

# wwPDB X-ray Structure Validation Summary Report (i)

#### Aug 20, 2023 – 06:41 AM EDT

PDB ID : 2HKL

Title : Crystal structure of Enterococcus faecium L,D-transpeptidase C442S mutant Authors : Delfosse, V.; Hugonnet, J.-E.; Magnet, S.; Mainardi, J.-L.; Arthur, M.; Mayer,

C.

Deposited on : 2006-07-05

Resolution : 2.60 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 (i) 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 (1)) were used in the production of this report:

 $Mol Probity \quad : \quad 4.02b\text{--}467$ 

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.35

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$ 

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

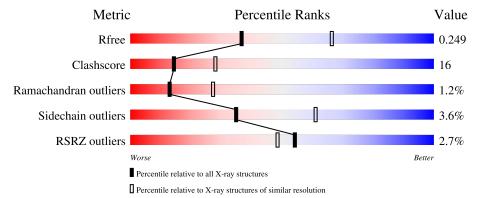
Validation Pipeline (wwPDB-VP) : 2.35

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$ 

The reported resolution of this entry is 2.60 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 <=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.

	Cham	Length	Quality of chain				
1	Δ	250	70%	26%			
1	11	200	70% 3%	20%	••		
1	В	250	67%	30%	•••		
1	$\mathbf{C}$	250	69%	28%			



# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6210 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.

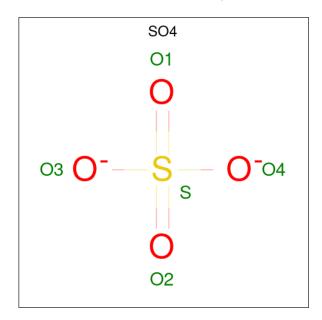
• Molecule 1 is a protein called L,D-TRANSPEPTIDASE.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	248	Total	С	N	О	S	0	0	0
1	A	240	1941	1231	313	391	6	U	0	
1	D	248	Total	С	N	О	S	0	0	0
1	В	240	1941	1231	313	391	6	U	U	
1	С	240	Total	С	N	О	S	0	0	0
	248	1941	1231	313	391	6	U	U		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	442	SER	CYS	engineered mutation	UNP Q3Y185
В	442	SER	CYS	engineered mutation	UNP Q3Y185
С	442	SER	CYS	engineered mutation	UNP Q3Y185

• Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	В	1	Total O S 5 4 1	0	0
2	С	1	Total O S 5 4 1	0	0

### • Molecule 3 is water.

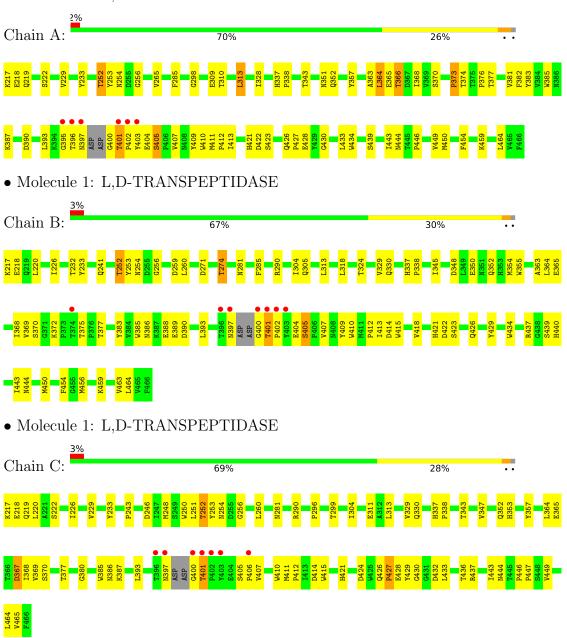
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	137	Total O 137 137	0	0
3	В	129	Total O 129 129	0	0
3	С	106	Total O 106 106	0	0



# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: L,D-TRANSPEPTIDASE





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	211.14Å 132.66Å 70.12Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $89.98^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	19.88 - 2.60	Depositor
resolution (A)	29.74 - 2.60	EDS
% Data completeness	89.4 (19.88-2.60)	Depositor
(in resolution range)	89.5 (29.74-2.60)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$< I/\sigma(I) > 1$	2.08 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
$R, R_{free}$	0.216 , $0.249$	Depositor
it, it free	0.210 , $0.249$	DCC
$R_{free}$ test set	2651 reflections $(5.00\%)$	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.0	Xtriage
Anisotropy	0.651	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.34, 45.8	EDS
L-test for twinning <sup>2</sup>	$< L > = 0.48, < L^2> = 0.31$	Xtriage
Estimated twinning fraction	0.028  for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6210	wwPDB-VP
Average B, all atoms $(Å^2)$	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.98% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $<L^2>$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

## 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: 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	
IVIOI	Moi Chain		# Z  > 5	RMSZ	# Z  > 5
1	A	0.36	0/1991	0.60	0/2716
1	В	0.35	0/1991	0.60	0/2716
1	С	0.35	0/1991	0.60	0/2716
All	All	0.35	0/5973	0.60	0/8148

There are no bond length outliers.

There are no bond angle outliers.

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	1941	0	1856	57	0
1	В	1941	0	1856	66	0
1	С	1941	0	1856	57	0
2	A	5	0	0	0	0
2	В	5	0	0	0	0
2	С	5	0	0	0	0
3	A	137	0	0	3	0
3	В	129	0	0	1	0
3	С	106	0	0	5	0
All	All	6210	0	5568	177	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 16.

The worst 5 of 177 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{aligned}$
1:C:407:VAL:HG11	1:C:421:HIS:HB2	1.38	1.03
1:B:407:VAL:HG21	1:B:421:HIS:HB2	1.54	0.87
1:A:407:VAL:HG11	1:A:421:HIS:HB2	1.56	0.87
1:C:352:GLN:NE2	1:C:370:SER:H	1.76	0.83
1:A:387:LYS:HG2	1:A:411:MET:HE2	1.64	0.80

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	Perce	entiles
1	A	244/250 (98%)	223 (91%)	16 (7%)	5 (2%)	7	14
1	В	244/250 (98%)	221 (91%)	21 (9%)	2 (1%)	19	39
1	С	244/250 (98%)	218 (89%)	24 (10%)	2 (1%)	19	39
All	All	732/750 (98%)	662 (90%)	61 (8%)	9 (1%)	13	27

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	401	THR
1	В	401	THR
1	С	401	THR
1	A	439	SER
1	В	405	SER



#### 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	214/218 (98%)	209 (98%)	5 (2%)	50 75		
1	В	214/218 (98%)	209 (98%)	5 (2%)	50 75		
1	С	214/218 (98%)	201 (94%)	13 (6%)	18 38		
All	All	642/654 (98%)	619 (96%)	23 (4%)	35 61		

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	С	252	THR
1	С	367	ASP
1	С	330	GLN
1	С	424	ASP
1	В	252	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	С	353	HIS
1	С	352	GLN
1	В	337	HIS
1	С	337	HIS
1	В	330	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 monosaccharides 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 Typ	Type	Chain	Res	Link	Bond lengths			Bond angles		
	туре	Chain			Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
2	SO4	В	2	-	4,4,4	0.24	0	6,6,6	0.06	0
2	SO4	С	3	-	4,4,4	0.24	0	6,6,6	0.04	0
2	SO4	A	1	-	4,4,4	0.26	0	6,6,6	0.08	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,  $95^{th}$  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 $>$	$\#\mathrm{RSRZ}{>}2$		$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q < 0.9
1	A	$248/250 \ (99\%)$	-0.30	6 (2%) 59	53	31, 46, 76, 97	0
1	В	248/250 (99%)	-0.25	7 (2%) 53	46	30, 46, 77, 104	0
1	С	248/250 (99%)	-0.25	7 (2%) 53	46	32, 50, 81, 105	0
All	All	744/750 (99%)	-0.27	20 (2%) 54	48	30, 47, 80, 105	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type	RSRZ
1	В	401	THR	4.6
1	В	403	TYR	4.4
1	В	402	PRO	4.2
1	A	402	PRO	4.1
1	С	401	THR	3.9

## 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,  $95^{th}$  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	$\mathbf{B} ext{-}\mathbf{factors}(\mathring{\mathbf{A}}^2)$	Q < 0.9
2	SO4	В	2	5/5	0.97	0.12	73,74,75,75	0
2	SO4	С	3	5/5	0.98	0.11	80,81,82,82	0
2	SO4	A	1	5/5	0.99	0.11	79,80,80,80	0

# 6.5 Other polymers (i)

There are no such residues in this entry.

