



# wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 03:39 PM GMT

PDB ID : 2ONJ  
Title : Structure of the multidrug ABC transporter Sav1866 from *S. aureus* in complex with AMP-PNP  
Authors : Dawson, R.J.P.; Locher, K.P.  
Deposited on : 2007-01-24  
Resolution : 3.40 Å(reported)

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

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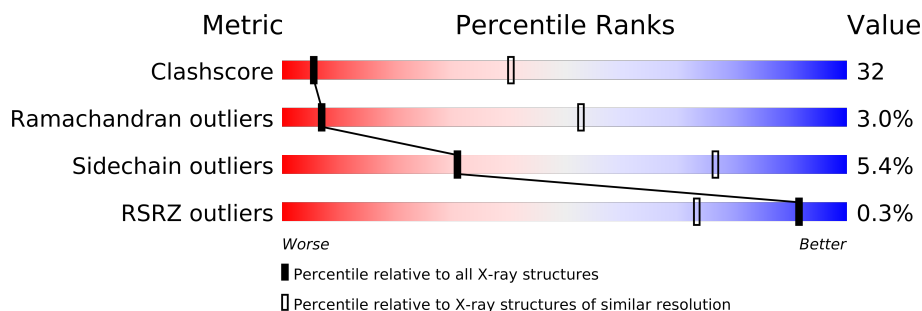
The following versions of software and data (see [references](#)) were used in the production of this report:

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

The reported resolution of this entry is 3.40 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))
Clashscore	79885	1214 (3.50-3.30)
Ramachandran outliers	78287	1177 (3.50-3.30)
Sidechain outliers	78261	1177 (3.50-3.30)
RSRZ outliers	66119	1017 (3.52-3.28)

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	578	
1	B	578	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9254 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.

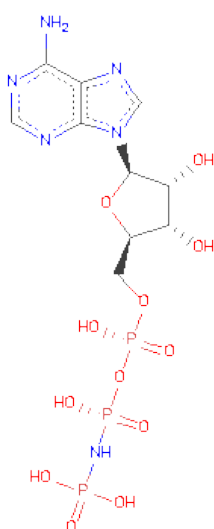
- Molecule 1 is a protein called Multidrug export ATP-binding/permease protein SAV1866.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	578	Total	C	N	O	S	0	0	0
			4584	2967	774	834	9			
1	B	578	Total	C	N	O	S	0	0	0
			4584	2967	774	834	9			

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Na	0	0
			2	2		
2	A	2	Total	Na	0	0
			2	2		

- Molecule 3 is PHOSPHOAMINOPHOSPHONICACID-ADENYLATE ESTER (three-letter code: ANP) (formula:  $C_{10}H_{17}N_6O_{12}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 4 is water.

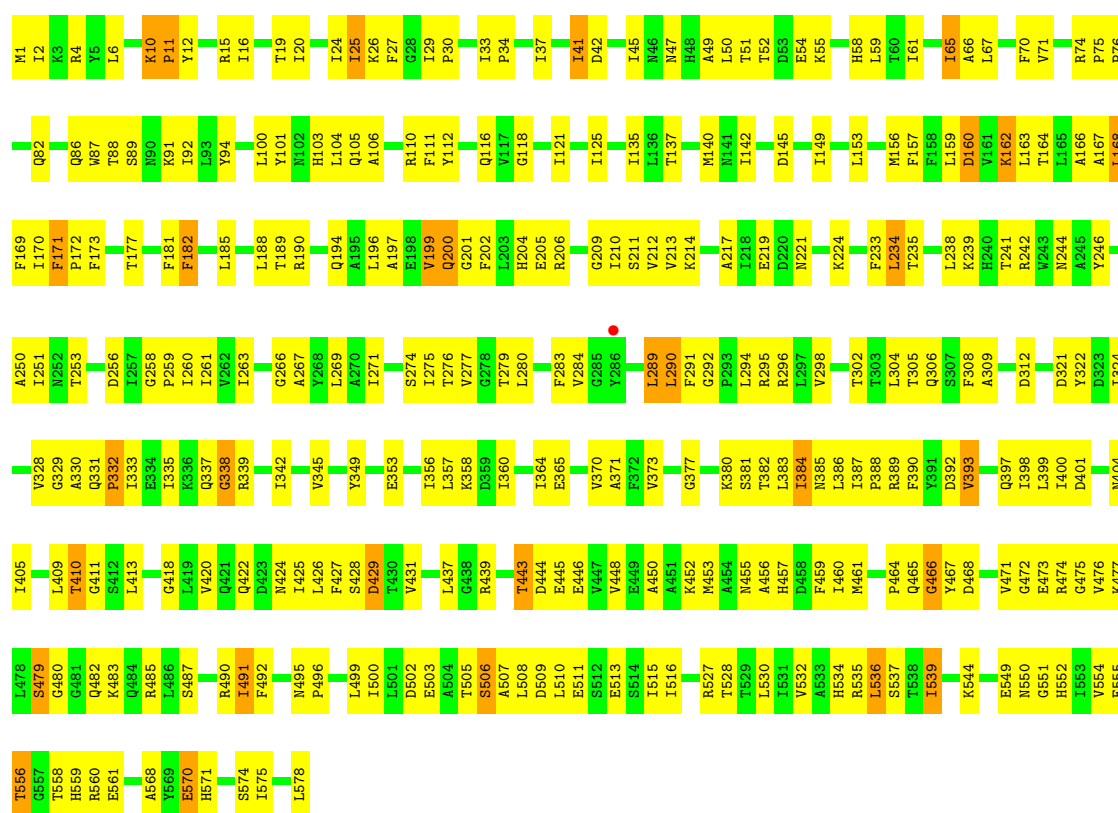
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total	O	0	0
			10	10		
4	B	10	Total	O	0	0
			10	10		

### 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.

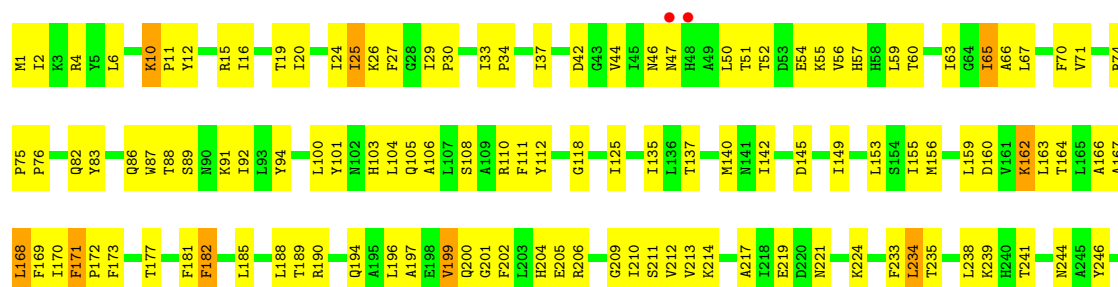
- Molecule 1: Multidrug export ATP-binding/permease protein SAV1866

Chain A:



- Molecule 1: Multidrug export ATP-binding/permease protein SAV1866

Chain B:



G551	E473	L399	D323	A250
H552	R474	I400	I324	I251
T553	G475	D401		T252
V554	V476		V328	T253
E555	K477	N404	G329	
T556	L478	I405	A330	
G557	S479	L409	Q331	
T558	G481	G480	P332	I257
H559	G482	T410	I333	G258
E560	K483	G411	E334	P259
E561	Q484	L412	I335	I260
	R485	L413	K336	V261
A568	L486	G418	Q337	I263
V569	S487	L419	G338	G264
E570		V420	R339	V265
H571	R490	Q421	I342	G266
I575	I491	D422		A267
	F492	D423	V345	Y268
		D424		L269
N495		I425	Y349	A270
P496		L426		I271
		F427	E353	S272
L499		S428		G273
I500		D429	I356	S274
L501		T430	I357	I275
D502		V431	K358	T276
E503			D559	V277
A504		L437	I360	G278
T505		G438	I364	T279
S506		R439	E365	L280
A507		T443		F283
L508		D444	E368	
D509		E445	T369	Y286
E510		E446	V370	L287
S512		V447	A371	E288
E513		V448	P372	L289
S514		E449	V373	L290
I515		A450		F291
I516		K451	G377	G292
		K452	G378	P293
R527		M453	G379	L294
T528		A454	K380	R295
T529		N455	S381	P296
L530		A456	T382	L297
I531		H457	L383	V298
V532		D458	I384	
A533		F459	N385	T302
H534		I460	L386	T303
R535		M461	T387	L304
L536			P388	T305
S537		P464	R389	Q306
T538		T538	F390	S307
I539		G466	Y391	F308
		Y467	D392	A309
K544		D468	V393	
				D312
E549		V471	Q397	
N550		G472	I398	D321
				Y322

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	160.96Å 104.45Å 181.39Å 90.00° 98.23° 90.00°	Depositor
Resolution (Å)	20.00 – 3.40 29.59 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-3.40) 99.9 (29.59-3.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.58 (at 3.39Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.254 , 0.278 0.255 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	101.1	Xtriage
Anisotropy	0.613	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 87.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 41082 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9254	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.42	0/4669	0.66	1/6328 (0.0%)
1	B	0.42	0/4669	0.67	1/6328 (0.0%)
All	All	0.42	0/9338	0.67	2/12656 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	234	LEU	CA-CB-CG	6.64	130.56	115.30
1	A	234	LEU	CB-CG-CD1	-5.28	102.03	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 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	4584	0	4713	327	0
1	B	4584	0	4714	332	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	31	0	12	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	31	0	12	9	0
4	A	10	0	0	3	0
4	B	10	0	0	3	0
All	All	9254	0	9451	598	0

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 32.

The worst 5 of 598 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:15:ARG:HD2	1:A:15:ARG:H	1.05	1.19
1:A:52:THR:HA	1:A:55:LYS:HE2	1.18	1.17
1:A:94:TYR:CD1	1:B:234:LEU:HD21	1.79	1.16
1:A:234:LEU:HD21	1:B:94:TYR:CD1	1.84	1.13
1:A:94:TYR:CD1	1:B:234:LEU:CD2	2.36	1.08

There are no symmetry-related clashes.

## 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	576/578 (100%)	463 (80%)	95 (16%)	18 (3%)	7	52
1	B	576/578 (100%)	458 (80%)	102 (18%)	16 (3%)	8	54
All	All	1152/1156 (100%)	921 (80%)	197 (17%)	34 (3%)	7	53

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	ILE
1	A	338	GLY
1	A	506	SER
1	B	25	ILE
1	B	182	PHE

### 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	499/499 (100%)	473 (95%)	26 (5%)	32	77
1	B	499/499 (100%)	471 (94%)	28 (6%)	30	75
All	All	998/998 (100%)	944 (95%)	54 (5%)	31	77

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	556	THR
1	B	199	VAL
1	B	536	LEU
1	A	570	GLU
1	B	82	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	465	GLN
1	B	47	ASN
1	B	397	GLN
1	A	397	GLN
1	A	455	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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	ANP	A	701	2	33,33,33	5.67	25 (75%)	51,52,52	3.92	22 (43%)
3	ANP	B	700	2	33,33,33	5.73	22 (66%)	51,52,52	3.95	23 (45%)

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	ANP	A	701	2	-	0/18/38/38	0/1/3/3
3	ANP	B	700	2	-	0/18/38/38	0/1/3/3

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	ANP	PG-O1G	16.41	1.66	1.46
3	B	700	ANP	PG-O1G	15.22	1.65	1.46
3	B	700	ANP	PB-N3B	14.74	1.77	1.64
3	A	701	ANP	PB-O3A	12.10	1.76	1.59
3	B	700	ANP	PB-O3A	12.06	1.76	1.59

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	ANP	C4'-O4'-C1'	-16.26	92.08	109.75
3	B	700	ANP	C4'-O4'-C1'	-15.86	92.53	109.75
3	A	701	ANP	PB-N3B-PG	-10.61	112.22	130.07
3	B	700	ANP	PB-N3B-PG	-10.39	112.59	130.07
3	B	700	ANP	N3-C2-N1	-10.39	120.03	128.71

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	578/578 (100%)	-0.22	1 (0%) 93 77	55, 120, 187, 200	0
1	B	578/578 (100%)	-0.23	3 (0%) 88 61	52, 117, 194, 200	0
All	All	1156/1156 (100%)	-0.22	4 (0%) 91 73	52, 119, 189, 200	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	286	TYR	2.4
1	B	48	HIS	2.3
1	B	47	ASN	2.2
1	B	578	LEU	2.0

### 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( $\text{\AA}^2$ )	Q<0.9
2	NA	B	910	1/1	0.20	0.68	132,132,132,132	0
2	NA	A	900	1/1	0.19	-0.11	125,125,125,125	0
3	ANP	B	700	31/31	0.20	-0.34	74,74,74,74	0
2	NA	B	901	1/1	0.23	-0.44	64,64,64,64	0
3	ANP	A	701	31/31	0.19	-0.55	80,80,80,80	0
2	NA	A	911	1/1	0.15	-1.19	63,63,63,63	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.