wwPDB EM Validation Summary Report (i)

May 25, 2025 – 12:17 AM JST

PDB ID	:	9L40 / pdb_00009l40
EMDB ID	:	EMD-62801
Title	:	kinase of ATR bound VE-822 state
Authors	:	Wang, G.
Deposited on	:	2024-12-19
Resolution	:	2.87 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 (i) 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 (i)) were used in the production of this report:

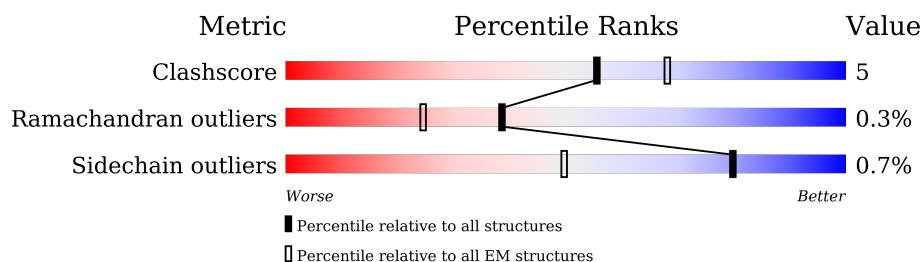|		
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 2.87 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	Percentile Ranks	Value
Clashscore		5
Ramachandran outliers		0.3%
Sidechain outliers		0.7%

Worse   *Better*

▌Percentile relative to all structures
▯Percentile relative to all EM structures

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 <=5%

| Mol	Chain	Length	Quality of chain
1	A	2644	44% 5% 50%
1	B	2644	45% 5% 50%

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 35331 atoms, of which 16354 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	1322	Total	C	H	N	O	S	0	0
			17716	5944	8256	1690	1772	54		
1	B	1322	Total	C	H	N	O	S	0	0
			17475	5875	8090	1683	1774	53		

- Molecule 2 is VE-822 (CCD ID: A1EIE) (formula: $C_{24}H_{25}N_5O_3S$) (labeled as "Ligand of Interest" by depositor).

A1EIE
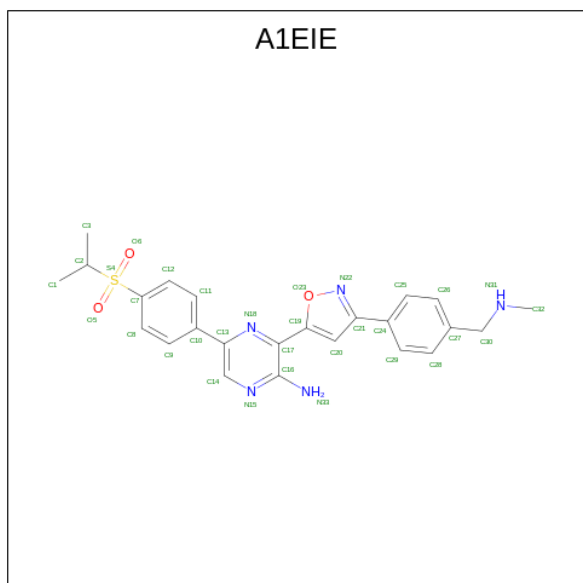
Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	H	N	O	S	0
			35	24	2	5	3	1	
2	A	1	Total	C	H	N	O	S	0
			35	24	2	5	3	1	
2	B	1	Total	C	H	N	O	S	0
			35	24	2	5	3	1	
2	B	1	Total	C	H	N	O	S	0
			35	24	2	5	3	1	

3 Residue-property plots ⓘ

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.

• Molecule 1: Serine/threonine-protein kinase ATR

Chain A:

• Molecule 1: Serine/threonine-protein kinase ATR

Chain B:

45% 5% 50%

Labeled residues (lower rows):

L1281, I1331, Q1349, L1353, C1354, C1357, I1364, D1365, T1376, R1402, A1406, L1425, Y1428, D1429, C1430, H1440, P1447, V1450, R1451

L1454, E1455, P1456, H1457, L1458, K1463, S1464, K1476, P1477, I1478, G1484, L1498, K1501, M1553, H1558, T1566, Q1567, S1571, D1572, L1573, S1577, T1580, S1583, L1588, K1595, A1598, A1601

S1619, V1629, L1633, P1637, Q1638, D1639, T1640, H1657, H1709, L1712, G1713, L1714, L1715, A1718, H1735, Y1736, V1740, L1744, H1760, E1776, L1804, K1813, R1814, Q1845, Q1869, D1879, R1895, R1905, K1912, E1922

Q1926 S1927 L1945 L1952 W1962 K1966 K1978 P1991 E1992 G1993 K1994 N1995 M1996 S2018 K2024 Y2025 T2029 E2034 L2042 Y2045 Y2046 R2066 Y2078 Y2102 K2121 S2152 H2153 F2157 F2168 M2161 M2179 T2180 A2181 M2189 R2193

L2198 D2231 G2232 S2233 S2234 M2239 L2259 V2265 F2286 W2290 D2298 K2308 P2309 D2318 D2335 D2352 A2416 E2419 K2420 L2421 R2425 H2437 M2466 I2470 L2471 R2476 N2496 E2509 H2517 N2521 C2536 M2540 R2541 R2547 E2548

P2549 L2550 M2551 F2557 L2558 H2559 H2572 SER LYS ALA PRO LEU ASN GLU T2580 E2630 M2636 M2644

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	162505	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 $(e^-/\text{Å}^2)$	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: A1EIE

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	0.55	14/9645 (0.1%)	0.61	26/13121 (0.2%)
1	B	0.52	12/9565 (0.1%)	0.59	16/13021 (0.1%)
All	All	0.54	26/19210 (0.1%)	0.60	42/26142 (0.2%)

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	2
1	B	0	4
All	All	0	6

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1457	HIS	ND1-CE1	5.27	1.37	1.32
1	A	1558	HIS	ND1-CE1	5.21	1.37	1.32
1	B	1760	HIS	ND1-CE1	5.20	1.37	1.32
1	B	2153	HIS	ND1-CE1	5.20	1.37	1.32
1	A	1302	HIS	ND1-CE1	5.17	1.37	1.32

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1477	PRO	N-CA-CB	9.79	109.31	102.65
1	A	1735	HIS	CB-CG-CD2	-6.67	122.53	131.20
1	A	1457	HIS	CB-CG-CD2	-6.66	122.54	131.20
1	A	1862	HIS	CB-CG-CD2	-6.66	122.54	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1760	HIS	CB-CG-CD2	-6.65	122.55	131.20

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1929	ARG	Sidechain
1	A	2425	ARG	Sidechain
1	B	1566	THR	Peptide
1	B	1952	LEU	Peptide
1	B	2425	ARG	Sidechain

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	9460	8256	8273	85	0
1	B	9385	8090	8122	83	0
2	A	66	4	0	1	0
2	B	66	4	0	2	0
All	All	18977	16354	16395	169	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 5.

The worst 5 of 169 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:B:1455:GLU:O	1:B:1458:LEU:N	2.02	0.92
1:B:1354:CYS:HA	1:B:1357:CYS:SG	2.16	0.86
1:B:1573:LEU:O	1:B:1577:SER:OG	1.99	0.81
1:A:1403:ALA:O	1:A:1407:TYR:N	2.16	0.79
1:B:1945:LEU:HG	2:B:2702:A1EIE:C32	2.13	0.78

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	1310/2644 (50%)	1233 (94%)	72 (6%)	5 (0%)	30	58
1	B	1312/2644 (50%)	1249 (95%)	61 (5%)	2 (0%)	44	71
All	All	2622/5288 (50%)	2482 (95%)	133 (5%)	7 (0%)	38	63

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2307	GLN
1	B	2308	LYS
1	A	1478	ILE
1	A	2305	SER
1	A	2328	PRO

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	823/2363 (35%)	816 (99%)	7 (1%)	75	91
1	B	808/2363 (34%)	804 (100%)	4 (0%)	86	95
All	All	1631/4726 (34%)	1620 (99%)	11 (1%)	80	93

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1978	LYS

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Mol	Chain	Res	Type
1	B	2308	LYS
1	B	2425	ARG
1	B	2335	ASP
1	A	2310	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1891	GLN
1	B	1970	HIS
1	B	2621	HIS
1	B	2307	GLN
1	B	2437	HIS

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 ⓘ

4 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	A1EIE	A	2702	-	33,36,36	0.64	1 (3%)	43,52,52	0.72	2 (4%)
2	A1EIE	B	2702	-	33,36,36	0.64	2 (6%)	43,52,52	0.61	1 (2%)
2	A1EIE	A	2701	-	33,36,36	0.66	2 (6%)	43,52,52	0.75	1 (2%)
2	A1EIE	B	2701	-	33,36,36	0.62	1 (3%)	43,52,52	0.67	1 (2%)

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	A1EIE	A	2702	-	-	7/22/27/27	0/4/4/4
2	A1EIE	B	2702	-	-	8/22/27/27	0/4/4/4
2	A1EIE	A	2701	-	-	6/22/27/27	0/4/4/4
2	A1EIE	B	2701	-	-	5/22/27/27	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2701	A1EIE	C30-N31	2.22	1.49	1.46
2	B	2702	A1EIE	C17-C16	-2.22	1.42	1.45
2	A	2702	A1EIE	C30-N31	2.12	1.49	1.46
2	B	2701	A1EIE	C30-N31	2.09	1.49	1.46
2	B	2702	A1EIE	C30-N31	2.07	1.49	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2701	A1EIE	C19-C17-N18	-3.41	108.74	115.09
2	B	2701	A1EIE	C19-C17-N18	-2.63	110.21	115.09
2	A	2702	A1EIE	C19-C17-N18	-2.25	110.92	115.09
2	A	2702	A1EIE	C20-C19-C17	2.04	135.34	129.21
2	B	2702	A1EIE	C16-C17-N18	2.04	121.30	119.92

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2701	A1EIE	C1-C2-S4-C7
2	A	2701	A1EIE	C1-C2-S4-O5

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Mol	Chain	Res	Type	Atoms
2	A	2701	A1EIE	C1-C2-S4-O6
2	A	2701	A1EIE	C3-C2-S4-C7
2	A	2701	A1EIE	C3-C2-S4-O5

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2702	A1EIE	2	0
2	A	2701	A1EIE	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 then 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 A1EIE A 2702

Bond lengths

Bond angles

Torsions

Rings

Ligand A1EIE B 2702

Bond lengths

Bond angles

Torsions

Rings

Ligand A1EIE A 2701

Bond lengths

Bond angles

Torsions

Rings

Ligand A1EIE B 2701

Bond lengths

Bond angles

Torsions

Rings
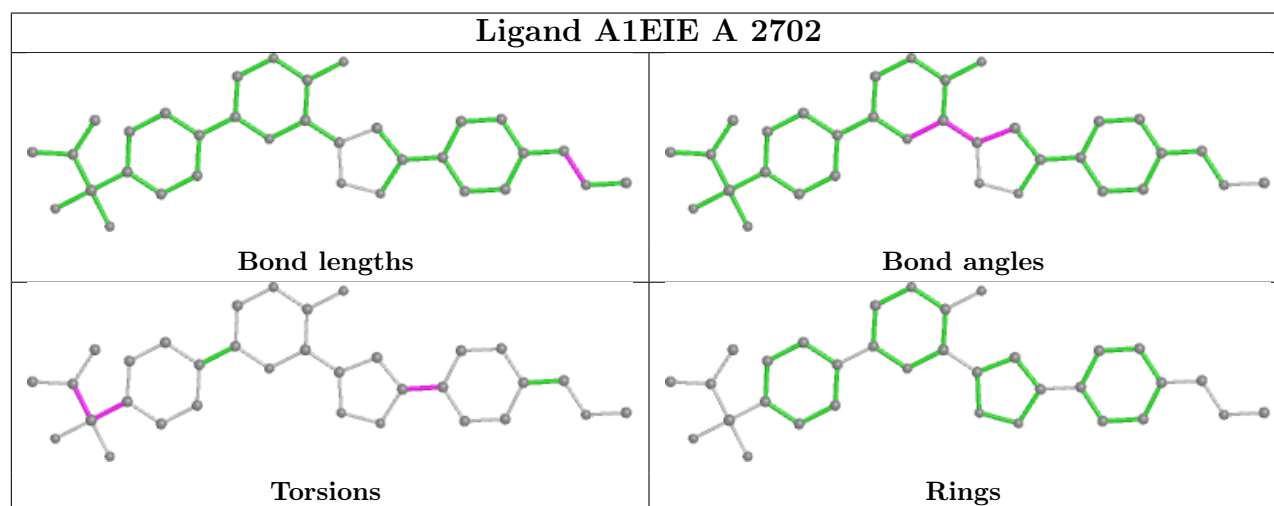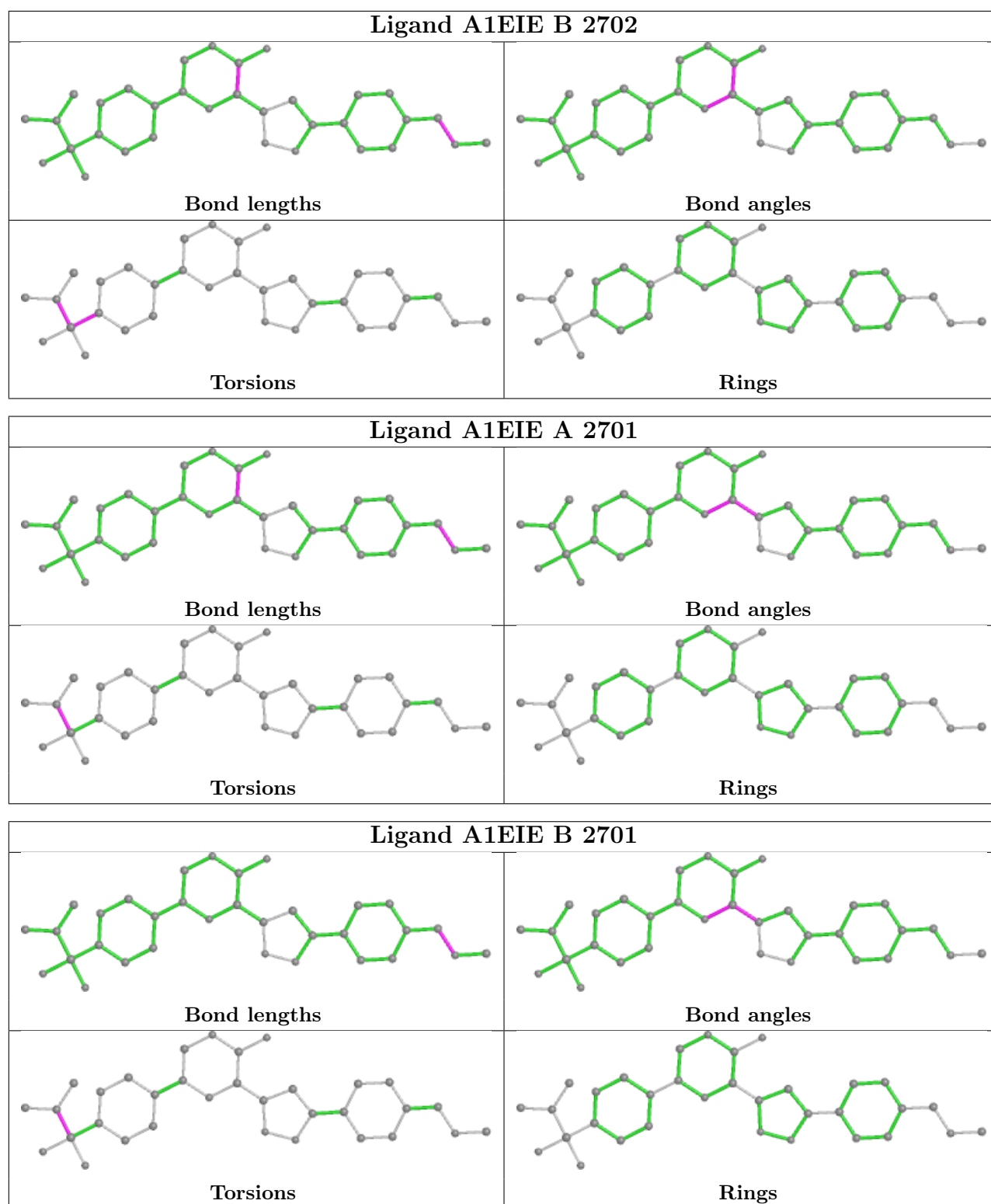
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.