



## wwPDB EM Validation Summary Report ⓘ

Jun 13, 2024 – 02:26 PM JST

PDB ID : 8XUV  
EMDB ID : EMD-38685  
Title : Cryo-EM structure of tomato NRC2 filament  
Authors : Sun, Y.; Ma, S.C.; Chai, J.J.  
Deposited on : 2024-01-14  
Resolution : 3.60 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](mailto: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>.

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

EMDB validation analysis	: <b>FAILED</b>
Mogul	: 1.8.5 (274361), CSD as541be (2020)
MolProbity	: 4.02b-467
buster-report	: 1.1.7 (2018)
Percentile statistics	: 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	: <b>FAILED</b>
Ideal geometry (proteins)	: Engh & Huber (2001)
Ideal geometry (DNA, RNA)	: Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: 2.36.2



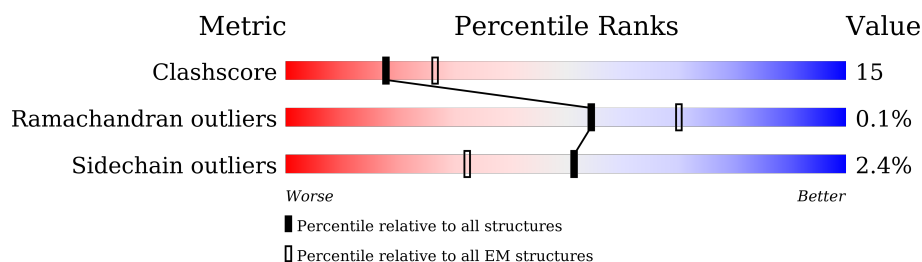
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826




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  $\geq 3$ , 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	885	69% 30% .
1	B	885	67% 32% .
1	C	885	68% 31% .
1	D	885	74% 26% .
1	E	885	66% 32% .
1	F	885	69% 29% .
1	G	885	73% 26% .
1	H	885	72% 27% .
1	I	885	70% 30% .

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Mol	Chain	Length	Quality of chain
1	J	885	 68%31%.
1	K	885	 69%30%.
1	L	885	 71%28%.



## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 86208 atoms, of which 0 are hydrogens and 0 are deuteriums.

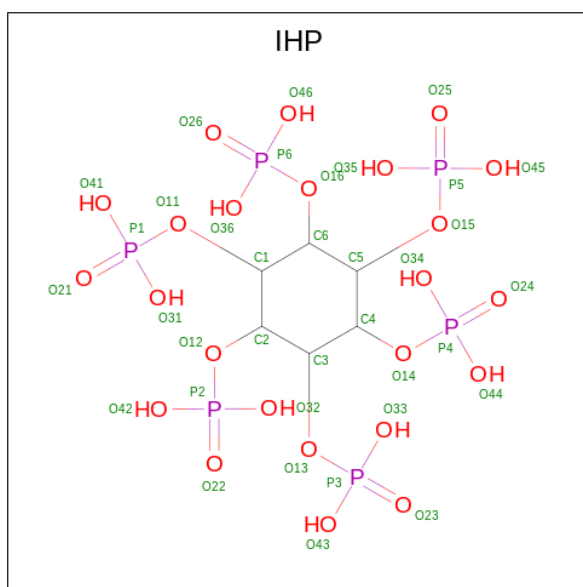
In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NRC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	885	Total 7121	C 4544	N 1237	O 1308	S 32	0	0
1	B	885	Total 7121	C 4544	N 1237	O 1308	S 32	0	0
1	C	885	Total 7121	C 4544	N 1237	O 1308	S 32	0	0
1	D	885	Total 7121	C 4544	N 1237	O 1308	S 32	0	0
1	E	885	Total 7121	C 4544	N 1237	O 1308	S 32	0	0
1	F	885	Total 7121	C 4544	N 1237	O 1308	S 32	0	0
1	G	885	Total 7121	C 4544	N 1237	O 1308	S 32	0	0
1	H	885	Total 7121	C 4544	N 1237	O 1308	S 32	0	0
1	I	885	Total 7121	C 4544	N 1237	O 1308	S 32	0	0
1	J	885	Total 7121	C 4544	N 1237	O 1308	S 32	0	0
1	K	885	Total 7121	C 4544	N 1237	O 1308	S 32	0	0
1	L	885	Total 7121	C 4544	N 1237	O 1308	S 32	0	0

- Molecule 2 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula:  $C_6H_{18}O_{24}P_6$ ) (labeled as "Ligand of Interest" by depositor).

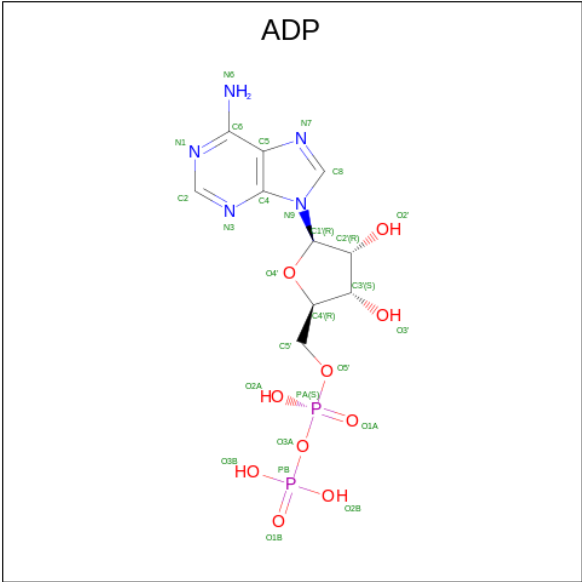




Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	O	P	0
			36	6	24	6	
2	B	1	Total	C	O	P	0
			36	6	24	6	
2	C	1	Total	C	O	P	0
			36	6	24	6	
2	D	1	Total	C	O	P	0
			36	6	24	6	
2	E	1	Total	C	O	P	0
			36	6	24	6	
2	F	1	Total	C	O	P	0
			36	6	24	6	
2	G	1	Total	C	O	P	0
			36	6	24	6	
2	H	1	Total	C	O	P	0
			36	6	24	6	
2	I	1	Total	C	O	P	0
			36	6	24	6	
2	J	1	Total	C	O	P	0
			36	6	24	6	
2	K	1	Total	C	O	P	0
			36	6	24	6	
2	L	1	Total	C	O	P	0
			36	6	24	6	

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





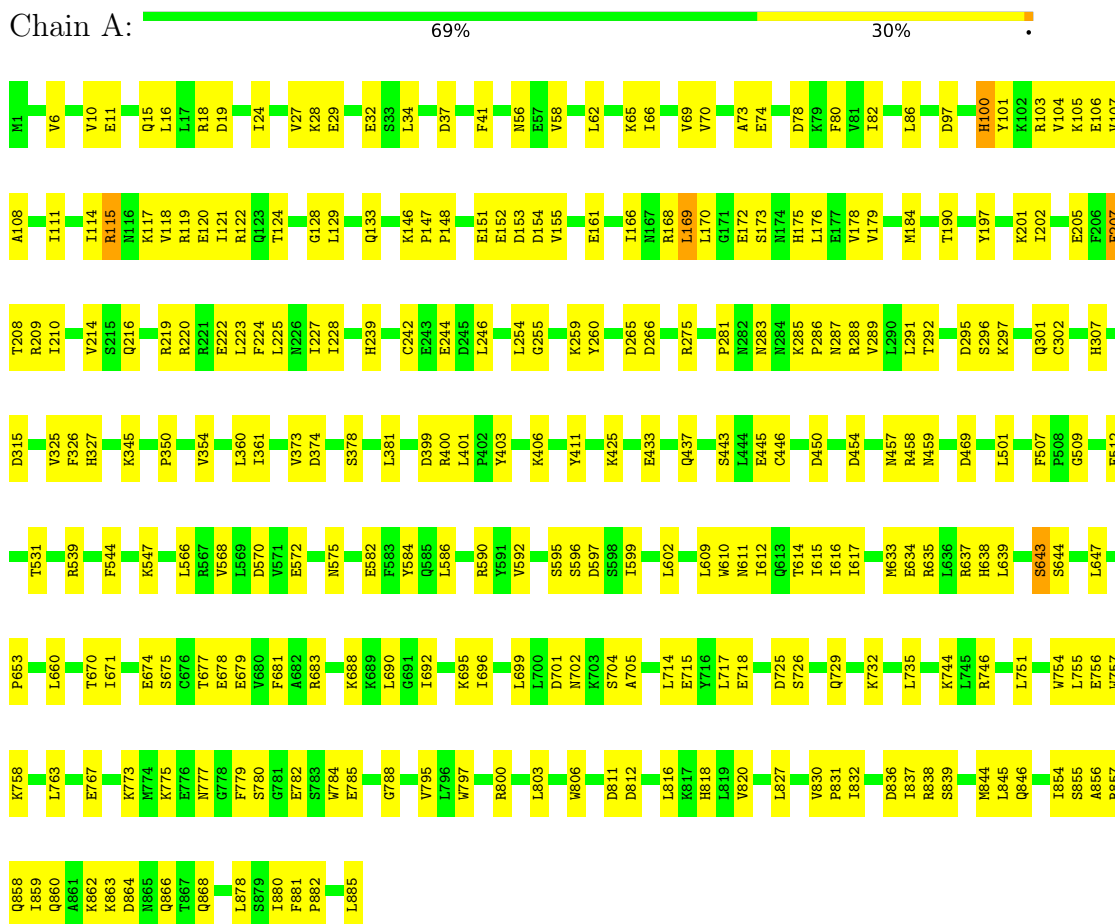
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	G	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	H	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	I	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	J	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	K	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	L	1	Total	C	N	O	P	0
			27	10	5	10	2	



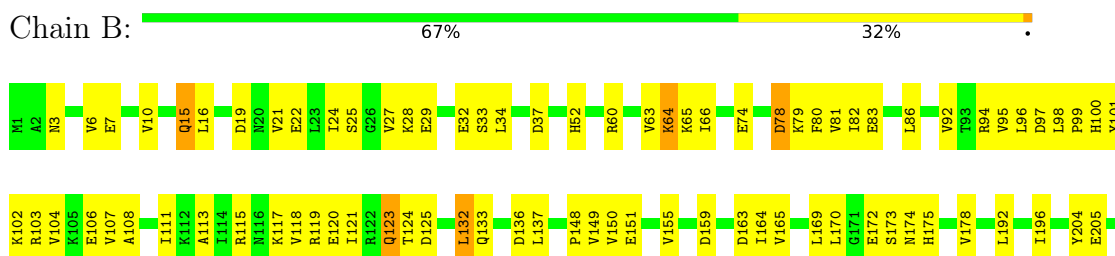
### 3 Residue-property plots

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: NRC2



#### • Molecule 1: NRC2



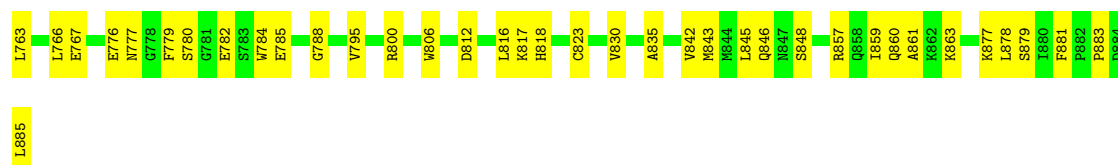






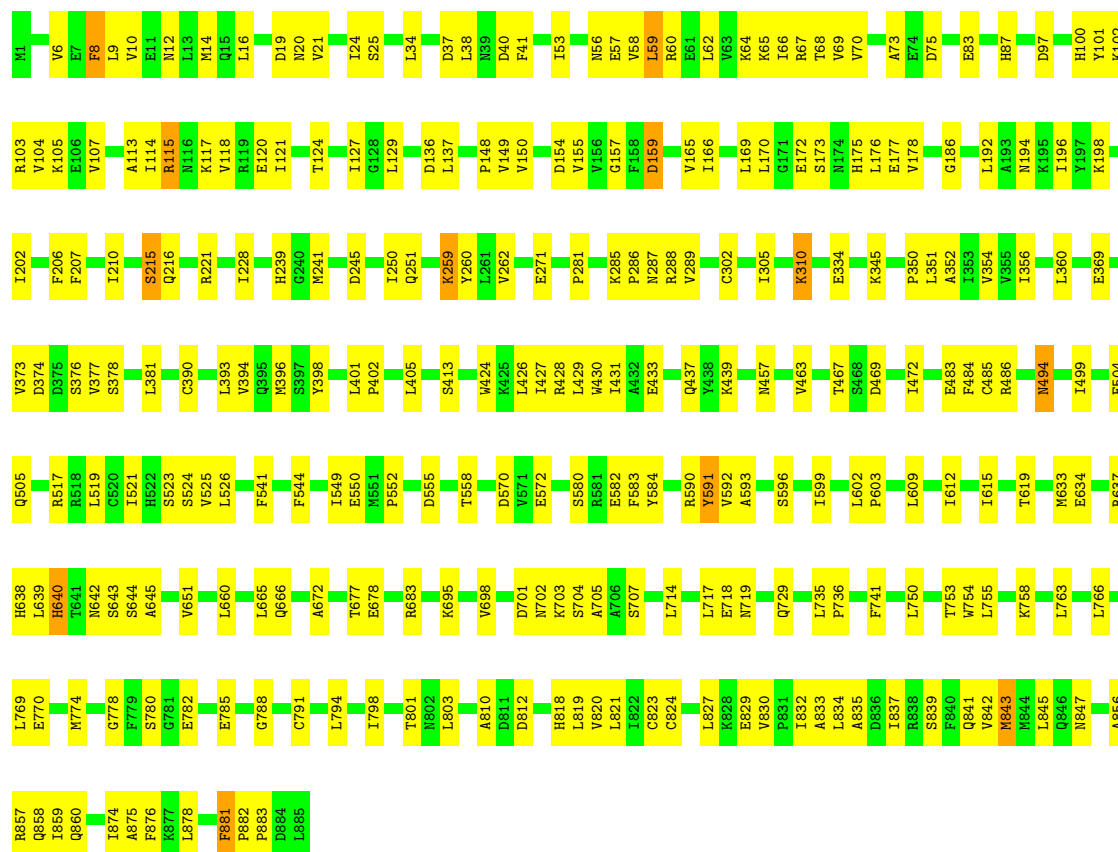






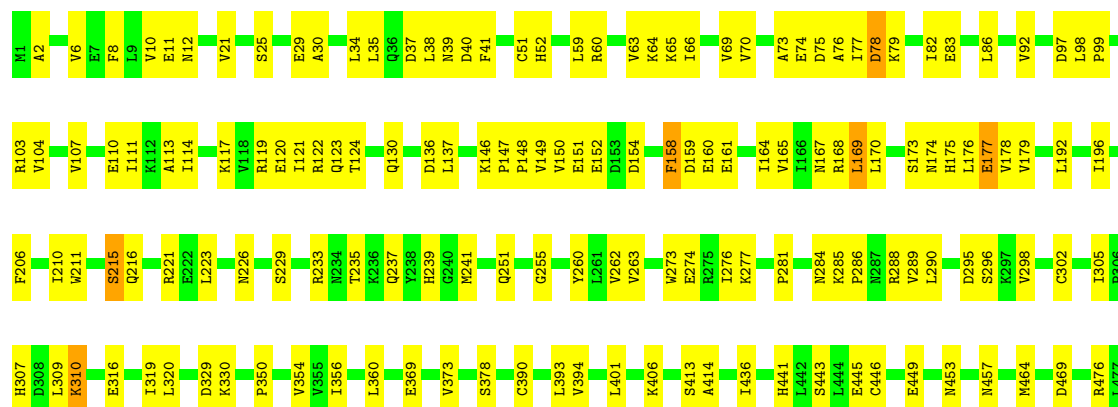
• Molecule 1: NRC2

Chain F: 69% 29% .



• Molecule 1: NRC2

Chain G: 73% 26% .

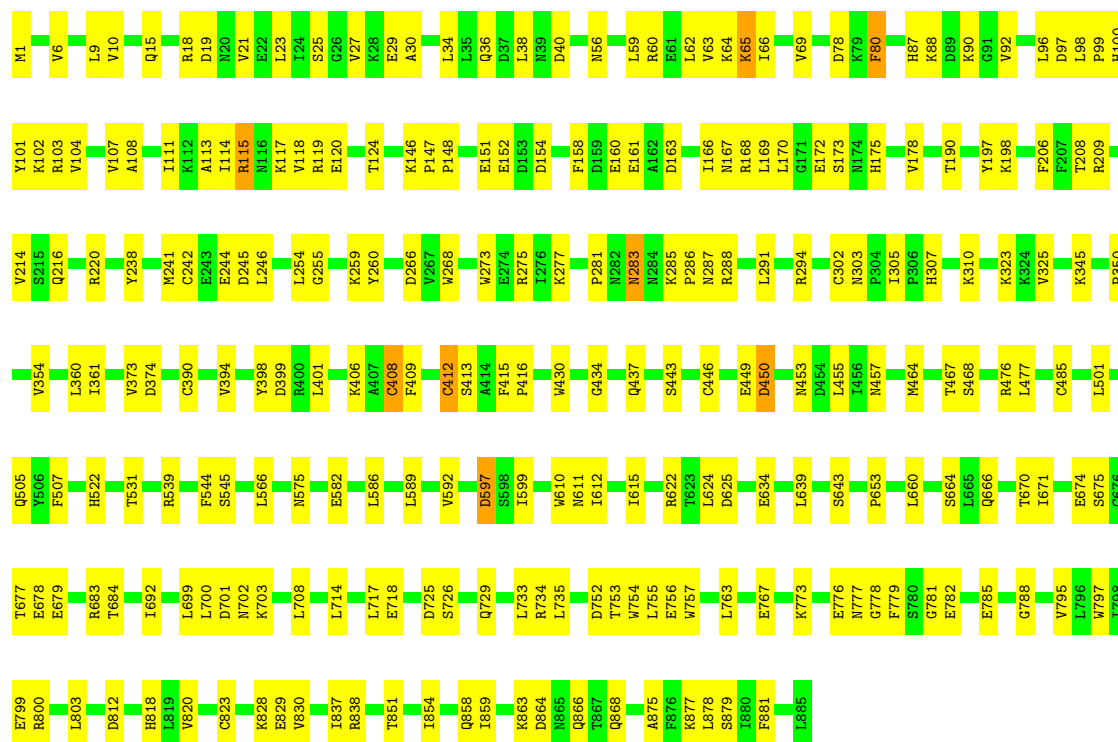






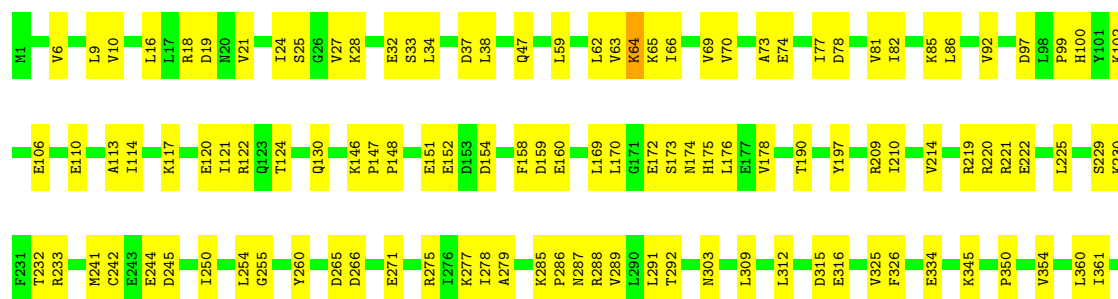
• Molecule 1: NRC2

Chain H: 72% 27%



• Molecule 1: NRC2

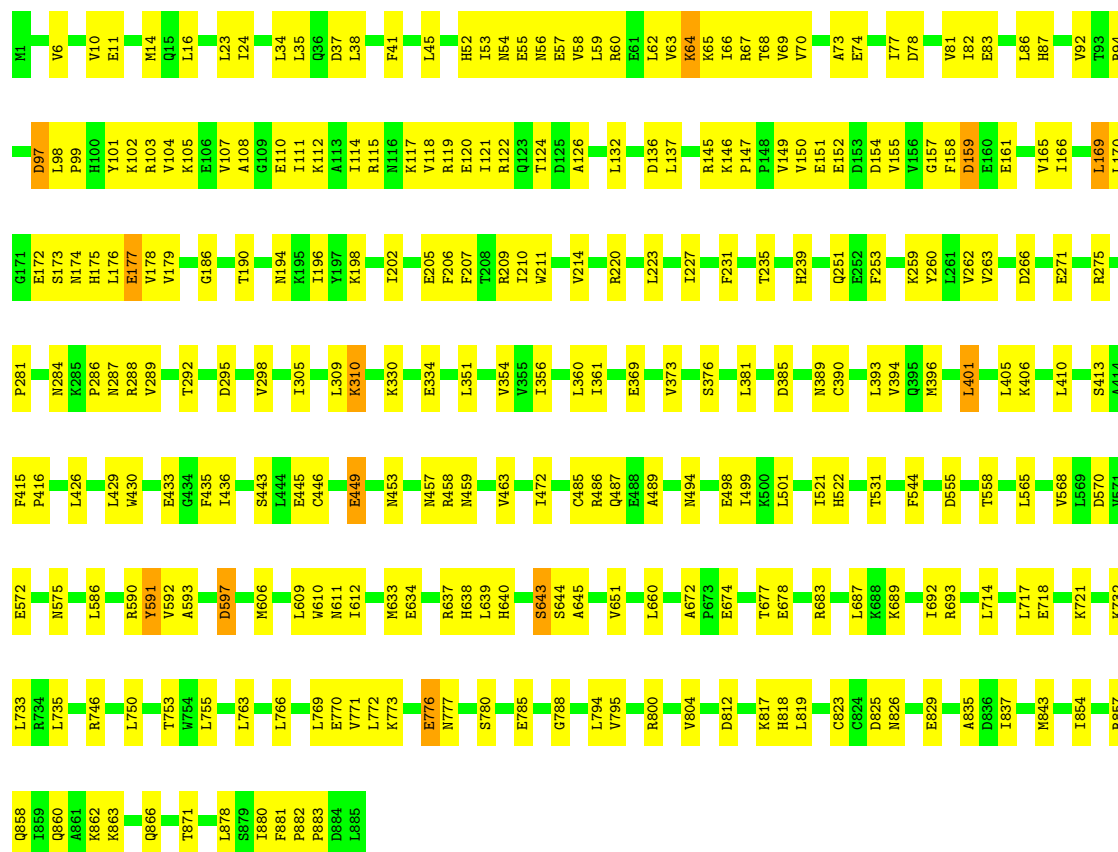
Chain I: 70% 30%





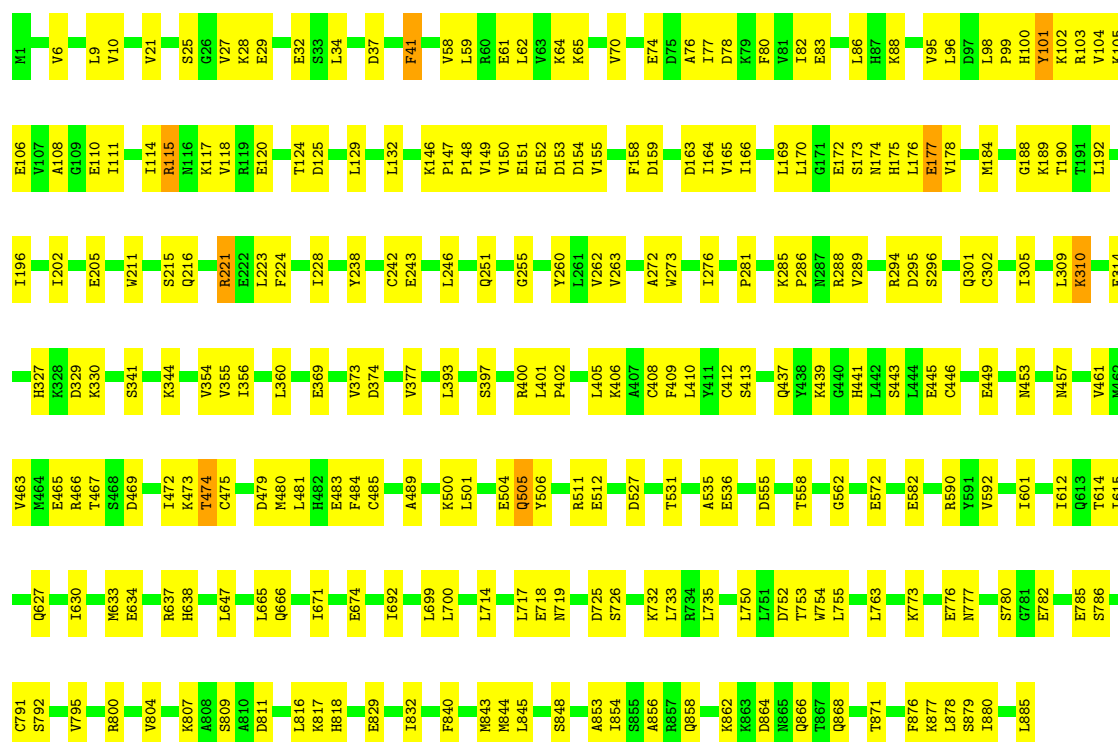






• Molecule 1: NRC2

Chain L: 71% 28%





## 4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-55.85°, rise=64.04 Å, axial sym=C3	Depositor
Number of segments used	280426	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IHP, 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	0.31	0/7260	0.51	0/9803
1	B	0.34	0/7260	0.54	0/9803
1	C	0.30	0/7260	0.54	0/9803
1	D	0.30	0/7260	0.51	0/9803
1	E	0.33	0/7260	0.52	0/9803
1	F	0.31	0/7260	0.52	0/9803
1	G	0.31	0/7260	0.51	0/9803
1	H	0.32	0/7260	0.53	0/9803
1	I	0.32	0/7260	0.51	0/9803
1	J	0.32	0/7260	0.52	0/9803
1	K	0.33	0/7260	0.53	0/9803
1	L	0.30	0/7260	0.51	0/9803
All	All	0.32	0/87120	0.52	0/117636

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	7121	0	7283	225	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	7121	0	7283	232	0
1	C	7121	0	7283	210	0
1	D	7121	0	7283	190	0
1	E	7121	0	7283	236	0
1	F	7121	0	7283	233	0
1	G	7121	0	7283	176	0
1	H	7121	0	7283	193	0
1	I	7121	0	7283	227	0
1	J	7121	0	7283	213	0
1	K	7121	0	7283	249	0
1	L	7121	0	7283	214	0
2	A	36	0	6	0	0
2	B	36	0	6	0	0
2	C	36	0	6	0	0
2	D	36	0	6	1	0
2	E	36	0	6	0	0
2	F	36	0	6	0	0
2	G	36	0	6	0	0
2	H	36	0	6	2	0
2	I	36	0	6	2	0
2	J	36	0	6	0	0
2	K	36	0	6	1	0
2	L	36	0	6	1	0
3	A	27	0	12	5	0
3	B	27	0	12	4	0
3	C	27	0	12	3	0
3	D	27	0	12	6	0
3	E	27	0	12	1	0
3	F	27	0	12	4	0
3	G	27	0	12	1	0
3	H	27	0	12	3	0
3	I	27	0	12	3	0
3	J	27	0	12	3	0
3	K	27	0	12	4	0
3	L	27	0	12	7	0
All	All	86208	0	87612	2593	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 15.

The worst 5 of 2593 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:H:34:LEU:O	1:H:38:LEU:HD12	1.40	1.19
1:B:169:LEU:HD12	1:B:170:LEU:HG	1.26	1.07
1:B:254:LEU:HD11	1:B:260:TYR:CG	1.90	1.07
1:A:634:GLU:OE1	1:A:635:ARG:NH2	1.88	1.06
1:B:169:LEU:HD12	1:B:170:LEU:CG	1.93	0.98

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	883/885 (100%)	813 (92%)	70 (8%)	0	100	100
1	B	883/885 (100%)	820 (93%)	63 (7%)	0	100	100
1	C	883/885 (100%)	843 (96%)	39 (4%)	1 (0%)	51	83
1	D	883/885 (100%)	835 (95%)	48 (5%)	0	100	100
1	E	883/885 (100%)	806 (91%)	74 (8%)	3 (0%)	41	75
1	F	883/885 (100%)	834 (94%)	49 (6%)	0	100	100
1	G	883/885 (100%)	839 (95%)	44 (5%)	0	100	100
1	H	883/885 (100%)	818 (93%)	64 (7%)	1 (0%)	51	83
1	I	883/885 (100%)	824 (93%)	59 (7%)	0	100	100
1	J	883/885 (100%)	804 (91%)	78 (9%)	1 (0%)	51	83
1	K	883/885 (100%)	821 (93%)	61 (7%)	1 (0%)	51	83
1	L	883/885 (100%)	836 (95%)	47 (5%)	0	100	100
All	All	10596/10620 (100%)	9893 (93%)	696 (7%)	7 (0%)	54	83

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	408	CYS

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Mol	Chain	Res	Type
1	E	409	PHE
1	H	65	LYS
1	K	147	PRO
1	J	107	VAL

### 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	797/797 (100%)	782 (98%)	15 (2%)	57	80
1	B	797/797 (100%)	779 (98%)	18 (2%)	50	76
1	C	797/797 (100%)	773 (97%)	24 (3%)	41	71
1	D	797/797 (100%)	783 (98%)	14 (2%)	59	81
1	E	797/797 (100%)	767 (96%)	30 (4%)	33	66
1	F	797/797 (100%)	780 (98%)	17 (2%)	53	78
1	G	797/797 (100%)	781 (98%)	16 (2%)	55	79
1	H	797/797 (100%)	780 (98%)	17 (2%)	53	78
1	I	797/797 (100%)	783 (98%)	14 (2%)	59	81
1	J	797/797 (100%)	768 (96%)	29 (4%)	35	67
1	K	797/797 (100%)	778 (98%)	19 (2%)	49	75
1	L	797/797 (100%)	782 (98%)	15 (2%)	57	80
All	All	9564/9564 (100%)	9336 (98%)	228 (2%)	51	75

5 of 228 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	791	CYS
1	L	310	LYS
1	H	294	ARG
1	L	242	CYS
1	K	169	LEU



Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	453	ASN
1	K	478	HIS
1	F	478	HIS
1	E	588	HIS
1	K	640	HIS

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

24 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	$\# Z  > 2$
3	ADP	J	902	-	24,29,29	0.73	0	29,45,45	0.78	0
3	ADP	H	902	-	24,29,29	0.74	0	29,45,45	0.82	1 (3%)
2	IHP	D	901	-	36,36,36	0.76	0	54,60,60	0.56	0
2	IHP	F	901	-	36,36,36	0.73	0	54,60,60	0.56	0
3	ADP	D	902	-	24,29,29	0.71	0	29,45,45	0.85	1 (3%)
3	ADP	B	902	-	24,29,29	0.72	0	29,45,45	0.78	1 (3%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ADP	K	902	-	24,29,29	0.67	0	29,45,45	0.92	2 (6%)
3	ADP	A	902	-	24,29,29	0.79	0	29,45,45	0.79	1 (3%)
2	IHP	E	901	-	36,36,36	1.45	6 (16%)	54,60,60	0.65	1 (1%)
3	ADP	L	902	-	24,29,29	0.70	0	29,45,45	0.88	0
3	ADP	E	902	-	24,29,29	0.71	0	29,45,45	0.70	1 (3%)
3	ADP	F	902	-	24,29,29	0.70	1 (4%)	29,45,45	0.79	1 (3%)
2	IHP	G	901	-	36,36,36	0.75	0	54,60,60	0.61	0
2	IHP	K	901	-	36,36,36	1.44	6 (16%)	54,60,60	0.61	0
2	IHP	B	901	-	36,36,36	0.76	0	54,60,60	0.60	0
2	IHP	I	901	-	36,36,36	1.42	6 (16%)	54,60,60	0.59	0
2	IHP	L	901	-	36,36,36	1.43	6 (16%)	54,60,60	0.64	1 (1%)
2	IHP	C	901	-	36,36,36	1.48	6 (16%)	54,60,60	0.57	0
2	IHP	J	901	-	36,36,36	0.74	0	54,60,60	0.54	0
2	IHP	H	901	-	36,36,36	1.45	6 (16%)	54,60,60	0.73	2 (3%)
3	ADP	I	902	-	24,29,29	0.73	1 (4%)	29,45,45	0.78	1 (3%)
3	ADP	C	902	-	24,29,29	0.95	1 (4%)	29,45,45	1.41	4 (13%)
3	ADP	G	902	-	24,29,29	0.69	0	29,45,45	0.92	2 (6%)
2	IHP	A	901	-	36,36,36	0.74	0	54,60,60	0.63	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
3	ADP	J	902	-	-	1/12/32/32	0/3/3/3
3	ADP	H	902	-	-	5/12/32/32	0/3/3/3
2	IHP	D	901	-	-	8/30/54/54	0/1/1/1
2	IHP	F	901	-	-	8/30/54/54	0/1/1/1
3	ADP	D	902	-	-	5/12/32/32	0/3/3/3
3	ADP	B	902	-	-	1/12/32/32	0/3/3/3
3	ADP	K	902	-	-	4/12/32/32	0/3/3/3
3	ADP	A	902	-	-	5/12/32/32	0/3/3/3
2	IHP	E	901	-	-	18/30/54/54	0/1/1/1
3	ADP	L	902	-	-	5/12/32/32	0/3/3/3
3	ADP	E	902	-	-	6/12/32/32	0/3/3/3
3	ADP	F	902	-	-	9/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IHP	G	901	-	-	13/30/54/54	0/1/1/1
2	IHP	K	901	-	-	12/30/54/54	0/1/1/1
2	IHP	B	901	-	-	15/30/54/54	0/1/1/1
2	IHP	I	901	-	-	7/30/54/54	0/1/1/1
2	IHP	L	901	-	-	14/30/54/54	0/1/1/1
2	IHP	C	901	-	-	7/30/54/54	0/1/1/1
2	IHP	J	901	-	-	7/30/54/54	0/1/1/1
2	IHP	H	901	-	-	16/30/54/54	0/1/1/1
3	ADP	I	902	-	-	4/12/32/32	0/3/3/3
3	ADP	C	902	-	-	5/12/32/32	0/3/3/3
3	ADP	G	902	-	-	7/12/32/32	0/3/3/3
2	IHP	A	901	-	-	11/30/54/54	0/1/1/1

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	901	IHP	P4-O14	3.41	1.65	1.59
2	H	901	IHP	P5-O15	3.28	1.65	1.59
2	K	901	IHP	P6-O16	3.27	1.65	1.59
2	C	901	IHP	P6-O16	3.23	1.65	1.59
2	C	901	IHP	P4-O14	3.20	1.65	1.59

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	902	ADP	N3-C2-N1	-3.61	123.03	128.68
3	C	902	ADP	PA-O3A-PB	-3.11	122.16	132.83
2	H	901	IHP	C4-C3-C2	2.69	116.31	110.41
3	C	902	ADP	C3'-C2'-C1'	2.43	104.64	100.98
3	G	902	ADP	C5-C6-N6	2.39	123.98	120.35

There are no chirality outliers.

5 of 193 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	IHP	C1-C2-O12-P2
2	A	901	IHP	C3-C2-O12-P2
2	A	901	IHP	C2-C3-O13-P3
2	A	901	IHP	C3-O13-P3-O43

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Mol	Chain	Res	Type	Atoms
2	A	901	IHP	C4-O14-P4-O24

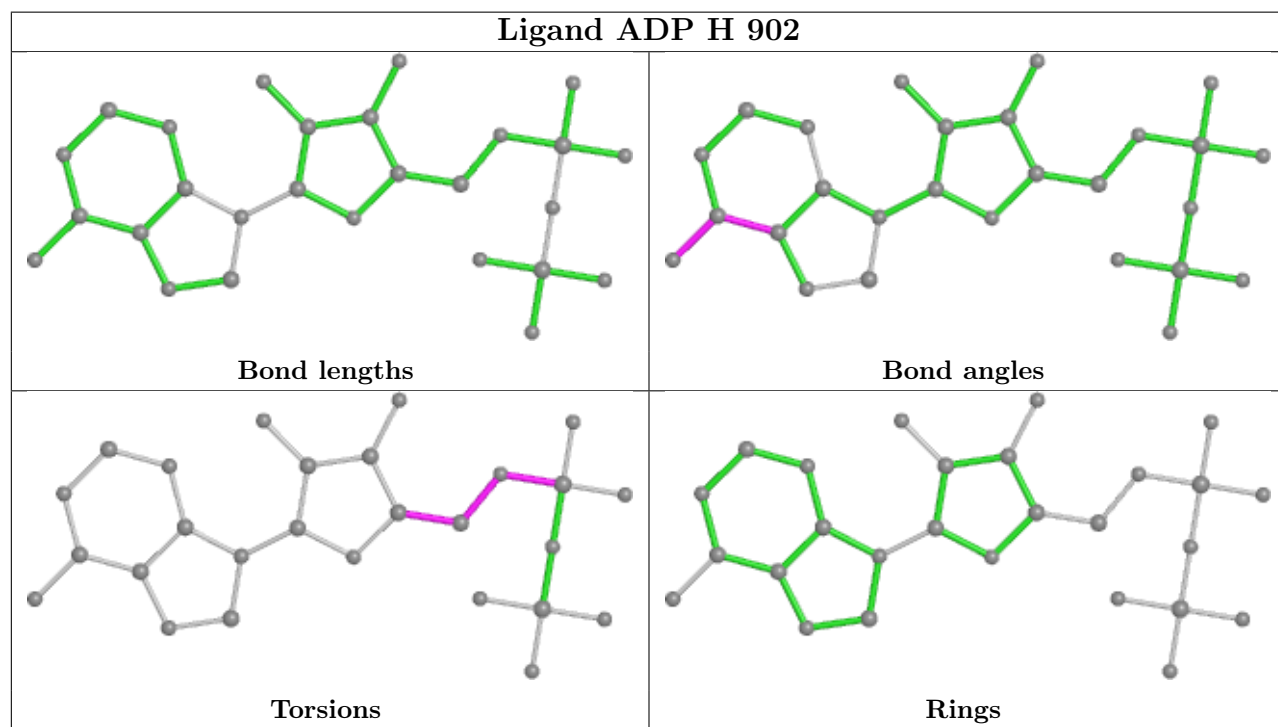
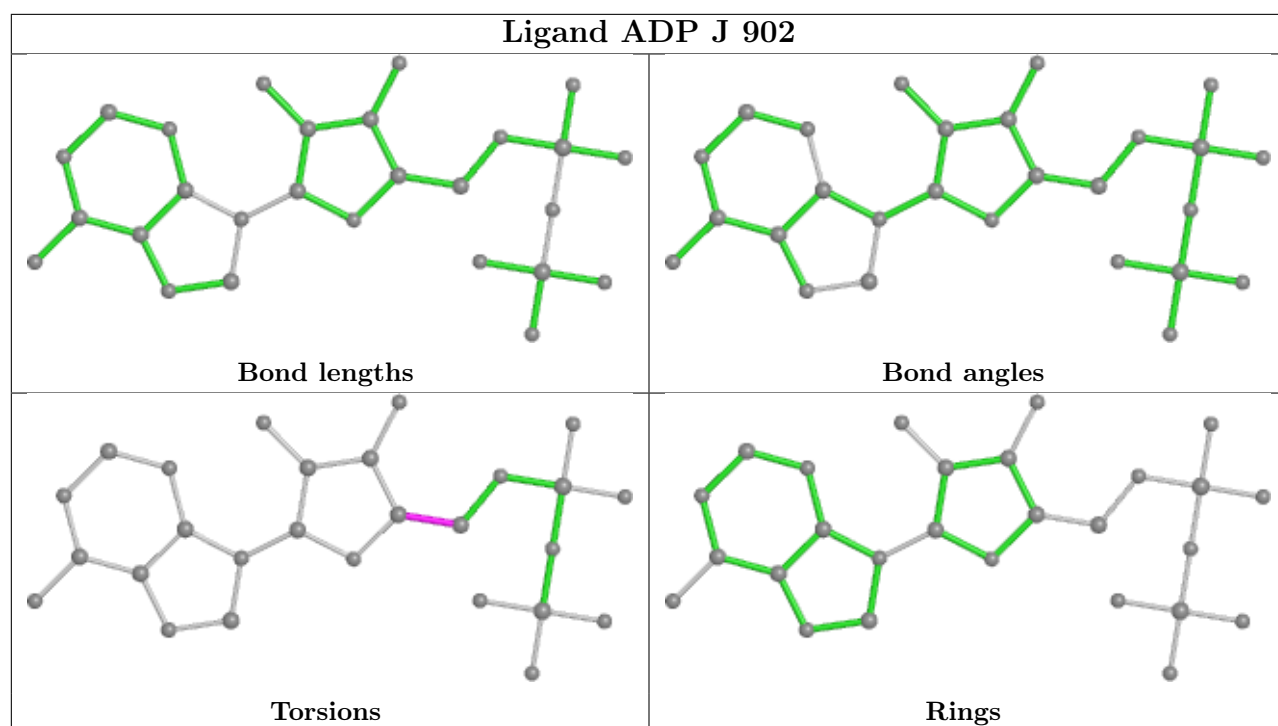
There are no ring outliers.

17 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	902	ADP	3	0
3	H	902	ADP	3	0
2	D	901	IHP	1	0
3	D	902	ADP	6	0
3	B	902	ADP	4	0
3	K	902	ADP	4	0
3	A	902	ADP	5	0
3	L	902	ADP	7	0
3	E	902	ADP	1	0
3	F	902	ADP	4	0
2	K	901	IHP	1	0
2	I	901	IHP	2	0
2	L	901	IHP	1	0
2	H	901	IHP	2	0
3	I	902	ADP	3	0
3	C	902	ADP	3	0
3	G	902	ADP	1	0

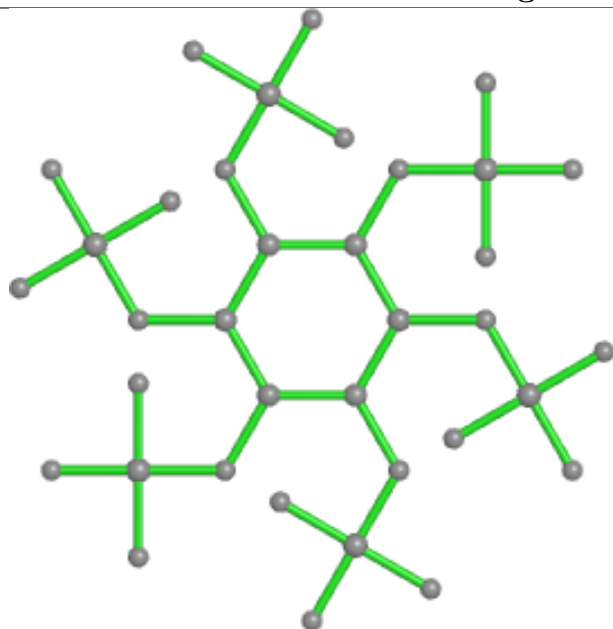
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



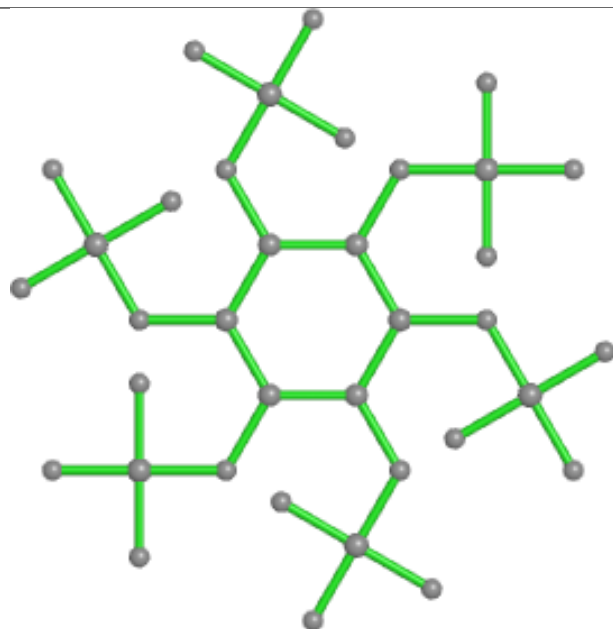




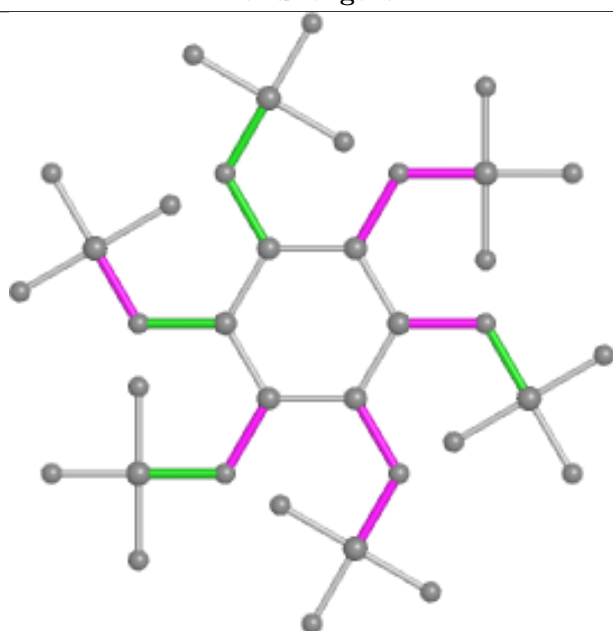
## Ligand IHP D 901



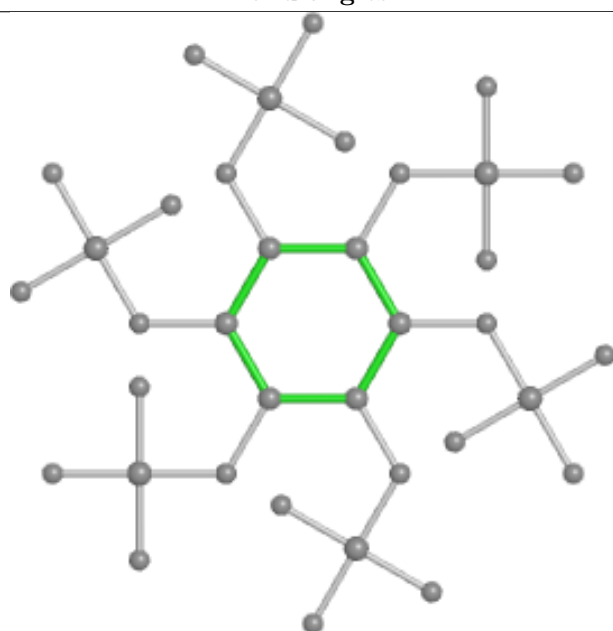
Bond lengths



Bond angles



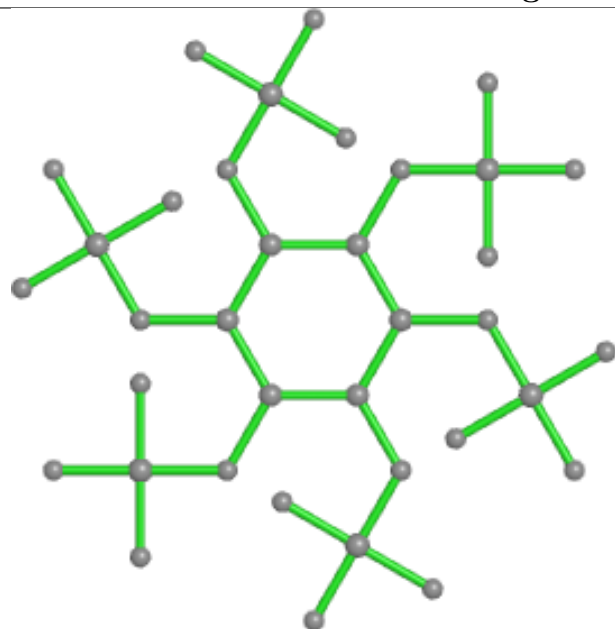
Torsions



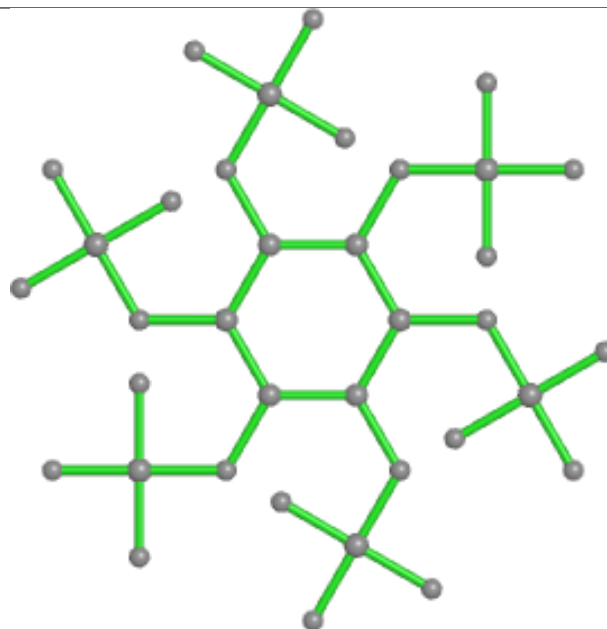
Rings



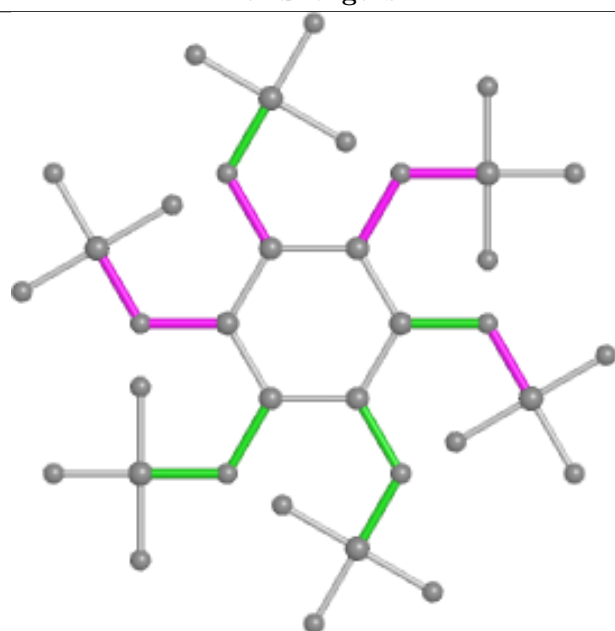
## Ligand IHP F 901



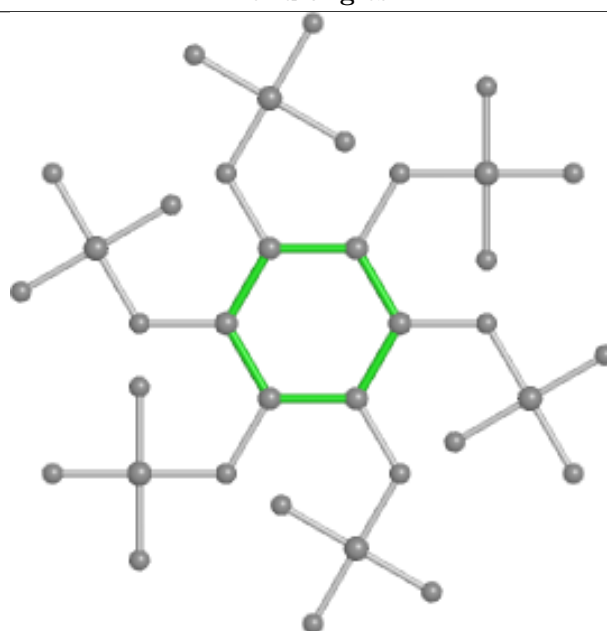
Bond lengths



Bond angles

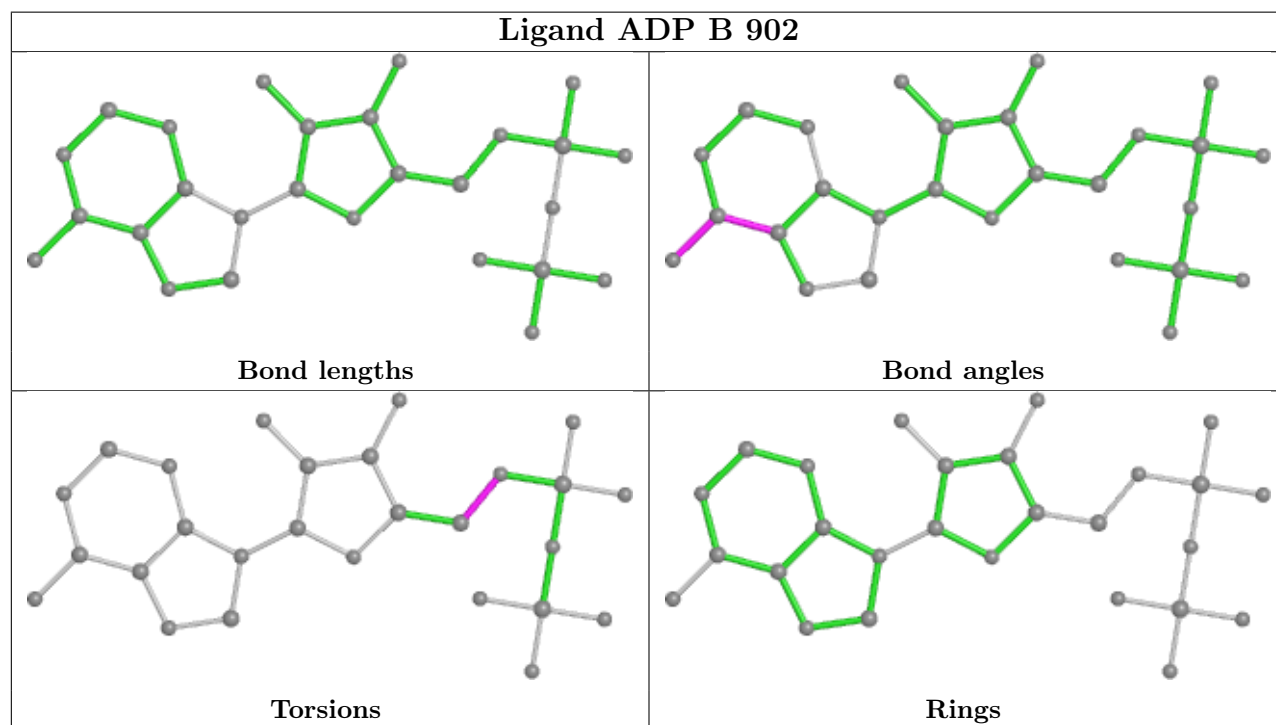
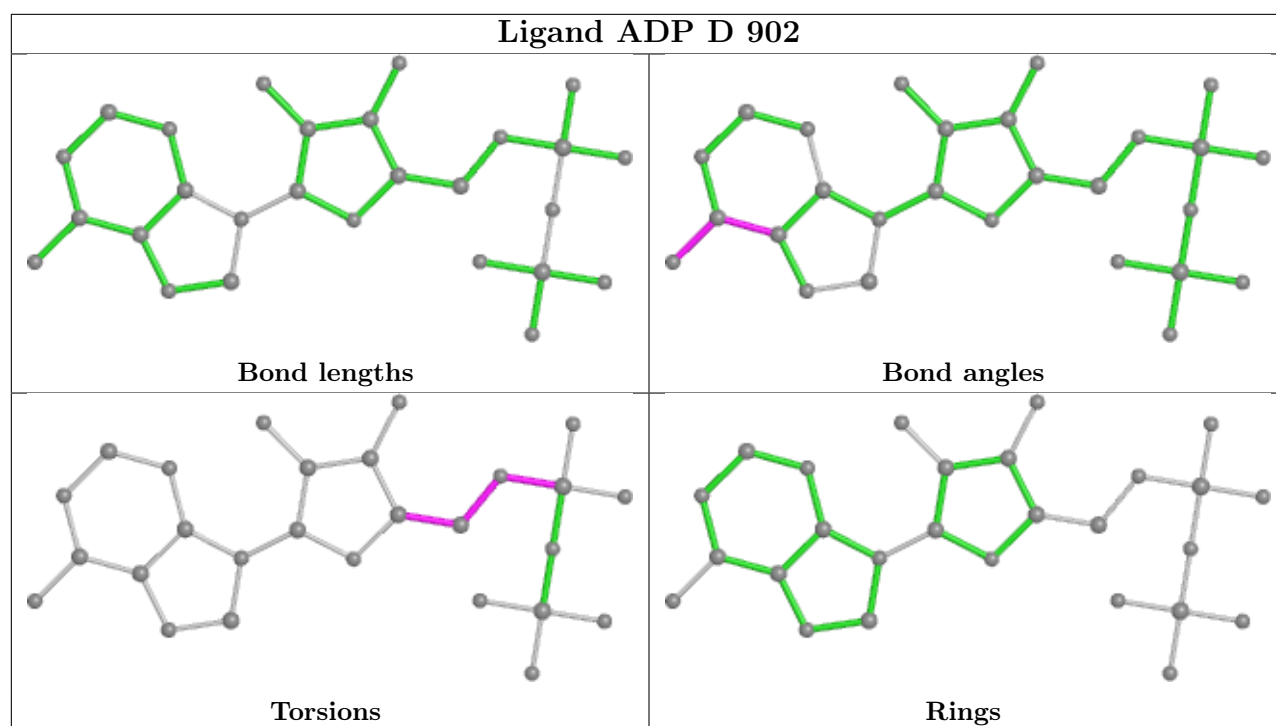


Torsions

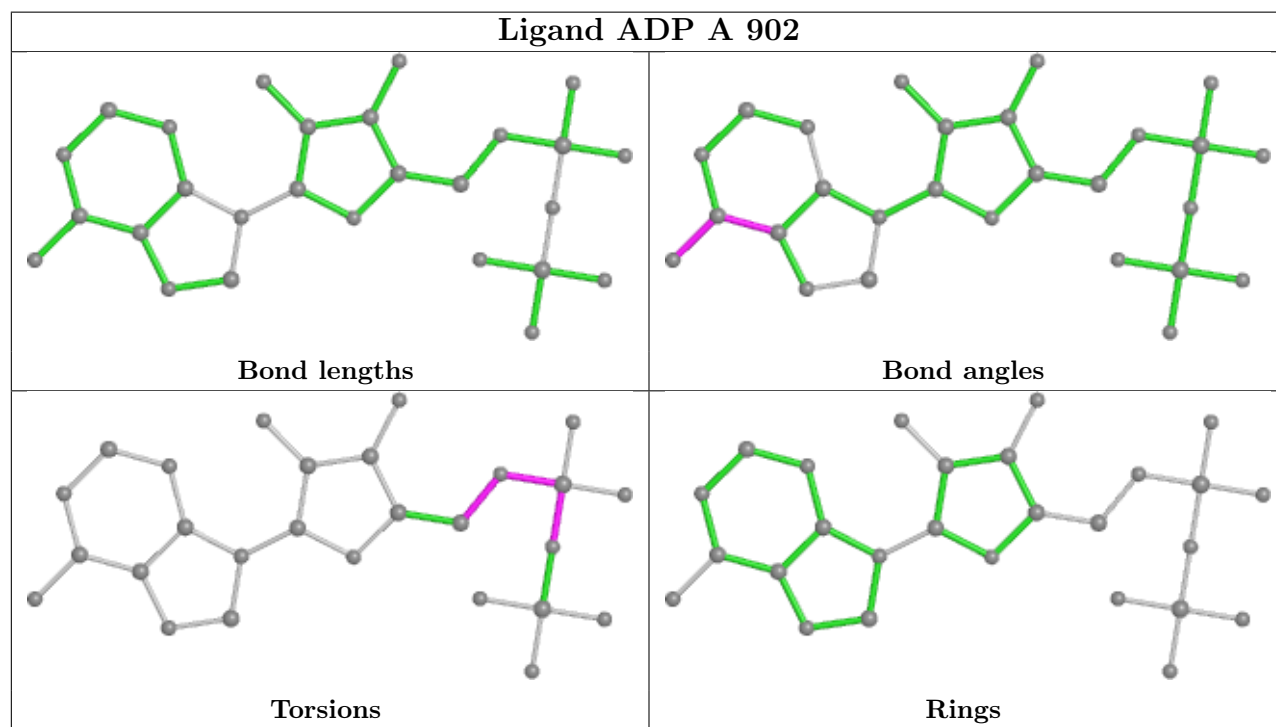
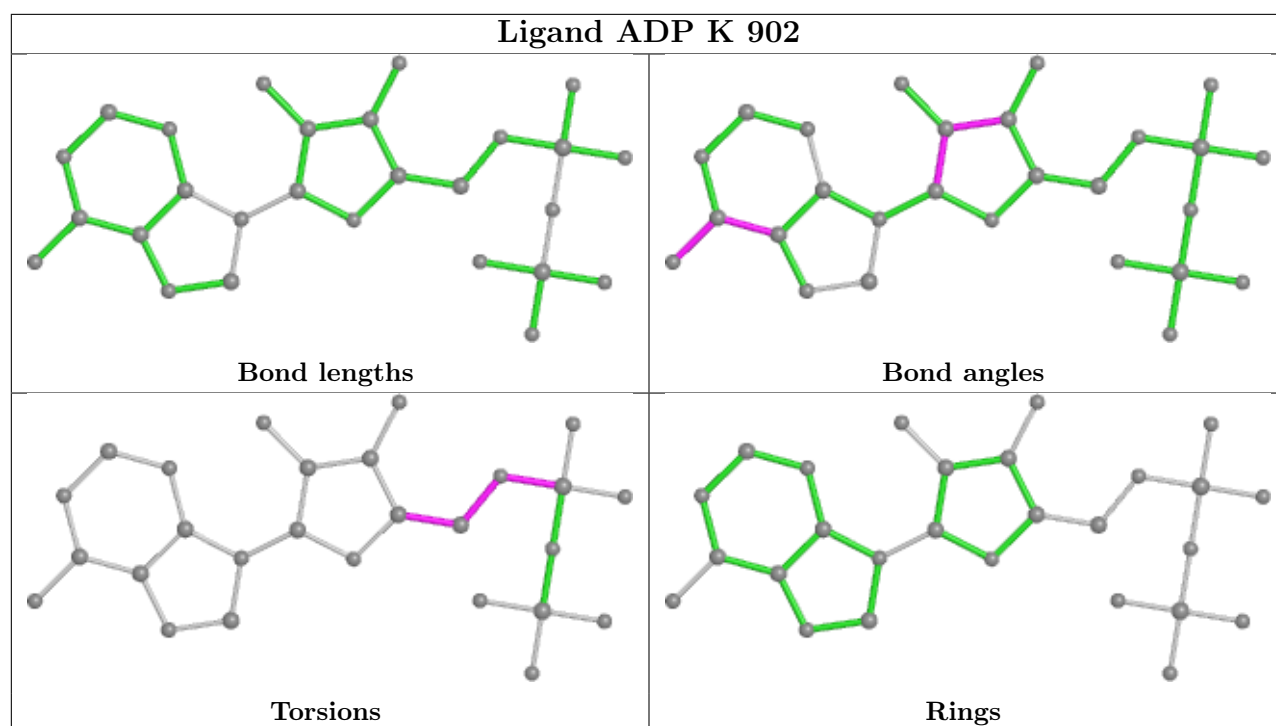


Rings



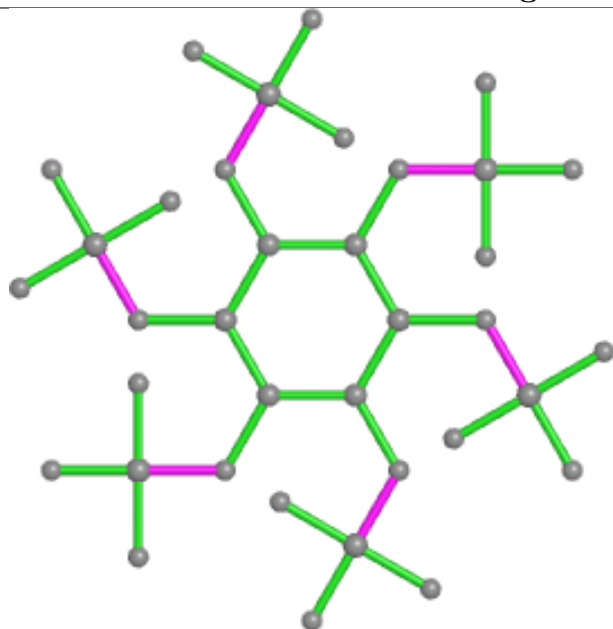




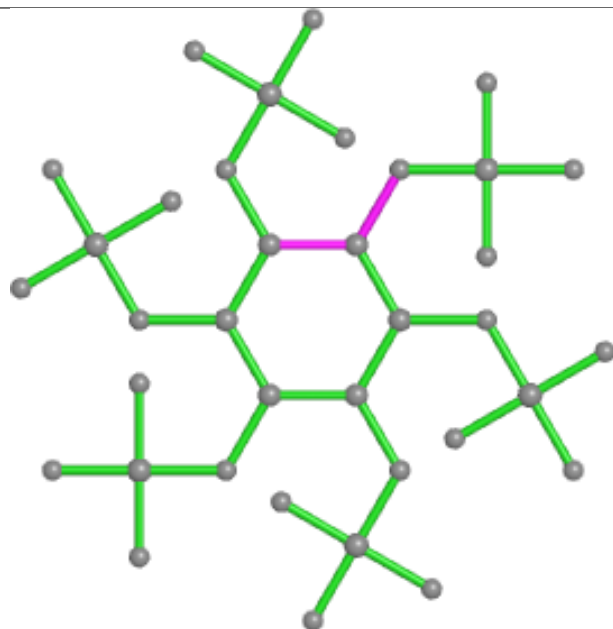




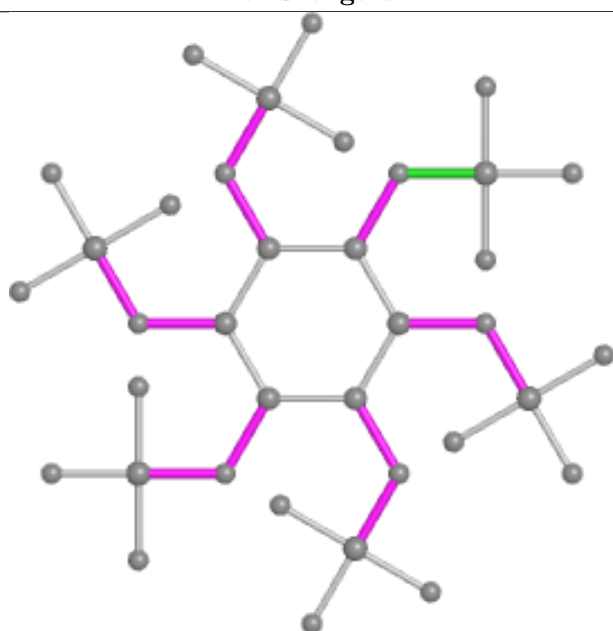
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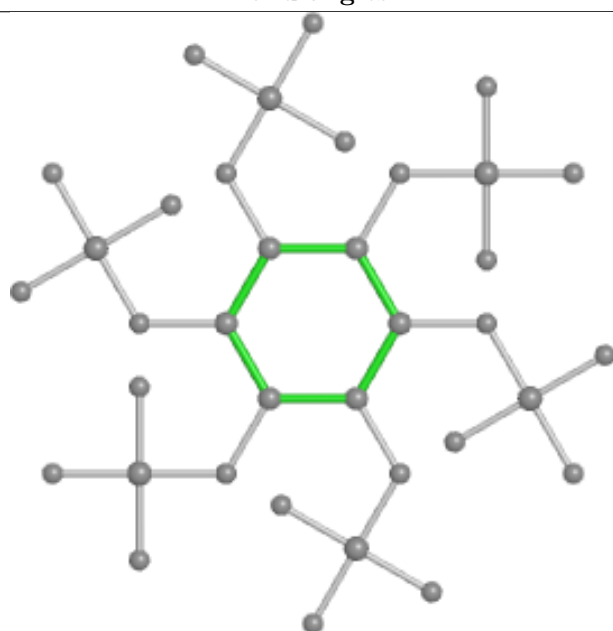
Bond lengths



Bond angles

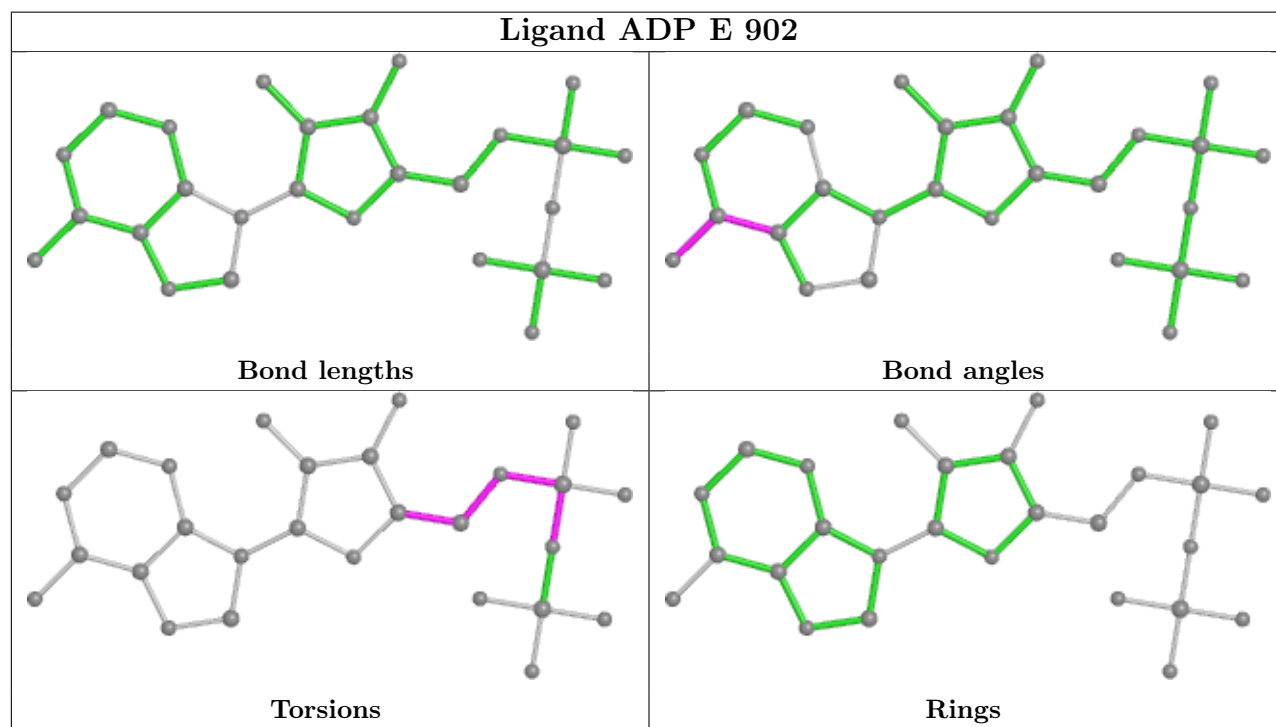
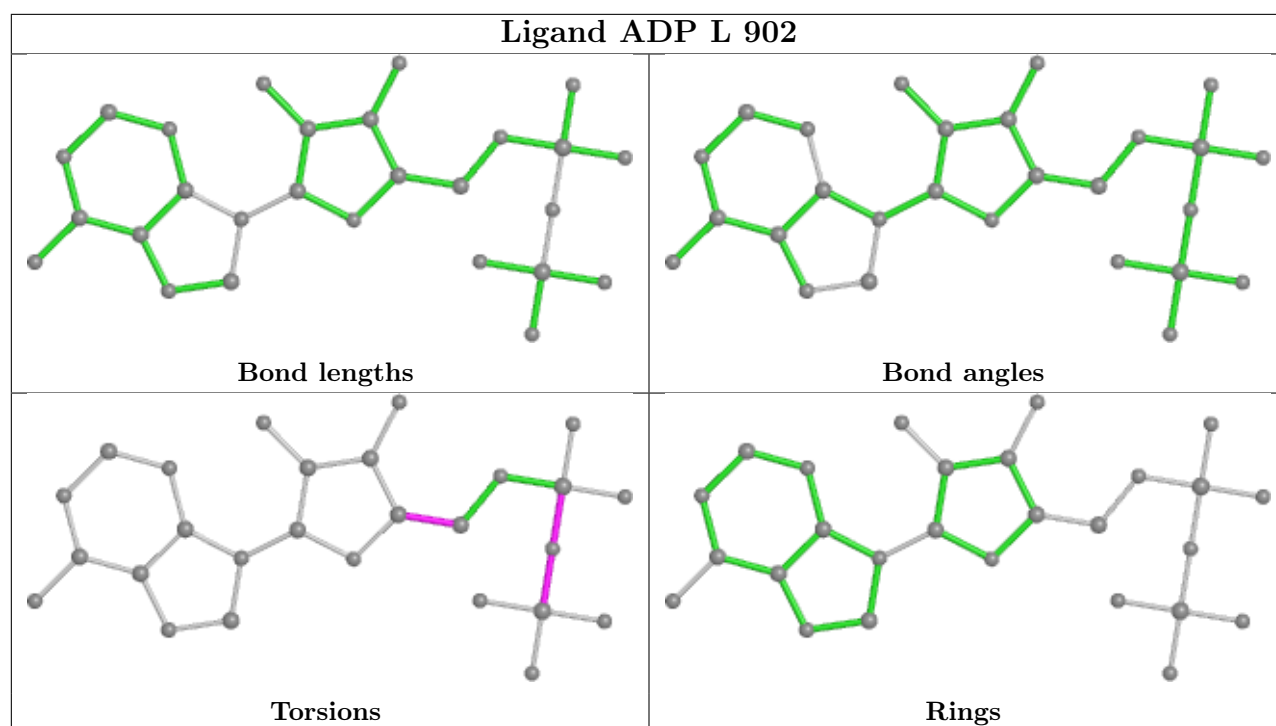


Torsions

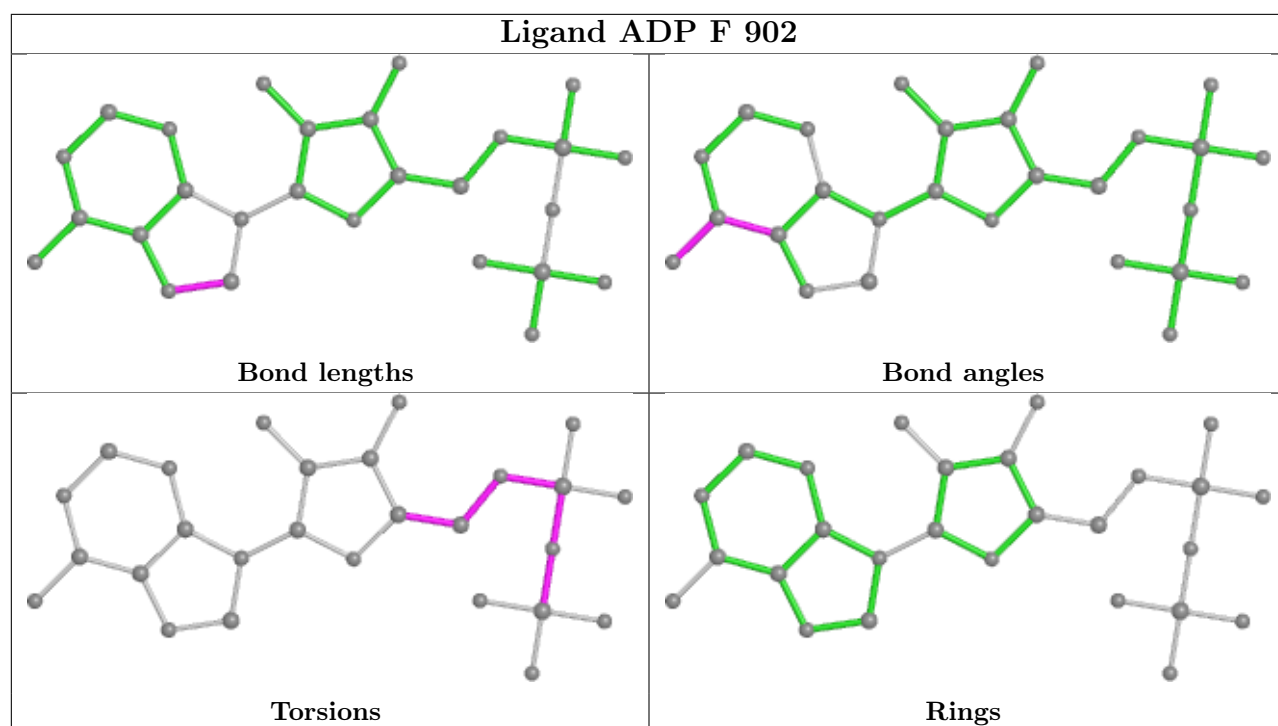


Rings



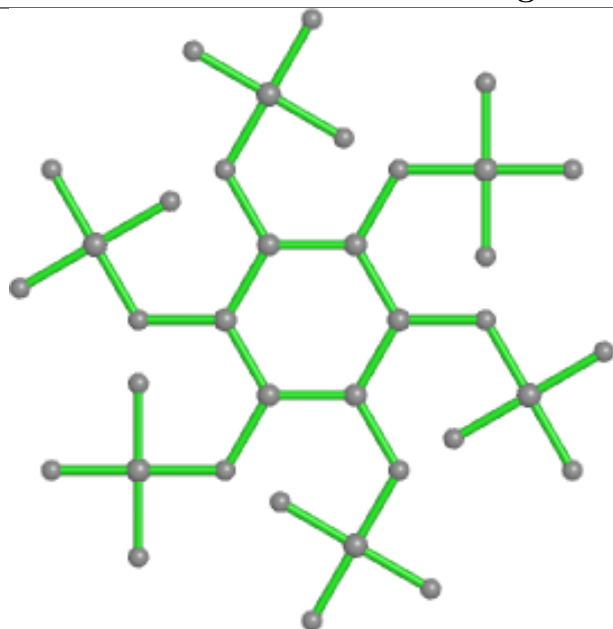




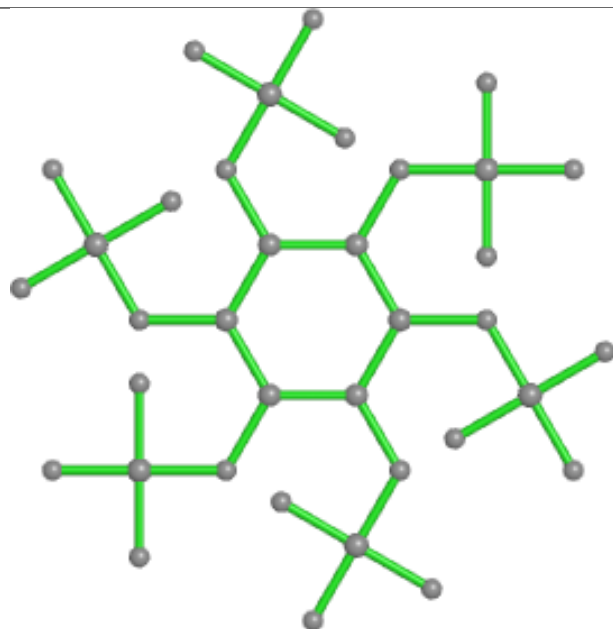




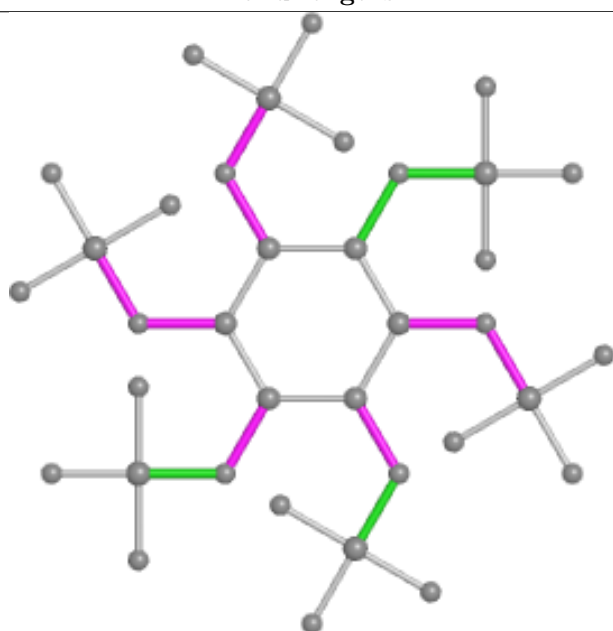
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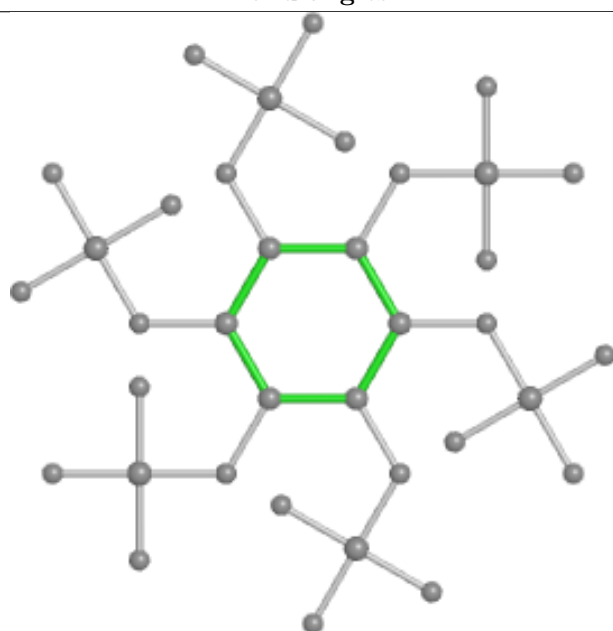
Bond lengths



Bond angles



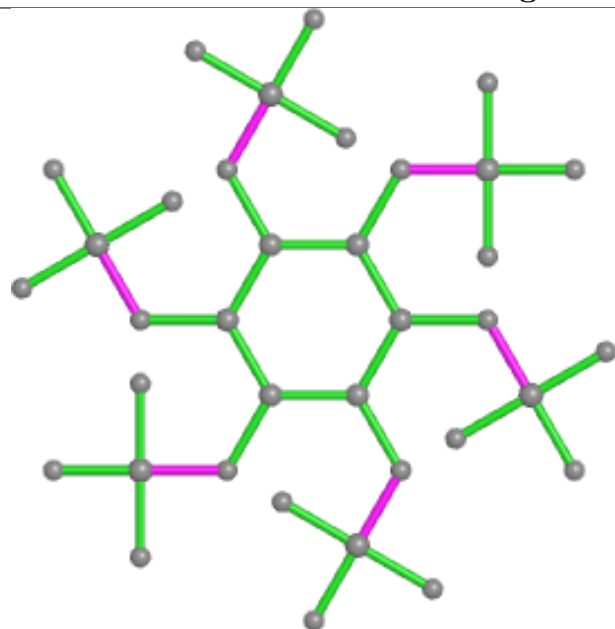
Torsions



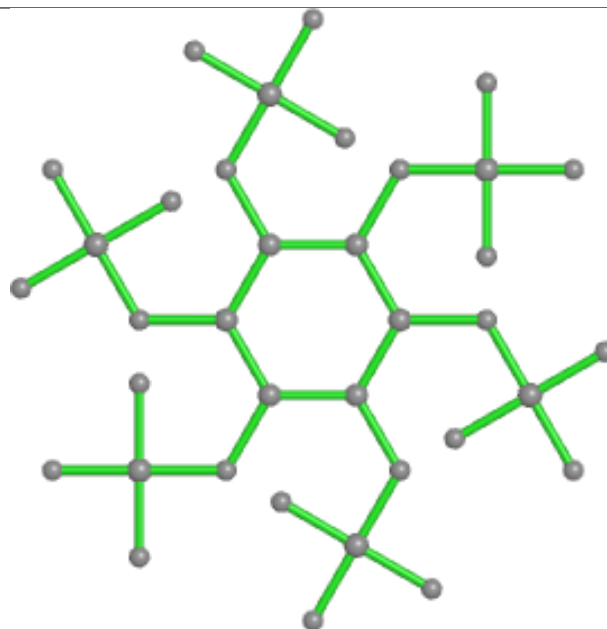
Rings



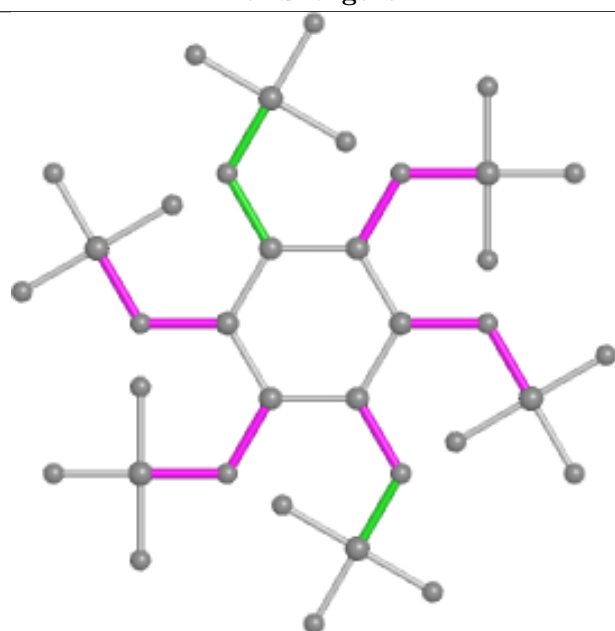
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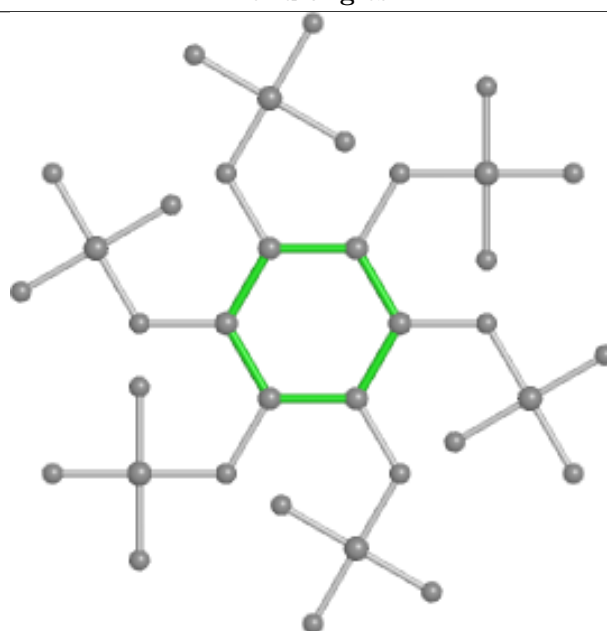
Bond lengths



Bond angles



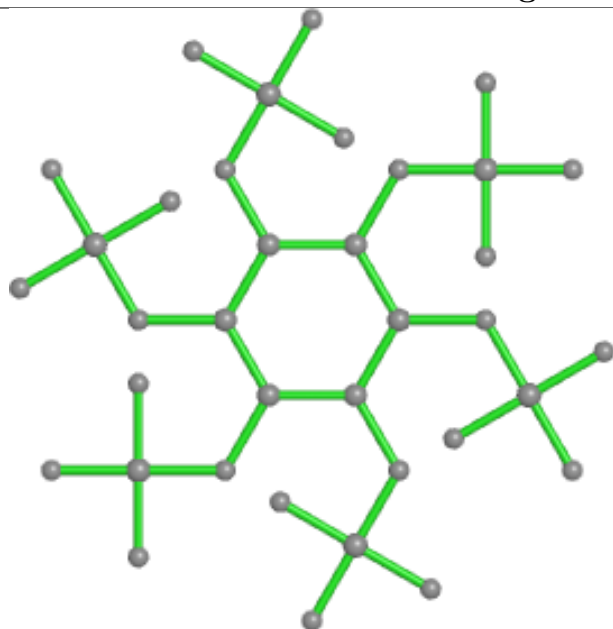
Torsions



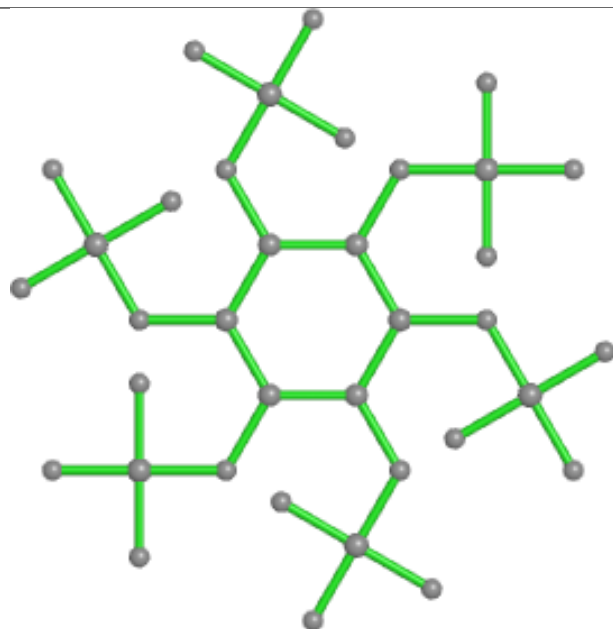
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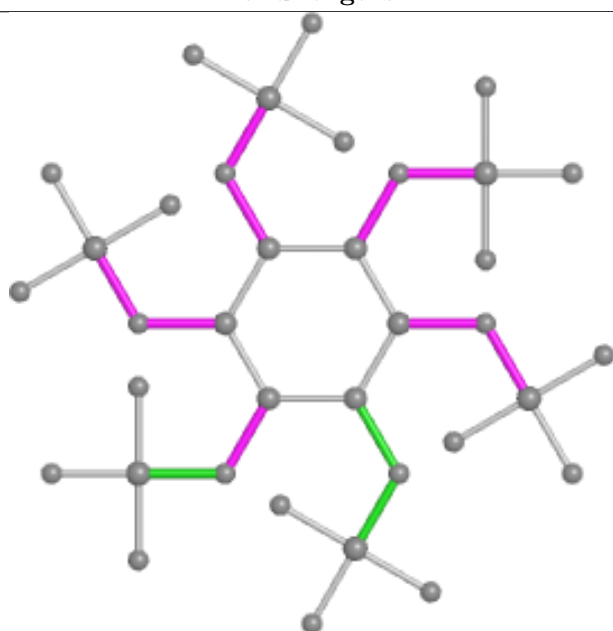
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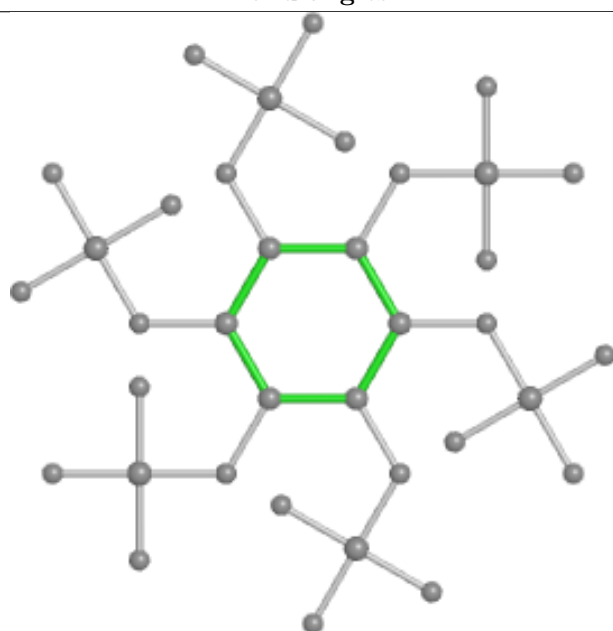
Bond lengths



Bond angles



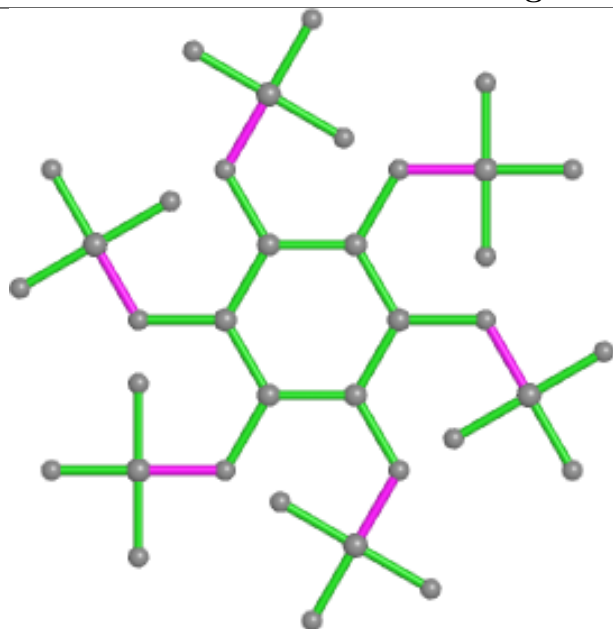
Torsions



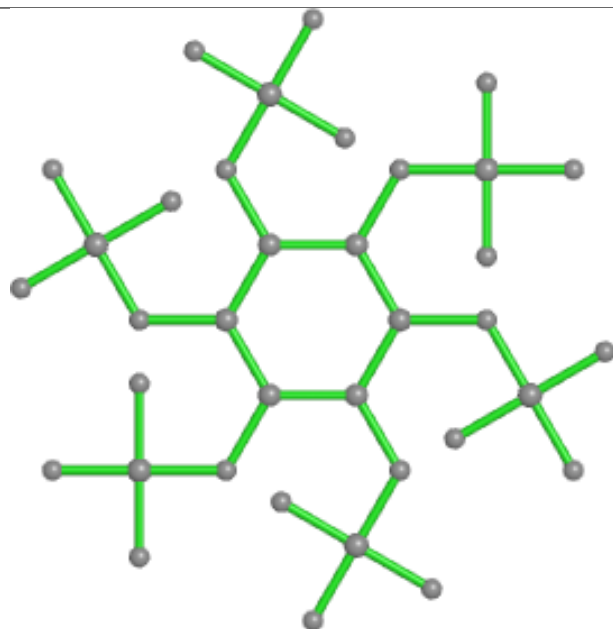
Rings



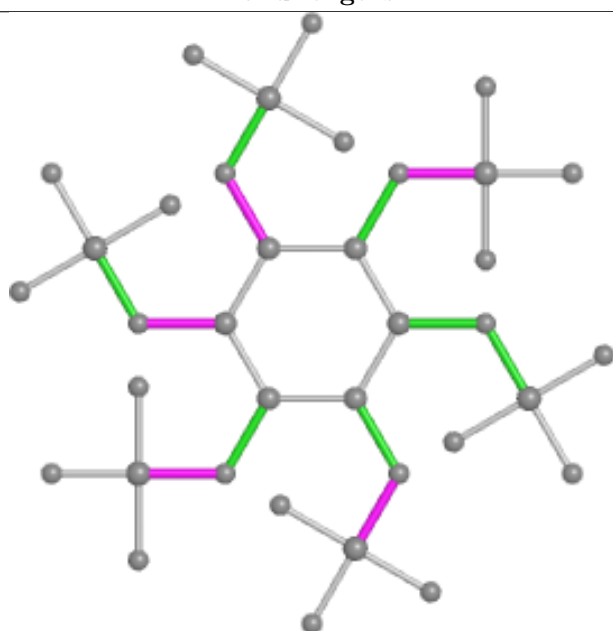
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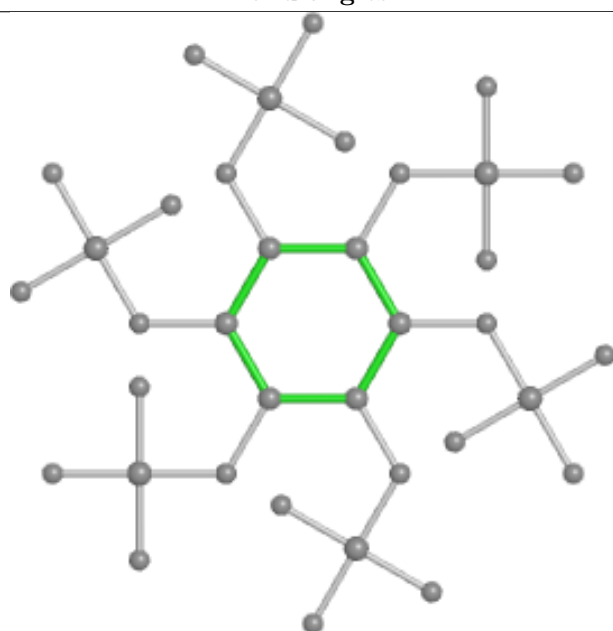
Bond lengths



Bond angles



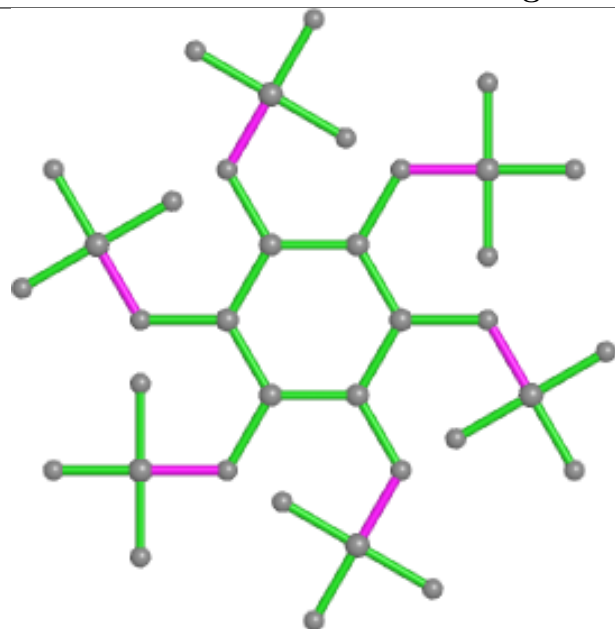
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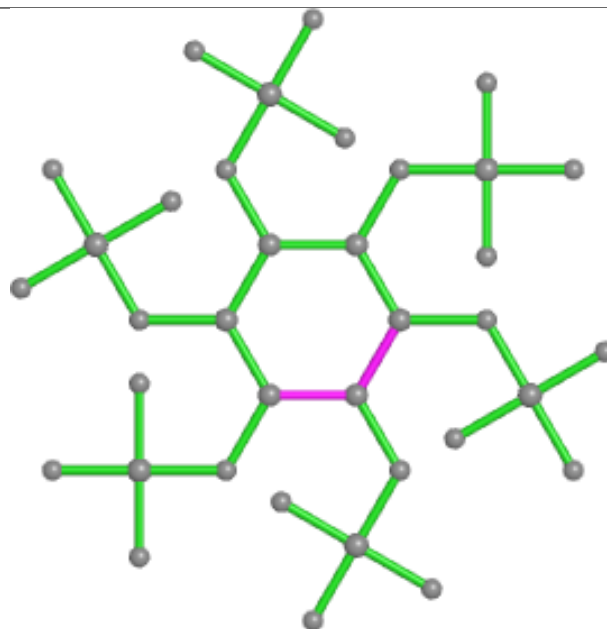
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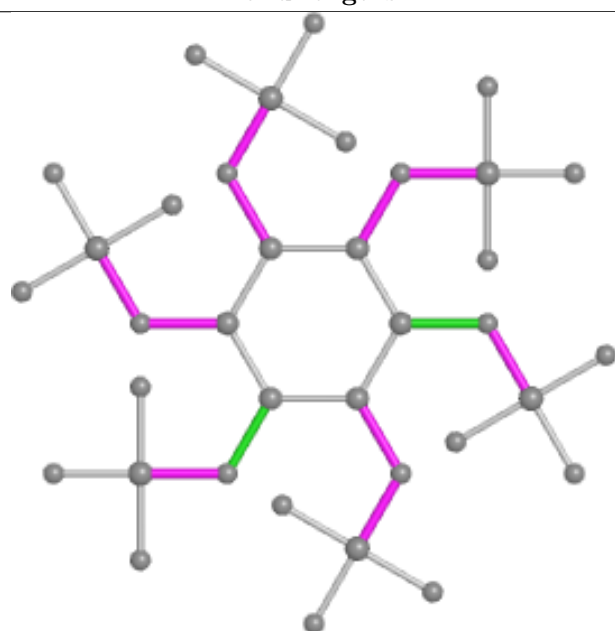
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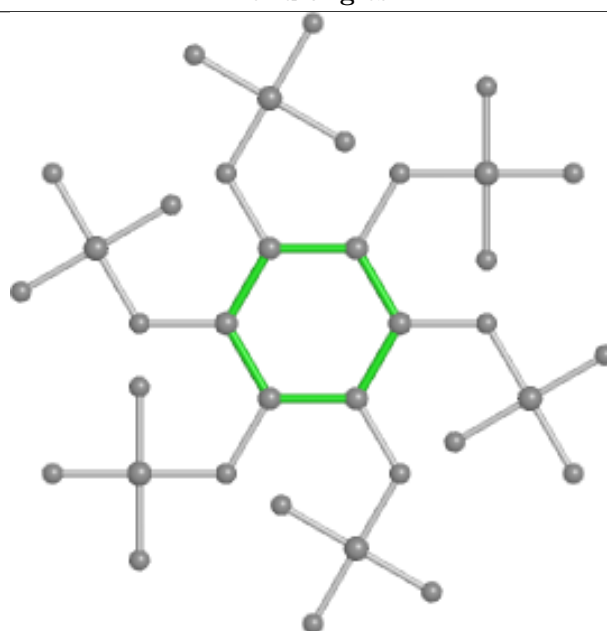
Bond lengths



Bond angles



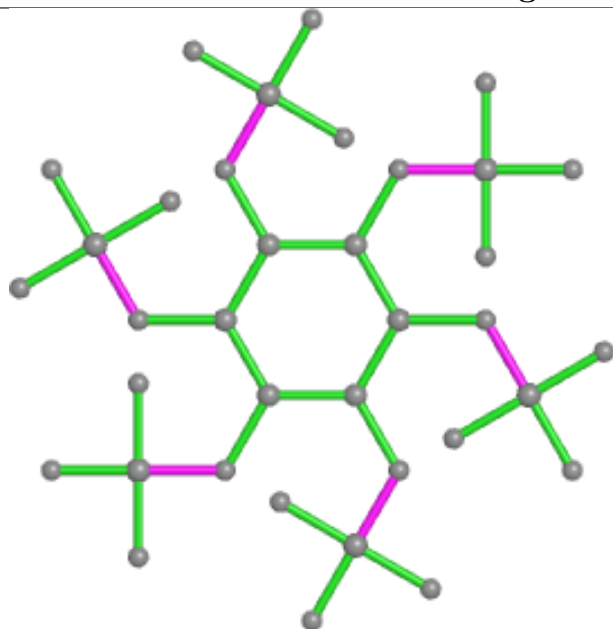
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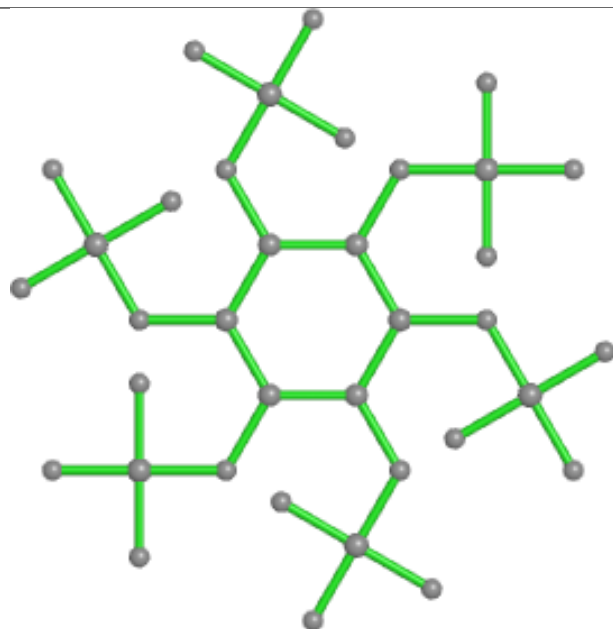
Rings



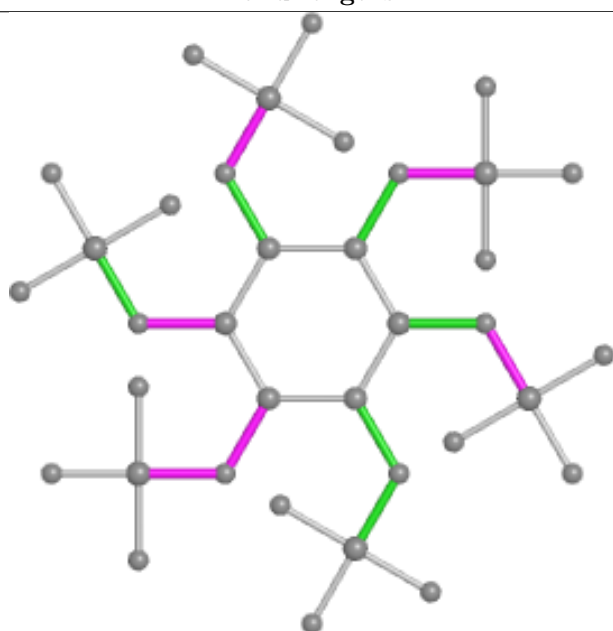
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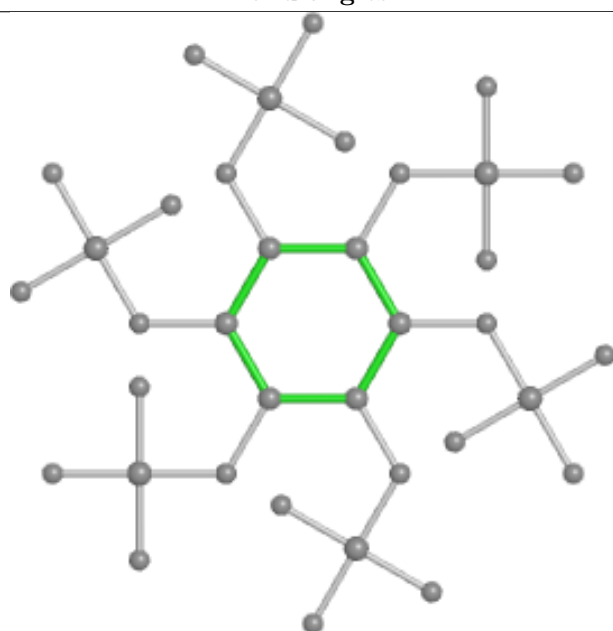
Bond lengths



Bond angles



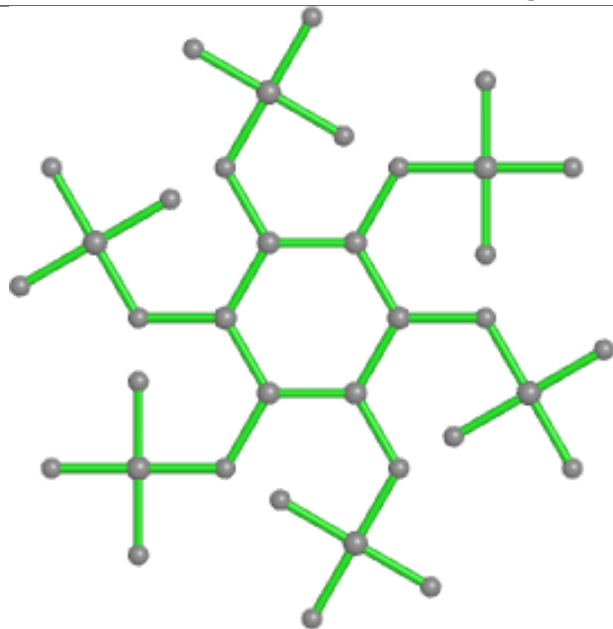
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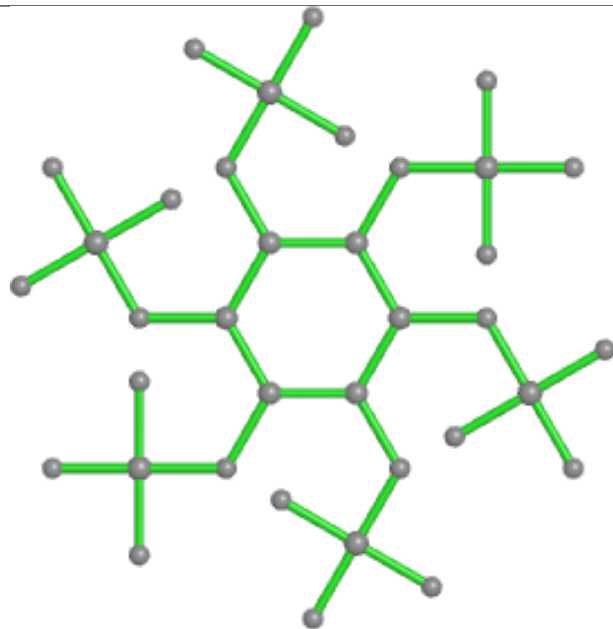
Rings



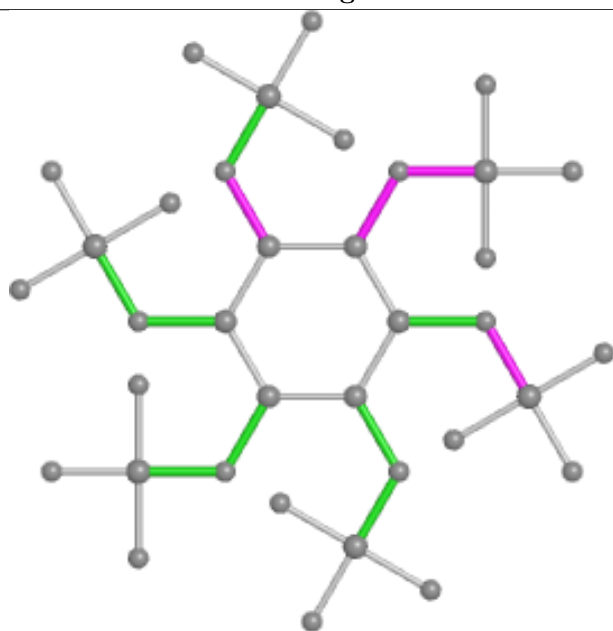
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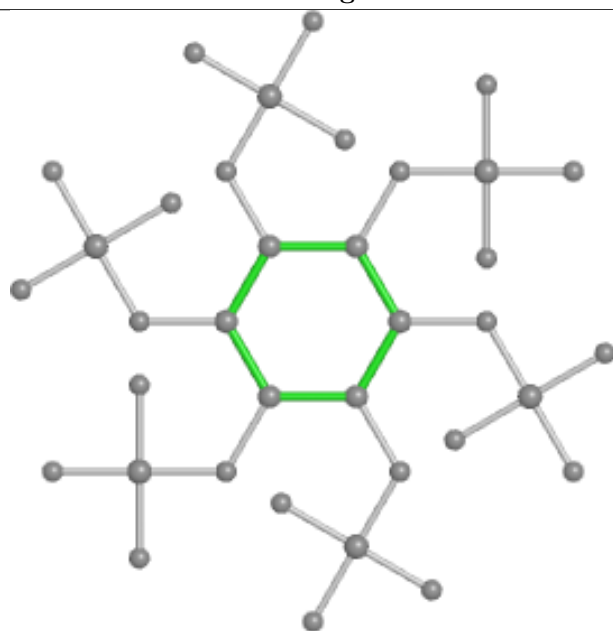
Bond lengths



Bond angles



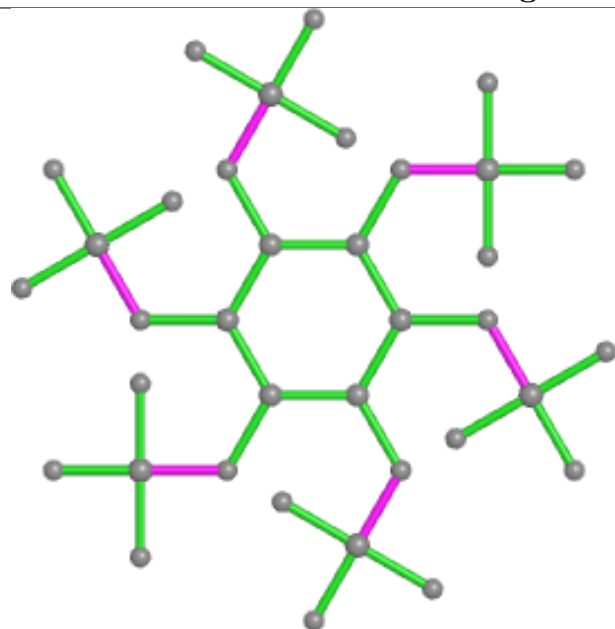
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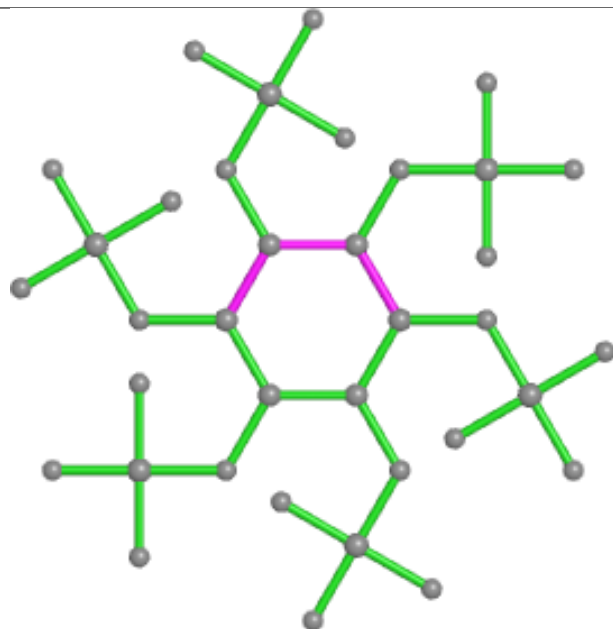
Rings



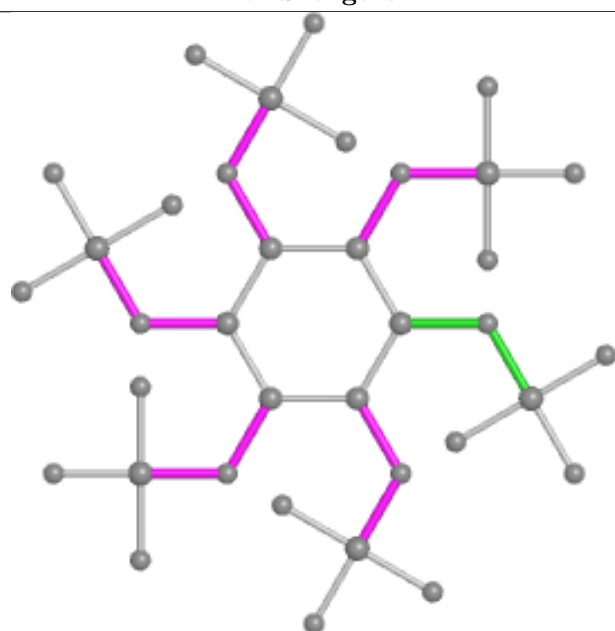
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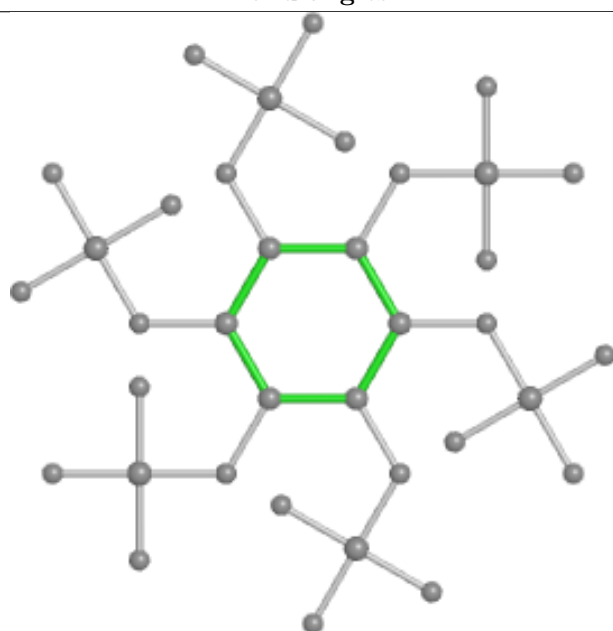
Bond lengths



Bond angles



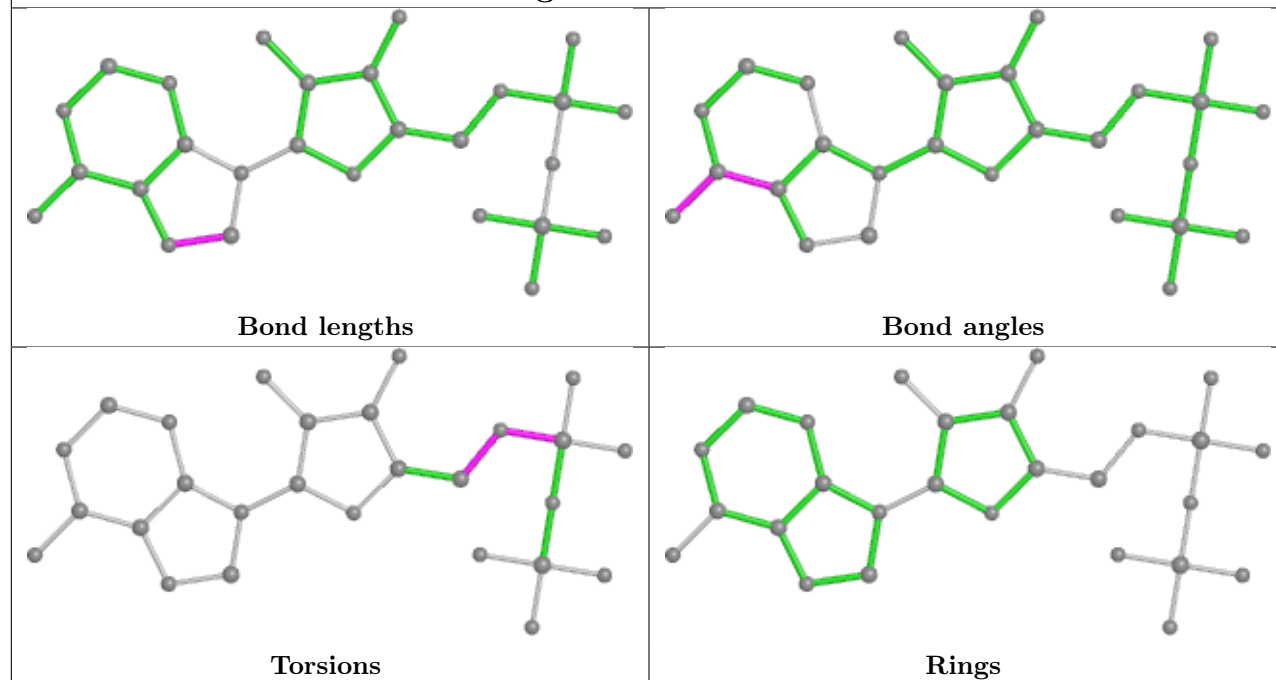
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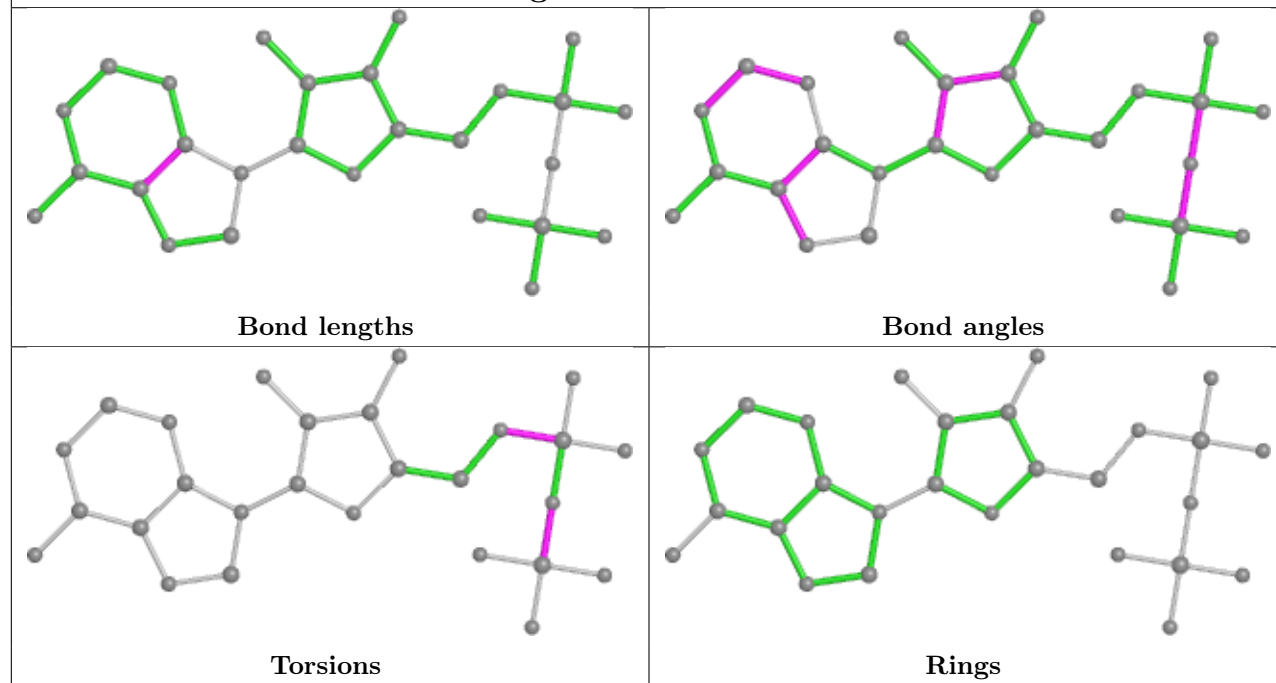
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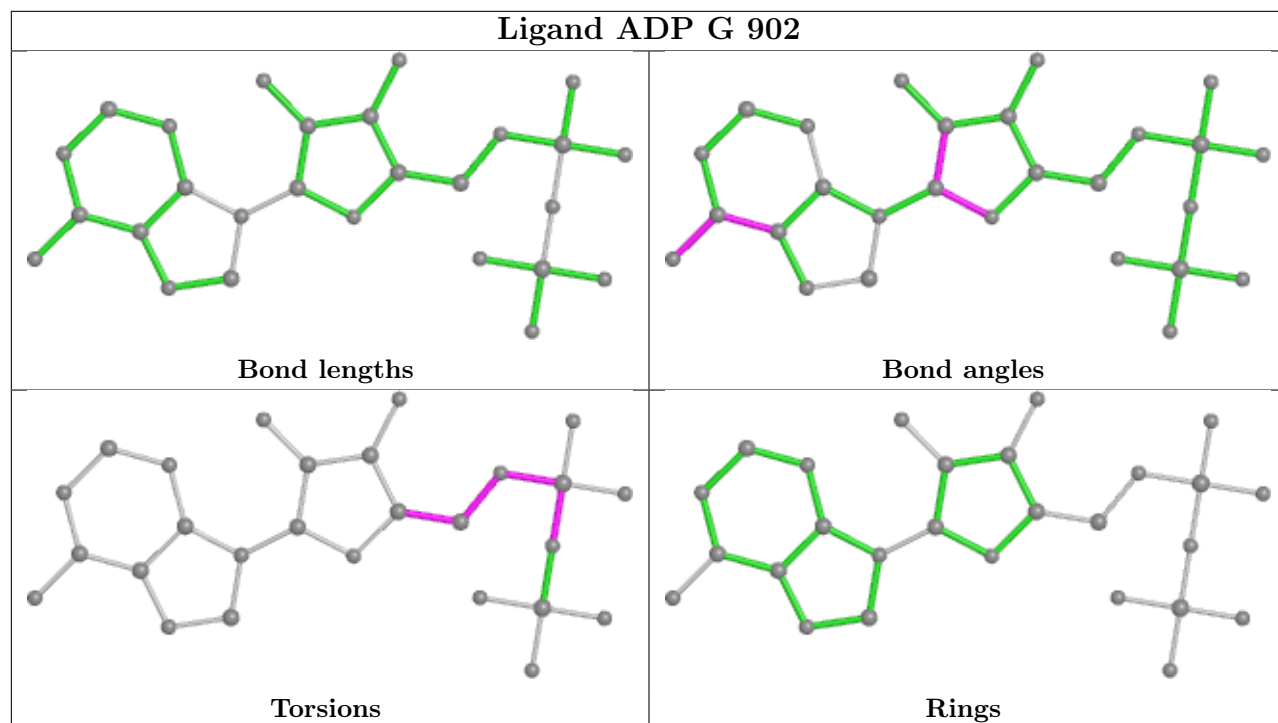
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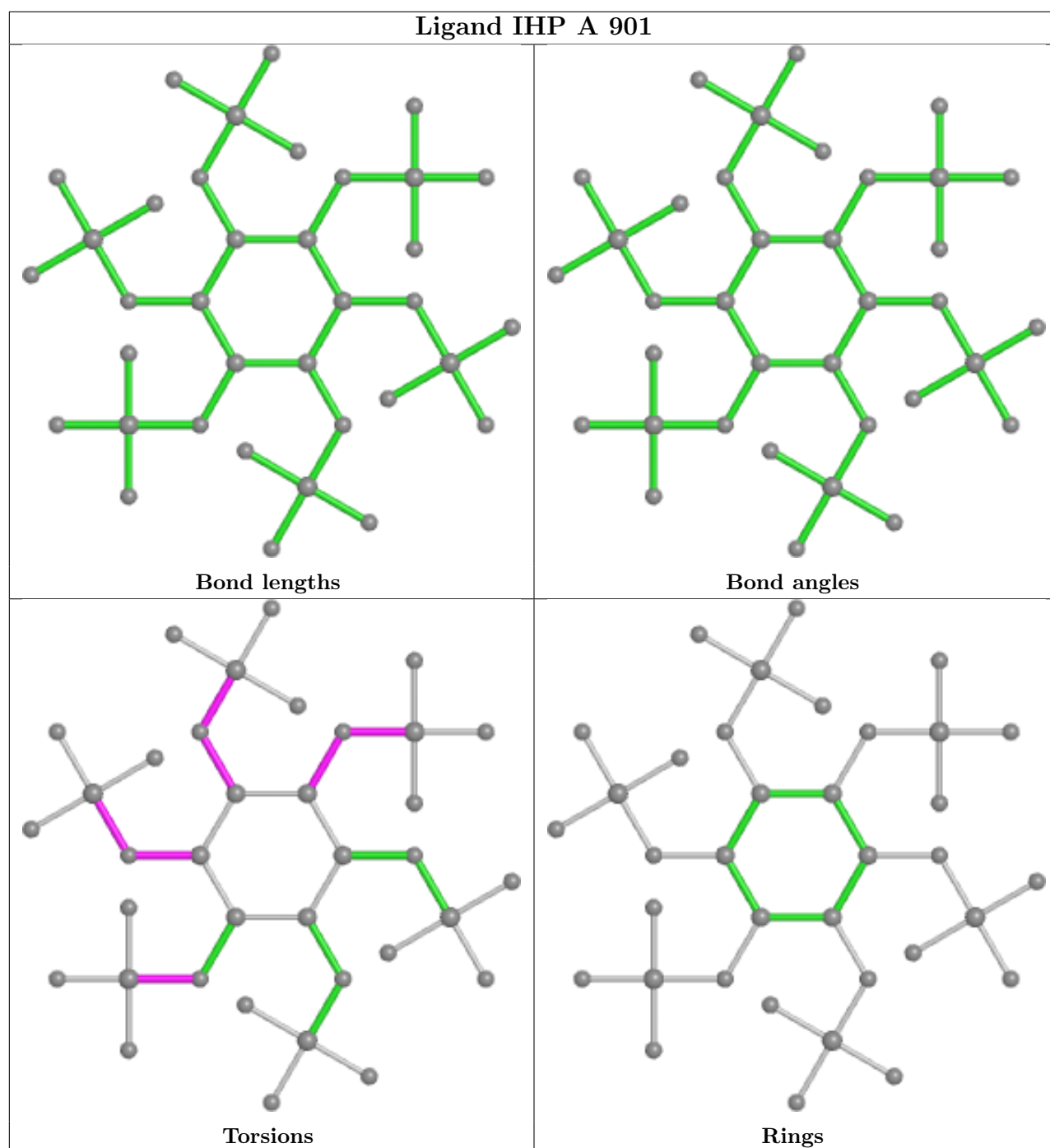
## Ligand ADP C 902











## 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.