



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 06:21 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 X-ray Structure 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/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

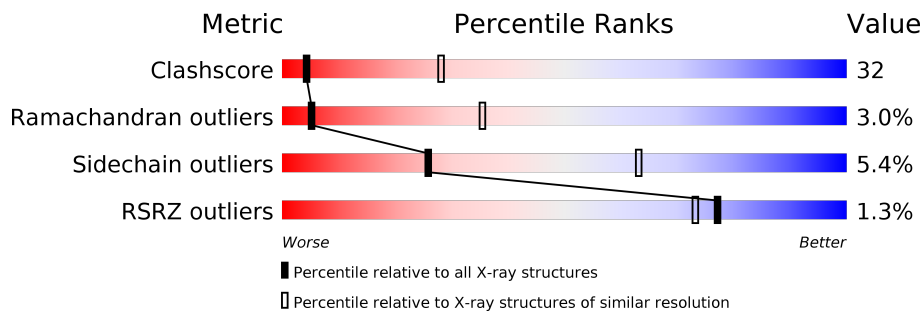
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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	112137	1832 (3.50-3.30)
Ramachandran outliers	110173	1789 (3.50-3.30)
Sidechain outliers	110143	1789 (3.50-3.30)
RSRZ outliers	101464	1709 (3.50-3.30)

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. 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	578	<div> <div>49%</div> <div>46%</div> <div>5%</div> </div>
1	B	578	<div> <div>48%</div> <div>48%</div> <div>5%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ANP	B	700	-	-	X	-

## 2 Entry composition [i](#)

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

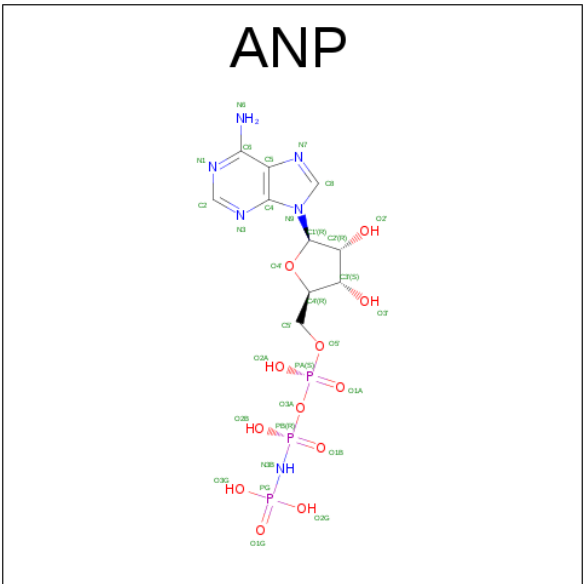
- Molecule 1 is a protein called Multidrug export ATP-binding/permease protein SAV1866.

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 PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).



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		

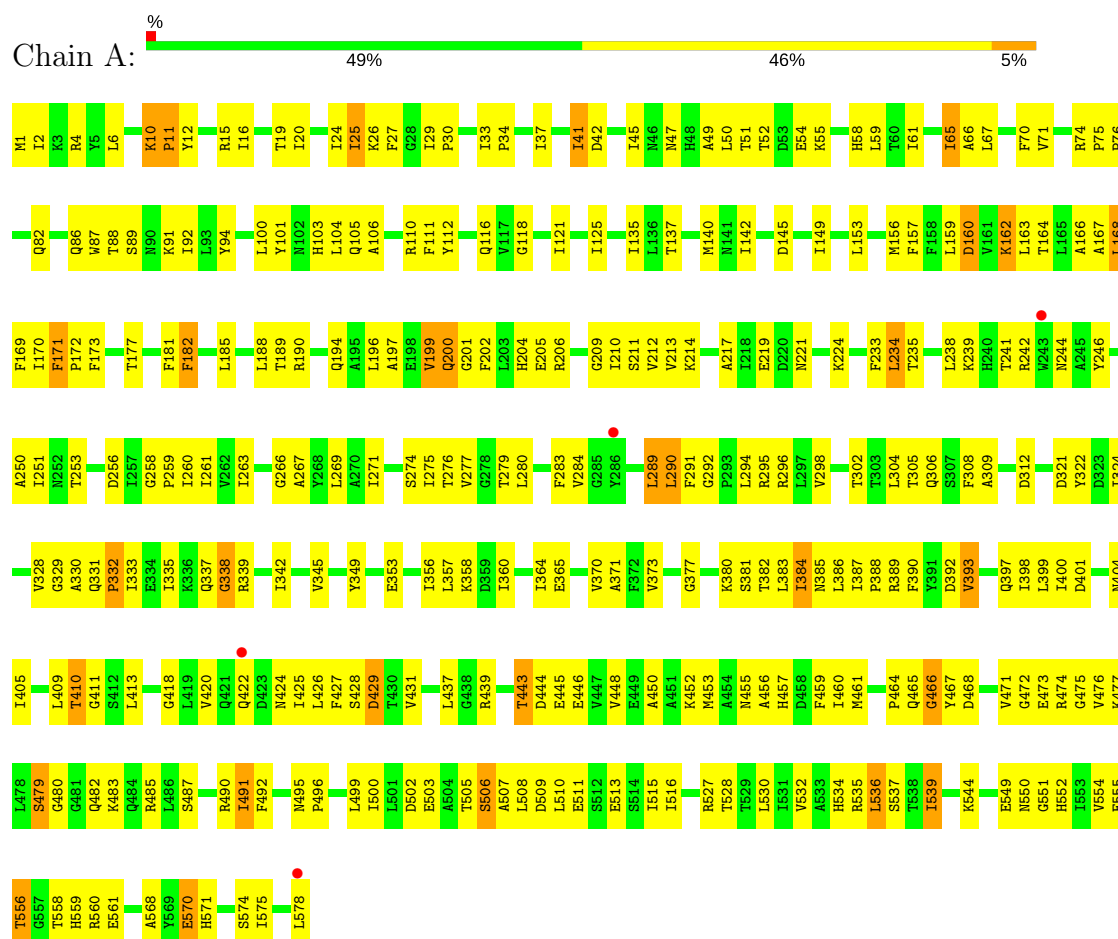
- Molecule 4 is water.

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

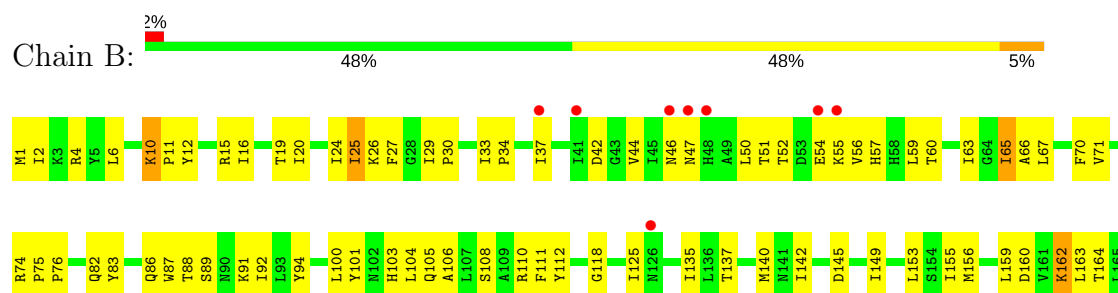
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Multidrug export ATP-binding/permease protein SAV1866



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



E549	W471	Q397	D321	Y246	A166
N550	C472	I398	Y322		A167
G551	C473	L399	D323	A250	L168
H552	R474	I400	I324	I251	F169
F553	C475	D401		N252	I170
V554	V476		V328	T253	F171
E555	K477	N404	G329		P172
T556	L478	I405	A330	D256	F173
G557	S479	G531	Q331	I257	
T558	C480	L409	P332	G258	T177
H559	G481	T410	I333	P259	
R560	Q482	G411	E334	I260	F181
E561	K483	S412	I335	I261	F182
	Q484	K336	Q337	V262	
A568	R485		Q337	I263	L185
F569	L486	G418	G338	G264	
E570	S487	L419	R339	V265	L188
H571		V420		G266	T189
	R490	Q421	I342	A267	R190
I575	L491	Q422		V268	
	F492	D423	V345	L269	Q194
L578	N496	N424		A270	A195
	P496	I425	Y349	I271	L196
		L426		G272	A197
	L499	S428	E353	S273	E198
	I500	D429		S274	V199
L501	L501	T430	I356	I275	Q200
D502	D502	V431	K357	T276	G201
E503			K358	V277	F202
A504	L437		D359	G278	L203
T505	G438	I360	I360	T279	H204
S506	R439		I364	L280	E205
A507			E365		R206
L508	T443			F283	
D509	D444		E368		G209
L510	E445		I369	Y286	I210
E511	E446		V370	L287	S211
S512	S512	V447	A371	E288	V212
E513	V448	V448	F372	L289	V213
S514	E449	S473		L290	K214
I515	A450			F291	
I516	A451		G377	G292	A217
	K452		G378	F293	T218
R527	M453		G379	L294	E219
T528	A454		K380	R295	D220
T529	N455		S381	R296	N221
L530	A456		T382	L297	
E531	H457		L383	V298	K224
V532	D458		I384		
A533	F459		N385	T302	F233
H534	I460		L386	T303	L234
R535	M461		I387	T305	T235
			P388	Q306	L238
L536		P464	R389	S307	K239
S537	Q465		F390	F308	H240
T538	G466		Y391	A309	T241
I539			D392		
	Y467				N245
K544	D468		V393	D312	A246

## 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 0.251 , (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> )	0.25 , 79.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	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.

<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: 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 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	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
3	B	31	0	12	9	0
4	A	10	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	10	0	0	3	0
All	All	9254	0	9451	598	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 32.

The worst 5 of 598 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: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 [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	576/578 (100%)	463 (80%)	95 (16%)	18 (3%)	5	35
1	B	576/578 (100%)	458 (80%)	102 (18%)	16 (3%)	6	37
All	All	1152/1156 (100%)	921 (80%)	197 (17%)	34 (3%)	5	35

5 of 34 Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
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%)	27	64
1	B	499/499 (100%)	471 (94%)	28 (6%)	25	62
All	All	998/998 (100%)	944 (95%)	54 (5%)	26	63

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 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](#)

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	29,33,33	5.62	20 (68%)	28,52,52	4.68	15 (53%)
3	ANP	B	700	2	29,33,33	5.57	17 (58%)	28,52,52	4.71	14 (50%)

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	-	0/13/38/38	0/3/3/3
3	ANP	B	700	2	-	0/13/38/38	0/3/3/3

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	700	ANP	O4'-C4'	-3.94	1.36	1.45
3	A	701	ANP	O4'-C4'	-3.44	1.37	1.45
3	B	700	ANP	C8-N7	-2.93	1.29	1.34
3	A	701	ANP	C8-N7	-2.82	1.29	1.34
3	B	700	ANP	PA-O1A	2.08	1.58	1.50

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	ANP	C4'-O4'-C1'	-16.62	92.08	109.77
3	B	700	ANP	C4'-O4'-C1'	-16.20	92.53	109.77
3	B	700	ANP	N3-C2-N1	-10.14	120.03	128.86
3	A	701	ANP	N3-C2-N1	-9.08	120.95	128.86
3	B	700	ANP	PA-O3A-PB	-8.84	101.18	132.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	701	ANP	8	0
3	B	700	ANP	9	0

## 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<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%)	-0.41	4 (0%) 87 85	55, 120, 187, 200	0
1	B	578/578 (100%)	-0.41	11 (1%) 67 63	52, 117, 194, 200	0
All	All	1156/1156 (100%)	-0.41	15 (1%) 77 73	52, 119, 189, 200	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	47	ASN	5.7
1	B	46	ASN	5.4
1	B	48	HIS	3.7
1	A	578	LEU	3.6
1	B	578	LEU	3.6

### 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. 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NA	B	910	1/1	0.91	0.17	0.95	132,132,132,132	0
3	ANP	B	700	31/31	0.87	0.20	-0.19	74,74,74,74	0
3	ANP	A	701	31/31	0.89	0.18	-0.37	80,80,80,80	0
2	NA	A	911	1/1	0.73	0.15	-0.97	63,63,63,63	0
2	NA	A	900	1/1	0.84	0.09	-1.41	125,125,125,125	0
2	NA	B	901	1/1	0.81	0.20	-	64,64,64,64	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.