

Supporting Information for

Cofactor-free ActVA-Orf6 monooxygenase catalysis via proton-coupled electron transfer: A QM/MM study

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1. Computational details

The experimental investigations on the steady-state kinetic properties indicated that the oxidation of phenols to quinones catalyzed ActVA-Orf6 monooxygenase was performed at 303.15 K (30 °C) and gives the reaction rate constant value of $k_{\text{cat}} = 4.17 * 10^{-2} \text{ s}^{-1}$. The reaction rate constant can be used to estimate the free energy barrier (ΔG^\ddagger) of the whole enzymic oxygenation reaction, whose value was calculated based on the classical transition state theory with the following equation:

$$k_{\text{cat}} = \nu \exp(-\Delta G^\ddagger / RT) \quad (1)$$

where ν is the frequency factor and computes by the equation of $\nu = k_B T / h$, in which k_B is the Boltzmann constant, h is the Planck constant, and T is the temperature. In equation (1), the free energy barrier (ΔG^\ddagger) refers to the free energy barrier of the whole catalytic reaction. On the basis of equation (1), the free energy barrier is computed as follows:

$$\Delta G^\ddagger = -RT \ln\left(\frac{k_{\text{cat}}}{\nu}\right) \quad (2)$$

According to the relationship of the free energy barrier (ΔG^\ddagger) with its experimental reaction rate constant $k_{\text{cat}} = 4.17 * 10^{-2} \text{ s}^{-1}$ in equation (2), the estimated free energy barrier is equal to 19.7 kcal/mol. The value of our calculated energy barrier of 20.7 kcal/mol is very close to the energy barrier (19.7 kcal/mol) estimated by experiments, thus indicating that our calculation results are reasonable and reliable.

2. MD/QM/MM simulation results

2.1 Hydrogen-bonding interactions between the substrate and residues

From **Figure 2**, we know that the dominant electrostatic interactions of the sidechains of residues Asn62, Trp66, and Arg86 are existing during the MD simulations. To figure out whether the dominant electrostatic interactions are hydrogen-bonding interactions, the distances of the possible hydrogen bonds were tracked over the entire MD simulations. It can be seen from **Figs. S1-2** that the hydrogen bond of Trp66@N ϵ -H ϵ ...O8@DDHK⁻ are always existing over the whole MD simulations; while the two hydrogen bonds of Arg86@N ϵ -H ϵ ...O15@DDHK⁻ and Arg86@N η -H η ...O16@DDHK⁻ were formed after about 40 ns MD simulation times, and they are stably existing over the following MD equilibrium simulations (about 80 ns), indicating that the substrate can be stabilized by forming hydrogen-bonding interactions with the two residues Trp66 and Arg86. Obviously, the angles for the Trp66@N ϵ -H ϵ ...O8@DDHK⁻, Arg86@N ϵ -H ϵ ...O15@DDHK⁻, and Arg86@N η -H η ...O16@DDHK⁻ are separately floated around 150°, 138°, and 138°, while their corresponding distances are floated around 3.0, 3.5, and 3.5 Å, respectively. All the analyses demonstrated that DDHK⁻ is well anchored at the binding site

of the ActVA-Orf6 enzyme.

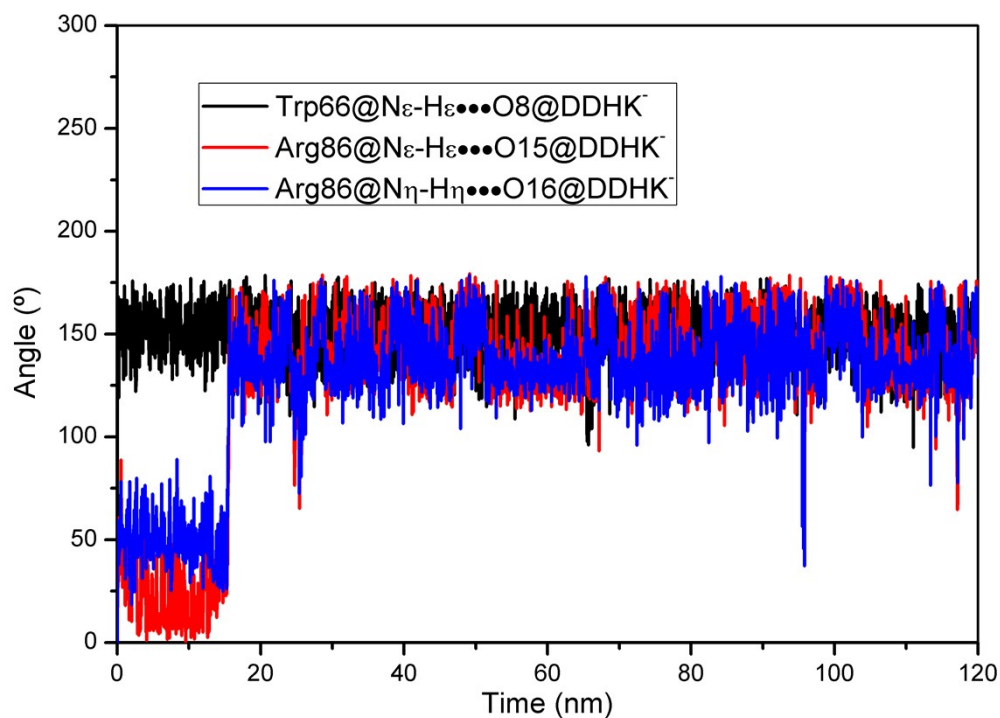


Fig. S1 Angles for the three hydrogen bonds between substrate DDHK^- and residues Trp66 and Arg86 related to the corresponding starting structures for the entire MD simulations (unit: $^\circ$).

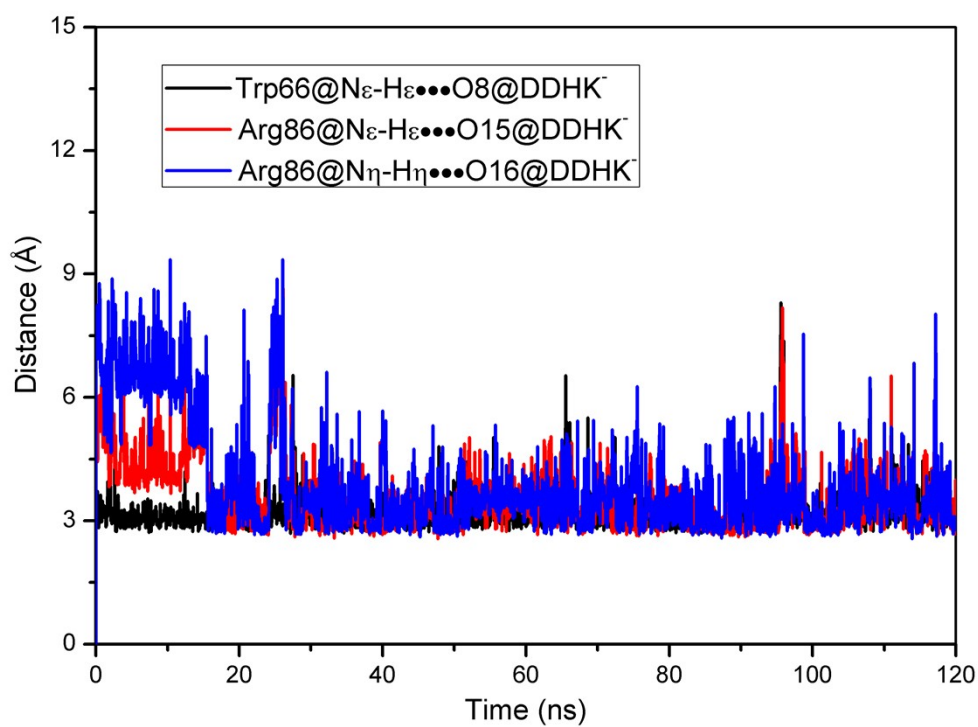
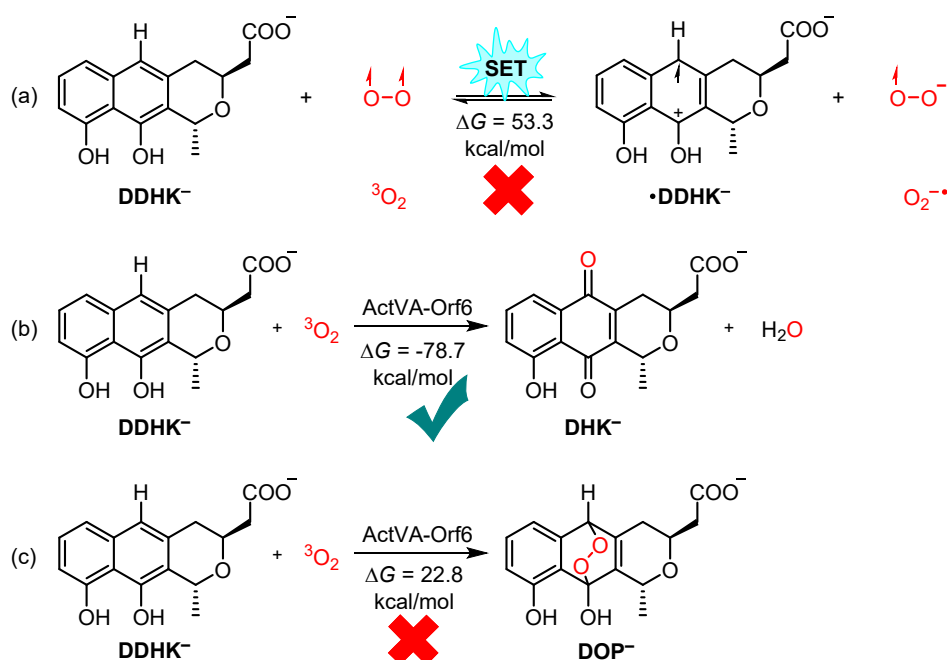


Fig. S2 Distances for the three hydrogen bonds between substrate DDHK^- and residues Trp66 and Arg86 related to the corresponding starting structures for the entire MD simulation (unit: \AA).

2.2 The possible path B associated with SET process

Since the substrate is identified to exist in a negative deprotonated state in the active center of enzyme catalysis, it is likely to occur an intermolecular single electron transfer (SET) process, monooxygenation reaction, or dioxygenation reaction for substrate **DDHK⁻** with triplet O₂. As shown in **Scheme S1**, the relative Gibbs free energy for the SET process, monooxygenation reaction, and dioxygenation reaction are 53.3, -78.7, and 22.8 kcal/mol, respectively, in the QM computational modeling, indicating the endothermic dioxygenation reaction associated with endothermic SET process is impossible to happen under experimental condition. Meanwhile, the relative energy (19.7 kcal/mol, see **Table S2**) of dioxygenation product **¹SP** is extremely higher than that (-103.5 kcal/mol, see **Table S2**) of monooxygenation product **¹EP** in the QM/MM computational modeling, meaning that monooxygenation product **¹EP** is more energetically preferred in both thermodynamics and dynamics. Thereby, the possible **path B** associated with the SET process for the production of dioxygenation product is unnecessary to investigate and calculate in detail for the QM/MM calculations.



Scheme S1. (a) The possible intermolecular single electron transfer process for substrate **DDHK⁻** associated with the related thermodynamic data. ActVA-Orf6 catalyzed oxidation reaction affording (b) monooxygenation product **DHK⁻** rather than (c) deoxygenation product **DOP⁻**. All the above structures are computed at the level B3LYP/6-31G(d,p)/CPCM_{water} of theory (energy unit: kcal/mol).

2.3 IRC analyses of all the transition states

To ensure whether the transition states can connect their relevant reactants and products, the intrinsic reaction coordinate (IRC) calculations have been conducted for the energetically favorable **path A** including the proton transfer accompanied by electron transfer (PCET), diradical complexation, and dehydration processes. As suggested by the calculated IRC results in **Figs. S3-5**, the energy differences between all the IRC-TSS/products and IRC-reactants in the scanning diagram of open-shell triplet transition state ${}^3\text{TS1}$, open-shell singlet transition state ${}^{\text{OS}}\text{TS2}$, and closed-shell singlet transition state ${}^1\text{TS3}$ are very close to their corresponding values in energy profiles **Figure 8**. In addition, all the 3D-structures in **Figures 3, 5, 7** revealed that the transition states ${}^3\text{TS1}/{}^{\text{OS}}\text{TS2}/{}^1\text{TS3}$ are indeed connecting their reactants and products, respectively. In other words, the ${}^3\text{ES0}$, ${}^3\text{TS1}$, and ${}^3\text{M1}$ are in the same conformational space, the same conclusion can be obtained in comparisons of the ${}^{\text{OS}}\text{M1}/{}^{\text{OS}}\text{TS2}/{}^1\text{M2}$ and ${}^1\text{TS3}/{}^1\text{EP}$ conformations.

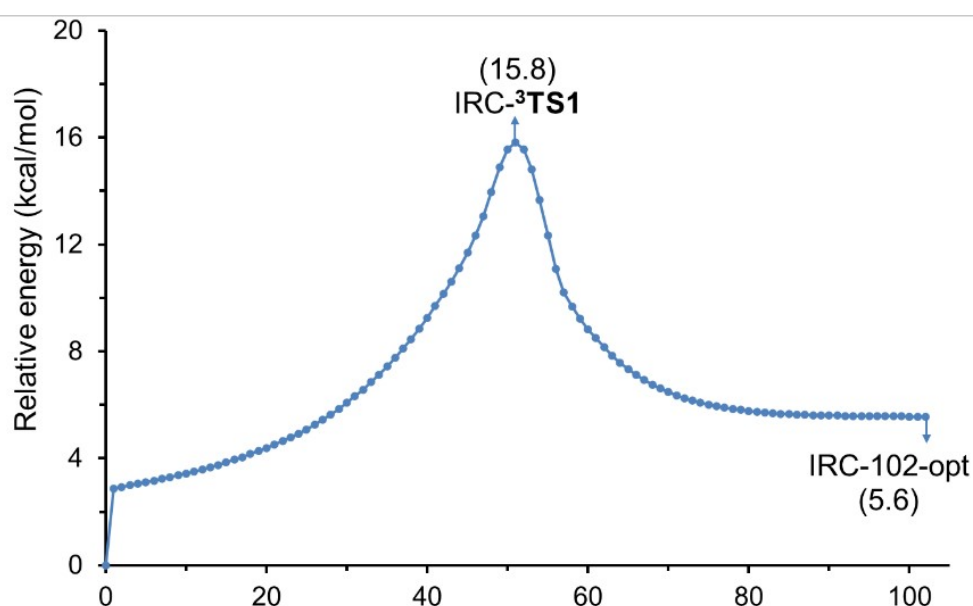


Fig. S3 The IRC results of open-shell triplet transition state ${}^3\text{TS1}$ calculated at the ONIOM[B3LYP/6-31G(d,p):AMBER] theory level (unit: kcal/mol).

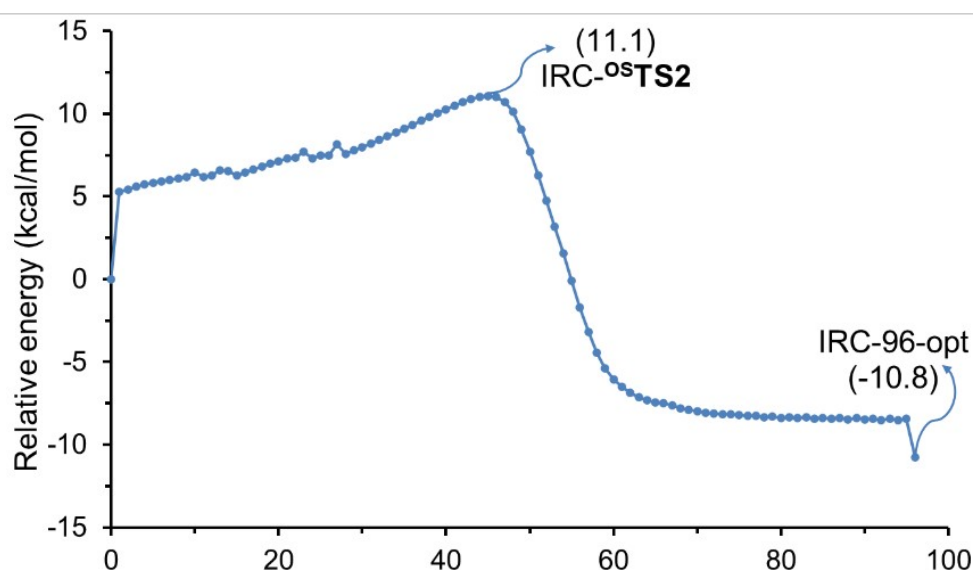


Fig. S4 The IRC results of open-shell singlet transition state ⁰TS2 calculated at the ONIOM[UB3LYP/6-31G(d,p):AMBER] theory level (unit: kcal/mol).

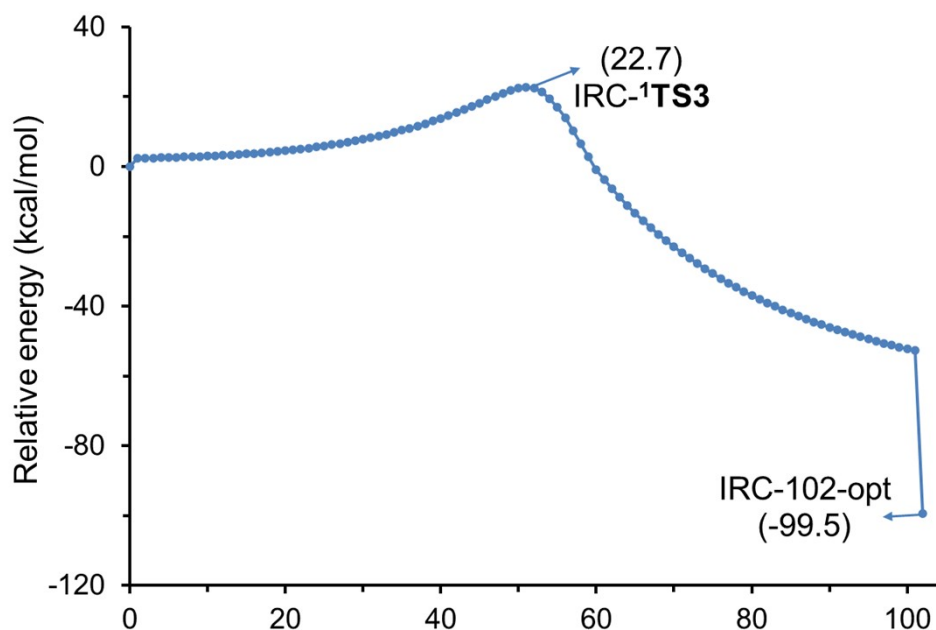


Fig. S5 The IRC results of closed-shell singlet transition state ¹TS3 calculated at the ONIOM[B3LYP/6-31G(d,p):AMBER] theory level (unit: kcal/mol).

2.4 Test results of computational methods

To check whether the aforementioned calculation method (*i.e.*, B3LYP) and level (*i.e.*, L1 level) can obtain reliable results, we additionally performed calculations on the key transition states of the diradical complexation and dehydration steps by using other DFT methods (such as, M06-2X-D3, B3PW91-D3, and B3LYP-D3) at different levels. The calculated results are summarized in **Tables S1-2**. Apparently, the relative energy barriers *via* transition states ⁰TS2/¹TS3 computed at the computational levels of L2~L4/L3~L4 are close to those (10.6/20.7 kcal/mol) computed at the L1 level. Thus, the selected computational method and level should be reliable for the studied system in this work.

Table S1. Comparisons of the relative energies for selected stationary points at different computational levels Ln = L1~L4 (Unit: kcal/mol)

Level	L1	L2	L3	L4
⁰ SM1	0.0	0.0	0.0	0.0
⁰ TS2	10.6	11.8	10.1	10.8

L1: ONIOM[B3LYP-D3/6-311++G(2df,2pd):AMBER]/ONIOM[B3LYP/6-31G(d,p):AMBER];
L2: ONIOM[M06-2X-D3/6-311++G(2df,2pd):AMBER]/ONIOM[B3LYP/6-31G(d,p):AMBER];
L3: ONIOM[B3PW91-D3/6-311++G(2df,2pd):AMBER]/ONIOM[B3LYP/6-31G(d,p):AMBER];
L4: ONIOM[B3LYP-D3/6-311++G(2df,2pd):AMBER]/ONIOM[B3LYP-D3/6-31G(d,p):AMBER].

Table S2. Comparisons of the relative energies for selected stationary points at different computational levels $L_n = L1, L3\sim L4$ (Unit: kcal/mol)

Level	L1	L3	L4
¹M2	0.0	0.0	0.0
¹TS3	20.7	19.2	20.4

L1: ONIOM[B3LYP-D3/6-311++G(2df,2pd):AMBER]//ONIOM[B3LYP/6-31G(d,p):AMBER];
L3: ONIOM[B3PW91-D3/6-311++G(2df,2pd):AMBER]//ONIOM[B3LYP/6-31G(d,p):AMBER];
L4: ONIOM[B3LYP-D3/6-311++G(2df,2pd):AMBER]//ONIOM[B3LYP-D3/6-31G(d,p):AMBER].

Table S3. Comparisons of the relative energy barriers and entropic changes of the three processes calculated at the L1 level of theory (Unit: kcal/mol)

	ΔAE	ΔAG	$-TAS$
³TS1-³ES0	15.5	16.9	2.9
^{0S}TS2-^{0S}M1	10.6	12.5	2.9
¹TS3-¹M2	20.7	21.0	0.6

3 Cartesian coordinates and energy values of optimized structures

3.1 Relative energies of the optimized structures by DFT

Table S4. The single-point energies (SPE), zero-point correction (ZPC), zero-point correction energies (ZPE=SPE+ZPC), and relative energies (ΔE) of the stationary points involved in the enzyme catalytic cycle, which are computed at the ONIOM[(U)B3LYP-D3/6-311++G(2df,2pd):AMBER]//ONIOM[(U)B3LYP/6-31G(d,p):AMBER] theory level.

	SPE (a.u.)	ZPC (a.u.)	ZPE (a.u.)	ΔE (kcal/mol)
³ES0	-2190.8980915	5.5581410	-2185.3399505	0.0
³TS1	-2190.8680115	5.5527580	-2185.3152535	15.5
³M1	-2190.8854007	5.5585000	-2185.3269007	8.2
^{0S}M1	-2190.8853291	5.5584380	-2185.3268911	8.2
^{0S}TS2	-2190.8721544	5.5621820	-2185.3099724	18.8
¹M2	-2190.9036590	5.5630270	-2185.3406320	-0.4
¹TS3	-2190.8627150	5.5551620	-2185.3075530	20.3
¹EP	-2191.0668933	5.5620730	-2185.5048203	-103.5
¹SP	-2190.8980915	5.5645380	-2185.3085265	19.7

Table S5. The single-point energies (SPE), Gibbs free energy correction (GFEC), Gibbs free energies (GFE=SPE+GFEC), entropy parameters (TAS), and relative Gibbs free energies ($\Delta\Delta G$) of the stationary points involved in the enzyme catalytic cycle, which are computed at the ONIOM[(U)B3LYP-D3/6-311++G(2df,2pd):AMBER]//ONIOM[(U)B3LYP/6-31G(d,p):AMBER] theory level.

SPE (a.u.)	GFEC (a.u.)	GFE (a.u.)	TAS (kcal/mol)	$\Delta\Delta G$ (kcal/mol)
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³ ES0	-2190.8980915	5.2012090	-2185.6968825	433.6347267	0.0
³ TS1	-2190.8680115	5.1981830	-2185.6698285	430.7131549	16.9
⁰ S ^M 1	-2190.8853291	5.2028480	-2185.6824811	432.0870301	0.0
⁰ S ^{TS} 2	-2190.8721544	5.2095510	-2185.6626034	429.1991492	12.5
¹ M2	-2190.9036590	5.2107590	-2185.6929000	429.3544853	0.0
¹ TS3	-2190.8627150	5.2033730	-2185.6593420	428.7587816	21.0

Table S6. The single-point energies (SPE), Gibbs free energy correction (GFEC), and relative Gibbs free energies (GFE=SPE+GFEC) of the stationary points involved in the QM modeling, which are computed at the B3LYP/6-31G(d,p)/CPCM_{water} level of theory.

	SPE (a.u.)	GFEC (a.u.)	GFE (a.u.)
DDHK⁻	-995.0368612	0.2370220	-994.7998392
³ O ₂	-150.3201360	-0.0161990	-150.3363350
•DDHK⁻	-994.8520540	0.2358870	-994.6161670
O ₂ ^{•-}	-150.4180477	-0.0170100	-150.4350577
DHK⁻	-1069.0549503	0.2170740	-1068.8378763
H₂O	-76.4267734	0.0029970	-76.4237764
DOP⁻	-1145.3431769	0.2434080	-1145.0997689

Table S7. The single-point energies (SPE), zero-point correction energies (ZPE=SPE+ZPC), and relative energies (ΔE) of the stationary points involved in the QM/MM calculations, which are computed at different computational levels (L1~L4).

Level	SPE (a.u.)	ZPC (a.u.)	ZPE (a.u.)	ΔE (kcal/mol)
Level L1				
⁰ S ^M 1	-2190.8853291	5.5584380	-2185.3268911	0.0
⁰ S ^{TS} 2	-2190.8721544	5.5621820	-2185.3099724	10.6
Level L2				
⁰ S ^M 1	-2189.8879856	5.5584380	-2184.3295476	0.0
⁰ S ^{TS} 2	-2189.8729116	5.5621820	-2184.3107296	11.8
Level L3				
⁰ S ^M 1	-2190.0361075	5.5584380	-2184.4776695	0.0
⁰ S ^{TS} 2	-2190.0238166	5.5621820	-2184.4616346	10.1
Level L4				
⁰ S ^M 1	-2190.8852594	5.5595390	-2185.3257204	0.0
⁰ S ^{TS} 2	-2190.8720020	5.5635190	-2185.3084830	10.8
Level L3				
¹ M2	-2190.0585758	5.5630270	-2184.4955488	0.0
¹ TS3	-2190.0201235	5.5551620	-2184.4649615	19.2
Level L4				
¹ M2	-2190.9035127	5.5643620	-2185.3391507	0.0
¹ TS3	-2190.8630263	5.5563010	-2185.3067253	20.4

3.2 The Cartesian coordinates of QM- and QM/MM-optimized stationary points

DDHK⁻

-1 1

C	-2.93317300	-2.50762400	0.04210600
H	-2.54092200	-3.52006600	0.03015900
C	-4.28596300	-2.27381400	0.14777700
H	-4.97922500	-3.10653300	0.22414000
C	-4.79280500	-0.95824700	0.15212000
H	-5.85916600	-0.77145500	0.22585200
C	-3.94125000	0.12906700	0.05587000
O	-4.50754800	1.36614900	0.05484800
H	-3.79256400	2.02537900	-0.03212500
C	-2.52144400	-0.07309300	-0.03950600
C	-1.56390100	0.98078900	-0.12558000
O	-2.06702600	2.27421900	-0.05390300
H	-1.53055000	2.88695100	-0.57658600
C	-2.02445300	-1.42010900	-0.05873500
C	-0.62939800	-1.63355400	-0.19502600
H	-0.26471600	-2.65729300	-0.22768500
C	0.26704900	-0.59125000	-0.29733900
C	1.74273700	-0.85367600	-0.50430700
H	2.06288200	-1.73834300	0.05164000
H	1.92458300	-1.05478700	-1.57024900
C	-0.20184100	0.75251400	-0.23211700
C	0.78828000	1.91576700	-0.25305900
C	0.88177800	2.63619100	1.10471400
H	1.59399800	3.46303800	1.03086000
H	1.21511800	1.95500800	1.89200500
H	-0.09086100	3.03847600	1.39970100
H	0.46250200	2.65336000	-1.00227900
O	2.07666400	1.52210300	-0.71885800
C	2.60320100	0.33471400	-0.08754200
H	2.56079500	0.44242900	1.00337400
C	4.06194300	0.20615800	-0.49694900
H	4.55979900	1.16763200	-0.31259500
H	4.13709400	0.02874400	-1.57728000
C	4.86528400	-0.89934900	0.25364100
O	4.32230100	-1.42469400	1.26548800
O	6.00623100	-1.14770800	-0.21699200

³O₂

0 3

O	0.00000000	0.00000000	0.60715800
O	0.00000000	0.00000000	-0.60715800

•DDHK-

0 2

C	-2.93106000	-2.48902200	0.02335900
H	-2.54085400	-3.50081700	0.00762100
C	-4.30892300	-2.26446000	0.11760400
H	-4.99097200	-3.10480300	0.17949500
C	-4.80674200	-0.97276900	0.12811500
H	-5.86973000	-0.77236600	0.19667100
C	-3.93260900	0.14101500	0.04629800
O	-4.51662900	1.33273700	0.05733100
H	-3.84349500	2.04021600	-0.01151100
C	-2.52082300	-0.05913000	-0.03966300
C	-1.57446000	0.99658200	-0.12044500
O	-2.09042700	2.24663300	-0.11064500
H	-1.44397200	2.94320900	-0.29723300
C	-2.02698000	-1.40321900	-0.05704600
C	-0.64128600	-1.62190600	-0.16552500
H	-0.27140000	-2.64233100	-0.18705700
C	0.27536300	-0.56245900	-0.24422600
C	1.74496900	-0.85407100	-0.39306600
H	2.04714500	-1.68824900	0.24590200
H	1.92750700	-1.16496600	-1.43192400
C	-0.18451500	0.76169000	-0.20127000
C	0.80327500	1.92383600	-0.24865300
C	0.91196000	2.66018900	1.10179800
H	1.61746400	3.48801100	0.99779600
H	1.26272300	1.99120700	1.89070000
H	-0.05102400	3.06771200	1.42354200
H	0.46039700	2.64237400	-1.00761600
O	2.07498600	1.51458600	-0.72665200
C	2.61932900	0.35162500	-0.06391600
H	2.61249000	0.50830700	1.02132900
C	4.06113500	0.19553500	-0.51982800

H	4.58199900	1.14888100	-0.36676200
H	4.09374600	0.00076600	-1.59928100
C	4.86296900	-0.91856700	0.21650600
O	4.28496100	-1.52353000	1.16335500
O	6.03440300	-1.10372100	-0.20112900

O₂⁻

-1 2

O	0.00000000	0.00000000	0.67472000
O	0.00000000	0.00000000	-0.67472000

DHK⁻

-1 1

C	3.60121600	1.89687400	0.18872300
C	4.87085300	1.29814700	0.19611100
C	5.01044000	-0.07592700	0.07832500
C	3.87085600	-0.89412400	-0.05030900
O	4.04701300	-2.21827000	-0.16579800
C	2.58490700	-0.30259800	-0.05367100
C	1.38995600	-1.13809100	-0.18257600
O	1.48204500	-2.37789200	-0.31281300
C	2.46904700	1.10165300	0.06466600
C	1.11943200	1.73209800	0.05083200
C	-0.07427400	0.84860700	-0.07981100
C	-1.42098100	1.51634400	-0.12487500
C	0.05512200	-0.49662600	-0.17521400
C	-1.15718400	-1.39533100	-0.33794200
C	-1.42622700	-2.26277100	0.90470200
O	-2.30665000	-0.65210200	-0.72781400
C	-2.56133700	0.51730000	0.07629500
C	-3.92496000	1.04994700	-0.32816700
C	-5.11106600	0.13593900	0.10454900
O	-6.07177400	0.05384200	-0.70547500
O	-5.01408600	-0.40696600	1.23944200
H	3.48625400	2.97082000	0.27615000
H	5.75658200	1.91796900	0.29284700
H	5.98695500	-0.54811600	0.08045000
H	3.13872800	-2.61155600	-0.25231600

H	-1.46026600	2.30786600	0.63091000
H	-1.52541600	2.02238400	-1.09523900
H	-0.58418500	-2.93281800	1.08890300
H	-2.32492800	-2.86105300	0.73167400
H	-1.58225300	-1.65026300	1.79662500
H	-0.95520100	-2.06842400	-1.17927900
H	-2.62044300	0.22650100	1.13213400
H	-3.95387200	1.21492800	-1.41117200
H	-4.06406200	2.02967700	0.15046800
O	0.97936600	2.95056600	0.14346000

H₂O

0 1

O	0.00000000	0.12022300	0.00000000
H	0.75671100	-0.48088700	0.00000000
H	-0.75671100	-0.48090000	0.00000000

DOP⁻

-1 1

C	2.95316800	-1.98247900	-1.13805000
H	2.81766200	-3.05484700	-1.23574900
C	3.90560100	-1.30264700	-1.91240900
H	4.50885400	-1.85210900	-2.62881700
C	4.09419500	0.06906000	-1.77668300
H	4.83395000	0.59359200	-2.37295700
C	3.33085100	0.81058200	-0.85640700
O	3.57852100	2.14550900	-0.75797000
H	3.00390100	2.51247900	-0.06332900
C	2.35695300	0.14161600	-0.11020900
C	1.43805500	0.69846200	0.95273900
O	1.70518300	2.03578500	1.21226200
H	1.10532400	2.37725900	1.89231700
C	2.18282400	-1.24387300	-0.25059500
C	1.13121100	-1.76056400	0.70495100
H	1.02653500	-2.84729200	0.70649100
C	-0.16503300	-1.00342800	0.52834600
C	-1.50625300	-1.63611300	0.30409900
H	-1.44085300	-2.41365000	-0.46805600

H	-1.84243500	-2.13868300	1.22281100
C	-0.00387100	0.31878600	0.67304500
C	-1.16155600	1.28887500	0.65699300
C	-1.12725600	2.24916700	-0.54247600
H	-0.20467700	2.83651200	-0.53592000
H	-1.97831800	2.93383800	-0.49006000
H	-1.17565800	1.70148400	-1.48734800
H	-1.13540400	1.89455400	1.57467800
O	-2.40115100	0.58446700	0.74315400
C	-2.51760500	-0.56429300	-0.12550200
H	-2.30721000	-0.25906500	-1.15795900
C	-3.96645900	-1.01585100	-0.06829100
H	-4.27050700	-1.16442900	0.97405000
H	-4.03828100	-1.99450000	-0.56410000
C	-4.96346100	-0.05238000	-0.78171200
O	-6.11012200	0.03604800	-0.26805300
O	-4.54489900	0.51589600	-1.82759900
O	1.80989100	-0.00908800	2.21590700
O	1.61369300	-1.46045200	2.06816500

³ES0 (QM, triplet)

0 3

N-N--0.415700(PDBName=N,ResName=ASN,ResNum=173)	0	-5.719962	3.001333	-
2.300634 L				
H-H-0.271900(PDBName=H,ResName=ASN,ResNum=173)	0	-5.902406	2.589924	-
3.211160 L				
C-CX-0.014300(PDBName=CA,ResName=ASN,ResNum=173)	0	-6.044609	2.202427	-
1.115021 L				
H-H1-0.104800(PDBName=HA,ResName=ASN,ResNum=173)	0	-6.221461	2.864880	-
0.268503 L				
C-2C--0.204100(PDBName=CB,ResName=ASN,ResNum=173)	0	-7.339855	1.411159	-
1.381890 H				
H-HC-0.079700(PDBName=HB2,ResName=ASN,ResNum=173)	0	-8.149313	2.116641	-
1.551865 H				
H-HC-0.079700(PDBName=HB3,ResName=ASN,ResNum=173)	0	-7.211608	0.816616	-
2.290836 H				
C-C-0.713000(PDBName=CG,ResName=ASN,ResNum=173)	0	-7.726860	0.511783	-
0.208405 H				

O-O--0.593100(PDBName=OD1,ResName=ASN,ResNum=173)	0	-8.527523	0.831224
0.657844 H			
N-N--0.919100(PDBName=ND2,ResName=ASN,ResNum=173)	0	-7.085946	-0.696066 -
0.173051 H			
H-H-0.419600(PDBName=HD21,ResName=ASN,ResNum=173)	0	-7.241068	-1.312041
0.611410 H			
H-H-0.419600(PDBName=HD22,ResName=ASN,ResNum=173)	0	-6.365723	-0.970445 -
0.826398 H			
C-C-0.597300(PDBName=C,ResName=ASN,ResNum=173)	0	-4.901277	1.234267 -
0.757402 L			
O-O--0.567900(PDBName=O,ResName=ASN,ResNum=173)	0	-4.429082	0.513094 -
1.636017 L			
N-N--0.415700(PDBName=N,ResName=TRP,ResNum=177)	0	-5.949190	-8.129755
5.621130 L			
H-H-0.271900(PDBName=H,ResName=TRP,ResNum=177)	0	-5.060079	-8.381814
5.198536 L			
C-CX--0.027500(PDBName=CA,ResName=TRP,ResNum=177)	0	-6.833033	-9.249441
5.953710 L			
H-H1-0.112300(PDBName=HA,ResName=TRP,ResNum=177)	0	-7.602971	-8.910399
6.646205 L			
C-CT--0.005000(PDBName=CB,ResName=TRP,ResNum=177)	0	-7.512046	-9.729855
4.656953 H			
H-HC-0.033900(PDBName=HB2,ResName=TRP,ResNum=177)	0	-6.708253	-10.081690
4.003501 H			
H-HC-0.033900(PDBName=HB3,ResName=TRP,ResNum=177)	0	-8.097057	-10.621500
4.914410 H			
C-C*--0.141500(PDBName=CG,ResName=TRP,ResNum=177)	0	-8.399910	-8.769941
3.921520 H			
C-CW--0.163800(PDBName=CD1,ResName=TRP,ResNum=177)	0	-8.066598	-7.892131
2.916445 H			
H-H4-0.206200(PDBName=HD1,ResName=TRP,ResNum=177)	0	-7.109959	-7.730277
2.436844 H			
N-NA--0.341800(PDBName=NE1,ResName=TRP,ResNum=177)	0	-9.170167	-7.145521
2.541657 H			
H-H-0.341200(PDBName=HE1,ResName=TRP,ResNum=177)	0	-9.221358	-6.514127
1.750756 H			
C-CN-0.138000(PDBName=CE2,ResName=TRP,ResNum=177)	0	-10.250389	-7.538149
3.304056 H			

C-CA--0.260100(PDBName=CZ2,ResName=TRP,ResNum=177)	0	-11.574165	-7.081173
3.317371 H			
H-HA-0.157200(PDBName=HZ2,ResName=TRP,ResNum=177)	0	-11.908041	-6.289567
2.653873 H			
C-CA--0.113400(PDBName=CH2,ResName=TRP,ResNum=177)	0	-12.445109	-7.664425
4.229774 H			
H-HA-0.141700(PDBName=HH2,ResName=TRP,ResNum=177)	0	-13.459323	-7.288008
4.306104 H			
C-CA--0.197200(PDBName=CZ3,ResName=TRP,ResNum=177)	0	-12.032398	-8.718100
5.069697 H			
H-HA-0.144700(PDBName=HZ3,ResName=TRP,ResNum=177)	0	-12.744764	-9.178006
5.748945 H			
C-CA--0.238700(PDBName=CE3,ResName=TRP,ResNum=177)	0	-10.721822	-9.171559
5.047746 H			
H-HA-0.170000(PDBName=HE3,ResName=TRP,ResNum=177)	0	-10.413183	-9.992547
5.688552 H			
C-CB-0.124300(PDBName=CD2,ResName=TRP,ResNum=177)	0	-9.799864	-8.561592
4.182563 H			
C-C-0.597300(PDBName=C,ResName=TRP,ResNum=177)	0	-6.067100	-10.411744
6.612080 L			
O-O--0.567900(PDBName=O,ResName=TRP,ResNum=177)	0	-4.863194	-10.586277
6.400202 L			
N-N--0.347900(PDBName=N,ResName=ARG,ResNum=197)	0	-18.574799	-1.570571 -
5.149329 L			
H-H-0.274700(PDBName=H,ResName=ARG,ResNum=197)	0	-18.911406	-2.431020 -
4.724816 L			
C-CX--0.263700(PDBName=CA,ResName=ARG,ResNum=197)	0	-17.940519	-1.642098 -
6.480321 L			
H-H1-0.156000(PDBName=HA,ResName=ARG,ResNum=197)	0	-16.923391	-1.250494 -
6.423220 L			
C-C8--0.000700(PDBName=CB,ResName=ARG,ResNum=197)	0	-17.892065	-3.094419 -
6.991821 L			
H-HC-0.032700(PDBName=HB2,ResName=ARG,ResNum=197)	0	-18.885475	-3.543166 -
6.942130 L			
H-HC-0.032700(PDBName=HB3,ResName=ARG,ResNum=197)	0	-17.609432	-3.057280 -
8.044191 L			
C-C8-0.039000(PDBName=CG,ResName=ARG,ResNum=197)	0	-16.892859	-3.992679 -
6.238574 L			

H-HC-0.028500(PDBName=HG2,ResName=ARG,ResNum=197) 0 -16.013296 -3.415650 -
 5.952061 L
 H-HC-0.028500(PDBName=HG3,ResName=ARG,ResNum=197) 0 -17.357233 -4.367998 -
 5.329702 L
 C-C8-0.048600(PDBName=CD,ResName=ARG,ResNum=197) 0 -16.448721 -5.188061 -
 7.090435 H
 H-H1-0.068700(PDBName=HD2,ResName=ARG,ResNum=197) 0 -15.896495 -5.875221 -
 6.433337 H
 H-H1-0.068700(PDBName=HD3,ResName=ARG,ResNum=197) 0 -17.346657 -5.708894 -
 7.447806 H
 N-N2--0.529500(PDBName=NE,ResName=ARG,ResNum=197) 0 -15.611160 -4.721267 -
 8.184643 H
 H-H-0.345600(PDBName=HE,ResName=ARG,ResNum=197) 0 -15.292651 -3.681715 -
 8.181073 H
 C-CA-0.807600(PDBName=CZ,ResName=ARG,ResNum=197) 0 -15.044371 -5.502700 -
 9.079013 H
 N-N2--0.862700(PDBName=NH1,ResName=ARG,ResNum=197) 0 -15.346058 -6.842846 -
 9.232407 H
 H-H-0.447800(PDBName=HH11,ResName=ARG,ResNum=197) 0 -15.837013 -7.276214 -
 8.431215 H
 H-H-0.447800(PDBName=HH12,ResName=ARG,ResNum=197) 0 -14.490640 -7.399091 -
 9.359768 H
 N-N2--0.862700(PDBName=NH2,ResName=ARG,ResNum=197) 0 -14.228884 -4.940598 -
 9.989617 H
 H-H-0.447800(PDBName=HH21,ResName=ARG,ResNum=197) 0 -13.715923 -4.075014 -
 9.737352 H
 H-H-0.447800(PDBName=HH22,ResName=ARG,ResNum=197) 0 -13.719763 -5.603464 -
 10.582604 H
 C-C-0.734100(PDBName=C,ResName=ARG,ResNum=197) 0 -18.687346 -0.780087 -
 7.493668 L
 O-O--0.589400(PDBName=O,ResName=ARG,ResNum=197) 0 -18.064486 -0.056101 -
 8.280253 L
 C-CJ--0.316472(PDBName=C1,ResName=DHK,ResNum=225) 0 -12.494039 -2.101170
 0.513855 H
 H-HK-0.158183(PDBName=H2,ResName=DHK,ResNum=225) 0 -13.177780 -1.265380
 0.626305 H
 C-CJ--0.090287(PDBName=C3,ResName=DHK,ResNum=225) 0 -11.949264 -2.724531
 1.612459 H

H-HK-0.142318(PDBName=H4,ResName=DHK,ResNum=225)	0	-12.198079	-2.390107
2.615039 H			
C-CJ--0.390043(PDBName=C5,ResName=DHK,ResNum=225)	0	-11.055993	-3.804042
1.457610 H			
H-HK-0.190546(PDBName=H6,ResName=DHK,ResNum=225)	0	-10.610779	-4.282751
2.323240 H			
C-CJ-0.446965(PDBName=C7,ResName=DHK,ResNum=225)	0	-10.732065	-4.279992
0.200116 H			
O-OX--0.642443(PDBName=O8,ResName=DHK,ResNum=225)	0	-9.872399	-5.338319
0.125251 H			
H-HY-0.433577(PDBName=H9,ResName=DHK,ResNum=225)	0	-9.757731	-5.567186 -
0.820660 H			
C-CJ--0.168157(PDBName=C10,ResName=DHK,ResNum=225)	0	-11.281773	-3.662698 -
0.973682 H			
C-CJ-0.254614(PDBName=C11,ResName=DHK,ResNum=225)	0	-10.977249	-4.060472 -
2.312462 H			
O-OX--0.544517(PDBName=O12,ResName=DHK,ResNum=225)	0	-10.121063	-5.144546 -
2.471631 H			
H-HY-0.383602(PDBName=H13,ResName=DHK,ResNum=225)	0	-9.411983	-4.940895 -
3.118273 H			
C-CJ-0.213075(PDBName=C14,ResName=DHK,ResNum=225)	0	-12.156342	-2.537866 -
0.794518 H			
C-CJ--0.377966(PDBName=C15,ResName=DHK,ResNum=225)	0	-12.617040	-1.845636 -
1.944565 H			
H-HK-0.179148(PDBName=H16,ResName=DHK,ResNum=225)	0	-13.219449	-0.951189 -
1.801255 H			
C-CJ-0.165502(PDBName=C17,ResName=DHK,ResNum=225)	0	-12.285292	-2.244378 -
3.222842 H			
C-CZ--0.111477(PDBName=C18,ResName=DHK,ResNum=225)	0	-12.654767	-1.409190 -
4.425389 H			
H-H8-0.032583(PDBName=H19,ResName=DHK,ResNum=225)	0	-13.604172	-0.893456 -
4.250157 H			
H-H8-0.032583(PDBName=H20,ResName=DHK,ResNum=225)	0	-11.888415	-0.632704 -
4.548034 H			
C-CJ--0.377452(PDBName=C21,ResName=DHK,ResNum=225)	0	-11.506932	-3.418318 -
3.421463 H			
C-CZ-0.692240(PDBName=C22,ResName=DHK,ResNum=225)	0	-11.328427	-3.996116 -
4.824144 H			

C-CZ--0.555194(PDBName=C23,ResName=DHK,ResNum=225) 0 -12.196198 -5.249267 -
 5.001420 H
 H-H8-0.129933(PDBName=H24,ResName=DHK,ResNum=225) 0 -11.929837 -6.003341 -
 4.253715 H
 H-H8-0.129933(PDBName=H25,ResName=DHK,ResNum=225) 0 -12.049748 -5.691355 -
 5.991362 H
 H-H8-0.129933(PDBName=H26,ResName=DHK,ResNum=225) 0 -13.260434 -5.028694 -
 4.874337 H
 H-H9--0.039392(PDBName=H27,ResName=DHK,ResNum=225) 0 -10.282672 -4.276097 -
 4.986617 H
 O-OI--0.712638(PDBName=O28,ResName=DHK,ResNum=225) 0 -11.581114 -3.051353 -
 5.870697 H
 C-CZ-0.665570(PDBName=C29,ResName=DHK,ResNum=225) 0 -12.751990 -2.239907 -
 5.700785 H
 H-H9--0.064844(PDBName=H30,ResName=DHK,ResNum=225) 0 -13.647490 -2.876108 -
 5.639119 H
 C-CZ--0.289485(PDBName=C31,ResName=DHK,ResNum=225) 0 -12.858468 -1.381324 -
 6.971919 H
 H-H8-0.039536(PDBName=H32,ResName=DHK,ResNum=225) 0 -11.854764 -1.038928 -
 7.234604 H
 H-H8-0.039536(PDBName=H33,ResName=DHK,ResNum=225) 0 -13.498089 -0.517718 -
 6.763493 H
 C-CV-0.810685(PDBName=C34,ResName=DHK,ResNum=225) 0 -13.493324 -2.195776 -
 8.097599 H
 O-O5--0.794847(PDBName=O35,ResName=DHK,ResNum=225) 0 -12.758713 -2.733399 -
 8.963612 H
 O-O5--0.794847(PDBName=O36,ResName=DHK,ResNum=225) 0 -14.767693 -2.289606 -
 8.038546 H
 O-O5--0.000000(PDBName=O1,ResName=OXY,ResNum=226) 0 -7.851870 -3.196025 -
 1.745639 H
 O-O5--0.000000(PDBName=O2,ResName=OXY,ResNum=226) 0 -8.719309 -2.343961 -
 1.698649 H
 O-OW--0.834000(PDBName=O,ResName=WAT,ResNum=425) 0 -10.252428 0.374415 -
 2.376807 H
 H-HW-0.417000(PDBName=H1,ResName=WAT,ResNum=425) 0 -10.533042 -0.521214 -
 2.142348 H
 H-HW-0.417000(PDBName=H2,ResName=WAT,ResNum=425) 0 -10.546181 0.882954 -
 1.597674 H

O-OW--0.834000(PDBName=O,ResName=WAT,ResNum=639) 0 -7.936436 -4.745215 -
4.300049 H
H-HW-0.417000(PDBName=H1,ResName=WAT,ResNum=639) 0 -7.212736 -4.101807 -
4.397622 H
H-HW-0.417000(PDBName=H2,ResName=WAT,ResNum=639) 0 -7.528931 -5.600709 -
4.513141 H

³TS1 (QM, triplet)

0 3

N-N--0.415700(PDBName=N,ResName=ASN,ResNum=173) 0 -5.728884 3.007224 -
2.306096 L
H-H-0.271900(PDBName=H,ResName=ASN,ResNum=173) 0 -5.901763 2.594881 -
3.217862 L
C-CX-0.014300(PDBName=CA,ResName=ASN,ResNum=173) 0 -6.060779 2.209125 -
1.122380 L
H-H1-0.104800(PDBName=HA,ResName=ASN,ResNum=173) 0 -6.220501 2.872076 -
0.272102 L
C-2C--0.204100(PDBName=CB,ResName=ASN,ResNum=173) 0 -7.362380 1.428595 -
1.371959 H
H-HC-0.079700(PDBName=HB2,ResName=ASN,ResNum=173) 0 -8.164449 2.140698 -
1.552712 H
H-HC-0.079700(PDBName=HB3,ResName=ASN,ResNum=173) 0 -7.241952 0.813486 -
2.267471 H
C-C-0.713000(PDBName=CG,ResName=ASN,ResNum=173) 0 -7.713872 0.588400 -
0.143045 H
O-O--0.593100(PDBName=OD1,ResName=ASN,ResNum=173) 0 -8.168077 1.074429
0.886272 H
N-N--0.919100(PDBName=ND2,ResName=ASN,ResNum=173) 0 -7.406850 -0.733890 -
0.242271 H
H-H-0.419600(PDBName=HD21,ResName=ASN,ResNum=173) 0 -7.584476 -1.327067
0.554395 H
H-H-0.419600(PDBName=HD22,ResName=ASN,ResNum=173) 0 -7.104299 -1.204400 -
1.084954 H
C-C-0.597300(PDBName=C,ResName=ASN,ResNum=173) 0 -4.937914 1.217516 -
0.773194 L
O-O--0.567900(PDBName=O,ResName=ASN,ResNum=173) 0 -4.447883 0.522721 -
1.663556 L
N-N--0.415700(PDBName=N,ResName=TRP,ResNum=177) 0 -5.951209 -8.133992

5.617613 L			
H-H-0.271900(PDBName=H,ResName=TRP,ResNum=177)	0	-5.061085	-8.384959
5.196519 L			
C-CX--0.027500(PDBName=CA,ResName=TRP,ResNum=177)	0	-6.833905	-9.254259
5.949429 L			
H-H1-0.112300(PDBName=HA,ResName=TRP,ResNum=177)	0	-7.605188	-8.916157
6.640967 L			
C-CT--0.005000(PDBName=CB,ResName=TRP,ResNum=177)	0	-7.510674	-9.737246
4.652856 H			
H-HC-0.033900(PDBName=HB2,ResName=TRP,ResNum=177)	0	-6.705246	-10.076880
3.995354 H			
H-HC-0.033900(PDBName=HB3,ResName=TRP,ResNum=177)	0	-8.085560	-10.636050
4.907683 H			
C-C*--0.141500(PDBName=CG,ResName=TRP,ResNum=177)	0	-8.411051	-8.782799
3.926238 H			
C-CW--0.163800(PDBName=CD1,ResName=TRP,ResNum=177)	0	-8.090756	-7.893971
2.927395 H			
H-H4-0.206200(PDBName=HD1,ResName=TRP,ResNum=177)	0	-7.137917	-7.716483
2.446083 H			
N-NA--0.341800(PDBName=NE1,ResName=TRP,ResNum=177)	0	-9.205210	-7.156108
2.564521 H			
H-H-0.341200(PDBName=HE1,ResName=TRP,ResNum=177)	0	-9.267407	-6.514746
1.785184 H			
C-CN-0.138000(PDBName=CE2,ResName=TRP,ResNum=177)	0	-10.277806	-7.564854
3.328851 H			
C-CA--0.260100(PDBName=CZ2,ResName=TRP,ResNum=177)	0	-11.605645	-7.121015
3.355272 H			
H-HA-0.157200(PDBName=HZ2,ResName=TRP,ResNum=177)	0	-11.954705	-6.332874
2.695437 H			
C-CA--0.113400(PDBName=CH2,ResName=TRP,ResNum=177)	0	-12.464247	-7.716994
4.271429 H			
H-HA-0.141700(PDBName=HH2,ResName=TRP,ResNum=177)	0	-13.480583	-7.349695
4.360421 H			
C-CA--0.197200(PDBName=CZ3,ResName=TRP,ResNum=177)	0	-12.035845	-8.773392
5.099424 H			
H-HA-0.144700(PDBName=HZ3,ResName=TRP,ResNum=177)	0	-12.738350	-9.244357
5.781141 H			
C-CA--0.238700(PDBName=CE3,ResName=TRP,ResNum=177)	0	-10.722000	-9.216196

5.061986 H
H-HA-0.170000(PDBName=HE3,ResName=TRP,ResNum=177) 0 -10.401712 -10.040956
5.691668 H
C-CB-0.124300(PDBName=CD2,ResName=TRP,ResNum=177) 0 -9.811852 -8.590756
4.195912 H
C-C-0.597300(PDBName=C,ResName=TRP,ResNum=177) 0 -6.066990 -10.413872
6.609499 L
O-O--0.567900(PDBName=O,ResName=TRP,ResNum=177) 0 -4.863040 -10.588074
6.397610 L
N-N--0.347900(PDBName=N,ResName=ARG,ResNum=197) 0 -18.573160 -1.568531 -
5.149021 L
H-H-0.274700(PDBName=H,ResName=ARG,ResNum=197) 0 -18.909277 -2.428891 -
4.724009 L
C-CX--0.263700(PDBName=CA,ResName=ARG,ResNum=197) 0 -17.938873 -1.641202 -
6.479746 L
H-H1-0.156000(PDBName=HA,ResName=ARG,ResNum=197) 0 -16.921228 -1.250740 -
6.422524 L
C-C8--0.000700(PDBName=CB,ResName=ARG,ResNum=197) 0 -17.891581 -3.094047 -
6.990035 L
H-HC-0.032700(PDBName=HB2,ResName=ARG,ResNum=197) 0 -18.885939 -3.540918 -
6.942909 L
H-HC-0.032700(PDBName=HB3,ResName=ARG,ResNum=197) 0 -17.606165 -3.058156 -
8.041655 L
C-C8-0.039000(PDBName=CG,ResName=ARG,ResNum=197) 0 -16.896469 -3.994192 -
6.233541 L
H-HC-0.028500(PDBName=HG2,ResName=ARG,ResNum=197) 0 -16.019951 -3.417449 -
5.937671 L
H-HC-0.028500(PDBName=HG3,ResName=ARG,ResNum=197) 0 -17.366779 -4.374600 -
5.329955 L
C-C8-0.048600(PDBName=CD,ResName=ARG,ResNum=197) 0 -16.444370 -5.185071 -
7.087283 H
H-H1-0.068700(PDBName=HD2,ResName=ARG,ResNum=197) 0 -15.896882 -5.875266 -
6.429258 H
H-H1-0.068700(PDBName=HD3,ResName=ARG,ResNum=197) 0 -17.339266 -5.704629 -
7.453945 H
N-N2--0.529500(PDBName=NE,ResName=ARG,ResNum=197) 0 -15.598962 -4.712327 -
8.172443 H
H-H-0.345600(PDBName=HE,ResName=ARG,ResNum=197) 0 -15.279692 -3.674764 -

8.158883 H
C-CA-0.807600(PDBName=CZ,ResName=ARG,ResNum=197) 0 -15.036583 -5.489048 -
9.074632 H
N-N2--0.862700(PDBName=NH1,ResName=ARG,ResNum=197) 0 -15.345779 -6.826383 -
9.238291 H
H-H-0.447800(PDBName=HH11,ResName=ARG,ResNum=197) 0 -15.838232 -7.263863 -
8.440269 H
H-H-0.447800(PDBName=HH12,ResName=ARG,ResNum=197) 0 -14.493218 -7.385975 -
9.370354 H
N-N2--0.862700(PDBName=NH2,ResName=ARG,ResNum=197) 0 -14.218337 -4.923986 -
9.979735 H
H-H-0.447800(PDBName=HH21,ResName=ARG,ResNum=197) 0 -13.703705 -4.060839 -
9.722095 H
H-H-0.447800(PDBName=HH22,ResName=ARG,ResNum=197) 0 -13.715398 -5.583373 -
10.581721 H
C-C-0.734100(PDBName=C,ResName=ARG,ResNum=197) 0 -18.685303 -0.779500 -
7.493601 L
O-O--0.589400(PDBName=O,ResName=ARG,ResNum=197) 0 -18.062412 -0.055384 -
8.280028 L
C-CJ--0.316472(PDBName=C1,ResName=DHK,ResNum=225) 0 -12.496018 -1.918826
0.539057 H
H-HK-0.158183(PDBName=H2,ResName=DHK,ResNum=225) 0 -13.094320 -1.019260
0.638773 H
C-CJ--0.090287(PDBName=C3,ResName=DHK,ResNum=225) 0 -12.021169 -2.584689
1.664596 H
H-HK-0.142318(PDBName=H4,ResName=DHK,ResNum=225) 0 -12.248672 -2.209285
2.657140 H
C-CJ--0.390043(PDBName=C5,ResName=DHK,ResNum=225) 0 -11.239817 -3.733456
1.537011 H
H-HK-0.190546(PDBName=H6,ResName=DHK,ResNum=225) 0 -10.850463 -4.247282
2.409040 H
C-CJ-0.446965(PDBName=C7,ResName=DHK,ResNum=225) 0 -10.948979 -4.254583
0.267356 H
O-OX--0.642443(PDBName=O8,ResName=DHK,ResNum=225) 0 -10.207053 -5.376228
0.194457 H
H-HY-0.433577(PDBName=H9,ResName=DHK,ResNum=225) 0 -10.116653 -5.594464 -
0.771893 H
C-CJ--0.168157(PDBName=C10,ResName=DHK,ResNum=225) 0 -11.434356 -3.605142 -

0.900389 H
C-CJ-0.254614(PDBName=C11,ResName=DHK,ResNum=225) 0 -11.128633 -4.079522 -
2.223911 H
O-OX--0.544517(PDBName=O12,ResName=DHK,ResNum=225) 0 -10.413614 -5.180568 -
2.360036 H
H-HY-0.383602(PDBName=H13,ResName=DHK,ResNum=225) 0 -9.428903 -5.016771 -
3.106955 H
C-CJ-0.213075(PDBName=C14,ResName=DHK,ResNum=225) 0 -12.188216 -2.400686 -
0.751284 H
C-CJ--0.377966(PDBName=C15,ResName=DHK,ResNum=225) 0 -12.565251 -1.687991 -
1.919888 H
H-HK-0.179148(PDBName=H16,ResName=DHK,ResNum=225) 0 -13.073087 -0.734422 -
1.803019 H
C-CJ-0.165502(PDBName=C17,ResName=DHK,ResNum=225) 0 -12.273425 -2.151848 -
3.201668 H
C-CZ--0.111477(PDBName=C18,ResName=DHK,ResNum=225) 0 -12.582495 -1.314460 -
4.416231 H
H-H8-0.032583(PDBName=H19,ResName=DHK,ResNum=225) 0 -13.470316 -0.700511 -
4.237376 H
H-H8-0.032583(PDBName=H20,ResName=DHK,ResNum=225) 0 -11.740685 -0.625173 -
4.559169 H
C-CJ--0.377452(PDBName=C21,ResName=DHK,ResNum=225) 0 -11.634276 -3.386756 -
3.370970 H
C-CZ-0.692240(PDBName=C22,ResName=DHK,ResNum=225) 0 -11.519863 -4.022008 -
4.747802 H
C-CZ--0.555194(PDBName=C23,ResName=DHK,ResNum=225) 0 -12.482080 -5.215228 -
4.872661 H
H-H8-0.129933(PDBName=H24,ResName=DHK,ResNum=225) 0 -12.250378 -5.978889 -
4.122839 H
H-H8-0.129933(PDBName=H25,ResName=DHK,ResNum=225) 0 -12.383066 -5.677198 -
5.859652 H
H-H8-0.129933(PDBName=H26,ResName=DHK,ResNum=225) 0 -13.525186 -4.915573 -
4.733798 H
H-H9--0.039392(PDBName=H27,ResName=DHK,ResNum=225) 0 -10.499930 -4.385883 -
4.896152 H
O-OI--0.712638(PDBName=O28,ResName=DHK,ResNum=225) 0 -11.711305 -3.101560 -
5.823790 H
C-CZ-0.665570(PDBName=C29,ResName=DHK,ResNum=225) 0 -12.790682 -2.169455 -

5.662316 H
H-H9--0.064844(PDBName=H30,ResName=DHK,ResNum=225) 0 -13.744434 -2.709547 -
5.566222 H
C-CZ--0.289485(PDBName=C31,ResName=DHK,ResNum=225) 0 -12.836820 -1.351740 -
6.960784 H
H-H8-0.039536(PDBName=H32,ResName=DHK,ResNum=225) 0 -11.816153 -1.058973 -
7.218723 H
H-H8-0.039536(PDBName=H33,ResName=DHK,ResNum=225) 0 -13.444049 -0.456374 -
6.791582 H
C-CV-0.810685(PDBName=C34,ResName=DHK,ResNum=225) 0 -13.483708 -2.179826 -
8.071798 H
O-O5--0.794847(PDBName=O35,ResName=DHK,ResNum=225) 0 -12.755218 -2.721500 -
8.939891 H
O-O5--0.794847(PDBName=O36,ResName=DHK,ResNum=225) 0 -14.756979 -2.275093 -
8.000040 H
O-O5--0.000000(PDBName=O1,ResName=OXY,ResNum=226) 0 -7.811936 -2.784702 -
2.348226 H
O-O5--0.000000(PDBName=O2,ResName=OXY,ResNum=226) 0 -9.039622 -2.361999 -
2.196195 H
O-OW--0.834000(PDBName=O,ResName=WAT,ResNum=425) 0 -10.269114 0.344320 -
2.366267 H
H-HW-0.417000(PDBName=H1,ResName=WAT,ResNum=425) 0 -9.759726 -0.435091 -
2.086281 H
H-HW-0.417000(PDBName=H2,ResName=WAT,ResNum=425) 0 -10.618417 0.698894 -
1.528148 H
O-OW--0.834000(PDBName=O,ResName=WAT,ResNum=639) 0 -8.492190 -4.672644 -
3.709237 H
H-HW-0.417000(PDBName=H1,ResName=WAT,ResNum=639) 0 -8.026510 -3.854095 -
3.114651 H
H-HW-0.417000(PDBName=H2,ResName=WAT,ResNum=639) 0 -7.868958 -5.390227 -
3.902719 H

³M1 (QM, triplet)

0 3
N-N--0.415700(PDBName=N,ResName=ASN,ResNum=173) 0 -5.726325 3.005919 -
2.304850 L
H-H-0.271900(PDBName=H,ResName=ASN,ResNum=173) 0 -5.901888 2.594961 -
3.216772 L

C-CX-0.014300(PDBName=CA,ResName=ASN,ResNum=173)	0	-6.056473	2.206844	-
1.121113 L				
H-H1-0.104800(PDBName=HA,ResName=ASN,ResNum=173)	0	-6.223154	2.868752	-
0.271481 L				
C-2C--0.204100(PDBName=CB,ResName=ASN,ResNum=173)	0	-7.353077	1.419614	-
1.378279 H				
H-HC-0.079700(PDBName=HB2,ResName=ASN,ResNum=173)	0	-8.158750	2.125347	-
1.564824 H				
H-HC-0.079700(PDBName=HB3,ResName=ASN,ResNum=173)	0	-7.221149	0.805068	-
2.272912 H				
C-C-0.713000(PDBName=CG,ResName=ASN,ResNum=173)	0	-7.717952	0.571537	-
0.159331 H				
O-O--0.593100(PDBName=OD1,ResName=ASN,ResNum=173)	0	-8.290947	1.025483	
0.823599 H				
N-N--0.919100(PDBName=ND2,ResName=ASN,ResNum=173)	0	-7.286829	-0.720114	-
0.207500 H				
H-H-0.419600(PDBName=HD21,ResName=ASN,ResNum=173)	0	-7.481177	-1.323381	
0.577452 H				
H-H-0.419600(PDBName=HD22,ResName=ASN,ResNum=173)	0	-6.884832	-1.166296	-
1.019420 H				
C-C-0.597300(PDBName=C,ResName=ASN,ResNum=173)	0	-4.927464	1.221886	-
0.770830 L				
O-O--0.567900(PDBName=O,ResName=ASN,ResNum=173)	0	-4.449060	0.515483	-
1.658543 L				
N-N--0.415700(PDBName=N,ResName=TRP,ResNum=177)	0	-5.951860	-8.133713	
5.614807 L				
H-H-0.271900(PDBName=H,ResName=TRP,ResNum=177)	0	-5.061587	-8.385807	
5.194705 L				
C-CX--0.027500(PDBName=CA,ResName=TRP,ResNum=177)	0	-6.835849	-9.253718	
5.945447 L				
H-H1-0.112300(PDBName=HA,ResName=TRP,ResNum=177)	0	-7.606872	-8.915706	
6.637281 L				
C-CT--0.005000(PDBName=CB,ResName=TRP,ResNum=177)	0	-7.513359	-9.732611	
4.647122 H				
H-HC-0.033900(PDBName=HB2,ResName=TRP,ResNum=177)	0	-6.707554	-10.062673	
3.985275 H				
H-HC-0.033900(PDBName=HB3,ResName=TRP,ResNum=177)	0	-8.081315	-10.636892	
4.897937 H				

C-C*--0.141500(PDBName=CG,ResName=TRP,ResNum=177)	0	-8.423646	-8.780162
3.928881 H			
C-CW--0.163800(PDBName=CD1,ResName=TRP,ResNum=177)	0	-8.116341	-7.882039
2.933982 H			
H-H4-0.206200(PDBName=HD1,ResName=TRP,ResNum=177)	0	-7.167849	-7.692874
2.448603 H			
N-NA--0.341800(PDBName=NE1,ResName=TRP,ResNum=177)	0	-9.239541	-7.150831
2.582707 H			
H-H-0.341200(PDBName=HE1,ResName=TRP,ResNum=177)	0	-9.311992	-6.500093
1.812594 H			
C-CN-0.138000(PDBName=CE2,ResName=TRP,ResNum=177)	0	-10.304159	-7.573464
3.350027 H			
C-CA--0.260100(PDBName=CZ2,ResName=TRP,ResNum=177)	0	-11.634741	-7.139350
3.387868 H			
H-HA-0.157200(PDBName=HZ2,ResName=TRP,ResNum=177)	0	-11.993558	-6.352658
2.731806 H			
C-CA--0.113400(PDBName=CH2,ResName=TRP,ResNum=177)	0	-12.482462	-7.747254
4.306317 H			
H-HA-0.141700(PDBName=HH2,ResName=TRP,ResNum=177)	0	-13.500616	-7.387868
4.405483 H			
C-CA--0.197200(PDBName=CZ3,ResName=TRP,ResNum=177)	0	-12.041125	-8.806580
5.123717 H			
H-HA-0.144700(PDBName=HZ3,ResName=TRP,ResNum=177)	0	-12.735571	-9.287399
5.806809 H			
C-CA--0.238700(PDBName=CE3,ResName=TRP,ResNum=177)	0	-10.724673	-9.240178
5.073851 H			
H-HA-0.170000(PDBName=HE3,ResName=TRP,ResNum=177)	0	-10.394488	-10.067823
5.694453 H			
C-CB-0.124300(PDBName=CD2,ResName=TRP,ResNum=177)	0	-9.824761	-8.601535
4.206882 H			
C-C-0.597300(PDBName=C,ResName=TRP,ResNum=177)	0	-6.068890	-10.414528
6.605774 L			
O-O--0.567900(PDBName=O,ResName=TRP,ResNum=177)	0	-4.865327	-10.589291
6.392098 L			
N-N--0.347900(PDBName=N,ResName=ARG,ResNum=197)	0	-18.572107	-1.568971 -
5.150127 L			
H-H-0.274700(PDBName=H,ResName=ARG,ResNum=197)	0	-18.907602	-2.429291 -
4.724526 L			

C-CX--0.263700(PDBName=CA,ResName=ARG,ResNum=197) 0 -17.938877 -1.642244 -
 6.481395 L
 H-H1-0.156000(PDBName=HA,ResName=ARG,ResNum=197) 0 -16.920641 -1.253241 -
 6.424840 L
 C-C8--0.000700(PDBName=CB,ResName=ARG,ResNum=197) 0 -17.894089 -3.095036 -
 6.992493 L
 H-HC-0.032700(PDBName=HB2,ResName=ARG,ResNum=197) 0 -18.889099 -3.540379 -
 6.945016 L
 H-HC-0.032700(PDBName=HB3,ResName=ARG,ResNum=197) 0 -17.609371 -3.058917 -
 8.044300 L
 C-C8-0.039000(PDBName=CG,ResName=ARG,ResNum=197) 0 -16.899979 -3.997618 -
 6.237592 L
 H-HC-0.028500(PDBName=HG2,ResName=ARG,ResNum=197) 0 -16.022526 -3.422430 -
 5.941956 L
 H-HC-0.028500(PDBName=HG3,ResName=ARG,ResNum=197) 0 -17.370222 -4.377865 -
 5.333897 L
 C-C8-0.048600(PDBName=CD,ResName=ARG,ResNum=197) 0 -16.449911 -5.188719 -
 7.092283 H
 H-H1-0.068700(PDBName=HD2,ResName=ARG,ResNum=197) 0 -15.902125 -5.879276 -
 6.434972 H
 H-H1-0.068700(PDBName=HD3,ResName=ARG,ResNum=197) 0 -17.345661 -5.707444 -
 7.458123 H
 N-N2--0.529500(PDBName=NE,ResName=ARG,ResNum=197) 0 -15.605272 -4.716506 -
 8.178283 H
 H-H-0.345600(PDBName=HE,ResName=ARG,ResNum=197) 0 -15.286731 -3.679615 -
 8.165725 H
 C-CA-0.807600(PDBName=CZ,ResName=ARG,ResNum=197) 0 -15.039974 -5.493626 -
 9.078424 H
 N-N2--0.862700(PDBName=NH1,ResName=ARG,ResNum=197) 0 -15.346841 -6.831593 -
 9.240549 H
 H-H-0.447800(PDBName=HH11,ResName=ARG,ResNum=197) 0 -15.840356 -7.268702 -
 8.442976 H
 H-H-0.447800(PDBName=HH12,ResName=ARG,ResNum=197) 0 -14.493354 -7.390278 -
 9.370337 H
 N-N2--0.862700(PDBName=NH2,ResName=ARG,ResNum=197) 0 -14.221317 -4.928581 -
 9.983121 H
 H-H-0.447800(PDBName=HH21,ResName=ARG,ResNum=197) 0 -13.708072 -4.063787 -
 9.726517 H

H-H-0.447800(PDBName=HH22,ResName=ARG,ResNum=197) 0 -13.716653 -5.588553 -
10.583080 H
C-C-0.734100(PDBName=C,ResName=ARG,ResNum=197) 0 -18.685205 -0.779584 -
7.494439 L
O-O--0.589400(PDBName=O,ResName=ARG,ResNum=197) 0 -18.062490 -0.055464 -
8.281033 L
C-CJ--0.316472(PDBName=C1,ResName=DHK,ResNum=225) 0 -12.601273 -1.801071
0.538990 H
H-HK-0.158183(PDBName=H2,ResName=DHK,ResNum=225) 0 -13.159305 -0.874420
0.622061 H
C-CJ--0.090287(PDBName=C3,ResName=DHK,ResNum=225) 0 -12.171979 -2.477961
1.679051 H
H-HK-0.142318(PDBName=H4,ResName=DHK,ResNum=225) 0 -12.393852 -2.079729
2.663931 H
C-CJ--0.390043(PDBName=C5,ResName=DHK,ResNum=225) 0 -11.445009 -3.662204
1.576098 H
H-HK-0.190546(PDBName=H6,ResName=DHK,ResNum=225) 0 -11.092579 -4.184322
2.458977 H
C-CJ-0.446965(PDBName=C7,ResName=DHK,ResNum=225) 0 -11.160010 -4.209630
0.311505 H
O-OX--0.642443(PDBName=O8,ResName=DHK,ResNum=225) 0 -10.465504 -5.359210
0.247009 H
H-HY-0.433577(PDBName=H9,ResName=DHK,ResNum=225) 0 -10.377652 -5.571250 -
0.729017 H
C-CJ--0.168157(PDBName=C10,ResName=DHK,ResNum=225) 0 -11.604250 -3.551493 -
0.861181 H
C-CJ-0.254614(PDBName=C11,ResName=DHK,ResNum=225) 0 -11.316536 -4.090971 -
2.178421 H
O-OX--0.544517(PDBName=O12,ResName=DHK,ResNum=225) 0 -10.645617 -5.176431 -
2.291612 H
H-HY-0.383602(PDBName=H13,ResName=DHK,ResNum=225) 0 -9.229853 -5.079045 -
3.317754 H
C-CJ-0.213075(PDBName=C14,ResName=DHK,ResNum=225) 0 -12.301995 -2.314261 -
0.740294 H
C-CJ--0.377966(PDBName=C15,ResName=DHK,ResNum=225) 0 -12.634391 -1.608698 -
1.928000 H
H-HK-0.179148(PDBName=H16,ResName=DHK,ResNum=225) 0 -13.094196 -0.628300 -
1.837485 H

C-CJ-0.165502(PDBName=C17,ResName=DHK,ResNum=225) 0 -12.352659 -2.114738 -
 3.205440 H
 C-CZ--0.111477(PDBName=C18,ResName=DHK,ResNum=225) 0 -12.612637 -1.279656 -
 4.433114 H
 H-H8-0.032583(PDBName=H19,ResName=DHK,ResNum=225) 0 -13.482442 -0.634779 -
 4.276251 H
 H-H8-0.032583(PDBName=H20,ResName=DHK,ResNum=225) 0 -11.746484 -0.620475 -
 4.573008 H
 C-CJ--0.377452(PDBName=C21,ResName=DHK,ResNum=225) 0 -11.786116 -3.378115 -
 3.350619 H
 C-CZ-0.692240(PDBName=C22,ResName=DHK,ResNum=225) 0 -11.628467 -4.023589 -
 4.714714 H
 C-CZ--0.555194(PDBName=C23,ResName=DHK,ResNum=225) 0 -12.585448 -5.216266 -
 4.874879 H
 H-H8-0.129933(PDBName=H24,ResName=DHK,ResNum=225) 0 -12.379843 -5.979614 -
 4.117260 H
 H-H8-0.129933(PDBName=H25,ResName=DHK,ResNum=225) 0 -12.449368 -5.677737 -
 5.857739 H
 H-H8-0.129933(PDBName=H26,ResName=DHK,ResNum=225) 0 -13.633372 -4.916388 -
 4.776024 H
 H-H9--0.039392(PDBName=H27,ResName=DHK,ResNum=225) 0 -10.602758 -4.389125 -
 4.814419 H
 O-OI--0.712638(PDBName=O28,ResName=DHK,ResNum=225) 0 -11.775730 -3.108468 -
 5.804419 H
 C-CZ-0.665570(PDBName=C29,ResName=DHK,ResNum=225) 0 -12.830216 -2.146125 -
 5.669252 H
 H-H9--0.064844(PDBName=H30,ResName=DHK,ResNum=225) 0 -13.799764 -2.657568 -
 5.574730 H
 C-CZ--0.289485(PDBName=C31,ResName=DHK,ResNum=225) 0 -12.842056 -1.347972 -
 6.979844 H
 H-H8-0.039536(PDBName=H32,ResName=DHK,ResNum=225) 0 -11.812815 -1.079240 -
 7.229723 H
 H-H8-0.039536(PDBName=H33,ResName=DHK,ResNum=225) 0 -13.433966 -0.438281 -
 6.833123 H
 C-CV-0.810685(PDBName=C34,ResName=DHK,ResNum=225) 0 -13.490060 -2.180994 -
 8.086157 H
 O-O5--0.794847(PDBName=O35,ResName=DHK,ResNum=225) 0 -12.762837 -2.723487 -
 8.954842 H

O-O5--0.794847(PDBName=O36,ResName=DHK,ResNum=225) 0 -14.762870 -2.277841 -
8.011148 H
O-O5--0.000000(PDBName=O1,ResName=OXY,ResNum=226) 0 -7.717439 -2.798266 -
2.273576 H
O-O5--0.000000(PDBName=O2,ResName=OXY,ResNum=226) 0 -8.969522 -2.363902 -
2.171909 H
O-OW--0.834000(PDBName=O,ResName=WAT,ResNum=425) 0 -10.245875 0.314997 -
2.287080 H
H-HW-0.417000(PDBName=H1,ResName=WAT,ResNum=425) 0 -9.736233 -0.451108 -
1.974963 H
H-HW-0.417000(PDBName=H2,ResName=WAT,ResNum=425) 0 -10.586470 0.709579 -
1.463515 H
O-OW--0.834000(PDBName=O,ResName=WAT,ResNum=639) 0 -8.441190 -4.750118 -
3.813388 H
H-HW-0.417000(PDBName=H1,ResName=WAT,ResNum=639) 0 -7.810792 -3.617331 -
2.870250 H
H-HW-0.417000(PDBName=H2,ResName=WAT,ResNum=639) 0 -7.924322 -5.528168 -
4.073482 H

osM1 (QM, open-shell singlet)

0 1
N-N--0.415700(PDBName=N,ResName=ASN,ResNum=173) 0 -5.726613 3.006197 -
2.303931 L
H-H-0.271900(PDBName=H,ResName=ASN,ResNum=173) 0 -5.902910 2.593995 -
3.215147 L
C-CX-0.014300(PDBName=CA,ResName=ASN,ResNum=173) 0 -6.055437 2.209939 -
1.118060 L
H-H1-0.104800(PDBName=HA,ResName=ASN,ResNum=173) 0 -6.216038 2.873881 -
0.268851 L
C-2C--0.204100(PDBName=CB,ResName=ASN,ResNum=173) 0 -7.356093 1.427200 -
1.366704 H
H-HC-0.079700(PDBName=HB2,ResName=ASN,ResNum=173) 0 -8.160135 2.135996 -
1.549324 H
H-HC-0.079700(PDBName=HB3,ResName=ASN,ResNum=173) 0 -7.232170 0.810446 -
2.260926 H
C-C-0.713000(PDBName=CG,ResName=ASN,ResNum=173) 0 -7.714317 0.584709 -
0.141686 H
O-O--0.593100(PDBName=OD1,ResName=ASN,ResNum=173) 0 -8.258587 1.049600

0.852367 H
N-N--0.919100(PDBName=ND2,ResName=ASN,ResNum=173) 0 -7.316757 -0.716435 -
0.202206 H
H-H-0.419600(PDBName=HD21,ResName=ASN,ResNum=173) 0 -7.495193 -1.314550
0.590449 H
H-H-0.419600(PDBName=HD22,ResName=ASN,ResNum=173) 0 -6.913699 -1.165228 -
1.012207 H
C-C-0.597300(PDBName=C,ResName=ASN,ResNum=173) 0 -4.929477 1.221118 -
0.769703 L
O-O--0.567900(PDBName=O,ResName=ASN,ResNum=173) 0 -4.454506 0.513364 -
1.658074 L
N-N--0.415700(PDBName=N,ResName=TRP,ResNum=177) 0 -5.951558 -8.133886
5.615096 L
H-H-0.271900(PDBName=H,ResName=TRP,ResNum=177) 0 -5.061220 -8.385942
5.195102 L
C-CX--0.027500(PDBName=CA,ResName=TRP,ResNum=177) 0 -6.835624 -9.253858
5.945337 L
H-H1-0.112300(PDBName=HA,ResName=TRP,ResNum=177) 0 -7.606814 -8.916016
6.637073 L
C-CT--0.005000(PDBName=CB,ResName=TRP,ResNum=177) 0 -7.512797 -9.732341
4.646696 H
H-HC-0.033900(PDBName=HB2,ResName=TRP,ResNum=177) 0 -6.706730 -10.060371
3.984177 H
H-HC-0.033900(PDBName=HB3,ResName=TRP,ResNum=177) 0 -8.079204 -10.637836
4.896678 H
C-C*--0.141500(PDBName=CG,ResName=TRP,ResNum=177) 0 -8.425318 -8.780769
3.930101 H
C-CW--0.163800(PDBName=CD1,ResName=TRP,ResNum=177) 0 -8.120889 -7.881954
2.934700 H
H-H4-0.206200(PDBName=HD1,ResName=TRP,ResNum=177) 0 -7.173576 -7.692162
2.447337 H
N-NA--0.341800(PDBName=NE1,ResName=TRP,ResNum=177) 0 -9.246548 -7.155023
2.583240 H
H-H-0.341200(PDBName=HE1,ResName=TRP,ResNum=177) 0 -9.322042 -6.497925
1.818901 H
C-CN-0.138000(PDBName=CE2,ResName=TRP,ResNum=177) 0 -10.308728 -7.578059
3.353584 H
C-CA--0.260100(PDBName=CZ2,ResName=TRP,ResNum=177) 0 -11.639567 -7.144850

3.393791 H			
H-HA-0.157200(PDBName=HZ2,ResName=TRP,ResNum=177)	0	-11.998846	-6.356576
2.739853 H			
C-CA--0.113400(PDBName=CH2,ResName=TRP,ResNum=177)	0	-12.485317	-7.754341
4.312948 H			
H-HA-0.141700(PDBName=HH2,ResName=TRP,ResNum=177)	0	-13.503590	-7.396083
4.414910 H			
C-CA--0.197200(PDBName=CZ3,ResName=TRP,ResNum=177)	0	-12.041674	-8.814614
5.127993 H			
H-HA-0.144700(PDBName=HZ3,ResName=TRP,ResNum=177)	0	-12.734655	-9.297394
5.811187 H			
C-CA--0.238700(PDBName=CE3,ResName=TRP,ResNum=177)	0	-10.724818	-9.246568
5.076202 H			
H-HA-0.170000(PDBName=HE3,ResName=TRP,ResNum=177)	0	-10.393312	-10.074922
5.695093 H			
C-CB-0.124300(PDBName=CD2,ResName=TRP,ResNum=177)	0	-9.826398	-8.605463
4.209465 H			
C-C-0.597300(PDBName=C,ResName=TRP,ResNum=177)	0	-6.068779	-10.414696
6.605641 L			
O-O--0.567900(PDBName=O,ResName=TRP,ResNum=177)	0	-4.865241	-10.589577
6.391933 L			
N-N--0.347900(PDBName=N,ResName=ARG,ResNum=197)	0	-18.571983	-1.569177 -
5.150303 L			
H-H-0.274700(PDBName=H,ResName=ARG,ResNum=197)	0	-18.907656	-2.429479 -
4.724805 L			
C-CX--0.263700(PDBName=CA,ResName=ARG,ResNum=197)	0	-17.938862	-1.642432 -
6.481638 L			
H-H1-0.156000(PDBName=HA,ResName=ARG,ResNum=197)	0	-16.920544	-1.253635 -
6.425136 L			
C-C8--0.000700(PDBName=CB,ResName=ARG,ResNum=197)	0	-17.894424	-3.095144 -
6.993058 L			
H-HC-0.032700(PDBName=HB2,ResName=ARG,ResNum=197)	0	-18.889545	-3.540246 -
6.945677 L			
H-HC-0.032700(PDBName=HB3,ResName=ARG,ResNum=197)	0	-17.609739	-3.058854 -
8.044869 L			
C-C8-0.039000(PDBName=CG,ResName=ARG,ResNum=197)	0	-16.900545	-3.998257 -
6.238527 L			
H-HC-0.028500(PDBName=HG2,ResName=ARG,ResNum=197)	0	-16.023142	-3.423345 -

5.942318 L
H-HC-0.028500(PDBName=HG3,ResName=ARG,ResNum=197) 0 -17.371046 -4.379033 -
5.335176 L
C-C8-0.048600(PDBName=CD,ResName=ARG,ResNum=197) 0 -16.450441 -5.188869 -
7.093882 H
H-H1-0.068700(PDBName=HD2,ResName=ARG,ResNum=197) 0 -15.903022 -5.879876 -
6.436730 H
H-H1-0.068700(PDBName=HD3,ResName=ARG,ResNum=197) 0 -17.346184 -5.707185 -
7.460288 H
N-N2--0.529500(PDBName=NE,ResName=ARG,ResNum=197) 0 -15.605267 -4.716472 -
8.179461 H
H-H-0.345600(PDBName=HE,ResName=ARG,ResNum=197) 0 -15.285596 -3.679219 -
8.166728 H
C-CA-0.807600(PDBName=CZ,ResName=ARG,ResNum=197) 0 -15.040243 -5.494090 -
9.079340 H
N-N2--0.862700(PDBName=NH1,ResName=ARG,ResNum=197) 0 -15.348025 -6.832037 -
9.241566 H
H-H-0.447800(PDBName=HH11,ResName=ARG,ResNum=197) 0 -15.841396 -7.268773 -
8.443653 H
H-H-0.447800(PDBName=HH12,ResName=ARG,ResNum=197) 0 -14.494636 -7.391061 -
9.370968 H
N-N2--0.862700(PDBName=NH2,ResName=ARG,ResNum=197) 0 -14.220736 -4.930244 -
9.983860 H
H-H-0.447800(PDBName=HH21,ResName=ARG,ResNum=197) 0 -13.707443 -4.065148 -
9.728652 H
H-H-0.447800(PDBName=HH22,ResName=ARG,ResNum=197) 0 -13.716453 -5.590608 -
10.583655 H
C-C-0.734100(PDBName=C,ResName=ARG,ResNum=197) 0 -18.685152 -0.779534 -
7.494496 L
O-O--0.589400(PDBName=O,ResName=ARG,ResNum=197) 0 -18.062424 -0.055322 -
8.280987 L
C-CJ--0.316472(PDBName=C1,ResName=DHK,ResNum=225) 0 -12.605432 -1.795294
0.543820 H
H-HK-0.158183(PDBName=H2,ResName=DHK,ResNum=225) 0 -13.166658 -0.870420
0.626388 H
C-CJ--0.090287(PDBName=C3,ResName=DHK,ResNum=225) 0 -12.173478 -2.469635
1.684094 H
H-HK-0.142318(PDBName=H4,ResName=DHK,ResNum=225) 0 -12.394822 -2.070538

2.668758 H
C-CJ--0.390043(PDBName=C5,ResName=DHK,ResNum=225) 0 -11.444267 -3.652686
1.581552 H
H-HK-0.190546(PDBName=H6,ResName=DHK,ResNum=225) 0 -11.090791 -4.174307
2.464317 H
C-CJ-0.446965(PDBName=C7,ResName=DHK,ResNum=225) 0 -11.160183 -4.201524
0.317387 H
O-OX--0.642443(PDBName=O8,ResName=DHK,ResNum=225) 0 -10.461643 -5.348873
0.254438 H
H-HY-0.433577(PDBName=H9,ResName=DHK,ResNum=225) 0 -10.376711 -5.564454 -
0.720692 H
C-CJ--0.168157(PDBName=C10,ResName=DHK,ResNum=225) 0 -11.608103 -3.546906 -
0.855565 H
C-CJ-0.254614(PDBName=C11,ResName=DHK,ResNum=225) 0 -11.324082 -4.089472 -
2.172852 H
O-OX--0.544517(PDBName=O12,ResName=DHK,ResNum=225) 0 -10.652307 -5.173842 -
2.285382 H
H-HY-0.383602(PDBName=H13,ResName=DHK,ResNum=225) 0 -9.233993 -5.082991 -
3.318460 H
C-CJ-0.213075(PDBName=C14,ResName=DHK,ResNum=225) 0 -12.307516 -2.310382 -
0.735553 H
C-CJ--0.377966(PDBName=C15,ResName=DHK,ResNum=225) 0 -12.643077 -1.607671 -
1.923242 H
H-HK-0.179148(PDBName=H16,ResName=DHK,ResNum=225) 0 -13.106709 -0.628923 -
1.833772 H
C-CJ-0.165502(PDBName=C17,ResName=DHK,ResNum=225) 0 -12.363440 -2.115695 -
3.201184 H
C-CZ--0.111477(PDBName=C18,ResName=DHK,ResNum=225) 0 -12.624972 -1.280941 -
4.428575 H
H-H8-0.032583(PDBName=H19,ResName=DHK,ResNum=225) 0 -13.498123 -0.640267 -
4.273080 H
H-H8-0.032583(PDBName=H20,ResName=DHK,ResNum=225) 0 -11.761119 -0.617920 -
4.564637 H
C-CJ--0.377452(PDBName=C21,ResName=DHK,ResNum=225) 0 -11.795800 -3.378034 -
3.345545 H
C-CZ-0.692240(PDBName=C22,ResName=DHK,ResNum=225) 0 -11.635162 -4.022930 -
4.709702 H
C-CZ--0.555194(PDBName=C23,ResName=DHK,ResNum=225) 0 -12.590335 -5.216397 -

4.873454 H
H-H8-0.129933(PDBName=H24,ResName=DHK,ResNum=225) 0 -12.385151 -5.980245 -
4.116152 H
H-H8-0.129933(PDBName=H25,ResName=DHK,ResNum=225) 0 -12.450968 -5.676882 -
5.856341 H
H-H8-0.129933(PDBName=H26,ResName=DHK,ResNum=225) 0 -13.639063 -4.918547 -
4.776853 H
H-H9--0.039392(PDBName=H27,ResName=DHK,ResNum=225) 0 -10.609034 -4.387795 -
4.806838 H
O-OI--0.712638(PDBName=O28,ResName=DHK,ResNum=225) 0 -11.779528 -3.106614 -
5.798640 H
C-CZ-0.665570(PDBName=C29,ResName=DHK,ResNum=225) 0 -12.836336 -2.146465 -
5.666164 H
H-H9--0.064844(PDBName=H30,ResName=DHK,ResNum=225) 0 -13.805036 -2.660030 -
5.575516 H
C-CZ--0.289485(PDBName=C31,ResName=DHK,ResNum=225) 0 -12.845531 -1.347122 -
6.976294 H
H-H8-0.039536(PDBName=H32,ResName=DHK,ResNum=225) 0 -11.815911 -1.077287 -
7.223462 H
H-H8-0.039536(PDBName=H33,ResName=DHK,ResNum=225) 0 -13.438602 -0.438073 -
6.830550 H
C-CV-0.810685(PDBName=C34,ResName=DHK,ResNum=225) 0 -13.490361 -2.180459 -
8.084187 H
O-O5--0.794847(PDBName=O35,ResName=DHK,ResNum=225) 0 -12.761515 -2.721664 -
8.952114 H
O-O5--0.794847(PDBName=O36,ResName=DHK,ResNum=225) 0 -14.763334 -2.278872 -
8.010726 H
O-O5--0.000000(PDBName=O1,ResName=OXY,ResNum=226) 0 -7.724405 -2.806432 -
2.258836 H
O-O5--0.000000(PDBName=O2,ResName=OXY,ResNum=226) 0 -8.975233 -2.363227 -
2.178399 H
O-OW--0.834000(PDBName=O,ResName=WAT,ResNum=425) 0 -10.261424 0.326367 -
2.307459 H
H-HW-0.417000(PDBName=H1,ResName=WAT,ResNum=425) 0 -9.735981 -0.431644 -
2.002856 H
H-HW-0.417000(PDBName=H2,ResName=WAT,ResNum=425) 0 -10.611807 0.704141 -
1.479639 H
O-OW--0.834000(PDBName=O,ResName=WAT,ResNum=639) 0 -8.447515 -4.752677 -

3.815614 H
H-HW-0.417000(PDBName=H1,ResName=WAT,ResNum=639) 0 -7.811655 -3.619075 -
2.862920 H
H-HW-0.417000(PDBName=H2,ResName=WAT,ResNum=639) 0 -7.930473 -5.530653 -
4.076001 H

o^sTS2 (QM, open-shell singlet)

0 1
N-N--0.415700(PDBName=N,ResName=ASN,ResNum=173) 0 -5.755714 3.028518 -
2.304654 L
H-H-0.271900(PDBName=H,ResName=ASN,ResNum=173) 0 -5.928169 2.606244 -
3.212034 L
C-CX-0.014300(PDBName=CA,ResName=ASN,ResNum=173) 0 -6.119047 2.267715 -
1.108762 L
H-H1-0.104800(PDBName=HA,ResName=ASN,ResNum=173) 0 -6.189121 2.943401 -
0.256641 L
C-2C--0.204100(PDBName=CB,ResName=ASN,ResNum=173) 0 -7.495750 1.618337 -
1.309302 H
H-HC-0.079700(PDBName=HB2,ResName=ASN,ResNum=173) 0 -8.229739 2.402807 -
1.488965 H
H-HC-0.079700(PDBName=HB3,ResName=ASN,ResNum=173) 0 -7.456816 0.966437 -
2.186809 H
C-C-0.713000(PDBName=CG,ResName=ASN,ResNum=173) 0 -7.913422 0.863268 -
0.049729 H
O-O--0.593100(PDBName=OD1,ResName=ASN,ResNum=173) 0 -8.354884 1.432138
0.942437 H
N-N--0.919100(PDBName=ND2,ResName=ASN,ResNum=173) 0 -7.708764 -0.483649 -
0.075947 H
H-H-0.419600(PDBName=HD21,ResName=ASN,ResNum=173) 0 -7.998744 -1.016782
0.730280 H
H-H-0.419600(PDBName=HD22,ResName=ASN,ResNum=173) 0 -7.488771 -1.010406 -
0.908945 H
C-C-0.597300(PDBName=C,ResName=ASN,ResNum=173) 0 -5.066648 1.193274 -
0.794972 L
O-O--0.567900(PDBName=O,ResName=ASN,ResNum=173) 0 -4.661013 0.466036 -
1.701395 L
N-N--0.415700(PDBName=N,ResName=TRP,ResNum=177) 0 -5.959463 -8.140234
5.607978 L

H-H-0.271900(PDBName=H,ResName=TRP,ResNum=177) 5.183634 L	0	-5.070423	-8.389431
C-CX--0.027500(PDBName=CA,ResName=TRP,ResNum=177) 5.947580 L	0	-6.837074	-9.261393
H-H1-0.112300(PDBName=HA,ResName=TRP,ResNum=177) 6.635504 L	0	-7.610740	-8.921600
C-CT--0.005000(PDBName=CB,ResName=TRP,ResNum=177) 4.656993 H	0	-7.509729	-9.763539
H-HC-0.033900(PDBName=HB2,ResName=TRP,ResNum=177) 4.004832 H	0	-6.702010	-10.107638
H-HC-0.033900(PDBName=HB3,ResName=TRP,ResNum=177) 4.922758 H	0	-8.080410	-10.661972
C-C*--0.141500(PDBName=CG,ResName=TRP,ResNum=177) 3.916594 H	0	-8.414669	-8.826253
C-CW--0.163800(PDBName=CD1,ResName=TRP,ResNum=177) 2.892747 H	0	-8.102319	-7.964862
H-H4-0.206200(PDBName=HD1,ResName=TRP,ResNum=177) 2.398522 H	0	-7.153593	-7.801424
N-NA--0.341800(PDBName=NE1,ResName=TRP,ResNum=177) 2.521696 H	0	-9.217741	-7.231859
H-H-0.341200(PDBName=HE1,ResName=TRP,ResNum=177) 1.675427 H	0	-9.309221	-6.684583
C-CN-0.138000(PDBName=CE2,ResName=TRP,ResNum=177) 3.300486 H	0	-10.286675	-7.627484
C-CA--0.260100(PDBName=CZ2,ResName=TRP,ResNum=177) 3.324577 H	0	-11.614728	-7.184266
H-HA-0.157200(PDBName=HZ2,ResName=TRP,ResNum=177) 2.646574 H	0	-11.969209	-6.414075
C-CA--0.113400(PDBName=CH2,ResName=TRP,ResNum=177) 4.262142 H	0	-12.466299	-7.756815
H-HA-0.141700(PDBName=HH2,ResName=TRP,ResNum=177) 4.350860 H	0	-13.481418	-7.386706
C-CA--0.197200(PDBName=CZ3,ResName=TRP,ResNum=177) 5.112060 H	0	-12.032034	-8.792875
H-HA-0.144700(PDBName=HZ3,ResName=TRP,ResNum=177) 5.808583 H	0	-12.730010	-9.248640
C-CA--0.238700(PDBName=CE3,ResName=TRP,ResNum=177) 5.076595 H	0	-10.718037	-9.235256

H-HA-0.170000(PDBName=HE3,ResName=TRP,ResNum=177)	0	-10.393772	-10.047357
5.719885 H			
C-CB-0.124300(PDBName=CD2,ResName=TRP,ResNum=177)	0	-9.814280	-8.629293
4.190735 H			
C-C-0.597300(PDBName=C,ResName=TRP,ResNum=177)	0	-6.065892	-10.411493
6.615463 L			
O-O--0.567900(PDBName=O,ResName=TRP,ResNum=177)	0	-4.860689	-10.582538
6.407865 L			
N-N--0.347900(PDBName=N,ResName=ARG,ResNum=197)	0	-18.570494	-1.580939 -
5.157025 L			
H-H-0.274700(PDBName=H,ResName=ARG,ResNum=197)	0	-18.900854	-2.441812 -
4.728498 L			
C-CX--0.263700(PDBName=CA,ResName=ARG,ResNum=197)	0	-17.936497	-1.652929 -
6.488646 L			
H-H1-0.156000(PDBName=HA,ResName=ARG,ResNum=197)	0	-16.918980	-1.262599 -
6.430310 L			
C-C8--0.000700(PDBName=CB,ResName=ARG,ResNum=197)	0	-17.889368	-3.104432 -
7.002948 L			
H-HC-0.032700(PDBName=HB2,ResName=ARG,ResNum=197)	0	-18.882996	-3.552639 -
6.952113 L			
H-HC-0.032700(PDBName=HB3,ResName=ARG,ResNum=197)	0	-17.608368	-3.065567 -
8.055692 L			
C-C8-0.039000(PDBName=CG,ResName=ARG,ResNum=197)	0	-16.889111	-4.005397 -
6.254919 L			
H-HC-0.028500(PDBName=HG2,ResName=ARG,ResNum=197)	0	-16.002409	-3.433015 -
5.981411 L			
H-HC-0.028500(PDBName=HG3,ResName=ARG,ResNum=197)	0	-17.346960	-4.371546 -
5.338792 L			
C-C8-0.048600(PDBName=CD,ResName=ARG,ResNum=197)	0	-16.462650	-5.208987 -
7.104687 H			
H-H1-0.068700(PDBName=HD2,ResName=ARG,ResNum=197)	0	-15.911045	-5.897401 -
6.448569 H			
H-H1-0.068700(PDBName=HD3,ResName=ARG,ResNum=197)	0	-17.368063	-5.722902 -
7.452547 H			
N-N2--0.529500(PDBName=NE,ResName=ARG,ResNum=197)	0	-15.629931	-4.755959 -
8.208643 H			
H-H-0.345600(PDBName=HE,ResName=ARG,ResNum=197)	0	-15.293994	-3.736122 -
8.200943 H			

C-CA-0.807600(PDBName=CZ,ResName=ARG,ResNum=197) 0 -15.070566 -5.548749 -
 9.102657 H
 N-N2--0.862700(PDBName=NH1,ResName=ARG,ResNum=197) 0 -15.385834 -6.886881 -
 9.242233 H
 H-H-0.447800(PDBName=HH11,ResName=ARG,ResNum=197) 0 -15.878890 -7.309291 -
 8.436408 H
 H-H-0.447800(PDBName=HH12,ResName=ARG,ResNum=197) 0 -14.535964 -7.452510 -
 9.365224 H
 N-N2--0.862700(PDBName=NH2,ResName=ARG,ResNum=197) 0 -14.254909 -5.002642 -
 10.017491 H
 H-H-0.447800(PDBName=HH21,ResName=ARG,ResNum=197) 0 -13.735221 -4.128087 -
 9.784350 H
 H-H-0.447800(PDBName=HH22,ResName=ARG,ResNum=197) 0 -13.753519 -5.676059 -
 10.605517 H
 C-C-0.734100(PDBName=C,ResName=ARG,ResNum=197) 0 -18.682467 -0.789276 -
 7.501502 L
 O-O--0.589400(PDBName=O,ResName=ARG,ResNum=197) 0 -18.057610 -0.069154 -
 8.290025 L
 C-CJ--0.316472(PDBName=C1,ResName=DHK,ResNum=225) 0 -11.546889 -1.825889
 0.338377 H
 H-HK-0.158183(PDBName=H2,ResName=DHK,ResNum=225) 0 -11.797826 -0.771753
 0.404457 H
 C-CJ--0.090287(PDBName=C3,ResName=DHK,ResNum=225) 0 -11.267983 -2.569635
 1.483767 H
 H-HK-0.142318(PDBName=H4,ResName=DHK,ResNum=225) 0 -11.348834 -2.105286
 2.460374 H
 C-CJ--0.390043(PDBName=C5,ResName=DHK,ResNum=225) 0 -10.870068 -3.902212
 1.392485 H
 H-HK-0.190546(PDBName=H6,ResName=DHK,ResNum=225) 0 -10.613491 -4.470718
 2.279686 H
 C-CJ-0.446965(PDBName=C7,ResName=DHK,ResNum=225) 0 -10.773585 -4.526697
 0.137554 H
 O-OX--0.642443(PDBName=O8,ResName=DHK,ResNum=225) 0 -10.338064 -5.800472
 0.082257 H
 H-HY-0.433577(PDBName=H9,ResName=DHK,ResNum=225) 0 -10.315926 -6.052211 -
 0.883012 H
 C-CJ--0.168157(PDBName=C10,ResName=DHK,ResNum=225) 0 -11.128105 -3.815011 -
 1.029980 H

C-CJ-0.254614(PDBName=C11,ResName=DHK,ResNum=225) 0 -11.064510 -4.437020 -
 2.350889 H
 O-OX--0.544517(PDBName=O12,ResName=DHK,ResNum=225) 0 -10.565605 -5.596685 -
 2.479770 H
 H-HY-0.383602(PDBName=H13,ResName=DHK,ResNum=225) 0 -8.997718 -5.229362 -
 3.460184 H
 C-CJ-0.213075(PDBName=C14,ResName=DHK,ResNum=225) 0 -11.482990 -2.446945 -
 0.919888 H
 C-CJ--0.377966(PDBName=C15,ResName=DHK,ResNum=225) 0 -11.684934 -1.717350 -
 2.127795 H
 H-HK-0.179148(PDBName=H16,ResName=DHK,ResNum=225) 0 -11.874485 -0.651299 -
 2.054645 H
 C-CJ-0.165502(PDBName=C17,ResName=DHK,ResNum=225) 0 -11.849234 -2.369128 -
 3.383670 H
 C-CZ--0.111477(PDBName=C18,ResName=DHK,ResNum=225) 0 -12.272909 -1.541687 -
 4.564411 H
 H-H8-0.032583(PDBName=H19,ResName=DHK,ResNum=225) 0 -13.125904 -0.911900 -
 4.282800 H
 H-H8-0.032583(PDBName=H20,ResName=DHK,ResNum=225) 0 -11.460442 -0.847504 -
 4.812562 H
 C-CJ--0.377452(PDBName=C21,ResName=DHK,ResNum=225) 0 -11.559275 -3.705867 -
 3.513011 H
 C-CZ-0.692240(PDBName=C22,ResName=DHK,ResNum=225) 0 -11.649428 -4.404854 -
 4.856957 H
 C-CZ--0.555194(PDBName=C23,ResName=DHK,ResNum=225) 0 -12.792575 -5.425150 -
 4.907364 H
 H-H8-0.129933(PDBName=H24,ResName=DHK,ResNum=225) 0 -12.638562 -6.204186 -
 4.153099 H
 H-H8-0.129933(PDBName=H25,ResName=DHK,ResNum=225) 0 -12.814493 -5.915950 -
 5.886469 H
 H-H8-0.129933(PDBName=H26,ResName=DHK,ResNum=225) 0 -13.768706 -4.966122 -
 4.725901 H
 H-H9--0.039392(PDBName=H27,ResName=DHK,ResNum=225) 0 -10.705894 -4.932369 -
 5.023881 H
 O-OI--0.712638(PDBName=O28,ResName=DHK,ResNum=225) 0 -11.726478 -3.480187 -
 5.953986 H
 C-CZ-0.665570(PDBName=C29,ResName=DHK,ResNum=225) 0 -12.652782 -2.396247 -
 5.771017 H

H-H9--0.064844(PDBName=H30,ResName=DHK,ResNum=225) 0 -13.667619 -2.792667 -
5.623205 H

C-CZ--0.289485(PDBName=C31,ResName=DHK,ResNum=225) 0 -12.644350 -1.583674 -
7.072147 H

H-H8-0.039536(PDBName=H32,ResName=DHK,ResNum=225) 0 -11.604825 -1.413097 -
7.363935 H

H-H8-0.039536(PDBName=H33,ResName=DHK,ResNum=225) 0 -13.131608 -0.621255 -
6.879948 H

C-CV-0.810685(PDBName=C34,ResName=DHK,ResNum=225) 0 -13.414940 -2.312402 -
8.171246 H

O-O5--0.794847(PDBName=O35,ResName=DHK,ResNum=225) 0 -12.762556 -2.858029 -
9.098762 H

O-O5--0.794847(PDBName=O36,ResName=DHK,ResNum=225) 0 -14.683567 -2.327870 -
8.039585 H

O-O5--0.000000(PDBName=O1,ResName=OXY,ResNum=226) 0 -8.703354 -2.413679 -
2.172842 H

O-O5--0.000000(PDBName=O2,ResName=OXY,ResNum=226) 0 -9.472283 -1.390539 -
2.631651 H

O-OW--0.834000(PDBName=O,ResName=WAT,ResNum=425) 0 -10.525110 0.971137 -
1.650658 H

H-HW-0.417000(PDBName=H1,ResName=WAT,ResNum=425) 0 -9.937379 0.196502 -
1.633271 H

H-HW-0.417000(PDBName=H2,ResName=WAT,ResNum=425) 0 -10.487217 1.325875 -
0.747428 H

O-OW--0.834000(PDBName=O,ResName=WAT,ResNum=639) 0 -8.431925 -4.542381 -
3.860892 H

H-HW-0.417000(PDBName=H1,ResName=WAT,ResNum=639) 0 -8.594034 -3.062182 -
2.924186 H

H-HW-0.417000(PDBName=H2,ResName=WAT,ResNum=639) 0 -7.596506 -4.964937 -
4.104335 H

¹M2 (QM, closed-shell singlet)

0 1

N-N--0.415700(PDBName=N,ResName=ASN,ResNum=173) 0 -5.786907 3.041908 -
2.277794 L

H-H-0.271900(PDBName=H,ResName=ASN,ResNum=173) 0 -5.967610 2.594810 -
3.171902 L

C-CX-0.014300(PDBName=CA,ResName=ASN,ResNum=173) 0 -6.150368 2.323803 -

1.045249 L
H-H1-0.104800(PDBName=HA,ResName=ASN,ResNum=173) 0 -6.085826 3.011785 -
0.204540 L
C-2C--0.204100(PDBName=CB,ResName=ASN,ResNum=173) 0 -7.609126 1.837970 -
1.114105 H
H-HC-0.079700(PDBName=HB2,ResName=ASN,ResNum=173) 0 -8.242332 2.679434 -
1.416066 H
H-HC-0.079700(PDBName=HB3,ResName=ASN,ResNum=173) 0 -7.713797 1.077209 -
1.894823 H
C-C-0.713000(PDBName=CG,ResName=ASN,ResNum=173) 0 -8.121315 1.286709
0.218015 H
O-O--0.593100(PDBName=OD1,ResName=ASN,ResNum=173) 0 -7.512159 1.297942
1.269315 H
N-N--0.919100(PDBName=ND2,ResName=ASN,ResNum=173) 0 -9.363806 0.658836
0.139387 H
H-H-0.419600(PDBName=HD21,ResName=ASN,ResNum=173) 0 -9.762433 0.465504
1.051517 H
H-H-0.419600(PDBName=HD22,ResName=ASN,ResNum=173) 0 -10.051610 1.013496 -
0.517557 H
C-C-0.597300(PDBName=C,ResName=ASN,ResNum=173) 0 -5.155211 1.181934 -
0.775333 L
O-O--0.567900(PDBName=O,ResName=ASN,ResNum=173) 0 -4.808979 0.459217 -
1.708146 L
N-N--0.415700(PDBName=N,ResName=TRP,ResNum=177) 0 -5.947859 -8.128705
5.630683 L
H-H-0.271900(PDBName=H,ResName=TRP,ResNum=177) 0 -5.061603 -8.377466
5.199889 L
C-CX--0.027500(PDBName=CA,ResName=TRP,ResNum=177) 0 -6.829749 -9.249033
5.963149 L
H-H1-0.112300(PDBName=HA,ResName=TRP,ResNum=177) 0 -7.597502 -8.910807
6.658200 L
C-CT--0.005000(PDBName=CB,ResName=TRP,ResNum=177) 0 -7.513304 -9.727639
4.668610 H
H-HC-0.033900(PDBName=HB2,ResName=TRP,ResNum=177) 0 -6.714494 -10.103771
4.023060 H
H-HC-0.033900(PDBName=HB3,ResName=TRP,ResNum=177) 0 -8.119336 -10.603350
4.931895 H
C-C*-0.141500(PDBName=CG,ResName=TRP,ResNum=177) 0 -8.372850 -8.755255

3.915565 H			
C-CW--0.163800(PDBName=CD1,ResName=TRP,ResNum=177)	0	-8.005437	-7.898431
2.904660 H			
H-H4-0.206200(PDBName=HD1,ResName=TRP,ResNum=177)	0	-7.038809	-7.762479
2.437443 H			
N-NA--0.341800(PDBName=NE1,ResName=TRP,ResNum=177)	0	-9.087574	-7.135070
2.502147 H			
H-H-0.341200(PDBName=HE1,ResName=TRP,ResNum=177)	0	-9.113009	-6.514492
1.702963 H			
C-CN-0.138000(PDBName=CE2,ResName=TRP,ResNum=177)	0	-10.188001	-7.495584
3.250492 H			
C-CA--0.260100(PDBName=CZ2,ResName=TRP,ResNum=177)	0	-11.504629	-7.019669
3.228586 H			
H-HA-0.157200(PDBName=HZ2,ResName=TRP,ResNum=177)	0	-11.816261	-6.240988
2.539088 H			
C-CA--0.113400(PDBName=CH2,ResName=TRP,ResNum=177)	0	-12.404484	-7.573826
4.131340 H			
H-HA-0.141700(PDBName=HH2,ResName=TRP,ResNum=177)	0	-13.415998	-7.184492
4.174207 H			
C-CA--0.197200(PDBName=CZ3,ResName=TRP,ResNum=177)	0	-12.024088	-8.615733
5.000341 H			
H-HA-0.144700(PDBName=HZ3,ResName=TRP,ResNum=177)	0	-12.757462	-9.052155
5.672620 H			
C-CA--0.238700(PDBName=CE3,ResName=TRP,ResNum=177)	0	-10.720062	-9.089645
5.013170 H			
H-HA-0.170000(PDBName=HE3,ResName=TRP,ResNum=177)	0	-10.437021	-9.901824
5.676892 H			
C-CB-0.124300(PDBName=CD2,ResName=TRP,ResNum=177)	0	-9.771849	-8.513199
4.153311 H			
C-C-0.597300(PDBName=C,ResName=TRP,ResNum=177)	0	-6.062323	-10.411599
6.617424 L			
O-O--0.567900(PDBName=O,ResName=TRP,ResNum=177)	0	-4.857789	-10.584369
6.407983 L			
N-N--0.347900(PDBName=N,ResName=ARG,ResNum=197)	0	-18.559383	-1.591138 -
5.140368 L			
H-H-0.274700(PDBName=H,ResName=ARG,ResNum=197)	0	-18.890316	-2.457490 -
4.723458 L			
C-CX--0.263700(PDBName=CA,ResName=ARG,ResNum=197)	0	-17.922943	-1.650150 -

6.471444 L
H-H1-0.156000(PDBName=HA,ResName=ARG,ResNum=197) 0 -16.906759 -1.257114 -
6.409374 L
C-C8--0.000700(PDBName=CB,ResName=ARG,ResNum=197) 0 -17.868917 -3.099319 -
6.992194 L
H-HC-0.032700(PDBName=HB2,ResName=ARG,ResNum=197) 0 -18.861261 -3.551096 -
6.946234 L
H-HC-0.032700(PDBName=HB3,ResName=ARG,ResNum=197) 0 -17.585007 -3.055164 -
8.043894 L
C-C8-0.039000(PDBName=CG,ResName=ARG,ResNum=197) 0 -16.868097 -4.001249 -
6.245431 L
H-HC-0.028500(PDBName=HG2,ResName=ARG,ResNum=197) 0 -15.979691 -3.430408 -
5.973550 L
H-HC-0.028500(PDBName=HG3,ResName=ARG,ResNum=197) 0 -17.323814 -4.367031 -
5.328490 L
C-C8-0.048600(PDBName=CD,ResName=ARG,ResNum=197) 0 -16.446489 -5.206012 -
7.095881 H
H-H1-0.068700(PDBName=HD2,ResName=ARG,ResNum=197) 0 -15.898399 -5.898180 -
6.440437 H
H-H1-0.068700(PDBName=HD3,ResName=ARG,ResNum=197) 0 -17.354328 -5.716421 -
7.443414 H
N-N2--0.529500(PDBName=NE,ResName=ARG,ResNum=197) 0 -15.612127 -4.754515 -
8.198187 H
H-H-0.345600(PDBName=HE,ResName=ARG,ResNum=197) 0 -15.274856 -3.727071 -
8.192938 H
C-CA-0.807600(PDBName=CZ,ResName=ARG,ResNum=197) 0 -15.056985 -5.547509 -
9.092799 H
N-N2--0.862700(PDBName=NH1,ResName=ARG,ResNum=197) 0 -15.382425 -6.881947 -
9.243682 H
H-H-0.447800(PDBName=HH11,ResName=ARG,ResNum=197) 0 -15.881999 -7.306007 -
8.442920 H
H-H-0.447800(PDBName=HH12,ResName=ARG,ResNum=197) 0 -14.536535 -7.453534 -
9.369841 H
N-N2--0.862700(PDBName=NH2,ResName=ARG,ResNum=197) 0 -14.232411 -4.999901 -
10.000570 H
H-H-0.447800(PDBName=HH21,ResName=ARG,ResNum=197) 0 -13.698972 -4.143741 -
9.741216 H
H-H-0.447800(PDBName=HH22,ResName=ARG,ResNum=197) 0 -13.731337 -5.671945 -

10.590427 H
C-C-0.734100(PDBName=C,ResName=ARG,ResNum=197) 0 -18.669752 -0.784388 -
7.482839 L
O-O--0.589400(PDBName=O,ResName=ARG,ResNum=197) 0 -18.045708 -0.053784 -
8.262884 L
C-CJ--0.316472(PDBName=C1,ResName=DHK,ResNum=225) 0 -11.968027 -1.747290
0.456414 H
H-HK-0.158183(PDBName=H2,ResName=DHK,ResNum=225) 0 -12.529681 -0.822500
0.550257 H
C-CJ--0.090287(PDBName=C3,ResName=DHK,ResNum=225) 0 -11.592460 -2.482049
1.589077 H
H-HK-0.142318(PDBName=H4,ResName=DHK,ResNum=225) 0 -11.864585 -2.126750
2.578942 H
C-CJ--0.390043(PDBName=C5,ResName=DHK,ResNum=225) 0 -10.866166 -3.659721
1.468668 H
H-HK-0.190546(PDBName=H6,ResName=DHK,ResNum=225) 0 -10.552897 -4.219633
2.342805 H
C-CJ-0.446965(PDBName=C7,ResName=DHK,ResNum=225) 0 -10.528546 -4.144405
0.195793 H
O-OX--0.642443(PDBName=O8,ResName=DHK,ResNum=225) 0 -9.831578 -5.294937
0.106185 H
H-HY-0.433577(PDBName=H9,ResName=DHK,ResNum=225) 0 -9.672500 -5.455157 -
0.863791 H
C-CJ--0.168157(PDBName=C10,ResName=DHK,ResNum=225) 0 -10.926952 -3.424536 -
0.958779 H
C-CJ-0.254614(PDBName=C11,ResName=DHK,ResNum=225) 0 -10.649172 -3.955553 -
2.305295 H
O-OX--0.544517(PDBName=O12,ResName=DHK,ResNum=225) 0 -9.908592 -4.955498 -
2.444220 H
H-HY-0.383602(PDBName=H13,ResName=DHK,ResNum=225) 0 -8.052989 -4.745524 -
3.777091 H
C-CJ-0.213075(PDBName=C14,ResName=DHK,ResNum=225) 0 -11.623726 -2.210541 -
0.808855 H
C-CJ--0.377966(PDBName=C15,ResName=DHK,ResNum=225) 0 -11.885724 -1.368662 -
2.032777 H
H-HK-0.179148(PDBName=H16,ResName=DHK,ResNum=225) 0 -12.817368 -0.805596 -
1.905993 H
C-CJ-0.165502(PDBName=C17,ResName=DHK,ResNum=225) 0 -11.870163 -2.110994 -

3.340814 H
C-CZ--0.111477(PDBName=C18,ResName=DHK,ResNum=225) 0 -12.404707 -1.374815 -
4.531456 H
H-H8-0.032583(PDBName=H19,ResName=DHK,ResNum=225) 0 -13.356828 -0.893258 -
4.277043 H
H-H8-0.032583(PDBName=H20,ResName=DHK,ResNum=225) 0 -11.707268 -0.560980 -
4.769875 H
C-CJ--0.377452(PDBName=C21,ResName=DHK,ResNum=225) 0 -11.286379 -3.320212 -
3.474208 H
C-CZ-0.692240(PDBName=C22,ResName=DHK,ResNum=225) 0 -11.194682 -4.027438 -
4.817783 H
C-CZ--0.555194(PDBName=C23,ResName=DHK,ResNum=225) 0 -12.084921 -5.271670 -
4.868048 H
H-H8-0.129933(PDBName=H24,ResName=DHK,ResNum=225) 0 -11.819378 -5.963852 -
4.063086 H
H-H8-0.129933(PDBName=H25,ResName=DHK,ResNum=225) 0 -11.951445 -5.804414 -
5.813597 H
H-H8-0.129933(PDBName=H26,ResName=DHK,ResNum=225) 0 -13.145621 -5.022891 -
4.756871 H
H-H9--0.039392(PDBName=H27,ResName=DHK,ResNum=225) 0 -10.153251 -4.326633 -
4.972991 H
O-OI--0.712638(PDBName=O28,ResName=DHK,ResNum=225) 0 -11.477884 -3.153655 -
5.922487 H
C-CZ-0.665570(PDBName=C29,ResName=DHK,ResNum=225) 0 -12.597652 -2.282255 -
5.744970 H
H-H9--0.064844(PDBName=H30,ResName=DHK,ResNum=225) 0 -13.518278 -2.868338 -
5.600248 H
C-CZ--0.289485(PDBName=C31,ResName=DHK,ResNum=225) 0 -12.732787 -1.470221 -
7.042444 H
H-H8-0.039536(PDBName=H32,ResName=DHK,ResNum=225) 0 -11.727742 -1.173845 -
7.351541 H
H-H8-0.039536(PDBName=H33,ResName=DHK,ResNum=225) 0 -13.333427 -0.577722 -
6.837546 H
C-CV-0.810685(PDBName=C34,ResName=DHK,ResNum=225) 0 -13.432270 -2.287125 -
8.125377 H
O-O5--0.794847(PDBName=O35,ResName=DHK,ResNum=225) 0 -12.731747 -2.870823 -
8.990615 H
O-O5--0.794847(PDBName=O36,ResName=DHK,ResNum=225) 0 -14.706668 -2.328541 -

8.040352 H
O-O5--0.000000(PDBName=O1,ResName=OXY,ResNum=226) 0 -9.589272 -0.834505 -
2.183789 H
O-O5--0.000000(PDBName=O2,ResName=OXY,ResNum=226) 0 -10.924357 -0.268769 -
2.114707 H
O-OW--0.834000(PDBName=O,ResName=WAT,ResNum=425) 0 -13.840593 0.948605 -
0.767251 H
H-HW-0.417000(PDBName=H1,ResName=WAT,ResNum=425) 0 -13.182767 1.373844 -
0.179778 H
H-HW-0.417000(PDBName=H2,ResName=WAT,ResNum=425) 0 -14.610015 0.888627 -
0.185717 H
O-OW--0.834000(PDBName=O,ResName=WAT,ResNum=639) 0 -7.719996 -4.661079 -
4.680052 H
H-HW-0.417000(PDBName=H1,ResName=WAT,ResNum=639) 0 -9.314699 -0.708318 -
1.246652 H
H-HW-0.417000(PDBName=H2,ResName=WAT,ResNum=639) 0 -6.976257 -4.035127 -
4.627835 H

¹TS3 (QM, closed-shell singlet)

0 1
N-N--0.415700(PDBName=N,ResName=ASN,ResNum=173) 0 -5.728160 2.998852 -
2.313299 L
H-H-0.271900(PDBName=H,ResName=ASN,ResNum=173) 0 -5.897433 2.601095 -
3.232227 L
C-CX-0.014300(PDBName=CA,ResName=ASN,ResNum=173) 0 -6.045297 2.159243 -
1.152530 L
H-H1-0.104800(PDBName=HA,ResName=ASN,ResNum=173) 0 -6.278656 2.787322 -
0.291672 L
C-2C--0.204100(PDBName=CB,ResName=ASN,ResNum=173) 0 -7.274743 1.291482 -
1.483445 H
H-HC-0.079700(PDBName=HB2,ResName=ASN,ResNum=173) 0 -8.131899 1.950438 -
1.621721 H
H-HC-0.079700(PDBName=HB3,ResName=ASN,ResNum=173) 0 -7.087584 0.761350 -
2.421225 H
C-C-0.713000(PDBName=CG,ResName=ASN,ResNum=173) 0 -7.596844 0.322516 -
0.342213 H
O-O--0.593100(PDBName=OD1,ResName=ASN,ResNum=173) 0 -8.084210 0.694198
0.712655 H

N-N--0.919100(PDBName=ND2,ResName=ASN,ResNum=173)	0	-7.291319	-0.990726	-
0.592016 H				
H-H-0.419600(PDBName=HD21,ResName=ASN,ResNum=173)	0	-7.355378	-1.629233	
0.190453 H				
H-H-0.419600(PDBName=HD22,ResName=ASN,ResNum=173)	0	-6.634287	-1.256771	-
1.311226 H				
C-C-0.597300(PDBName=C,ResName=ASN,ResNum=173)	0	-4.873236	1.230850	-
0.788153 L				
O-O--0.567900(PDBName=O,ResName=ASN,ResNum=173)	0	-4.327224	0.581302	-
1.679129 L				
N-N--0.415700(PDBName=N,ResName=TRP,ResNum=177)	0	-5.953648	-8.135755	
5.612489 L				
H-H-0.271900(PDBName=H,ResName=TRP,ResNum=177)	0	-5.068276	-8.388657	
5.182489 L				
C-CX--0.027500(PDBName=CA,ResName=TRP,ResNum=177)	0	-6.835984	-9.253475	
5.954172 L				
H-H1-0.112300(PDBName=HA,ResName=TRP,ResNum=177)	0	-7.599586	-8.910554	
6.651534 L				
C-CT--0.005000(PDBName=CB,ResName=TRP,ResNum=177)	0	-7.527126	-9.736313	
4.664360 H				
H-HC-0.033900(PDBName=HB2,ResName=TRP,ResNum=177)	0	-6.734481	-10.144513	
4.030418 H				
H-HC-0.033900(PDBName=HB3,ResName=TRP,ResNum=177)	0	-8.153889	-10.593185	
4.941695 H				
C-C*-0.141500(PDBName=CG,ResName=TRP,ResNum=177)	0	-8.361646	-8.764253	
3.880522 H				
C-CW--0.163800(PDBName=CD1,ResName=TRP,ResNum=177)	0	-7.972322	-7.959485	
2.834854 H				
H-H4-0.206200(PDBName=HD1,ResName=TRP,ResNum=177)	0	-7.001556	-7.866014	
2.365784 H				
N-NA--0.341800(PDBName=NE1,ResName=TRP,ResNum=177)	0	-9.034107	-7.188120	
2.394784 H				
H-H-0.341200(PDBName=HE1,ResName=TRP,ResNum=177)	0	-9.063310	-6.650018	
1.536394 H				
C-CN-0.138000(PDBName=CE2,ResName=TRP,ResNum=177)	0	-10.146185	-7.497316	
3.150225 H				
C-CA--0.260100(PDBName=CZ2,ResName=TRP,ResNum=177)	0	-11.451593	-6.995141	
3.093795 H				

H-HA-0.157200(PDBName=HZ2,ResName=TRP,ResNum=177)	0	-11.733699	-6.235554
2.371265 H			
C-CA--0.113400(PDBName=CH2,ResName=TRP,ResNum=177)	0	-12.372048	-7.495607
4.006611 H			
H-HA-0.141700(PDBName=HH2,ResName=TRP,ResNum=177)	0	-13.377334	-7.087882
4.019242 H			
C-CA--0.197200(PDBName=CZ3,ResName=TRP,ResNum=177)	0	-12.020282	-8.506472
4.923627 H			
H-HA-0.144700(PDBName=HZ3,ResName=TRP,ResNum=177)	0	-12.770081	-8.901516
5.603442 H			
C-CA--0.238700(PDBName=CE3,ResName=TRP,ResNum=177)	0	-10.724979	-9.002031
4.974357 H			
H-HA-0.170000(PDBName=HE3,ResName=TRP,ResNum=177)	0	-10.464232	-9.788167
5.677673 H			
C-CB-0.124300(PDBName=CD2,ResName=TRP,ResNum=177)	0	-9.757137	-8.482561
4.099447 H			
C-C-0.597300(PDBName=C,ResName=TRP,ResNum=177)	0	-6.065279	-10.415839
6.610067 L			
O-O--0.567900(PDBName=O,ResName=TRP,ResNum=177)	0	-4.860833	-10.586997
6.398365 L			
N-N--0.347900(PDBName=N,ResName=ARG,ResNum=197)	0	-18.549547	-1.580084 -
5.131071 L			
H-H-0.274700(PDBName=H,ResName=ARG,ResNum=197)	0	-18.890238	-2.441826 -
4.712235 L			
C-CX--0.263700(PDBName=CA,ResName=ARG,ResNum=197)	0	-17.914560	-1.647227 -
6.462974 L			
H-H1-0.156000(PDBName=HA,ResName=ARG,ResNum=197)	0	-16.899141	-1.251835 -
6.403506 L			
C-C8--0.000700(PDBName=CB,ResName=ARG,ResNum=197)	0	-17.857166	-3.098879 -
6.977351 L			
H-HC-0.032700(PDBName=HB2,ResName=ARG,ResNum=197)	0	-18.847256	-3.554637 -
6.922761 L			
H-HC-0.032700(PDBName=HB3,ResName=ARG,ResNum=197)	0	-17.580297	-3.057982 -
8.031109 L			
C-C8-0.039000(PDBName=CG,ResName=ARG,ResNum=197)	0	-16.846968	-3.994048 -
6.234906 L			
H-HC-0.028500(PDBName=HG2,ResName=ARG,ResNum=197)	0	-15.956671	-3.419190 -
5.977409 L			

H-HC-0.028500(PDBName=HG3,ResName=ARG,ResNum=197) 0 -17.294106 -4.352247 -
5.309702 L
C-C8-0.048600(PDBName=CD,ResName=ARG,ResNum=197) 0 -16.430569 -5.204190 -
7.082386 H
H-H1-0.068700(PDBName=HD2,ResName=ARG,ResNum=197) 0 -15.874154 -5.890778 -
6.428482 H
H-H1-0.068700(PDBName=HD3,ResName=ARG,ResNum=197) 0 -17.340549 -5.718239 -
7.418461 H
N-N2--0.529500(PDBName=NE,ResName=ARG,ResNum=197) 0 -15.608136 -4.759050 -
8.197847 H
H-H-0.345600(PDBName=HE,ResName=ARG,ResNum=197) 0 -15.272055 -3.740175 -
8.202228 H
C-CA-0.807600(PDBName=CZ,ResName=ARG,ResNum=197) 0 -15.051320 -5.555954 -
9.090468 H
N-N2--0.862700(PDBName=NH1,ResName=ARG,ResNum=197) 0 -15.365615 -6.894298 -
9.225412 H
H-H-0.447800(PDBName=HH11,ResName=ARG,ResNum=197) 0 -15.864814 -7.315126 -
8.422886 H
H-H-0.447800(PDBName=HH12,ResName=ARG,ResNum=197) 0 -14.516518 -7.460364 -
9.346593 H
N-N2--0.862700(PDBName=NH2,ResName=ARG,ResNum=197) 0 -14.238388 -5.013765 -
10.009724 H
H-H-0.447800(PDBName=HH21,ResName=ARG,ResNum=197) 0 -13.714374 -4.137848 -
9.783489 H
H-H-0.447800(PDBName=HH22,ResName=ARG,ResNum=197) 0 -13.741013 -5.691153 -
10.596926 H
C-C-0.734100(PDBName=C,ResName=ARG,ResNum=197) 0 -18.664944 -0.788092 -
7.477999 L
O-O--0.589400(PDBName=O,ResName=ARG,ResNum=197) 0 -18.043152 -0.062324 -
8.264161 L
C-CJ--0.316472(PDBName=C1,ResName=DHK,ResNum=225) 0 -11.210892 -1.649141
0.253221 H
H-HK-0.158183(PDBName=H2,ResName=DHK,ResNum=225) 0 -11.509354 -0.613308
0.355089 H
C-CJ--0.090287(PDBName=C3,ResName=DHK,ResNum=225) 0 -10.856719 -2.409316
1.363793 H
H-HK-0.142318(PDBName=H4,ResName=DHK,ResNum=225) 0 -10.935866 -1.969668
2.349787 H

C-CJ--0.390043(PDBName=C5,ResName=DHK,ResNum=225) 0 -10.420157 -3.727150
1.238229 H
H-HK-0.190546(PDBName=H6,ResName=DHK,ResNum=225) 0 -10.130774 -4.309888
2.105951 H
C-CJ-0.446965(PDBName=C7,ResName=DHK,ResNum=225) 0 -10.350698 -4.313046 -
0.027602 H
O-OX--0.642443(PDBName=O8,ResName=DHK,ResNum=225) 0 -9.901240 -5.580960 -
0.136985 H
H-HY-0.433577(PDBName=H9,ResName=DHK,ResNum=225) 0 -9.947151 -5.809276 -
1.113435 H
C-CJ--0.168157(PDBName=C10,ResName=DHK,ResNum=225) 0 -10.775382 -3.579519 -
1.171498 H
C-CJ-0.254614(PDBName=C11,ResName=DHK,ResNum=225) 0 -10.778820 -4.213693 -
2.491625 H
O-OX--0.544517(PDBName=O12,ResName=DHK,ResNum=225) 0 -10.323019 -5.375753 -
2.640526 H
H-HY-0.383602(PDBName=H13,ResName=DHK,ResNum=225) 0 -12.643096 1.540375 -
2.108674 H
C-CJ-0.213075(PDBName=C14,ResName=DHK,ResNum=225) 0 -11.181057 -2.234745 -
1.014175 H
C-CJ--0.377966(PDBName=C15,ResName=DHK,ResNum=225) 0 -11.680176 -1.499547 -
2.201305 H
H-HK-0.179148(PDBName=H16,ResName=DHK,ResNum=225) 0 -13.012920 -1.612360 -
2.011254 H
C-CJ-0.165502(PDBName=C17,ResName=DHK,ResNum=225) 0 -11.690003 -2.175139 -
3.508472 H
C-CZ--0.111477(PDBName=C18,ResName=DHK,ResNum=225) 0 -12.128050 -1.385138 -
4.705837 H
H-H8-0.032583(PDBName=H19,ResName=DHK,ResNum=225) 0 -12.954523 -0.716356 -
4.440823 H
H-H8-0.032583(PDBName=H20,ResName=DHK,ResNum=225) 0 -11.299360 -0.738732 -
5.010806 H
C-CJ--0.377452(PDBName=C21,ResName=DHK,ResNum=225) 0 -11.329713 -3.483831 -
3.630668 H
C-CZ-0.692240(PDBName=C22,ResName=DHK,ResNum=225) 0 -11.398761 -4.211471 -
4.963743 H
C-CZ--0.555194(PDBName=C23,ResName=DHK,ResNum=225) 0 -12.479077 -5.297367 -
4.979058 H

H-H8-0.129933(PDBName=H24,ResName=DHK,ResNum=225) 0 -12.273367 -6.041203 -
 4.203140 H
 H-H8-0.129933(PDBName=H25,ResName=DHK,ResNum=225) 0 -12.482913 -5.818110 -
 5.942846 H
 H-H8-0.129933(PDBName=H26,ResName=DHK,ResNum=225) 0 -13.478922 -4.888954 -
 4.801197 H
 H-H9--0.039392(PDBName=H27,ResName=DHK,ResNum=225) 0 -10.431456 -4.693953 -
 5.136988 H
 O-OI--0.712638(PDBName=O28,ResName=DHK,ResNum=225) 0 -11.558554 -3.315921 -
 6.078073 H
 C-CZ-0.665570(PDBName=C29,ResName=DHK,ResNum=225) 0 -12.532869 -2.284146 -
 5.869538 H
 H-H9--0.064844(PDBName=H30,ResName=DHK,ResNum=225) 0 -13.518000 -2.724597 -
 5.657764 H
 C-CZ--0.289485(PDBName=C31,ResName=DHK,ResNum=225) 0 -12.624795 -1.499133 -
 7.182345 H
 H-H8-0.039536(PDBName=H32,ResName=DHK,ResNum=225) 0 -11.605729 -1.292746 -
 7.516215 H
 H-H8-0.039536(PDBName=H33,ResName=DHK,ResNum=225) 0 -13.149458 -0.556483 -
 6.991044 H
 C-CV-0.810685(PDBName=C34,ResName=DHK,ResNum=225) 0 -13.399094 -2.289171 -
 8.233286 H
 O-O5--0.794847(PDBName=O35,ResName=DHK,ResNum=225) 0 -12.749723 -2.859958 -
 9.148441 H
 O-O5--0.794847(PDBName=O36,ResName=DHK,ResNum=225) 0 -14.663751 -2.325467 -
 8.076610 H
 O-O5--0.000000(PDBName=O1,ResName=OXY,ResNum=226) 0 -12.792982 0.711706 -
 1.597746 H
 O-O5--0.000000(PDBName=O2,ResName=OXY,ResNum=226) 0 -11.474138 -0.165694 -
 2.231597 H
 O-OW--0.834000(PDBName=O,ResName=WAT,ResNum=425) 0 -12.276533 3.214219 -
 2.730482 H
 H-HW-0.417000(PDBName=H1,ResName=WAT,ResNum=425) 0 -11.620142 3.362731 -
 3.426535 H
 H-HW-0.417000(PDBName=H2,ResName=WAT,ResNum=425) 0 -11.953089 3.717911 -
 1.969358 H
 O-OW--0.834000(PDBName=O,ResName=WAT,ResNum=639) 0 -14.201480 -1.212039 -
 1.777758 H

H-HW-0.417000(PDBName=H1,ResName=WAT,ResNum=639) 0 -13.821699 -0.216813 -
 1.747983 H
 H-HW-0.417000(PDBName=H2,ResName=WAT,ResNum=639) 0 -14.344289 -1.440937 -
 0.844052 H

¹EP (QM, closed-shell singlet)

0 1

N-N--0.415700(PDBName=N,ResName=ASN,ResNum=173) 0 -5.750929 3.016889 -
 2.299828 L
 H-H-0.271900(PDBName=H,ResName=ASN,ResNum=173) 0 -5.934411 2.601072 -
 3.208106 L
 C-CX-0.014300(PDBName=CA,ResName=ASN,ResNum=173) 0 -6.084678 2.226295 -
 1.109680 L
 H-H1-0.104800(PDBName=HA,ResName=ASN,ResNum=173) 0 -6.190821 2.891990 -
 0.254220 L
 C-2C--0.204100(PDBName=CB,ResName=ASN,ResNum=173) 0 -7.433791 1.525016 -
 1.332479 H
 H-HC-0.079700(PDBName=HB2,ResName=ASN,ResNum=173) 0 -8.183459 2.304098 -
 1.511840 H
 H-HC-0.079700(PDBName=HB3,ResName=ASN,ResNum=173) 0 -7.364451 0.908780 -
 2.233379 H
 C-C-0.713000(PDBName=CG,ResName=ASN,ResNum=173) 0 -7.871776 0.683035 -
 0.124864 H
 O-O--0.593100(PDBName=OD1,ResName=ASN,ResNum=173) 0 -7.626493 0.993761
 1.033060 H
 N-N--0.919100(PDBName=ND2,ResName=ASN,ResNum=173) 0 -8.554724 -0.451824 -
 0.454843 H
 H-H-0.419600(PDBName=HD21,ResName=ASN,ResNum=173) 0 -8.961492 -0.965966
 0.313521 H
 H-H-0.419600(PDBName=HD22,ResName=ASN,ResNum=173) 0 -8.998027 -0.538466 -
 1.363790 H
 C-C-0.597300(PDBName=C,ResName=ASN,ResNum=173) 0 -4.971972 1.212027 -
 0.785985 L
 O-O--0.567900(PDBName=O,ResName=ASN,ResNum=173) 0 -4.430666 0.594885 -
 1.701952 L
 N-N--0.415700(PDBName=N,ResName=TRP,ResNum=177) 0 -5.949992 -8.137188
 5.621311 L
 H-H-0.271900(PDBName=H,ResName=TRP,ResNum=177) 0 -5.067159 -8.385904

5.183394 L			
C-CX--0.027500(PDBName=CA,ResName=TRP,ResNum=177)	0	-6.830007	-9.256979
5.959408 L			
H-H1-0.112300(PDBName=HA,ResName=TRP,ResNum=177)	0	-7.595917	-8.917085
6.655560 L			
C-CT--0.005000(PDBName=CB,ResName=TRP,ResNum=177)	0	-7.517289	-9.742677
4.669922 H			
H-HC-0.033900(PDBName=HB2,ResName=TRP,ResNum=177)	0	-6.721563	-10.134995
4.030075 H			
H-HC-0.033900(PDBName=HB3,ResName=TRP,ResNum=177)	0	-8.132158	-10.609446
4.942617 H			
C-C*--0.141500(PDBName=CG,ResName=TRP,ResNum=177)	0	-8.366193	-8.771873
3.903361 H			
C-CW--0.163800(PDBName=CD1,ResName=TRP,ResNum=177)	0	-7.986427	-7.932977
2.882503 H			
H-H4-0.206200(PDBName=HD1,ResName=TRP,ResNum=177)	0	-7.016258	-7.812222
2.418520 H			
N-NA--0.341800(PDBName=NE1,ResName=TRP,ResNum=177)	0	-9.058537	-7.163790
2.464977 H			
H-H-0.341200(PDBName=HE1,ResName=TRP,ResNum=177)	0	-9.078896	-6.582034
1.636900 H			
C-CN-0.138000(PDBName=CE2,ResName=TRP,ResNum=177)	0	-10.167082	-7.506611
3.211334 H			
C-CA--0.260100(PDBName=CZ2,ResName=TRP,ResNum=177)	0	-11.479064	-7.019114
3.175681 H			
H-HA-0.157200(PDBName=HZ2,ResName=TRP,ResNum=177)	0	-11.778463	-6.242646
2.478586 H			
C-CA--0.113400(PDBName=CH2,ResName=TRP,ResNum=177)	0	-12.389242	-7.553994
4.079530 H			
H-HA-0.141700(PDBName=HH2,ResName=TRP,ResNum=177)	0	-13.397829	-7.155828
4.110228 H			
C-CA--0.197200(PDBName=CZ3,ResName=TRP,ResNum=177)	0	-12.022379	-8.586075
4.965945 H			
H-HA-0.144700(PDBName=HZ3,ResName=TRP,ResNum=177)	0	-12.763370	-9.006795
5.639925 H			
C-CA--0.238700(PDBName=CE3,ResName=TRP,ResNum=177)	0	-10.722063	-9.069589
4.994493 H			
H-HA-0.170000(PDBName=HE3,ResName=TRP,ResNum=177)	0	-10.449081	-9.872956

5.673163 H
C-CB-0.124300(PDBName=CD2,ResName=TRP,ResNum=177) 0 -9.764414 -8.514421
4.130886 H
C-C-0.597300(PDBName=C,ResName=TRP,ResNum=177) 0 -6.060263 -10.417411
6.613511 L
O-O--0.567900(PDBName=O,ResName=TRP,ResNum=177) 0 -4.854736 -10.587404
6.407421 L
N-N--0.347900(PDBName=N,ResName=ARG,ResNum=197) 0 -18.559090 -1.590836 -
5.163523 L
H-H-0.274700(PDBName=H,ResName=ARG,ResNum=197) 0 -18.876518 -2.458083 -
4.737742 L
C-CX--0.263700(PDBName=CA,ResName=ARG,ResNum=197) 0 -17.923410 -1.652204 -
6.495061 L
H-H1-0.156000(PDBName=HA,ResName=ARG,ResNum=197) 0 -16.906561 -1.260232 -
6.433534 L
C-C8--0.000700(PDBName=CB,ResName=ARG,ResNum=197) 0 -17.871502 -3.100991 -
7.017886 L
H-HC-0.032700(PDBName=HB2,ResName=ARG,ResNum=197) 0 -18.864500 -3.551377 -
6.972151 L
H-HC-0.032700(PDBName=HB3,ResName=ARG,ResNum=197) 0 -17.587627 -3.055605 -
8.069601 L
C-C8-0.039000(PDBName=CG,ResName=ARG,ResNum=197) 0 -16.871881 -4.006478 -
6.274397 L
H-HC-0.028500(PDBName=HG2,ResName=ARG,ResNum=197) 0 -15.982364 -3.437319 -
6.002842 L
H-HC-0.028500(PDBName=HG3,ResName=ARG,ResNum=197) 0 -17.328419 -4.372243 -
5.357288 L
C-C8-0.048600(PDBName=CD,ResName=ARG,ResNum=197) 0 -16.452940 -5.210432 -
7.128498 H
H-H1-0.068700(PDBName=HD2,ResName=ARG,ResNum=197) 0 -15.909881 -5.907261 -
6.474085 H
H-H1-0.068700(PDBName=HD3,ResName=ARG,ResNum=197) 0 -17.361700 -5.715884 -
7.480780 H
N-N2--0.529500(PDBName=NE,ResName=ARG,ResNum=197) 0 -15.611956 -4.760164 -
8.227244 H
H-H-0.345600(PDBName=HE,ResName=ARG,ResNum=197) 0 -15.288850 -3.733193 -
8.235198 H
C-CA-0.807600(PDBName=CZ,ResName=ARG,ResNum=197) 0 -15.033338 -5.554208 -

9.107079 H
N-N2--0.862700(PDBName=NH1,ResName=ARG,ResNum=197) 0 -15.341472 -6.892325 -
9.250792 H
H-H-0.447800(PDBName=HH11,ResName=ARG,ResNum=197) 0 -15.854906 -7.317889 -
8.460030 H
H-H-0.447800(PDBName=HH12,ResName=ARG,ResNum=197) 0 -14.491228 -7.457391 -
9.366626 H
N-N2--0.862700(PDBName=NH2,ResName=ARG,ResNum=197) 0 -14.199665 -5.007325 -
10.005783 H
H-H-0.447800(PDBName=HH21,ResName=ARG,ResNum=197) 0 -13.680608 -4.137725 -
9.763742 H
H-H-0.447800(PDBName=HH22,ResName=ARG,ResNum=197) 0 -13.696880 -5.678842 -
10.594541 H
C-C-0.734100(PDBName=C,ResName=ARG,ResNum=197) 0 -18.671993 -0.786176 -
7.503878 L
O-O--0.589400(PDBName=O,ResName=ARG,ResNum=197) 0 -18.051126 -0.054405 -
8.285158 L
O-OW--0.834000(PDBName=O,ResName=WAT,ResNum=425) 0 -10.208853 0.022089 -
2.875572 H
H-HW-0.417000(PDBName=H1,ResName=WAT,ResNum=425) 0 -10.744331 0.673368 -
2.376706 H
H-HW-0.417000(PDBName=H2,ResName=WAT,ResNum=425) 0 -9.667893 0.573481 -
3.456997 H
O-OW--0.834000(PDBName=O,ResName=WAT,ResNum=639) 0 -13.063990 0.973590
0.561795 H
H-HW-0.417000(PDBName=H1,ResName=WAT,ResNum=639) 0 -11.803622 3.205756
2.252909 H
H-HW-0.417000(PDBName=H2,ResName=WAT,ResNum=639) 0 -13.011053 1.462969
1.411977 H

'SP (QM, closed-shell singlet)

0 1
N-N--0.415700(PDBName=N,ResName=ASN,ResNum=173) 0 -5.757761 3.031872 -
2.311914 L
H-H-0.271900(PDBName=H,ResName=ASN,ResNum=173) 0 -5.941383 2.631634 -
3.226715 L
C-CX-0.014300(PDBName=CA,ResName=ASN,ResNum=173) 0 -6.113213 2.233228 -
1.136917 L

H-H1-0.104800(PDBName=HA,ResName=ASN,ResNum=173) 0.279663 L	0	-6.258199	2.891184	-
C-2C--0.204100(PDBName=CB,ResName=ASN,ResNum=173) 1.400017 H	0	-7.433696	1.487007	-
H-HC-0.079700(PDBName=HB2,ResName=ASN,ResNum=173) 1.559721 H	0	-8.224699	2.220696	-
H-HC-0.079700(PDBName=HB3,ResName=ASN,ResNum=173) 2.314037 H	0	-7.323177	0.896217	-
C-C-0.713000(PDBName=CG,ResName=ASN,ResNum=173) 0.192506 H	0	-7.794872	0.618838	-
O-O--0.593100(PDBName=OD1,ResName=ASN,ResNum=173) 0.876661 H	0	-8.152090	1.092178	
N-N--0.919100(PDBName=ND2,ResName=ASN,ResNum=173) 0.360736 H	0	-7.576549	-0.720450	-
H-H-0.419600(PDBName=HD21,ResName=ASN,ResNum=173) 0.375828 H	0	-7.889468	-1.336588	
H-H-0.419600(PDBName=HD22,ResName=ASN,ResNum=173) 1.272606 H	0	-7.511014	-1.144608	-
C-C-0.597300(PDBName=C,ResName=ASN,ResNum=173) 0.799045 L	0	-5.002749	1.222056	-
O-O--0.567900(PDBName=O,ResName=ASN,ResNum=173) 1.702613 L	0	-4.495771	0.555922	-
N-N--0.415700(PDBName=N,ResName=TRP,ResNum=177) 5.636287 L	0	-5.929369	-8.131503	
H-H-0.271900(PDBName=H,ResName=TRP,ResNum=177) 5.220560 L	0	-5.033651	-8.371002	
C-CX--0.027500(PDBName=CA,ResName=TRP,ResNum=177) 5.941633 L	0	-6.805496	-9.263651	
H-H1-0.112300(PDBName=HA,ResName=TRP,ResNum=177) 6.603273 L	0	-7.608837	-8.940283	
C-CT--0.005000(PDBName=CB,ResName=TRP,ResNum=177) 4.622174 H	0	-7.417679	-9.762193	
H-HC-0.033900(PDBName=HB2,ResName=TRP,ResNum=177) 3.955543 H	0	-6.578333	-9.978159	
H-HC-0.033900(PDBName=HB3,ResName=TRP,ResNum=177) 4.831712 H	0	-7.890522	-10.729314	
C-C*-0.141500(PDBName=CG,ResName=TRP,ResNum=177) 3.949604 H	0	-8.424084	-8.884163	

C-CW--0.163800(PDBName=CD1,ResName=TRP,ResNum=177)	0	-8.240684	-7.929851
2.978862 H			
H-H4-0.206200(PDBName=HD1,ResName=TRP,ResNum=177)	0	-7.332711	-7.632355
2.470827 H			
N-NA--0.341800(PDBName=NE1,ResName=TRP,ResNum=177)	0	-9.441319	-7.303117
2.688144 H			
H-H-0.341200(PDBName=HE1,ResName=TRP,ResNum=177)	0	-9.599735	-6.675249
1.909041 H			
C-CN-0.138000(PDBName=CE2,ResName=TRP,ResNum=177)	0	-10.431313	-7.855449
3.473856 H			
C-CA--0.260100(PDBName=CZ2,ResName=TRP,ResNum=177)	0	-11.796653	-7.566246
3.583199 H			
H-HA-0.157200(PDBName=HZ2,ResName=TRP,ResNum=177)	0	-12.275813	-6.813750
2.968035 H			
C-CA--0.113400(PDBName=CH2,ResName=TRP,ResNum=177)	0	-12.535653	-8.280789
4.517207 H			
H-HA-0.141700(PDBName=HH2,ResName=TRP,ResNum=177)	0	-13.574225	-8.021945
4.671405 H			
C-CA--0.197200(PDBName=CZ3,ResName=TRP,ResNum=177)	0	-11.962668	-9.317066
5.277448 H			
H-HA-0.144700(PDBName=HZ3,ResName=TRP,ResNum=177)	0	-12.578563	-9.886549
5.968537 H			
C-CA--0.238700(PDBName=CE3,ResName=TRP,ResNum=177)	0	-10.615368	-9.615999
5.149707 H			
H-HA-0.170000(PDBName=HE3,ResName=TRP,ResNum=177)	0	-10.176169	-10.433966
5.711090 H			
C-CB-0.124300(PDBName=CD2,ResName=TRP,ResNum=177)	0	-9.823248	-8.857176
4.276481 H			
C-C-0.597300(PDBName=C,ResName=TRP,ResNum=177)	0	-6.050790	-10.414271
6.622122 L			
O-O--0.567900(PDBName=O,ResName=TRP,ResNum=177)	0	-4.843857	-10.589316
6.428915 L			
N-N--0.347900(PDBName=N,ResName=ARG,ResNum=197)	0	-18.574156	-1.568145 -
5.147197 L			
H-H-0.274700(PDBName=H,ResName=ARG,ResNum=197)	0	-18.909555	-2.428246 -
4.721270 L			
C-CX--0.263700(PDBName=CA,ResName=ARG,ResNum=197)	0	-17.939369	-1.641349 -
6.477751 L			

H-H1-0.156000(PDBName=HA,ResName=ARG,ResNum=197) 0 -16.921465 -1.251599 -
 6.419609 L
 C-C8--0.000700(PDBName=CB,ResName=ARG,ResNum=197) 0 -17.892807 -3.094119 -
 6.988514 L
 H-HC-0.032700(PDBName=HB2,ResName=ARG,ResNum=197) 0 -18.888010 -3.539356 -
 6.943886 L
 H-HC-0.032700(PDBName=HB3,ResName=ARG,ResNum=197) 0 -17.605192 -3.058118 -
 8.039504 L
 C-C8-0.039000(PDBName=CG,ResName=ARG,ResNum=197) 0 -16.900837 -3.996963 -
 6.230864 L
 H-HC-0.028500(PDBName=HG2,ResName=ARG,ResNum=197) 0 -16.022572 -3.422934 -
 5.934099 L
 H-HC-0.028500(PDBName=HG3,ResName=ARG,ResNum=197) 0 -17.373182 -4.375696 -
 5.327732 L
 C-C8-0.048600(PDBName=CD,ResName=ARG,ResNum=197) 0 -16.452517 -5.189984 -
 7.083826 H
 H-H1-0.068700(PDBName=HD2,ResName=ARG,ResNum=197) 0 -15.908187 -5.881935 -
 6.425118 H
 H-H1-0.068700(PDBName=HD3,ResName=ARG,ResNum=197) 0 -17.348801 -5.706390 -
 7.451396 H
 N-N2--0.529500(PDBName=NE,ResName=ARG,ResNum=197) 0 -15.604320 -4.720685 -
 8.168340 H
 H-H-0.345600(PDBName=HE,ResName=ARG,ResNum=197) 0 -15.273649 -3.688240 -
 8.145592 H
 C-CA-0.807600(PDBName=CZ,ResName=ARG,ResNum=197) 0 -15.042213 -5.498157 -
 9.070371 H
 N-N2--0.862700(PDBName=NH1,ResName=ARG,ResNum=197) 0 -15.360337 -6.832735 -
 9.241489 H
 H-H-0.447800(PDBName=HH11,ResName=ARG,ResNum=197) 0 -15.857123 -7.269505 -
 8.445615 H
 H-H-0.447800(PDBName=HH12,ResName=ARG,ResNum=197) 0 -14.509676 -7.396551 -
 9.369871 H
 N-N2--0.862700(PDBName=NH2,ResName=ARG,ResNum=197) 0 -14.214175 -4.935289 -
 9.967414 H
 H-H-0.447800(PDBName=HH21,ResName=ARG,ResNum=197) 0 -13.688561 -4.081310 -
 9.696179 H
 H-H-0.447800(PDBName=HH22,ResName=ARG,ResNum=197) 0 -13.715750 -5.595938 -
 10.571720 H

C-C-0.734100(PDBName=C,ResName=ARG,ResNum=197) 7.491904 L	0	-18.684425	-0.778351	-
O-O--0.589400(PDBName=O,ResName=ARG,ResNum=197) 8.278735 L	0	-18.059708	-0.056423	-
C-CJ--0.316472(PDBName=C1,ResName=DHK,ResNum=225) 0.427789 H	0	-12.732234	-2.363417	
H-HK-0.158183(PDBName=H2,ResName=DHK,ResNum=225) 0.525750 H	0	-13.285189	-1.435104	
C-CJ--0.090287(PDBName=C3,ResName=DHK,ResNum=225) 1.482302 H	0	-12.668038	-3.279967	
H-HK-0.142318(PDBName=H4,ResName=DHK,ResNum=225) 2.403952 H	0	-13.210445	-3.096111	
C-CJ--0.390043(PDBName=C5,ResName=DHK,ResNum=225) 1.383978 H	0	-11.877802	-4.419728	
H-HK-0.190546(PDBName=H6,ResName=DHK,ResNum=225) 2.227526 H	0	-11.779588	-5.090180	
C-CJ-0.446965(PDBName=C7,ResName=DHK,ResNum=225) 0.209985 H	0	-11.162961	-4.701390	
O-OX--0.642443(PDBName=O8,ResName=DHK,ResNum=225) 0.203108 H	0	-10.347629	-5.795593	
H-HY-0.433577(PDBName=H9,ResName=DHK,ResNum=225) 0.656521 H	0	-9.885496	-5.827460	-
C-CJ--0.168157(PDBName=C10,ResName=DHK,ResNum=225) 0.881399 H	0	-11.292532	-3.839415	-
C-CJ-0.254614(PDBName=C11,ResName=DHK,ResNum=225) 2.151848 H	0	-10.469754	-3.827729	-
O-OX--0.544517(PDBName=O12,ResName=DHK,ResNum=225) 2.283879 H	0	-9.667855	-4.948133	-
H-HY-0.383602(PDBName=H13,ResName=DHK,ResNum=225) 2.949614 H	0	-8.958988	-4.786746	-
C-CJ-0.213075(PDBName=C14,ResName=DHK,ResNum=225) 0.731817 H	0	-12.026045	-2.653095	-
C-CJ--0.377966(PDBName=C15,ResName=DHK,ResNum=225) 1.836386 H	0	-11.710844	-1.687083	-
H-HK-0.179148(PDBName=H16,ResName=DHK,ResNum=225) 1.697173 H	0	-12.119545	-0.687457	-
C-CJ-0.165502(PDBName=C17,ResName=DHK,ResNum=225) 3.207525 H	0	-11.912050	-2.255346	-

C-CZ--0.111477(PDBName=C18,ResName=DHK,ResNum=225) 0 -12.532088 -1.489915 -
 4.334032 H
 H-H8-0.032583(PDBName=H19,ResName=DHK,ResNum=225) 0 -13.527109 -1.116187 -
 4.059133 H
 H-H8-0.032583(PDBName=H20,ResName=DHK,ResNum=225) 0 -11.915055 -0.599765 -
 4.514909 H
 C-CJ--0.377452(PDBName=C21,ResName=DHK,ResNum=225) 0 -11.269915 -3.417072 -
 3.379197 H
 C-CZ-0.692240(PDBName=C22,ResName=DHK,ResNum=225) 0 -11.209631 -4.109048 -
 4.721832 H
 C-CZ--0.555194(PDBName=C23,ResName=DHK,ResNum=225) 0 -12.108658 -5.346731 -
 4.764138 H
 H-H8-0.129933(PDBName=H24,ResName=DHK,ResNum=225) 0 -11.826700 -6.043637 -
 3.967914 H
 H-H8-0.129933(PDBName=H25,ResName=DHK,ResNum=225) 0 -12.011852 -5.875890 -
 5.717557 H
 H-H8-0.129933(PDBName=H26,ResName=DHK,ResNum=225) 0 -13.160918 -5.089191 -
 4.613224 H
 H-H9--0.039392(PDBName=H27,ResName=DHK,ResNum=225) 0 -10.178289 -4.417995 -
 4.927701 H
 O-OI--0.712638(PDBName=O28,ResName=DHK,ResNum=225) 0 -11.514805 -3.203561 -
 5.797289 H
 C-CZ-0.665570(PDBName=C29,ResName=DHK,ResNum=225) 0 -12.657839 -2.351946 -
 5.598068 H
 H-H9--0.064844(PDBName=H30,ResName=DHK,ResNum=225) 0 -13.565008 -2.967803 -
 5.507991 H
 C-CZ--0.289485(PDBName=C31,ResName=DHK,ResNum=225) 0 -12.776436 -1.487267 -
 6.866402 H
 H-H8-0.039536(PDBName=H32,ResName=DHK,ResNum=225) 0 -11.771571 -1.158313 -
 7.143335 H
 H-H8-0.039536(PDBName=H33,ResName=DHK,ResNum=225) 0 -13.393077 -0.613264 -
 6.632348 H
 C-CV-0.810685(PDBName=C34,ResName=DHK,ResNum=225) 0 -13.444911 -2.254133 -
 8.006938 H
 O-O5--0.794847(PDBName=O35,ResName=DHK,ResNum=225) 0 -12.724460 -2.795557 -
 8.884009 H
 O-O5--0.794847(PDBName=O36,ResName=DHK,ResNum=225) 0 -14.721834 -2.298220 -
 7.961292 H

O-O5--0.000000(PDBName=O1,ResName=OXY,ResNum=226) 0 -9.499880 -2.696930 -
1.925732 H
O-O5--0.000000(PDBName=O2,ResName=OXY,ResNum=226) 0 -10.239441 -1.459231 -
1.684716 H
O-OW--0.834000(PDBName=O,ResName=WAT,ResNum=425) 0 -10.677197 1.011583 -
2.627310 H
H-HW-0.417000(PDBName=H1,ResName=WAT,ResNum=425) 0 -10.133425 0.244631 -
2.385858 H
H-HW-0.417000(PDBName=H2,ResName=WAT,ResNum=425) 0 -10.976048 1.342451 -
1.757371 H
O-OW--0.834000(PDBName=O,ResName=WAT,ResNum=639) 0 -7.673061 -4.710906 -
4.218192 H
H-HW-0.417000(PDBName=H1,ResName=WAT,ResNum=639) 0 -6.971976 -4.058452 -
4.403930 H
H-HW-0.417000(PDBName=H2,ResName=WAT,ResNum=639) 0 -7.277669 -5.566762 -
4.449720 H

^oM1 (L4)

0 1

N-N--0.415700(PDBName=N,ResName=ASN,ResNum=173) 0 -5.737309 3.010909 -
2.313060 L
H-H-0.271900(PDBName=H,ResName=ASN,ResNum=173) 0 -5.907265 2.609623 -
3.230405 L
C-CX-0.014300(PDBName=CA,ResName=ASN,ResNum=173) 0 -6.091741 2.197879 -
1.145626 L
H-H1-0.104800(PDBName=HA,ResName=ASN,ResNum=173) 0 -6.278759 2.846546 -
0.289559 L
C-2C--0.204100(PDBName=CB,ResName=ASN,ResNum=173) 0 -7.379637 1.411376 -
1.455257 H
H-HC-0.079700(PDBName=HB2,ResName=ASN,ResNum=173) 0 -8.184889 2.114771 -
1.652720 H
H-HC-0.079700(PDBName=HB3,ResName=ASN,ResNum=173) 0 -7.216425 0.812995 -
2.356179 H
C-C-0.713000(PDBName=CG,ResName=ASN,ResNum=173) 0 -7.817830 0.528226 -
0.287474 H
O-O--0.593100(PDBName=OD1,ResName=ASN,ResNum=173) 0 -8.564377 0.929001
0.600174 H
N-N--0.919100(PDBName=ND2,ResName=ASN,ResNum=173) 0 -7.299919 -0.730810 -

0.268842 H			
H-H-0.419600(PDBName=HD21,ResName=ASN,ResNum=173)	0	-7.630476	-1.365846
0.442886 H			
H-H-0.419600(PDBName=HD22,ResName=ASN,ResNum=173)	0	-6.818472	-1.162699 -
1.045201 H			
C-C-0.597300(PDBName=C,ResName=ASN,ResNum=173)	0	-4.966681	1.210573 -
0.792228 L			
O-O--0.567900(PDBName=O,ResName=ASN,ResNum=173)	0	-4.489667	0.503392 -
1.680220 L			
N-N--0.415700(PDBName=N,ResName=TRP,ResNum=177)	0	-5.952887	-8.130648
5.618852 L			
H-H-0.271900(PDBName=H,ResName=TRP,ResNum=177)	0	-5.064770	-8.385143
5.195737 L			
C-CX--0.027500(PDBName=CA,ResName=TRP,ResNum=177)	0	-6.839893	-9.246734
5.953134 L			
H-H1-0.112300(PDBName=HA,ResName=TRP,ResNum=177)	0	-7.604034	-8.904858
6.650552 L			
C-CT--0.005000(PDBName=CB,ResName=TRP,ResNum=177)	0	-7.529131	-9.719215
4.658139 H			
H-HC-0.033900(PDBName=HB2,ResName=TRP,ResNum=177)	0	-6.736997	-10.122591
4.020250 H			
H-HC-0.033900(PDBName=HB3,ResName=TRP,ResNum=177)	0	-8.159997	-10.575605
4.927501 H			
C-C*-0.141500(PDBName=CG,ResName=TRP,ResNum=177)	0	-8.359943	-8.739192
3.881062 H			
C-CW--0.163800(PDBName=CD1,ResName=TRP,ResNum=177)	0	-7.968180	-7.923904
2.845004 H			
H-H4-0.206200(PDBName=HD1,ResName=TRP,ResNum=177)	0	-6.995209	-7.823373
2.382153 H			
N-NA--0.341800(PDBName=NE1,ResName=TRP,ResNum=177)	0	-9.032645	-7.151558
2.409625 H			
H-H-0.341200(PDBName=HE1,ResName=TRP,ResNum=177)	0	-9.059731	-6.587566
1.570251 H			
C-CN-0.138000(PDBName=CE2,ResName=TRP,ResNum=177)	0	-10.146938	-7.472210
3.156650 H			
C-CA--0.260100(PDBName=CZ2,ResName=TRP,ResNum=177)	0	-11.457409	-6.984139
3.094817 H			
H-HA-0.157200(PDBName=HZ2,ResName=TRP,ResNum=177)	0	-11.748412	-6.232872

2.368297 H
C-CA--0.113400(PDBName=CH2,ResName=TRP,ResNum=177) 0 -12.375230 -7.494590
4.005272 H
H-HA-0.141700(PDBName=HH2,ResName=TRP,ResNum=177) 0 -13.383559 -7.095058
4.015666 H
C-CA--0.197200(PDBName=CZ3,ResName=TRP,ResNum=177) 0 -12.017980 -8.505091
4.921041 H
H-HA-0.144700(PDBName=HZ3,ResName=TRP,ResNum=177) 0 -12.766297 -8.906406
5.598601 H
C-CA--0.238700(PDBName=CE3,ResName=TRP,ResNum=177) 0 -10.719776 -8.993856
4.970152 H
H-HA-0.170000(PDBName=HE3,ResName=TRP,ResNum=177) 0 -10.451366 -9.782160
5.667897 H
C-CB-0.124300(PDBName=CD2,ResName=TRP,ResNum=177) 0 -9.755555 -8.462681
4.099467 H
C-C-0.597300(PDBName=C,ResName=TRP,ResNum=177) 0 -6.072030 -10.412625
6.606711 L
O-O--0.567900(PDBName=O,ResName=TRP,ResNum=177) 0 -4.868948 -10.587261
6.389941 L
N-N--0.347900(PDBName=N,ResName=ARG,ResNum=197) 0 -18.567184 -1.559773 -
5.133966 L
H-H-0.274700(PDBName=H,ResName=ARG,ResNum=197) 0 -18.897896 -2.422069 -
4.708502 L
C-CX--0.263700(PDBName=CA,ResName=ARG,ResNum=197) 0 -17.924006 -1.629992 -
6.459900 L
H-H1-0.156000(PDBName=HA,ResName=ARG,ResNum=197) 0 -16.913931 -1.220948 -
6.397516 L
C-C8--0.000700(PDBName=CB,ResName=ARG,ResNum=197) 0 -17.843300 -3.087361 -
6.952500 L
H-HC-0.032700(PDBName=HB2,ResName=ARG,ResNum=197) 0 -18.828295 -3.554774 -
6.904594 L
H-HC-0.032700(PDBName=HB3,ResName=ARG,ResNum=197) 0 -17.551813 -3.058797 -
8.002571 L
C-C8-0.039000(PDBName=CG,ResName=ARG,ResNum=197) 0 -16.832096 -3.953124 -
6.174929 L
H-HC-0.028500(PDBName=HG2,ResName=ARG,ResNum=197) 0 -15.969796 -3.352035 -
5.886409 L
H-HC-0.028500(PDBName=HG3,ResName=ARG,ResNum=197) 0 -17.297688 -4.325778 -

5.265603 L
C-C8-0.048600(PDBName=CD,ResName=ARG,ResNum=197) 0 -16.348574 -5.150424 -
7.002498 H
H-H1-0.068700(PDBName=HD2,ResName=ARG,ResNum=197) 0 -15.782254 -5.814496 -
6.333240 H
H-H1-0.068700(PDBName=HD3,ResName=ARG,ResNum=197) 0 -17.230947 -5.698591 -
7.358241 H
N-N2--0.529500(PDBName=NE,ResName=ARG,ResNum=197) 0 -15.517639 -4.678263 -
8.098251 H
H-H-0.345600(PDBName=HE,ResName=ARG,ResNum=197) 0 -15.215945 -3.634122 -
8.098874 H
C-CA-0.807600(PDBName=CZ,ResName=ARG,ResNum=197) 0 -14.982383 -5.450837 -
9.019335 H
N-N2--0.862700(PDBName=NH1,ResName=ARG,ResNum=197) 0 -15.297055 -6.787452 -
9.181908 H
H-H-0.447800(PDBName=HH11,ResName=ARG,ResNum=197) 0 -15.780232 -7.229206 -
8.381142 H
H-H-0.447800(PDBName=HH12,ResName=ARG,ResNum=197) 0 -14.449095 -7.349524 -
9.329947 H
N-N2--0.862700(PDBName=NH2,ResName=ARG,ResNum=197) 0 -14.188281 -4.881550 -
9.943679 H
H-H-0.447800(PDBName=HH21,ResName=ARG,ResNum=197) 0 -13.669290 -4.019117 -
9.694261 H
H-H-0.447800(PDBName=HH22,ResName=ARG,ResNum=197) 0 -13.701463 -5.536971 -
10.562857 H
C-C-0.734100(PDBName=C,ResName=ARG,ResNum=197) 0 -18.675800 -0.784769 -
7.485285 L
O-O--0.589400(PDBName=O,ResName=ARG,ResNum=197) 0 -18.055456 -0.066046 -
8.278714 L
C-CJ--0.316472(PDBName=C1,ResName=DHK,ResNum=225) 0 -11.922064 -1.881186
0.525695 H
H-HK-0.158183(PDBName=H2,ResName=DHK,ResNum=225) 0 -12.386427 -0.911564
0.668302 H
C-CJ--0.090287(PDBName=C3,ResName=DHK,ResNum=225) 0 -11.401579 -2.583162
1.610070 H
H-HK-0.142318(PDBName=H4,ResName=DHK,ResNum=225) 0 -11.489098 -2.172433
2.609822 H
C-CJ--0.390043(PDBName=C5,ResName=DHK,ResNum=225) 0 -10.757611 -3.806707

1.429499 H
H-HK-0.190546(PDBName=H6,ResName=DHK,ResNum=225) 0 -10.329374 -4.349094
2.265167 H
C-CJ-0.446965(PDBName=C7,ResName=DHK,ResNum=225) 0 -10.653647 -4.362191
0.143258 H
O-OX--0.642443(PDBName=O8,ResName=DHK,ResNum=225) 0 -10.027025 -5.545572
0.004167 H
H-HY-0.433577(PDBName=H9,ResName=DHK,ResNum=225) 0 -10.062912 -5.767234 -
0.971473 H
C-CJ--0.168157(PDBName=C10,ResName=DHK,ResNum=225) 0 -11.201423 -3.681932 -
0.971147 H
C-CJ-0.254614(PDBName=C11,ResName=DHK,ResNum=225) 0 -11.073194 -4.215886 -
2.313227 H
O-OX--0.544517(PDBName=O12,ResName=DHK,ResNum=225) 0 -10.467606 -5.329525 -
2.505833 H
H-HY-0.383602(PDBName=H13,ResName=DHK,ResNum=225) 0 -9.082821 -5.126911 -
3.497623 H
C-CJ-0.213075(PDBName=C14,ResName=DHK,ResNum=225) 0 -11.814859 -2.410891 -
0.775497 H
C-CJ--0.377966(PDBName=C15,ResName=DHK,ResNum=225) 0 -12.253387 -1.684970 -
1.915481 H
H-HK-0.179148(PDBName=H16,ResName=DHK,ResNum=225) 0 -12.658211 -0.689390 -
1.769059 H
C-CJ-0.165502(PDBName=C17,ResName=DHK,ResNum=225) 0 -12.119022 -2.187102 -
3.218508 H
C-CZ--0.111477(PDBName=C18,ResName=DHK,ResNum=225) 0 -12.465906 -1.323739 -
4.404500 H
H-H8-0.032583(PDBName=H19,ResName=DHK,ResNum=225) 0 -13.330112 -0.692009 -
4.176151 H
H-H8-0.032583(PDBName=H20,ResName=DHK,ResNum=225) 0 -11.619470 -0.647788 -
4.579916 H
C-CJ--0.377452(PDBName=C21,ResName=DHK,ResNum=225) 0 -11.604608 -3.461502 -
3.428554 H
C-CZ-0.692240(PDBName=C22,ResName=DHK,ResNum=225) 0 -11.554522 -4.078978 -
4.811036 H
C-CZ--0.555194(PDBName=C23,ResName=DHK,ResNum=225) 0 -12.576864 -5.218010 -
4.942619 H
H-H8-0.129933(PDBName=H24,ResName=DHK,ResNum=225) 0 -12.357770 -6.010949 -

4.219738 H
H-H8-0.129933(PDBName=H25,ResName=DHK,ResNum=225) 0 -12.530158 -5.650520 -
5.946782 H
H-H8-0.129933(PDBName=H26,ResName=DHK,ResNum=225) 0 -13.598520 -4.868798 -
4.764498 H
H-H9--0.039392(PDBName=H27,ResName=DHK,ResNum=225) 0 -10.553580 -4.488821 -
4.973782 H
O-OI--0.712638(PDBName=O28,ResName=DHK,ResNum=225) 0 -11.718055 -3.127820 -
5.865801 H
C-CZ-0.665570(PDBName=C29,ResName=DHK,ResNum=225) 0 -12.749971 -2.154024 -
5.653376 H
H-H9--0.064844(PDBName=H30,ResName=DHK,ResNum=225) 0 -13.723417 -2.653699 -
5.534264 H
C-CZ--0.289485(PDBName=C31,ResName=DHK,ResNum=225) 0 -12.799814 -1.316893 -
6.936278 H
H-H8-0.039536(PDBName=H32,ResName=DHK,ResNum=225) 0 -11.778605 -1.027704 -
7.195716 H
H-H8-0.039536(PDBName=H33,ResName=DHK,ResNum=225) 0 -13.404223 -0.422785 -
6.752292 H
C-CV-0.810685(PDBName=C34,ResName=DHK,ResNum=225) 0 -13.452387 -2.138123 -
8.047250 H
O-O5--0.794847(PDBName=O35,ResName=DHK,ResNum=225) 0 -12.727637 -2.684914 -
8.914526 H
O-O5--0.794847(PDBName=O36,ResName=DHK,ResNum=225) 0 -14.725595 -2.230840 -
7.970662 H
O-O5--0.000000(PDBName=O1,ResName=OXY,ResNum=226) 0 -7.682512 -2.818806 -
2.328558 H
O-O5--0.000000(PDBName=O2,ResName=OXY,ResNum=226) 0 -8.924258 -2.345545 -
2.314083 H
O-OW--0.834000(PDBName=O,ResName=WAT,ResNum=425) 0 -10.203074 0.311533 -
2.084248 H
H-HW-0.417000(PDBName=H1,ResName=WAT,ResNum=425) 0 -9.682421 -0.501023 -
1.970019 H
H-HW-0.417000(PDBName=H2,ResName=WAT,ResNum=425) 0 -10.292305 0.637993 -
1.172997 H
O-OW--0.834000(PDBName=O,ResName=WAT,ResNum=639) 0 -8.298872 -4.742006 -
3.960679 H
H-HW-0.417000(PDBName=H1,ResName=WAT,ResNum=639) 0 -7.748592 -3.613389 -

2.962253 H
H-HW-0.417000(PDBName=H2,ResName=WAT,ResNum=639) 0 -7.732200 -5.488827 -
4.208514 H

OSTS2 (L4)

0 1
N-N--0.415700(PDBName=N,ResName=ASN,ResNum=173) 0 -5.757116 3.026149 -
2.309052 L
H-H-0.271900(PDBName=H,ResName=ASN,ResNum=173) 0 -5.925573 2.611073 -
3.220445 L
C-CX-0.014300(PDBName=CA,ResName=ASN,ResNum=173) 0 -6.124401 2.247762 -
1.123925 L
H-H1-0.104800(PDBName=HA,ResName=ASN,ResNum=173) 0 -6.228560 2.914796 -
0.268166 L
C-2C--0.204100(PDBName=CB,ResName=ASN,ResNum=173) 0 -7.477292 1.557603 -
1.360682 H
H-HC-0.079700(PDBName=HB2,ResName=ASN,ResNum=173) 0 -8.235136 2.320046 -
1.535191 H
H-HC-0.079700(PDBName=HB3,ResName=ASN,ResNum=173) 0 -7.406279 0.926506 -
2.251680 H
C-C-0.713000(PDBName=CG,ResName=ASN,ResNum=173) 0 -7.908959 0.761599 -
0.130422 H
O-O--0.593100(PDBName=OD1,ResName=ASN,ResNum=173) 0 -8.386229 1.300112
0.863197 H
N-N--0.919100(PDBName=ND2,ResName=ASN,ResNum=173) 0 -7.706355 -0.583667 -
0.191161 H
H-H-0.419600(PDBName=HD21,ResName=ASN,ResNum=173) 0 -8.045609 -1.144351
0.576793 H
H-H-0.419600(PDBName=HD22,ResName=ASN,ResNum=173) 0 -7.462169 -1.082817 -
1.033551 H
C-C-0.597300(PDBName=C,ResName=ASN,ResNum=173) 0 -5.052727 1.195315 -
0.801149 L
O-O--0.567900(PDBName=O,ResName=ASN,ResNum=173) 0 -4.622705 0.479475 -
1.705416 L
N-N--0.415700(PDBName=N,ResName=TRP,ResNum=177) 0 -5.956688 -8.133509
5.617840 L
H-H-0.271900(PDBName=H,ResName=TRP,ResNum=177) 0 -5.069053 -8.386018
5.192522 L

C-CX--0.027500(PDBName=CA,ResName=TRP,ResNum=177)	0	-6.840170	-9.250485
5.955323 L			
H-H1-0.112300(PDBName=HA,ResName=TRP,ResNum=177)	0	-7.607135	-8.908356
6.649437 L			
C-CT--0.005000(PDBName=CB,ResName=TRP,ResNum=177)	0	-7.524206	-9.735999
4.663356 H			
H-HC-0.033900(PDBName=HB2,ResName=TRP,ResNum=177)	0	-6.728779	-10.139036
4.029472 H			
H-HC-0.033900(PDBName=HB3,ResName=TRP,ResNum=177)	0	-8.150345	-10.594317
4.937817 H			
C-C*--0.141500(PDBName=CG,ResName=TRP,ResNum=177)	0	-8.360133	-8.768242
3.878737 H			
C-CW--0.163800(PDBName=CD1,ResName=TRP,ResNum=177)	0	-7.975261	-7.967869
2.829602 H			
H-H4-0.206200(PDBName=HD1,ResName=TRP,ResNum=177)	0	-7.004574	-7.870992
2.361255 H			
N-NA--0.341800(PDBName=NE1,ResName=TRP,ResNum=177)	0	-9.042855	-7.202318
2.389040 H			
H-H-0.341200(PDBName=HE1,ResName=TRP,ResNum=177)	0	-9.089359	-6.694879
1.515276 H			
C-CN-0.138000(PDBName=CE2,ResName=TRP,ResNum=177)	0	-10.154337	-7.518700
3.143708 H			
C-CA--0.260100(PDBName=CZ2,ResName=TRP,ResNum=177)	0	-11.466538	-7.035696
3.080924 H			
H-HA-0.157200(PDBName=HZ2,ResName=TRP,ResNum=177)	0	-11.764532	-6.300044
2.341410 H			
C-CA--0.113400(PDBName=CH2,ResName=TRP,ResNum=177)	0	-12.377254	-7.531976
4.006382 H			
H-HA-0.141700(PDBName=HH2,ResName=TRP,ResNum=177)	0	-13.385450	-7.132666
4.018432 H			
C-CA--0.197200(PDBName=CZ3,ResName=TRP,ResNum=177)	0	-12.012779	-8.527321
4.935419 H			
H-HA-0.144700(PDBName=HZ3,ResName=TRP,ResNum=177)	0	-12.756248	-8.919566
5.623509 H			
C-CA--0.238700(PDBName=CE3,ResName=TRP,ResNum=177)	0	-10.713470	-9.013210
4.983523 H			
H-HA-0.170000(PDBName=HE3,ResName=TRP,ResNum=177)	0	-10.439682	-9.791873
5.689520 H			

C-CB-0.124300(PDBName=CD2,ResName=TRP,ResNum=177)	0	-9.755731	-8.492719
4.099798 H			
C-C-0.597300(PDBName=C,ResName=TRP,ResNum=177)	0	-6.070085	-10.409867
6.614034 L			
O-O--0.567900(PDBName=O,ResName=TRP,ResNum=177)	0	-4.866044	-10.582647
6.401036 L			
N-N--0.347900(PDBName=N,ResName=ARG,ResNum=197)	0	-18.563185	-1.573145 -
5.143365 L			
H-H-0.274700(PDBName=H,ResName=ARG,ResNum=197)	0	-18.891630	-2.435783 -
4.716712 L			
C-CX--0.263700(PDBName=CA,ResName=ARG,ResNum=197)	0	-17.919933	-1.641601 -
6.470296 L			
H-H1-0.156000(PDBName=HA,ResName=ARG,ResNum=197)	0	-16.910633	-1.231353 -
6.406554 L			
C-C8--0.000700(PDBName=CB,ResName=ARG,ResNum=197)	0	-17.837479	-3.097198 -
6.968774 L			
H-HC-0.032700(PDBName=HB2,ResName=ARG,ResNum=197)	0	-18.821140	-3.567204 -
6.917508 L			
H-HC-0.032700(PDBName=HB3,ResName=ARG,ResNum=197)	0	-17.550329	-3.064277 -
8.019997 L			
C-C8-0.039000(PDBName=CG,ResName=ARG,ResNum=197)	0	-16.819672	-3.963526 -
6.201271 L			
H-HC-0.028500(PDBName=HG2,ResName=ARG,ResNum=197)	0	-15.945428	-3.367080 -
5.940057 L			
H-HC-0.028500(PDBName=HG3,ResName=ARG,ResNum=197)	0	-17.270489	-4.317868 -
5.276880 L			
C-C8-0.048600(PDBName=CD,ResName=ARG,ResNum=197)	0	-16.365494	-5.177517 -
7.022373 H			
H-H1-0.068700(PDBName=HD2,ResName=ARG,ResNum=197)	0	-15.794782	-5.838763 -
6.354255 H			
H-H1-0.068700(PDBName=HD3,ResName=ARG,ResNum=197)	0	-17.260204	-5.719582 -
7.355431 H			
N-N2--0.529500(PDBName=NE,ResName=ARG,ResNum=197)	0	-15.548423	-4.731016 -
8.139744 H			
H-H-0.345600(PDBName=HE,ResName=ARG,ResNum=197)	0	-15.230722	-3.703156 -
8.155723 H			
C-CA-0.807600(PDBName=CZ,ResName=ARG,ResNum=197)	0	-15.017215	-5.523878 -
9.049569 H			

N-N2--0.862700(PDBName=NH1,ResName=ARG,ResNum=197) 0 -15.335817 -6.862176 -
 9.180885 H
 H-H-0.447800(PDBName=HH11,ResName=ARG,ResNum=197) 0 -15.818272 -7.285936 -
 8.370032 H
 H-H-0.447800(PDBName=HH12,ResName=ARG,ResNum=197) 0 -14.490620 -7.430470 -
 9.319985 H
 N-N2--0.862700(PDBName=NH2,ResName=ARG,ResNum=197) 0 -14.228576 -4.977581 -
 9.988575 H
 H-H-0.447800(PDBName=HH21,ResName=ARG,ResNum=197) 0 -13.705253 -4.102408 -
 9.770246 H
 H-H-0.447800(PDBName=HH22,ResName=ARG,ResNum=197) 0 -13.741394 -5.649722 -
 10.589710 H
 C-C-0.734100(PDBName=C,ResName=ARG,ResNum=197) 0 -18.671898 -0.794140 -
 7.494039 L
 O-O--0.589400(PDBName=O,ResName=ARG,ResNum=197) 0 -18.049793 -0.079331 -
 8.289551 L
 C-CJ--0.316472(PDBName=C1,ResName=DHK,ResNum=225) 0 -11.354738 -1.857007
 0.290208 H
 H-HK-0.158183(PDBName=H2,ResName=DHK,ResNum=225) 0 -11.596250 -0.801936
 0.370945 H
 C-CJ--0.090287(PDBName=C3,ResName=DHK,ResNum=225) 0 -11.000466 -2.602278
 1.412610 H
 H-HK-0.142318(PDBName=H4,ResName=DHK,ResNum=225) 0 -11.027280 -2.141191
 2.392030 H
 C-CJ--0.390043(PDBName=C5,ResName=DHK,ResNum=225) 0 -10.604327 -3.934114
 1.295615 H
 H-HK-0.190546(PDBName=H6,ResName=DHK,ResNum=225) 0 -10.289077 -4.504383
 2.162343 H
 C-CJ-0.446965(PDBName=C7,ResName=DHK,ResNum=225) 0 -10.588539 -4.556605
 0.036967 H
 O-OX--0.642443(PDBName=O8,ResName=DHK,ResNum=225) 0 -10.157333 -5.830822 -
 0.042692 H
 H-HY-0.433577(PDBName=H9,ResName=DHK,ResNum=225) 0 -10.206145 -6.091004 -
 1.004042 H
 C-CJ--0.168157(PDBName=C10,ResName=DHK,ResNum=225) 0 -11.016719 -3.843702 -
 1.105191 H
 C-CJ-0.254614(PDBName=C11,ResName=DHK,ResNum=225) 0 -11.015531 -4.457754 -
 2.429929 H

O-OX--0.544517(PDBName=O12,ResName=DHK,ResNum=225) 0 -10.543642 -5.626709 -
2.587454 H

H-HY-0.383602(PDBName=H13,ResName=DHK,ResNum=225) 0 -9.027594 -5.248556 -
3.586670 H

C-CJ-0.213075(PDBName=C14,ResName=DHK,ResNum=225) 0 -11.372476 -2.477383 -
0.969921 H

C-CJ--0.377966(PDBName=C15,ResName=DHK,ResNum=225) 0 -11.647217 -1.742691 -
2.156597 H

H-HK-0.179148(PDBName=H16,ResName=DHK,ResNum=225) 0 -11.847415 -0.680905 -
2.065049 H

C-CJ-0.165502(PDBName=C17,ResName=DHK,ResNum=225) 0 -11.820132 -2.375605 -
3.416645 H

C-CZ--0.111477(PDBName=C18,ResName=DHK,ResNum=225) 0 -12.246236 -1.530362 -
4.581616 H

H-H8-0.032583(PDBName=H19,ResName=DHK,ResNum=225) 0 -13.092288 -0.896634 -
4.289548 H

H-H8-0.032583(PDBName=H20,ResName=DHK,ResNum=225) 0 -11.426084 -0.842919 -
4.822341 H

C-CJ--0.377452(PDBName=C21,ResName=DHK,ResNum=225) 0 -11.524003 -3.708510 -
3.570303 H

C-CZ-0.692240(PDBName=C22,ResName=DHK,ResNum=225) 0 -11.640904 -4.388792 -
4.920392 H

C-CZ--0.555194(PDBName=C23,ResName=DHK,ResNum=225) 0 -12.809963 -5.379315 -
4.962970 H

H-H8-0.129933(PDBName=H24,ResName=DHK,ResNum=225) 0 -12.654390 -6.174976 -
4.226188 H

H-H8-0.129933(PDBName=H25,ResName=DHK,ResNum=225) 0 -12.870338 -5.845075 -
5.952762 H

H-H8-0.129933(PDBName=H26,ResName=DHK,ResNum=225) 0 -13.767367 -4.896814 -
4.746909 H

H-H9--0.039392(PDBName=H27,ResName=DHK,ResNum=225) 0 -10.712077 -4.934696 -
5.105831 H

O-OI--0.712638(PDBName=O28,ResName=DHK,ResNum=225) 0 -11.715099 -3.449786 -
6.004030 H

C-CZ-0.665570(PDBName=C29,ResName=DHK,ResNum=225) 0 -12.635810 -2.365706 -
5.797096 H

H-H9--0.064844(PDBName=H30,ResName=DHK,ResNum=225) 0 -13.652088 -2.759605 -
5.651465 H

C-CZ--0.289485(PDBName=C31,ResName=DHK,ResNum=225) 0 -12.627034 -1.536811 -
 7.084742 H
 H-H8-0.039536(PDBName=H32,ResName=DHK,ResNum=225) 0 -11.586860 -1.359024 -
 7.368542 H
 H-H8-0.039536(PDBName=H33,ResName=DHK,ResNum=225) 0 -13.124668 -0.581509 -
 6.886158 H
 C-CV-0.810685(PDBName=C34,ResName=DHK,ResNum=225) 0 -13.388446 -2.273349 -
 8.181788 H
 O-O5--0.794847(PDBName=O35,ResName=DHK,ResNum=225) 0 -12.733201 -2.828263 -
 9.100484 H
 O-O5--0.794847(PDBName=O36,ResName=DHK,ResNum=225) 0 -14.657328 -2.294276 -
 8.048532 H
 O-O5--0.000000(PDBName=O1,ResName=OXY,ResNum=226) 0 -8.683351 -2.477542 -
 2.282351 H
 O-O5--0.000000(PDBName=O2,ResName=OXY,ResNum=226) 0 -9.414615 -1.421595 -
 2.715382 H
 O-OW--0.834000(PDBName=O,ResName=WAT,ResNum=425) 0 -10.467665 0.892668 -
 1.590846 H
 H-HW-0.417000(PDBName=H1,ResName=WAT,ResNum=425) 0 -9.884598 0.115497 -
 1.623623 H
 H-HW-0.417000(PDBName=H2,ResName=WAT,ResNum=425) 0 -10.372319 1.229614 -
 0.685316 H
 O-OW--0.834000(PDBName=O,ResName=WAT,ResNum=639) 0 -8.467953 -4.562367 -
 4.000270 H
 H-HW-0.417000(PDBName=H1,ResName=WAT,ResNum=639) 0 -8.606769 -3.120946 -
 3.044276 H
 H-HW-0.417000(PDBName=H2,ResName=WAT,ResNum=639) 0 -7.616102 -4.974830 -
 4.200898 H

¹M2 (L4)

0 1

N-N--0.415700(PDBName=N,ResName=ASN,ResNum=173) 0 -5.790989 3.042514 -
 2.282342 L
 H-H-0.271900(PDBName=H,ResName=ASN,ResNum=173) 0 -5.968702 2.598886 -
 3.178789 L
 C-CX-0.014300(PDBName=CA,ResName=ASN,ResNum=173) 0 -6.161775 2.318340 -
 1.055269 L
 H-H1-0.104800(PDBName=HA,ResName=ASN,ResNum=173) 0 -6.110510 3.005642 -

0.212492 L
C-2C--0.204100(PDBName=CB,ResName=ASN,ResNum=173) 0 -7.614391 1.811765 -
1.138071 H
H-HC-0.079700(PDBName=HB2,ResName=ASN,ResNum=173) 0 -8.257695 2.641838 -
1.449055 H
H-HC-0.079700(PDBName=HB3,ResName=ASN,ResNum=173) 0 -7.702380 1.041938 -
1.912369 H
C-C-0.713000(PDBName=CG,ResName=ASN,ResNum=173) 0 -8.127843 1.268475
0.198620 H
O-O--0.593100(PDBName=OD1,ResName=ASN,ResNum=173) 0 -7.543015 1.351650
1.261674 H
N-N--0.919100(PDBName=ND2,ResName=ASN,ResNum=173) 0 -9.327856 0.571199
0.112751 H
H-H-0.419600(PDBName=HD21,ResName=ASN,ResNum=173) 0 -9.741282 0.369562
1.015056 H
H-H-0.419600(PDBName=HD22,ResName=ASN,ResNum=173) 0 -10.009634 0.828290 -
0.593880 H
C-C-0.597300(PDBName=C,ResName=ASN,ResNum=173) 0 -5.162454 1.181765 -
0.780706 L
O-O--0.567900(PDBName=O,ResName=ASN,ResNum=173) 0 -4.816321 0.454222 -
1.710058 L
N-N--0.415700(PDBName=N,ResName=TRP,ResNum=177) 0 -5.945391 -8.126106
5.635612 L
H-H-0.271900(PDBName=H,ResName=TRP,ResNum=177) 0 -5.059591 -8.377447
5.205416 L
C-CX--0.027500(PDBName=CA,ResName=TRP,ResNum=177) 0 -6.831395 -9.243522
5.966289 L
H-H1-0.112300(PDBName=HA,ResName=TRP,ResNum=177) 0 -7.595689 -8.903777
6.664366 L
C-CT--0.005000(PDBName=CB,ResName=TRP,ResNum=177) 0 -7.520385 -9.712765
4.670519 H
H-HC-0.033900(PDBName=HB2,ResName=TRP,ResNum=177) 0 -6.729518 -10.123716
4.036092 H
H-HC-0.033900(PDBName=HB3,ResName=TRP,ResNum=177) 0 -8.159229 -10.563541
4.938894 H
C-C*--0.141500(PDBName=CG,ResName=TRP,ResNum=177) 0 -8.338503 -8.725506
3.889589 H
C-CW--0.163800(PDBName=CD1,ResName=TRP,ResNum=177) 0 -7.929804 -7.909360

2.860633 H			
H-H4-0.206200(PDBName=HD1,ResName=TRP,ResNum=177)	0	-6.951250	-7.814102
2.408568 H			
N-NA--0.341800(PDBName=NE1,ResName=TRP,ResNum=177)	0	-8.983940	-7.130370
2.415130 H			
H-H-0.341200(PDBName=HE1,ResName=TRP,ResNum=177)	0	-8.989483	-6.546336
1.589218 H			
C-CN-0.138000(PDBName=CE2,ResName=TRP,ResNum=177)	0	-10.107869	-7.443824
3.149013 H			
C-CA--0.260100(PDBName=CZ2,ResName=TRP,ResNum=177)	0	-11.415479	-6.950390
3.070752 H			
H-HA-0.157200(PDBName=HZ2,ResName=TRP,ResNum=177)	0	-11.695113	-6.200231
2.338409 H			
C-CA--0.113400(PDBName=CH2,ResName=TRP,ResNum=177)	0	-12.348159	-7.458339
3.967579 H			
H-HA-0.141700(PDBName=HH2,ResName=TRP,ResNum=177)	0	-13.356110	-7.057181
3.961683 H			
C-CA--0.197200(PDBName=CZ3,ResName=TRP,ResNum=177)	0	-12.007008	-8.470125
4.888111 H			
H-HA-0.144700(PDBName=HZ3,ResName=TRP,ResNum=177)	0	-12.766067	-8.868459
5.555453 H			
C-CA--0.238700(PDBName=CE3,ResName=TRP,ResNum=177)	0	-10.711654	-8.965176
4.953406 H			
H-HA-0.170000(PDBName=HE3,ResName=TRP,ResNum=177)	0	-10.455816	-9.754644
5.654840 H			
C-CB-0.124300(PDBName=CD2,ResName=TRP,ResNum=177)	0	-9.733848	-8.439210
4.094650 H			
C-C-0.597300(PDBName=C,ResName=TRP,ResNum=177)	0	-6.064623	-10.411129
6.615977 L			
O-O--0.567900(PDBName=O,ResName=TRP,ResNum=177)	0	-4.860793	-10.584889
6.403168 L			
N-N--0.347900(PDBName=N,ResName=ARG,ResNum=197)	0	-18.548225	-1.573575 -
5.126728 L			
H-H-0.274700(PDBName=H,ResName=ARG,ResNum=197)	0	-18.889254	-2.436021 -
4.709780 L			
C-CX--0.263700(PDBName=CA,ResName=ARG,ResNum=197)	0	-17.908564	-1.639263 -
6.455454 L			
H-H1-0.156000(PDBName=HA,ResName=ARG,ResNum=197)	0	-16.896748	-1.234761 -

6.394177 L
C-C8--0.000700(PDBName=CB,ResName=ARG,ResNum=197) 0 -17.835583 -3.093891 -
6.958235 L
H-HC-0.032700(PDBName=HB2,ResName=ARG,ResNum=197) 0 -18.822535 -3.557160 -
6.909192 L
H-HC-0.032700(PDBName=HB3,ResName=ARG,ResNum=197) 0 -17.548697 -3.059352 -
8.009430 L
C-C8-0.039000(PDBName=CG,ResName=ARG,ResNum=197) 0 -16.825193 -3.972063 -
6.194362 L
H-HC-0.028500(PDBName=HG2,ResName=ARG,ResNum=197) 0 -15.946980 -3.384217 -
5.925807 L
H-HC-0.028500(PDBName=HG3,ResName=ARG,ResNum=197) 0 -17.281105 -4.331270 -
5.274365 L
C-C8-0.048600(PDBName=CD,ResName=ARG,ResNum=197) 0 -16.378948 -5.181945 -
7.025869 H
H-H1-0.068700(PDBName=HD2,ResName=ARG,ResNum=197) 0 -15.816651 -5.855435 -
6.362655 H
H-H1-0.068700(PDBName=HD3,ResName=ARG,ResNum=197) 0 -17.277451 -5.713784 -
7.365969 H
N-N2--0.529500(PDBName=NE,ResName=ARG,ResNum=197) 0 -15.555211 -4.731131 -
8.135849 H
H-H-0.345600(PDBName=HE,ResName=ARG,ResNum=197) 0 -15.230257 -3.697927 -
8.142476 H
C-CA-0.807600(PDBName=CZ,ResName=ARG,ResNum=197) 0 -15.023366 -5.519803 -
9.047165 H
N-N2--0.862700(PDBName=NH1,ResName=ARG,ResNum=197) 0 -15.354505 -6.853303 -
9.199590 H
H-H-0.447800(PDBName=HH11,ResName=ARG,ResNum=197) 0 -15.847010 -7.281632 -
8.397104 H
H-H-0.447800(PDBName=HH12,ResName=ARG,ResNum=197) 0 -14.512162 -7.427311 -
9.337386 H
N-N2--0.862700(PDBName=NH2,ResName=ARG,ResNum=197) 0 -14.219095 -4.967535 -
9.971480 H
H-H-0.447800(PDBName=HH21,ResName=ARG,ResNum=197) 0 -13.675920 -4.116957 -
9.714449 H
H-H-0.447800(PDBName=HH22,ResName=ARG,ResNum=197) 0 -13.730777 -5.636602 -
10.575316 H
C-C-0.734100(PDBName=C,ResName=ARG,ResNum=197) 0 -18.660666 -0.787789 -

7.476338 L
O-O--0.589400(PDBName=O,ResName=ARG,ResNum=197) 0 -18.039824 -0.062713 -
8.263846 L
C-CJ--0.316472(PDBName=C1,ResName=DHK,ResNum=225) 0 -11.668061 -1.745113
0.425866 H
H-HK-0.158183(PDBName=H2,ResName=DHK,ResNum=225) 0 -12.135232 -0.772199
0.538449 H
C-CJ--0.090287(PDBName=C3,ResName=DHK,ResNum=225) 0 -11.303713 -2.499965
1.548424 H
H-HK-0.142318(PDBName=H4,ResName=DHK,ResNum=225) 0 -11.506218 -2.118827
2.544791 H
C-CJ--0.390043(PDBName=C5,ResName=DHK,ResNum=225) 0 -10.681482 -3.732836
1.406804 H
H-HK-0.190546(PDBName=H6,ResName=DHK,ResNum=225) 0 -10.375726 -4.314519
2.268970 H
C-CJ-0.446965(PDBName=C7,ResName=DHK,ResNum=225) 0 -10.440558 -4.248181
0.124154 H
O-OX--0.642443(PDBName=O8,ResName=DHK,ResNum=225) 0 -9.843929 -5.452492
0.020794 H
H-HY-0.433577(PDBName=H9,ResName=DHK,ResNum=225) 0 -9.746825 -5.641340 -
0.951771 H
C-CJ--0.168157(PDBName=C10,ResName=DHK,ResNum=225) 0 -10.830837 -3.506158 -
1.019299 H
C-CJ-0.254614(PDBName=C11,ResName=DHK,ResNum=225) 0 -10.646780 -4.062236 -
2.372892 H
O-OX--0.544517(PDBName=O12,ResName=DHK,ResNum=225) 0 -10.008383 -5.127501 -
2.529572 H
H-HY-0.383602(PDBName=H13,ResName=DHK,ResNum=225) 0 -8.176355 -4.932191 -
3.810262 H
C-CJ-0.213075(PDBName=C14,ResName=DHK,ResNum=225) 0 -11.426651 -2.242950 -
0.849059 H
C-CJ--0.377966(PDBName=C15,ResName=DHK,ResNum=225) 0 -11.691803 -1.394710 -
2.066598 H
H-HK-0.179148(PDBName=H16,ResName=DHK,ResNum=225) 0 -12.586376 -0.783877 -
1.906026 H
C-CJ-0.165502(PDBName=C17,ResName=DHK,ResNum=225) 0 -11.773378 -2.139013 -
3.367481 H
C-CZ--0.111477(PDBName=C18,ResName=DHK,ResNum=225) 0 -12.325041 -1.373854 -

4.530265 H
 H-H8-0.032583(PDBName=H19,ResName=DHK,ResNum=225) 0 -13.249617 -0.860953 -
 4.235729 H
 H-H8-0.032583(PDBName=H20,ResName=DHK,ResNum=225) 0 -11.609251 -0.581393 -
 4.784372 H
 C-CJ--0.377452(PDBName=C21,ResName=DHK,ResNum=225) 0 -11.265430 -3.378566 -
 3.521354 H
 C-CZ-0.692240(PDBName=C22,ResName=DHK,ResNum=225) 0 -11.266249 -4.085216 -
 4.866154 H
 C-CZ--0.555194(PDBName=C23,ResName=DHK,ResNum=225) 0 -12.247906 -5.259426 -
 4.886907 H
 H-H8-0.129933(PDBName=H24,ResName=DHK,ResNum=225) 0 -11.989586 -5.983611 -
 4.107864 H
 H-H8-0.129933(PDBName=H25,ResName=DHK,ResNum=225) 0 -12.205367 -5.776803 -
 5.849662 H
 H-H8-0.129933(PDBName=H26,ResName=DHK,ResNum=225) 0 -13.278919 -4.933162 -
 4.714711 H
 H-H9--0.039392(PDBName=H27,ResName=DHK,ResNum=225) 0 -10.252995 -4.452653 -
 5.051661 H
 O-OI--0.712638(PDBName=O28,ResName=DHK,ResNum=225) 0 -11.523766 -3.187754 -
 5.956958 H
 C-CZ-0.665570(PDBName=C29,ResName=DHK,ResNum=225) 0 -12.593257 -2.263165 -
 5.743358 H
 H-H9--0.064844(PDBName=H30,ResName=DHK,ResNum=225) 0 -13.539717 -2.802497 -
 5.582650 H
 C-CZ--0.289485(PDBName=C31,ResName=DHK,ResNum=225) 0 -12.716263 -1.438553 -
 7.030411 H
 H-H8-0.039536(PDBName=H32,ResName=DHK,ResNum=225) 0 -11.707869 -1.148770 -
 7.334189 H
 H-H8-0.039536(PDBName=H33,ResName=DHK,ResNum=225) 0 -13.314110 -0.545314 -
 6.821622 H
 C-CV-0.810685(PDBName=C34,ResName=DHK,ResNum=225) 0 -13.414540 -2.256703 -
 8.110517 H
 O-O5--0.794847(PDBName=O35,ResName=DHK,ResNum=225) 0 -12.714132 -2.846309 -
 8.970881 H
 O-O5--0.794847(PDBName=O36,ResName=DHK,ResNum=225) 0 -14.688641 -2.300720 -
 8.021222 H
 O-O5--0.000000(PDBName=O1,ResName=OXY,ResNum=226) 0 -9.367932 -0.978280 -

2.201579 H
O-O5--0.000000(PDBName=O2,ResName=OXY,ResNum=226) 0 -10.676025 -0.350629 -
2.196278 H
O-OW--0.834000(PDBName=O,ResName=WAT,ResNum=425) 0 -13.762369 0.657107 -
0.751665 H
H-HW-0.417000(PDBName=H1,ResName=WAT,ResNum=425) 0 -13.228084 1.260548 -
0.195784 H
H-HW-0.417000(PDBName=H2,ResName=WAT,ResNum=425) 0 -14.204526 0.113310 -
0.086350 H
O-OW--0.834000(PDBName=O,ResName=WAT,ResNum=639) 0 -7.938555 -4.649242 -
4.702581 H
H-HW-0.417000(PDBName=H1,ResName=WAT,ResNum=639) 0 -9.125553 -0.850730 -
1.255776 H
H-HW-0.417000(PDBName=H2,ResName=WAT,ResNum=639) 0 -7.136369 -4.109166 -
4.603052 H

1TS3 (L4)
0 1
N-N--0.415700(PDBName=N,ResName=ASN,ResNum=173) 0 -5.730069 2.996981 -
2.315334 L
H-H-0.271900(PDBName=H,ResName=ASN,ResNum=173) 0 -5.898887 2.605598 -
3.237137 L
C-CX-0.014300(PDBName=CA,ResName=ASN,ResNum=173) 0 -6.052990 2.143991 -
1.163789 L
H-H1-0.104800(PDBName=HA,ResName=ASN,ResNum=173) 0 -6.308309 2.760487 -
0.300703 L
C-2C--0.204100(PDBName=CB,ResName=ASN,ResNum=173) 0 -7.264128 1.260424 -
1.527981 H
H-HC-0.079700(PDBName=HB2,ResName=ASN,ResNum=173) 0 -8.128308 1.907804 -
1.675395 H
H-HC-0.079700(PDBName=HB3,ResName=ASN,ResNum=173) 0 -7.049684 0.749473 -
2.470618 H
C-C-0.713000(PDBName=CG,ResName=ASN,ResNum=173) 0 -7.618720 0.257831 -
0.423618 H
O-O--0.593100(PDBName=OD1,ResName=ASN,ResNum=173) 0 -8.206104 0.587079
0.595669 H
N-N--0.919100(PDBName=ND2,ResName=ASN,ResNum=173) 0 -7.251764 -1.037568 -
0.672126 H

H-H-0.419600(PDBName=HD21,ResName=ASN,ResNum=173)	0	-7.390162	-1.704717
0.075845 H			
H-H-0.419600(PDBName=HD22,ResName=ASN,ResNum=173)	0	-6.534550	-1.275137 -
1.341992 H			
C-C-0.597300(PDBName=C,ResName=ASN,ResNum=173)	0	-4.871977	1.228776 -
0.795154 L			
O-O--0.567900(PDBName=O,ResName=ASN,ResNum=173)	0	-4.326957	0.574897 -
1.683455 L			
N-N--0.415700(PDBName=N,ResName=TRP,ResNum=177)	0	-5.944140	-8.126862
5.630936 L			
H-H-0.271900(PDBName=H,ResName=TRP,ResNum=177)	0	-5.059946	-8.384815
5.201556 L			
C-CX--0.027500(PDBName=CA,ResName=TRP,ResNum=177)	0	-6.836218	-9.239614
5.962270 L			
H-H1-0.112300(PDBName=HA,ResName=TRP,ResNum=177)	0	-7.597708	-8.895423
6.661244 L			
C-CT--0.005000(PDBName=CB,ResName=TRP,ResNum=177)	0	-7.529142	-9.702851
4.664656 H			
H-HC-0.033900(PDBName=HB2,ResName=TRP,ResNum=177)	0	-6.747971	-10.166241
4.054156 H			
H-HC-0.033900(PDBName=HB3,ResName=TRP,ResNum=177)	0	-8.209471	-10.517680
4.943313 H			
C-C*-0.141500(PDBName=CG,ResName=TRP,ResNum=177)	0	-8.290057	-8.707166
3.832540 H			
C-CW--0.163800(PDBName=CD1,ResName=TRP,ResNum=177)	0	-7.828361	-7.971698
2.765428 H			
H-H4-0.206200(PDBName=HD1,ResName=TRP,ResNum=177)	0	-6.838925	-7.946571
2.327921 H			
N-NA--0.341800(PDBName=NE1,ResName=TRP,ResNum=177)	0	-8.836478	-7.170012
2.254084 H			
H-H-0.341200(PDBName=HE1,ResName=TRP,ResNum=177)	0	-8.832893	-6.718152
1.347934 H			
C-CN-0.138000(PDBName=CE2,ResName=TRP,ResNum=177)	0	-9.988816	-7.400377
2.978284 H			
C-CA--0.260100(PDBName=CZ2,ResName=TRP,ResNum=177)	0	-11.270558	-6.860814
2.828909 H			
H-HA-0.157200(PDBName=HZ2,ResName=TRP,ResNum=177)	0	-11.485208	-6.136906
2.049055 H			

C-CA--0.113400(PDBName=CH2,ResName=TRP,ResNum=177)	0	-12.250949	-7.288265
3.716663 H			
H-HA-0.141700(PDBName=HH2,ResName=TRP,ResNum=177)	0	-13.247333	-6.863471
3.647105 H			
C-CA--0.197200(PDBName=CZ3,ResName=TRP,ResNum=177)	0	-11.973876	-8.252710
4.708125 H			
H-HA-0.144700(PDBName=HZ3,ResName=TRP,ResNum=177)	0	-12.769693	-8.585208
5.368866 H			
C-CA--0.238700(PDBName=CE3,ResName=TRP,ResNum=177)	0	-10.698525	-8.784107
4.851525 H			
H-HA-0.170000(PDBName=HE3,ResName=TRP,ResNum=177)	0	-10.492405	-9.534524
5.610798 H			
C-CB-0.124300(PDBName=CD2,ResName=TRP,ResNum=177)	0	-9.677337	-8.350082
3.990497 H			
C-C-0.597300(PDBName=C,ResName=TRP,ResNum=177)	0	-6.069263	-10.411794
6.612221 L			
O-O--0.567900(PDBName=O,ResName=TRP,ResNum=177)	0	-4.865969	-10.585861
6.395989 L			
N-N--0.347900(PDBName=N,ResName=ARG,ResNum=197)	0	-18.551508	-1.581964 -
5.130253 L			
H-H-0.274700(PDBName=H,ResName=ARG,ResNum=197)	0	-18.890064	-2.443614 -
4.709299 L			
C-CX--0.263700(PDBName=CA,ResName=ARG,ResNum=197)	0	-17.912916	-1.650656 -
6.460012 L			
H-H1-0.156000(PDBName=HA,ResName=ARG,ResNum=197)	0	-16.901485	-1.245542 -
6.399912 L			
C-C8--0.000700(PDBName=CB,ResName=ARG,ResNum=197)	0	-17.837723	-3.106141 -
6.961830 L			
H-HC-0.032700(PDBName=HB2,ResName=ARG,ResNum=197)	0	-18.822691	-3.572839 -
6.906238 L			
H-HC-0.032700(PDBName=HB3,ResName=ARG,ResNum=197)	0	-17.556738	-3.071674 -
8.014713 L			
C-C8-0.039000(PDBName=CG,ResName=ARG,ResNum=197)	0	-16.818712	-3.979894 -
6.203804 L			
H-HC-0.028500(PDBName=HG2,ResName=ARG,ResNum=197)	0	-15.937630	-3.389378 -
5.951513 L			
H-HC-0.028500(PDBName=HG3,ResName=ARG,ResNum=197)	0	-17.263918	-4.329902 -
5.274594 L			

C-C8-0.048600(PDBName=CD,ResName=ARG,ResNum=197) 0 -16.379618 -5.197849 -
 7.028805 H
 H-H1-0.068700(PDBName=HD2,ResName=ARG,ResNum=197) 0 -15.805074 -5.860331 -
 6.365738 H
 H-H1-0.068700(PDBName=HD3,ResName=ARG,ResNum=197) 0 -17.280396 -5.736039 -
 7.352339 H
 N-N2--0.529500(PDBName=NE,ResName=ARG,ResNum=197) 0 -15.571237 -4.756727 -
 8.154854 H
 H-H-0.345600(PDBName=HE,ResName=ARG,ResNum=197) 0 -15.265130 -3.725668 -
 8.185947 H
 C-CA-0.807600(PDBName=CZ,ResName=ARG,ResNum=197) 0 -15.028817 -5.551951 -
 9.055690 H
 N-N2--0.862700(PDBName=NH1,ResName=ARG,ResNum=197) 0 -15.330950 -6.894406 -
 9.177331 H
 H-H-0.447800(PDBName=HH11,ResName=ARG,ResNum=197) 0 -15.820214 -7.316686 -
 8.370017 H
 H-H-0.447800(PDBName=HH12,ResName=ARG,ResNum=197) 0 -14.479925 -7.455374 -
 9.306580 H
 N-N2--0.862700(PDBName=NH2,ResName=ARG,ResNum=197) 0 -14.244336 -5.005512 -
 9.998374 H
 H-H-0.447800(PDBName=HH21,ResName=ARG,ResNum=197) 0 -13.732174 -4.119967 -
 9.792300 H
 H-H-0.447800(PDBName=HH22,ResName=ARG,ResNum=197) 0 -13.746935 -5.679014 -
 10.589847 H
 C-C-0.734100(PDBName=C,ResName=ARG,ResNum=197) 0 -18.666212 -0.799517 -
 7.480570 L
 O-O--0.589400(PDBName=O,ResName=ARG,ResNum=197) 0 -18.046148 -0.076958 -
 8.271150 L
 C-CJ--0.316472(PDBName=C1,ResName=DHK,ResNum=225) 0 -10.615019 -1.659681
 0.020743 H
 H-HK-0.158183(PDBName=H2,ResName=DHK,ResNum=225) 0 -10.751146 -0.589255
 0.116919 H
 C-CJ--0.090287(PDBName=C3,ResName=DHK,ResNum=225) 0 -10.173988 -2.430649
 1.091682 H
 H-HK-0.142318(PDBName=H4,ResName=DHK,ResNum=225) 0 -9.992625 -1.951182
 2.041563 H
 C-CJ--0.390043(PDBName=C5,ResName=DHK,ResNum=225) 0 -9.947859 -3.801460
 0.970489 H

H-HK-0.190546(PDBName=H6,ResName=DHK,ResNum=225) 0 -9.611627 -4.398408
1.811531 H
C-CJ-0.446965(PDBName=C7,ResName=DHK,ResNum=225) 0 -10.139385 -4.425546 -
0.262492 H
O-OX--0.642443(PDBName=O8,ResName=DHK,ResNum=225) 0 -9.870624 -5.743827 -
0.365677 H
H-HY-0.433577(PDBName=H9,ResName=DHK,ResNum=225) 0 -10.061877 -5.998401 -
1.314995 H
C-CJ--0.168157(PDBName=C10,ResName=DHK,ResNum=225) 0 -10.626378 -3.670870 -
1.366121 H
C-CJ-0.254614(PDBName=C11,ResName=DHK,ResNum=225) 0 -10.852513 -4.320584 -
2.658603 H
O-OX--0.544517(PDBName=O12,ResName=DHK,ResNum=225) 0 -10.560969 -5.531262 -
2.825104 H
H-HY-0.383602(PDBName=H13,ResName=DHK,ResNum=225) 0 -12.481877 1.470380 -
2.112137 H
C-CJ-0.213075(PDBName=C14,ResName=DHK,ResNum=225) 0 -10.852581 -2.283987 -
1.204874 H
C-CJ--0.377966(PDBName=C15,ResName=DHK,ResNum=225) 0 -11.472698 -1.539690 -
2.321875 H
H-HK-0.179148(PDBName=H16,ResName=DHK,ResNum=225) 0 -12.747775 -1.687230 -
1.922007 H
C-CJ-0.165502(PDBName=C17,ResName=DHK,ResNum=225) 0 -11.672197 -2.213420 -
3.608911 H
C-CZ--0.111477(PDBName=C18,ResName=DHK,ResNum=225) 0 -12.160989 -1.386761 -
4.756203 H
H-H8-0.032583(PDBName=H19,ResName=DHK,ResNum=225) 0 -12.952413 -0.706109 -
4.421691 H
H-H8-0.032583(PDBName=H20,ResName=DHK,ResNum=225) 0 -11.334677 -0.748514 -
5.082447 H
C-CJ--0.377452(PDBName=C21,ResName=DHK,ResNum=225) 0 -11.420623 -3.544138 -
3.753676 H
C-CZ-0.692240(PDBName=C22,ResName=DHK,ResNum=225) 0 -11.638224 -4.254096 -
5.076965 H
C-CZ--0.555194(PDBName=C23,ResName=DHK,ResNum=225) 0 -12.826471 -5.219804 -
5.036463 H
H-H8-0.129933(PDBName=H24,ResName=DHK,ResNum=225) 0 -12.631884 -6.011378 -
4.305297 H

H-H8-0.129933(PDBName=H25,ResName=DHK,ResNum=225) 0 -12.963416 -5.690073 -
6.017289 H
H-H8-0.129933(PDBName=H26,ResName=DHK,ResNum=225) 0 -13.757943 -4.717751 -
4.758539 H
H-H9--0.039392(PDBName=H27,ResName=DHK,ResNum=225) 0 -10.737023 -4.834333 -
5.299954 H
O-OI--0.712638(PDBName=O28,ResName=DHK,ResNum=225) 0 -11.753732 -3.332197 -
6.172718 H
C-CZ-0.665570(PDBName=C29,ResName=DHK,ResNum=225) 0 -12.649986 -2.240207 -
5.920155 H
H-H9--0.064844(PDBName=H30,ResName=DHK,ResNum=225) 0 -13.658732 -2.617589 -
5.699964 H
C-CZ--0.289485(PDBName=C31,ResName=DHK,ResNum=225) 0 -12.708464 -1.437784 -
7.219420 H
H-H8-0.039536(PDBName=H32,ResName=DHK,ResNum=225) 0 -11.681531 -1.231043 -
7.526834 H
H-H8-0.039536(PDBName=H33,ResName=DHK,ResNum=225) 0 -13.241335 -0.499087 -
7.033264 H
C-CV-0.810685(PDBName=C34,ResName=DHK,ResNum=225) 0 -13.453673 -2.243266 -
8.275082 H
O-O5--0.794847(PDBName=O35,ResName=DHK,ResNum=225) 0 -12.790110 -2.807482 -
9.181890 H
O-O5--0.794847(PDBName=O36,ResName=DHK,ResNum=225) 0 -14.716954 -2.310712 -
8.114340 H
O-O5--0.000000(PDBName=O1,ResName=OXY,ResNum=226) 0 -12.530685 0.644476 -
1.579049 H
O-O5--0.000000(PDBName=O2,ResName=OXY,ResNum=226) 0 -11.277647 -0.205431 -
2.365812 H
O-OW--0.834000(PDBName=O,ResName=WAT,ResNum=425) 0 -12.213340 3.166481 -
2.692199 H
H-HW-0.417000(PDBName=H1,ResName=WAT,ResNum=425) 0 -11.562229 3.331059 -
3.389674 H
H-HW-0.417000(PDBName=H2,ResName=WAT,ResNum=425) 0 -11.867027 3.625709 -
1.912810 H
O-OW--0.834000(PDBName=O,ResName=WAT,ResNum=639) 0 -13.872582 -1.348535 -
1.414819 H
H-HW-0.417000(PDBName=H1,ResName=WAT,ResNum=639) 0 -13.560203 -0.347963 -
1.484228 H

H-HW-0.417000(PDBName=H2,ResName=WAT,ResNum=639) 0 -13.737500 -1.565471 -
0.476015 H