



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 02:40 am BST

PDB ID : 4IYA  
Title : Structure of the Y250A mutant of the PANTON-VALENTINE LEUCOCIDIN  
S component from STAPHYLOCOCCUS AUREUS  
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Deposited on : 2013-01-28  
Resolution : 1.55 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

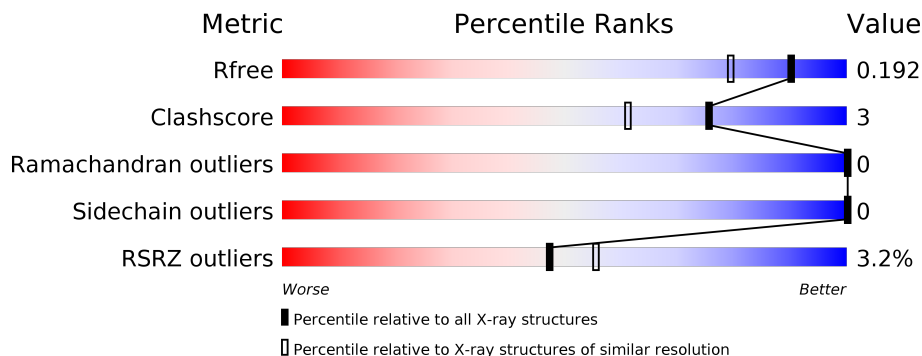
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.55 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	1483 (1.56-1.56)
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (1.56-1.56)

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	292	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2640 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.

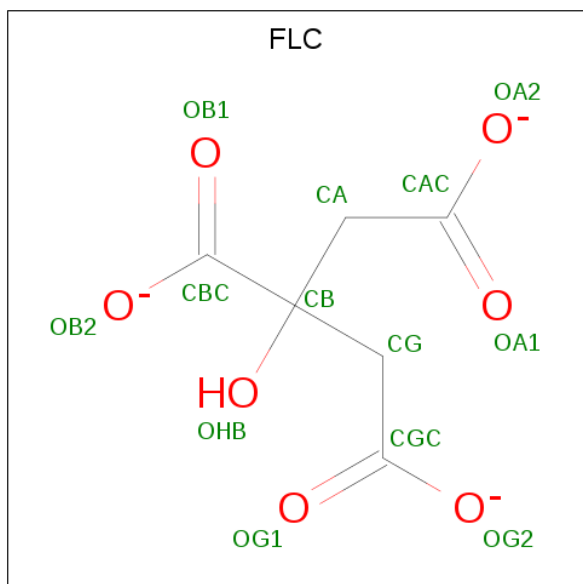
- Molecule 1 is a protein called LukS-PV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	283	2300	1447	398	450	5	0	7	0

There are 9 discrepancies between the modelled and reference sequences:

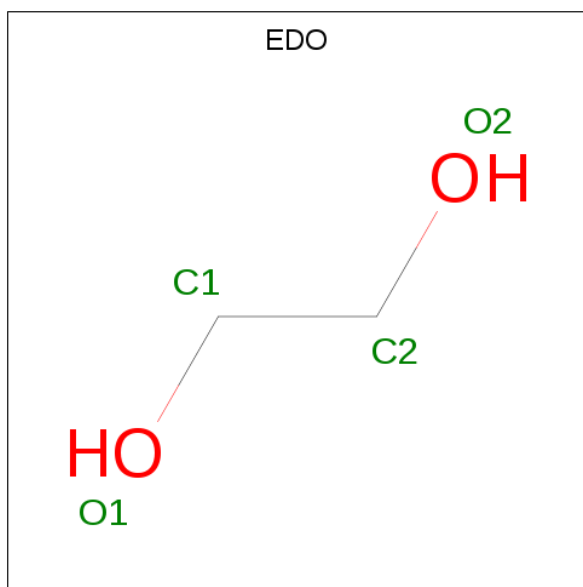
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	EXPRESSION TAG	UNP O80066
A	-6	PRO	-	EXPRESSION TAG	UNP O80066
A	-5	LEU	-	EXPRESSION TAG	UNP O80066
A	-4	GLY	-	EXPRESSION TAG	UNP O80066
A	-3	SER	-	EXPRESSION TAG	UNP O80066
A	-2	PRO	-	EXPRESSION TAG	UNP O80066
A	-1	GLU	-	EXPRESSION TAG	UNP O80066
A	0	PHE	-	EXPRESSION TAG	UNP O80066
A	250	ALA	TYR	ENGINEERED MUTATION	UNP O80066

- Molecule 2 is CITRATE ANION (three-letter code: FLC) (formula: C<sub>6</sub>H<sub>5</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	A	1	Total	C	O	0	1
			26	12	14		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

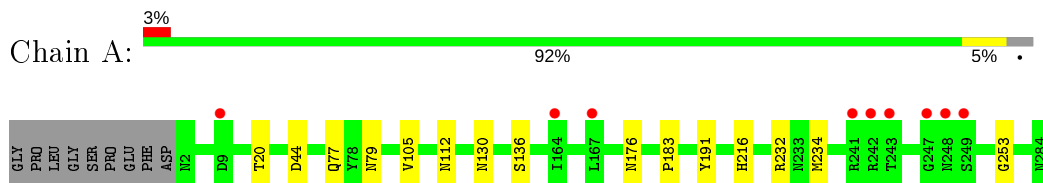
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	297	Total	O	0	0
			297	297		

### 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: LukS-PV



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.34Å 89.32Å 38.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.69 – 1.55 34.79 – 1.55	Depositor EDS
% Data completeness (in resolution range)	99.8 (22.69-1.55) 99.7 (34.79-1.55)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.91 (at 1.55Å)	Xtrriage
Refinement program	BUSTER 2.10.0	Depositor
R, $R_{free}$	0.165 , 0.189 0.166 , 0.192	Depositor DCC
$R_{free}$ test set	2161 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.0	Xtrriage
Anisotropy	0.451	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 55.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.014 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	2640	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.60% 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: FLC, EDO

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	0.49	0/2358	0.65	0/3197

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	2300	0	2147	11	0
2	A	39	0	15	3	0
3	A	4	0	6	0	0
4	A	297	0	0	2	0
All	All	2640	0	2168	14	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 3.

All (14) 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)
2:A:302[A]:FLC:CBC	2:A:302[A]:FLC:OG1	2.43	0.67
1:A:112:ASN:HA	1:A:130:ASN:HD22	1.62	0.64
1:A:20[B]:THR:HG22	4:A:623:HOH:O	2.09	0.53
1:A:232:ARG:HD3	1:A:234[B]:MET:SD	2.51	0.51
1:A:176:ASN:ND2	1:A:253:GLY:H	2.09	0.49
1:A:216:HIS:HE1	4:A:446:HOH:O	1.96	0.49
1:A:232:ARG:CD	1:A:234[B]:MET:SD	3.05	0.44
1:A:77:GLN:HE21	1:A:79:ASN:ND2	2.16	0.44
1:A:44:ASP:OD2	1:A:216:HIS:HD2	2.01	0.43
1:A:176:ASN:HD21	1:A:253:GLY:H	1.66	0.42
1:A:183:PRO:HB3	1:A:191:TYR:CE1	2.55	0.42
2:A:302[A]:FLC:OG1	2:A:302[A]:FLC:OB1	2.37	0.42
1:A:105:VAL:O	1:A:136:SER:HA	2.20	0.41
2:A:302[B]:FLC:OHB	2:A:302[B]:FLC:OG2	2.31	0.41

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	288/292 (99%)	278 (96%)	10 (4%)	0	100 100

There are no Ramachandran outliers to report.

### 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	249/259 (96%)	249 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	79	ASN
1	A	104	ASN
1	A	126	ASN
1	A	130	ASN
1	A	176	ASN
1	A	216	HIS
1	A	276	HIS

### 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](#)

4 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
2	FLC	A	302[A]	-	3,12,12	0.63	0	3,17,17	0.39	0
2	FLC	A	301	-	3,12,12	0.52	0	3,17,17	0.81	0
2	FLC	A	302[B]	-	3,12,12	0.51	0	3,17,17	0.16	0
3	EDO	A	303	-	3,3,3	0.72	0	2,2,2	0.38	0

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	FLC	A	302[A]	-	-	3/6/16/16	-
2	FLC	A	301	-	-	1/6/16/16	-
2	FLC	A	302[B]	-	-	3/6/16/16	-
3	EDO	A	303	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	302[A]	FLC	CBC-CB-CG-CGC
2	A	302[B]	FLC	CBC-CB-CG-CGC
2	A	302[A]	FLC	OHB-CB-CG-CGC
2	A	302[B]	FLC	CA-CB-CG-CGC
2	A	302[B]	FLC	OHB-CB-CG-CGC
2	A	301	FLC	OHB-CB-CG-CGC
2	A	302[A]	FLC	CA-CB-CG-CGC

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	302[A]	FLC	2	0
2	A	302[B]	FLC	1	0

## 5.7 Other polymers

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 [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	283/292 (96%)	-0.11	9 (3%) 47 55	11, 18, 32, 52	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	247	GLY	5.2
1	A	243	THR	4.6
1	A	167	LEU	3.6
1	A	248	ASN	3.5
1	A	241	ARG	3.4
1	A	242	ARG	3.3
1	A	249	SER	3.0
1	A	9	ASP	2.1
1	A	164	ILE	2.0

### 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	FLC	A	302[A]	13/13	0.86	0.20	67,68,68,68	13
2	FLC	A	302[B]	13/13	0.86	0.20	11,19,24,24	13
3	EDO	A	303	4/4	0.91	0.09	20,23,28,33	0
2	FLC	A	301	13/13	0.96	0.08	14,17,19,20	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.