

SUPPORTING INFORMATION FOR WORLD WIDE WEB EDITION**Structural Definition of the Active Site and Catalytic Mechanism of 3,4-Dihydroxy-2-Butanone 4-Phosphate Synthase**

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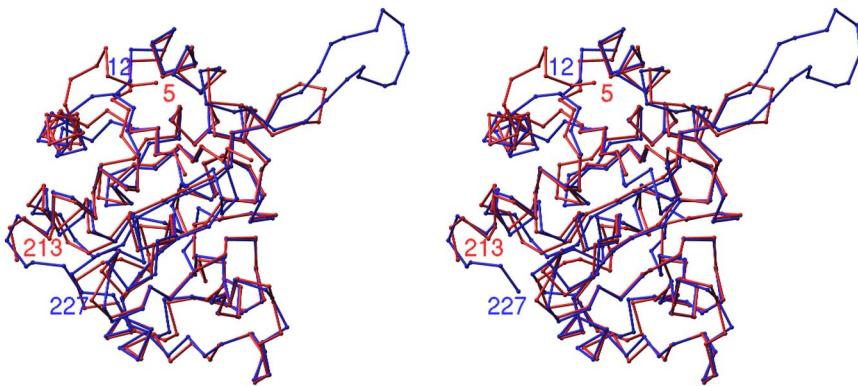


FIGURE S1: Stereoview of an overlay of $\text{C}\alpha$ traces for the *E. coli* DS (red) and the *M. grisea* DS (blue). The rmsd between the $\text{C}\alpha$ atoms of the two proteins is 1.0 Å for the 193 atoms used in the alignment.

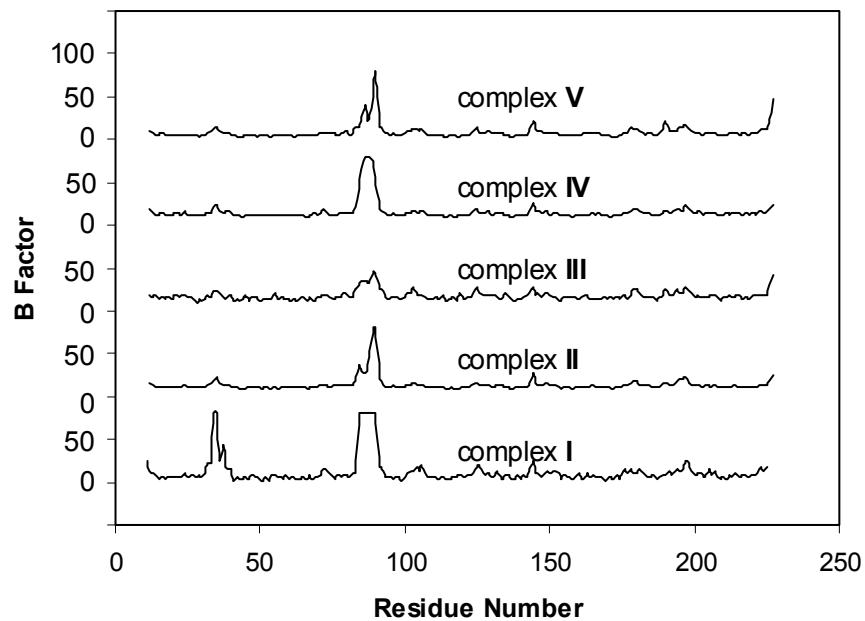


FIGURE S2: B factors of the C α atoms of DS. The B factor scale is 0-100 for each of the complexes **I-V**. The B factors values were set to 80 for residues 84-90 of complex **I** because there is insufficient electron density to make residue assignments.

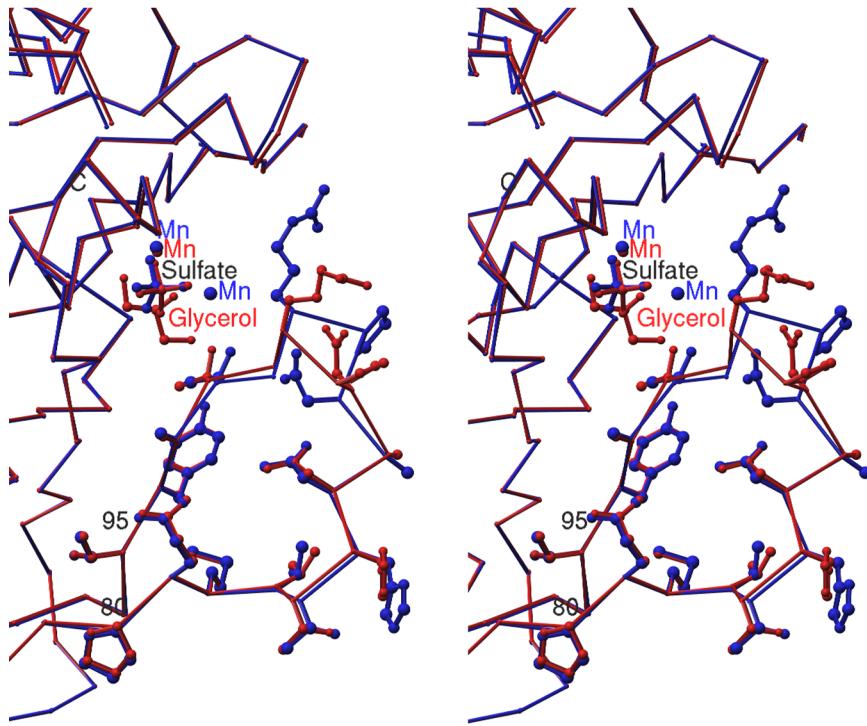


FIGURE S3: Different orientations of a loop of DS. Stereoview of the complexes **III** (blue) and **IV** (red) in the mismatched loop region (residues 80-95). The side chains of the loop region are shown in the same color codes.

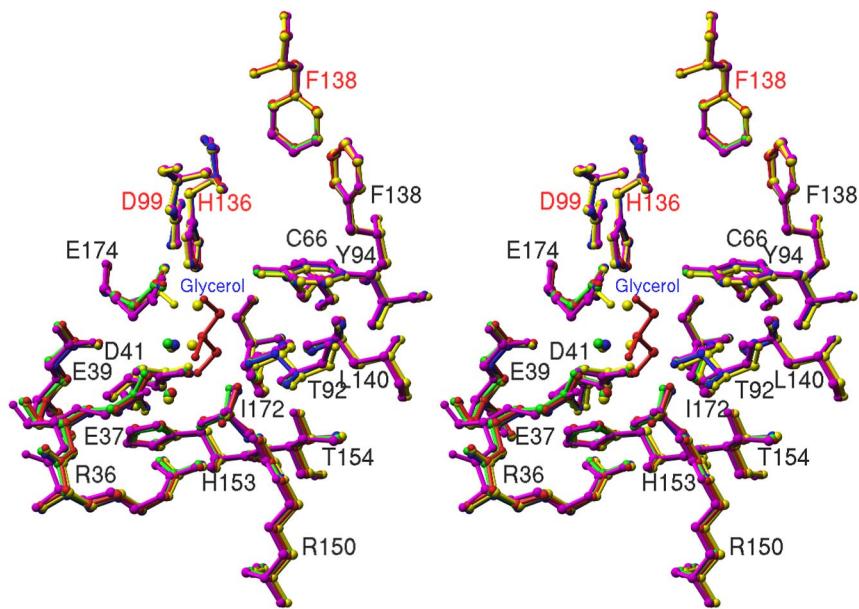


FIGURE S4: Overlay of the active site residues in complexes **I-V**. The stereoview has the following coloring scheme: complex **I** (magenta), complex **II** (green), complex **III** (blue), complex **IV** (red) and complex **V** (yellow).

	50		151		200
{d64620}	-----	MILKRVTE ALEAYKNGEM LIVMDDEDRE NEGDLVLAGI	{d64620}	LIAKGGVLA RTGHTEASVD LCKLAGLKPV SVICEIMKED GSMARRGDKF	
{c81404}	-----	-MKFVSVEO AIKDQAGKM LIVMVAEDE NEGDLIFPAQ	{c81404}	LIAKGGVLE RTGHTEOTWD LCKLAGLKGA CVICEIVKDN GMARRED..	
{a38159}	-MNQTLSSF G.TPVERVEN ALAALREGRM VMVLLDDEDR NEGDMIFFPAE		{a38159}	LRAQAGGVLT RGHTTEATID LMMLAGFKPA GVLCETL.N DD.....	
{e64091}	-MNQSILSPF GNTAAERVLN AINAFKNCTG VLVLDDDEDR NEGDLIFPAAE		{e64091}	LRAANGVLT RGHTTEASVD LARLAGFKEA GVICEIT..N DD.....	
{c35081}	MSSTSLLDEP G.TPVQRVBD AIEALKRNGLG VLLMDDDEDR NEGDLIFSAQ		{c35081}	LVAKTNGVLA RGHTTEGTID MYLNLVPs GILCELT.N PD.....	
{h81104}	----- MSHISPIPL ILADIAGKGM VIITDAEDE NEGDLILMAAQ		{h81104}	LRAQGGVLV RGHTTEAVGD LQMNLIPs SVICEII..N DD.....	
{jc1188}	----- -MASHSAAK IIIDIQRGMRM VILMDDESRE NEGDLIASE		{jc1188}	LMAQHGGVLI RGHTTEAGCD VARLAGELPS SVIEIL..N ED.....	
{s50973}	----- -MFTPIDA AIEHFQKNP K VIVMDDAGR NEGDLICAAE		{s50973}	LRAADGGVLQ RGHTTEAVGD LCKLGLSLPV AVIGELVN..D DEGQT..	
{t39940}	----- -MLASIESV AVNDPRDKPF LIVLDDETRE NEGDLIIAGC		{t39940}	LRARDGGVLQ RDGHTEAVGD LCKLAGLIPV GAICELVR..E EEDGL..	
{mgds}	----- MPSTDST PKNSFDAIPV VIQAFKNQEF VVVLDDPSRE NEADLIIAAE		{mgds}	LRAVAGGVR RRGHTEAGVE LCRLAGKPV AVISEIVDDE QVEGEVRAVRA	
{g81514}	----- -MIE TREEV GSANFSVLER AIEDLRAGKF VIVVDEASRE DEGDLIAGE		{g81514}	LASSPGGVQI LASSPGGVQI RGHTTESTWD LMLAGLQPC GVLAELV..N ED.....	
{b71477}	----- -MFT CEAGIASVQQ AIKDVAEKGK VIVIDAASRE NEGDLILAGE		{b71477}	LISPGGGAVQI RPHTHEAAMD LMLAGLQPC GIFAELV..N PD.....	
{b81740}	----- -MVT CEAGIASVQQ AIKDIAKGK VIVIDRSE NEGDLILAGE		{b81740}	LVSPGGGVVK RPHTHEASD LMLAGLQPC GIFAELV..N AD.....	
{c70331}	----- MSER EEFKFNTVVE AIEIDIQRGK M VIVVDDPDR NEGDLVMAAE		{c70331}	LKARPGGVLE RGHTTEASVD LARLAGLYPA GVICEI..M ED.....	
{e45545}	----- -MFPIPIEB ALDALKKGBV IIVVDDPDR NEGDFVALAE		{e45545}	LIAKGGVLU RGHTTEAVGD LAAACGSPGA GVICEI..M ED.....	
{c75629}	----- -MFDADIA ALADIAGKAG VVVLDDENRE NEGDLICAAQ		{c75629}	LRAKTCGVLU RGHTTEAVGD LSRLAGLYPA GVICEI..QN AD.....	
{a75553}	----- MS DSITLSTPD LLAELRAGR VILVLDENRE NEGDLLMPAA		{a75553}	LVARPGGGVLR RGHTTEAGCD LARLAGFAPV GVICEI..MG DD.....	
{d70902}	----- -MTRLDSSVER AVADIAAGKA VIVIDDDRE NEGDLFVAAE		{d70902}	LRAKDGGLVLR RGHTTEAVGD LARMAGLQPA GAICEIVSQQK DE.....	
{e72207}	----- -MEE LREAFEEGKP VILID.RNE NEADFVPPAQ		{e72207}	IGGI..GFQR RGHTTEASLE ISELAGFSRH AVITEILDEK	
Consensus	----- D-----R-----E-----D-----		Consensus	----- G-----R-GHTE-----E-----	
	3 33 3 4			1 1 1111	
	2 67 9 1			4 5 5555	
				6 0 2345	
	51	100		201	250
{d64620}	FSTPEKINFN ATHARGLICV SLTKDLAKKF ELPPM.... .VSVNDSNHE		{d64620}	...L SDFPALHNLK TLVYSDLISY RLENESLLMK FCQEEERFLK	
{c81404}	FSTQEKFVNFM IKEARGVCVV ALDETLLAKKF ELPLM.... .VPKNTNSNHE		{c81404}L EIPCQKHDLN MIAVSDLIEY RLKHESLKL EKKSQSVLAG	
{a38159}	TMTVQBMALT IRHGSSIVCL CITEDRRKQL DLEMM.... .VENNTASYG		{a38159}L CTMARAPCIE IEPANKHNLN LVTIEDLVAY ROHMSVKPAA NRCLQYCLNQ	
{e64091}	TITPEQMAKL IRYGSGIVCL CITEDRCOOL DLPPM.... .VHEHNSVNUK		{e64091}L CTMARAPEI VEFAKKPGVS VLTIEDLVEY RLAHN.....	
{c35081}	HLTEAQMALM IREGSGIVCL CLTERANWNL DLPPM.... .VKDNKSNQ		{c35081}L CTMALKPTEI EFPARRCHGK VLTIEDIVDY RTCGIDLNEY KGGLVREWSW	
{h81104}	FVTPEAINFM IKHARGLICV PMDGEVMVKL GLPMPM.... .TQKNGAQYG		{h81104}L GTMARNPDL MKPAEHEHKL IGTIADLIEY RSRTESLLED MGNAQVPTFW	
{jc1188}	MVTPEAINFM ATHRGGLICL TLSKARCKTL NLFPM.... .LQGNNDNFS		{jc1188}L GSJNARPPOL EI PAEHHKGLK LGTIADLIEY RTQOESHIER ISEYELNTY	
{s50973}	NVSTEQMAPL VRHSGSVCA PMTNATADLPEL FESNDDDRHG		{s50973}L ...MRMLNDI QAFGKKGKIP LISIEELAQY LKR.....	
{t39940}	KVTTEQMAPL VRHSGSVCA PMTGERLDSL EIPMM.... .VNNDNEDMR		{t39940}L ...MSRPDDI ISPGKKGKIG VITIESLKS YIKGRM.....	
{mgds}	SVTTEQMAPL VRHSGSVCA PLTPTERTIAL DLQPM.... .VTHNADPRG		{mgds}L AGPMLRDGEVIAFARPGKLG VCITYEDMIAH VEKTEGKLET NGSC*	
{g81514}	KITTEKMFPL LQHTVGCVCA ALSLQRLLS DLPPM.... .NCRCPK		{g81514}L YSMMLRPOI LEFARKHNIA VIVPTSIIAH RMLSDRLVST ISARALPTIY	
{b71477}	KVSTEKMFPL LSHTTGIVCA SLRSREQAKS DLPPM.... .NOQCAF		{b71477}L HSMMRQQVQI LAFPAEHQDIT VITVDDLLITY RYTVDLSVLT ISARALPTK	
{b81740}	KVSAEKKMFPL LSHTTGIVCA SVTRTEQARVL DLPPM.... .NOQCAF		{b81740}L HSMMRQQQI LDPAEHQHGT VITVDDLLITY RWTFDLSVLT VSSARALPTK	
{c70331}	KVTPPEAINFM AKYGRGLICL SLTPERCEOL DLHPPM.... .T...PMNTDDPKG		{c70331}L CTMARPDLE MEFAKPHKLNK IIITIADLKY RLRLRETLLVER VASAHLPTFW	
{e45545}	HATPEVINFM ATHRGGLICL PLSEEIADRL DLHPPM.... .EHNTDSHH		{e45545}L CTMARVPDL IEIAKHKQKL MITIKDQIY RYNLTTLVER EVDITLPTDP	
{s75629}	TAFTPALVNFM AVEARGLICL AMTDGRDLDR DLHPPM.... .SKNTDSNQ		{s75629}L GSJNARPPEL VEYARKHQLK LISIADLISY RLQHDFEVQR ETICEPPSQF	
{t55553}	TAOTPWNFM ARBGRGLICL TLTPERARRL DLHPPM.... .VGAG AYQGTDPPNG		{t55553}L GEMSLRPLD LARGEHKHGLK VGSIETALLAY RMHEDDPMEP VAAEALPTRF	
{d70902}	KATPEMVAFM VRYTSGYLCV PLDGAICDRL GLLPM.... .YAVNQDKHG		{d70902}L GSMAHTDEL RVFADEHGILA LITIADLIEW RRKHEKHIER VAAEALPTRH	
{e72207}	LITEDVSWSPF VTYKGKFCV TADEE.... DL..LKGRCV KLSNN.... YG		{e72207}L GNSHNLDVY LKLSKFKSPL VLEMDDDWRE FVKKRKLMMK KAETALPTD	
Consensus	-----G-C-----		Consensus		
	6 6				
	3 6				
	101	150		251	300
{d64620}	TAFTVSIDAK E...ARTGIS AFERHLTIE LCKDTTK.PS DFVRPGHVF		{d64620}	HQTQCYTFLD H.QQKHNHYAF ...KFKGAKT HDLAPLVRFH PIKEDFDLFT	
{c81404}	TAFTITVDAK D...ATTGVS AYERNMTIQI FADDNAK.AS DFVRPGHVF		{c81404}	CFAEKFFIFSD H.NQTQHIAPI .CFKDIKK ..CENVKFH ISGSDFELL	
{a38159}	TGFTVTIEAA... EGVTGTVS AADRITTVS D.SDGAK.PS DLNRPGHVFP		{a38159}	ETEVVAGFGF YFSLLCKMLI PLLFL-----	
{e64091}	TAFTVTIEAA... KGVTGTVS AADRVTTIQI AJADNAV.LT DLHRPGHVFP		{e64091}	-----	
{c35081}	TAFTVSIKAA... EGVTGTVS AKDRVTITV ATYFDQK.PE DLARPGHVFP		{c35081}S-----	
{h81104}	TNTPTISIEAA... HGTTGTVS AADRALTIQI AVSPVTAK.PE DIVPQGHIPP		{h81104}	GEFPQHQVYD KLSGETHML VKGTPAA... .DTETLVRVH EPFSVMDPFIQ	
{jc1188}	TPPTISIEAA... KVVTGTVS ASDRAKTVLA AVAPNAK.ST DIVPQGHIPP		{jc1188}	GIFTLVLYTD TIDNQAHFAL CKGEIQA... .KAATLVRVH VKDTLKDILQ	
{s50973}	TAYTITVDAV... Q.GTTGTVS AHDRSMTCA LADSSST.PK SPLKPGHICP		{s50973}	-----	
{t39940}	TAYAVTLDYA... N.GTTGTVS AHDRAILTRQ LANPEVTSR BFPNRPGHIVP		{t39940}	-----	
{mgds}	TAYTIVSVDAA... HPSTTTGIGS AHDRALACRM LAAPDA.QPS HFRPRGHVF		{mgds}(mgds)	
{g81514}	TPFTIVSVDAA... HGVTGTVS AADRTKVKQD LADPKSE.PE DFISPGHFP		{g81514}	GDFITIHYYES LLGEGMQHML VKGNV... A GKSNLVLRVH SECVTGDIIG	
{b71477}	TAFTIVSVDAS... SGVTTGVS ASDRTTRVQD LADPAAT.AE SFVRPGHVFP		{b71477}	GDFSIHRYYES IIDGTQHFAVL VKGDI... .R EQEAVPVRVH SECVTGDIIG	
{b81740}	TAFTIVSVDAS... SGTTGTVS AADRTKVKQD LSDPTSI.SQ SFVRPGHVFP		{b81740}	GEFFIHYKYE IIDGTHEFAVL VKGDI... .R EQESVVRVH SECVTGDIIG	
{c70331}	TYFCVSIDAA... PKHGTGTTGIGS AYDRALTIK AISPDAK.PS DFVRPGHVFP		{c70331}	GEFFIHYKYE IIDGTHEFAVL VKGDI... .R EQESVVRVH SECVTGDIIG	
{e45545}	TAFTVSIKAA... PHLOVTTGIGS AEDRARTIQI AINPVT.R.PE DLSPRGHIPP		{e45545}	GTFKVKVGYTN EVDGEKEHFAV VMGD.V... PP GEEPVLRVH SECVTGDPVG	
{s75629}	TAFTVSIKAA... PHLOVTTGIGS AEDRARTIQI AINPVT.R.PE DLSPRGHIPP		{s75629}	GEFKLYAYRN LLQDTEHIAI VKGDP... .EP CQQPVMVRMII SECVTGDALG	
{a75553}	TAFTVSIKAA... HSSNNTGIGS AYDRAATIAA LLEDTSQ.PT DFPRPGHIPP		{a75553}	-----	
{d70902}	TAFTVSIKAA... RNCIGTGIS ASDRATTMRL ADLPTSV.AD DFTPRGHVPP		{d70902}	GEFRALIGTS IYEDVEHIAL VRGEITAGPNA DGDVVLRVH SECVTGDVPG	
{e72207}	ANFVPPVD... WGTGTTGIGS ALRAETCKR LAR.GRHY FPRYRGHVT		{e72207}	GVEKVWSPEH HLZGKEHFAI VKEPL.... .EDPVAVRVH SECVTGDVLS	
Consensus	-----TG-S A--R-----		Consensus		
	11 1 1	111			
	00 1 1 1	333			
	78 0 1 4	456			

FIGURE S5: Sequence alignment of 19 species of DS. Identical residues are indicated by the consensus. The *M. grisea* sequence number is immediately below the consensus (identical) residue. Species key for the pir files: {d64620} *Helicobacter pylori*, {c81404} *Campylobacter jejuni*, {a38159} *Escherichia coli*, {e64091} *Haemophilus influenzae*, {c35081} *Vibrio harveyi*, {h81104} *Neisseria meningitidis*, {jc1188} *Photobacterium leiognathi*, {s50973} *Saccharomyces cerevisiae*, {t39940} *Schizosaccharomyces pombe*, {mgds} *Magnapothe grisea*, {g81514} *Chlamydia pneumoniae*, {b71477} *Chlamydia trachomatis*, {b81740} *Chlamydia muridarum*, {c70331} *Aquifex aeolicus*, {s45545} *Bacillus subtilis*, {s75629} *Synechocystis sp.*, {a75553} *Deinococcus radiodurans*, {d70902} *Mycobacterium tuberculosis*, and {e72207} *Thermotoga maritima*.