



## wwPDB EM Validation Summary Report ⓘ

Feb 24, 2025 – 06:07 pm GMT

PDB ID : 8R2N  
EMDB ID : EMD-18852  
Title : Structure of the BeeR filament  
Authors : Bergeron, J.R.C.; Kollman, J.M.  
Deposited on : 2023-11-07  
Resolution : 3.10 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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<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	: <b>FAILED</b>
Mogul	: 1.8.4, CSD as541be (2020)
MolProbity	: 4.02b-467
buster-report	: 1.1.7 (2018)
Percentile statistics	: 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	: <b>FAILED</b>
Ideal geometry (proteins)	: Engh & Huber (2001)
Ideal geometry (DNA, RNA)	: Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: 2.41

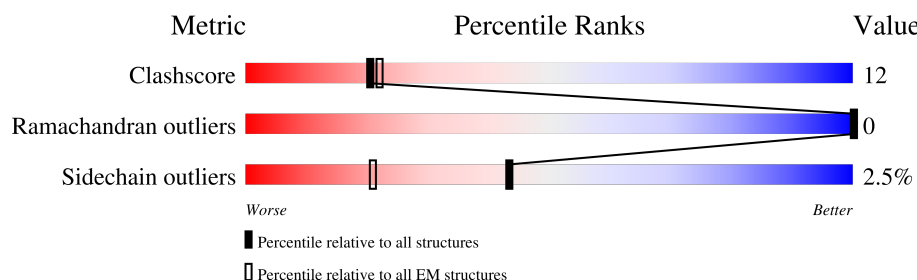
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.10 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	386	67% 23% • 9%
1	B	386	62% 29% • 9%
1	C	386	66% 24% • 9%
1	D	386	69% 22% • 9%
1	E	386	69% 22% 9%
1	F	386	66% 25% • 9%
1	G	386	65% 26% 9%
1	H	386	67% 24% • 9%
1	I	386	71% 20% • 9%

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Mol	Chain	Length	Quality of chain
1	J	386	 68%23%9%
1	K	386	 65%25%9%
1	L	386	 65%27%9%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 33237 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 Actin/actin family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	353	Total	C	N	O	S	4	0
			2692	1703	480	504	5		
1	B	353	Total	C	N	O	S	4	0
			2692	1703	480	504	5		
1	C	353	Total	C	N	O	S	4	0
			2692	1703	480	504	5		
1	D	353	Total	C	N	O	S	4	0
			2692	1703	480	504	5		
1	E	353	Total	C	N	O	S	4	0
			2692	1703	480	504	5		
1	F	353	Total	C	N	O	S	4	0
			2692	1703	480	504	5		
1	G	353	Total	C	N	O	S	4	0
			2692	1703	480	504	5		
1	H	353	Total	C	N	O	S	4	0
			2692	1703	480	504	5		
1	I	353	Total	C	N	O	S	4	0
			2692	1703	480	504	5		
1	J	353	Total	C	N	O	S	4	0
			2692	1703	480	504	5		
1	K	353	Total	C	N	O	S	4	0
			2692	1703	480	504	5		
1	L	353	Total	C	N	O	S	4	0
			2692	1703	480	504	5		

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total 31	C 10	N 5	O 13	P 3	0
2	B	1	Total 31	C 10	N 5	O 13	P 3	0
2	C	1	Total 31	C 10	N 5	O 13	P 3	0
2	D	1	Total 31	C 10	N 5	O 13	P 3	0
2	E	1	Total 31	C 10	N 5	O 13	P 3	0
2	F	1	Total 31	C 10	N 5	O 13	P 3	0
2	G	1	Total 31	C 10	N 5	O 13	P 3	0
2	H	1	Total 31	C 10	N 5	O 13	P 3	0
2	I	1	Total 31	C 10	N 5	O 13	P 3	0
2	J	1	Total 31	C 10	N 5	O 13	P 3	0
2	K	1	Total 31	C 10	N 5	O 13	P 3	0
2	L	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total Ca 1 1	0
3	B	1	Total Ca 1 1	0
3	C	1	Total Ca 1 1	0
3	D	1	Total Ca 1 1	0
3	E	1	Total Ca 1 1	0
3	F	1	Total Ca 1 1	0
3	G	1	Total Ca 1 1	0
3	H	1	Total Ca 1 1	0
3	I	1	Total Ca 1 1	0
3	J	1	Total Ca 1 1	0
3	K	1	Total Ca 1 1	0
3	L	1	Total Ca 1 1	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	AltConf
4	A	45	Total O 45 45	0
4	B	46	Total O 46 46	0
4	C	46	Total O 46 46	0
4	D	47	Total O 47 47	0
4	E	46	Total O 46 46	0
4	F	46	Total O 46 46	0
4	G	45	Total O 45 45	0
4	H	47	Total O 47 47	0

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Mol	Chain	Residues	Atoms		AltConf
4	I	45	Total 45	O 45	0
4	J	47	Total 47	O 47	0
4	K	45	Total 45	O 45	0
4	L	44	Total 44	O 44	0

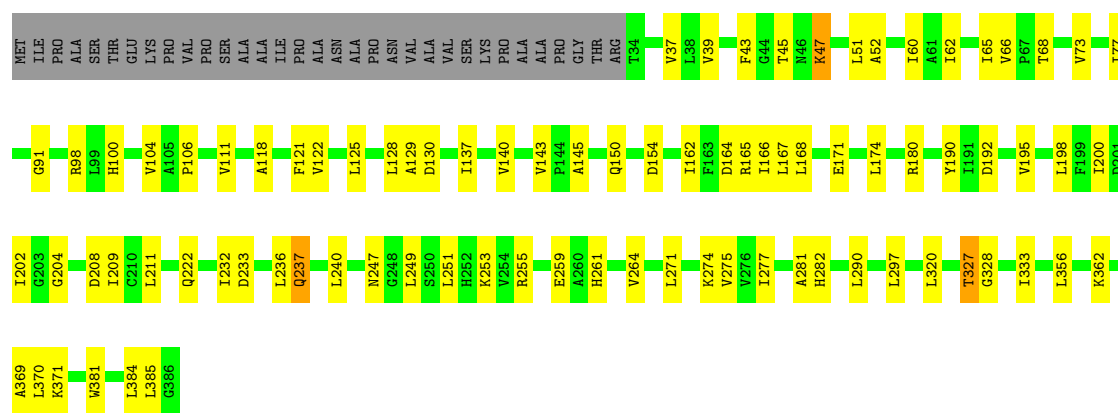






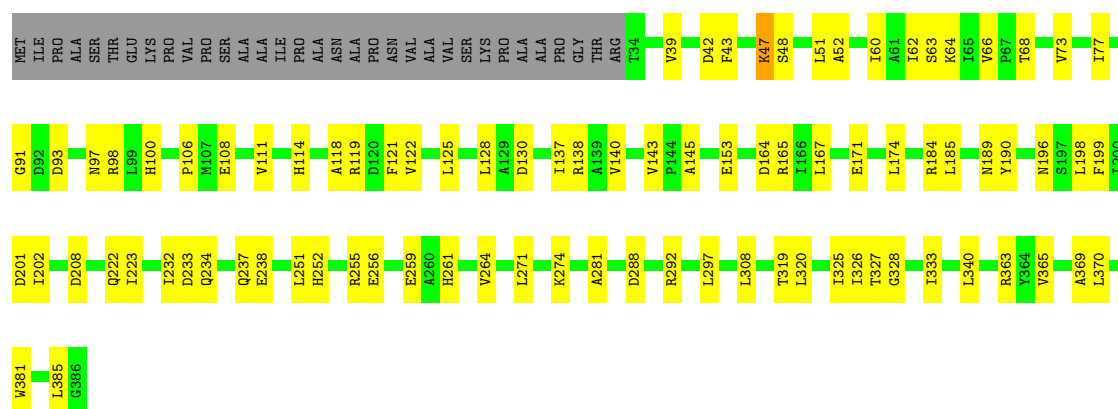
- Molecule 1: Actin/actin family protein

Chain D: 69% 22% 9%



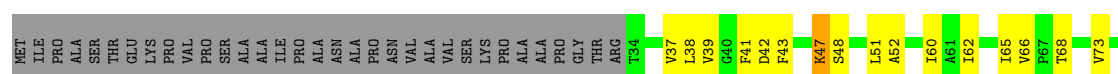
- Molecule 1: Actin/actin family protein

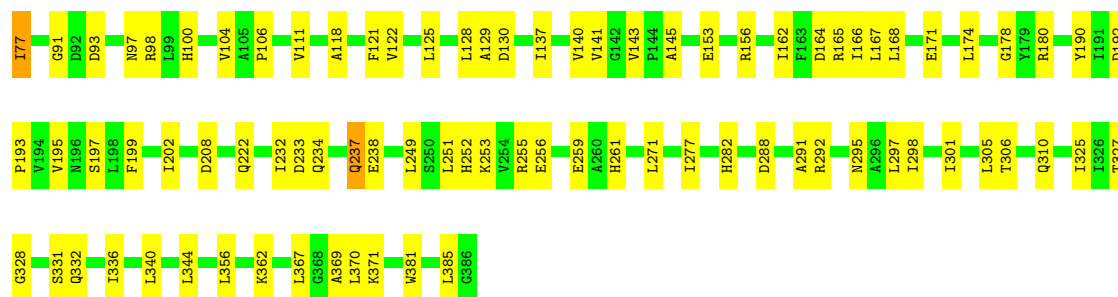
Chain E: 69% 22% 9%



- Molecule 1: Actin/actin family protein

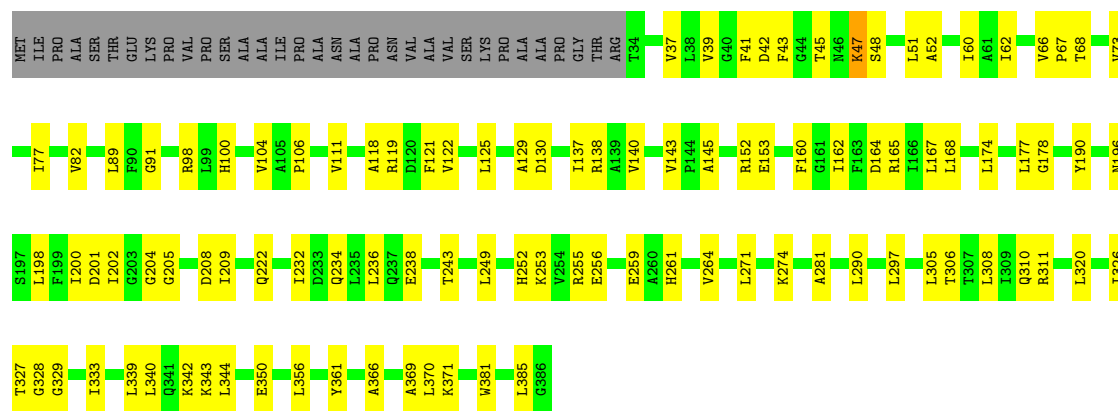
Chain F: 66% 25% 9%





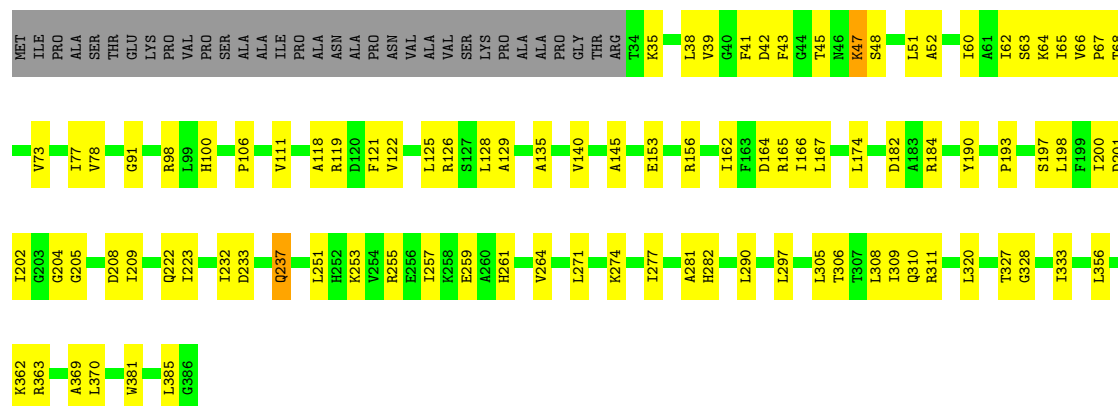
- Molecule 1: Actin/actin family protein

Chain G: 65% 26% 9%



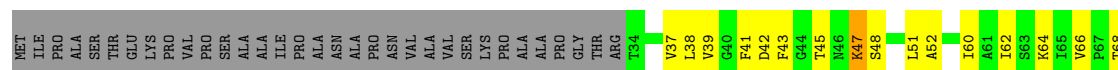
- Molecule 1: Actin/actin family protein

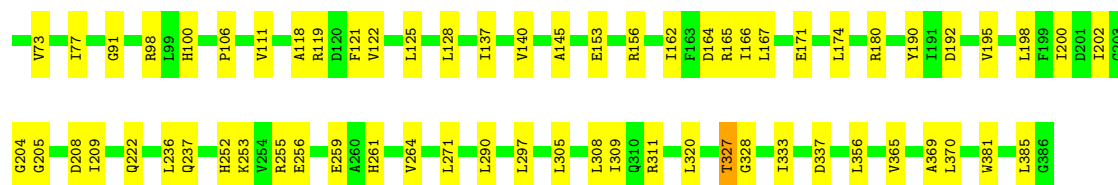
Chain H: 67% 24% 9%



- Molecule 1: Actin/actin family protein

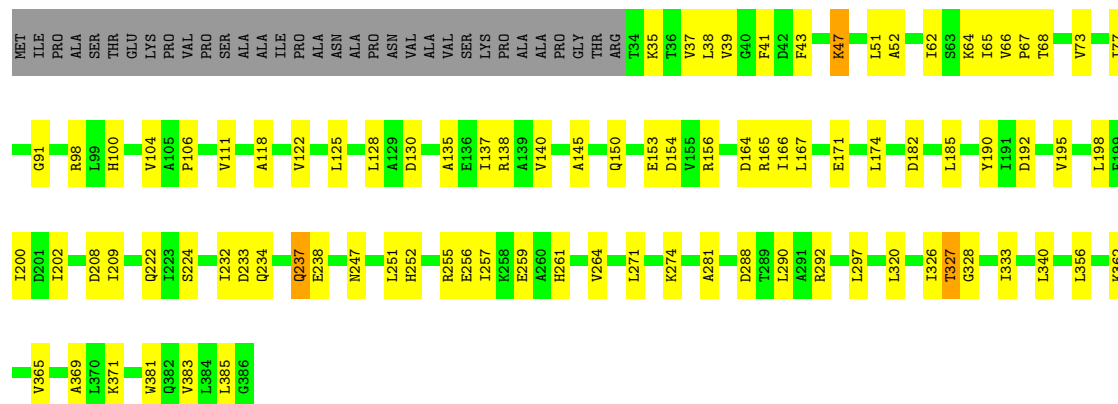
Chain I: 71% 20% 9%





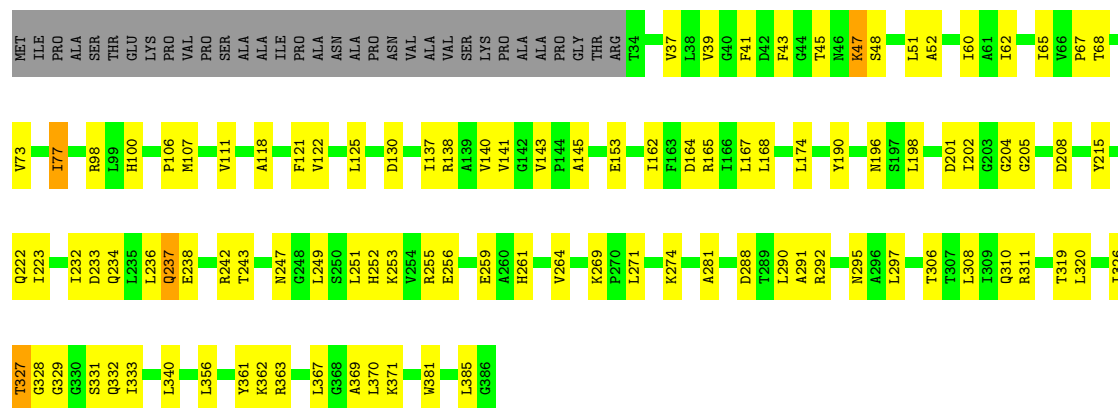
• Molecule 1: Actin/actin family protein

Chain J: 68% 23% 9%



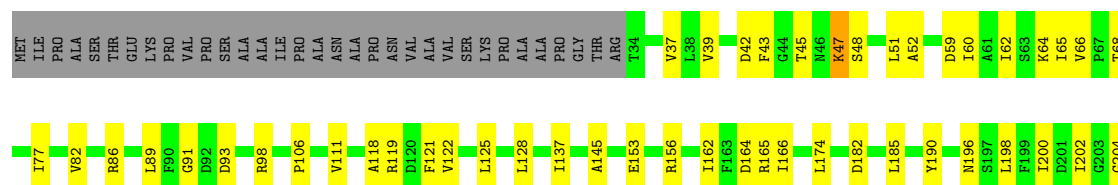
• Molecule 1: Actin/actin family protein

Chain K: 65% 25% 9%



• Molecule 1: Actin/actin family protein

Chain L: 65% 27% 9%



G205	I206	S207	D208	I209	Q222	I232	D233	Q234	Q237	E238	L249	H252	K253	V284	R285	E286	I287	K288	E289	A290	L291	N295	A296	L297	L305	T306	T307	L308	I309	Q310	R311	T319	L320	L321	I326
T327	G328	G329	I333	L340	L344	P352	L356	D360	Y361	K362	R363	A369	L370	R374	W381	L385	G386																		

## 4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=126.5°, rise=17.4 Å, axial sym=C1	Depositor
Number of segments used	882189	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{Å}^2$ )	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k 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: ATP, CA

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	0.27	0/2749	0.43	0/3729
1	B	0.28	0/2749	0.44	0/3729
1	C	0.27	0/2749	0.44	0/3729
1	D	0.27	0/2749	0.44	0/3729
1	E	0.28	0/2749	0.44	0/3729
1	F	0.27	0/2749	0.44	0/3729
1	G	0.27	0/2749	0.44	0/3729
1	H	0.27	0/2749	0.44	0/3729
1	I	0.27	0/2749	0.44	0/3729
1	J	0.27	0/2749	0.44	0/3729
1	K	0.27	0/2749	0.44	0/3729
1	L	0.28	0/2749	0.44	0/3729
All	All	0.27	0/32988	0.44	0/44748

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 [i](#)

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	2692	0	2747	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2692	0	2747	76	0
1	C	2692	0	2747	64	0
1	D	2692	0	2747	58	0
1	E	2692	0	2747	59	0
1	F	2692	0	2747	65	0
1	G	2692	0	2747	72	0
1	H	2692	0	2747	67	0
1	I	2692	0	2747	54	0
1	J	2692	0	2747	58	0
1	K	2692	0	2747	71	0
1	L	2692	0	2747	68	0
2	A	31	0	11	0	0
2	B	31	0	11	4	0
2	C	31	0	11	3	0
2	D	31	0	11	3	0
2	E	31	0	11	0	0
2	F	31	0	11	1	0
2	G	31	0	11	4	0
2	H	31	0	11	4	0
2	I	31	0	11	4	0
2	J	31	0	11	1	0
2	K	31	0	11	3	0
2	L	31	0	11	4	0
3	A	1	0	0	1	0
3	B	1	0	0	1	0
3	C	1	0	0	1	0
3	D	1	0	0	1	0
3	E	1	0	0	1	0
3	F	1	0	0	1	0
3	G	1	0	0	1	0
3	H	1	0	0	1	0
3	I	1	0	0	1	0
3	J	1	0	0	1	0
3	K	1	0	0	1	0
3	L	1	0	0	1	0
4	A	45	0	0	10	0
4	B	46	0	0	9	0
4	C	46	0	0	8	0
4	D	47	0	0	9	0
4	E	46	0	0	10	0
4	F	46	0	0	11	0
4	G	45	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	47	0	0	11	0
4	I	45	0	0	9	0
4	J	47	0	0	11	0
4	K	45	0	0	9	0
4	L	44	0	0	10	0
All	All	33237	0	33096	783	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 783 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:L:190:TYR:CE1	4:L:506:HOH:O	1.79	1.35
3:F:401:CA:CA	4:F:507:HOH:O	1.04	1.31
1:J:190:TYR:CE1	4:J:506:HOH:O	1.84	1.31
3:H:401:CA:CA	4:H:515:HOH:O	0.95	1.30
1:K:190:TYR:CE1	4:K:506:HOH:O	1.80	1.29

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	355/386 (92%)	342 (96%)	13 (4%)	0	100	100
1	B	355/386 (92%)	339 (96%)	16 (4%)	0	100	100
1	C	355/386 (92%)	343 (97%)	12 (3%)	0	100	100
1	D	355/386 (92%)	340 (96%)	15 (4%)	0	100	100
1	E	355/386 (92%)	341 (96%)	14 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	355/386 (92%)	341 (96%)	14 (4%)	0	100	100
1	G	355/386 (92%)	341 (96%)	14 (4%)	0	100	100
1	H	355/386 (92%)	341 (96%)	14 (4%)	0	100	100
1	I	355/386 (92%)	341 (96%)	14 (4%)	0	100	100
1	J	355/386 (92%)	340 (96%)	15 (4%)	0	100	100
1	K	355/386 (92%)	341 (96%)	14 (4%)	0	100	100
1	L	355/386 (92%)	341 (96%)	14 (4%)	0	100	100
All	All	4260/4632 (92%)	4091 (96%)	169 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	285/305 (93%)	279 (98%)	6 (2%)	48	72
1	B	285/305 (93%)	279 (98%)	6 (2%)	48	72
1	C	285/305 (93%)	276 (97%)	9 (3%)	34	63
1	D	285/305 (93%)	278 (98%)	7 (2%)	42	69
1	E	285/305 (93%)	281 (99%)	4 (1%)	62	81
1	F	285/305 (93%)	276 (97%)	9 (3%)	34	63
1	G	285/305 (93%)	279 (98%)	6 (2%)	48	72
1	H	285/305 (93%)	277 (97%)	8 (3%)	38	66
1	I	285/305 (93%)	277 (97%)	8 (3%)	38	66
1	J	285/305 (93%)	277 (97%)	8 (3%)	38	66
1	K	285/305 (93%)	278 (98%)	7 (2%)	42	69
1	L	285/305 (93%)	280 (98%)	5 (2%)	54	76
All	All	3420/3660 (93%)	3337 (98%)	83 (2%)	43	70

5 of 83 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	47	LYS
1	K	43	PHE
1	I	180	ARG
1	J	47	LYS
1	K	237	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	246	ASN
1	L	196	ASN
1	E	196	ASN
1	F	196	ASN
1	F	234	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](#)

Of 24 ligands modelled in this entry, 12 are monoatomic - leaving 12 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
2	ATP	I	400	3	26,33,33	0.92	1 (3%)	31,52,52	1.45	5 (16%)
2	ATP	H	400	3	26,33,33	0.92	1 (3%)	31,52,52	1.44	5 (16%)
2	ATP	L	400	3	26,33,33	0.91	1 (3%)	31,52,52	1.43	5 (16%)
2	ATP	J	400	3	26,33,33	0.92	1 (3%)	31,52,52	1.45	5 (16%)
2	ATP	F	400	3	26,33,33	0.91	1 (3%)	31,52,52	1.49	5 (16%)
2	ATP	C	400	3	26,33,33	0.92	1 (3%)	31,52,52	1.40	5 (16%)
2	ATP	D	400	3	26,33,33	0.91	1 (3%)	31,52,52	1.46	5 (16%)
2	ATP	B	400	3	26,33,33	0.91	1 (3%)	31,52,52	1.45	5 (16%)
2	ATP	A	400	3	26,33,33	0.91	1 (3%)	31,52,52	1.40	5 (16%)
2	ATP	G	400	3	26,33,33	0.91	1 (3%)	31,52,52	1.44	5 (16%)
2	ATP	K	400	3	26,33,33	0.90	1 (3%)	31,52,52	1.43	5 (16%)
2	ATP	E	400	3	26,33,33	0.91	1 (3%)	31,52,52	1.45	5 (16%)

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	ATP	I	400	3	-	4/18/38/38	0/3/3/3
2	ATP	H	400	3	-	4/18/38/38	0/3/3/3
2	ATP	L	400	3	-	4/18/38/38	0/3/3/3
2	ATP	J	400	3	-	3/18/38/38	0/3/3/3
2	ATP	F	400	3	-	3/18/38/38	0/3/3/3
2	ATP	C	400	3	-	7/18/38/38	0/3/3/3
2	ATP	D	400	3	-	4/18/38/38	0/3/3/3
2	ATP	B	400	3	-	4/18/38/38	0/3/3/3
2	ATP	A	400	3	-	4/18/38/38	0/3/3/3
2	ATP	G	400	3	-	4/18/38/38	0/3/3/3
2	ATP	K	400	3	-	4/18/38/38	0/3/3/3
2	ATP	E	400	3	-	3/18/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	ATP	C5-C4	2.41	1.47	1.40
2	I	400	ATP	C5-C4	2.40	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	400	ATP	C5-C4	2.40	1.47	1.40
2	D	400	ATP	C5-C4	2.40	1.47	1.40
2	H	400	ATP	C5-C4	2.40	1.47	1.40

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	400	ATP	C3'-C2'-C1'	3.31	105.96	100.98
2	B	400	ATP	C3'-C2'-C1'	3.31	105.96	100.98
2	I	400	ATP	C3'-C2'-C1'	3.29	105.93	100.98
2	G	400	ATP	C3'-C2'-C1'	3.28	105.92	100.98
2	L	400	ATP	C3'-C2'-C1'	3.26	105.88	100.98

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	400	ATP	C5'-O5'-PA-O1A
2	A	400	ATP	C5'-O5'-PA-O2A
2	B	400	ATP	C5'-O5'-PA-O1A
2	B	400	ATP	C5'-O5'-PA-O2A
2	C	400	ATP	C5'-O5'-PA-O1A

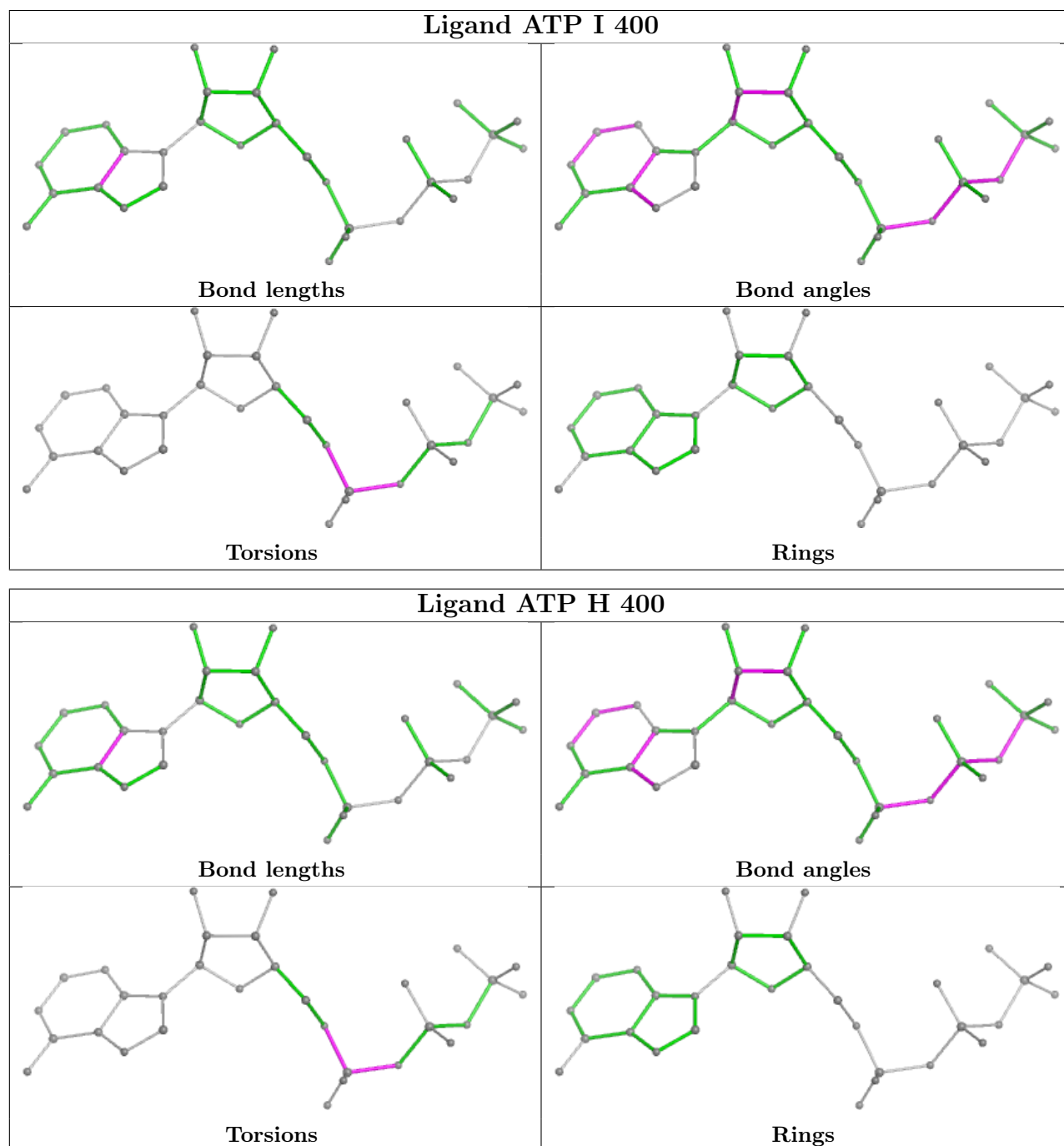
There are no ring outliers.

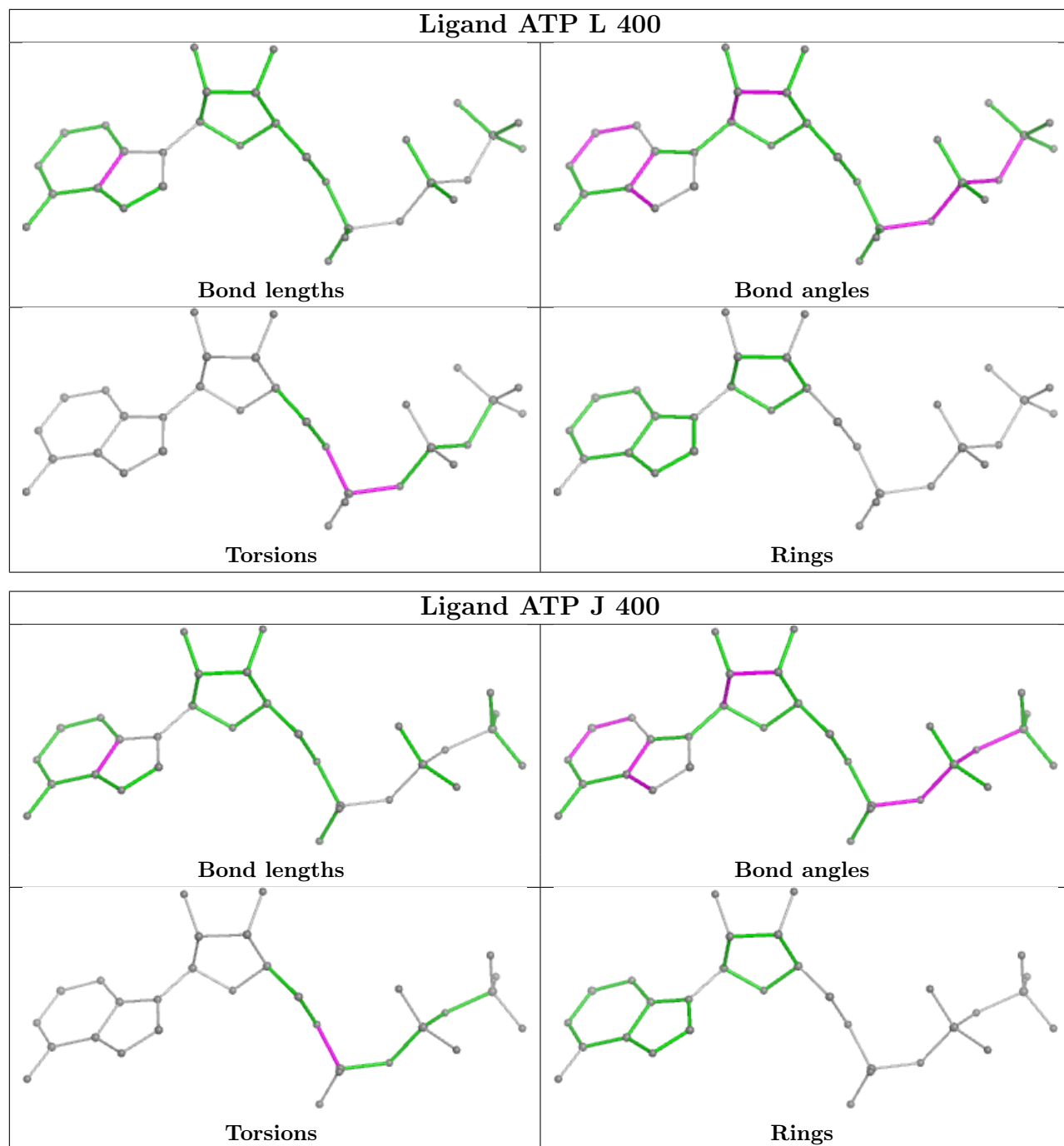
10 monomers are involved in 31 short contacts:

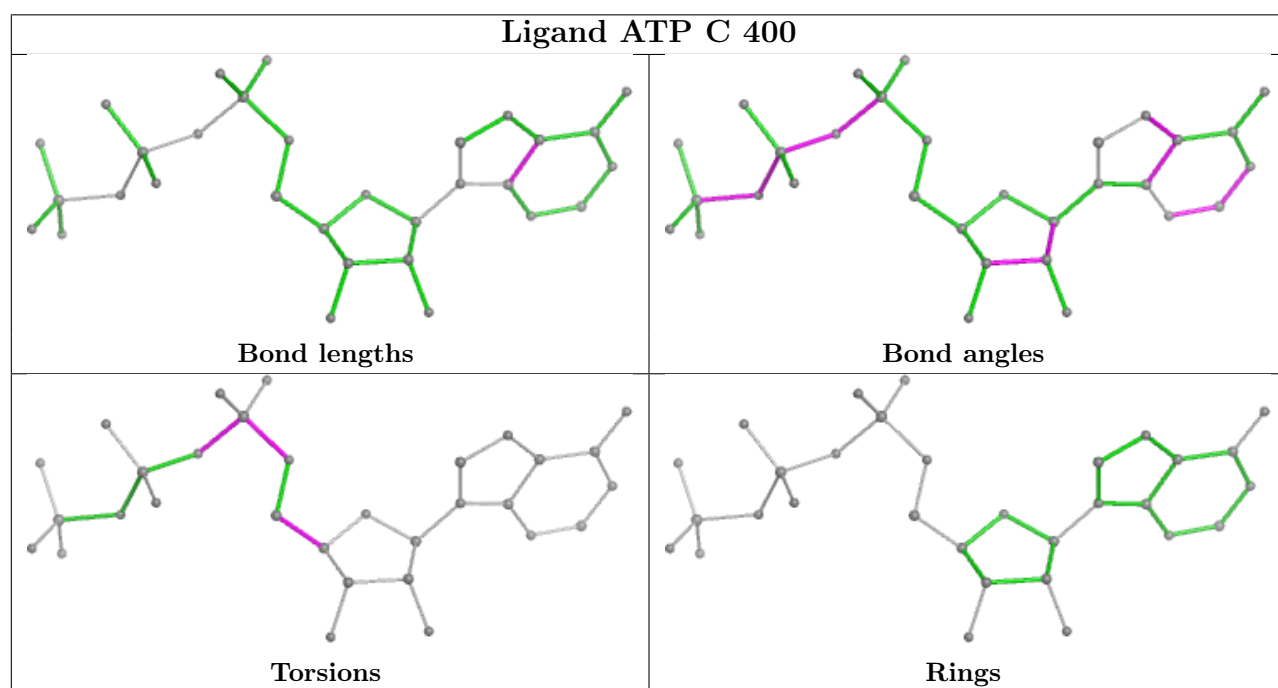
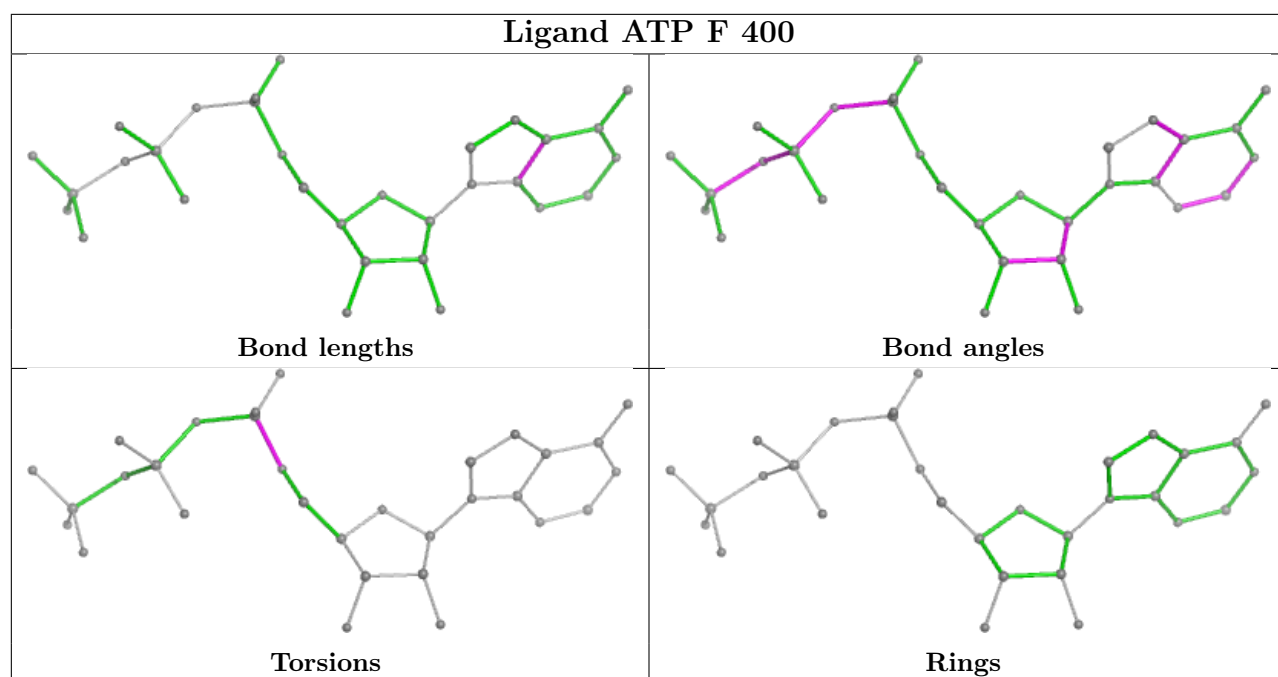
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	400	ATP	4	0
2	H	400	ATP	4	0
2	L	400	ATP	4	0
2	J	400	ATP	1	0
2	F	400	ATP	1	0
2	C	400	ATP	3	0
2	D	400	ATP	3	0
2	B	400	ATP	4	0
2	G	400	ATP	4	0
2	K	400	ATP	3	0

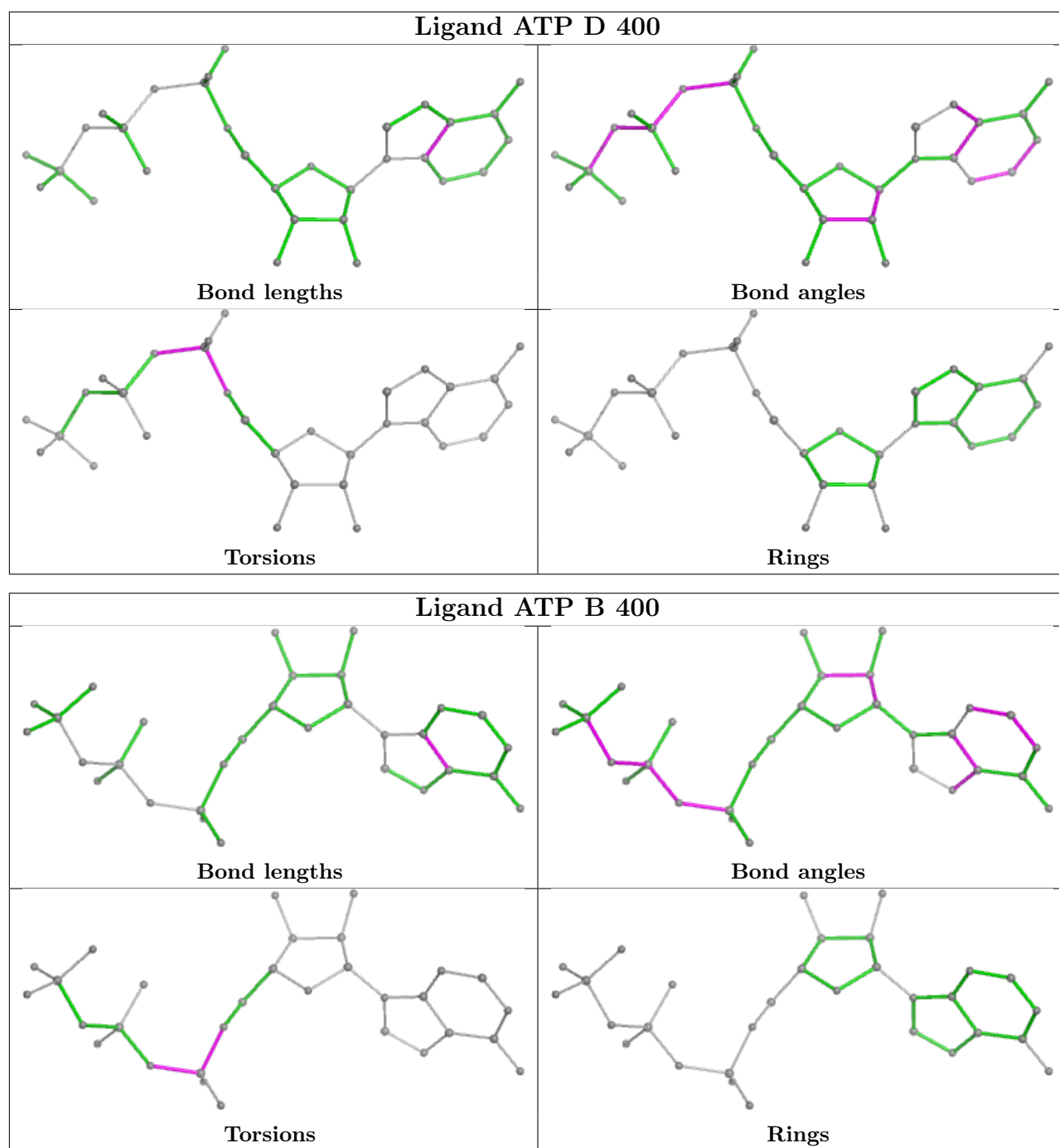
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

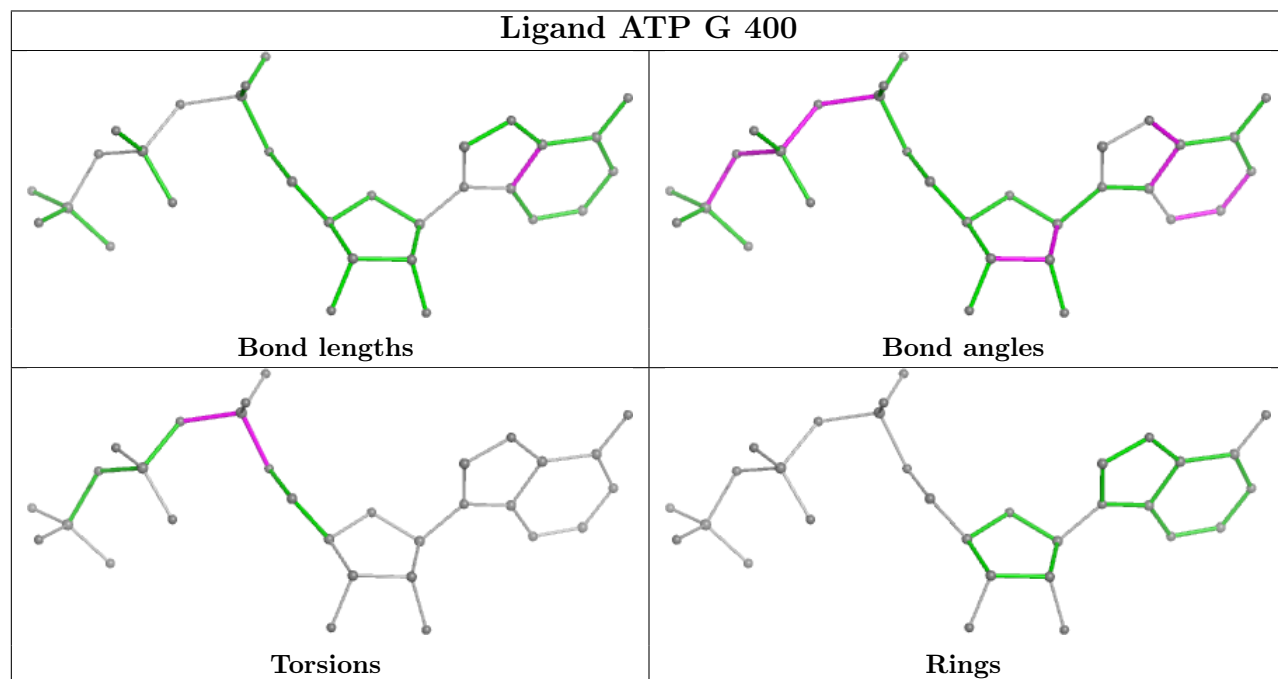
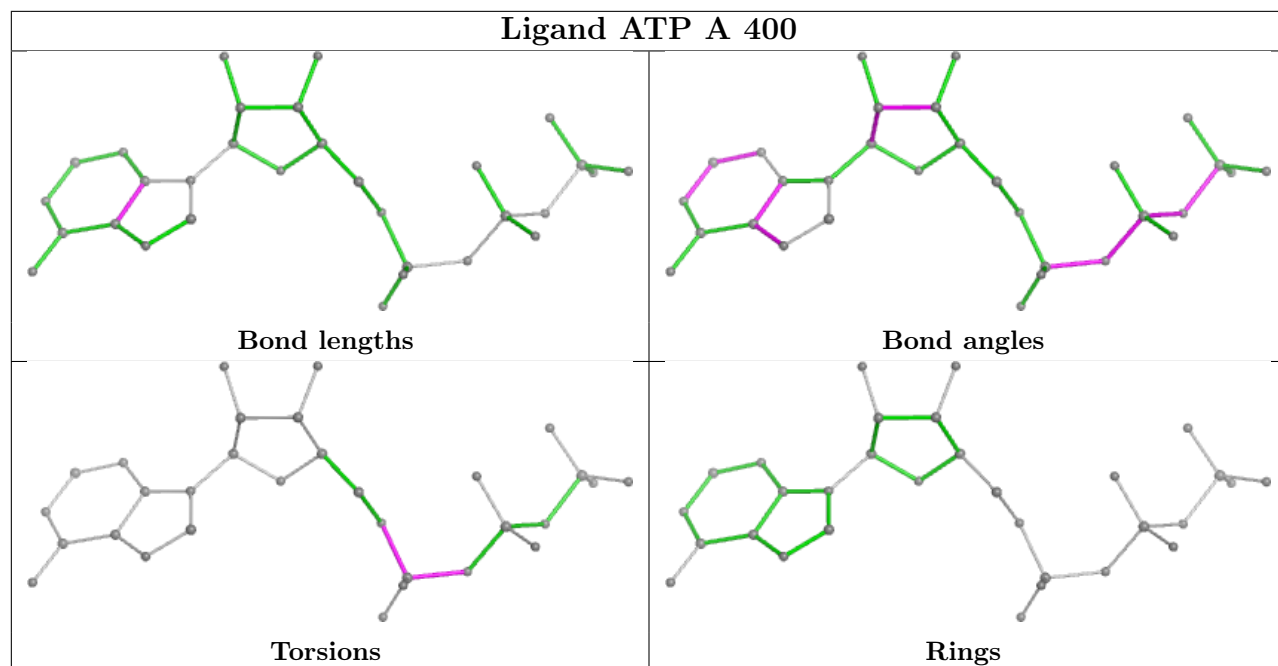


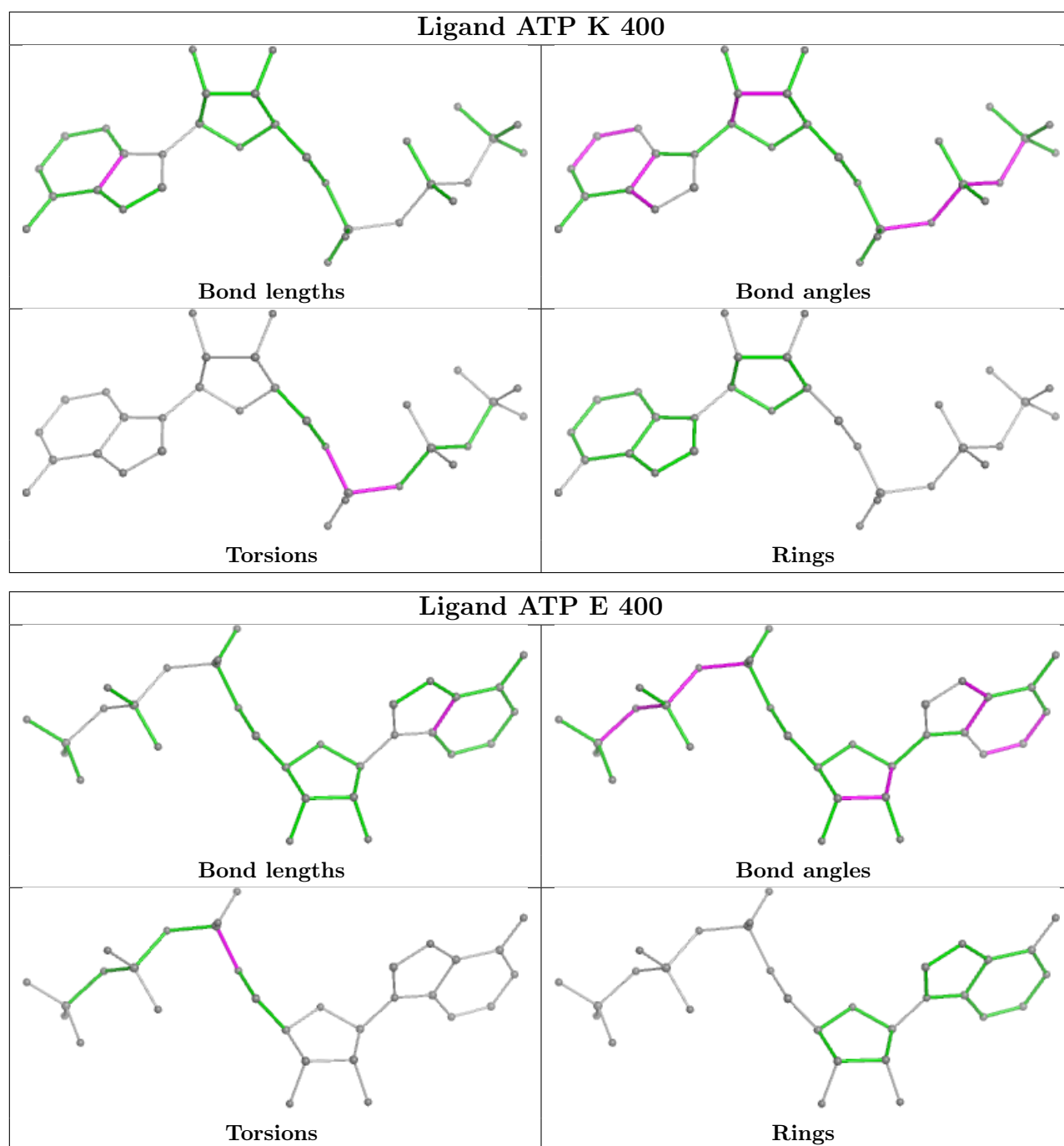












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.