

56248  
2R5V AChain A, Hydroxymandelate Synthase Crystal Structure  
AC660972UE630 [uncultured soil bacterium]  
CAC48371putative hydroxyphenyl pyruvate dioxygenase [Ampicillatopsis balhincynina]  
AM80551HmaS3 [Streptomyces toyoensis]  
CAD9119putative hydroxymandelate synthase [Monomurata sp. ATCC 39727]  
AM8183hydroxyphenyl pyruvate dioxygenase [Streptomyces lavenderulae]  
ZP\_046564844-hydroxyphenylpyruvate dioxygenase [Streptomyces roseosporus MREU 15998]  
YP\_003342414-hydroxyphenylpyruvate dioxygenase [Streptosporangium roseum DSM 40021]  
CAG15040hnaS3 protein [Actinoplanes teichomyeticus]  
CAG53378hnaS3 protein [Actinoplanes teichomyeticus]  
YP\_0031022694-hydroxyphenylpyruvate dioxygenase [Actinosynnema mirum DSM 43827]  
YP\_0011595494-hydroxyphenylpyruvate dioxygenase [Salinispora tropica CMB-440]  
YP\_003383684-hydroxyphenylpyruvate dioxygenase [Kribbella flavida DSM 17836]  
ZP\_064002134-hydroxyphenylpyruvate dioxygenase [Micromonospora sp. L5]  
ZP\_062154194-hydroxyphenylpyruvate dioxygenase [Micromonospora aurantiaca ATCC 27023]  
YP\_48115504-hydroxyphenylpyruvate dioxygenase [Frankia sp. Cc13]  
ZP\_05235754-hydroxyphenylpyruvic acid dioxygenase [Streptomyces lividans TK64]  
**MF\_6274484-hydroxyphenylpyruvic acid dioxygenase [Streptomyces coelicolor 3121]**  
AM859484-hydroxyphenylpyruvate dioxygenase [Caenulitpora acidiphila DSM 44828]  
AB059484-hydroxyphenylpyruvate dioxygenase [Streptomyces fungitidicus]  
YP\_0011593144-hydroxyphenylpyruvate dioxygenase [Salinispora tropica CMB-440]  
YP\_0015975014-hydroxyphenylpyruvate dioxygenase [Salinispora arenicola CMB-205]  
ZP\_04604114-hydroxyphenylpyruvate dioxygenase [Micromonospora sp. ATCC 39149]

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CAG15040hnaS3 protein [Actinoplanes teichomyeticus]  
CAG53378hnaS3 protein [Actinoplanes teichomyeticus]  
YP\_0031022694-hydroxyphenylpyruvate dioxygenase [Actinosynnema mirum DSM 43827]  
YP\_0011595494-hydroxyphenylpyruvate dioxygenase [Salinispora tropica CMB-440]  
YP\_003383684-hydroxyphenylpyruvate dioxygenase [Kribbella flavida DSM 17836]  
ZP\_064002134-hydroxyphenylpyruvate dioxygenase [Micromonospora sp. L5]  
ZP\_062154194-hydroxyphenylpyruvate dioxygenase [Micromonospora aurantiaca ATCC 27023]  
YP\_48115504-hydroxyphenylpyruvate dioxygenase [Frankia sp. Cc13]  
ZP\_05235754-hydroxyphenylpyruvic acid dioxygenase [Streptomyces lividans TK64]  
**MF\_6274484-hydroxyphenylpyruvic acid dioxygenase [Streptomyces coelicolor 3121]**  
AM859484-hydroxyphenylpyruvate dioxygenase [Caenulitpora acidiphila DSM 44828]  
AB059484-hydroxyphenylpyruvate dioxygenase [Streptomyces fungitidicus]  
YP\_0011593144-hydroxyphenylpyruvate dioxygenase [Salinispora tropica CMB-440]  
YP\_0015975014-hydroxyphenylpyruvate dioxygenase [Salinispora arenicola CMB-205]  
ZP\_04604114-hydroxyphenylpyruvate dioxygenase [Micromonospora sp. ATCC 39149]

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2R5V AChain A, Hydroxymandelate Synthase Crystal Structure  
AC660972UE630 [uncultured soil bacterium]  
CAC48371putative hydroxyphenyl pyruvate dioxygenase [Ampicillatopsis balhincynina]  
AM80551HmaS3 [Streptomyces toyoensis]  
CAD9119putative hydroxymandelate synthase [Monomurata sp. ATCC 39727]  
AM8183hydroxyphenyl pyruvate dioxygenase [Streptomyces lavenderulae]  
ZP\_046564844-hydroxyphenylpyruvate dioxygenase [Streptomyces roseosporus MREU 15998]  
YP\_003342414-hydroxyphenylpyruvate dioxygenase [Streptosporangium roseum DSM 40021]  
CAG15040hnaS3 protein [Actinoplanes teichomyeticus]  
CAG53378hnaS3 protein [Actinoplanes teichomyeticus]  
YP\_0031022694-hydroxyphenylpyruvate dioxygenase [Actinosynnema mirum DSM 43827]  
YP\_0011595494-hydroxyphenylpyruvate dioxygenase [Salinispora tropica CMB-440]  
YP\_003383684-hydroxyphenylpyruvate dioxygenase [Kribbella flavida DSM 17836]  
ZP\_064002134-hydroxyphenylpyruvate dioxygenase [Micromonospora sp. L5]  
ZP\_062154194-hydroxyphenylpyruvate dioxygenase [Micromonospora aurantiaca ATCC 27023]  
YP\_48115504-hydroxyphenylpyruvate dioxygenase [Frankia sp. Cc13]  
ZP\_05235754-hydroxyphenylpyruvic acid dioxygenase [Streptomyces lividans TK64]  
**MF\_6274484-hydroxyphenylpyruvic acid dioxygenase [Streptomyces coelicolor 3121]**  
AM859484-hydroxyphenylpyruvate dioxygenase [Caenulitpora acidiphila DSM 44828]  
AB059484-hydroxyphenylpyruvate dioxygenase [Streptomyces fungitidicus]  
YP\_0011593144-hydroxyphenylpyruvate dioxygenase [Salinispora tropica CMB-440]  
YP\_0015975014-hydroxyphenylpyruvate dioxygenase [Salinispora arenicola CMB-205]  
ZP\_04604114-hydroxyphenylpyruvate dioxygenase [Micromonospora sp. ATCC 39149]

56248  
 2850\_sChain\_b, Hydroxymandelate Synthase Crystal Structure  
 ACJ609720E630 [uncultured soil bacterium]  
 CAC48371pevative hydroxyphenyl pyruvate dioxygenase [Amycolabopsis bialkaycina]  
 AM80835HmaS [Streptomyces toyoensis]  
 CMO21197pevative hydroxymandelate synthase [Monomastax sp. ATCC 39727]  
 AMK8183hydroxyphenyl pyruvate dioxygenase [Streptomyces lavendulae]  
 ZP\_0465968484-hydroxyphenylpyruvate dioxygenase [Streptomyces roseosporus DBEL 15998]  
 YP\_0033424184-hydroxyphenylpyruvate dioxygenase [Streptopirangium roseum DSM 43021]  
 C8615040HmaS protein [Actinoplanes teichomyeticus]  
 CAE53278HmaS protein [Actinoplanes teichomyeticus]  
 YP\_0031022694-hydroxyphenylpyruvate dioxygenase [Actinosynnema mirum DSM 43827]  
 YP\_0011593494-hydroxyphenylpyruvate dioxygenase [Salinispora tropica CM8-440]  
 YP\_0033838684-hydroxyphenylpyruvate dioxygenase [Kribbella flavida DSM 17836]  
 ZP\_064002134-hydroxyphenylpyruvate dioxygenase [Micromonospora sp. L5]  
 ZP\_062154194-hydroxyphenylpyruvate dioxygenase [Micromonospora aurantiaca ATCC 27029]  
 YP\_4818504-hydroxyphenylpyruvate dioxygenase [Frankia sp. Ccl3]  
 ZP\_05825754-hydroxyphenylpyruvic acid dioxygenase [Streptomyces lividans TK24]  
**WP\_6274424-hydroxyphenylpyruvic acid dioxygenase [Streptomyces coelicolor A3(2)]**  
 YP\_0031140044-hydroxyphenylpyruvate dioxygenase [Catenulispora acidiphila DSM 44828]  
 AB0659484-hydroxyphenylpyruvate dioxygenase [Streptomyces fungitidicus]  
 YP\_0011592144-hydroxyphenylpyruvate dioxygenase [Salinispora tropica CM8-440]  
 YP\_0015757014-hydroxyphenylpyruvate dioxygenase [Salinispora arenicola CM8-205]  
 ZP\_04604114-hydroxyphenylpyruvate dioxygenase [Micromonospora sp. ATCC 39149]

Legend:

\* metal binding

x conserved among Hms

+ conserved among Hms and HppD

- pointing outside the active site, backbone lines binding pocket

276 ERIT--L-----QTHSLDILRATWOLANEDHGGLPIITASTHERHTIFFIEHGGAGTFS SKKALVEMLERT 347  
 276 ERIT--L-----QTHSLDILRATWOLANEDHGGLPIITASTHERHTIFFIEHGGAGTFS SKKALVEMLERT 347  
 276 ERIT--L-----ATHSLDILRATWOLANEDHGGLPIITASTHERHTIFFIEHGGAGTFS SKKALVEMLERT 347  
 275 ERIT--L-----ETHSLDILRATWOLANEDHGGLPIITASTHERHTIFFIEHGGAGTFS SKKALVEMLERT 346  
 275 ERIT--L-----ETHSLDILRATWOLANEDHGGLPIITASTHERHTIFFIEHGGAGTFS SKKALVEMLERT 346  
 281 ER1A--L-----SESDIDLRATWOLANEDHGGLPIITASTHERHTIFFIEHGGAGTFS SKKALVEMLERT 362  
 281 ER1A--L-----RSHVDDLRATWOLANEDHGGLPIITASTHERHTIFFIEHGGAGTFS SKKALVEMLERT 362  
 281 ER1A--L-----RSHVDDLRATWOLANEDHGGLPIITASTHERHTIFFIEHGGAGTFS SKKALVEMLERT 362  
 261 GRD--L-----ATHSIFTRITQLLANEDHGGLPIITASTHERHTIFFIEHGGAGTFS AMKALVEMLERL 332  
 282 DR1R--L-----GRHSITLAAADILANEDHGGLPIITASTHERHTIFFIEHGGAGTFS SKKALVEMLERL 348  
 285 EMD--L-----GRSDDELRLANEDHGGLPIITASTHERHTIFFIEHGGAGTFS GAKALVEMLERL 348  
 277 DR1Q--L-----TRHSVTLSLAWLANEDHGGLPIITASTHERHTIFFIEHGGAGTFS SKKALVEMLERL 346  
 275 DR1Q--L-----TRHSVTLSLAWLANEDHGGLPIITASTHERHTIFFIEHGGAGTFS SKKALVEMLERL 346  
 275 DR1Q--L-----TRHSVTLSLAWLANEDHGGLPIITASTHERHTIFFIEHGGAGTFS SKKALVEMLERL 346  
 270 DR1Q--P-----TRVSTLALAWLANEDHGGLPIITASTHERHTIFFIEHGGAGTFS SKKALVEMLERL 341  
 285 AMD--L-----AKYDDELRESILANEDHGGLPIITASTHERHTIFFIEHGGAGTFS GAKALVEMLERL 356  
 282 ER0G--E-----LQTFIDELQELGLANEDHGGLPIITASTHERHTIFFIEHGGAGTFS SKKALVEMLERL 352  
 280 QR0G--R-----LQAFVDELRESILANEDHGGLPIITASTHERHTIFFIEHGGAGTFS SKKALVEMLERL 351  
 280 QR0G--R-----LQAFVDELRESILANEDHGGLPIITASTHERHTIFFIEHGGAGTFS SKKALVEMLERL 351  
 280 QR0G--R-----LQAFVDELRESILANEDHGGLPIITASTHERHTIFFIEHGGAGTFS SKKALVEMLERL 351  
 280 QR0G--P-----GQVDFDELRESILANEDHGGLPIITASTHERHTIFFIEHGGAGTFS SKKALVEMLERL 351  
 283 ER0G--A-----MADALDELRESILANEDHGGLPIITASTHERHTIFFIEHGGAGTFS SKKALVEMLERL 354  
 295 ER0G--A-----MADALDELRESILANEDHGGLPIITASTHERHTIFFIEHGGAGTFS SKKALVEMLERL 367  
 279 ER1G-----HDFDDELRESILANEDHGGLPIITASTHERHTIFFIEHGGAGTFS SKKALVEMLERL 350  
 278 GR1G--P-----GQVDFDELRESILANEDHGGLPIITASTHERHTIFFIEHGGAGTFS SKKALVEMLERL 349  
 302 TR0G--R-----VQGSVDDELRESILANEDHGGLPIITASTHERHTIFFIEHGGAGTFS SKKALVEMLERL 373  
 280 TR0G--R-----VQGSVDDELRESILANEDHGGLPIITASTHERHTIFFIEHGGAGTFS SKKALVEMLERL 351  
 177 ER0G--P-----VQGSVDDELRESILANEDHGGLPIITASTHERHTIFFIEHGGAGTFS SKKALVEMLERL 246

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