Supporting Information

On the Yellow-Green Bioluminescence of the Firefly, *Photinus Pyralis*: SAC-CI Study

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Preliminary computational models: Model A and Model B

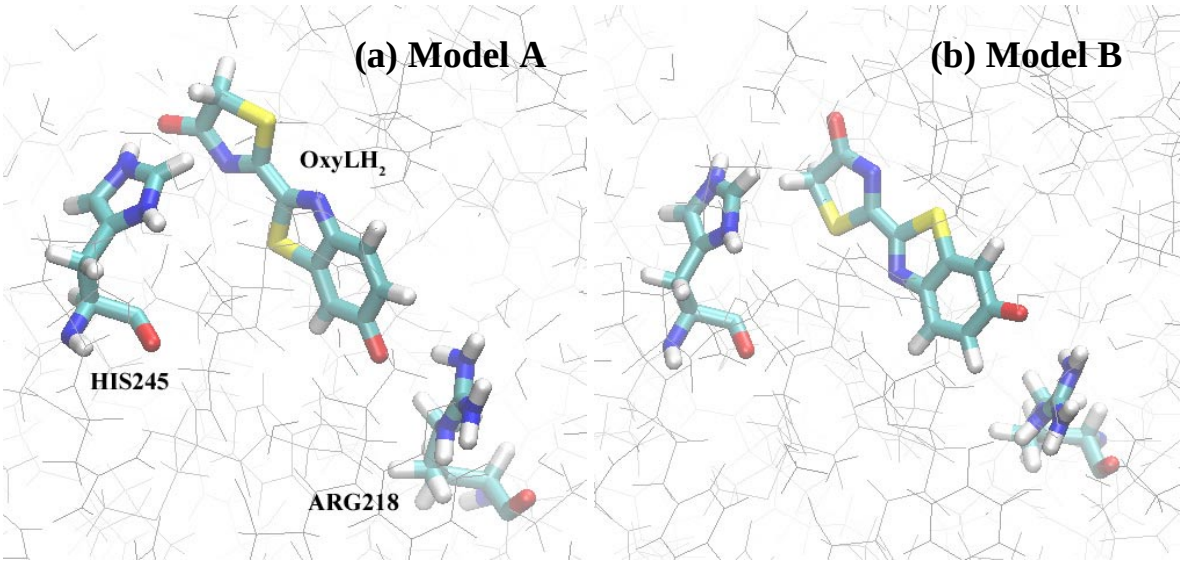

Figure S1. Snap shots taken from MD simulations for (a) model **A** and (b) model **B**. $OxyLH_2$. The graphics were drawn using VMD.[1]

For the computational models of Luc containing $OxyLH_2$ ($OxyLH_2$-Luc), we constructed two structures, models A and B, which are different in the orientation of $OxyLH_2$ as shown in Figure S1. In the model A, $OxyLH_2$ is placed in the pocket, so that its carbonyl oxygen in thiazolinone and hydroxybenzothiazole rings can interact with His245 and Arg218, respectively. Model B has the opposite orientation. The results of the MD simulations showed that model A is much more stable than model B, because of the hydrogen-bonding between $OxyLH_2$ and the histidine.

On the accuracy of the CIS geometry

Since the computational model for the Luc active site includes some neighboring residues, it is too large to perform geometry optimization using the SAC-CI method. The geometry of the first excited state was therefore optimized using the CI-Single (CIS) method, and single-point SAC-CI calculations were performed for obtaining fluorescence energy. Since the wave functions of the first excited states were well described by the one-electron transitions from HOMOs to LUMOs, the CIS geometries were qualitatively correct. Actually, we also performed the geometry optimization at the SAC-CI/6-31g* level for the first excited state of keto-s-trans(-1) and enol-s-trans(-1) in a gas phase. The LevelOne set of thresholds (1.0×10^{-5} and 1.0×10^{-6} hartree for the SAC and SAC-CI wave functions, respectively) was used for the perturbation selection of the double excitation operators in the SAC and SAC-CI wave functions. With the CIS and SAC-CI geometries, the calculated fluorescence energies of the keto form were 1.97 and 1.84 eV, respectively, and for the enol form, they were 2.04 and 2.01 eV, respectively. The correlation effect on the geometry of the excited state was very small (0.03 eV) in the enol form, while it was not negligible in the keto form (0.13 eV = 3.07 kcal/mol). However, such differences were fortunately small enough not to affect the conclusions of the present paper.

In Table S1, the bond distances of the first excited state of keto-s-trans(-1) and enol-s-trans(-1) in a gas phase are summarized. The bond indices were graphically shown in Figure S2. The RMS deviation between the CIS and SAC-CI results was 0.014 and 0.010 Å in the keto and enol forms,

respectively. The largest deviation is in the R6 bond in both keto and enol forms, and the CIS bond length is about 0.03 Å shorter than the SAC-CI one.

Table S1 The bond distances optimized using CIS and SAC-CI method.

Bond	keto-s-trans(-1)			enol-s-trans(-1)		
indices[a]	CIS/6-31g*	SAC-CI/6-31g*	Δ	CIS/D95(d)	SAC-CI/6-31g*	Δ
1	1.203	1.208	0.005	1.353	1.356	0.003
2	1.358	1.363	0.005	1.328	1.330	0.002
3	1.308	1.306	-0.002	1.333	1.333	0.000
4	1.410	1.430	0.020	1.406	1.417	0.011
5	1.331	1.311	-0.020	1.337	1.319	-0.018
6	1.343	1.377	0.034	1.342	1.367	0.025
7	1.427	1.415	-0.012	1.429	1.416	-0.013
8	1.353	1.370	0.017	1.359	1.371	0.012
9	1.463	1.458	-0.005	1.467	1.459	-0.008
10	1.221	1.238	0.017	1.230	1.237	0.007
11	1.460	1.457	-0.003	1.461	1.460	-0.001
12	1.359	1.380	0.021	1.363	1.376	0.013
13	1.422	1.408	-0.014	1.428	1.416	-0.012
14	1.766	1.762	-0.004	1.766	1.762	-0.004
15	1.763	1.768	0.005	1.770	1.773	0.003
16	1.776	1.782	0.006	1.756	1.762	0.006
17	1.806	1.812	0.006	1.742	1.750	0.008
18	1.541	1.544	0.003	1.372	1.371	-0.001
RMS			0.014			0.010

[a] See Figure S2

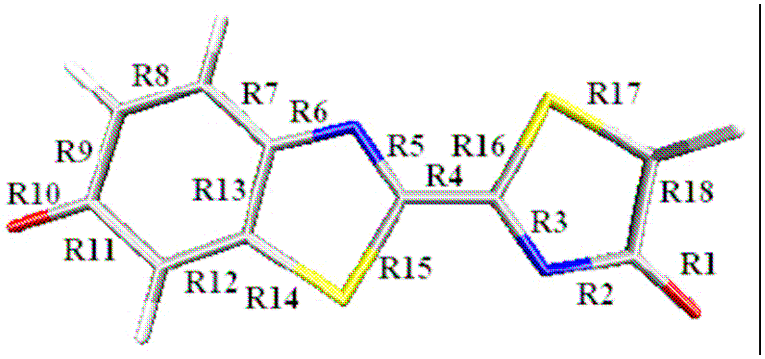

Figure S2. Bond indices corresponding the notation in Table

On the accuracy of the SAC/SAC-CI method

We briefly describe the accuracy of the SAC/SAC-CI method. The details can be found elsewhere in a previous review.[2] The SAC theory[3] is the cluster expansion approach. The SAC method is size-

extensive, which means the method can be applicable to large systems. When we apply the variational principle to Schroedinger equation with the SAC wave function, we obtain the variational SAC equation, which implies the following important property. Based on the SAC wave function, we can define a set of basis functions for describing the excited states; this basis function satisfies orthogonality and Hamiltonian orthogonality to the ground-state SAC wave function. Therefore, the excited state wave function can be expanded by a linear combination of these basis functions, which is the SAC-CI theory.[4] It is evident that the SAC-CI wave function satisfies the orthogonality and Hamiltonian-orthogonality to the ground state. Because of this theoretical foundation, the SAC/SAC-CI method performs quite well for both ground and excited states, which has been confirmed by comparing the SAC-CI results with the full-CI one (exact limit within a given basis set),[5] and also by applying to numerous examples.[2] Another important property of the SAC-CI method is that we can study various electronic states in the same accuracy.

The SAC-CI method has been developed mainly by our laboratory, both in theories and algorithms, and has been successfully applied to various chemical phenomena involving more than 170 molecules. The SAC-CI method has been applied to a wide variety of chemistry; electronic excitation spectroscopy of valence, Rydberg and inner-core states, ionization (photo-electron) spectroscopy in outer-valence, inner-valence and core regions, molecular spectroscopies including multi-electron processes, molecular structure and spectroscopic constants in the excited states, electronic structures of adsorbates, catalytic reactions and surface sciences, photochemical reaction dynamics, biological photochemistry and electron transfer, atmospheric chemistry, molecular interactions, and ESR hyperfine splitting constants.[2] The size of the applied system ranges from small atoms and molecules to biologically important systems composed of more than hundred atoms. Through these applications, the SAC-CI method has been established to be a reliable method for studying the electronic structure of atoms and molecules in their ground, excited, ionized and electron-attached states. In Figure S3, we show an example of SAC-CI result for the retinal proteins.[6]

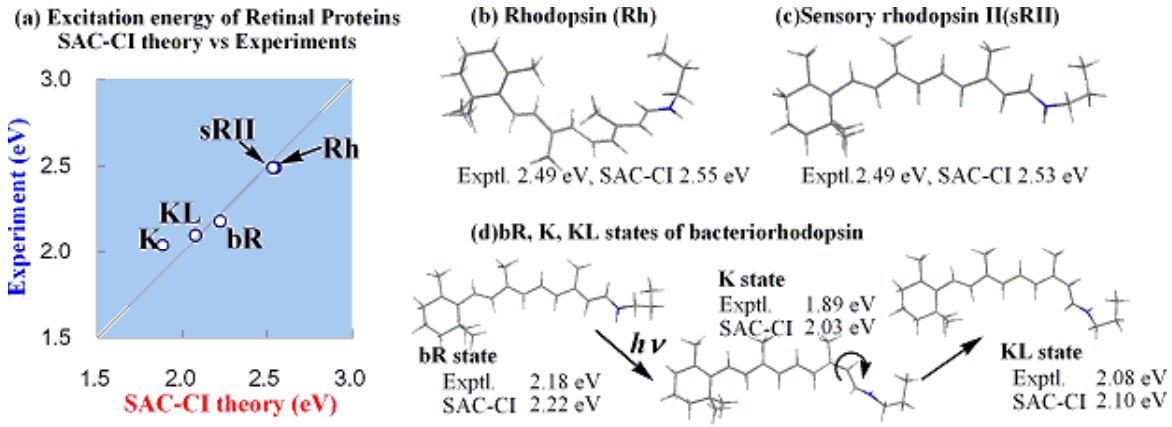

Figure S3. Excitation energy of retinal proteins. (a)SAC-CI theoretical excitation energies are compared with the experimental values. Structures and excitation energies of (b)rhodopsin, (c)sensory rhodopsin II, and (d)bR, K, and KL states of bacteriorhodopsin.

On the choice of basis sets for geometry optimization and SAC-CI calculation

We used D95(d) basis sets for the SAC-CI calculation, whereas 6-31G and 6-31G(d) basis sets were used for the geometry optimizations in protein. This is because the integral calculation with 6-31G(d) sets is faster than that with D95(d) sets in the Gaussian program.[7] In our experiences, both 6-31G(d) and D95(d) give the optimized structures for the excited state similar to each other. However, D95(d) is better basis set for calculating the excitation or emission energies. To show numerical evidence, we performed three calculations with different combinations of basis sets: 6-31G(d)//6-31G(d), D95(d)//6-31G(d), and D95(d)//D95(d). "Basis A"//"Basis B" denotes SAC-CI calculation was performed with the basis A, while CIS optimization was carried out with the basis B.

As Figure S4 shows, both 6-31G(d) and D95(d) sets give optimized geometries very similar to each other. Table S2 shows the SAC-CI results with the three combinations. The D95(d)//6-31G(d) and D95(d)//D95(d) combinations give only 0.02 eV of deviation in the emission energy. However, 6-31G(d)//6-31G(d) calculation gives slightly higher emission energy (~0.1 eV). Therefore, D95(d)//6-31G(d) combination is a reasonable choice in terms of the accuracy and the computing time.

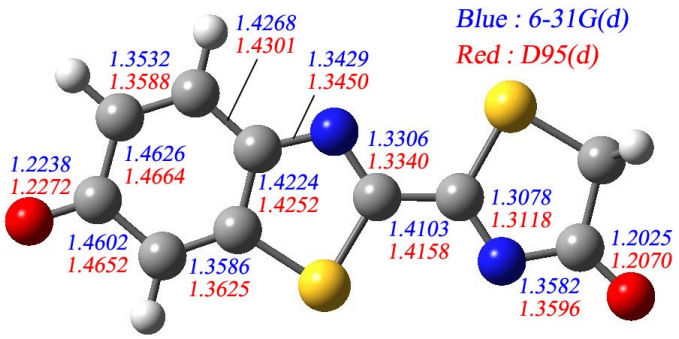

Figure S4. The CIS optimized geometries with 6-31G(d) (blue) and D95(d) (red) basis ests.

Table S2. The emission energies of keto-s-trans(-1) calculated by using three different combinations of basis sets.

	Optimization	Emission energy / eV	
	CIS	SAC-CI	
6-31G(d)//6-31G(d)	6-31G(d)	6-31G(d)	2.06
D95(d)//6-31G(d)	6-31G(d)	D95(d)	1.98
D95(d)//D95(d)	D95(d)	D95(d)	1.96

Structures and potential energies of the first excited state of $OxyLH_2$ in DMSO solution

Structures of $OxyLH_2$ in the first excited state were calculated with the solvent effect. In Table S3, emission energies at CIS/D95(d) plus PCM(DMSO) level were summarized. We considered two models. The first one is "tight ion-pair" model in which the K^+ ion is directly attached to $OxyLH_2$ ("K^+ / PCM (DMSO)" in Table S3). The second one is "separated ion-pair" model in which the K^+ ion is separated by a DMSO molecule ("DMSO + K^+ / PCM (DMSO)" in Table S3). In Figure S5, the optimized structures were shown. As shown in Table S3, the additional DMSO molecule gives only minor change in the emission energies. With the explicit DMSO, emission energies become slightly small by 0.03-0.05 eV.

Table S3. CIS emission energies of $OxyLH_2$ calculated with the "tight ion-pair" model and "solvent-separated ion-pair" models

Molecule	Solvation Model	Emission Energy / eV
keto-s-trans(-1)	K^+ / PCM (DMSO)	3.10
	DMSO + K^+ / PCM (DMSO)	3.07
enol-s-trans(-1)	K^+ / PCM (DMSO)	3.04
	DMSO + K^+ / PCM (DMSO)	3.00
enol-s-trans(-1)'	K^+ / PCM (DMSO)	3.11
	DMSO + K^+ / PCM (DMSO)	3.06
enol-s-trans(-2)	K^+ / PCM (DMSO)	3.01
	DMSO + K^+ / PCM (DMSO)	2.97

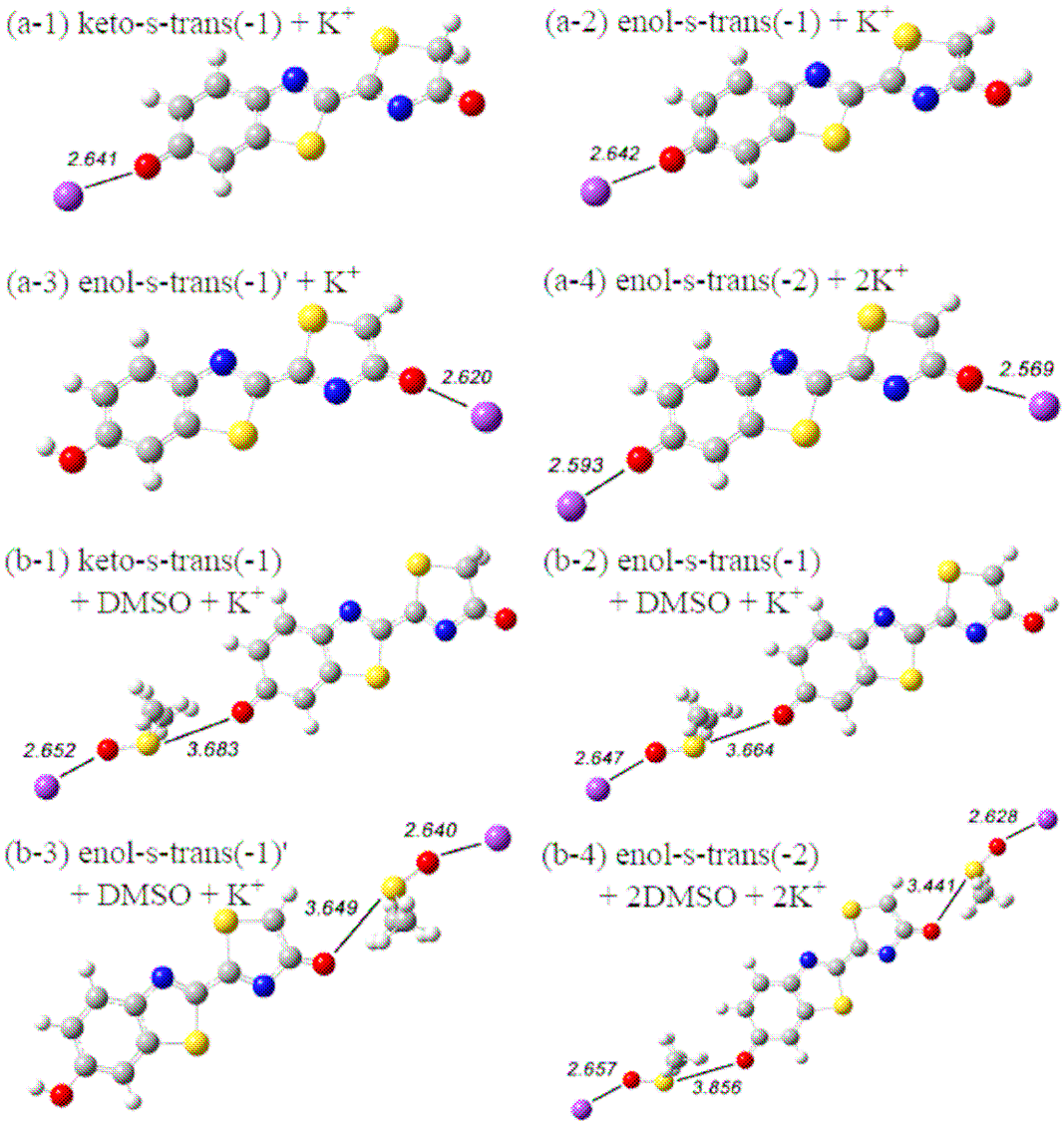

Figure S5. Optimized structures of the excited state of $OxyLH_2$ in K^+/DMSO solution. (a-1)-(a-4)"Tight ion-pair model". (b-1)-(b-4)"Separated ion-pair model" including DMSO molecule between $OxyLH_2$ and K^+.

Coordinate of the model A-a and model A-b

Followings are cartesian coordinates for the QM region of the CIS optimized structures (models A-a and A-b).

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HEADER    OXYLUCIFERIN-AMP-LUCIFERASE COMPLEX WORKING MODEL A-a
REMARK

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ATOM      4  NH1 ARG   218      17.301  84.136  43.753  1.00  0.00           N
ATOM      5  NH2 ARG   218      17.691  82.048  43.118  1.00  0.00           N
ATOM      6  HD  ARG   218      16.898  85.697  41.393  1.00  0.00           H
ATOM      7  HD  ARG   218      18.643  85.466  41.572  1.00  0.00           H
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HETATM   13  HDM ARG   218      17.834  85.109  40.010  1.00  0.00           H
ATOM     14  CB  HIS   245       4.714  85.621  42.330  1.00  0.00           C
ATOM     15  CG  HIS   245       5.086  86.551  43.453  1.00  0.00           C
ATOM     16  ND1 HIS   245       5.744  86.205  44.619  1.00  0.00           N
ATOM     17  CD2 HIS   245       4.611  87.820  43.591  1.00  0.00           C
ATOM     18  CE1 HIS   245       5.659  87.260  45.456  1.00  0.00           C
ATOM     19  NE2 HIS   245       4.976  88.251  44.848  1.00  0.00           N
ATOM     20  HB  HIS   245       4.787  84.596  42.680  1.00  0.00           H
ATOM     21  HB  HIS   245       3.662  85.795  42.098  1.00  0.00           H
ATOM     22  HD1 HIS   245       6.024  85.258  44.880  1.00  0.00           H
ATOM     23  HD2 HIS   245       3.952  88.338  42.909  1.00  0.00           H
ATOM     24  HE1 HIS   245       5.902  87.251  46.515  1.00  0.00           H
ATOM     25  HE2 HIS   245       4.464  89.009  45.325  1.00  0.00           H
HETATM   26  HDM HIS   245       5.388  85.771  41.500  1.00  0.00           H
ATOM     27  N   PHE   247       9.589  85.214  43.346  1.00  0.00           N
ATOM     28  CA  PHE   247      10.267  84.085  43.992  1.00  0.00           C
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ATOM     33  CD1 PHE   247      11.709  82.486  46.119  1.00  0.00           C
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ATOM     36  CE2 PHE   247      10.295  81.458  48.308  1.00  0.00           C
ATOM     37  CZ  PHE   247      11.632  81.090  48.102  1.00  0.00           C
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HETATM   46  HDM PHE   247      10.178  83.207  43.369  1.00  0.00           H
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ATOM     48  C   GLY   341      11.674  91.718  47.691  1.00  0.00           C
ATOM     49  O   GLY   341      10.724  91.417  48.410  1.00  0.00           O
ATOM     50  HA  GLY   341      13.789  91.578  47.374  1.00  0.00           H
ATOM     51  HA  GLY   341      12.898  90.051  47.177  1.00  0.00           H
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ATOM     62  HA  SER   347      13.874  88.468  43.572  1.00  0.00           H
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HETATM   77  HDM ALA   348      17.040  89.360  46.845  1.00  0.00           H
TER
HETATM   78  OW  HOH    45       7.526  89.768  43.419  1.00  0.00           O
HETATM   79  HW  HOH    45       8.112  89.725  44.197  1.00  0.00           H
HETATM   80  HW  HOH    45       7.184  90.680  43.542  1.00  0.00           H
TER
HETATM   81  C2D OLU     1      10.698  87.907  46.189  1.00  0.00           C
HETATM   82  C2N OLU     1       9.650  88.632  46.800  1.00  0.00           C
HETATM   83  N3N OLU     1       8.964  89.526  46.131  1.00  0.00           N
HETATM   84  S1N OLU     1       9.227  88.363  48.475  1.00  0.00           S
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HETATM   86  C4N OLU     1       8.081  90.210  46.918  1.00  0.00           C
HETATM   87  O4N OLU     1       7.370  91.094  46.519  1.00  0.00           O
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HETATM   92  S3D OLU     1      11.004  88.118  44.468  1.00  0.00           S
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HETATM  107  C5* AMP     2       0.028  89.832  47.046  1.00  0.00           C
HETATM  108  H5* AMP     2      -0.590  89.814  46.147  1.00  0.00           H
HETATM  109  H5* AMP     2       0.581  90.772  47.067  1.00  0.00           H
HETATM  110  HDM AMP     2      -0.508  89.845  47.984  1.00  0.00           H
END


HEADER   OXYLUCIFERIN-AMP-LUCIFERASE COMPLEX WORKING MODEL A-b
REMARK
ATOM      1  CD  ARG   218      17.752  85.039  41.026  1.00  0.00           C
ATOM      2  NE  ARG   218      17.552  83.646  41.479  1.00  0.00           N
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ATOM      3  CZ  ARG   218      17.575  83.265  42.743  1.00  0.00           C
ATOM      4  NH1 ARG   218      17.363  84.114  43.698  1.00  0.00           N
ATOM      5  NH2 ARG   218      17.783  82.031  43.082  1.00  0.00           N
ATOM      6  HD  ARG   218      16.900  85.651  41.323  1.00  0.00           H
ATOM      7  HD  ARG   218      18.643  85.432  41.518  1.00  0.00           H
ATOM      8  HE  ARG   218      17.424  82.924  40.785  1.00  0.00           H
ATOM      9  HH  ARG   218      16.633  84.772  43.457  1.00  0.00           H
ATOM     10  HH  ARG   218      17.375  83.761  44.649  1.00  0.00           H
ATOM     11  HH  ARG   218      17.813  81.281  42.397  1.00  0.00           H
ATOM     12  HH  ARG   218      17.837  81.761  44.058  1.00  0.00           H
HETATM   13  HDM ARG   218      17.847  85.058  39.950  1.00  0.00           H
ATOM     14  CB  HIS   245       4.780  85.728  42.348  1.00  0.00           C
ATOM     15  CG  HIS   245       5.335  86.536  43.492  1.00  0.00           C
ATOM     16  ND1 HIS   245       6.017  86.031  44.583  1.00  0.00           N
ATOM     17  CD2 HIS   245       5.161  87.874  43.695  1.00  0.00           C
ATOM     18  CE1 HIS   245       6.237  87.042  45.445  1.00  0.00           C
ATOM     19  NE2 HIS   245       5.742  88.174  44.910  1.00  0.00           N
ATOM     20  HB  HIS   245       4.740  84.685  42.657  1.00  0.00           H
ATOM     21  HB  HIS   245       3.754  86.051  42.169  1.00  0.00           H
ATOM     22  HD1 HIS   245       6.136  85.038  44.788  1.00  0.00           H
ATOM     23  HD2 HIS   245       4.587  88.554  43.078  1.00  0.00           H
ATOM     24  HE1 HIS   245       6.629  86.950  46.454  1.00  0.00           H
ATOM     25  HE2 HIS   245       5.698  89.082  45.382  1.00  0.00           H
HETATM   26  HDM HIS   245       5.421  85.836  41.486  1.00  0.00           H
ATOM     27  N   PHE   247       9.633  85.175  43.319  1.00  0.00           N
ATOM     28  CA  PHE   247      10.327  84.062  43.984  1.00  0.00           C
ATOM     29  HN  PHE   247       8.901  85.659  43.815  1.00  0.00           H
ATOM     30  HA  PHE   247      11.375  84.328  44.067  1.00  0.00           H
ATOM     31  CB  PHE   247       9.788  83.863  45.411  1.00  0.00           C
ATOM     32  CG  PHE   247      10.500  82.848  46.306  1.00  0.00           C
ATOM     33  CD1 PHE   247      11.879  82.586  46.220  1.00  0.00           C
ATOM     34  CD2 PHE   247       9.758  82.203  47.304  1.00  0.00           C
ATOM     35  CE1 PHE   247      12.515  81.730  47.140  1.00  0.00           C
ATOM     36  CE2 PHE   247      10.361  81.277  48.258  1.00  0.00           C
ATOM     37  CZ  PHE   247      11.788  81.103  48.167  1.00  0.00           C
ATOM     38  HB  PHE   247       8.737  83.583  45.343  1.00  0.00           H
ATOM     39  HB  PHE   247       9.826  84.823  45.925  1.00  0.00           H
ATOM     40  HD  PHE   247      12.470  83.057  45.455  1.00  0.00           H
ATOM     41  HD  PHE   247       8.703  82.419  47.389  1.00  0.00           H
ATOM     42  HE  PHE   247      13.579  81.558  47.065  1.00  0.00           H
ATOM     43  HE  PHE   247       9.788  80.787  49.030  1.00  0.00           H
ATOM     44  HZ  PHE   247      12.296  80.461  48.871  1.00  0.00           H
HETATM   45  HDM PHE   247       9.910  85.462  42.316  1.00  0.00           H
HETATM   46  HDM PHE   247      10.214  83.164  43.395  1.00  0.00           H
ATOM     47  CA  GLY   341      13.275  91.870  48.015  1.00  0.00           C
ATOM     48  C   GLY   341      11.875  92.430  47.821  1.00  0.00           C
ATOM     49  O   GLY   341      11.023  92.337  48.701  1.00  0.00           O
ATOM     50  HA  GLY   341      13.994  92.685  47.934  1.00  0.00           H
ATOM     51  HA  GLY   341      13.474  91.134  47.236  1.00  0.00           H
HETATM   52  HDM GLY   341      13.344  91.401  48.985  1.00  0.00           H
ATOM     53  N   LEU   342      11.639  92.976  46.641  1.00  0.00           N
ATOM     54  CA  LEU   342      10.309  93.277  46.135  1.00  0.00           C
ATOM     55  HN  LEU   342      12.392  92.973  45.959  1.00  0.00           H
ATOM     56  HA  LEU   342       9.547  92.786  46.746  1.00  0.00           H
HETATM   57  HDM LEU   342      10.146  94.344  46.163  1.00  0.00           H
HETATM   58  HDM LEU   342      10.222  92.926  45.118  1.00  0.00           H
ATOM     59  CA  SER   347      14.849  88.876  43.401  1.00  0.00           C
ATOM     60  C   SER   347      15.379  89.441  44.706  1.00  0.00           C
ATOM     61  O   SER   347      15.665  90.636  44.808  1.00  0.00           O
ATOM     62  HA  SER   347      13.870  88.483  43.630  1.00  0.00           H
ATOM     63  CB  SER   347      15.737  87.747  42.853  1.00  0.00           C
ATOM     64  OG  SER   347      17.023  88.168  42.460  1.00  0.00           O
ATOM     65  HB  SER   347      15.239  87.298  41.992  1.00  0.00           H
ATOM     66  HB  SER   347      15.865  86.989  43.622  1.00  0.00           H
ATOM     67  HG  SER   347      17.669  87.865  43.123  1.00  0.00           H
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HETATM   68  HDM SER   347      14.760  89.657  42.660  1.00  0.00           H
ATOM     69  N   ALA   348      15.491  88.582  45.719  1.00  0.00           N
ATOM     70  CA  ALA   348      16.051  88.959  47.005  1.00  0.00           C
ATOM     71  HN  ALA   348      15.172  87.632  45.607  1.00  0.00           H
ATOM     72  HA  ALA   348      15.388  89.703  47.444  1.00  0.00           H
ATOM     73  CB  ALA   348      16.051  87.730  47.907  1.00  0.00           C
ATOM     74  HB  ALA   348      16.394  88.003  48.906  1.00  0.00           H
ATOM     75  HB  ALA   348      16.702  86.956  47.502  1.00  0.00           H
ATOM     76  HB  ALA   348      15.038  87.340  47.978  1.00  0.00           H
HETATM   77  HDM ALA   348      17.038  89.372  46.862  1.00  0.00           H
TER
HETATM   78  OW  HOH    45       8.023  89.221  43.178  1.00  0.00           O
HETATM   79  HW  HOH    45       8.377  89.240  44.083  1.00  0.00           H
HETATM   80  HW  HOH    45       7.584  90.090  43.113  1.00  0.00           H
TER
HETATM   81  C2* OLU     1      10.710  87.969  46.174  1.00  0.00           C
HETATM   82  C2  OLU     1       9.574  88.601  46.736  1.00  0.00           C
HETATM   83  N3  OLU     1       8.799  89.383  46.012  1.00  0.00           N
HETATM   84  S1  OLU     1       9.093  88.294  48.389  1.00  0.00           S
HETATM   85  C5  OLU     1       7.704  89.430  48.160  1.00  0.00           C
HETATM   86  C4  OLU     1       7.725  89.851  46.696  1.00  0.00           C
HETATM   87  O4  OLU     1       6.839  90.521  46.211  1.00  0.00           O
HETATM   88  H5  OLU     1       7.852  90.309  48.764  1.00  0.00           H
HETATM   89  H5  OLU     1       6.746  88.988  48.410  1.00  0.00           H
HETATM   90  N1* OLU     1      11.551  87.191  46.847  1.00  0.00           N
HETATM   91  C9* OLU     1      12.389  86.568  45.998  1.00  0.00           C
HETATM   92  S3* OLU     1      10.989  88.104  44.446  1.00  0.00           S
HETATM   93  C4* OLU     1      12.207  86.853  44.617  1.00  0.00           C
HETATM   94  C5* OLU     1      12.912  86.234  43.629  1.00  0.00           C
HETATM   95  C6* OLU     1      13.968  85.299  43.974  1.00  0.00           C
HETATM   96  O6* OLU     1      14.675  84.782  43.097  1.00  0.00           O
HETATM   97  C8* OLU     1      13.422  85.655  46.353  1.00  0.00           C
HETATM   98  C7* OLU     1      14.189  85.067  45.392  1.00  0.00           C
HETATM   99  H5* OLU     1      12.743  86.444  42.591  1.00  0.00           H
HETATM  100  H8* OLU     1      13.576  85.429  47.391  1.00  0.00           H
HETATM  101  H7* OLU     1      14.957  84.368  45.666  1.00  0.00           H
HETATM  102  P   AMP     2       2.152  89.105  45.287  1.00  0.00           P
HETATM  103  OP  AMP     2       0.705  88.879  45.239  1.00  0.00           O
HETATM  104  OP  AMP     2       2.912  87.938  45.733  1.00  0.00           O
HETATM  105  OP  AMP     2       2.705  89.803  44.127  1.00  0.00           O
HETATM  106  O5* AMP     2       2.390  90.169  46.411  1.00  0.00           O
HETATM  107  C5* AMP     2       1.642  90.198  47.609  1.00  0.00           C
HETATM  108  H5* AMP     2       1.801  89.282  48.177  1.00  0.00           H
HETATM  109  H5* AMP     2       0.581  90.301  47.375  1.00  0.00           H
HETATM  110  HDM AMP     2       1.959  91.037  48.211  1.00  0.00           H
HETATM  111  N9  AMP     2       5.402  92.576  49.295  1.00  0.00           N
HETATM  112  C8  AMP     2       6.354  93.366  48.692  1.00  0.00           C
HETATM  113  N7  AMP     2       7.569  93.178  49.133  1.00  0.00           N
HETATM  114  C5  AMP     2       7.398  92.224  50.147  1.00  0.00           C
HETATM  115  C6  AMP     2       8.271  91.513  51.010  1.00  0.00           C
HETATM  116  N6  AMP     2       9.584  91.586  50.985  1.00  0.00           N
HETATM  117  N1  AMP     2       7.814  90.599  51.867  1.00  0.00           N
HETATM  118  C2  AMP     2       6.508  90.386  51.886  1.00  0.00           C
HETATM  119  N3  AMP     2       5.571  90.950  51.138  1.00  0.00           N
HETATM  120  C4  AMP     2       6.081  91.865  50.264  1.00  0.00           C
HETATM  121  H8  AMP     2       6.117  94.070  47.904  1.00  0.00           H
HETATM  122  H61 AMP     2      10.007  92.133  50.239  1.00  0.00           H
HETATM  123  H62 AMP     2      10.096  90.863  51.453  1.00  0.00           H
HETATM  124  H2  AMP     2       6.162  89.645  52.593  1.00  0.00           H
HETATM  125  HDM AMP     2       4.337  92.534  49.118  1.00  0.00           H
END
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The following coordinates are for the amino acids having the averaged deviation more than 0.4 Å from the X-ray structure (See Table 1). OxyLH_2 and AMP are also included.

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HEADER   OXYLUCIFERIN-AMP-LUCIFERASE COMPLEX WORKING MODEL A-a
REMARK
ATOM   3105  N   SER   198       3.336  94.012  40.695  1.00  0.00           N
ATOM   3106  CA  SER   198       3.637  94.595  42.027  1.00  0.00           C
ATOM   3107  C   SER   198       2.549  95.573  42.493  1.00  0.00           C
ATOM   3108  O   SER   198       1.636  95.828  41.725  1.00  0.00           O
ATOM   3109  HN  SER   198       3.041  94.665  39.980  1.00  0.00           H
ATOM   3110  HA  SER   198       3.722  93.794  42.762  1.00  0.00           H
ATOM   3111  CB  SER   198       4.950  95.361  41.963  1.00  0.00           C
ATOM   3112  OG  SER   198       5.433  95.552  43.279  1.00  0.00           O
ATOM   3113  HB  SER   198       4.792  96.313  41.445  1.00  0.00           H
ATOM   3114  HB  SER   198       5.664  94.772  41.401  1.00  0.00           H
ATOM   3115  HG  SER   198       6.094  96.295  43.272  1.00  0.00           H
ATOM   3380  N   ARG   218      20.810  87.547  38.562  1.00  0.00           N
ATOM   3381  CA  ARG   218      20.188  86.491  39.355  1.00  0.00           C
ATOM   3382  C   ARG   218      20.860  85.135  39.116  1.00  0.00           C
ATOM   3383  O   ARG   218      21.035  84.344  40.068  1.00  0.00           O
ATOM   3384  HN  ARG   218      20.231  88.108  37.942  1.00  0.00           H
ATOM   3385  HA  ARG   218      20.330  86.718  40.411  1.00  0.00           H
ATOM   3386  CB  ARG   218      18.658  86.439  39.070  1.00  0.00           C
ATOM   3387  CG  ARG   218      17.907  85.200  39.565  1.00  0.00           C
ATOM   3388  CD  ARG   218      17.743  85.083  41.086  1.00  0.00           C
ATOM   3389  NE  ARG   218      17.530  83.689  41.531  1.00  0.00           N
ATOM   3390  CZ  ARG   218      17.518  83.292  42.792  1.00  0.00           C
ATOM   3391  NH1 ARG   218      17.301  84.136  43.753  1.00  0.00           N
ATOM   3392  NH2 ARG   218      17.691  82.048  43.118  1.00  0.00           N
ATOM   3393  HB  ARG   218      18.474  86.477  38.007  1.00  0.00           H
ATOM   3394  HB  ARG   218      18.192  87.329  39.500  1.00  0.00           H
ATOM   3395  HG  ARG   218      18.437  84.348  39.183  1.00  0.00           H
ATOM   3396  HG  ARG   218      16.927  85.184  39.095  1.00  0.00           H
ATOM   3397  HD  ARG   218      16.898  85.697  41.393  1.00  0.00           H
ATOM   3398  HD  ARG   218      18.643  85.466  41.572  1.00  0.00           H
ATOM   3399  HE  ARG   218      17.419  82.962  40.838  1.00  0.00           H
ATOM   3400  HH  ARG   218      16.493  84.695  43.493  1.00  0.00           H
ATOM   3401  HH  ARG   218      17.312  83.753  44.694  1.00  0.00           H
ATOM   3402  HH  ARG   218      17.757  81.300  42.432  1.00  0.00           H
ATOM   3403  HH  ARG   218      17.725  81.771  44.093  1.00  0.00           H
ATOM   3811  N   HIS   245       5.076  84.757  40.103  1.00  0.00           N
ATOM   3812  CA  HIS   245       5.523  85.793  41.038  1.00  0.00           C
ATOM   3813  C   HIS   245       7.042  85.697  41.207  1.00  0.00           C
ATOM   3814  O   HIS   245       7.625  84.659  40.892  1.00  0.00           O
ATOM   3815  HN  HIS   245       5.211  83.789  40.369  1.00  0.00           H
ATOM   3816  HA  HIS   245       5.303  86.785  40.637  1.00  0.00           H
ATOM   3817  CB  HIS   245       4.714  85.621  42.330  1.00  0.00           C
ATOM   3818  CG  HIS   245       5.086  86.551  43.453  1.00  0.00           C
ATOM   3819  ND1 HIS   245       5.744  86.205  44.619  1.00  0.00           N
ATOM   3820  CD2 HIS   245       4.611  87.820  43.591  1.00  0.00           C
ATOM   3821  CE1 HIS   245       5.659  87.260  45.456  1.00  0.00           C
ATOM   3822  NE2 HIS   245       4.976  88.251  44.848  1.00  0.00           N
ATOM   3823  HB  HIS   245       4.787  84.596  42.680  1.00  0.00           H
ATOM   3824  HB  HIS   245       3.662  85.795  42.098  1.00  0.00           H
ATOM   3825  HD1 HIS   245       6.024  85.258  44.880  1.00  0.00           H
ATOM   3826  HD2 HIS   245       3.952  88.338  42.909  1.00  0.00           H
ATOM   3827  HE1 HIS   245       5.902  87.251  46.515  1.00  0.00           H
ATOM   3828  HE2 HIS   245       4.464  89.009  45.325  1.00  0.00           H
ATOM   4953  N   SER   314      12.193  80.996  52.520  1.00  0.00           N
ATOM   4954  CA  SER   314      11.256  82.070  52.166  1.00  0.00           C
ATOM   4955  C   SER   314      11.826  82.983  51.075  1.00  0.00           C
ATOM   4956  O   SER   314      11.069  83.718  50.435  1.00  0.00           O
ATOM   4957  HN  SER   314      12.960  81.224  53.147  1.00  0.00           H
ATOM   4958  HA  SER   314      10.338  81.628  51.780  1.00  0.00           H
ATOM   4959  CB  SER   314      10.893  82.894  53.399  1.00  0.00           C
ATOM   4960  OG  SER   314      11.929  83.782  53.741  1.00  0.00           O
ATOM   4961  HB  SER   314      10.715  82.225  54.238  1.00  0.00           H
ATOM   4962  HB  SER   314       9.986  83.464  53.193  1.00  0.00           H
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ATOM   4963  HG  SER   314      11.501  84.636  53.968  1.00  0.00           H
ATOM   4964  N   GLY   315      13.148  82.913  50.852  1.00  0.00           N
ATOM   4965  CA  GLY   315      13.888  83.520  49.744  1.00  0.00           C
ATOM   4966  C   GLY   315      14.014  85.040  49.825  1.00  0.00           C
ATOM   4967  O   GLY   315      15.119  85.560  49.909  1.00  0.00           O
ATOM   4968  HN  GLY   315      13.668  82.337  51.505  1.00  0.00           H
ATOM   4969  HA  GLY   315      14.894  83.099  49.719  1.00  0.00           H
ATOM   4970  HA  GLY   315      13.397  83.270  48.806  1.00  0.00           H
ATOM   4971  N   GLY   316      12.885  85.746  49.758  1.00  0.00           N
ATOM   4972  CA  GLY   316      12.787  87.209  49.770  1.00  0.00           C
ATOM   4973  C   GLY   316      11.637  87.770  50.609  1.00  0.00           C
ATOM   4974  O   GLY   316      11.533  88.986  50.736  1.00  0.00           O
ATOM   4975  HN  GLY   316      12.037  85.196  49.676  1.00  0.00           H
ATOM   4976  HA  GLY   316      13.713  87.633  50.149  1.00  0.00           H
ATOM   4977  HA  GLY   316      12.662  87.573  48.754  1.00  0.00           H
ATOM   5355  N   GLY   341      13.255  90.602  49.161  1.00  0.00           N
ATOM   5356  CA  GLY   341      12.988  90.957  47.776  1.00  0.00           C
ATOM   5357  C   GLY   341      11.674  91.718  47.691  1.00  0.00           C
ATOM   5358  O   GLY   341      10.724  91.417  48.410  1.00  0.00           O
ATOM   5359  HN  GLY   341      12.450  90.313  49.714  1.00  0.00           H
ATOM   5360  HA  GLY   341      13.789  91.578  47.374  1.00  0.00           H
ATOM   5361  HA  GLY   341      12.898  90.051  47.177  1.00  0.00           H
ATOM   5362  N   LEU   342      11.610  92.667  46.767  1.00  0.00           N
ATOM   5363  CA  LEU   342      10.356  93.205  46.257  1.00  0.00           C
ATOM   5364  C   LEU   342      10.261  92.810  44.784  1.00  0.00           C
ATOM   5365  O   LEU   342      11.272  92.469  44.160  1.00  0.00           O
ATOM   5366  HN  LEU   342      12.423  92.798  46.172  1.00  0.00           H
ATOM   5367  HA  LEU   342       9.506  92.761  46.776  1.00  0.00           H
ATOM   5368  CB  LEU   342      10.313  94.735  46.444  1.00  0.00           C
ATOM   5369  CG  LEU   342      10.464  95.233  47.893  1.00  0.00           C
ATOM   5370  CD1 LEU   342      10.530  96.762  47.901  1.00  0.00           C
ATOM   5371  CD2 LEU   342       9.288  94.796  48.768  1.00  0.00           C
ATOM   5372  HB  LEU   342       9.360  95.098  46.062  1.00  0.00           H
ATOM   5373  HB  LEU   342      11.100  95.179  45.836  1.00  0.00           H
ATOM   5374  HG  LEU   342      11.390  94.853  48.322  1.00  0.00           H
ATOM   5375  HD1 LEU   342      10.627  97.123  48.925  1.00  0.00           H
ATOM   5376  HD1 LEU   342       9.621  97.178  47.464  1.00  0.00           H
ATOM   5377  HD1 LEU   342      11.390  97.099  47.324  1.00  0.00           H
ATOM   5378  HD2 LEU   342       9.386  95.235  49.760  1.00  0.00           H
ATOM   5379  HD2 LEU   342       9.288  93.711  48.872  1.00  0.00           H
ATOM   5380  HD2 LEU   342       8.351  95.119  48.317  1.00  0.00           H
ATOM   5381  N   THR   343       9.079  92.918  44.185  1.00  0.00           N
ATOM   5382  CA  THR   343       8.937  92.705  42.740  1.00  0.00           C
ATOM   5383  C   THR   343       9.932  93.562  41.962  1.00  0.00           C
ATOM   5384  O   THR   343      10.618  93.056  41.068  1.00  0.00           O
ATOM   5385  HN  THR   343       8.271  93.166  44.742  1.00  0.00           H
ATOM   5386  HA  THR   343       9.144  91.658  42.522  1.00  0.00           H
ATOM   5387  CB  THR   343       7.531  93.040  42.260  1.00  0.00           C
ATOM   5388  OG1 THR   343       6.561  92.374  43.034  1.00  0.00           O
ATOM   5389  CG2 THR   343       7.355  92.611  40.806  1.00  0.00           C
ATOM   5390  HB  THR   343       7.387  94.114  42.350  1.00  0.00           H
ATOM   5391  HG1 THR   343       6.022  93.062  43.448  1.00  0.00           H
ATOM   5392  HG2 THR   343       7.542  91.540  40.725  1.00  0.00           H
ATOM   5393  HG2 THR   343       8.061  93.148  40.165  1.00  0.00           H
ATOM   5394  HG2 THR   343       6.340  92.822  40.475  1.00  0.00           H
ATOM   5438  N   SER   347      14.692  89.871  42.334  1.00  0.00           N
ATOM   5439  CA  SER   347      14.859  88.842  43.342  1.00  0.00           C
ATOM   5440  C   SER   347      15.389  89.405  44.650  1.00  0.00           C
ATOM   5441  O   SER   347      15.652  90.602  44.752  1.00  0.00           O
ATOM   5442  HN  SER   347      15.389  90.607  42.316  1.00  0.00           H
ATOM   5443  HA  SER   347      13.874  88.468  43.572  1.00  0.00           H
ATOM   5444  CB  SER   347      15.732  87.703  42.797  1.00  0.00           C
ATOM   5445  OG  SER   347      17.014  88.129  42.390  1.00  0.00           O
ATOM   5446  HB  SER   347      15.224  87.253  41.943  1.00  0.00           H
ATOM   5447  HB  SER   347      15.862  86.947  43.568  1.00  0.00           H
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ATOM   5448  HG  SER   347      17.663  87.855  43.061  1.00  0.00           H
ATOM   5459  N   ILE   349      17.665  90.703  47.554  1.00  0.00           N
ATOM   5460  CA  ILE   349      18.942  91.449  47.573  1.00  0.00           C
ATOM   5461  C   ILE   349      19.605  91.525  48.955  1.00  0.00           C
ATOM   5462  O   ILE   349      20.742  91.985  49.108  1.00  0.00           O
ATOM   5463  HN  ILE   349      16.857  91.085  48.040  1.00  0.00           H
ATOM   5464  HA  ILE   349      19.625  90.866  46.976  1.00  0.00           H
ATOM   5465  CB  ILE   349      18.851  92.834  46.883  1.00  0.00           C
ATOM   5466  CG1 ILE   349      18.383  94.013  47.758  1.00  0.00           C
ATOM   5467  CG2 ILE   349      18.019  92.770  45.597  1.00  0.00           C
ATOM   5468  CD  ILE   349      17.015  93.845  48.422  1.00  0.00           C
ATOM   5469  HB  ILE   349      19.867  93.085  46.575  1.00  0.00           H
ATOM   5470  HG1 ILE   349      18.352  94.908  47.136  1.00  0.00           H
ATOM   5471  HG1 ILE   349      19.123  94.191  48.539  1.00  0.00           H
ATOM   5472  HG2 ILE   349      18.091  93.708  45.051  1.00  0.00           H
ATOM   5473  HG2 ILE   349      16.972  92.580  45.825  1.00  0.00           H
ATOM   5474  HG2 ILE   349      18.386  91.962  44.977  1.00  0.00           H
ATOM   5475  HD  ILE   349      16.736  94.773  48.919  1.00  0.00           H
ATOM   5476  HD  ILE   349      17.065  93.058  49.171  1.00  0.00           H
ATOM   5477  HD  ILE   349      16.249  93.605  47.686  1.00  0.00           H
HETATM 9568  C2D OLU     1      10.698  87.907  46.189  1.00  0.00           C
HETATM 9569  C2N OLU     1       9.650  88.632  46.800  1.00  0.00           C
HETATM 9570  N3N OLU     1       8.964  89.526  46.131  1.00  0.00           N
HETATM 9571  S1N OLU     1       9.227  88.363  48.475  1.00  0.00           S
HETATM 9572  C5N OLU     1       8.086  89.768  48.382  1.00  0.00           C
HETATM 9573  C4N OLU     1       8.081  90.210  46.918  1.00  0.00           C
HETATM 9574  O4N OLU     1       7.370  91.094  46.519  1.00  0.00           O
HETATM 9575  H5N OLU     1       8.461  90.579  48.987  1.00  0.00           H
HETATM 9576  H5N OLU     1       7.089  89.492  48.697  1.00  0.00           H
HETATM 9577  N1D OLU     1      11.503  87.061  46.830  1.00  0.00           N
HETATM 9578  C9D OLU     1      12.337  86.466  45.964  1.00  0.00           C
HETATM 9579  S3D OLU     1      11.004  88.118  44.468  1.00  0.00           S
HETATM 9580  C4D OLU     1      12.189  86.824  44.591  1.00  0.00           C
HETATM 9581  C5D OLU     1      12.893  86.220  43.594  1.00  0.00           C
HETATM 9582  C6D OLU     1      13.914  85.241  43.914  1.00  0.00           C
HETATM 9583  O6D OLU     1      14.626  84.733  43.032  1.00  0.00           O
HETATM 9584  C8D OLU     1      13.341  85.511  46.300  1.00  0.00           C
HETATM 9585  C7D OLU     1      14.102  84.947  45.325  1.00  0.00           C
HETATM 9586  H5D OLU     1      12.746  86.468  42.560  1.00  0.00           H
HETATM 9587  H8D OLU     1      13.470  85.246  47.331  1.00  0.00           H
HETATM 9588  H7D OLU     1      14.854  84.219  45.579  1.00  0.00           H
HETATM 9589  P   AMP     2       1.858  88.455  45.784  1.00  0.00           P
HETATM 9590  OP  AMP     2       0.925  88.355  44.655  1.00  0.00           O
HETATM 9591  OP  AMP     2       2.500  87.182  46.140  1.00  0.00           O
HETATM 9592  OP  AMP     2       2.761  89.610  45.746  1.00  0.00           O
HETATM 9593  O5* AMP     2       0.933  88.739  47.020  1.00  0.00           O
HETATM 9594  C5* AMP     2       0.028  89.832  47.046  1.00  0.00           C
HETATM 9595  C4* AMP     2      -0.898  89.745  48.271  1.00  0.00           C
HETATM 9596  O4* AMP     2      -1.530  88.464  48.263  1.00  0.00           O
HETATM 9597  C3* AMP     2      -0.162  89.902  49.613  1.00  0.00           C
HETATM 9598  O2* AMP     2      -1.016  90.452  50.621  1.00  0.00           O
HETATM 9599  C2* AMP     2       0.151  88.444  49.957  1.00  0.00           C
HETATM 9600  O2* AMP     2       0.271  88.260  51.356  1.00  0.00           O
HETATM 9601  C1* AMP     2      -1.078  87.726  49.392  1.00  0.00           C
HETATM 9602  N9  AMP     2      -0.807  86.314  49.034  1.00  0.00           N
HETATM 9603  C8  AMP     2       0.243  85.780  48.327  1.00  0.00           C
HETATM 9604  N7  AMP     2       0.214  84.473  48.198  1.00  0.00           N
HETATM 9605  C5  AMP     2      -0.969  84.128  48.886  1.00  0.00           C
HETATM 9606  C6  AMP     2      -1.665  82.923  49.176  1.00  0.00           C
HETATM 9607  N6  AMP     2      -1.333  81.712  48.783  1.00  0.00           N
HETATM 9608  N1  AMP     2      -2.781  82.917  49.905  1.00  0.00           N
HETATM 9609  C2  AMP     2      -3.265  84.084  50.304  1.00  0.00           C
HETATM 9610  N3  AMP     2      -2.728  85.282  50.135  1.00  0.00           N
HETATM 9611  C4  AMP     2      -1.579  85.242  49.402  1.00  0.00           C
HETATM 9612  H5* AMP     2      -0.590  89.814  46.147  1.00  0.00           H
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HETATM 9613  H5* AMP     2       0.581  90.772  47.067  1.00  0.00           H
HETATM 9614  H4* AMP     2      -1.653  90.527  48.185  1.00  0.00           H
HETATM 9615  H3* AMP     2       0.753  90.490  49.515  1.00  0.00           H
HETATM 9616  HO* AMP     2      -0.917  91.422  50.664  1.00  0.00           H
HETATM 9617  H2* AMP     2       1.059  88.133  49.438  1.00  0.00           H
HETATM 9618  HO* AMP     2      -0.261  88.973  51.740  1.00  0.00           H
HETATM 9619  H1* AMP     2      -1.862  87.752  50.153  1.00  0.00           H
HETATM 9620  H8  AMP     2       1.018  86.411  47.911  1.00  0.00           H
HETATM 9621  H61 AMP     2      -0.633  81.605  48.059  1.00  0.00           H
HETATM 9622  H62 AMP     2      -2.003  80.996  48.997  1.00  0.00           H
HETATM 9623  H2  AMP     2      -4.181  84.052  50.877  1.00  0.00           H

HEADER   OXYLUCIFERIN-AMP-LUCIFERASE COMPLEX WORKING MODEL A-b
REMARK
ATOM   3105  N   SER   198       3.286  93.907  40.803  1.00  0.00           N
ATOM   3106  CA  SER   198       3.560  94.390  42.171  1.00  0.00           C
ATOM   3107  C   SER   198       2.474  95.379  42.597  1.00  0.00           C
ATOM   3108  O   SER   198       1.751  95.867  41.735  1.00  0.00           O
ATOM   3109  HN  SER   198       2.908  94.602  40.167  1.00  0.00           H
ATOM   3110  HA  SER   198       3.577  93.550  42.869  1.00  0.00           H
ATOM   3111  CB  SER   198       4.903  95.116  42.225  1.00  0.00           C
ATOM   3112  OG  SER   198       5.333  95.185  43.568  1.00  0.00           O
ATOM   3113  HB  SER   198       4.804  96.122  41.814  1.00  0.00           H
ATOM   3114  HB  SER   198       5.629  94.572  41.628  1.00  0.00           H
ATOM   3115  HG  SER   198       6.237  95.586  43.584  1.00  0.00           H
ATOM   3380  N   ARG   218      20.810  87.547  38.562  1.00  0.00           N
ATOM   3381  CA  ARG   218      20.188  86.491  39.355  1.00  0.00           C
ATOM   3382  C   ARG   218      20.860  85.135  39.116  1.00  0.00           C
ATOM   3383  O   ARG   218      21.035  84.344  40.068  1.00  0.00           O
ATOM   3384  HN  ARG   218      20.226  88.102  37.943  1.00  0.00           H
ATOM   3385  HA  ARG   218      20.329  86.716  40.412  1.00  0.00           H
ATOM   3386  CB  ARG   218      18.658  86.439  39.070  1.00  0.00           C
ATOM   3387  CG  ARG   218      17.935  85.145  39.506  1.00  0.00           C
ATOM   3388  CD  ARG   218      17.752  85.039  41.026  1.00  0.00           C
ATOM   3389  NE  ARG   218      17.552  83.646  41.479  1.00  0.00           N
ATOM   3390  CZ  ARG   218      17.575  83.265  42.743  1.00  0.00           C
ATOM   3391  NH1 ARG   218      17.363  84.114  43.698  1.00  0.00           N
ATOM   3392  NH2 ARG   218      17.783  82.031  43.082  1.00  0.00           N
ATOM   3393  HB  ARG   218      18.475  86.550  38.012  1.00  0.00           H
ATOM   3394  HB  ARG   218      18.181  87.293  39.555  1.00  0.00           H
ATOM   3395  HG  ARG   218      18.468  84.271  39.134  1.00  0.00           H
ATOM   3396  HG  ARG   218      16.958  85.126  39.030  1.00  0.00           H
ATOM   3397  HD  ARG   218      16.900  85.651  41.323  1.00  0.00           H
ATOM   3398  HD  ARG   218      18.643  85.432  41.518  1.00  0.00           H
ATOM   3399  HE  ARG   218      17.424  82.924  40.785  1.00  0.00           H
ATOM   3400  HH  ARG   218      16.633  84.772  43.457  1.00  0.00           H
ATOM   3401  HH  ARG   218      17.375  83.761  44.649  1.00  0.00           H
ATOM   3402  HH  ARG   218      17.813  81.281  42.397  1.00  0.00           H
ATOM   3403  HH  ARG   218      17.837  81.761  44.058  1.00  0.00           H
ATOM   3811  N   HIS   245       5.088  84.789  40.113  1.00  0.00           N
ATOM   3812  CA  HIS   245       5.563  85.845  41.030  1.00  0.00           C
ATOM   3813  C   HIS   245       7.082  85.717  41.195  1.00  0.00           C
ATOM   3814  O   HIS   245       7.625  84.659  40.892  1.00  0.00           O
ATOM   3815  HN  HIS   245       5.214  83.831  40.417  1.00  0.00           H
ATOM   3816  HA  HIS   245       5.366  86.836  40.614  1.00  0.00           H
ATOM   3817  CB  HIS   245       4.780  85.728  42.348  1.00  0.00           C
ATOM   3818  CG  HIS   245       5.335  86.536  43.492  1.00  0.00           C
ATOM   3819  ND1 HIS   245       6.017  86.031  44.583  1.00  0.00           N
ATOM   3820  CD2 HIS   245       5.161  87.874  43.695  1.00  0.00           C
ATOM   3821  CE1 HIS   245       6.237  87.042  45.445  1.00  0.00           C
ATOM   3822  NE2 HIS   245       5.742  88.174  44.910  1.00  0.00           N
ATOM   3823  HB  HIS   245       4.740  84.685  42.657  1.00  0.00           H
ATOM   3824  HB  HIS   245       3.754  86.051  42.169  1.00  0.00           H
ATOM   3825  HD1 HIS   245       6.136  85.038  44.788  1.00  0.00           H
ATOM   3826  HD2 HIS   245       4.587  88.554  43.078  1.00  0.00           H
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ATOM   3827  HE1 HIS   245       6.629  86.950  46.454  1.00  0.00           H
ATOM   3828  HE2 HIS   245       5.698  89.082  45.382  1.00  0.00           H
ATOM   4953  N   SER   314      12.193  80.996  52.520  1.00  0.00           N
ATOM   4954  CA  SER   314      11.220  82.119  52.177  1.00  0.00           C
ATOM   4955  C   SER   314      11.813  83.058  51.127  1.00  0.00           C
ATOM   4956  O   SER   314      11.073  83.782  50.456  1.00  0.00           O
ATOM   4957  HN  SER   314      12.952  81.218  53.159  1.00  0.00           H
ATOM   4958  HA  SER   314      10.316  81.680  51.757  1.00  0.00           H
ATOM   4959  CB  SER   314      10.830  82.914  53.395  1.00  0.00           C
ATOM   4960  OG  SER   314      11.880  83.758  53.845  1.00  0.00           O
ATOM   4961  HB  SER   314      10.556  82.237  54.199  1.00  0.00           H
ATOM   4962  HB  SER   314       9.963  83.530  53.150  1.00  0.00           H
ATOM   4963  HG  SER   314      11.484  84.649  53.951  1.00  0.00           H
ATOM   4964  N   GLY   315      13.143  83.016  50.964  1.00  0.00           N
ATOM   4965  CA  GLY   315      13.931  83.600  49.877  1.00  0.00           C
ATOM   4966  C   GLY   315      14.058  85.121  49.897  1.00  0.00           C
ATOM   4967  O   GLY   315      15.171  85.632  49.884  1.00  0.00           O
ATOM   4968  HN  GLY   315      13.649  82.444  51.627  1.00  0.00           H
ATOM   4969  HA  GLY   315      14.935  83.175  49.901  1.00  0.00           H
ATOM   4970  HA  GLY   315      13.471  83.327  48.931  1.00  0.00           H
ATOM   4971  N   GLY   316      12.934  85.837  49.916  1.00  0.00           N
ATOM   4972  CA  GLY   316      12.857  87.302  49.816  1.00  0.00           C
ATOM   4973  C   GLY   316      11.655  87.932  50.526  1.00  0.00           C
ATOM   4974  O   GLY   316      11.585  89.156  50.631  1.00  0.00           O
ATOM   4975  HN  GLY   316      12.069  85.309  49.897  1.00  0.00           H
ATOM   4976  HA  GLY   316      13.761  87.740  50.227  1.00  0.00           H
ATOM   4977  HA  GLY   316      12.807  87.587  48.769  1.00  0.00           H
ATOM   5355  N   GLY   341      13.360  91.250  49.321  1.00  0.00           N
ATOM   5356  CA  GLY   341      13.275  91.870  48.015  1.00  0.00           C
ATOM   5357  C   GLY   341      11.875  92.430  47.821  1.00  0.00           C
ATOM   5358  O   GLY   341      11.023  92.337  48.701  1.00  0.00           O
ATOM   5359  HN  GLY   341      12.480  91.128  49.814  1.00  0.00           H
ATOM   5360  HA  GLY   341      13.994  92.685  47.934  1.00  0.00           H
ATOM   5361  HA  GLY   341      13.474  91.134  47.236  1.00  0.00           H
ATOM   5362  N   LEU   342      11.639  92.976  46.641  1.00  0.00           N
ATOM   5363  CA  LEU   342      10.309  93.277  46.135  1.00  0.00           C
ATOM   5364  C   LEU   342      10.239  92.703  44.724  1.00  0.00           C
ATOM   5365  O   LEU   342      11.267  92.369  44.124  1.00  0.00           O
ATOM   5366  HN  LEU   342      12.392  92.973  45.959  1.00  0.00           H
ATOM   5367  HA  LEU   342       9.547  92.786  46.746  1.00  0.00           H
ATOM   5368  CB  LEU   342      10.035  94.797  46.123  1.00  0.00           C
ATOM   5369  CG  LEU   342      10.089  95.502  47.494  1.00  0.00           C
ATOM   5370  CD1 LEU   342      11.493  96.021  47.819  1.00  0.00           C
ATOM   5371  CD2 LEU   342       9.162  96.719  47.497  1.00  0.00           C
ATOM   5372  HB  LEU   342       9.031  94.935  45.718  1.00  0.00           H
ATOM   5373  HB  LEU   342      10.728  95.288  45.440  1.00  0.00           H
ATOM   5374  HG  LEU   342       9.764  94.817  48.276  1.00  0.00           H
ATOM   5375  HD1 LEU   342      11.468  96.462  48.811  1.00  0.00           H
ATOM   5376  HD1 LEU   342      11.798  96.772  47.092  1.00  0.00           H
ATOM   5377  HD1 LEU   342      12.213  95.208  47.835  1.00  0.00           H
ATOM   5378  HD2 LEU   342       9.207  97.216  48.468  1.00  0.00           H
ATOM   5379  HD2 LEU   342       8.134  96.395  47.333  1.00  0.00           H
ATOM   5380  HD2 LEU   342       9.447  97.421  46.714  1.00  0.00           H
ATOM   5381  N   THR   343       9.051  92.687  44.133  1.00  0.00           N
ATOM   5382  CA  THR   343       8.941  92.490  42.686  1.00  0.00           C
ATOM   5383  C   THR   343       9.866  93.452  41.911  1.00  0.00           C
ATOM   5384  O   THR   343      10.543  92.989  40.996  1.00  0.00           O
ATOM   5385  HN  THR   343       8.229  92.962  44.654  1.00  0.00           H
ATOM   5386  HA  THR   343       9.273  91.478  42.459  1.00  0.00           H
ATOM   5387  CB  THR   343       7.474  92.600  42.274  1.00  0.00           C
ATOM   5388  OG1 THR   343       6.756  91.519  42.823  1.00  0.00           O
ATOM   5389  CG2 THR   343       7.313  92.446  40.776  1.00  0.00           C
ATOM   5390  HB  THR   343       7.070  93.544  42.620  1.00  0.00           H
ATOM   5391  HG1 THR   343       6.002  91.855  43.359  1.00  0.00           H
ATOM   5392  HG2 THR   343       7.740  91.487  40.485  1.00  0.00           H
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ATOM   5393  HG2 THR   343       7.838  93.241  40.261  1.00  0.00           H
ATOM   5394  HG2 THR   343       6.260  92.487  40.507  1.00  0.00           H
ATOM   5438  N   SER   347      14.670  89.912  42.404  1.00  0.00           N
ATOM   5439  CA  SER   347      14.849  88.876  43.401  1.00  0.00           C
ATOM   5440  C   SER   347      15.379  89.441  44.706  1.00  0.00           C
ATOM   5441  O   SER   347      15.665  90.636  44.808  1.00  0.00           O
ATOM   5442  HN  SER   347      15.334  90.679  42.419  1.00  0.00           H
ATOM   5443  HA  SER   347      13.870  88.483  43.630  1.00  0.00           H
ATOM   5444  CB  SER   347      15.737  87.747  42.853  1.00  0.00           C
ATOM   5445  OG  SER   347      17.023  88.168  42.460  1.00  0.00           O
ATOM   5446  HB  SER   347      15.239  87.298  41.992  1.00  0.00           H
ATOM   5447  HB  SER   347      15.865  86.989  43.622  1.00  0.00           H
ATOM   5448  HG  SER   347      17.669  87.865  43.123  1.00  0.00           H
ATOM   5459  N   ILE   349      17.665  90.703  47.554  1.00  0.00           N
ATOM   5460  CA  ILE   349      18.942  91.449  47.573  1.00  0.00           C
ATOM   5461  C   ILE   349      19.605  91.525  48.955  1.00  0.00           C
ATOM   5462  O   ILE   349      20.742  91.985  49.108  1.00  0.00           O
ATOM   5463  HN  ILE   349      16.887  91.069  48.096  1.00  0.00           H
ATOM   5464  HA  ILE   349      19.623  90.863  46.978  1.00  0.00           H
ATOM   5465  CB  ILE   349      18.851  92.834  46.883  1.00  0.00           C
ATOM   5466  CG1 ILE   349      18.383  94.013  47.758  1.00  0.00           C
ATOM   5467  CG2 ILE   349      18.019  92.770  45.597  1.00  0.00           C
ATOM   5468  CD  ILE   349      17.015  93.845  48.422  1.00  0.00           C
ATOM   5469  HB  ILE   349      19.867  93.085  46.575  1.00  0.00           H
ATOM   5470  HG1 ILE   349      18.352  94.908  47.135  1.00  0.00           H
ATOM   5471  HG1 ILE   349      19.123  94.193  48.538  1.00  0.00           H
ATOM   5472  HG2 ILE   349      18.099  93.704  45.046  1.00  0.00           H
ATOM   5473  HG2 ILE   349      16.971  92.591  45.826  1.00  0.00           H
ATOM   5474  HG2 ILE   349      18.379  91.956  44.981  1.00  0.00           H
ATOM   5475  HD  ILE   349      16.720  94.781  48.893  1.00  0.00           H
ATOM   5476  HD  ILE   349      17.072  93.080  49.192  1.00  0.00           H
ATOM   5477  HD  ILE   349      16.254  93.577  47.692  1.00  0.00           H
HETATM 9568  C2* OLU     1      10.710  87.969  46.174  1.00  0.00           C
HETATM 9569  C2  OLU     1       9.574  88.601  46.736  1.00  0.00           C
HETATM 9570  N3  OLU     1       8.799  89.383  46.012  1.00  0.00           N
HETATM 9571  S1  OLU     1       9.093  88.294  48.389  1.00  0.00           S
HETATM 9572  C5  OLU     1       7.704  89.430  48.160  1.00  0.00           C
HETATM 9573  C4  OLU     1       7.725  89.851  46.696  1.00  0.00           C
HETATM 9574  O4  OLU     1       6.839  90.521  46.211  1.00  0.00           O
HETATM 9575  H5  OLU     1       7.852  90.309  48.764  1.00  0.00           H
HETATM 9576  H5  OLU     1       6.746  88.988  48.410  1.00  0.00           H
HETATM 9577  N1* OLU     1      11.551  87.191  46.847  1.00  0.00           N
HETATM 9578  C9* OLU     1      12.389  86.568  45.998  1.00  0.00           C
HETATM 9579  S3* OLU     1      10.989  88.104  44.446  1.00  0.00           S
HETATM 9580  C4* OLU     1      12.207  86.853  44.617  1.00  0.00           C
HETATM 9581  C5* OLU     1      12.912  86.234  43.629  1.00  0.00           C
HETATM 9582  C6* OLU     1      13.968  85.299  43.974  1.00  0.00           C
HETATM 9583  O6* OLU     1      14.675  84.782  43.097  1.00  0.00           O
HETATM 9584  C8* OLU     1      13.422  85.655  46.353  1.00  0.00           C
HETATM 9585  C7* OLU     1      14.189  85.067  45.392  1.00  0.00           C
HETATM 9586  H5* OLU     1      12.743  86.444  42.591  1.00  0.00           H
HETATM 9587  H8* OLU     1      13.576  85.429  47.391  1.00  0.00           H
HETATM 9588  H7* OLU     1      14.957  84.368  45.666  1.00  0.00           H
HETATM 9589  P   AMP     2       2.152  89.105  45.287  1.00  0.00           P
HETATM 9590  OP  AMP     2       0.705  88.879  45.239  1.00  0.00           O
HETATM 9591  OP  AMP     2       2.912  87.938  45.733  1.00  0.00           O
HETATM 9592  OP  AMP     2       2.705  89.803  44.127  1.00  0.00           O
HETATM 9593  O5* AMP     2       2.390  90.169  46.411  1.00  0.00           O
HETATM 9594  C5* AMP     2       1.642  90.198  47.609  1.00  0.00           C
HETATM 9595  C4* AMP     2       2.089  91.409  48.432  1.00  0.00           C
HETATM 9596  O4* AMP     2       3.423  91.242  48.893  1.00  0.00           O
HETATM 9597  C3* AMP     2       2.054  92.724  47.631  1.00  0.00           C
HETATM 9598  O2* AMP     2       1.090  93.619  48.172  1.00  0.00           O
HETATM 9599  C2* AMP     2       3.477  93.273  47.798  1.00  0.00           C
HETATM 9600  O2* AMP     2       3.512  94.688  47.928  1.00  0.00           O
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HETATM 9601  C1* AMP     2       3.937  92.551  49.063  1.00  0.00           C
HETATM 9602  N9  AMP     2       5.402  92.576  49.295  1.00  0.00           N
HETATM 9603  C8  AMP     2       6.354  93.366  48.692  1.00  0.00           C
HETATM 9604  N7  AMP     2       7.569  93.178  49.133  1.00  0.00           N
HETATM 9605  C5  AMP     2       7.398  92.224  50.147  1.00  0.00           C
HETATM 9606  C6  AMP     2       8.271  91.513  51.010  1.00  0.00           C
HETATM 9607  N6  AMP     2       9.584  91.586  50.985  1.00  0.00           N
HETATM 9608  N1  AMP     2       7.814  90.599  51.867  1.00  0.00           N
HETATM 9609  C2  AMP     2       6.508  90.386  51.886  1.00  0.00           C
HETATM 9610  N3  AMP     2       5.571  90.950  51.138  1.00  0.00           N
HETATM 9611  C4  AMP     2       6.081  91.865  50.264  1.00  0.00           C
HETATM 9612  H5* AMP     2       1.801  89.282  48.177  1.00  0.00           H
HETATM 9613  H5* AMP     2       0.581  90.301  47.375  1.00  0.00           H
HETATM 9614  H4* AMP     2       1.432  91.511  49.297  1.00  0.00           H
HETATM 9615  H3* AMP     2       1.854  92.544  46.575  1.00  0.00           H
HETATM 9616  HO* AMP     2       0.571  93.943  47.414  1.00  0.00           H
HETATM 9617  H2* AMP     2       4.083  92.942  46.951  1.00  0.00           H
HETATM 9618  HO* AMP     2       2.660  94.959  48.303  1.00  0.00           H
HETATM 9619  H1* AMP     2       3.449  93.014  49.915  1.00  0.00           H
HETATM 9620  H8  AMP     2       6.117  94.070  47.904  1.00  0.00           H
HETATM 9621  H61 AMP     2      10.007  92.133  50.239  1.00  0.00           H
HETATM 9622  H62 AMP     2      10.096  90.863  51.453  1.00  0.00           H
HETATM 9623  H2  AMP     2       6.162  89.645  52.593  1.00  0.00           H
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