



Full wwPDB EM Model Validation Report ⓘ

Feb 23, 2020 – 07:44 PM EST

PDB ID : 6T24
EMDB ID : EMD-10366
Title : Cryo-EM structure of jasplakinolide-stabilized F-actin (aged)
Authors : Pospich, S.; Merino, F.; Raunser, S.
Deposited on : 2019-10-07
Resolution : 3.70 Å (reported)
Based on initial model : 6T23

This is a Full wwPDB EM Model Validation 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.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
buster-report : 1.1.7 (2018)
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) : 2.8

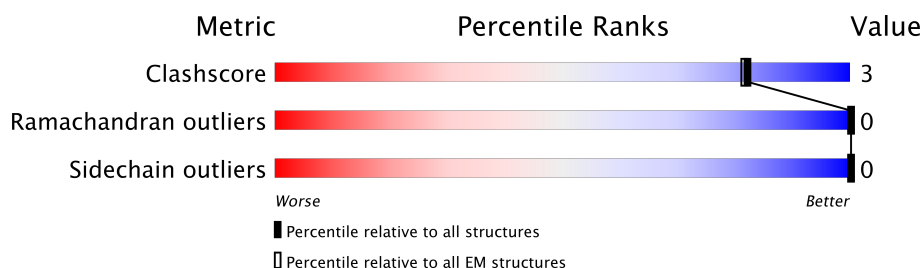
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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 and their fit to the map. 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 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	375	92% 7% .
1	B	375	92% 7% .
1	C	375	92% 7% .
1	D	375	92% 7% .
1	E	375	92% 7% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	A	377	-	X	X	-
3	PO4	B	377	-	X	X	-
3	PO4	C	377	-	X	X	-
3	PO4	D	377	-	X	X	-
3	PO4	E	377	-	X	X	-

2 Entry composition [i](#)

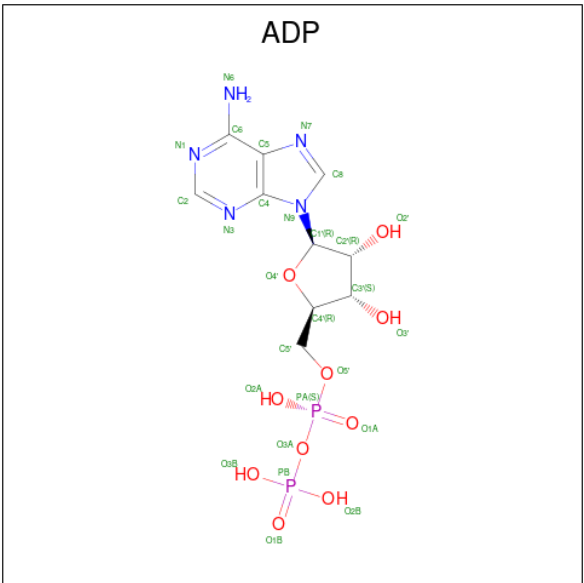
There are 5 unique types of molecules in this entry. The entry contains 14910 atoms, of which 0 are hydrogens and 0 are deuteriums.

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, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	371	Total	C	N	O	S	0	0
			2900	1837	489	553	21		
1	B	371	Total	C	N	O	S	0	0
			2900	1837	489	553	21		
1	C	371	Total	C	N	O	S	0	0
			2900	1837	489	553	21		
1	D	371	Total	C	N	O	S	0	0
			2900	1837	489	553	21		
1	E	371	Total	C	N	O	S	0	0
			2900	1837	489	553	21		

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by author).



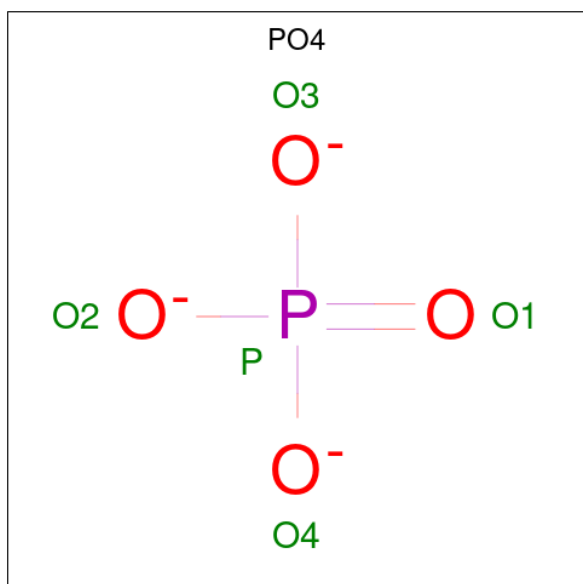
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

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Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P) (labeled as "Ligand of Interest" by author).

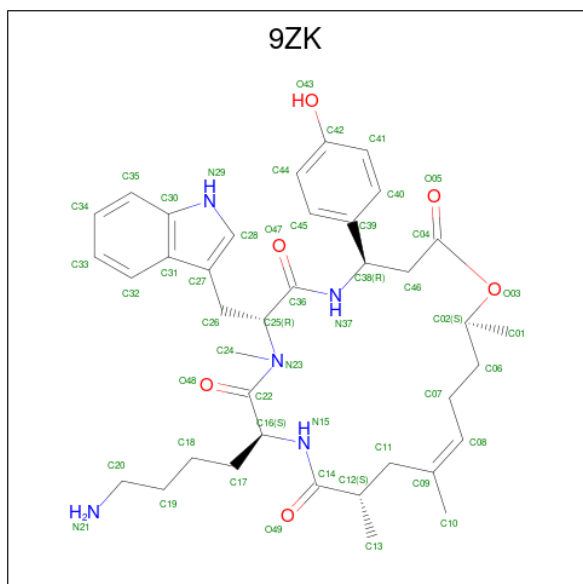


Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	O	P	0
			5	4	1	
3	B	1	Total	O	P	0
			5	4	1	
3	C	1	Total	O	P	0
			5	4	1	
3	D	1	Total	O	P	0
			5	4	1	
3	E	1	Total	O	P	0
			5	4	1	

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total	Mg	0
			1	1	
4	A	1	Total	Mg	0
			1	1	
4	D	1	Total	Mg	0
			1	1	
4	C	1	Total	Mg	0
			1	1	
4	E	1	Total	Mg	0
			1	1	

- Molecule 5 is (4 {R},7 {R},10 {S},13 {S},15 {E},19 {S})-10-(4-azanylbutyl)-4-(4-hydroxyphenyl)-7-(1 {H}-indol-3-ylmethyl)-8,13,15,19-tetramethyl-1-oxa-5,8,11-triazacyclononadec-15-ene-2,6,9,12-tetrone (three-letter code: 9ZK) (formula: C₃₈H₅₁N₅O₆) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			49	38	5	6	
5	B	1	Total	C	N	O	0
			49	38	5	6	
5	C	1	Total	C	N	O	0
			49	38	5	6	
5	D	1	Total	C	N	O	0
			49	38	5	6	
5	E	1	Total	C	N	O	0
			49	38	5	6	

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: Actin, alpha skeletal muscle

Chain A: 



- Molecule 1: Actin, alpha skeletal muscle

Chain B: 



- Molecule 1: Actin, alpha skeletal muscle

Chain C: 



- Molecule 1: Actin, alpha skeletal muscle

Chain D: 



- Molecule 1: Actin, alpha skeletal muscle

Chain E: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	352285	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	88	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, HIC, 9ZK, MG, ADP

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	1.03	4/2950 (0.1%)	0.93	11/3994 (0.3%)
1	B	1.03	3/2950 (0.1%)	0.93	11/3994 (0.3%)
1	C	1.03	3/2950 (0.1%)	0.93	11/3994 (0.3%)
1	D	1.03	3/2950 (0.1%)	0.93	11/3994 (0.3%)
1	E	1.03	4/2950 (0.1%)	0.93	11/3994 (0.3%)
All	All	1.03	17/14750 (0.1%)	0.93	55/19970 (0.3%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	253	GLU	CD-OE1	-6.31	1.18	1.25
1	D	253	GLU	CD-OE1	-6.30	1.18	1.25
1	E	253	GLU	CD-OE1	-6.29	1.18	1.25
1	C	253	GLU	CD-OE1	-6.29	1.18	1.25
1	B	253	GLU	CD-OE1	-6.24	1.18	1.25
1	B	306	TYR	CB-CG	-5.12	1.44	1.51
1	D	306	TYR	CB-CG	-5.12	1.44	1.51
1	B	255	PHE	CB-CG	-5.09	1.42	1.51
1	A	306	TYR	CB-CG	-5.09	1.44	1.51
1	D	255	PHE	CB-CG	-5.08	1.42	1.51
1	C	306	TYR	CB-CG	-5.08	1.44	1.51
1	E	255	PHE	CB-CG	-5.08	1.42	1.51
1	C	255	PHE	CB-CG	-5.07	1.42	1.51
1	E	306	TYR	CB-CG	-5.06	1.44	1.51
1	A	255	PHE	CB-CG	-5.06	1.42	1.51
1	A	270	GLU	CD-OE2	-5.04	1.20	1.25
1	E	270	GLU	CD-OE2	-5.02	1.20	1.25

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	39	ARG	NE-CZ-NH1	10.22	125.41	120.30
1	C	39	ARG	NE-CZ-NH1	10.20	125.40	120.30
1	B	39	ARG	NE-CZ-NH1	10.18	125.39	120.30
1	A	39	ARG	NE-CZ-NH1	10.17	125.39	120.30
1	E	39	ARG	NE-CZ-NH1	10.16	125.38	120.30
1	D	62	ARG	NE-CZ-NH2	-7.78	116.41	120.30
1	A	62	ARG	NE-CZ-NH2	-7.75	116.42	120.30
1	E	62	ARG	NE-CZ-NH2	-7.73	116.44	120.30
1	C	62	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	B	62	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	E	312	ARG	NE-CZ-NH2	-7.05	116.78	120.30
1	D	312	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	A	312	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	C	312	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	B	312	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	E	254	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	A	254	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	D	254	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	C	254	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	E	183	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	B	183	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	B	254	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	C	183	ARG	NE-CZ-NH2	-6.53	117.04	120.30
1	A	183	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	D	183	ARG	NE-CZ-NH2	-6.47	117.07	120.30
1	E	62	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	B	62	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	C	62	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	A	62	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	D	62	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	A	210	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	E	210	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	E	39	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	D	39	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	C	39	ARG	NE-CZ-NH2	-6.15	117.23	120.30
1	D	210	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	C	210	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	A	39	ARG	NE-CZ-NH2	-6.11	117.24	120.30
1	B	39	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	B	210	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	A	116	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	B	116	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	C	116	ARG	NE-CZ-NH1	5.63	123.12	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	116	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	D	116	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	210	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	C	210	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	D	210	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	B	210	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	E	210	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	C	198	TYR	CB-CG-CD1	-5.07	117.96	121.00
1	B	198	TYR	CB-CG-CD1	-5.07	117.96	121.00
1	A	198	TYR	CB-CG-CD1	-5.05	117.97	121.00
1	D	198	TYR	CB-CG-CD1	-5.03	117.98	121.00
1	E	198	TYR	CB-CG-CD1	-5.01	118.00	121.00

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	2900	0	2872	16	0
1	B	2900	0	2872	16	0
1	C	2900	0	2872	16	0
1	D	2900	0	2872	16	0
1	E	2900	0	2872	15	0
2	A	27	0	12	4	0
2	B	27	0	12	4	0
2	C	27	0	12	4	0
2	D	27	0	12	4	0
2	E	27	0	12	4	0
3	A	5	0	0	5	0
3	B	5	0	0	5	0
3	C	5	0	0	5	0
3	D	5	0	0	5	0
3	E	5	0	0	4	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
5	A	49	0	0	0	0
5	B	49	0	0	0	0
5	C	49	0	0	0	0
5	D	49	0	0	0	0
5	E	49	0	0	0	0
All	All	14910	0	14420	79	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 3.

All (79) 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:E:14:SER:N	3:E:377:PO4:O1	2.10	0.84
1:D:14:SER:N	3:D:377:PO4:O1	2.10	0.83
1:B:14:SER:N	3:B:377:PO4:O1	2.10	0.83
1:A:14:SER:N	3:A:377:PO4:O1	2.10	0.83
1:C:14:SER:N	3:C:377:PO4:O1	2.10	0.82
1:A:14:SER:CB	3:A:377:PO4:O1	2.34	0.76
1:E:14:SER:CB	3:E:377:PO4:O1	2.34	0.76
1:C:14:SER:CB	3:C:377:PO4:O1	2.34	0.76
1:B:14:SER:CB	3:B:377:PO4:O1	2.34	0.76
1:D:14:SER:CB	3:D:377:PO4:O1	2.34	0.76
1:C:305:MET:HB2	2:C:376:ADP:C6	2.25	0.72
1:D:305:MET:HB2	2:D:376:ADP:C6	2.25	0.72
1:A:305:MET:HB2	2:A:376:ADP:C6	2.25	0.71
1:B:305:MET:HB2	2:B:376:ADP:C6	2.25	0.71
1:E:305:MET:HB2	2:E:376:ADP:C6	2.25	0.71
1:B:14:SER:HB3	3:B:377:PO4:O1	1.94	0.68
1:A:14:SER:HB3	3:A:377:PO4:O1	1.94	0.68
1:C:14:SER:HB3	3:C:377:PO4:O1	1.94	0.68
1:E:14:SER:HB3	3:E:377:PO4:O1	1.94	0.67
1:D:14:SER:HB3	3:D:377:PO4:O1	1.94	0.67
1:C:305:MET:HB3	2:C:376:ADP:N6	2.12	0.65
1:D:305:MET:HB3	2:D:376:ADP:N6	2.12	0.64
1:A:305:MET:HB3	2:A:376:ADP:N6	2.12	0.63
1:B:305:MET:HB3	2:B:376:ADP:N6	2.12	0.63
1:E:305:MET:HB3	2:E:376:ADP:N6	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:305:MET:CB	2:E:376:ADP:C6	2.89	0.56
1:C:305:MET:CB	2:C:376:ADP:C6	2.89	0.56
1:D:305:MET:CB	2:D:376:ADP:C6	2.89	0.56
1:B:305:MET:CB	2:B:376:ADP:C6	2.89	0.55
1:A:305:MET:CB	2:A:376:ADP:C6	2.89	0.55
1:E:187:ASP:OD2	1:E:191:LYS:NZ	2.41	0.54
1:B:187:ASP:OD2	1:B:191:LYS:NZ	2.41	0.53
1:A:187:ASP:OD2	1:A:191:LYS:NZ	2.41	0.53
1:C:187:ASP:OD2	1:C:191:LYS:NZ	2.41	0.53
1:D:187:ASP:OD2	1:D:191:LYS:NZ	2.41	0.53
1:E:305:MET:CB	2:E:376:ADP:N6	2.73	0.51
1:A:305:MET:CB	2:A:376:ADP:N6	2.74	0.51
1:B:305:MET:CB	2:B:376:ADP:N6	2.74	0.50
1:C:305:MET:CB	2:C:376:ADP:N6	2.74	0.50
1:D:305:MET:CB	2:D:376:ADP:N6	2.74	0.50
1:D:25:ASP:OD1	1:D:25:ASP:N	2.45	0.49
1:B:14:SER:H	3:B:377:PO4:P	2.36	0.47
1:A:96:VAL:HG21	1:A:101:HIS:CD2	2.50	0.47
1:C:96:VAL:HG21	1:C:101:HIS:CD2	2.50	0.47
1:A:25:ASP:N	1:A:25:ASP:OD1	2.45	0.46
1:E:96:VAL:HG21	1:E:101:HIS:CD2	2.50	0.46
1:B:96:VAL:HG21	1:B:101:HIS:CD2	2.50	0.46
1:D:96:VAL:HG21	1:D:101:HIS:CD2	2.50	0.46
1:C:14:SER:H	3:C:377:PO4:P	2.36	0.46
1:E:25:ASP:N	1:E:25:ASP:OD1	2.45	0.46
1:B:6:THR:O	1:B:101:HIS:HB3	2.16	0.46
1:C:6:THR:O	1:C:101:HIS:HB3	2.16	0.46
1:A:6:THR:O	1:A:101:HIS:HB3	2.16	0.46
1:D:14:SER:H	3:D:377:PO4:P	2.36	0.46
1:A:14:SER:H	3:A:377:PO4:P	2.36	0.45
1:D:6:THR:O	1:D:101:HIS:HB3	2.16	0.45
1:E:6:THR:O	1:E:101:HIS:HB3	2.16	0.45
1:C:25:ASP:OD1	1:C:25:ASP:N	2.45	0.44
1:A:332:PRO:O	1:A:335:ARG:HG3	2.19	0.43
1:D:332:PRO:O	1:D:335:ARG:HG3	2.19	0.43
1:E:332:PRO:O	1:E:335:ARG:HG3	2.19	0.42
1:B:332:PRO:O	1:B:335:ARG:HG3	2.19	0.42
1:B:14:SER:CA	3:B:377:PO4:O1	2.67	0.42
1:A:14:SER:CA	3:A:377:PO4:O1	2.67	0.42
1:B:25:ASP:N	1:B:25:ASP:OD1	2.45	0.42
1:A:7:ALA:HA	1:A:102:PRO:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:332:PRO:O	1:C:335:ARG:HG3	2.19	0.42
1:C:7:ALA:HA	1:C:102:PRO:HG2	2.02	0.42
1:E:14:SER:H	3:E:377:PO4:P	2.36	0.41
1:B:7:ALA:HA	1:B:102:PRO:HG2	2.02	0.41
1:D:14:SER:CA	3:D:377:PO4:O1	2.67	0.41
1:E:7:ALA:HA	1:E:102:PRO:HG2	2.02	0.41
1:C:14:SER:CA	3:C:377:PO4:O1	2.67	0.41
1:D:7:ALA:HA	1:D:102:PRO:HG2	2.02	0.41
1:C:111:ASN:HB3	1:C:112:PRO:HD2	2.04	0.40
1:E:111:ASN:HB3	1:E:112:PRO:HD2	2.04	0.40
1:D:111:ASN:HB3	1:D:112:PRO:HD2	2.04	0.40
1:A:111:ASN:HB3	1:A:112:PRO:HD2	2.03	0.40
1:B:111:ASN:HB3	1:B:112:PRO:HD2	2.04	0.40

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	368/375 (98%)	366 (100%)	2 (0%)	0	100	100
1	B	368/375 (98%)	366 (100%)	2 (0%)	0	100	100
1	C	368/375 (98%)	366 (100%)	2 (0%)	0	100	100
1	D	368/375 (98%)	366 (100%)	2 (0%)	0	100	100
1	E	368/375 (98%)	366 (100%)	2 (0%)	0	100	100
All	All	1840/1875 (98%)	1830 (100%)	10 (0%)	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	313/317 (99%)	313 (100%)	0	100	100
1	B	313/317 (99%)	313 (100%)	0	100	100
1	C	313/317 (99%)	313 (100%)	0	100	100
1	D	313/317 (99%)	313 (100%)	0	100	100
1	E	313/317 (99%)	313 (100%)	0	100	100
All	All	1565/1585 (99%)	1565 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

5 non-standard protein/DNA/RNA residues 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
1	HIC	A	73	1	9,11,12	1.25	1 (11%)	6,14,16	1.28	1 (16%)
1	HIC	B	73	1	9,11,12	1.26	1 (11%)	6,14,16	1.29	1 (16%)
1	HIC	C	73	1	9,11,12	1.25	1 (11%)	6,14,16	1.29	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	HIC	D	73	1	9,11,12	1.25	1 (11%)	6,14,16	1.29	1 (16%)
1	HIC	E	73	1	9,11,12	1.26	1 (11%)	6,14,16	1.29	1 (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
1	HIC	A	73	1	-	1/4/6/8	0/1/1/1
1	HIC	B	73	1	-	1/4/6/8	0/1/1/1
1	HIC	C	73	1	-	1/4/6/8	0/1/1/1
1	HIC	D	73	1	-	1/4/6/8	0/1/1/1
1	HIC	E	73	1	-	1/4/6/8	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	73	HIC	CA-C	2.81	1.53	1.50
1	E	73	HIC	CA-C	2.81	1.53	1.50
1	C	73	HIC	CA-C	2.79	1.53	1.50
1	A	73	HIC	CA-C	2.79	1.53	1.50
1	D	73	HIC	CA-C	2.77	1.53	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	73	HIC	O-C-CA	-2.55	118.15	124.98
1	C	73	HIC	O-C-CA	-2.53	118.19	124.98
1	D	73	HIC	O-C-CA	-2.53	118.20	124.98
1	B	73	HIC	O-C-CA	-2.52	118.21	124.98
1	A	73	HIC	O-C-CA	-2.52	118.22	124.98

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	73	HIC	CA-CB-CG-ND1
1	C	73	HIC	CA-CB-CG-ND1
1	B	73	HIC	CA-CB-CG-ND1
1	A	73	HIC	CA-CB-CG-ND1

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Mol	Chain	Res	Type	Atoms
1	E	73	HIC	CA-CB-CG-ND1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 5 are monoatomic - leaving 15 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	ADP	A	376	4	24,29,29	1.38	4 (16%)	25,45,45	1.41	5 (20%)
3	PO4	A	377	4	4,4,4	2.09	2 (50%)	6,6,6	1.87	2 (33%)
5	9ZK	A	379	-	51,52,52	3.65	30 (58%)	64,71,71	2.50	20 (31%)
2	ADP	B	376	4	24,29,29	1.38	3 (12%)	25,45,45	1.42	5 (20%)
3	PO4	B	377	4	4,4,4	2.09	2 (50%)	6,6,6	1.88	2 (33%)
5	9ZK	B	379	-	51,52,52	3.65	30 (58%)	64,71,71	2.50	20 (31%)
2	ADP	C	376	4	24,29,29	1.38	4 (16%)	25,45,45	1.42	5 (20%)
3	PO4	C	377	4	4,4,4	2.09	2 (50%)	6,6,6	1.88	2 (33%)
5	9ZK	C	379	-	51,52,52	3.65	30 (58%)	64,71,71	2.50	20 (31%)
2	ADP	D	376	4	24,29,29	1.38	4 (16%)	25,45,45	1.42	5 (20%)
3	PO4	D	377	4	4,4,4	2.09	2 (50%)	6,6,6	1.88	2 (33%)
5	9ZK	D	379	-	51,52,52	3.65	30 (58%)	64,71,71	2.50	20 (31%)
2	ADP	E	376	4	24,29,29	1.38	3 (12%)	25,45,45	1.42	5 (20%)
3	PO4	E	377	4	4,4,4	2.09	2 (50%)	6,6,6	1.87	2 (33%)
5	9ZK	E	379	-	51,52,52	3.65	30 (58%)	64,71,71	2.50	20 (31%)

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	ADP	A	376	4	-	6/12/32/32	0/3/3/3
5	9ZK	A	379	-	-	13/58/59/59	0/3/4/4
2	ADP	B	376	4	-	6/12/32/32	0/3/3/3
5	9ZK	B	379	-	-	13/58/59/59	0/3/4/4
2	ADP	C	376	4	-	6/12/32/32	0/3/3/3
5	9ZK	C	379	-	-	13/58/59/59	0/3/4/4
2	ADP	D	376	4	-	6/12/32/32	0/3/3/3
5	9ZK	D	379	-	-	13/58/59/59	0/3/4/4
2	ADP	E	376	4	-	6/12/32/32	0/3/3/3
5	9ZK	E	379	-	-	13/58/59/59	0/3/4/4

All (178) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	379	9ZK	C40-C39	7.83	1.51	1.39
5	C	379	9ZK	C40-C39	7.79	1.51	1.39
5	B	379	9ZK	C40-C39	7.77	1.51	1.39
5	A	379	9ZK	C40-C39	7.77	1.51	1.39
5	E	379	9ZK	C40-C39	7.76	1.51	1.39
5	E	379	9ZK	C22-N23	7.68	1.53	1.35
5	D	379	9ZK	C22-N23	7.67	1.53	1.35
5	C	379	9ZK	C22-N23	7.66	1.53	1.35
5	B	379	9ZK	C22-N23	7.65	1.53	1.35
5	A	379	9ZK	C22-N23	7.63	1.53	1.35
5	E	379	9ZK	C45-C39	7.31	1.50	1.39
5	A	379	9ZK	C45-C39	7.31	1.50	1.39
5	C	379	9ZK	C45-C39	7.26	1.50	1.39
5	B	379	9ZK	C45-C39	7.25	1.50	1.39
5	D	379	9ZK	C45-C39	7.25	1.50	1.39
5	B	379	9ZK	C45-C44	6.01	1.49	1.38
5	A	379	9ZK	C45-C44	6.01	1.49	1.38
5	C	379	9ZK	C45-C44	5.99	1.49	1.38
5	D	379	9ZK	C45-C44	5.98	1.49	1.38
5	E	379	9ZK	C45-C44	5.97	1.49	1.38
5	D	379	9ZK	C39-C38	5.72	1.60	1.52
5	C	379	9ZK	C39-C38	5.70	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	379	9ZK	C39-C38	5.70	1.60	1.52
5	E	379	9ZK	C39-C38	5.69	1.60	1.52
5	A	379	9ZK	C39-C38	5.69	1.60	1.52
5	B	379	9ZK	C36-N37	5.41	1.46	1.34
5	C	379	9ZK	C36-N37	5.40	1.46	1.34
5	D	379	9ZK	C36-N37	5.39	1.46	1.34
5	A	379	9ZK	C36-N37	5.39	1.46	1.34
5	E	379	9ZK	C34-C35	5.37	1.49	1.36
5	D	379	9ZK	C34-C35	5.36	1.49	1.36
5	E	379	9ZK	C36-N37	5.36	1.45	1.34
5	C	379	9ZK	C34-C35	5.35	1.48	1.36
5	A	379	9ZK	C34-C35	5.35	1.48	1.36
5	A	379	9ZK	C14-N15	5.34	1.45	1.34
5	B	379	9ZK	C34-C35	5.34	1.48	1.36
5	C	379	9ZK	C14-N15	5.32	1.45	1.34
5	E	379	9ZK	C14-N15	5.32	1.45	1.34
5	B	379	9ZK	C14-N15	5.32	1.45	1.34
5	D	379	9ZK	C14-N15	5.31	1.45	1.34
5	B	379	9ZK	C25-N23	5.29	1.56	1.47
5	A	379	9ZK	C25-N23	5.28	1.56	1.47
5	C	379	9ZK	C25-N23	5.27	1.56	1.47
5	D	379	9ZK	C25-N23	5.25	1.56	1.47
5	E	379	9ZK	C25-N23	5.24	1.56	1.47
5	A	379	9ZK	C32-C31	5.16	1.52	1.42
5	B	379	9ZK	C32-C31	5.14	1.52	1.42
5	C	379	9ZK	C32-C31	5.14	1.52	1.42
5	D	379	9ZK	C32-C31	5.12	1.52	1.42
5	E	379	9ZK	C32-C31	5.12	1.52	1.42
5	E	379	9ZK	C44-C42	5.08	1.48	1.38
5	B	379	9ZK	C44-C42	5.07	1.48	1.38
5	C	379	9ZK	C44-C42	5.05	1.48	1.38
5	D	379	9ZK	C44-C42	5.04	1.48	1.38
5	A	379	9ZK	C44-C42	5.04	1.48	1.38
5	E	379	9ZK	C33-C32	4.97	1.48	1.36
5	C	379	9ZK	C33-C32	4.94	1.48	1.36
5	A	379	9ZK	C33-C32	4.93	1.48	1.36
5	B	379	9ZK	C33-C32	4.93	1.48	1.36
5	A	379	9ZK	C16-C22	4.93	1.62	1.53
5	C	379	9ZK	C16-C22	4.93	1.62	1.53
5	E	379	9ZK	C16-C22	4.92	1.62	1.53
5	B	379	9ZK	C16-C22	4.91	1.62	1.53
5	D	379	9ZK	C33-C32	4.90	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	379	9ZK	C16-C22	4.90	1.62	1.53
5	D	379	9ZK	C35-C30	4.83	1.50	1.41
5	C	379	9ZK	C35-C30	4.82	1.50	1.41
5	E	379	9ZK	C35-C30	4.80	1.50	1.41
5	A	379	9ZK	C35-C30	4.80	1.50	1.41
5	B	379	9ZK	C35-C30	4.79	1.50	1.41
5	B	379	9ZK	C41-C42	4.40	1.47	1.38
5	D	379	9ZK	C41-C42	4.40	1.47	1.38
5	E	379	9ZK	C41-C42	4.39	1.47	1.38
5	C	379	9ZK	C41-C42	4.38	1.47	1.38
5	D	379	9ZK	C38-N37	4.37	1.52	1.46
5	A	379	9ZK	C41-C42	4.36	1.47	1.38
5	A	379	9ZK	C38-N37	4.36	1.52	1.46
5	B	379	9ZK	C38-N37	4.36	1.52	1.46
5	E	379	9ZK	C38-N37	4.35	1.52	1.46
5	C	379	9ZK	C38-N37	4.34	1.52	1.46
5	D	379	9ZK	C41-C40	4.29	1.46	1.38
5	E	379	9ZK	C41-C40	4.29	1.46	1.38
5	B	379	9ZK	C41-C40	4.27	1.46	1.38
5	A	379	9ZK	C41-C40	4.27	1.46	1.38
5	C	379	9ZK	C41-C40	4.26	1.46	1.38
5	B	379	9ZK	C11-C09	4.04	1.59	1.51
5	A	379	9ZK	C11-C09	4.03	1.59	1.51
5	C	379	9ZK	C11-C09	4.01	1.59	1.51
5	D	379	9ZK	C11-C09	4.00	1.59	1.51
5	E	379	9ZK	C11-C09	3.97	1.59	1.51
5	D	379	9ZK	C11-C12	3.94	1.61	1.53
5	A	379	9ZK	C11-C12	3.93	1.61	1.53
5	C	379	9ZK	C11-C12	3.91	1.61	1.53
5	E	379	9ZK	C11-C12	3.91	1.61	1.53
5	B	379	9ZK	C33-C34	3.89	1.48	1.38
5	A	379	9ZK	C33-C34	3.89	1.48	1.38
5	B	379	9ZK	C11-C12	3.88	1.61	1.53
5	C	379	9ZK	C33-C34	3.88	1.48	1.38
5	D	379	9ZK	C33-C34	3.86	1.48	1.38
2	E	376	ADP	PB-O3A	-3.86	1.54	1.60
5	E	379	9ZK	C33-C34	3.85	1.48	1.38
2	C	376	ADP	PB-O3A	-3.83	1.54	1.60
2	B	376	ADP	PB-O3A	-3.82	1.54	1.60
2	D	376	ADP	PB-O3A	-3.80	1.54	1.60
2	A	376	ADP	PB-O3A	-3.80	1.54	1.60
5	B	379	9ZK	C24-N23	3.66	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	379	9ZK	C24-N23	3.64	1.54	1.46
5	C	379	9ZK	C24-N23	3.62	1.54	1.46
5	A	379	9ZK	C24-N23	3.61	1.54	1.46
5	E	379	9ZK	C24-N23	3.61	1.54	1.46
5	A	379	9ZK	C46-C38	3.58	1.62	1.53
5	B	379	9ZK	C46-C38	3.55	1.62	1.53
5	E	379	9ZK	C46-C38	3.55	1.62	1.53
5	C	379	9ZK	C46-C38	3.55	1.62	1.53
5	D	379	9ZK	C46-C38	3.54	1.62	1.53
5	D	379	9ZK	O47-C36	-3.39	1.16	1.23
5	A	379	9ZK	O47-C36	-3.38	1.16	1.23
5	B	379	9ZK	O47-C36	-3.37	1.16	1.23
5	C	379	9ZK	O47-C36	-3.37	1.16	1.23
5	E	379	9ZK	O47-C36	-3.34	1.16	1.23
5	D	379	9ZK	O03-C04	3.06	1.43	1.34
5	E	379	9ZK	O03-C04	3.05	1.43	1.34
5	C	379	9ZK	O03-C04	3.05	1.43	1.34
5	B	379	9ZK	O03-C04	3.04	1.43	1.34
5	A	379	9ZK	O03-C04	3.03	1.43	1.34
3	A	377	PO4	P-O3	-2.98	1.45	1.54
3	D	377	PO4	P-O3	-2.96	1.45	1.54
3	E	377	PO4	P-O3	-2.95	1.45	1.54
5	A	379	9ZK	C26-C25	2.95	1.60	1.54
3	C	377	PO4	P-O3	-2.95	1.45	1.54
5	E	379	9ZK	C26-C25	2.94	1.60	1.54
3	B	377	PO4	P-O3	-2.94	1.45	1.54
5	C	379	9ZK	C26-C25	2.94	1.60	1.54
5	B	379	9ZK	C26-C25	2.93	1.60	1.54
5	D	379	9ZK	C26-C25	2.91	1.60	1.54
2	A	376	ADP	C4-N3	-2.70	1.31	1.35
2	C	376	ADP	C4-N3	-2.65	1.32	1.35
2	E	376	ADP	C4-N3	-2.64	1.32	1.35
2	B	376	ADP	C4-N3	-2.64	1.32	1.35
2	D	376	ADP	C4-N3	-2.63	1.32	1.35
5	E	379	9ZK	C12-C14	2.51	1.58	1.51
5	D	379	9ZK	C12-C14	2.50	1.58	1.51
5	C	379	9ZK	C12-C14	2.49	1.58	1.51
5	A	379	9ZK	C12-C14	2.48	1.58	1.51
5	B	379	9ZK	C12-C14	2.48	1.58	1.51
5	E	379	9ZK	C08-C09	2.36	1.38	1.33
5	C	379	9ZK	C08-C09	2.33	1.38	1.33
5	D	379	9ZK	C08-C09	2.33	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	379	9ZK	C08-C09	2.31	1.38	1.33
5	A	379	9ZK	C08-C09	2.29	1.38	1.33
5	A	379	9ZK	C01-C02	2.22	1.59	1.51
5	B	379	9ZK	C01-C02	2.22	1.59	1.51
5	C	379	9ZK	C01-C02	2.22	1.59	1.51
5	E	379	9ZK	C01-C02	2.22	1.59	1.51
5	D	379	9ZK	C01-C02	2.21	1.59	1.51
3	D	377	PO4	P-O2	-2.21	1.47	1.54
3	B	377	PO4	P-O2	-2.21	1.47	1.54
3	C	377	PO4	P-O2	-2.20	1.47	1.54
3	A	377	PO4	P-O2	-2.18	1.48	1.54
3	E	377	PO4	P-O2	-2.18	1.48	1.54
5	E	379	9ZK	C06-C02	2.16	1.59	1.52
5	A	379	9ZK	C06-C02	2.15	1.59	1.52
5	E	379	9ZK	O49-C14	-2.15	1.19	1.23
5	B	379	9ZK	C06-C02	2.15	1.59	1.52
5	A	379	9ZK	O49-C14	-2.15	1.19	1.23
5	C	379	9ZK	C06-C02	2.14	1.59	1.52
5	B	379	9ZK	O49-C14	-2.14	1.19	1.23
5	D	379	9ZK	O49-C14	-2.14	1.19	1.23
5	C	379	9ZK	O49-C14	-2.14	1.19	1.23
5	D	379	9ZK	C06-C02	2.13	1.59	1.52
2	D	376	ADP	C5-N7	-2.04	1.32	1.39
2	C	376	ADP	C5-N7	-2.03	1.32	1.39
2	A	376	ADP	C5-N7	-2.03	1.32	1.39
2	B	376	ADP	C5-N7	-2.02	1.32	1.39
2	E	376	ADP	C5-N7	-2.02	1.32	1.39
2	A	376	ADP	O4'-C4'	-2.00	1.40	1.45
2	C	376	ADP	O4'-C4'	-2.00	1.40	1.45
2	D	376	ADP	O4'-C4'	-2.00	1.40	1.45

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	379	9ZK	C02-O03-C04	8.38	128.47	117.90
5	A	379	9ZK	C02-O03-C04	8.38	128.46	117.90
5	E	379	9ZK	C02-O03-C04	8.37	128.45	117.90
5	C	379	9ZK	C02-O03-C04	8.37	128.45	117.90
5	B	379	9ZK	C02-O03-C04	8.36	128.44	117.90
5	D	379	9ZK	C13-C12-C14	7.78	121.16	109.32
5	A	379	9ZK	C13-C12-C14	7.76	121.12	109.32
5	C	379	9ZK	C13-C12-C14	7.75	121.11	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	379	9ZK	C13-C12-C14	7.75	121.10	109.32
5	E	379	9ZK	C13-C12-C14	7.74	121.08	109.32
5	B	379	9ZK	C16-N15-C14	6.17	134.91	121.66
5	A	379	9ZK	C16-N15-C14	6.15	134.87	121.66
5	C	379	9ZK	C16-N15-C14	6.14	134.84	121.66
5	D	379	9ZK	C16-N15-C14	6.14	134.84	121.66
5	E	379	9ZK	C16-N15-C14	6.13	134.82	121.66
5	A	379	9ZK	O03-C04-C46	5.03	120.80	111.45
5	B	379	9ZK	O03-C04-C46	5.03	120.79	111.45
5	E	379	9ZK	O03-C04-C46	5.02	120.78	111.45
5	C	379	9ZK	O03-C04-C46	5.02	120.78	111.45
5	A	379	9ZK	C12-C14-N15	-5.01	111.05	116.42
5	D	379	9ZK	O03-C04-C46	5.01	120.75	111.45
5	E	379	9ZK	C12-C14-N15	-5.00	111.06	116.42
5	C	379	9ZK	C12-C14-N15	-4.99	111.07	116.42
5	D	379	9ZK	C12-C14-N15	-4.98	111.08	116.42
5	B	379	9ZK	C12-C14-N15	-4.97	111.09	116.42
5	B	379	9ZK	C38-C46-C04	4.17	121.57	112.87
5	E	379	9ZK	C38-C46-C04	4.17	121.57	112.87
5	C	379	9ZK	C38-C46-C04	4.16	121.53	112.87
5	A	379	9ZK	C38-C46-C04	4.15	121.52	112.87
5	D	379	9ZK	C38-C46-C04	4.15	121.52	112.87
5	D	379	9ZK	C16-C22-N23	3.96	127.73	119.36
5	A	379	9ZK	C16-C22-N23	3.95	127.71	119.36
5	C	379	9ZK	C16-C22-N23	3.94	127.69	119.36
5	B	379	9ZK	C16-C22-N23	3.94	127.69	119.36
5	E	379	9ZK	C46-C38-C39	3.93	120.62	111.61
5	E	379	9ZK	C16-C22-N23	3.93	127.65	119.36
5	B	379	9ZK	C46-C38-C39	3.92	120.60	111.61
5	C	379	9ZK	C46-C38-C39	3.92	120.59	111.61
5	A	379	9ZK	C46-C38-C39	3.91	120.58	111.61
5	D	379	9ZK	C46-C38-C39	3.91	120.57	111.61
5	E	379	9ZK	C38-N37-C36	3.84	129.07	123.23
5	B	379	9ZK	C38-N37-C36	3.82	129.04	123.23
5	C	379	9ZK	C38-N37-C36	3.82	129.04	123.23
5	D	379	9ZK	C38-N37-C36	3.80	129.01	123.23
5	A	379	9ZK	C38-N37-C36	3.78	128.99	123.23
5	A	379	9ZK	O48-C22-C16	-3.48	113.50	119.67
5	C	379	9ZK	O03-C02-C06	3.47	114.22	106.89
5	D	379	9ZK	O48-C22-C16	-3.46	113.52	119.67
5	B	379	9ZK	O03-C02-C06	3.46	114.20	106.89
5	A	379	9ZK	O03-C02-C06	3.46	114.20	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	379	9ZK	O03-C02-C06	3.46	114.20	106.89
5	B	379	9ZK	O48-C22-C16	-3.46	113.53	119.67
5	C	379	9ZK	O48-C22-C16	-3.45	113.55	119.67
5	E	379	9ZK	O03-C02-C06	3.44	114.16	106.89
5	E	379	9ZK	O48-C22-C16	-3.43	113.58	119.67
3	B	377	PO4	O4-P-O2	3.40	118.92	107.99
3	D	377	PO4	O4-P-O2	3.39	118.90	107.99
3	E	377	PO4	O4-P-O2	3.39	118.89	107.99
3	C	377	PO4	O4-P-O2	3.38	118.88	107.99
3	A	377	PO4	O4-P-O2	3.38	118.86	107.99
2	D	376	ADP	N3-C2-N1	-3.13	123.64	128.68
2	E	376	ADP	N3-C2-N1	-3.12	123.65	128.68
2	B	376	ADP	N3-C2-N1	-3.12	123.66	128.68
2	C	376	ADP	N3-C2-N1	-3.10	123.68	128.68
2	A	376	ADP	N3-C2-N1	-3.09	123.70	128.68
5	D	379	9ZK	C06-C07-C08	2.97	120.23	112.26
5	E	379	9ZK	C06-C07-C08	2.96	120.21	112.26
5	A	379	9ZK	C06-C07-C08	2.96	120.20	112.26
5	C	379	9ZK	C06-C07-C08	2.95	120.19	112.26
5	B	379	9ZK	C06-C07-C08	2.95	120.18	112.26
5	A	379	9ZK	C07-C08-C09	2.56	133.95	127.67
5	D	379	9ZK	C07-C08-C09	2.54	133.91	127.67
5	C	379	9ZK	C07-C08-C09	2.54	133.91	127.67
5	B	379	9ZK	C07-C08-C09	2.53	133.90	127.67
5	D	379	9ZK	C39-C38-N37	-2.53	107.23	111.99
5	E	379	9ZK	C07-C08-C09	2.52	133.87	127.67
5	C	379	9ZK	C39-C38-N37	-2.52	107.24	111.99
5	B	379	9ZK	C39-C38-N37	-2.52	107.25	111.99
5	E	379	9ZK	C39-C38-N37	-2.52	107.25	111.99
5	A	379	9ZK	C39-C38-N37	-2.51	107.27	111.99
5	D	379	9ZK	C45-C39-C38	2.47	126.30	120.82
2	D	376	ADP	PA-O3A-PB	-2.46	124.75	132.57
5	C	379	9ZK	C45-C39-C38	2.46	126.27	120.82
5	B	379	9ZK	C45-C39-C38	2.45	126.26	120.82
2	E	376	ADP	PA-O3A-PB	-2.45	124.78	132.57
2	B	376	ADP	PA-O3A-PB	-2.45	124.79	132.57
2	C	376	ADP	PA-O3A-PB	-2.45	124.79	132.57
5	E	379	9ZK	C45-C39-C38	2.45	126.25	120.82
5	A	379	9ZK	C45-C39-C38	2.45	126.25	120.82
2	A	376	ADP	PA-O3A-PB	-2.45	124.79	132.57
5	A	379	9ZK	C17-C16-C22	2.37	115.70	109.80
5	E	379	9ZK	C17-C16-C22	2.36	115.69	109.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	379	9ZK	C17-C16-C22	2.36	115.69	109.80
5	C	379	9ZK	C17-C16-C22	2.36	115.68	109.80
5	D	379	9ZK	C17-C16-C22	2.35	115.67	109.80
5	E	379	9ZK	C36-C25-N23	2.29	116.30	109.97
5	A	379	9ZK	C36-C25-N23	2.29	116.29	109.97
5	B	379	9ZK	O05-C04-C46	-2.28	119.59	124.71
5	E	379	9ZK	O05-C04-C46	-2.28	119.61	124.71
5	C	379	9ZK	C36-C25-N23	2.28	116.25	109.97
5	D	379	9ZK	C36-C25-N23	2.27	116.25	109.97
5	B	379	9ZK	C36-C25-N23	2.27	116.24	109.97
5	C	379	9ZK	O05-C04-C46	-2.26	119.64	124.71
5	A	379	9ZK	O05-C04-C46	-2.26	119.64	124.71
5	D	379	9ZK	O05-C04-C46	-2.25	119.66	124.71
2	B	376	ADP	C4-C5-N7	-2.25	107.05	109.40
2	A	376	ADP	C4-C5-N7	-2.25	107.06	109.40
2	E	376	ADP	C4-C5-N7	-2.23	107.08	109.40
2	C	376	ADP	C4-C5-N7	-2.22	107.08	109.40
2	D	376	ADP	C4-C5-N7	-2.22	107.09	109.40
5	B	379	9ZK	O47-C36-N37	-2.17	118.85	122.92
5	C	379	9ZK	O47-C36-N37	-2.17	118.86	122.92
5	E	379	9ZK	O47-C36-N37	-2.17	118.86	122.92
5	A	379	9ZK	O47-C36-N37	-2.16	118.88	122.92
2	C	376	ADP	C4'-O4'-C1'	2.15	112.07	109.83
2	A	376	ADP	C4'-O4'-C1'	2.15	112.07	109.83
2	E	376	ADP	C4'-O4'-C1'	2.15	112.07	109.83
5	D	379	9ZK	O47-C36-N37	-2.14	118.91	122.92
2	B	376	ADP	C4'-O4'-C1'	2.14	112.06	109.83
2	D	376	ADP	C4'-O4'-C1'	2.13	112.05	109.83
2	E	376	ADP	C2-N1-C6	2.08	122.36	118.77
2	B	376	ADP	C2-N1-C6	2.07	122.36	118.77
5	A	379	9ZK	C32-C31-C30	2.07	120.91	118.17
2	D	376	ADP	C2-N1-C6	2.07	122.35	118.77
5	E	379	9ZK	C32-C31-C30	2.06	120.90	118.17
3	D	377	PO4	O4-P-O1	-2.05	103.37	110.88
5	C	379	9ZK	C32-C31-C30	2.05	120.88	118.17
2	C	376	ADP	C2-N1-C6	2.05	122.31	118.77
3	B	377	PO4	O4-P-O1	-2.05	103.40	110.88
3	A	377	PO4	O4-P-O1	-2.04	103.41	110.88
3	C	377	PO4	O4-P-O1	-2.04	103.41	110.88
5	B	379	9ZK	C32-C31-C30	2.04	120.87	118.17
3	E	377	PO4	O4-P-O1	-2.04	103.43	110.88
5	D	379	9ZK	C32-C31-C30	2.03	120.86	118.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	376	ADP	C2-N1-C6	2.02	122.27	118.77

There are no chirality outliers.

All (95) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	379	9ZK	C39-C38-C46-C04
2	A	376	ADP	C5'-O5'-PA-O2A
2	A	376	ADP	C5'-O5'-PA-O3A
5	B	379	9ZK	C39-C38-C46-C04
2	C	376	ADP	C5'-O5'-PA-O2A
2	C	376	ADP	C5'-O5'-PA-O3A
2	E	376	ADP	C5'-O5'-PA-O2A
2	E	376	ADP	C5'-O5'-PA-O3A
5	C	379	9ZK	C39-C38-C46-C04
5	A	379	9ZK	C39-C38-C46-C04
2	B	376	ADP	C5'-O5'-PA-O2A
2	B	376	ADP	C5'-O5'-PA-O3A
2	D	376	ADP	C5'-O5'-PA-O2A
2	D	376	ADP	C5'-O5'-PA-O3A
5	D	379	9ZK	C39-C38-C46-C04
5	E	379	9ZK	N37-C38-C46-C04
5	B	379	9ZK	N37-C38-C46-C04
5	C	379	9ZK	N37-C38-C46-C04
5	A	379	9ZK	N37-C38-C46-C04
5	D	379	9ZK	N37-C38-C46-C04
5	E	379	9ZK	O05-C04-O03-C02
5	B	379	9ZK	O05-C04-O03-C02
5	C	379	9ZK	O05-C04-O03-C02
5	A	379	9ZK	O05-C04-O03-C02
5	D	379	9ZK	O05-C04-O03-C02
5	E	379	9ZK	C46-C04-O03-C02
5	B	379	9ZK	C46-C04-O03-C02
5	C	379	9ZK	C46-C04-O03-C02
5	A	379	9ZK	C46-C04-O03-C02
5	D	379	9ZK	C46-C04-O03-C02
5	E	379	9ZK	C01-C02-C06-C07
5	B	379	9ZK	C01-C02-C06-C07
5	C	379	9ZK	C01-C02-C06-C07
5	A	379	9ZK	C01-C02-C06-C07
5	D	379	9ZK	C01-C02-C06-C07
5	E	379	9ZK	C46-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
5	E	379	9ZK	C46-C38-C39-C45
5	B	379	9ZK	C46-C38-C39-C40
5	B	379	9ZK	C46-C38-C39-C45
5	C	379	9ZK	C46-C38-C39-C40
5	C	379	9ZK	C46-C38-C39-C45
5	A	379	9ZK	C46-C38-C39-C40
5	A	379	9ZK	C46-C38-C39-C45
5	D	379	9ZK	C46-C38-C39-C40
5	D	379	9ZK	C46-C38-C39-C45
2	A	376	ADP	C3'-C4'-C5'-O5'
2	C	376	ADP	C3'-C4'-C5'-O5'
2	E	376	ADP	C3'-C4'-C5'-O5'
2	B	376	ADP	C3'-C4'-C5'-O5'
2	D	376	ADP	C3'-C4'-C5'-O5'
2	A	376	ADP	C5'-O5'-PA-O1A
2	C	376	ADP	C5'-O5'-PA-O1A
2	E	376	ADP	C5'-O5'-PA-O1A
2	B	376	ADP	C5'-O5'-PA-O1A
2	D	376	ADP	C5'-O5'-PA-O1A
5	E	379	9ZK	C11-C12-C14-O49
5	B	379	9ZK	C11-C12-C14-O49
5	C	379	9ZK	C11-C12-C14-O49
5	A	379	9ZK	C11-C12-C14-O49
5	D	379	9ZK	C11-C12-C14-O49
5	E	379	9ZK	O03-C02-C06-C07
5	B	379	9ZK	O03-C02-C06-C07
5	C	379	9ZK	O03-C02-C06-C07
5	A	379	9ZK	O03-C02-C06-C07
5	D	379	9ZK	O03-C02-C06-C07
2	A	376	ADP	O4'-C4'-C5'-O5'
2	C	376	ADP	O4'-C4'-C5'-O5'
2	E	376	ADP	O4'-C4'-C5'-O5'
2	B	376	ADP	O4'-C4'-C5'-O5'
2	D	376	ADP	O4'-C4'-C5'-O5'
5	E	379	9ZK	C10-C09-C11-C12
5	B	379	9ZK	C10-C09-C11-C12
5	C	379	9ZK	C10-C09-C11-C12
5	A	379	9ZK	C10-C09-C11-C12
5	D	379	9ZK	C10-C09-C11-C12
5	E	379	9ZK	N37-C38-C39-C40
5	E	379	9ZK	N37-C38-C39-C45
5	B	379	9ZK	N37-C38-C39-C40

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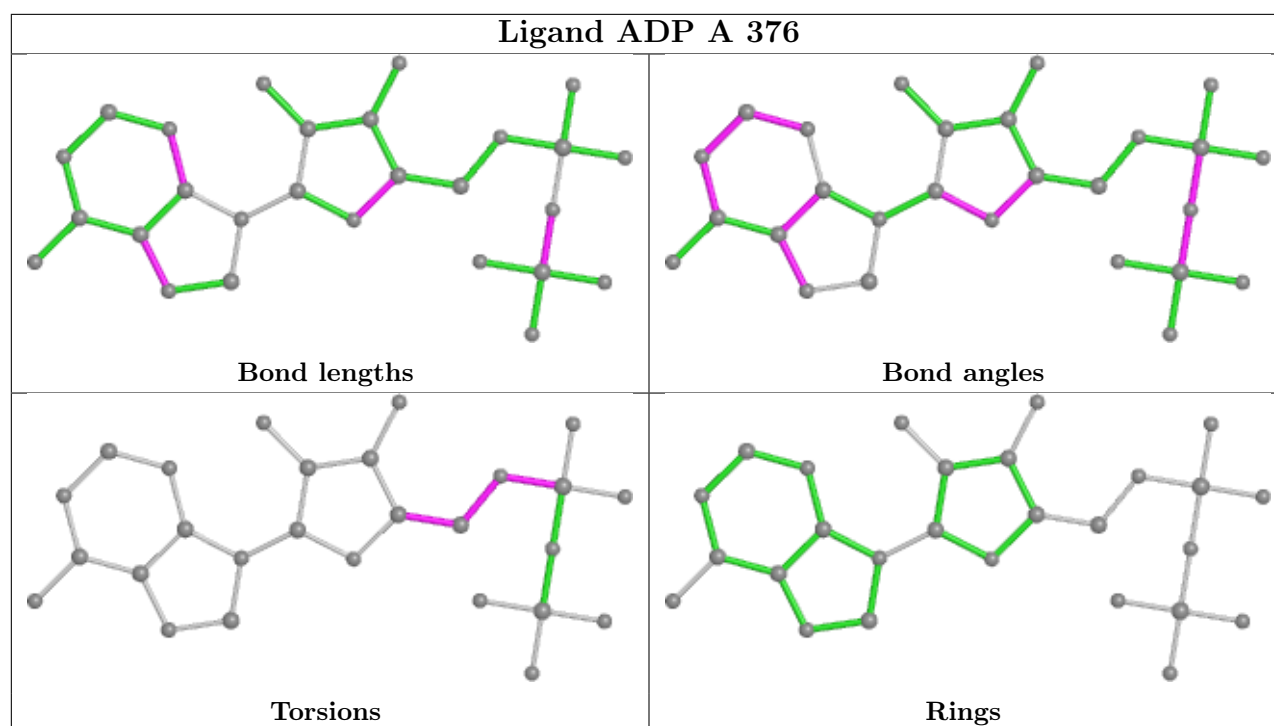
Mol	Chain	Res	Type	Atoms
5	B	379	9ZK	N37-C38-C39-C45
5	C	379	9ZK	N37-C38-C39-C40
5	C	379	9ZK	N37-C38-C39-C45
5	A	379	9ZK	N37-C38-C39-C40
5	A	379	9ZK	N37-C38-C39-C45
5	D	379	9ZK	N37-C38-C39-C40
5	D	379	9ZK	N37-C38-C39-C45
5	E	379	9ZK	C11-C12-C14-N15
5	B	379	9ZK	C11-C12-C14-N15
5	C	379	9ZK	C11-C12-C14-N15
5	A	379	9ZK	C11-C12-C14-N15
5	D	379	9ZK	C11-C12-C14-N15
2	A	376	ADP	C4'-C5'-O5'-PA
2	C	376	ADP	C4'-C5'-O5'-PA
2	E	376	ADP	C4'-C5'-O5'-PA
2	B	376	ADP	C4'-C5'-O5'-PA
2	D	376	ADP	C4'-C5'-O5'-PA

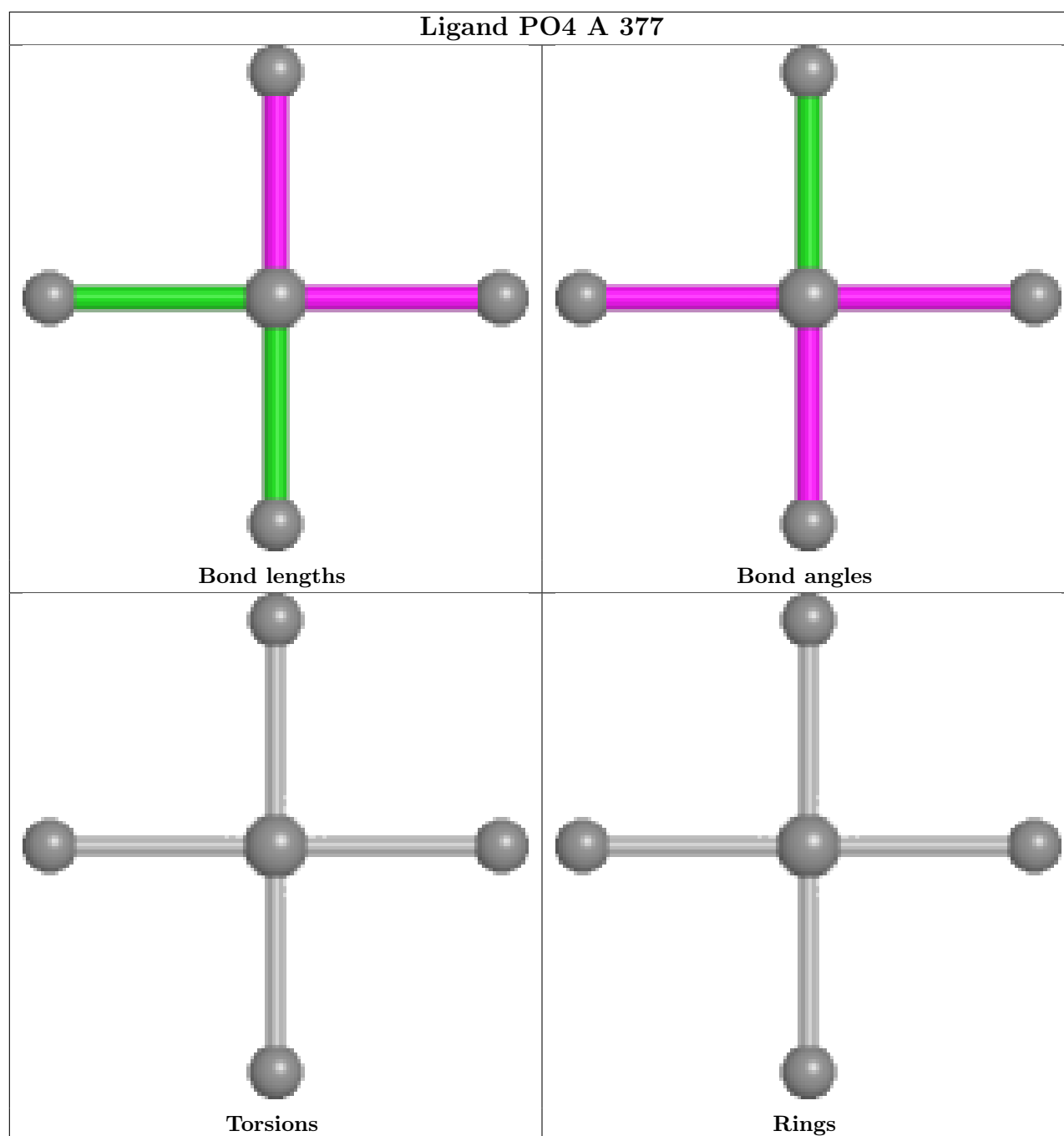
There are no ring outliers.

5 monomers are involved in 20 short contacts:

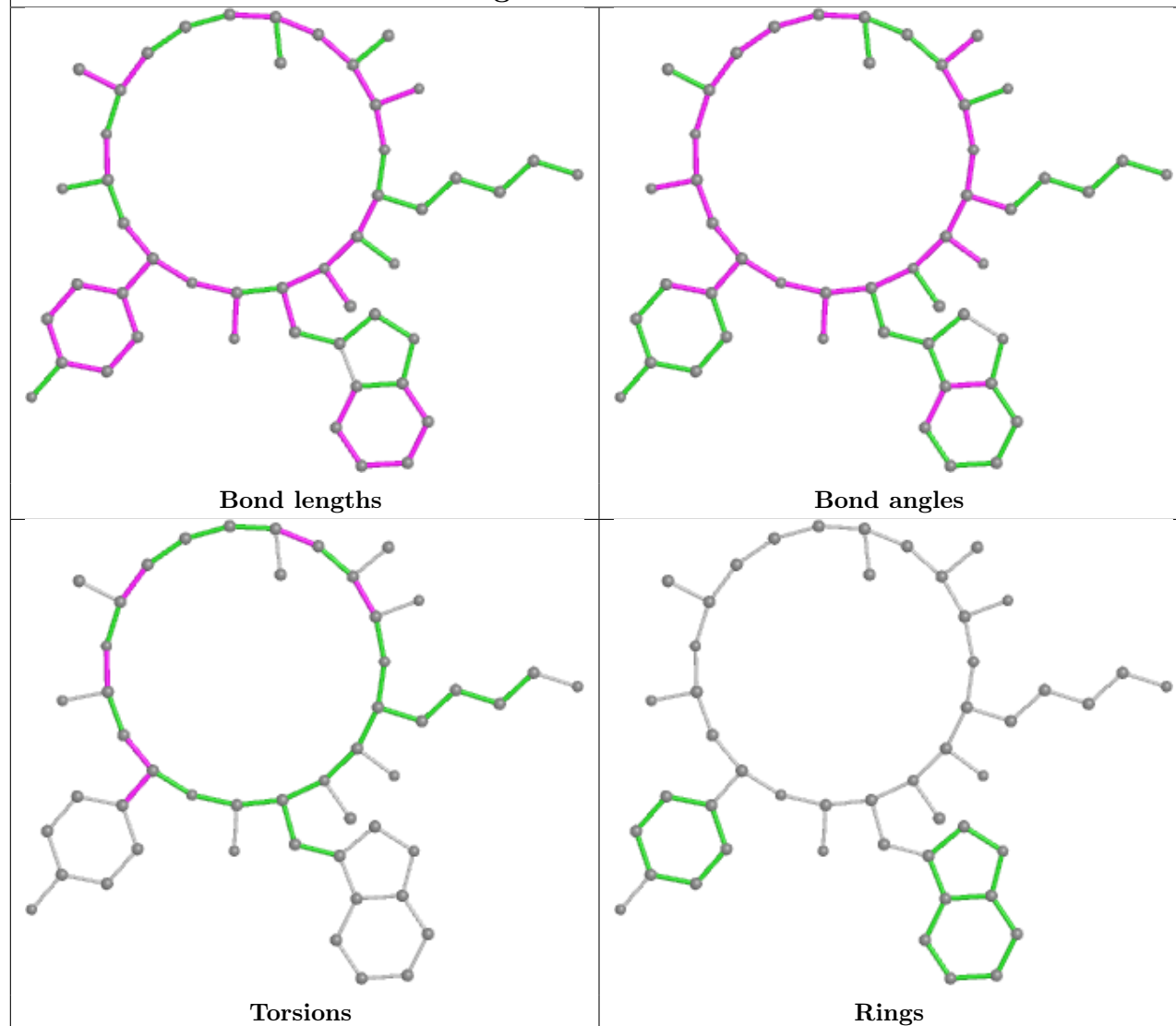
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	376	ADP	4	0
2	B	376	ADP	4	0
2	C	376	ADP	4	0
2	D	376	ADP	4	0
2	E	376	ADP	4	0

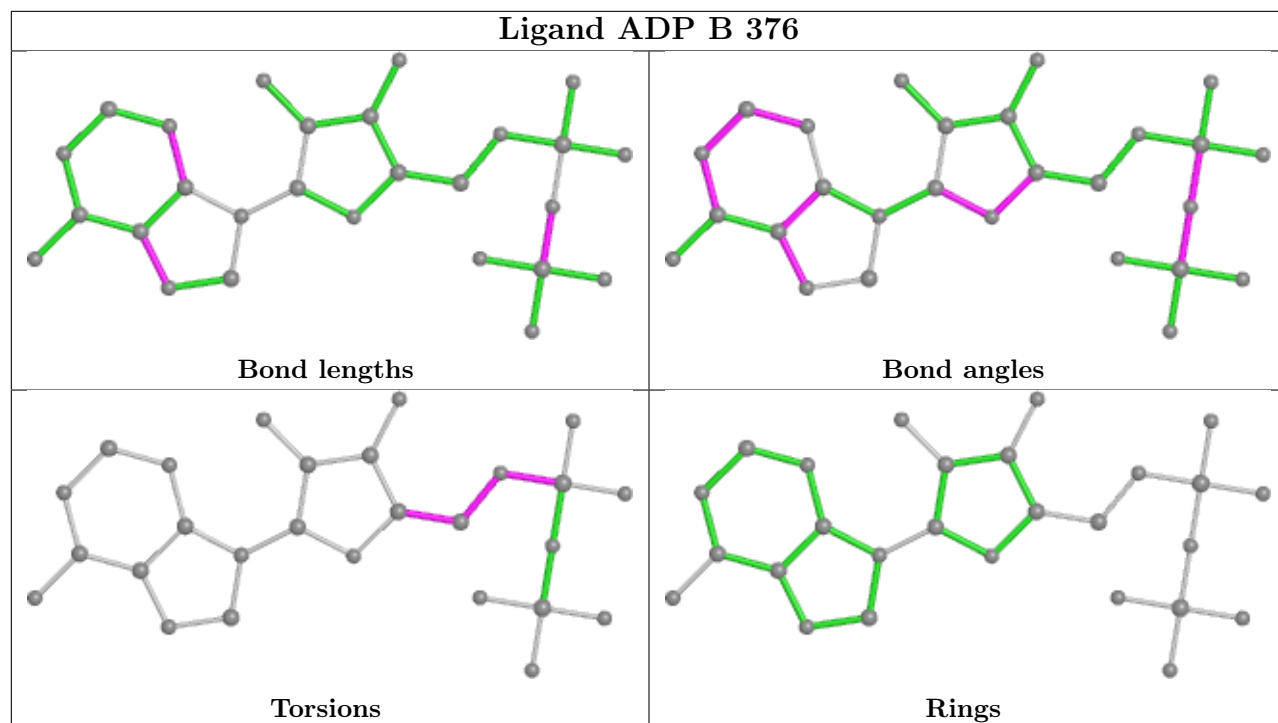
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

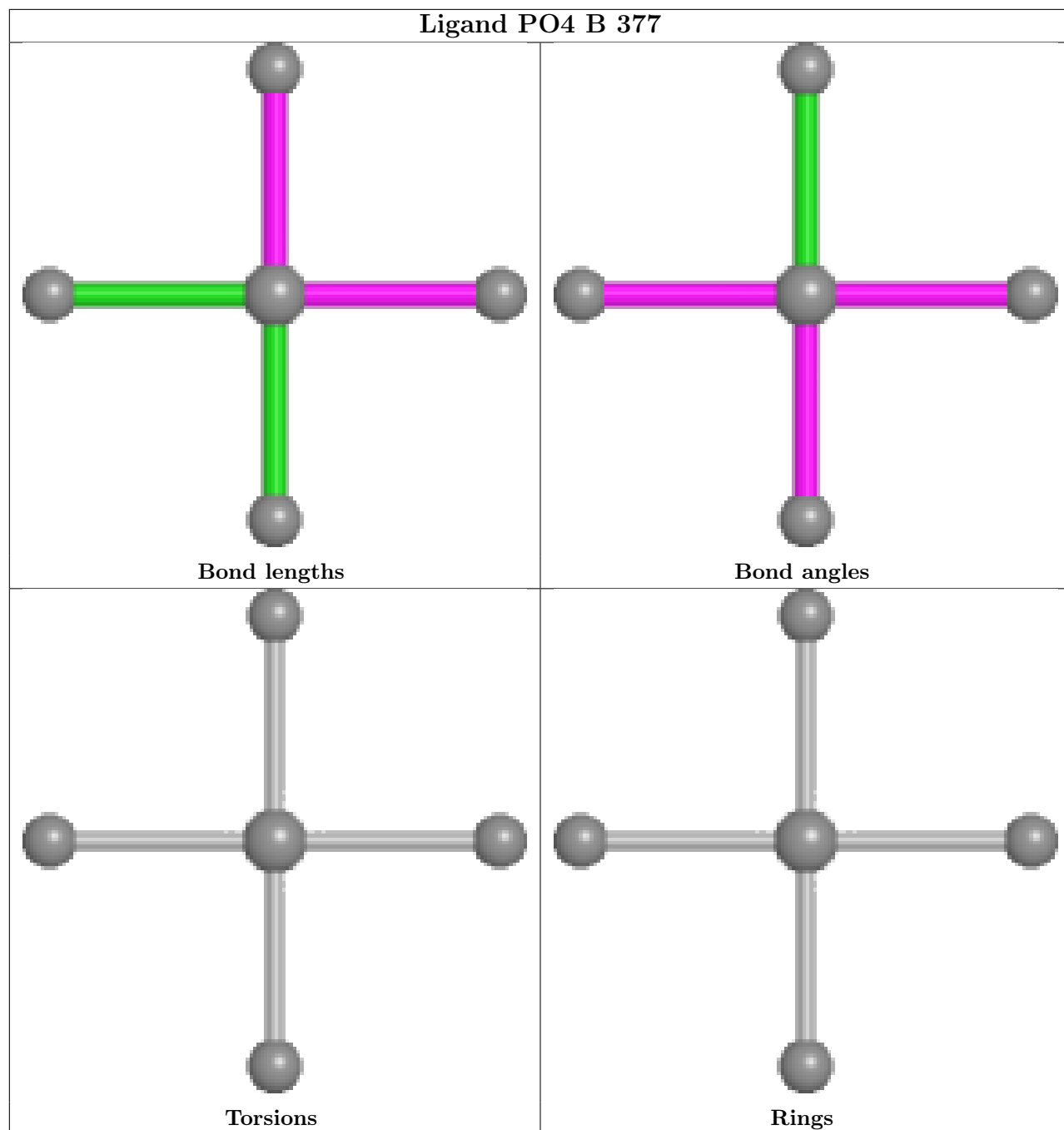




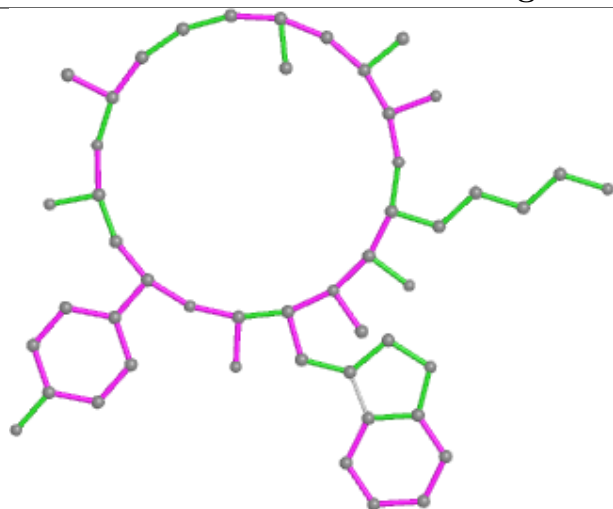
Ligand 9ZK A 379



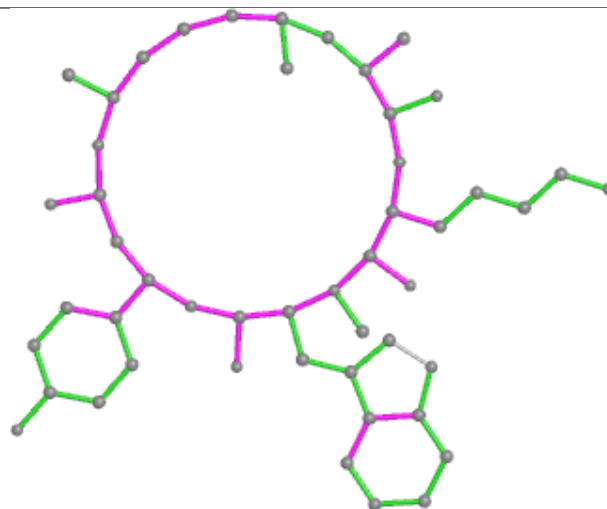




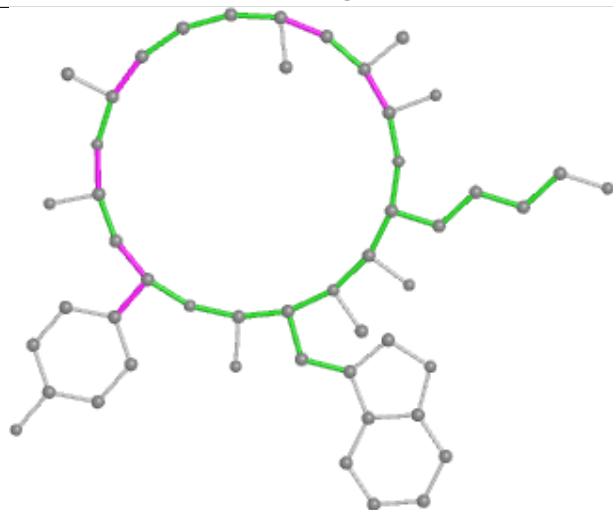
Ligand 9ZK B 379



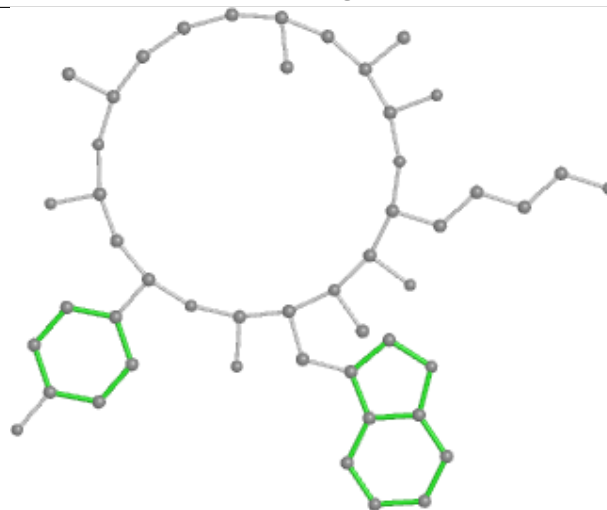
Bond lengths



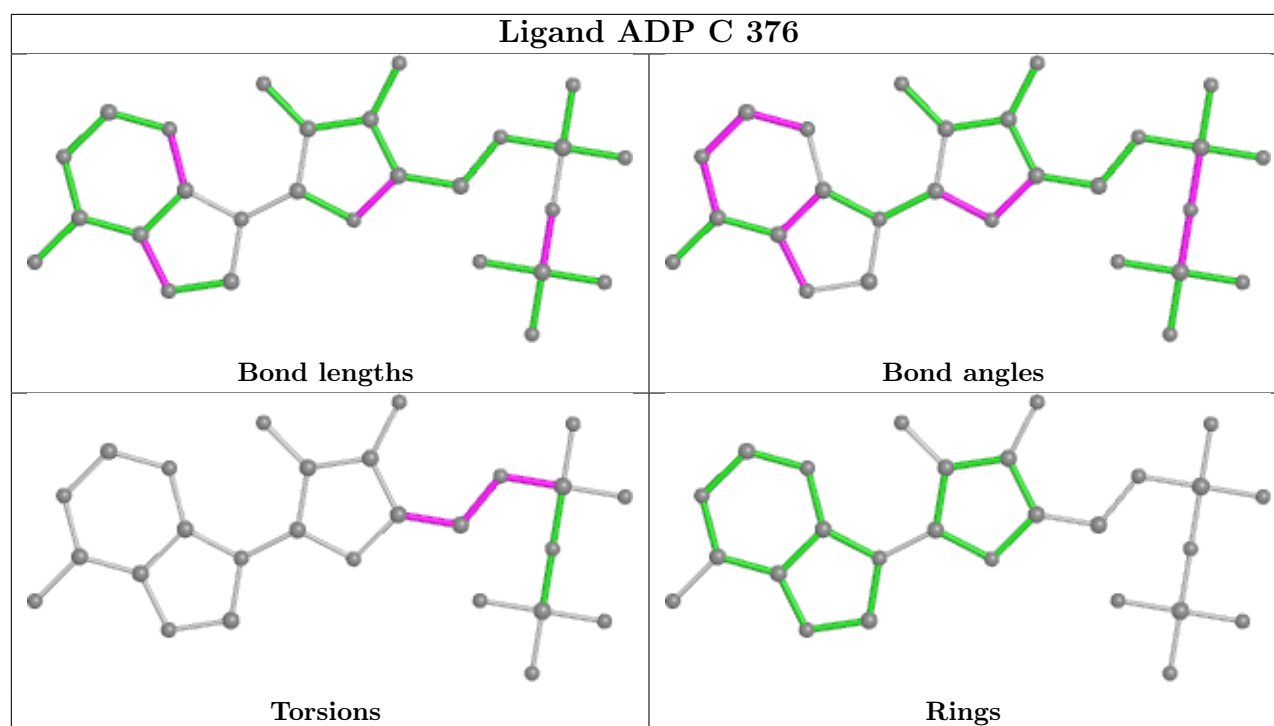
Bond angles

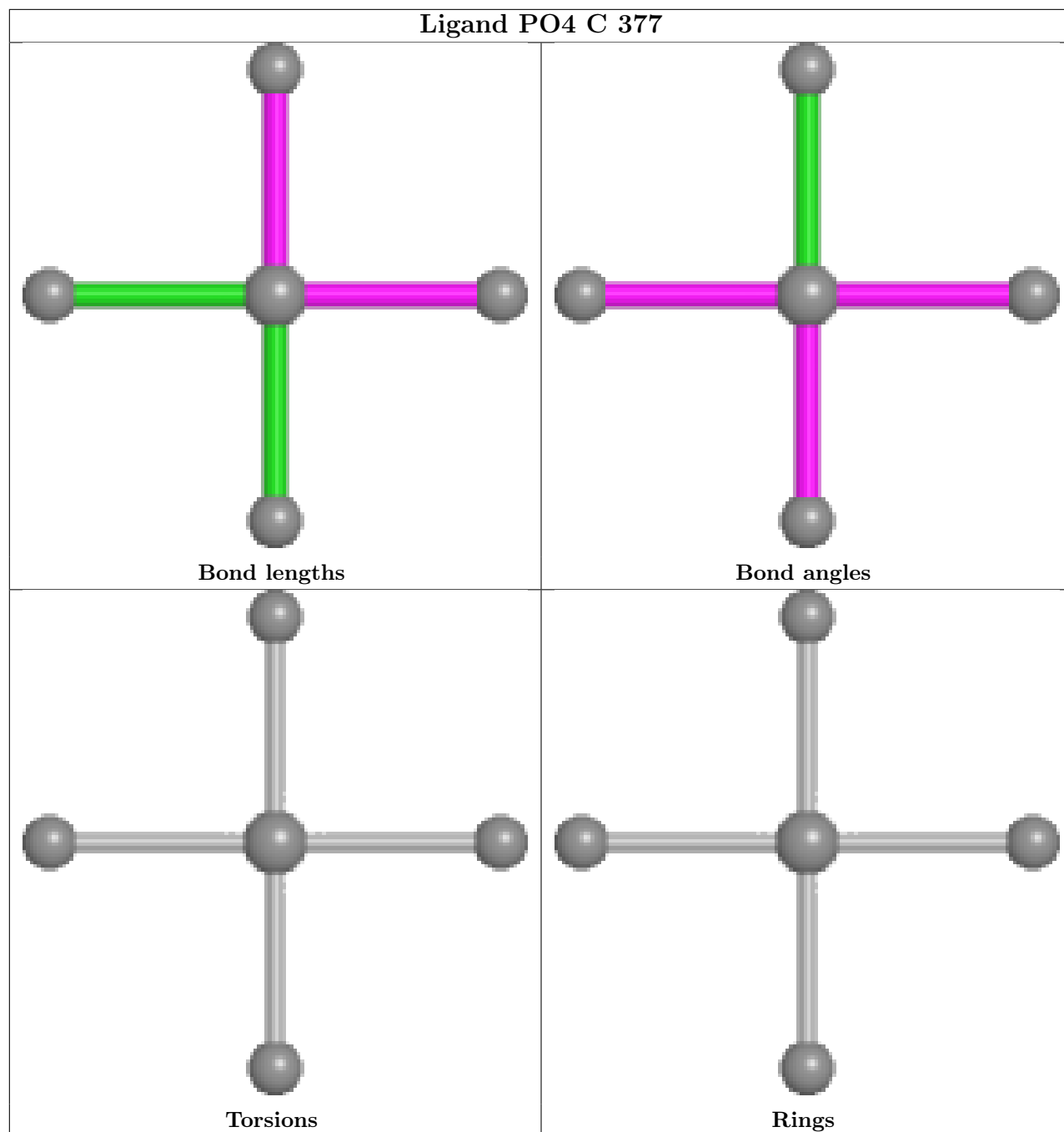


Torsions

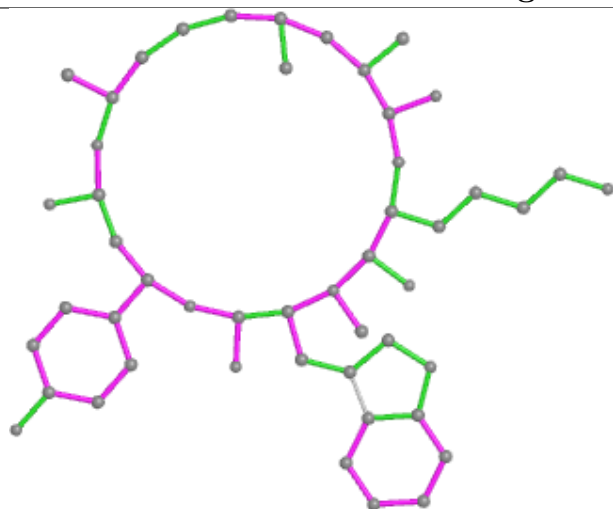


Rings

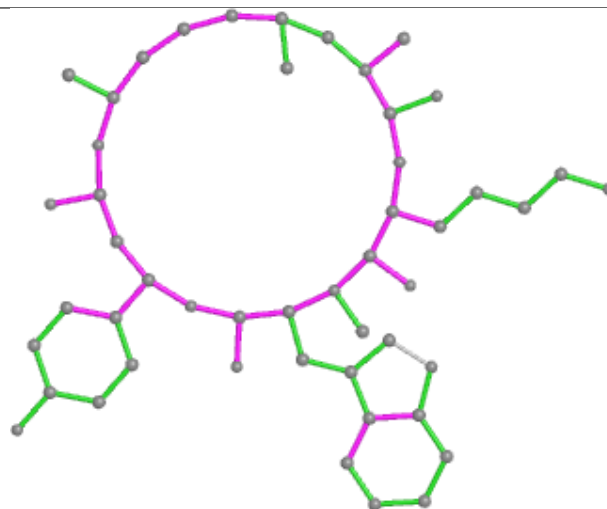




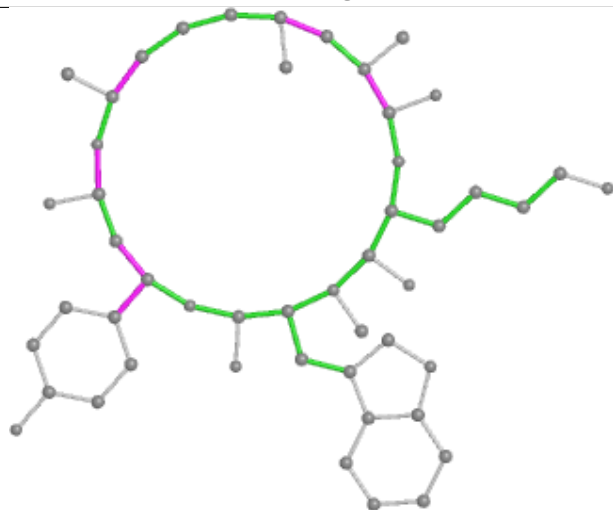
Ligand 9ZK C 379



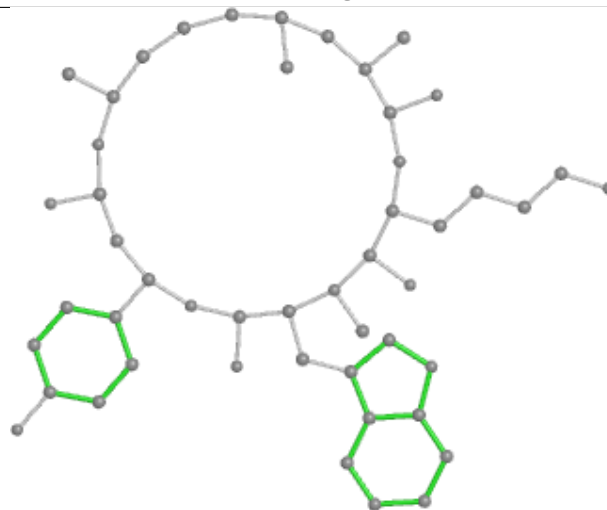
Bond lengths



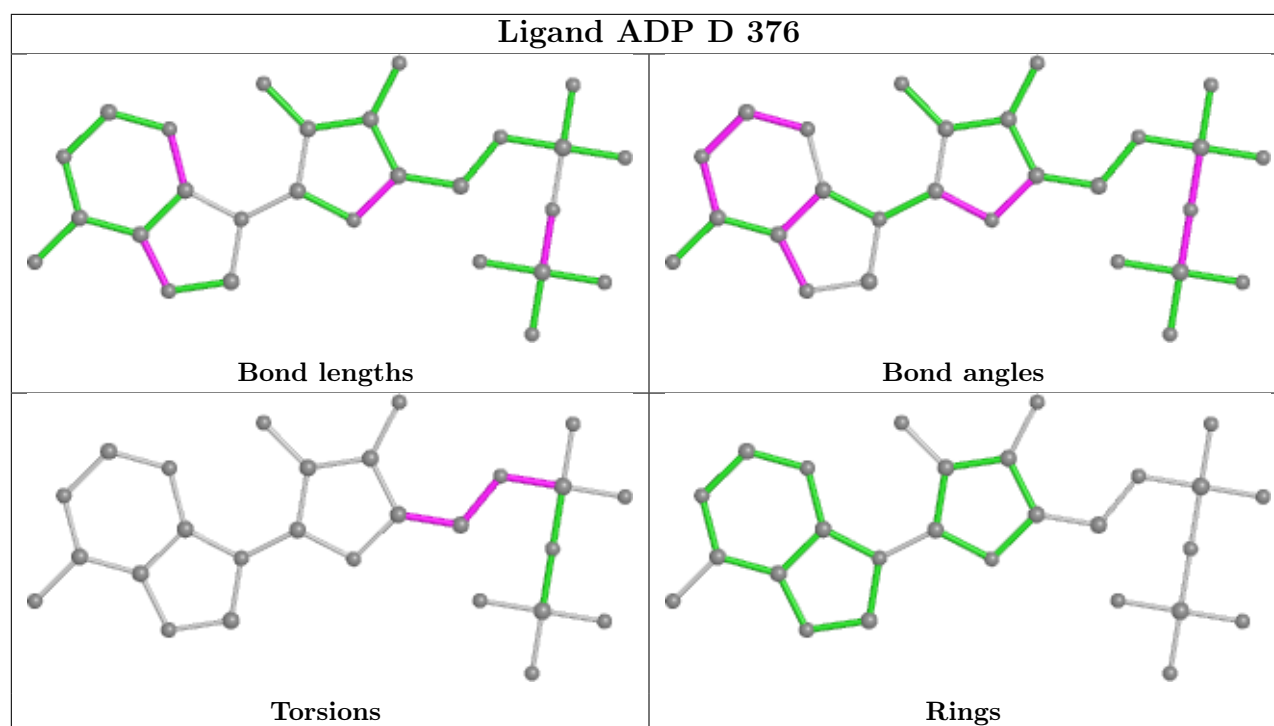
Bond angles

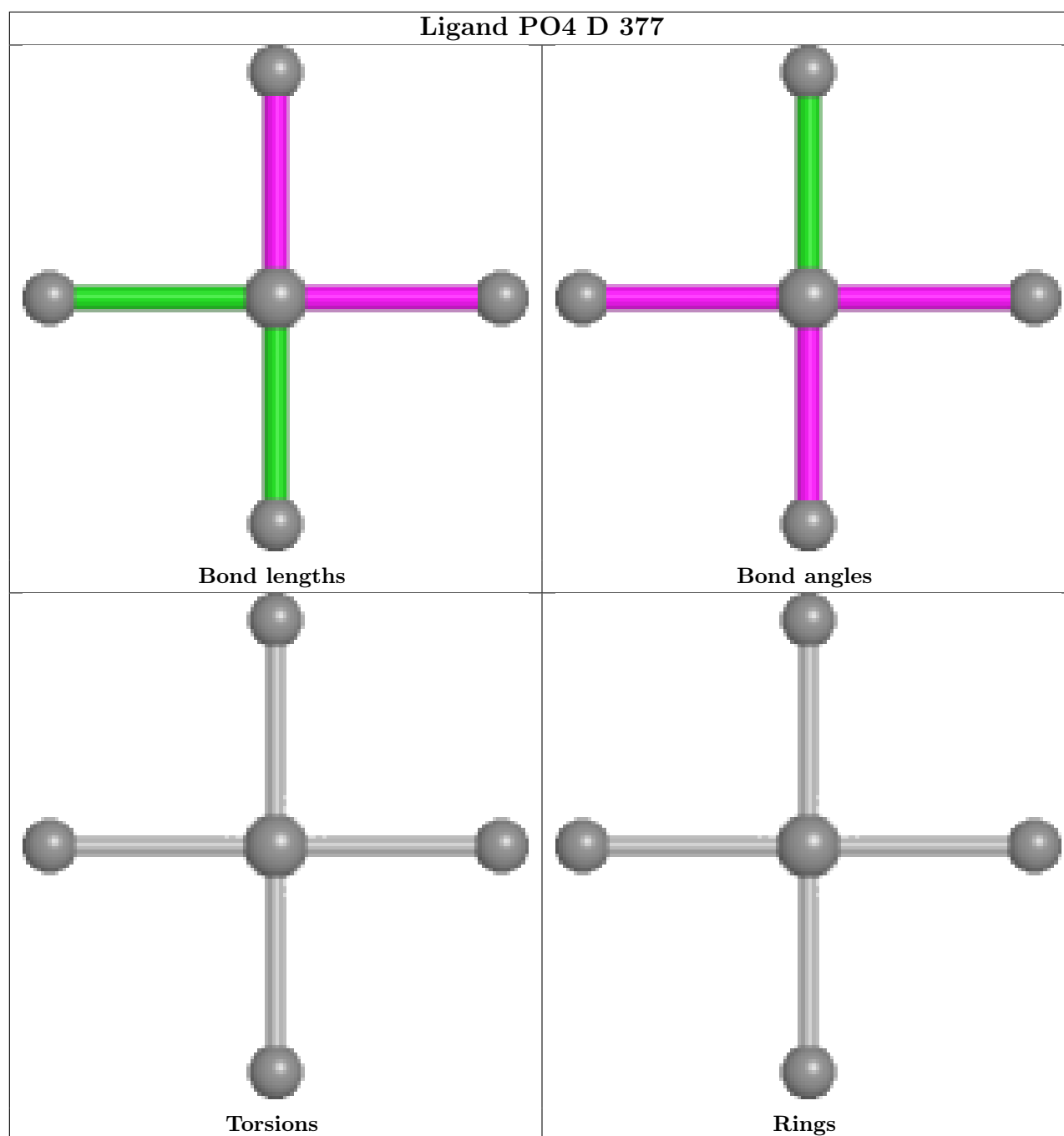


Torsions

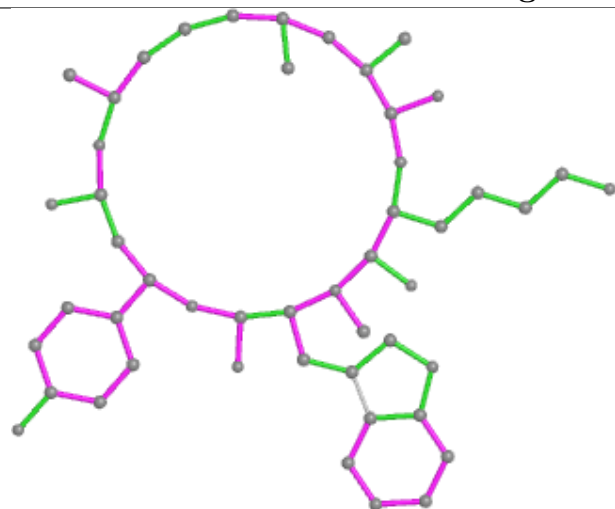


Rings

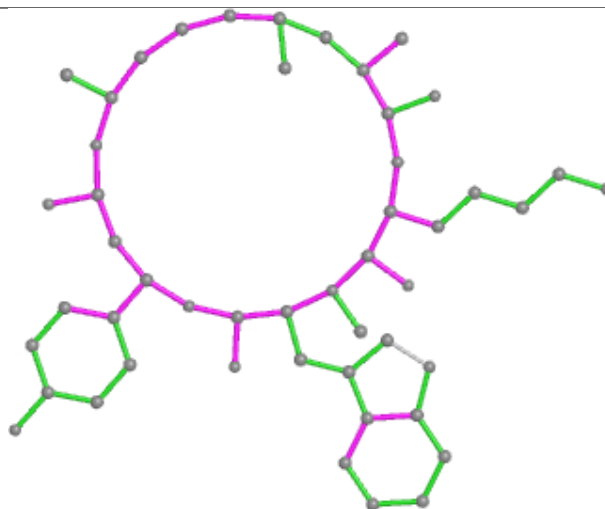




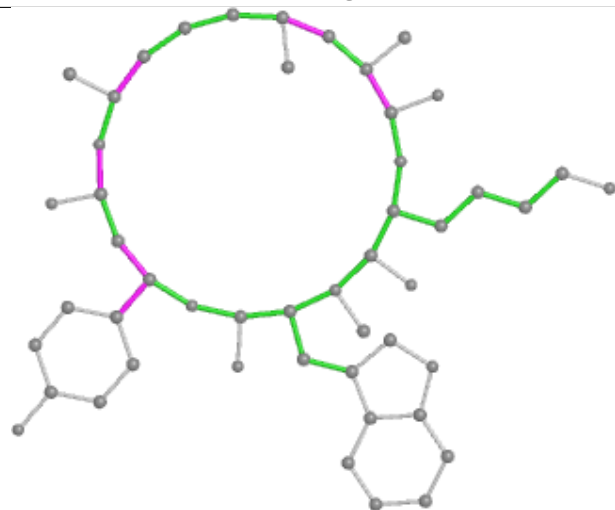
Ligand 9ZK D 379



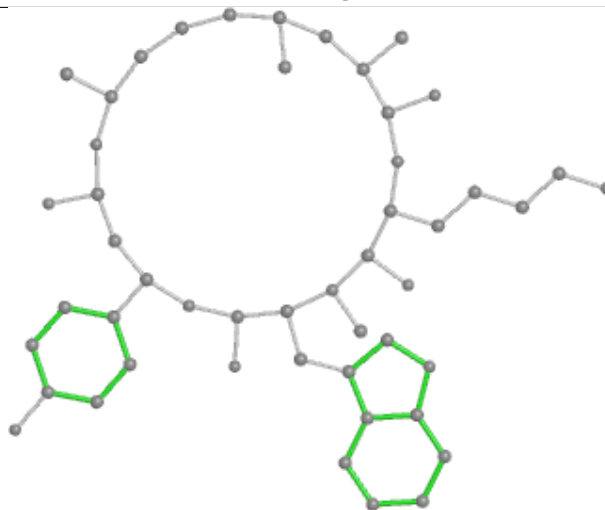
Bond lengths



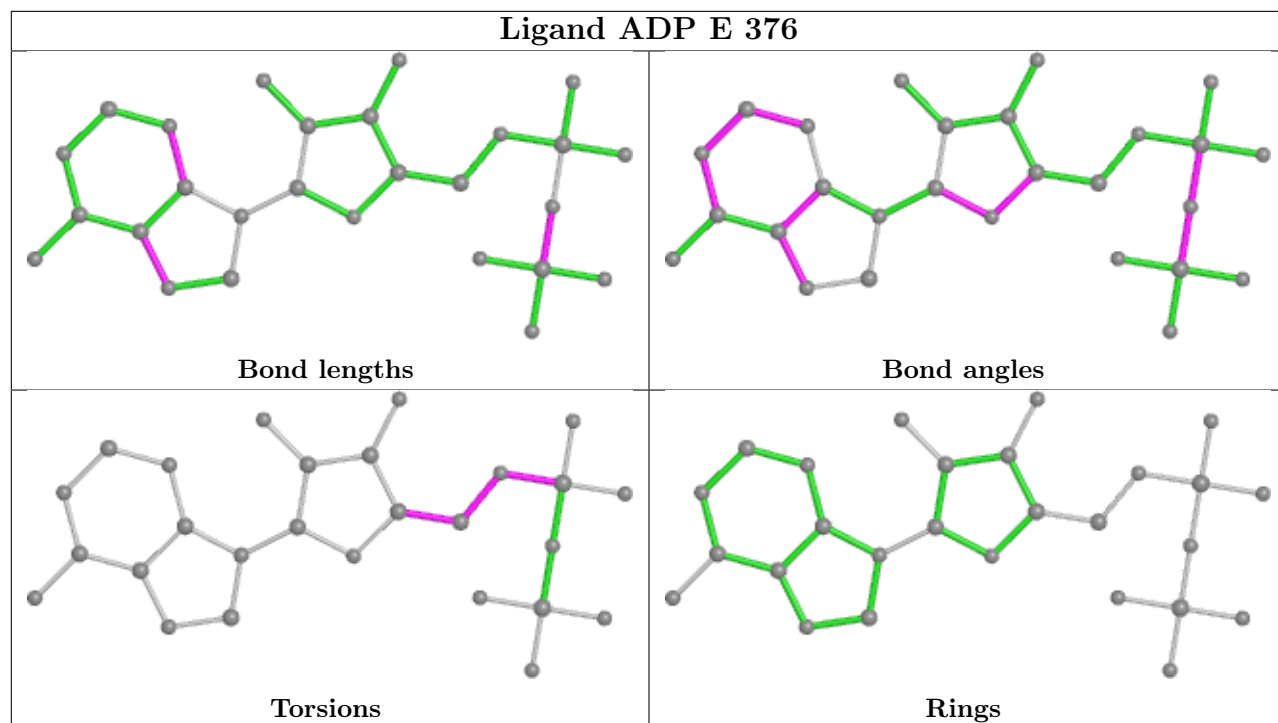
Bond angles

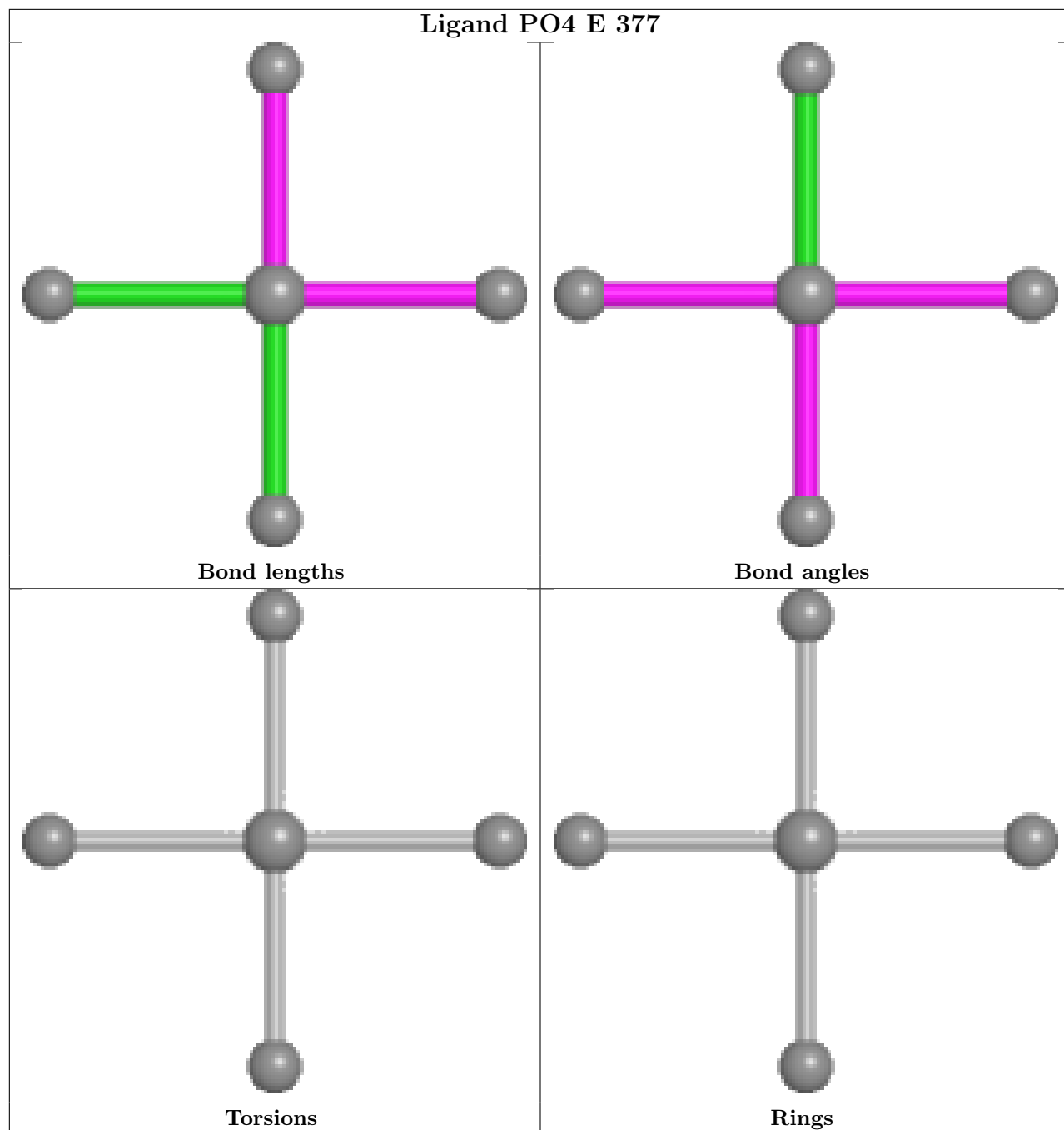


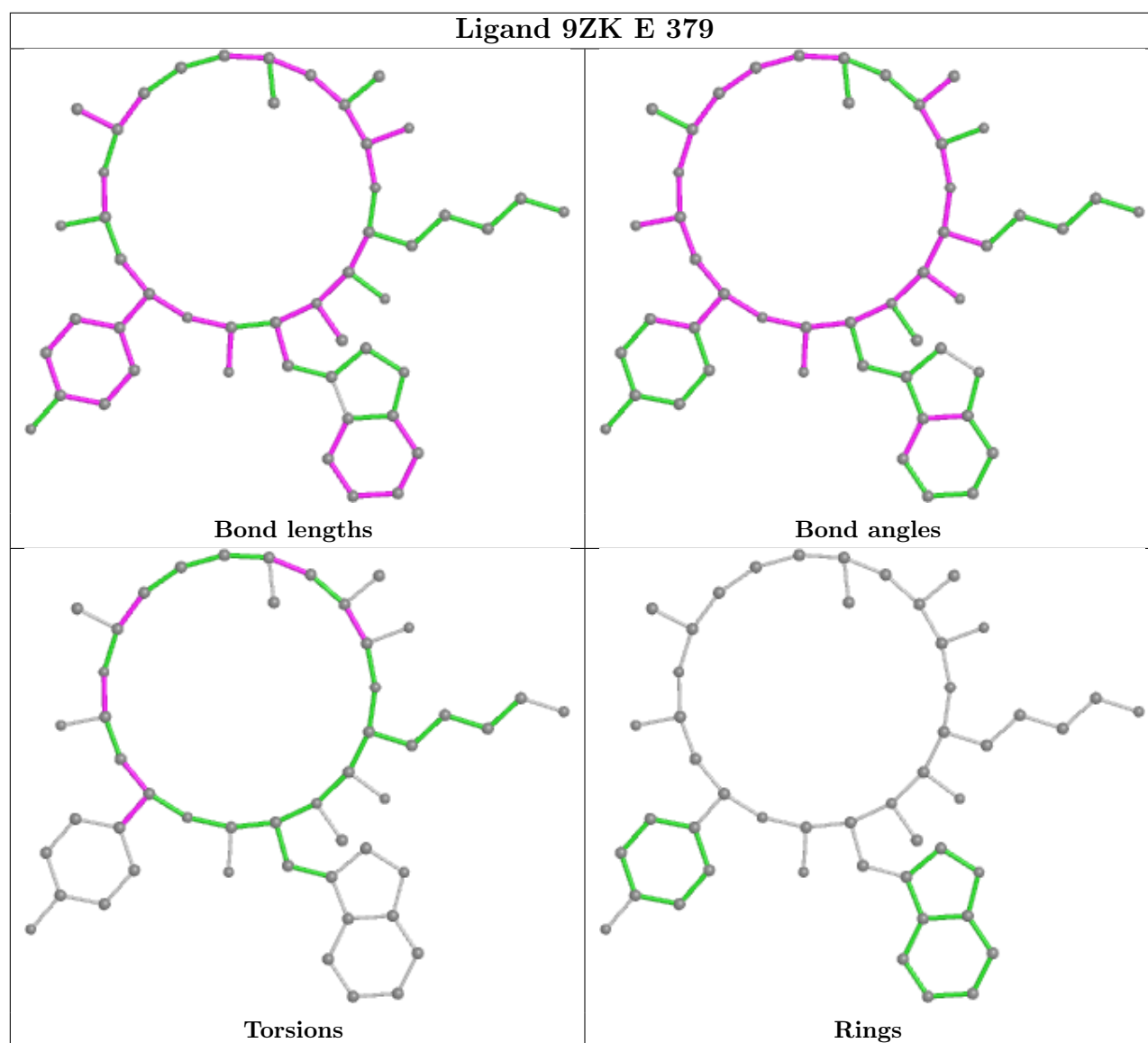
Torsions



Rings







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.