



wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 10:25 am BST

PDB ID : 1LCU
Title : Polylysine Induces an Antiparallel Actin Dimer that Nucleates Filament Assembly: Crystal Structure at 3.5 Å Resolution
Authors : Bubb, M.R.; Govindasamy, L.; Yarmola, E.G.; Vorobiev, S.M.; Almo, S.C.; Somasundaram, T.; Chapman, M.S.; Agbandje-Mckenna, M.; McKenna, R.
Deposited on : 2002-04-06
Resolution : 3.50 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
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)	:	2.11

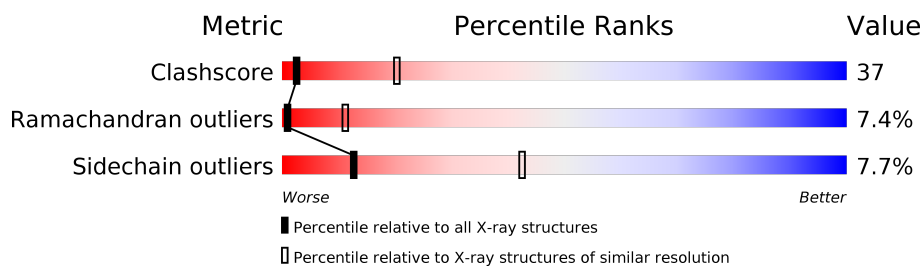
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)

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 ≥ 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 was not executed.

Mol	Chain	Length	Quality of chain
1	A	371	
1	B	371	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5936 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 Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	361	Total	C	N	O	S	0	0	0
			2829	1794	476	540	19			
1	B	371	Total	C	N	O	S	0	0	0
			2896	1835	488	552	21			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	56	VAL	GLY	CONFLICT	UNP P68135
A	60	GLY	LYS	CONFLICT	UNP P68135
B	1056	VAL	GLY	CONFLICT	UNP P68135
B	1060	GLY	LYS	CONFLICT	UNP P68135

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	3	Total	Ca	0	0
			3	3		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

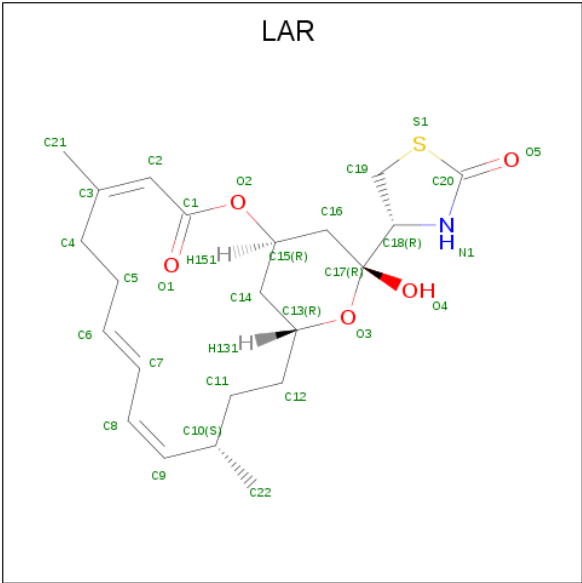
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		
3	A	2	Total	Cl	0	0
			2	2		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 5 is LATRUNCULIN A (three-letter code: LAR) (formula: C₂₂H₃₁NO₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			29	22	1	5	1		
5	B	1	Total	C	N	O	S	0	0
			29	22	1	5	1		

- Molecule 6 is water.

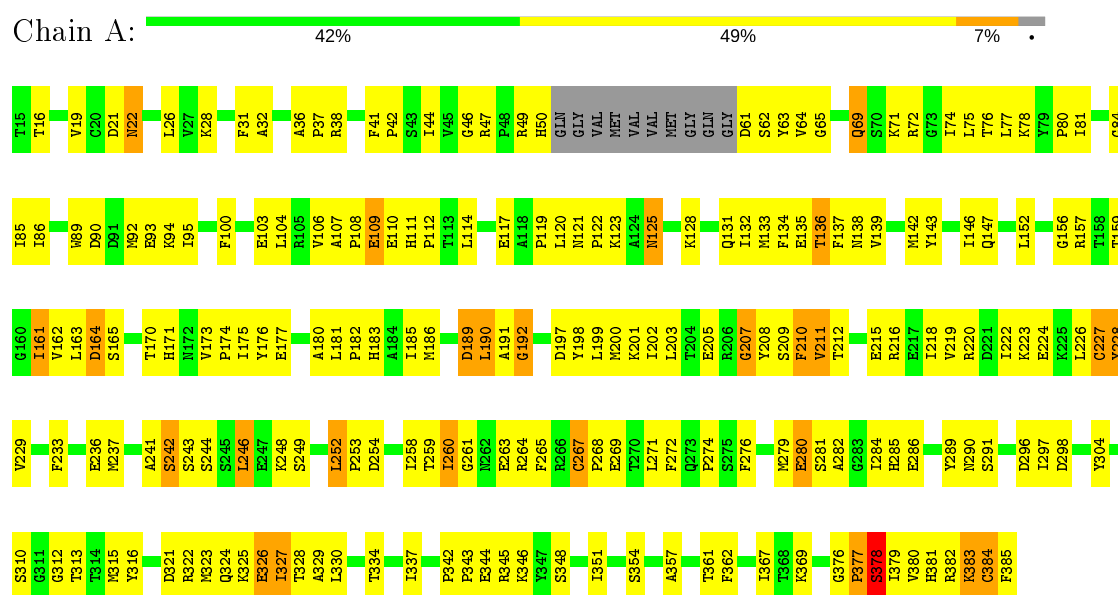
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	41	Total 41	O 41	0	0
6	B	43	Total 43	O 43	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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 was not executed.

- Molecule 1: Actin, alpha skeletal muscle



K1325	E1326	I1327	T1328	A1329	L1330	A1331	F1332	I1337	I1340	A1341	P1342	P1343	E1344	R1345	K1346	V1347	S1348	V1349	M1350	I1351	G1352	G1353	S1354	I1355	L1356	A1357	S1358	T1361	F1362	Q1363	Q1364	M1365	T1368	K1369	Q1370	E1371	Y1372	G1376	P1377	S1378	I1379	V1380	H1381	R1382	K1383	C1384	F1385
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4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.46Å 103.03Å 126.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.50	Depositor
% Data completeness (in resolution range)	88.8 (30.00-3.50)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.196 , 0.266	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5936	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA, ATP, LAR, CL

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	0.43	0/2891	0.67	0/3919
1	B	0.42	0/2959	0.65	0/4011
All	All	0.42	0/5850	0.66	0/7930

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2829	0	2795	216	0
1	B	2896	0	2866	209	0
2	A	3	0	0	0	0
2	B	1	0	0	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
4	A	31	0	12	2	0
4	B	31	0	12	1	0
5	A	29	0	31	1	0
5	B	29	0	31	1	0
6	A	41	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	43	0	0	11	0
All	All	5936	0	5747	427	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 37.

The worst 5 of 427 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:383:LYS:HD2	1:A:384:CYS:H	0.92	1.08
1:A:383:LYS:H	1:A:383:LYS:HE2	1.23	1.02
1:A:383:LYS:HD2	1:A:384:CYS:N	1.77	0.98
1:B:1351:ILE:HD12	1:B:1351:ILE:H	1.32	0.93
1:B:1376:GLY:O	1:B:1379:ILE:HG22	1.69	0.93

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 X-ray entries followed by that with respect to entries of similar resolution.

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	357/371 (96%)	277 (78%)	58 (16%)	22 (6%)	1	15
1	B	369/371 (100%)	277 (75%)	60 (16%)	32 (9%)	1	9
All	All	726/742 (98%)	554 (76%)	118 (16%)	54 (7%)	1	11

5 of 54 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	210	PHE
1	A	211	VAL
1	A	242	SER

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Mol	Chain	Res	Type
1	A	280	GLU
1	A	281	SER

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 X-ray entries followed by that with respect to entries of similar resolution.

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	307/314 (98%)	287 (94%)	20 (6%)	17	50
1	B	314/314 (100%)	286 (91%)	28 (9%)	9	37
All	All	621/628 (99%)	573 (92%)	48 (8%)	13	42

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1049	ARG
1	B	1139	VAL
1	B	1368	THR
1	B	1061	ASP
1	B	1094	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	364	GLN
1	B	1069	GLN
1	B	1363	GLN
1	A	381	HIS
1	B	1051	GLN

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 7 are 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	$\# Z > 2$
5	LAR	A	411	-	30,31,31	1.14	3 (10%)	32,43,43	1.72	5 (15%)
5	LAR	B	1411	-	30,31,31	1.20	4 (13%)	32,43,43	1.53	3 (9%)
4	ATP	B	1390	2	26,33,33	2.23	12 (46%)	31,52,52	3.05	10 (32%)
4	ATP	A	390	2	26,33,33	2.18	11 (42%)	31,52,52	3.14	9 (29%)

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
5	LAR	A	411	-	-	4/23/51/51	0/2/3/3
5	LAR	B	1411	-	-	4/23/51/51	0/2/3/3
4	ATP	B	1390	2	-	2/18/38/38	0/3/3/3
4	ATP	A	390	2	-	1/18/38/38	0/3/3/3

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	390	ATP	C4-N3	5.54	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1390	ATP	C4-N3	4.77	1.42	1.35
4	B	1390	ATP	O4'-C1'	4.75	1.47	1.41
4	B	1390	ATP	O5'-C5'	-4.40	1.27	1.44
4	A	390	ATP	O5'-C5'	-4.34	1.28	1.44

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	390	ATP	O5'-C5'-C4'	11.66	149.12	108.99
4	B	1390	ATP	O5'-C5'-C4'	11.59	148.89	108.99
4	A	390	ATP	O5'-PA-O1A	-7.11	81.27	109.07
4	B	1390	ATP	O5'-PA-O1A	-7.10	81.31	109.07
4	A	390	ATP	PA-O5'-C5'	5.90	156.28	121.68

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1411	LAR	O3-C17-C18-C19
5	A	411	LAR	O3-C17-C18-C19
5	A	411	LAR	C3-C4-C5-C6
4	B	1390	ATP	PG-O3B-PB-O2B
4	A	390	ATP	PG-O3B-PB-O2B

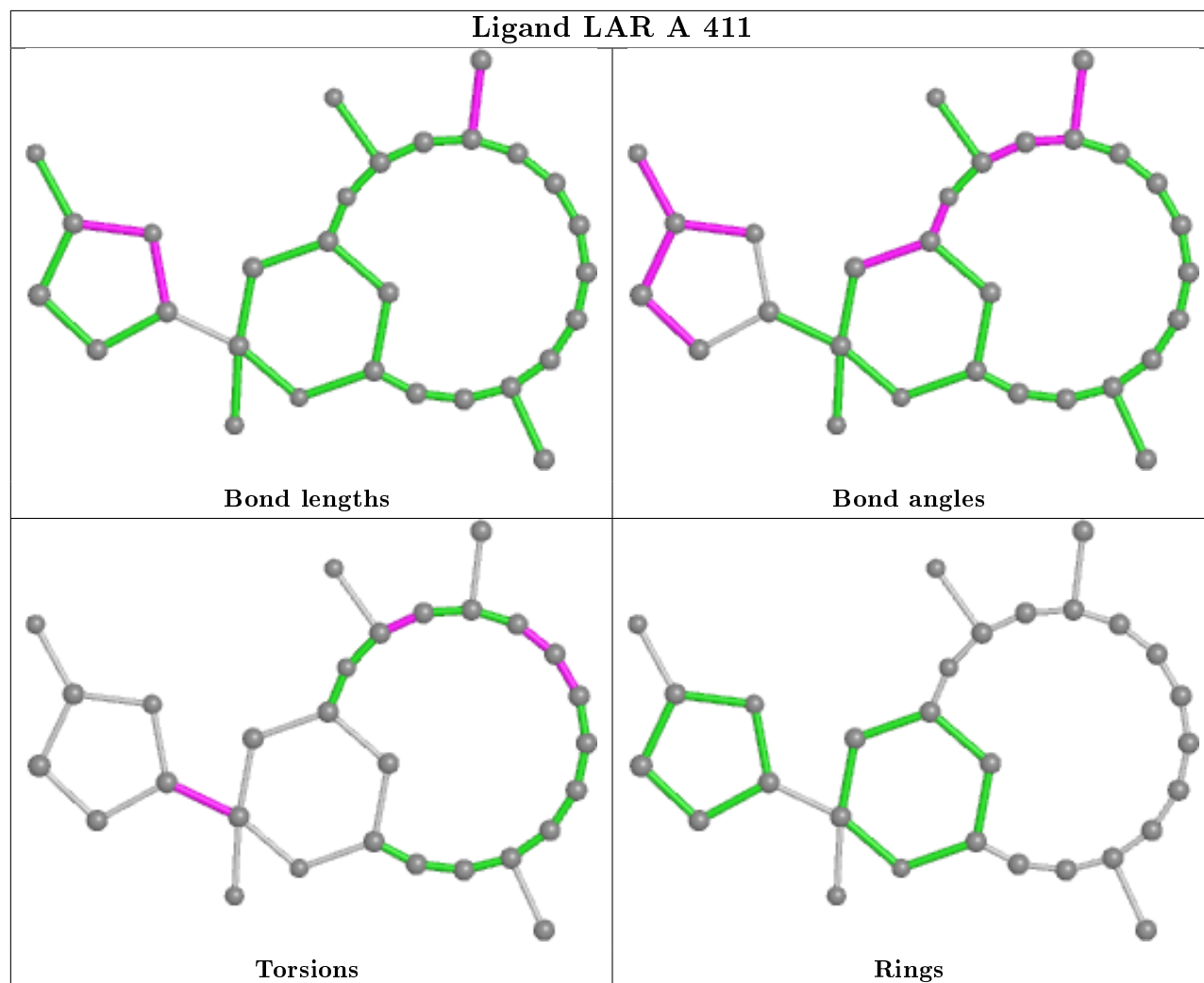
There are no ring outliers.

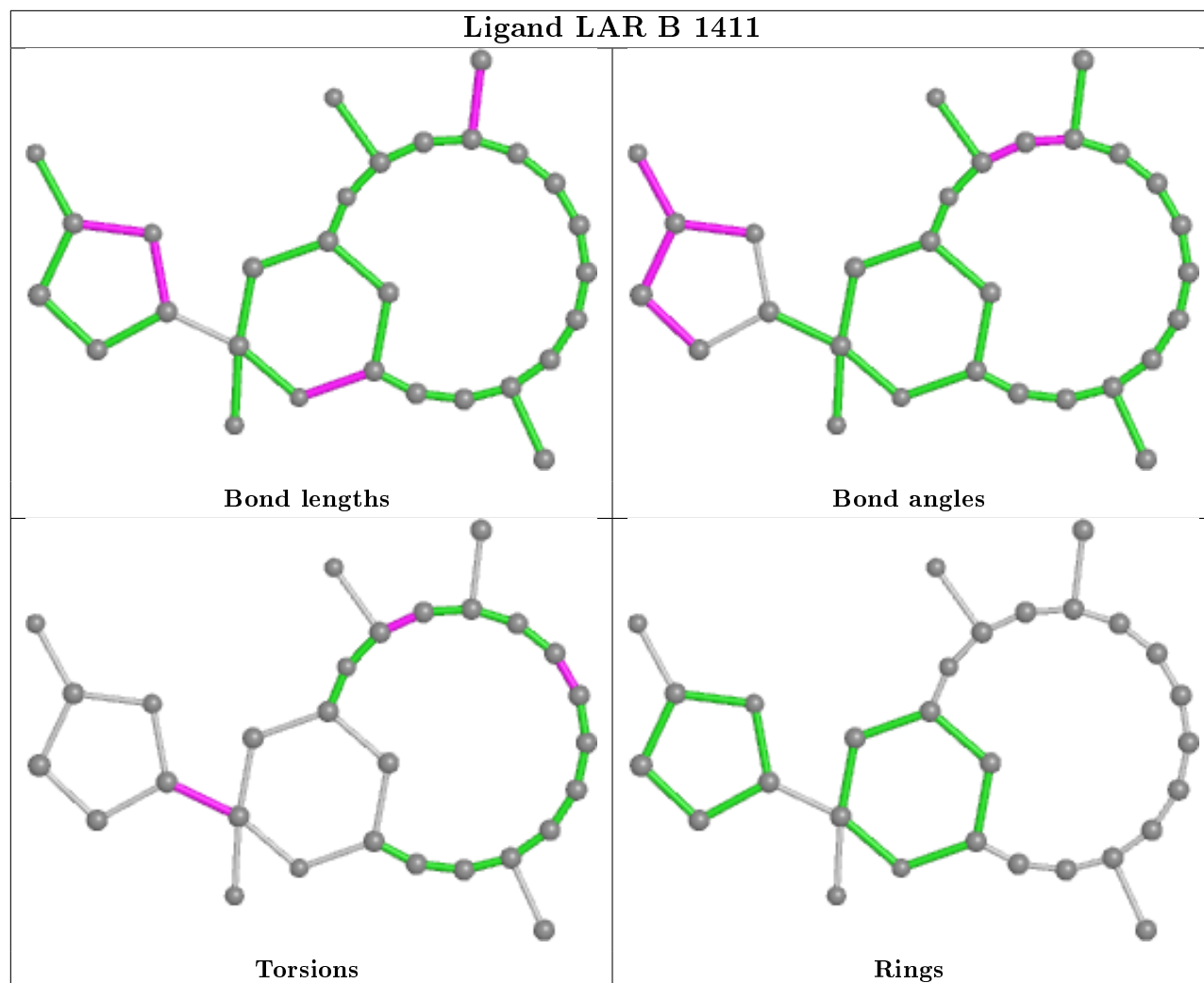
4 monomers are involved in 5 short contacts:

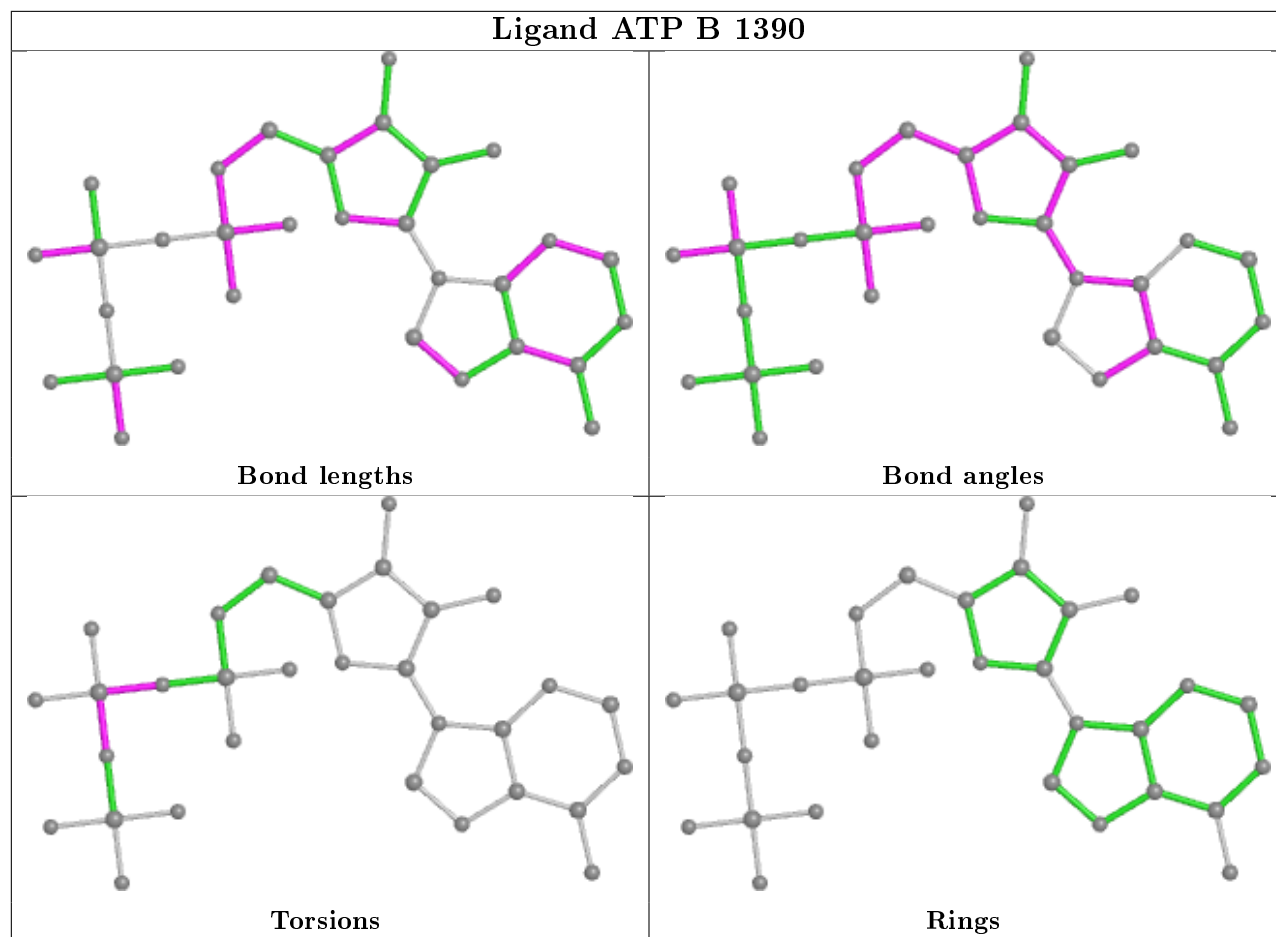
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	411	LAR	1	0
5	B	1411	LAR	1	0
4	B	1390	ATP	1	0
4	A	390	ATP	2	0

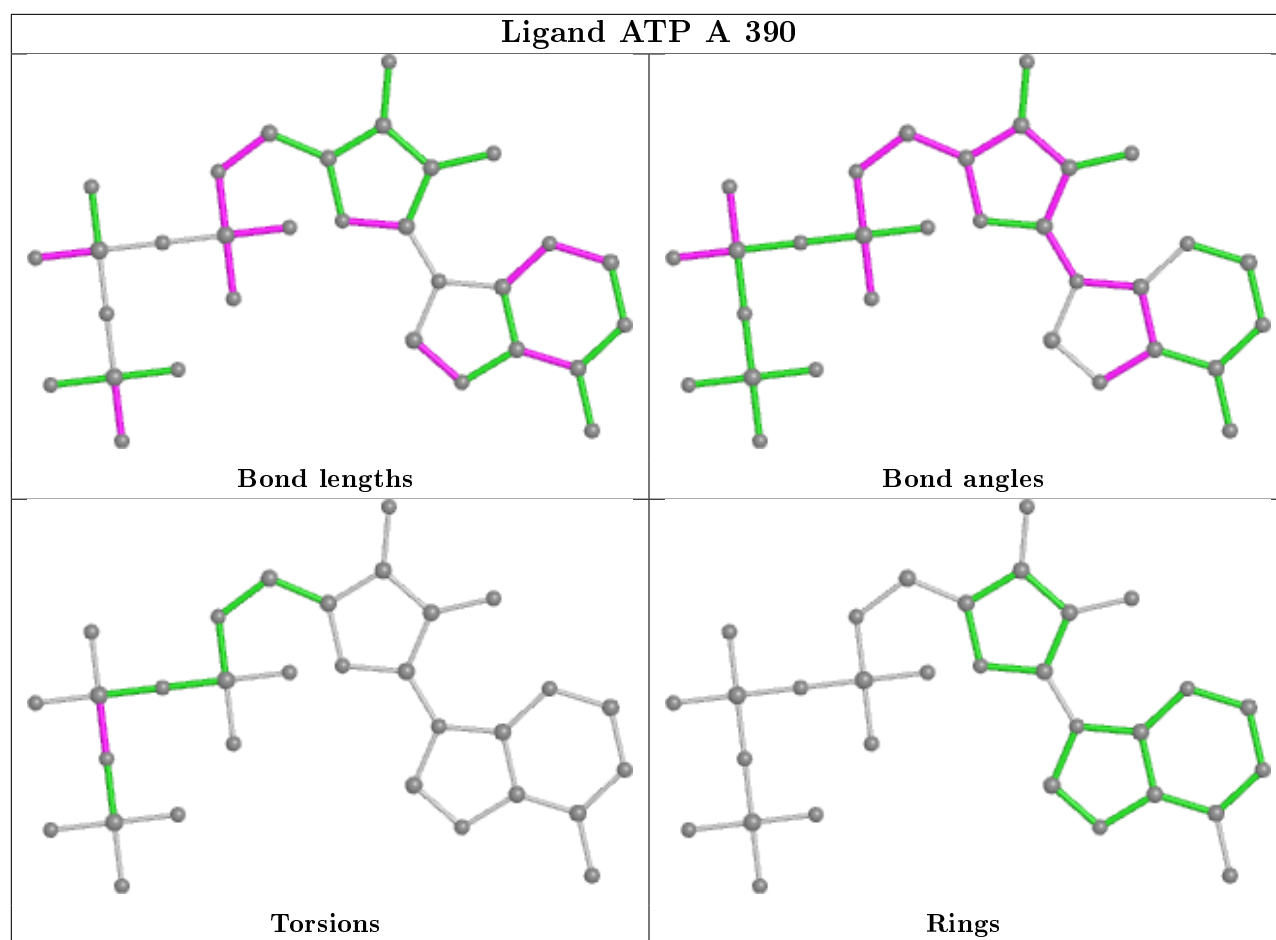
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.