



wwPDB EM Validation Summary Report ⓘ

May 25, 2025 – 12:15 AM JST

PDB ID : 9L4B / pdb_00009l4b
EMDB ID : EMD-62808
Title : Kinase domain of ATR bound with RP-3500
Authors : Wang, G.
Deposited on : 2024-12-20
Resolution : 3.20 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

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>.

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

EMDB validation analysis : **FAILED**
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 : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

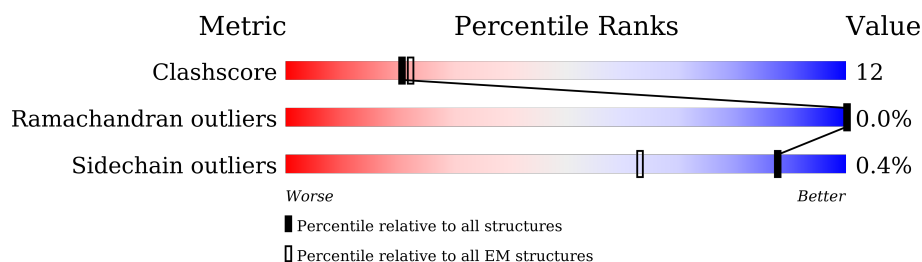
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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 ≥ 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	A	2644	
1	B	2644	

2 Entry composition [i](#)

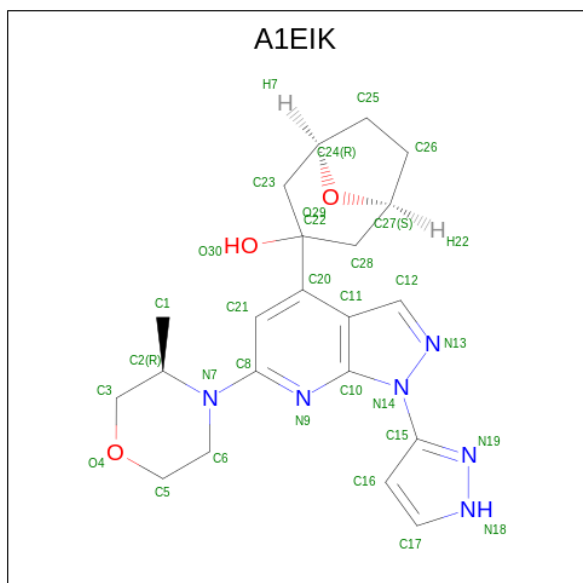
There are 3 unique types of molecules in this entry. The entry contains 40347 atoms, of which 19645 are hydrogens and 0 are deuteriums.

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 Serine/threonine-protein kinase ATR.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1335	Total	C	H	N	O	S	0	0
			19911	6499	9651	1785	1913	63		
1	B	1334	Total	C	H	N	O	S	0	0
			20372	6610	9994	1792	1907	69		

- Molecule 2 is RP-3500 (CCD ID: A1EIK) (formula: $C_{21}H_{26}N_6O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			30	21	6	3	
2	B	1	Total	C	N	O	0
			30	21	6	3	

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		AltConf
3	A	2	Total 2	O 2	0
3	B	2	Total 2	O 2	0

- Molecule 1: Serine/threonine-protein kinase ATR

Response	Percentage
Used	37%
Not used	13%
Don't know	50%

[illegible]

L2550	E2436	C2336	C2226	L2091	M1889	V1692	I1564	R1461	L1352	LEU	ARG
M2551	F2427	R2337	N2227	L2091	M1889	V1692	M1585	Y1462	L1352	LYS	CYS
L2554	L2428	L2338	K2228	D2096	N1892	I1695	T1566	S1465	L1353	LYS	LEU
K2555	F2341	F2341	S2235	T2099	E1898	L1712	I1569	Q1466	C1354	ILE	ASP
H2559	T2435	T2345	T2236	K2100	P1899	M1743	L1573	Y1479	E1355	ALA	HIS
H2560	H2437	R2346	L2237	V2113	I1900	M1743	S1577	S1480	G1356	VAL	CYS
P2561	E2438	K2347	M2239	Q2114	R1904	Q1748	S1577	S1481	D1365	LEU	LEU
L2562	P2439	C2348	K2247	M2115	R1905	L1749	V1581	K1482	G1367	GLN	GLY
K2567	L2441	R2350	E2251	R2116	L1908	Q1755	L1585	G1484	R1368	TYR	LEU
P2568	T2443	D2352	L2259	L2139	N1911	V1759	F1596	F1487	L1369	ARG	LEU
M2464	M2464	S2355	L2260	T2140	N1911	V1759	F1596	F1488	F1392	LYS	SER
V2467	V2467	R2358	P2261	A2141	S1927	T1767	A1601	A1488	T1396	THR	HIS
Q2468	Q2468	E2359	L2262	F2142	S1927	T1767	A1601	A1489	L1396	THR	VAL
Y2469	Y2469	L2360	V2285	Q2144	H1937	M1771	GLY	W1494	A1403	THR	VAL
I2470	I2470	H2361	T2269	L2145	N1942	L1781	LYS	Y1497	A1406	THR	ALA
L2471	L2471	T2362	T2269	T2146	L1945	D1785	HIS	L1498	Y1407	LEU	LEU
G2472	G2472	T2362	L2270	S2147	L1946	L1786	LYS	K1501	A1413	LEU	LEU
L2473	L2473	V2367	P2271	R2148	N1946	L1786	SER	V1502	Q1414	HIS	HIS
G2478	G2478	D2372	L2274	T2149	E1949	R1803	ASN	A1507	D1415	ILE	ILE
E2479	E2479	E2373	G2275	C2150	E1949	R1803	ASN	S1508	S1416	GLN	GLN
N2480	N2480	C2374	T2276	H2151	W1962	T1817	ARG	S1508	Y1419	PRO	PRO
L2481	L2481	W2379	N2279	T2164	W1962	T1817	ASN	F1511	Y1420	LYS	LYS
L2482	L2482	W2379	H2280	T2164	S1965	A1818	VAL	T1512	I1421	THR	THR
L2486	L2486	W2382	A2281	F2168	S1965	V1826	VAL	C1513	Q1422	ALA	ALA
V2491	V2491	G2385	F2286	L2169	Q1971	R1827	SER	C1514	E1423	ALA	ALA
H2492	H2492	R2386	G2295	Q2174	V1975	T1831	MET	S1515	L1424	ILE	ILE
L2498	L2498	R2387	F2296	T2180	V1975	T1831	VAL	I1516	L1425	HIS	HIS
F2499	F2499	T2391	F2296	A2181	K2026	L1834	S1619	F1522	R1431	TYR	TYR
E2506	E2506	R2392	M2299	V2182	L2042	S1838	T1620	GLY	GLY	LEU	LEU
V2507	V2507	L2393	V2300	S2183	A2043	S1838	Y1623	MET	GLY	ILE	ILE
R2514	R2514	V2399	E2301	M2189	K2044	V1852	E1624	GLY	THR	ILE	ILE
L2515	L2515	W2400	I2302	R2190	Y2045	R1853	Y1626	ASN	ASN	GLY	GLY
T2516	T2516	M2401	I2302	V2191	Y2046	L1857	V1629	P1530	GLY	ARG	ARG
M2519	M2519	L2411	S2305	M2192	L2049	C1858	I1632	H1831	PRO	ASP	ASP
V2520	V2520	K2413	Q2307	R2193	M2088	E1859	F1632	I1532	GLY	ALA	ALA
N2521	N2521	S2414	K2311	K2200	E2059	L1860	L1635	L1533	VAL	VAL	VAL
G2522	G2522	A2415	L2312	K2200	Q2061	I1864	I1636	V1534	Q1441	GLN	GLN
M2523	M2523	L2416	S2313	M2204	H2071	H1870	R1647	V1536	L1442	ASP	ASP
R2534	R2534	L2417	L2314	K2205	F2072	PRO	GLY	L1537	W1443	PHE	PHE
Q2535	Q2535	S2418	K2315	L2208	S2075	GLY	Y1651	L1538	V1450	TYR	TYR
V2538	V2538	K2420	L2323	L2208	L2076	SER	L1673	D1544	L1454	PHE	PHE
L2421	L2421	L2421	T2219	T2219	L2076	SER	Q1677	Y1548	E1455	LEU	LEU
M2543	M2543	K2422	C2326	L2223	Y2084	S1876	W1883	Y1549	P1456	PRO	PRO
E2548	E2548	V2423	P2327	E2224	M2087	W1883	A1682	D1559	H1457	ASP	ASP
P2549	P2549	R2425	P2328	L2225	P2088	V1884	D1687	D1559	L1458	HIS	HIS
M2544	M2544	R2425	L2225	L2225	P2088	A1885	D1687	T1460	M1459	PRO	PRO

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	102467	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 BIOQUANTUM (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: A1EIK

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	0.36	0/10488	0.42	0/14230
1	B	0.39	2/10604 (0.0%)	0.52	12/14369 (0.1%)
All	All	0.38	2/21092 (0.0%)	0.48	12/28599 (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	1
1	B	0	5
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2225	LEU	C-O	-7.56	1.15	1.24
1	B	2373	GLU	C-O	-6.06	1.16	1.24

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2226	CYS	CB-CA-C	-13.30	88.25	110.85
1	B	2225	LEU	CA-C-O	-12.97	107.34	120.70
1	B	2326	CYS	N-CA-CB	9.85	125.70	109.94
1	B	2578	ASN	O-C-N	-9.71	109.68	122.59
1	B	2227	ASN	N-CA-C	-8.75	102.78	113.19

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2363	ARG	Sidechain
1	B	1354	CYS	Peptide
1	B	1465	SER	Peptide
1	B	2225	LEU	Mainchain
1	B	2578	ASN	Mainchain

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	10260	9651	9686	200	0
1	B	10378	9994	10051	276	0
2	A	30	0	0	3	0
2	B	30	0	0	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
All	All	20702	19645	19737	476	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 12.

The worst 5 of 476 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:2327:LYS:HZ2	2:A:2701:A1EIK:C16	1.71	1.01
1:B:1304:LEU:HD22	1:B:1354:CYS:SG	2.05	0.96
1:A:1319:ILE:O	1:A:1323:THR:OG1	1.85	0.95
1:B:2276:THR:OG1	1:B:2279:ASN:OD1	1.88	0.91
1:B:2328:PRO:HA	1:B:2374:CYS:HB2	1.60	0.83

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	A	1327/2644 (50%)	1274 (96%)	53 (4%)	0	100	100
1	B	1326/2644 (50%)	1262 (95%)	63 (5%)	1 (0%)	48	80
All	All	2653/5288 (50%)	2536 (96%)	116 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2567	LYS

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	A	1037/2363 (44%)	1034 (100%)	3 (0%)	91	96
1	B	1075/2363 (46%)	1069 (99%)	6 (1%)	84	92
All	All	2112/4726 (45%)	2103 (100%)	9 (0%)	88	94

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2480	ASN
1	B	2580	THR
1	B	1466	GLN
1	B	2225	LEU
1	B	2327	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	2437	HIS
1	B	2480	ASN
1	B	2600	GLN
1	A	2492	HIS
1	A	2408	GLN

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	$\# Z > 2$
2	A1EIK	A	2701	-	31,35,35	0.73	1 (3%)	33,53,53	1.28	3 (9%)
2	A1EIK	B	2701	-	31,35,35	0.76	2 (6%)	33,53,53	1.39	3 (9%)

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	A1EIK	A	2701	-	-	0/10/44/44	0/7/6/6
2	A1EIK	B	2701	-	-	0/10/44/44	0/7/6/6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2701	A1EIK	C15-N14	-2.22	1.40	1.44
2	A	2701	A1EIK	C15-N14	-2.07	1.40	1.44
2	B	2701	A1EIK	C11-C10	-2.00	1.38	1.43

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2701	A1EIK	O4-C3-C2	-5.75	95.25	111.48
2	A	2701	A1EIK	O4-C3-C2	-4.57	98.57	111.48
2	B	2701	A1EIK	C21-C20-C11	-3.15	116.58	119.98
2	A	2701	A1EIK	C21-C20-C11	-3.10	116.63	119.98
2	B	2701	A1EIK	C8-N9-C10	-2.18	115.52	118.75

There are no chirality outliers.

There are no torsion outliers.

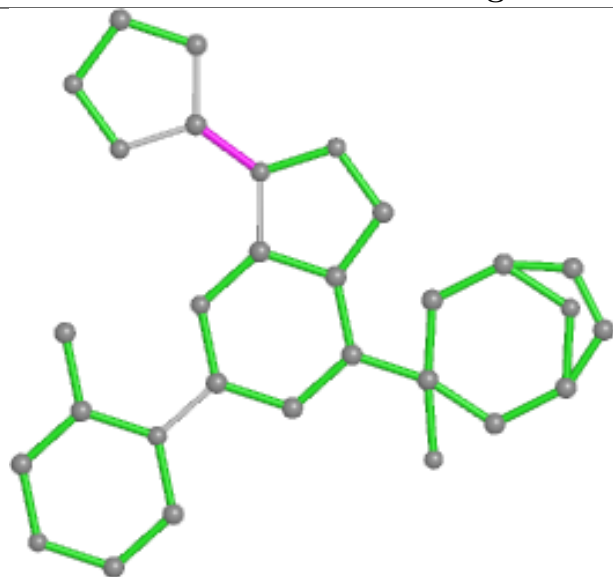
There are no ring outliers.

2 monomers are involved in 4 short contacts:

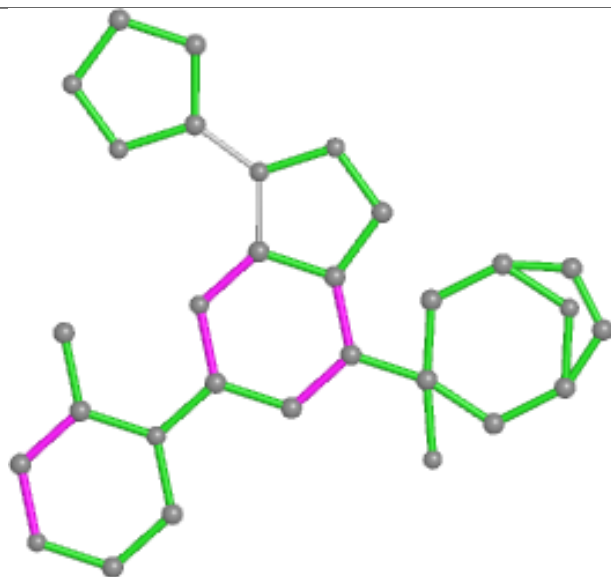
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2701	A1EIK	3	0
2	B	2701	A1EIK	1	0

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.

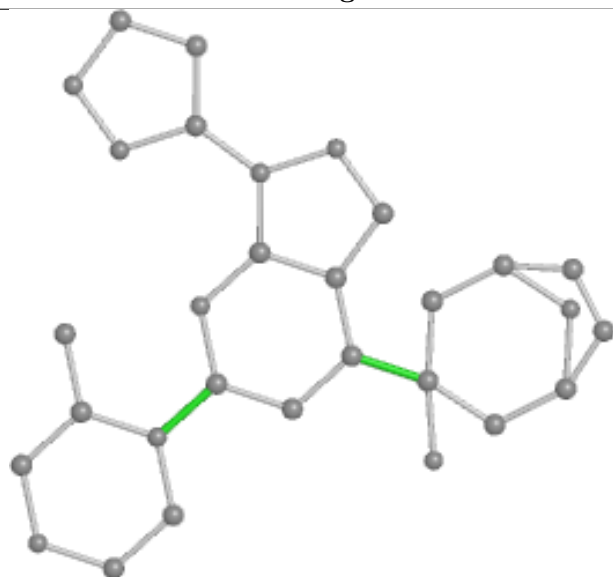
Ligand A1EIK A 2701



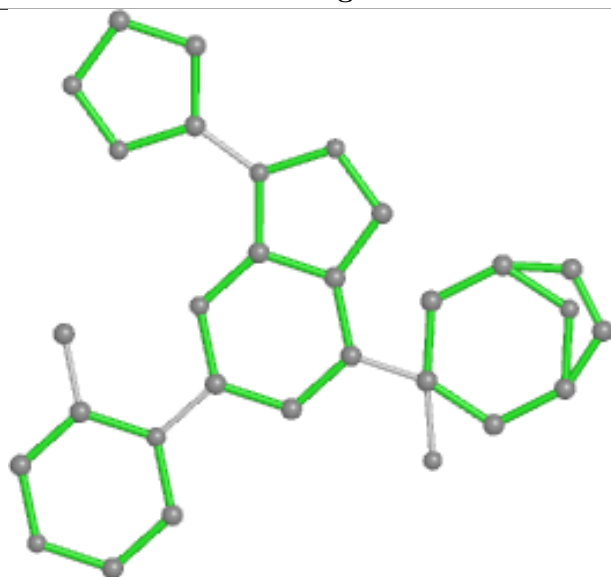
Bond lengths



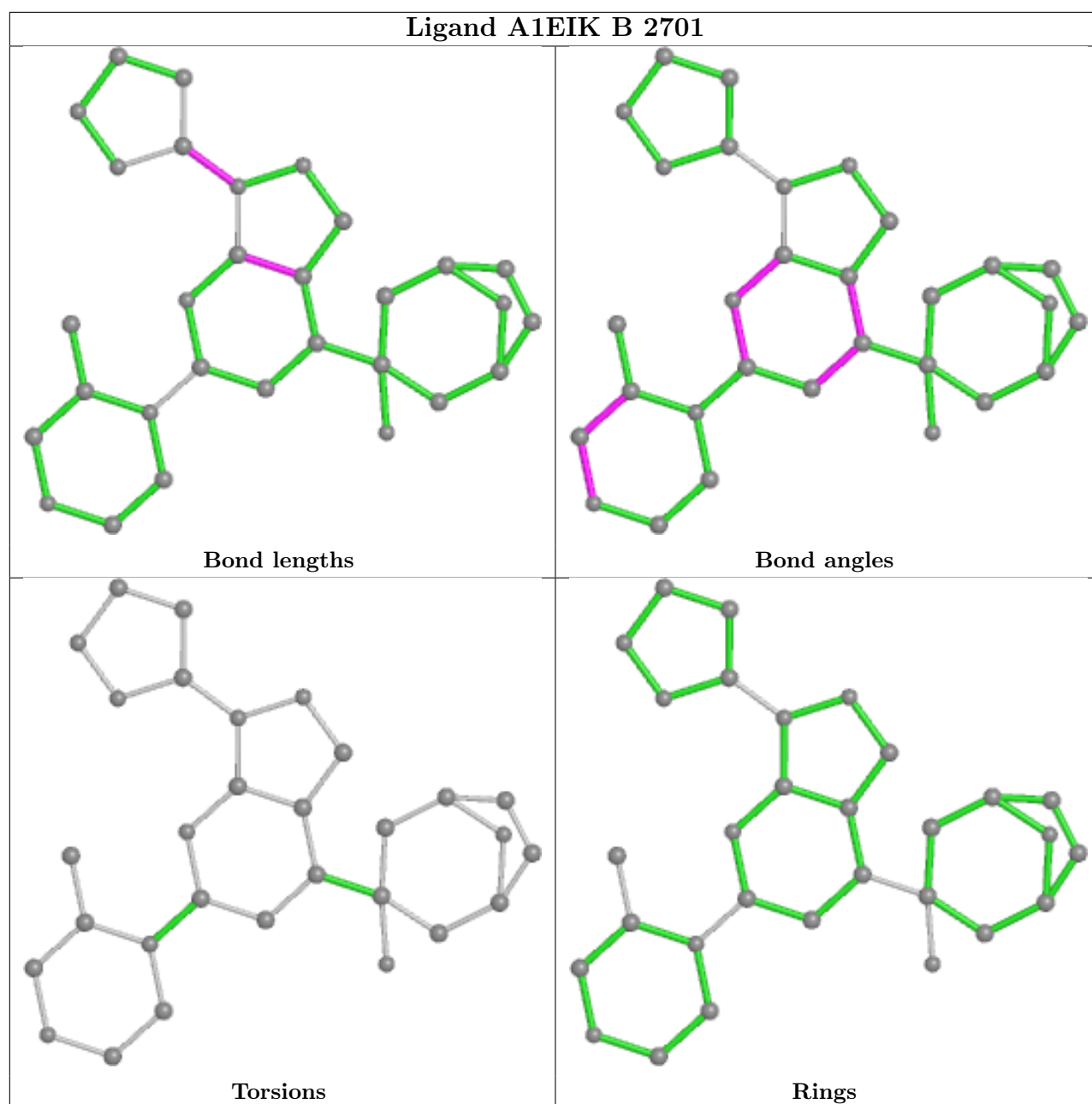
Bond angles



Torsions



Rings



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.