



# wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 1ZUJ  
Title : The crystal structure of the Lactococcus lactis MG1363 DpsA protein  
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Deposited on : 2005-05-31  
Resolution : 2.90 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](mailto: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.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

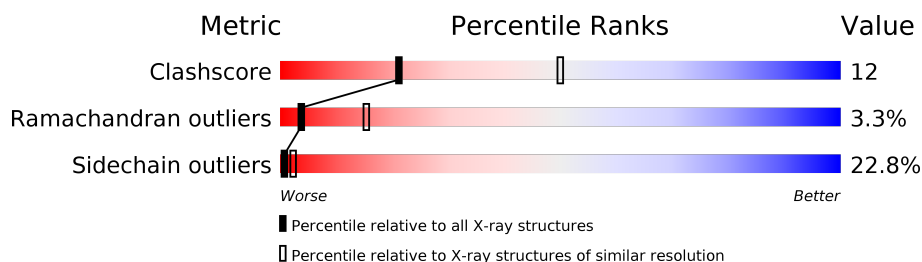
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	179	
1	B	179	
1	C	179	
1	D	179	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5589 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 hypothetical protein Llacc01001955.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	168	Total	C	N	O	S	0	0	0
			1386	900	221	263	2			
1	B	168	Total	C	N	O	S	0	0	0
			1386	900	221	263	2			
1	C	168	Total	C	N	O	S	0	0	0
			1386	900	221	263	2			
1	D	168	Total	C	N	O	S	0	0	0
			1386	900	221	263	2			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	O	0	0
			3	3		
2	B	6	Total	O	0	0
			6	6		
2	C	19	Total	O	0	0
			19	19		
2	D	17	Total	O	0	0
			17	17		

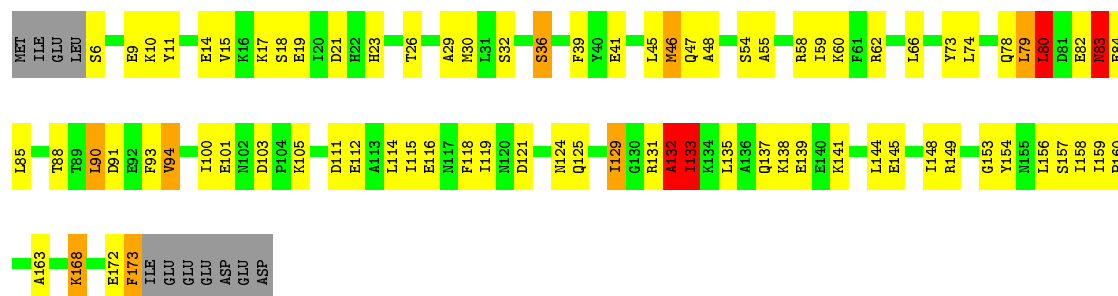
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

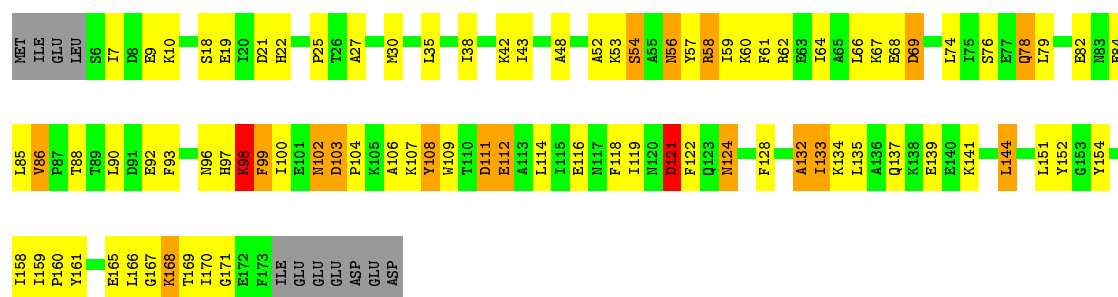
- Molecule 1: hypothetical protein Llacc01001955

Chain A: 



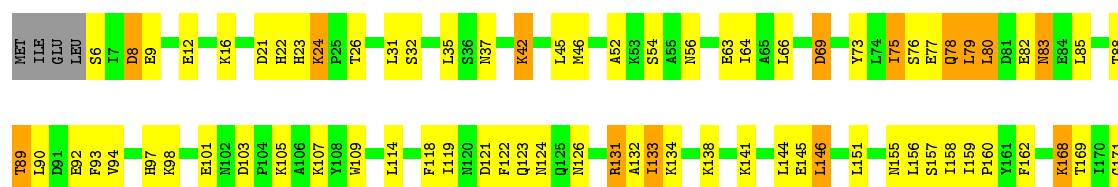
- Molecule 1: hypothetical protein Llacc01001955

Chain B: 



- Molecule 1: hypothetical protein Llacc01001955

Chain C: 



E172	F173
ILE	GLU
GLU	GLU
GLU	ASP
ASP	ASP

● Molecule 1: hypothetical protein Llacc01001955



MET	ILE	GLU	LEU	S6	I7	D8	E14	V15	K16	K17	H22	H23	K24	P25	T26	K30	L31	S32	H33	N37	Y40	E41	K42	M46	Y51	A52	K53	Y57	F61	R62	K67	E68	D69	E70	Y73	L74	E77	Q78	L79	N83	E84	L85	T88	T89	L90
D91	S95	N96	H97	K98	A106	K107	V108	W109	E116	H117	F118	I119	M120	D121	F122	Q123	M124	I129	A132	T133	K134	K138	I148	Y154	M155	L156	S157	I158	T159	P160	Y161	F162	A163	I170	G171	E172	F173	ILE	GLU	GLU	GLU	ASP	GLU	ASP	

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.84Å 131.84Å 325.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.90	Depositor
% Data completeness (in resolution range)	87.1 (15.00-2.90)	Depositor
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.253 , 0.322	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5589	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

## 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	0.56	0/1417	0.76	5/1909 (0.3%)
1	B	0.54	0/1417	0.79	4/1909 (0.2%)
1	C	0.65	0/1417	0.85	5/1909 (0.3%)
1	D	0.77	0/1417	0.93	3/1909 (0.2%)
All	All	0.64	0/5668	0.84	17/7636 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	3
1	D	0	2
All	All	0	7

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	91	ASP	CB-CG-OD2	7.11	124.70	118.30
1	B	21	ASP	CB-CG-OD2	6.68	124.32	118.30
1	A	111	ASP	CB-CG-OD2	6.35	124.02	118.30
1	B	121	ASP	CB-CG-OD2	6.11	123.80	118.30
1	C	103	ASP	CB-CG-OD2	5.84	123.55	118.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	132	ALA	Peptide
1	B	132	ALA	Peptide
1	C	131	ARG	Peptide
1	C	132	ALA	Peptide
1	C	24	LYS	Peptide

## 5.2 Too-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 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	1386	0	1366	43	0
1	B	1386	0	1366	36	0
1	C	1386	0	1366	30	0
1	D	1386	0	1366	32	0
2	A	3	0	0	0	0
2	B	6	0	0	0	0
2	C	19	0	0	0	0
2	D	17	0	0	1	0
All	All	5589	0	5464	133	0

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 12.

The worst 5 of 133 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:C:156:LEU:O	1:C:160:PRO:CD	2.15	0.94
1:A:154:TYR:CE2	1:A:158:ILE:HD11	2.07	0.90
1:C:156:LEU:O	1:C:160:PRO:HD3	1.71	0.88
1:A:41:GLU:OE1	1:A:121:ASP:HB3	1.81	0.80
1:C:107:LYS:NZ	1:D:14:GLU:OE2	2.15	0.79

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	166/179 (93%)	136 (82%)	25 (15%)	5 (3%)	4	17
1	B	166/179 (93%)	133 (80%)	25 (15%)	8 (5%)	2	8
1	C	166/179 (93%)	140 (84%)	19 (11%)	7 (4%)	3	10
1	D	166/179 (93%)	153 (92%)	11 (7%)	2 (1%)	13	40
All	All	664/716 (93%)	562 (85%)	80 (12%)	22 (3%)	4	15

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	132	ALA
1	B	103	ASP
1	B	167	GLY
1	C	133	ILE

### 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	148/159 (93%)	113 (76%)	35 (24%)	1	2
1	B	148/159 (93%)	108 (73%)	40 (27%)	0	1
1	C	148/159 (93%)	116 (78%)	32 (22%)	1	3
1	D	148/159 (93%)	120 (81%)	28 (19%)	1	4
All	All	592/636 (93%)	457 (77%)	135 (23%)	1	2

5 of 135 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	107	LYS
1	C	8	ASP
1	D	91	ASP
1	B	108	TYR
1	B	135	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	102	ASN
1	C	22	HIS
1	D	96	ASN
1	B	96	ASN
1	D	120	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.