Lipids

Write str: LMG (add residue 5464 of 4ub6) DGD SQD LHG

Unknown ligand UNL: 3wu2 residue 5379, residue 5362

Table

Description automatically generated with medium confidence

Cofactors

Write str: BCR

CLA HEM PHO PL9

Proteins

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| seg id\* | c\*\* |  | missing | 4ub6 | psfge guess | N | C | D/E | HSP | LYS | HSE |
| A | A | D1/psbA | 1-10 N |  | -- | ACE | CTER |  | 92 304 337 |  | 195 252 |
| B | B | CP47 |  |  |  | GLYP | CTER | D380 E387 E405 | 343 |  | 157 201 |
| C | C | CP43 | 19-22 N |  | 19-22 | NTER | CTER | E413 | 74 398 |  |  |
| D | D | D2 | 11 N | E11 |  | NTER | CTER | E242 E343 |  |  | 61 87 189 336 (HSK) |
| E | E | b559a | 2-3 N |  | 2-3 | NTER | CTER |  |  |  |  |
| F | F | b559b | 2-11 N |  | -- | ACE | CTER |  |  |  |  |
| G | H | psbH |  |  |  | NTER | CTER |  |  |  |  |
| H | I | psbI | 37-38 C | L37E38 |  | NTER | CTER |  |  |  |  |
| I | J | psbJ | 1-4 N | S3E4(23) | 1-2 | NTER | CTER |  |  |  |  |
| J | K | psbK |  |  |  | NTER | CTER |  |  |  |  |
| K | L | psbL |  |  |  | NTER | CTER |  |  |  |  |
| L | M | psbM | 34-36 C | K34 | 35-36 | NTER | CTER |  |  |  |  |
| M | O | psbO |  |  |  | NTER | CTER | D102 D224 E97 | 228 |  | 231 |
| N | T | psbT | 31-32 C |  | 31-32 | NTER | CTER |  |  |  |  |
| O | U | psbU | 1-7 N |  | -- | ACE | CTER |  | 81 |  |  |
| P | V | psbV |  |  |  | NTER | CTER |  |  | 47 134 | 118 |
| Q | X | psbX | 40-41 C | S40 | 41 | NTER | CTER |  |  |  |  |
| R | Y | psbY | 17-19 N | V18I19 | 17 | NTER | CTER |  |  |  |  |
| S | Z | psbZ |  |  |  | NTER | CTER |  |  |  |  |

\*the default segname in the charmmgui output – we modified it later.

\*\*the chain id in 3wu2 and our system

No lipid modification to amino acids (<https://www.tandfonline.com/doi/full/10.1080/09687680802680090?cookieSet=1>, <https://nph.onlinelibrary.wiley.com/doi/pdf/10.1111/nph.13085> ) (D1 has S-acyl, but removed after assembled into PSII)

Amino acid modifications:

FME mutate to MET (removed after translocation)

HSK mutate to HSE (doesn’t exist in 4ub6)