

Supporting Information

A Single Site Mutation Can Induce a Functional Promiscuity in Homoserine Kinase

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QM region Coordinates.

QM region coordinates of a QM/MM optimised geometry of Homoserine kinase complexed with the native substrate (RC, TS, and PC) following the previous proposed pathway for phosphoryl transfer mechanism (Kinase Activity).

QM region coordinates of a QM/MM optimised geometry of Homoserine kinase complexed with the native substrate (RC, TS, IM, and PC) following a newly proposed pathway via H138 for phosphoryl transfer mechanism (Kinase Activity).

QM region coordinates of a QM/MM optimised geometry of H138L Homoserine kinase complexed with the native substrate (RC, TS, IM, and PC) following hydrolysis of ATP (ATPase Activity).

QM region coordinates of a QM/MM optimised geometry of Homoserine kinase complexed with the native substrate (RC, TS, and PC) following the previous proposed pathway for phosphoryl transfer mechanism (Kinase Activity) including H138 in the QM-region.

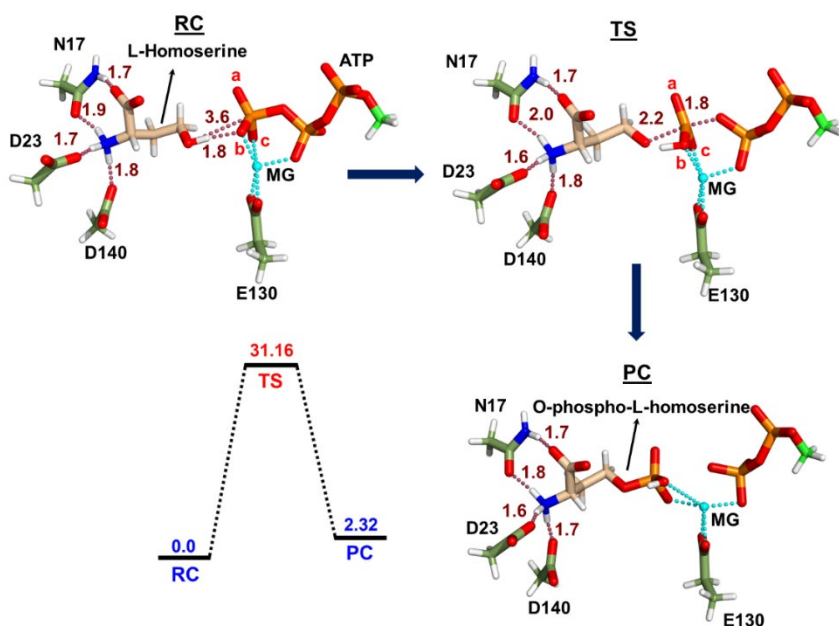


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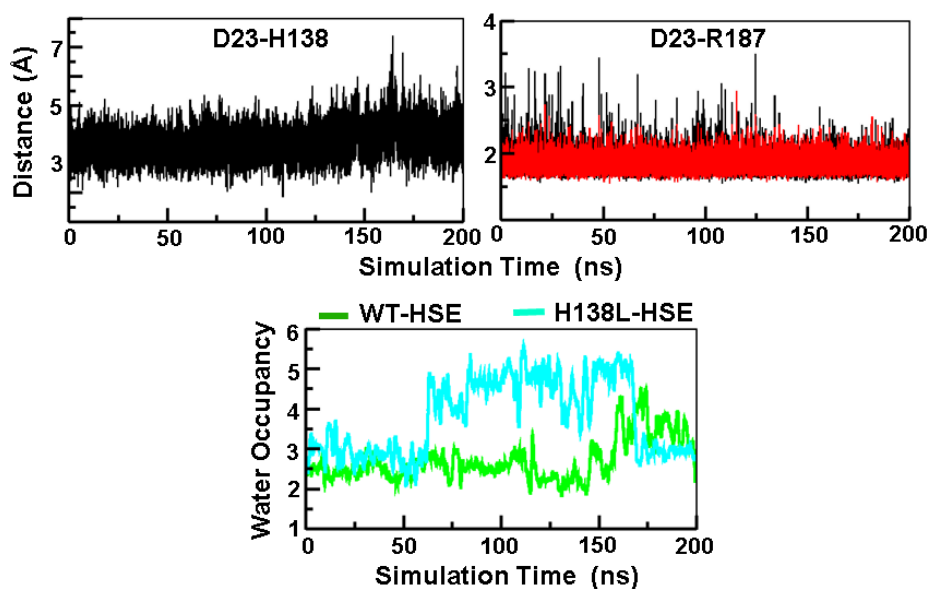


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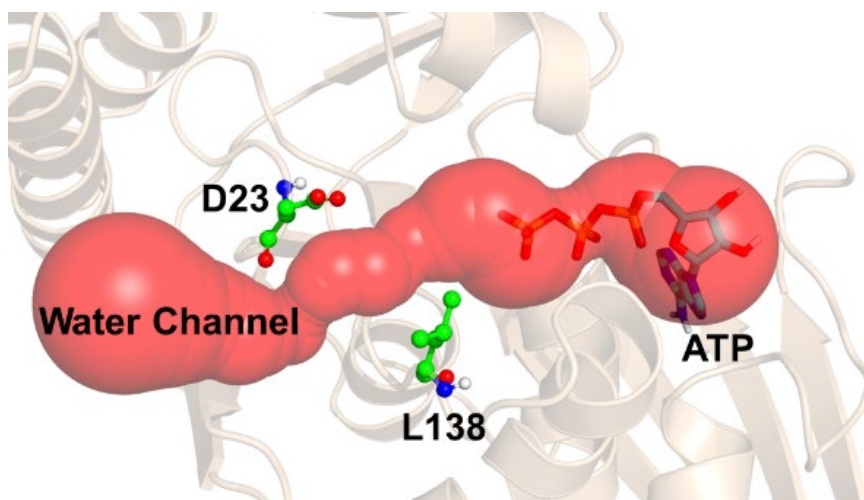


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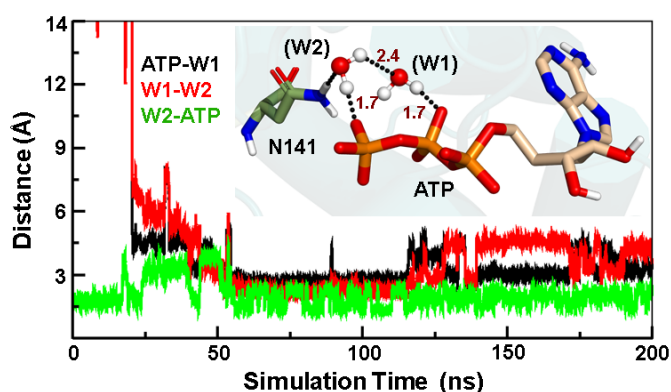


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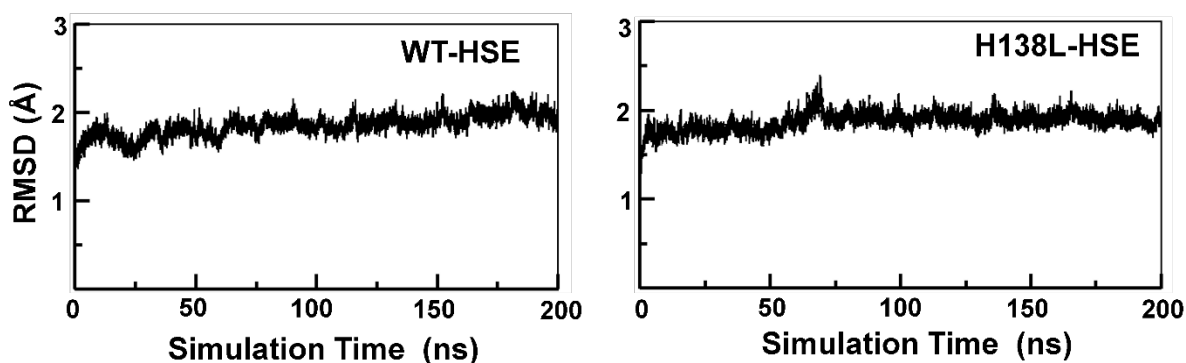


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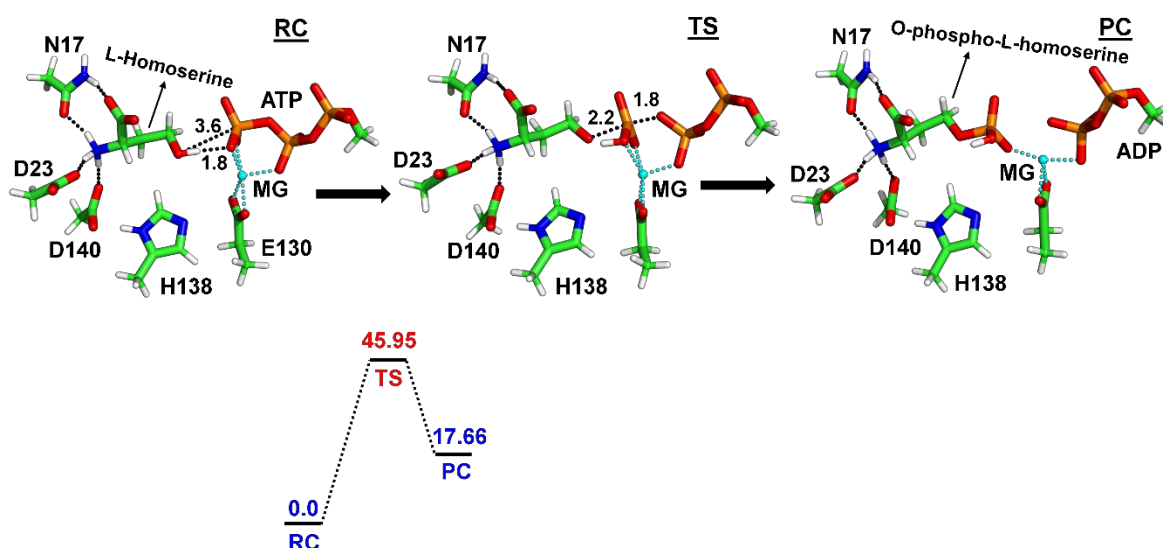


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Table1: Potential energy barrier corresponding to different pathways proposed in WT and H138L Homoserine Kinase (HSK)

Different Pathways	Energy Barrier (in kcal/mol)
Already proposed pathway for phosphoryl transfer (without H138) in HSK	31.16
Newly proposed pathway for phosphoryl transfer in HSK	18.25
ATPase pathway in H138L HSK	22.45

Table2: pKa value of Histidine in crystal structure

	pKa
His 138	4.01
His 163	5.14

QM-Optimised Coordinates

WT-Homoserine **kinase-previous**
proposed mechanism

RC

C	48.3156311	35.7826910	42.1493265
H	48.7444337	34.8303254	41.8079858
H	49.0310993	36.2448407	42.8515704
C	47.0008620	35.5478012	42.8908525
O	46.3100131	36.4889298	43.2935529
N	46.6960607	34.2619030	43.0993533
H	45.8625281	34.0741922	43.6844961
H	47.3187329	33.5248162	42.7657132
C	44.5505465	40.0263743	46.9744855
H	45.3477732	40.4212547	47.6176322
H	43.7035583	40.7283205	47.0770946
C	44.0450404	38.6756188	47.5166307
O	43.5764789	37.8278941	46.6913825
O	44.0084297	38.5284462	48.7582681
C	33.7438255	36.8401293	42.9909837
H	33.3551779	37.8500257	42.8285270
H	34.3057876	36.8568439	43.9374083
C	34.6990764	36.4488259	41.8691170
H	34.1914727	36.1922466	40.9228062
H	35.3603034	37.2959922	41.6211611
C	35.6163813	35.2924786	42.2084900
O	36.4452660	34.8888441	41.3369915
O	35.5507636	34.7094369	43.3320754
C	42.3725391	40.8340730	41.5397938
H	43.3221218	40.5879300	41.0409243
H	42.4608782	41.8376812	41.9829677
C	42.0953160	39.8072768	42.6603471
O	41.4833100	40.2173404	43.6766478
O	42.5371331	38.6372775	42.4819839
Mg	36.8672540	33.2758428	42.5542795
P	38.6462549	31.3753817	42.5251306
O	39.9916932	30.7163264	42.4939055
O	38.2330147	32.2434595	43.7749424
O	38.2299685	32.2789483	41.3183834
P	35.9359431	30.3744175	42.0950667
O	35.6570570	29.9968368	40.6561719
O	35.5140849	31.7907624	42.5307034
O	37.5022143	30.1422866	42.4636267
P	35.3293478	27.7220449	43.3010365
O	36.7421407	27.2366110	43.1783402
O	34.5100962	27.3290782	44.5001439
O	35.2035039	29.3697220	43.1412100

O	34.5339678	27.2329112	41.9282931
C	33.2975771	27.7753013	41.5383754
N	43.5911189	36.7055503	44.2334834
C	42.7030963	35.5271655	44.4467785
C	43.4436759	34.3979012	45.1981057
C	42.1768126	34.9968843	43.1089929
O	42.7977692	33.7814719	46.0631144
O	44.6260837	34.1562738	44.8283809
C	41.1816540	33.8503396	43.2432924
O	40.0855217	34.2413974	44.0566757
H	39.4406189	33.4967432	44.0551393
H	43.1510657	37.4119958	43.5872106
H	43.7399692	37.1990442	45.1543283
H	44.5286774	36.4346615	43.8632172
H	40.8391115	33.5717262	42.2299396
H	41.6844163	32.9613585	43.6627016
H	41.7319808	35.8372899	42.5491405
H	43.0328846	34.6305016	42.5204213
H	41.8594102	35.8632027	45.0646386
H	48.2128374	36.4553212	41.2978166
H	44.8935331	40.0347974	45.9399052
H	32.9034862	36.1591177	43.1255945
H	41.6077450	40.9240112	40.7683871
H	33.3321044	28.8547178	41.3909476
H	33.0159922	27.3317502	40.5833678
H	32.4822385	27.5899034	42.2376020

TS

C	48.1775267	35.7743100	42.2284857
H	48.6020623	34.8178962	41.8953313
H	48.8896935	36.2290870	42.9387917
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H	47.1673057	33.5256466	42.8483456
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H	45.2825595	40.3083794	47.6620463
H	43.6748111	40.7745454	47.1156577
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O	43.4200454	37.8348168	46.6647267
O	43.6915421	38.5844406	48.7450684
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PC

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H	33.0836430	27.3728942	40.6225267
H	32.5400013	27.6026981	42.2752053

WT-Homoserine kinase-Newly proposed mechanism including H138

RC

C	45.1156788	29.4604731	28.1686789
H	44.0604300	29.3227294	27.8970619
H	45.7276951	29.0696030	27.3374225
C	45.4540912	28.6778899	29.4330809
O	46.5577162	28.7746794	29.9766842
N	44.4869754	27.8672442	29.8841910
H	44.7508240	27.2289733	30.6615224
H	43.6203133	27.7499273	29.3707204
C	51.2750544	27.5132177	31.2242817
H	51.8706561	27.2429419	30.3428070
H	51.9776334	27.7105783	32.0535699
C	50.4619722	26.2969204	31.6857215
O	49.4792194	26.4986971	32.4926066
O	50.8661337	25.1725233	31.3702838
C	47.3299485	28.8999747	42.1724191
H	48.1103883	29.6011836	42.5022405
H	47.8198850	28.1422509	41.5434666

C	46.2506502	29.6119307	41.3504863
H	45.5491743	30.2051960	41.9619522
H	46.7141826	30.3402647	40.6703887
C	45.4100375	28.7002193	40.4700955
O	44.3883163	29.1634681	39.8768469
O	45.7183378	27.4757897	40.3332733
C	50.8378309	28.3507805	38.1891923
H	51.5608392	28.2914125	37.3641173
H	50.8038245	27.3443379	38.6362387
C	49.4895884	28.7326664	37.6754671
N	49.3031071	29.4793378	36.5298464
H	49.9991369	29.8230170	35.8439850
C	47.9798000	29.7344368	36.4192395
H	47.5740004	30.2863183	35.5741980
N	47.2958310	29.1993745	37.4191292
C	48.2266066	28.5565619	38.2043296
H	47.9356971	27.9932829	39.0896236
C	49.3333957	32.9839842	33.9593005
H	48.6085876	33.2347998	33.1721220
H	50.3111824	33.4226315	33.7062558
C	49.5348220	31.4586768	34.0594014
O	48.6319705	30.7182694	33.6056106
O	50.5991877	31.0591935	34.6255173
Mg	43.9173752	27.1732730	39.3628530
P	42.3966443	26.0151902	37.6341018
O	41.8562302	25.6760914	36.2768958
O	43.7956678	25.5280161	38.1088291
O	42.3641625	27.5271257	38.0774433
P	41.3991456	25.5504840	40.3548500
O	40.1454246	26.2489907	40.8248279
O	42.7354106	26.2388001	40.7430218
O	41.3276996	25.3109373	38.7454916
P	40.3518996	22.8582084	40.8695776
O	39.7634833	22.7749067	39.4980607
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O	41.5225666	24.0521335	40.9548201
O	39.1798777	23.5335727	41.8529189
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N	47.3874472	28.0832844	32.6593369
C	46.4862768	27.3356991	33.5880237
C	45.9294517	26.0789653	32.8712789
C	45.3505533	28.2343932	34.0992100
O	45.6541682	26.2131761	31.6406035
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O	45.4558610	27.3972577	36.4187064
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H	47.7077960	28.9870166	33.0503990

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TS

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C 47.3425113 28.9326734 42.1889815
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C	47.1098740	28.8665373	42.1126075
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H	47.5540924	28.1182364	41.4411620
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H	45.2698938	30.1042035	42.0787017
H	46.2691795	30.2549060	40.6569417
C	45.0029462	28.5573277	40.6309538
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C	50.8336159	28.4021728	38.0855692
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Mg	43.4766785	26.9628486	39.4975775
P	43.9929719	26.7022672	36.7344519
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P	40.3790665	22.8007217	40.8349476
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H138L-Homoserine kinase-ATPase activity

RC

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C	47.1978293	31.3631264	39.7230420	O	43.4403319	33.1209854	38.1309141
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O	48.9233016	30.2883982	42.1470081	H	41.3435781	33.8398014	36.9799678
C	46.7866895	32.4244324	38.7110341	H	42.0106712	35.3765475	36.4320341
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H	49.2454817	29.9853993	38.3043108	H	44.3928370	30.7470087	43.1826949
H	47.1027295	32.1241863	37.7000261	Mg	44.6266385	36.0811932	41.9982271
H	45.6858368	32.4888961	38.6989967	P	44.0271884	33.5762802	42.5407318
H	46.7597389	30.3952036	39.4213152	O	44.7432825	32.1338037	42.0816454
H	46.7661834	31.6165897	40.7047791	O	45.4418125	34.3249834	42.7123957
H	49.1095211	32.0942642	40.4055508	O	43.3878965	34.5155432	41.4608685
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H	47.1103454	34.3622541	42.0721146	O	41.6323042	35.6227851	44.6581785
H	47.7732368	34.1363947	40.7000876	O	43.9068887	36.5386732	43.8234576
O	43.2528283	31.2663113	40.5999115	O	43.5709872	33.9945795	44.1748577
H	44.2695768	31.7429933	41.5423100	P	43.2631754	34.8061958	47.5290372
H	43.3076420	31.9385946	39.8957159	O	43.1837911	33.3166082	47.3459801
O	41.0373807	35.7046483	41.9635668	O	44.0790730	35.4175608	48.6499902
H	41.1388600	35.5988749	42.9317531	O	43.7376700	35.5822763	46.1521879
H	41.7652838	35.1357043	41.6329103	O	41.6864143	35.3226146	47.6791793
O	42.3175725	32.5591604	42.4573728	C	41.2562121	36.6546965	47.5264142
H	42.6604389	31.7508816	41.3697576	N	49.4534045	30.9047174	38.6831492
H	42.2960169	32.0784192	43.2985614	C	48.6713852	31.1439285	39.9451162
H	46.2790414	40.6475098	41.4930044	C	48.8465145	29.9584328	40.9286575
H	44.6503657	35.4585940	36.3296863	C	47.1679009	31.2942787	39.6868959
H	45.1863530	28.2953678	42.7048240	O	48.8179430	28.8051002	40.4232184
H	41.7139918	37.1244763	46.6377474	O	48.9083564	30.2539201	42.1370775
H	40.1967300	36.6344188	47.3523647	C	46.7459819	32.3498222	38.6717461
H	41.4949203	37.2752808	48.3519665	O	47.2599422	33.6298044	38.9992746

IM

C	46.5180099	40.1564060	40.5498718	H	49.2517267	31.5959457	37.9248723
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H	47.3695757	39.4803267	40.6758413	H	49.2517231	29.9641927	38.2937873
C	45.3681444	39.3613368	39.9381854	H	47.0786270	32.0580645	37.6632778
H	44.4300802	39.9333624	39.8565349	H	45.6438230	32.3935601	38.6509833
H	45.6504406	39.0558248	38.9142783	H	46.7635692	30.3165807	39.3688020
C	45.0532617	38.0693080	40.6676942	H	46.7083921	31.5318390	40.6605166
O	43.9318628	37.5142054	40.5408229	H	49.0538472	32.0674517	40.3979099
O	45.9403877	37.5326413	41.4193088	O	47.8650839	34.2905538	41.6032675
C	44.4378446	35.1835420	37.3586462	H	46.9777385	34.2246423	42.0498877
H	45.3411132	34.7219026	37.7790624	H	47.6543486	34.0665644	40.6732563
				O	42.7717995	31.3725195	40.4445142
				H	44.1062335	31.6560614	41.4745765

H 42.9391509 32.1391755 39.8619715
 O 40.9721206 35.6727104 42.0025360
 H 41.1309510 35.6512917 42.9699247
 H 41.7452821 35.1665672 41.6670734
 O 42.4556164 32.5817137 42.6678323
 H 42.3961569 31.7770209 41.2830335
 H 42.2825307 32.4036982 43.6116333
 H 46.2706806 40.6075320 41.5107988
 H 44.6312767 35.4461517 36.3186043
 H 45.2117656 28.2164908 42.6827499
 H 41.6902074 37.1600473 46.6636653
 H 40.1758447 36.6678734 47.3825402
 H 41.4837537 37.2941415 48.3792929

PC

C 46.4548665 40.0722190 40.5924048
 H 46.8224526 40.8437289 39.9015321
 H 47.2787590 39.3640260 40.7300381
 C 45.2695296 39.3039312 40.0073303
 H 44.3446299 39.8974290 39.9378758
 H 45.5371200 38.9884298 38.9818675
 C 44.9421478 38.0139679 40.7389480
 O 43.7662829 37.5739640 40.7799504
 O 45.8841194 37.3456157 41.2977878
 C 44.6076185 35.2514017 37.2673948
 H 45.5176758 34.7896604 37.6738322
 H 44.4178860 36.1644366 37.8568857
 C 43.4579341 34.2625008 37.4501965
 O 43.6352600 33.1781230 38.0221096
 N 42.2491273 34.6019932 36.9677009
 H 41.5094405 33.8907164 36.9480801
 H 42.1488566 35.4339583 36.3844861
 C 45.0033849 29.3265711 43.2877374
 H 45.3541676 29.0571341 44.3016621
 H 45.7598867 30.0120040 42.8657796
 O 43.7109268 29.8912215 43.3138206
 H 43.7388780 30.8318811 43.0157528
 Mg 44.5741035 35.9323714 41.9545539
 P 44.3168765 33.2967857 41.5546916
 O 44.7664993 32.3684325 40.3173563
 O 45.5389862 33.9894380 42.2245889
 O 43.4496401 34.4879443 41.0117667
 P 43.0899805 35.3893907 44.6987049

O 41.6265396 35.7835141 44.5860831
 O 44.0410276 36.2307860 43.8129091
 O 43.3082304 33.8349821 44.5751802
 P 43.2563253 34.8688815 47.6028537
 O 43.2232840 33.3745248 47.4937311
 O 44.0782121 35.5278307 48.6895691
 O 43.6696466 35.6450398 46.2070941
 O 41.6670137 35.3520405 47.7337690
 C 41.2247695 36.6777861 47.5624555
 N 49.7323310 30.8371390 38.5407092
 C 48.9245276 31.0893289 39.7837979
 C 49.0522522 29.9239611 40.8019395
 C 47.4424795 31.2369217 39.4483983
 O 48.9958649 28.7599441 40.3282343
 O 49.1030734 30.2514968 42.0026224
 C 47.0992602 32.3021787 38.4201268
 O 47.5850078 33.5739103 38.8126938
 H 48.0974626 34.0004025 38.0555738
 H 49.5656306 31.5519625 37.7971554
 H 50.7608791 30.8375580 38.7268384
 H 49.4945900 29.9092410 38.1387658
 H 47.4983095 32.0189261 37.4353254
 H 46.0077549 32.3444547 38.3161498
 H 47.0534892 30.2637665 39.1012479
 H 46.9186006 31.4683931 40.3853325
 H 49.2939100 32.0190751 40.2342990
 O 48.1282819 34.2445935 41.4145902
 H 47.2259041 34.1112191 41.7878272
 H 47.9853446 34.0231548 40.4691545
 O 41.7019797 32.1406542 40.3390302
 H 44.3730005 32.6852617 39.4668418
 H 42.0458125 33.0127282 40.0899797
 O 40.9454480 35.2129212 42.0397882
 H 41.1704429 35.4440243 42.9726978
 H 41.7948696 34.9161020 41.6520351
 O 43.4976774 32.3884516 42.5063725
 H 42.1026413 32.0301756 41.2242866
 H 43.2536180 33.2780215 43.7275634
 H 46.2338947 40.5555075 41.5440722
 H 44.7807982 35.5034968 36.2211997
 H 45.0198098 28.4280002 42.6709978
 H 41.6529844 37.1769028 46.6932135
 H 40.1438565 36.6815389 47.4221696
 H 41.4525948 37.3250858 48.409312

**WT-Homoserine kinase-previous
proposed mechanism including H138**

RC

C	48.3190864	35.8048849	42.1758109
H	48.7415948	34.8483557	41.8381451
H	49.0398915	36.2689038	42.8714161
C	47.0070476	35.5811106	42.9274028
O	46.3261613	36.5281684	43.3316514
N	46.6948892	34.2975119	43.1416893
H	45.8619132	34.1166959	43.7324966
H	47.3098574	33.5561871	42.8037211
C	44.5316700	40.0772546	47.0435591
H	45.3623646	40.3562277	47.7062426
H	43.7623277	40.8587411	47.1738895
C	43.8833268	38.7736858	47.5624559
O	43.4816228	37.9095232	46.7067487
O	43.6889931	38.6778452	48.7872471
C	33.7463232	36.8457044	42.9353966
H	33.3615550	37.8585876	42.7816052
H	34.3442115	36.8646255	43.8586003
C	34.6640830	36.4425633	41.7846600
H	34.1272469	36.1923622	40.8524501
H	35.3284804	37.2828154	41.5251059
C	35.5734478	35.2757130	42.1118680
O	36.4151026	34.8780162	41.2454153
O	35.4824250	34.6845702	43.2238122
C	37.7592012	40.5732130	44.9582385
H	38.6743702	41.1502930	44.7514962
H	37.6166806	40.6131920	46.0510416
C	37.9216089	39.1674647	44.4579287
N	39.1415348	38.6785641	44.0531006
H	40.0330998	39.2062043	44.0508783
C	38.9758664	37.3845475	43.6908591
H	39.7946491	36.7364605	43.3863382
N	37.7131501	37.0041566	43.8142868
C	37.0470600	38.1075545	44.2947670
H	35.9858600	38.0652311	44.5293679
C	42.3354441	40.9110569	41.5412581
H	43.2908673	40.6632565	41.0554621
H	42.4116495	41.9185492	41.9780554
C	42.0389113	39.8911459	42.6575424
O	41.3600599	40.3072817	43.6409615
O	42.4974006	38.7300561	42.5255951
Mg	36.8493100	33.2955000	42.5160820
P	38.6476186	31.4022114	42.5171967

O	39.9982681	30.7516592	42.4942181
O	38.2299609	32.2789783	43.7568107
O	38.2244690	32.2847295	41.2975853
P	35.9468004	30.3721143	42.0933991
O	35.6701256	29.9786906	40.6578763
O	35.5114609	31.7857453	42.5170898
O	37.5139113	30.1552956	42.4668031
P	35.3366798	27.7205875	43.3037508
O	36.7475474	27.2285691	43.1818577
O	34.5152543	27.3285413	44.5022886
O	35.2183507	29.3665544	43.1453370
O	34.5388007	27.2308062	41.9316701
C	33.3036756	27.7761407	41.5429468
N	43.6163309	36.7530292	44.3132477
C	42.7331373	35.5697538	44.5303878
C	43.4786998	34.4525956	45.2935975
C	42.2206083	35.0230534	43.1935187
O	42.8583833	33.8813141	46.2058577
O	44.6379555	34.1675710	44.8801717
C	41.2520194	33.8527860	43.3297551
O	40.1474548	34.2252206	44.1374725
H	39.4775182	33.5051064	44.0838688
H	43.1780282	37.4391367	43.6574730
H	43.7376049	37.2672617	45.2370383
H	44.5577698	36.4858530	43.9510239
H	40.9204260	33.5603710	42.3167947
H	41.7744313	32.9761805	43.7533559
H	41.7508336	35.8479399	42.6299389
H	43.0878442	34.6764986	42.6090158
H	41.8892798	35.9084623	45.1454290
H	48.2155766	36.4717336	41.3198519
H	44.8832267	40.0785242	46.0118259
H	32.9064064	36.1707522	43.0998547
H	36.9070161	41.0993572	44.5280988
H	41.5732392	40.9874198	40.7658359
H	33.3399218	28.8560222	41.3993876
H	33.0216517	27.3365535	40.5862375
H	32.4873474	27.5897915	42.2407643

TS

C	48.1822859	35.7751221	42.2260627
H	48.6075936	34.8192271	41.8923232
H	48.8949093	36.2308464	42.9353365
C	46.8551296	35.5501071	42.9562790
O	46.1549800	36.4865373	43.3482651

H	33.9820320	36.1674146	40.7558617	H	44.7880142	36.7270574	44.0408957
H	35.3353585	37.0725654	41.4207419	H	41.9909717	33.7882572	41.6039895
C	35.3890358	35.0145282	41.8775983	H	42.5436899	33.1342403	43.1551827
O	35.9224625	34.4575081	40.8670938	H	42.4164876	36.0988063	42.3055053
O	35.5154587	34.5346730	43.0346855	H	43.8691997	35.0926437	42.5278649
C	37.7660074	40.5660034	44.9599756	H	41.9859014	36.0028698	44.7567074
H	38.6775501	41.1568975	44.7768019	H	48.2699118	36.4959352	41.2758667
H	37.6124179	40.5754843	46.0520213	H	44.9334363	40.1389381	46.0634420
C	37.9399449	39.1761392	44.4199228	H	32.9139430	36.1193220	43.0882149
N	39.1590015	38.7092551	43.9851748	H	36.9140839	41.0969080	44.5352007
H	40.0480632	39.2326235	44.0121717	H	41.5404215	40.8963555	40.7215543
C	38.9900278	37.4307793	43.5613617	H	33.3656653	28.8551342	41.4461747
H	39.8040483	36.8079305	43.1899577	H	33.0596339	27.3434882	40.6209822
N	37.7299730	37.0450496	43.6790495	H	32.5210018	27.5797506	42.2746056
C	37.0674129	38.1211312	44.2174200				
H	36.0068948	38.0647400	44.4564396				
C	42.3300051	40.8667579	41.4723865				
H	43.2741775	40.6124964	40.9674125				
H	42.4025665	41.8946487	41.8606793				
C	42.0988431	39.9001275	42.6470192				
O	41.4298233	40.3320955	43.6262051				
O	42.6087700	38.7525490	42.5636719				
Mg	36.6193662	32.9352856	42.1921380				
P	39.6337061	32.9684285	42.9895183				
O	40.3627070	31.7409734	42.4888402				
O	39.0696727	32.7574148	44.5032488				
O	38.4952705	33.5644451	42.1796147				
P	35.8432582	30.4336815	42.0449726				
O	35.6829677	29.7919900	40.6638715				
O	34.9876543	31.7214356	42.2424539				
O	37.2672805	30.9114344	42.4184096				
P	35.3972195	27.7517144	43.3232352				
O	36.8066588	27.2418519	43.1712331				
O	34.6087440	27.3155257	44.5355967				
O	35.2775036	29.3721321	43.1956945				
O	34.5718359	27.2264922	41.9706935				
C	33.3401483	27.7739790	41.5822607				
N	43.8231013	36.9432712	44.3759294				
C	42.9681768	35.7261836	44.3521131				
C	43.5600393	34.5895181	45.2143377				
C	42.8454875	35.2717502	42.8954644				
O	42.7986664	34.0077498	46.0235896				
O	44.7593760	34.2863110	45.0009174				
C	42.0485715	34.0007233	42.6846783				
O	40.7443049	34.1721039	43.2299544				
H	39.5423703	33.2653908	45.2136876				
H	43.3978161	37.6602818	43.7390125				
H	43.8549326	37.3835440	45.3505479				