wwPDB EM Validation Summary Report ⓘ

Apr 1, 2025 – 08:51 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 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:

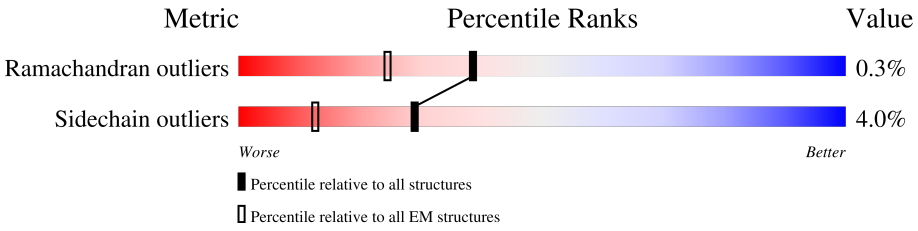
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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 <=5%

Mol	Chain	Length	Quality of chain
1	C	377	95%
1	D	377	96%
1	E	377	95%
1	F	377	95%
1	G	377	95%
1	H	377	95%
1	I	377	95%
1	J	377	95%
1	K	377	96%
1	L	377	96%

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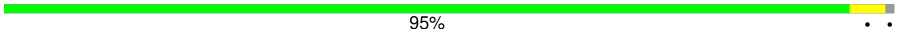
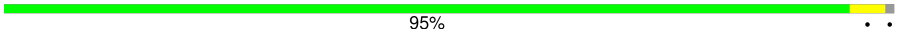
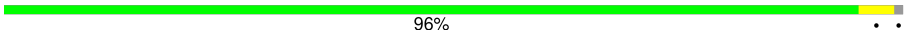
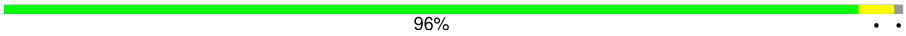
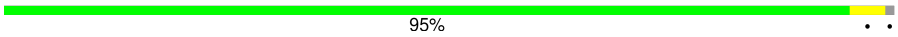
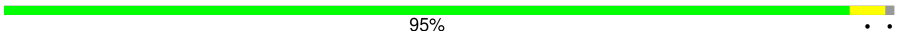
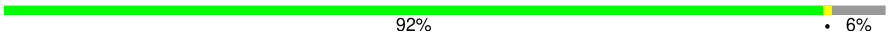
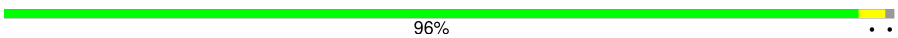
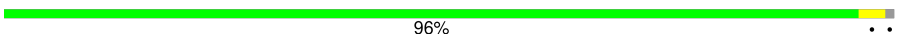
Mol	Chain	Length	Quality of chain
1	M	377	
1	N	377	
1	O	377	
1	P	377	
1	Q	377	
1	R	377	
2	W	285	
2	b	285	
2	e	285	
2	f	285	
2	g	285	
2	h	285	
2	i	285	
2	j	285	
3	X	288	
3	Y	288	
3	c	288	
3	d	288	
4	V	210	
4	a	210	
5	U	161	
5	Z	161	

2 Entry composition (i)

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			

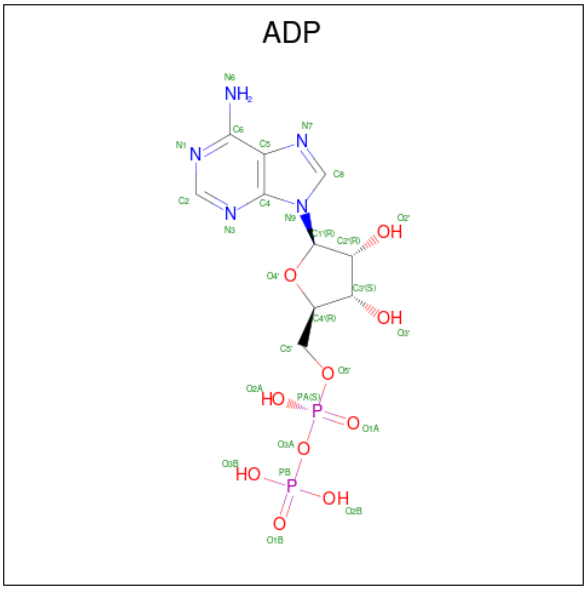
- Molecule 4 is a protein called Troponin I, cardiac muscle.

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

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

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

- 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	C	H	N	O	P	0
			39	10	12	5	10	2	
6	D	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
6	E	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
6	F	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
6	G	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
6	H	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

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

- 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 Mg 1 1	0
7	M	1	Total Mg 1 1	0
7	N	1	Total Mg 1 1	0
7	O	1	Total Mg 1 1	0
7	P	1	Total Mg 1 1	0
7	Q	1	Total Mg 1 1	0
7	R	1	Total Mg 1 1	0

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

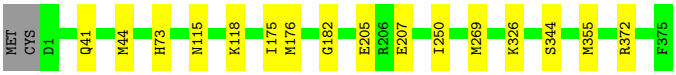
Mol	Chain	Residues	Atoms	AltConf
8	U	3	Total Ca 3 3	0
8	Z	3	Total Ca 3 3	0

3 Residue-property plots (i)

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:



• Molecule 1: Actin, alpha skeletal muscle

Chain D:

• Molecule 1: Actin, alpha skeletal muscle

Chain E:

• Molecule 1: Actin, alpha skeletal muscle

Chain F:

• Molecule 1: Actin, alpha skeletal muscle

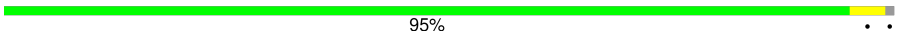
Chain G:

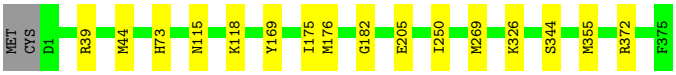
• Molecule 1: Actin, alpha skeletal muscle

Chain H:

• Molecule 1: Actin, alpha skeletal muscle

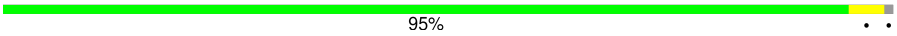
Chain I:





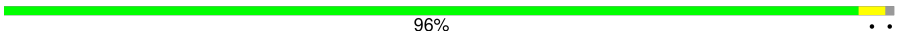
• Molecule 1: Actin, alpha skeletal muscle

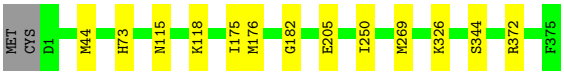
Chain J:



• Molecule 1: Actin, alpha skeletal muscle

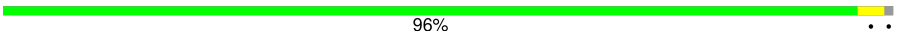
Chain K:





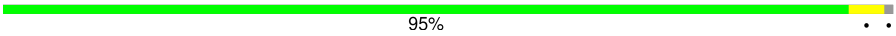
• Molecule 1: Actin, alpha skeletal muscle

Chain L:



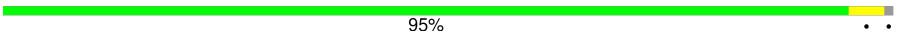
• Molecule 1: Actin, alpha skeletal muscle

Chain M:



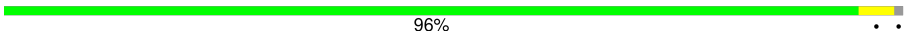
• Molecule 1: Actin, alpha skeletal muscle

Chain N:



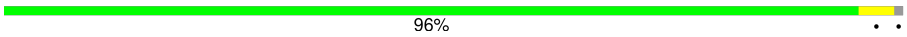
• Molecule 1: Actin, alpha skeletal muscle

Chain O:



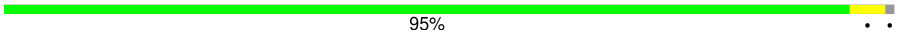
• Molecule 1: Actin, alpha skeletal muscle

Chain P:



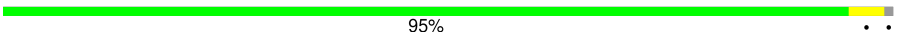
• Molecule 1: Actin, alpha skeletal muscle

Chain Q:



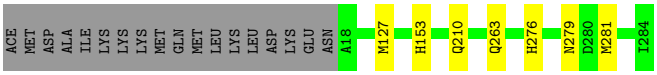
• Molecule 1: Actin, alpha skeletal muscle

Chain R:



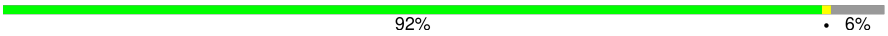
• Molecule 2: Tropomyosin alpha-1 chain

Chain e:



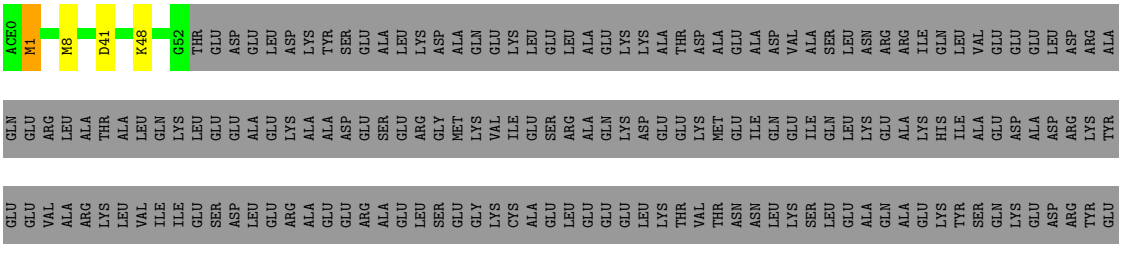
• Molecule 2: Tropomyosin alpha-1 chain

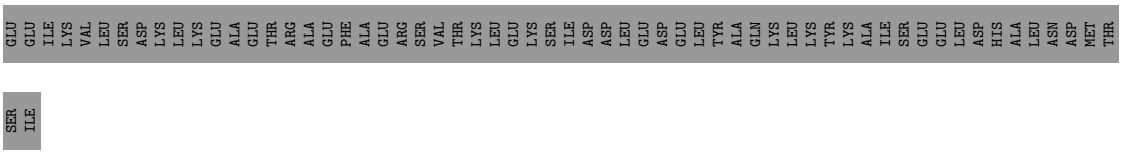
Chain f:



• Molecule 2: Tropomyosin alpha-1 chain

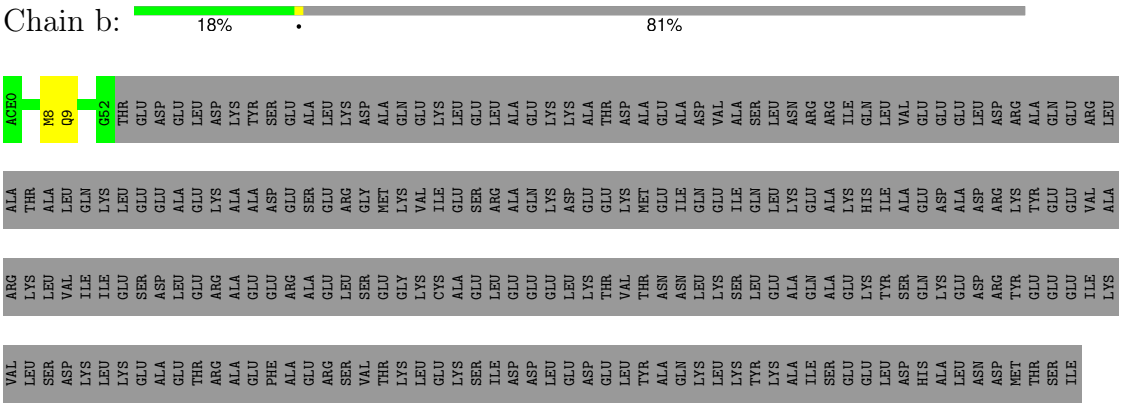
Chain W:





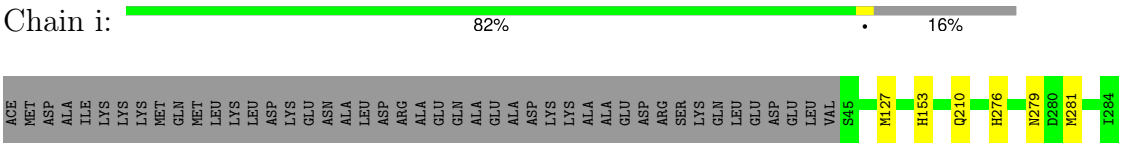
• Molecule 2: Tropomyosin alpha-1 chain

Chain b:



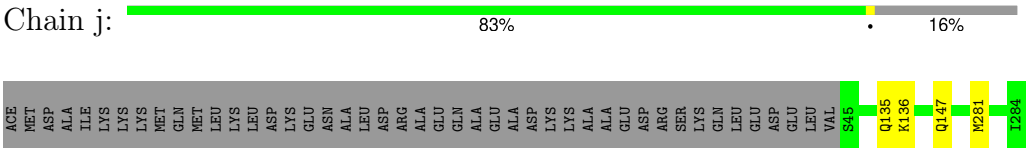
• Molecule 2: Tropomyosin alpha-1 chain

Chain i:



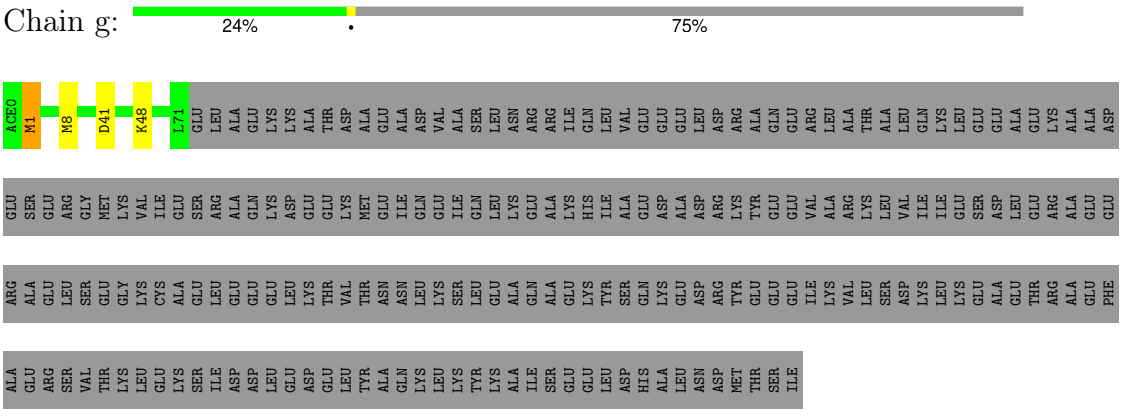
• Molecule 2: Tropomyosin alpha-1 chain

Chain j:



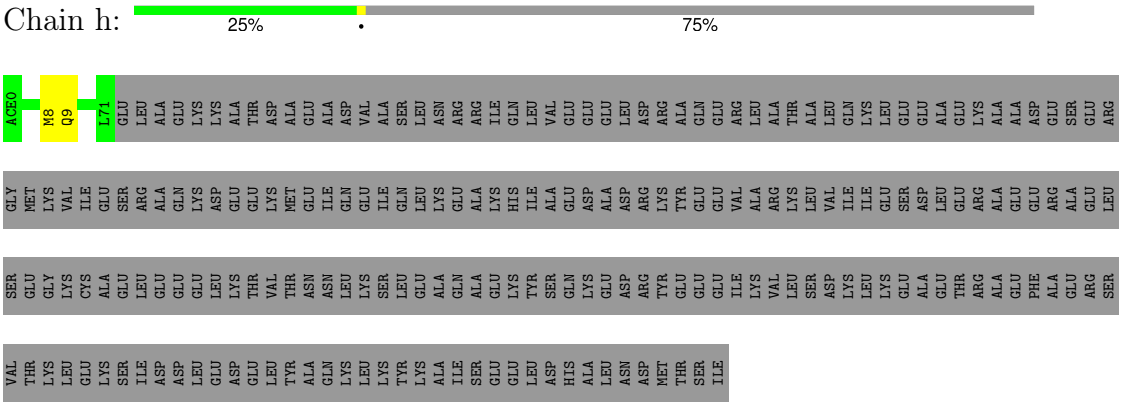
• Molecule 2: Tropomyosin alpha-1 chain

Chain g:



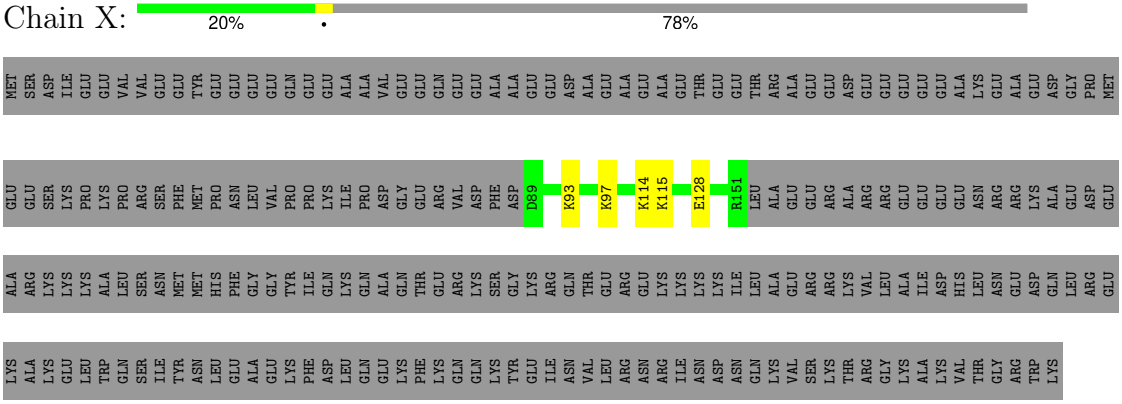
• Molecule 2: Tropomyosin alpha-1 chain

Chain h:



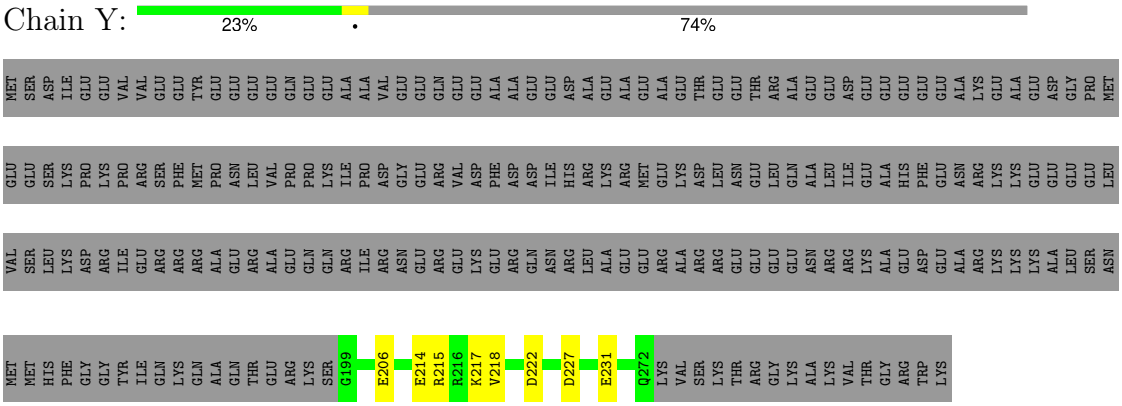
• Molecule 3: Isoform 6 of Troponin T, cardiac muscle

Chain X:



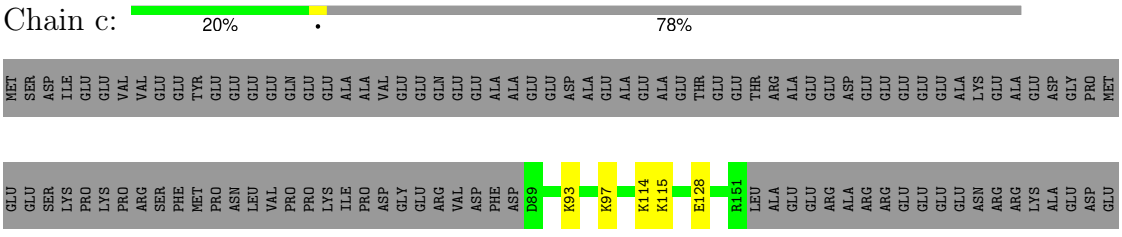
• Molecule 3: Isoform 6 of Troponin T, cardiac muscle

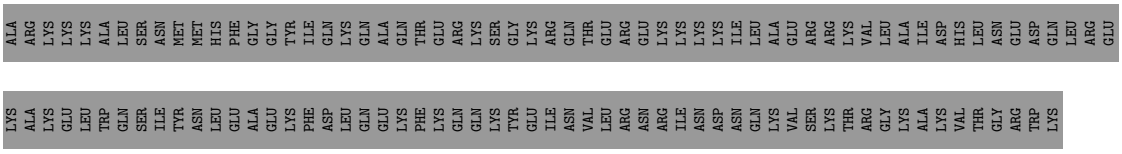
Chain Y:



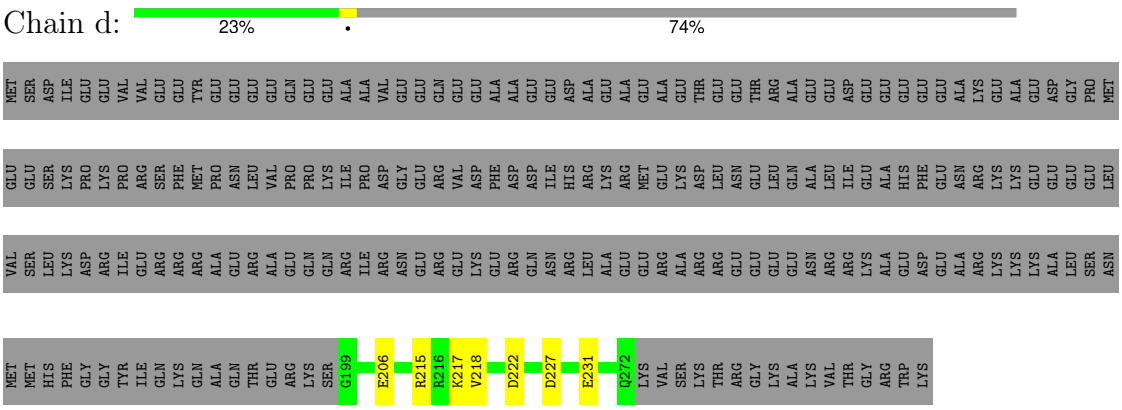
• Molecule 3: Isoform 6 of Troponin T, cardiac muscle

Chain c:

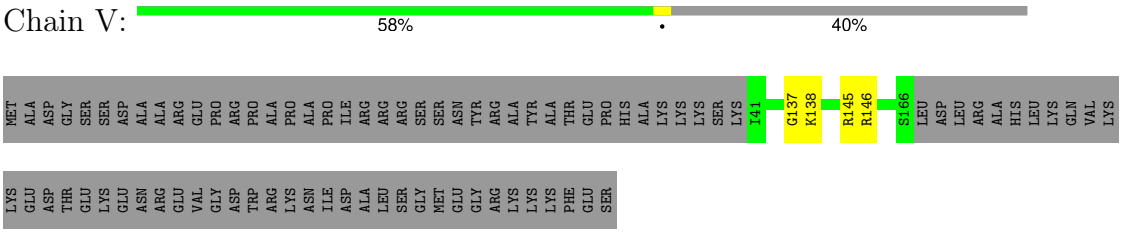




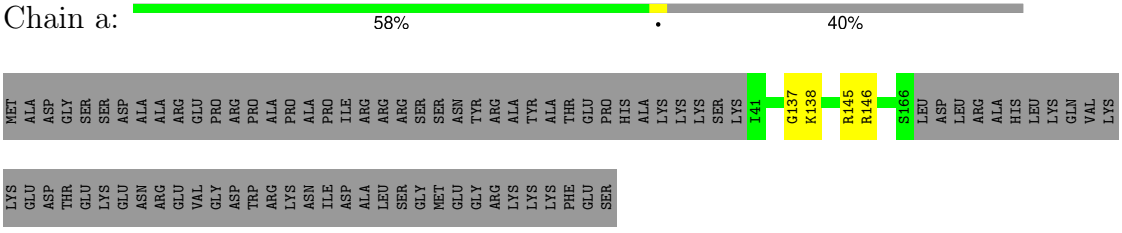
• Molecule 3: Isoform 6 of Troponin T, cardiac muscle



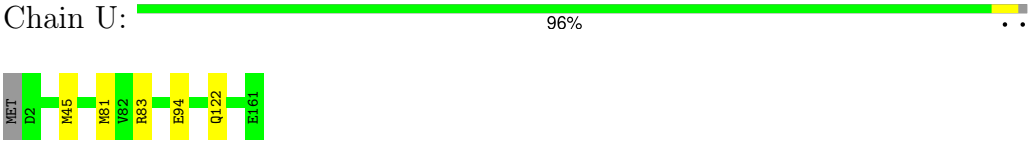
• Molecule 4: Troponin I, cardiac muscle



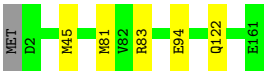
• Molecule 4: Troponin I, cardiac muscle



• Molecule 5: Troponin C, slow skeletal and cardiac muscles



• Molecule 5: Troponin C, slow skeletal and cardiac muscles


MET
D2
M45
M81
V82
R83
E94
Q122
E161

4 Experimental information (i)

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 ($e^-/Å^2$)	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(^{o})	Ideal(^{o})
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

5 of 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

5.3.2 Protein sidechains (i)

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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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

5 of 273 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	Y	231	GLU
5	U	122	GLN
3	d	215	ARG
1	J	205	GLU
1	J	166	TYR

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

The worst 5 of 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
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

There are no bond angle outliers.

There are no chirality outliers.

5 of 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

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
6	ADP	I	401	7	-	0/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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.

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

There are no chirality outliers.

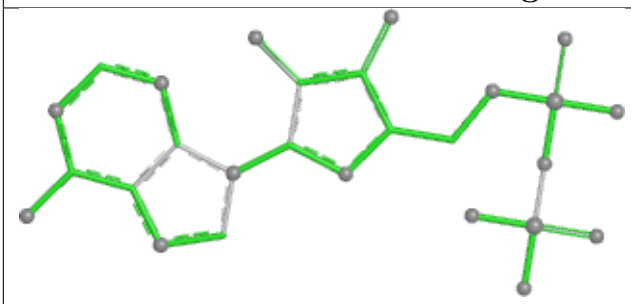
There are no torsion outliers.

There are no ring outliers.

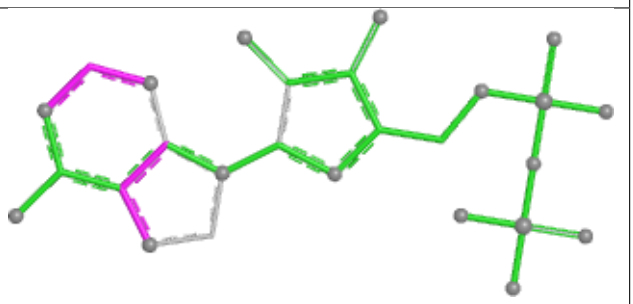
No monomer is involved in short contacts.

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

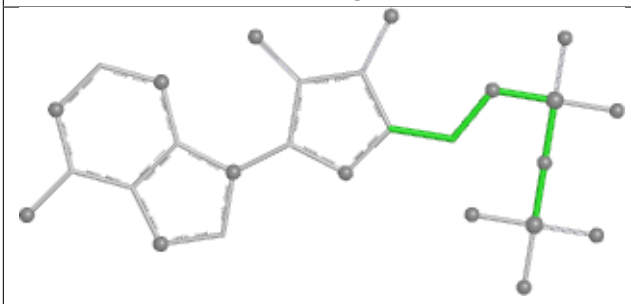
Ligand ADP D 401



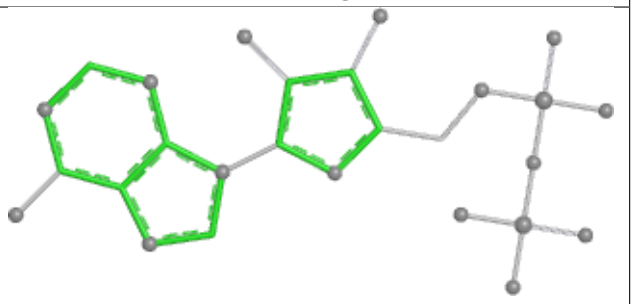
Bond lengths



Bond angles

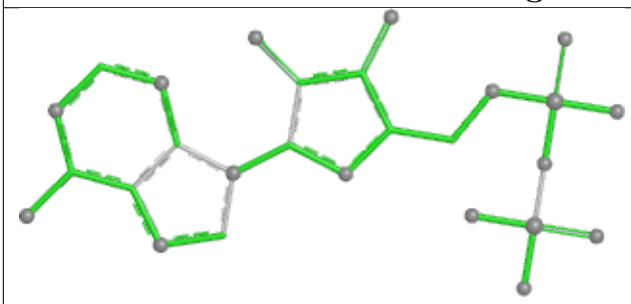


Torsions



Rings

Ligand ADP J 401



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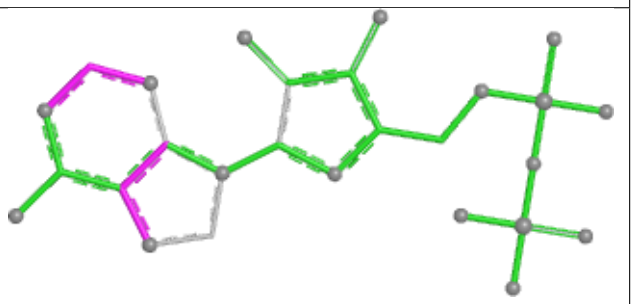

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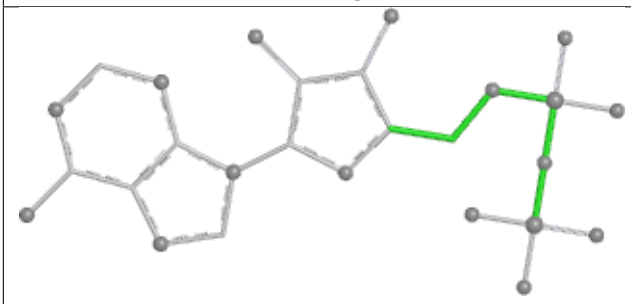

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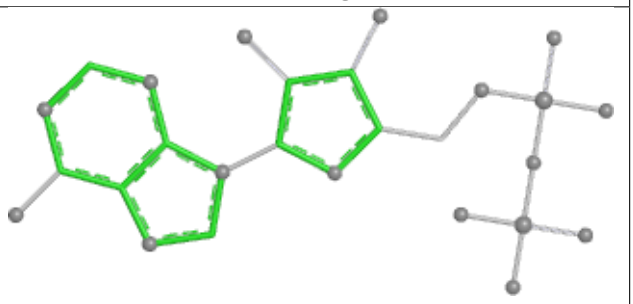

Rings

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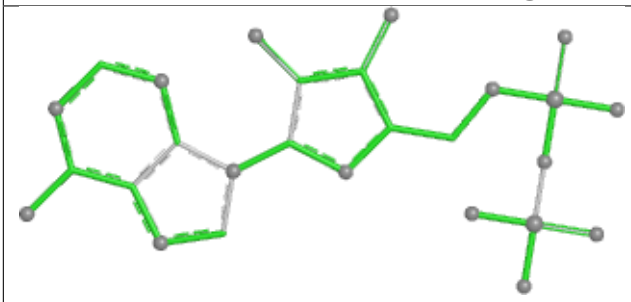

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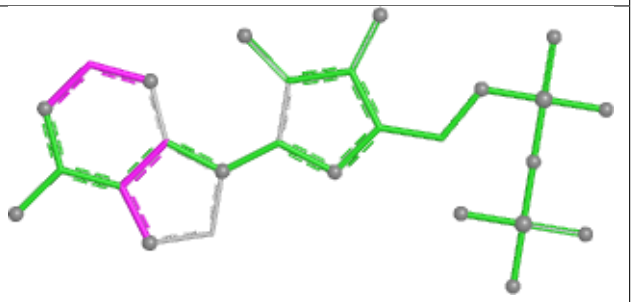
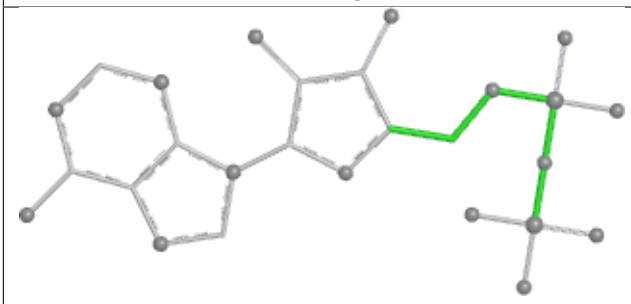


Bond angles



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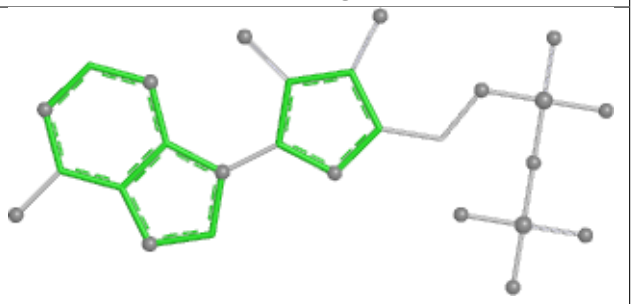

Rings

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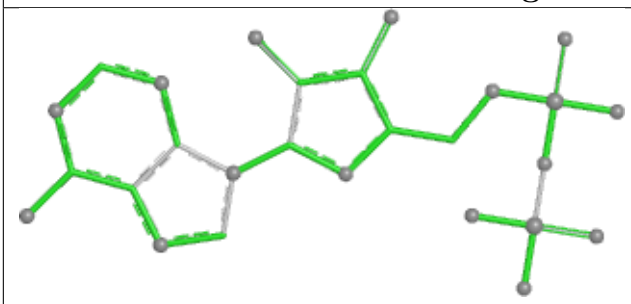

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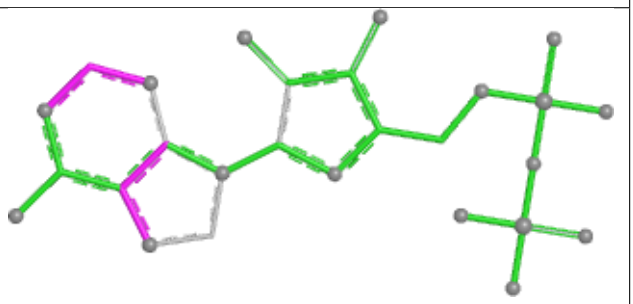

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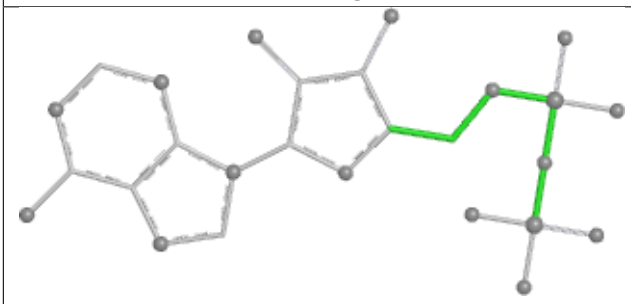

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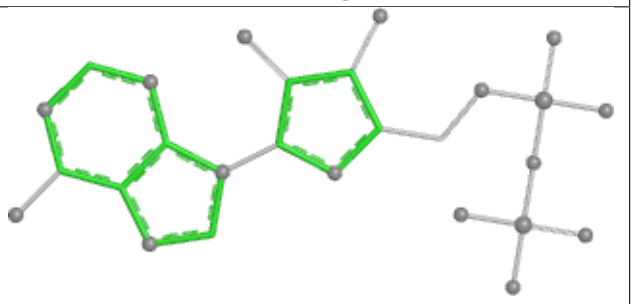

Rings

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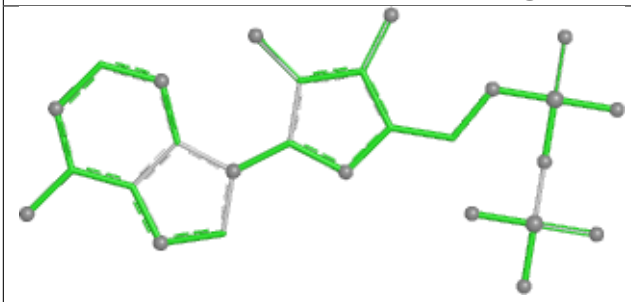

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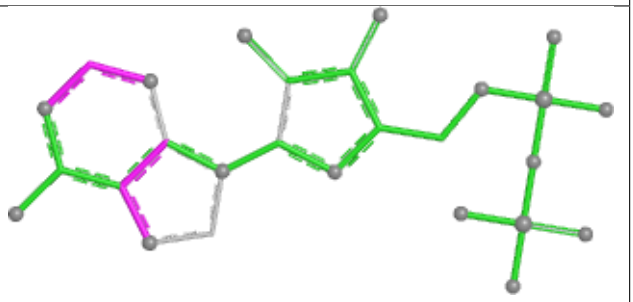

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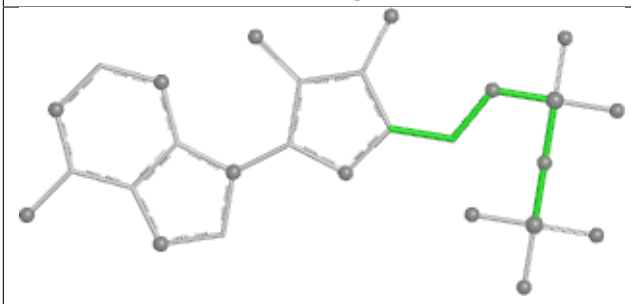

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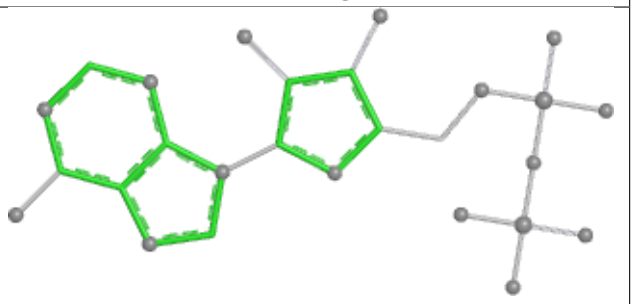

Rings

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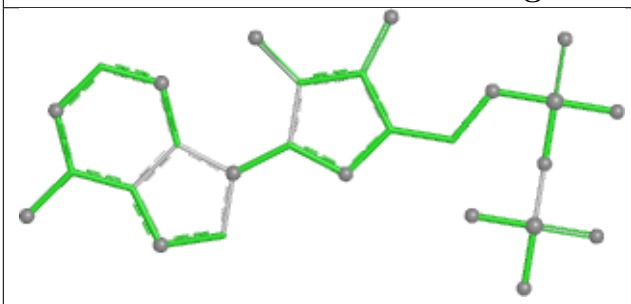

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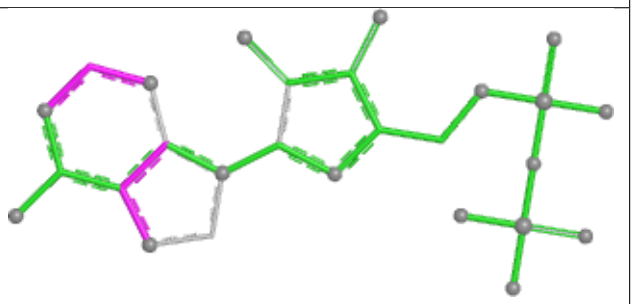

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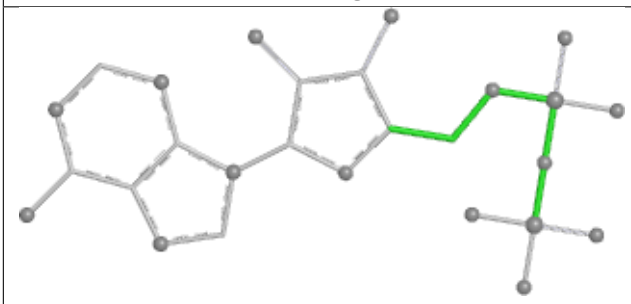

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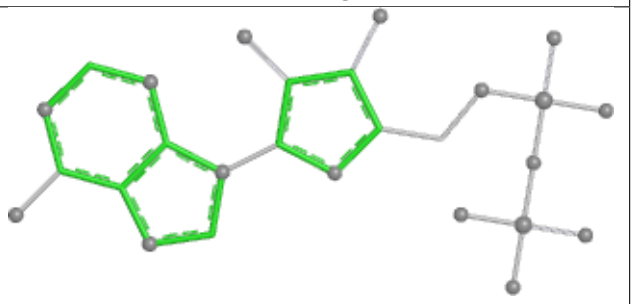

Rings

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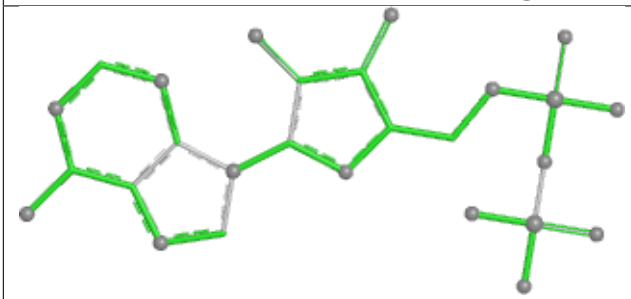

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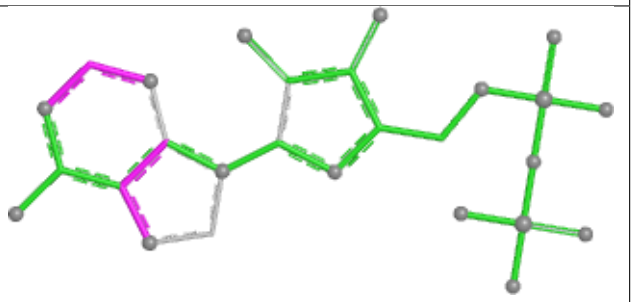

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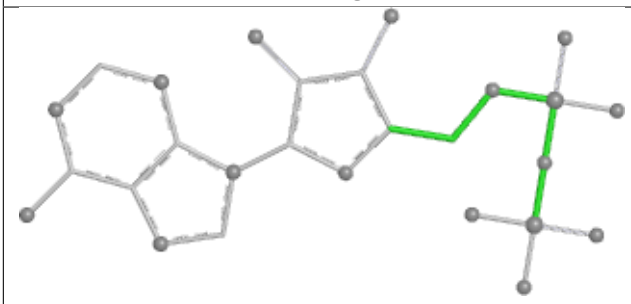

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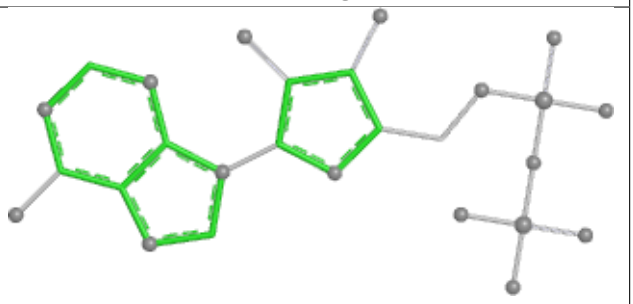

Rings

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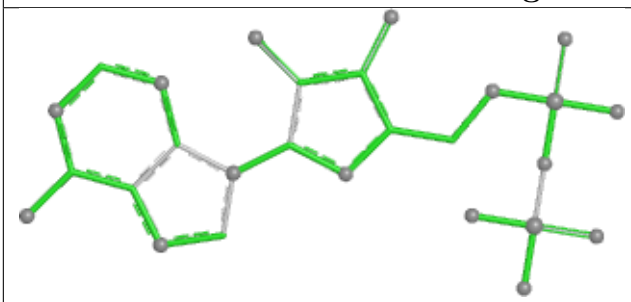

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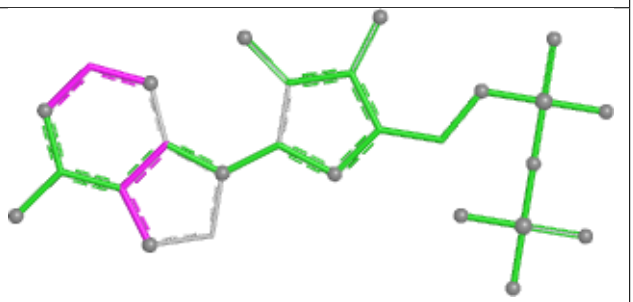

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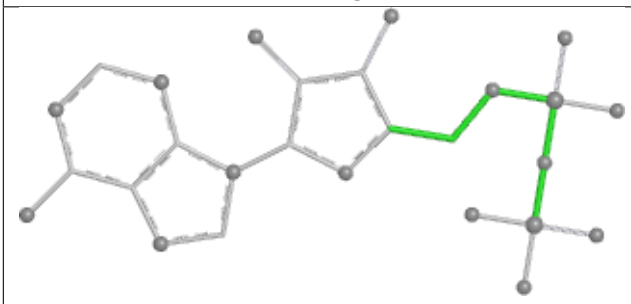
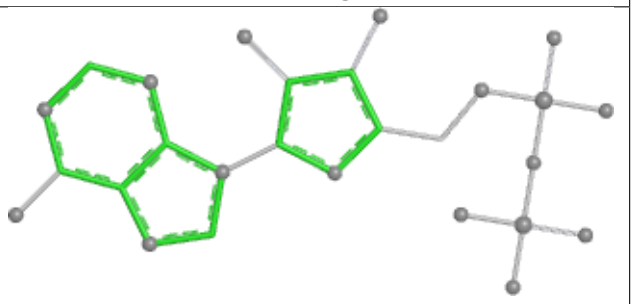
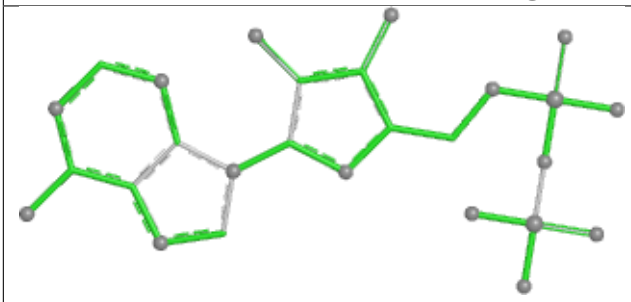


Torsions



Rings

Ligand ADP F 401



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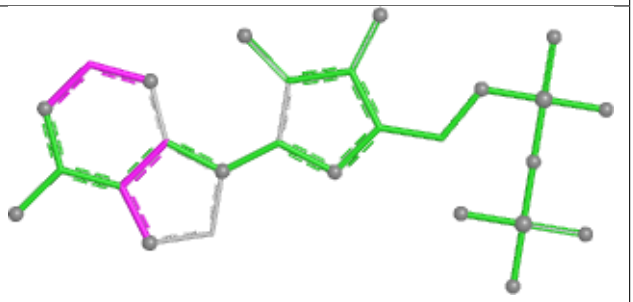

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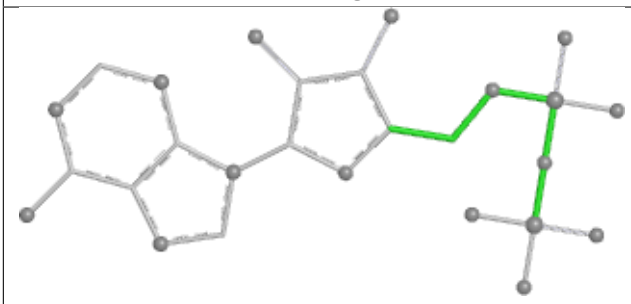

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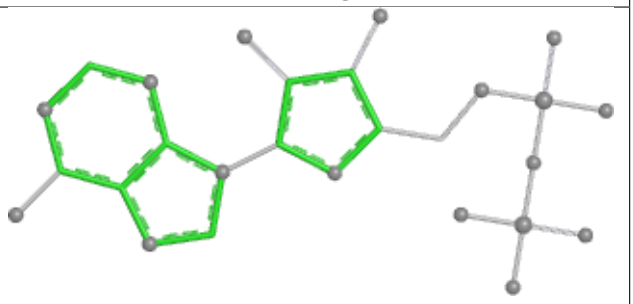
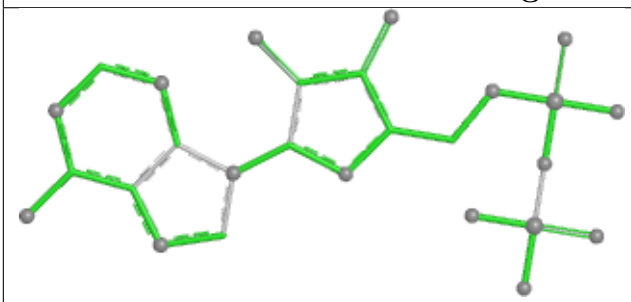


Rings

Ligand ADP R 401



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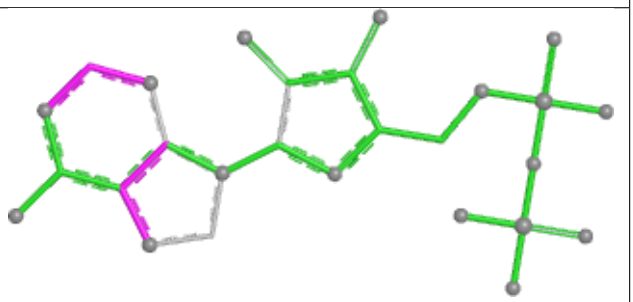

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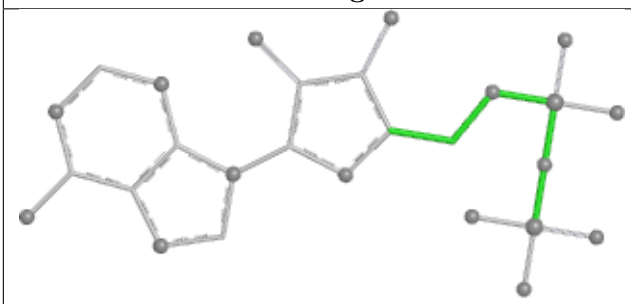

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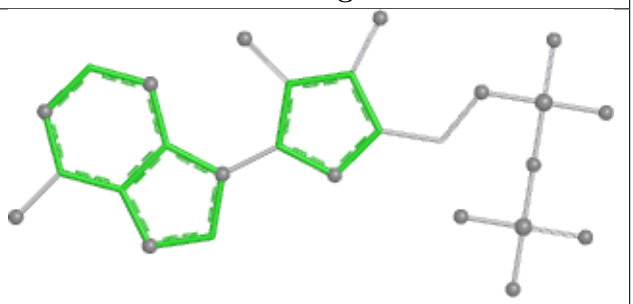
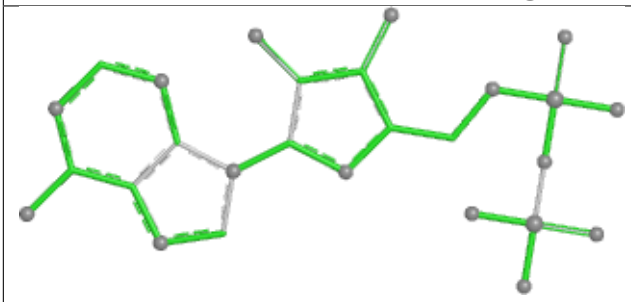


Rings

Ligand ADP O 401



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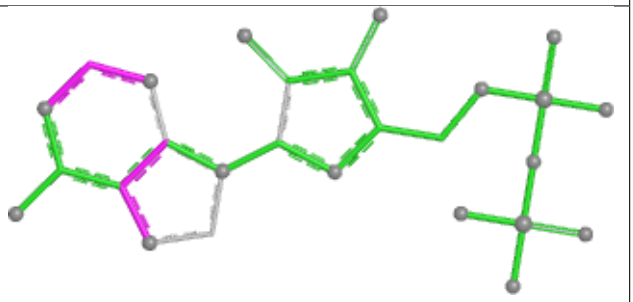

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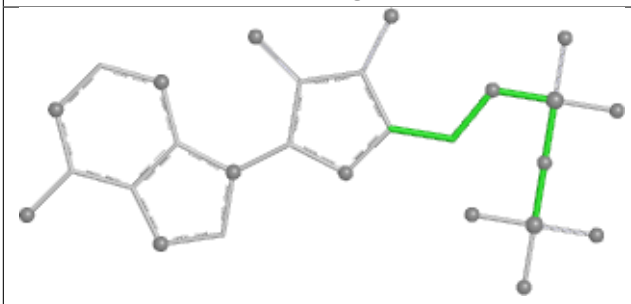

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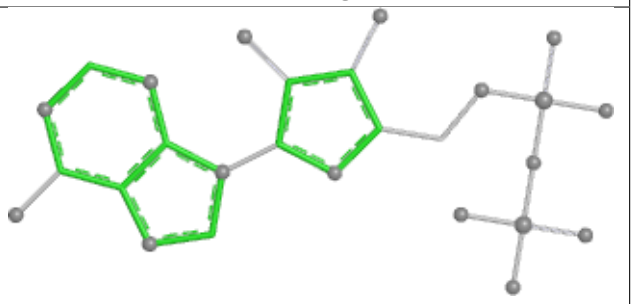
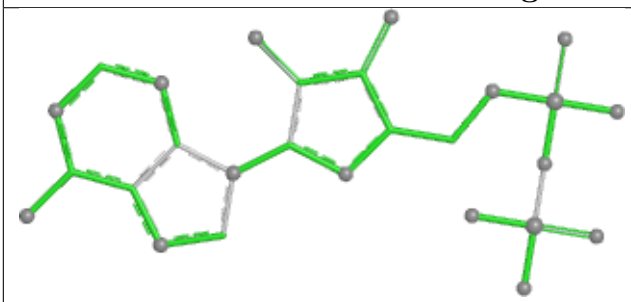
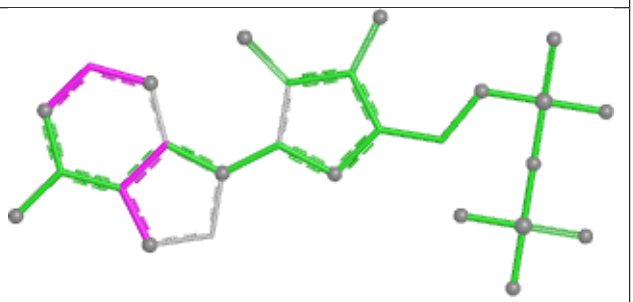


Rings

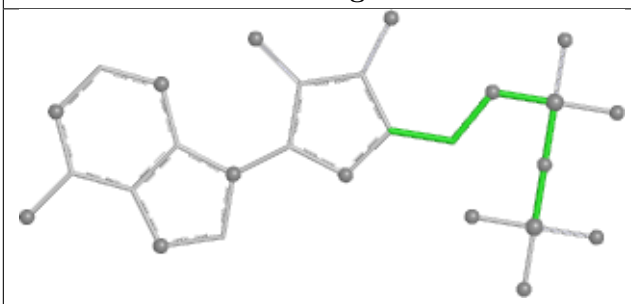
Ligand ADP H 401



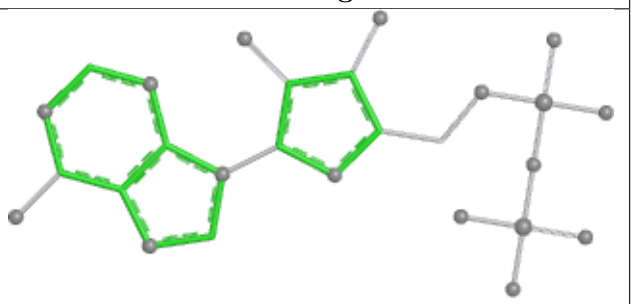
Bond lengths



Bond angles

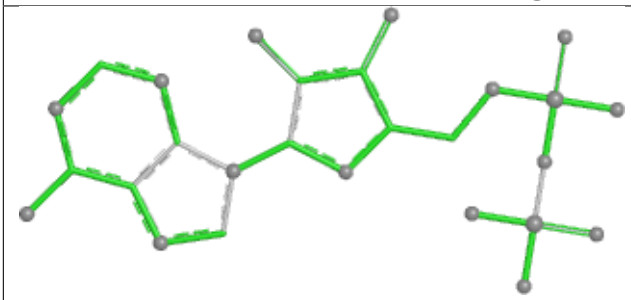


Torsions

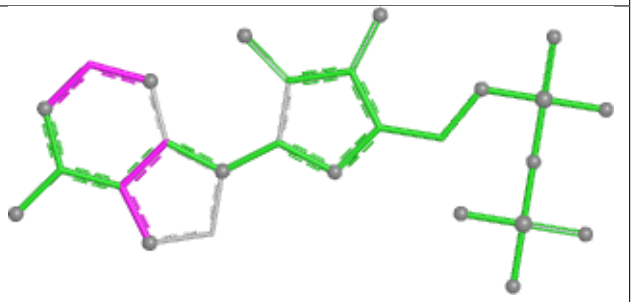


Rings

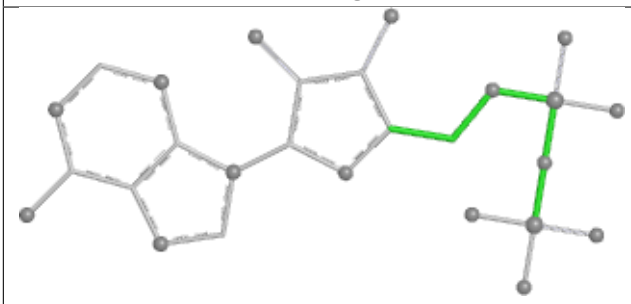
Ligand ADP I 401



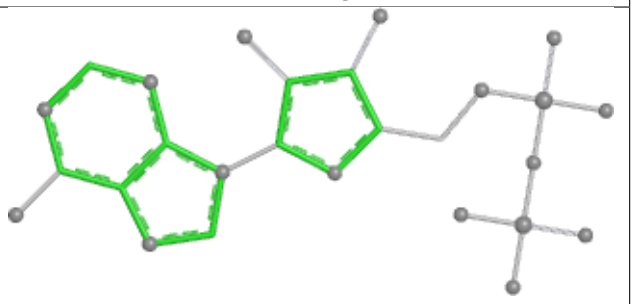
Bond lengths



Bond angles

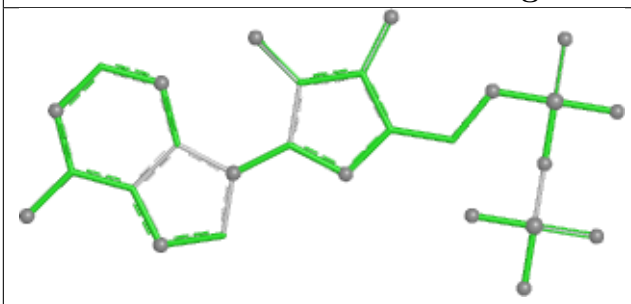


Torsions



Rings

Ligand ADP Q 401



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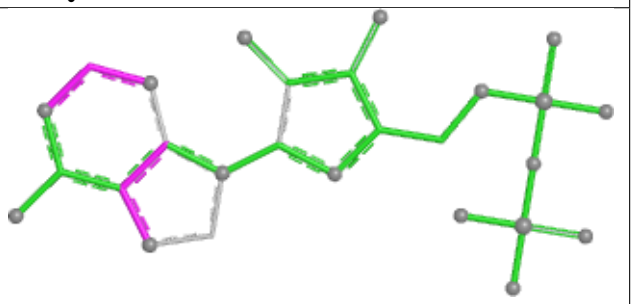
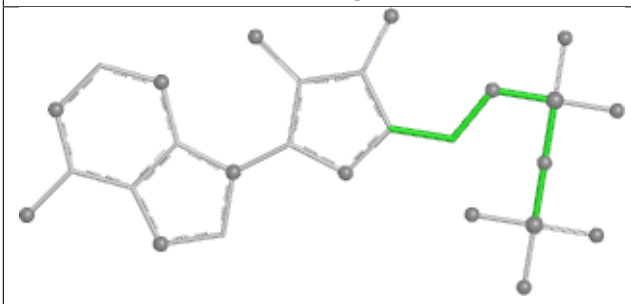
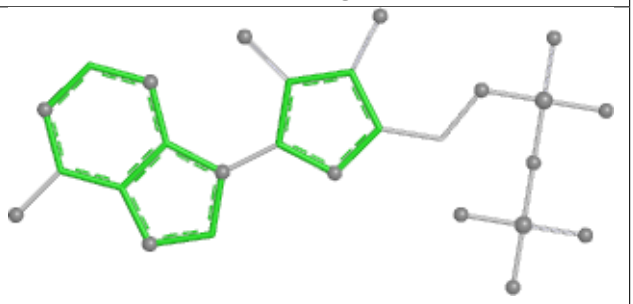


Bond angles

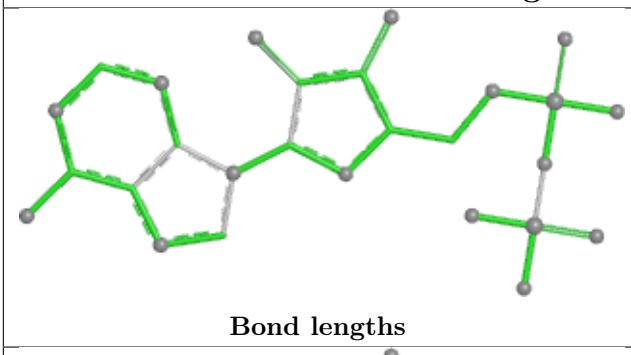


Torsions



Rings

Ligand ADP E 401



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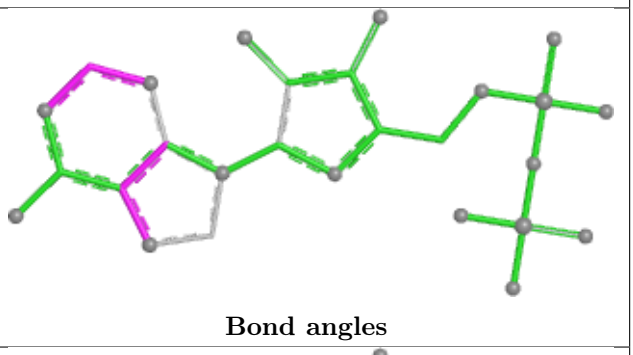
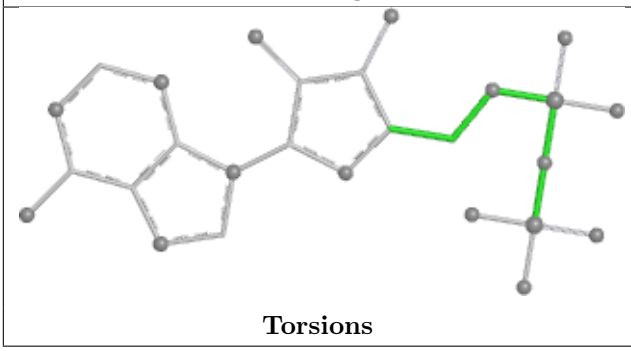
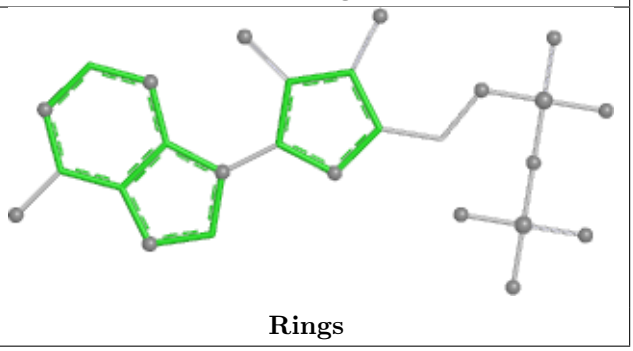


Bond angles

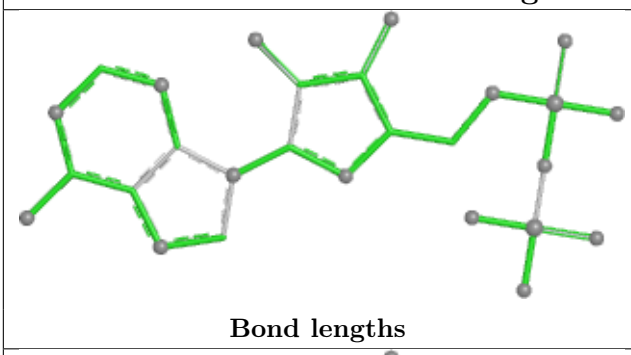


Torsions

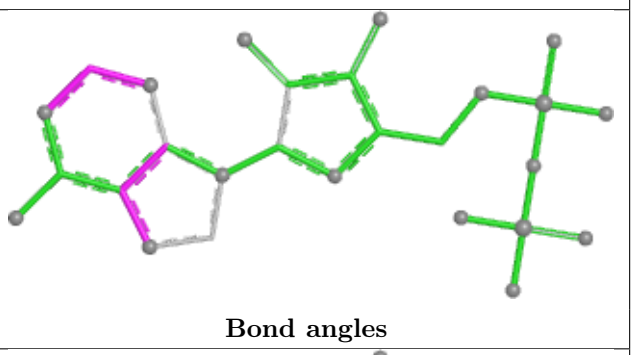


Rings

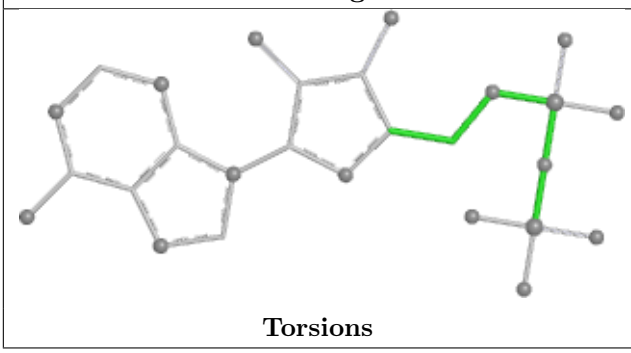
Ligand ADP G 401



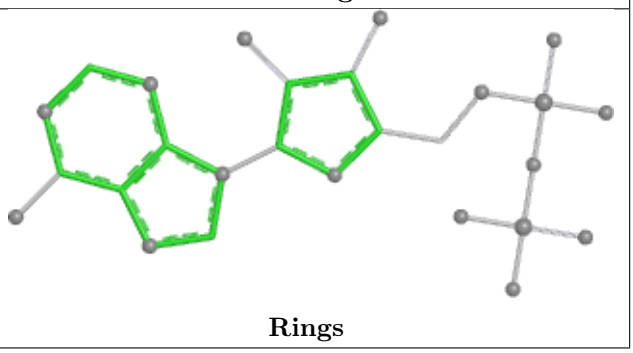
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

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 (i)

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

9 Map-model fit

This section was not generated.