



# wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 3ISZ  
Title : Crystal structure of mono-zinc form of succinyl-diaminopimelate desuccinylase from *Haemophilus influenzae*  
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Deposited on : 2009-08-27  
Resolution : 2.00 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
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

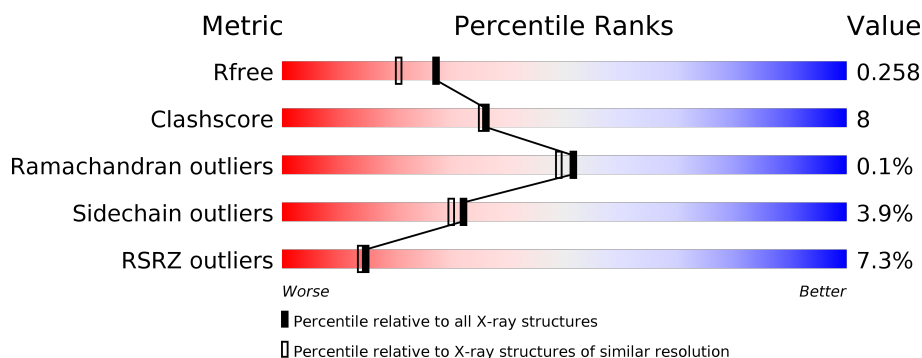
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	377	<div> <div>2%</div> <div>84%</div> <div>12%</div> <div>••</div> </div>
1	B	377	<div> <div>12%</div> <div>77%</div> <div>18%</div> <div>••</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6109 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 Succinyl-diaminopimelate desuccinylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	S	0	1	0
			2852	1804	480	553	15			
1	B	366	Total	C	N	O	S	0	2	0
			2844	1802	479	548	15			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	271	Total	O	0	0
			271	271		
4	B	130	Total	O	0	0
			130	130		

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). 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.

- Chain A:
- 
- 20% 84% 12% ..
- 1  
D11  
S19  
C25  
I28  
K35  
L36  
A53  
K54  
H55  
A65  
S80  
E113  
H122  
A127  
T137  
A138  
K139  
V146  
C159  
V160  
V161  
G162  
K175  
M185  
I191  
GLN  
GLY  
HIS  
VAL  
ALA  
TYR  
PRO  
H199  
L205  
Q213  
T217  
K222
- L232  
N236  
P245  
V246  
I247  
P248  
L251  
K269  
A273  
L276  
E277  
E286  
W287  
N288  
K292  
K297  
T306  
I313  
G314  
I315  
T316  
P317  
I331  
A332  
L333  
M334  
E340  
L344  
N352  
K362  
L374  
L375  
D376  
SER

- Chain B:
- 
- 12%
- 77%
- 18%

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.18Å 95.71Å 181.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.86 – 2.00 28.86 – 2.03	Depositor EDS
% Data completeness (in resolution range)	99.9 (28.86-2.00) 99.9 (28.86-2.03)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.43 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.5.0054	Depositor
R, $R_{free}$	0.202 , 0.254 0.206 , 0.258	Depositor DCC
$R_{free}$ test set	2608 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.6	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 51.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6109	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.36% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: ZN, SO4

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	0.86	0/2907	0.79	1/3939 (0.0%)
1	B	0.76	0/2899	0.75	0/3924
All	All	0.81	0/5806	0.77	1/7863 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	374	LEU	CA-CB-CG	5.21	127.28	115.30

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	2852	0	2839	40	0
1	B	2844	0	2833	58	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	271	0	0	4	0
4	B	130	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6109	0	5672	91	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 8.

The worst 5 of 91 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:247:ILE:HD11	1:B:233:GLN:NE2	1.92	0.84
1:B:80:SER:H	1:B:352:ASN:HD21	1.25	0.83
1:A:80:SER:H	1:A:352:ASN:HD21	1.28	0.82
1:B:272:VAL:HA	1:B:275:MET:HE2	1.65	0.77
1:A:137:THR:HG22	1:A:139:LYS:HG2	1.67	0.75

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	366/377 (97%)	358 (98%)	8 (2%)	0	100	100
1	B	362/377 (96%)	350 (97%)	11 (3%)	1 (0%)	41	37
All	All	728/754 (97%)	708 (97%)	19 (3%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	76	GLU



### 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	310/315 (98%)	298 (96%)	12 (4%)	32	30
1	B	308/315 (98%)	295 (96%)	13 (4%)	30	27
All	All	618/630 (98%)	593 (96%)	25 (4%)	32	29

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	344	LEU
1	B	19	SER
1	B	192	GLN
1	B	13	ILE
1	B	75	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	27	GLN
1	B	77	ASN
1	B	233	GLN
1	B	26	GLN
1	B	206	HIS

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z  > 2$
3	SO4	B	378	-	4,4,4	0.30	0	6,6,6	1.23	0
3	SO4	A	378	-	4,4,4	0.37	0	6,6,6	0.60	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	369/377 (97%)	0.08	9 (2%) 59 57	17, 26, 38, 51	0
1	B	366/377 (97%)	0.72	45 (12%) 4 3	20, 37, 55, 64	0
All	All	735/754 (97%)	0.39	54 (7%) 15 14	17, 30, 52, 64	0

The worst 5 of 54 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	199	HIS	5.6
1	B	136	ALA	5.0
1	B	137	THR	4.4
1	B	247	ILE	4.4
1	A	191	ILE	4.3

### 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 carbohydrates 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	ZN	B	1001	1/1	0.96	0.04	39,39,39,39	0
3	SO4	B	378	5/5	0.98	0.09	39,40,41,41	0
3	SO4	A	378	5/5	0.99	0.10	37,39,40,45	0
2	ZN	A	1001	1/1	1.00	0.04	24,24,24,24	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.