wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 04:53 AM 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

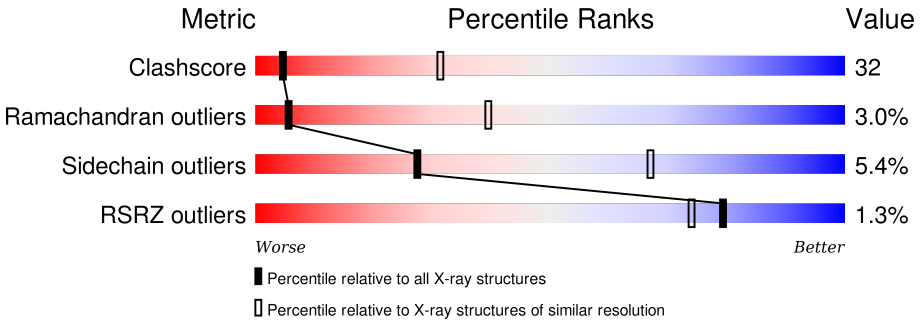
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (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 >=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 <=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	
1	B	578	

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

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.

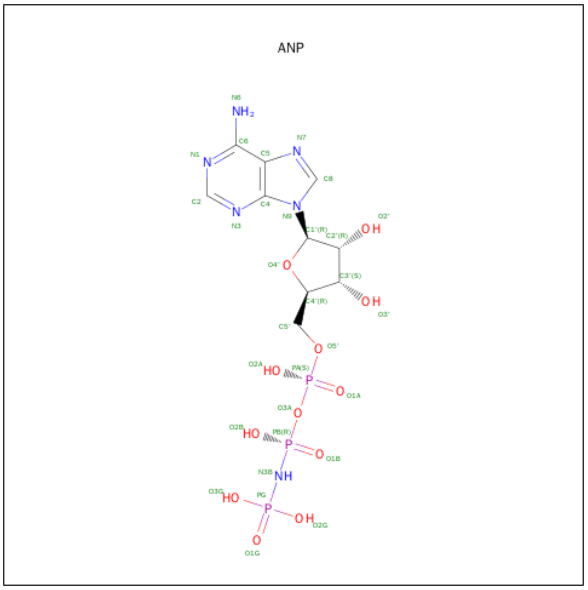
- Molecule 1 is a protein called Multidrug export ATP-binding/permease protein SAV1866.

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: $C_{10}H_{17}N_6O_{12}P_3$).



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.

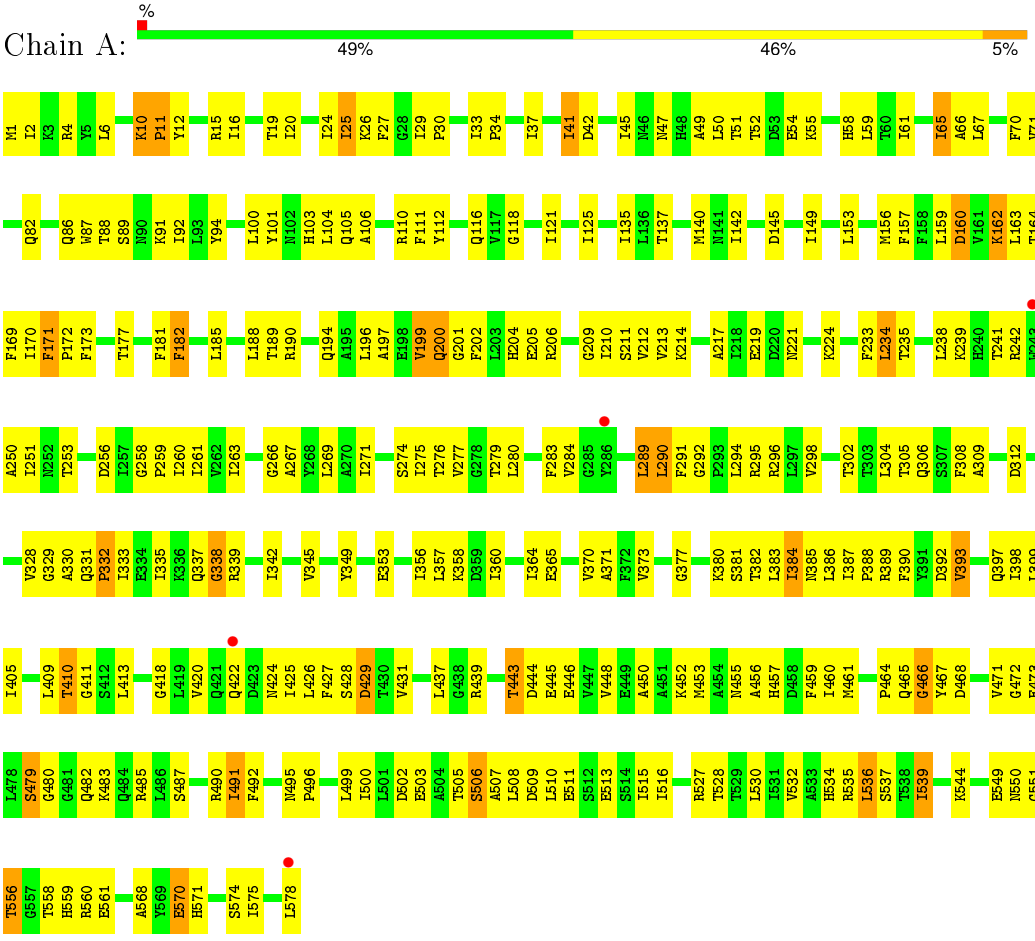
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total	O	0	0
			10	10		
4	B	10	Total	O	0	0
			10	10		

3 Residue-property plots (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 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.

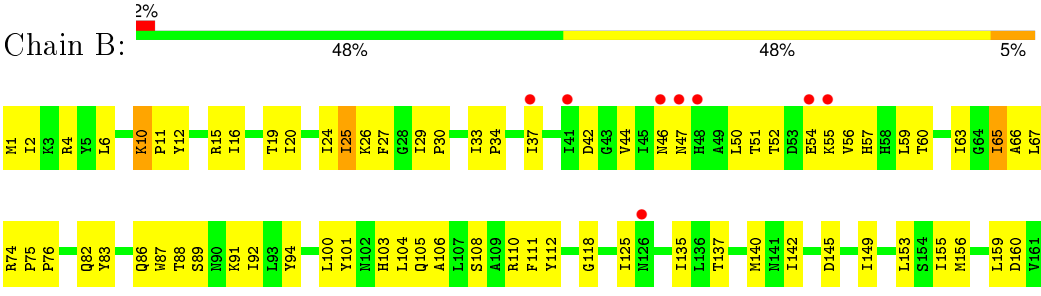
- Molecule 1: Multidrug export ATP-binding/permease protein SAV1866

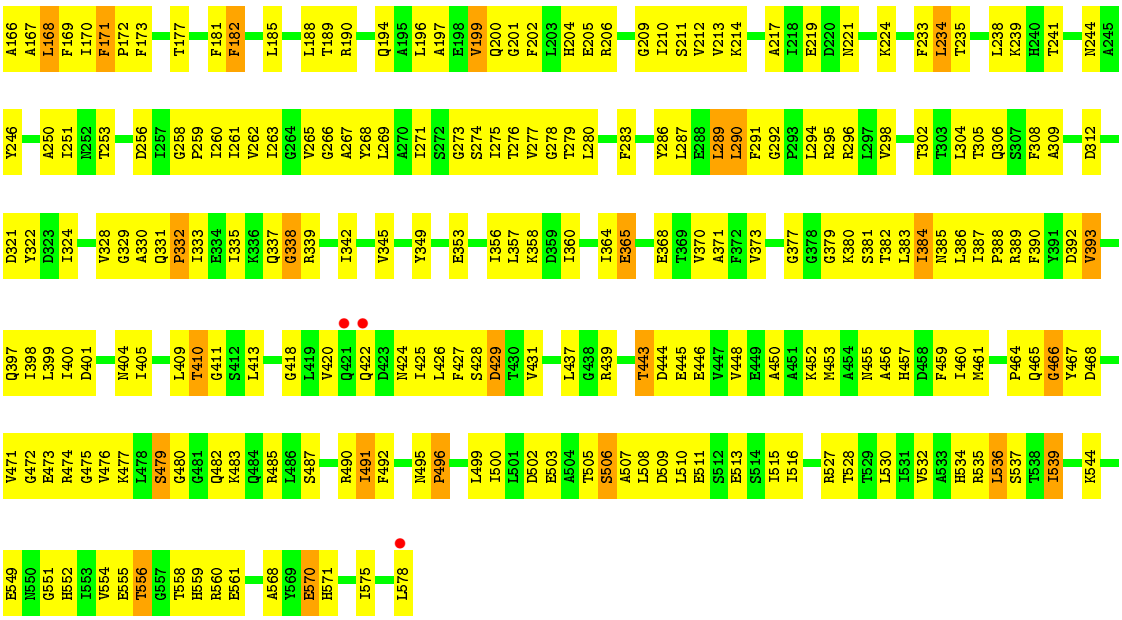
Chain A:



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

Chain B:




A166 A167 L168 F169 I170 F171 P172 F173 T177 F181 F182 L185 L188 T189 R190 Q194 A195 L196 A197 E198 Y199 Q200 G201 F202 L203 H204 E205 R206 G209 I210 S211 V212 V213 K214 A217 I218 E219 D220 N221 K224 F233 L234 T235 L238 K239 H240 T241 N244 A245
Y246 A250 I251 N252 T253 D256 I257 G258 P259 I260 I261 V262 I263 G264 V265 G266 A267 Y268 L269 A270 I271 S272 G273 S274 I275 T276 V277 G278 T279 L280 F283 Y286 L287 E288 L289 L290 F291 G292 P293 L294 R295 R296 L297 V298 T302 T303 L304 T305 Q306 S307 F308 A309 D312
D321 Y322 D323 I324 V328 G329 A330 Q331 P332 I333 E334 I335 K336 Q337 G338 R339 I342 V345 Y349 E353 I356 L357 K358 D359 I360 I364 E365 E368 T369 V370 A371 F372 V373 G377 G378 G379 K380 S381 T382 L383 I384 N385 L386 I387 P388 R389 F390 Y391 D392 V393
Q397 I398 L399 I400 D401 N404 I405 L409 T410 G411 S412 I413 G418 L419 V420 Q421 Q422 D423 N424 I425 L426 F427 S428 D429 T430 V431 L437 G438 R439 T443 D444 E445 E446 V447 Y448 E449 A450 A451 K452 M453 A454 N455 A456 H457 D458 F459 I460 M461 P464 Q465 G466 Y467 D468
V471 G472 E473 R474 G475 V476 K477 L478 S479 G480 G481 Q482 K483 Q484 R485 L486 S487 R490 I491 F492 N495 P496 L499 I500 L501 D502 E503 A504 T505 S506 A507 L508 D509 L510 E511 S512 E513 S514 I515 I516 R527 T528 T529 L530 I531 V532 A533 H534 R535 L536 S537 T538 I539 K544
E549 N550 G551 H552 I553 V554 E555 T556 G557 T558 H559 R560 E561 A568 Y569 E570 H571 I575 L578

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	2.58 (at 3.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.254 , 0.278 0.247 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	101.1	Xtriage
Anisotropy	0.613	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 79.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 41082 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9254	wwPDB-VP
Average B, all atoms (Å^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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(^{o})	Ideal(^{o})
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

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 39
1	B	576/578 (100%)	458 (80%)	102 (18%)	16 (3%)	6 41
All	All	1152/1156 (100%)	921 (80%)	197 (17%)	34 (3%)	5 39

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 (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	499/499 (100%)	473 (95%)	26 (5%)	29	68
1	B	499/499 (100%)	471 (94%)	28 (6%)	26	66
All	All	998/998 (100%)	944 (95%)	54 (5%)	27	67

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 (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)

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	27,33,33	5.72	18 (66%)	30,52,52	4.55	15 (50%)
3	ANP	B	700	2	27,33,33	5.65	17 (62%)	30,52,52	4.62	14 (46%)

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	-	0/12/38/38	0/3/3/3
3	ANP	B	700	2	-	0/12/38/38	0/3/3/3

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	700	ANP	O4'-C4'	-3.87	1.36	1.45
3	A	701	ANP	O4'-C4'	-3.38	1.37	1.45
3	B	700	ANP	C8-N7	-2.83	1.29	1.34
3	A	701	ANP	C8-N7	-2.72	1.29	1.34
3	B	700	ANP	PA-O1A	2.06	1.58	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	701	ANP	C4'-O4'-C1'	-16.05	92.08	109.72
3	B	700	ANP	C4'-O4'-C1'	-15.65	92.53	109.72
3	B	700	ANP	N3-C2-N1	-11.58	120.03	128.89
3	A	701	ANP	N3-C2-N1	-10.38	120.95	128.89
3	B	700	ANP	PA-O3A-PB	-9.39	101.18	132.67

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

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^{th} 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^2)	Q<0.9
1	A	578/578 (100%)	-0.39	4 (0%)	89	85	55, 120, 187, 200	0
1	B	578/578 (100%)	-0.40	11 (1%)	70	64	52, 117, 194, 200	0
All	All	1156/1156 (100%)	-0.40	15 (1%)	79	74	52, 119, 189, 200	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	47	ASN	5.8
1	B	46	ASN	5.5
1	B	48	HIS	3.8
1	A	578	LEU	3.7
1	B	578	LEU	3.7

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^{th} 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(Å^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.