



# Full wwPDB X-ray Structure Validation Report i

Feb 26, 2014 – 04:58 PM GMT

PDB ID : 3V8K  
Title : Crystal structure of Staphylococcus aureus biotin protein ligase in complex with biotin  
Authors : Yap, M.Y.; Pendini, N.R.  
Deposited on : 2011-12-23  
Resolution : 3.23 Å (reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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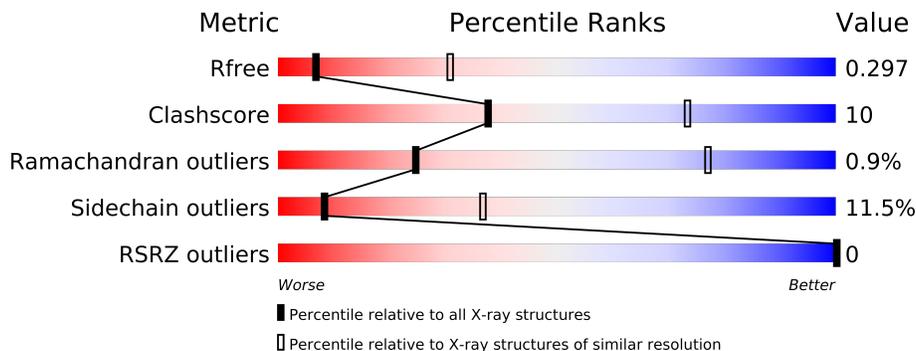
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance i

The reported resolution of this entry is 3.23 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))
$R_{free}$	66092	1080 (3.30-3.18)
Clashscore	79885	1369 (3.30-3.18)
Ramachandran outliers	78287	1342 (3.30-3.18)
Sidechain outliers	78261	1340 (3.30-3.18)
RSRZ outliers	66119	1081 (3.30-3.18)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	329	<span style="color: red;">█</span> <span style="color: orange;">█</span> <span style="color: yellow;">█</span> <span style="color: green;">█</span>

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 2651 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

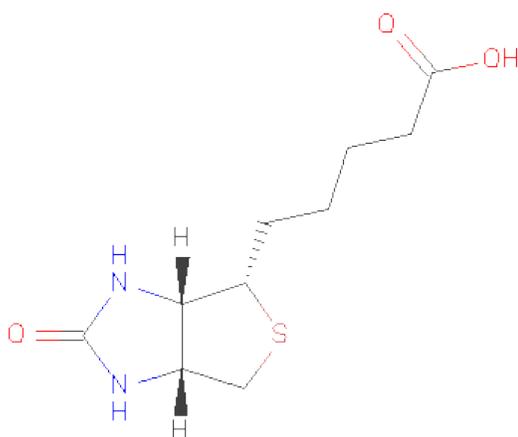
- Molecule 1 is a protein called Biotin ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	322	2610	1657	449	498	6	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	HIS	-	EXPRESSION TAG	UNP C8N5A9
A	-5	HIS	-	EXPRESSION TAG	UNP C8N5A9
A	-4	HIS	-	EXPRESSION TAG	UNP C8N5A9
A	-3	HIS	-	EXPRESSION TAG	UNP C8N5A9
A	-2	HIS	-	EXPRESSION TAG	UNP C8N5A9
A	-1	HIS	-	EXPRESSION TAG	UNP C8N5A9

- Molecule 2 is BIOTIN (three-letter code: BTN) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>2</sub>O<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	16	10	2	3	1	0	0

- Molecule 3 is water.

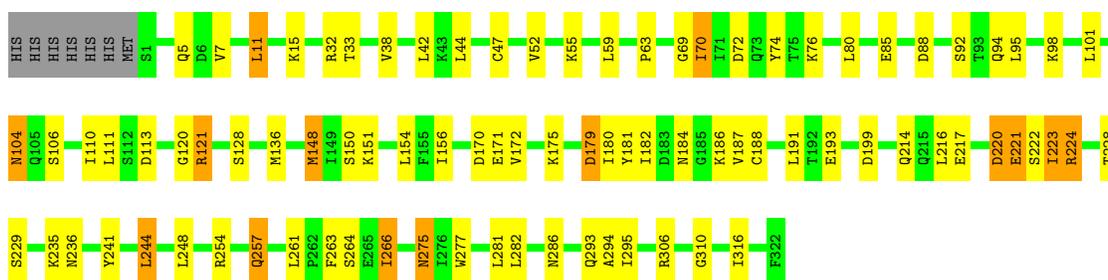
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	25	25	25	0	0

### 3 Residue-property plots

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.

- Molecule 1: Biotin ligase

Chain A:



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.27Å 94.27Å 130.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.80 – 3.23 19.80 – 3.23	Depositor EDS
% Data completeness (in resolution range)	98.7 (19.80-3.23) 98.8 (19.80-3.23)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.49 (at 3.22Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.202 , 0.268 0.274 , 0.297	Depositor DCC
$R_{free}$ test set	465 reflections (4.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	63.1	Xtrriage
Anisotropy	0.010	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 9.5	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Outliers	0 of 9798 reflections	Xtrriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	2651	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: BTN

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	0/2660	0.63	0/3587

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2610	0	2573	51	1
2	A	16	0	15	3	0
3	A	25	0	0	5	1
All	All	2651	0	2588	52	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (52) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:121:ARG:HG2	1:A:121:ARG:HH11	1.15	1.05

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:5:GLN:HE21	1:A:69:GLY:H	1.22	0.87
1:A:104:ASN:HD22	1:A:106:SER:H	1.26	0.82
1:A:15:LYS:HD3	3:A:615:HOH:O	1.79	0.82
1:A:121:ARG:CG	1:A:121:ARG:HH11	2.00	0.67
1:A:120:GLY:HA2	2:A:500:BTN:H92	1.78	0.65
1:A:217:GLU:HA	1:A:224:ARG:HH21	1.61	0.64
1:A:175:LYS:HD3	1:A:181:TYR:HE1	1.63	0.63
1:A:121:ARG:NH1	1:A:121:ARG:HG2	1.95	0.62
1:A:214:GLN:HB2	1:A:229:SER:HB3	1.81	0.62
1:A:151:LYS:HA	1:A:154:LEU:HD12	1.83	0.60
1:A:222:SER:HA	3:A:618:HOH:O	2.02	0.59
1:A:220:ASP:HB3	1:A:221:GLU:HG3	1.87	0.56
1:A:85:GLU:HB2	1:A:110:ILE:HG12	1.87	0.55
1:A:5:GLN:NE2	1:A:69:GLY:H	2.00	0.55
1:A:104:ASN:HD22	1:A:106:SER:N	2.02	0.53
1:A:171:GLU:HG2	3:A:612:HOH:O	2.07	0.53
1:A:98:LYS:HA	1:A:101:LEU:HD23	1.91	0.52
1:A:52:VAL:HG23	1:A:55:LYS:HB3	1.93	0.50
1:A:111:LEU:HD23	1:A:136:MET:HB2	1.92	0.50
1:A:281:LEU:HD11	1:A:294:ALA:HB2	1.95	0.49
1:A:120:GLY:CA	2:A:500:BTN:H92	2.43	0.48
1:A:94:GLN:NE2	1:A:193:GLU:OE1	2.47	0.48
1:A:104:ASN:ND2	1:A:106:SER:H	2.03	0.47
1:A:7:VAL:HG21	1:A:38:VAL:HG11	1.97	0.47
1:A:275:ASN:C	1:A:275:ASN:HD22	2.17	0.47
1:A:52:VAL:CG2	1:A:55:LYS:HB3	2.45	0.47
1:A:92:SER:HB3	1:A:95:LEU:HG	1.96	0.46
1:A:257:GLN:HG2	1:A:261:LEU:HD12	1.96	0.46
1:A:175:LYS:HD3	1:A:181:TYR:CE1	2.46	0.46
1:A:42:LEU:O	1:A:47:CYS:HB2	2.15	0.46
1:A:221:GLU:HA	1:A:222:SER:HA	1.62	0.46
1:A:148:MET:HG3	3:A:602:HOH:O	2.17	0.44
1:A:244:LEU:HD22	1:A:248:LEU:HG	1.98	0.44
1:A:74:TYR:N	1:A:74:TYR:CD1	2.85	0.44
1:A:74:TYR:H	1:A:74:TYR:HD1	1.65	0.44
1:A:172:VAL:HG22	1:A:182:ILE:HG12	2.00	0.44
1:A:148:MET:HG2	3:A:619:HOH:O	2.19	0.43
1:A:223:ILE:H	1:A:223:ILE:HG13	1.55	0.42
1:A:121:ARG:CG	1:A:121:ARG:NH1	2.70	0.42
1:A:150:SER:HB3	1:A:316:ILE:HD11	2.00	0.42
1:A:263:PHE:O	1:A:266:ILE:N	2.53	0.42
1:A:306:ARG:NH1	1:A:310:GLY:HA2	2.35	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:500:BTN:HN2	2:A:500:BTN:H72	1.61	0.41
1:A:263:PHE:O	1:A:264:SER:C	2.57	0.41
1:A:69:GLY:O	1:A:72:ASP:HB2	2.20	0.41
1:A:179:ASP:OD1	1:A:186:LYS:NZ	2.45	0.41
1:A:180:ILE:O	1:A:187:VAL:HG12	2.21	0.41
1:A:187:VAL:HA	1:A:228:THR:O	2.21	0.41
1:A:70:ILE:HG12	1:A:241:TYR:CE2	2.56	0.40
1:A:88:ASP:O	1:A:113:ASP:HB2	2.22	0.40
1:A:11:LEU:HD12	1:A:11:LEU:HA	1.82	0.40

All (1) 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	Distance(Å)	Clash(Å)
1:A:286:ASN:O	3:A:617:HOH:O[6_555]	2.15	0.05

## 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	320/329 (97%)	287 (90%)	30 (9%)	3 (1%)	25 77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	220	ASP
1	A	224	ARG
1	A	63	PRO

### 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	287/295 (97%)	254 (88%)	33 (12%)	8 37

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	32	ARG
1	A	33	THR
1	A	44	LEU
1	A	59	LEU
1	A	70	ILE
1	A	76	LYS
1	A	80	LEU
1	A	104	ASN
1	A	121	ARG
1	A	128	SER
1	A	148	MET
1	A	156	ILE
1	A	170	ASP
1	A	179	ASP
1	A	184	ASN
1	A	188	CYS
1	A	191	LEU
1	A	199	ASP
1	A	216	LEU
1	A	221	GLU
1	A	223	ILE
1	A	235	LYS
1	A	236	ASN
1	A	244	LEU
1	A	254	ARG
1	A	257	GLN
1	A	266	ILE
1	A	275	ASN
1	A	277	TRP
1	A	282	LEU
1	A	293	GLN
1	A	295	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	68	GLN
1	A	104	ASN
1	A	123	ASN
1	A	143	ASN
1	A	178	ASN
1	A	184	ASN
1	A	211	ASN
1	A	275	ASN

### 5.3.3 RNA [i](#)

There are no RNA chains 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](#)

1 ligand 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	BTN	A	500	-	17,17,17	1.71	2 (11%)	23,23,23	1.85	3 (13%)

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	BTN	A	500	-	-	0/7/28/28	0/0/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	BTN	C10-C11	-5.32	1.36	1.50
2	A	500	BTN	C2-S1	-2.33	1.78	1.82

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	BTN	C2-C4-N2	-5.84	104.97	113.27
2	A	500	BTN	C6-C5-N1	-4.45	104.31	112.56
2	A	500	BTN	C9-C10-C11	3.13	123.05	114.51

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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

### 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	322/329 (97%)	0.02	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	30, 52, 71, 86	0

There are no RSRZ outliers to report.

### 6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates

There are no carbohydrates in this entry.

### 6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	BTN	A	500	16/16	0.19	-0.06	33,35,45,45	0

### 6.5 Other polymers

There are no such residues in this entry.