



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 06:34 AM UTC

PDB ID : 6KN8 / pdb_00006kn8
EMDB ID : EMD-0729
Title : Structure of human cardiac thin filament in the calcium bound state
Authors : Fujii, T.; Yamada, Y.; Namba, K.
Deposited on : 2019-08-03
Resolution : 4.80 Å(reported)

This is a wwPDB EM Validation Summary 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

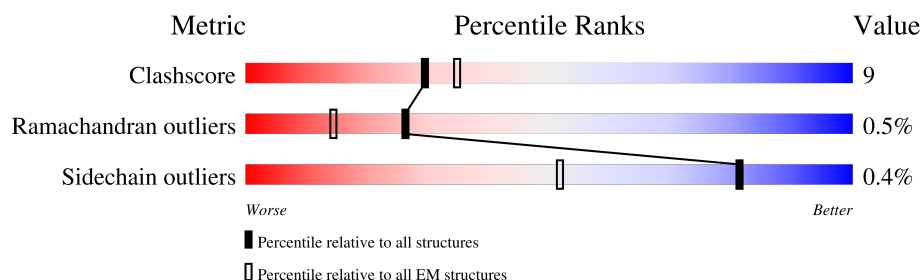
1 Overall quality at a glance

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.



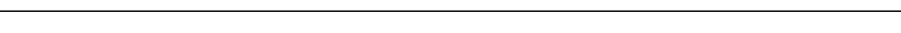
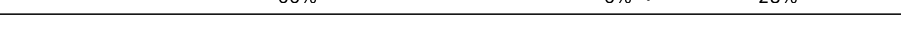
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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	A	375	
1	B	375	
1	C	375	
1	D	375	
1	E	375	
1	F	375	
1	G	375	
1	H	375	
1	I	375	

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Mol	Chain	Length	Quality of chain
1	J	375	 86% 13% .
1	K	375	 82% 17% .
1	L	375	 83% 16% .
1	M	375	 89% 10% .
1	N	375	 87% 12% .
1	O	375	 83% 15% .
2	P	274	 81% 17% .
2	Q	274	 78% 18% .
2	W	274	 83% 15% .
2	X	274	 80% 17% .
3	R	31	 87% 13%
3	S	31	 87% 13%
3	Y	31	 87% 13%
3	Z	31	 87% 13%
4	T	174	 66% 6% . 28%
4	a	174	 65% 7% . 28%
5	U	126	 91% 7% .
5	b	126	 91% 7% .
6	V	160	 91% 9%
6	c	160	 88% 12%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 60966 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	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	B	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	C	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	D	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	E	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	F	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	G	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	H	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	I	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	J	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	K	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	L	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	M	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	N	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	O	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	274	Total	C	N	O	S	0	0
			2207	1347	376	480	4		
2	Q	274	Total	C	N	O	S	0	0
			2207	1347	376	480	4		
2	W	274	Total	C	N	O	S	0	0
			2207	1347	376	480	4		
2	X	274	Total	C	N	O	S	0	0
			2207	1347	376	480	4		

- Molecule 3 is a protein called Tropomyosin alpha-1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	R	31	Total	C	N	O	S	0	0
			243	147	43	50	3		
3	S	31	Total	C	N	O	S	0	0
			243	147	43	50	3		
3	Y	31	Total	C	N	O	S	0	0
			243	147	43	50	3		
3	Z	31	Total	C	N	O	S	0	0
			243	147	43	50	3		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-1	ALA	-	expression tag	UNP P09493
R	0	SER	-	expression tag	UNP P09493
S	-1	ALA	-	expression tag	UNP P09493
S	0	SER	-	expression tag	UNP P09493
Y	-1	ALA	-	expression tag	UNP P09493
Y	0	SER	-	expression tag	UNP P09493
Z	-1	ALA	-	expression tag	UNP P09493
Z	0	SER	-	expression tag	UNP P09493

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

Mol	Chain	Residues	Atoms				AltConf	Trace
4	T	126	Total	C	N	O	0	0
			1101	673	219	209		
4	a	126	Total	C	N	O	0	0
			1101	673	219	209		

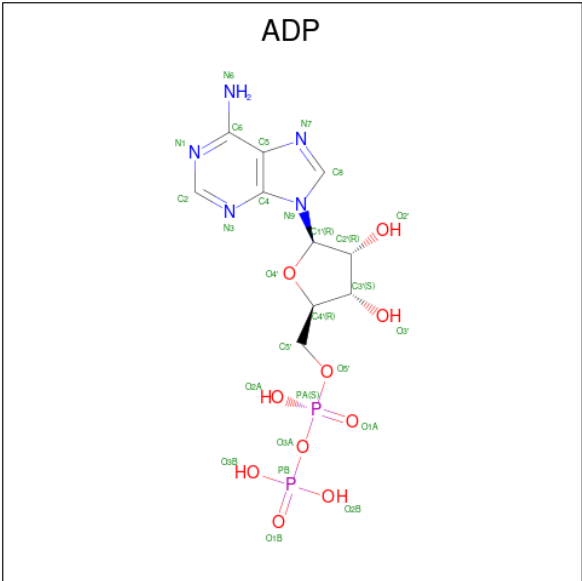
- Molecule 5 is a protein called Troponin I, cardiac muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	U	126	Total	C	N	O	S	0	0
			1009	624	193	188	4		
5	b	126	Total	C	N	O	S	0	0
			1009	624	193	188	4		

- Molecule 6 is a protein called Troponin C, slow skeletal and cardiac muscles.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	V	160	Total	C	N	O	S	0	0
			1273	788	195	278	12		
6	c	160	Total	C	N	O	S	0	0
			1273	788	195	278	12		

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

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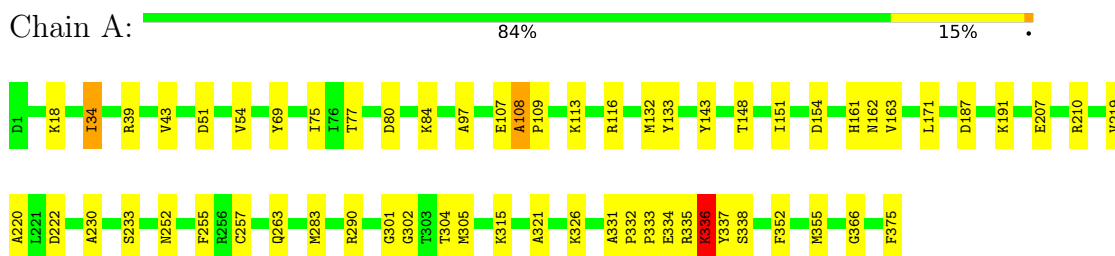
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Mol	Chain	Residues	Atoms					AltConf
7	G	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	H	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	I	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	J	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	K	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	L	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	M	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	N	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	O	1	Total	C	N	O	P	0
			27	10	5	10	2	

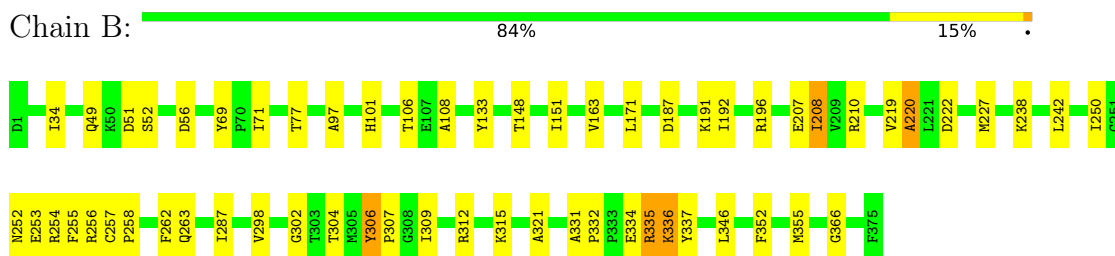
3 Residue-property plots

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.

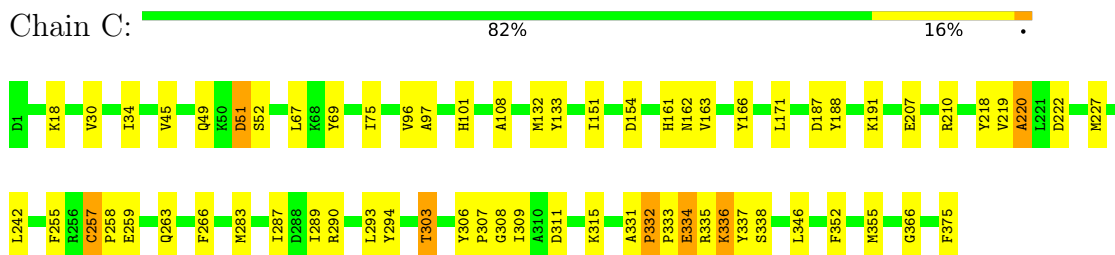
- Molecule 1: Actin, alpha skeletal muscle



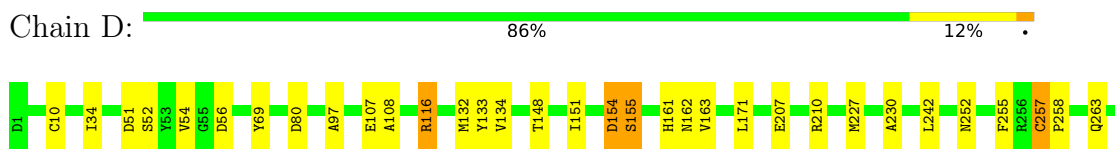
- Molecule 1: Actin, alpha skeletal muscle



- Molecule 1: Actin, alpha skeletal muscle



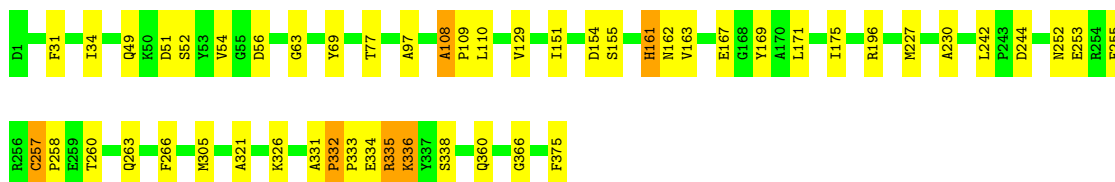
- Molecule 1: Actin, alpha skeletal muscle





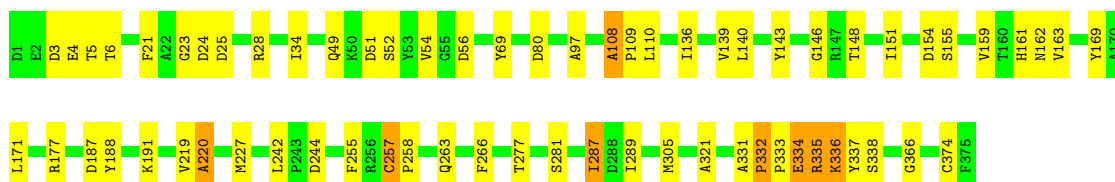
- Molecule 1: Actin, alpha skeletal muscle

Chain E: 86% 12% .



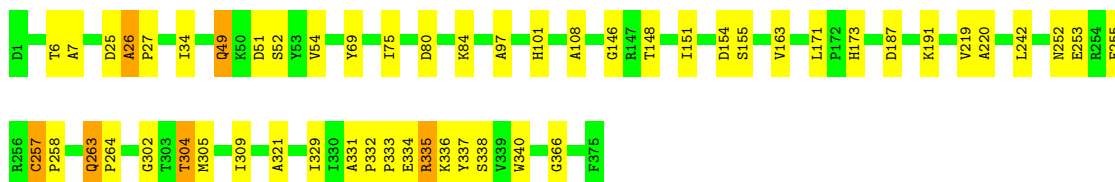
- Molecule 1: Actin, alpha skeletal muscle

Chain F: 82% 15% .



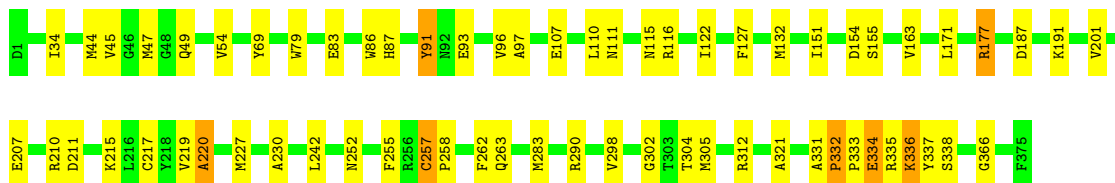
- Molecule 1: Actin, alpha skeletal muscle

Chain G: 86% 13% .



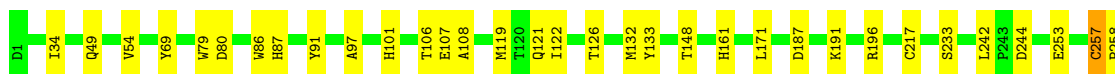
- Molecule 1: Actin, alpha skeletal muscle

Chain H: 83% 15% .



- Molecule 1: Actin, alpha skeletal muscle

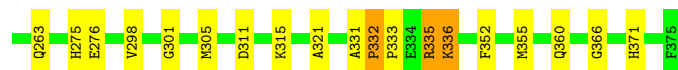
Chain I: 85% 14% .





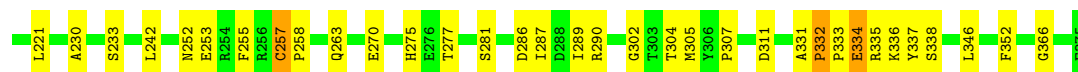
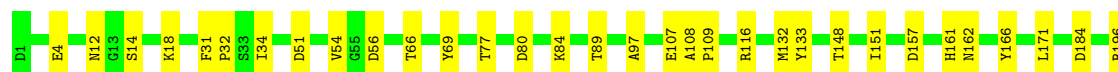
- Molecule 1: Actin, alpha skeletal muscle

Chain J: 86% 13%



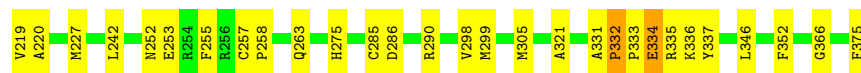
- Molecule 1: Actin, alpha skeletal muscle

Chain K: 82% 17%



- Molecule 1: Actin, alpha skeletal muscle

Chain L: 83% 16%



- Molecule 1: Actin, alpha skeletal muscle

Chain M: 89% 10%



- Molecule 1: Actin, alpha skeletal muscle

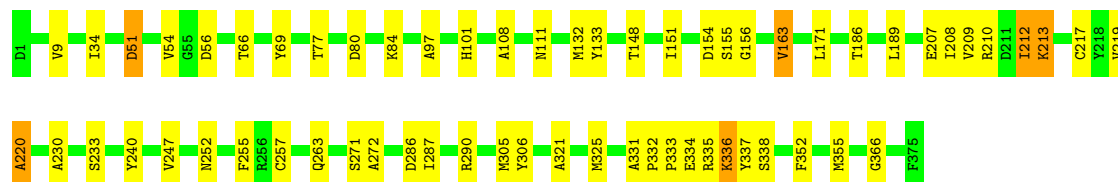
Chain N: 87% 12%





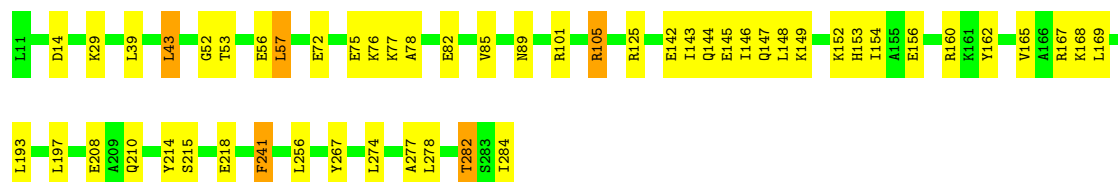
- Molecule 1: Actin, alpha skeletal muscle

Chain O: 83% 15% .



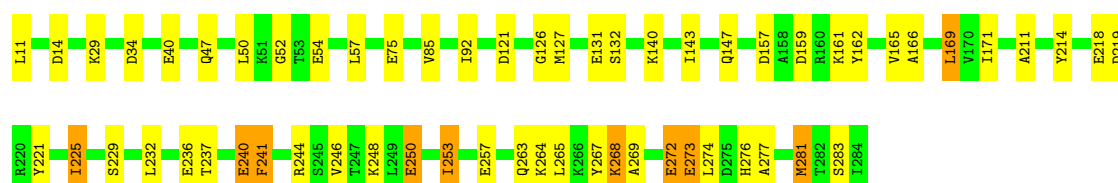
- Molecule 2: Tropomyosin alpha-1 chain

Chain P: 81% 17% .



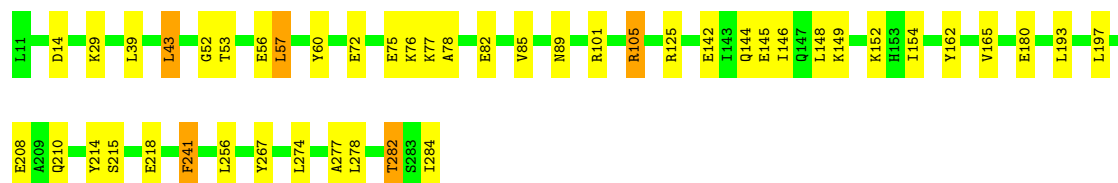
- Molecule 2: Tropomyosin alpha-1 chain

Chain Q: 78% 18% .



- Molecule 2: Tropomyosin alpha-1 chain

Chain W: 83% 15% .



- Molecule 2: Tropomyosin alpha-1 chain

Chain X: 80% 17% .





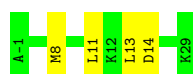
- Molecule 3: Tropomyosin alpha-1 chain

Chain R: 87% 13%



- Molecule 3: Tropomyosin alpha-1 chain

Chain S: 87% 13%



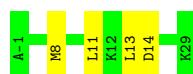
- Molecule 3: Tropomyosin alpha-1 chain

Chain Y: 87% 13%



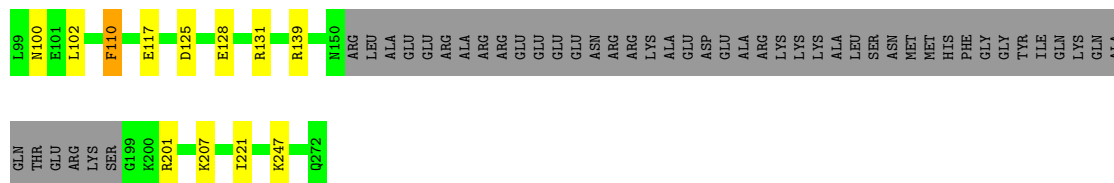
- Molecule 3: Tropomyosin alpha-1 chain

Chain Z: 87% 13%



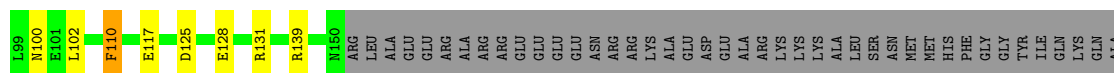
- Molecule 4: Troponin T, cardiac muscle

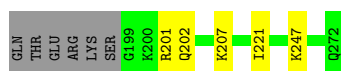
Chain T: 66% 6% 28%



- Molecule 4: Troponin T, cardiac muscle

Chain a: 65% 7% 28%





- Molecule 5: Troponin I, cardiac muscle

Chain U: 91% 7%



- Molecule 5: Troponin I, cardiac muscle

Chain b: 91% 7%



- Molecule 6: Troponin C, slow skeletal and cardiac muscles

Chain V: 91% 9%



- Molecule 6: Troponin C, slow skeletal and cardiac muscles

Chain c: 88% 12%



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)	Not provided	
Maximum defocus (nm)	Not provided	
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: ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.91	0/2996	1.31	35/4058 (0.9%)
1	B	0.89	0/2996	1.27	33/4058 (0.8%)
1	C	0.95	1/2996 (0.0%)	1.29	36/4058 (0.9%)
1	D	0.92	1/2996 (0.0%)	1.32	42/4058 (1.0%)
1	E	0.90	0/2996	1.31	40/4058 (1.0%)
1	F	0.91	0/2996	1.31	33/4058 (0.8%)
1	G	0.92	0/2996	1.32	37/4058 (0.9%)
1	H	0.90	0/2996	1.33	38/4058 (0.9%)
1	I	0.93	1/2996 (0.0%)	1.31	35/4058 (0.9%)
1	J	0.91	1/2996 (0.0%)	1.32	36/4058 (0.9%)
1	K	0.91	0/2996	1.31	33/4058 (0.8%)
1	L	0.93	1/2996 (0.0%)	1.30	37/4058 (0.9%)
1	M	0.92	0/2996	1.30	35/4058 (0.9%)
1	N	0.91	0/2996	1.32	35/4058 (0.9%)
1	O	0.94	0/2996	1.35	40/4058 (1.0%)
2	P	1.37	0/2215	1.32	15/2954 (0.5%)
2	Q	1.37	2/2215 (0.1%)	1.38	23/2954 (0.8%)
2	W	1.37	0/2215	1.32	15/2954 (0.5%)
2	X	1.37	2/2215 (0.1%)	1.38	22/2954 (0.7%)
3	R	1.39	1/242 (0.4%)	1.26	2/316 (0.6%)
3	S	1.32	1/242 (0.4%)	1.20	0/316
3	Y	1.39	1/242 (0.4%)	1.26	2/316 (0.6%)
3	Z	1.33	1/242 (0.4%)	1.20	0/316
4	T	0.97	0/1108	1.08	5/1466 (0.3%)
4	a	0.97	0/1108	1.08	5/1466 (0.3%)
5	U	0.94	2/1015 (0.2%)	1.11	6/1352 (0.4%)
5	b	0.93	2/1015 (0.2%)	1.10	6/1352 (0.4%)
6	V	0.94	0/1286	1.16	7/1719 (0.4%)
6	c	0.94	0/1286	1.15	7/1719 (0.4%)
All	All	1.01	17/61586 (0.0%)	1.30	660/83024 (0.8%)

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	161	HIS	CB-CG	-6.32	1.41	1.50
3	S	8	MET	SD-CE	-6.28	1.63	1.79
3	Z	8	MET	SD-CE	-6.27	1.63	1.79
3	R	4	ILE	CA-CB	-6.16	1.47	1.54
3	Y	4	ILE	CA-CB	-6.12	1.47	1.54

The worst 5 of 660 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	163	VAL	N-CA-C	10.97	117.54	107.56
1	N	331	ALA	CA-C-N	10.10	126.93	119.66
1	N	331	ALA	C-N-CA	10.10	126.93	119.66
1	L	163	VAL	N-CA-C	8.84	117.52	107.89
1	C	263	GLN	CA-C-N	8.59	128.24	119.82

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	2933	0	2894	57	0
1	B	2933	0	2894	49	0
1	C	2933	0	2894	89	0
1	D	2933	0	2894	45	0
1	E	2933	0	2894	52	0
1	F	2933	0	2894	101	0
1	G	2933	0	2894	38	0
1	H	2933	0	2894	72	0
1	I	2933	0	2894	61	0
1	J	2933	0	2894	49	0
1	K	2933	0	2894	71	0
1	L	2933	0	2894	69	0
1	M	2933	0	2894	34	0
1	N	2933	0	2894	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	2933	0	2894	70	0
2	P	2207	0	2200	87	0
2	Q	2207	0	2200	78	0
2	W	2207	0	2200	80	0
2	X	2207	0	2200	62	0
3	R	243	0	255	2	0
3	S	243	0	255	2	0
3	Y	243	0	255	2	0
3	Z	243	0	255	2	0
4	T	1101	0	1120	20	0
4	a	1101	0	1120	29	0
5	U	1009	0	1064	37	0
5	b	1009	0	1064	10	0
6	V	1273	0	1201	37	0
6	c	1273	0	1201	50	0
7	A	27	0	12	1	0
7	B	27	0	12	0	0
7	C	27	0	12	0	0
7	D	27	0	12	0	0
7	E	27	0	12	0	0
7	F	27	0	12	1	0
7	G	27	0	12	0	0
7	H	27	0	12	0	0
7	I	27	0	12	0	0
7	J	27	0	12	0	0
7	K	27	0	12	1	0
7	L	27	0	12	0	0
7	M	27	0	12	6	0
7	N	27	0	12	2	0
7	O	27	0	12	5	0
All	All	60966	0	60180	1115	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 9.

The worst 5 of 1115 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:M:305:MET:CE	1:M:335:ARG:HG3	1.33	1.57
1:F:305:MET:CE	1:F:335:ARG:HB2	1.35	1.53
1:M:306:TYR:CZ	7:M:401:ADP:H2	1.35	1.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:305:MET:HE2	1:F:335:ARG:CB	1.52	1.39
1:B:252:ASN:HA	1:B:255:PHE:CE2	1.59	1.36

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	373/375 (100%)	361 (97%)	10 (3%)	2 (0%)	24	63
1	B	373/375 (100%)	360 (96%)	9 (2%)	4 (1%)	11	45
1	C	373/375 (100%)	362 (97%)	7 (2%)	4 (1%)	11	45
1	D	373/375 (100%)	361 (97%)	10 (3%)	2 (0%)	24	63
1	E	373/375 (100%)	363 (97%)	7 (2%)	3 (1%)	16	52
1	F	373/375 (100%)	361 (97%)	7 (2%)	5 (1%)	9	41
1	G	373/375 (100%)	358 (96%)	13 (4%)	2 (0%)	24	63
1	H	373/375 (100%)	362 (97%)	8 (2%)	3 (1%)	16	52
1	I	373/375 (100%)	361 (97%)	9 (2%)	3 (1%)	16	52
1	J	373/375 (100%)	357 (96%)	13 (4%)	3 (1%)	16	52
1	K	373/375 (100%)	358 (96%)	13 (4%)	2 (0%)	24	63
1	L	373/375 (100%)	360 (96%)	11 (3%)	2 (0%)	24	63
1	M	373/375 (100%)	362 (97%)	9 (2%)	2 (0%)	24	63
1	N	373/375 (100%)	363 (97%)	8 (2%)	2 (0%)	24	63
1	O	373/375 (100%)	359 (96%)	12 (3%)	2 (0%)	24	63
2	P	272/274 (99%)	272 (100%)	0	0	100	100
2	Q	272/274 (99%)	272 (100%)	0	0	100	100
2	W	272/274 (99%)	272 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	X	272/274 (99%)	272 (100%)	0	0	100	100
3	R	29/31 (94%)	29 (100%)	0	0	100	100
3	S	29/31 (94%)	29 (100%)	0	0	100	100
3	Y	29/31 (94%)	29 (100%)	0	0	100	100
3	Z	29/31 (94%)	29 (100%)	0	0	100	100
4	T	122/174 (70%)	122 (100%)	0	0	100	100
4	a	122/174 (70%)	122 (100%)	0	0	100	100
5	U	124/126 (98%)	122 (98%)	2 (2%)	0	100	100
5	b	124/126 (98%)	122 (98%)	2 (2%)	0	100	100
6	V	158/160 (99%)	156 (99%)	2 (1%)	0	100	100
6	c	158/160 (99%)	156 (99%)	2 (1%)	0	100	100
All	All	7607/7765 (98%)	7412 (97%)	154 (2%)	41 (0%)	26	63

5 of 41 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	155	SER
1	J	155	SER
1	L	155	SER
1	M	155	SER
1	O	155	SER

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	318/318 (100%)	317 (100%)	1 (0%)	86	84
1	B	318/318 (100%)	313 (98%)	5 (2%)	55	69
1	C	318/318 (100%)	317 (100%)	1 (0%)	86	84
1	D	318/318 (100%)	316 (99%)	2 (1%)	78	81
1	E	318/318 (100%)	316 (99%)	2 (1%)	78	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	318/318 (100%)	316 (99%)	2 (1%)	78	81
1	G	318/318 (100%)	316 (99%)	2 (1%)	78	81
1	H	318/318 (100%)	316 (99%)	2 (1%)	78	81
1	I	318/318 (100%)	316 (99%)	2 (1%)	78	81
1	J	318/318 (100%)	316 (99%)	2 (1%)	78	81
1	K	318/318 (100%)	317 (100%)	1 (0%)	86	84
1	L	318/318 (100%)	317 (100%)	1 (0%)	86	84
1	M	318/318 (100%)	317 (100%)	1 (0%)	86	84
1	N	318/318 (100%)	318 (100%)	0	100	100
1	O	318/318 (100%)	315 (99%)	3 (1%)	70	77
2	P	236/236 (100%)	236 (100%)	0	100	100
2	Q	236/236 (100%)	236 (100%)	0	100	100
2	W	236/236 (100%)	236 (100%)	0	100	100
2	X	236/236 (100%)	236 (100%)	0	100	100
3	R	25/25 (100%)	25 (100%)	0	100	100
3	S	25/25 (100%)	25 (100%)	0	100	100
3	Y	25/25 (100%)	25 (100%)	0	100	100
3	Z	25/25 (100%)	25 (100%)	0	100	100
4	T	117/157 (74%)	117 (100%)	0	100	100
4	a	117/157 (74%)	117 (100%)	0	100	100
5	U	106/106 (100%)	106 (100%)	0	100	100
5	b	106/106 (100%)	106 (100%)	0	100	100
6	V	141/141 (100%)	141 (100%)	0	100	100
6	c	141/141 (100%)	141 (100%)	0	100	100
All	All	6542/6622 (99%)	6515 (100%)	27 (0%)	81	83

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	336	LYS
1	I	287	ILE
1	O	163	VAL
1	H	336	LYS
1	I	336	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	371	HIS
2	Q	47	GLN
2	X	47	GLN
1	H	115	ASN
1	H	92	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

15 ligands 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	$\# Z > 2$
7	ADP	A	401	-	28,29,29	1.90	8 (28%)	43,45,45	1.94	10 (23%)
7	ADP	K	401	-	28,29,29	1.76	8 (28%)	43,45,45	2.03	12 (27%)
7	ADP	L	401	-	28,29,29	1.87	9 (32%)	43,45,45	1.95	10 (23%)
7	ADP	I	401	-	28,29,29	1.75	7 (25%)	43,45,45	1.88	11 (25%)
7	ADP	O	401	-	28,29,29	1.81	7 (25%)	43,45,45	1.98	11 (25%)
7	ADP	E	401	-	28,29,29	1.75	6 (21%)	43,45,45	1.89	8 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	ADP	F	401	-	28,29,29	1.83	8 (28%)	43,45,45	1.87	9 (20%)
7	ADP	G	401	-	28,29,29	1.86	10 (35%)	43,45,45	1.95	10 (23%)
7	ADP	M	401	-	28,29,29	1.93	10 (35%)	43,45,45	2.04	10 (23%)
7	ADP	H	401	-	28,29,29	1.71	8 (28%)	43,45,45	1.85	8 (18%)
7	ADP	C	401	-	28,29,29	1.88	10 (35%)	43,45,45	1.98	10 (23%)
7	ADP	J	401	-	28,29,29	1.73	6 (21%)	43,45,45	1.94	9 (20%)
7	ADP	N	401	-	28,29,29	1.75	8 (28%)	43,45,45	2.08	11 (25%)
7	ADP	B	401	-	28,29,29	1.87	8 (28%)	43,45,45	1.92	10 (23%)
7	ADP	D	401	-	28,29,29	1.87	10 (35%)	43,45,45	1.99	10 (23%)

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
7	ADP	A	401	-	-	5/16/32/32	0/3/3/3
7	ADP	K	401	-	-	6/16/32/32	0/3/3/3
7	ADP	L	401	-	-	2/16/32/32	0/3/3/3
7	ADP	I	401	-	-	5/16/32/32	0/3/3/3
7	ADP	O	401	-	-	2/16/32/32	0/3/3/3
7	ADP	E	401	-	-	5/16/32/32	0/3/3/3
7	ADP	F	401	-	-	2/16/32/32	0/3/3/3
7	ADP	G	401	-	-	7/16/32/32	0/3/3/3
7	ADP	M	401	-	-	5/16/32/32	0/3/3/3
7	ADP	H	401	-	-	3/16/32/32	0/3/3/3
7	ADP	C	401	-	-	8/16/32/32	0/3/3/3
7	ADP	J	401	-	-	2/16/32/32	0/3/3/3
7	ADP	N	401	-	-	3/16/32/32	0/3/3/3
7	ADP	B	401	-	-	3/16/32/32	0/3/3/3
7	ADP	D	401	-	-	6/16/32/32	0/3/3/3

The worst 5 of 123 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	401	ADP	C5-C4	4.68	1.47	1.39
7	L	401	ADP	C5-C4	4.54	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	401	ADP	C5-C4	4.42	1.47	1.39
7	G	401	ADP	C5-C4	4.39	1.46	1.39
7	A	401	ADP	C5-C4	4.29	1.46	1.39

The worst 5 of 149 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	401	ADP	C5-C4-N3	-5.76	118.79	126.72
7	O	401	ADP	C5-C4-N3	-5.69	118.89	126.72
7	D	401	ADP	C5-C4-N3	-5.61	118.99	126.72
7	B	401	ADP	C5-C4-N3	-5.60	119.00	126.72
7	C	401	ADP	C5-C4-N3	-5.58	119.03	126.72

There are no chirality outliers.

5 of 64 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	401	ADP	C5'-O5'-PA-O1A
7	B	401	ADP	C5'-O5'-PA-O2A
7	B	401	ADP	C5'-O5'-PA-O3A
7	C	401	ADP	PA-O3A-PB-O2B
7	C	401	ADP	C5'-O5'-PA-O1A

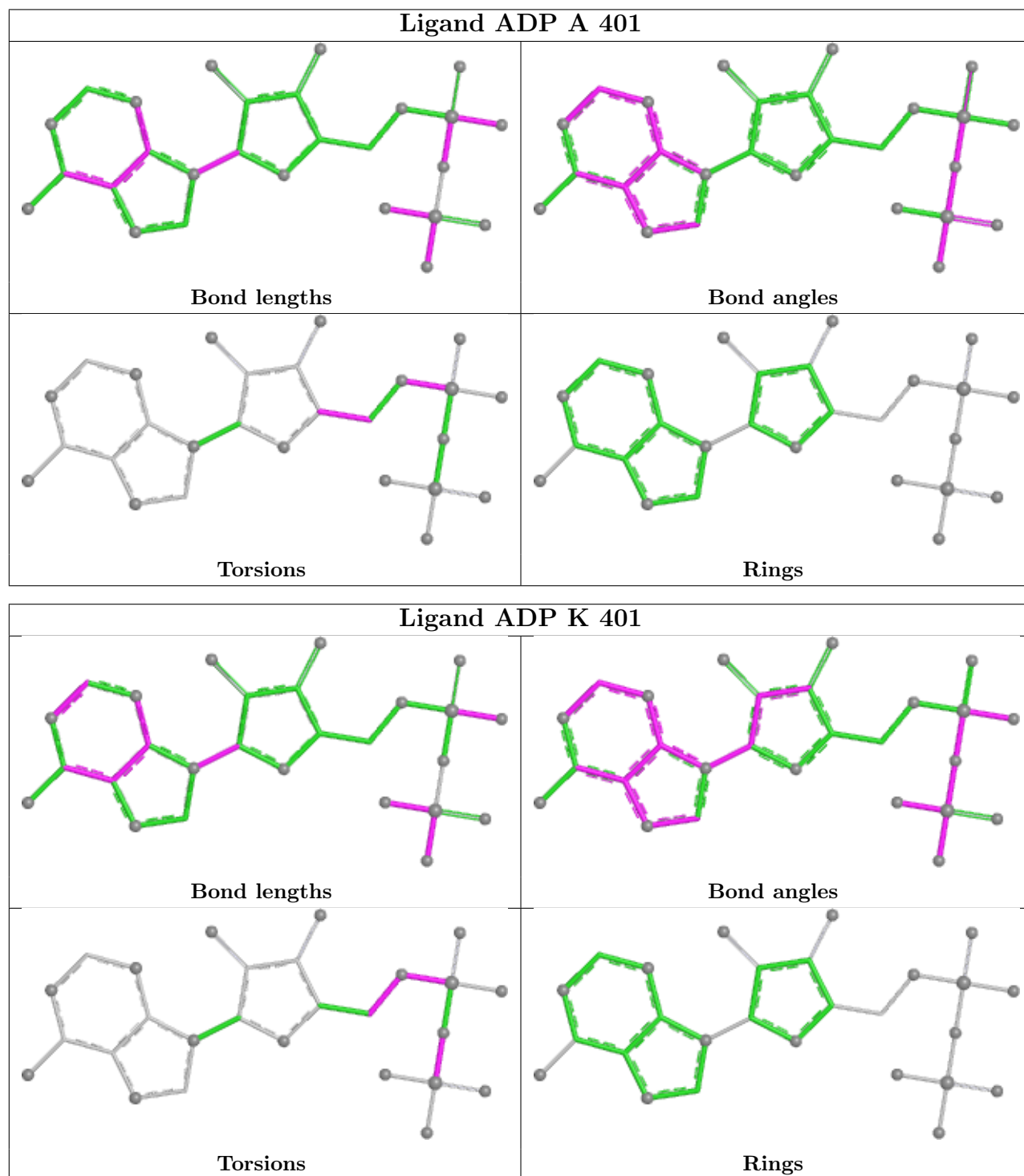
There are no ring outliers.

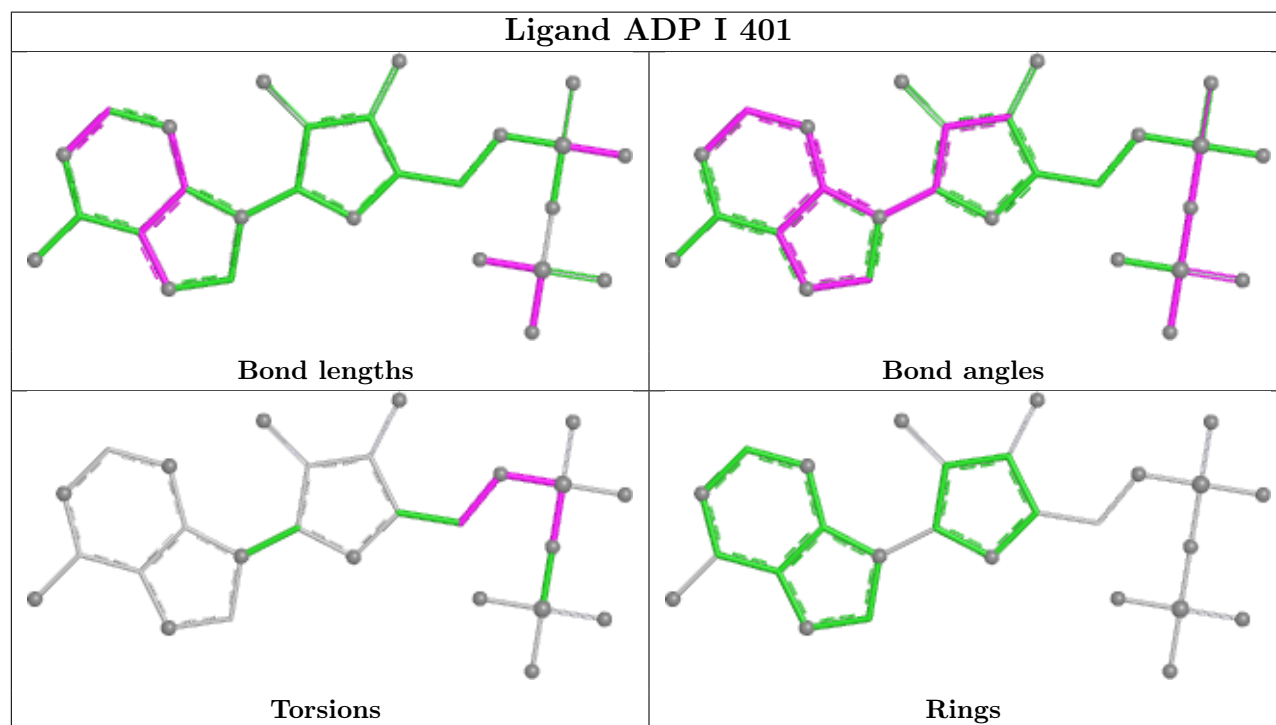
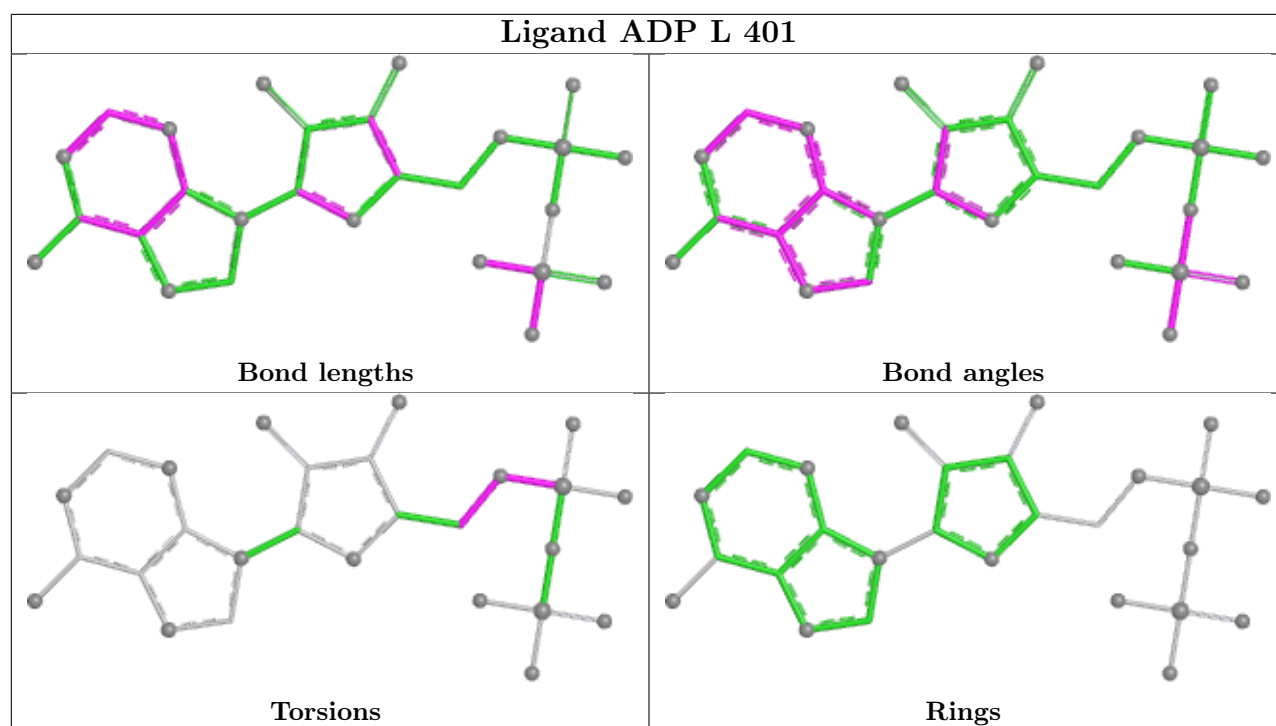
6 monomers are involved in 16 short contacts:

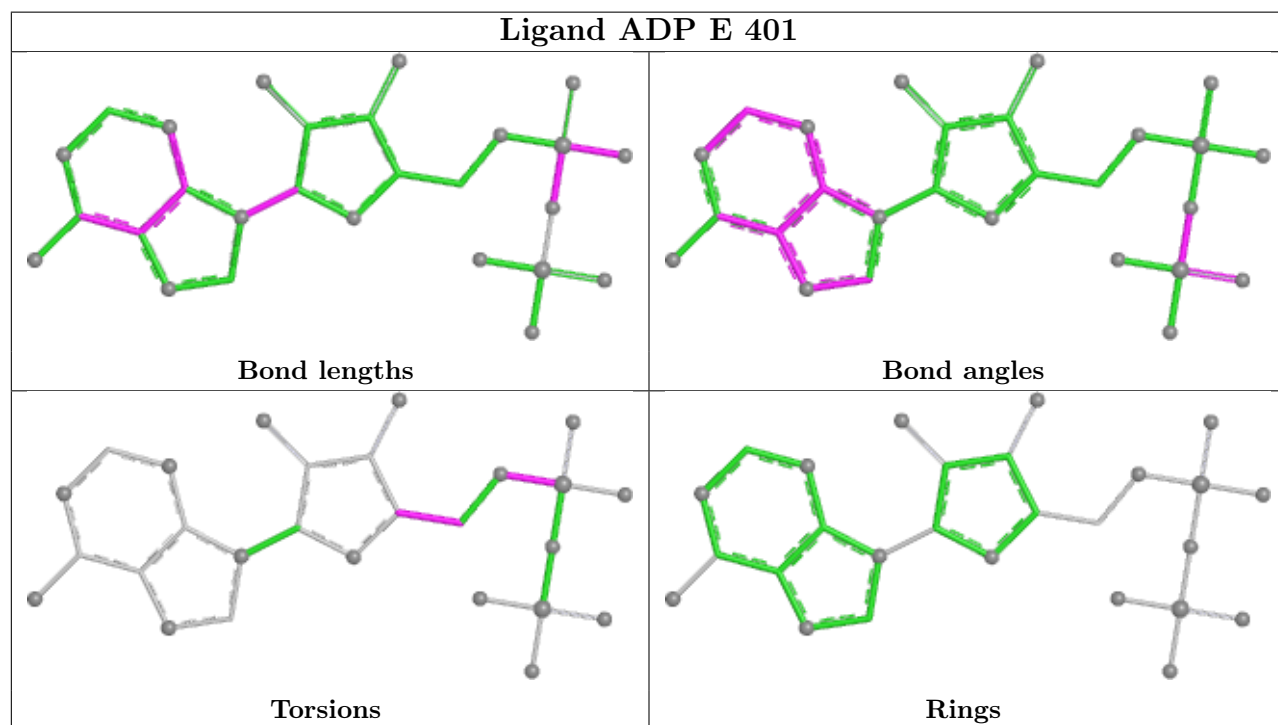
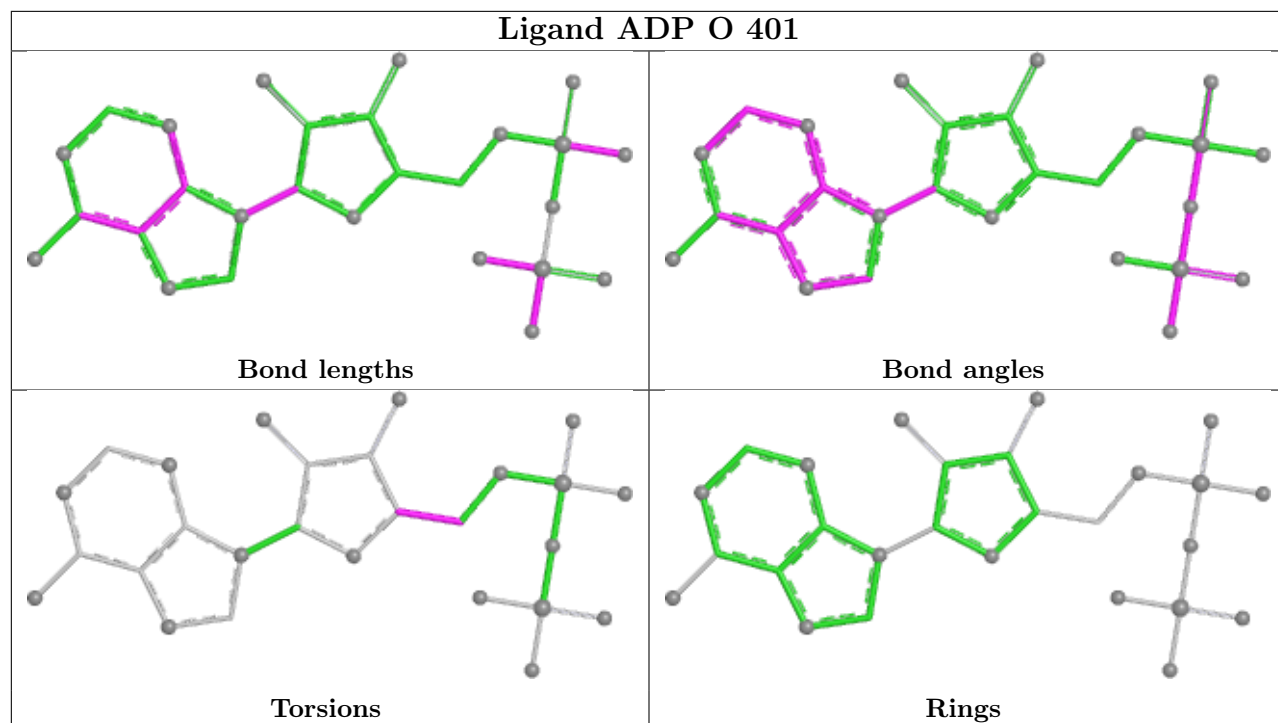
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	401	ADP	1	0
7	K	401	ADP	1	0
7	O	401	ADP	5	0
7	F	401	ADP	1	0
7	M	401	ADP	6	0
7	N	401	ADP	2	0

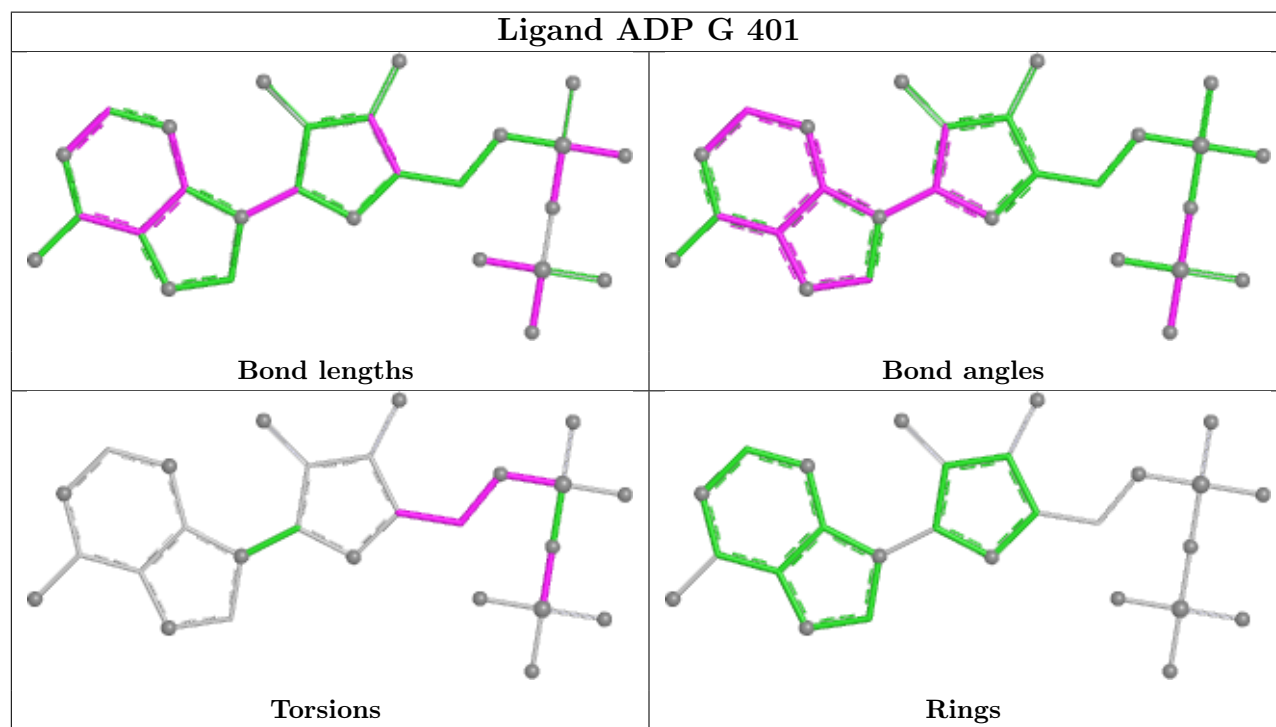
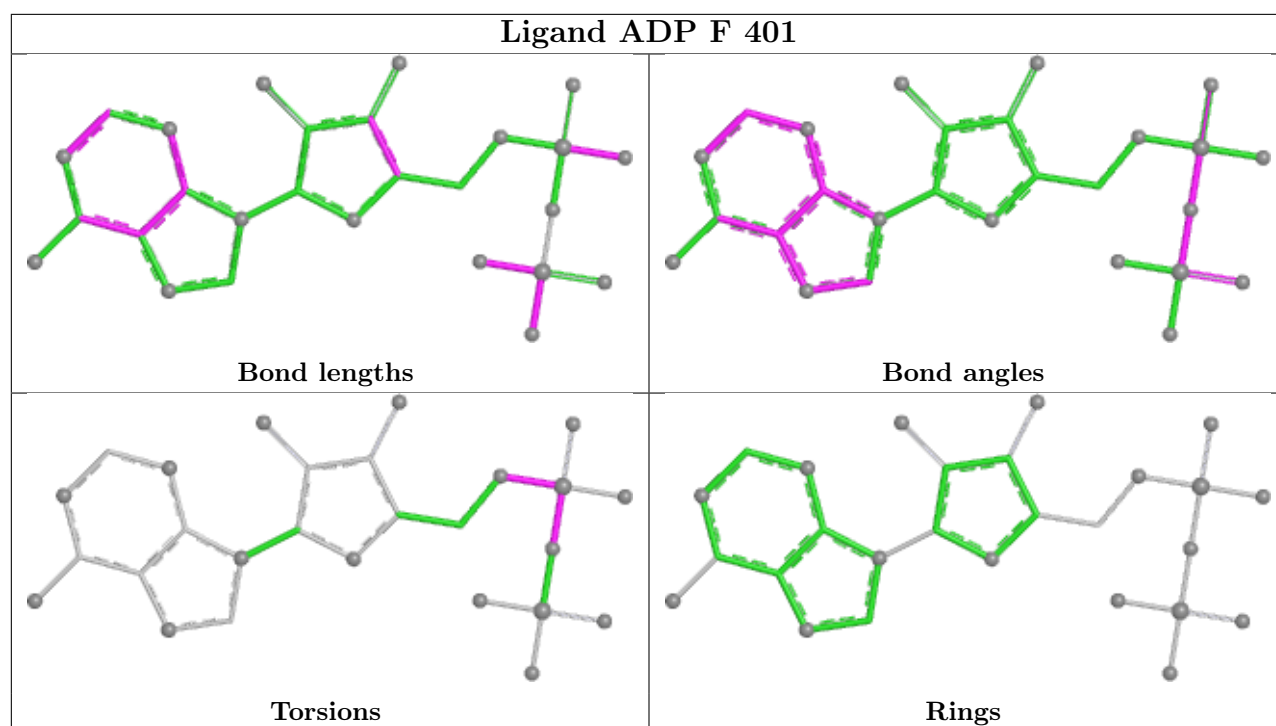
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

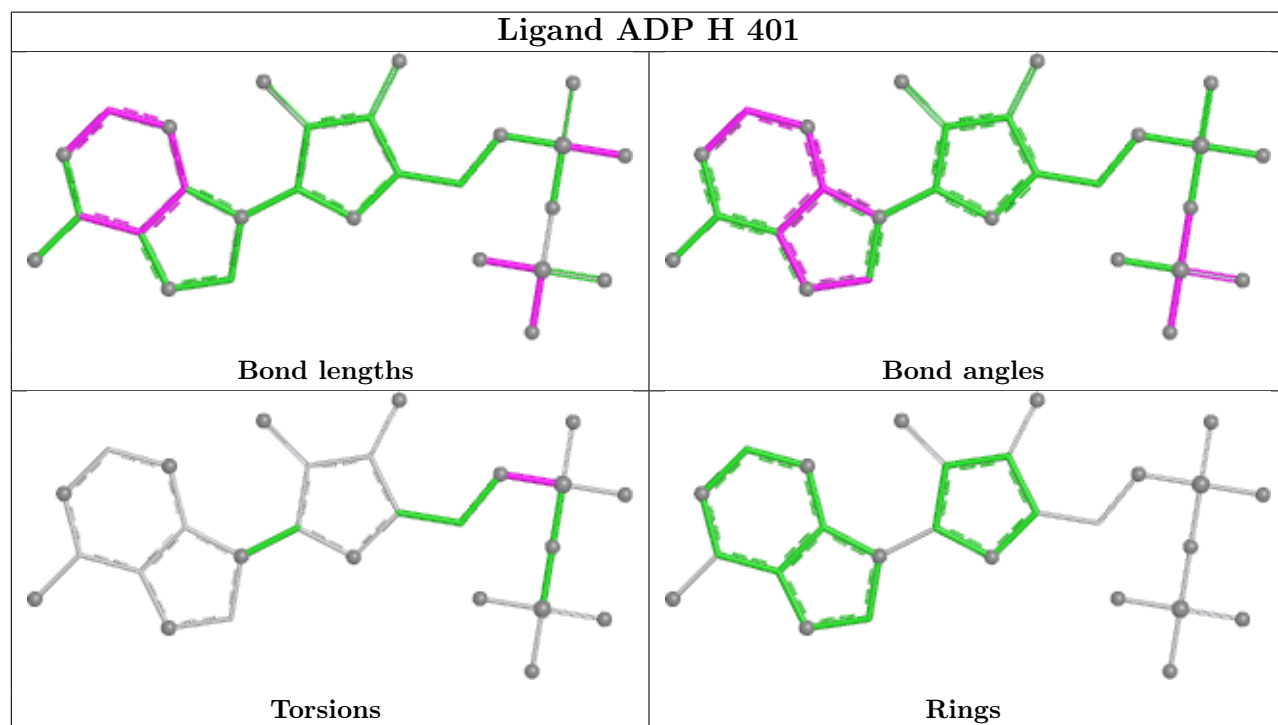
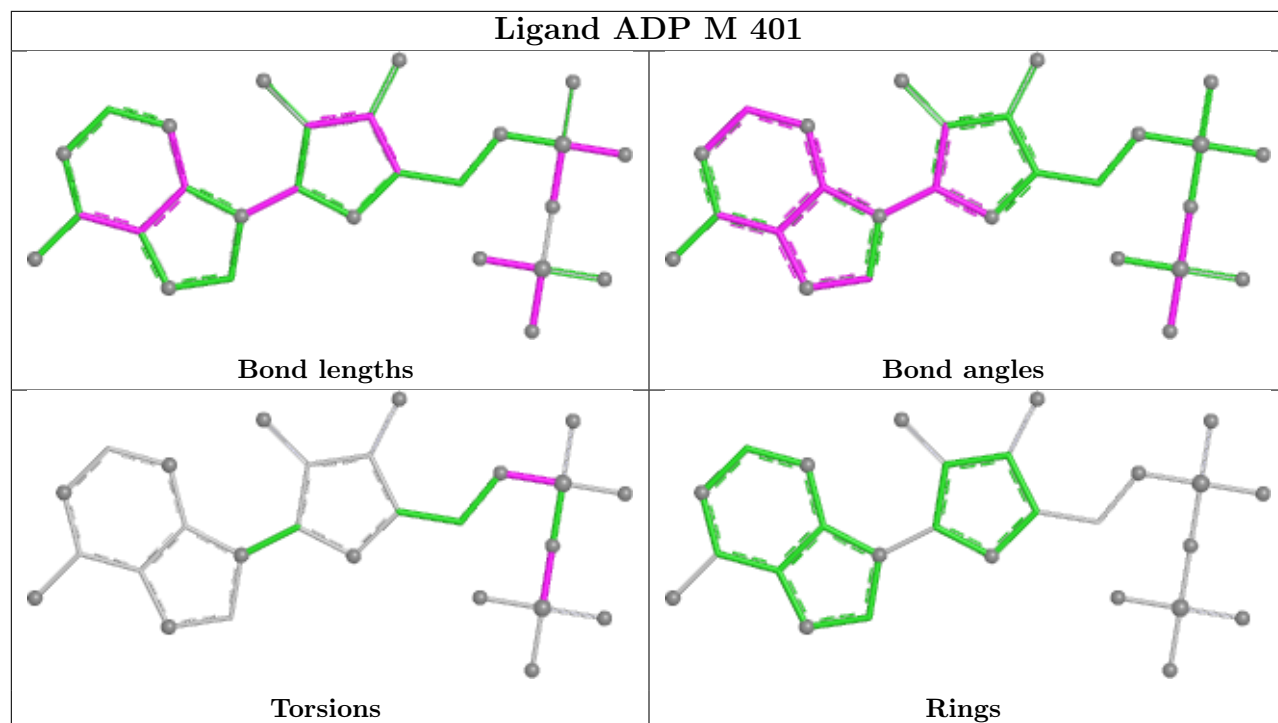
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

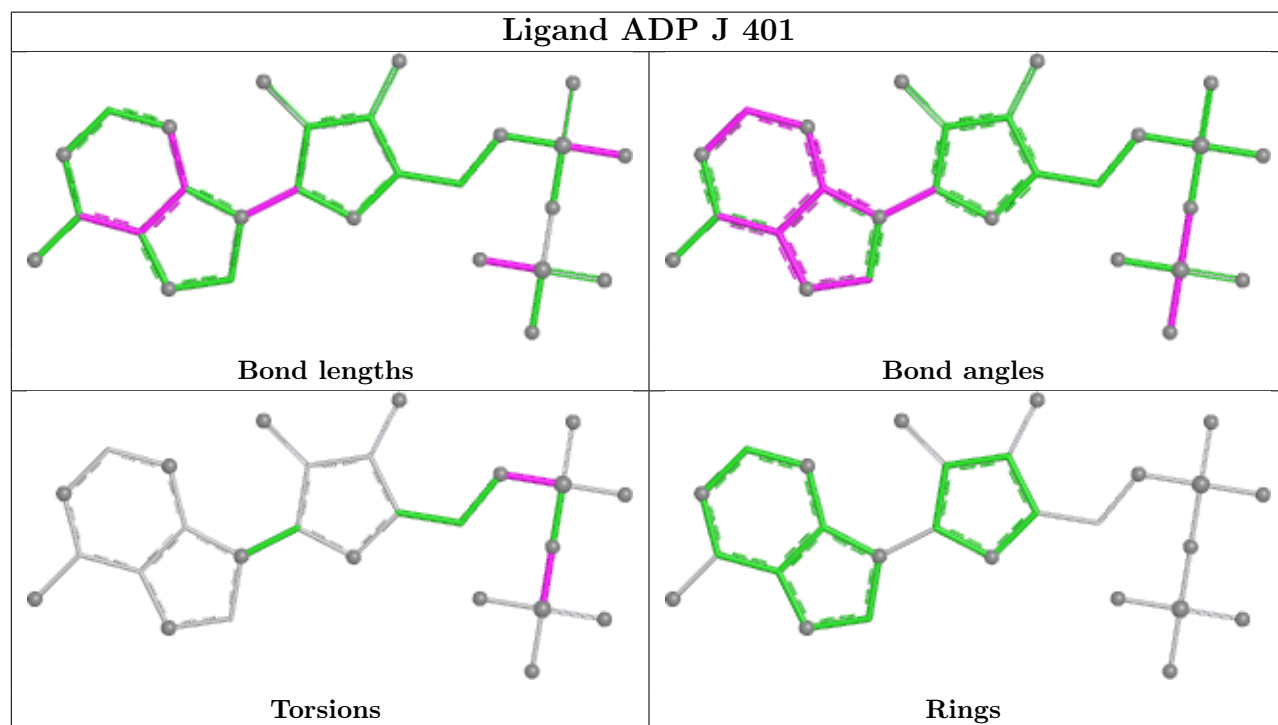
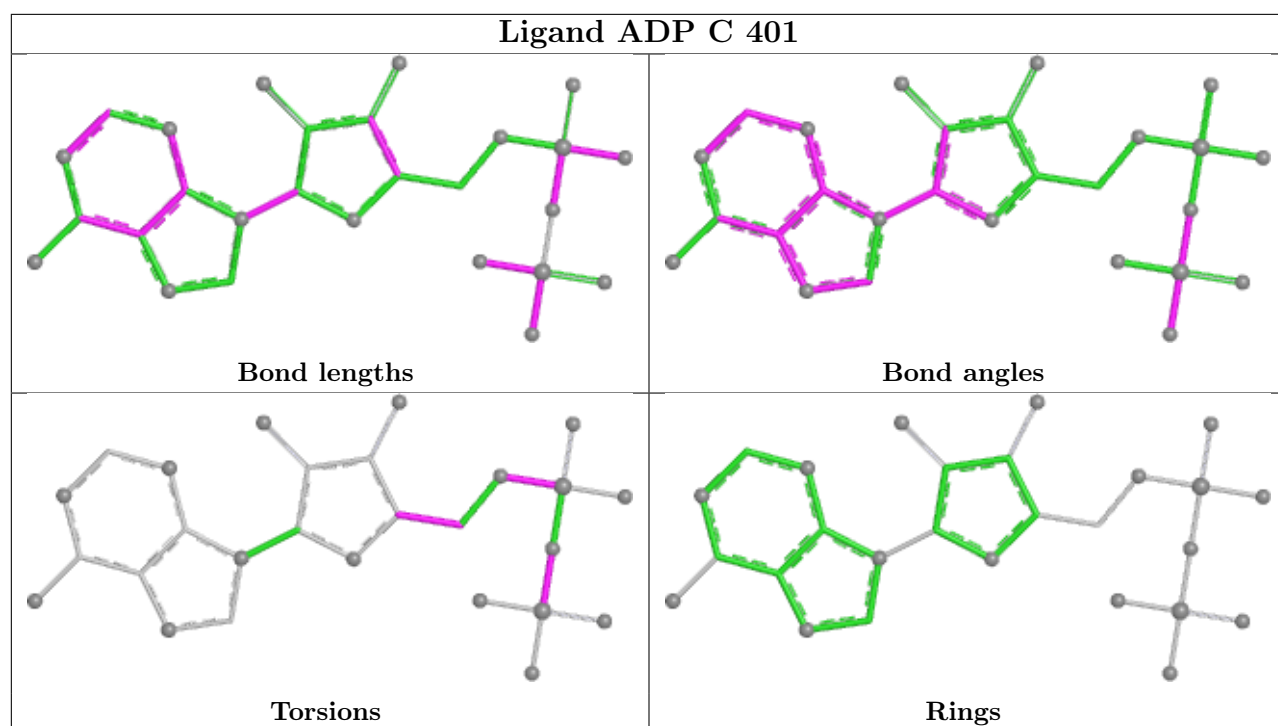


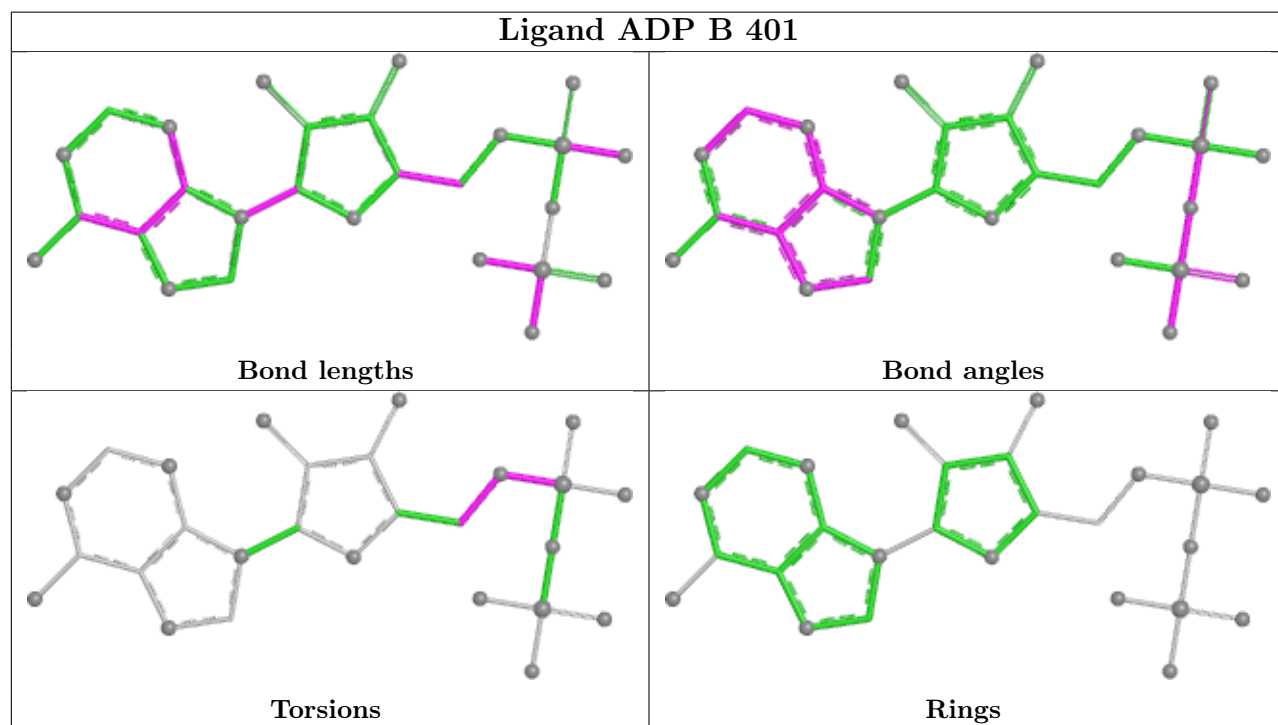
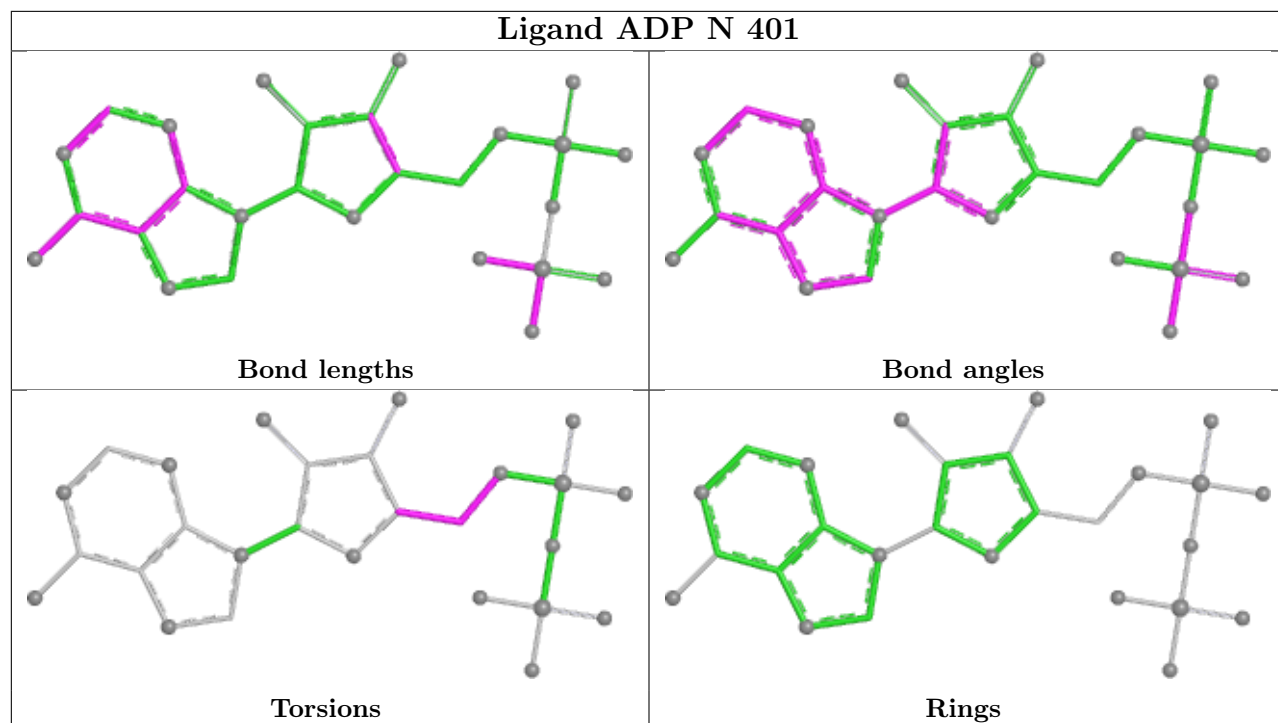


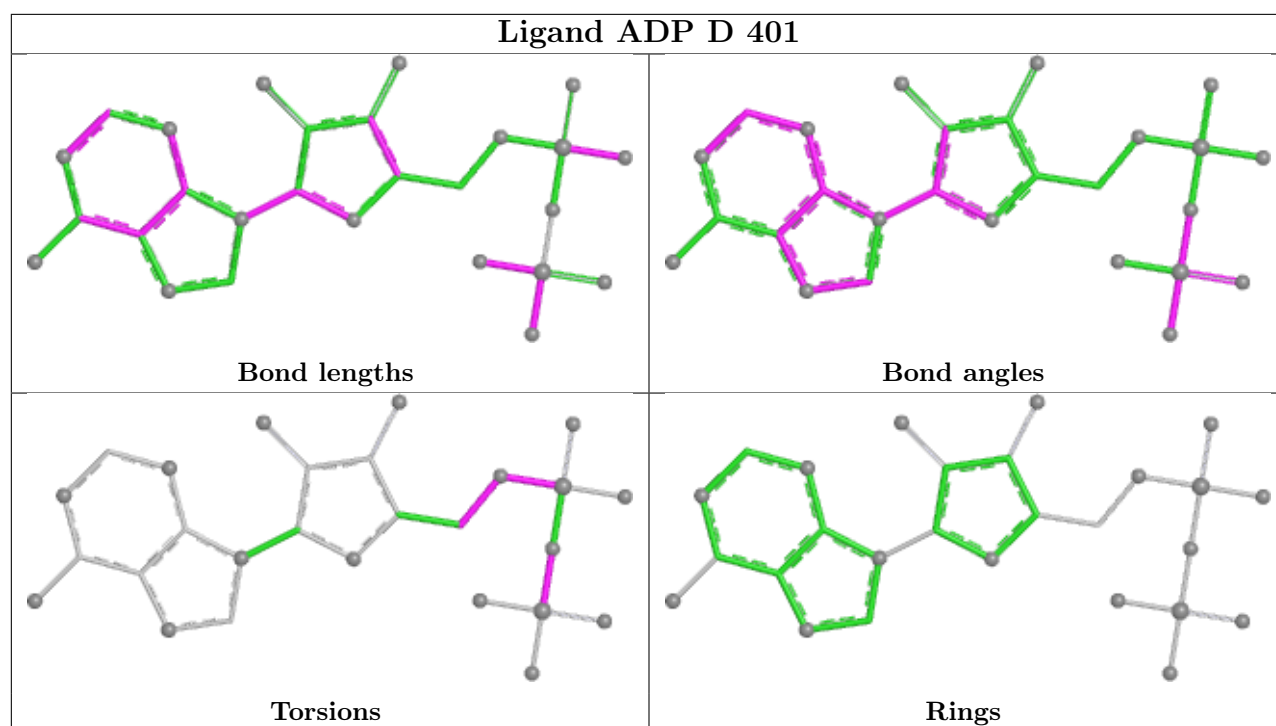












5.7 Other polymers [i](#)

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.