



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Oct 15, 2019 – 11:27 PM EDT

PDB ID : 4A7L
EMDB ID: : EMD-1989
Title : Structure of the Actin-Tropomyosin-Myosin Complex (rigor ATM 1)
Authors : Behrmann, E.; Mueller, M.; Penczek, P.A.; Mannherz, H.G.; Manstein, D.J.;
Raunser, S.
Deposited on : 2011-11-14
Resolution : 8.10 Å(reported)
Based on PDB ID : 3MFP, 1LKX

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

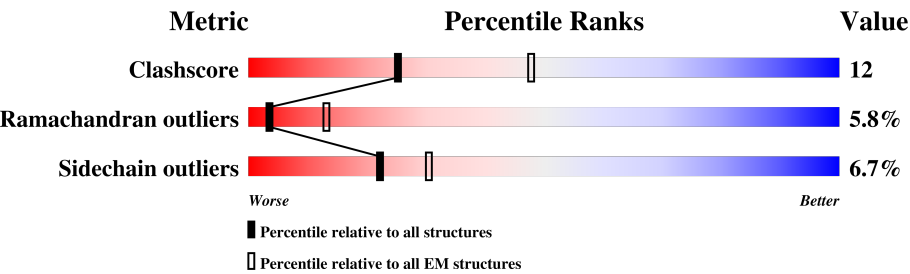
MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 8.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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	71% 21% 6% .
1	D	375	69% 23% 5% .
1	E	375	70% 22% 5% .
1	F	375	70% 22% 6% .
1	I	375	70% 22% 5% .
2	B	136	97% .
2	H	136	96% .
3	C	697	78% 17% . .
3	G	697	76% 18% . .

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Mol	Chain	Length	Quality of chain
3	J	697	<div><div></div><div>77%</div><div>18%</div><div>• •</div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 33500 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 SKELETON MUSCLE.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		
1	D	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		
1	E	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		
1	F	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		
1	I	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		

- Molecule 2 is a protein called TROPOMYOSIN 1 ALPHA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	136	Total	C	N	O	S	0	0
			1104	673	189	239	3		
2	H	136	Total	C	N	O	S	0	0
			1104	673	189	239	3		

- Molecule 3 is a protein called MYOSIN IE HEAVY CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	689	Total	C	N	O	S	0	0
			5494	3469	946	1048	31		
3	G	689	Total	C	N	O	S	0	0
			5494	3469	946	1048	31		
3	J	689	Total	C	N	O	S	0	0
			5494	3469	946	1048	31		

There are 9 discrepancies between the modelled and reference sequences:

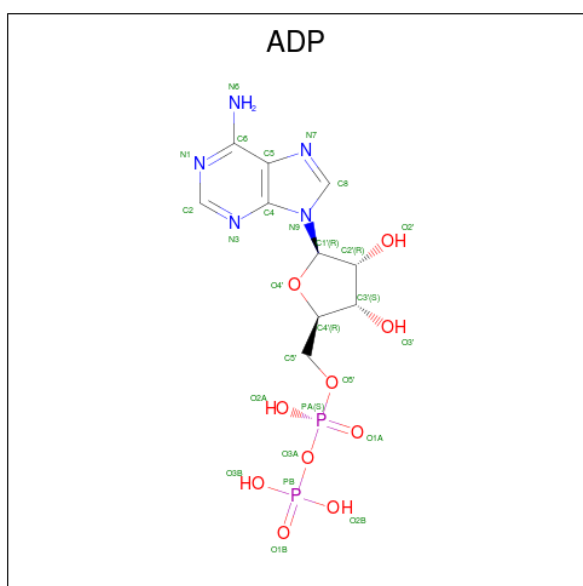
Chain	Residue	Modelled	Actual	Comment	Reference
C	77	MET	ILE	conflict	UNP Q03479

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Chain	Residue	Modelled	Actual	Comment	Reference
C	215	ASP	ASN	conflict	UNP Q03479
C	334	GLU	SER	engineered mutation	UNP Q03479
G	77	MET	ILE	conflict	UNP Q03479
G	215	ASP	ASN	conflict	UNP Q03479
G	334	GLU	SER	engineered mutation	UNP Q03479
J	77	MET	ILE	conflict	UNP Q03479
J	215	ASP	ASN	conflict	UNP Q03479
J	334	GLU	SER	engineered mutation	UNP Q03479

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	I	1	Total	C	N	O	P	0
			27	10	5	10	2	

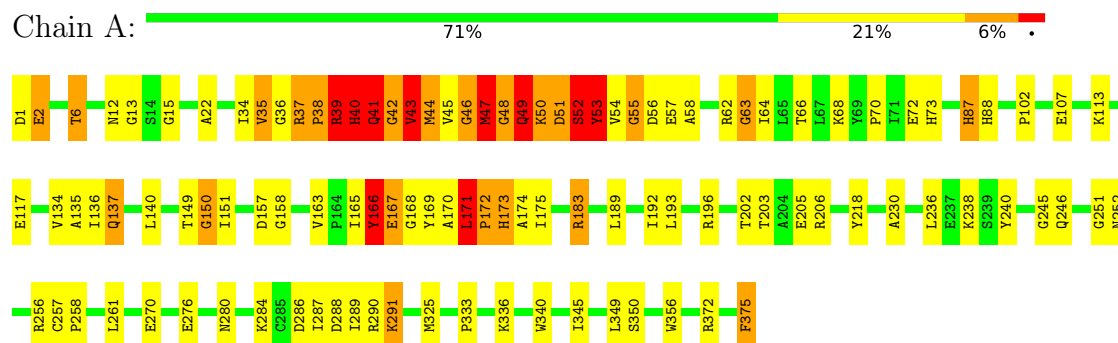
- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
5	I	1	Total 1	Ca 1	0
5	A	1	Total 1	Ca 1	0
5	D	1	Total 1	Ca 1	0
5	F	1	Total 1	Ca 1	0
5	E	1	Total 1	Ca 1	0

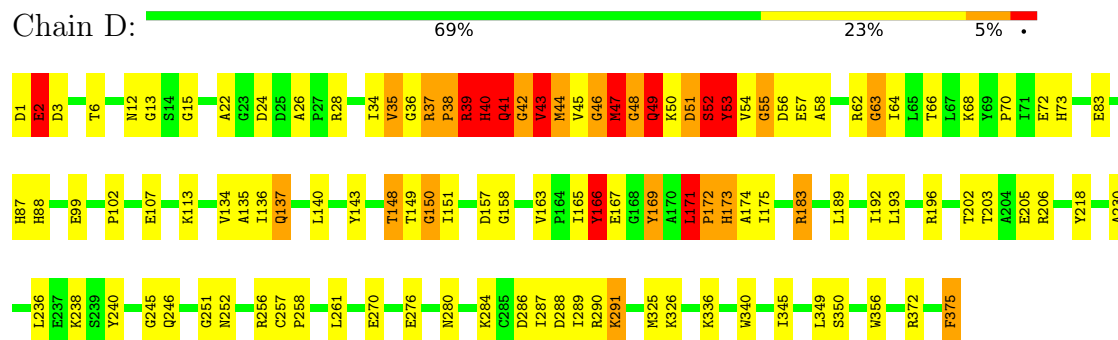
3 Residue-property plots

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.

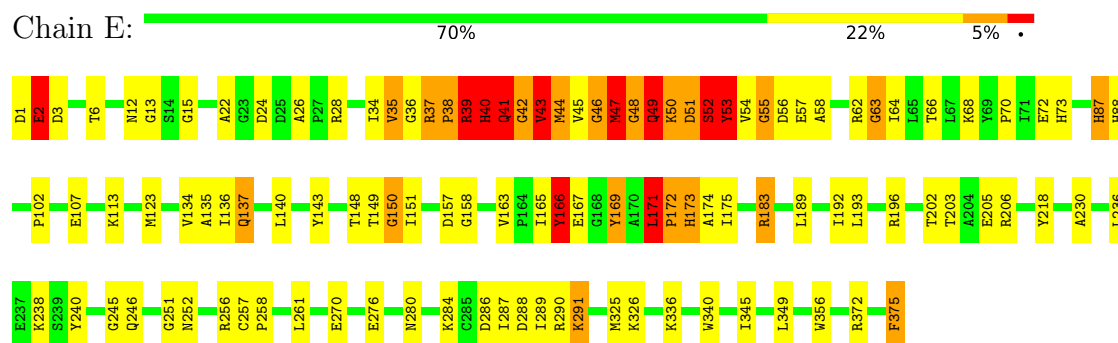
• Molecule 1: ACTIN, ALPHA SKELETON MUSCLE



• Molecule 1: ACTIN, ALPHA SKELETON MUSCLE

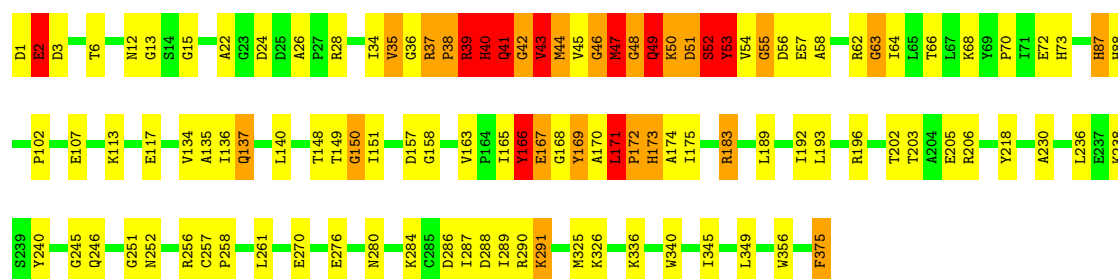


• Molecule 1: ACTIN, ALPHA SKELETON MUSCLE



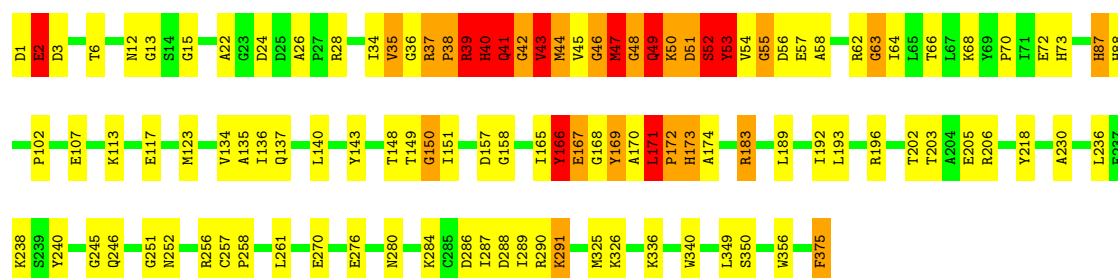
• Molecule 1: ACTIN, ALPHA SKELETON MUSCLE

Chain F:  70% 22% 6% .



- Molecule 1: ACTIN, ALPHA SKELETON MUSCLE

Chain I:  70% 22% 5% .



- Molecule 2: TROPOMYOSIN 1 ALPHA

Chain B:  97% .




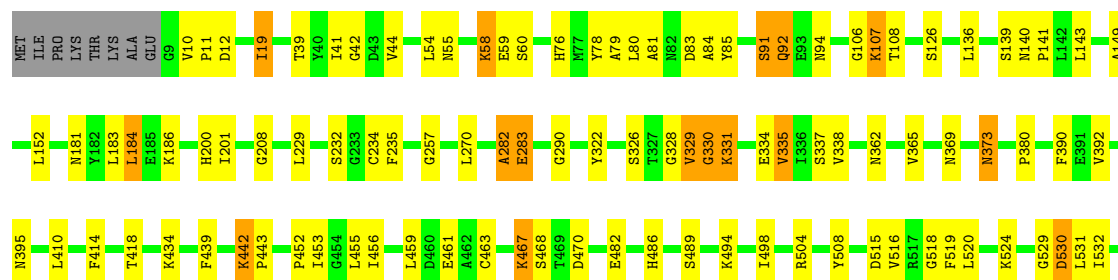
- Molecule 2: TROPOMYOSIN 1 ALPHA

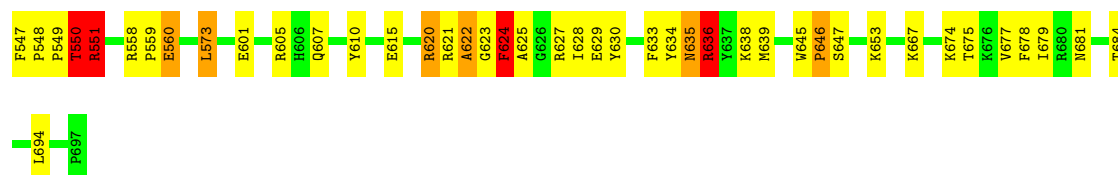
Chain H:  96% .



- Molecule 3: MYOSIN IE HEAVY CHAIN

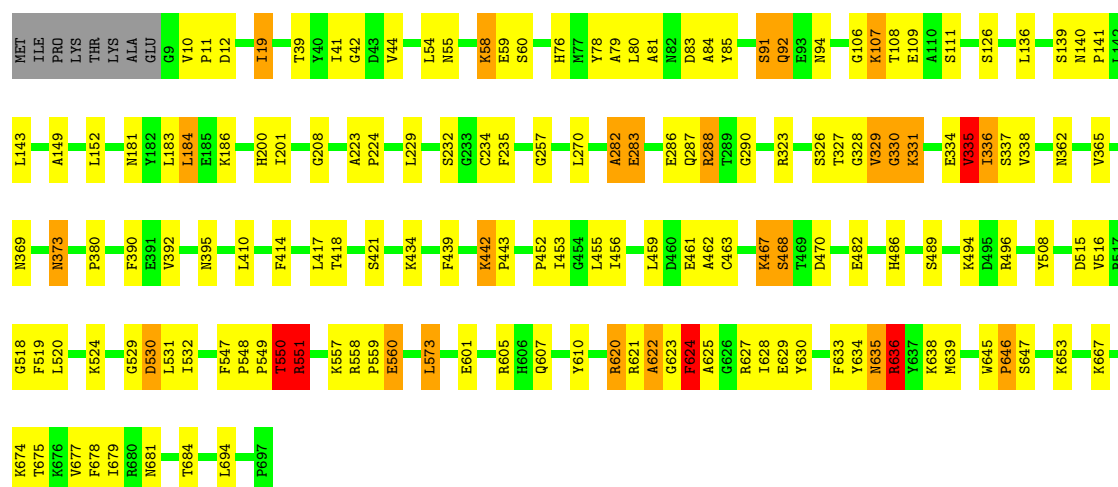
Chain C:  78% 17% . .





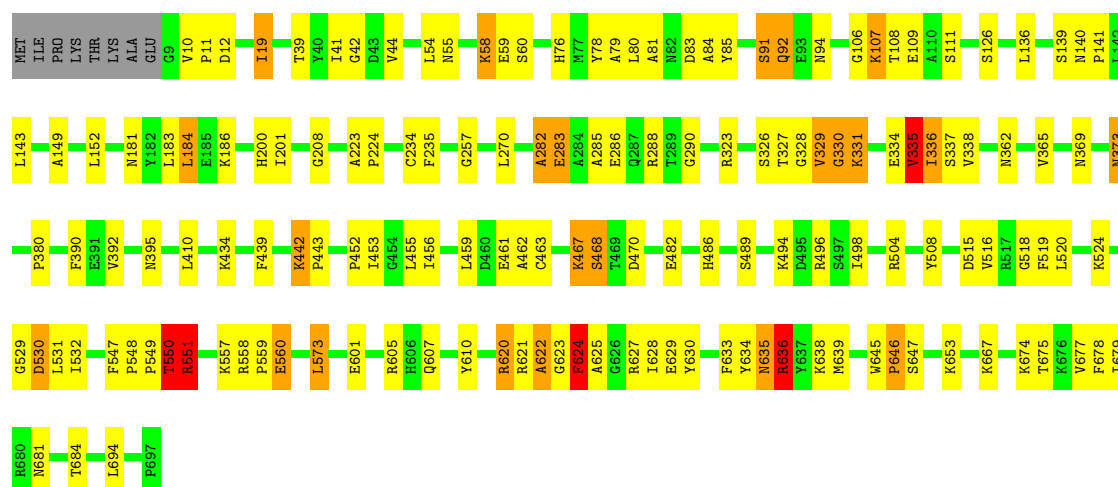
● Molecule 3: MYOSIN IE HEAVY CHAIN

Chain G: 76% 18%



● Molecule 3: MYOSIN IE HEAVY CHAIN

Chain J: 77% 18%



4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=Not provided°, rise=Not provided Å, axial sym=Not provided	Depositor
Number of segments used	5555	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH PARTICLE	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.7	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	169644	Depositor
Image detector	TVIPS TEMCAM-F816 (8k x 8k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	0.97	18/2984 (0.6%)	0.72	15/4040 (0.4%)
1	D	0.93	17/2984 (0.6%)	0.68	13/4040 (0.3%)
1	E	0.93	17/2984 (0.6%)	0.71	15/4040 (0.4%)
1	F	0.93	17/2984 (0.6%)	0.71	15/4040 (0.4%)
1	I	0.93	17/2984 (0.6%)	0.71	15/4040 (0.4%)
2	B	0.36	0/1107	0.31	0/1471
2	H	0.21	0/1107	0.33	0/1471
3	C	0.26	0/5594	0.39	0/7539
3	G	0.22	0/5594	0.38	0/7539
3	J	0.22	0/5594	0.38	0/7539
All	All	0.65	86/33916 (0.3%)	0.55	73/45759 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	I	0	1
All	All	0	5

The worst 5 of 86 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	166	TYR	CD2-CE2	19.09	1.68	1.39
1	E	166	TYR	CD2-CE2	19.08	1.68	1.39
1	A	166	TYR	CD2-CE2	19.07	1.68	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	166	TYR	CD2-CE2	19.05	1.68	1.39
1	D	166	TYR	CD2-CE2	19.03	1.67	1.39

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	39	ARG	NE-CZ-NH2	-9.45	115.58	120.30
1	E	149	THR	C-N-CA	9.42	142.07	122.30
1	E	39	ARG	NE-CZ-NH2	-9.41	115.59	120.30
1	F	39	ARG	NE-CZ-NH2	-9.40	115.60	120.30
1	I	149	THR	C-N-CA	9.40	142.04	122.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	40	HIS	Sidechain
1	D	40	HIS	Sidechain
1	E	40	HIS	Sidechain
1	F	40	HIS	Sidechain
1	I	40	HIS	Sidechain

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	2934	0	2895	150	0
1	D	2934	0	2895	131	0
1	E	2934	0	2895	125	0
1	F	2934	0	2895	123	0
1	I	2934	0	2895	127	0
2	B	1104	0	1104	3	0
2	H	1104	0	1104	18	0
3	C	5494	0	5492	79	0
3	G	5494	0	5492	89	0
3	J	5494	0	5492	97	0
4	A	27	0	12	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	27	0	12	4	0
4	E	27	0	12	4	0
4	F	27	0	12	4	0
4	I	27	0	12	4	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	I	1	0	0	0	0
All	All	33500	0	33219	834	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 834 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:D:54:VAL:HG22	1:D:55:GLY:H	1.10	1.14
1:A:54:VAL:HG22	1:A:55:GLY:H	1.10	1.10
1:I:54:VAL:HG22	1:I:55:GLY:H	1.10	1.10
1:F:54:VAL:HG22	1:F:55:GLY:H	1.10	1.08
1:E:54:VAL:HG22	1:E:55:GLY:H	1.10	1.07

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	372/375 (99%)	289 (78%)	55 (15%)	28 (8%)	1	17
1	D	372/375 (99%)	288 (77%)	56 (15%)	28 (8%)	1	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	372/375 (99%)	289 (78%)	55 (15%)	28 (8%)	1	17
1	F	372/375 (99%)	289 (78%)	55 (15%)	28 (8%)	1	17
1	I	372/375 (99%)	289 (78%)	55 (15%)	28 (8%)	1	17
2	B	134/136 (98%)	134 (100%)	0	0	100	100
2	H	134/136 (98%)	134 (100%)	0	0	100	100
3	C	687/697 (99%)	574 (84%)	78 (11%)	35 (5%)	2	25
3	G	687/697 (99%)	573 (83%)	80 (12%)	34 (5%)	2	26
3	J	687/697 (99%)	574 (84%)	79 (12%)	34 (5%)	2	26
All	All	4189/4238 (99%)	3433 (82%)	513 (12%)	243 (6%)	3	23

5 of 243 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	GLY
1	A	43	VAL
1	A	47	MET
1	A	49	GLN
1	A	51	ASP

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	317/317 (100%)	289 (91%)	28 (9%)	11	37
1	D	317/317 (100%)	289 (91%)	28 (9%)	11	37
1	E	317/317 (100%)	286 (90%)	31 (10%)	9	32
1	F	317/317 (100%)	286 (90%)	31 (10%)	9	32
1	I	317/317 (100%)	286 (90%)	31 (10%)	9	32
2	B	118/118 (100%)	118 (100%)	0	100	100
2	H	118/118 (100%)	118 (100%)	0	100	100
3	C	609/616 (99%)	580 (95%)	29 (5%)	28	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	G	609/616 (99%)	575 (94%)	34 (6%)	23	54
3	J	609/616 (99%)	575 (94%)	34 (6%)	23	54
All	All	3648/3669 (99%)	3402 (93%)	246 (7%)	22	48

5 of 246 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	291	LYS
1	F	218	TYR
3	J	373	ASN
1	E	356	TRP
1	F	53	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	354	GLN
3	G	76	HIS
3	J	362	ASN
1	F	88	HIS
1	F	225	ASN

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	2.99	3 (33%)	6,14,16	2.08	3 (50%)
1	HIC	D	73	1	9,11,12	3.00	2 (22%)	6,14,16	2.07	3 (50%)
1	HIC	E	73	1	9,11,12	2.99	3 (33%)	6,14,16	2.08	3 (50%)
1	HIC	F	73	1	9,11,12	2.98	3 (33%)	6,14,16	2.08	3 (50%)
1	HIC	I	73	1	9,11,12	2.99	3 (33%)	6,14,16	2.08	3 (50%)

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	-	2/4/6/8	0/1/1/1
1	HIC	D	73	1	-	2/4/6/8	0/1/1/1
1	HIC	E	73	1	-	2/4/6/8	0/1/1/1
1	HIC	F	73	1	-	2/4/6/8	0/1/1/1
1	HIC	I	73	1	-	2/4/6/8	0/1/1/1

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	73	HIC	CA-C	7.84	1.60	1.50
1	A	73	HIC	CA-C	7.81	1.60	1.50
1	I	73	HIC	CA-C	7.80	1.60	1.50
1	E	73	HIC	CA-C	7.79	1.60	1.50
1	F	73	HIC	CA-C	7.74	1.60	1.50

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	73	HIC	CB-CA-C	-3.62	104.43	111.41
1	D	73	HIC	CB-CA-C	-3.62	104.44	111.41
1	E	73	HIC	CB-CA-C	-3.62	104.44	111.41
1	A	73	HIC	CB-CA-C	-3.61	104.45	111.41
1	F	73	HIC	CB-CA-C	-3.60	104.47	111.41

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	73	HIC	N-CA-CB-CG
1	D	73	HIC	C-CA-CB-CG
1	A	73	HIC	N-CA-CB-CG
1	A	73	HIC	C-CA-CB-CG
1	I	73	HIC	N-CA-CB-CG

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	73	HIC	2	0
1	D	73	HIC	2	0
1	E	73	HIC	2	0
1	F	73	HIC	2	0
1	I	73	HIC	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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
4	ADP	A	376	-	24,29,29	1.13	1 (4%)	25,45,45	1.45	4 (16%)
4	ADP	D	376	-	24,29,29	1.13	1 (4%)	25,45,45	1.44	4 (16%)
4	ADP	E	376	-	24,29,29	1.12	1 (4%)	25,45,45	1.45	4 (16%)
4	ADP	F	376	-	24,29,29	1.13	1 (4%)	25,45,45	1.45	4 (16%)
4	ADP	I	376	-	24,29,29	1.13	2 (8%)	25,45,45	1.46	4 (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
4	ADP	A	376	-	-	0/12/32/32	0/3/3/3
4	ADP	D	376	-	-	0/12/32/32	0/3/3/3
4	ADP	E	376	-	-	0/12/32/32	0/3/3/3
4	ADP	F	376	-	-	0/12/32/32	0/3/3/3
4	ADP	I	376	-	-	0/12/32/32	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	376	ADP	C2-N1	2.97	1.39	1.33
4	D	376	ADP	C2-N1	2.95	1.39	1.33
4	I	376	ADP	C2-N1	2.94	1.39	1.33
4	F	376	ADP	C2-N1	2.93	1.39	1.33
4	E	376	ADP	C2-N1	2.89	1.39	1.33

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	376	ADP	C4-C5-N7	3.96	113.52	109.40
4	I	376	ADP	C4-C5-N7	3.94	113.50	109.40
4	F	376	ADP	C4-C5-N7	3.92	113.49	109.40
4	A	376	ADP	C4-C5-N7	3.89	113.45	109.40
4	D	376	ADP	C4-C5-N7	3.87	113.43	109.40

There are no chirality outliers.

There are no torsion outliers.

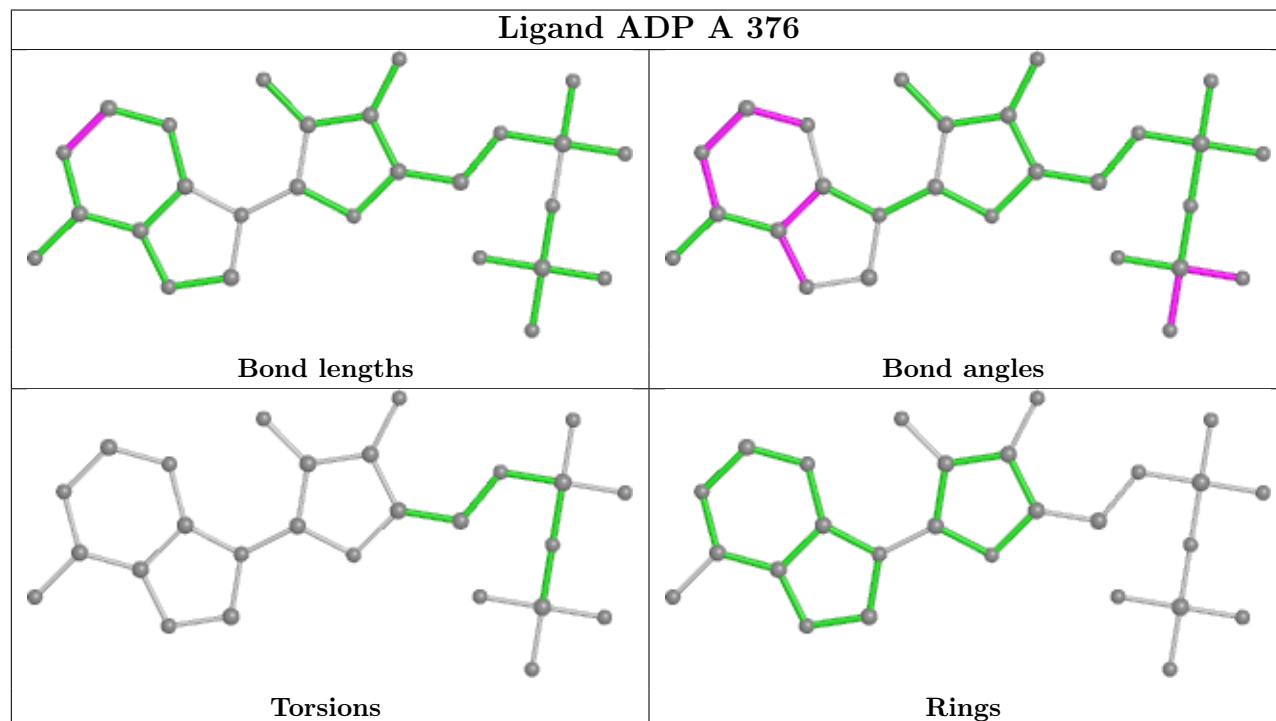
There are no ring outliers.

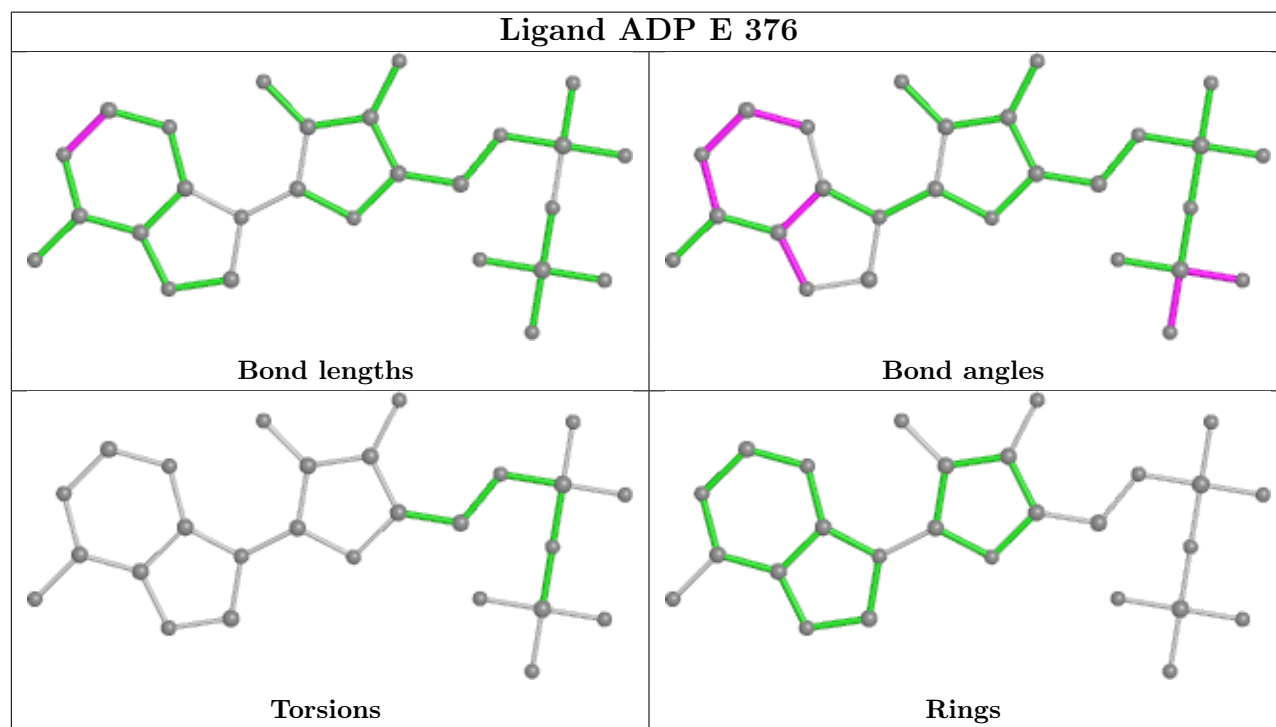
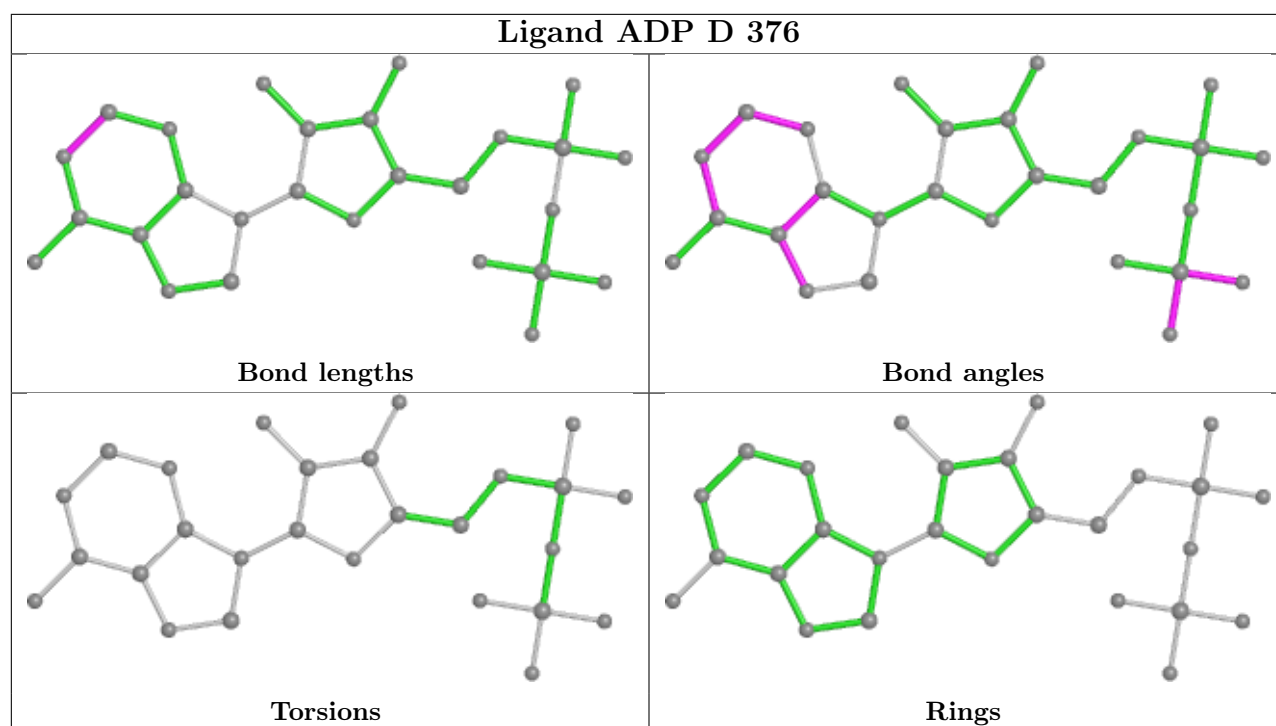
5 monomers are involved in 20 short contacts:

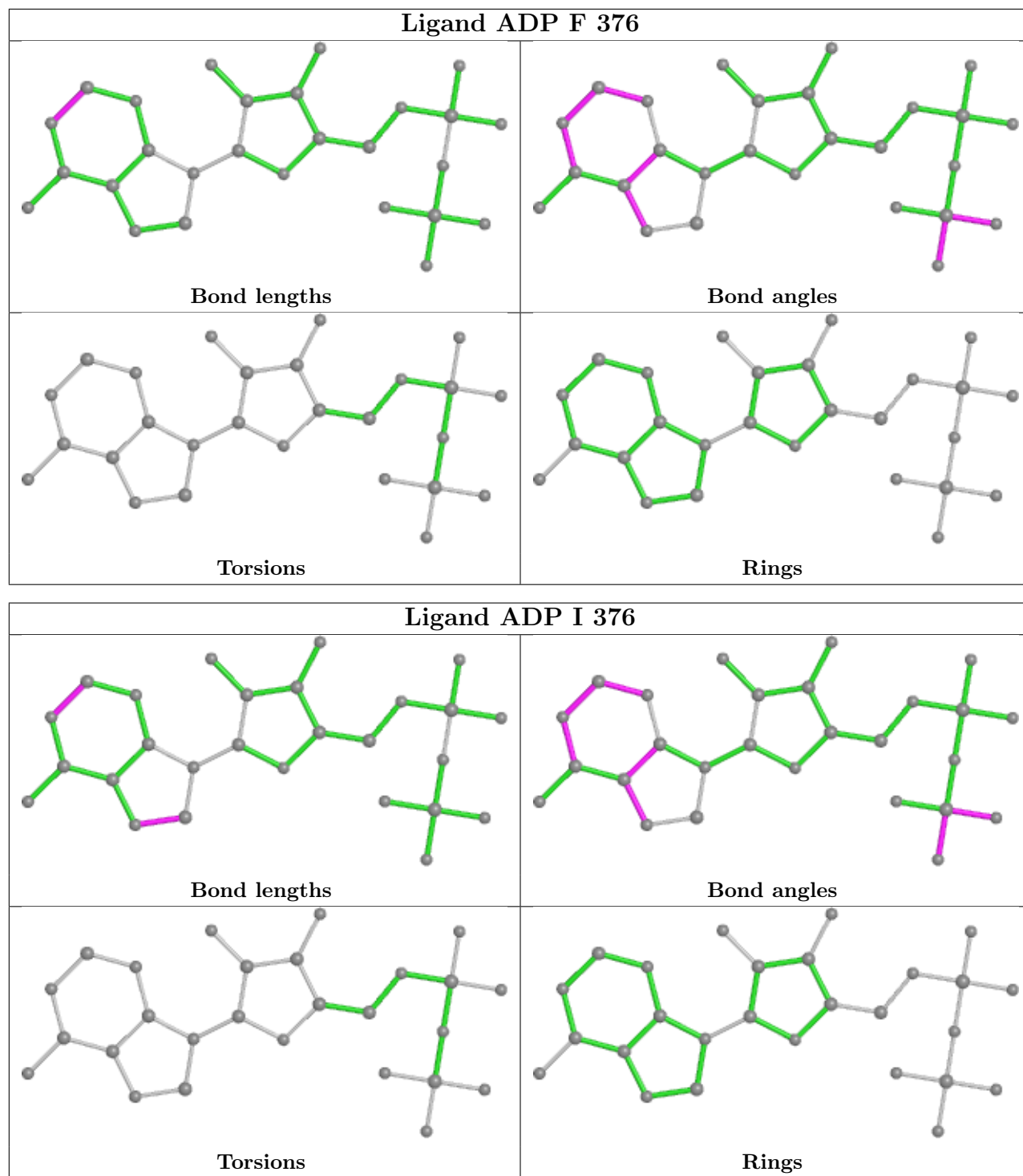
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	376	ADP	4	0
4	D	376	ADP	4	0
4	E	376	ADP	4	0
4	F	376	ADP	4	0
4	I	376	ADP	4	0

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.







5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.