wwPDB EM Validation Summary Report (i)

Jun 13, 2024 – 02:13 PM JST

PDB ID	:	8XUO
EMDB ID	:	EMD-38679
Title	:	Cryo-EM structure of tomato NRC2 dimer
Authors	:	Sun, Y.; Ma, S.C.; Chai, J.J.
Deposited on	:	2024-01-13
Resolution	:	2.84 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 (i) 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 (1)) were used in the production of this report:

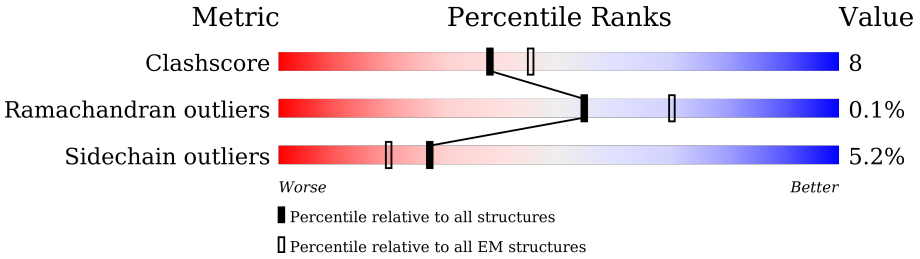
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.84 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 >=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	A	752	79% 20% •
1	G	752	77% 22% •

2 Entry composition (i)

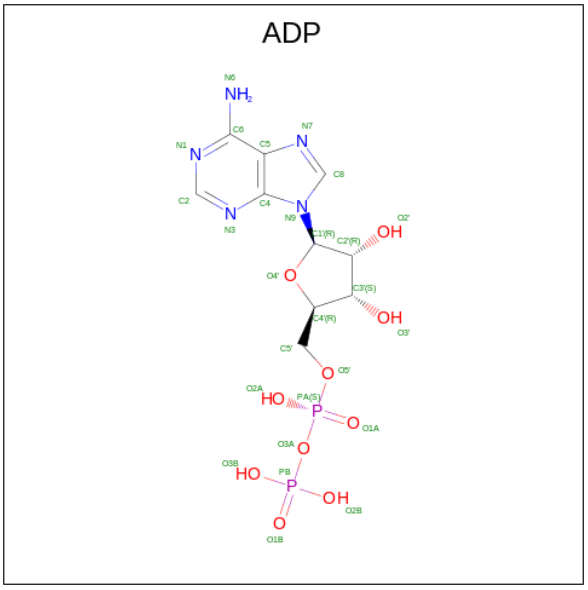
There are 3 unique types of molecules in this entry. The entry contains 12254 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

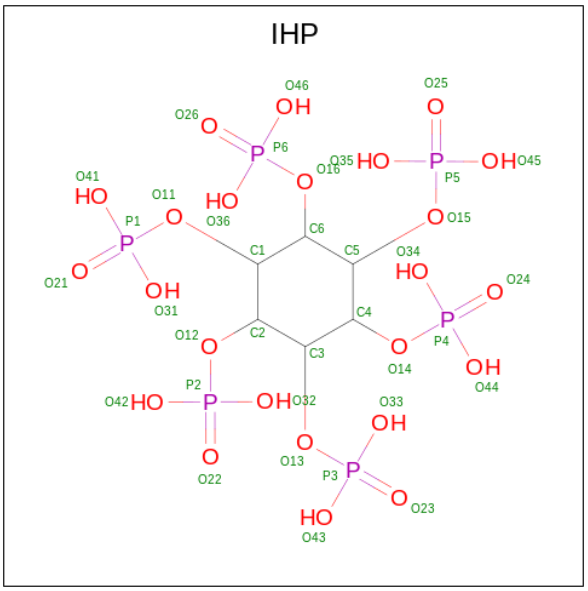
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	752	6064	3878	1046	1111	29	0	0
1	G	752	6064	3878	1046	1111	29	0	0

- Molecule 2 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
			Total	C	N	O	P	
2	A	1	27	10	5	10	2	0
2	G	1	27	10	5	10	2	0

- Molecule 3 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).



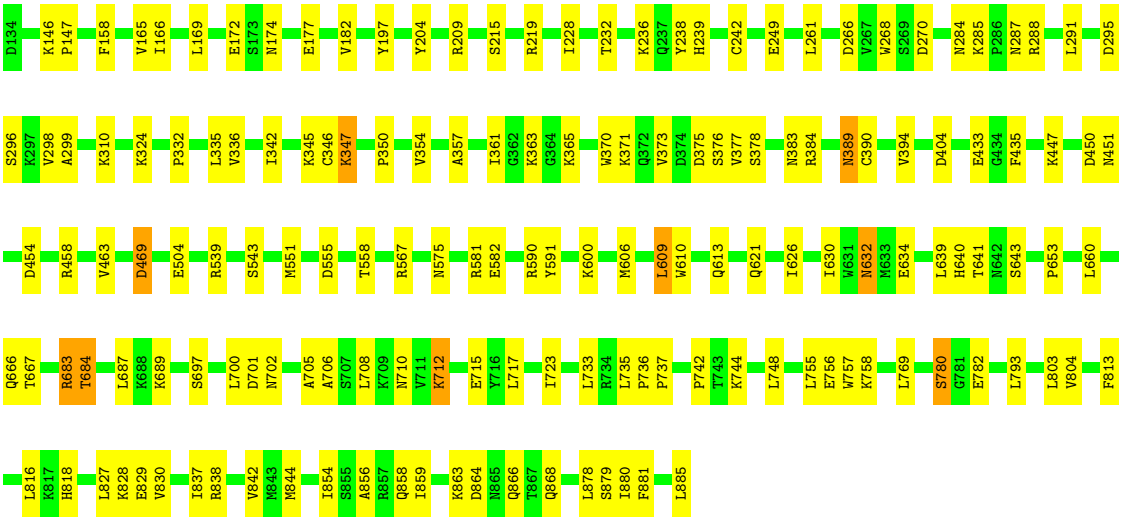
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	P	0
			36	6	24	6	
3	G	1	Total	C	O	P	0
			36	6	24	6	

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.

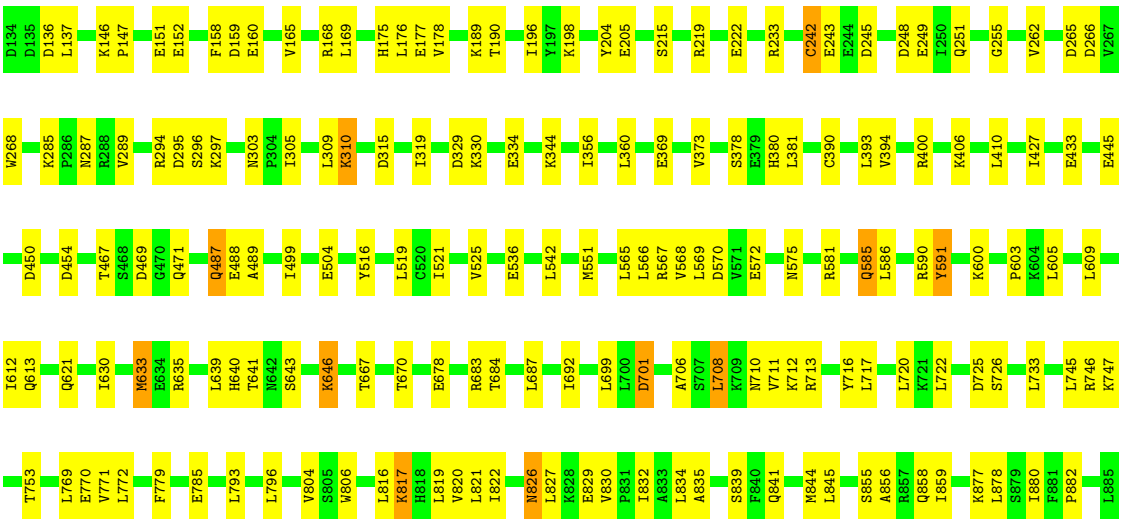
- Molecule 1: NRC2

Chain A: 79% 20%



- Molecule 1: NRC2

Chain G: 77% 22%



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	560935	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 ($e^-/Å^2$)	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: ADP, IHP

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	0.28	0/6194	0.52	0/8369
1	G	0.27	0/6194	0.52	0/8369
All	All	0.27	0/12388	0.52	0/16738

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	6064	0	6171	96	0
1	G	6064	0	6171	103	0
2	A	27	0	12	0	0
2	G	27	0	12	2	0
3	A	36	0	6	0	0
3	G	36	0	6	1	0
All	All	12254	0	12378	199	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 8.

The worst 5 of 199 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:A:712:LYS:O	1:A:712:LYS:NZ	1.97	0.96
1:A:758:LYS:O	1:A:758:LYS:NZ	2.10	0.83
1:A:700:LEU:HD12	1:A:733:LEU:HD22	1.65	0.79
1:G:712:LYS:O	1:G:712:LYS:NZ	2.11	0.79
1:A:653:PRO:HD3	1:A:660:LEU:HD11	1.68	0.76

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	750/752 (100%)	730 (97%)	19 (2%)	1 (0%)	51	75
1	G	750/752 (100%)	727 (97%)	23 (3%)	0	100	100
All	All	1500/1504 (100%)	1457 (97%)	42 (3%)	1 (0%)	54	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	347	LYS

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	A	682/682 (100%)	647 (95%)	35 (5%)	24	45
1	G	682/682 (100%)	646 (95%)	36 (5%)	22	43
All	All	1364/1364 (100%)	1293 (95%)	71 (5%)	27	44

5 of 71 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	633	MET
1	G	643	SER
1	G	779	PHE
1	A	632	ASN
1	A	610	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	537	HIS
1	G	710	ASN
1	G	826	ASN
1	A	710	ASN
1	A	174	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	IHP	A	902	-	36,36,36	1.49	6 (16%)	54,60,60	0.68	1 (1%)
3	IHP	G	902	-	36,36,36	1.47	6 (16%)	54,60,60	0.85	3 (5%)
2	ADP	A	901	-	24,29,29	0.93	1 (4%)	29,45,45	1.47	4 (13%)
2	ADP	G	901	-	24,29,29	0.91	1 (4%)	29,45,45	1.41	5 (17%)

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	IHP	A	902	-	-	7/30/54/54	0/1/1/1
3	IHP	G	902	-	-	9/30/54/54	0/1/1/1
2	ADP	A	901	-	-	3/12/32/32	0/3/3/3
2	ADP	G	901	-	-	7/12/32/32	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	902	IHP	P4-O14	3.29	1.65	1.59
3	G	902	IHP	P1-O11	3.24	1.65	1.59
3	A	902	IHP	P5-O15	3.23	1.65	1.59
3	A	902	IHP	P3-O13	3.19	1.65	1.59
3	A	902	IHP	P6-O16	3.15	1.65	1.59

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	901	ADP	N3-C2-N1	-3.74	122.83	128.68
2	A	901	ADP	PA-O3A-PB	-3.58	120.56	132.83
2	G	901	ADP	N3-C2-N1	-3.48	123.24	128.68
3	G	902	IHP	C5-C4-C3	3.47	118.00	110.41
2	G	901	ADP	PA-O3A-PB	-3.46	120.94	132.83

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	ADP	C5'-O5'-PA-O1A
2	A	901	ADP	C5'-O5'-PA-O2A
2	G	901	ADP	C5'-O5'-PA-O3A
2	G	901	ADP	O4'-C4'-C5'-O5'
2	G	901	ADP	C3'-C4'-C5'-O5'

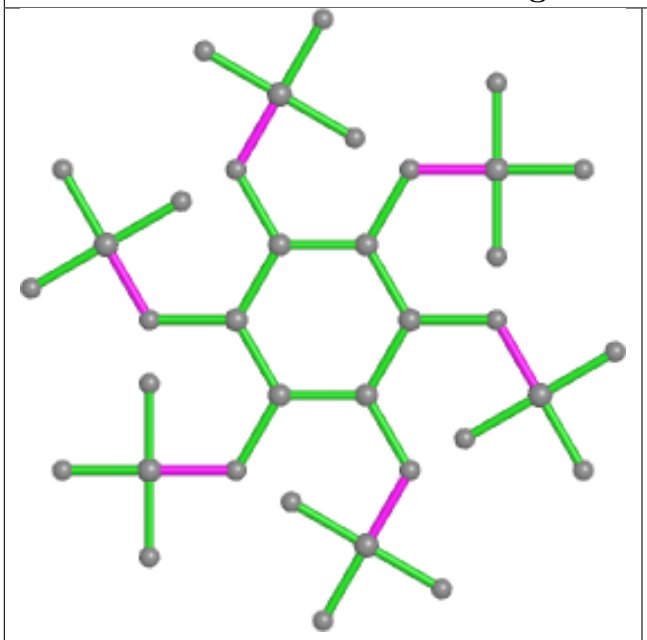
There are no ring outliers.

2 monomers are involved in 3 short contacts:

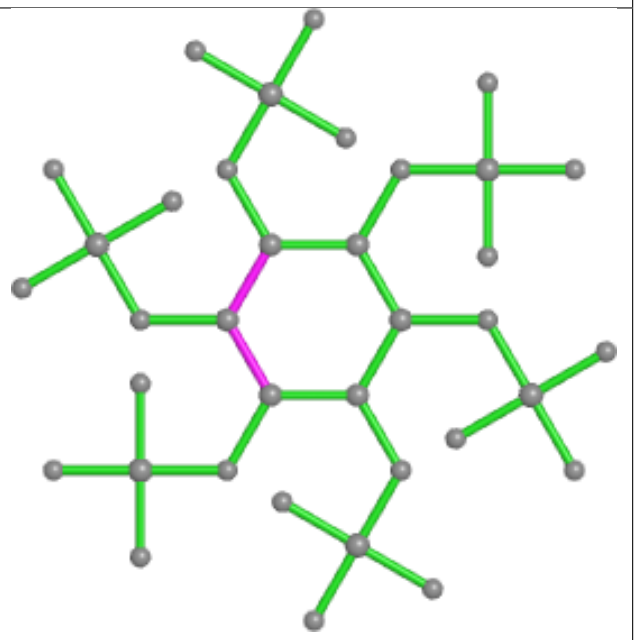
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	902	IHP	1	0
2	G	901	ADP	2	0

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 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.

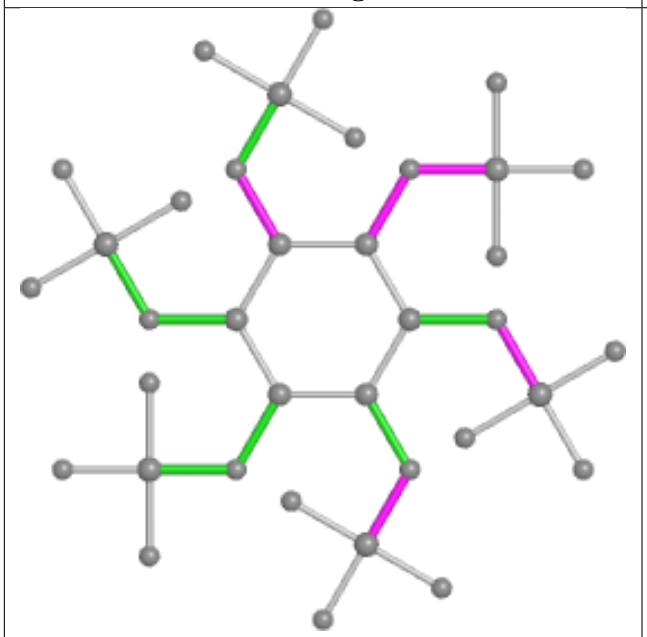
Ligand IHP A 902



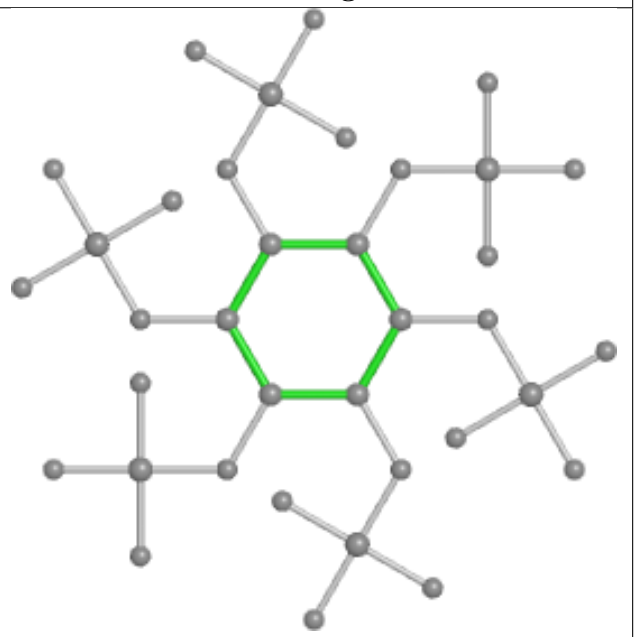
Bond lengths



Bond angles

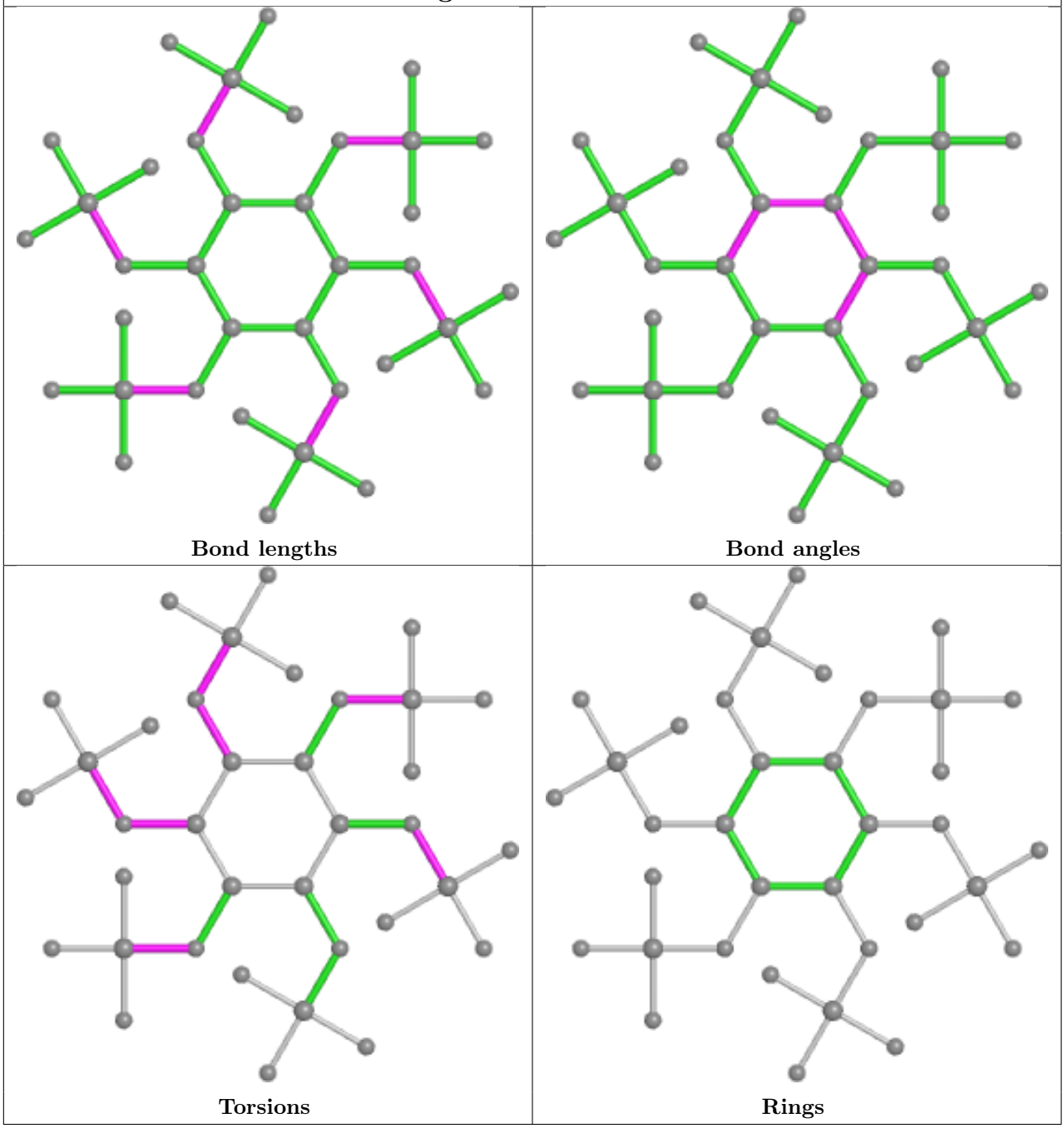


Torsions

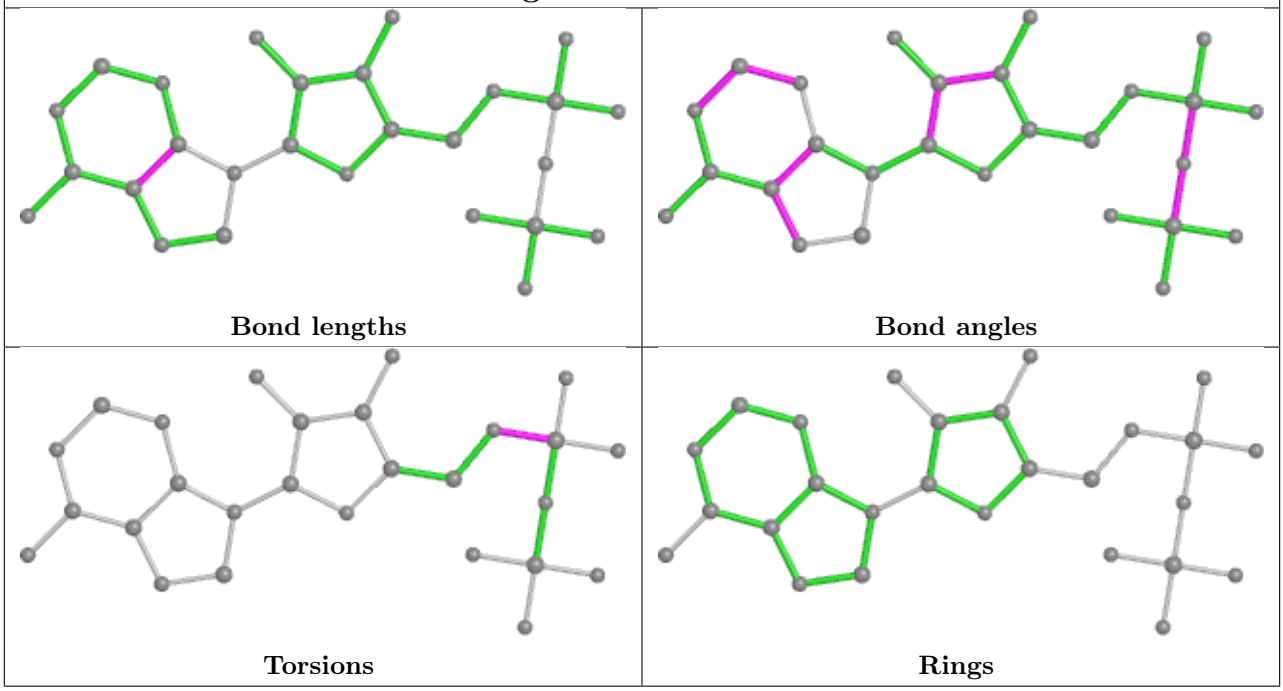


Rings

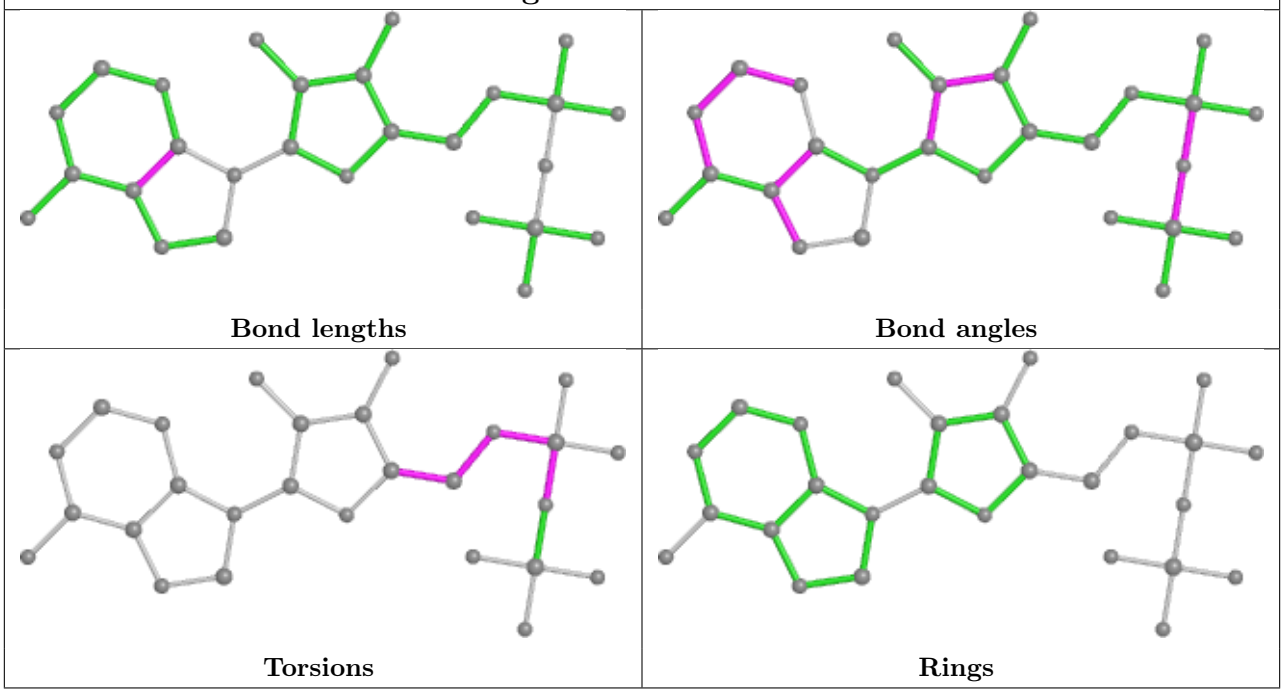
Ligand IHP G 902



Ligand ADP A 901



Ligand ADP G 901



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.