



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 03:00 am BST

PDB ID : 3X03  
Title : Crystal structure of PIP4KIIBETA complex with AMPPNP  
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Deposited on : 2014-10-09  
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (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

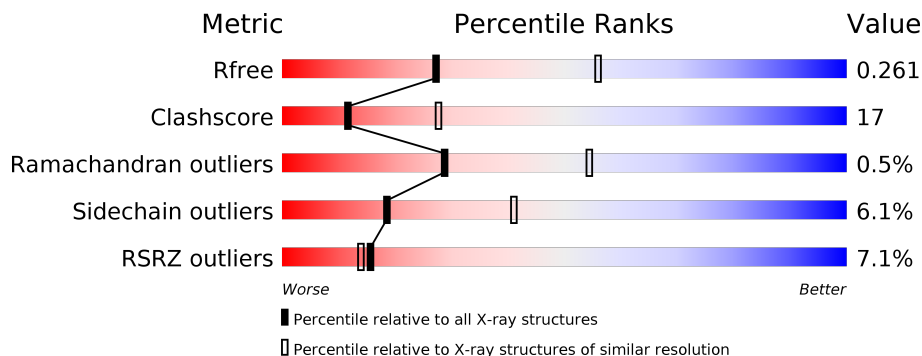
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 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	393	
1	B	393	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5237 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.

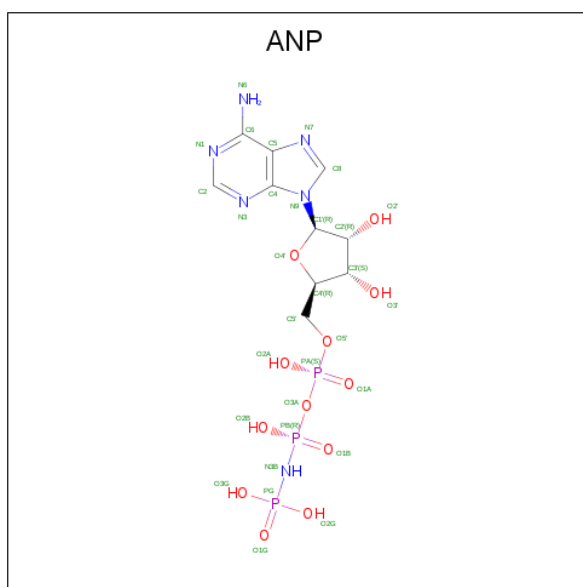
- Molecule 1 is a protein called Phosphatidylinositol 5-phosphate 4-kinase type-2 beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	320	2629	1672	448	495	14	0	0	0
1	B	302	2490	1595	426	456	13	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	GLY	-	EXPRESSION TAG	UNP P78356
A	25	PRO	-	EXPRESSION TAG	UNP P78356
A	26	ASN	-	EXPRESSION TAG	UNP P78356
A	27	CYS	-	EXPRESSION TAG	UNP P78356
A	28	ALA	-	EXPRESSION TAG	UNP P78356
A	29	PRO	-	EXPRESSION TAG	UNP P78356
A	30	GLY	-	EXPRESSION TAG	UNP P78356
B	24	GLY	-	EXPRESSION TAG	UNP P78356
B	25	PRO	-	EXPRESSION TAG	UNP P78356
B	26	ASN	-	EXPRESSION TAG	UNP P78356
B	27	CYS	-	EXPRESSION TAG	UNP P78356
B	28	ALA	-	EXPRESSION TAG	UNP P78356
B	29	PRO	-	EXPRESSION TAG	UNP P78356
B	30	GLY	-	EXPRESSION TAG	UNP P78356

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	11	Total	O	0	0
			11	11		
3	B	14	Total	O	0	0
			14	14		





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.64Å 182.98Å 106.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.18 – 2.70 91.49 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.6 (53.18-2.70) 98.7 (91.49-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.18 (at 2.69Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.3_928)	Depositor
R, $R_{free}$	0.234 , 0.280 0.218 , 0.261	Depositor DCC
$R_{free}$ test set	1451 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	75.6	Xtrriage
Anisotropy	0.146	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 75.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.005 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.012 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5237	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	89.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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: 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	0.83	0/2682	0.82	1/3608 (0.0%)
1	B	0.81	2/2542 (0.1%)	0.81	1/3418 (0.0%)
All	All	0.82	2/5224 (0.0%)	0.81	2/7026 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	83	LEU	N-CA	5.20	1.56	1.46
1	B	207	HIS	C-N	-5.09	1.22	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	271	LEU	O-C-N	5.49	131.49	122.70
1	B	208	ARG	N-CA-CB	-5.44	100.81	110.60

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	2629	0	2601	91	0
1	B	2490	0	2472	87	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	62	0	22	10	0
2	B	31	0	11	2	0
3	A	11	0	0	0	0
3	B	14	0	0	2	0
All	All	5237	0	5106	180	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 17.

All (180) 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:281:LEU:HD22	1:A:411:MET:SD	1.87	1.12
1:B:411:MET:O	1:B:414:ILE:HG12	1.51	1.11
1:A:281:LEU:CD2	1:A:411:MET:SD	2.47	1.03
1:A:56:GLU:HG3	1:A:57:LEU:N	1.75	1.02
1:B:251:HIS:ND1	1:B:416:THR:HG21	1.78	0.98
1:A:53:THR:O	1:A:56:GLU:HG2	1.66	0.93
1:B:281:LEU:HD22	1:B:411:MET:SD	2.10	0.92
2:A:501:ANP:PG	2:A:501:ANP:O1A	2.30	0.89
1:B:281:LEU:HB2	1:B:407:PHE:HZ	1.43	0.83
1:B:251:HIS:ND1	1:B:416:THR:CG2	2.44	0.81
1:A:407:PHE:CE2	1:A:411:MET:HG3	2.16	0.80
1:B:335:ARG:HG3	1:B:336:PHE:N	1.96	0.79
1:A:56:GLU:HG3	1:A:57:LEU:H	1.47	0.79
1:A:128:ASN:HB3	1:A:140:LEU:HD23	1.69	0.75
1:A:53:THR:O	1:A:56:GLU:CG	2.34	0.75
1:B:411:MET:O	1:B:414:ILE:CG1	2.32	0.74
1:A:357:SER:OG	1:A:358:PRO:HD2	1.87	0.74
1:A:77:ILE:HG13	1:B:77:ILE:HD11	1.72	0.72
1:B:268:VAL:CG1	1:B:404:SER:HB2	2.21	0.71
1:A:415:LEU:O	1:A:415:LEU:HD23	1.91	0.70
1:A:258:LYS:NZ	1:A:262:GLU:OE2	2.24	0.70
1:A:53:THR:HA	1:A:56:GLU:HG2	1.73	0.69
1:A:268:VAL:HG12	1:A:404:SER:HB2	1.76	0.68
1:B:99:CYS:N	1:B:100:PRO:CD	2.57	0.68
1:A:281:LEU:HD23	1:A:411:MET:SD	2.35	0.65
1:A:56:GLU:CG	1:A:57:LEU:N	2.56	0.65
1:A:141:THR:CG2	1:A:145:ARG:HA	2.27	0.64
1:B:210:THR:HG22	1:B:211:VAL:N	2.12	0.64
1:B:157:VAL:HA	1:B:186:MET:HE1	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:VAL:HG12	1:B:404:SER:HB2	1.81	0.62
1:A:160:MET:HE1	1:A:164:LEU:HD13	1.82	0.61
1:B:212:HIS:O	1:B:213:ARG:HG2	2.00	0.61
1:A:129:SER:HG	1:A:139:PHE:HD1	1.49	0.60
1:B:94:LYS:HB2	1:B:190:THR:HB	1.83	0.60
1:B:47:MET:HE3	1:B:125:ALA:HA	1.84	0.60
1:B:219:GLY:N	1:B:240:ASP:OD2	2.35	0.59
1:B:47:MET:CE	1:B:125:ALA:HA	2.31	0.59
1:B:228:ASP:OD1	1:B:228:ASP:N	2.33	0.59
1:B:281:LEU:HB2	1:B:407:PHE:CZ	2.33	0.58
1:A:155:GLU:N	1:A:155:GLU:OE1	2.33	0.58
1:A:188:ARG:NH1	2:A:502:ANP:O4'	2.36	0.58
1:A:204:VAL:HG23	2:A:501:ANP:N6	2.19	0.58
1:A:53:THR:C	1:A:56:GLU:HG2	2.24	0.58
1:B:279:TYR:O	1:B:403:TYR:OH	2.22	0.58
1:B:287:ASP:OD2	1:B:359:LYS:HD3	2.04	0.58
1:A:281:LEU:CB	1:A:411:MET:SD	2.92	0.57
1:A:51:ASN:HB2	1:A:122:THR:HG21	1.86	0.57
1:B:78:LYS:HD2	1:B:94:LYS:HE2	1.85	0.57
1:A:270:PHE:CZ	1:A:274:LEU:HD11	2.39	0.57
1:B:277:MET:HG3	1:B:278:ASP:OD2	2.06	0.56
1:A:69:ASP:HB3	1:B:83:LEU:HD13	1.87	0.56
1:B:240:ASP:HB3	1:B:410:PHE:CZ	2.40	0.56
1:A:229:LYS:HG2	1:A:233:LYS:HZ2	1.71	0.56
1:A:53:THR:CA	1:A:56:GLU:HG2	2.36	0.55
1:A:268:VAL:HG13	1:A:279:TYR:OH	2.06	0.55
2:A:501:ANP:N3B	2:A:501:ANP:O1A	2.30	0.55
1:A:264:LEU:HD11	1:A:407:PHE:HE2	1.72	0.55
1:A:229:LYS:HG2	1:A:233:LYS:NZ	2.22	0.55
1:B:288:VAL:CG1	1:B:339:PRO:HB2	2.37	0.55
1:B:236:PRO:HB2	1:B:238:PHE:CZ	2.42	0.54
1:B:250:LEU:HD22	1:B:363:TYR:CD2	2.43	0.53
1:A:350:ALA:HB2	1:A:364:PHE:CE2	2.43	0.53
1:A:287:ASP:OD2	1:A:359:LYS:HD3	2.08	0.53
1:B:336:PHE:O	1:B:336:PHE:CD2	2.62	0.53
1:B:277:MET:O	1:B:278:ASP:HB2	2.09	0.53
1:B:251:HIS:CE1	1:B:416:THR:HG21	2.44	0.53
1:B:43:LEU:HD21	1:B:140:LEU:HD11	1.91	0.53
1:A:157:VAL:HG21	1:A:197:TYR:CD2	2.43	0.52
1:B:177:ASN:ND2	1:B:263:LYS:HD2	2.24	0.52
1:B:40:GLU:HB3	1:B:42:ILE:HG22	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:VAL:HG23	2:B:501:ANP:N6	2.24	0.52
1:B:282:LEU:HB2	1:B:368:ILE:HD13	1.90	0.52
1:A:186:MET:HG3	1:A:199:VAL:HG22	1.92	0.52
1:A:217:LEU:HB2	1:A:411:MET:CE	2.40	0.52
1:A:80:ASP:O	1:B:76:LYS:HB2	2.09	0.52
1:A:56:GLU:CG	1:A:57:LEU:H	2.17	0.51
1:B:283:VAL:HG12	1:B:284:GLY:N	2.25	0.51
1:B:191:VAL:O	1:B:192:ASP:HB2	2.10	0.51
2:A:502:ANP:C3'	2:A:502:ANP:PA	2.99	0.50
1:A:77:ILE:HD12	3:B:614:HOH:O	2.11	0.50
1:B:236:PRO:CB	1:B:238:PHE:CZ	2.94	0.50
2:A:501:ANP:O1A	2:A:501:ANP:O3G	2.30	0.50
2:A:501:ANP:O1B	2:A:501:ANP:O1G	2.30	0.50
1:B:233:LYS:HG2	1:B:234:ASP:N	2.26	0.50
1:A:216:ASP:C	1:A:217:LEU:HD23	2.31	0.49
1:A:216:ASP:O	1:A:217:LEU:HD23	2.12	0.49
1:B:214:LYS:HD2	1:B:235:LEU:CD1	2.43	0.49
1:B:43:LEU:HD21	1:B:140:LEU:CD1	2.43	0.49
1:B:120:SER:O	1:B:142:THR:HB	2.12	0.48
1:B:213:ARG:HD2	1:B:238:PHE:HE1	1.76	0.48
1:B:79:VAL:O	1:B:92:ARG:HA	2.13	0.48
1:A:99:CYS:N	1:A:100:PRO:CD	2.76	0.48
1:A:225:GLU:CG	1:A:241:ASN:HB2	2.44	0.48
1:B:110:PHE:CD1	1:B:182:GLN:HB3	2.47	0.48
1:B:81:ASN:O	1:B:91:SER:HB3	2.13	0.48
1:A:160:MET:CE	1:A:164:LEU:HD13	2.44	0.48
1:B:127:ILE:HG13	1:B:141:THR:HG22	1.94	0.48
1:A:227:SER:O	1:A:231:LYS:HG3	2.13	0.48
1:A:213:ARG:NH1	1:A:246:GLU:OE1	2.47	0.47
1:A:295:GLU:O	1:A:295:GLU:CD	2.53	0.47
1:A:77:ILE:CG1	1:B:77:ILE:HD11	2.42	0.47
1:B:250:LEU:CD2	1:B:363:TYR:CD2	2.97	0.47
1:A:141:THR:HG21	1:A:145:ARG:HA	1.95	0.47
1:B:210:THR:CG2	1:B:211:VAL:N	2.77	0.47
1:B:227:SER:OG	1:B:230:GLU:N	2.44	0.47
1:B:371:LEU:C	1:B:372:THR:HG23	2.34	0.47
1:B:124:SER:HB3	1:B:143:TYR:CG	2.50	0.47
1:B:216:ASP:OD1	1:B:280:SER:CB	2.63	0.47
1:B:335:ARG:CG	1:B:336:PHE:N	2.69	0.47
1:A:139:PHE:CE2	2:A:501:ANP:H1'	2.49	0.47
1:B:110:PHE:CE1	1:B:182:GLN:HB3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:ALA:O	1:B:275:LYS:N	2.47	0.46
1:B:411:MET:C	1:B:414:ILE:HG12	2.30	0.46
1:B:214:LYS:HG3	1:B:235:LEU:HD11	1.97	0.46
1:A:137:THR:HB	1:A:138:ARG:HB3	1.98	0.46
1:B:189:LEU:HD12	1:B:189:LEU:N	2.30	0.46
1:A:264:LEU:O	1:A:268:VAL:HG23	2.16	0.46
1:A:160:MET:O	1:A:164:LEU:HB2	2.16	0.46
1:A:97:GLU:HG3	1:A:187:TYR:CE2	2.51	0.45
1:B:349:TYR:CD1	1:B:366:ALA:HB2	2.51	0.45
1:B:236:PRO:HB2	1:B:238:PHE:CE1	2.51	0.45
1:A:110:PHE:CD1	1:A:182:GLN:HB3	2.52	0.45
1:B:235:LEU:HD13	1:B:235:LEU:O	2.17	0.45
1:A:274:LEU:O	1:A:276:ILE:HG13	2.16	0.45
1:A:166:LYS:HD3	1:A:274:LEU:CD2	2.47	0.45
1:B:99:CYS:N	1:B:100:PRO:HD3	2.32	0.44
1:A:189:LEU:N	1:A:189:LEU:HD12	2.32	0.44
1:B:223:ALA:O	1:B:224:ARG:HG3	2.17	0.44
1:A:220:SER:HB3	1:A:222:VAL:HG23	2.00	0.44
1:A:217:LEU:CB	1:A:411:MET:HE1	2.47	0.44
1:A:270:PHE:CE1	1:A:274:LEU:HD11	2.52	0.44
1:A:80:ASP:HB3	1:A:92:ARG:HE	1.82	0.44
1:B:213:ARG:HH22	1:B:246:GLU:HG3	1.83	0.44
1:A:215:TYR:HB3	1:A:217:LEU:HD21	1.99	0.44
1:B:214:LYS:HB2	1:B:236:PRO:O	2.18	0.44
1:B:261:LEU:HB3	1:B:265:LYS:HE2	2.00	0.43
1:A:268:VAL:CG1	1:A:404:SER:HA	2.48	0.43
1:A:106:LEU:HD23	1:A:106:LEU:HA	1.89	0.43
1:A:282:LEU:O	1:A:365:MET:HA	2.19	0.43
1:A:278:ASP:N	1:A:403:TYR:CE1	2.86	0.43
1:B:177:ASN:HD21	1:B:263:LYS:HD2	1.82	0.43
1:B:255:GLU:O	1:B:259:ASN:OD1	2.37	0.42
1:A:179:LEU:HG	1:A:263:LYS:HB3	2.00	0.42
2:B:501:ANP:O1G	2:B:501:ANP:O1B	2.37	0.42
1:A:217:LEU:HB2	1:A:411:MET:HE1	2.02	0.42
1:A:42:ILE:H	1:A:42:ILE:HD12	1.83	0.42
1:B:283:VAL:CG1	1:B:284:GLY:N	2.83	0.42
1:A:272:ALA:HB2	1:A:404:SER:HB3	2.01	0.42
1:A:98:TYR:O	1:A:99:CYS:C	2.57	0.42
1:A:129:SER:OG	1:A:139:PHE:HD1	2.02	0.42
1:A:141:THR:HG22	1:A:142:THR:O	2.19	0.42
1:A:139:PHE:CZ	2:A:501:ANP:HI'	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:LEU:HB2	1:A:411:MET:HE3	2.00	0.42
1:A:225:GLU:HG2	1:A:241:ASN:HB2	2.00	0.42
1:B:124:SER:HB3	1:B:143:TYR:CB	2.49	0.42
1:B:51:ASN:HB2	1:B:122:THR:HG21	2.01	0.42
1:B:250:LEU:HD23	1:B:363:TYR:CE2	2.54	0.42
1:B:71:PHE:CE2	1:B:165:LYS:HA	2.55	0.41
1:A:281:LEU:HB2	1:A:411:MET:SD	2.60	0.41
1:B:79:VAL:HG13	3:B:614:HOH:O	2.19	0.41
1:A:141:THR:HG22	1:A:142:THR:N	2.34	0.41
1:A:77:ILE:HG13	1:B:77:ILE:CD1	2.45	0.41
1:B:216:ASP:O	1:B:239:LYS:HA	2.20	0.41
1:A:272:ALA:HB2	1:A:404:SER:CB	2.51	0.41
1:A:281:LEU:HB3	1:A:411:MET:SD	2.60	0.41
1:A:123:ARG:HG3	1:A:123:ARG:NH1	2.36	0.41
1:A:124:SER:HB3	1:A:143:TYR:CG	2.56	0.41
1:B:40:GLU:OE1	1:B:138:ARG:NH2	2.53	0.41
1:B:243:PHE:CD2	1:B:243:PHE:C	2.94	0.41
1:A:350:ALA:HA	1:A:363:TYR:O	2.21	0.41
1:A:407:PHE:CD2	1:A:407:PHE:C	2.93	0.41
2:A:501:ANP:O1A	2:A:501:ANP:O1G	2.39	0.41
1:B:159:GLU:HA	1:B:159:GLU:OE2	2.20	0.41
1:A:54:ILE:HG21	1:A:118:GLN:HB2	2.03	0.40
1:B:336:PHE:CD2	1:B:336:PHE:C	2.93	0.40
1:A:298:VAL:O	1:A:302:ALA:HB2	2.21	0.40
1:A:170:PHE:CE1	1:A:180:LEU:HD12	2.57	0.40
1:A:79:VAL:O	1:A:92:ARG:HA	2.22	0.40
1:B:47:MET:HE1	1:B:125:ALA:N	2.37	0.40
1:B:40:GLU:O	1:B:43:LEU:HB2	2.22	0.40

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	312/393 (79%)	295 (95%)	15 (5%)	2 (1%)	25	50
1	B	290/393 (74%)	272 (94%)	17 (6%)	1 (0%)	41	66
All	All	602/786 (77%)	567 (94%)	32 (5%)	3 (0%)	29	54

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	358	PRO
1	B	358	PRO
1	A	339	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	297/352 (84%)	280 (94%)	17 (6%)	20	44
1	B	280/352 (80%)	262 (94%)	18 (6%)	17	39
All	All	577/704 (82%)	542 (94%)	35 (6%)	18	41

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	ILE
1	A	123	ARG
1	A	127	ILE
1	A	137	THR
1	A	165	LYS
1	A	173	GLU
1	A	174	CYS
1	A	177	ASN
1	A	202	ARG
1	A	222	VAL
1	A	240	ASP
1	A	248	GLN
1	A	280	SER

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Mol	Chain	Res	Type
1	A	348	VAL
1	A	351	MET
1	A	404	SER
1	A	415	LEU
1	B	39	SER
1	B	42	ILE
1	B	56	GLU
1	B	76	LYS
1	B	77	ILE
1	B	80	ASP
1	B	87	GLU
1	B	104	ARG
1	B	150	LYS
1	B	227	SER
1	B	228	ASP
1	B	234	ASP
1	B	240	ASP
1	B	256	SER
1	B	281	LEU
1	B	289	ASP
1	B	336	PHE
1	B	356	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	207	HIS

### 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

3 ligands are modelled in this entry.

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	501	-	29,33,33	2.17	12 (41%)	31,52,52	2.82	7 (22%)
2	ANP	B	501	-	29,33,33	2.17	11 (37%)	31,52,52	2.69	8 (25%)
2	ANP	A	502	-	29,33,33	2.52	14 (48%)	31,52,52	3.45	17 (54%)

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	501	-	-	5/14/38/38	0/3/3/3
2	ANP	B	501	-	-	5/14/38/38	0/3/3/3
2	ANP	A	502	-	-	8/14/38/38	0/3/3/3

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	ANP	PB-O1B	6.57	1.56	1.46
2	A	502	ANP	PB-O1B	5.60	1.55	1.46
2	A	501	ANP	PB-O1B	5.56	1.55	1.46
2	A	502	ANP	PA-O2A	3.86	1.73	1.55
2	A	502	ANP	C2'-C1'	-3.86	1.47	1.53
2	B	501	ANP	C5'-C4'	3.73	1.63	1.51
2	A	501	ANP	C5'-C4'	3.66	1.63	1.51
2	A	502	ANP	PA-O5'	3.56	1.73	1.59
2	A	502	ANP	C2'-C3'	-3.40	1.44	1.53
2	A	501	ANP	O3'-C3'	-3.39	1.35	1.43
2	A	502	ANP	PG-O1G	3.38	1.51	1.46
2	A	502	ANP	PB-O3A	-3.32	1.54	1.59
2	A	502	ANP	C6-N6	3.25	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	502	ANP	O3'-C3'	-3.06	1.35	1.43
2	A	501	ANP	O4'-C1'	-3.01	1.36	1.41
2	B	501	ANP	PG-O1G	2.98	1.50	1.46
2	A	502	ANP	C3'-C4'	2.95	1.60	1.53
2	A	502	ANP	PB-N3B	2.82	1.70	1.63
2	A	501	ANP	C2'-C1'	-2.79	1.49	1.53
2	B	501	ANP	PA-O2A	2.75	1.68	1.55
2	B	501	ANP	C2'-C3'	-2.72	1.45	1.53
2	B	501	ANP	C6-N6	2.71	1.43	1.34
2	A	502	ANP	PA-O1A	2.65	1.60	1.50
2	B	501	ANP	O3'-C3'	-2.61	1.36	1.43
2	A	501	ANP	PB-O3A	-2.55	1.55	1.59
2	A	501	ANP	O2'-C2'	-2.52	1.37	1.43
2	A	501	ANP	C2'-C3'	-2.41	1.46	1.53
2	B	501	ANP	PA-O5'	2.41	1.69	1.59
2	A	501	ANP	C8-N7	-2.37	1.30	1.34
2	A	502	ANP	C2-N3	2.30	1.35	1.32
2	A	501	ANP	PA-O2A	2.22	1.65	1.55
2	A	501	ANP	C5-N7	-2.20	1.31	1.39
2	A	501	ANP	C6-C5	-2.17	1.35	1.43
2	B	501	ANP	O2'-C2'	-2.17	1.37	1.43
2	A	502	ANP	PG-N3B	2.12	1.68	1.63
2	B	501	ANP	C2-N3	2.08	1.35	1.32
2	B	501	ANP	PA-O1A	2.03	1.58	1.50

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	ANP	O5'-PA-O1A	-8.86	74.43	109.07
2	B	501	ANP	O5'-PA-O1A	-7.68	79.08	109.07
2	A	502	ANP	O5'-PA-O1A	-7.56	79.53	109.07
2	A	502	ANP	O2A-PA-O1A	-7.20	76.63	112.24
2	B	501	ANP	O2A-PA-O1A	-7.18	76.72	112.24
2	A	501	ANP	O2A-PA-O1A	-6.84	78.42	112.24
2	A	502	ANP	N3-C2-N1	-6.76	118.11	128.68
2	B	501	ANP	N3-C2-N1	-6.29	118.85	128.68
2	A	501	ANP	N3-C2-N1	-5.94	119.39	128.68
2	A	502	ANP	O2A-PA-O5'	5.40	132.85	107.75
2	A	502	ANP	C5'-C4'-C3'	5.05	134.09	115.18
2	A	501	ANP	C3'-C2'-C1'	4.37	107.55	100.98
2	A	502	ANP	N6-C6-N1	4.23	127.34	118.57
2	A	502	ANP	PA-O3A-PB	-3.99	118.57	132.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	502	ANP	C5-C6-N6	-3.94	114.37	120.35
2	A	502	ANP	O4'-C1'-C2'	3.88	112.60	106.93
2	B	501	ANP	C5'-C4'-C3'	3.76	129.27	115.18
2	A	501	ANP	O4'-C4'-C5'	3.64	121.34	109.37
2	A	502	ANP	C1'-N9-C4	-3.56	120.39	126.64
2	A	502	ANP	O3'-C3'-C4'	3.56	121.33	111.05
2	B	501	ANP	O4'-C4'-C5'	3.46	120.76	109.37
2	A	502	ANP	C2-N1-C6	3.35	124.49	118.75
2	A	501	ANP	O4'-C1'-C2'	3.34	111.80	106.93
2	A	502	ANP	O2'-C2'-C1'	-3.20	99.04	110.85
2	A	502	ANP	C3'-C2'-C1'	2.95	105.43	100.98
2	A	501	ANP	C5'-C4'-C3'	2.85	125.86	115.18
2	B	501	ANP	C2-N1-C6	2.65	123.29	118.75
2	A	502	ANP	O3G-PG-O1G	-2.63	106.83	113.45
2	A	502	ANP	O5'-C5'-C4'	-2.61	100.01	108.99
2	B	501	ANP	PA-O3A-PB	-2.58	123.54	132.62
2	A	502	ANP	O1B-PB-N3B	-2.36	108.29	111.77
2	B	501	ANP	C3'-C2'-C1'	2.03	104.04	100.98

There are no chirality outliers.

All (18) torsion outliers are listed below:

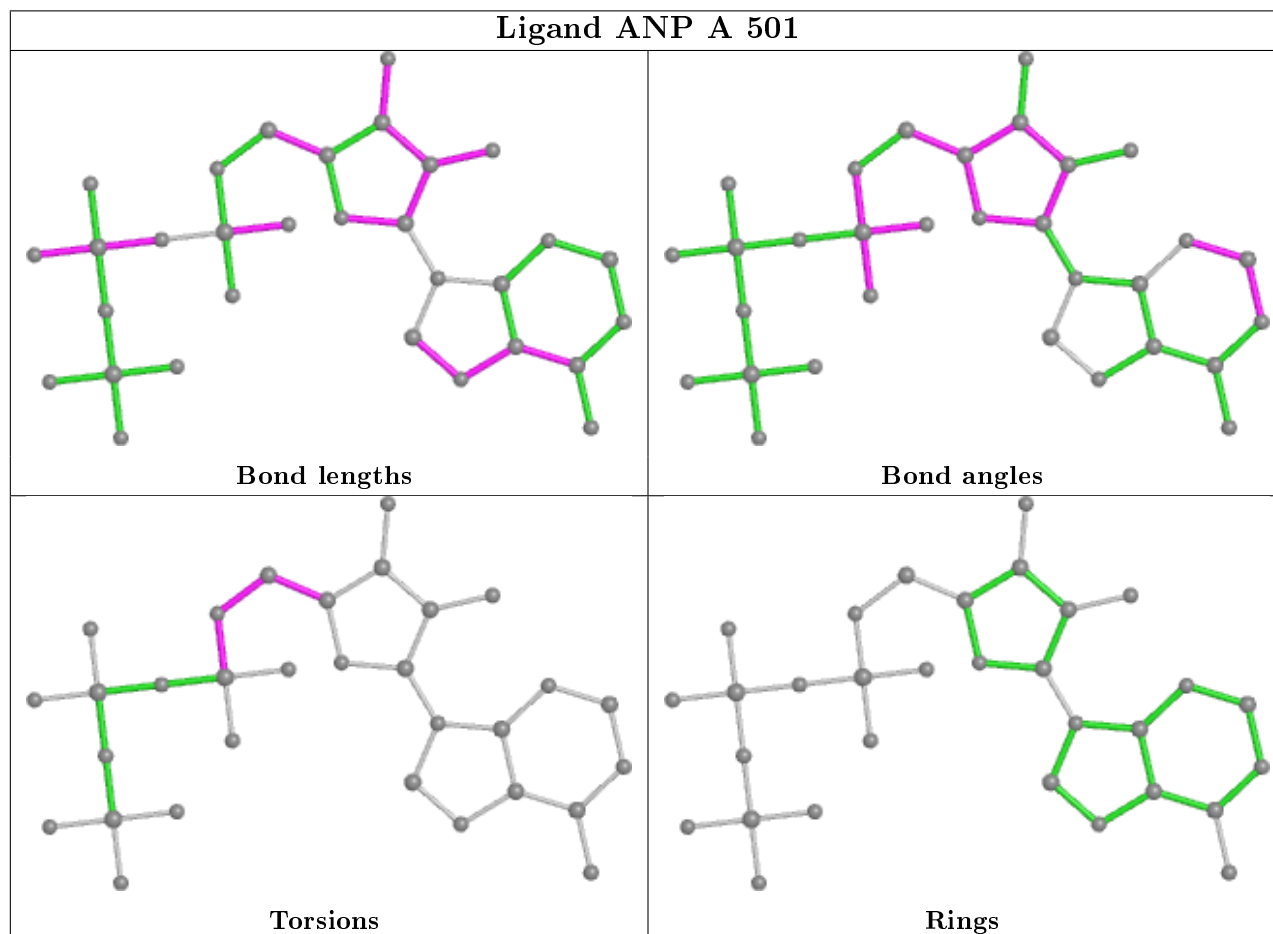
Mol	Chain	Res	Type	Atoms
2	A	501	ANP	C5'-O5'-PA-O1A
2	A	501	ANP	C5'-O5'-PA-O2A
2	A	501	ANP	C5'-O5'-PA-O3A
2	A	501	ANP	C4'-C5'-O5'-PA
2	A	501	ANP	O4'-C4'-C5'-O5'
2	B	501	ANP	PA-O3A-PB-O1B
2	B	501	ANP	C5'-O5'-PA-O3A
2	A	502	ANP	PB-N3B-PG-O1G
2	A	502	ANP	PG-N3B-PB-O1B
2	A	502	ANP	PG-N3B-PB-O3A
2	A	502	ANP	PA-O3A-PB-O2B
2	A	502	ANP	C5'-O5'-PA-O1A
2	A	502	ANP	C4'-C5'-O5'-PA
2	B	501	ANP	C3'-C4'-C5'-O5'
2	A	502	ANP	O4'-C4'-C5'-O5'
2	B	501	ANP	C5'-O5'-PA-O1A
2	B	501	ANP	O4'-C4'-C5'-O5'
2	A	502	ANP	PB-O3A-PA-O1A

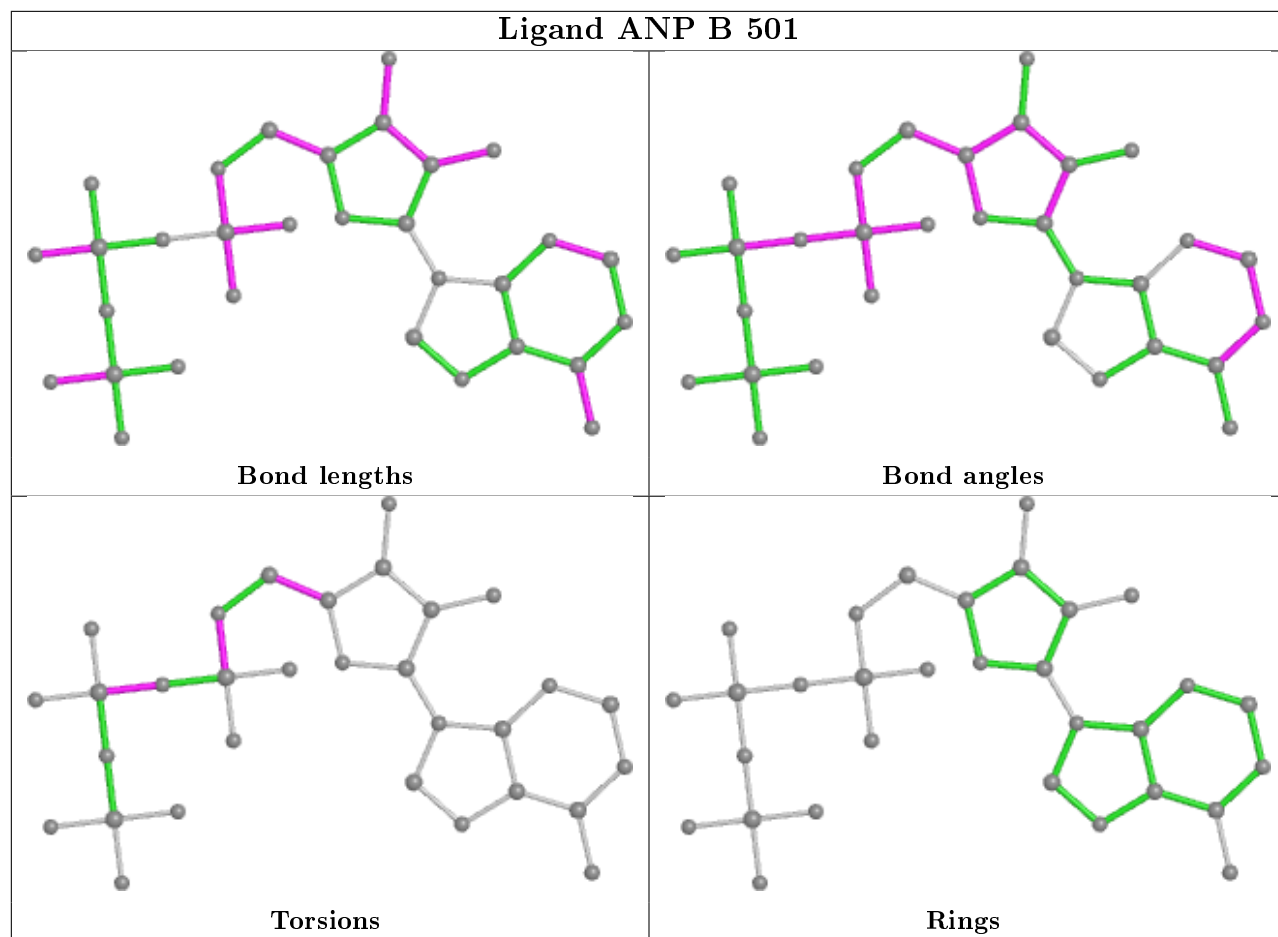
There are no ring outliers.

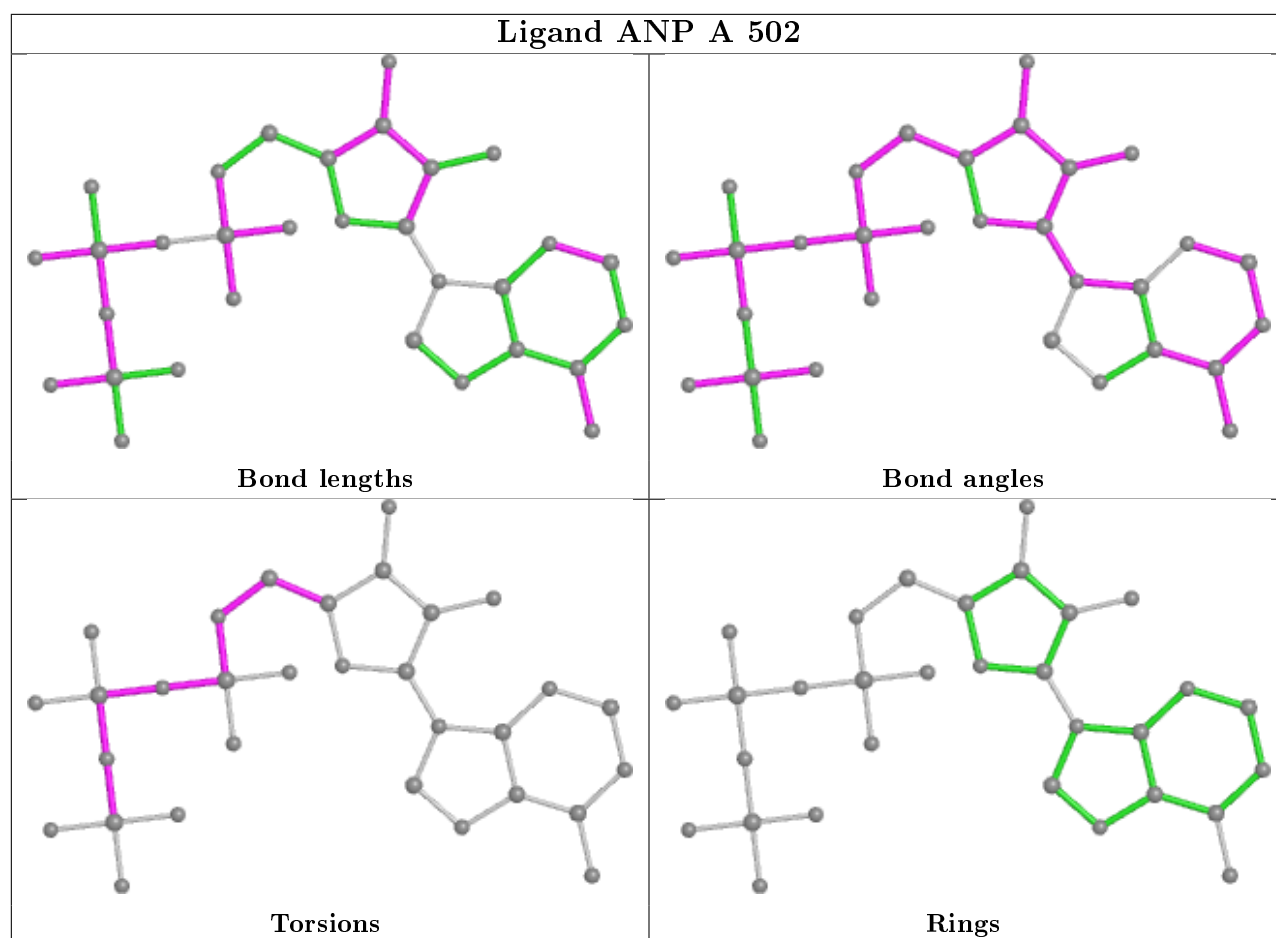
3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	ANP	8	0
2	B	501	ANP	2	0
2	A	502	ANP	2	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

### 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	320/393 (81%)	0.78	11 (3%) 45 45	39, 78, 132, 181	0
1	B	302/393 (76%)	1.00	33 (10%) 5 4	28, 86, 158, 173	0
All	All	622/786 (79%)	0.89	44 (7%) 16 14	28, 81, 151, 181	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	251	HIS	5.7
1	B	400	PRO	5.5
1	B	238	PHE	4.3
1	B	413	ASN	4.3
1	B	250	LEU	4.2
1	B	215	TYR	4.2
1	B	233	LYS	4.2
1	B	230	GLU	4.0
1	B	354	HIS	3.9
1	B	224	ARG	3.5
1	B	246	GLU	3.3
1	B	265	LYS	3.2
1	A	405	LYS	3.2
1	A	402	GLN	3.1
1	A	304	ASP	3.1
1	B	235	LEU	3.1
1	A	274	LEU	3.0
1	B	336	PHE	2.9
1	B	407	PHE	2.9
1	B	86	LYS	2.8
1	B	258	LYS	2.8
1	B	411	MET	2.7
1	B	241	ASN	2.6
1	A	296	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	268	VAL	2.6
1	A	414	ILE	2.6
1	B	245	ASN	2.6
1	A	403	TYR	2.5
1	B	36	PHE	2.5
1	A	291	ALA	2.5
1	B	277	MET	2.3
1	B	33	VAL	2.3
1	B	229	LYS	2.3
1	B	285	ILE	2.2
1	B	415	LEU	2.2
1	B	416	THR	2.2
1	A	411	MET	2.1
1	B	34	LYS	2.1
1	B	270	PHE	2.1
1	B	406	ARG	2.1
1	A	56	GLU	2.1
1	B	363	TYR	2.1
1	A	188	ARG	2.0
1	B	100	PRO	2.0

## 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](#)

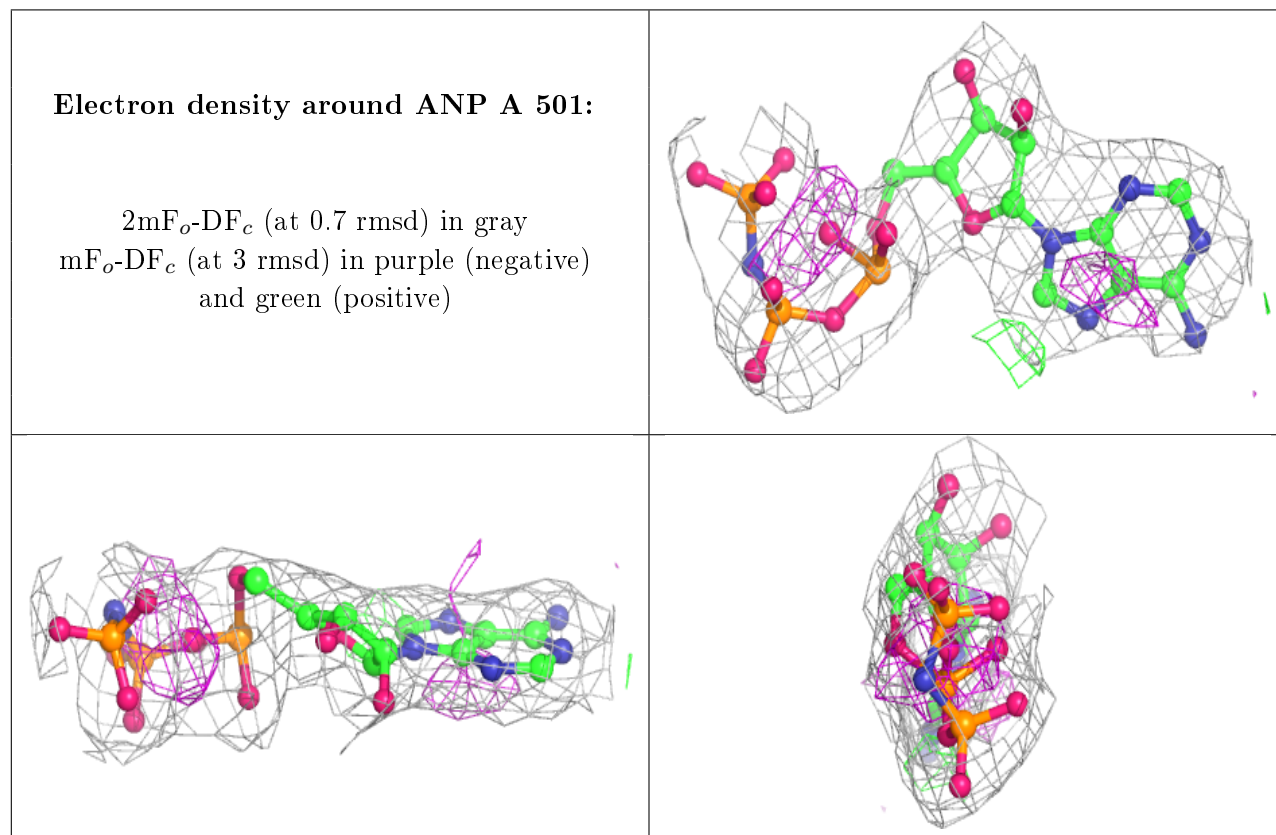
There are no carbohydrates in this entry.

## 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, 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ANP	A	501	31/31	0.80	0.21	69,117,221,271	0
2	ANP	A	502	31/31	0.80	0.22	41,87,161,228	0
2	ANP	B	501	31/31	0.81	0.23	110,129,249,301	0

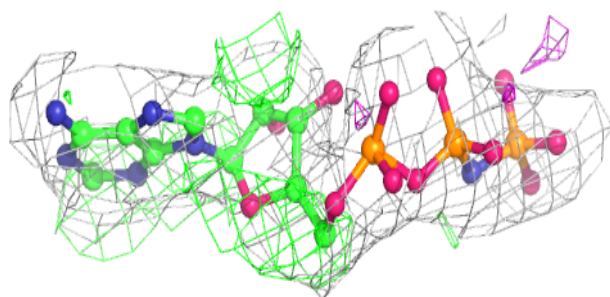
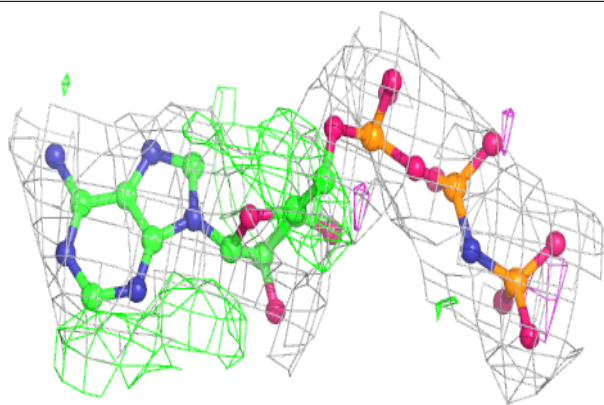
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



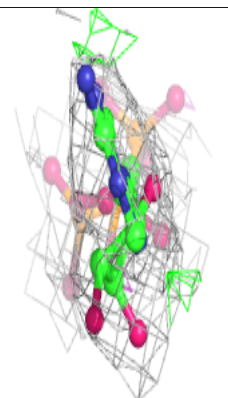
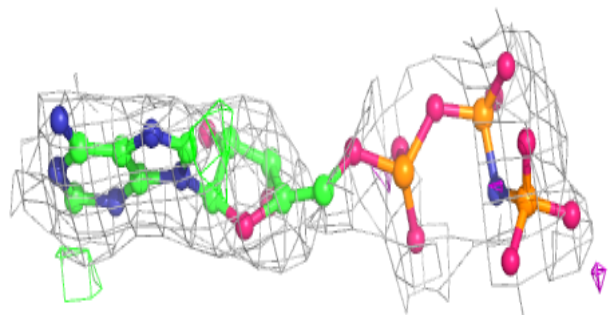
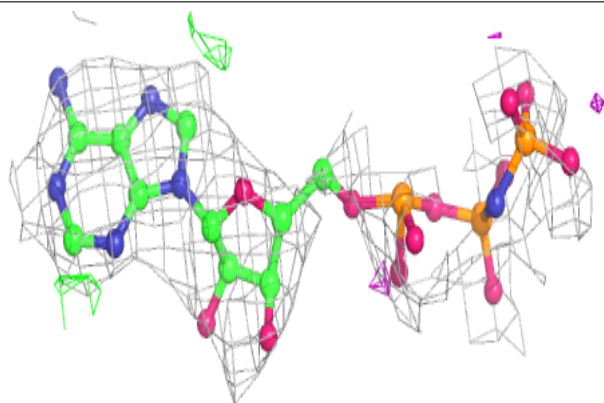


**Electron density around ANP A 502:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around ANP B 501:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.