



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:29 AM GMT

PDB ID : 3ETF  
Title : Crystal structure of a putative succinate-semialdehyde dehydrogenase from salmonella typhimurium lt2  
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Deposited on : 2008-10-07  
Resolution : 1.85 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

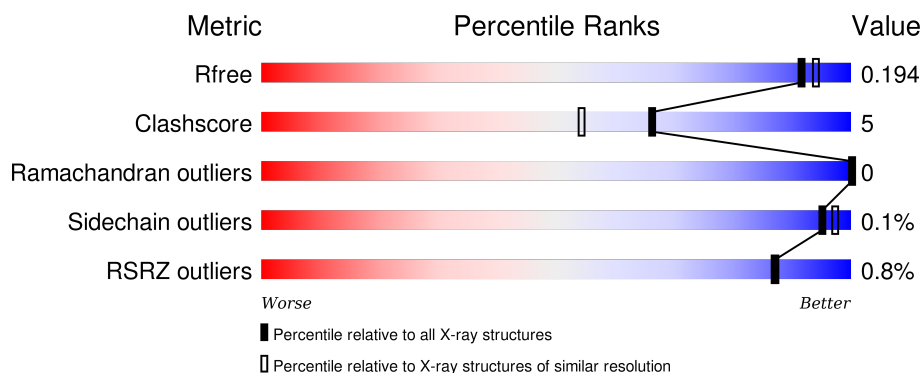
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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))
$R_{free}$	91344	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (1.86-1.86)

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. 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	462	<div> <div>90%</div> <div>9% .</div> </div>
1	B	462	<div> <div>90%</div> <div>8% .</div> </div>
1	C	462	<div> <div>90%</div> <div>8% .</div> </div>
1	D	462	<div> <div>90%</div> <div>8% .</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15906 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 Putative succinate-semialdehyde dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	457	Total	C	N	O	S	Se	11	15	0
			3523	2218	622	663	8	12			
1	B	456	Total	C	N	O	S	Se	8	11	0
			3482	2190	615	656	9	12			
1	C	455	Total	C	N	O	S	Se	6	12	0
			3485	2195	612	658	8	12			
1	D	454	Total	C	N	O	S	Se	14	7	0
			3431	2158	608	645	8	12			


- Molecule 2 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	527	Total	O	0	0
			527	527		
2	B	493	Total	O	0	0
			493	493		
2	C	518	Total	O	0	0
			518	518		
2	D	447	Total	O	0	0
			447	447		

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $RSRZ > 2$ ). 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:
- 
- 90% 9%
- MSE THR MSE MSE THR A46 T77 Q29 V50 R53 L64 S93 G104 M107 L127 G128 F138 P139 L140 R141 Q142 Y143 L144 R145 M155 K160 H161 A162 P163 V208 V214 A219 Q223 L228 C231 V243 Q262 Q266 V276
- M297 E303 L307 A311 D317 Y347 P357 F362 R363 D388 E407 L448 V462

- Chain B:
- 
- 90% 8%
- 98%
- Residues: MSE, THR, MSE, THR, ALA, Q7, Q29, Q52, S93, L108, Q119, L127, Q128, I133, P139, L144, R145, H155, K160, H161, A162, R174, A191, V208, V214, L228, C231, E234, V243, Q266, V276, M297, A311, P317, Q322, K339, Y347, P357, F362, R363, Q364, K377, D402, E407, C414, E442, L448, N460, R461, V462.

- Chain C: 

- Chain D: 
- | Model | Category |
|-------|----------|
| NSE   | Green    |
| TTR   | Green    |
| NSE   | Green    |
| NSE   | Green    |
| TTR   | Green    |
| ALA   | Green    |
| TTR   | Green    |
| GLN   | Green    |
| A9    | Red      |
| M23   | Yellow   |
| Q29   | Red      |
| M79   | Green    |
| G80   | Green    |
| K31   | Yellow   |
| Q119  | Green    |
| L127  | Green    |
| G128  | Green    |
| V129  | Green    |
| P139  | Green    |
| R145  | Green    |
| H155  | Green    |
| S156  | Green    |
| H161  | Green    |
| A162  | Green    |
| V208  | Green    |
| V214  | Green    |
| A219  | Green    |
| Q223  | Green    |
| L228  | Green    |
| K229  | Green    |
| K230  | Green    |
| C231  | Green    |
| D239  | Green    |
| E250  | Green    |
| Y261  | Green    |
| Q262  | Green    |
| Q266  | Green    |
| R287  | Green    |
| L307  | Green    |

A311	D317	D322	D364	S394	I397	M408	C414	L443	M460	M461	M462
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	133.88Å 133.88Å 247.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 1.85 29.84 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.00-1.85) 99.8 (29.84-1.85)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.59 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.167 , 0.194 0.168 , 0.194	Depositor DCC
$R_{free}$ test set	10912 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.9	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 50.1	EDS
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 217377 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15906	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.65	0/3572	0.68	1/4825 (0.0%)
1	B	0.60	1/3533 (0.0%)	0.67	0/4775
1	C	0.63	0/3536	0.67	1/4780 (0.0%)
1	D	0.56	0/3482	0.65	0/4708
All	All	0.61	1/14123 (0.0%)	0.67	2/19088 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	377	LYS	CD-CE	5.41	1.64	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	363	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	C	215	ARG	CA-CB-CG	5.13	124.68	113.40

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	3523	0	3503	40	1
1	B	3482	0	3445	33	0
1	C	3485	0	3452	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3431	0	3406	40	0
2	A	527	0	0	4	2
2	B	493	0	0	3	1
2	C	518	0	0	7	3
2	D	447	0	0	8	1
All	All	15906	0	13806	135	4

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 5.

The worst 5 of 135 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:107:MSE:CE	1:A:448:LEU:HD22	1.47	1.43
1:A:107:MSE:HE3	1:A:448:LEU:CD2	1.68	1.22
1:D:414:CYS:HB3	2:D:749:HOH:O	1.45	1.15
1:A:317:ASP:OD2	1:C:317:ASP:OD2	1.69	1.08
1:B:234:GLU:HG3	1:B:442:GLU:OE2	1.56	1.06

All (4) 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)
1:A:303[B]:GLU:OE2	2:C:979:HOH:O[5_665]	1.88	0.32
2:A:598:HOH:O	2:C:979:HOH:O[5_665]	1.91	0.29
2:A:837:HOH:O	2:B:974:HOH:O[5_665]	1.99	0.21
2:C:1198:HOH:O	2:D:763:HOH:O[5_565]	2.08	0.12

## 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	470/462 (102%)	460 (98%)	10 (2%)	0	100	100
1	B	465/462 (101%)	453 (97%)	12 (3%)	0	100	100
1	C	465/462 (101%)	455 (98%)	10 (2%)	0	100	100
1	D	459/462 (99%)	448 (98%)	11 (2%)	0	100	100
All	All	1859/1848 (101%)	1816 (98%)	43 (2%)	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	350/325 (108%)	349 (100%)	1 (0%)	94	94
1	B	345/325 (106%)	345 (100%)	0	100	100
1	C	346/325 (106%)	345 (100%)	1 (0%)	94	94
1	D	340/325 (105%)	340 (100%)	0	100	100
All	All	1381/1300 (106%)	1379 (100%)	2 (0%)	95	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	C	8	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	266	GLN
1	B	364	GLN
1	D	266	GLN
1	B	321	GLN
1	C	119	GLN

### 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 [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	445/462 (96%)	-0.47	4 (0%) 85 85	12, 18, 26, 47	2 (0%)
1	B	444/462 (96%)	-0.35	4 (0%) 85 85	15, 21, 31, 45	2 (0%)
1	C	443/462 (95%)	-0.46	4 (0%) 85 85	12, 19, 27, 39	3 (0%)
1	D	442/462 (95%)	-0.40	2 (0%) 91 91	14, 23, 32, 38	4 (0%)
All	All	1774/1848 (95%)	-0.42	14 (0%) 87 87	12, 20, 30, 47	11 (0%)

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	8	GLN	4.9
1	C	462	VAL	4.7
1	B	7	THR	4.4
1	A	6	ALA	4.3
1	A	462	VAL	3.8

### 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.