



wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 01:20 am BST

PDB ID : 4YIY
Title : Structure of MRB1590 bound to AMP-PNP
Authors : Shaw, P.L.R.; Schumacher, M.A.
Deposited on : 2015-03-02
Resolution : 3.02 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

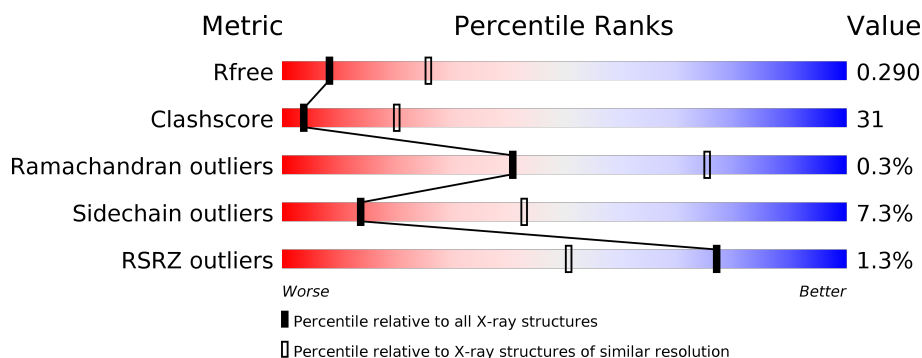
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.02 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}	130704	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)

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	680	<div> <div>%</div> <div> <div></div> <div>44%</div> <div>36%</div> <div>5%</div> <div>15%</div> </div> </div>
1	B	680	<div> <div>%</div> <div> <div></div> <div>47%</div> <div>33%</div> <div>5%</div> <div>15%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8916 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 kRNA Editing A6 Specific Protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	577	Total	C	N	O	S	0	0	0
			4416	2763	782	845	26			
1	A	577	Total	C	N	O	S	0	0	0
			4418	2763	783	846	26			

There are 46 discrepancies between the modelled and reference sequences:

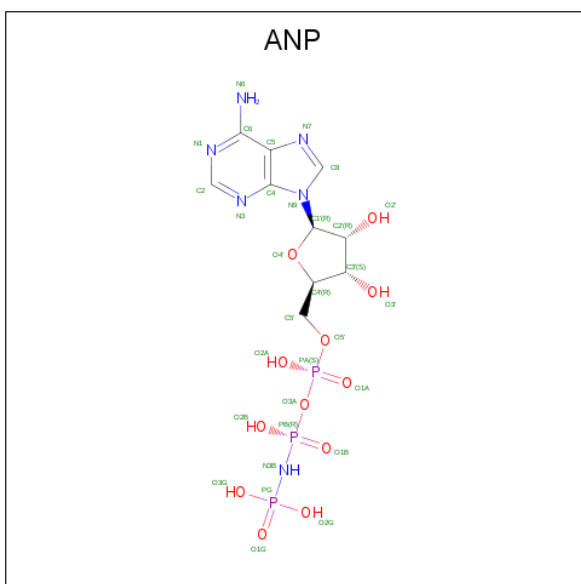
Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	MET	-	initiating methionine	UNP Q57ZF2
B	-10	HIS	-	expression tag	UNP Q57ZF2
B	-9	HIS	-	expression tag	UNP Q57ZF2
B	-8	HIS	-	expression tag	UNP Q57ZF2
B	-7	HIS	-	expression tag	UNP Q57ZF2
B	-6	HIS	-	expression tag	UNP Q57ZF2
B	-5	HIS	-	expression tag	UNP Q57ZF2
B	-4	SER	-	expression tag	UNP Q57ZF2
B	-3	SER	-	expression tag	UNP Q57ZF2
B	-2	GLY	-	expression tag	UNP Q57ZF2
B	-1	VAL	-	expression tag	UNP Q57ZF2
B	0	ASP	-	expression tag	UNP Q57ZF2
B	1	LEU	-	expression tag	UNP Q57ZF2
B	2	GLY	-	expression tag	UNP Q57ZF2
B	3	THR	-	expression tag	UNP Q57ZF2
B	4	GLU	-	expression tag	UNP Q57ZF2
B	5	ASN	-	expression tag	UNP Q57ZF2
B	6	LEU	-	expression tag	UNP Q57ZF2
B	7	TYR	-	expression tag	UNP Q57ZF2
B	8	PHE	-	expression tag	UNP Q57ZF2
B	9	GLN	-	expression tag	UNP Q57ZF2
B	10	SER	-	expression tag	UNP Q57ZF2
B	242	GLU	VAL	conflict	UNP Q57ZF2
A	-11	MET	-	initiating methionine	UNP Q57ZF2
A	-10	HIS	-	expression tag	UNP Q57ZF2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	HIS	-	expression tag	UNP Q57ZF2
A	-8	HIS	-	expression tag	UNP Q57ZF2
A	-7	HIS	-	expression tag	UNP Q57ZF2
A	-6	HIS	-	expression tag	UNP Q57ZF2
A	-5	HIS	-	expression tag	UNP Q57ZF2
A	-4	SER	-	expression tag	UNP Q57ZF2
A	-3	SER	-	expression tag	UNP Q57ZF2
A	-2	GLY	-	expression tag	UNP Q57ZF2
A	-1	VAL	-	expression tag	UNP Q57ZF2
A	0	ASP	-	expression tag	UNP Q57ZF2
A	1	LEU	-	expression tag	UNP Q57ZF2
A	2	GLY	-	expression tag	UNP Q57ZF2
A	3	THR	-	expression tag	UNP Q57ZF2
A	4	GLU	-	expression tag	UNP Q57ZF2
A	5	ASN	-	expression tag	UNP Q57ZF2
A	6	LEU	-	expression tag	UNP Q57ZF2
A	7	TYR	-	expression tag	UNP Q57ZF2
A	8	PHE	-	expression tag	UNP Q57ZF2
A	9	GLN	-	expression tag	UNP Q57ZF2
A	10	SER	-	expression tag	UNP Q57ZF2
A	242	GLU	VAL	conflict	UNP Q57ZF2

- Molecule 2 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
2	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Mg	0	0
			2	2		
3	A	2	Total	Mg	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	12	Total	O	0	0
			12	12		
4	A	4	Total	O	0	0
			4	4		

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 ($\text{RSRZ} > 2$). 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.

[illegible]

Chain A:

Residue	Count	Percentage
MET	1	1%
HIS	1	
HIS	1	
HIS	1	
HIS	1	
HIS	1	
SER	1	
SER	1	
VAL	1	
ASP	1	
LEU	1	
GLY	1	
THR	1	
GLU	1	
ASN	1	
LEU	1	
TRP	1	
PHE	1	
GLN	1	
SER	1	
ARG	1	
GLY	1	
GLY	1	
ARG	1	
GLY	1	
GLY	1	
GLY	1	
ARG	1	
GLY	1	
HIS	1	
SER	1	
HIS	1	
THR	1	
HIS	1	
ASN	1	
ASN	1	
ASN	1	
ALA	1	
PRO	1	
PRO	1	
MET	1	
GLU	1	
ARG	1	
GLY	1	
GLY	1	
HIS	1	
MET	1	
PRO	1	
SER	1	
ASN	1	
ASN	1	
GLU	1	
GLY	1	
ALA	1	
ALA	1	
ILE	1	
SER	1	
SER	1	
GLY	1	
SER	1	

L638	P639	R640	G641	F642	R647	H648	I649	G652	A653	A654	L655	M656	R657	L658	R659	T660	L661	R662	T663	V664	T665	ALA	LYS	ARG																															
GLU	GLY	T533	K534	E556	E560	Q563	I567	A568	Q569	L573	L574	Y575	D576	G577	E578	PRO	R580	I581	V582	P583	E584	M585	T586	T587	K588	L595	P596	V601	C602	GLU	ILE	GLN	ARG	GLY	LYS	F609	F613	S614	H623	K627	E630	L631	R632	T633	P634	S635	C636	Y637							
S452	S453	I454	M455	V456	I457	G458	S460	S461	Q462	Y463	Q466	A467	R468	V469	V470	Y476	D480	C481	T482	A485	I488	S493	LEU	PRO	ALA	LEU	ASN	PRO	PRO	GLU	ILE	GLY	ASP	THR	ALA	S505	V506	D510	V511	N512	S520	F521	T522	T523	V524	R525	ARG	ARG	ARG	GLY	ARG				
N370	N378	F379	F380	V381	T382	A383	D384	A385	S386	T389	S390	Q391	I395	M396	E397	A398	L399	E400	L401	L405	L406	L407	L408	D409	E410	L417	M418	Y419	R420	D421	M424	L427	V428	P429	R430	A431	Q432	E433	P434	I435	T436	P437	F438	V439	R441	V442	L445	N448	H449						
G296	K297	G301	P305	L308	T309	L310	G313	G314	G315	F316	H317	G318	K319	M396	E397	A398	L399	L322	R324	V328	G329	I330	Y331	N332	H333	V334	P335	D336	L337	G338	R339	V342	V343	V344	D345	K350	I351	R352	A353	E354	D355	R356	R357	H360	D363	I364	S365	P366	F367	I368	N369				
I201	D202	H204	G205	A206	T207	D208	I209	F210	F211	I212	E213	L214	V215	P216	L217	Q220	C221	V222	L225	N226	E227	L230	H231	Q232	H233	V234	T235	C236	V237	H238	D239	Q240	E241	E242	L243	R244	S245	N246	L247	L248	Y252	I261	L262	P263	P283	L286	E287	P293	H294	S295					
L115	C126	R127	A130	A131	E132	D133	F134	I135	L136	R137	I147	P148	R149	R150	A154	V155	Q156	R159	P160	S161	Q162	H163	V164	L165	V170	G171	L172	V173	K174	ALA	HIS	GLN	GLN	LYS	SER	GLY	MET	GLN	ALA	E185	I188	R191	V192	K193	L194	P195	GLY	HIS	G198	R199	R200				
THR	GLY	PHE	S52	P53	L54	M55	D56	F57	F58	H59	S60	V61	E62	G63	R64	N65	Y66	L69	R70	S71	L72	T73	N74	E75	T76	Y77	Q78	I79	S80	E81	N82	V83	R84	C85	T86	F87	L88	S89	I90	Q91	S92	D93	P94	P95	A96	P97	G98	R102	L103	V104	C105	P106	S110	K113	V114

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	103.18 Å 71.52 Å 103.54 Å 90.00° 120.03° 90.00°	Depositor
Resolution (Å)	44.82 – 3.02 44.82 – 3.02	Depositor EDS
% Data completeness (in resolution range)	97.6 (44.82-3.02) 97.6 (44.82-3.02)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 3.01 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.233 , 0.297 0.251 , 0.290	Depositor DCC
R_{free} test set	2004 reflections (7.87%)	wwPDB-VP
Wilson B-factor (Å ²)	51.2	Xtriage
Anisotropy	0.781	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 14.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.036 for l,k,-h-l 0.036 for -h-l,k,h 0.047 for h,-k,-h-l 0.378 for l,-k,h 0.044 for -h-l,-k,l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	8916	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.19% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.78	1/4495 (0.0%)	0.82	13/6091 (0.2%)
1	B	0.77	0/4494	0.81	11/6091 (0.2%)
All	All	0.77	1/8989 (0.0%)	0.82	24/12182 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	634	PRO	N-CD	-13.53	1.28	1.47

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	631	LEU	N-CA-C	-10.11	83.70	111.00
1	B	657	ARG	CB-CA-C	-8.28	93.84	110.40
1	A	533	THR	N-CA-CB	-6.89	97.22	110.30
1	A	631	LEU	CB-CA-C	6.47	122.50	110.20
1	A	75	GLU	N-CA-C	-6.30	93.99	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	336	ASP	Peptide
1	B	336	ASP	Peptide
1	B	96	ALA	Peptide

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	4418	0	4382	258	50
1	B	4416	0	4381	305	50
2	A	31	0	13	4	0
2	B	31	0	13	7	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	4	0	0	3	0
4	B	12	0	0	4	0
All	All	8916	0	8789	544	50

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 31.

The worst 5 of 544 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:B:114:VAL:HG23	1:B:115:LEU:CD1	1.70	1.21
1:B:576:ASP:OD2	1:B:634:PRO:HD2	1.03	1.19
1:A:57:PHE:O	1:A:60:SER:HB2	1.38	1.17
1:A:244:ARG:NH2	1:A:332:ASN:OD1	1.78	1.16
1:B:366:PRO:HG2	1:B:396:MET:HE3	1.27	1.16

The worst 5 of 50 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	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:GLY:C	1:A:580:ARG:NH1[2_455]	0.27	1.93
1:B:69:LEU:C	1:A:632:ARG:NH2[2_455]	0.39	1.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:ARG:CA	1:A:632:ARG:NE[2_455]	0.55	1.65
1:B:584:GLU:CD	1:A:64:ARG:NE[2_455]	0.57	1.63
1:B:584:GLU:CG	1:A:64:ARG:NH2[2_455]	0.63	1.57

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	563/680 (83%)	535 (95%)	28 (5%)	0	100	100
1	B	563/680 (83%)	534 (95%)	26 (5%)	3 (0%)	29	66
All	All	1126/1360 (83%)	1069 (95%)	54 (5%)	3 (0%)	41	75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	68	GLU
1	B	410	GLU
1	B	579	PRO

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	491/567 (87%)	455 (93%)	36 (7%)	14	43
1	B	491/567 (87%)	455 (93%)	36 (7%)	14	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	982/1134 (87%)	910 (93%)	72 (7%)	14	43

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	567	ILE
1	A	81	GLU
1	A	574	LEU
1	B	632	ARG
1	A	58	PHE

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	B	333	HIS
1	B	369	ASN
1	A	281	GLN
1	B	281	GLN
1	B	332	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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
2	ANP	A	701	3	29,33,33	1.98	9 (31%)	31,52,52	2.99	11 (35%)
2	ANP	B	701	3	29,33,33	1.86	5 (17%)	31,52,52	1.89	8 (25%)

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	ANP	A	701	3	-	7/14/38/38	0/3/3/3
2	ANP	B	701	3	-	6/14/38/38	0/3/3/3

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	ANP	PG-N3B	4.66	1.75	1.63
2	B	701	ANP	PB-N3B	4.61	1.75	1.63
2	A	701	ANP	PB-O2B	-4.54	1.44	1.56
2	A	701	ANP	PG-O3G	-4.33	1.45	1.56
2	B	701	ANP	PB-O1B	3.36	1.51	1.46

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	ANP	O1G-PG-N3B	-11.17	95.32	111.77
2	A	701	ANP	O2B-PB-O1B	6.96	124.52	109.92
2	B	701	ANP	O1G-PG-N3B	-4.83	104.65	111.77
2	A	701	ANP	O1B-PB-N3B	-4.49	105.15	111.77
2	B	701	ANP	O2B-PB-O1B	4.05	118.41	109.92

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	ANP	PB-N3B-PG-O1G
2	A	701	ANP	PG-N3B-PB-O1B

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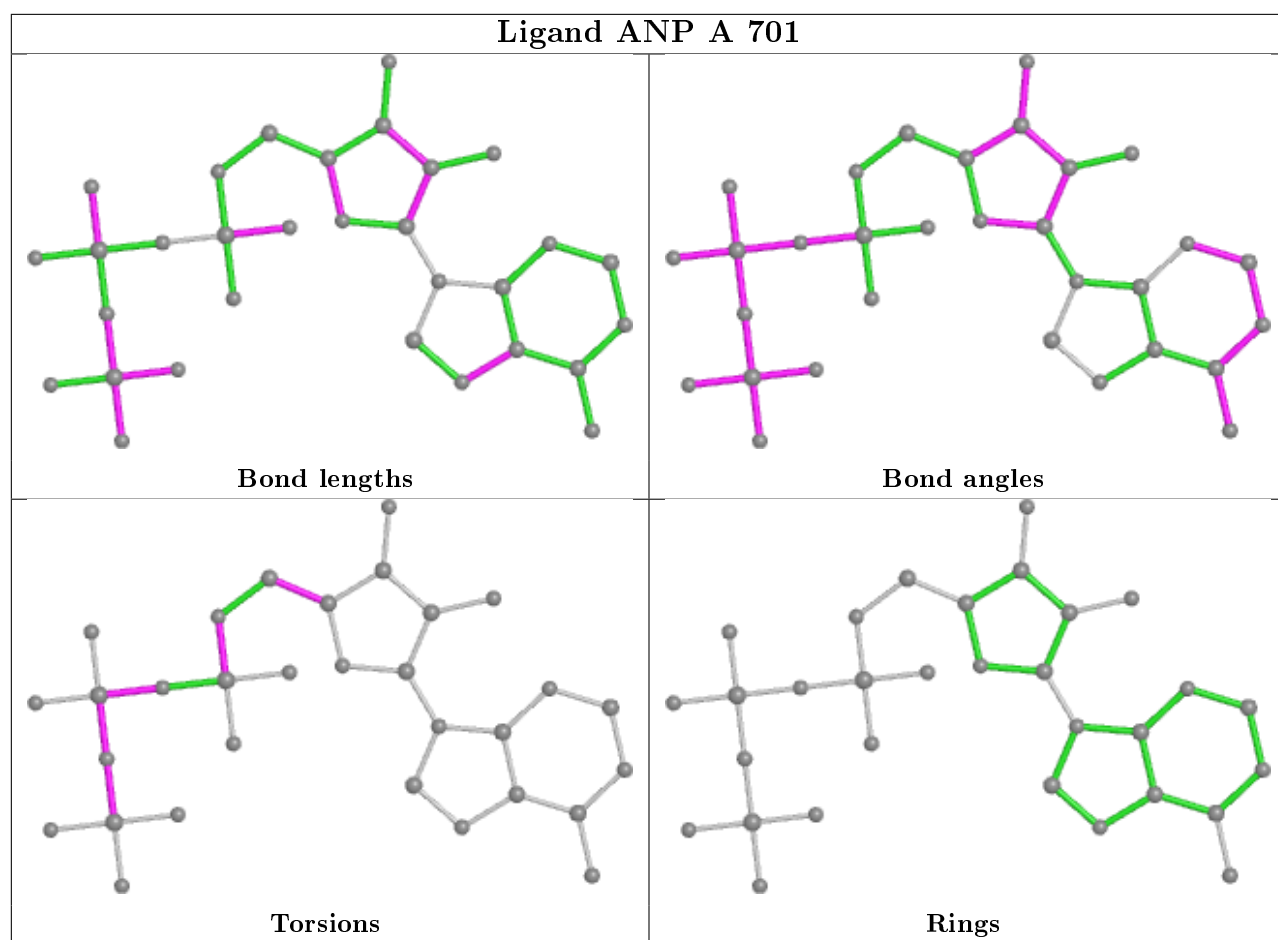
Mol	Chain	Res	Type	Atoms
2	A	701	ANP	PA-O3A-PB-O1B
2	A	701	ANP	C5'-O5'-PA-O1A
2	B	701	ANP	PB-N3B-PG-O1G

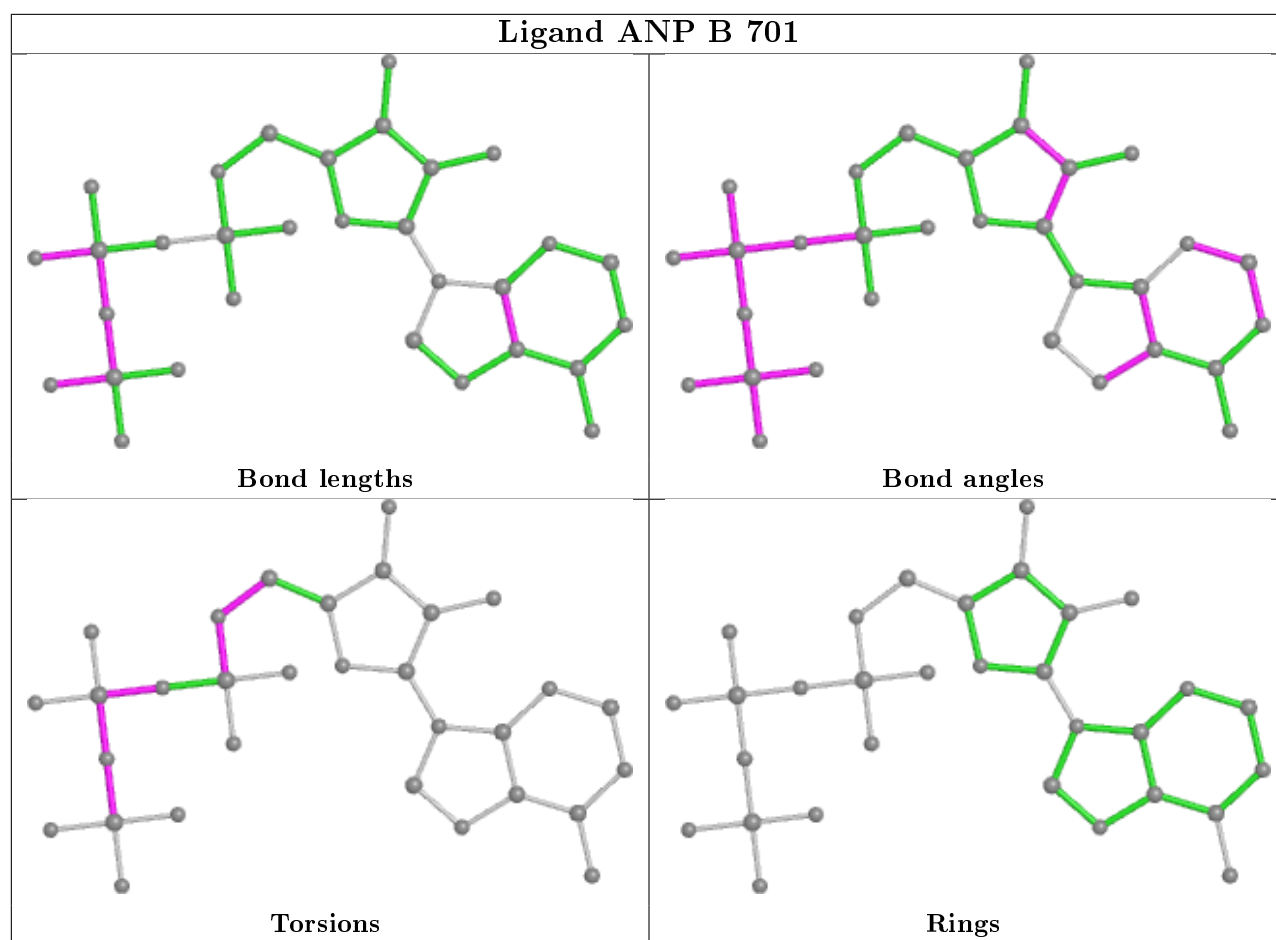
There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	ANP	4	0
2	B	701	ANP	7	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	577/680 (84%)	0.06	8 (1%) 75 48	26, 43, 72, 80	0
1	B	577/680 (84%)	-0.01	7 (1%) 79 53	26, 42, 75, 81	0
All	All	1154/1360 (84%)	0.03	15 (1%) 77 51	26, 42, 73, 81	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	79	ILE	5.3
1	A	70	ARG	4.8
1	A	427	LEU	3.1
1	B	114	VAL	3.0
1	B	72	LEU	3.0

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](#)

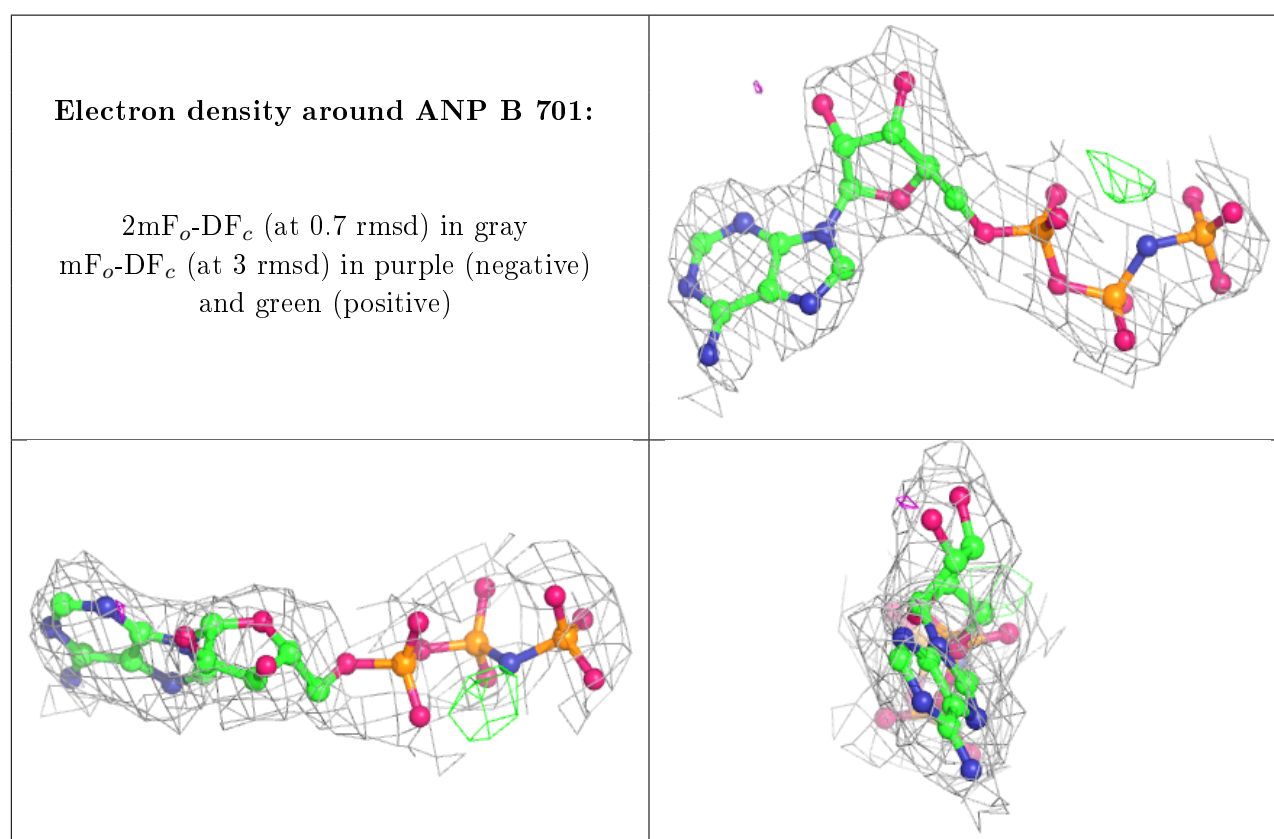
There are no carbohydrates in this entry.

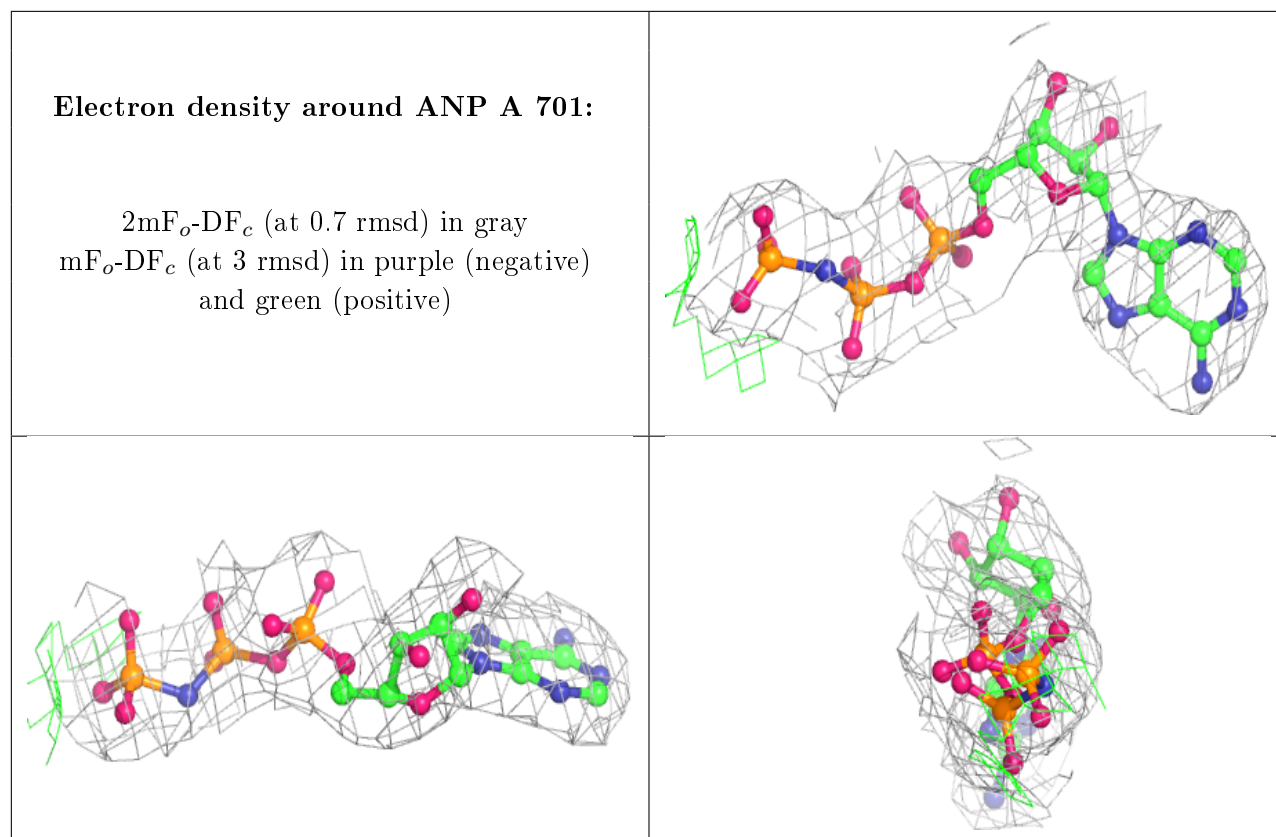
6.4 Ligands [i](#)

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
3	MG	B	703	1/1	0.78	0.18	37,37,37,37	0
3	MG	A	702	1/1	0.91	0.09	45,45,45,45	0
2	ANP	B	701	31/31	0.93	0.18	36,37,40,40	0
2	ANP	A	701	31/31	0.95	0.17	36,40,44,45	0
3	MG	B	702	1/1	0.96	0.13	43,43,43,43	0
3	MG	A	703	1/1	0.97	0.16	79,79,79,79	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.