



## wwPDB EM Validation Summary Report ⓘ

Jul 16, 2025 – 02:21 AM JST

PDB ID : 9IZ0 / pdb\_00009iz0  
EMDB ID : EMD-61006  
Title : ATM/Tel1 bound to CHK2 peptide  
Authors : Wang, P.  
Deposited on : 2024-07-31  
Resolution : 3.63 Å(reported)

This is a wwPDB EM Validation Summary 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/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis	: <b>FAILED</b>
Mogul	: 1.8.5 (274361), CSD as541be (2020)
MolProbity	: 4-5-2 with Phenix2.0rc1
buster-report	: 1.1.7 (2018)
Percentile statistics	: 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	: <b>FAILED</b>
Ideal geometry (proteins)	: Engh & Huber (2001)
Ideal geometry (DNA, RNA)	: Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: 2.44

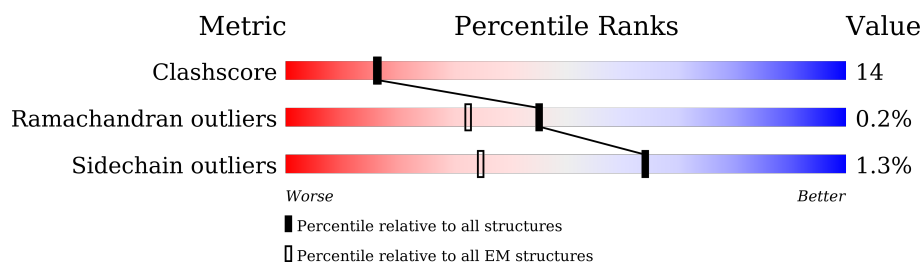
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.63 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	F	8	62% 38%
2	A	2812	68% 18% 14%
2	B	2812	68% 18% 14%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 32048 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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.

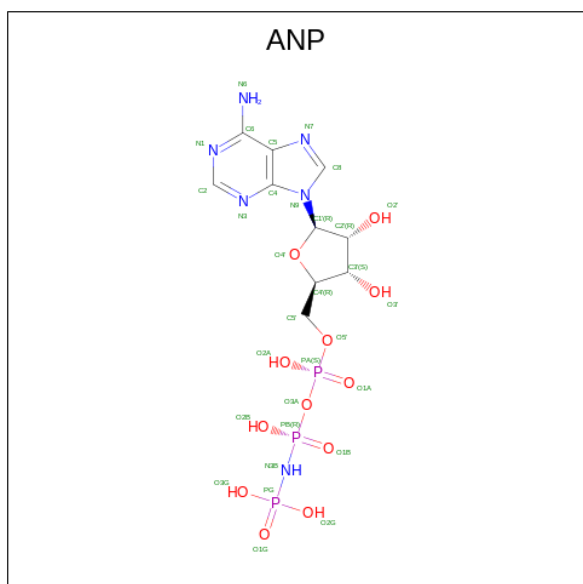
- Molecule 1 is a protein called VAL-SER-THR-GLN-GLU-LEU-TYR-SER.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	F	8	Total	C	N	O	0	0
			64	40	9	15		

- Molecule 2 is a protein called Serine/threonine-protein kinase tel1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	2430	Total	C	N	O	S	0	0
			15929	10030	2839	3040	20		
2	B	2424	Total	C	N	O	S	0	0
			15993	10091	2847	3035	20		

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



*Continued from previous page...*

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



- Molecule 2: Serine/threonine-protein kinase tel1

Chain B:



MET	THR	SER	LEU	ASN	ASP	ILE	VAL	ASN	LYS	LEU	SER	SER	LYS	ILE	LYS	THR	ARG	SER	ASP	ALA	ALA	LEU	GLN	ASN	LEU	ARG	SER	SER	TYR	ILE	ILE	TYR	SER	ARG	ARG	ASN	GLY	ASN	SER	LEU	SER	ASN	GLN	GLU	ASP	ALA	ALA	LEU	ILE	ILE	GLU	LYS	GLU	TRP	TYR
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Y2165	I2053	F1967	E1785	L1685	A1588	I1474	V1370	LYS	D1043	GLY	ALA	ILE
M2167	A2060	Y1968	F1790	L1686	L1591	E1475	L1371	TYR	F1047	CYS	SER	SER
A2169	V2063	A1969	F1790	S1687	L1591	E1475	L1371	GLN	GLN	TYR	GLN	ALA
N2174	V2063	D1973	I1793	Y1689	Y1595	N1478	R1375	ARG	S1066	PHE	GLN	HIS
S2178	L2066	K1975	H1794	M1690	ASP	H1485	Q1384	ASN	I1066	GLY	ASN	GLY
L2181	S2067	F1976	H1794	V1691	T1597	PHE	L1386	ILE	R1093	SER	GLN	LYS
T2182	L2070	L1977	Y1819	GLY	L1598	LEU	L1387	ILE	S1094	ASP	LYS	ARG
M2188	D2075	R1978	Y1820	S1694	L1599	K1488	L1388	ASP	K1102	GLU	GLN	ILE
Y2192	L2076	R1979	E1825	I1697	D1600	R1489	GLU	ASP	L1103	T806	LYS	SER
F2193	A2077	Q1984	M1830	I1698	I1603	I1490	I1390	ALA	F716	THR	LYS	LYS
E2194	D2086	F1985	M1830	I1698	I1603	I1490	I1390	LEU	S417	CYS	ALA	SER
L2199	D2086	M1986	M1830	I1698	I1603	I1490	I1390	LEU	S417	GLN	GLN	GLN
Q2200	S2089	A1835	A1835	I1702	M1809	F1500	K1399	GLN	S491	PHE	HIS	SER
L2201	S2090	S1841	S1841	H1703	PHE	W1501	P1400	GLU	S491	GLN	ASP	GLU
L2202	L2093	P1842	P1842	L1704	GLU	Q1502	F1403	VAL	M493	VAL	VAL	GLN
E2203	L2093	I1845	I1845	E1708	GLY	L1512	F1403	SER	L503	ARG	LEU	LEU
R2204	L2106	M1857	M1857	N1715	HIS	W1520	ASP	THR	A504	VAL	GLN	ASP
SER	E2107	K1997	K1997	K1716	Q1617	C1521	TYR	GLY	A505	VAL	ILE	ILE
VAL	E2108	Q1998	Q1998	Q1717	F1625	Y1523	F1406	GLU	A505	ALA	SER	SER
ASN	S2109	ASP	ASP	Q1718	P1626	K1524	F1412	ASN	S507	ALA	TYR	TYR
ALA	L2110	GLU	GLU	K1719	K1627	A1525	L1417	THR	T515	LEU	LEU	LEU
ILE	N2114	G1961	G1961	V1722	I1630	I1528	C1420	THR	P517	LEU	ARG	ARG
VAL	L2117	M1879	M1879	I1725	I1631	I1528	TYR	GLY	L523	GLY	THR	THR
ASN	L2121	S1896	S1896	I1726	S1634	L1535	ILE	LEU	L523	PHE	CYS	CYS
ALA	E2122	E1898	E1898	L1730	D1635	M1543	THR	GLY	N527	LEU	LEU	LEU
ASN	Y2123	S1902	S1902	L1730	PHE	I1543	GLY	ARG	I546	PRO	ILE	ILE
MET	L2126	A1903	A1903	I1730	LYS	M1543	THR	PRO	L574	TYR	LEU	LEU
LYS	L2126	W1904	W1904	C1742	T1638	F1547	K1427	LYS	L574	ASN	VAL	VAL
GLU	W2129	L1916	L1916	I1745	Q1647	F1548	A1430	PRO	V576	ASN	GLY	GLY
LYS	L2130	K1919	K1919	L1746	K1650	P1551	T1431	ILE	G577	THR	THR	THR
MET	Y2131	L1925	L1925	Y1747	L1651	E1552	Q1432	PHE	Q578	ARG	HIS	HIS
L2218	T2132	L1925	L1925	Y1748	L1651	I1553	F1434	SER	W588	ASN	ASN	ALA
H2222	S2135	L1925	L1925	L1749	D1657	D1564	F1435	LEU	H502	VAL	SER	ALA
M2226	E2136	R1926	R1926	R1750	S1658	P1565	F1438	THR	PHE	THR	SER	ALA
I2230	K2137	F1927	F1927	R1751	S1658	P1565	D1439	PRO	W651	PRO	ASN	ASN
I2231	E2139	E1928	E1928	Q1752	M1661	ARG	GLY	ASN	F361	ASN	ASN	ILE
R2234	L2140	L1930	L1930	L1758	T1663	CYS	Y1441	LEU	F361	ASN	ASN	ALA
E2236	Y2141	Y1933	Y1933	N1759	K1664	ASP	T1442	PRO	F365	LEU	ALA	ALA
Y2236	SER	Y1942	Y1942	E1782	E1665	THR	A1444	VAL	I386	VAL	GLU	GLU
M2239	K2143	K1952	K1952	Y1786	E1666	LYS	L1445	THR	Y387	PHE	THR	THR
S2244	Y2145	M1959	M1959	V1786	L1670	THR	L1446	ASN	P389	TYR	TYR	TYR
K2245	L2150	E1960	E1960	S1772	S1678	E1573	F1447	LEU	I394	ASN	VAL	VAL
Q2249	N2153	L1965	L1965	T1777	T1680	E1576	N1448	SER	T399	CYS	ASP	ASP
	T2164	L1966	L1966	C1781	H1681	K1577	F1455	GLN	VAL	GLN	GLU	GLU
					S1682	L1578	L1456	THR	D788	SER	LEU	LEU
							R1457	LYS	M1223	PRO	GLU	GLU
							I1460	LYS	K791	GLU	PRO	PRO

SER	G2763	E2766	R2769	A2770	I2771	L2772	R2775	V2784	V2788	G2789	E2790	R2793	I2794	A2795	G2807	W2808	S2809	ALA	PHE	GLN																																				
	D2572			L2573						E2574				T2575							L2576	L2577	K2578	V2579	R2585	H2593	F2594	F2595	L2596	E2597	S2598	Y2599	A2600	D2601	P2602	V2603	Q2604	W2605	T2608	Y2612	G2629	D2630	R2631	N2635	L2636	D2639	G2643	H2647	I2648	D2649	L2652	E2655	K2659	L2660	V2666	R2669
V2686	F2687	E2702	L2706	S2707	V2708	L2709	E2710	V2711	L2712	R2713	V2714	L2717	F2718	S2719	Y2720	L2721	L2722	S2723	P2724	L2725	R2726	R2727	M2728	K2729	L2730	Q2731	K2732	M2733	GLN	LEU	GLU	ASN	PHE	ASN	GLN	PRO	GLU	SER	GLY	ASN	ILE	THR	THR	ASP	ALA	SER	ARG	ASP	PRO	LYS	ILE	GLN	ARG	ASN	ASN	VAL
A2362	V2363		K2364	K2365	L2366	L2367	D2368	L2369	L2370	K2371	S2372	N2373	S2377	L2383	F2387	F2388	N2389	Y2390	D2403	S2404	T2405	S2406	F2407	L2417	K2418	V2419	D2420	L2425	P2426	P2427	I2428	T2429	M2430	N2431	V2446	F2449	D2450	D2451	T2452	I2453	H2454	F2455	A2456	S2457	G2458	I2459	N2460	A2461	P2462	K2463	V2464	I2465				
S2250	A2251	H2253	Y2254	L2255	K2256	C2257	L2258	K2259	I2268	S2269	R2270	T2273	L2276	E2283	L2284	L2288	Q2289	Y2290	Y2291	L2292	F2300	I2301	P2302	F2304	A2309	R2310	L2311	M2312	V2315	SER	K2317	F2318	Q2319	Y2327	P2334	Y2335	L2341	V2345	L2354	D2355	A2356	G2357	S2358	R2359	Y2360	R2361										



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	64713	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

## 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	F	0.67	0/64	0.74	0/86
2	A	0.20	1/16139 (0.0%)	0.43	10/22100 (0.0%)
2	B	0.15	0/16185	0.36	3/22124 (0.0%)
All	All	0.18	1/32388 (0.0%)	0.39	13/44310 (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
2	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2658	LYS	CA-C	-12.38	1.36	1.52

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2334	PRO	CA-N-CD	-9.86	98.20	112.00
2	A	2661	PRO	N-CA-C	-6.93	103.89	113.53
2	B	2334	PRO	CA-N-CD	-6.40	103.04	112.00
2	B	2458	GLY	N-CA-C	-5.92	104.83	113.48
2	A	2457	SER	N-CA-C	5.72	117.84	108.52

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	2657	GLY	Mainchain

## 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	F	64	0	59	6	0
2	A	15929	0	12395	416	0
2	B	15993	0	12577	381	0
3	A	31	0	13	3	0
3	B	31	0	13	4	0
All	All	32048	0	25057	799	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 14.

The worst 5 of 799 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)
2:A:2195:LYS:HD3	2:A:2229:PHE:HB2	1.56	0.88
2:A:2018:LEU:HB3	2:A:2037:ARG:HH22	1.38	0.88
2:B:2459:ILE:HG22	2:B:2459:ILE:O	1.73	0.86
2:A:1399:LYS:HG3	2:A:1400:PRO:HD3	1.59	0.84
2:A:1492:MET:HE3	2:A:1492:MET:H	1.41	0.84

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 PDB entries followed by that with respect to all EM entries.

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	F	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
2	A	2372/2812 (84%)	2222 (94%)	142 (6%)	8 (0%)	37	66
2	B	2330/2812 (83%)	2190 (94%)	137 (6%)	3 (0%)	48	78
All	All	4708/5632 (84%)	4417 (94%)	280 (6%)	11 (0%)	45	72

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	1571	LYS
2	A	2640	LYS
2	A	2658	LYS
2	A	2462	PRO
2	A	2562	ARG

### 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 PDB entries followed by that with respect to all EM entries.

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	F	8/8 (100%)	8 (100%)	0	100	100
2	A	1106/2621 (42%)	1090 (99%)	16 (1%)	62	78
2	B	1126/2621 (43%)	1113 (99%)	13 (1%)	67	80
All	All	2240/5250 (43%)	2211 (99%)	29 (1%)	64	79

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	2660	LEU
2	B	2730	LYS
2	B	1599	LEU
2	B	2726	ARG
2	B	1456	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	1744	ASN
2	B	1957	ASN
2	B	1879	ASN
2	B	1996	ASN
2	A	2332	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 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	$\# Z  > 2$
3	ANP	A	2901	-	29,33,33	1.09	4 (13%)	31,52,52	1.10	2 (6%)
3	ANP	B	2901	-	29,33,33	1.09	4 (13%)	31,52,52	1.05	2 (6%)

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	2901	-	-	5/14/38/38	0/3/3/3
3	ANP	B	2901	-	-	7/14/38/38	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2901	ANP	PG-N3B	2.47	1.69	1.63
3	B	2901	ANP	PG-O1G	2.45	1.50	1.46
3	A	2901	ANP	PG-N3B	2.44	1.69	1.63
3	A	2901	ANP	PG-O1G	2.39	1.49	1.46
3	A	2901	ANP	PB-O3A	-2.36	1.56	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2901	ANP	PB-O3A-PA	-3.84	119.09	132.62
3	B	2901	ANP	PB-O3A-PA	-3.61	119.91	132.62
3	A	2901	ANP	C5-C6-N6	2.29	123.83	120.35
3	B	2901	ANP	C5-C6-N6	2.28	123.81	120.35

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2901	ANP	PB-N3B-PG-O1G
3	A	2901	ANP	O4'-C4'-C5'-O5'
3	B	2901	ANP	PB-N3B-PG-O1G
3	B	2901	ANP	C5'-O5'-PA-O3A
3	A	2901	ANP	C3'-C4'-C5'-O5'

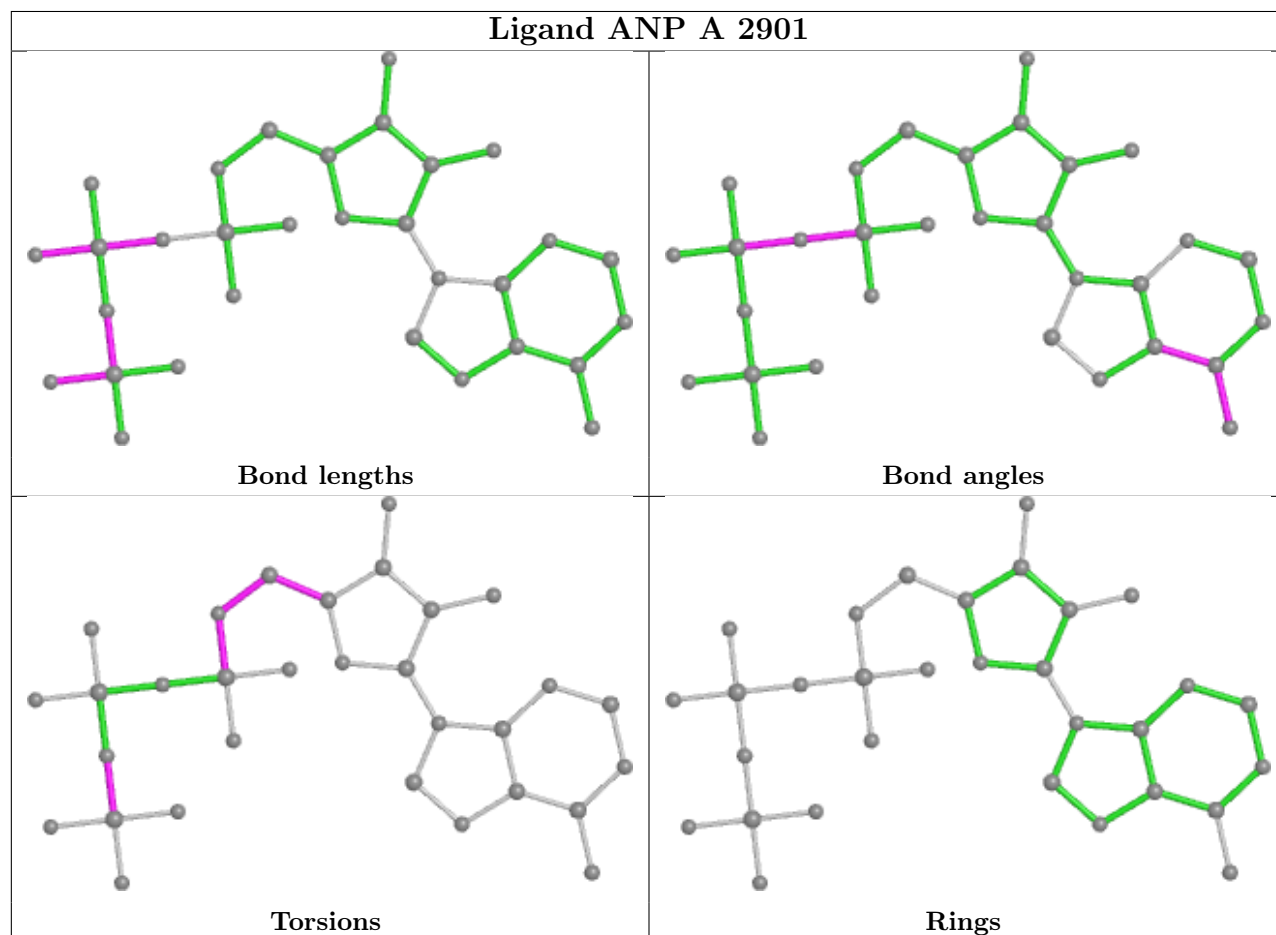
There are no ring outliers.

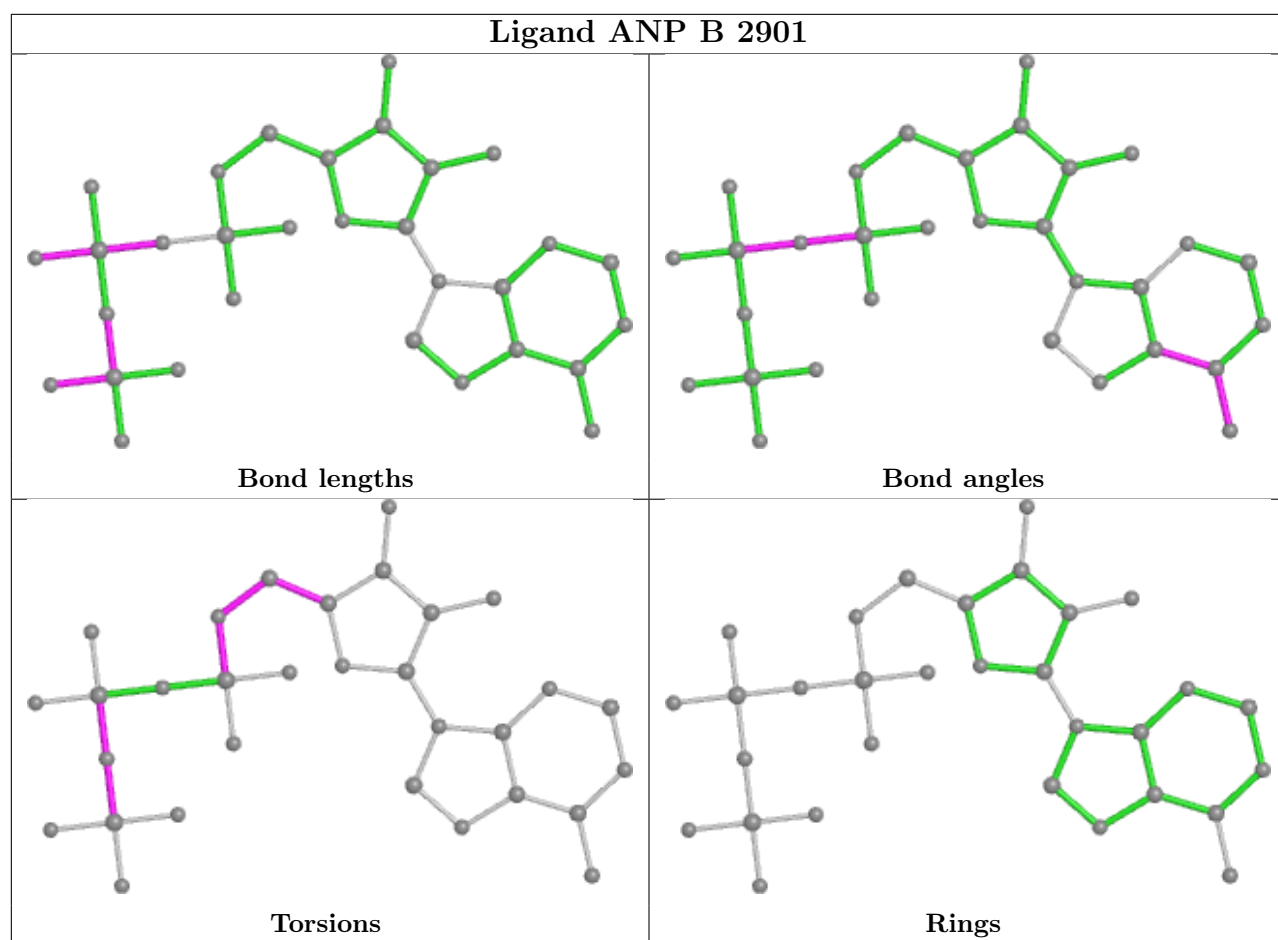
2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2901	ANP	3	0
3	B	2901	ANP	4	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.