



Full wwPDB EM Validation Report ⓘ

Apr 1, 2025 – 08:55 PM EDT

PDB ID : 7UTI / pdb_00007uti
EMDB ID : EMD-0729
Title : ALTERNATIVE MODELING OF TROPOMYOSIN IN HUMAN CARDIAC
THIN FILAMENT IN THE CALCIUM BOUND STATE
Authors : Rynkiewicz, M.J.; Pavadai, E.; Lehman, W.
Deposited on : 2022-04-27
Resolution : 4.80 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev117
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

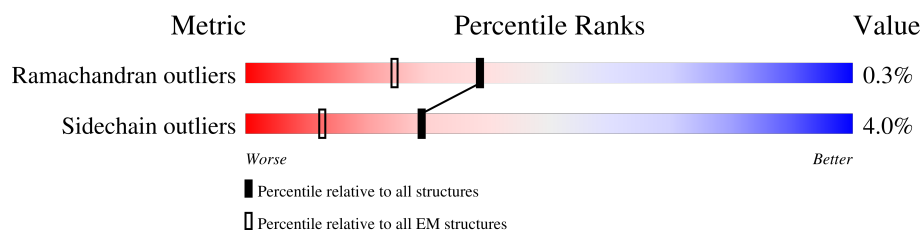
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.80 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.



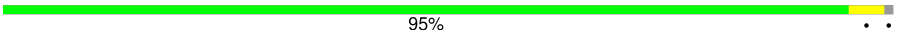
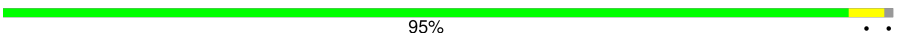

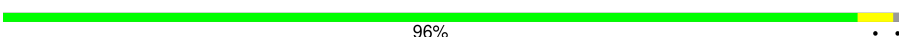
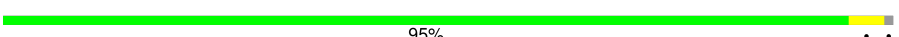








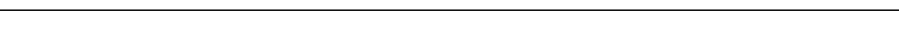
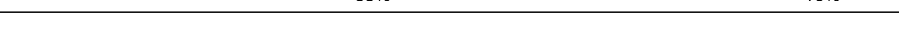
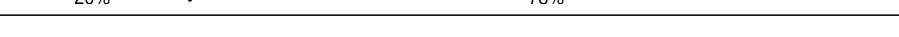





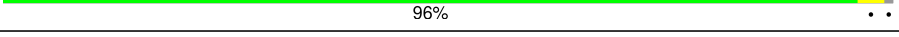
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	C	377	
1	D	377	
1	E	377	
1	F	377	
1	G	377	
1	H	377	
1	I	377	
1	J	377	
1	K	377	
1	L	377	

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Mol	Chain	Length	Quality of chain
1	M	377	 95%
1	N	377	 95%
1	O	377	 96%
1	P	377	 96%
1	Q	377	 95%
1	R	377	 95%
2	W	285	 17% 81%
2	b	285	 18% 81%
2	e	285	 91% 6%
2	f	285	 92% 6%
2	g	285	 24% 75%
2	h	285	 25% 75%
2	i	285	 82% 16%
2	j	285	 83% 16%
3	X	288	 20% 78%
3	Y	288	 23% 74%
3	c	288	 20% 78%
3	d	288	 23% 74%
4	V	210	 58% 40%
4	a	210	 58% 40%
5	U	161	 96%
5	Z	161	 96%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 128171 atoms, of which 63663 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	C	375	Total	C	H	N	O	S	0	0
			5827	1855	2893	493	565	21		
1	D	375	Total	C	H	N	O	S	0	0
			5827	1855	2893	493	565	21		
1	E	375	Total	C	H	N	O	S	0	0
			5827	1855	2893	493	565	21		
1	F	375	Total	C	H	N	O	S	0	0
			5827	1855	2893	493	565	21		
1	G	375	Total	C	H	N	O	S	0	0
			5827	1855	2893	493	565	21		
1	H	375	Total	C	H	N	O	S	0	0
			5827	1855	2893	493	565	21		
1	I	375	Total	C	H	N	O	S	0	0
			5827	1855	2893	493	565	21		
1	J	375	Total	C	H	N	O	S	0	0
			5827	1855	2893	493	565	21		
1	K	375	Total	C	H	N	O	S	0	0
			5827	1855	2893	493	565	21		
1	L	375	Total	C	H	N	O	S	0	0
			5827	1855	2893	493	565	21		
1	M	375	Total	C	H	N	O	S	0	0
			5827	1855	2893	493	565	21		
1	N	375	Total	C	H	N	O	S	0	0
			5827	1855	2893	493	565	21		
1	O	375	Total	C	H	N	O	S	0	0
			5827	1855	2893	493	565	21		
1	P	375	Total	C	H	N	O	S	0	0
			5827	1855	2893	493	565	21		
1	Q	375	Total	C	H	N	O	S	0	0
			5827	1855	2893	493	565	21		
1	R	375	Total	C	H	N	O	S	0	0
			5827	1855	2893	493	565	21		

- Molecule 2 is a protein called Tropomyosin alpha-1 chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	e	267	Total	C	H	N	O	S	0	0
			4284	1310	2136	366	468	4		
2	f	267	Total	C	H	N	O	S	0	0
			4284	1310	2136	366	468	4		
2	W	53	Total	C	H	N	O	S	0	0
			858	255	442	74	84	3		
2	b	53	Total	C	H	N	O	S	0	0
			858	255	442	74	84	3		
2	i	240	Total	C	H	N	O	S	0	0
			3869	1185	1932	328	420	4		
2	j	240	Total	C	H	N	O	S	0	0
			3869	1185	1932	328	420	4		
2	g	72	Total	C	H	N	O	S	0	0
			1160	350	589	97	121	3		
2	h	72	Total	C	H	N	O	S	0	0
			1160	350	589	97	121	3		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
e	0	ACE	-	acetylation	UNP P09493
f	0	ACE	-	acetylation	UNP P09493
W	0	ACE	-	acetylation	UNP P09493
b	0	ACE	-	acetylation	UNP P09493
i	0	ACE	-	acetylation	UNP P09493
j	0	ACE	-	acetylation	UNP P09493
g	0	ACE	-	acetylation	UNP P09493
h	0	ACE	-	acetylation	UNP P09493

- Molecule 3 is a protein called Isoform 6 of Troponin T, cardiac muscle.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	X	63	Total	C	H	N	O	S	0	0
			1123	332	564	120	106	1		
3	Y	74	Total	C	H	N	O		0	0
			1306	401	663	123	119			
3	c	63	Total	C	H	N	O	S	0	0
			1123	332	564	120	106	1		
3	d	74	Total	C	H	N	O		0	0
			1306	401	663	123	119			

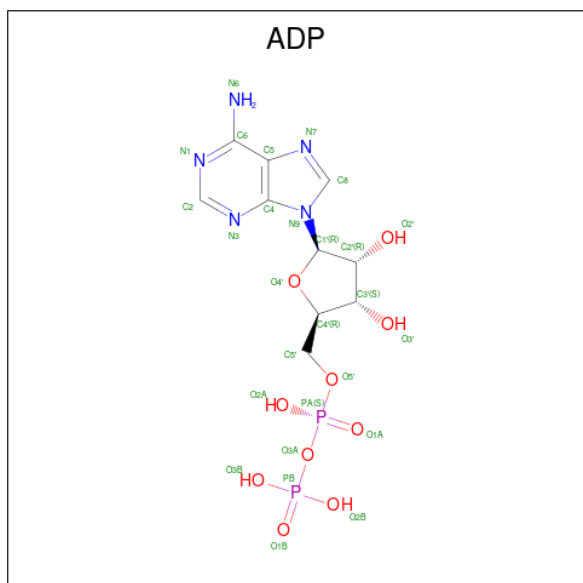
- Molecule 4 is a protein called Troponin I, cardiac muscle.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	V	126	Total 2073	C 624	H 1065	N 193	O 187	S 4	0	0
4	a	126	Total 2072	C 624	H 1064	N 193	O 187	S 4	0	0

- Molecule 5 is a protein called Troponin C, slow skeletal and cardiac muscles.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	U	160	Total 2474	C 788	H 1201	N 195	O 278	S 12	0	0
5	Z	160	Total 2474	C 788	H 1201	N 195	O 278	S 12	0	0

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms						AltConf
6	C	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
6	D	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
6	E	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
6	F	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
6	G	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
6	H	1	Total 39	C 10	H 12	N 5	O 10	P 2	0

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Mol	Chain	Residues	Atoms						AltConf
6	I	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
6	J	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
6	K	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
6	L	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
6	M	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
6	N	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
6	O	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
6	P	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
6	Q	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
6	R	1	Total 39	C 10	H 12	N 5	O 10	P 2	0

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
7	C	1	Total	Mg	0
			1	1	
7	D	1	Total	Mg	0
			1	1	
7	E	1	Total	Mg	0
			1	1	
7	F	1	Total	Mg	0
			1	1	
7	G	1	Total	Mg	0
			1	1	
7	H	1	Total	Mg	0
			1	1	
7	I	1	Total	Mg	0
			1	1	
7	J	1	Total	Mg	0
			1	1	
7	K	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
7	L	1	Total 1	Mg 1	0
7	M	1	Total 1	Mg 1	0
7	N	1	Total 1	Mg 1	0
7	O	1	Total 1	Mg 1	0
7	P	1	Total 1	Mg 1	0
7	Q	1	Total 1	Mg 1	0
7	R	1	Total 1	Mg 1	0

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
8	U	3	Total 3	Ca 3	0
8	Z	3	Total 3	Ca 3	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 C:  95%



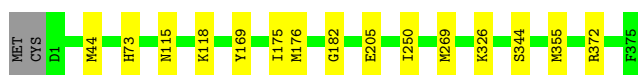
- Molecule 1: Actin, alpha skeletal muscle

Chain D:  96%



- Molecule 1: Actin, alpha skeletal muscle

Chain E:  95%



- Molecule 1: Actin, alpha skeletal muscle

Chain F:  95%



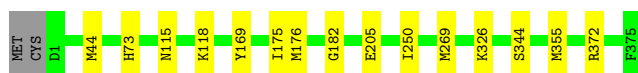
- Molecule 1: Actin, alpha skeletal muscle

Chain G:  95%



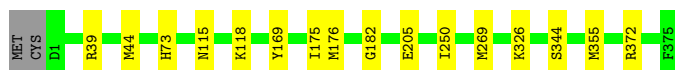
- Molecule 1: Actin, alpha skeletal muscle

Chain H:  95%



- Molecule 1: Actin, alpha skeletal muscle

Chain I: 95%



- Molecule 1: Actin, alpha skeletal muscle

Chain J: 95%



- Molecule 1: Actin, alpha skeletal muscle

Chain K: 96%



- Molecule 1: Actin, alpha skeletal muscle

Chain L: 96%



- Molecule 1: Actin, alpha skeletal muscle

Chain M: 95%



- Molecule 1: Actin, alpha skeletal muscle

Chain N: 95%



- Molecule 1: Actin, alpha skeletal muscle

Chain O: 96%



- Molecule 1: Actin, alpha skeletal muscle

Chain P: 96%



- Molecule 1: Actin, alpha skeletal muscle

Chain Q: 95%



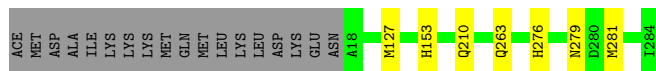
- Molecule 1: Actin, alpha skeletal muscle

Chain R: 95%



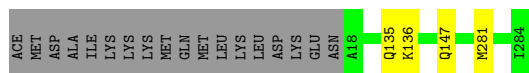
- Molecule 2: Tropomyosin alpha-1 chain

Chain e: 91%



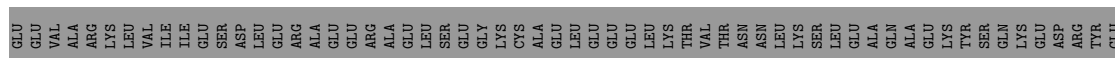
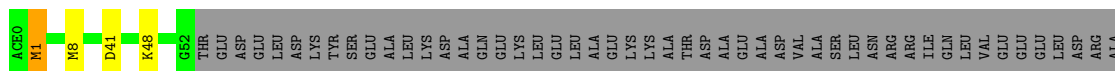
- Molecule 2: Tropomyosin alpha-1 chain

Chain f: 92%

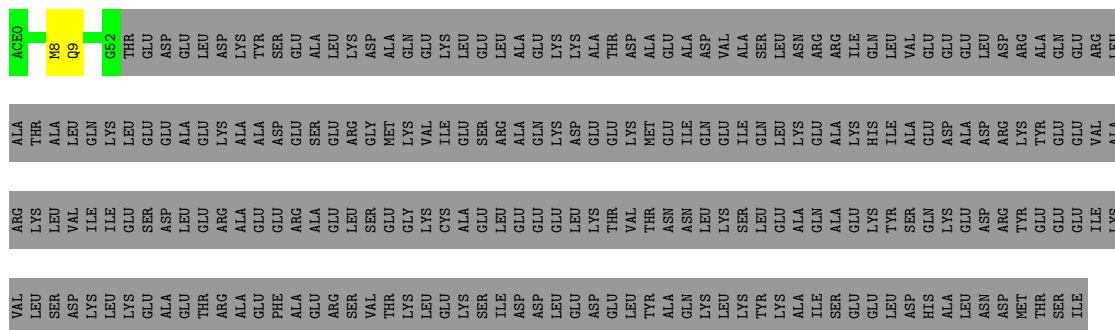


- Molecule 2: Tropomyosin alpha-1 chain

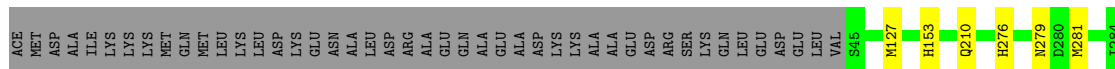
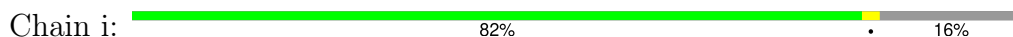
Chain W: 17%



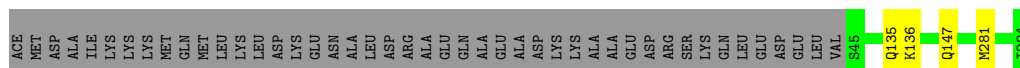
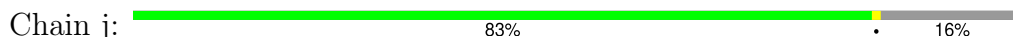
- Molecule 2: Tropomyosin alpha-1 chain



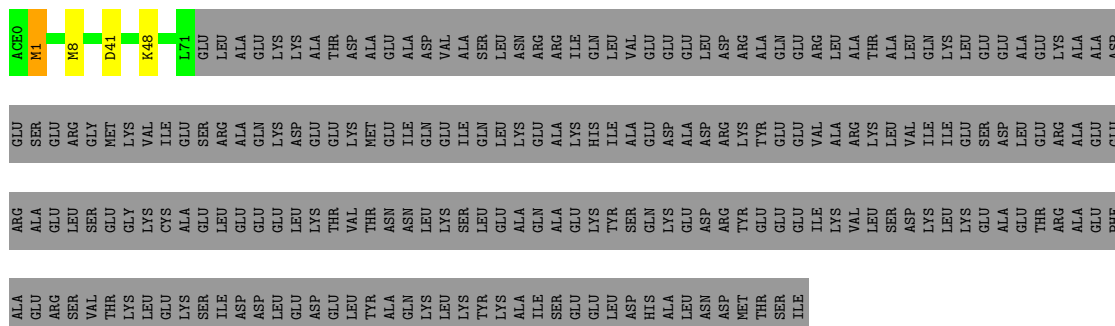
- Molecule 2: Tropomyosin alpha-1 chain



- Molecule 2: Tropomyosin alpha-1 chain



- Molecule 2: Tropomyosin alpha-1 chain

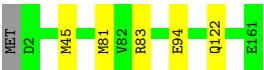


- Molecule 2: Tropomyosin alpha-1 chain

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LYS	ALA	GLU	MET
ALA	ARG	GLU	SER
LYS	LYS	SER	LIE
GLU	LYS	PRO	GLU
LEU	LYS	ALA	GLU
THR	LEU	PRO	VAL
GLN	LEU	ARG	VAL
SER	SER	ASN	GLU
GLN	ASN	SER	GLU
TYR	MET	PHE	GLU
TYR	MET	MET	TYR
LEU	LEU	PRO	GLU
ASN	GLU	ASN	GLU
ALA	GLY	LEU	GLU
GLU	GLY	VAL	GLU
GLU	TYR	PRO	GLN
LYS	LIE	PRO	GLU
PHE	LIE	PRO	GLU
ASP	GLN	LYS	GLU
LEU	LYS	LIE	ALA
LEU	LYS	ILE	ALA
GLN	GLN	PRO	ALA
GLU	ALA	ASP	VAL
GLU	GLN	GLY	GLU
PHE	THR	GLU	GLU
LYS	GLU	ARG	GLN
GLN	ARG	VAL	GLU
GLN	LYS	ASP	GLU
LYS	SER	PHE	ALA
TYR	GLY	ASP	ALA
GLU	LYS	D89	GLU
ILE	ARG	K93	GLU
ASN	GLN	K97	ASP
VAL	THR	K114	ALA
LEU	GLU	K115	ALA
LEU	ARG	E128	ALA
ASN	ASN	R151	THR
ASP	LYS	LEU	GLU
ASN	LIE	ALA	THR
ASN	LEU	ALA	ARG
GLN	GLU	GLU	ALA
LYS	VAL	ARG	GLU
VAL	SER	ARG	GLU
LYS	ARG	ALA	GLU
THR	LYS	ARG	ASP
ARG	VAL	ARG	GLU
GLY	LEU	ARG	GLU
LYS	ALA	GLU	GLU
ALA	ILE	GLU	GLU
LYS	ASP	GLU	GLU
VAL	HIS	LEU	ALA
THR	LEU	ASN	LYS
GLY	ASN	ARG	GLU
ARG	GLU	ARG	ALA
TRP	ASP	LYS	GLU
LYS	GLN	ALA	ASP
	LEU	GLU	GLY
	ARG	ASP	PRO
	GLN	THR	MET

[illegible][illegible]



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	23374	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 200	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	65	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (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: ACE, MG, ADP, HIC, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	C	0.26	0/2984	0.56	0/4040
1	D	0.26	0/2984	0.56	0/4040
1	E	0.28	0/2984	0.57	0/4040
1	F	0.26	0/2984	0.56	0/4040
1	G	0.27	0/2984	0.56	0/4040
1	H	0.27	0/2984	0.56	0/4040
1	I	0.26	0/2984	0.55	0/4040
1	J	0.27	0/2984	0.56	0/4040
1	K	0.26	0/2984	0.56	0/4040
1	L	0.26	0/2984	0.56	0/4040
1	M	0.26	0/2984	0.56	0/4040
1	N	0.26	0/2984	0.56	0/4040
1	O	0.26	0/2984	0.56	0/4040
1	P	0.27	0/2984	0.56	0/4040
1	Q	0.26	0/2984	0.56	0/4040
1	R	0.26	0/2984	0.56	0/4040
2	W	0.27	0/413	0.60	0/543
2	b	0.25	0/413	0.49	0/543
2	e	0.27	0/2156	0.51	1/2876 (0.0%)
2	f	0.28	0/2156	0.47	0/2876
2	g	0.26	0/569	0.54	0/752
2	h	0.25	0/569	0.46	0/752
2	i	0.28	0/1945	0.51	1/2594 (0.0%)
2	j	0.28	0/1945	0.47	0/2594
3	X	0.26	0/561	0.65	0/739
3	Y	0.33	0/649	0.62	0/861
3	c	0.26	0/561	0.65	0/739
3	d	0.34	0/649	0.63	0/861
4	V	0.26	0/1014	0.57	0/1352
4	a	0.25	0/1014	0.56	0/1352
5	U	0.28	0/1286	0.52	0/1719
5	Z	0.28	0/1286	0.52	0/1719

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.27	0/64930	0.55	2/87512 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	i	127	MET	CG-SD-CE	5.68	109.29	100.20
2	e	127	MET	CG-SD-CE	5.68	109.29	100.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	C	372/377 (99%)	352 (95%)	19 (5%)	1 (0%)	37	72
1	D	372/377 (99%)	352 (95%)	19 (5%)	1 (0%)	37	72
1	E	372/377 (99%)	351 (94%)	20 (5%)	1 (0%)	37	72
1	F	372/377 (99%)	352 (95%)	19 (5%)	1 (0%)	37	72
1	G	372/377 (99%)	352 (95%)	19 (5%)	1 (0%)	37	72
1	H	372/377 (99%)	352 (95%)	19 (5%)	1 (0%)	37	72
1	I	372/377 (99%)	351 (94%)	20 (5%)	1 (0%)	37	72
1	J	372/377 (99%)	352 (95%)	19 (5%)	1 (0%)	37	72
1	K	372/377 (99%)	352 (95%)	19 (5%)	1 (0%)	37	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	372/377 (99%)	352 (95%)	19 (5%)	1 (0%)	37	72
1	M	372/377 (99%)	352 (95%)	19 (5%)	1 (0%)	37	72
1	N	372/377 (99%)	352 (95%)	19 (5%)	1 (0%)	37	72
1	O	372/377 (99%)	352 (95%)	19 (5%)	1 (0%)	37	72
1	P	372/377 (99%)	352 (95%)	19 (5%)	1 (0%)	37	72
1	Q	372/377 (99%)	352 (95%)	19 (5%)	1 (0%)	37	72
1	R	372/377 (99%)	352 (95%)	19 (5%)	1 (0%)	37	72
2	W	51/285 (18%)	50 (98%)	0	1 (2%)	6	31
2	b	51/285 (18%)	51 (100%)	0	0	100	100
2	e	265/285 (93%)	265 (100%)	0	0	100	100
2	f	265/285 (93%)	265 (100%)	0	0	100	100
2	g	70/285 (25%)	69 (99%)	0	1 (1%)	9	40
2	h	70/285 (25%)	70 (100%)	0	0	100	100
2	i	238/285 (84%)	238 (100%)	0	0	100	100
2	j	238/285 (84%)	238 (100%)	0	0	100	100
3	X	61/288 (21%)	61 (100%)	0	0	100	100
3	Y	72/288 (25%)	70 (97%)	2 (3%)	0	100	100
3	c	61/288 (21%)	61 (100%)	0	0	100	100
3	d	72/288 (25%)	70 (97%)	2 (3%)	0	100	100
4	V	124/210 (59%)	117 (94%)	5 (4%)	2 (2%)	8	37
4	a	124/210 (59%)	117 (94%)	5 (4%)	2 (2%)	8	37
5	U	158/161 (98%)	140 (89%)	18 (11%)	0	100	100
5	Z	158/161 (98%)	140 (89%)	18 (11%)	0	100	100
All	All	8030/10206 (79%)	7652 (95%)	356 (4%)	22 (0%)	38	72

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	182	GLY
1	D	182	GLY
1	E	182	GLY
1	F	182	GLY
1	G	182	GLY
1	H	182	GLY

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Mol	Chain	Res	Type
1	I	182	GLY
1	J	182	GLY
1	K	182	GLY
1	L	182	GLY
1	M	182	GLY
1	N	182	GLY
1	O	182	GLY
1	P	182	GLY
1	Q	182	GLY
1	R	182	GLY
2	W	1	MET
4	V	138	LYS
2	g	1	MET
4	a	138	LYS
4	V	137	GLY
4	a	137	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	C	317/319 (99%)	303 (96%)	14 (4%)	24	46
1	D	317/319 (99%)	306 (96%)	11 (4%)	31	52
1	E	317/319 (99%)	304 (96%)	13 (4%)	26	48
1	F	317/319 (99%)	304 (96%)	13 (4%)	26	48
1	G	317/319 (99%)	304 (96%)	13 (4%)	26	48
1	H	317/319 (99%)	304 (96%)	13 (4%)	26	48
1	I	317/319 (99%)	303 (96%)	14 (4%)	24	46
1	J	317/319 (99%)	303 (96%)	14 (4%)	24	46
1	K	317/319 (99%)	306 (96%)	11 (4%)	31	52
1	L	317/319 (99%)	306 (96%)	11 (4%)	31	52
1	M	317/319 (99%)	304 (96%)	13 (4%)	26	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	317/319 (99%)	304 (96%)	13 (4%)	26	48
1	O	317/319 (99%)	305 (96%)	12 (4%)	28	49
1	P	317/319 (99%)	305 (96%)	12 (4%)	28	49
1	Q	317/319 (99%)	304 (96%)	13 (4%)	26	48
1	R	317/319 (99%)	304 (96%)	13 (4%)	26	48
2	W	44/245 (18%)	40 (91%)	4 (9%)	7	24
2	b	44/245 (18%)	42 (96%)	2 (4%)	23	45
2	e	229/245 (94%)	223 (97%)	6 (3%)	41	60
2	f	229/245 (94%)	225 (98%)	4 (2%)	56	72
2	g	61/245 (25%)	57 (93%)	4 (7%)	14	35
2	h	61/245 (25%)	59 (97%)	2 (3%)	33	53
2	i	208/245 (85%)	203 (98%)	5 (2%)	44	63
2	j	208/245 (85%)	204 (98%)	4 (2%)	52	70
3	X	59/256 (23%)	54 (92%)	5 (8%)	8	27
3	Y	69/256 (27%)	61 (88%)	8 (12%)	4	17
3	c	59/256 (23%)	54 (92%)	5 (8%)	8	27
3	d	69/256 (27%)	62 (90%)	7 (10%)	6	21
4	V	106/176 (60%)	104 (98%)	2 (2%)	52	70
4	a	106/176 (60%)	104 (98%)	2 (2%)	52	70
5	U	141/142 (99%)	136 (96%)	5 (4%)	31	52
5	Z	141/142 (99%)	136 (96%)	5 (4%)	31	52
All	All	6906/8724 (79%)	6633 (96%)	273 (4%)	29	48

All (273) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	41	GLN
1	C	44	MET
1	C	115	ASN
1	C	118	LYS
1	C	175	ILE
1	C	176	MET
1	C	205	GLU
1	C	207	GLU
1	C	250	ILE

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Mol	Chain	Res	Type
1	C	269	MET
1	C	326	LYS
1	C	344	SER
1	C	355	MET
1	C	372	ARG
1	D	44	MET
1	D	115	ASN
1	D	118	LYS
1	D	175	ILE
1	D	176	MET
1	D	205	GLU
1	D	250	ILE
1	D	269	MET
1	D	326	LYS
1	D	344	SER
1	D	372	ARG
1	E	44	MET
1	E	115	ASN
1	E	118	LYS
1	E	169	TYR
1	E	175	ILE
1	E	176	MET
1	E	205	GLU
1	E	250	ILE
1	E	269	MET
1	E	326	LYS
1	E	344	SER
1	E	355	MET
1	E	372	ARG
1	F	44	MET
1	F	115	ASN
1	F	118	LYS
1	F	169	TYR
1	F	175	ILE
1	F	176	MET
1	F	205	GLU
1	F	250	ILE
1	F	269	MET
1	F	326	LYS
1	F	344	SER
1	F	355	MET
1	F	372	ARG

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Mol	Chain	Res	Type
1	G	44	MET
1	G	115	ASN
1	G	118	LYS
1	G	175	ILE
1	G	176	MET
1	G	205	GLU
1	G	250	ILE
1	G	269	MET
1	G	326	LYS
1	G	344	SER
1	G	355	MET
1	G	361	GLU
1	G	372	ARG
1	H	44	MET
1	H	115	ASN
1	H	118	LYS
1	H	169	TYR
1	H	175	ILE
1	H	176	MET
1	H	205	GLU
1	H	250	ILE
1	H	269	MET
1	H	326	LYS
1	H	344	SER
1	H	355	MET
1	H	372	ARG
1	I	39	ARG
1	I	44	MET
1	I	115	ASN
1	I	118	LYS
1	I	169	TYR
1	I	175	ILE
1	I	176	MET
1	I	205	GLU
1	I	250	ILE
1	I	269	MET
1	I	326	LYS
1	I	344	SER
1	I	355	MET
1	I	372	ARG
1	J	44	MET
1	J	115	ASN

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Mol	Chain	Res	Type
1	J	118	LYS
1	J	166	TYR
1	J	175	ILE
1	J	176	MET
1	J	205	GLU
1	J	250	ILE
1	J	269	MET
1	J	326	LYS
1	J	344	SER
1	J	355	MET
1	J	361	GLU
1	J	372	ARG
1	K	44	MET
1	K	115	ASN
1	K	118	LYS
1	K	175	ILE
1	K	176	MET
1	K	205	GLU
1	K	250	ILE
1	K	269	MET
1	K	326	LYS
1	K	344	SER
1	K	372	ARG
1	L	44	MET
1	L	115	ASN
1	L	118	LYS
1	L	175	ILE
1	L	176	MET
1	L	205	GLU
1	L	250	ILE
1	L	269	MET
1	L	326	LYS
1	L	344	SER
1	L	372	ARG
1	M	44	MET
1	M	115	ASN
1	M	118	LYS
1	M	175	ILE
1	M	176	MET
1	M	205	GLU
1	M	250	ILE
1	M	269	MET

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Mol	Chain	Res	Type
1	M	326	LYS
1	M	344	SER
1	M	355	MET
1	M	361	GLU
1	M	372	ARG
1	N	44	MET
1	N	115	ASN
1	N	118	LYS
1	N	166	TYR
1	N	175	ILE
1	N	176	MET
1	N	205	GLU
1	N	250	ILE
1	N	269	MET
1	N	326	LYS
1	N	344	SER
1	N	355	MET
1	N	372	ARG
1	O	44	MET
1	O	115	ASN
1	O	118	LYS
1	O	175	ILE
1	O	176	MET
1	O	205	GLU
1	O	250	ILE
1	O	269	MET
1	O	326	LYS
1	O	344	SER
1	O	355	MET
1	O	372	ARG
1	P	44	MET
1	P	115	ASN
1	P	118	LYS
1	P	175	ILE
1	P	176	MET
1	P	205	GLU
1	P	250	ILE
1	P	269	MET
1	P	326	LYS
1	P	344	SER
1	P	355	MET
1	P	372	ARG

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Mol	Chain	Res	Type
1	Q	44	MET
1	Q	115	ASN
1	Q	118	LYS
1	Q	166	TYR
1	Q	175	ILE
1	Q	176	MET
1	Q	205	GLU
1	Q	250	ILE
1	Q	269	MET
1	Q	326	LYS
1	Q	344	SER
1	Q	355	MET
1	Q	372	ARG
1	R	37	ARG
1	R	44	MET
1	R	115	ASN
1	R	118	LYS
1	R	169	TYR
1	R	175	ILE
1	R	176	MET
1	R	205	GLU
1	R	250	ILE
1	R	269	MET
1	R	326	LYS
1	R	344	SER
1	R	372	ARG
2	e	153	HIS
2	e	210	GLN
2	e	263	GLN
2	e	276	HIS
2	e	279	ASN
2	e	281	MET
2	f	135	GLN
2	f	136	LYS
2	f	147	GLN
2	f	281	MET
2	W	1	MET
2	W	8	MET
2	W	41	ASP
2	W	48	LYS
2	b	8	MET
2	b	9	GLN

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Mol	Chain	Res	Type
3	X	93	LYS
3	X	97	LYS
3	X	114	LYS
3	X	115	LYS
3	X	128	GLU
3	Y	206	GLU
3	Y	214	GLU
3	Y	215	ARG
3	Y	217	LYS
3	Y	218	VAL
3	Y	222	ASP
3	Y	227	ASP
3	Y	231	GLU
4	V	145	ARG
4	V	146	ARG
5	U	45	MET
5	U	81	MET
5	U	83	ARG
5	U	94	GLU
5	U	122	GLN
2	i	153	HIS
2	i	210	GLN
2	i	276	HIS
2	i	279	ASN
2	i	281	MET
2	j	135	GLN
2	j	136	LYS
2	j	147	GLN
2	j	281	MET
2	g	1	MET
2	g	8	MET
2	g	41	ASP
2	g	48	LYS
2	h	8	MET
2	h	9	GLN
3	c	93	LYS
3	c	97	LYS
3	c	114	LYS
3	c	115	LYS
3	c	128	GLU
3	d	206	GLU
3	d	215	ARG

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Mol	Chain	Res	Type
3	d	217	LYS
3	d	218	VAL
3	d	222	ASP
3	d	227	ASP
3	d	231	GLU
4	a	145	ARG
4	a	146	ARG
5	Z	45	MET
5	Z	81	MET
5	Z	83	ARG
5	Z	94	GLU
5	Z	122	GLN

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

16 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	C	73	1	8,11,12	1.67	2 (25%)	5,14,16	0.91	0
1	HIC	G	73	1	8,11,12	1.65	2 (25%)	5,14,16	0.91	0
1	HIC	P	73	1	8,11,12	1.67	2 (25%)	5,14,16	0.92	0
1	HIC	H	73	1	8,11,12	1.66	2 (25%)	5,14,16	0.91	0
1	HIC	E	73	1	8,11,12	1.64	1 (12%)	5,14,16	0.89	0
1	HIC	M	73	1	8,11,12	1.67	2 (25%)	5,14,16	0.91	0
1	HIC	R	73	1	8,11,12	1.67	2 (25%)	5,14,16	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	HIC	F	73	1	8,11,12	1.67	2 (25%)	5,14,16	0.89	0
1	HIC	Q	73	1	8,11,12	1.66	2 (25%)	5,14,16	0.90	0
1	HIC	D	73	1	8,11,12	1.66	2 (25%)	5,14,16	0.90	0
1	HIC	K	73	1	8,11,12	1.65	2 (25%)	5,14,16	0.92	0
1	HIC	O	73	1	8,11,12	1.65	1 (12%)	5,14,16	0.90	0
1	HIC	J	73	1	8,11,12	1.65	2 (25%)	5,14,16	0.89	0
1	HIC	N	73	1	8,11,12	1.65	1 (12%)	5,14,16	0.89	0
1	HIC	L	73	1	8,11,12	1.65	2 (25%)	5,14,16	0.88	0
1	HIC	I	73	1	8,11,12	1.66	2 (25%)	5,14,16	0.92	0

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	C	73	1	-	2/5/6/8	0/1/1/1
1	HIC	G	73	1	-	2/5/6/8	0/1/1/1
1	HIC	P	73	1	-	2/5/6/8	0/1/1/1
1	HIC	H	73	1	-	2/5/6/8	0/1/1/1
1	HIC	E	73	1	-	2/5/6/8	0/1/1/1
1	HIC	M	73	1	-	2/5/6/8	0/1/1/1
1	HIC	R	73	1	-	2/5/6/8	0/1/1/1
1	HIC	F	73	1	-	2/5/6/8	0/1/1/1
1	HIC	Q	73	1	-	2/5/6/8	0/1/1/1
1	HIC	D	73	1	-	2/5/6/8	0/1/1/1
1	HIC	K	73	1	-	2/5/6/8	0/1/1/1
1	HIC	O	73	1	-	2/5/6/8	0/1/1/1
1	HIC	J	73	1	-	2/5/6/8	0/1/1/1
1	HIC	N	73	1	-	2/5/6/8	0/1/1/1
1	HIC	L	73	1	-	2/5/6/8	0/1/1/1
1	HIC	I	73	1	-	2/5/6/8	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	73	HIC	CD2-CG	3.69	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	73	HIC	CD2-CG	3.69	1.41	1.36
1	C	73	HIC	CD2-CG	3.67	1.41	1.36
1	F	73	HIC	CD2-CG	3.67	1.41	1.36
1	Q	73	HIC	CD2-CG	3.67	1.41	1.36
1	R	73	HIC	CD2-CG	3.67	1.41	1.36
1	D	73	HIC	CD2-CG	3.66	1.41	1.36
1	O	73	HIC	CD2-CG	3.66	1.41	1.36
1	E	73	HIC	CD2-CG	3.66	1.41	1.36
1	I	73	HIC	CD2-CG	3.64	1.41	1.36
1	K	73	HIC	CD2-CG	3.64	1.41	1.36
1	N	73	HIC	CD2-CG	3.64	1.41	1.36
1	H	73	HIC	CD2-CG	3.63	1.41	1.36
1	G	73	HIC	CD2-CG	3.63	1.41	1.36
1	J	73	HIC	CD2-CG	3.62	1.41	1.36
1	L	73	HIC	CD2-CG	3.62	1.41	1.36
1	F	73	HIC	CZ-NE2	-2.05	1.42	1.48
1	I	73	HIC	CZ-NE2	-2.05	1.42	1.48
1	L	73	HIC	CZ-NE2	-2.04	1.42	1.48
1	R	73	HIC	CZ-NE2	-2.03	1.42	1.48
1	M	73	HIC	CZ-NE2	-2.02	1.42	1.48
1	H	73	HIC	CZ-NE2	-2.02	1.42	1.48
1	G	73	HIC	CZ-NE2	-2.02	1.42	1.48
1	C	73	HIC	CZ-NE2	-2.01	1.42	1.48
1	Q	73	HIC	CZ-NE2	-2.01	1.42	1.48
1	D	73	HIC	CZ-NE2	-2.01	1.42	1.48
1	K	73	HIC	CZ-NE2	-2.01	1.42	1.48
1	J	73	HIC	CZ-NE2	-2.00	1.42	1.48
1	P	73	HIC	CZ-NE2	-2.00	1.42	1.48

There are no bond angle outliers.

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	73	HIC	CA-CB-CG-ND1
1	C	73	HIC	CA-CB-CG-CD2
1	D	73	HIC	CA-CB-CG-ND1
1	D	73	HIC	CA-CB-CG-CD2
1	E	73	HIC	CA-CB-CG-ND1
1	E	73	HIC	CA-CB-CG-CD2
1	F	73	HIC	CA-CB-CG-ND1

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Mol	Chain	Res	Type	Atoms
1	F	73	HIC	CA-CB-CG-CD2
1	G	73	HIC	CA-CB-CG-ND1
1	G	73	HIC	CA-CB-CG-CD2
1	H	73	HIC	CA-CB-CG-ND1
1	H	73	HIC	CA-CB-CG-CD2
1	I	73	HIC	CA-CB-CG-ND1
1	I	73	HIC	CA-CB-CG-CD2
1	J	73	HIC	CA-CB-CG-ND1
1	J	73	HIC	CA-CB-CG-CD2
1	K	73	HIC	CA-CB-CG-ND1
1	K	73	HIC	CA-CB-CG-CD2
1	L	73	HIC	CA-CB-CG-ND1
1	L	73	HIC	CA-CB-CG-CD2
1	M	73	HIC	CA-CB-CG-ND1
1	M	73	HIC	CA-CB-CG-CD2
1	N	73	HIC	CA-CB-CG-ND1
1	N	73	HIC	CA-CB-CG-CD2
1	O	73	HIC	CA-CB-CG-ND1
1	O	73	HIC	CA-CB-CG-CD2
1	P	73	HIC	CA-CB-CG-ND1
1	P	73	HIC	CA-CB-CG-CD2
1	Q	73	HIC	CA-CB-CG-ND1
1	Q	73	HIC	CA-CB-CG-CD2
1	R	73	HIC	CA-CB-CG-ND1
1	R	73	HIC	CA-CB-CG-CD2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 38 ligands modelled in this entry, 22 are monoatomic - leaving 16 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	$\# Z > 2$
6	ADP	D	401	7	24,29,29	0.90	0	29,45,45	1.20	2 (6%)
6	ADP	J	401	7	24,29,29	0.90	0	29,45,45	1.20	2 (6%)
6	ADP	K	401	7	24,29,29	0.90	0	29,45,45	1.21	2 (6%)
6	ADP	C	401	7	24,29,29	0.90	0	29,45,45	1.20	2 (6%)
6	ADP	N	401	7	24,29,29	0.90	0	29,45,45	1.20	2 (6%)
6	ADP	L	401	7	24,29,29	0.91	0	29,45,45	1.19	2 (6%)
6	ADP	M	401	7	24,29,29	0.90	0	29,45,45	1.20	2 (6%)
6	ADP	P	401	7	24,29,29	0.90	0	29,45,45	1.20	2 (6%)
6	ADP	F	401	7	24,29,29	0.91	0	29,45,45	1.20	2 (6%)
6	ADP	R	401	7	24,29,29	0.91	0	29,45,45	1.20	2 (6%)
6	ADP	O	401	7	24,29,29	0.90	0	29,45,45	1.20	2 (6%)
6	ADP	H	401	7	24,29,29	0.90	0	29,45,45	1.20	2 (6%)
6	ADP	I	401	7	24,29,29	0.91	0	29,45,45	1.20	2 (6%)
6	ADP	Q	401	7	24,29,29	0.90	0	29,45,45	1.20	2 (6%)
6	ADP	E	401	7	24,29,29	0.90	0	29,45,45	1.20	2 (6%)
6	ADP	G	401	7	24,29,29	0.92	0	29,45,45	1.20	2 (6%)

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
6	ADP	D	401	7	-	0/12/32/32	0/3/3/3
6	ADP	J	401	7	-	0/12/32/32	0/3/3/3
6	ADP	K	401	7	-	0/12/32/32	0/3/3/3
6	ADP	C	401	7	-	0/12/32/32	0/3/3/3
6	ADP	N	401	7	-	0/12/32/32	0/3/3/3
6	ADP	L	401	7	-	0/12/32/32	0/3/3/3
6	ADP	M	401	7	-	0/12/32/32	0/3/3/3
6	ADP	P	401	7	-	0/12/32/32	0/3/3/3
6	ADP	F	401	7	-	0/12/32/32	0/3/3/3
6	ADP	R	401	7	-	0/12/32/32	0/3/3/3
6	ADP	O	401	7	-	0/12/32/32	0/3/3/3
6	ADP	H	401	7	-	0/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ADP	I	401	7	-	0/12/32/32	0/3/3/3
6	ADP	Q	401	7	-	0/12/32/32	0/3/3/3
6	ADP	E	401	7	-	0/12/32/32	0/3/3/3
6	ADP	G	401	7	-	0/12/32/32	0/3/3/3

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	K	401	ADP	N3-C2-N1	-3.65	123.72	128.67
6	Q	401	ADP	N3-C2-N1	-3.64	123.73	128.67
6	E	401	ADP	N3-C2-N1	-3.64	123.73	128.67
6	F	401	ADP	N3-C2-N1	-3.64	123.73	128.67
6	P	401	ADP	N3-C2-N1	-3.63	123.74	128.67
6	C	401	ADP	N3-C2-N1	-3.63	123.75	128.67
6	G	401	ADP	N3-C2-N1	-3.63	123.75	128.67
6	I	401	ADP	N3-C2-N1	-3.63	123.75	128.67
6	N	401	ADP	N3-C2-N1	-3.62	123.77	128.67
6	D	401	ADP	N3-C2-N1	-3.61	123.77	128.67
6	J	401	ADP	N3-C2-N1	-3.61	123.77	128.67
6	R	401	ADP	N3-C2-N1	-3.61	123.77	128.67
6	M	401	ADP	N3-C2-N1	-3.59	123.80	128.67
6	O	401	ADP	N3-C2-N1	-3.59	123.81	128.67
6	L	401	ADP	N3-C2-N1	-3.58	123.81	128.67
6	H	401	ADP	N3-C2-N1	-3.57	123.82	128.67
6	K	401	ADP	C4-C5-N7	-2.62	106.57	109.34
6	R	401	ADP	C4-C5-N7	-2.61	106.58	109.34
6	L	401	ADP	C4-C5-N7	-2.61	106.58	109.34
6	Q	401	ADP	C4-C5-N7	-2.61	106.58	109.34
6	H	401	ADP	C4-C5-N7	-2.60	106.59	109.34
6	J	401	ADP	C4-C5-N7	-2.59	106.60	109.34
6	C	401	ADP	C4-C5-N7	-2.59	106.60	109.34
6	I	401	ADP	C4-C5-N7	-2.58	106.61	109.34
6	M	401	ADP	C4-C5-N7	-2.58	106.61	109.34
6	O	401	ADP	C4-C5-N7	-2.58	106.61	109.34
6	E	401	ADP	C4-C5-N7	-2.58	106.61	109.34
6	G	401	ADP	C4-C5-N7	-2.58	106.61	109.34
6	N	401	ADP	C4-C5-N7	-2.58	106.62	109.34
6	D	401	ADP	C4-C5-N7	-2.57	106.62	109.34
6	P	401	ADP	C4-C5-N7	-2.56	106.64	109.34
6	F	401	ADP	C4-C5-N7	-2.55	106.64	109.34

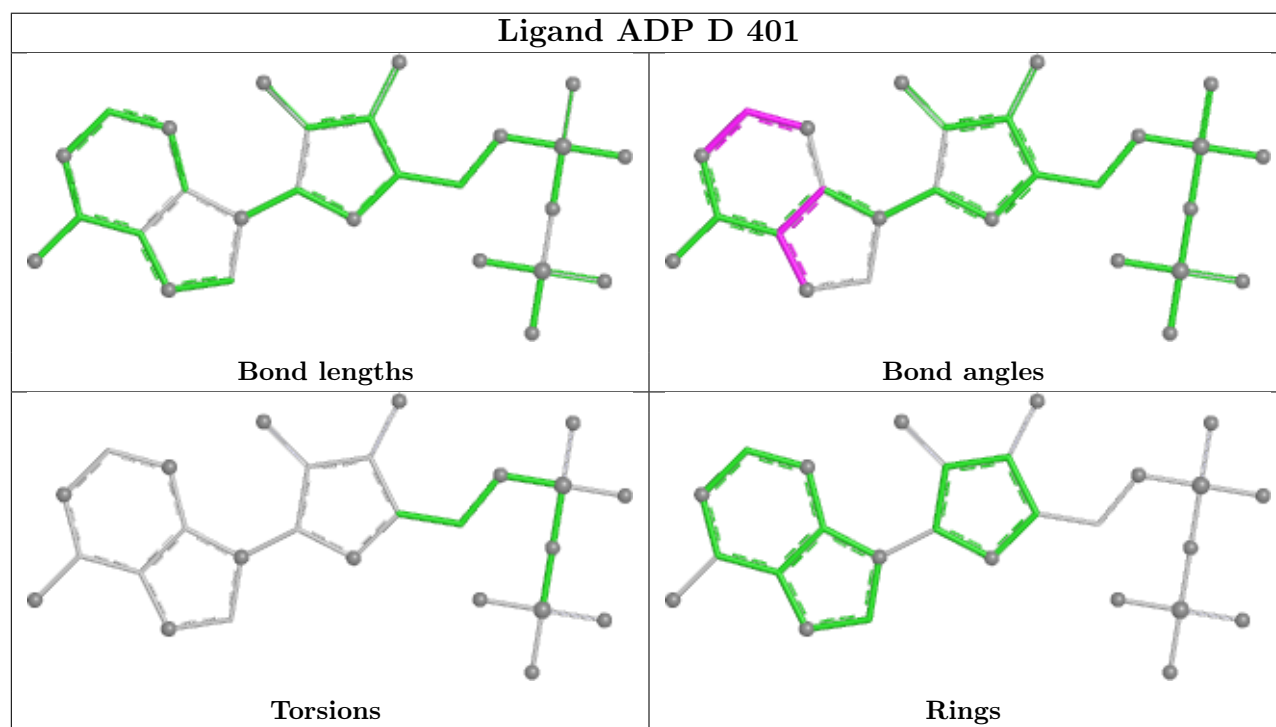
There are no chirality outliers.

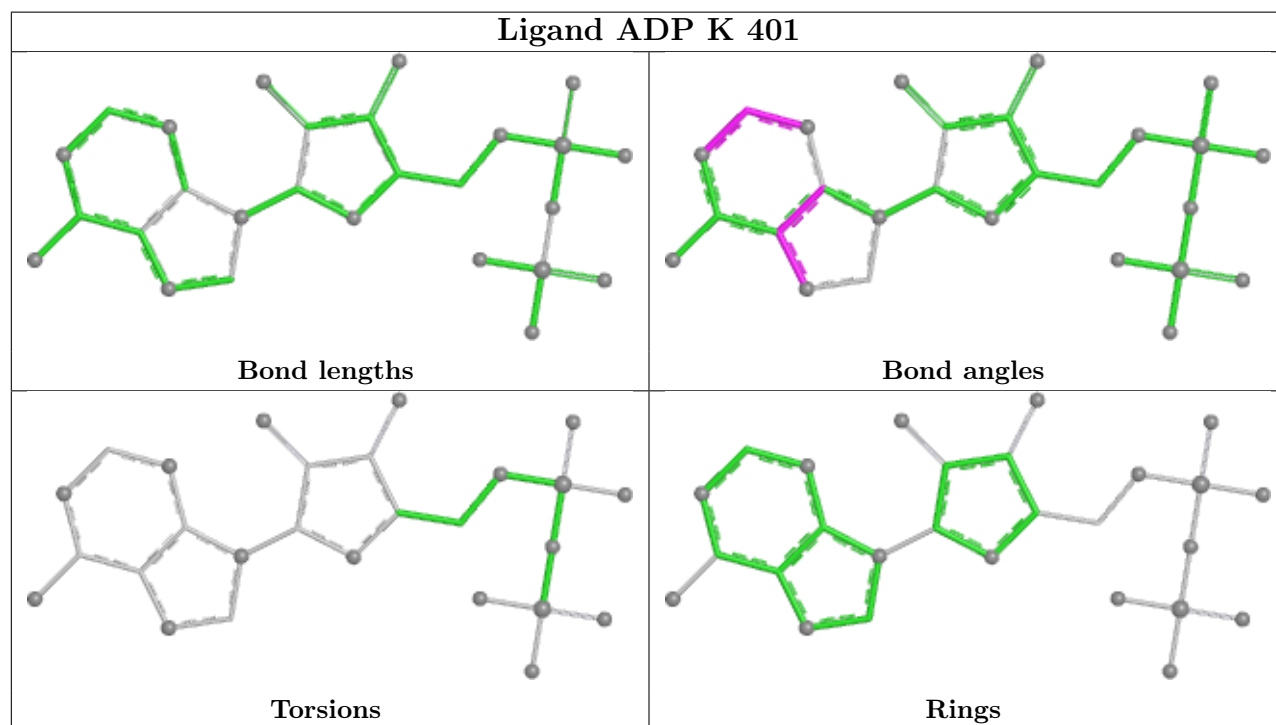
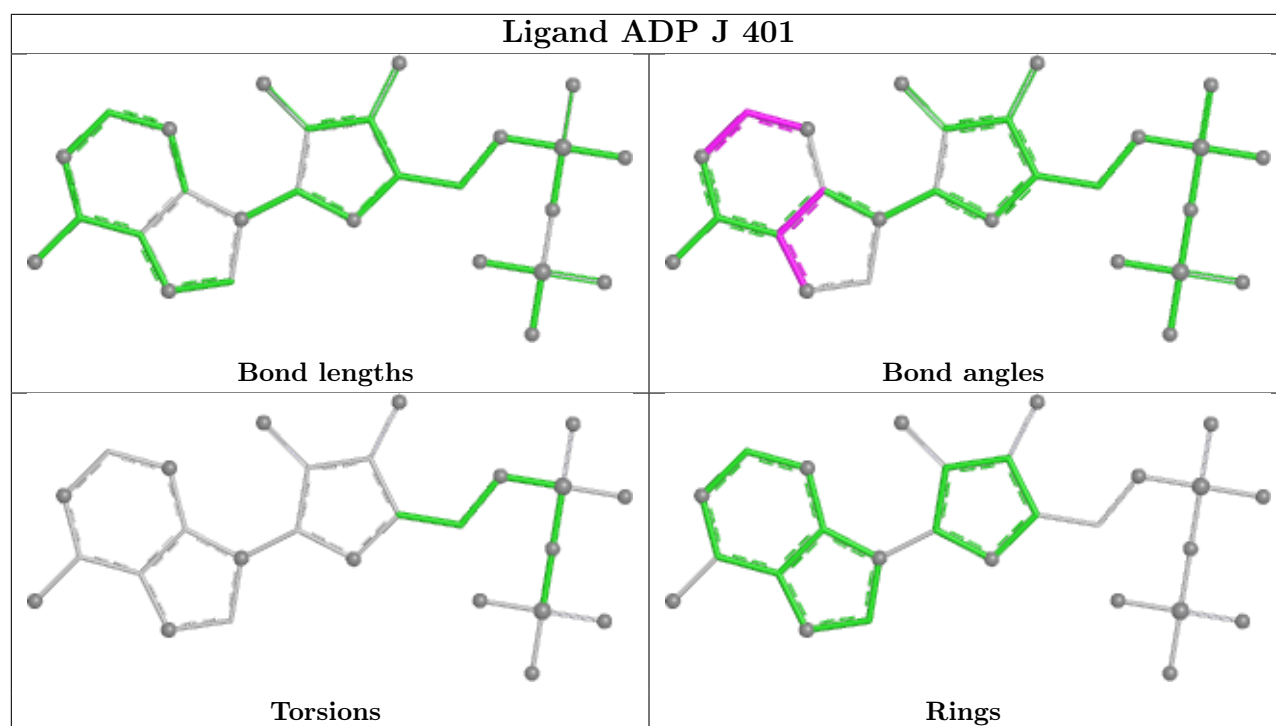
There are no torsion outliers.

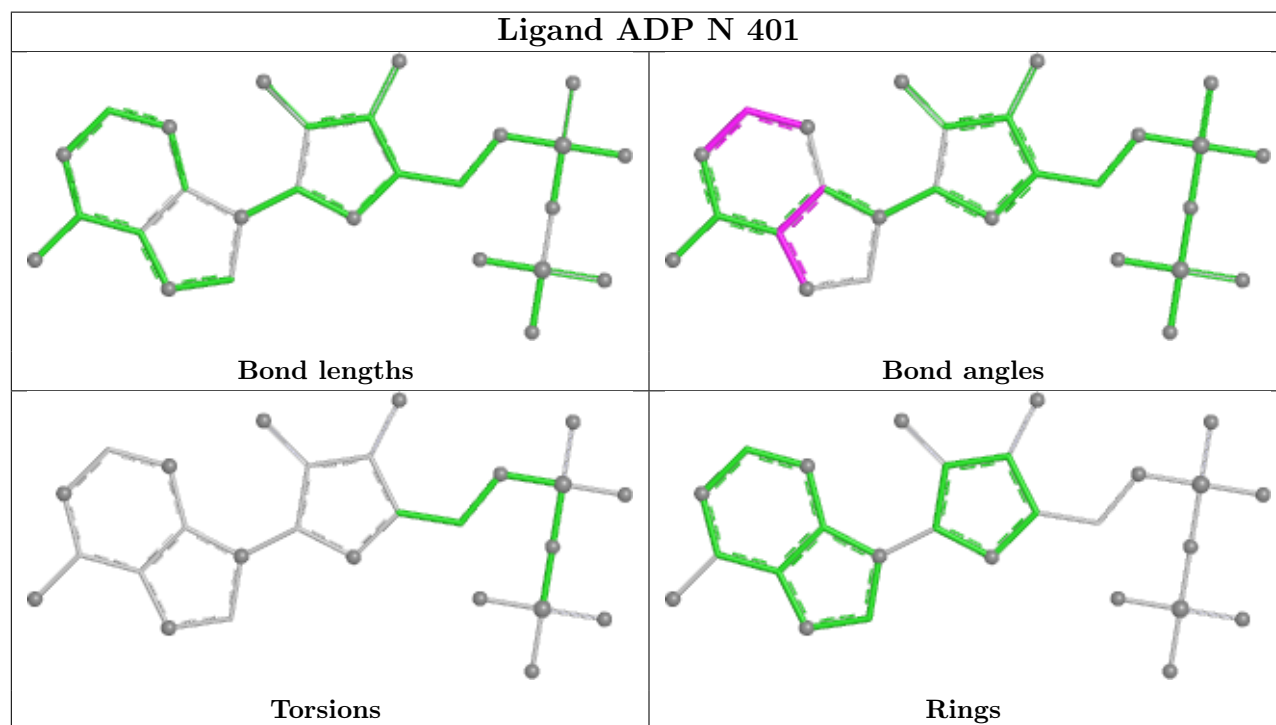
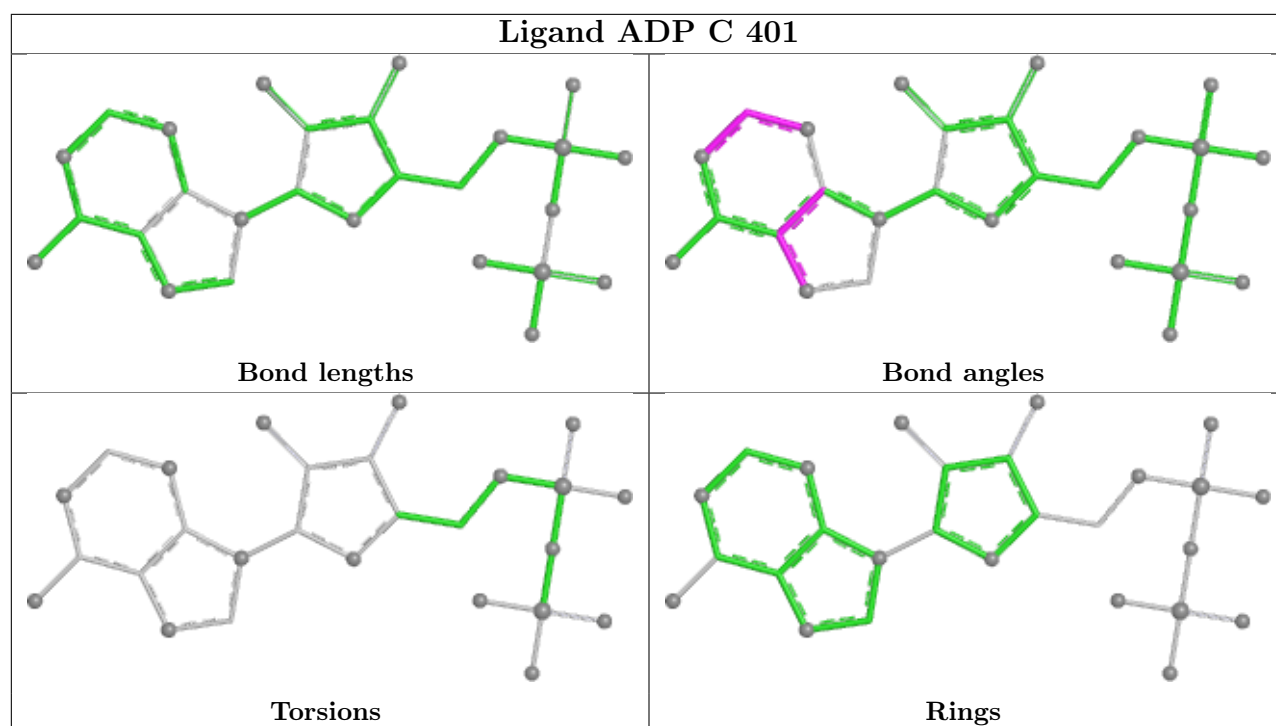
There are no ring outliers.

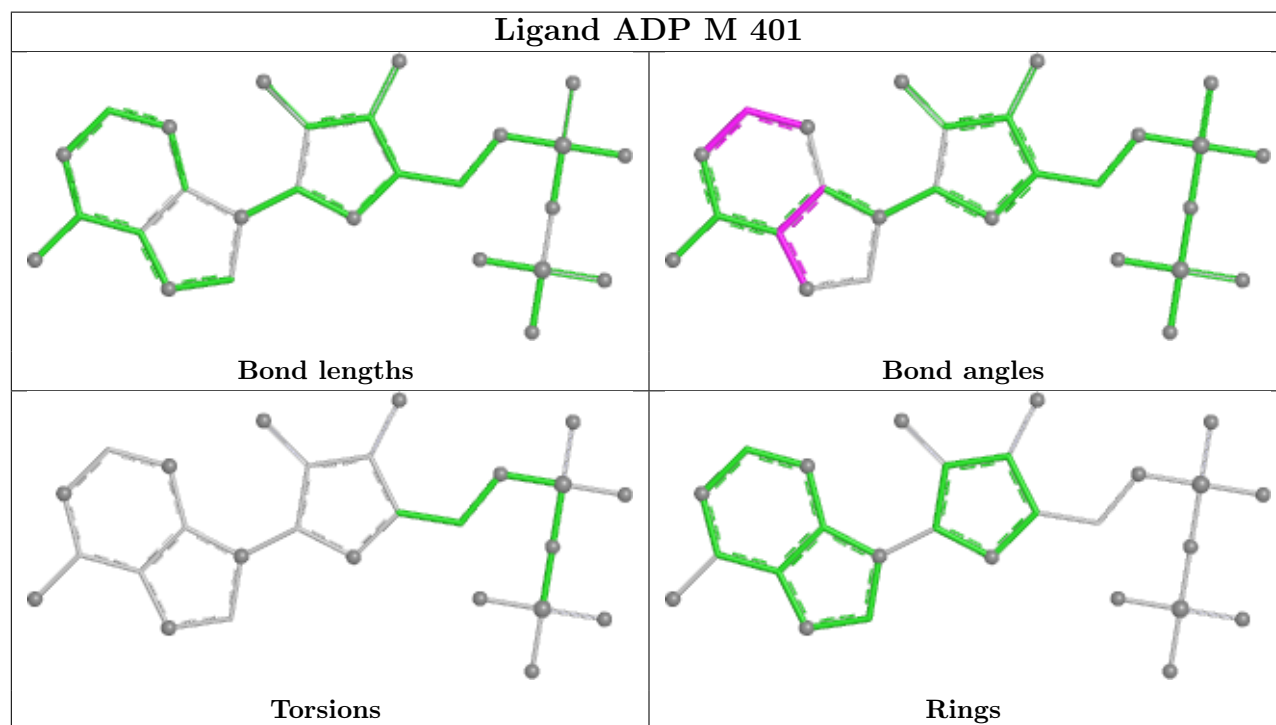
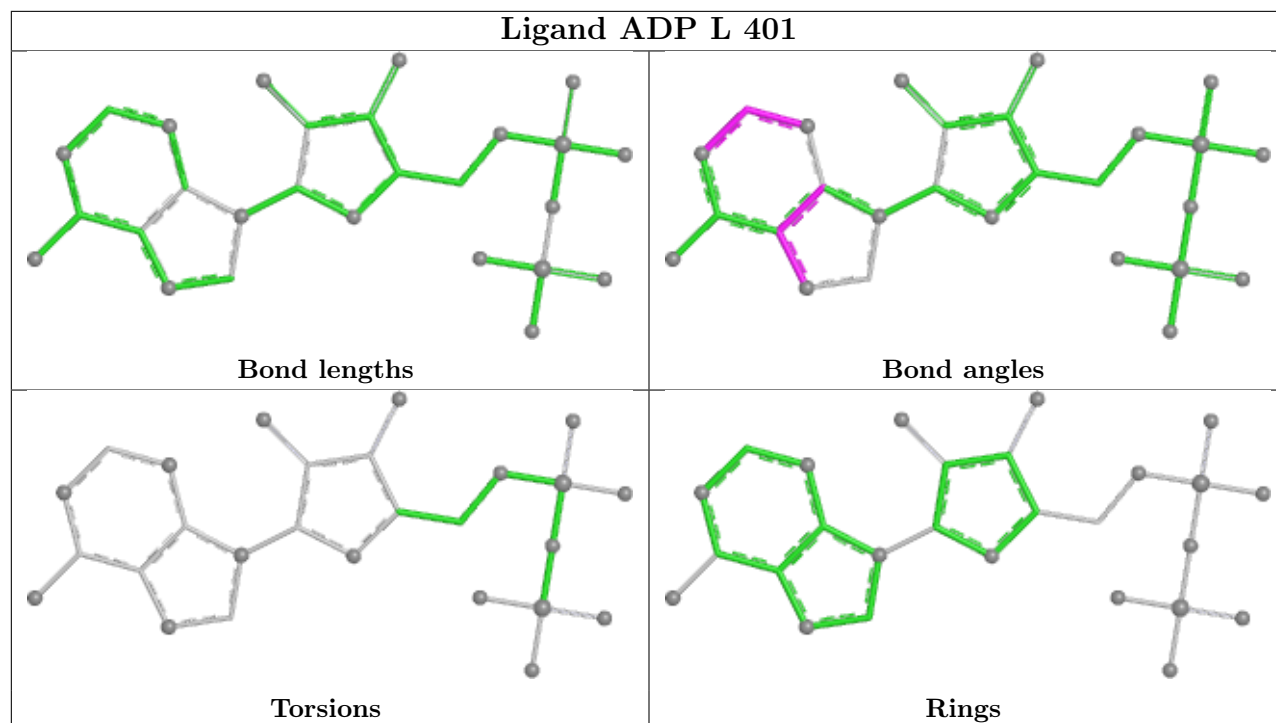
No monomer is involved in short contacts.

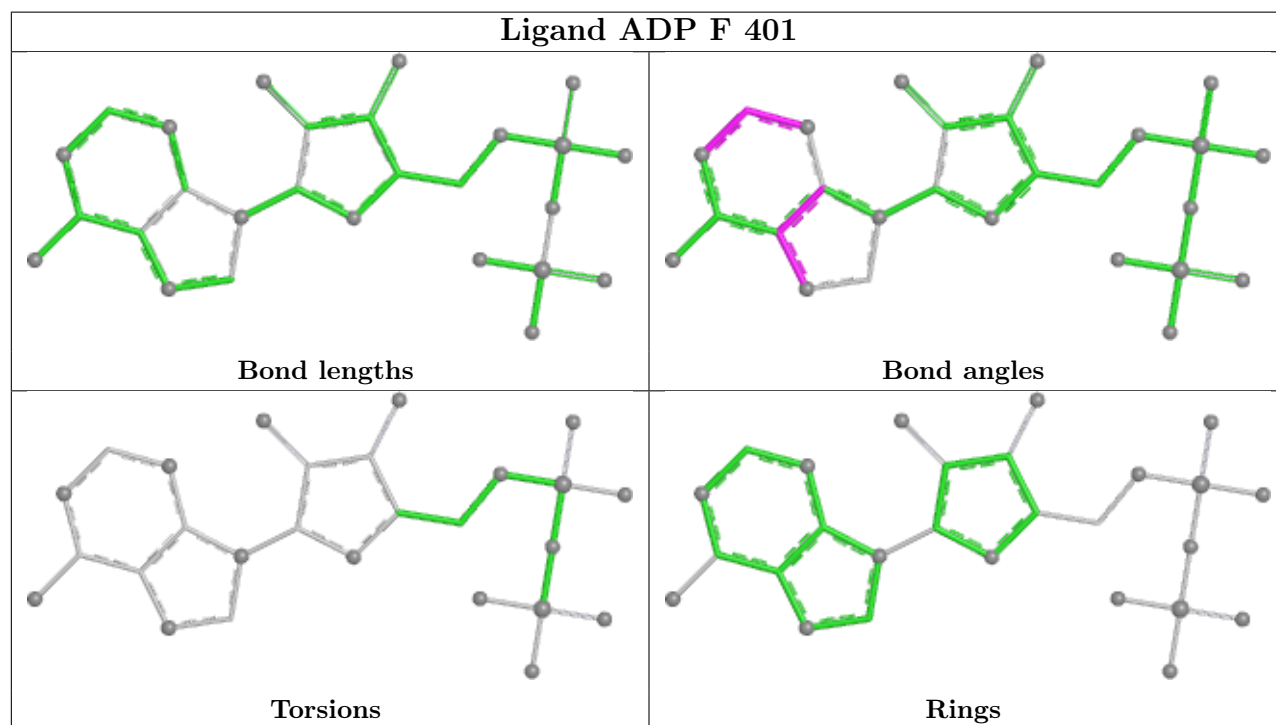
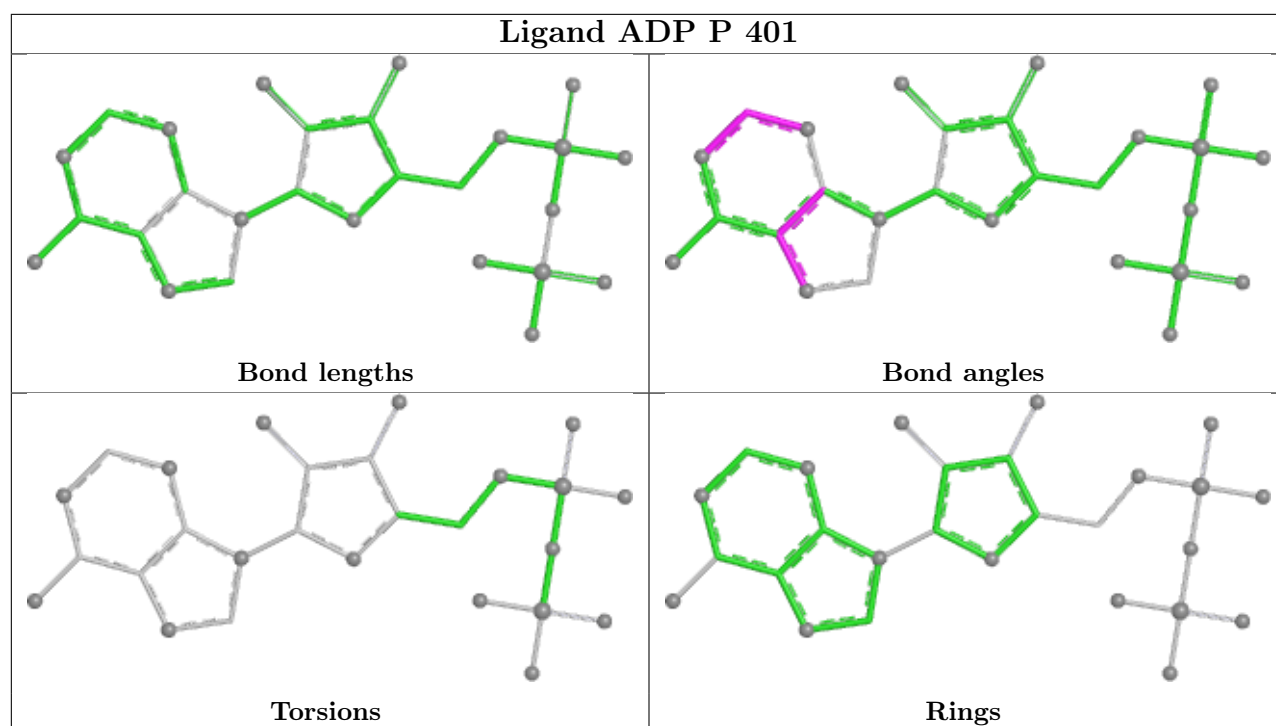
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

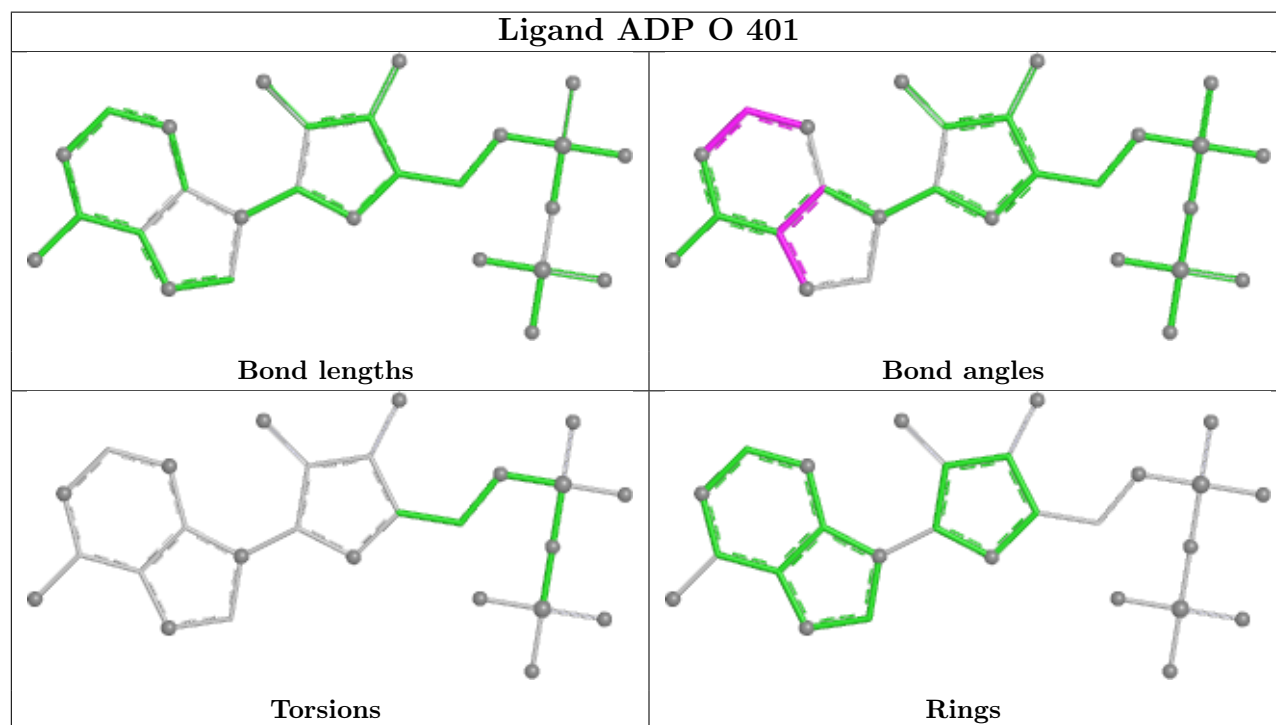
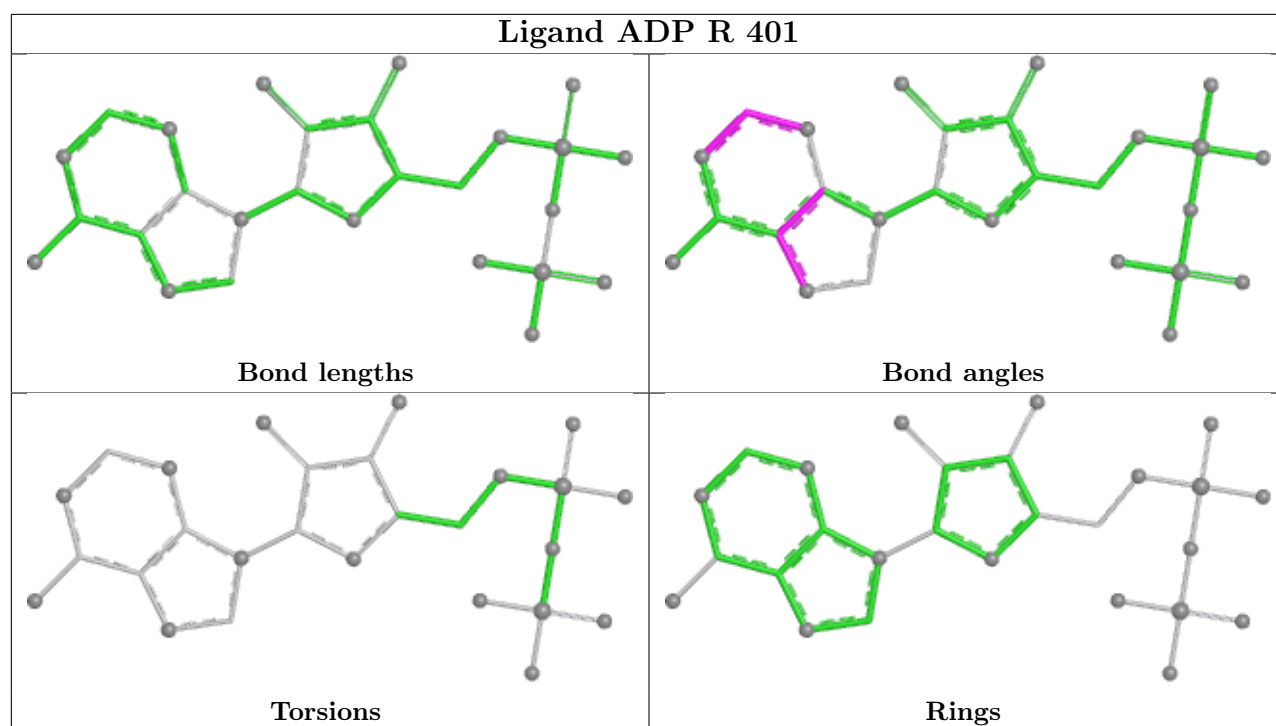


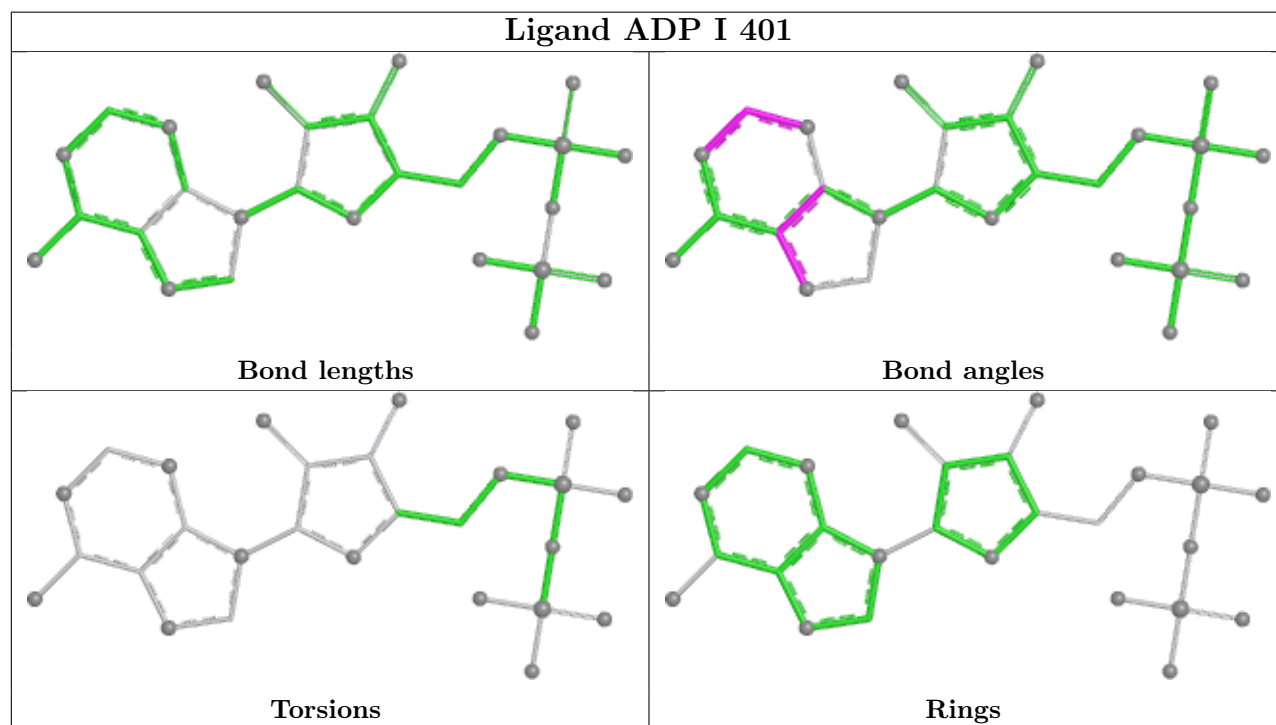
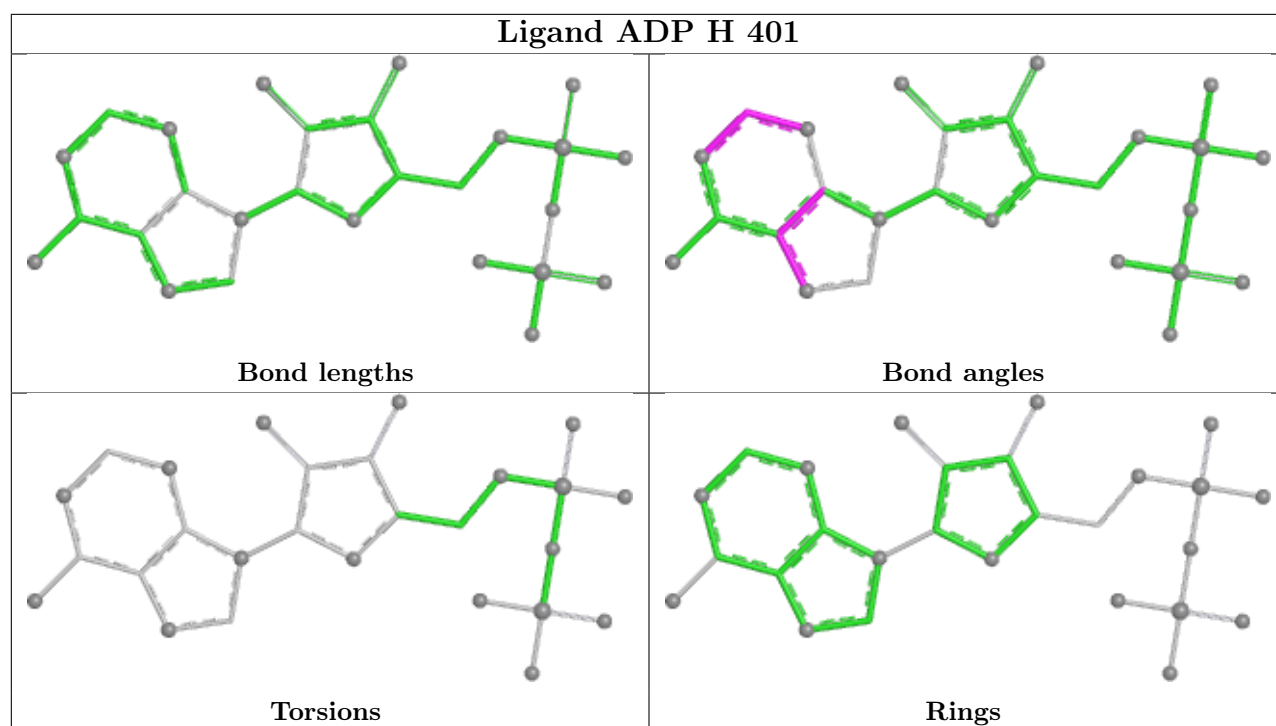


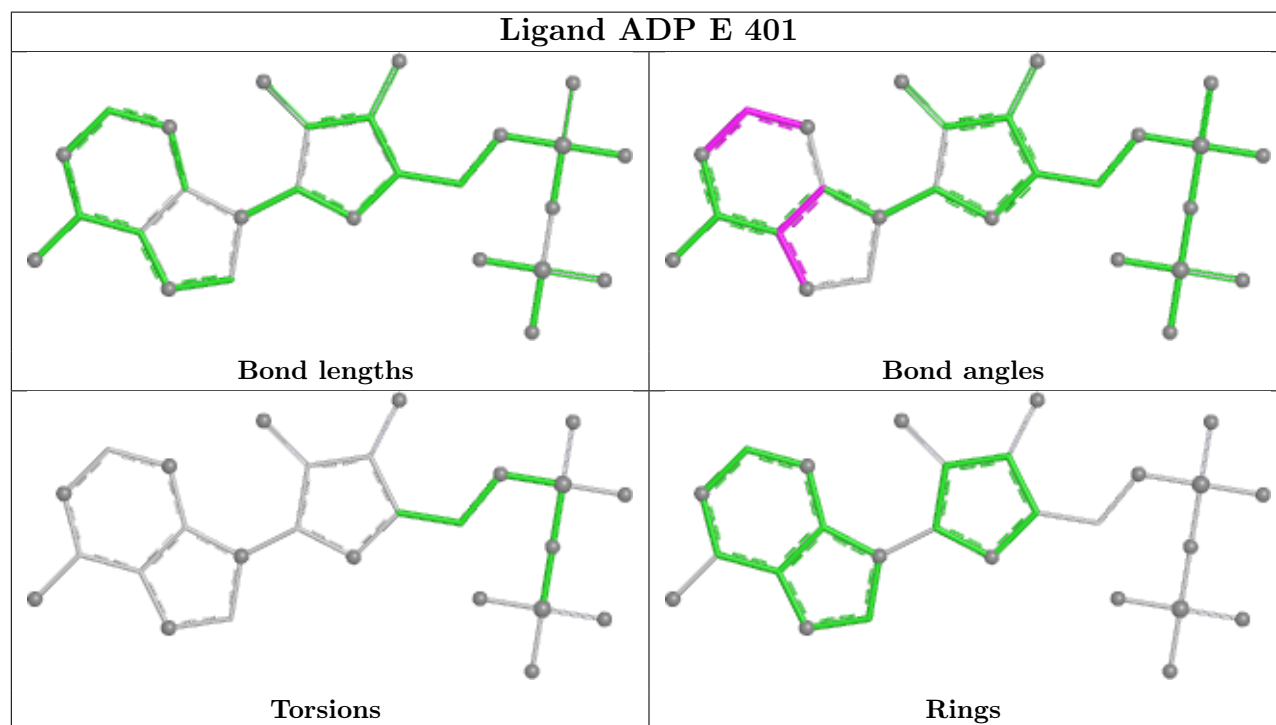
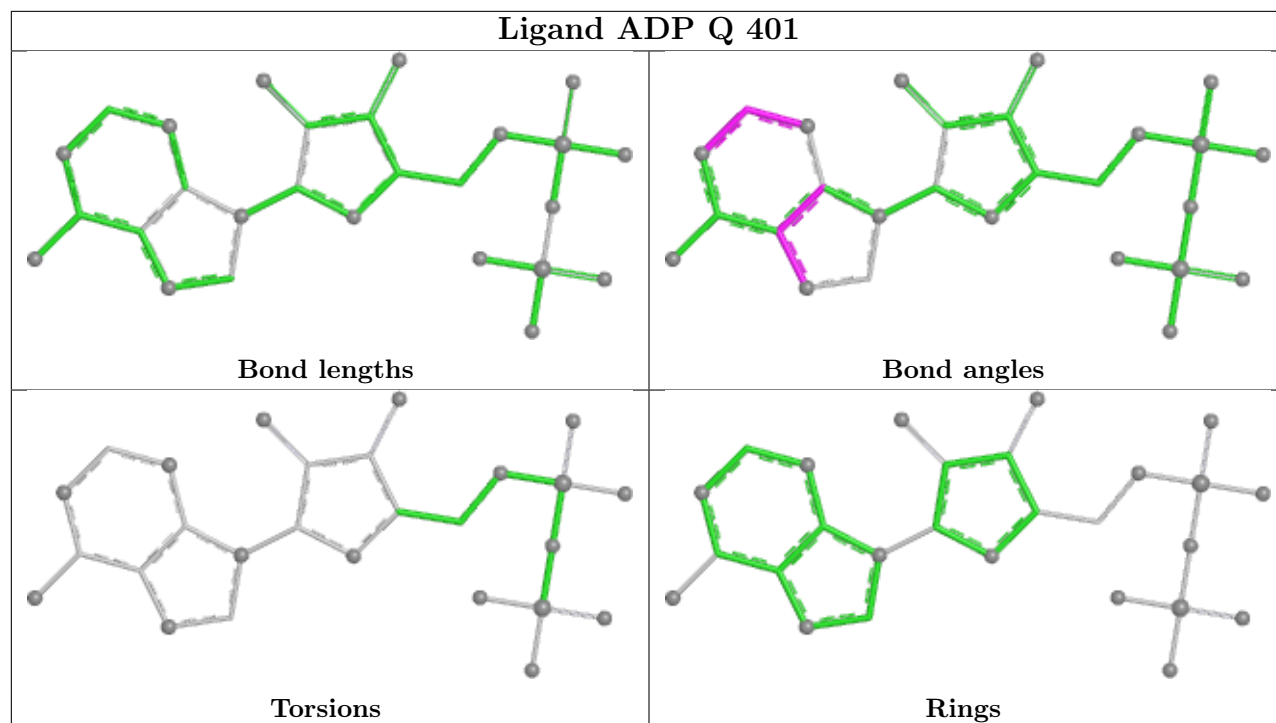


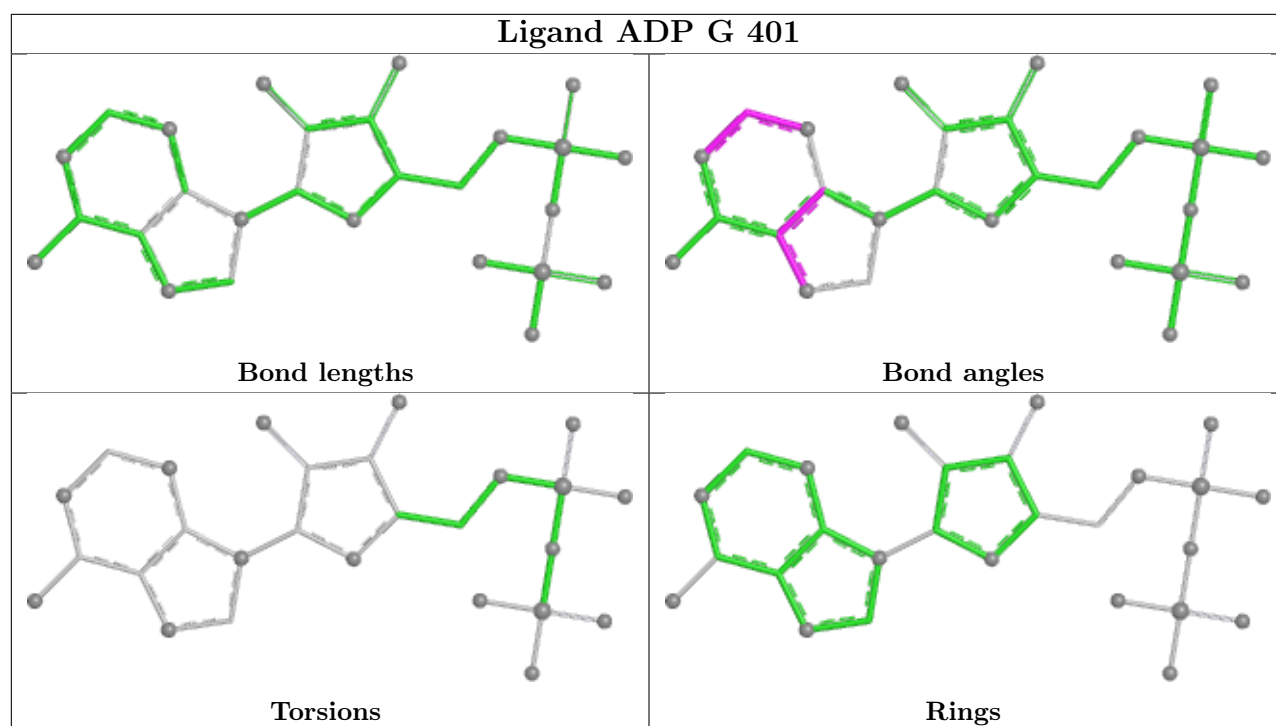












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-0729. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit ⓘ

This section was not generated.