



wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 01:33 am BST

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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

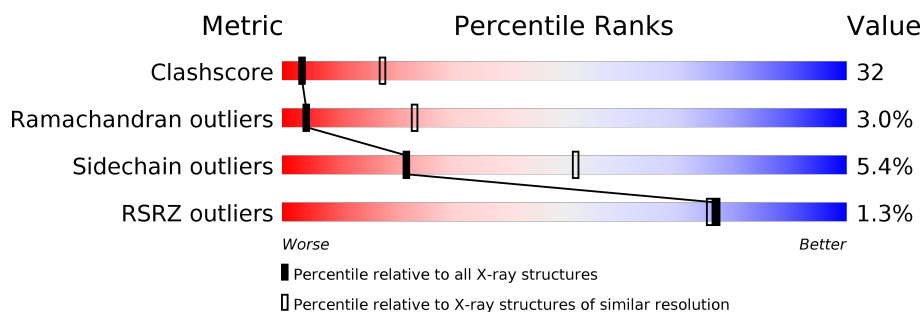
1 Overall quality at a glance

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	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (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 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	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.

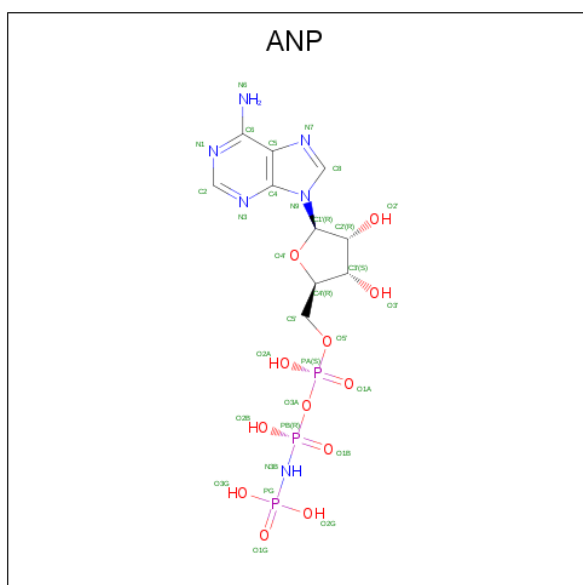
- Molecule 1 is a protein called Multidrug export ATP-binding/permease protein SAV1866.

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



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

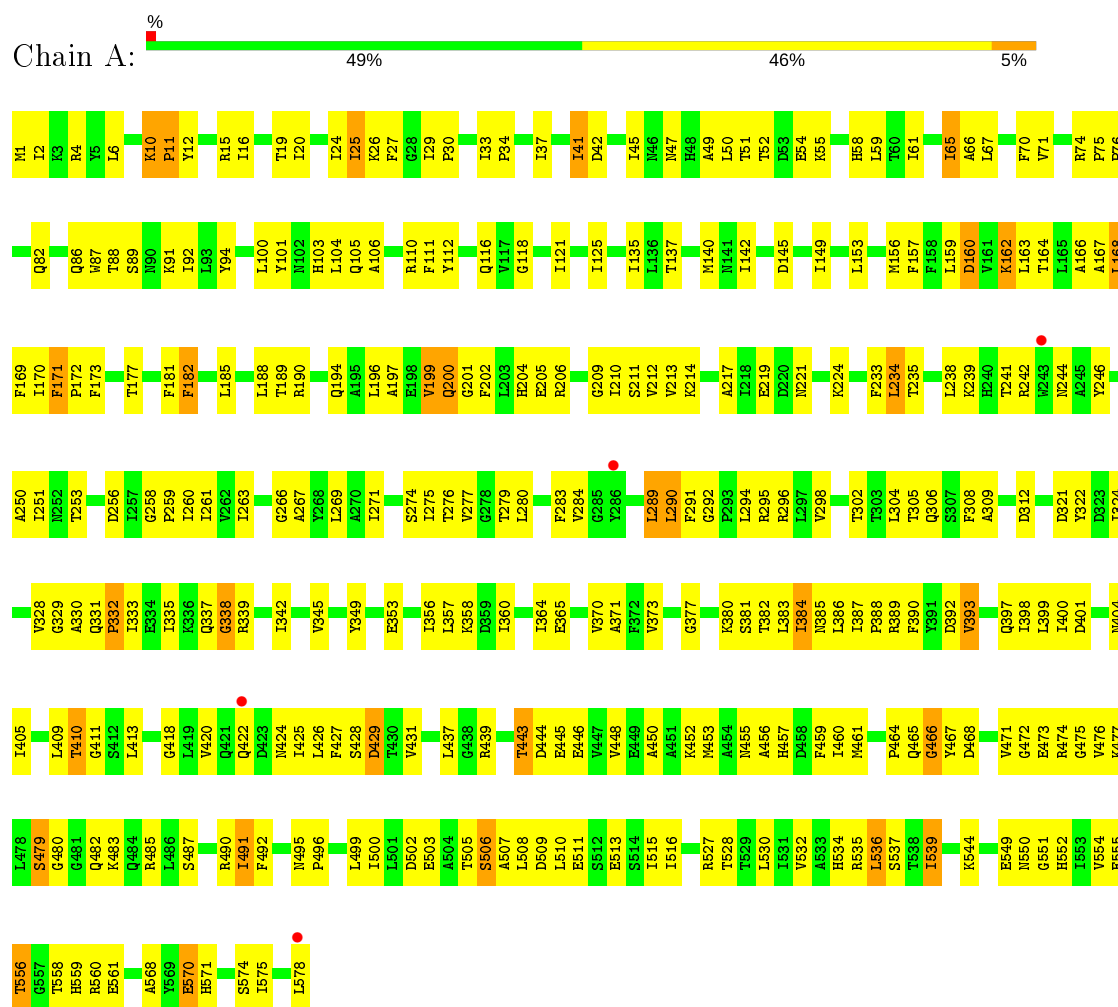
- Molecule 4 is water.

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

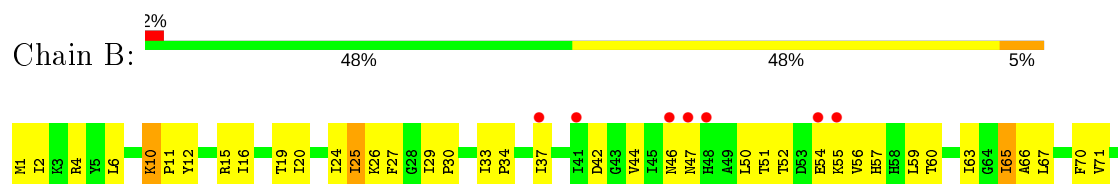
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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	V471	Q397	D321	Y246	A166	R74
M550	G472	I398	Y322		A167	P75
G551	E473	L399	D323	A250	L168	P76
H552	R474	I400	I324	I251	F169	
T553	G475	D401		N252	I170	Q82
V554	V476	N404	V328	T253	F171	Y83
E555	K477	L405	G329		P172	
T556	L478	I405	A330	D256	F173	Q86
G557	S479	Q331	Q331	L257		W87
T558	G480	L409	P332	G258	T177	T88
H559	G481	T410	L333	P259		S89
R560	Q482	G411	E334	L260	F181	N90
E561	K483	L413	L335	I261	F182	K91
	Q484	L413	K336	V262	L185	I92
A568	R485	Q337	Q337	L263		L93
Y569	L486	G418	G338	G264	L185	Y94
E570	S487	L419	R339	V265	L188	L100
H571	R490	V420		G266	T189	
	I491	Q421	I342	A267	R190	Y101
I575	F492	Q422		Y268		H102
		N423	V345	L269	Q194	H103
L578	M495	D424	Y349	A270	A195	L104
	P496	L425		I271	L196	Q105
		F427	E353	S272	A197	A106
		S428		G273	E198	L107
	L499	D429	I356	S274	V199	A109
I501	L500	L430	L357	L275	Q200	R110
D502	D502	V431	K358	T276	G201	F111
E503	E503		D359	V277	F202	Y112
A504	L437		L360	G278	L203	
T505	G438			T279	H204	
S506	R439		I364	L280	E205	G118
A507		E365			R206	
L508	T443	E368		F283	I125	
D509	D444		E368		G209	N126
L510	E445	T369		Y286	T210	
E511	E446	V370		L287	S211	I135
S512	V447	A371	E288	L289	V212	L136
E513	V448	F372	L290	L289	V213	T137
S514	E449	V373		F291	K214	
I515	A450			G292	A217	M140
I516	A451		G377	P293	L218	N141
	K452	G378		L294	E219	L142
R527	M453	G379	K380	R295	D220	D145
T528	A454	R296		R296	N221	
T529	N455	S381	S381	L297		I149
L530	A456	T382		V298	K224	
I531	H457	L383				
V532	D458	L384		T302		L153
A533	F459	N385		T303	F233	S154
H534	L460	L386		L304	L234	I155
R535	M461	L387		T305	T235	M156
		P388		Q306	L238	L159
L536	P464	R389		S307	K239	D160
S537	Q465	F390		F308	V161	
T538	G466	Y391		A309	K162	L163
I539	Y467	D392			T241	L164
	D468	V393		D312	N244	T165
K544					G245	

4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 3.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.254 , 0.278 0.245 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
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
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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 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.*

¹Intensities estimated from amplitudes.

²Theoretical 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%)	4	23
1	B	576/578 (100%)	458 (80%)	102 (18%)	16 (3%)	5	24
All	All	1152/1156 (100%)	921 (80%)	197 (17%)	34 (3%)	4	23

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%)	23	53
1	B	499/499 (100%)	471 (94%)	28 (6%)	21	51
All	All	998/998 (100%)	944 (95%)	54 (5%)	22	52

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	4.90	20 (68%)	31,52,52	3.20	18 (58%)
3	ANP	B	700	2	29,33,33	4.88	19 (65%)	31,52,52	3.23	16 (51%)

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	-	8/14/38/38	0/3/3/3
3	ANP	B	700	2	-	8/14/38/38	0/3/3/3

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	ANP	PB-O3A	13.63	1.76	1.59
3	B	700	ANP	PB-O3A	13.58	1.76	1.59
3	A	701	ANP	PG-O1G	12.83	1.66	1.46
3	B	700	ANP	PG-O1G	11.89	1.65	1.46
3	B	700	ANP	PB-O1B	8.94	1.60	1.46

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	700	ANP	PA-O3A-PB	-8.93	101.18	132.62
3	A	701	ANP	PA-O3A-PB	-8.67	102.08	132.62
3	B	700	ANP	O3A-PB-N3B	-6.97	87.24	106.59
3	A	701	ANP	O3A-PB-N3B	-6.86	87.57	106.59
3	B	700	ANP	N3-C2-N1	-5.54	120.03	128.68

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

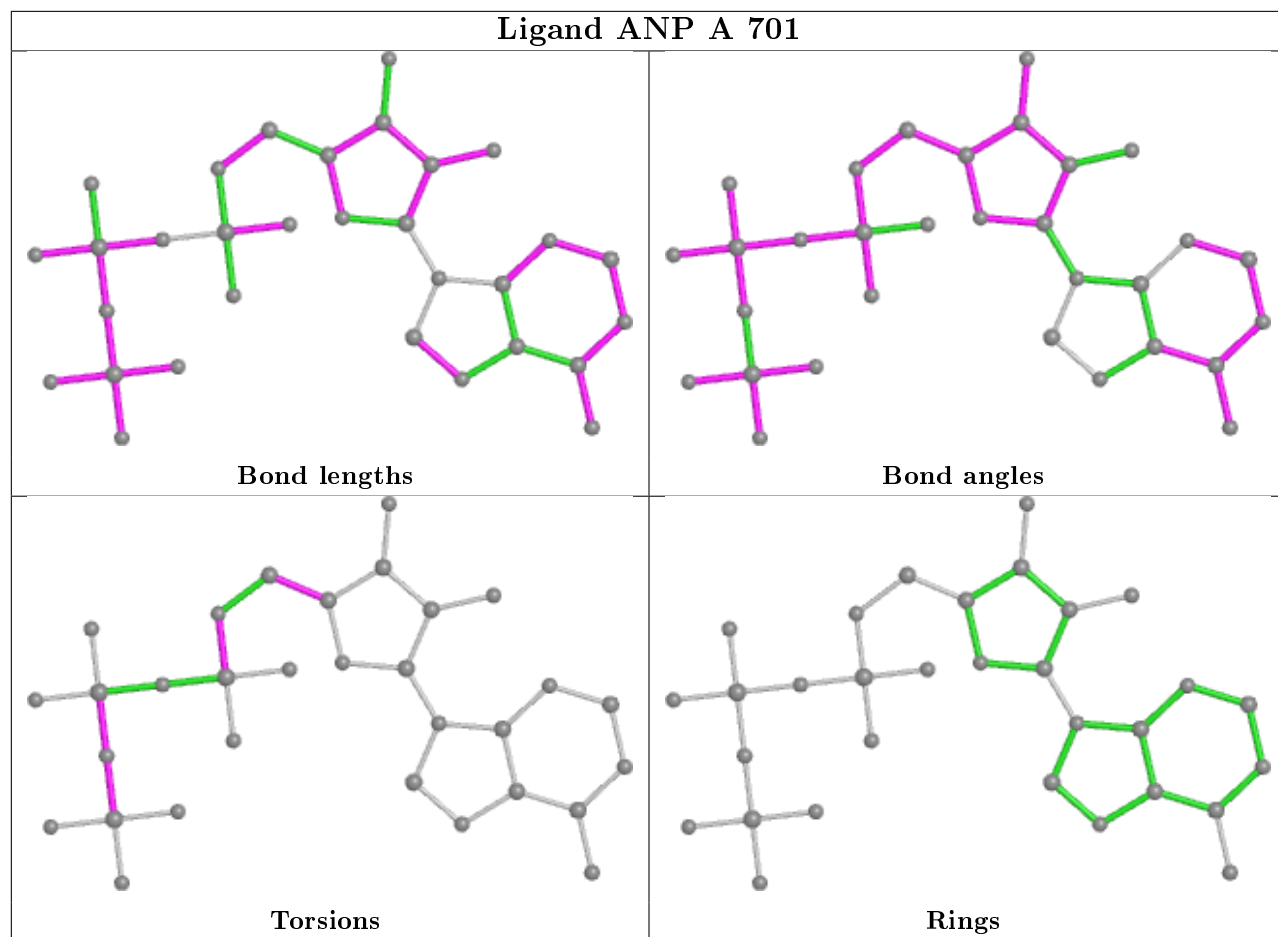
Mol	Chain	Res	Type	Atoms
3	A	701	ANP	PB-N3B-PG-O1G
3	A	701	ANP	PG-N3B-PB-O1B
3	A	701	ANP	PG-N3B-PB-O3A
3	A	701	ANP	C5'-O5'-PA-O1A
3	A	701	ANP	C5'-O5'-PA-O2A

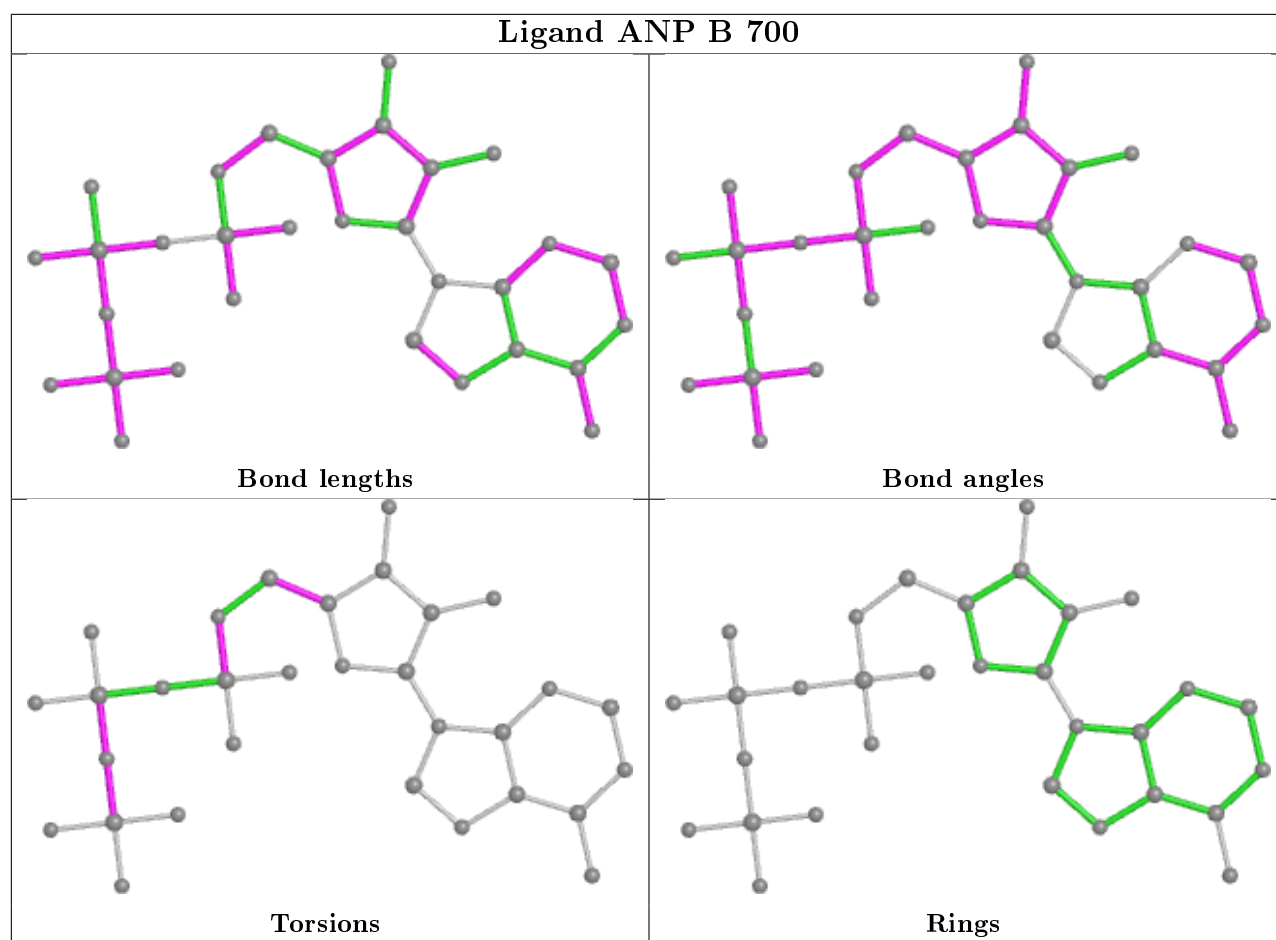
There are no ring outliers.

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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, 95th 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%)	-0.41	4 (0%) 87 87	55, 120, 187, 200	0
1	B	578/578 (100%)	-0.41	11 (1%) 66 65	52, 117, 194, 200	0
All	All	1156/1156 (100%)	-0.41	15 (1%) 77 76	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	5.4
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](#)

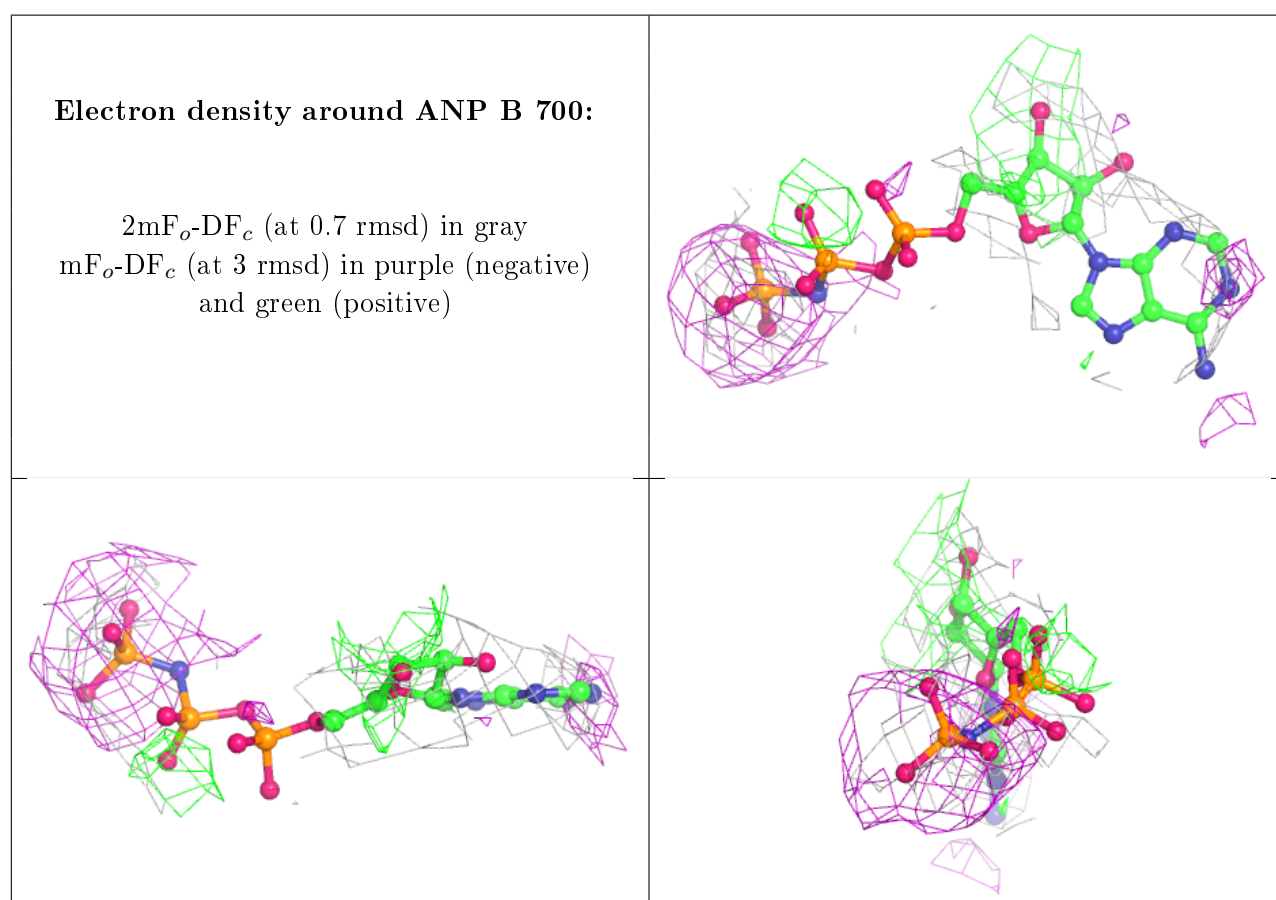
There are no carbohydrates in this entry.

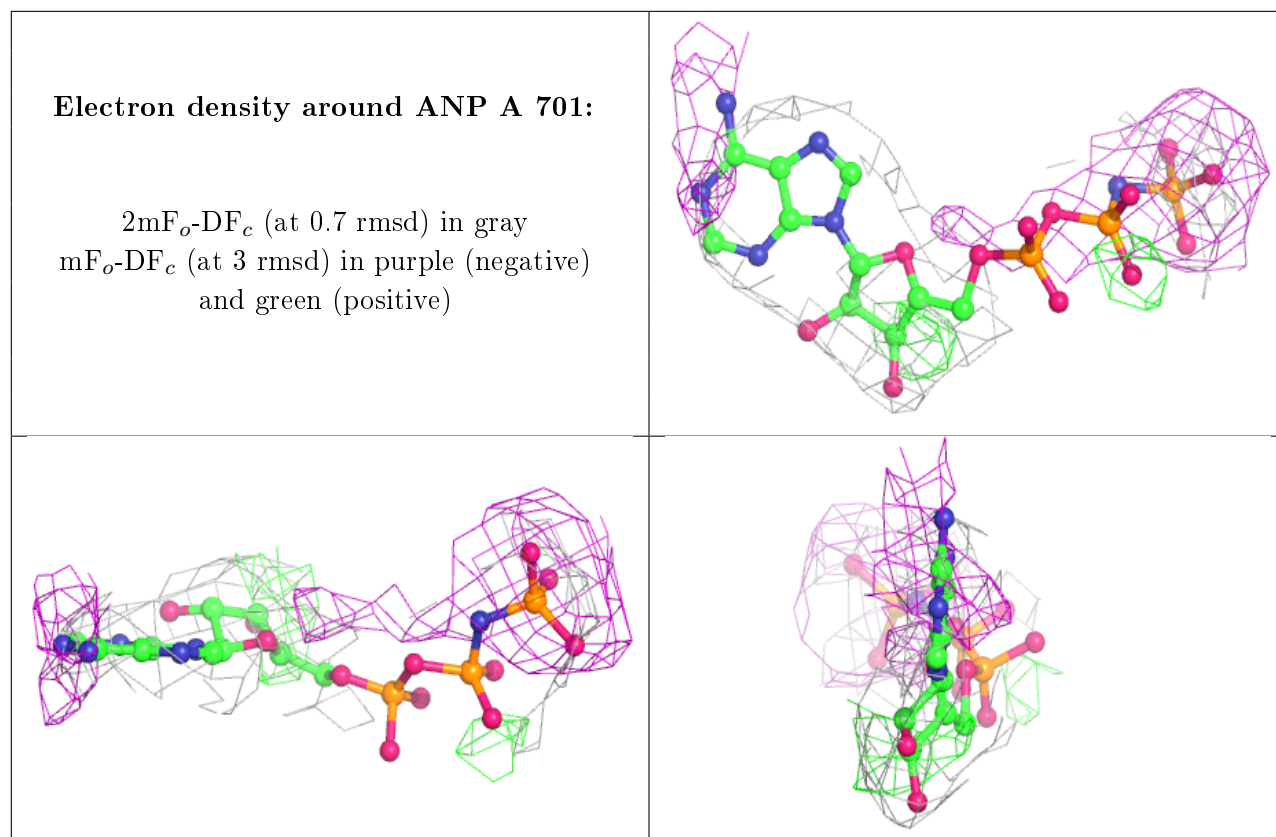
6.4 Ligands [i](#)

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. The B-factors column lists the minimum, median, 95th 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	B-factors(\AA^2)	Q<0.9
2	NA	A	911	1/1	0.73	0.15	63,63,63,63	0
2	NA	B	901	1/1	0.81	0.20	64,64,64,64	0
2	NA	A	900	1/1	0.84	0.09	125,125,125,125	0
3	ANP	B	700	31/31	0.87	0.20	74,74,74,74	0
3	ANP	A	701	31/31	0.89	0.18	80,80,80,80	0
2	NA	B	910	1/1	0.91	0.17	132,132,132,132	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers [i](#)

There are no such residues in this entry.