (deg)

| Bond            | Squid     | Mouse      |
|-----------------|-----------|------------|
|                 | Rhodopsin | Melanopsin |
| C5=C6-C7=C8     | -45.47    | -42.597    |
| C6-C7=C8-C9     | -173.51   | -175.141   |
| C7=C8-C9=C10    | 160.06    | 172.509    |
| C8-C9=C10-C11   | 178.90    | 171.266    |
| C9=C10-C11=C12  | 168.89    | 167.832    |
| C10-C11=C12-C13 | -17.26    | -22.069    |
| C11=C12-C13=C14 | 165.77    | 163.759    |
| C12-C13=C14-C15 | 176.11    | 172.100    |
| C13=C14-C15=N   | 163.17    | 166.761    |
| C14-C15=N-C     | 179.55    | 178.601    |

#### IV. ONIOM (QM/MM) where QM=B3LYP/6-31G\*; MM= AMBER96; optimized Cartesian coordinates (in Å).

##### Retinal geometry of squid rhodopsin (490 nm)

51 Atoms

|   |           |           |           |
|---|-----------|-----------|-----------|
| N | 9.796233  | 38.054782 | 57.858373 |
| H | 8.874230  | 38.327781 | 58.190451 |
| H | 9.949860  | 37.043264 | 57.784239 |
| C | 17.131212 | 44.828289 | 61.316098 |
| C | 18.532048 | 44.846576 | 60.654834 |
| C | 18.870817 | 46.259227 | 60.126053 |
| H | 19.906116 | 46.277020 | 59.772084 |
| H | 18.779472 | 47.006821 | 60.922821 |
| H | 18.237644 | 46.559165 | 59.284186 |
| C | 18.548568 | 43.860266 | 59.463264 |
| H | 18.399492 | 42.824057 | 59.788053 |
| H | 19.506550 | 43.917572 | 58.932764 |
| H | 17.755349 | 44.100632 | 58.751135 |
| C | 16.912775 | 44.359680 | 62.574668 |
| C | 15.608993 | 44.463847 | 63.332561 |
| H | 15.119096 | 43.483846 | 63.410627 |
| H | 14.902069 | 45.168229 | 62.891403 |
| H | 15.819203 | 44.788952 | 64.362000 |
| C | 19.631556 | 44.455889 | 61.667449 |
| H | 19.860961 | 45.321078 | 62.302797 |
| H | 20.550740 | 44.232709 | 61.115124 |
| C | 19.220124 | 43.289667 | 62.561279 |
| H | 18.961602 | 42.416279 | 61.948123 |
| H | 20.049083 | 42.987873 | 63.210366 |
| C | 18.004888 | 43.701138 | 63.388020 |
| H | 17.572340 | 42.835050 | 63.909033 |
| H | 18.305715 | 44.399838 | 64.183154 |
| C | 16.029066 | 45.291883 | 60.462118 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | 16.203974 | 46.156939 | 59.824983 |
| C | 14.869973 | 44.599724 | 60.325323 |
| H | 14.771476 | 43.680386 | 60.893245 |
| C | 13.772753 | 44.876468 | 59.427957 |
| C | 13.645232 | 46.232245 | 58.791031 |
| H | 14.483039 | 46.425287 | 58.111967 |
| H | 13.676323 | 47.020597 | 59.551211 |
| H | 12.721317 | 46.331297 | 58.215712 |
| C | 12.925458 | 43.821423 | 59.175028 |
| H | 13.167594 | 42.897372 | 59.686577 |
| C | 11.761487 | 43.797790 | 58.360372 |
| H | 11.313150 | 44.752256 | 58.089777 |
| C | 11.061109 | 42.678445 | 57.961636 |
| H | 10.061518 | 42.853916 | 57.567039 |
| C | 11.469136 | 41.306496 | 57.959251 |
| C | 12.906167 | 40.878555 | 58.117623 |
| H | 13.087954 | 40.474542 | 59.121559 |
| H | 13.595416 | 41.701705 | 57.942621 |
| H | 13.152791 | 40.094901 | 57.395900 |
| C | 10.472504 | 40.349016 | 57.793664 |
| H | 9.437313  | 40.675394 | 57.796475 |
| C | 10.729282 | 38.979201 | 57.692339 |
| H | 11.721453 | 38.619755 | 57.440379 |

##### Retinal geometry of mouse melanopsin (447 nm)

51 Atoms

|   |          |           |           |
|---|----------|-----------|-----------|
| N | 9.536555 | 37.770705 | 58.055030 |
| H | 8.652185 | 38.035166 | 58.506020 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | 9.663435  | 36.762490 | 57.921536 |
| C | 16.896084 | 44.580690 | 61.786132 |
| C | 18.358192 | 44.786896 | 61.322341 |
| C | 18.566113 | 46.269721 | 60.935087 |
| H | 19.613902 | 46.434563 | 60.665674 |
| H | 18.320884 | 46.930397 | 61.775062 |
| H | 17.967183 | 46.571643 | 60.072391 |
| C | 18.649815 | 43.881527 | 60.105541 |
| H | 18.701231 | 42.830259 | 60.410656 |
| H | 19.613400 | 44.145544 | 59.657082 |
| H | 17.875110 | 43.969477 | 59.339211 |
| C | 16.574050 | 44.111854 | 63.019571 |
| C | 15.181455 | 44.063435 | 63.598212 |
| H | 14.808043 | 43.033520 | 63.650082 |
| H | 14.455235 | 44.659683 | 63.042434 |
| H | 15.218442 | 44.431866 | 64.634084 |
| C | 19.373618 | 44.450753 | 62.437242 |
| H | 19.473228 | 45.323616 | 63.091085 |
| H | 20.360131 | 44.282930 | 61.990588 |
| C | 18.942312 | 43.256586 | 63.283238 |
| H | 18.805268 | 42.372106 | 62.645830 |
| H | 19.715611 | 43.001970 | 64.013196 |
| C | 17.624085 | 43.588667 | 63.977149 |
| H | 17.212995 | 42.705492 | 64.487803 |
| H | 17.794607 | 44.332410 | 64.774947 |
| C | 15.890171 | 44.909756 | 60.763936 |
| H | 16.105047 | 45.753516 | 60.112549 |
| C | 14.799379 | 44.155628 | 60.485922 |
| H | 14.626657 | 43.273588 | 61.092688 |
| C | 13.831180 | 44.374326 | 59.430754 |
| C | 13.923933 | 45.608065 | 58.575660 |
| H | 14.870607 | 45.602746 | 58.025708 |
| H | 13.913291 | 46.520925 | 59.182327 |
| H | 13.125844 | 45.664238 | 57.833565 |
| C | 12.894633 | 43.389228 | 59.240190 |
| H | 13.011245 | 42.498232 | 59.850922 |
| C | 11.737365 | 43.422707 | 58.400698 |
| H | 11.371285 | 44.396256 | 58.083790 |
| C | 10.954095 | 42.351096 | 58.054642 |
| H | 9.968790  | 42.567740 | 57.651687 |
| C | 11.300848 | 40.958731 | 58.058937 |
| C | 12.738963 | 40.491129 | 58.061467 |
| H | 12.990353 | 39.958233 | 58.987196 |
| H | 13.431241 | 41.323099 | 57.954979 |
| H | 12.917668 | 39.802974 | 57.226767 |
| C | 10.263723 | 40.042115 | 58.003495 |
| H | 9.239572  | 40.390368 | 58.100933 |
| C | 10.473911 | 38.667940 | 57.839762 |
| H | 11.434242 | 38.303403 | 57.485884 |

### Retinal geometry of bovine rhodopsin (495 nm)

#### 51 Atoms

|   |           |           |           |
|---|-----------|-----------|-----------|
| N | 45.694430 | 12.502870 | 16.364385 |
| H | 45.807918 | 13.373397 | 16.914726 |
| H | 46.444345 | 12.305347 | 15.688714 |
| C | 35.568625 | 7.669884  | 17.142234 |
| C | 34.995010 | 6.241890  | 17.288725 |
| C | 33.702505 | 6.321771  | 18.128443 |
| H | 32.952901 | 6.975493  | 17.676432 |
| H | 33.929950 | 6.733959  | 19.112773 |
| H | 33.266081 | 5.325390  | 18.272255 |
| C | 35.970925 | 5.283604  | 18.004033 |
| H | 36.198759 | 5.598337  | 19.027142 |
| H | 36.916052 | 5.188017  | 17.461361 |
| H | 35.523240 | 4.284771  | 18.068614 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 35.223538 | 8.465664  | 16.095637 |
| C | 35.575557 | 9.928031  | 15.962908 |
| H | 36.372887 | 10.073718 | 15.222171 |
| H | 35.894625 | 10.387829 | 16.898835 |
| H | 34.692141 | 10.470690 | 15.602100 |
| C | 34.716811 | 5.663125  | 15.885088 |
| H | 34.261306 | 4.670450  | 15.988319 |
| H | 35.678087 | 5.520899  | 15.369712 |
| C | 33.821342 | 6.567984  | 15.042812 |
| H | 32.824641 | 6.620010  | 15.492403 |
| H | 33.692457 | 6.135658  | 14.042543 |
| C | 34.397880 | 7.983650  | 14.926069 |
| H | 35.031968 | 8.065493  | 14.028753 |
| H | 33.585097 | 8.708361  | 14.775229 |
| C | 36.432612 | 8.157183  | 18.218899 |
| H | 36.147971 | 7.894226  | 19.236736 |
| C | 37.574754 | 8.860050  | 17.991401 |
| H | 37.851853 | 9.007029  | 16.952494 |
| C | 38.486832 | 9.440215  | 18.944544 |
| C | 38.191727 | 9.389086  | 20.419274 |
| H | 37.438774 | 8.633720  | 20.641006 |
| H | 37.808565 | 10.345121 | 20.785965 |
| H | 39.092373 | 9.147788  | 20.990478 |
| C | 39.627532 | 10.034788 | 18.447995 |
| H | 39.795602 | 9.960811  | 17.379603 |
| C | 40.533658 | 10.815884 | 19.212458 |
| H | 40.175547 | 11.114086 | 20.194388 |
| C | 41.752051 | 11.354073 | 18.857318 |
| H | 42.133455 | 12.116700 | 19.526857 |
| C | 42.634430 | 11.026008 | 17.784490 |
| C | 42.379761 | 9.826035  | 16.903419 |
| H | 41.716662 | 10.084853 | 16.067383 |
| H | 41.901359 | 9.025744  | 17.471605 |
| H | 43.297345 | 9.421118  | 16.472648 |
| C | 43.752532 | 11.847084 | 17.616102 |
| H | 43.894133 | 12.691885 | 18.287052 |
| C | 44.715035 | 11.652702 | 16.622000 |
| H | 44.680531 | 10.768083 | 15.991591 |

### Retinal geometry of G89Q mutant in bovine rhodopsin (481 nm)

#### 51 Atoms

|   |           |           |           |
|---|-----------|-----------|-----------|
| N | 45.703702 | 12.547579 | 16.397008 |
| H | 45.798153 | 13.420060 | 16.948515 |
| H | 46.460402 | 12.359470 | 15.726177 |
| C | 35.566823 | 7.663189  | 17.134140 |
| C | 34.976945 | 6.243572  | 17.296092 |
| C | 33.695275 | 6.346527  | 18.149956 |
| H | 32.942163 | 6.992959  | 17.693294 |
| H | 33.936137 | 6.779354  | 19.122385 |
| H | 33.256346 | 5.355480  | 18.320644 |
| C | 35.950178 | 5.278854  | 18.006785 |
| H | 36.188698 | 5.594798  | 19.027106 |
| H | 36.890095 | 5.174061  | 17.456379 |
| H | 35.494355 | 4.284128  | 18.077921 |
| C | 35.227206 | 8.454329  | 16.082277 |
| C | 35.594714 | 9.911349  | 15.935536 |
| H | 36.383520 | 10.043106 | 15.183150 |
| H | 35.930920 | 10.374018 | 16.863924 |
| H | 34.712749 | 10.461268 | 15.582097 |
| C | 34.675798 | 5.657484  | 15.900328 |
| H | 34.207358 | 4.672519  | 16.017026 |
| H | 35.629399 | 5.496137  | 15.376384 |
| C | 33.787592 | 6.569625  | 15.058211 |
| H | 32.796416 | 6.646288  | 15.516465 |
| H | 33.640448 | 6.129839  | 14.063669 |

|   |           |           |           |   |           |           |           |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | 34.390856 | 7.971958  | 14.920526 | C | 40.541124 | 10.796788 | 19.204042 |
| H | 35.024910 | 8.028786  | 14.021130 | H | 40.180866 | 11.087439 | 20.187307 |
| H | 33.591870 | 8.709929  | 14.760913 | C | 41.755120 | 11.348514 | 18.853008 |
| C | 36.437170 | 8.148578  | 18.206283 | H | 42.126322 | 12.111321 | 19.528107 |
| H | 36.149801 | 7.893908  | 19.225444 | C | 42.644878 | 11.034159 | 17.782820 |
| C | 37.586181 | 8.839670  | 17.976867 | C | 42.404216 | 9.838480  | 16.891732 |
| H | 37.866820 | 8.979327  | 16.937929 | H | 41.740890 | 10.097675 | 16.055968 |
| C | 38.498442 | 9.418106  | 18.930867 | H | 41.931819 | 9.029015  | 17.452104 |
| C | 38.200856 | 9.367253  | 20.405336 | H | 43.326450 | 9.445797  | 16.459415 |
| H | 37.443685 | 8.615672  | 20.625373 | C | 43.757917 | 11.865015 | 17.626960 |
| H | 37.822303 | 10.324330 | 20.773376 | H | 43.887410 | 12.707784 | 18.303102 |
| H | 39.099456 | 9.121205  | 20.977686 | C | 44.731215 | 11.685132 | 16.641207 |
| C | 39.640588 | 10.012831 | 18.436786 | H | 44.712851 | 10.802351 | 16.007253 |
| H | 39.811859 | 9.939519  | 17.369039 |   |           |           |           |

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