



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 11:33 PM GMT

PDB ID : 3K3P
Title : Crystal Structure of the Apo Form of D-Alanine:D-Alanine Ligase (DDL) from Streptococcus mutans
Authors : Lu, Y.
Deposited on : 2009-10-03
Resolution : 2.23 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

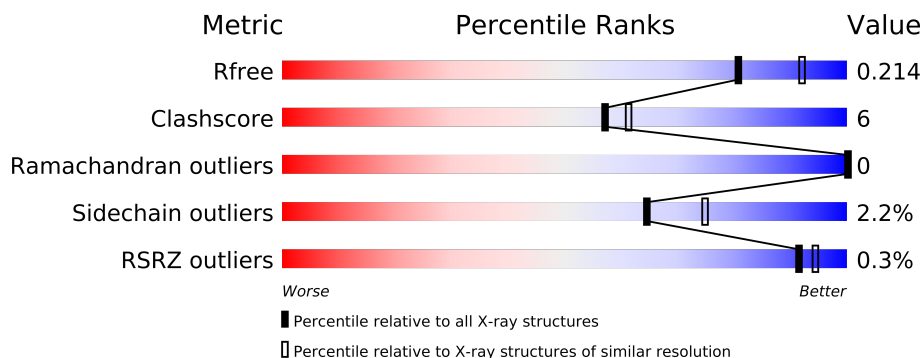
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance



The reported resolution of this entry is 2.23 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1112 (2.26-2.22)
Clashscore	79885	1317 (2.26-2.22)
Ramachandran outliers	78287	1282 (2.26-2.22)
Sidechain outliers	78261	1282 (2.26-2.22)
RSRZ outliers	66119	1112 (2.26-2.22)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	383	
1	B	383	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5080 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called D-alanine–D-alanine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	0	0
			2463	1572	389	488	14			
1	B	318	Total	C	N	O	S	1	0	0
			2467	1574	390	489	14			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-33	MET	-	EXPRESSION TAG	UNP P95803
A	-32	GLY	-	EXPRESSION TAG	UNP P95803
A	-31	SER	-	EXPRESSION TAG	UNP P95803
A	-30	SER	-	EXPRESSION TAG	UNP P95803
A	-29	HIS	-	EXPRESSION TAG	UNP P95803
A	-28	HIS	-	EXPRESSION TAG	UNP P95803
A	-27	HIS	-	EXPRESSION TAG	UNP P95803
A	-26	HIS	-	EXPRESSION TAG	UNP P95803
A	-25	HIS	-	EXPRESSION TAG	UNP P95803
A	-24	HIS	-	EXPRESSION TAG	UNP P95803
A	-23	SER	-	EXPRESSION TAG	UNP P95803
A	-22	SER	-	EXPRESSION TAG	UNP P95803
A	-21	GLY	-	EXPRESSION TAG	UNP P95803
A	-20	LEU	-	EXPRESSION TAG	UNP P95803
A	-19	VAL	-	EXPRESSION TAG	UNP P95803
A	-18	PRO	-	EXPRESSION TAG	UNP P95803
A	-17	ARG	-	EXPRESSION TAG	UNP P95803
A	-16	GLY	-	EXPRESSION TAG	UNP P95803
A	-15	SER	-	EXPRESSION TAG	UNP P95803
A	-14	HIS	-	EXPRESSION TAG	UNP P95803
A	-13	MET	-	EXPRESSION TAG	UNP P95803
A	-12	ALA	-	EXPRESSION TAG	UNP P95803
A	-11	SER	-	EXPRESSION TAG	UNP P95803
A	-10	MET	-	EXPRESSION TAG	UNP P95803
A	-9	THR	-	EXPRESSION TAG	UNP P95803

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	GLY	-	EXPRESSION TAG	UNP P95803
A	-7	GLY	-	EXPRESSION TAG	UNP P95803
A	-6	GLN	-	EXPRESSION TAG	UNP P95803
A	-5	GLN	-	EXPRESSION TAG	UNP P95803
A	-4	MET	-	EXPRESSION TAG	UNP P95803
A	-3	GLY	-	EXPRESSION TAG	UNP P95803
A	-2	ARG	-	EXPRESSION TAG	UNP P95803
A	-1	GLY	-	EXPRESSION TAG	UNP P95803
A	0	SER	-	EXPRESSION TAG	UNP P95803
B	-33	MET	-	EXPRESSION TAG	UNP P95803
B	-32	GLY	-	EXPRESSION TAG	UNP P95803
B	-31	SER	-	EXPRESSION TAG	UNP P95803
B	-30	SER	-	EXPRESSION TAG	UNP P95803
B	-29	HIS	-	EXPRESSION TAG	UNP P95803
B	-28	HIS	-	EXPRESSION TAG	UNP P95803
B	-27	HIS	-	EXPRESSION TAG	UNP P95803
B	-26	HIS	-	EXPRESSION TAG	UNP P95803
B	-25	HIS	-	EXPRESSION TAG	UNP P95803
B	-24	HIS	-	EXPRESSION TAG	UNP P95803
B	-23	SER	-	EXPRESSION TAG	UNP P95803
B	-22	SER	-	EXPRESSION TAG	UNP P95803
B	-21	GLY	-	EXPRESSION TAG	UNP P95803
B	-20	LEU	-	EXPRESSION TAG	UNP P95803
B	-19	VAL	-	EXPRESSION TAG	UNP P95803
B	-18	PRO	-	EXPRESSION TAG	UNP P95803
B	-17	ARG	-	EXPRESSION TAG	UNP P95803
B	-16	GLY	-	EXPRESSION TAG	UNP P95803
B	-15	SER	-	EXPRESSION TAG	UNP P95803
B	-14	HIS	-	EXPRESSION TAG	UNP P95803
B	-13	MET	-	EXPRESSION TAG	UNP P95803
B	-12	ALA	-	EXPRESSION TAG	UNP P95803
B	-11	SER	-	EXPRESSION TAG	UNP P95803
B	-10	MET	-	EXPRESSION TAG	UNP P95803
B	-9	THR	-	EXPRESSION TAG	UNP P95803
B	-8	GLY	-	EXPRESSION TAG	UNP P95803
B	-7	GLY	-	EXPRESSION TAG	UNP P95803
B	-6	GLN	-	EXPRESSION TAG	UNP P95803
B	-5	GLN	-	EXPRESSION TAG	UNP P95803
B	-4	MET	-	EXPRESSION TAG	UNP P95803
B	-3	GLY	-	EXPRESSION TAG	UNP P95803
B	-2	ARG	-	EXPRESSION TAG	UNP P95803
B	-1	GLY	-	EXPRESSION TAG	UNP P95803

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	SER	-	EXPRESSION TAG	UNP P95803

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	71	Total O 71 71	0	0
2	B	79	Total O 79 79	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	79.50Å 79.50Å 109.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	17.58 – 2.23 17.58 – 2.23	Depositor EDS
% Data completeness (in resolution range)	99.9 (17.58-2.23) 99.9 (17.58-2.23)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.23Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.196 , 0.248 0.195 , 0.214	Depositor DCC
R_{free} test set	1921 reflections (5.39%)	DCC
Wilson B-factor (Å ²)	29.0	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 24.6	EDS
Estimated twinning fraction	0.013 for -h,-k,l 0.487 for h,-h-k,-l 0.015 for -k,-h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 37611 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5080	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.05	2/2499 (0.1%)	0.93	1/3381 (0.0%)
1	B	1.03	1/2503 (0.0%)	0.94	2/3386 (0.1%)
All	All	1.04	3/5002 (0.1%)	0.94	3/6767 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	85	GLU	CB-CG	-5.70	1.41	1.52
1	A	298	VAL	CB-CG1	5.68	1.64	1.52
1	A	170	VAL	CB-CG2	5.05	1.63	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	B	344	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	B	189	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2463	0	2481	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2467	0	2484	36	0
2	A	71	0	0	1	0
2	B	79	0	0	1	0
All	All	5080	0	4965	63	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (63) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:235:ILE:O	1:A:236:VAL:HG12	1.60	1.02
1:A:149:LEU:HD13	1:A:158:LYS:HG3	1.64	0.79
1:B:176:ASN:HD22	1:B:203:ASP:HB2	1.50	0.75
1:B:173:LYS:HE2	1:B:207:LEU:HD23	1.68	0.75
1:B:288:CYS:SG	1:B:303:LEU:CD1	2.75	0.74
1:B:288:CYS:SG	1:B:303:LEU:HD13	2.31	0.71
1:B:340:MET:HE1	1:B:343:LYS:HD3	1.72	0.69
1:B:99:GLU:HB2	1:B:126:MET:HE1	1.76	0.65
1:A:235:ILE:O	1:A:236:VAL:CG1	2.43	0.63
1:A:288:CYS:SG	1:A:303:LEU:HD13	2.38	0.63
1:B:310:THR:HG22	1:B:313:SER:HB3	1.81	0.62
1:A:340:MET:HE1	1:A:343:LYS:HD3	1.80	0.62
1:B:288:CYS:SG	1:B:303:LEU:HD12	2.40	0.60
1:B:149:LEU:HD13	1:B:158:LYS:HG3	1.84	0.60
1:A:99:GLU:HB2	1:A:126:MET:HE1	1.84	0.60
1:B:16:GLU:OE1	1:B:95:GLY:HA3	2.02	0.59
1:A:344:ARG:HG2	1:A:344:ARG:O	2.04	0.57
1:B:72:ILE:HG21	1:B:75:GLN:HE21	1.68	0.57
1:B:103:ILE:HG22	1:B:104:GLN:OE1	2.06	0.56
1:B:41:TYR:HE1	1:B:51:LYS:HG3	1.72	0.55
1:A:288:CYS:SG	1:A:303:LEU:CD1	2.96	0.53
1:A:105:GLY:HA2	1:A:119:ILE:HD11	1.91	0.53
1:B:255:MET:HE1	1:B:314:MET:HG2	1.91	0.52
1:A:45:GLN:H	1:A:68:ASN:HD21	1.55	0.52
1:B:96:PRO:O	1:B:97:MET:HB2	2.09	0.52
1:B:310:THR:CG2	1:B:313:SER:HB3	2.41	0.50
1:B:255:MET:CE	1:B:314:MET:HG2	2.41	0.50
1:A:219:VAL:HG22	1:A:232:PRO:HG3	1.93	0.50
1:B:103:ILE:HG22	1:B:104:GLN:CD	2.32	0.50
1:B:45:GLN:H	1:B:68:ASN:HD21	1.58	0.50
1:B:41:TYR:CE1	1:B:51:LYS:HG3	2.47	0.49
1:B:39:LYS:HG2	1:B:54:GLU:HG2	1.93	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:31:ILE:HD11	1:A:36:PHE:CD2	2.48	0.49
1:B:105:GLY:HA2	1:B:119:ILE:HD11	1.95	0.49
1:A:118:ASN:HB2	2:A:381:HOH:O	2.14	0.48
1:A:236:VAL:HA	1:A:254:THR:CG2	2.44	0.47
1:A:99:GLU:C	1:A:126:MET:HE2	2.35	0.47
1:B:93:LEU:HD12	1:B:103:ILE:HG12	1.96	0.47
1:A:10:TYR:CE1	1:A:65:LEU:HB3	2.50	0.47
1:A:40:THR:HG1	1:A:52:THR:HG1	1.59	0.47
1:A:153:GLU:CD	1:A:158:LYS:HE3	2.35	0.46
1:B:50:ILE:HG21	1:B:66:MET:SD	2.55	0.46
1:B:99:GLU:C	1:B:126:MET:HE2	2.36	0.46
1:B:147:VAL:HG21	1:B:162:VAL:HA	1.98	0.45
1:A:101:GLY:HA2	1:A:104:GLN:OE1	2.17	0.44
1:A:173:LYS:HE2	1:A:207:LEU:HD23	1.98	0.44
1:A:104:GLN:O	1:A:108:GLU:HG3	2.17	0.44
1:B:217:ILE:CG2	1:B:232:PRO:HB3	2.46	0.44
1:A:14:SER:O	1:A:17:ARG:NH1	2.50	0.44
1:B:68:ASN:HD22	1:B:71:ILE:HD11	1.82	0.44
1:B:103:ILE:CG2	1:B:104:GLN:N	2.80	0.43
1:B:224:ASN:HB3	1:B:340:MET:HE3	2.01	0.43
1:A:315:TYR:HB3	1:A:316:PRO:HD3	1.99	0.43
1:A:313:SER:O	1:A:316:PRO:HD2	2.18	0.43
1:B:14:SER:O	1:B:17:ARG:NH1	2.50	0.42
1:A:111:LYS:HD2	1:B:46:ALA:O	2.19	0.42
1:B:234:GLU:O	1:B:255:MET:HA	2.20	0.42
1:A:106:PHE:HA	1:B:106:PHE:HB2	2.02	0.41
1:B:118:ASN:HB2	2:B:382:HOH:O	2.20	0.41
1:B:153:GLU:OE1	1:B:158:LYS:HE3	2.21	0.41
1:A:117:THR:HB	1:A:121:SER:OG	2.21	0.41
1:A:233:GLY:HA3	1:A:314:MET:HE1	2.02	0.40
1:A:344:ARG:O	1:A:344:ARG:CG	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	307/383 (80%)	301 (98%)	6 (2%)	0	100	100
1	B	308/383 (80%)	297 (96%)	11 (4%)	0	100	100
All	All	615/766 (80%)	598 (97%)	17 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	276/330 (84%)	270 (98%)	6 (2%)	64	75
1	B	276/330 (84%)	270 (98%)	6 (2%)	64	75
All	All	552/660 (84%)	540 (98%)	12 (2%)	64	75

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LYS
1	A	90	PHE
1	A	236	VAL
1	A	288	CYS
1	A	302	GLU
1	A	326	TYR
1	B	51	LYS
1	B	85	GLU
1	B	90	PHE
1	B	103	ILE
1	B	288	CYS
1	B	326	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	75	GLN

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Mol	Chain	Res	Type
1	A	133	GLN
1	B	35	ASN
1	B	58	GLN
1	B	68	ASN
1	B	75	GLN
1	B	133	GLN
1	B	176	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	317/383 (82%)	-0.50	1 (0%) 91 94	17, 27, 44, 56	19 (5%)
1	B	318/383 (83%)	-0.51	1 (0%) 91 94	17, 27, 44, 55	19 (5%)
All	All	635/766 (82%)	-0.51	2 (0%) 91 94	17, 27, 44, 56	38 (5%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	236	VAL	3.6
1	B	236	VAL	2.2

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.