



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2018 – 08:14 pm GMT

PDB ID : 3T5Y  
Title : Crystal structure of CerJ from Streptomyces tendae - malonic acid covalently linked to the catalytic Cystein C116  
Authors : Zocher, G.; Bretschneider, T.; Hertweck, C.; Stehle, T.  
Deposited on : 2011-07-28  
Resolution : 2.12 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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

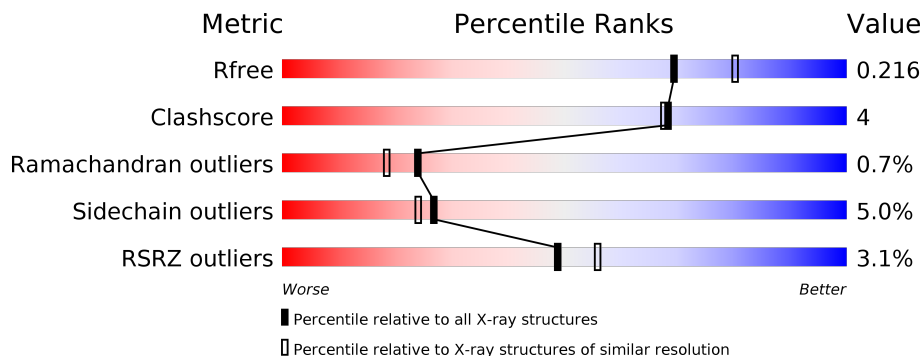
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.12 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))
$R_{free}$	111664	5449 (2.14-2.10)
Clashscore	122126	5972 (2.14-2.10)
Ramachandran outliers	120053	5914 (2.14-2.10)
Sidechain outliers	120020	5915 (2.14-2.10)
RSRZ outliers	108989	5321 (2.14-2.10)

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	357	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 5%; height: 10px; background-color: red;"></div> <div style="position: absolute; top: -10px; left: 5%; width: 83%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: -10px; left: 88%; width: 11%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: -10px; left: 99%; width: 4%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>83%</span> <span>11%</span> <span>• •</span> </div> </div>
2	B	357	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 5%; height: 10px; background-color: red;"></div> <div style="position: absolute; top: -10px; left: 5%; width: 83%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: -10px; left: 88%; width: 10%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: -10px; left: 99%; width: 4%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>5%</span> <span>83%</span> <span>10%</span> <span>• •</span> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5362 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 CerJ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	3	0
			2538	1592	457	481	8			

- Molecule 2 is a protein called CerJ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	342	Total	C	N	O	S	0	0	0
			2519	1577	455	479	8			

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



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		

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

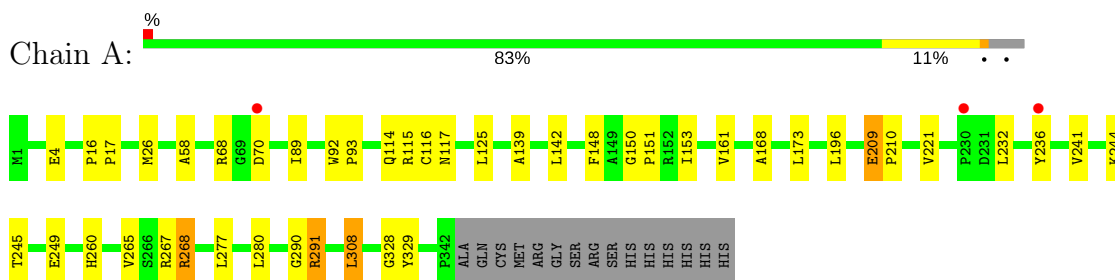
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	181	Total	O	0	0
			181	181		
4	B	112	Total	O	0	0
			112	112		

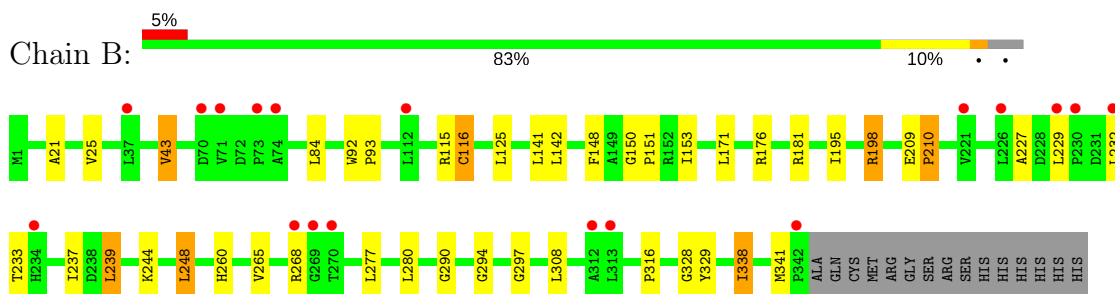
### 3 Residue-property plots [i](#)

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 ( $RSRZ > 2$ ). 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.

- Molecule 1: CerJ



- Molecule 2: CerJ



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.04Å 106.04Å 121.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.41 – 2.12 29.41 – 2.12	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.41-2.12) 99.8 (29.41-2.12)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.14 (at 2.12Å)	Xtriage
Refinement program	REFMAC - Rigid Body	Depositor
R, $R_{free}$	0.168 , 0.208 0.176 , 0.216	Depositor DCC
$R_{free}$ test set	1994 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.7	Xtriage
Anisotropy	0.532	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 47.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5362	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	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.*

<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

### 5.1 Standard geometry

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

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	0.72	0/2604	0.81	5/3556 (0.1%)
2	B	0.64	0/2561	0.79	2/3496 (0.1%)
All	All	0.68	0/5165	0.80	7/7052 (0.1%)

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	5
2	B	0	6
All	All	0	11

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	291	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	A	209	GLU	C-N-CD	-6.04	107.31	120.60
2	B	329	TYR	N-CA-CB	5.94	121.30	110.60
1	A	267	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	A	329	TYR	N-CA-CB	5.22	120.00	110.60

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	150	GLY	Mainchain,Peptide...

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Mol	Chain	Res	Type	Group
1	A	209	GLU	Peptide
1	A	328	GLY	Mainchain,Peptide
2	B	116	MCS	Mainchain
2	B	150	GLY	Mainchain

## 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	2538	0	2490	24	0
2	B	2519	0	2466	18	0
3	A	8	0	6	2	0
3	B	4	0	3	0	0
4	A	181	0	0	2	0
4	B	112	0	0	0	0
All	All	5362	0	4965	41	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 4.

The worst 5 of 41 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:114:GLN:NE2	1:A:117:ASN:HD22	1.70	0.90
2:B:43:VAL:HG22	2:B:294:GLY:HA3	1.70	0.72
1:A:114:GLN:HE21	1:A:117:ASN:HD22	1.41	0.69
2:B:229:LEU:HD12	2:B:232:LEU:CD1	2.24	0.67
1:A:277:LEU:O	1:A:277:LEU:HD23	1.94	0.66

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	343/357 (96%)	330 (96%)	10 (3%)	3 (1%)	19	13
2	B	339/357 (95%)	327 (96%)	10 (3%)	2 (1%)	27	22
All	All	682/714 (96%)	657 (96%)	20 (3%)	5 (1%)	24	18

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	210	PRO
2	B	210	PRO
1	A	115	ARG
1	A	151	PRO
2	B	151	PRO

### 5.3.2 Protein sidechains [i](#)

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	252/262 (96%)	242 (96%)	10 (4%)	34	33
2	B	247/261 (95%)	232 (94%)	15 (6%)	20	17
All	All	499/523 (95%)	474 (95%)	25 (5%)	27	24

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

Mol	Chain	Res	Type
2	B	125	LEU

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Mol	Chain	Res	Type
2	B	142	LEU
2	B	338	ILE
2	B	141	LEU
2	B	171	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	114	GLN
1	A	301	GLN
1	A	307	HIS
2	B	260	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	MCS	B	116	2	8,11,12	1.79	3 (37%)	5,13,15	8.01	5 (100%)

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	MCS	B	116	2	-	0/6/11/13	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	116	MCS	CAG-CAK	2.23	1.57	1.50
2	B	116	MCS	CAK-SAI	2.44	1.82	1.76
2	B	116	MCS	CA-C	2.96	1.54	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	116	MCS	O-C-CA	-2.97	116.81	124.96
2	B	116	MCS	OAC-CAK-CAG	-2.82	118.47	123.35
2	B	116	MCS	OAC-CAK-SAI	-2.06	119.80	122.60
2	B	116	MCS	CAG-CAK-SAI	6.79	121.55	113.58
2	B	116	MCS	CB-SAI-CAK	15.93	113.71	101.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	116	MCS	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

3 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
3	ACT	A	358	-	1,3,3	2.28	1 (100%)	0,3,3	0.00	-
3	ACT	A	359	-	1,3,3	1.86	0	0,3,3	0.00	-
3	ACT	B	358	-	1,3,3	1.63	0	0,3,3	0.00	-

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
3	ACT	A	358	-	-	0/0/0/0	0/0/0/0
3	ACT	A	359	-	-	0/0/0/0	0/0/0/0
3	ACT	B	358	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	358	ACT	CH3-C	2.28	1.51	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	358	ACT	1	0
3	A	359	ACT	1	0

## 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	342/357 (95%)	-0.07	3 (0%) 84 86	34, 44, 62, 78	0
2	B	341/357 (95%)	0.25	18 (5%) 26 32	33, 52, 76, 88	1 (0%)
All	All	683/714 (95%)	0.09	21 (3%) 49 56	33, 47, 71, 88	1 (0%)

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	342	PRO	4.1
1	A	70	ASP	3.8
2	B	230	PRO	3.7
2	B	269	GLY	3.6
2	B	70	ASP	3.6

### 6.2 Non-standard residues in protein, DNA, RNA chains [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(Å <sup>2</sup> )	Q<0.9
2	MCS	B	116	12/13	0.93	0.17	41,48,60,61	0

### 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(Å <sup>2</sup> )	Q<0.9
3	ACT	B	358	4/4	0.86	0.27	42,45,45,46	4
3	ACT	A	359	4/4	0.91	0.25	34,37,40,45	4
3	ACT	A	358	4/4	0.97	0.12	48,49,49,52	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.