



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Sep 17, 2019 – 09:40 AM EDT

PDB ID : 6U3E
EMDB ID: : EMD-20628
Title : Best fitting antiparallel model for Volume 1 of truncated dimeric Cytohesin-3
(Grp1; amino acids 14-399)
Authors : Das, S.; Lambright, D.G.
Deposited on : 2019-08-21
Resolution : 53.00 Å (reported)
Based on PDB ID : 2R09

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB 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.

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

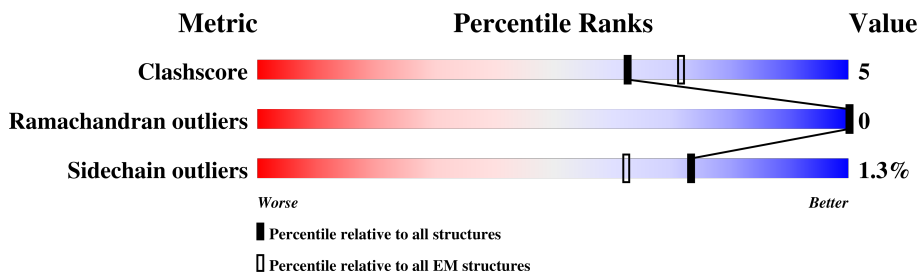
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 53.00 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	397	 92% 7% .
1	B	397	 91% 9% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6594 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 Cytohesin-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	397	Total	C	N	O	S	0	0
			3269	2065	574	614	16		
1	B	397	Total	C	N	O	S	0	0
			3269	2065	574	614	16		

There are 32 discrepancies between the modelled and reference sequences:

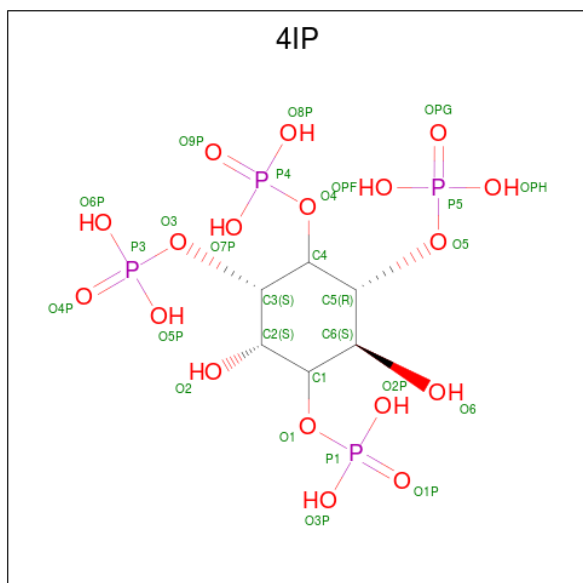
Chain	Residue	Modelled	Actual	Comment	Reference
A	3	MET	-	expression tag	UNP O43739
A	4	GLY	-	expression tag	UNP O43739
A	5	HIS	-	expression tag	UNP O43739
A	6	HIS	-	expression tag	UNP O43739
A	7	HIS	-	expression tag	UNP O43739
A	8	HIS	-	expression tag	UNP O43739
A	9	HIS	-	expression tag	UNP O43739
A	10	HIS	-	expression tag	UNP O43739
A	11	GLY	-	expression tag	UNP O43739
A	12	SER	-	expression tag	UNP O43739
A	63	TYR	THR	conflict	UNP O43739
A	68	ALA	LYS	conflict	UNP O43739
A	125	ASP	GLU	conflict	UNP O43739
A	220	THR	ALA	conflict	UNP O43739
A	260	TYR	HIS	conflict	UNP O43739
A	?	-	GLY	deletion	UNP O43739
B	3	MET	-	expression tag	UNP O43739
B	4	GLY	-	expression tag	UNP O43739
B	5	HIS	-	expression tag	UNP O43739
B	6	HIS	-	expression tag	UNP O43739
B	7	HIS	-	expression tag	UNP O43739
B	8	HIS	-	expression tag	UNP O43739
B	9	HIS	-	expression tag	UNP O43739
B	10	HIS	-	expression tag	UNP O43739
B	11	GLY	-	expression tag	UNP O43739
B	12	SER	-	expression tag	UNP O43739

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Chain	Residue	Modelled	Actual	Comment	Reference
B	63	TYR	THR	conflict	UNP O43739
B	68	ALA	LYS	conflict	UNP O43739
B	125	ASP	GLU	conflict	UNP O43739
B	220	THR	ALA	conflict	UNP O43739
B	260	TYR	HIS	conflict	UNP O43739
B	?	-	GLY	deletion	UNP O43739

- Molecule 2 is INOSITOL-(1,3,4,5)-TETRAKISPHOSPHATE (three-letter code: 4IP) (formula: $C_6H_{16}O_{18}P_4$).

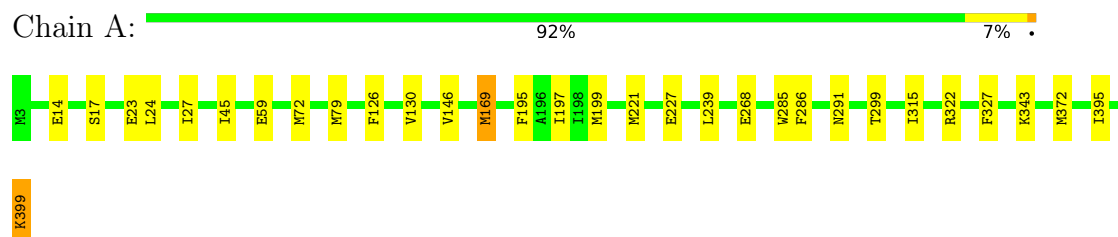


Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	O	P	0
			28	6	18	4	
2	B	1	Total	C	O	P	0
			28	6	18	4	

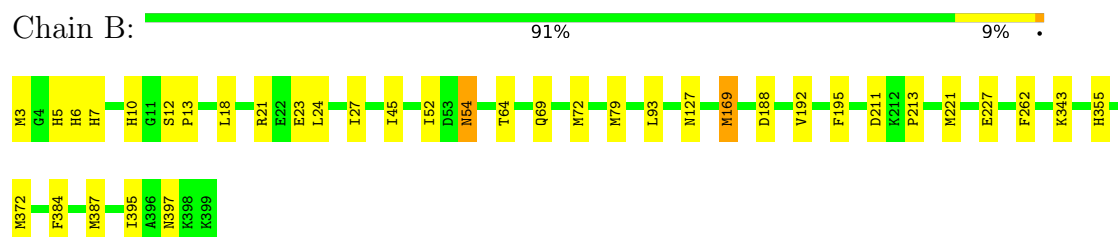
3 Residue-property plots [i](#)

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.

- Molecule 1: Cytohesin-3



- Molecule 1: Cytohesin-3



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	2052	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI/PHILIPS CM120T	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30.0	Depositor
Minimum defocus (nm)	-1200	Depositor
Maximum defocus (nm)	-3200	Depositor
Magnification	28000	Depositor
Image detector	TVIPS TEMCAM-F224 (2k x 2k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 4IP

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.67	6/3340 (0.2%)	0.63	0/4500
1	B	0.66	7/3340 (0.2%)	0.62	0/4500
All	All	0.66	13/6680 (0.2%)	0.62	0/9000

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	64	THR	C-N	11.15	1.59	1.34
1	A	169	MET	CG-SD	6.97	1.99	1.81
1	B	387	MET	CG-SD	6.90	1.99	1.81
1	A	221	MET	CG-SD	6.24	1.97	1.81
1	B	169	MET	CG-SD	5.81	1.96	1.81

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	3269	0	3217	30	0
1	B	3269	0	3217	48	0
2	A	28	0	8	0	0
2	B	28	0	8	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6594	0	6450	62	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 62 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:192:VAL:HG21	1:B:395:ILE:CD1	1.14	1.55
1:B:192:VAL:CG2	1:B:395:ILE:CD1	1.87	1.49
1:B:192:VAL:CG2	1:B:395:ILE:HD11	1.42	1.49
1:B:192:VAL:HG23	1:B:395:ILE:HD11	1.11	1.05
1:B:192:VAL:HG21	1:B:395:ILE:HD12	0.96	0.96

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	395/397 (100%)	389 (98%)	6 (2%)	0	100	100
1	B	395/397 (100%)	389 (98%)	6 (2%)	0	100	100
All	All	790/794 (100%)	778 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	358/358 (100%)	352 (98%)	6 (2%)	63	83
1	B	358/358 (100%)	355 (99%)	3 (1%)	83	92
All	All	716/716 (100%)	707 (99%)	9 (1%)	73	86

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

Mol	Chain	Res	Type
1	A	343	LYS
1	B	343	LYS
1	B	7	HIS
1	A	291	ASN
1	A	399	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	10	HIS
1	B	355	HIS
1	B	54	ASN
1	A	291	ASN
1	B	127	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry

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	4IP	A	400	-	28,28,28	0.78	0	42,46,46	0.93	0
2	4IP	B	401	-	28,28,28	0.78	0	42,46,46	1.03	3 (7%)

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	4IP	A	400	-	-	2/20/44/44	0/1/1/1
2	4IP	B	401	-	-	4/20/44/44	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	4IP	O8P-P4-O7P	2.33	116.63	107.57
2	B	401	4IP	OPH-P5-OPF	2.27	116.41	107.57
2	B	401	4IP	O6P-P3-O5P	2.23	116.23	107.57

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	400	4IP	C1-O1-P1-O3P
2	A	400	4IP	C5-O5-P5-OPH
2	B	401	4IP	C1-O1-P1-O3P
2	B	401	4IP	C5-O5-P5-OPH
2	B	401	4IP	C1-O1-P1-O2P

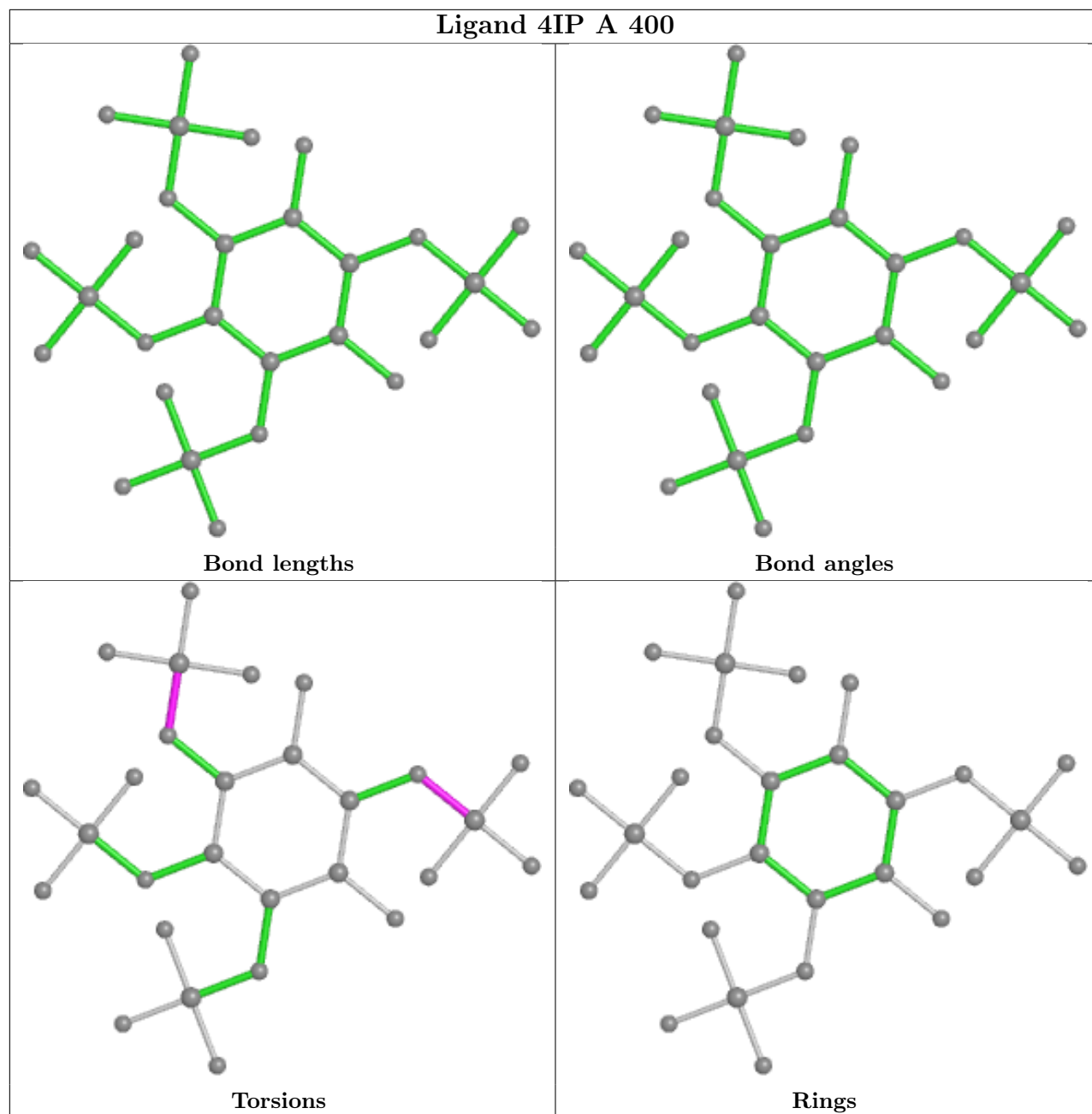
There are no ring outliers.

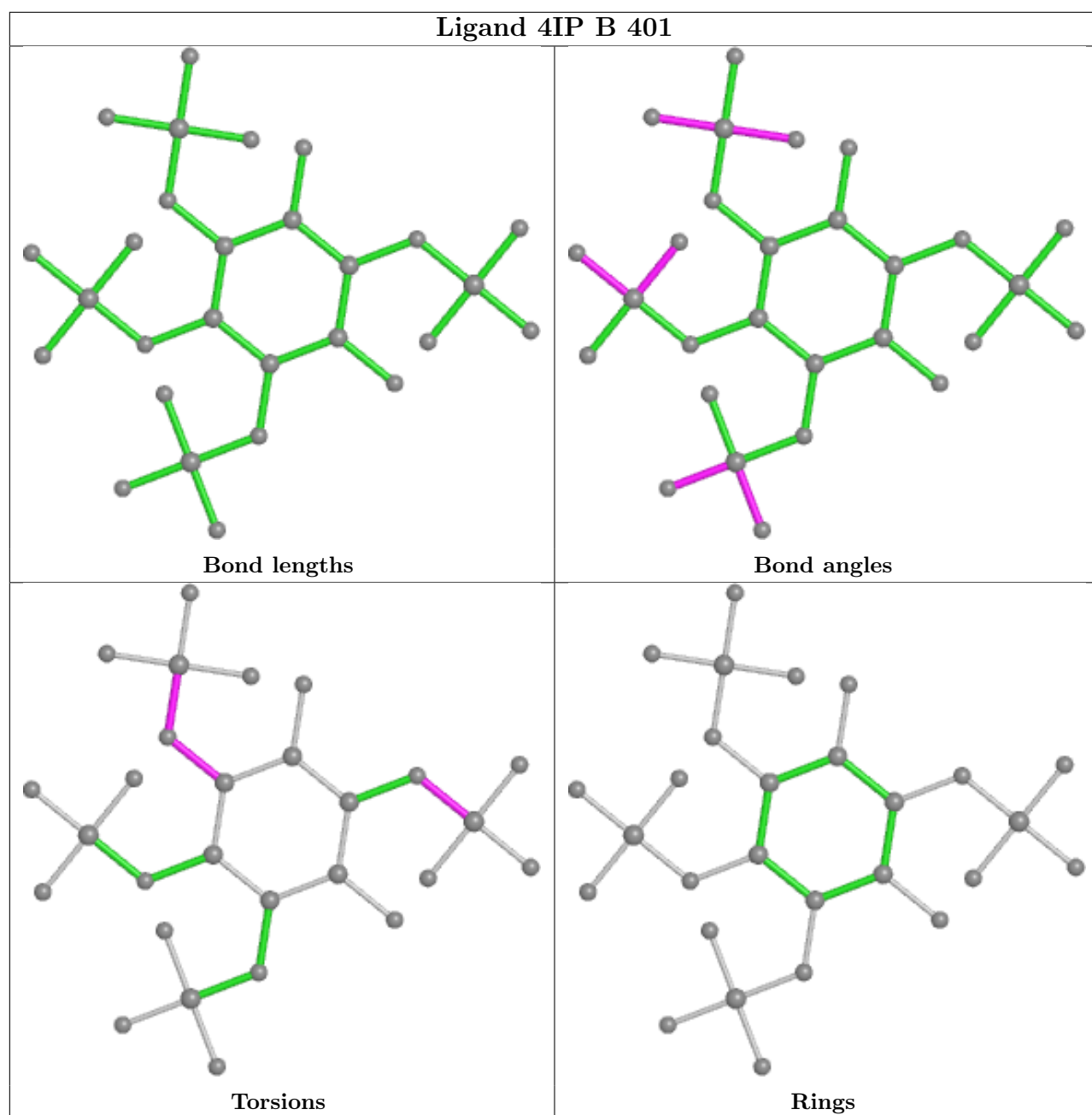
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	4IP	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.

Ligand 4IP A 400





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.