



Full wwPDB EM Model Validation Report ⓘ

Feb 27, 2020 – 03:48 PM EST

PDB ID : 6T25
EMDB ID : EMD-10367
Title : Cryo-EM structure of phalloidin-Alexa Flour-546-stabilized F-actin (copolymerized)
Authors : Pospich, S.; Merino, F.; Raunser, S.
Deposited on : 2019-10-07
Resolution : 3.60 Å(reported)
Based on initial model : 5OOD

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:

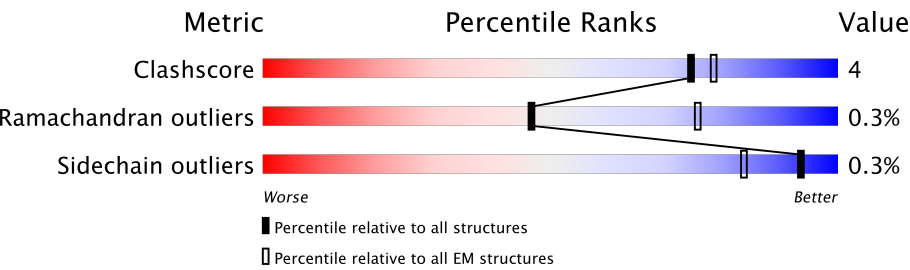
MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
buster-report : 1.1.7 (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.8

1 Overall quality at a glance i

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.



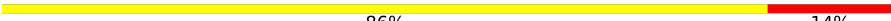
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains 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% . .
1	B	375	93% . .
1	C	375	93% . .
1	D	375	93% . .
1	E	375	92% 5% .
2	F	7	86% 14%
2	G	7	86% 14%
2	H	7	86% 14%
2	I	7	86% 14%

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Mol	Chain	Length	Quality of chain
2	J	7	 86% 14%

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
2	DTH	F	4	-	-	X	-
2	HYP	F	6	-	-	X	-
2	DTH	G	4	-	-	X	-
2	HYP	G	6	-	-	X	-
2	DTH	H	4	-	-	X	-
2	HYP	H	6	-	-	X	-
2	DTH	I	4	-	-	X	-
2	HYP	I	6	-	-	X	-
2	DTH	J	4	-	-	X	-
2	HYP	J	6	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14590 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	362	Total	C	N	O	S	0	0
			2835	1795	479	543	18		
1	B	362	Total	C	N	O	S	0	0
			2835	1795	479	543	18		
1	C	362	Total	C	N	O	S	0	0
			2835	1795	479	543	18		
1	D	362	Total	C	N	O	S	0	0
			2835	1795	479	543	18		
1	E	362	Total	C	N	O	S	0	0
			2835	1795	479	543	18		

- Molecule 2 is a protein called phalloidin.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	7	Total	C	N	O	S	0	0
			55	35	8	11	1		
2	G	7	Total	C	N	O	S	0	0
			55	35	8	11	1		
2	H	7	Total	C	N	O	S	0	0
			55	35	8	11	1		
2	I	7	Total	C	N	O	S	0	0
			55	35	8	11	1		
2	J	7	Total	C	N	O	S	0	0
			55	35	8	11	1		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by author).



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

- 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	

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:  92%



- Molecule 1: Actin, alpha skeletal muscle

Chain B:  93%



- Molecule 1: Actin, alpha skeletal muscle

Chain C:  93%



- Molecule 1: Actin, alpha skeletal muscle

Chain D:  93%




- Molecule 1: Actin, alpha skeletal muscle

Chain E:  92% 5%




- Molecule 2: phalloidin

Chain F:  86% 14%


W1	T2	A3	T4	C5	P6	A7
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- Molecule 2: phalloidin

Chain G:  86% 14%


W1	T2	A3	T4	C5	P6	A7
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- Molecule 2: phalloidin

Chain H:  86% 14%

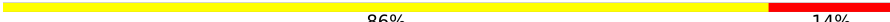
W1	T2	A3	T4	C5	P6	A7
----	----	----	----	----	----	----

- Molecule 2: phalloidin

Chain I:  86% 14%

W1	T2	A3	T4	C5	P6	A7
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- Molecule 2: phalloidin

Chain J:  86% 14%

W1	T2	A3	T4	C5	P6	A7
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	719053	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 ($e^-/\text{\AA}^2$)	92	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: MG, DTH, ADP, EEP, HYP, HIC

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	0.99	0/2883	0.76	5/3906 (0.1%)
1	B	0.99	0/2883	0.76	5/3906 (0.1%)
1	C	0.99	0/2883	0.76	5/3906 (0.1%)
1	D	0.99	0/2883	0.76	5/3906 (0.1%)
1	E	0.99	0/2883	0.76	5/3906 (0.1%)
2	F	1.00	0/28	1.55	0/33
2	G	0.99	0/28	1.55	0/33
2	H	0.99	0/28	1.54	0/33
2	I	0.99	0/28	1.54	0/33
2	J	0.99	0/28	1.55	0/33
All	All	0.99	0/14555	0.77	25/19695 (0.1%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	62	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	A	62	ARG	NE-CZ-NH2	-8.19	116.20	120.30
1	B	62	ARG	NE-CZ-NH2	-8.18	116.21	120.30
1	C	62	ARG	NE-CZ-NH2	-8.18	116.21	120.30
1	D	62	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	C	166	TYR	CB-CG-CD1	-6.37	117.18	121.00
1	A	166	TYR	CB-CG-CD1	-6.36	117.19	121.00
1	B	166	TYR	CB-CG-CD1	-6.33	117.20	121.00
1	E	166	TYR	CB-CG-CD1	-6.31	117.21	121.00
1	D	166	TYR	CB-CG-CD1	-6.31	117.21	121.00
1	D	39	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	C	39	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	E	39	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	39	ARG	NE-CZ-NH1	5.64	123.12	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	39	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	D	39	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	C	39	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	B	312	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	C	312	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	E	312	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	D	312	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	A	312	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	E	39	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	39	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	B	39	ARG	NE-CZ-NH2	-5.10	117.75	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	2835	0	2802	10	0
1	B	2835	0	2802	10	0
1	C	2835	0	2802	10	0
1	D	2835	0	2802	9	0
1	E	2835	0	2802	11	0
2	F	55	0	37	10	0
2	G	55	0	37	10	0
2	H	55	0	37	10	0
2	I	55	0	37	11	0
2	J	55	0	37	11	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
3	C	27	0	12	0	0
3	D	27	0	12	0	0
3	E	27	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1	0	0	0	0
4	E	1	0	0	0	0
All	All	14590	0	14255	102	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 4.

All (102) 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)
2:I:2:EPP:N	2:I:2:EPP:O1	2.13	0.82
2:J:2:EPP:O1	2:J:2:EPP:N	2.13	0.80
2:G:2:EPP:O1	2:G:2:EPP:N	2.13	0.80
2:H:2:EPP:N	2:H:2:EPP:O1	2.13	0.79
2:F:2:EPP:N	2:F:2:EPP:O1	2.13	0.78
2:I:6:HYP:O	2:I:7:ALA:C	2.30	0.70
2:G:6:HYP:O	2:G:7:ALA:C	2.30	0.69
2:J:6:HYP:O	2:J:7:ALA:C	2.31	0.69
2:H:6:HYP:O	2:H:7:ALA:C	2.30	0.68
2:F:6:HYP:O	2:F:7:ALA:C	2.31	0.67
2:F:3:ALA:O	2:F:4:DTH:O	2.13	0.66
2:H:3:ALA:O	2:H:4:DTH:O	2.13	0.66
2:J:3:ALA:O	2:J:4:DTH:O	2.13	0.66
2:I:3:ALA:O	2:I:4:DTH:O	2.13	0.66
2:G:3:ALA:O	2:G:4:DTH:O	2.13	0.66
2:F:5:CYS:SG	2:F:6:HYP:N	2.72	0.62
2:G:5:CYS:SG	2:G:6:HYP:N	2.72	0.62
2:H:5:CYS:SG	2:H:6:HYP:N	2.72	0.62
2:I:5:CYS:SG	2:I:6:HYP:N	2.72	0.61
2:J:5:CYS:SG	2:J:6:HYP:N	2.72	0.57
1:E:352:PHE:CG	1:E:352:PHE:O	2.60	0.55
1:B:352:PHE:O	1:B:352:PHE:CG	2.60	0.54
1:C:352:PHE:O	1:C:352:PHE:CG	2.60	0.54
2:F:4:DTH:OG1	2:F:5:CYS:N	2.40	0.54
1:D:352:PHE:CG	1:D:352:PHE:O	2.60	0.54
1:A:352:PHE:CG	1:A:352:PHE:O	2.60	0.53
2:I:4:DTH:OG1	2:I:5:CYS:N	2.40	0.53
2:H:4:DTH:OG1	2:H:5:CYS:N	2.40	0.53
2:G:4:DTH:OG1	2:G:5:CYS:N	2.40	0.52
2:J:4:DTH:OG1	2:J:5:CYS:N	2.40	0.52
2:I:1:TRP:N	2:I:6:HYP:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1:TRP:N	2:F:6:HYP:O	2.45	0.50
2:G:1:TRP:N	2:G:6:HYP:O	2.45	0.50
2:J:1:TRP:N	2:J:6:HYP:O	2.45	0.49
2:H:1:TRP:N	2:H:6:HYP:O	2.45	0.49
2:H:4:DTH:O	2:H:5:CYS:SG	2.71	0.49
2:G:4:DTH:O	2:G:5:CYS:SG	2.71	0.49
2:I:4:DTH:O	2:I:5:CYS:SG	2.71	0.49
1:A:352:PHE:CD2	1:A:352:PHE:O	2.66	0.48
1:B:352:PHE:O	1:B:352:PHE:CD2	2.66	0.48
1:E:352:PHE:CD2	1:E:352:PHE:O	2.66	0.48
2:F:4:DTH:O	2:F:5:CYS:SG	2.71	0.48
2:J:4:DTH:O	2:J:5:CYS:SG	2.71	0.48
2:I:4:DTH:C	2:I:5:CYS:O	2.62	0.48
1:D:352:PHE:CD2	1:D:352:PHE:O	2.66	0.48
2:G:4:DTH:C	2:G:5:CYS:O	2.62	0.48
1:C:352:PHE:O	1:C:352:PHE:CD2	2.66	0.48
2:J:4:DTH:C	2:J:5:CYS:O	2.62	0.47
2:H:4:DTH:C	2:H:5:CYS:O	2.62	0.47
2:G:4:DTH:O	2:G:5:CYS:O	2.33	0.47
2:J:4:DTH:O	2:J:5:CYS:O	2.33	0.47
2:I:4:DTH:O	2:I:5:CYS:O	2.33	0.46
2:F:4:DTH:C	2:F:5:CYS:O	2.62	0.46
1:C:99:GLU:N	1:C:99:GLU:OE1	2.38	0.46
1:E:99:GLU:N	1:E:99:GLU:OE1	2.38	0.46
2:F:4:DTH:O	2:F:5:CYS:O	2.33	0.46
1:A:99:GLU:OE1	1:A:99:GLU:N	2.38	0.46
1:C:78:ASN:OD1	1:C:78:ASN:C	2.54	0.46
1:D:78:ASN:OD1	1:D:78:ASN:C	2.54	0.46
2:H:4:DTH:O	2:H:5:CYS:O	2.33	0.45
1:E:78:ASN:C	1:E:78:ASN:OD1	2.54	0.45
1:E:192:ILE:O	1:E:195:GLU:HG2	2.17	0.45
1:A:78:ASN:C	1:A:78:ASN:OD1	2.54	0.44
1:B:78:ASN:OD1	1:B:78:ASN:C	2.54	0.44
1:A:192:ILE:O	1:A:195:GLU:HG2	2.17	0.44
1:C:192:ILE:O	1:C:195:GLU:HG2	2.17	0.44
1:B:192:ILE:O	1:B:195:GLU:HG2	2.17	0.44
1:A:252:ASN:C	1:A:252:ASN:OD1	2.57	0.44
1:D:252:ASN:OD1	1:D:252:ASN:C	2.57	0.44
1:D:192:ILE:O	1:D:195:GLU:HG2	2.17	0.43
1:E:252:ASN:OD1	1:E:252:ASN:C	2.57	0.43
1:A:257:CYS:HB3	1:A:258:PRO:CD	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:ASN:OD1	1:C:252:ASN:C	2.57	0.43
1:E:37:ARG:HA	1:E:38:PRO:HD3	1.92	0.43
1:C:257:CYS:HB3	1:C:258:PRO:CD	2.49	0.42
1:B:252:ASN:OD1	1:B:252:ASN:C	2.57	0.42
1:E:257:CYS:HB3	1:E:258:PRO:CD	2.49	0.42
1:C:222:ASP:C	1:C:222:ASP:OD1	2.58	0.42
1:E:222:ASP:OD1	1:E:222:ASP:C	2.58	0.42
1:A:222:ASP:C	1:A:222:ASP:OD1	2.58	0.42
2:F:1:TRP:O	2:F:6:HYP:O	2.38	0.42
1:D:257:CYS:HB3	1:D:258:PRO:CD	2.49	0.42
2:H:1:TRP:O	2:H:6:HYP:O	2.38	0.42
1:D:253:GLU:H	1:D:253:GLU:CD	2.23	0.42
1:E:253:GLU:CD	1:E:253:GLU:H	2.23	0.41
2:J:1:TRP:O	2:J:6:HYP:O	2.38	0.41
1:B:253:GLU:CD	1:B:253:GLU:H	2.23	0.41
1:B:222:ASP:C	1:B:222:ASP:OD1	2.58	0.41
1:C:253:GLU:H	1:C:253:GLU:CD	2.23	0.41
1:A:253:GLU:CD	1:A:253:GLU:H	2.23	0.41
1:B:257:CYS:HB3	1:B:258:PRO:CD	2.49	0.41
1:C:330:ILE:HD12	1:C:330:ILE:N	2.36	0.41
1:D:222:ASP:OD1	1:D:222:ASP:C	2.58	0.41
2:G:1:TRP:O	2:G:6:HYP:O	2.38	0.41
1:B:330:ILE:HD12	1:B:330:ILE:N	2.36	0.41
2:J:2:EEP:O	2:J:3:ALA:HB2	2.21	0.41
1:D:330:ILE:N	1:D:330:ILE:HD12	2.36	0.41
2:I:1:TRP:O	2:I:6:HYP:O	2.38	0.41
1:B:99:GLU:OE1	1:B:99:GLU:N	2.38	0.40
1:E:330:ILE:N	1:E:330:ILE:HD12	2.36	0.40
1:A:332:PRO:HA	1:A:333:PRO:HD3	1.91	0.40
2:I:2:EEP:O	2:I:3:ALA:HB2	2.21	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	357/375 (95%)	348 (98%)	9 (2%)	0	100	100
1	B	357/375 (95%)	348 (98%)	9 (2%)	0	100	100
1	C	357/375 (95%)	348 (98%)	9 (2%)	0	100	100
1	D	357/375 (95%)	348 (98%)	9 (2%)	0	100	100
1	E	357/375 (95%)	348 (98%)	9 (2%)	0	100	100
2	F	2/7 (29%)	0	1 (50%)	1 (50%)	0	0
2	G	2/7 (29%)	0	1 (50%)	1 (50%)	0	0
2	H	2/7 (29%)	0	1 (50%)	1 (50%)	0	0
2	I	2/7 (29%)	0	1 (50%)	1 (50%)	0	0
2	J	2/7 (29%)	0	1 (50%)	1 (50%)	0	0
All	All	1795/1910 (94%)	1740 (97%)	50 (3%)	5 (0%)	47	78

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	5	CYS
2	G	5	CYS
2	H	5	CYS
2	I	5	CYS
2	J	5	CYS

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	306/317 (96%)	306 (100%)	0	100	100
1	B	306/317 (96%)	306 (100%)	0	100	100
1	C	306/317 (96%)	306 (100%)	0	100	100
1	D	306/317 (96%)	306 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	306/317 (96%)	306 (100%)	0	100	100
2	F	2/2 (100%)	1 (50%)	1 (50%)	0	0
2	G	2/2 (100%)	1 (50%)	1 (50%)	0	0
2	H	2/2 (100%)	1 (50%)	1 (50%)	0	0
2	I	2/2 (100%)	1 (50%)	1 (50%)	0	0
2	J	2/2 (100%)	1 (50%)	1 (50%)	0	0
All	All	1540/1595 (97%)	1535 (100%)	5 (0%)	93	98

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	5	CYS
2	G	5	CYS
2	H	5	CYS
2	I	5	CYS
2	J	5	CYS

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	246	GLN
1	B	246	GLN
1	C	246	GLN
1	D	246	GLN
1	E	246	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

20 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	1.24	1 (11%)	6,14,16	1.03	1 (16%)
1	HIC	B	73	1	9,11,12	1.23	1 (11%)	6,14,16	1.03	1 (16%)
1	HIC	C	73	1	9,11,12	1.22	1 (11%)	6,14,16	1.03	1 (16%)
1	HIC	D	73	1	9,11,12	1.22	1 (11%)	6,14,16	1.03	1 (16%)
1	HIC	E	73	1	9,11,12	1.23	1 (11%)	6,14,16	1.03	1 (16%)
2	EEP	F	2	2	9,9,10	1.27	1 (11%)	7,12,14	1.21	0
2	DTH	F	4	2	6,6,7	0.48	0	6,7,9	1.62	1 (16%)
2	HYP	F	6	2	7,8,9	0.53	0	5,10,12	1.19	1 (20%)
2	EEP	G	2	2	9,9,10	1.27	1 (11%)	7,12,14	1.22	0
2	DTH	G	4	2	6,6,7	0.48	0	6,7,9	1.61	1 (16%)
2	HYP	G	6	2	7,8,9	0.53	0	5,10,12	1.19	1 (20%)
2	EEP	H	2	2	9,9,10	1.26	1 (11%)	7,12,14	1.22	0
2	DTH	H	4	2	6,6,7	0.48	0	6,7,9	1.62	1 (16%)
2	HYP	H	6	2	7,8,9	0.54	0	5,10,12	1.17	1 (20%)
2	EEP	I	2	2	9,9,10	1.27	1 (11%)	7,12,14	1.22	0
2	DTH	I	4	2	6,6,7	0.48	0	6,7,9	1.62	1 (16%)
2	HYP	I	6	2	7,8,9	0.53	0	5,10,12	1.18	1 (20%)
2	EEP	J	2	2	9,9,10	1.26	1 (11%)	7,12,14	1.22	0
2	DTH	J	4	2	6,6,7	0.48	0	6,7,9	1.61	1 (16%)
2	HYP	J	6	2	7,8,9	0.53	0	5,10,12	1.18	1 (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
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
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
2	EEP	F	2	2	-	0/8/10/12	-
2	DTH	F	4	2	-	1/5/6/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HYP	F	6	2	-	0/0/11/13	0/1/1/1
2	EEP	G	2	2	-	0/8/10/12	-
2	DTH	G	4	2	-	1/5/6/8	-
2	HYP	G	6	2	-	0/0/11/13	0/1/1/1
2	EEP	H	2	2	-	0/8/10/12	-
2	DTH	H	4	2	-	1/5/6/8	-
2	HYP	H	6	2	-	0/0/11/13	0/1/1/1
2	EEP	I	2	2	-	0/8/10/12	-
2	DTH	I	4	2	-	1/5/6/8	-
2	HYP	I	6	2	-	0/0/11/13	0/1/1/1
2	EEP	J	2	2	-	0/8/10/12	-
2	DTH	J	4	2	-	1/5/6/8	-
2	HYP	J	6	2	-	0/0/11/13	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	73	HIC	CD2-NE2	-2.69	1.34	1.38
1	E	73	HIC	CD2-NE2	-2.69	1.34	1.38
1	A	73	HIC	CD2-NE2	-2.66	1.34	1.38
1	C	73	HIC	CD2-NE2	-2.65	1.34	1.38
1	D	73	HIC	CD2-NE2	-2.63	1.34	1.38
2	G	2	EEP	CB-CA	-2.55	1.51	1.54
2	I	2	EEP	CB-CA	-2.52	1.51	1.54
2	F	2	EEP	CB-CA	-2.49	1.51	1.54
2	H	2	EEP	CB-CA	-2.47	1.51	1.54
2	J	2	EEP	CB-CA	-2.47	1.51	1.54

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	4	DTH	O-C-CA	-2.98	118.30	125.11
2	F	4	DTH	O-C-CA	-2.97	118.32	125.11
2	G	4	DTH	O-C-CA	-2.97	118.33	125.11
2	H	4	DTH	O-C-CA	-2.96	118.34	125.11
2	J	4	DTH	O-C-CA	-2.95	118.37	125.11
2	F	6	HYP	O-C-CA	-2.53	119.33	125.11
2	G	6	HYP	O-C-CA	-2.52	119.35	125.11
2	J	6	HYP	O-C-CA	-2.51	119.37	125.11
2	H	6	HYP	O-C-CA	-2.50	119.40	125.11
2	I	6	HYP	O-C-CA	-2.49	119.41	125.11
1	A	73	HIC	O-C-CA	-2.22	119.03	124.98

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	E	73	HIC	O-C-CA	-2.20	119.07	124.98
1	B	73	HIC	O-C-CA	-2.20	119.08	124.98
1	D	73	HIC	O-C-CA	-2.20	119.09	124.98
1	C	73	HIC	O-C-CA	-2.19	119.10	124.98

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	4	DTH	C-CA-CB-OG1
2	F	4	DTH	C-CA-CB-OG1
2	H	4	DTH	C-CA-CB-OG1
2	I	4	DTH	C-CA-CB-OG1
2	J	4	DTH	C-CA-CB-OG1

There are no ring outliers.

15 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	2	EEP	1	0
2	F	4	DTH	5	0
2	F	6	HYP	4	0
2	G	2	EEP	1	0
2	G	4	DTH	5	0
2	G	6	HYP	4	0
2	H	2	EEP	1	0
2	H	4	DTH	5	0
2	H	6	HYP	4	0
2	I	2	EEP	2	0
2	I	4	DTH	5	0
2	I	6	HYP	4	0
2	J	2	EEP	2	0
2	J	4	DTH	5	0
2	J	6	HYP	4	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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
3	ADP	A	376	4	24,29,29	1.31	3 (12%)	25,45,45	1.45	5 (20%)
3	ADP	B	376	4	24,29,29	1.30	3 (12%)	25,45,45	1.46	5 (20%)
3	ADP	C	376	4	24,29,29	1.30	2 (8%)	25,45,45	1.46	5 (20%)
3	ADP	D	376	4	24,29,29	1.30	3 (12%)	25,45,45	1.45	5 (20%)
3	ADP	E	376	4	24,29,29	1.31	3 (12%)	25,45,45	1.45	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
3	ADP	A	376	4	-	3/12/32/32	0/3/3/3
3	ADP	B	376	4	-	3/12/32/32	0/3/3/3
3	ADP	C	376	4	-	3/12/32/32	0/3/3/3
3	ADP	D	376	4	-	3/12/32/32	0/3/3/3
3	ADP	E	376	4	-	3/12/32/32	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	376	ADP	PB-O3A	-3.32	1.55	1.60
3	E	376	ADP	PB-O3A	-3.29	1.55	1.60
3	C	376	ADP	PB-O3A	-3.28	1.55	1.60
3	B	376	ADP	PB-O3A	-3.27	1.55	1.60
3	D	376	ADP	PB-O3A	-3.24	1.55	1.60
3	B	376	ADP	C4-N3	-2.71	1.31	1.35
3	C	376	ADP	C4-N3	-2.71	1.31	1.35
3	D	376	ADP	C4-N3	-2.70	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	376	ADP	C4-N3	-2.69	1.31	1.35
3	A	376	ADP	C4-N3	-2.66	1.31	1.35
3	E	376	ADP	O4'-C4'	-2.04	1.40	1.45
3	A	376	ADP	O4'-C4'	-2.02	1.40	1.45
3	D	376	ADP	O4'-C4'	-2.00	1.40	1.45
3	B	376	ADP	O4'-C4'	-2.00	1.40	1.45

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	376	ADP	N3-C2-N1	-3.18	123.56	128.68
3	C	376	ADP	N3-C2-N1	-3.16	123.59	128.68
3	D	376	ADP	N3-C2-N1	-3.15	123.60	128.68
3	A	376	ADP	N3-C2-N1	-3.14	123.61	128.68
3	E	376	ADP	N3-C2-N1	-3.13	123.63	128.68
3	D	376	ADP	PA-O3A-PB	-2.59	124.34	132.57
3	E	376	ADP	PA-O3A-PB	-2.59	124.34	132.57
3	C	376	ADP	PA-O3A-PB	-2.59	124.36	132.57
3	A	376	ADP	PA-O3A-PB	-2.58	124.36	132.57
3	B	376	ADP	PA-O3A-PB	-2.58	124.38	132.57
3	B	376	ADP	C4-C5-N7	-2.43	106.86	109.40
3	A	376	ADP	C4-C5-N7	-2.41	106.89	109.40
3	C	376	ADP	C4-C5-N7	-2.40	106.90	109.40
3	E	376	ADP	C4-C5-N7	-2.39	106.91	109.40
3	D	376	ADP	C4-C5-N7	-2.37	106.93	109.40
3	B	376	ADP	C2-N1-C6	2.10	122.41	118.77
3	D	376	ADP	C2-N1-C6	2.09	122.39	118.77
3	C	376	ADP	C1'-N9-C4	-2.09	123.02	126.64
3	C	376	ADP	C2-N1-C6	2.08	122.37	118.77
3	A	376	ADP	C2-N1-C6	2.08	122.36	118.77
3	E	376	ADP	C1'-N9-C4	-2.07	123.05	126.64
3	E	376	ADP	C2-N1-C6	2.05	122.33	118.77
3	B	376	ADP	C1'-N9-C4	-2.05	123.10	126.64
3	A	376	ADP	C1'-N9-C4	-2.04	123.11	126.64
3	D	376	ADP	C1'-N9-C4	-2.04	123.12	126.64

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	376	ADP	C5'-O5'-PA-O1A
3	A	376	ADP	C5'-O5'-PA-O3A

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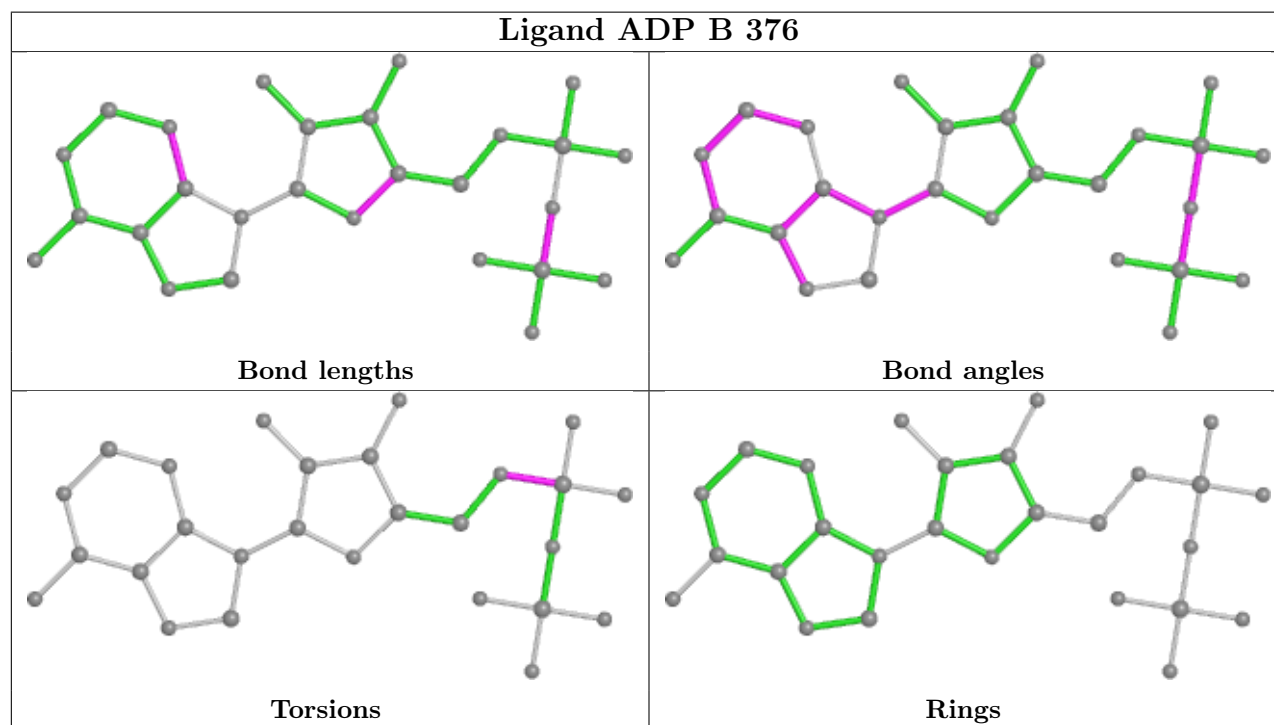
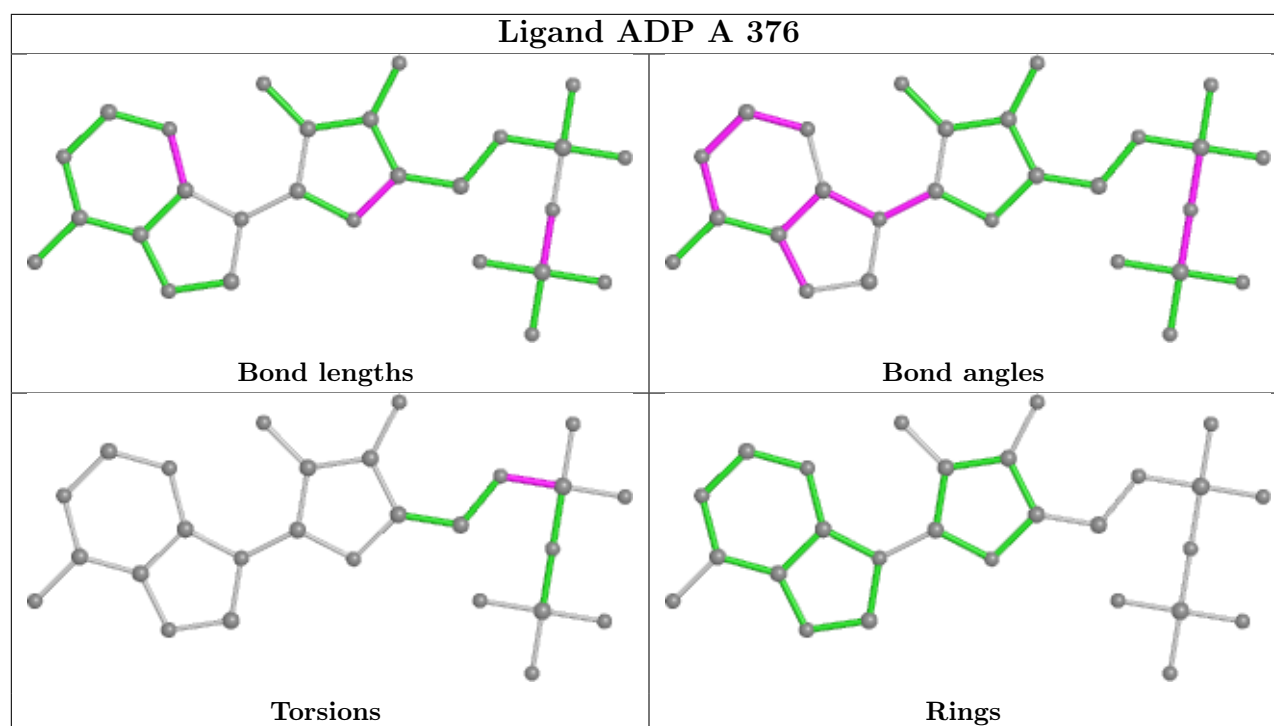
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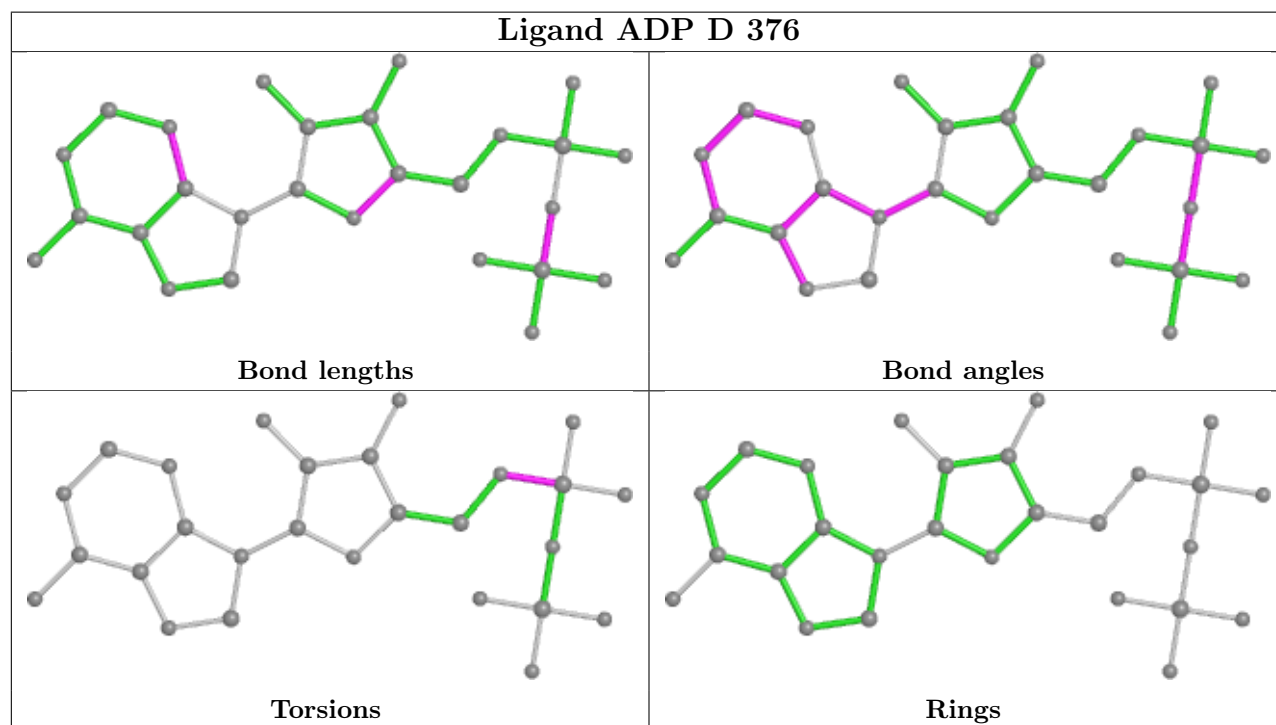
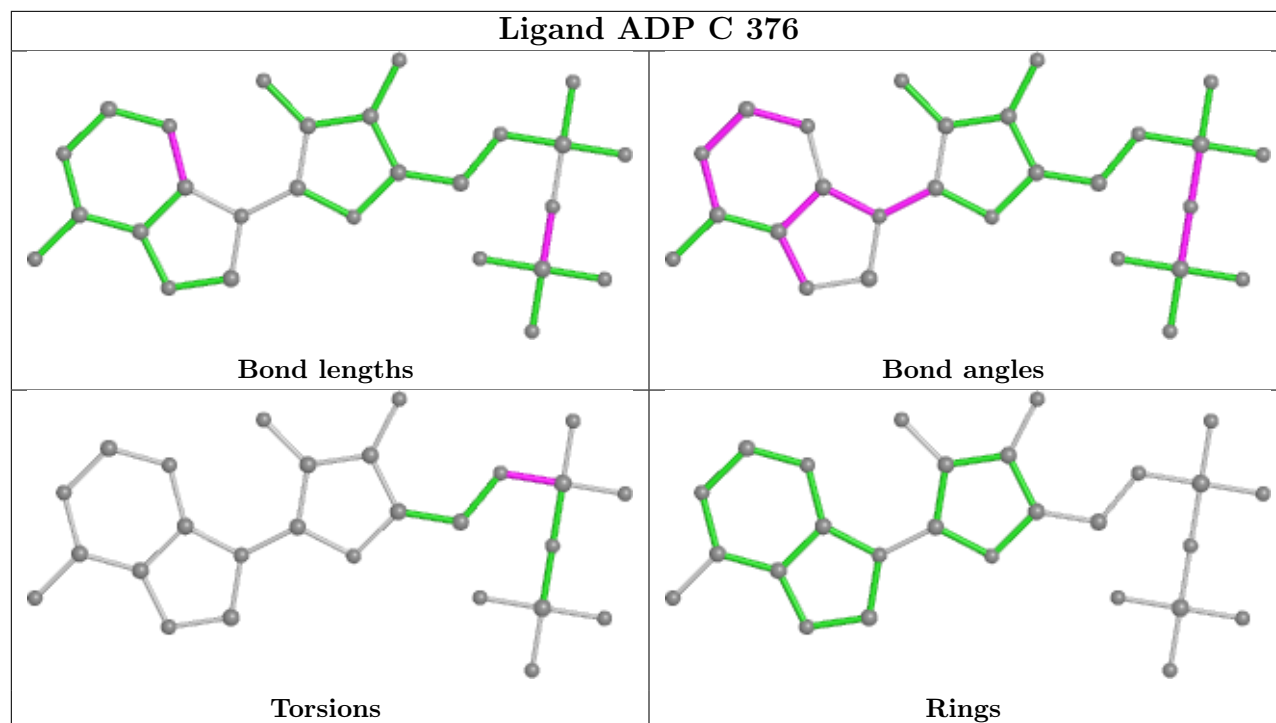
Mol	Chain	Res	Type	Atoms
3	C	376	ADP	C5'-O5'-PA-O1A
3	C	376	ADP	C5'-O5'-PA-O3A
3	E	376	ADP	C5'-O5'-PA-O1A
3	E	376	ADP	C5'-O5'-PA-O3A
3	D	376	ADP	C5'-O5'-PA-O1A
3	D	376	ADP	C5'-O5'-PA-O3A
3	B	376	ADP	C5'-O5'-PA-O1A
3	B	376	ADP	C5'-O5'-PA-O3A
3	A	376	ADP	C5'-O5'-PA-O2A
3	C	376	ADP	C5'-O5'-PA-O2A
3	E	376	ADP	C5'-O5'-PA-O2A
3	D	376	ADP	C5'-O5'-PA-O2A
3	B	376	ADP	C5'-O5'-PA-O2A

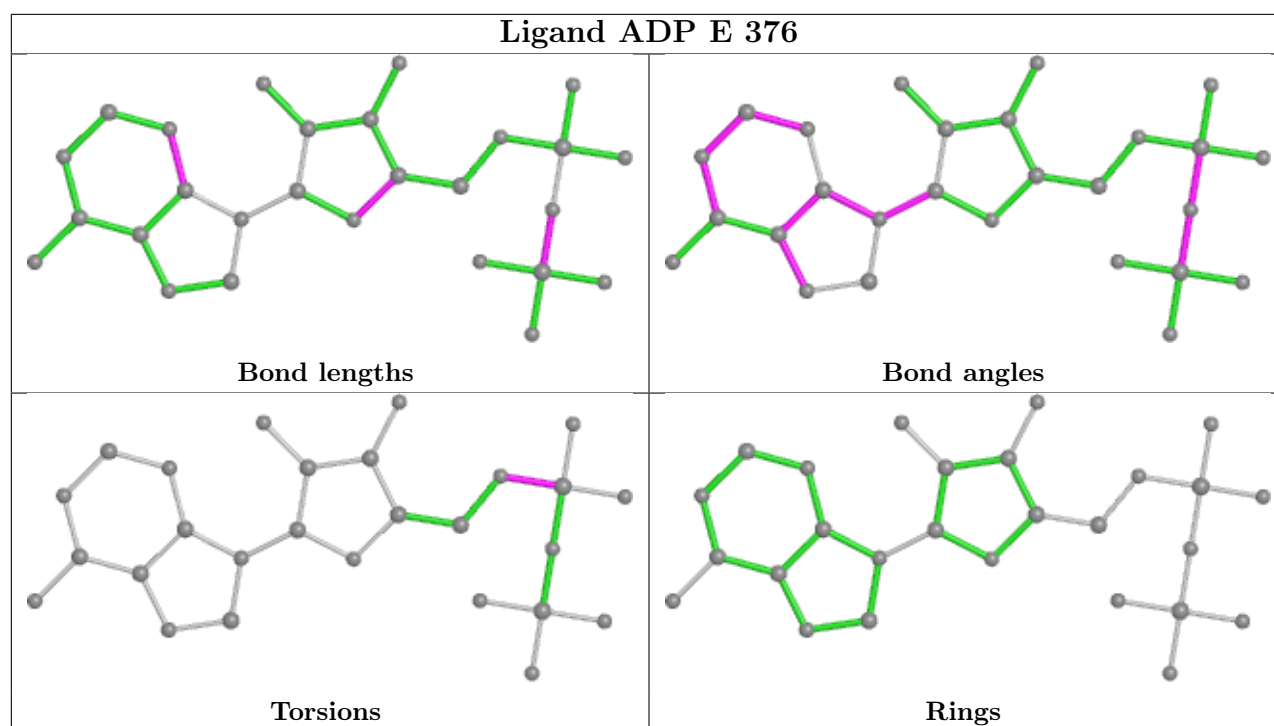
There are no ring outliers.

No monomer is involved in short contacts.

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.