



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 03:33 PM BST

PDB ID : 4D4I  
Title : Understanding bi-specificity of A-domains  
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Deposited on : 2014-10-29  
Resolution : 2.00 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 : **FAILED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.14.4.dev1

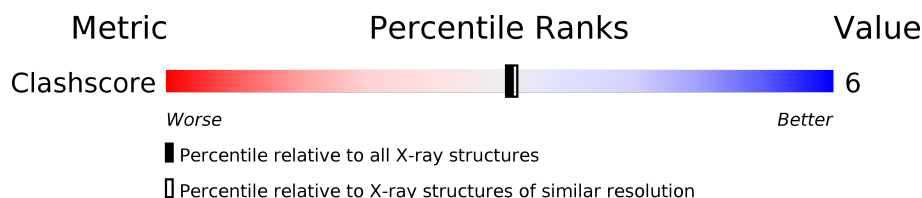
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	9178 (2.00-2.00)

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  $\geq 3$ , 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  $\leq 5\%$

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	573	 76% 8% 16%

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
2	ARG	A	1491	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4064 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.

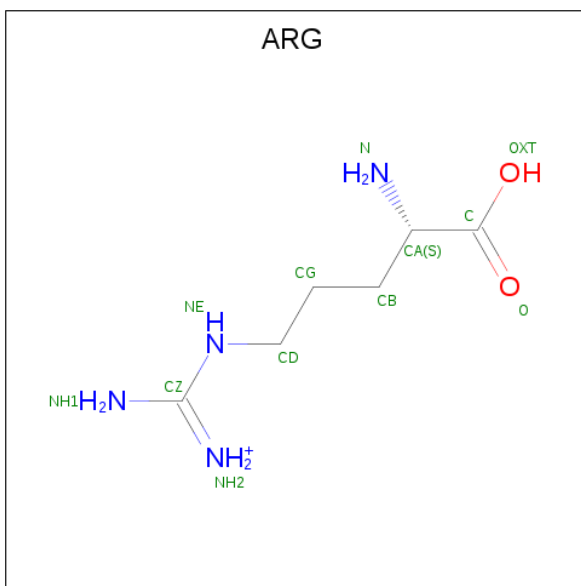
- Molecule 1 is a protein called APNAA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	481	3838	2458	638	732	10	0	8	0

There are 26 discrepancies between the modelled and reference sequences:

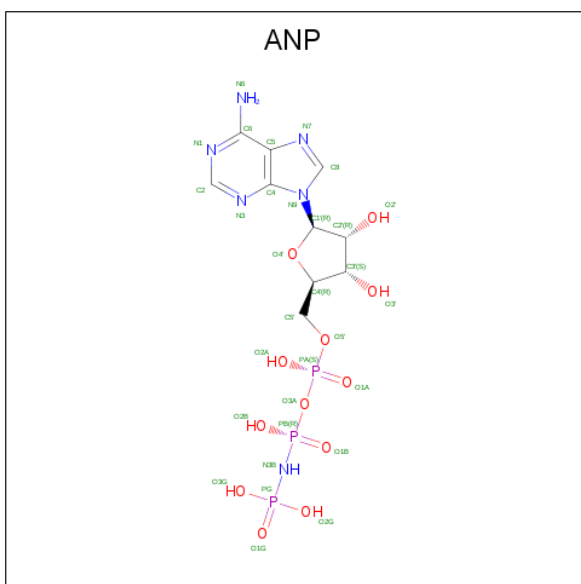
Chain	Residue	Modelled	Actual	Comment	Reference
A	-25	MET	-	expression tag	UNP G0WVH3
A	-24	LYS	-	expression tag	UNP G0WVH3
A	-23	HIS	-	expression tag	UNP G0WVH3
A	-22	HIS	-	expression tag	UNP G0WVH3
A	-21	HIS	-	expression tag	UNP G0WVH3
A	-20	HIS	-	expression tag	UNP G0WVH3
A	-19	HIS	-	expression tag	UNP G0WVH3
A	-18	HIS	-	expression tag	UNP G0WVH3
A	-17	PRO	-	expression tag	UNP G0WVH3
A	-16	MET	-	expression tag	UNP G0WVH3
A	-15	SER	-	expression tag	UNP G0WVH3
A	-14	ASP	-	expression tag	UNP G0WVH3
A	-13	TYR	-	expression tag	UNP G0WVH3
A	-12	ASP	-	expression tag	UNP G0WVH3
A	-11	ILE	-	expression tag	UNP G0WVH3
A	-10	PRO	-	expression tag	UNP G0WVH3
A	-9	THR	-	expression tag	UNP G0WVH3
A	-8	THR	-	expression tag	UNP G0WVH3
A	-7	GLU	-	expression tag	UNP G0WVH3
A	-6	ASN	-	expression tag	UNP G0WVH3
A	-5	LEU	-	expression tag	UNP G0WVH3
A	-4	TYR	-	expression tag	UNP G0WVH3
A	-3	PHE	-	expression tag	UNP G0WVH3
A	-2	GLN	-	expression tag	UNP G0WVH3
A	-1	GLY	-	expression tag	UNP G0WVH3
A	0	ALA	-	expression tag	UNP G0WVH3

- Molecule 2 is ARGinine (three-letter code: ARG) (formula:  $C_6H_{15}N_4O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			12	6	4	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	1
			62	20	12	24	6		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		

- Molecule 6 is water.

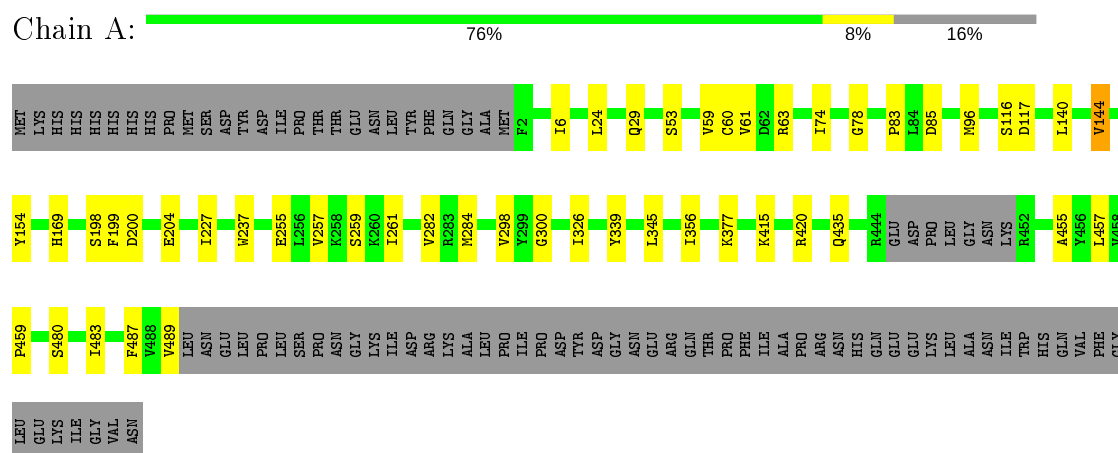
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	145	Total	O	0	0
			145	145		

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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.

Note EDS failed to run properly.

- Molecule 1: APNAA1



## 4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.42Å 82.69Å 90.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.94 – 2.00	Depositor
% Data completeness (in resolution range)	100.0 (60.94-2.00)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.34 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.190 , 0.245	Depositor
Wilson B-factor (Å <sup>2</sup> )	29.0	Xtriage
Anisotropy	0.518	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4064	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% 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: GOL, 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	0.61	0/3933	0.73	2/5357 (0.0%)

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	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	144	VAL	CB-CA-C	-5.06	101.79	111.40
1	A	200	ASP	CB-CG-OD1	5.02	122.82	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	116	SER	Peptide
1	A	117[A]	ASP	Peptide
1	A	117[B]	ASP	Peptide

### 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	3838	0	3896	40	0
2	A	12	0	12	6	0
3	A	62	0	26	7	0
4	A	6	0	8	1	0
5	A	1	0	0	0	0
6	A	145	0	0	8	0
All	All	4064	0	3942	44	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 6.

All (44) 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:300:GLY:O	2:A:1491:ARG:N	1.71	1.24
2:A:1491:ARG:NH2	6:A:2096:HOH:O	1.68	0.93
3:A:1490[A]:ANP:O3G	6:A:2068:HOH:O	1.88	0.91
1:A:435:GLN:HB2	6:A:2144:HOH:O	1.79	0.82
1:A:345:LEU:O	4:A:1492:GOL:O3	2.07	0.72
1:A:457:LEU:O	1:A:489:VAL:HA	1.92	0.69
1:A:204:GLU:OE1	2:A:1491:ARG:NH1	2.26	0.69
1:A:63:ARG:NH1	6:A:2035:HOH:O	2.15	0.66
1:A:377:LYS:HE3	6:A:2135:HOH:O	1.98	0.63
1:A:259:SER:HB2	1:A:261:ILE:HG13	1.80	0.62
1:A:6:ILE:H	1:A:169:HIS:HD2	1.46	0.61
1:A:298:VAL:O	2:A:1491:ARG:HG2	2.02	0.60
1:A:24[B]:LEU:HD23	1:A:29:GLN:HB3	1.86	0.58
1:A:53:SER:HA	1:A:78:GLY:O	2.05	0.56
1:A:59[A]:VAL:HG12	1:A:61:VAL:HG22	1.88	0.55
1:A:24[A]:LEU:CD2	1:A:237:TRP:CZ3	2.92	0.53
1:A:480:SER:HA	1:A:483:ILE:HD12	1.93	0.51
1:A:60:CYS:SG	6:A:2032:HOH:O	2.12	0.49
1:A:169:HIS:HE1	6:A:2039:HOH:O	1.96	0.49
1:A:24[A]:LEU:HD22	1:A:237:TRP:CZ3	2.47	0.49
1:A:435:GLN:CB	6:A:2144:HOH:O	2.51	0.49
2:A:1491:ARG:OXT	2:A:1491:ARG:HG3	2.15	0.47
1:A:85:ASP:HB2	1:A:198:SER:OG	2.15	0.46
1:A:24[A]:LEU:CD2	1:A:237:TRP:CH2	2.99	0.46
1:A:420:ARG:HB3	3:A:1490[A]:ANP:PG	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:GLY:HA2	1:A:144:VAL:HG13	1.98	0.45
1:A:227:ILE:HB	1:A:255:GLU:HG2	1.99	0.44
1:A:415:LYS:NZ	3:A:1490[B]:ANP:O2B	2.30	0.44
1:A:420:ARG:HB3	3:A:1490[A]:ANP:O2G	2.18	0.43
1:A:96:MET:HE3	1:A:154:TYR:HB2	2.00	0.43
1:A:459:PRO:CD	1:A:489:VAL:HG13	2.48	0.43
1:A:282:VAL:HG21	1:A:326:ILE:HG13	2.00	0.43
2:A:1491:ARG:OXT	3:A:1490[B]:ANP:O1G	2.38	0.42
1:A:59[B]:VAL:HG23	1:A:83:PRO:HA	2.00	0.42
1:A:455:ALA:HB3	1:A:487:PHE:CD2	2.54	0.42
1:A:420:ARG:HB3	3:A:1490[A]:ANP:N3B	2.34	0.42
1:A:199:PHE:HB3	3:A:1490[B]:ANP:PG	2.60	0.41
1:A:24[A]:LEU:HD21	1:A:237:TRP:CZ3	2.56	0.41
1:A:257:VAL:HG11	1:A:284:MET:HG2	2.03	0.40
1:A:59[A]:VAL:CG2	1:A:74:ILE:CD1	2.99	0.40
1:A:140:LEU:HD12	1:A:140:LEU:N	2.35	0.40
1:A:459:PRO:HD2	1:A:489:VAL:HG13	2.03	0.40
1:A:6:ILE:H	1:A:169:HIS:CD2	2.33	0.40
1:A:339:TYR:O	1:A:356:ILE:HA	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 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

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	1490[A]	5	29,33,33	2.10	6 (20%)	31,52,52	2.05	5 (16%)
3	ANP	A	1490[B]	5	29,33,33	1.95	7 (24%)	31,52,52	1.81	8 (25%)
4	GOL	A	1492	-	5,5,5	0.19	0	5,5,5	0.77	0
2	ARG	A	1491	-	7,11,11	0.54	0	6,13,13	0.62	0

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	1490[A]	5	-	2/14/38/38	0/3/3/3
3	ANP	A	1490[B]	5	-	4/14/38/38	0/3/3/3
4	GOL	A	1492	-	-	0/4/4/4	-
2	ARG	A	1491	-	-	1/7/11/11	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1490[A]	ANP	PB-N3B	5.52	1.77	1.63
3	A	1490[A]	ANP	PG-N3B	5.36	1.77	1.63
3	A	1490[B]	ANP	PG-N3B	4.58	1.75	1.63
3	A	1490[A]	ANP	PB-O1B	4.51	1.53	1.46
3	A	1490[B]	ANP	PB-N3B	4.30	1.74	1.63
3	A	1490[B]	ANP	PG-O1G	3.70	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1490[B]	ANP	PB-O3A	3.64	1.63	1.59
3	A	1490[B]	ANP	PB-O1B	3.62	1.51	1.46
3	A	1490[A]	ANP	PG-O1G	3.18	1.51	1.46
3	A	1490[A]	ANP	PB-O3A	2.45	1.62	1.59
3	A	1490[A]	ANP	PG-O3G	-2.23	1.50	1.56
3	A	1490[B]	ANP	C5-C4	2.13	1.46	1.40
3	A	1490[B]	ANP	C2'-C1'	-2.04	1.50	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1490[A]	ANP	O1G-PG-N3B	-7.30	101.01	111.77
3	A	1490[B]	ANP	O1B-PB-N3B	-4.79	104.72	111.77
3	A	1490[A]	ANP	O2B-PB-O1B	4.66	119.68	109.92
3	A	1490[A]	ANP	N3-C2-N1	-4.35	121.88	128.68
3	A	1490[B]	ANP	N3-C2-N1	-3.93	122.53	128.68
3	A	1490[B]	ANP	O2B-PB-O1B	3.45	117.15	109.92
3	A	1490[B]	ANP	O3G-PG-O2G	3.13	115.98	107.64
3	A	1490[B]	ANP	O1G-PG-N3B	-2.58	107.98	111.77
3	A	1490[A]	ANP	O1B-PB-N3B	-2.52	108.06	111.77
3	A	1490[A]	ANP	C2-N1-C6	2.51	123.04	118.75
3	A	1490[B]	ANP	C2-N1-C6	2.45	122.95	118.75
3	A	1490[B]	ANP	C4-C5-N7	-2.40	106.89	109.40
3	A	1490[B]	ANP	O2B-PB-O3A	2.32	112.39	104.64

There are no chirality outliers.

All (7) torsion outliers are listed below:

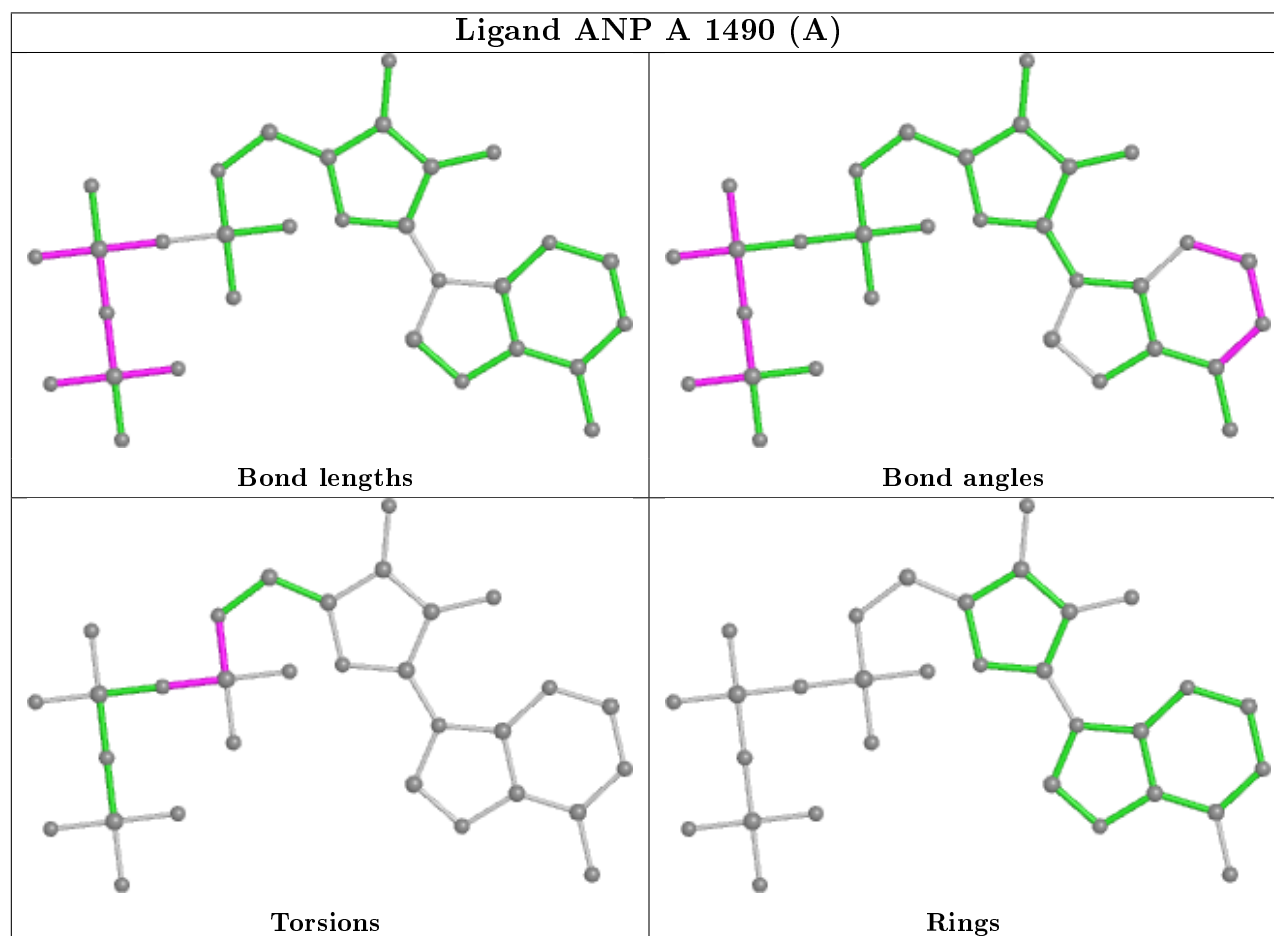
Mol	Chain	Res	Type	Atoms
3	A	1490[B]	ANP	PB-N3B-PG-O1G
3	A	1490[B]	ANP	PG-N3B-PB-O1B
3	A	1490[B]	ANP	C5'-O5'-PA-O1A
3	A	1490[B]	ANP	C5'-O5'-PA-O3A
3	A	1490[A]	ANP	PB-O3A-PA-O1A
2	A	1491	ARG	CG-CD-NE-CZ
3	A	1490[A]	ANP	C5'-O5'-PA-O1A

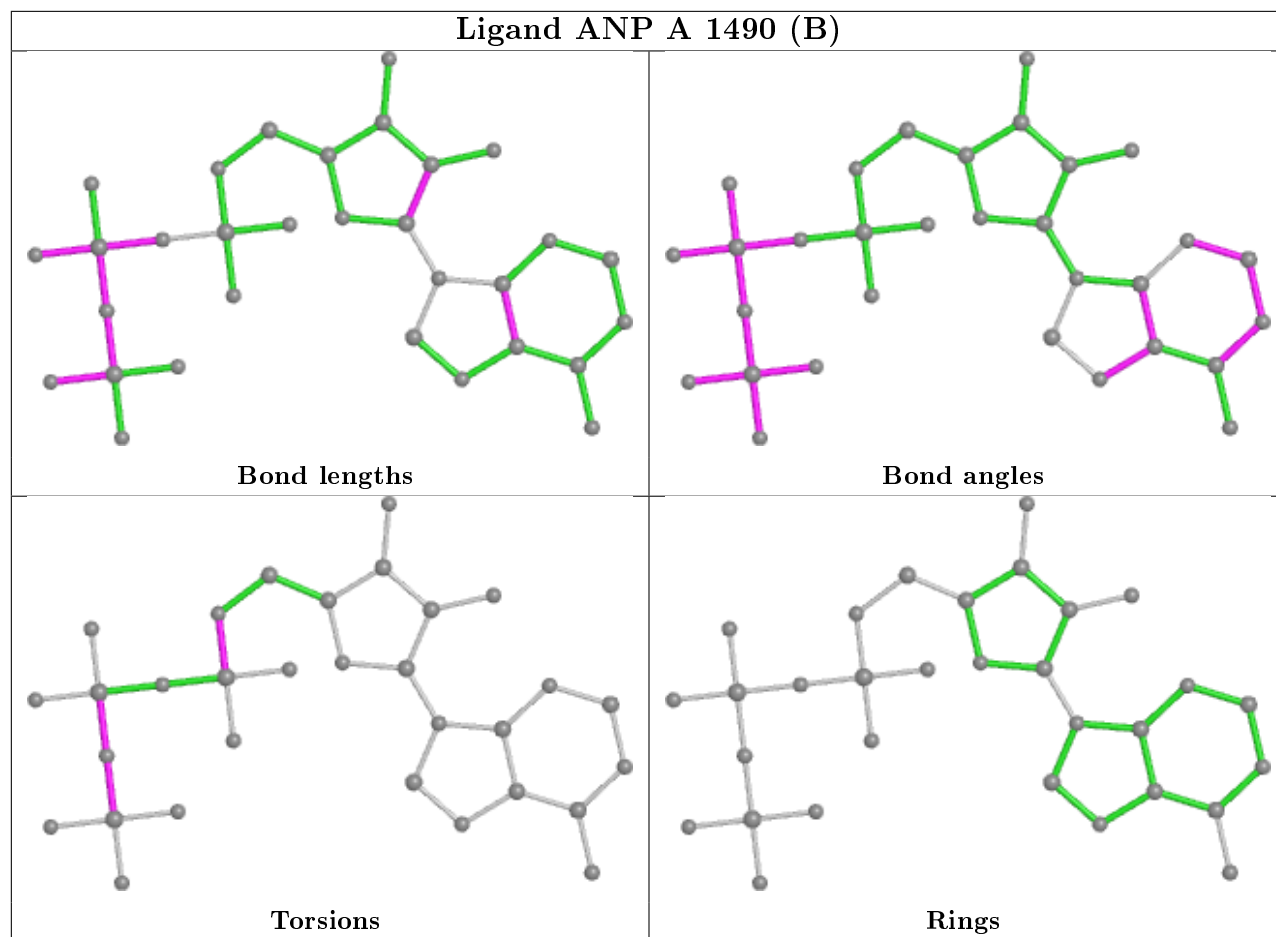
There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1490[A]	ANP	4	0
3	A	1490[B]	ANP	3	0
4	A	1492	GOL	1	0
2	A	1491	ARG	6	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

EDS failed to run properly - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

### 6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

### 6.4 Ligands

EDS failed to run properly - this section is therefore empty.

### 6.5 Other polymers

EDS failed to run properly - this section is therefore empty.