



## wwPDB EM Validation Summary Report ⓘ

May 25, 2025 – 12:33 AM JST

PDB ID : 9L4D / pdb\_00009l4d  
EMDB ID : EMD-62811  
Title : ATR-ATRIP bound with RP-3500  
Authors : Wang, G.  
Deposited on : 2024-12-20  
Resolution : 3.79 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 : **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

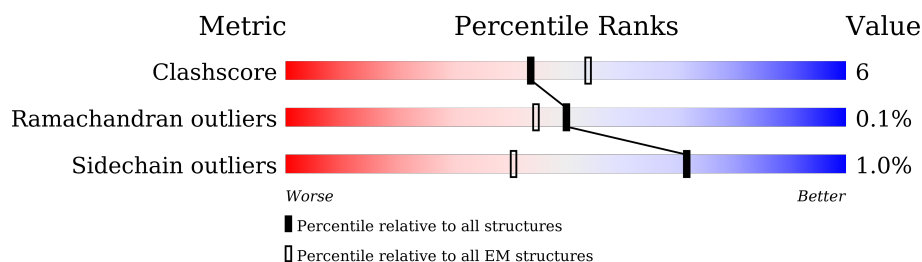
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.79 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	A	2637	
1	B	2637	
2	C	491	
2	D	491	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 67221 atoms, of which 29861 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.

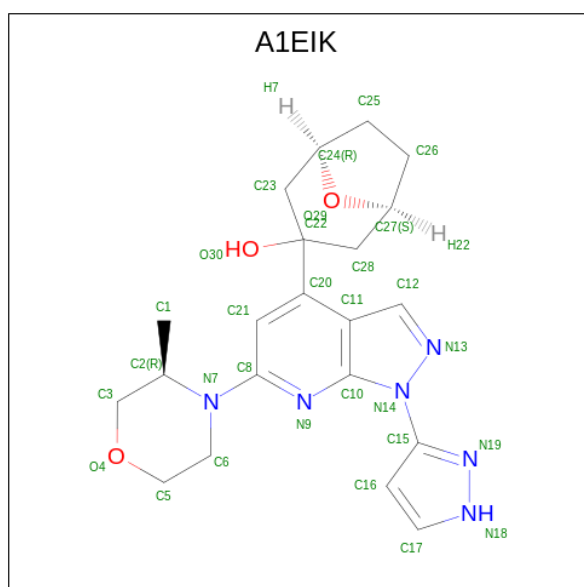
- Molecule 1 is a protein called Serine/threonine-protein kinase ATR.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	2473	Total	C	H	N	O	S	0	0
			26772	9217	11475	2847	3181	52		
1	B	2497	Total	C	H	N	O	S	0	0
			31311	10642	14272	3025	3281	91		

- Molecule 2 is a protein called ATR-interacting protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	382	Total	C	H	N	O	S	0	0
			4498	1510	2026	462	485	15		
2	C	382	Total	C	H	N	O	S	0	0
			4579	1521	2088	461	485	24		

- Molecule 3 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
3	A	1	Total	C	N	O	0
			30	21	6	3	
3	B	1	Total	C	N	O	0
			30	21	6	3	

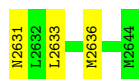
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	C	1	Total	Zn	0
			1	1	



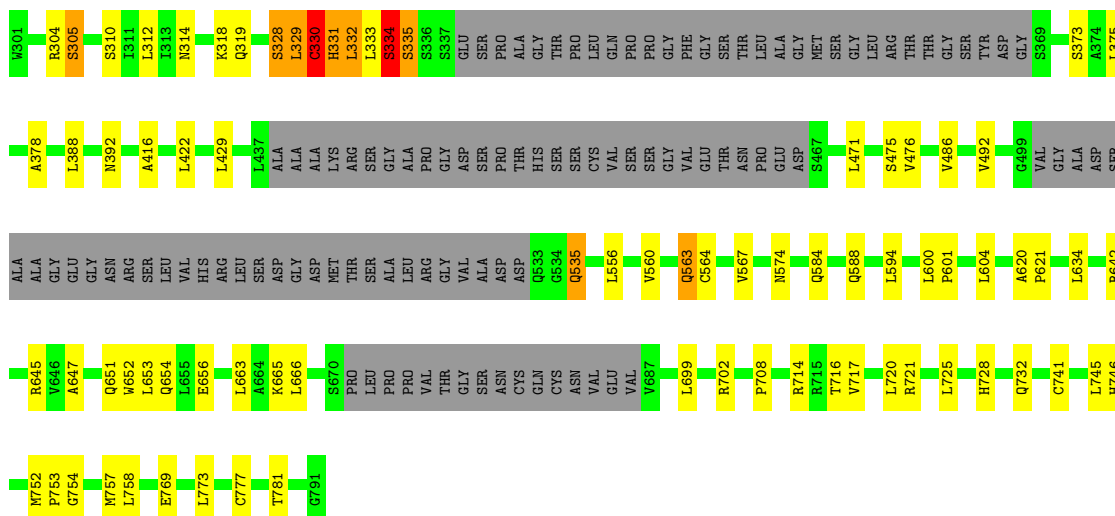
81% 13% 5%





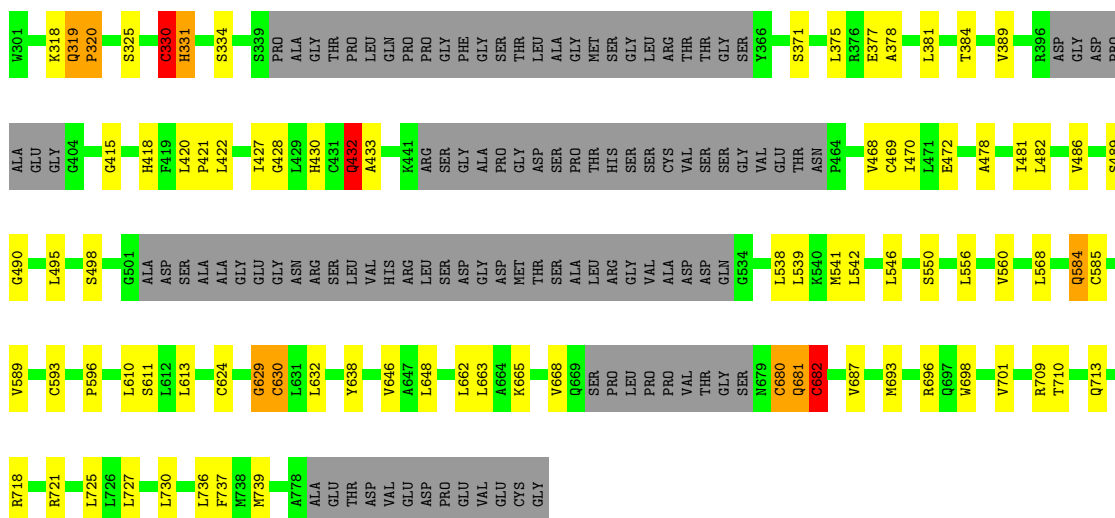
• Molecule 2: ATR-interacting protein

Chain D: 62% 14% 22%



• Molecule 2: ATR-interacting protein

Chain C: 61% 15% 22%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	77631	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: ZN, 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	0.34	10/15382 (0.1%)	0.50	16/21057 (0.1%)
1	B	0.38	6/17289 (0.0%)	0.62	38/23571 (0.2%)
2	C	0.45	2/2513 (0.1%)	0.82	12/3426 (0.4%)
2	D	0.69	6/2493 (0.2%)	0.72	7/3401 (0.2%)
All	All	0.40	24/37677 (0.1%)	0.60	73/51455 (0.1%)

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	3
1	B	0	5
2	D	0	2
All	All	0	10

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	330	CYS	C-O	-23.55	0.93	1.24
2	D	330	CYS	C-N	-5.83	1.25	1.33
1	B	751	HIS	ND1-CE1	5.61	1.38	1.32
1	B	737	HIS	ND1-CE1	5.45	1.38	1.32
1	B	830	HIS	ND1-CE1	5.42	1.38	1.32

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	682	CYS	N-CA-CB	14.97	132.13	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	330	CYS	N-CA-CB	14.64	134.69	110.39
1	B	1188	PHE	CB-CA-C	-13.90	89.17	110.02
1	B	1189	PRO	N-CA-C	-13.87	94.82	113.40
1	B	1767	THR	CA-CB-OG1	-11.30	92.64	109.60

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2333	ARG	Sidechain
1	A	2475	ASP	Mainchain
1	A	2547	ARG	Sidechain
1	B	1194	ARG	Sidechain
1	B	1767	THR	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	15297	11475	11498	103	0
1	B	17039	14272	14390	220	0
2	C	2491	2088	2096	56	0
2	D	2472	2026	2034	55	0
3	A	30	0	0	1	0
3	B	30	0	0	0	0
4	C	1	0	0	0	0
All	All	37360	29861	30018	424	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.

The worst 5 of 424 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:D:330:CYS:O	2:D:331:HIS:C	2.08	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:330:CYS:O	2:D:330:CYS:SG	2.35	0.84
1:B:2514:ARG:HG3	1:B:2519:MET:HE1	1.62	0.82
1:A:2366:ALA:HB1	1:A:2368:ILE:HD11	1.62	0.81
2:C:680:CYS:C	2:C:682:CYS:H	1.88	0.81

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	A	2451/2637 (93%)	2313 (94%)	136 (6%)	2 (0%)	48	79
1	B	2471/2637 (94%)	2327 (94%)	142 (6%)	2 (0%)	48	79
2	C	370/491 (75%)	341 (92%)	27 (7%)	2 (0%)	25	58
2	D	372/491 (76%)	336 (90%)	35 (9%)	1 (0%)	37	69
All	All	5664/6256 (90%)	5317 (94%)	340 (6%)	7 (0%)	50	79

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	557	LEU
2	D	329	LEU
2	C	318	LYS
1	A	2328	PRO
2	C	629	GLY

### 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 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	1021/2358 (43%)	1013 (99%)	8 (1%)	79	84
1	B	1387/2358 (59%)	1376 (99%)	11 (1%)	79	84
2	C	207/417 (50%)	201 (97%)	6 (3%)	37	58
2	D	194/417 (46%)	190 (98%)	4 (2%)	48	66
All	All	2809/5550 (51%)	2780 (99%)	29 (1%)	71	80

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

Mol	Chain	Res	Type
1	B	2327	LYS
2	C	630	CYS
1	B	2380	VAL
2	C	432	GLN
1	B	2377	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	2480	ASN
2	D	657	GLN
1	B	2517	HIS
2	D	424	GLN
2	C	584	GLN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 3 ligands modelled in this entry, 1 is 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
3	A1EIK	B	2701	-	31,35,35	0.80	1 (3%)	33,53,53	1.51	4 (12%)
3	A1EIK	A	2701	-	31,35,35	0.71	0	33,53,53	1.14	5 (15%)

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	A1EIK	B	2701	-	-	2/10/44/44	0/7/6/6
3	A1EIK	A	2701	-	-	4/10/44/44	0/7/6/6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2701	A1EIK	C15-N14	-2.25	1.40	1.44

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2701	A1EIK	O4-C3-C2	-5.84	94.99	111.48
3	A	2701	A1EIK	C21-C20-C11	-3.56	116.14	119.98
3	B	2701	A1EIK	C21-C20-C11	-3.25	116.47	119.98
3	B	2701	A1EIK	C8-N9-C10	-2.71	114.74	118.75
3	A	2701	A1EIK	C8-N9-C10	-2.48	115.09	118.75

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2701	A1EIK	C21-C8-N7-C2
3	A	2701	A1EIK	N9-C8-N7-C2
3	A	2701	A1EIK	N9-C8-N7-C6
3	A	2701	A1EIK	C21-C8-N7-C6
3	B	2701	A1EIK	C21-C8-N7-C2

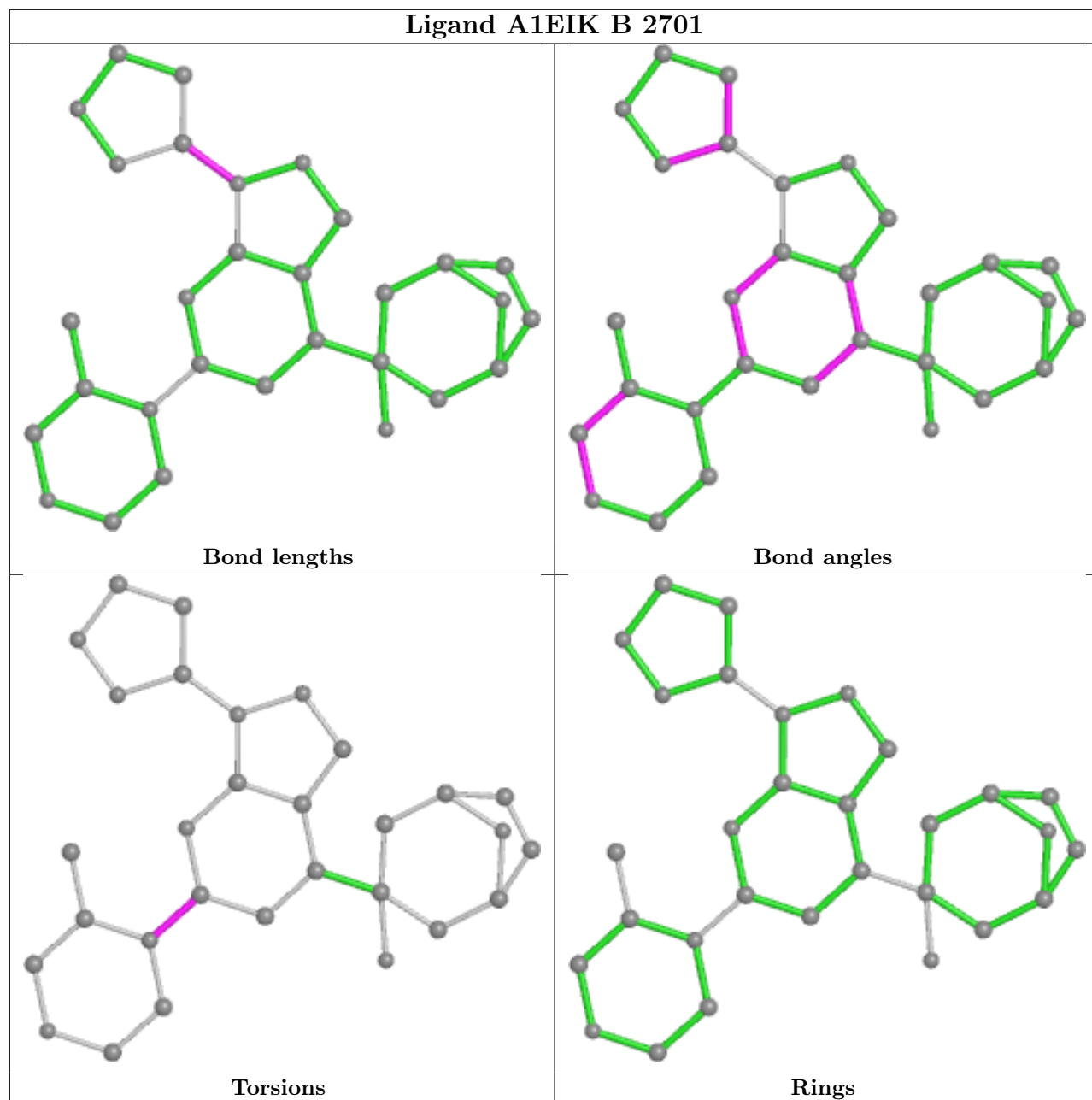
There are no ring outliers.

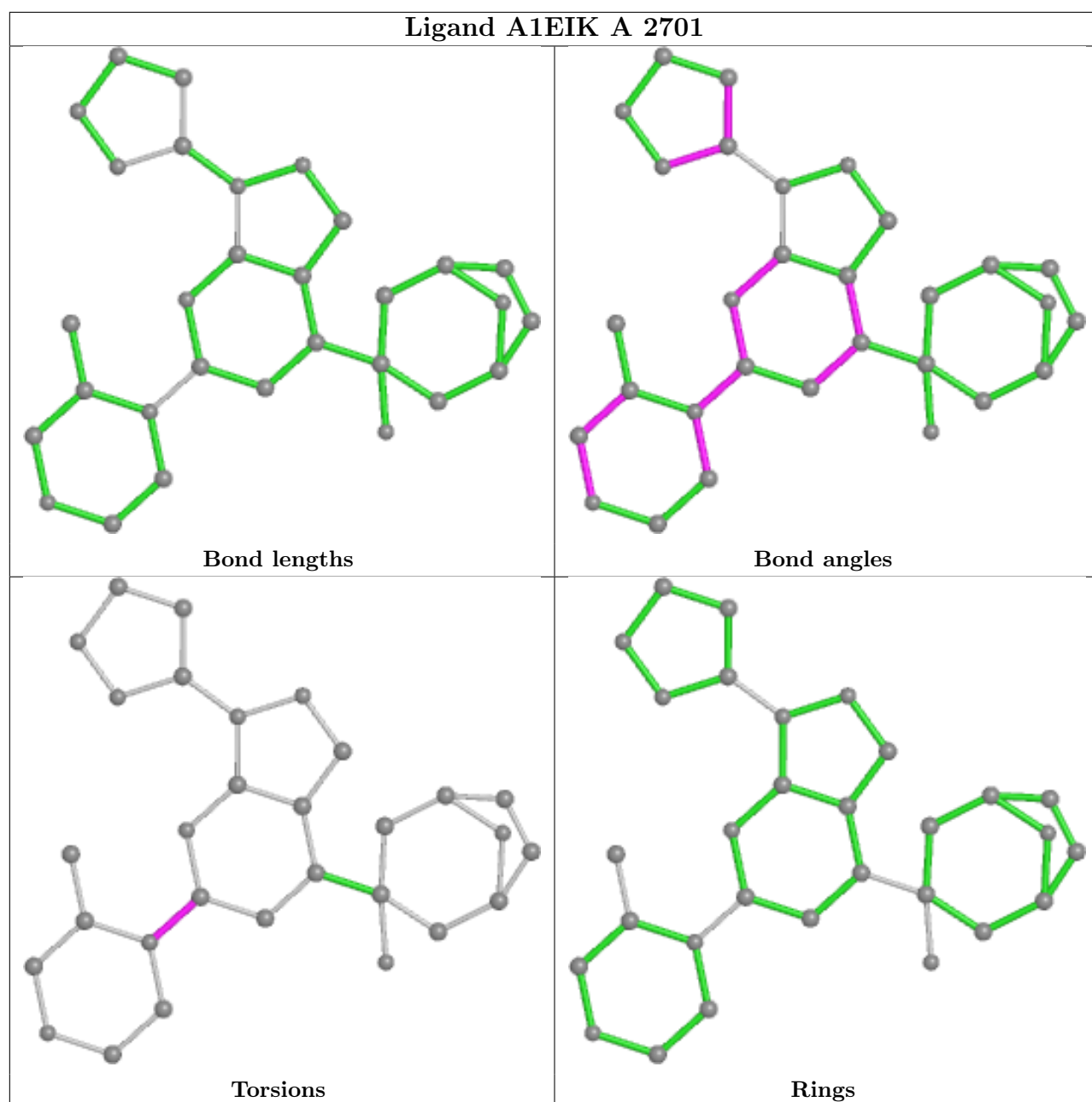
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	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 B 2701





## 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.