PDB ID : 4PZP
RCSB ID : RCSB085421
TITLE   : Substrate-free structure of D-alanine carrier protein ligase DltA
          from Bacillus cereus
AUTHORS : L.Du, M.Atila, Y.Luo

The following geometrical and stereochemical features have been calculated
for your structure.

CLOSE CONTACTS

==> Close contacts in same asymmetric unit. Distances smaller than 2.2
Angstroms are considered as close contacts.

none

==> Close contacts based on crystal symmetry. Distances smaller than 2.2
Angstroms are considered as close contacts.

none

BOND DISTANCES AND ANGLES

Bond and angle checks are performed by first computing the average rms
error for all bonds and angles relative to standard values for nucleotide
units [L. Clowney et al., Geometric Parameters in Nucleic Acids: Nitrogenous
Bases, J.Am.Chem.Soc. 1996, 118, 509-518; A. Gelbin et al., Geometric
Parameters in Nucleic Acids: Sugar and Phosphate Constituents, J.Am.Chem.Soc.
1996, 118, 519-529] and amino acid units [R.A. Engh and R. Huber, Structure
quality and target parameters, International Tables for Crystallography,
Volume F, 2001, 382-392]. Any bond or angle which deviates from the
dictionary values by more than six times this computed rms error is
identified as an outlier.

==> Covalent Bond Lengths:

The overall RMS deviation for covalent bonds relative to the standard
dictionary is   0.010 Angstroms

All covalent bonds lie within a 6.0*RMSD range about the
standard dictionary values.

==> Covalent Angle Values:

The overall RMS deviation for covalent angles relative to the standard
dictionary is   1.6 degrees.

All covalent bond angles lie within a 6.0*RMSD range about the
standard dictionary values.

TORSION ANGLES

The torsion angle distributions have been checked. To view these reports,
please refer to the ADIT Validation Server at http://deposit.pdb.org/validate.

==> The following table contains a list of torsion angles outside the expected
Ramachandran regions [GJ. Kleywegt and TA. Jones, PHI/PSI-chology:
Ramachandran Revisited, Structure 1996, 4, 1395 - 1400].

Residue	Chain	Sequence	PSI	PHI
ARG	A	23	-120.77	50.05

HIS	A	59	−92.33	−129.47
ALA	A	105	34.93	−94.74
THR	A	106	−163.52	167.31
VAL	A	110	101.53	−55.80
ASP	A	112	82.16	33.35
GLN	A	183	−120.41	−84.04
GLU	A	271	−169.91	−161.30
THR	A	300	74.20	55.19
VAL	A	301	−66.06	69.64
LYS	A	317	−75.39	−97.52
ASP	A	336	149.56	119.39
TYR	A	423	−5.58	79.67

CHIRALITY

The chirality has been checked. O1P, O2P, and hydrogen atoms which do not follow the convention defined in the IUBMB (Liebecq, C. Compendium of Biochemical Nomenclature and Related Documents, 2nd ed.; Portland Press: London and Chapel Hill, 1992) and IUPAC nomenclature (J.L. Markley, A. Bax, Y. Arata, C.W. Hilbers, R. Kaptein, B.D. Sykes, P.E. Wright and K. Wuthrich, Recommendations for the Presentation of NMR Structures of Proteins and Nucleic Acids, Pure & Appl. Chem., Vol. 70, pp. 117−142, 1998) have been standardized. Any other stereochemical violations are listed below.

none

SOLVENT

The following solvent molecules are further than 3.5 Angstroms away from macromolecule atoms in the asymmetric unit that are available for hydrogen bonding. Solvent molecules in extended hydration shells separated by 3.5 Angstroms or less are not listed.

HETATM 3793	O	HOH A 950	−2.546	−3.336	30.488	1.00 36.24	DIST =	3.94	A
HETATM 3795	O	HOH A 952	18.370	−3.733	−0.638	1.00 25.91	DIST =	4.85	A
HETATM 3799	O	HOH A 956	−16.878	−17.396	6.246	1.00 31.41	DIST =	5.32	A
HETATM 3805	O	HOH A 962	3.805	0.454	40.252	1.00 38.82	DIST =	5.25	A
HETATM 3806	O	HOH A 963	17.185	−2.274	24.817	1.00 31.72	DIST =	4.03	A
HETATM 3817	O	HOH A 974	10.646	−28.842	22.448	1.00 29.89	DIST =	3.84	A
HETATM 3823	O	HOH A 980	9.178	−31.923	24.980	1.00 28.54	DIST =	5.98	A
HETATM 3827	O	HOH A 984	10.228	8.702	6.294	1.00 30.03	DIST =	3.54	A
HETATM 3833	O	HOH A 990	24.128	−0.275	24.581	1.00 33.91	DIST =	3.85	A
HETATM 3837	O	HOH A 994	12.186	−33.945	13.696	1.00 34.56	DIST =	4.70	A
HETATM 3841	O	HOH A 998	15.287	−39.843	2.501	1.00 40.35	DIST =	4.29	A
HETATM 3848	O	HOH A1005	17.135	3.395	23.813	1.00 37.64	DIST =	5.18	A
HETATM 3852	O	HOH A1009	25.741	−28.547	−21.782	1.00 38.77	DIST =	5.54	A
HETATM 3854	O	HOH A1011	19.480	−2.757	30.230	1.00 32.31	DIST =	3.80	A
HETATM 3859	O	HOH A1016	−10.496	−13.212	−0.749	1.00 47.60	DIST =	4.62	A
HETATM 3862	O	HOH A1019	−15.198	−21.782	2.386	1.00 36.22	DIST =	5.52	A
HETATM 3863	O	HOH A1020	4.350	9.284	44.454	1.00 40.69	DIST =	3.76	A
HETATM 3867	O	HOH A1024	16.769	−1.530	22.049	1.00 34.64	DIST =	3.62	A
HETATM 3868	O	HOH A1025	−7.044	−28.650	1.984	1.00 34.13	DIST =	4.30	A
HETATM 3869	O	HOH A1026	8.775	−34.125	29.546	1.00 43.38	DIST =	10.46	A
HETATM 3870	O	HOH A1027	28.107	−25.561	−22.678	1.00 34.60	DIST =	5.28	A
HETATM 3875	O	HOH A1032	−2.020	14.928	40.388	1.00 31.05	DIST =	5.51	A
HETATM 3876	O	HOH A1033	31.668	−28.387	−23.327	1.00 34.09	DIST =	6.06	A
HETATM 3879	O	HOH A1036	26.484	−40.189	−8.625	1.00 42.23	DIST =	4.01	A
HETATM 3880	O	HOH A1037	25.732	−5.928	−17.661	1.00 37.33	DIST =	3.81	A
HETATM 3881	O	HOH A1038	12.519	3.260	−11.973	1.00 40.82	DIST =	4.49	A
HETATM 3882	O	HOH A1039	17.311	−8.855	34.618	1.00 35.37	DIST =	4.41	A
HETATM 3884	O	HOH A1041	28.483	−8.603	36.700	1.00 35.65	DIST =	3.62	A
HETATM 3885	O	HOH A1042	24.873	−12.752	36.008	1.00 39.45	DIST =	3.97	A
HETATM 3886	O	HOH A1043	−10.150	21.967	26.644	1.00 34.37	DIST =	3.56	A
HETATM 3888	O	HOH A1045	5.835	−34.265	24.505	1.00 46.09	DIST =	6.31	A
HETATM 3889	O	HOH A1046	20.977	−32.451	9.418	1.00 31.05	DIST =	5.35	A
HETATM 3890	O	HOH A1047	−3.453	−1.764	−6.334	1.00 41.52	DIST =	4.72	A
HETATM 3891	O	HOH A1048	23.332	3.513	21.715	1.00 37.52	DIST =	6.07	A
HETATM 3894	O	HOH A1051	11.518	−2.316	18.259	1.00 40.65	DIST =	3.55	A
HETATM 3900	O	HOH A1057	9.549	5.496	2.340	1.00 37.16	DIST =	5.89	A
HETATM 3901	O	HOH A1058	20.203	5.071	28.953	1.00 38.61	DIST =	6.47	A
HETATM 3902	O	HOH A1059	−8.532	−1.459	25.053	1.00 42.13	DIST =	4.45	A
HETATM 3906	O	HOH A1063	30.292	−10.784	−7.314	1.00 42.24	DIST =	3.71	A

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HETATM 3907  O   HOH A1064      10.476  22.281  13.486  1.00 41.61      DIST =   7.50 A
HETATM 3908  O   HOH A1065      17.343   0.640  33.151  1.00 43.33      DIST =   5.38 A
HETATM 3912  O   HOH A1069      41.761 -23.953  11.968  1.00 47.88      DIST =   4.58 A
HETATM 3913  O   HOH A1070       9.075   4.024  44.855  1.00 42.47      DIST =   4.26 A
HETATM 3915  O   HOH A1072      -7.448 -31.771  -2.357  1.00 42.28      DIST =   4.10 A
HETATM 3918  O   HOH A1075     -15.486 -15.683   3.890  1.00 44.64      DIST =   3.54 A
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We have replaced the coordinates for solvent molecules which could be translated back into the asymmetric unit. Please review all solvent molecules in your file and contact us if you have any serious objections.

MISSING RESIDUES

==> The following residues are missing:
(Note: The SEQ number starts from 1 for each chain according to SEQRES sequence record.)

RES	MOD	#C	SEQ
SER		A	153
GLY		A	154
SER		A	155
THR		A	156
GLY		A	157
ASN		A	158
PRO		A	159
PRO		A	363
GLU		A	364
LEU		A	365
THR		A	366
GLU		A	367
ARG		A	397
LEU		A	398
ASP		A	399
PHE		A	400
GLN		A	401
ILE		A	402
LYS		A	403
LEU		A	404
HIS		A	405
GLY		A	406
TYR		A	407
ARG		A	408
MET		A	409
GLU		A	410
LEU		A	411
GLU		A	412
GLU		A	413
LYS		A	433
LYS		A	434
GLY		A	435
GLU		A	436
LYS		A	437
TYR		A	438
ASP		A	439
TYR		A	440
VAL		A	502
THR		A	503
ALA		A	504
LEU		A	505
GLU		A	506
HIS		A	507
HIS		A	508
HIS		A	509
HIS		A	510
HIS		A	511
HIS		A	512

PDB Chain_ID: A

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SEQRES: ALA LYS LEU LEU GLU GLN ILE GLU LYS TRP ALA ALA GLU THR PRO
COORDS: ALA LYS LEU LEU GLU GLN ILE GLU LYS TRP ALA ALA GLU THR PRO
        1                                                      15

        16                                                     30
SEQRES: ASP GLN THR ALA PHE VAL TRP ARG ASP ALA LYS ILE THR TYR LYS
COORDS: ASP GLN THR ALA PHE VAL TRP ARG ASP ALA LYS ILE THR TYR LYS
        16                                                     30

        31                                                     45
SEQRES: GLN LEU LYS GLU ASP SER ASP ALA LEU ALA HIS TRP ILE SER SER
COORDS: GLN LEU LYS GLU ASP SER ASP ALA LEU ALA HIS TRP ILE SER SER
        31                                                     45

        46                                                     60
SEQRES: GLU TYR PRO ASP ASP ARG SER PRO ILE MET VAL TYR GLY HIS MET
COORDS: GLU TYR PRO ASP ASP ARG SER PRO ILE MET VAL TYR GLY HIS MET
        46                                                     60

        61                                                     75
SEQRES: GLN PRO GLU MET ILE ILE ASN PHE LEU GLY CYS VAL LYS ALA GLY
COORDS: GLN PRO GLU MET ILE ILE ASN PHE LEU GLY CYS VAL LYS ALA GLY
        61                                                     75

        76                                                     90
SEQRES: HIS ALA TYR ILE PRO VAL ASP LEU SER ILE PRO ALA ASP ARG VAL
COORDS: HIS ALA TYR ILE PRO VAL ASP LEU SER ILE PRO ALA ASP ARG VAL
        76                                                     90

        91                                                    105
SEQRES: GLN ARG ILE ALA GLU ASN SER GLY ALA LYS LEU LEU LEU SER ALA
COORDS: GLN ARG ILE ALA GLU ASN SER GLY ALA LYS LEU LEU LEU SER ALA
        91                                                    105

        106                                                   120
SEQRES: THR ALA VAL THR VAL THR ASP LEU PRO VAL ARG ILE VAL SER GLU
COORDS: THR ALA VAL THR VAL THR ASP LEU PRO VAL ARG ILE VAL SER GLU
        106                                                   120

        121                                                   135
SEQRES: ASP ASN LEU LYS ASP ILE PHE PHE THR HIS LYS GLY ASN THR PRO
COORDS: ASP ASN LEU LYS ASP ILE PHE PHE THR HIS LYS GLY ASN THR PRO
        121                                                   135

        136                                                   150
SEQRES: ASN PRO GLU HIS ALA VAL LYS GLY ASP GLU ASN PHE TYR ILE ILE
COORDS: ASN PRO GLU HIS ALA VAL LYS GLY ASP GLU ASN PHE TYR ILE ILE
        136                                                   150

        151                                                   165
SEQRES: TYR THR SER GLY SER THR GLY ASN PRO LYS GLY VAL GLN ILE THR
COORDS: TYR THR   ?   ?   ?   ?   ?   ?   ? LYS GLY VAL GLN ILE THR
        151                                                   165

        166                                                   180
SEQRES: TYR ASN CYS LEU VAL SER PHE THR LYS TRP ALA VAL GLU ASP PHE
COORDS: TYR ASN CYS LEU VAL SER PHE THR LYS TRP ALA VAL GLU ASP PHE
        166                                                   180

        181                                                   195
SEQRES: ASN LEU GLN THR GLY GLN VAL PHE LEU ASN GLN ALA PRO PHE SER
COORDS: ASN LEU GLN THR GLY GLN VAL PHE LEU ASN GLN ALA PRO PHE SER
        181                                                   195

        196                                                   210
SEQRES: PHE ASP LEU SER VAL MET ASP ILE TYR PRO SER LEU VAL THR GLY
COORDS: PHE ASP LEU SER VAL MET ASP ILE TYR PRO SER LEU VAL THR GLY
        196                                                   210

        211                                                   225
SEQRES: GLY THR LEU TRP ALA ILE ASP LYS ASP MET ILE ALA ARG PRO LYS
COORDS: GLY THR LEU TRP ALA ILE ASP LYS ASP MET ILE ALA ARG PRO LYS
        211                                                   225

        226                                                   240
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SEQRES: ASP LEU PHE ALA SER LEU GLU GLN SER ASP ILE GLN VAL TRP THR
COORDS: ASP LEU PHE ALA SER LEU GLU GLN SER ASP ILE GLN VAL TRP THR
        226                                                     240

        241                                                     255
SEQRES: SER THR PRO SER PHE ALA GLU MET CYS LEU MET GLU ALA SER PHE
COORDS: SER THR PRO SER PHE ALA GLU MET CYS LEU MET GLU ALA SER PHE
        241                                                     255

        256                                                     270
SEQRES: SER GLU SER MET LEU PRO ASN MET LYS THR PHE LEU PHE CYS GLY
COORDS: SER GLU SER MET LEU PRO ASN MET LYS THR PHE LEU PHE CYS GLY
        256                                                     270

        271                                                     285
SEQRES: GLU VAL LEU PRO ASN GLU VAL ALA ARG LYS LEU ILE GLU ARG PHE
COORDS: GLU VAL LEU PRO ASN GLU VAL ALA ARG LYS LEU ILE GLU ARG PHE
        271                                                     285

        286                                                     300
SEQRES: PRO LYS ALA THR ILE MET ASN THR TYR GLY PRO THR GLU ALA THR
COORDS: PRO LYS ALA THR ILE MET ASN THR TYR GLY PRO THR GLU ALA THR
        286                                                     300

        301                                                     315
SEQRES: VAL ALA VAL THR GLY ILE HIS VAL THR GLU GLU VAL LEU ASP GLN
COORDS: VAL ALA VAL THR GLY ILE HIS VAL THR GLU GLU VAL LEU ASP GLN
        301                                                     315

        316                                                     330
SEQRES: TYR LYS SER LEU PRO VAL GLY TYR CYS LYS SER ASP CYS ARG LEU
COORDS: TYR LYS SER LEU PRO VAL GLY TYR CYS LYS SER ASP CYS ARG LEU
        316                                                     330

        331                                                     345
SEQRES: LEU ILE MET LYS GLU ASP GLY THR ILE ALA PRO ASP GLY GLU LYS
COORDS: LEU ILE MET LYS GLU ASP GLY THR ILE ALA PRO ASP GLY GLU LYS
        331                                                     345

        346                                                     360
SEQRES: GLY GLU ILE VAL ILE VAL GLY PRO SER VAL SER VAL GLY TYR LEU
COORDS: GLY GLU ILE VAL ILE VAL GLY PRO SER VAL SER VAL GLY TYR LEU
        346                                                     360

        361                                                     375
SEQRES: GLY SER PRO GLU LEU THR GLU LYS ALA PHE THR MET ILE ASP GLY
COORDS: GLY SER   ?   ?   ?   ?   ? LYS ALA PHE THR MET ILE ASP GLY
        361                                                     375

        376                                                     390
SEQRES: GLU ARG ALA TYR LYS THR GLY ASP ALA GLY TYR VAL GLU ASN GLY
COORDS: GLU ARG ALA TYR LYS THR GLY ASP ALA GLY TYR VAL GLU ASN GLY
        376                                                     390

        391                                                     405
SEQRES: LEU LEU PHE TYR ASN GLY ARG LEU ASP PHE GLN ILE LYS LEU HIS
COORDS: LEU LEU PHE TYR ASN GLY   ?   ?   ?   ?   ?   ?   ?   ?   ?
        391                   396

        406                                                     420
SEQRES: GLY TYR ARG MET GLU LEU GLU GLU ILE GLU HIS HIS LEU ARG ALA
COORDS:   ?   ?   ?   ?   ?   ?   ?   ? ILE GLU HIS HIS LEU ARG ALA
                                      414                       420

        421                                                     435
SEQRES: CYS SER TYR VAL GLU GLY ALA VAL ILE VAL PRO ILE LYS LYS GLY
COORDS: CYS SER TYR VAL GLU GLY ALA VAL ILE VAL PRO ILE   ?   ?   ?
        421                                         432

        436                                                     450
SEQRES: GLU LYS TYR ASP TYR LEU LEU ALA VAL VAL VAL PRO GLY GLU HIS
COORDS:   ?   ?   ?   ?   ? LEU LEU ALA VAL VAL VAL PRO GLY GLU HIS
                        441                                     450

        451                                                     465
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SEQRES: SER PHE GLU LYS GLU PHE LYS LEU THR SER ALA ILE LYS LYS GLU
COORDS: SER PHE GLU LYS GLU PHE LYS LEU THR SER ALA ILE LYS LYS GLU
        451                                                     465

        466                                                     480
SEQRES: LEU ASN GLU ARG LEU PRO ASN TYR MET ILE PRO ARG LYS PHE MET
COORDS: LEU ASN GLU ARG LEU PRO ASN TYR MET ILE PRO ARG LYS PHE MET
        466                                                     480

        481                                                     495
SEQRES: TYR GLN SER SER ILE PRO MET THR PRO ASN GLY LYS VAL ASP ARG
COORDS: TYR GLN SER SER ILE PRO MET THR PRO ASN GLY LYS VAL ASP ARG
        481                                                     495

        496                                                     510
SEQRES: LYS LYS LEU LEU SER GLU VAL THR ALA LEU GLU HIS HIS HIS HIS
COORDS: LYS LYS LEU LEU SER GLU   ?   ?   ?   ?   ?   ?   ?   ?   ?
        496                 501

        511  512
SEQRES: HIS HIS
COORDS:   ?   ?
```