



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 25, 2024 – 06:43 PM EST

PDB ID : 3MFD
Title : The Structure of the Beta-lactamase superfamily domain of D-alanyl-D-alanine carboxypeptidase from *Bacillus subtilis*
Authors : Cuff, M.E.; Rakowski, E.; Buck, K.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2010-04-01
Resolution : 1.75 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.21
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.004 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

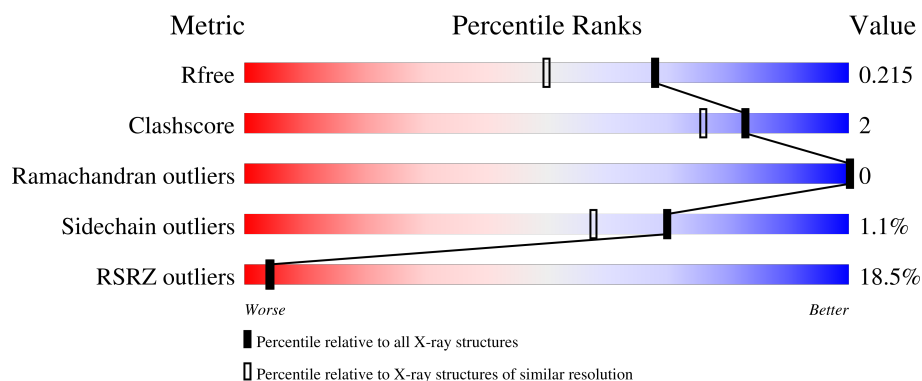
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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}	164625	2888 (1.76-1.76)
Clashscore	180529	3097 (1.76-1.76)
Ramachandran outliers	177936	3072 (1.76-1.76)
Sidechain outliers	177891	3072 (1.76-1.76)
RSRZ outliers	164620	2887 (1.76-1.76)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	334	<div> <div>18%</div> <div>94%</div> <div>.</div> <div>.</div> </div>
1	B	334	<div> <div>15%</div> <div>84%</div> <div>7%</div> <div>8%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CIT	A	1	-	X	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6071 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

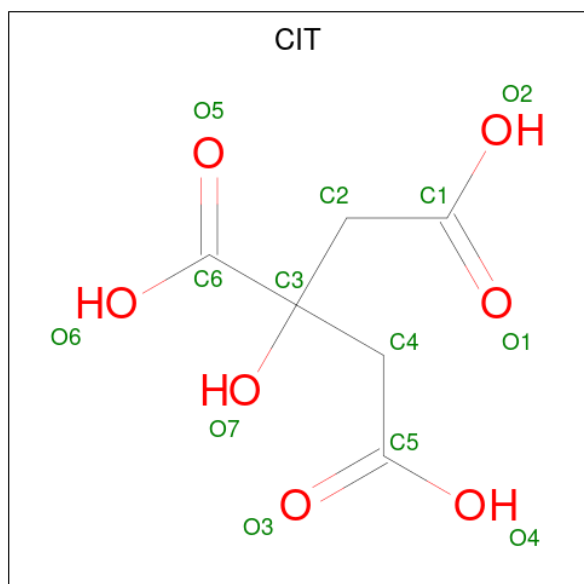
- Molecule 1 is a protein called D-alanyl-D-alanine carboxypeptidase dacB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	Se	0	18	0
			2696	1718	450	514	14			
1	B	306	Total	C	N	O	Se	0	16	0
			2518	1599	421	484	14			

There are 4 discrepancies between the modelled and reference sequences:

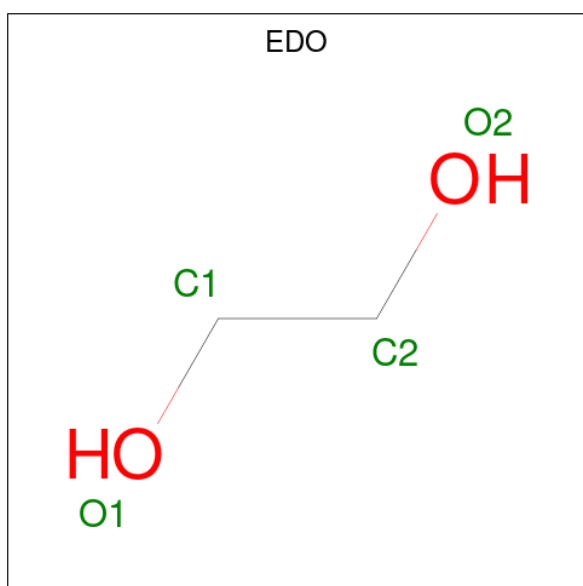
Chain	Residue	Modelled	Actual	Comment	Reference
A	25	SER	-	expression tag	UNP P35150
A	26	ASN	-	expression tag	UNP P35150
B	25	SER	-	expression tag	UNP P35150
B	26	ASN	-	expression tag	UNP P35150

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	A	1	Total	C	O	0	0
			13	6	7		
2	A	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	434	Total 434	O 434	0	0
4	B	339	Total 339	O 339	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	100.44Å 100.44Å 171.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.78 – 1.75 34.78 – 1.75	Depositor EDS
% Data completeness (in resolution range)	98.5 (34.78-1.75) 98.5 (34.78-1.75)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.89 (at 1.75Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.165 , 0.190 0.195 , 0.215	Depositor DCC
R_{free} test set	4388 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	23.3	Xtriage
Anisotropy	0.473	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 30.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6071	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CIT, EDO

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	0.68	0/2761	0.73	2/3691 (0.1%)
1	B	0.63	0/2560	0.67	1/3422 (0.0%)
All	All	0.66	0/5321	0.70	3/7113 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	259	MSE	CG-SE-CE	-11.53	73.54	98.90
1	B	106	ASP	CB-CG-OD1	5.74	123.47	118.30
1	A	118	ASP	CB-CG-OD1	5.52	123.27	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2696	0	2745	11	0
1	B	2518	0	2521	12	0
2	A	39	0	15	3	0
2	B	13	0	5	1	0
3	A	16	0	24	1	0
3	B	16	0	24	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	434	0	0	2	2
4	B	339	0	0	0	2
All	All	6071	0	5334	24	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 24 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162[B]:GLU:HA	1:A:162[B]:GLU:OE1	1.80	0.81
1:B:199[A]:GLU:HG3	1:B:199[A]:GLU:O	1.84	0.77
1:A:205:LYS:HD3	2:A:1:CIT:O6	1.89	0.71
1:A:28:ALA:N	4:A:759:HOH:O	2.27	0.67
1:B:314:LEU:HD23	1:B:332:VAL:CG1	2.26	0.65

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:727:HOH:O	4:B:646:HOH:O[8_565]	2.06	0.14
4:A:534:HOH:O	4:B:410:HOH:O[8_565]	2.12	0.08

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	342/334 (102%)	334 (98%)	8 (2%)	0	100	100
1	B	316/334 (95%)	306 (97%)	10 (3%)	0	100	100
All	All	658/668 (98%)	640 (97%)	18 (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	293/270 (108%)	293 (100%)	0	100	100
1	B	269/270 (100%)	261 (97%)	8 (3%)	36	15
All	All	562/540 (104%)	554 (99%)	8 (1%)	70	49

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	338	MSE
1	B	332	VAL
1	B	294[A]	ARG
1	B	280	LYS
1	B	294[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides in this entry.

5.6 Ligand geometry

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CIT	A	362	-	12,12,12	1.09	0	17,17,17	1.54	3 (17%)
3	EDO	A	361	-	3,3,3	0.42	0	2,2,2	0.36	0
3	EDO	B	360	-	3,3,3	0.47	0	2,2,2	0.39	0
3	EDO	A	359	-	3,3,3	0.56	0	2,2,2	0.33	0
3	EDO	B	359	-	3,3,3	0.36	0	2,2,2	0.38	0
3	EDO	A	363	-	3,3,3	0.44	0	2,2,2	0.19	0
3	EDO	B	362	-	3,3,3	0.48	0	2,2,2	0.14	0
2	CIT	A	364	-	12,12,12	1.15	0	17,17,17	1.86	5 (29%)
2	CIT	B	1	-	12,12,12	1.17	1 (8%)	17,17,17	1.71	3 (17%)
2	CIT	A	1	-	12,12,12	1.27	2 (16%)	17,17,17	2.16	6 (35%)
3	EDO	A	360	-	3,3,3	0.39	0	2,2,2	0.52	0
3	EDO	B	361	-	3,3,3	0.49	0	2,2,2	0.38	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CIT	A	362	-	-	10/16/16/16	-
3	EDO	A	361	-	-	0/1/1/1	-
3	EDO	B	360	-	-	1/1/1/1	-
3	EDO	A	359	-	-	1/1/1/1	-
3	EDO	B	359	-	-	0/1/1/1	-
3	EDO	A	363	-	-	0/1/1/1	-
3	EDO	B	362	-	-	1/1/1/1	-
2	CIT	A	364	-	-	7/16/16/16	-
2	CIT	B	1	-	-	3/16/16/16	-
2	CIT	A	1	-	-	11/16/16/16	-
3	EDO	A	360	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	361	-	-	0/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	CIT	O6-C6	-2.41	1.21	1.30
2	B	1	CIT	C2-C3	-2.25	1.51	1.54
2	A	1	CIT	O4-C5	-2.12	1.23	1.30

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	CIT	O6-C6-C3	4.19	121.18	113.14
2	A	1	CIT	O6-C6-C3	3.79	120.42	113.14
2	A	1	CIT	C2-C3-C6	3.78	118.39	110.03
2	A	362	CIT	O6-C6-C3	3.73	120.30	113.14
2	A	364	CIT	O4-C5-O3	-3.46	114.43	123.33

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	CIT	O7-C3-C6-O5
2	A	1	CIT	O7-C3-C6-O6
2	A	1	CIT	C4-C3-C6-O5
2	A	1	CIT	C4-C3-C6-O6
2	A	362	CIT	C1-C2-C3-C4

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	361	EDO	1	0
2	B	1	CIT	1	0
2	A	1	CIT	3	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

Warning: The R factor obtained from EDS is 0.2504, which does not match the depositor's R factor of 0.16456. Please interpret the results in this section carefully.

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	312/334 (93%)	0.84	61 (19%) 4 4	6, 15, 38, 65	18 (5%)
1	B	292/334 (87%)	0.67	51 (17%) 5 5	7, 14, 73, 93	16 (5%)
All	All	604/668 (90%)	0.76	112 (18%) 4 4	6, 15, 43, 93	34 (5%)

The worst 5 of 112 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	247	ILE	8.7
1	A	253	TRP	8.1
1	B	253	TRP	8.1
1	A	245	VAL	7.8
1	A	244	ALA	7.2

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CIT	A	362	13/13	0.45	0.25	77,79,81,82	0
3	EDO	B	360	4/4	0.49	0.30	81,82,82,82	0
3	EDO	B	362	4/4	0.65	0.22	77,78,78,78	0
2	CIT	A	364	13/13	0.68	0.21	67,70,72,74	0
3	EDO	B	361	4/4	0.72	0.17	46,48,48,49	0
3	EDO	A	361	4/4	0.74	0.32	76,76,77,77	0
3	EDO	A	359	4/4	0.75	0.23	54,56,56,56	0
3	EDO	B	359	4/4	0.78	0.18	68,68,68,69	0
3	EDO	A	360	4/4	0.79	0.15	44,47,49,50	0
2	CIT	B	1	13/13	0.81	0.13	25,30,37,37	0
2	CIT	A	1	13/13	0.82	0.16	17,37,44,45	13
3	EDO	A	363	4/4	0.84	0.16	50,50,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.