



Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Oct 9, 2019 – 12:47 PM EDT

PDB ID : 5OOC
EMDB ID: : EMD-3836
Title : Cryo-EM structure of jasplakinolide-stabilized F-actin in complex with ADP
Authors : Merino, F.; Pospich, S.; Funk, J.; Kuellmer, F.; Arndt, H.-D.; Bieling, P.;
Raunser, S.
Deposited on : 2017-08-07
Resolution : 3.60 Å(reported)

This is a Full wwPDB/EMDataBank EM Map/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.

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

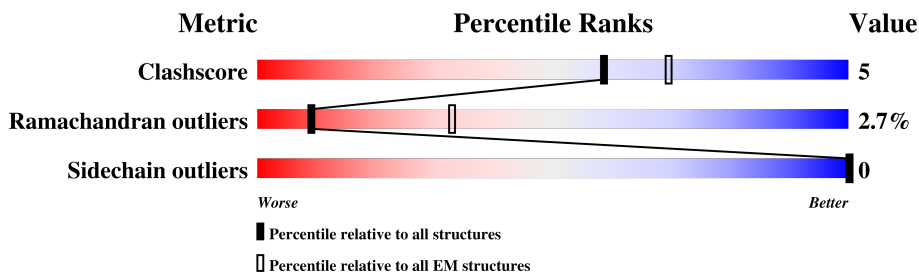
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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	375	91% 7% ..
1	B	375	91% 7% ..
1	C	375	91% 7% ..
1	D	375	91% 7% ..
1	E	375	91% 7% ..

2 Entry composition [i](#)

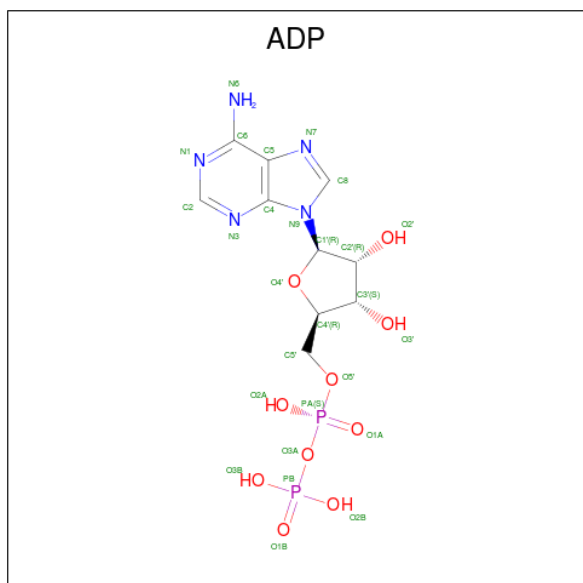
There are 4 unique types of molecules in this entry. The entry contains 14885 atoms, of which 0 are hydrogens and 0 are deuteriums.

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: $C_{10}H_{15}N_5O_{10}P_2$).



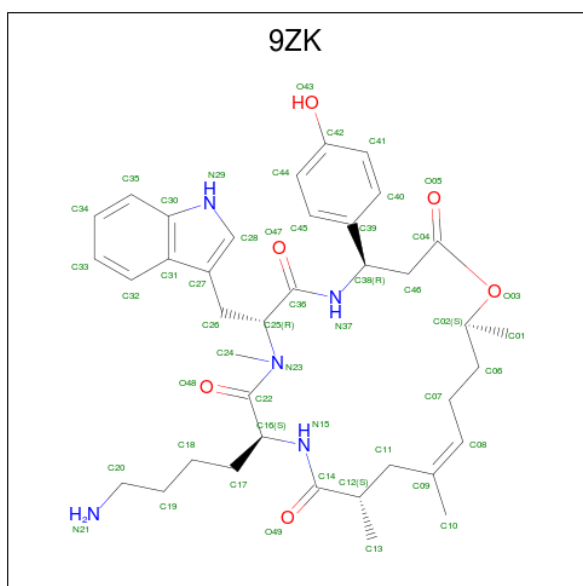
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

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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 (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-1 5-ene-2,6,9,12-tetrone (three-letter code: 9ZK) (formula: C₃₈H₅₁N₅O₆).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			98	76	10	12	
3	A	1	Total	C	N	O	0
			98	76	10	12	
3	B	1	Total	C	N	O	0
			49	38	5	6	
3	C	1	Total	C	N	O	0
			49	38	5	6	
3	D	1	Total	C	N	O	0
			49	38	5	6	

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

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

- 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
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	365209	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 ($e^-/\text{\AA}^2$)	71	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON II (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: MG, 9ZK, HIC, 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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.84	0/2950	0.73	4/3994 (0.1%)
1	B	0.84	0/2950	0.73	4/3994 (0.1%)
1	C	0.84	0/2950	0.73	4/3994 (0.1%)
1	D	0.84	0/2950	0.73	4/3994 (0.1%)
1	E	0.84	0/2950	0.73	4/3994 (0.1%)
All	All	0.84	0/14750	0.73	20/19970 (0.1%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	39	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	E	39	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	A	39	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	C	39	ARG	NE-CZ-NH1	7.19	123.89	120.30
1	B	39	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	D	39	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	B	39	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	A	39	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	C	39	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	E	39	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	D	177	ARG	NE-CZ-NH2	5.76	123.18	120.30
1	B	177	ARG	NE-CZ-NH2	5.75	123.17	120.30
1	A	177	ARG	NE-CZ-NH2	5.72	123.16	120.30
1	E	177	ARG	NE-CZ-NH2	5.72	123.16	120.30
1	C	177	ARG	NE-CZ-NH2	5.68	123.14	120.30
1	D	116	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	B	116	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	E	116	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	A	116	ARG	NE-CZ-NH2	-5.04	117.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	116	ARG	NE-CZ-NH2	-5.02	117.79	120.30

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	19	0
1	B	2900	0	2872	18	0
1	C	2900	0	2872	21	0
1	D	2900	0	2872	18	0
1	E	2900	0	2872	18	0
2	A	27	0	12	3	0
2	B	27	0	12	3	0
2	C	27	0	12	3	0
2	D	27	0	12	3	0
2	E	27	0	12	3	0
3	A	98	0	0	22	0
3	B	49	0	0	11	0
3	C	49	0	0	11	0
3	D	49	0	0	11	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
All	All	14885	0	14420	154	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.

All (154) 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)
3:A:404:9ZK:O05	3:A:404:9ZK:C45	2.19	0.90
3:C:403:9ZK:C45	3:C:403:9ZK:O05	2.19	0.90
3:B:403:9ZK:C45	3:B:403:9ZK:O05	2.19	0.89
3:A:402:9ZK:C45	3:A:402:9ZK:O05	2.19	0.89
3:B:403:9ZK:O47	3:B:403:9ZK:C24	2.21	0.89
3:D:403:9ZK:O05	3:D:403:9ZK:C45	2.19	0.89
3:A:404:9ZK:O47	3:A:404:9ZK:C24	2.21	0.88
3:D:403:9ZK:O47	3:D:403:9ZK:C24	2.21	0.86
3:A:402:9ZK:O47	3:A:402:9ZK:C24	2.21	0.86
3:C:403:9ZK:O47	3:C:403:9ZK:C24	2.21	0.84
3:A:402:9ZK:C46	3:A:402:9ZK:O47	2.25	0.83
3:A:404:9ZK:C46	3:A:404:9ZK:O47	2.25	0.80
3:D:403:9ZK:C24	3:D:403:9ZK:O49	2.30	0.80
3:A:402:9ZK:O49	3:A:402:9ZK:C24	2.30	0.80
3:B:403:9ZK:C24	3:B:403:9ZK:O49	2.30	0.79
3:C:403:9ZK:C24	3:C:403:9ZK:O49	2.30	0.79
3:A:404:9ZK:O49	3:A:404:9ZK:C24	2.30	0.79
3:B:403:9ZK:C46	3:B:403:9ZK:O47	2.25	0.79
3:B:403:9ZK:C45	3:B:403:9ZK:C04	2.63	0.76
3:A:402:9ZK:C04	3:A:402:9ZK:C45	2.63	0.75
3:C:403:9ZK:O47	3:C:403:9ZK:C46	2.25	0.74
3:D:403:9ZK:O47	3:D:403:9ZK:C46	2.25	0.73
3:C:403:9ZK:C45	3:C:403:9ZK:C04	2.63	0.73
3:A:402:9ZK:C10	3:A:402:9ZK:C14	2.67	0.72
3:D:403:9ZK:C45	3:D:403:9ZK:C04	2.63	0.72
3:B:403:9ZK:C14	3:B:403:9ZK:C10	2.67	0.72
3:A:404:9ZK:C10	3:A:404:9ZK:C14	2.67	0.72
3:A:404:9ZK:C04	3:A:404:9ZK:C45	2.63	0.71
3:D:403:9ZK:C14	3:D:403:9ZK:C10	2.67	0.70
3:A:404:9ZK:C39	3:A:404:9ZK:O05	2.40	0.70
3:D:403:9ZK:C39	3:D:403:9ZK:O05	2.40	0.70
3:A:402:9ZK:C39	3:A:402:9ZK:O05	2.40	0.69
3:B:403:9ZK:O05	3:B:403:9ZK:C39	2.40	0.68
3:C:403:9ZK:C10	3:C:403:9ZK:C14	2.67	0.68
3:C:403:9ZK:O05	3:C:403:9ZK:C39	2.40	0.67
1:B:253:GLU:H	1:B:253:GLU:CD	2.00	0.64
1:D:253:GLU:H	1:D:253:GLU:CD	2.00	0.64
1:A:253:GLU:CD	1:A:253:GLU:H	2.00	0.63
1:C:253:GLU:CD	1:C:253:GLU:H	2.01	0.63
1:E:253:GLU:CD	1:E:253:GLU:H	2.00	0.62
2:B:401:ADP:C8	2:B:401:ADP:H3'	2.40	0.56
2:C:401:ADP:C8	2:C:401:ADP:H3'	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:401:ADP:H3'	2:D:401:ADP:C8	2.40	0.56
2:A:401:ADP:C8	2:A:401:ADP:H3'	2.40	0.56
2:E:401:ADP:H3'	2:E:401:ADP:C8	2.40	0.56
1:D:207:GLU:HA	1:D:207:GLU:OE1	2.07	0.55
1:A:207:GLU:HA	1:A:207:GLU:OE1	2.07	0.55
1:B:207:GLU:HA	1:B:207:GLU:OE1	2.07	0.55
1:C:207:GLU:OE1	1:C:207:GLU:HA	2.07	0.55
1:E:207:GLU:OE1	1:E:207:GLU:HA	2.07	0.55
1:B:49:GLN:O	1:B:50:LYS:CB	2.56	0.53
1:A:49:GLN:O	1:A:50:LYS:CB	2.56	0.53
1:C:49:GLN:O	1:C:50:LYS:CB	2.56	0.53
1:D:49:GLN:O	1:D:50:LYS:CB	2.56	0.53
1:E:138:ALA:HB2	1:E:161:HIS:CE1	2.44	0.53
1:C:138:ALA:HB2	1:C:161:HIS:CE1	2.43	0.53
1:E:49:GLN:O	1:E:50:LYS:CB	2.56	0.53
1:D:138:ALA:HB2	1:D:161:HIS:CE1	2.43	0.53
1:A:138:ALA:HB2	1:A:161:HIS:CE1	2.44	0.53
1:B:138:ALA:HB2	1:B:161:HIS:CE1	2.44	0.52
3:A:402:9ZK:C09	3:A:402:9ZK:O49	2.57	0.52
3:C:403:9ZK:C09	3:C:403:9ZK:O49	2.57	0.52
3:D:403:9ZK:C09	3:D:403:9ZK:O49	2.57	0.52
2:B:401:ADP:H8	2:B:401:ADP:H3'	1.76	0.51
2:D:401:ADP:H3'	2:D:401:ADP:H8	1.76	0.51
3:A:404:9ZK:O49	3:A:404:9ZK:C09	2.57	0.50
2:E:401:ADP:H3'	2:E:401:ADP:H8	1.76	0.49
3:B:403:9ZK:C09	3:B:403:9ZK:O49	2.57	0.49
1:C:138:ALA:HB2	1:C:161:HIS:HE1	1.78	0.49
2:C:401:ADP:H8	2:C:401:ADP:H3'	1.76	0.48
3:A:402:9ZK:C46	3:A:402:9ZK:C06	2.91	0.48
1:D:138:ALA:HB2	1:D:161:HIS:HE1	1.78	0.48
3:D:403:9ZK:C06	3:D:403:9ZK:C46	2.91	0.48
1:B:138:ALA:HB2	1:B:161:HIS:HE1	1.78	0.48
3:C:403:9ZK:C06	3:C:403:9ZK:C46	2.91	0.48
2:A:401:ADP:H3'	2:A:401:ADP:H8	1.76	0.48
3:B:403:9ZK:C46	3:B:403:9ZK:C06	2.91	0.47
1:A:138:ALA:HB2	1:A:161:HIS:HE1	1.78	0.47
3:A:404:9ZK:C46	3:A:404:9ZK:C06	2.91	0.47
1:C:59:GLN:OE1	1:C:59:GLN:HA	2.15	0.47
1:E:59:GLN:HA	1:E:59:GLN:OE1	2.15	0.47
1:D:59:GLN:HA	1:D:59:GLN:OE1	2.15	0.47
1:A:40:HIS:ND1	1:C:173:HIS:ND1	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:ASP:C	1:C:244:ASP:OD1	2.53	0.46
2:E:401:ADP:C8	2:E:401:ADP:C3'	2.99	0.46
1:B:40:HIS:ND1	1:D:173:HIS:ND1	2.64	0.46
1:C:352:PHE:CG	1:C:352:PHE:O	2.69	0.46
1:E:5:THR:OG1	1:E:6:THR:N	2.48	0.46
2:B:401:ADP:C8	2:B:401:ADP:C3'	2.98	0.46
1:B:5:THR:OG1	1:B:6:THR:N	2.48	0.46
1:C:40:HIS:ND1	1:E:173:HIS:ND1	2.64	0.46
1:E:352:PHE:CG	1:E:352:PHE:O	2.69	0.46
1:A:59:GLN:HA	1:A:59:GLN:OE1	2.15	0.46
1:B:99:GLU:N	1:B:99:GLU:OE1	2.32	0.46
1:D:99:GLU:OE1	1:D:99:GLU:N	2.32	0.46
1:C:5:THR:OG1	1:C:6:THR:N	2.48	0.46
1:B:59:GLN:OE1	1:B:59:GLN:HA	2.15	0.46
1:B:244:ASP:OD1	1:B:244:ASP:C	2.53	0.45
1:A:352:PHE:CG	1:A:352:PHE:O	2.69	0.45
1:A:5:THR:OG1	1:A:6:THR:N	2.48	0.45
1:D:352:PHE:O	1:D:352:PHE:CG	2.69	0.45
1:B:352:PHE:O	1:B:352:PHE:CG	2.69	0.45
1:D:352:PHE:CD2	1:D:352:PHE:O	2.70	0.45
1:D:5:THR:OG1	1:D:6:THR:N	2.48	0.45
1:A:99:GLU:OE1	1:A:99:GLU:N	2.32	0.45
1:A:352:PHE:CD2	1:A:352:PHE:O	2.70	0.45
1:E:138:ALA:HB2	1:E:161:HIS:HE1	1.78	0.45
1:C:352:PHE:O	1:C:352:PHE:CD2	2.70	0.44
1:D:244:ASP:C	1:D:244:ASP:OD1	2.53	0.44
1:B:352:PHE:O	1:B:352:PHE:CD2	2.70	0.44
2:D:401:ADP:C3'	2:D:401:ADP:C8	2.99	0.44
2:C:401:ADP:C8	2:C:401:ADP:C3'	2.98	0.44
1:E:352:PHE:O	1:E:352:PHE:CD2	2.70	0.44
1:E:78:ASN:C	1:E:78:ASN:OD1	2.56	0.44
3:B:403:9ZK:C26	3:B:403:9ZK:O48	2.65	0.44
1:E:244:ASP:C	1:E:244:ASP:OD1	2.53	0.44
1:A:62:ARG:NE	1:C:288:ASP:OD2	2.51	0.44
1:B:62:ARG:NE	1:D:288:ASP:OD2	2.51	0.44
1:C:62:ARG:NE	1:E:288:ASP:OD2	2.51	0.44
1:D:78:ASN:OD1	1:D:78:ASN:C	2.56	0.43
1:C:78:ASN:C	1:C:78:ASN:OD1	2.56	0.43
1:C:99:GLU:N	1:C:99:GLU:OE1	2.32	0.43
3:A:404:9ZK:O48	3:A:404:9ZK:C26	2.65	0.43
1:D:39:ARG:HD3	1:E:270:GLU:OE1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ASN:OD1	1:A:78:ASN:C	2.56	0.43
1:B:78:ASN:OD1	1:B:78:ASN:C	2.56	0.43
1:A:244:ASP:C	1:A:244:ASP:OD1	2.53	0.43
3:C:403:9ZK:C26	3:C:403:9ZK:O48	2.65	0.42
3:D:403:9ZK:C27	3:D:403:9ZK:O48	2.67	0.42
1:A:39:ARG:HD3	1:B:270:GLU:OE1	2.19	0.42
3:B:403:9ZK:C27	3:B:403:9ZK:O48	2.67	0.42
1:E:99:GLU:OE1	1:E:99:GLU:N	2.32	0.42
1:B:39:ARG:HD3	1:C:270:GLU:OE1	2.19	0.42
3:A:404:9ZK:O48	3:A:404:9ZK:C27	2.67	0.42
1:C:48:GLY:O	1:C:50:LYS:N	2.53	0.42
1:E:207:GLU:OE1	1:E:207:GLU:CA	2.66	0.42
1:E:48:GLY:O	1:E:50:LYS:N	2.53	0.42
3:C:403:9ZK:C27	3:C:403:9ZK:O48	2.67	0.41
1:B:257:CYS:HB3	1:B:258:PRO:HD3	2.02	0.41
1:C:207:GLU:OE1	1:C:207:GLU:CA	2.66	0.41
1:C:39:ARG:HD3	1:D:270:GLU:OE1	2.19	0.41
1:D:48:GLY:O	1:D:50:LYS:N	2.53	0.41
3:A:402:9ZK:C27	3:A:402:9ZK:O48	2.67	0.41
1:E:257:CYS:HB3	1:E:258:PRO:HD3	2.02	0.41
1:B:48:GLY:O	1:B:50:LYS:N	2.53	0.41
1:A:207:GLU:CA	1:A:207:GLU:OE1	2.66	0.41
1:A:48:GLY:O	1:A:50:LYS:N	2.53	0.41
2:A:401:ADP:C3'	2:A:401:ADP:C8	2.99	0.41
3:A:402:9ZK:O48	3:A:402:9ZK:C26	2.65	0.41
3:D:403:9ZK:O48	3:D:403:9ZK:C26	2.65	0.41
1:C:257:CYS:HB3	1:C:258:PRO:HD3	2.02	0.40
1:D:257:CYS:HB3	1:D:258:PRO:HD3	2.02	0.40
1:A:257:CYS:HB3	1:A:258:PRO:HD3	2.02	0.40
1:A:16:LEU:HD23	1:A:16:LEU:N	2.37	0.40

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	368/375 (98%)	342 (93%)	16 (4%)	10 (3%)	5	40
1	B	368/375 (98%)	342 (93%)	16 (4%)	10 (3%)	5	40
1	C	368/375 (98%)	342 (93%)	16 (4%)	10 (3%)	5	40
1	D	368/375 (98%)	342 (93%)	16 (4%)	10 (3%)	5	40
1	E	368/375 (98%)	342 (93%)	16 (4%)	10 (3%)	5	40
All	All	1840/1875 (98%)	1710 (93%)	80 (4%)	50 (3%)	9	40

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	THR
1	A	43	VAL
1	A	50	LYS
1	B	6	THR
1	B	43	VAL
1	B	50	LYS
1	C	6	THR
1	C	43	VAL
1	C	50	LYS
1	D	6	THR
1	D	43	VAL
1	D	50	LYS
1	E	6	THR
1	E	43	VAL
1	E	50	LYS
1	A	41	GLN
1	A	97	ALA
1	B	41	GLN
1	B	97	ALA
1	C	41	GLN
1	C	97	ALA
1	D	41	GLN
1	D	97	ALA
1	E	41	GLN
1	E	97	ALA
1	A	49	GLN
1	B	49	GLN
1	C	49	GLN

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Mol	Chain	Res	Type
1	D	49	GLN
1	E	49	GLN
1	A	164	PRO
1	A	367	PRO
1	B	164	PRO
1	B	367	PRO
1	C	164	PRO
1	C	367	PRO
1	D	164	PRO
1	D	367	PRO
1	E	164	PRO
1	E	367	PRO
1	A	98	PRO
1	B	98	PRO
1	C	98	PRO
1	D	98	PRO
1	E	98	PRO
1	B	42	GLY
1	D	42	GLY
1	E	42	GLY
1	A	42	GLY
1	C	42	GLY

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	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. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	HIS
1	B	161	HIS
1	C	161	HIS
1	D	161	HIS
1	E	161	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	1.17	1 (11%)	6,14,16	1.18	1 (16%)
1	HIC	B	73	1	9,11,12	1.15	1 (11%)	6,14,16	1.18	1 (16%)
1	HIC	C	73	1	9,11,12	1.15	1 (11%)	6,14,16	1.18	1 (16%)
1	HIC	D	73	1	9,11,12	1.16	1 (11%)	6,14,16	1.18	1 (16%)
1	HIC	E	73	1	9,11,12	1.16	1 (11%)	6,14,16	1.18	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	-	0/4/6/8	0/1/1/1
1	HIC	B	73	1	-	0/4/6/8	0/1/1/1
1	HIC	C	73	1	-	0/4/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HIC	D	73	1	-	0/4/6/8	0/1/1/1
1	HIC	E	73	1	-	0/4/6/8	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	HIC	CD2-NE2	-2.60	1.34	1.38
1	E	73	HIC	CD2-NE2	-2.60	1.34	1.38
1	C	73	HIC	CD2-NE2	-2.60	1.34	1.38
1	D	73	HIC	CD2-NE2	-2.59	1.34	1.38
1	B	73	HIC	CD2-NE2	-2.58	1.34	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	73	HIC	O-C-CA	-2.11	119.31	124.98
1	A	73	HIC	O-C-CA	-2.11	119.31	124.98
1	E	73	HIC	O-C-CA	-2.10	119.35	124.98
1	C	73	HIC	O-C-CA	-2.10	119.35	124.98
1	B	73	HIC	O-C-CA	-2.09	119.39	124.98

There are no chirality outliers.

There are no torsion outliers.

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 15 ligands modelled in this entry, 5 are monoatomic - leaving 10 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	401	4	24,29,29	1.93	7 (29%)	25,45,45	1.71	5 (20%)
3	9ZK	A	402	-	51,52,52	1.88	15 (29%)	64,71,71	2.05	16 (25%)
3	9ZK	A	404	-	51,52,52	1.88	15 (29%)	64,71,71	2.05	16 (25%)
2	ADP	B	401	4	24,29,29	1.94	7 (29%)	25,45,45	1.71	5 (20%)
3	9ZK	B	403	-	51,52,52	1.89	15 (29%)	64,71,71	2.05	16 (25%)
2	ADP	C	401	4	24,29,29	1.93	7 (29%)	25,45,45	1.71	5 (20%)
3	9ZK	C	403	-	51,52,52	1.88	15 (29%)	64,71,71	2.05	16 (25%)
2	ADP	D	401	4	24,29,29	1.93	7 (29%)	25,45,45	1.71	5 (20%)
3	9ZK	D	403	-	51,52,52	1.88	15 (29%)	64,71,71	2.05	16 (25%)
2	ADP	E	401	4	24,29,29	1.93	7 (29%)	25,45,45	1.71	5 (20%)

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	401	4	-	5/12/32/32	0/3/3/3
3	9ZK	A	402	-	-	33/58/59/59	0/3/4/4
3	9ZK	A	404	-	-	33/58/59/59	0/3/4/4
2	ADP	B	401	4	-	5/12/32/32	0/3/3/3
3	9ZK	B	403	-	-	33/58/59/59	0/3/4/4
2	ADP	C	401	4	-	5/12/32/32	0/3/3/3
3	9ZK	C	403	-	-	33/58/59/59	0/3/4/4
2	ADP	D	401	4	-	5/12/32/32	0/3/3/3
3	9ZK	D	403	-	-	33/58/59/59	0/3/4/4
2	ADP	E	401	4	-	5/12/32/32	0/3/3/3

All (110) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	ADP	PB-O3A	-5.97	1.51	1.60
2	C	401	ADP	PB-O3A	-5.96	1.51	1.60
2	A	401	ADP	PB-O3A	-5.95	1.51	1.60
2	E	401	ADP	PB-O3A	-5.95	1.51	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	ADP	PB-O3A	-5.94	1.51	1.60
3	B	403	9ZK	C14-N15	4.22	1.43	1.34
3	A	402	9ZK	C14-N15	4.21	1.43	1.34
3	C	403	9ZK	C14-N15	4.20	1.43	1.34
3	A	404	9ZK	C14-N15	4.19	1.43	1.34
3	D	403	9ZK	C14-N15	4.17	1.43	1.34
3	B	403	9ZK	O47-C36	-4.13	1.15	1.23
2	B	401	ADP	C4-N3	-4.12	1.29	1.35
3	A	402	9ZK	O47-C36	-4.11	1.15	1.23
3	D	403	9ZK	O47-C36	-4.08	1.15	1.23
3	C	403	9ZK	O47-C36	-4.08	1.15	1.23
3	A	404	9ZK	O47-C36	-4.07	1.15	1.23
2	E	401	ADP	C4-N3	-4.04	1.30	1.35
2	A	401	ADP	C4-N3	-4.02	1.30	1.35
2	C	401	ADP	C4-N3	-4.00	1.30	1.35
2	D	401	ADP	C4-N3	-4.00	1.30	1.35
3	A	402	9ZK	C31-C30	-3.61	1.33	1.42
3	B	403	9ZK	C31-C30	-3.59	1.33	1.42
3	A	404	9ZK	C31-C30	-3.59	1.33	1.42
3	D	403	9ZK	C31-C30	-3.58	1.33	1.42
3	C	403	9ZK	C31-C30	-3.57	1.33	1.42
3	D	403	9ZK	C25-C36	-3.53	1.44	1.52
3	A	404	9ZK	C25-C36	-3.51	1.44	1.52
3	C	403	9ZK	C25-C36	-3.50	1.44	1.52
3	B	403	9ZK	C25-C36	-3.49	1.44	1.52
3	A	402	9ZK	C25-C36	-3.48	1.44	1.52
3	D	403	9ZK	C45-C39	-2.98	1.34	1.39
3	A	402	9ZK	C45-C39	-2.98	1.34	1.39
3	C	403	9ZK	C45-C39	-2.96	1.34	1.39
3	B	403	9ZK	C45-C39	-2.95	1.34	1.39
3	A	402	9ZK	C36-N37	2.93	1.40	1.34
3	D	403	9ZK	C36-N37	2.93	1.40	1.34
3	C	403	9ZK	C36-N37	2.91	1.40	1.34
3	A	404	9ZK	C45-C39	-2.91	1.34	1.39
3	B	403	9ZK	C36-N37	2.91	1.40	1.34
3	A	404	9ZK	C36-N37	2.90	1.40	1.34
3	B	403	9ZK	O48-C22	-2.89	1.17	1.22
3	A	404	9ZK	O48-C22	-2.88	1.17	1.22
3	B	403	9ZK	C22-N23	2.88	1.42	1.35
3	A	402	9ZK	O48-C22	-2.88	1.17	1.22
3	D	403	9ZK	C22-N23	2.87	1.42	1.35
3	D	403	9ZK	O48-C22	-2.87	1.17	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	403	9ZK	O49-C14	-2.87	1.17	1.23
3	A	404	9ZK	C22-N23	2.86	1.42	1.35
3	C	403	9ZK	O48-C22	-2.86	1.17	1.22
3	C	403	9ZK	O49-C14	-2.85	1.17	1.23
3	A	402	9ZK	C22-N23	2.85	1.42	1.35
3	A	404	9ZK	O49-C14	-2.84	1.17	1.23
3	A	402	9ZK	O49-C14	-2.84	1.17	1.23
3	C	403	9ZK	C22-N23	2.83	1.42	1.35
3	B	403	9ZK	C32-C31	-2.82	1.36	1.42
3	D	403	9ZK	O49-C14	-2.82	1.17	1.23
3	C	403	9ZK	C32-C31	-2.81	1.36	1.42
3	A	404	9ZK	C32-C31	-2.81	1.36	1.42
3	A	402	9ZK	C32-C31	-2.78	1.36	1.42
3	D	403	9ZK	C32-C31	-2.77	1.36	1.42
2	B	401	ADP	O4'-C4'	-2.70	1.38	1.45
2	C	401	ADP	O4'-C4'	-2.69	1.39	1.45
2	D	401	ADP	O4'-C4'	-2.68	1.39	1.45
2	A	401	ADP	O4'-C4'	-2.68	1.39	1.45
2	E	401	ADP	O4'-C4'	-2.67	1.39	1.45
3	D	403	9ZK	C28-N29	-2.58	1.31	1.36
3	C	403	9ZK	C28-N29	-2.57	1.31	1.36
3	A	404	9ZK	C28-N29	-2.56	1.31	1.36
3	B	403	9ZK	C28-N29	-2.56	1.31	1.36
3	A	402	9ZK	C28-N29	-2.55	1.31	1.36
3	A	402	9ZK	C35-C30	-2.55	1.37	1.41
3	D	403	9ZK	C35-C30	-2.54	1.37	1.41
3	A	404	9ZK	C35-C30	-2.53	1.37	1.41
3	C	403	9ZK	C35-C30	-2.51	1.37	1.41
3	B	403	9ZK	C35-C30	-2.50	1.37	1.41
3	A	404	9ZK	C40-C39	-2.43	1.35	1.39
3	B	403	9ZK	C40-C39	-2.43	1.35	1.39
3	D	403	9ZK	C40-C39	-2.41	1.35	1.39
3	C	403	9ZK	C40-C39	-2.36	1.35	1.39
3	A	402	9ZK	C40-C39	-2.35	1.35	1.39
2	A	401	ADP	C3'-C4'	-2.31	1.47	1.53
2	E	401	ADP	C3'-C4'	-2.28	1.47	1.53
3	D	403	9ZK	O03-C02	-2.28	1.43	1.47
3	B	403	9ZK	O03-C02	-2.28	1.43	1.47
3	A	402	9ZK	C25-N23	-2.27	1.43	1.47
3	C	403	9ZK	C25-N23	-2.27	1.43	1.47
2	B	401	ADP	C3'-C4'	-2.27	1.47	1.53
3	A	402	9ZK	O03-C02	-2.27	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	404	9ZK	O03-C02	-2.27	1.43	1.47
2	D	401	ADP	C5-N7	-2.26	1.31	1.39
2	C	401	ADP	C3'-C4'	-2.26	1.47	1.53
2	B	401	ADP	C5-N7	-2.26	1.31	1.39
3	C	403	9ZK	O03-C02	-2.25	1.43	1.47
2	C	401	ADP	C2-N1	-2.25	1.29	1.33
2	E	401	ADP	C5-N7	-2.25	1.31	1.39
2	D	401	ADP	C2-N1	-2.25	1.29	1.33
2	D	401	ADP	C3'-C4'	-2.25	1.47	1.53
2	A	401	ADP	C5-N7	-2.25	1.31	1.39
3	D	403	9ZK	C25-N23	-2.24	1.43	1.47
2	C	401	ADP	C5-N7	-2.24	1.31	1.39
2	B	401	ADP	C2-N1	-2.23	1.29	1.33
2	A	401	ADP	C2-N1	-2.22	1.29	1.33
3	B	403	9ZK	C25-N23	-2.22	1.43	1.47
2	E	401	ADP	C2-N1	-2.21	1.29	1.33
3	A	404	9ZK	C25-N23	-2.21	1.43	1.47
2	C	401	ADP	C2'-C3'	-2.05	1.48	1.53
2	B	401	ADP	C2'-C3'	-2.05	1.48	1.53
2	D	401	ADP	C2'-C3'	-2.03	1.48	1.53
2	A	401	ADP	C2'-C3'	-2.03	1.48	1.53
2	E	401	ADP	C2'-C3'	-2.02	1.48	1.53

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	9ZK	C38-N37-C36	-9.36	109.00	123.23
3	B	403	9ZK	C38-N37-C36	-9.36	109.01	123.23
3	C	403	9ZK	C38-N37-C36	-9.36	109.01	123.23
3	A	404	9ZK	C38-N37-C36	-9.35	109.02	123.23
3	D	403	9ZK	C38-N37-C36	-9.35	109.02	123.23
3	B	403	9ZK	C22-C16-N15	5.10	120.60	108.84
3	C	403	9ZK	C22-C16-N15	5.10	120.58	108.84
3	A	402	9ZK	C22-C16-N15	5.10	120.58	108.84
3	A	404	9ZK	C22-C16-N15	5.09	120.57	108.84
3	D	403	9ZK	C22-C16-N15	5.08	120.53	108.84
3	D	403	9ZK	O03-C04-C46	4.94	120.63	111.45
3	B	403	9ZK	O03-C04-C46	4.93	120.61	111.45
3	A	402	9ZK	O03-C04-C46	4.93	120.61	111.45
3	C	403	9ZK	O03-C04-C46	4.92	120.59	111.45
3	A	404	9ZK	O03-C04-C46	4.91	120.57	111.45
2	B	401	ADP	PA-O3A-PB	-4.65	117.80	132.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	ADP	PA-O3A-PB	-4.65	117.80	132.57
2	D	401	ADP	PA-O3A-PB	-4.64	117.82	132.57
2	C	401	ADP	PA-O3A-PB	-4.64	117.83	132.57
2	A	401	ADP	PA-O3A-PB	-4.64	117.83	132.57
2	C	401	ADP	O4'-C4'-C3'	-3.49	98.25	105.14
2	D	401	ADP	O4'-C4'-C3'	-3.48	98.26	105.14
2	B	401	ADP	O4'-C4'-C3'	-3.48	98.27	105.14
2	E	401	ADP	O4'-C4'-C3'	-3.47	98.28	105.14
2	A	401	ADP	O4'-C4'-C3'	-3.46	98.30	105.14
3	B	403	9ZK	C24-N23-C25	3.17	123.41	117.75
3	A	402	9ZK	C24-N23-C25	3.16	123.40	117.75
3	A	404	9ZK	C24-N23-C25	3.15	123.38	117.75
3	C	403	9ZK	C24-N23-C25	3.14	123.37	117.75
3	D	403	9ZK	C24-N23-C25	3.14	123.37	117.75
3	A	402	9ZK	O48-C22-N23	-2.79	116.98	121.71
3	D	403	9ZK	O48-C22-N23	-2.78	117.00	121.71
3	C	403	9ZK	O48-C22-N23	-2.77	117.00	121.71
3	A	404	9ZK	O48-C22-N23	-2.77	117.01	121.71
3	B	403	9ZK	O48-C22-N23	-2.75	117.04	121.71
3	D	403	9ZK	C17-C16-C22	-2.74	102.97	109.80
3	B	403	9ZK	C17-C16-C22	-2.72	103.02	109.80
3	A	404	9ZK	C17-C16-C22	-2.71	103.03	109.80
3	C	403	9ZK	C17-C16-C22	-2.71	103.03	109.80
3	A	402	9ZK	C17-C16-C22	-2.70	103.05	109.80
3	A	402	9ZK	C26-C25-C36	-2.60	104.50	110.92
3	B	403	9ZK	C18-C17-C16	-2.60	105.83	113.95
3	A	402	9ZK	C18-C17-C16	-2.59	105.84	113.95
3	C	403	9ZK	C18-C17-C16	-2.59	105.84	113.95
3	A	404	9ZK	C26-C25-C36	-2.59	104.53	110.92
3	C	403	9ZK	C26-C25-C36	-2.59	104.54	110.92
3	D	403	9ZK	C26-C25-C36	-2.59	104.54	110.92
3	B	403	9ZK	C26-C25-C36	-2.59	104.54	110.92
3	A	404	9ZK	C18-C17-C16	-2.58	105.88	113.95
3	D	403	9ZK	C18-C17-C16	-2.58	105.88	113.95
3	C	403	9ZK	C10-C09-C08	-2.51	117.16	123.68
3	D	403	9ZK	C10-C09-C08	-2.51	117.16	123.68
3	B	403	9ZK	C10-C09-C08	-2.51	117.16	123.68
3	A	402	9ZK	C10-C09-C08	-2.50	117.18	123.68
3	A	404	9ZK	C10-C09-C08	-2.50	117.19	123.68
2	C	401	ADP	C4-C5-N7	-2.46	106.83	109.40
3	A	402	9ZK	O03-C02-C06	2.45	112.06	106.89
2	A	401	ADP	C4-C5-N7	-2.45	106.85	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	403	9ZK	O03-C02-C06	2.44	112.05	106.89
3	D	403	9ZK	O03-C02-C06	2.44	112.03	106.89
3	A	404	9ZK	O03-C02-C06	2.43	112.03	106.89
2	E	401	ADP	C4-C5-N7	-2.43	106.87	109.40
3	B	403	9ZK	O03-C02-C06	2.43	112.02	106.89
2	D	401	ADP	C4-C5-N7	-2.41	106.88	109.40
2	B	401	ADP	C4-C5-N7	-2.40	106.89	109.40
3	D	403	9ZK	O05-C04-C46	-2.38	119.39	124.71
3	A	402	9ZK	O05-C04-C46	-2.35	119.44	124.71
3	C	403	9ZK	O05-C04-C46	-2.35	119.44	124.71
3	B	403	9ZK	O05-C04-C46	-2.35	119.44	124.71
3	A	404	9ZK	O05-C04-C46	-2.34	119.46	124.71
3	D	403	9ZK	O47-C36-N37	-2.30	118.61	122.92
3	A	404	9ZK	O47-C36-N37	-2.30	118.62	122.92
2	D	401	ADP	C5-C6-N6	2.29	123.98	120.38
2	A	401	ADP	C5-C6-N6	2.29	123.98	120.38
2	B	401	ADP	C5-C6-N6	2.29	123.98	120.38
3	A	402	9ZK	O47-C36-N37	-2.29	118.64	122.92
2	E	401	ADP	C5-C6-N6	2.28	123.97	120.38
3	B	403	9ZK	O47-C36-N37	-2.28	118.65	122.92
3	C	403	9ZK	O47-C36-N37	-2.28	118.65	122.92
2	C	401	ADP	C5-C6-N6	2.28	123.96	120.38
3	B	403	9ZK	C26-C27-C31	-2.27	122.72	126.25
3	C	403	9ZK	C26-C27-C31	-2.25	122.74	126.25
3	A	404	9ZK	C26-C27-C31	-2.24	122.76	126.25
3	A	402	9ZK	C26-C27-C31	-2.23	122.78	126.25
3	C	403	9ZK	C32-C31-C30	2.20	121.08	118.17
3	D	403	9ZK	C26-C27-C31	-2.19	122.83	126.25
3	B	403	9ZK	C01-C02-C06	-2.19	107.89	113.98
3	C	403	9ZK	C01-C02-C06	-2.19	107.91	113.98
3	A	404	9ZK	C01-C02-C06	-2.19	107.91	113.98
3	A	402	9ZK	C01-C02-C06	-2.18	107.92	113.98
3	D	403	9ZK	C01-C02-C06	-2.18	107.92	113.98
3	B	403	9ZK	C32-C31-C30	2.18	121.05	118.17
3	A	404	9ZK	C07-C08-C09	-2.17	122.33	127.67
3	A	402	9ZK	C07-C08-C09	-2.17	122.34	127.67
3	C	403	9ZK	C07-C08-C09	-2.16	122.36	127.67
3	D	403	9ZK	C07-C08-C09	-2.16	122.37	127.67
3	B	403	9ZK	C07-C08-C09	-2.16	122.37	127.67
3	A	402	9ZK	C32-C31-C30	2.15	121.02	118.17
3	A	404	9ZK	C32-C31-C30	2.13	120.99	118.17
3	D	403	9ZK	C32-C31-C30	2.13	120.99	118.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	ADP	N3-C2-N1	-2.12	125.27	128.68
2	B	401	ADP	N3-C2-N1	-2.09	125.30	128.68
2	C	401	ADP	N3-C2-N1	-2.08	125.32	128.68
2	A	401	ADP	N3-C2-N1	-2.08	125.32	128.68
2	E	401	ADP	N3-C2-N1	-2.08	125.33	128.68

There are no chirality outliers.

All (190) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	404	9ZK	C39-C38-C46-C04
3	A	404	9ZK	N37-C38-C46-C04
3	A	404	9ZK	C39-C38-N37-C36
3	A	404	9ZK	C46-C38-N37-C36
3	A	404	9ZK	C36-C25-C26-C27
3	A	404	9ZK	N23-C25-C26-C27
3	A	404	9ZK	C36-C25-N23-C24
3	A	404	9ZK	C22-C16-N15-C14
3	A	404	9ZK	C13-C12-C14-N15
3	A	404	9ZK	C13-C12-C14-O49
3	A	404	9ZK	C09-C11-C12-C14
3	A	404	9ZK	C46-C04-O03-C02
3	A	404	9ZK	O05-C04-O03-C02
2	C	401	ADP	C5'-O5'-PA-O2A
2	C	401	ADP	C5'-O5'-PA-O3A
2	C	401	ADP	O4'-C4'-C5'-O5'
2	C	401	ADP	C3'-C4'-C5'-O5'
3	D	403	9ZK	C39-C38-C46-C04
3	D	403	9ZK	N37-C38-C46-C04
3	D	403	9ZK	C39-C38-N37-C36
3	D	403	9ZK	C46-C38-N37-C36
3	D	403	9ZK	C36-C25-C26-C27
3	D	403	9ZK	N23-C25-C26-C27
3	D	403	9ZK	C36-C25-N23-C24
3	D	403	9ZK	C22-C16-N15-C14
3	D	403	9ZK	C13-C12-C14-N15
3	D	403	9ZK	C13-C12-C14-O49
3	D	403	9ZK	C09-C11-C12-C14
3	D	403	9ZK	C46-C04-O03-C02
3	D	403	9ZK	O05-C04-O03-C02
2	B	401	ADP	C5'-O5'-PA-O2A
2	B	401	ADP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
2	B	401	ADP	O4'-C4'-C5'-O5'
2	B	401	ADP	C3'-C4'-C5'-O5'
3	B	403	9ZK	C39-C38-C46-C04
3	B	403	9ZK	N37-C38-C46-C04
3	B	403	9ZK	C39-C38-N37-C36
3	B	403	9ZK	C46-C38-N37-C36
3	B	403	9ZK	C36-C25-C26-C27
3	B	403	9ZK	N23-C25-C26-C27
3	B	403	9ZK	C36-C25-N23-C24
3	B	403	9ZK	C22-C16-N15-C14
3	B	403	9ZK	C13-C12-C14-N15
3	B	403	9ZK	C13-C12-C14-O49
3	B	403	9ZK	C09-C11-C12-C14
3	B	403	9ZK	C46-C04-O03-C02
3	B	403	9ZK	O05-C04-O03-C02
2	D	401	ADP	C5'-O5'-PA-O2A
2	D	401	ADP	C5'-O5'-PA-O3A
2	D	401	ADP	O4'-C4'-C5'-O5'
2	D	401	ADP	C3'-C4'-C5'-O5'
3	A	402	9ZK	C39-C38-C46-C04
3	A	402	9ZK	N37-C38-C46-C04
3	A	402	9ZK	C39-C38-N37-C36
3	A	402	9ZK	C46-C38-N37-C36
3	A	402	9ZK	C36-C25-C26-C27
3	A	402	9ZK	N23-C25-C26-C27
3	A	402	9ZK	C36-C25-N23-C24
3	A	402	9ZK	C22-C16-N15-C14
3	A	402	9ZK	C13-C12-C14-N15
3	A	402	9ZK	C13-C12-C14-O49
3	A	402	9ZK	C09-C11-C12-C14
3	A	402	9ZK	C46-C04-O03-C02
3	A	402	9ZK	O05-C04-O03-C02
2	A	401	ADP	C5'-O5'-PA-O2A
2	A	401	ADP	C5'-O5'-PA-O3A
2	A	401	ADP	O4'-C4'-C5'-O5'
2	A	401	ADP	C3'-C4'-C5'-O5'
2	E	401	ADP	C5'-O5'-PA-O2A
2	E	401	ADP	C5'-O5'-PA-O3A
2	E	401	ADP	O4'-C4'-C5'-O5'
2	E	401	ADP	C3'-C4'-C5'-O5'
3	C	403	9ZK	C39-C38-C46-C04
3	C	403	9ZK	N37-C38-C46-C04

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Mol	Chain	Res	Type	Atoms
3	C	403	9ZK	C39-C38-N37-C36
3	C	403	9ZK	C46-C38-N37-C36
3	C	403	9ZK	C36-C25-C26-C27
3	C	403	9ZK	N23-C25-C26-C27
3	C	403	9ZK	C36-C25-N23-C24
3	C	403	9ZK	C22-C16-N15-C14
3	C	403	9ZK	C13-C12-C14-N15
3	C	403	9ZK	C13-C12-C14-O49
3	C	403	9ZK	C09-C11-C12-C14
3	C	403	9ZK	C46-C04-O03-C02
3	C	403	9ZK	O05-C04-O03-C02
3	A	404	9ZK	C26-C25-N23-C24
3	D	403	9ZK	C26-C25-N23-C24
3	B	403	9ZK	C26-C25-N23-C24
3	A	402	9ZK	C26-C25-N23-C24
3	C	403	9ZK	C26-C25-N23-C24
3	A	404	9ZK	C26-C25-N23-C22
3	D	403	9ZK	C26-C25-N23-C22
3	B	403	9ZK	C26-C25-N23-C22
3	A	402	9ZK	C26-C25-N23-C22
3	C	403	9ZK	C26-C25-N23-C22
3	A	404	9ZK	C46-C38-C39-C40
3	D	403	9ZK	C46-C38-C39-C40
3	B	403	9ZK	C46-C38-C39-C40
3	A	402	9ZK	C46-C38-C39-C40
3	C	403	9ZK	C46-C38-C39-C40
3	A	404	9ZK	C46-C38-C39-C45
3	D	403	9ZK	C46-C38-C39-C45
3	B	403	9ZK	C46-C38-C39-C45
3	A	402	9ZK	C46-C38-C39-C45
3	C	403	9ZK	C46-C38-C39-C45
3	A	404	9ZK	C22-C16-C17-C18
3	D	403	9ZK	C22-C16-C17-C18
3	B	403	9ZK	C22-C16-C17-C18
3	A	402	9ZK	C22-C16-C17-C18
3	C	403	9ZK	C22-C16-C17-C18
3	A	404	9ZK	C36-C25-N23-C22
3	D	403	9ZK	C36-C25-N23-C22
3	B	403	9ZK	C36-C25-N23-C22
3	A	402	9ZK	C36-C25-N23-C22
3	C	403	9ZK	C36-C25-N23-C22
3	A	404	9ZK	N37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
3	A	404	9ZK	N37-C38-C39-C45
3	D	403	9ZK	N37-C38-C39-C40
3	D	403	9ZK	N37-C38-C39-C45
3	B	403	9ZK	N37-C38-C39-C40
3	B	403	9ZK	N37-C38-C39-C45
3	A	402	9ZK	N37-C38-C39-C40
3	A	402	9ZK	N37-C38-C39-C45
3	C	403	9ZK	N37-C38-C39-C40
3	C	403	9ZK	N37-C38-C39-C45
3	A	404	9ZK	C18-C19-C20-N21
3	D	403	9ZK	C18-C19-C20-N21
3	B	403	9ZK	C18-C19-C20-N21
3	A	402	9ZK	C18-C19-C20-N21
3	C	403	9ZK	C18-C19-C20-N21
3	D	403	9ZK	C17-C18-C19-C20
3	B	403	9ZK	C17-C18-C19-C20
3	A	402	9ZK	C17-C18-C19-C20
3	C	403	9ZK	C17-C18-C19-C20
3	A	404	9ZK	C17-C18-C19-C20
3	A	404	9ZK	N15-C16-C17-C18
3	D	403	9ZK	N15-C16-C17-C18
3	B	403	9ZK	N15-C16-C17-C18
3	A	402	9ZK	N15-C16-C17-C18
3	C	403	9ZK	N15-C16-C17-C18
2	C	401	ADP	C5'-O5'-PA-O1A
2	B	401	ADP	C5'-O5'-PA-O1A
2	D	401	ADP	C5'-O5'-PA-O1A
2	A	401	ADP	C5'-O5'-PA-O1A
2	E	401	ADP	C5'-O5'-PA-O1A
3	A	404	9ZK	C02-C06-C07-C08
3	D	403	9ZK	C02-C06-C07-C08
3	B	403	9ZK	C02-C06-C07-C08
3	A	402	9ZK	C02-C06-C07-C08
3	C	403	9ZK	C02-C06-C07-C08
3	D	403	9ZK	C17-C16-C22-O48
3	A	404	9ZK	C17-C16-C22-O48
3	B	403	9ZK	C17-C16-C22-O48
3	A	402	9ZK	C17-C16-C22-O48
3	C	403	9ZK	C17-C16-C22-O48
3	A	404	9ZK	C25-C26-C27-C28
3	A	404	9ZK	C09-C11-C12-C13
3	D	403	9ZK	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
3	D	403	9ZK	C09-C11-C12-C13
3	B	403	9ZK	C25-C26-C27-C28
3	B	403	9ZK	C09-C11-C12-C13
3	A	402	9ZK	C25-C26-C27-C28
3	A	402	9ZK	C09-C11-C12-C13
3	C	403	9ZK	C25-C26-C27-C28
3	C	403	9ZK	C09-C11-C12-C13
3	A	404	9ZK	O03-C02-C06-C07
3	D	403	9ZK	O03-C02-C06-C07
3	B	403	9ZK	O03-C02-C06-C07
3	A	402	9ZK	O03-C02-C06-C07
3	C	403	9ZK	O03-C02-C06-C07
3	A	404	9ZK	C17-C16-C22-N23
3	D	403	9ZK	C17-C16-C22-N23
3	B	403	9ZK	C17-C16-C22-N23
3	A	402	9ZK	C17-C16-C22-N23
3	C	403	9ZK	C17-C16-C22-N23
3	B	403	9ZK	N15-C16-C22-O48
3	A	404	9ZK	N15-C16-C22-O48
3	D	403	9ZK	N15-C16-C22-O48
3	A	402	9ZK	N15-C16-C22-O48
3	C	403	9ZK	N15-C16-C22-O48
3	A	404	9ZK	N23-C25-C36-O47
3	D	403	9ZK	N23-C25-C36-O47
3	B	403	9ZK	N23-C25-C36-O47
3	A	402	9ZK	N23-C25-C36-O47
3	C	403	9ZK	N23-C25-C36-O47
3	A	404	9ZK	N15-C16-C22-N23
3	D	403	9ZK	N15-C16-C22-N23
3	B	403	9ZK	N15-C16-C22-N23
3	A	402	9ZK	N15-C16-C22-N23
3	C	403	9ZK	N15-C16-C22-N23

There are no ring outliers.

10 monomers are involved in 70 short contacts:

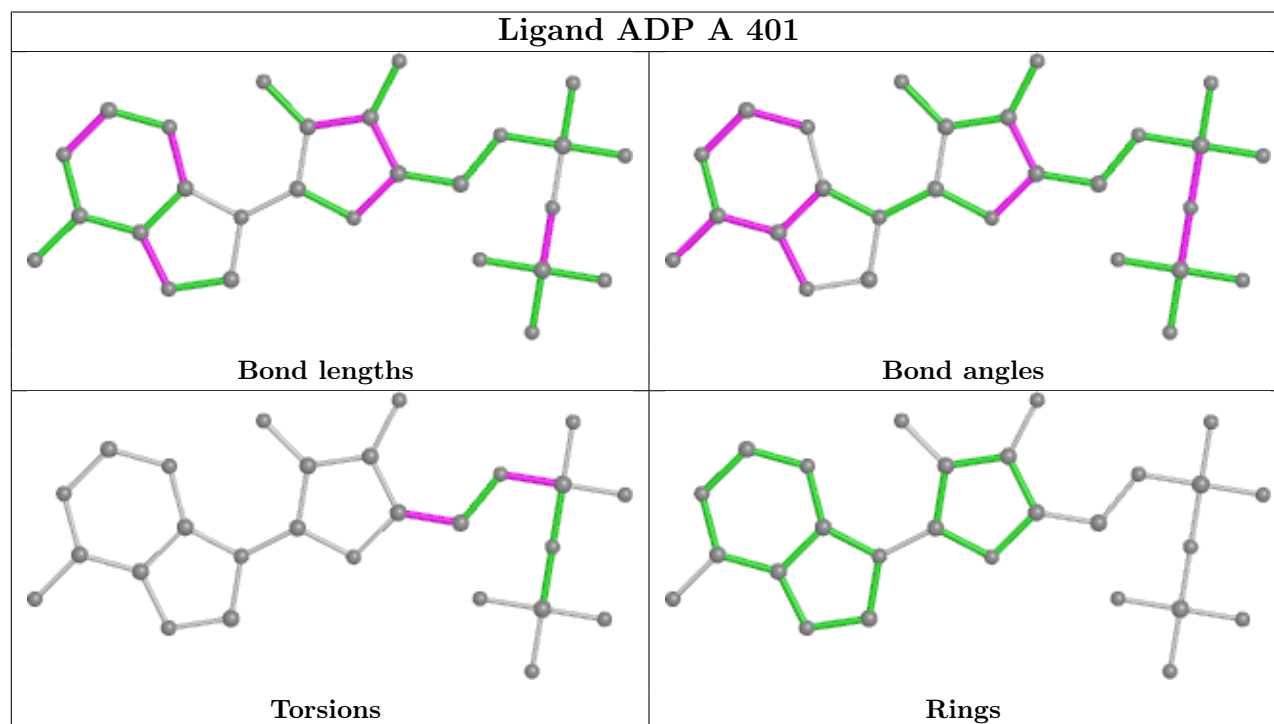
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	ADP	3	0
3	A	402	9ZK	11	0
3	A	404	9ZK	11	0
2	B	401	ADP	3	0
3	B	403	9ZK	11	0

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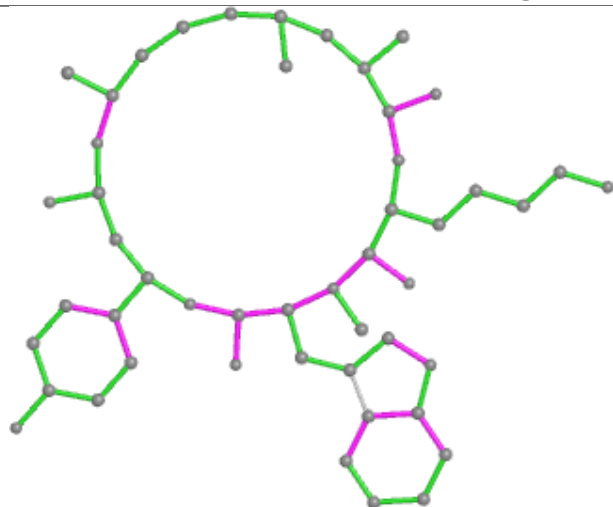
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	ADP	3	0
3	C	403	9ZK	11	0
2	D	401	ADP	3	0
3	D	403	9ZK	11	0
2	E	401	ADP	3	0

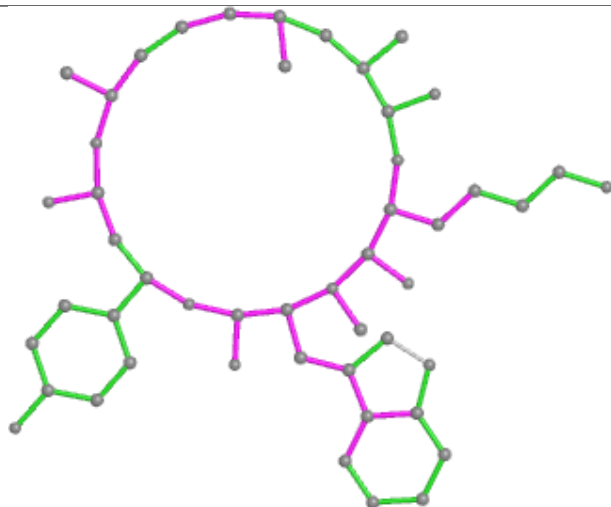
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



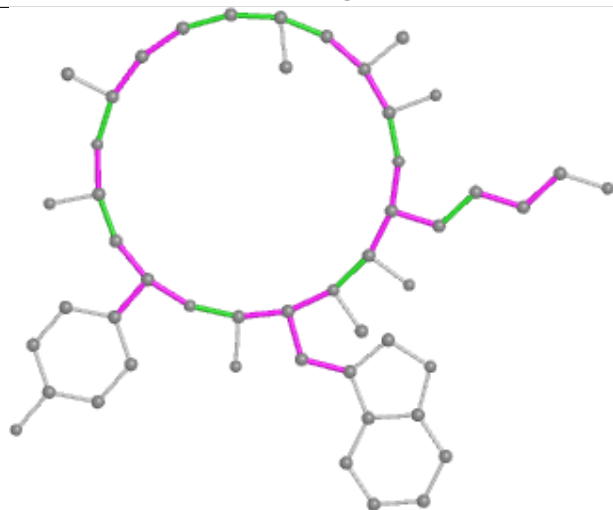
Ligand 9ZK A 402



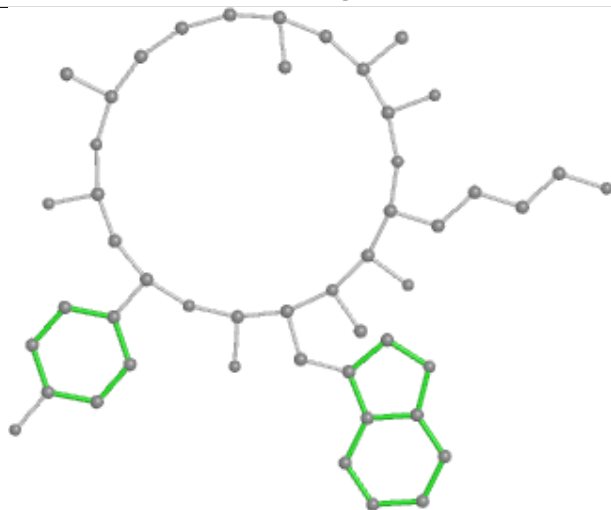
Bond lengths



Bond angles

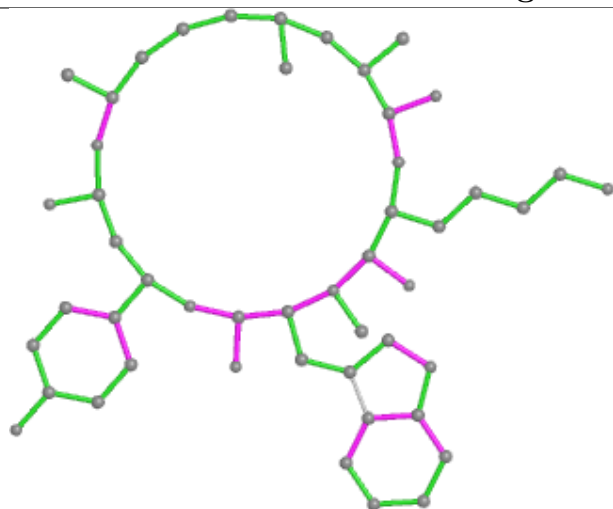


Torsions

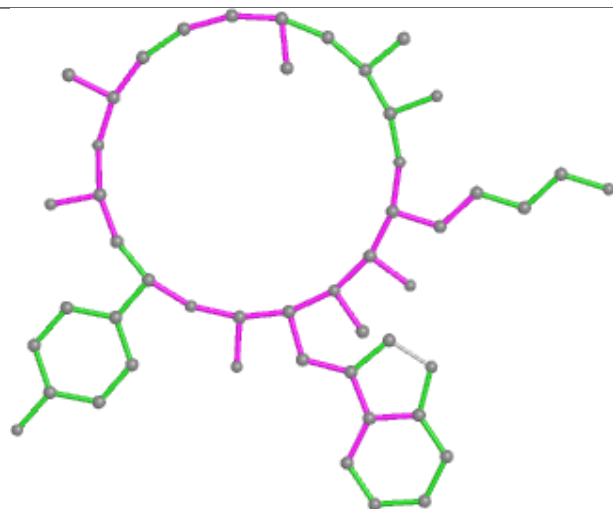


Rings

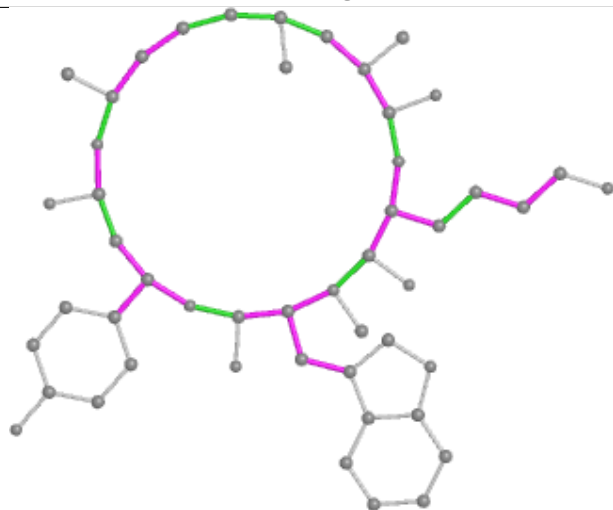
Ligand 9ZK A 404



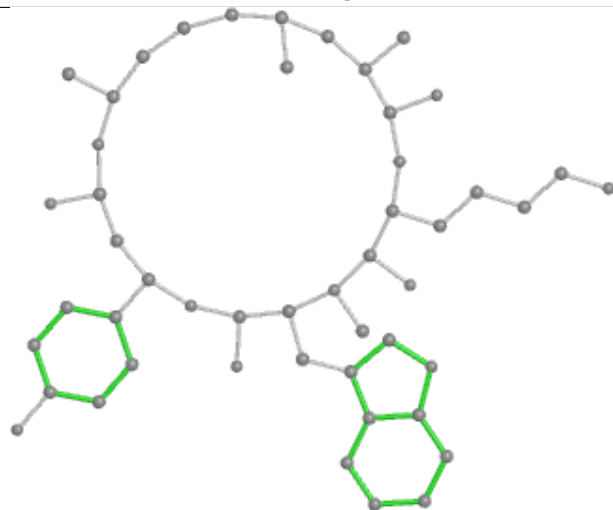
Bond lengths



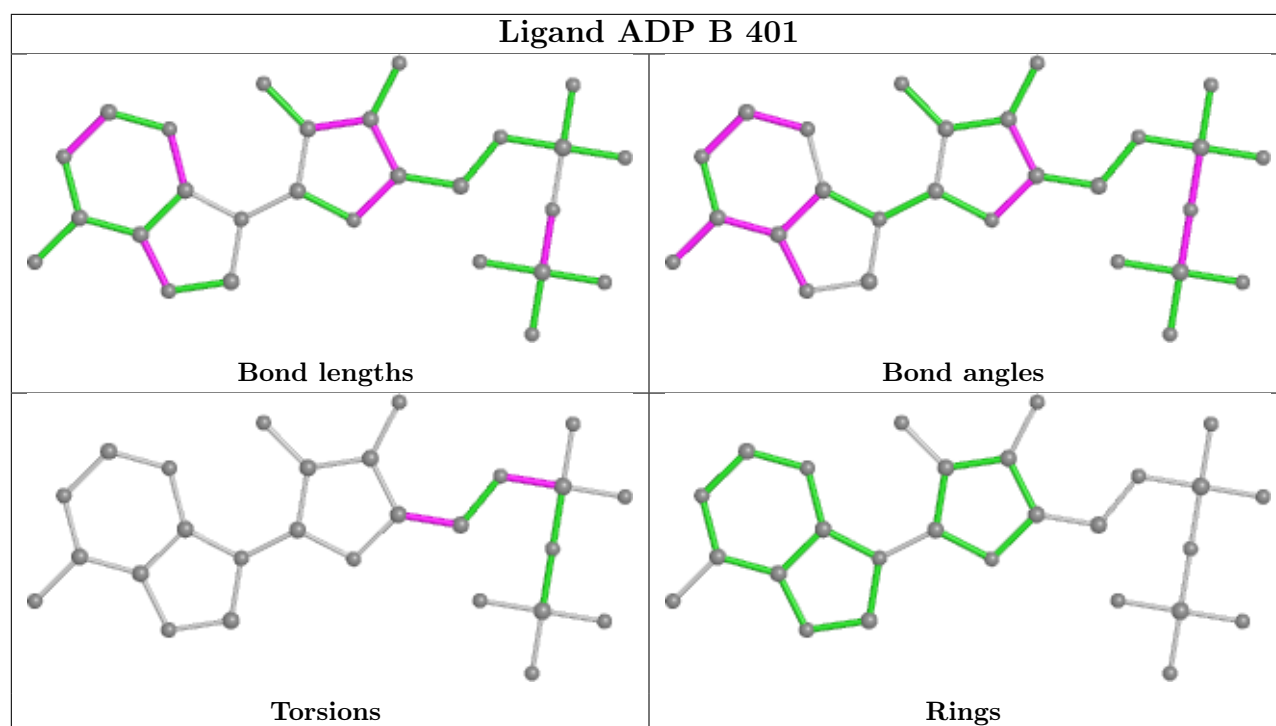
Bond angles



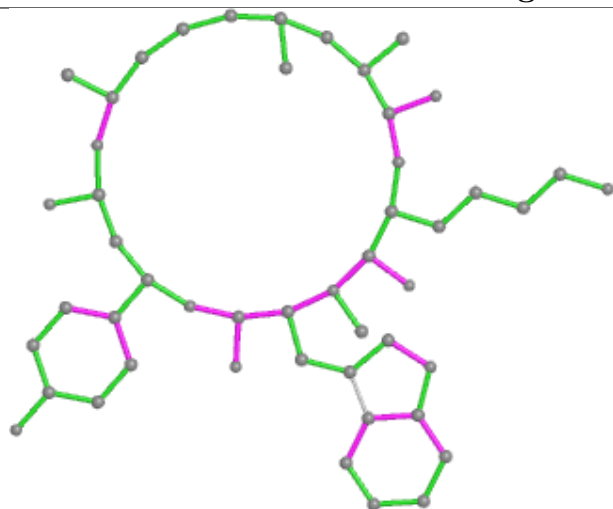
Torsions



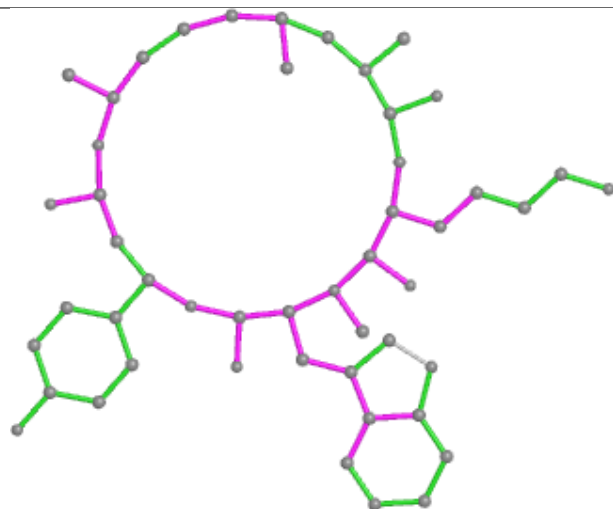
Rings



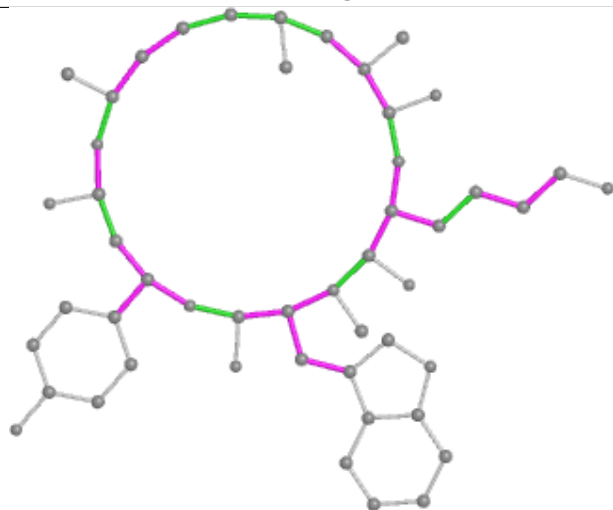
Ligand 9ZK B 403



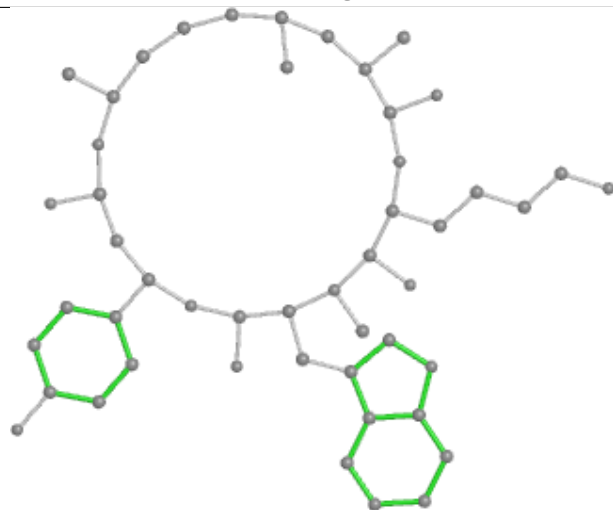
Bond lengths



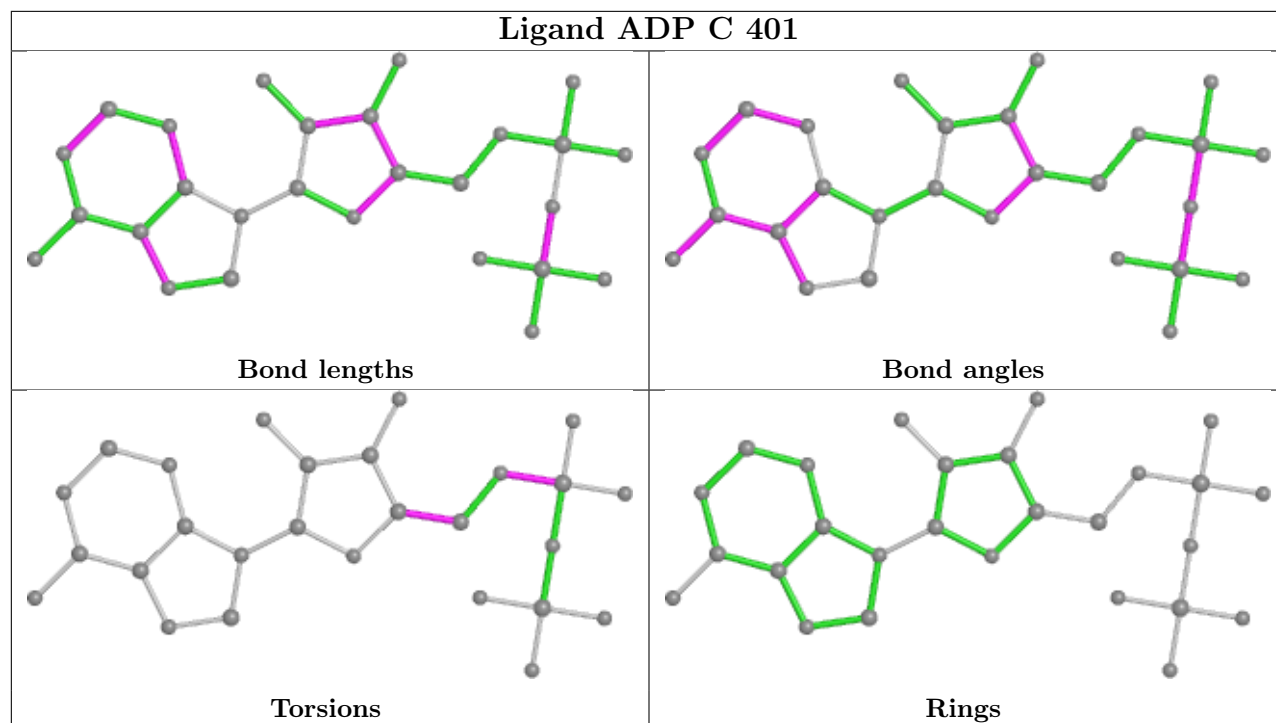
Bond angles



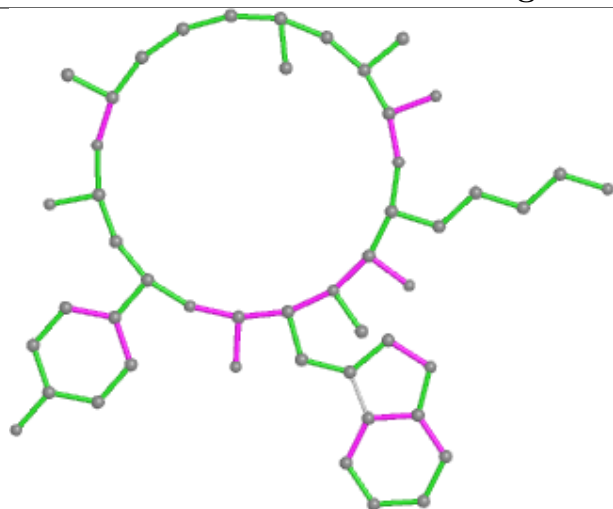
Torsions



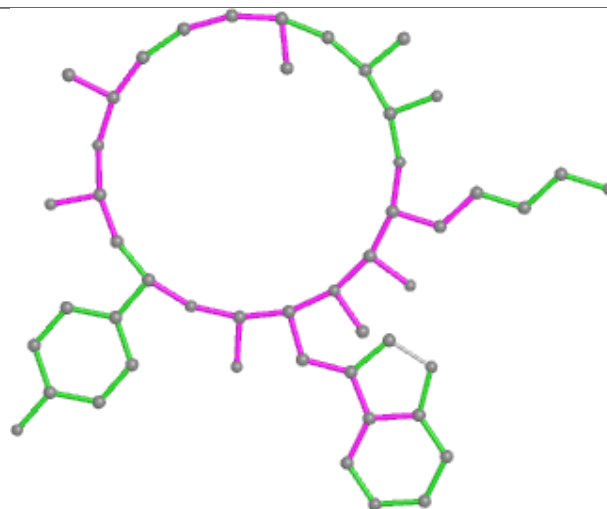
Rings



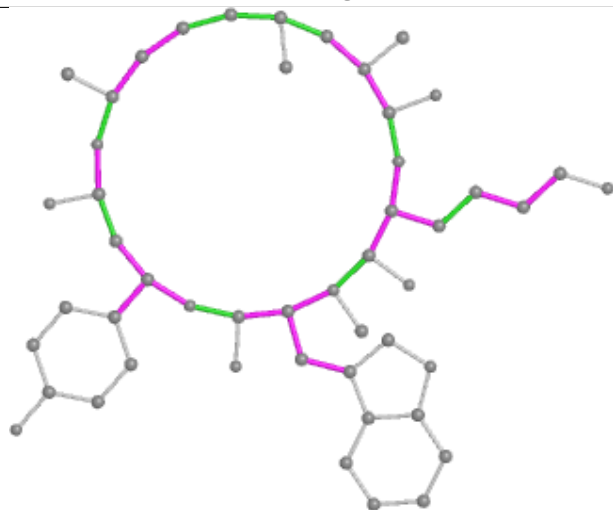
Ligand 9ZK C 403



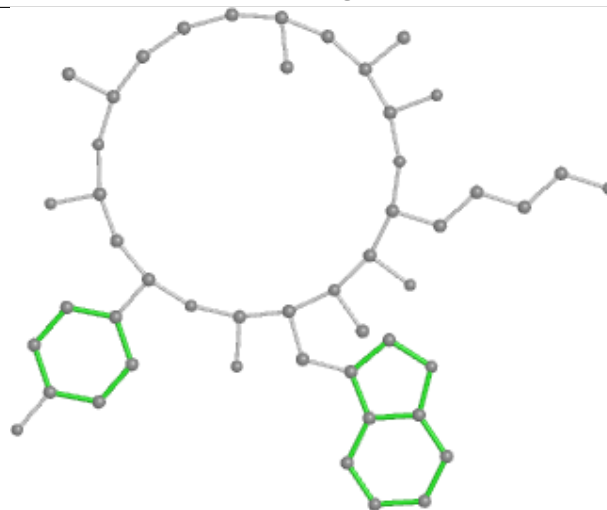
Bond lengths



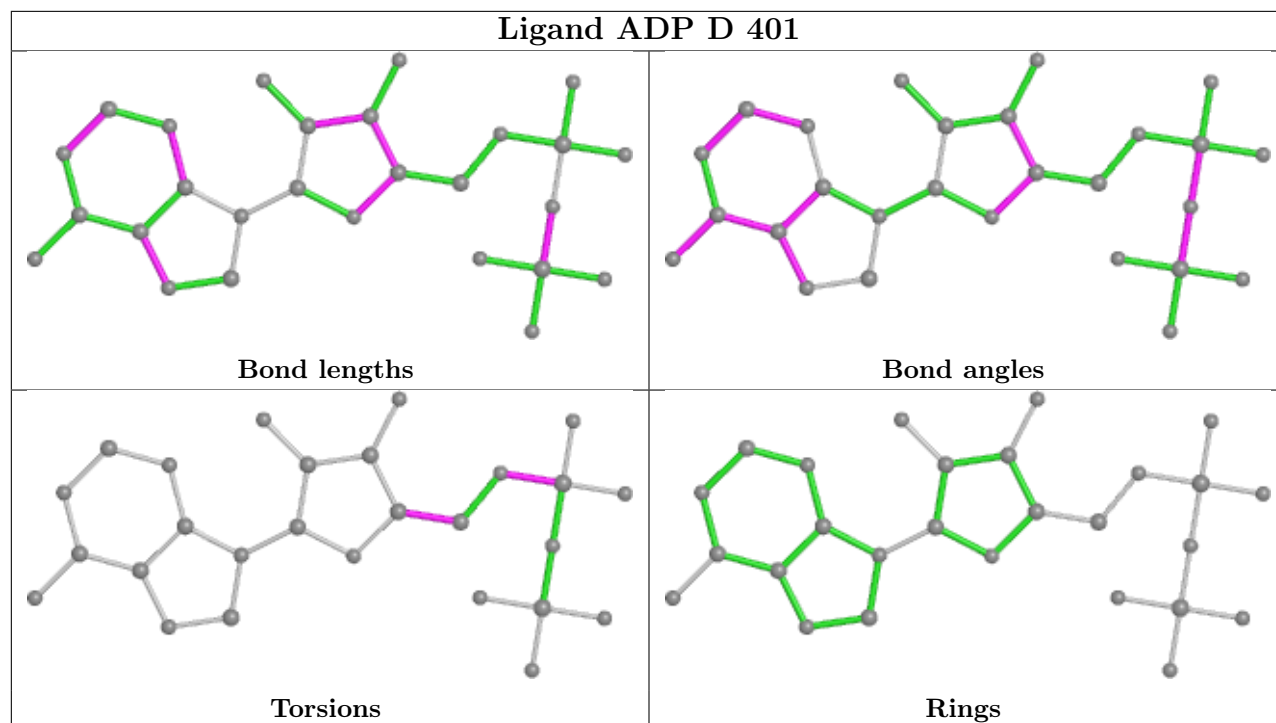
Bond angles



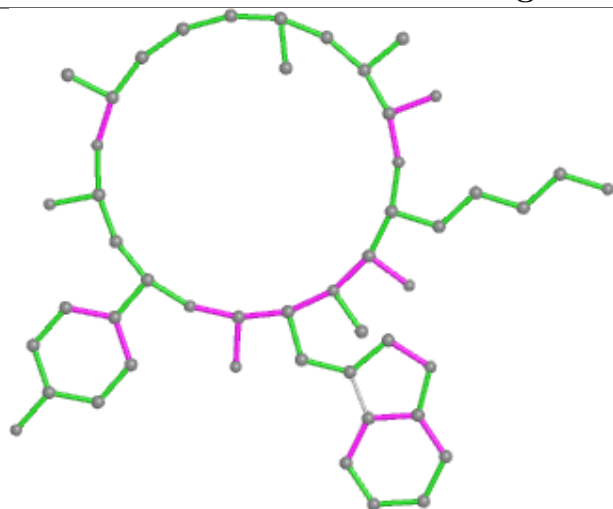
Torsions



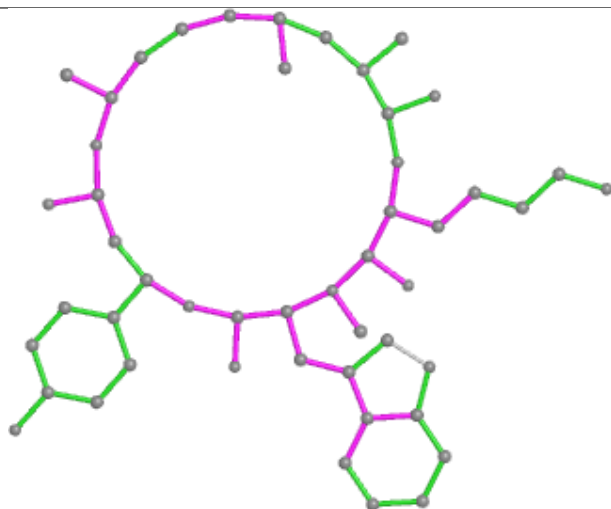
Rings



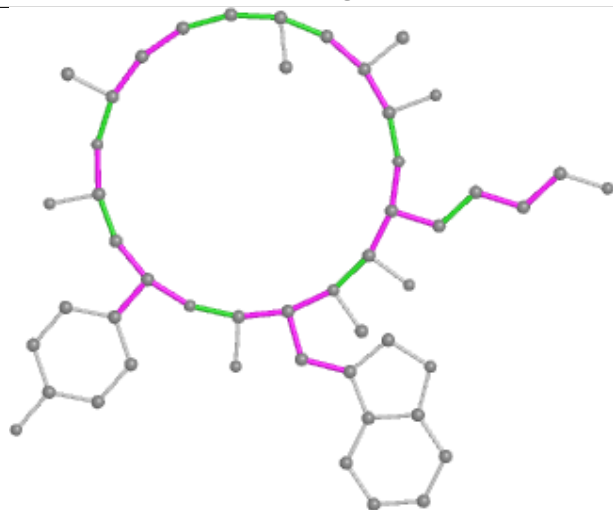
Ligand 9ZK D 403



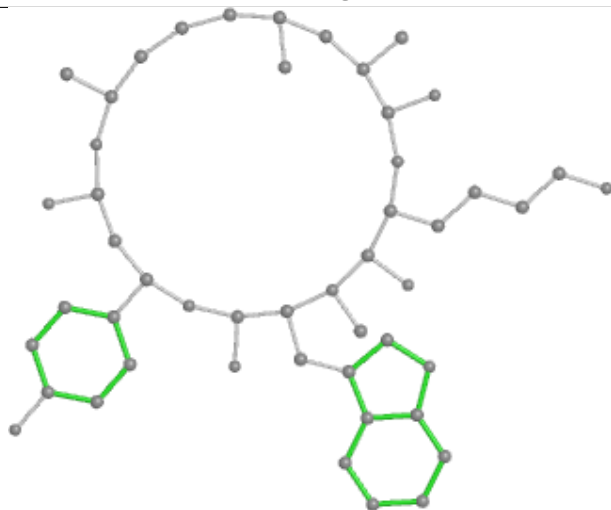
Bond lengths



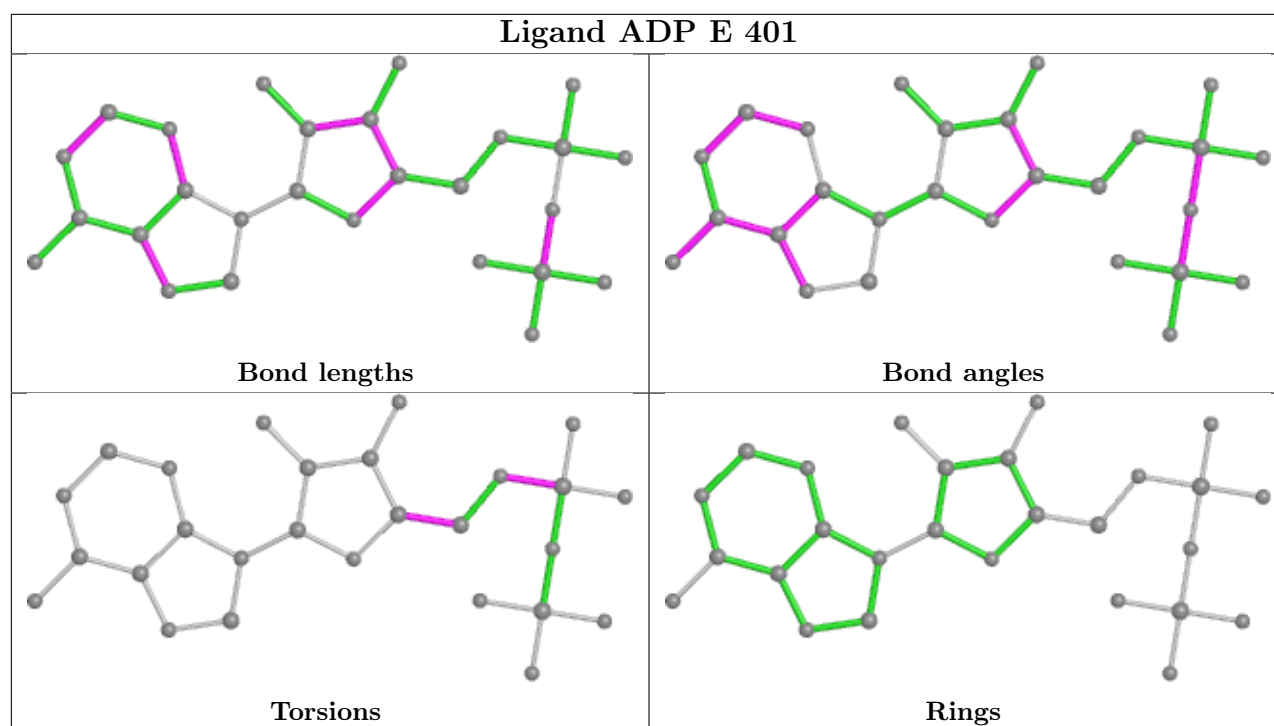
Bond angles



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.