



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 14, 2025 – 02:06 PM EDT

PDB ID : 9BSH / pdb\_00009bsh  
Title : Staphylococcus aureus exfoliative toxin A D164A variant  
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Deposited on : 2024-05-13  
Resolution : 1.35 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

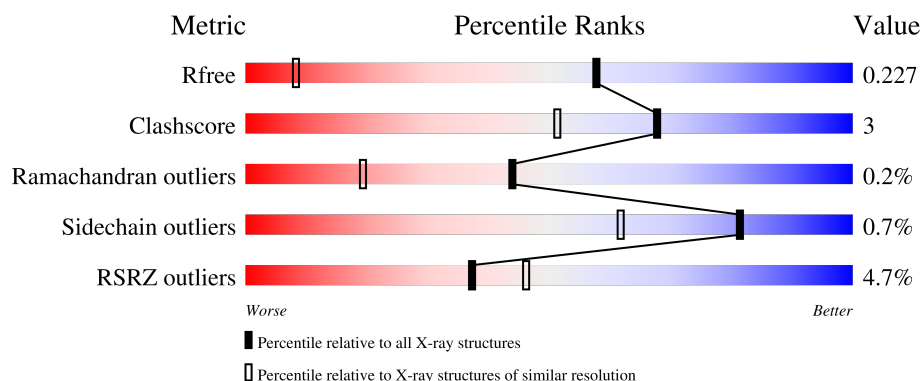
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.35 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))
$R_{free}$	164625	1089 (1.36-1.36)
Clashscore	180529	1157 (1.36-1.36)
Ramachandran outliers	177936	1146 (1.36-1.36)
Sidechain outliers	177891	1146 (1.36-1.36)
RSRZ outliers	164620	1088 (1.36-1.36)

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  $\geq 3$ , 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	280	
1	B	280	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4812 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 Exfoliative toxin A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	10	0
			1955	1236	337	381	1			
1	B	243	Total	C	N	O	S	0	7	0
			1950	1232	340	377	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	LYS	ASN	conflict	UNP P09331
A	202	ALA	ASP	engineered mutation	UNP P09331
B	34	LYS	ASN	conflict	UNP P09331
B	202	ALA	ASP	engineered mutation	UNP P09331

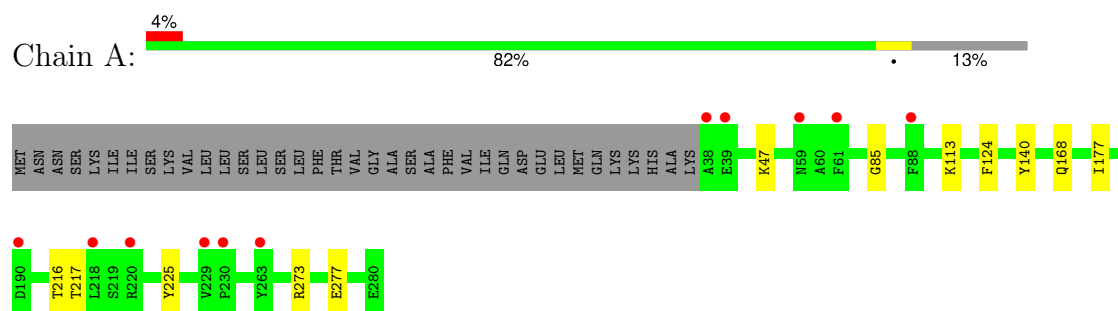
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	472	Total	O	0	0
			472	472		
2	B	435	Total	O	0	0
			435	435		

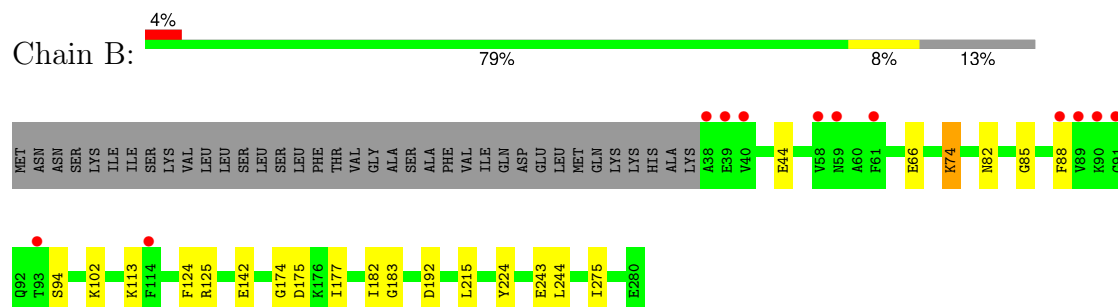
### 3 Residue-property plots [i](#)

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: Exfoliative toxin A



- Molecule 1: Exfoliative toxin A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.55Å 66.54Å 81.81Å 90.00° 94.17° 90.00°	Depositor
Resolution (Å)	51.57 – 1.35 51.57 – 1.35	Depositor EDS
% Data completeness (in resolution range)	96.4 (51.57-1.35) 96.4 (51.57-1.35)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.36 (at 1.35Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, $R_{free}$	0.199 , 0.227 0.199 , 0.227	Depositor DCC
$R_{free}$ test set	5740 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	11.5	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 35.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4812	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.01 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6673e-03.*

<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

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	0.37	0/2020	0.65	0/2724
1	B	0.38	0/2010	0.67	0/2708
All	All	0.37	0/4030	0.66	0/5432

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

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	1955	0	1960	10	0
1	B	1950	0	1944	17	0
2	A	472	0	0	4	0
2	B	435	0	0	8	0
All	All	4812	0	3904	27	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 (27) 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:216[B]:THR:HG21	1:A:225:TYR:HE2	1.35	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216[B]:THR:HG21	1:A:225:TYR:CE2	2.15	0.81
1:B:66:GLU:OE2	2:B:301:HOH:O	2.13	0.64
1:A:113:LYS:NZ	2:A:304:HOH:O	2.28	0.59
1:B:44[A]:GLU:OE1	2:B:302:HOH:O	2.18	0.56
1:B:88[B]:PHE:HD1	1:B:94:SER:HB3	1.74	0.52
1:A:168:GLN:HG2	2:A:471:HOH:O	2.10	0.52
1:A:47[A]:LYS:NZ	2:A:314:HOH:O	2.41	0.51
1:B:175:ASP:OD2	2:B:303:HOH:O	2.19	0.51
1:B:88[B]:PHE:CD1	1:B:94:SER:HB3	2.48	0.49
1:B:243:GLU:HB3	2:B:304:HOH:O	2.15	0.47
1:B:183:GLY:HA3	2:B:304:HOH:O	2.14	0.47
1:B:74:LYS:NZ	2:B:326:HOH:O	2.47	0.46
1:A:140:TYR:CE1	1:A:177[A]:ILE:HD11	2.51	0.45
1:B:85:GLY:HA3	1:B:124:PHE:CZ	2.53	0.44
1:B:192:ASP:HB2	1:B:215:LEU:HD12	2.00	0.43
1:B:244:LEU:O	2:B:304:HOH:O	2.21	0.43
1:A:85:GLY:HA3	1:A:124:PHE:CZ	2.54	0.43
1:B:74:LYS:CE	1:B:74:LYS:H	2.33	0.42
1:B:142:GLU:OE1	2:B:305:HOH:O	2.21	0.42
1:B:82:ASN:O	1:B:177:ILE:HG21	2.19	0.42
1:B:102:LYS:HA	1:B:174:GLY:HA3	2.01	0.42
1:A:47[B]:LYS:HD3	2:A:744:HOH:O	2.19	0.42
1:A:177[A]:ILE:HD13	1:A:177[A]:ILE:HA	1.88	0.41
1:A:273:ARG:O	1:A:277:GLU:HG3	2.20	0.41
1:B:182:ILE:HD13	1:B:275:ILE:HG21	2.03	0.40
1:B:215:LEU:HD23	1:B:224:TYR:HB3	2.04	0.40

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	251/280 (90%)	243 (97%)	6 (2%)	2 (1%)	16	3
1	B	248/280 (89%)	243 (98%)	5 (2%)	0	100	100
All	All	499/560 (89%)	486 (97%)	11 (2%)	2 (0%)	44	12

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	217[A]	THR
1	A	217[B]	THR

### 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	218/241 (90%)	218 (100%)	0	100	100
1	B	215/241 (89%)	211 (98%)	4 (2%)	52	21
All	All	433/482 (90%)	429 (99%)	4 (1%)	81	51

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	74	LYS
1	B	113[A]	LYS
1	B	113[B]	LYS
1	B	125	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	260	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 oligosaccharides 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

### 6.1 Protein, DNA and RNA chains

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	243/280 (86%)	0.35	11 (4%)	39 48	6, 13, 26, 52	10 (4%)
1	B	243/280 (86%)	0.37	12 (4%)	36 45	7, 13, 25, 44	7 (2%)
All	All	486/560 (86%)	0.36	23 (4%)	37 46	6, 13, 26, 52	17 (3%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	38	ALA	4.7
1	B	61	PHE	4.1
1	B	93	THR	3.7
1	A	88	PHE	3.5
1	A	220	ARG	3.5
1	A	38	ALA	3.5
1	B	114	PHE	3.1
1	A	39	GLU	2.8
1	A	61	PHE	2.7
1	B	39	GLU	2.5
1	B	40	VAL	2.5
1	B	90	LYS	2.4
1	B	88[A]	PHE	2.4
1	A	218	LEU	2.4
1	B	91	GLY	2.4
1	A	59	ASN	2.3
1	B	59	ASN	2.3
1	A	190	ASP	2.2
1	A	230	PRO	2.2
1	B	58	VAL	2.1
1	B	89	VAL	2.1
1	A	263	TYR	2.1
1	A	229	VAL	2.1

## 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.