

Supporting Info for “Converging Nuclear Magnetic Shielding Calculations with Respect to Basis and System Size in Protein Systems”

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This file contains (1) details of the experimental chemical shifts for 2AP and (2) Cartesian XYZ coordinates for the bare substrates and the different sized substrate/protein clusters used in the paper, in units of Angstroms.

1 Experimental Measurement of Select Chemical Shifts for the 2AP Quinonoid Intermediate

Sample Preparation: Selectively $^{13}\text{C}/^{15}\text{N}$ enriched PLP was synthesized and exchanged into *S. typhimurium* tryptophan synthase as previously described.[1] Microcrystals of the enzyme with labeled and unlabeled coenzyme were prepared and packed into a Bruker 4 mm magic-angle-spinning rotor (volume $\approx 80 \mu\text{L}$) with the aid of a bench top centrifuge (10,000 rpm); each rotor contained approximately 25-30 mg of protein. The 2AP quinonoid intermediate was formed *in situ* by the addition of 5 μL of 1.2 M L-serine (unlabeled, ^{15}N -labeled, or U- ^{13}C -labeled) and 8 μL of a concentrated stock solution of 2AP (unlabeled or ^{15}N -labeled) in acetonitrile.

NMR Experiments: Solid-state NMR experiments were performed at 9.4 T (400.37 MHz ^1H , 40.57 MHz ^{15}N) on a Bruker AVIII spectrometer equipped with an ^1H - ^{13}C - ^{15}N triple resonance 4 mm MAS probe spinning at a MAS rate of 8 kHz and with the bearing gas cooled to $-15 \text{ }^\circ\text{C}$, giving an effective sample temperature of $-5 \text{ }^\circ\text{C}$. Cross-polarization was accomplished at a ^1H spin-lock field of 45 kHz, a $^{13}\text{C}/^{15}\text{N}$ spin-lock field of 37 kHz (ramped ± 2 kHz), and a contact time of 2 ms; 85 kHz Spinal64 [2] ^1H decoupling was used throughout. ^{15}N spectra were acquired as the sum of 81,920 transients using a relaxation delay of 4 s, for a total acquisition time of 3 days 19 h. ^{15}N chemical shifts were referenced indirectly to $\text{NH}_3(\text{l})$ via an external solid-state sample of $^{15}\text{NH}_4\text{Cl}$ ($\delta[\text{NH}_3(\text{l})] = 39.3$ ppm) calibrated under MAS conditions. ^{13}C spectra were acquired as the sum of 16,384 transients acquired with a relaxation delay of 4 s, for a total acquisition time of 18 h. ^{13}C chemical shifts were referenced indirectly to TMS(l) via an external solid-state sample of adamantane ($\delta[\text{TMS}] = 38.48$ ppm) calibrated under MAS conditions.

Chemical Shifts: Chemical shifts were measured for N1, C2, and C3 on PLP (shown in black), N, C^α , C^β , and C' for the segment derived from serine (shown in blue), and N for the segment derived from 2AP (shown in red). These shifts are summarized below:

Linear Regression models: As described in the main text, the isotropic chemical shielding values were converted to chemical shifts via least-squares fitting for the carbon and nitrogen shieldings. The absolute shieldings, linear regression parameters, and resulting chemical shifts are provided here.

Table 1: Experimentally measured ^{13}C and ^{15}N chemical shifts for selected atoms in 2AP.

Site	Chemical Shift (ppm)
C^α (Ser)	105.1
C^β (Ser)	47.0
C' (Ser)	173.1
N (Ser)	298.6
N (2AP)	55.9
C2 (PLP)	144.6
C3 (PLP)	153.1
N1 (PLP)	265.0

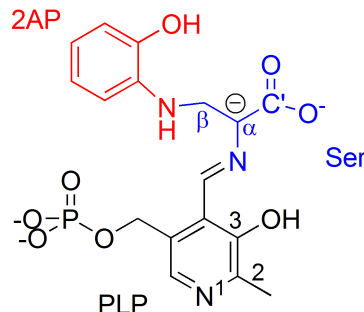


Table 2: ^{13}C Carbon chemical shieldings and shifts for selected atoms in 2AP.

	5 Å Cluster	7 Å Cluster	5 Å ONIOM	Experiment
<i>Chemical Shieldings:</i>				
C3 (PLP)	26.7	26.6	26.2	
C2 (PLP)	39.1	37.1	36.3	
C^α (Ser)	68.3	68.8	67.7	
C' (Ser)	2.5	2.7	2.3	
C^β (Ser)	126.7	126.9	126.3	
<i>Linear Regression Parameters:</i>				
Slope:	-1.0403	-1.0402	-1.0418	
Intercept:	179.51	179.09	178.51	
<i>Chemical Shifts:</i>				
C3 (PLP)	151.5	151.2	151.2	153.1
C2 (PLP)	139.2	140.9	140.7	144.6
C^α (Ser)	108.5	107.8	107.9	105.1
C' (Ser)	176.7	176.1	176.1	173.1
C^β (Ser)	47.1	46.9	46.9	47.0
C rms	3.4	2.6	2.7	

Table 3: ^{15}N Nitrogen chemical shieldings and shifts for selected atoms in 2AP.

	5 Å Cluster	7 Å Cluster	5 Å ONIOM	Experiment
<i>Chemical Shieldings:</i>				
N (Ser)	-80.5	-80.7	-80.7	
N (2AP)	177.4	177.2	177.3	
N1 (PLP)	-32.3	-34.9	-34.8	
<i>Linear Regression Parameters:</i>				
Slope:	-0.9578	-0.9549	-0.9547	
Intercept:	227.10	226.12	226.17	
<i>Chemical Shifts:</i>				
N (Ser)	304.2	303.2	303.2	298.6
N (2AP)	57.2	56.9	56.9	55.9
N1 (PLP)	258.1	259.4	259.4	265.0
N rms	5.2	4.2	4.3	

2 2AP system

2.1 2AP coenzyme/substrate only

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2AP coenzyme-substrate complex only

O	3.891392	-3.220755	-0.725068
C	4.310711	-2.075858	-0.116111
C	5.645943	-1.823861	0.228945
C	5.977446	-0.626483	0.880147
C	4.979548	0.314007	1.143125
C	3.650188	0.069253	0.773100
C	3.302772	-1.139979	0.169234
N	1.944591	-1.482886	-0.122198
O	1.615698	4.718715	-0.209624
P	0.900404	3.566888	-0.962364
O	1.854691	2.536140	-1.599124
O	-0.213032	4.109356	-1.877248
O	0.161834	2.573427	0.167627
C	-0.927718	3.036275	0.951474
C	-2.194024	2.247409	0.689015
C	-3.385049	2.932374	0.494501
N	-4.579713	2.361219	0.268415
C	-2.241361	0.828016	0.669102
C	-3.506564	0.220348	0.372756
O	-3.646114	-1.119623	0.256136
C	-4.631642	1.022022	0.190367
C	-5.969095	0.398403	-0.147458
C	-1.075168	0.015740	0.863988
N	-1.206247	-1.290857	0.742094
C	-0.238571	-2.210191	0.810519
C	-0.512045	-3.524336	0.256375
O	-1.697169	-3.822446	-0.143558
O	0.506022	-4.309608	0.148847
C	1.171187	-1.823699	1.143105
H	4.637150	-3.641851	-1.218106
H	6.409962	-2.581591	0.006514
H	7.011173	-0.440448	1.187817
H	5.233305	1.248173	1.645438
H	2.883587	0.816571	0.925837
H	-0.636022	2.955638	2.028168
H	-1.123414	4.099876	0.744307
H	-3.370981	4.032872	0.531222
H	-5.984128	-0.691259	0.043910
H	-6.202953	0.540554	-1.224387

H	-6.771955	0.888844	0.431277
H	-0.129746	0.497025	1.105969
H	1.673893	-2.656883	1.658707
H	1.200174	-0.937092	1.791381
H	-2.697197	-1.512388	0.405410
H	1.961505	-2.396316	-0.588773

2.2 2AP coenzyme/substrate in a 5 Å protein cluster.

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2AP surrounded by a 5 Å cut of tryptophan synthase

O	3.89139200	-3.22075500	-0.72506800
C	4.31071100	-2.07585800	-0.11611100
C	5.64594300	-1.82386100	0.22894500
C	5.97744600	-0.62648300	0.88014700
C	4.97954800	0.31400700	1.14312500
C	3.65018800	0.06925300	0.77310000
C	3.30277200	-1.13997900	0.16923400
N	1.94459100	-1.48288600	-0.12219800
O	1.61569800	4.71871500	-0.20962400
P	0.90040400	3.56688800	-0.96236400
O	1.85469100	2.53614000	-1.59912400
O	-0.21303200	4.10935600	-1.87724800
O	0.16183400	2.57342700	0.16762700
C	-0.92771800	3.03627500	0.95147400
C	-2.19402400	2.24740900	0.68901500
C	-3.38504900	2.93237400	0.49450100
N	-4.57971300	2.36121900	0.26841500
C	-2.24136100	0.82801600	0.66910200
C	-3.50656400	0.22034800	0.37275600
O	-3.64611400	-1.11962300	0.25613600
C	-4.63164200	1.02202200	0.19036700
C	-5.96909500	0.39840300	-0.14745800
C	-1.07516800	0.01574000	0.86398800
N	-1.20624700	-1.29085700	0.74209400
C	-0.23857100	-2.21019100	0.81051900
C	-0.51204500	-3.52433600	0.25637500
O	-1.69716900	-3.82244600	-0.14355800
O	0.50602200	-4.30960800	0.14884700
C	1.17118700	-1.82369900	1.14310500
H	4.63715000	-3.64185100	-1.21810600
H	6.40996200	-2.58159100	0.00651400
H	7.01117300	-0.44044800	1.18781700

H	5.23330500	1.24817300	1.64543800
H	2.88358700	0.81657100	0.92583700
H	-0.63602200	2.95563800	2.02816800
H	-1.12341400	4.09987600	0.74430700
H	-3.37098100	4.03287200	0.53122200
H	-5.98412800	-0.69125900	0.04391000
H	-6.20295300	0.54055400	-1.22438700
H	-6.77195500	0.88884400	0.43127700
H	-0.12974600	0.49702500	1.10596900
H	1.67389300	-2.65688300	1.65870700
H	1.20017400	-0.93709200	1.79138100
H	-2.69719700	-1.51238800	0.40541000
H	1.96150500	-2.39631600	-0.58877300
C	5.39506600	-8.14705800	-0.91263800
C	6.41485600	-7.17699700	-0.27371400
C	6.14280200	-5.66946400	-0.50921200
C	6.37036900	-5.17371800	-1.95198800
O	7.07761200	-5.83795500	-2.73028500
O	5.84194400	-4.08452000	-2.32232800
C	4.00810000	-7.53946700	-0.79463100
O	3.52402900	-6.92201600	-1.73754500
N	3.35152100	-7.72224300	0.33942000
C	2.11509500	-6.99237200	0.59633600
C	0.90473900	-7.74385100	-0.03054400
O	-0.20218500	-6.83380200	-0.14169300
C	0.49777300	-8.98438700	0.78402700
C	1.93678000	-6.74518400	2.10035400
O	2.41475500	-7.52332700	2.92586900
N	1.23560400	-5.65402700	2.43223400
C	0.93481400	-5.29770900	3.81983200
C	-0.55594600	-5.37719500	4.04445300
O	-1.04602100	-6.24073200	4.80428500
N	-1.28639200	-4.45214000	3.43260900
C	-2.75324400	-4.49823200	3.45725100
C	-3.35398100	-3.20386400	2.91003500
C	-3.31085300	-5.69530800	2.71757200
O	-4.47704800	-6.04604900	2.89361000
N	-2.48830200	-6.33330800	1.87679600
C	-2.98672600	-7.40226300	1.01973900
C	-3.61419400	-6.92928500	-0.29943500
O	-4.04065700	-7.76799100	-1.11983400
N	-3.69155900	-5.61656000	-0.53067600
C	-4.28455100	-5.07604600	-1.75684400
C	-4.76868800	-3.64050400	-1.57864000
C	-5.97850300	-3.53686300	-0.65082700

C	-7.19438800	-4.25530100	-1.21948400
O	-7.95129600	-4.89143200	-0.48733500
N	-7.40774100	-4.12368500	-2.52824600
C	-3.30694700	-5.17790500	-2.92397800
O	-3.69260600	-5.51403400	-4.03806700
N	-2.02467400	-4.93235100	-2.64622400
C	-1.01527300	-5.20030100	-3.66360300
C	0.33028000	-4.61862400	-3.26390100
C	1.37136400	-4.83877300	-4.32463400
N	1.28090300	-4.30605400	-5.58003200
C	2.32957100	-4.72839600	-6.30271700
N	3.07299900	-5.53408700	-5.53945100
C	2.50088800	-5.62639200	-4.31626700
C	-0.87989100	-6.67476000	-3.95504500
O	-0.73624600	-7.07314700	-5.12483000
N	-0.96179900	-7.51028800	-2.90443700
H	7.42578100	-7.42333000	-0.65206900
H	6.44356100	-7.35373000	0.82092100
H	5.11981200	-5.40550800	-0.17222500
H	6.82480000	-5.09684200	0.16652100
H	5.46276100	-9.14441100	-0.43863500
H	1.16671000	-8.06189700	-1.07033400
H	-0.30570000	-9.53670600	0.27667100
H	1.34998500	-9.66370200	0.90301500
H	0.13338800	-8.72001300	1.78548300
H	0.13834900	-5.92614200	-0.22770500
H	2.20255700	-5.99384200	0.06513700
H	3.84720100	-8.08001800	1.12973900
H	1.47341500	-5.96946200	4.53393600
H	1.32590800	-4.27343500	4.03247100
H	0.98202900	-4.97510700	1.69919600
H	-4.45227900	-3.24706400	2.95346000
H	-3.07700000	-3.02747700	1.85684600
H	-3.03414000	-2.32621500	3.49216300
H	-3.05161500	-4.59770100	4.53860600
H	-0.86512000	-3.76879200	2.82451800
H	-3.73590700	-8.01569000	1.56414400
H	-2.13773600	-8.08412900	0.78763500
H	-1.62323700	-5.91923600	1.58564700
H	-5.00732100	-3.21332100	-2.58212700
H	-3.94790600	-2.99854700	-1.18247800
H	-5.73459800	-3.94276500	0.35459800
H	-6.20193300	-2.45084800	-0.46978700
H	-8.03557900	-4.75026800	-2.97915800
H	-6.64278800	-3.81118200	-3.09375500

H	-5.17072400	-5.72349900	-2.00785300
H	-3.07113000	-4.96040300	-0.04545400
H	0.70785300	-5.04866200	-2.30911200
H	0.23419500	-3.52495800	-3.07968900
H	2.92715200	-6.18375200	-3.44948000
H	3.91719000	-5.97295700	-5.80293500
H	2.51131700	-4.42808500	-7.34012400
H	-1.34008300	-4.68858700	-4.61617400
H	-1.72083300	-4.51627900	-1.74574900
H	-1.19679902	-6.99078332	-2.08292018
H	5.64681200	-8.29149500	-1.98165300
C	-10.60779400	-2.79848300	-4.35970200
C	-9.61102200	-1.73599200	-3.93315300
O	-9.80558500	-1.12664500	-2.89423400
N	-8.58054000	-1.48566600	-4.74496000
C	-7.61116200	-0.41718900	-4.43405500
C	-6.62428300	-0.85139700	-3.35642300
C	-6.85340500	0.02204200	-5.66831300
O	-6.82569200	-0.69628400	-6.66809200
N	-6.21718500	1.18403600	-5.55091300
C	-5.38394900	1.77016100	-6.63080200
C	-4.80517400	3.11205900	-6.14003200
C	-3.71355000	2.94313900	-5.14694400
N	-3.96488100	2.50309000	-3.88340300
C	-2.80142400	2.40794200	-3.22407700
N	-1.80500600	2.71915700	-4.07779000
C	-2.33931900	3.02824400	-5.27671000
C	-4.26187300	0.83748000	-7.05279000
O	-3.72173800	0.96868600	-8.15681100
N	-3.86771200	-0.08571600	-6.16833400
C	-2.71705500	-1.00858700	-6.41947900
C	-2.56389200	-2.05305800	-5.29535300
C	-2.22727000	-1.41768600	-3.95064000
C	-0.83955700	-0.76338600	-3.90692400
C	-0.47734800	-0.43442600	-2.45655600
N	0.90365900	0.08452500	-2.22262600
C	-2.86172300	-1.73642600	-7.74653200
O	-1.83880200	-2.02936400	-8.41833500
H	-10.17400700	-3.80449600	-4.28018800
H	-11.49637600	-2.76558000	-3.70201100
H	-7.12608600	-1.37600200	-2.52824700
H	-5.84229700	-1.52280600	-3.74652200
H	-6.11945700	0.02109200	-2.89846300
H	-8.22244800	0.44020000	-4.02770100
H	-8.34715800	-2.13478100	-5.46675200

H	-4.40491500	3.66374700	-7.01437400
H	-5.60712400	3.75240900	-5.71598000
H	-1.75370800	3.31597700	-6.15428400
H	-0.84531400	2.81349500	-3.82541100
H	-2.70353500	2.15514400	-2.15663200
H	-6.04286300	1.95579400	-7.51728400
H	-6.36177000	1.74803100	-4.71348900
H	-3.49304700	-2.65216100	-5.19122300
H	-1.76405000	-2.77217700	-5.57959100
H	-2.29285000	-2.20005000	-3.16433300
H	-3.00451600	-0.66562300	-3.68578800
H	-0.08430900	-1.44961500	-4.35085700
H	-0.81753500	0.15060300	-4.53536800
H	-0.59899900	-1.36325500	-1.84690000
H	-1.21311500	0.28756000	-2.03116000
H	1.50305400	-0.16525000	-2.99936600
H	1.27342800	-0.37125800	-1.35972000
H	0.96821300	1.11963200	-2.07481600
H	-1.77187400	-0.39464300	-6.46391800
H	-4.00192200	0.07708100	-5.18581600
N	-4.19632700	-2.09853600	-8.24444700
H	-4.17923300	-2.80531800	-8.94307800
H	-4.83703500	-2.29953600	-7.50465300
H	-10.94966700	-2.65924900	-5.39285700
C	-1.12780000	-2.47151800	7.61431100
C	-0.46836900	-1.84175600	6.39204400
O	0.75814500	-1.95771000	6.23455900
N	-1.23069600	-1.16185100	5.53238700
C	-0.65454800	-0.60634000	4.31575600
C	0.20684200	0.62339600	4.53067500
O	0.95294300	1.01790900	3.62462500
N	0.07773600	1.25548800	5.70634800
C	0.92826100	2.38196500	6.04121400
C	0.09319300	3.49935800	6.67581500
C	-1.08528500	4.05362900	5.83559300
C	-1.70932800	5.23154400	6.59850000
C	-0.75194000	4.42552400	4.39261900
C	2.10275400	2.06535400	6.96081700
O	2.96201100	2.93614800	7.20801800
N	2.13895100	0.82660600	7.44983300
C	6.16358700	0.97069700	5.34760300
C	7.37382700	0.80390900	4.46858000
C	8.05172300	-0.41286700	4.41408300
C	9.16488400	-0.56990300	3.59149000
C	9.58436700	0.48366000	2.78142800

C	8.89861800	1.69235500	2.80651400
C	7.78122700	1.84059600	3.63809500
H	-0.41899915	-2.52513453	8.41407760
H	-0.04244800	-1.37642600	3.78727300
H	-1.47786300	-0.34335500	3.61020500
H	-2.24569600	-1.07744000	5.60815500
H	-0.31092700	3.16544300	7.65434500
H	0.77851200	4.34275900	6.90673100
H	-1.87297500	3.24546100	5.76199200
H	-2.61062200	5.59818500	6.08690900
H	-1.99826900	4.93880600	7.61545300
H	-1.00790800	6.07207200	6.67872200
H	-1.61815400	4.91914300	3.91469200
H	-0.50741700	3.55041700	3.75952600
H	0.10074100	5.11615700	4.34548400
H	1.38245900	2.80027800	5.09222600
H	-0.72390400	1.10607500	6.28299100
H	1.50716994	0.13343585	7.10289233
H	5.46103187	0.19110063	5.13892673
H	5.71036776	1.92045561	5.15408062
H	7.21805100	2.78624900	3.62383900
H	7.69016500	-1.25971400	5.01323900
H	9.20562200	2.51970500	2.15965000
H	9.66973300	-1.54084300	3.53907300
H	10.44056000	0.34881800	2.11010100
H	-1.96237352	-1.87413153	7.91682785
C	7.33175200	-4.01098400	-6.09637800
C	6.02749100	-3.19516800	-6.06148000
O	5.54593200	-2.69815500	-7.09437300
N	5.46861100	-3.05457800	-4.86229900
C	4.09558300	-2.55462200	-4.71844100
C	3.91182400	-1.09959100	-4.38154300
O	2.79453900	-0.65834900	-4.13915100
N	4.99556700	-0.33247100	-4.40788600
C	4.89618300	1.08686400	-4.06086200
C	4.99594300	1.29245600	-2.52718500
O	4.57209100	2.64078200	-2.21544900
C	6.42822100	1.11827500	-2.03053800
C	5.94832400	1.92039000	-4.80803800
O	6.84854000	1.34967100	-5.43779600
N	5.82717300	3.25505200	-4.73929900
H	7.38175841	-4.64072351	-5.23276494
H	3.51644300	-2.72914200	-5.65552800
H	3.60705700	-3.15831600	-3.91745200
H	5.83731000	-3.52964700	-4.01341500

H	4.32135800	0.56959000	-2.00222700
H	6.90869600	0.23412700	-2.47672600
H	6.43651100	0.97012000	-0.93723100
H	7.08101000	1.98520000	-2.23302000
H	3.62314100	2.57970200	-1.98878200
H	3.88630500	1.47264200	-4.39917000
H	5.92415500	-0.70528200	-4.53106100
H	5.29227331	3.67134621	-4.00405656
H	7.35132260	-4.61465746	-6.97960806
C	-2.11510000	8.85223600	2.47837300
C	-2.82916100	7.70297200	3.15402500
S	-3.19231500	6.30985500	2.09858400
C	-0.81914200	8.35315200	1.83260200
O	-0.70894400	8.21217900	0.60700100
N	0.19279600	8.16836600	2.66582100
C	1.55315500	7.79329600	2.24295900
C	2.53949200	8.99324900	2.34510900
C	3.91013600	8.56667700	1.81614600
C	2.04905900	10.18714900	1.54851700
C	2.02549700	6.59063000	3.05984700
O	2.39120100	6.71155100	4.24058200
N	2.04866800	5.42035100	2.41503800
C	2.62785100	4.18735700	2.99793200
C	4.03217800	4.08944000	2.44147900
O	5.00451100	4.29144000	3.12894500
N	4.14458600	3.77446500	1.17660000
C	5.42324600	3.91438100	0.47683200
C	5.37748500	5.07769000	-0.51605100
O	6.41669300	5.57605900	-0.95279600
N	4.17577600	5.49312500	-0.94580000
C	4.03273300	6.69159400	-1.80050500
C	3.32693800	6.51982900	-3.12344000
O	3.23001300	7.48815100	-3.87010000
N	2.79596400	5.31989100	-3.44565500
C	2.27115000	5.17126000	-4.81565300
C	2.16958500	3.71249900	-5.26737200
O	1.20898300	3.00032000	-4.53283000
C	0.92978200	5.87939100	-5.08344200
O	0.77098700	6.55195200	-6.12019700
N	-0.05554300	5.72720600	-4.20240100
C	-1.32839300	6.40345000	-4.48516600
C	-2.48890400	5.91814900	-3.57461500
C	-2.59162200	6.68684800	-2.23679900
O	-3.30831100	7.69334700	-2.16421600
N	-1.96382500	6.17671300	-1.17461300

C	-1.14558100	7.91403600	-4.43767800
O	-1.78423100	8.64451900	-5.21097700
N	-0.30577100	8.37552400	-3.49452100
H	-3.78527300	8.08446600	3.57101800
H	-2.25114900	7.37096900	4.04310100
H	-3.05552300	5.28515700	2.98375100
H	-1.92110400	9.66549400	3.20560100
H	2.64627900	9.28200700	3.41918700
H	3.85863800	8.26510100	0.75844000
H	4.63132100	9.39107200	1.88723100
H	4.31771300	7.72179400	2.38675600
H	1.85014400	9.92559500	0.49648100
H	2.79755400	10.99116600	1.54763600
H	1.12340700	10.61046500	1.96035800
H	1.50431700	7.52337700	1.14317900
H	0.05814600	8.27528700	3.64864600
H	1.98665500	3.31998200	2.71864500
H	2.63114300	4.22057400	4.11084500
H	1.75346200	5.32644300	1.42798200
H	5.64225400	2.96985000	-0.07202000
H	6.26881000	4.05559300	1.18423100
H	3.32608100	3.63648700	0.59825900
H	5.03699000	7.13423200	-2.00280000
H	3.47472800	7.45496800	-1.20510400
H	3.27680900	5.10266800	-0.59733400
H	1.92429600	3.68738900	-6.34881600
H	3.14456300	3.18754900	-5.13779600
H	1.06502100	2.19629000	-5.04649400
H	3.03269000	5.64312200	-5.49874300
H	2.53753500	4.63425400	-2.75974500
H	-2.40979500	4.83871200	-3.36049600
H	-3.43933000	6.05897900	-4.12663600
H	-1.28454700	5.41653600	-1.29560800
H	-2.01765100	6.63437400	-0.29041900
H	-1.63014900	6.12774000	-5.53312100
H	0.00158600	5.12198400	-3.35092200
H	-0.42467302	7.84621614	-2.65446416
H	-2.76609600	9.29405500	1.69319000
C	-7.24332200	4.71719100	-2.33572000
C	-5.83533900	4.80564600	-1.72522600
O	-5.89897900	4.55526300	-0.32836200
C	-7.78108800	3.29471700	-2.35724200
O	-7.41647600	2.51760700	-3.25239800
N	-8.62070600	2.91878800	-1.37910200
C	-9.19692900	1.56882000	-1.36022900

C	-10.45868800	1.46085700	-0.54645500
O	-10.82144400	2.40587200	0.15246500
N	-11.14325200	0.32530900	-0.68921800
H	-5.12776200	4.12116500	-2.23040100
H	-5.44483400	5.83781300	-1.80638800
H	-7.19393000	5.09381500	-3.37657800
H	-9.37384700	1.25003700	-2.41500000
H	-8.44343000	0.84949700	-0.95046500
H	-8.67461000	3.45735900	-0.52831800
H	-10.51233399	-0.45003366	-0.66117826
H	-7.93117000	5.40248800	-1.79842100
H	-5.64974800	3.63016100	-0.19202000
C	-7.54879700	-3.84178100	2.82150500
C	-7.16105000	-2.37380500	2.98428000
N	-6.81861300	-2.02524000	4.39642800
H	-7.96571185	-3.99472631	1.84801142
H	-6.67983719	-4.45520905	2.93775849
H	-7.97565500	-1.70142300	2.61914800
H	-6.28590100	-2.14665300	2.32439700
H	-7.64181000	-2.02864900	4.96461400
H	-6.36253100	-1.06213900	4.41725000
H	-6.16578600	-2.69653600	4.75799100
C	-5.12147700	3.65263100	4.90518500
C	-4.46230000	2.94414400	3.70307000
C	-3.63182500	1.68872100	4.04225200
C	-4.46105100	0.45795200	4.44673100
O	-5.66079800	0.39836200	4.08023200
O	-3.93287700	-0.45839500	5.13039300
C	-5.72645400	4.98539700	4.41491800
O	-5.32206800	6.07223000	4.86240300
N	-6.73937900	4.88699700	3.54444600
C	-7.41520000	6.02307000	2.90844900
C	-8.52029300	5.51739900	1.97701800
O	-8.06229900	4.40206500	1.19719100
C	-8.06395000	6.89840700	3.98141900
O	-8.16195300	8.14044700	3.80571300
H	-5.23450800	2.66986500	2.95494500
H	-3.78290800	3.67800300	3.20174400
H	-3.03139200	1.41173700	3.14774400
H	-2.89872100	1.95043100	4.84209000
H	-4.36615000	3.84704300	5.69314100
H	-9.38602700	5.09897100	2.52090500
H	-8.87707400	6.33456200	1.32286800
H	-6.66154700	6.63248600	2.33666500
H	-6.87991500	3.99152300	3.11185900

N	-8.57349500	6.28921500	5.21826300
H	-8.10099900	5.45536500	5.48345900
H	-8.62304700	6.94344500	5.96697500
H	-5.89881000	3.01439500	5.36638700
H	-7.35157200	4.72912400	0.63595700
C	-9.73754400	1.34911100	3.67370600
C	-8.63584000	1.18793600	2.63335200
C	-9.23931500	2.24456200	4.83091000
O	-9.37039300	3.49426200	4.76107900
H	-8.32609800	2.15857400	2.21882500
H	-8.97600200	0.56949300	1.78994200
H	-7.73917600	0.70978400	3.04964400
H	-10.05804600	0.36396500	4.06168200
N	-8.61202200	1.63613700	6.01299200
H	-8.05448200	0.85695700	5.73480900
H	-8.07349200	2.29509500	6.53333000
H	-10.63017100	1.81448800	3.21392700
C	4.89354400	-3.55337600	5.27712300
C	4.85194700	-3.06613500	3.86667800
C	4.50409300	-4.19703900	2.92550700
C	3.76829200	-1.99839000	3.92794200
H	3.89512749	-3.68927937	5.63711570
H	5.39821484	-2.83441057	5.88810259
H	5.82290300	-2.61278100	3.54977700
H	3.48719400	-1.64277300	2.92387200
H	2.85181100	-2.36383800	4.41829700
H	4.12924600	-1.11547700	4.48914700
H	5.34502900	-4.89624700	2.80761300
H	3.64074100	-4.77448000	3.28608500
H	4.25507500	-3.81733900	1.92171800
O	0.79376400	1.02002900	-6.55599700
O	-4.92465800	8.23320100	-0.04652300
O	-5.88929300	-3.84679400	-5.30282200
O	1.02763800	7.16836200	-1.27431000
O	0.49953500	-1.87111700	-6.77322700
O	3.32691600	-7.52125900	5.45288100
O	-8.57869700	-1.64945700	-0.16120300
O	2.41973700	-3.78428300	7.68434200
H	0.67802500	0.06457000	-6.44598500
H	1.48172400	1.14580800	-7.20063400
H	-4.68390100	7.48569600	0.49811000
H	-4.37987000	8.19920800	-0.84021800
H	-5.17744400	-4.43061800	-5.02646000
H	-5.53128200	-3.19588000	-5.90274900
H	1.15265100	6.23215300	-1.02234500

H	0.59566700	7.60877200	-0.53108700
H	0.72385100	-2.69230600	-6.31040500
H	-0.22044600	-2.04072800	-7.38869800
H	4.11336200	-7.85298000	5.03275400
H	2.70621600	-7.29744300	4.74414200
H	-7.64051600	-1.45555200	-0.24043400
H	-8.83948600	-2.18861800	-0.90035100
H	2.79530000	-3.36841600	8.45687100
H	2.67805100	-3.27525400	6.91729000
H	8.16909571	-3.34485046	-6.10102739
H	6.27179026	3.83335575	-5.42331674
H	-0.50527031	9.33843246	-3.31284185
H	-11.80793011	0.24120699	0.05316321
H	-8.27254022	-4.10403333	3.56468699
H	-1.66823906	-8.19634083	-3.07843113
H	6.45895450	0.91911087	6.37473343
H	5.41710506	-4.48567674	5.31711233
H	-1.46473384	-3.45717644	7.36966222
H	2.79790148	0.58997367	8.16382839

2.3 2AP coenzyme/substrate in a 7 Å protein cluster.

615

2AP surrounded by a 7 Ang cut of tryptophan synthase

O	3.891392	-3.220755	-0.725068
C	4.310711	-2.075858	-0.116111
C	5.645943	-1.823861	0.228945
C	5.977446	-0.626483	0.880147
C	4.979548	0.314007	1.143125
C	3.650188	0.069253	0.773100
C	3.302772	-1.139979	0.169234
N	1.944591	-1.482886	-0.122198
O	1.615698	4.718715	-0.209624
P	0.900404	3.566888	-0.962364
O	1.854691	2.536140	-1.599124
O	-0.213032	4.109356	-1.877248
O	0.161834	2.573427	0.167627
C	-0.927718	3.036275	0.951474
C	-2.194024	2.247409	0.689015
C	-3.385049	2.932374	0.494501
N	-4.579713	2.361219	0.268415
C	-2.241361	0.828016	0.669102

C	-3.506564	0.220348	0.372756
O	-3.646114	-1.119623	0.256136
C	-4.631642	1.022022	0.190367
C	-5.969095	0.398403	-0.147458
C	-1.075168	0.015740	0.863988
N	-1.206247	-1.290857	0.742094
C	-0.238571	-2.210191	0.810519
C	-0.512045	-3.524336	0.256375
O	-1.697169	-3.822446	-0.143558
O	0.506022	-4.309608	0.148847
C	1.171187	-1.823699	1.143105
H	4.637150	-3.641851	-1.218106
H	6.409962	-2.581591	0.006514
H	7.011173	-0.440448	1.187817
H	5.233305	1.248173	1.645438
H	2.883587	0.816571	0.925837
H	-0.636022	2.955638	2.028168
H	-1.123414	4.099876	0.744307
H	-3.370981	4.032872	0.531222
H	-5.984128	-0.691259	0.043910
H	-6.202953	0.540554	-1.224387
H	-6.771955	0.888844	0.431277
H	-0.129746	0.497025	1.105969
H	1.673893	-2.656883	1.658707
H	1.200174	-0.937092	1.791381
H	-2.697197	-1.512388	0.405410
H	1.961505	-2.396316	-0.588773
C	5.395066	-8.147058	-0.912638
C	6.414856	-7.176997	-0.273714
C	6.142802	-5.669464	-0.509212
C	6.370369	-5.173718	-1.951988
O	7.077612	-5.837955	-2.730285
O	5.841944	-4.084520	-2.322328
C	4.008100	-7.539467	-0.794631
O	3.524029	-6.922016	-1.737545
N	3.351521	-7.722243	0.339420
C	2.115095	-6.992372	0.596336
C	0.904739	-7.743851	-0.030544
O	-0.202185	-6.833802	-0.141693
C	0.497773	-8.984387	0.784027
C	1.936780	-6.745184	2.100354
O	2.414755	-7.523327	2.925869
N	1.235604	-5.654027	2.432234
C	0.934814	-5.297709	3.819832
C	-0.555946	-5.377195	4.044453

O	-1.046021	-6.240732	4.804285
N	-1.286392	-4.452140	3.432609
C	-2.753244	-4.498232	3.457251
C	-3.353981	-3.203864	2.910035
C	-3.310853	-5.695308	2.717572
O	-4.477048	-6.046049	2.893610
N	-2.488302	-6.333308	1.876796
C	-2.986726	-7.402263	1.019739
C	-3.614194	-6.929285	-0.299435
O	-4.040657	-7.767991	-1.119834
N	-3.691559	-5.616560	-0.530676
C	-4.284551	-5.076046	-1.756844
C	-4.768688	-3.640504	-1.578640
C	-5.978503	-3.536863	-0.650827
C	-7.194388	-4.255301	-1.219484
O	-7.951296	-4.891432	-0.487335
N	-7.407741	-4.123685	-2.528246
C	-3.306947	-5.177905	-2.923978
O	-3.692606	-5.514034	-4.038067
N	-2.024674	-4.932351	-2.646224
C	-1.015273	-5.200301	-3.663603
C	0.330280	-4.618624	-3.263901
C	1.371364	-4.838773	-4.324634
N	1.280903	-4.306054	-5.580032
C	2.329571	-4.728396	-6.302717
N	3.072999	-5.534087	-5.539451
C	2.500888	-5.626392	-4.316267
C	-0.879891	-6.674760	-3.955045
O	-0.736246	-7.073147	-5.124830
N	-0.961799	-7.510288	-2.904437
C	-0.971233	-8.993575	-3.039451
C	-2.157166	-9.453838	-3.886155
O	-1.989284	-10.214384	-4.847027
N	-3.357302	-8.962967	-3.555851
C	-4.550328	-9.258427	-4.369237
C	-5.836750	-8.660120	-3.723357
C	-6.980991	-8.562065	-4.741132
C	-6.244994	-9.496239	-2.501122
C	-4.380470	-8.813228	-5.831675
O	-4.660153	-9.606936	-6.767283
H	7.425781	-7.423330	-0.652069
H	6.443561	-7.353730	0.820921
H	5.119812	-5.405508	-0.172225
H	6.824800	-5.096842	0.166521
H	5.462761	-9.144411	-0.438635

H	1.166710	-8.061897	-1.070334
H	-0.305700	-9.536706	0.276671
H	1.349985	-9.663702	0.903015
H	0.133388	-8.720013	1.785483
H	0.138349	-5.926142	-0.227705
H	2.202557	-5.993842	0.065137
H	3.847201	-8.080018	1.129739
H	1.473415	-5.969462	4.533936
H	1.325908	-4.273435	4.032471
H	0.982029	-4.975107	1.699196
H	-4.452279	-3.247064	2.953460
H	-3.077000	-3.027477	1.856846
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N	-6.739379	4.886997	3.544446
C	-7.415200	6.023070	2.908449
C	-8.520293	5.517399	1.977018
O	-8.062299	4.402065	1.197191
C	-8.063950	6.898407	3.981419
O	-8.161953	8.140447	3.805713
H	-5.234508	2.669865	2.954945
H	-3.782908	3.678003	3.201744
H	-3.031392	1.411737	3.147744
H	-2.898721	1.950431	4.842090
H	-4.366150	3.847043	5.693141
H	-9.386027	5.098971	2.520905
H	-8.877074	6.334562	1.322868
H	-6.661547	6.632486	2.336665
H	-6.879915	3.991523	3.111859
N	-8.573495	6.289215	5.218263

H	-8.100999	5.455365	5.483459
H	-8.623047	6.943445	5.966975
H	-5.898810	3.014395	5.366387
H	-7.351572	4.729124	0.635957
C	-9.737544	1.349111	3.673706
C	-8.635840	1.187936	2.633352
C	-9.239315	2.244562	4.830910
O	-9.370393	3.494262	4.761079
H	-8.326098	2.158574	2.218825
H	-8.976002	0.569493	1.789942
H	-7.739176	0.709784	3.049644
H	-10.058046	0.363965	4.061682
N	-8.612022	1.636137	6.012992
H	-8.054482	0.856957	5.734809
H	-8.073492	2.295095	6.533330
H	-10.630171	1.814488	3.213927
C	7.191432	11.534671	-0.870592
C	5.992166	11.043510	-1.634523
N	4.958983	11.842850	-1.949284
C	4.066660	11.143796	-2.676040
N	4.525443	9.888816	-2.798075
C	5.717592	9.796270	-2.174327
H	7.873582	10.703706	-0.654594
H	6.894932	11.989831	0.082289
H	6.307469	8.876026	-2.112580
H	4.046662	9.110192	-3.240729
H	3.124582	11.544263	-3.066242
H	7.742276	12.287080	-1.448680
C	5.517300	-4.877852	5.682854
C	4.893544	-3.553376	5.277123
C	4.851947	-3.066135	3.866678
C	4.504093	-4.197039	2.925507
C	3.768292	-1.998390	3.927942
C	7.051823	-4.878054	5.480957
O	7.558893	-5.500146	4.511692
H	3.836614	-3.616439	5.648096
H	5.358976	-2.757612	5.903355
H	5.822903	-2.612781	3.549777
H	3.487194	-1.642773	2.923872
H	2.851811	-2.363838	4.418297
H	4.129246	-1.115477	4.489147
H	5.345029	-4.896247	2.807613
H	3.640741	-4.774480	3.286085
H	4.255075	-3.817339	1.921718
H	5.078925	-5.712748	5.099077

N	7.916594	-4.151558	6.421457
H	7.473177	-3.997161	7.297818
H	8.827985	-4.538573	6.507078
H	5.283259	-5.082931	6.746228
C	9.866521	-6.454318	1.750401
C	10.063276	-4.965643	2.021599
S	8.649895	-3.908941	1.653326
C	11.237817	-7.137602	1.737893
O	11.751595	-7.497717	0.646710
H	10.888594	-4.562683	1.394462
H	10.367512	-4.812228	3.074308
H	7.615326	-4.749170	1.794675
H	9.358076	-6.612559	0.774485
N	11.953881	-7.372917	3.000203
H	12.939097	-7.444651	2.880148
H	11.706124	-6.697380	3.688030
H	9.209458	-6.911719	2.517388
C	13.937772	-0.835126	1.097273
C	12.858132	-1.492812	0.242703
C	12.841490	-2.886158	0.039202
C	11.831666	-3.480972	-0.744115
C	10.825066	-2.699244	-1.295061
C	10.823308	-1.317360	-1.082953
C	11.829186	-0.724091	-0.310126
H	13.481862	-0.310088	1.945431
H	14.500911	-0.102970	0.506737
H	13.622113	-3.511385	0.482423
H	11.804373	0.356854	-0.130332
H	11.836943	-4.564926	-0.902806
H	10.024518	-0.701723	-1.515142
H	10.025584	-3.157499	-1.894669
H	14.645776	-1.573433	1.490947
O	0.793764	1.020029	-6.555997
O	-4.924658	8.233201	-0.046523
O	-5.889293	-3.846794	-5.302822
O	1.027638	7.168362	-1.274310
O	0.499535	-1.871117	-6.773227
O	3.326916	-7.521259	5.452881
O	-8.578697	-1.649457	-0.161203
O	2.419737	-3.784283	7.684342
H	0.678025	0.064570	-6.445985
H	1.481724	1.145808	-7.200634
H	-4.683901	7.485696	0.498110
H	-4.379870	8.199208	-0.840218
H	-5.177444	-4.430618	-5.026460

H	-5.531282	-3.195880	-5.902749
H	1.152651	6.232153	-1.022345
H	0.595667	7.608772	-0.531087
H	0.723851	-2.692306	-6.310405
H	-0.220446	-2.040728	-7.388698
H	4.113362	-7.852980	5.032754
H	2.706216	-7.297443	4.744142
H	-7.640516	-1.455552	-0.240434
H	-8.839486	-2.188618	-0.900351
H	2.795300	-3.368416	8.456871
H	2.678051	-3.275254	6.917290
Na	5.191120	5.146657	5.916166

3 F9 system

3.1 F9 substrate

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F9 substrate only

O	-0.25077700	2.15224400	3.11045800
S	0.02447700	2.56371400	1.71918700
O	0.33917400	3.96610200	1.43693900
N	-1.40422800	2.26346600	0.90668000
C	-1.95349900	0.90274300	0.95050500
C	-3.39717800	0.84044900	1.40814200
O	-3.80030400	-0.52586500	1.23543300
P	-5.23491300	-0.76369800	0.47055200
O	-5.26106700	0.13365800	-0.76513100
O	-6.30300500	-0.29072100	1.49266300
O	-5.29504800	-2.26446400	0.15999200
C	1.24009300	1.42272500	1.09589000
C	1.38591400	1.18098600	-0.29858000
C	2.33675700	0.27334000	-0.74272300
C	2.13623300	0.79819800	1.99034700
C	3.10836200	-0.09303400	1.54738300
C	3.18476900	-0.37120900	0.16650500
O	4.05684400	-1.31762200	-0.43280700
C	4.95987300	-2.01467900	0.26446000
F	5.63223900	-2.81111700	-0.59295100
F	5.85818200	-1.23117800	0.90294800
F	4.41181100	-2.81858400	1.20829600
H	-1.34026000	0.26957600	1.60126500
H	-1.91807100	0.45151900	-0.05087500
H	-3.49483800	1.12677900	2.46684600

H	-4.02553800	1.51783000	0.80708800
H	0.74657600	1.67826000	-1.03106600
H	2.43645500	0.04848500	-1.80463000
H	2.05153200	1.01098000	3.05569900
H	3.80194700	-0.53593700	2.26824900
H	-1.41832700	2.71444600	-0.02736200

3.2 F9 substrate in a 5 Å protein cluster

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F9 substrate in an 5 Angstrom protein complex

O	-0.25077700	2.15224400	3.11045800
S	0.02447700	2.56371400	1.71918700
O	0.33917400	3.96610200	1.43693900
N	-1.40422800	2.26346600	0.90668000
C	-1.95349900	0.90274300	0.95050500
C	-3.39717800	0.84044900	1.40814200
O	-3.80030400	-0.52586500	1.23543300
P	-5.23491300	-0.76369800	0.47055200
O	-5.26106700	0.13365800	-0.76513100
O	-6.30300500	-0.29072100	1.49266300
O	-5.29504800	-2.26446400	0.15999200
C	1.24009300	1.42272500	1.09589000
C	1.38591400	1.18098600	-0.29858000
C	2.33675700	0.27334000	-0.74272300
C	2.13623300	0.79819800	1.99034700
C	3.10836200	-0.09303400	1.54738300
C	3.18476900	-0.37120900	0.16650500
O	4.05684400	-1.31762200	-0.43280700
C	4.95987300	-2.01467900	0.26446000
F	5.63223900	-2.81111700	-0.59295100
F	5.85818200	-1.23117800	0.90294800
F	4.41181100	-2.81858400	1.20829600
H	-1.34026000	0.26957600	1.60126500
H	-1.91807100	0.45151900	-0.05087500
H	-3.49483800	1.12677900	2.46684600
H	-4.02553800	1.51783000	0.80708800
H	0.74657600	1.67826000	-1.03106600
H	2.43645500	0.04848500	-1.80463000
H	2.05153200	1.01098000	3.05569900
H	3.80194700	-0.53593700	2.26824900
H	-1.41832700	2.71444600	-0.02736200
C	-4.56527900	6.87148700	2.35399200
C	-3.78599200	5.63698800	1.83480900
C	-3.09698600	5.89439300	0.51694000

C -3.80629000 5.80577500 -0.68214500
C -3.20584400 6.12062100 -1.90155100
C -1.84925100 6.47976200 -1.93583200
C -1.13145900 6.56530400 -0.73832700
C -1.76160300 6.28640300 0.47308800
C -5.33267400 7.50456800 1.21136400
D -6.40769600 7.00553800 0.81817900
N -4.76740900 8.58346800 0.65829400
C -0.86556600 8.42968400 4.49289100
C -0.93643800 6.90776900 4.44560500
C 0.32022400 6.21226900 4.03525900
C 1.50816100 6.47225100 4.95323200
D 1.42141700 6.56600900 6.21902900
D 2.58871600 6.51866800 4.35903700
C -1.16858100 9.06217200 3.13226600
D -2.28207800 8.96103100 2.62378400
N -0.17434900 9.71661300 2.54783200
C 3.12759100 -1.99977500 -5.13404900
C 3.83413900 -1.63978700 -3.82618100
C 1.62715100 -1.74089600 -5.03757800
D 0.97250200 -2.13497600 -4.06634200
N 1.09480700 -1.07668100 -6.05542200
C -0.30945300 -0.66454100 -6.07851100
C -0.42288100 0.84678300 -6.28785600
C -0.06631500 1.61746400 -5.04677200
D -0.80528900 1.49102000 -4.03059200
D 0.96423700 2.35594900 -5.07986300
C -1.16619600 -1.38713200 -7.08631800
D -0.77938200 -1.56405800 -8.25055000
N -2.34266300 -1.82247000 -6.62116800
C -4.46394900 3.35651900 -6.72945500
C -3.66839000 3.07535200 -5.42957900
C -4.65057600 3.19716200 -4.24375500
C -4.13614700 2.66159600 -2.92342300
C -2.47619800 4.03054000 -5.30866800
C -3.64509300 3.66556800 -7.98835400
D -3.23924600 4.83744100 -8.20309300
C 4.00261400 6.86401600 0.50753900
C 2.67987800 6.10956500 0.19217100
C 2.85002600 4.69933800 -0.42929800
C 3.24239700 4.77780500 -1.91123400
C 3.75362500 3.74544500 0.33682000
C 4.77197000 7.22472700 -0.75703100
D 4.21994400 7.86059800 -1.68370500
N 6.04361600 6.82290600 -0.79043900

C 7.46182700 4.79938400 3.61733400
C 6.06076400 4.19947400 3.84961600
C 5.96368000 2.66682900 3.84445400
C 4.54418900 2.28679900 4.27364800
C 6.24198500 2.08228900 2.47818400
C 7.86566700 4.72363500 2.15416900
D 7.16421100 5.22974200 1.28363600
N 9.03811100 4.15633000 1.88987300
C 7.56806700 1.12338500 -1.00140700
C 6.27924300 1.27552200 -1.82051900
C 8.48333600 0.06240100 -1.61004300
D 8.34778900 -1.13670200 -1.31946600
N 9.43446200 0.49437200 -2.43337300
C 7.15370700 -3.24745800 6.36334200
C 7.04051400 -3.49867000 4.84404300
C 6.70351200 -2.19802800 4.08075700
C 5.28802700 -1.68780000 4.21146800
C 6.09944300 -4.66097900 4.56650000
C 7.48193500 -4.56718400 7.03177900
D 8.60728900 -5.10145200 6.85143900
C 3.58906400 -1.27243700 8.84907400
C 3.95302200 -0.81384900 7.43274800
C 2.76381000 -0.70333500 6.54373600
C 2.11565700 -1.84661000 6.04464200
C 0.96912000 -1.72050300 5.24938000
C 0.50392300 -0.46908100 4.91838900
D -0.62037400 -0.30405800 4.11754600
C 1.14004200 0.66798800 5.39911500
C 2.26229400 0.53232800 6.20779200
C 3.42801100 -2.78975700 8.87544600
D 4.36812300 -3.52905300 8.48271700
C 1.10215900 -6.07525500 5.94806700
C 2.09181400 -6.63897300 4.91180600
C 2.78449900 -5.77654800 3.89403200
C 3.68065000 -6.66101300 3.03414900
C 1.77294400 -4.99502400 3.04812000
C 0.11646000 -7.19110900 6.23241100
D 0.48912900 -8.20180900 6.85580600
N -1.10334500 -7.04762000 5.72854600
C -2.87589400 -2.66154300 -2.58158800
C -2.72502100 -1.13566700 -2.55778700
D -2.64912300 -0.60125700 -3.89201600
C -1.47143300 -0.75492800 -1.77409600
C -4.16549500 -3.00852000 -3.30302400
D -4.14698800 -3.27544600 -4.50978000

N -5.26239300 -3.09495100 -2.55179500
C -6.58306900 -3.24540600 -3.17339700
C -7.63827000 -3.72809700 -2.19914900
D -7.38343700 -4.63529800 -1.41920200
N -8.82589000 -3.12336200 -2.27005700
C -2.75342600 -2.29046800 6.07484900
C -2.67571000 -3.32284400 4.96986500
D -1.92825700 -4.32212800 5.09343000
N -3.40504400 -3.01865400 3.89966800
C -3.69746500 -3.82136900 2.70339600
C -2.60362000 -4.82053100 2.28175000
C -1.46265900 -4.23187600 1.46816100
C -0.95315100 -3.00380100 1.76891700
C 0.11075100 -2.48251700 1.07369700
C 0.65518800 -3.18392300 0.03909800
C 0.15834800 -4.41405300 -0.28705900
C -0.87490600 -4.95124600 0.42905800
C -4.99934300 -4.62863800 2.77618200
D -5.08832600 -5.57415500 3.46482400
N -5.99097600 -4.16163000 2.06836300
C -7.27651000 -4.85751700 1.99690800
C -8.25651800 -4.46658100 3.09212700
D -9.30589500 -5.09585300 3.18358500
N -7.93497700 -3.46407300 3.91190100
N -4.80396300 1.01426000 8.46676500
C -4.74361000 1.91075100 7.29728900
C -3.29401400 1.98318900 6.73623400
C -2.37949200 2.68524500 7.74503000
C -0.89564200 2.38810600 7.51883100
C -3.24943700 2.68791200 5.37822000
C -5.68131000 1.41483200 6.20454200
D -5.73789300 0.21281500 5.94183200
N -6.41991400 2.32602200 5.57489900
C -7.29876600 1.97214700 4.44837800
C -8.78761300 2.09189400 4.85875700
D -9.67911500 1.77831200 3.78077600
C -7.04046700 2.92544900 3.30131000
D -7.16122900 4.15005300 3.46867200
N -6.71691900 2.37212200 2.13112100
C -6.40975000 3.23293400 0.97476300
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D -8.19943100 3.95706000 -0.42900200
N -7.38112200 1.88336600 -0.76078900
C -8.26006300 1.63966900 -1.90480400
C -8.08269300 0.22029900 -2.43304300

O -6.77811500 0.05499200 -2.96725700
C -9.73442900 1.90343200 -1.62346500
O -10.42447200 2.42131600 -2.49358600
N -10.22257000 1.54802100 -0.42818200
C 11.72784300 -4.40633200 -4.48008200
C 11.00151900 -4.26044100 -3.15785400
O 11.63056500 -4.19368800 -2.11433900
N 9.66129900 -4.28200400 -3.18762900
C 8.95563700 -4.31850400 -1.91713500
C 7.49664700 -4.50793200 -2.34392200
C 7.42028100 -3.87326400 -3.72159400
C 8.74800400 -4.20999500 -4.34336600
C 9.39388000 -5.49485500 -1.03649300
O 9.77701900 -6.56443600 -1.54954300
N 9.35419200 -5.28206700 0.26606500
O -5.16834800 -0.17252500 -5.27647600
O 4.61777700 6.98493200 5.79610800
O 6.30108500 -5.25097900 0.92069800
O -8.92159900 -0.46128500 1.14561400
O 8.20881500 -2.78590400 0.96305400
O 3.86724300 -5.27627200 -0.25672700
O -5.79243400 -1.49414500 3.80322900
O 2.21155700 -7.48074300 -0.01451900
O -6.85120800 -2.03464200 -6.47503700
O 4.74500700 -5.23327500 -5.62294000
O 3.37166200 -5.03611900 -2.97840900
O 10.60230000 -3.01180900 5.06538300
O -7.20424800 -7.00180300 4.84833000
O -9.59026700 -1.82334600 -4.86835000
O 9.75596700 -1.26860200 2.56034900
O -5.26999700 -5.10256200 -6.12917000
O 9.03689100 0.85955900 3.44289500
O -1.01117100 3.17409600 -1.72949200
H -3.04051600 5.32595700 2.59568000
H -4.48821800 4.78032700 1.70129700
H -1.17951400 6.34304700 1.40577900
H -4.85522800 5.47267500 -0.67234100
H -0.05814100 6.80373300 -0.75093200
H -3.77719500 6.02150600 -2.83292300
H -1.35403400 6.67082800 -2.89310600
H -3.82018400 7.59639500 2.80634600
H -3.92320700 8.95072000 1.05732600
H -1.20632700 6.51764100 5.45342100
H -1.77109400 6.58735400 3.77721200
H 0.58103800 6.47189600 2.98522700

H 0.14224900 5.11689100 4.01927500
H 0.13691800 8.73831200 4.89306500
H 0.73004700 9.76504000 2.97155000
H 4.89045300 -1.94755600 -3.84647600
H 3.80779700 -0.55932400 -3.61675300
H 3.35754400 -2.15298500 -2.97763300
H 3.24576200 -3.11412100 -5.27288300
H 0.19026700 1.17092800 -7.15595200
H -1.46963300 1.09850800 -6.56905000
H -0.71042100 -0.86324900 -5.03651800
H 1.63883700 -0.74341600 -6.82321900
H -2.68883700 -1.44685500 -5.74412300
H -3.26321400 2.02837100 -5.44347600
H -2.78924600 5.08164200 -5.36132000
H -1.96070400 3.88418000 -4.34667900
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H -9.59152096 -3.36433385 -1.67361606
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H 10.04583768 -0.12822235 -2.92183595
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H -1.61606275 8.78715905 5.16658694
H -5.03413591 8.94683978 -0.23435246
H -5.26858062 6.60736327 3.11590111
H 7.94548927 -2.55168397 6.54740539
H 4.34775571 -0.96679713 9.53890815
H -11.19159426 1.69295205 -0.22821455
H -1.80146762 -7.74085491 5.90757160
H 1.61235283 -5.77024760 6.83777074
H -5.18142218 2.58795556 -6.92805629

3.3 F9 substrate in an 8 Å protein cluster

857

F9 substrate in an 8 Angstrom protein complex

O -0.25077700 2.15224400 3.11045800
S 0.02447700 2.56371400 1.71918700
O 0.33917400 3.96610200 1.43693900
N -1.40422800 2.26346600 0.90668000
C -1.95349900 0.90274300 0.95050500
C -3.39717800 0.84044900 1.40814200
O -3.80030400 -0.52586500 1.23543300
P -5.23491300 -0.76369800 0.47055200
O -5.26106700 0.13365800 -0.76513100
O -6.30300500 -0.29072100 1.49266300
O -5.29504800 -2.26446400 0.15999200

C 1.24009300 1.42272500 1.09589000
C 1.38591400 1.18098600 -0.29858000
C 2.33675700 0.27334000 -0.74272300
C 2.13623300 0.79819800 1.99034700
C 3.10836200 -0.09303400 1.54738300
C 3.18476900 -0.37120900 0.16650500
O 4.05684400 -1.31762200 -0.43280700
C 4.95987300 -2.01467900 0.26446000
F 5.63223900 -2.81111700 -0.59295100
F 5.85818200 -1.23117800 0.90294800
F 4.41181100 -2.81858400 1.20829600
H -1.34026000 0.26957600 1.60126500
H -1.91807100 0.45151900 -0.05087500
H -3.49483800 1.12677900 2.46684600
H -4.02553800 1.51783000 0.80708800
H 0.74657600 1.67826000 -1.03106600
H 2.43645500 0.04848500 -1.80463000
H 2.05153200 1.01098000 3.05569900
H 3.80194700 -0.53593700 2.26824900
H -1.41832700 2.71444600 -0.02736200
N -5.52642300 6.51053100 3.39523000
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C -3.78599200 5.63698800 1.83480900
C -3.09698600 5.89439300 0.51694000
C -3.80629000 5.80577500 -0.68214500
C -3.20584400 6.12062100 -1.90155100
C -1.84925100 6.47976200 -1.93583200
C -1.13145900 6.56530400 -0.73832700
C -1.76160300 6.28640300 0.47308800
C -5.33267400 7.50456800 1.21136400
O -6.40769600 7.00553800 0.81817900
N -4.76740900 8.58346800 0.65829400
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C -6.15631800 10.31437300 -0.59290900
C -7.49864800 9.87813100 -0.01455700
C -5.55580100 11.46479200 0.18556000
C -3.92467000 9.56422300 -1.41471700
O -2.84440100 9.76726300 -0.80211000
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C -0.86556600 8.42968400 4.49289100
C -0.93643800 6.90776900 4.44560500
C 0.32022400 6.21226900 4.03525900
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O 1.42141700 6.56600900 6.21902900
O 2.58871600 6.51866800 4.35903700

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C 7.17723300 -1.24289500 -8.53163200
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