wwPDB EM Validation Summary Report (i)

Apr 21, 2024 – 10:06 PM JST

PDB ID	:	8K1V
EMDB ID	:	EMD-36805
Title	:	Human TWIK-related acid-sensitive potassium channel TASK3 at pH 7.4, 5 mM KCl and 135 mM NaCl
Authors	:	Chen, S.; Lin, H.
Deposited on	:	2023-07-11
Resolution	:	3.48 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:

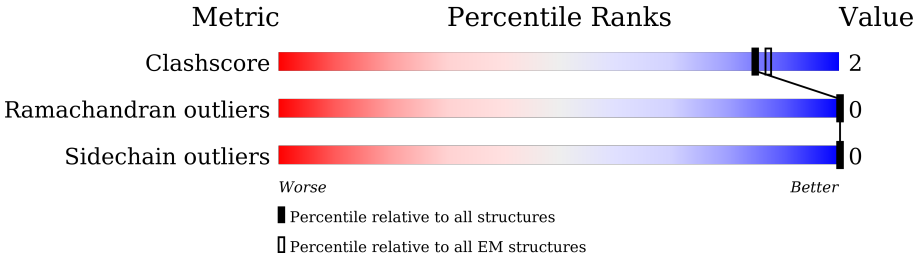
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.48 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	275	84% • 12%
1	B	275	84% • 12%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4059 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 Potassium channel subfamily K member 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	242	1921	1260	308	337	16	0	0
1	B	242	1921	1260	308	337	16	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	260	ASN	-	expression tag	UNP Q9NPC2
A	261	LEU	-	expression tag	UNP Q9NPC2
A	262	TYR	-	expression tag	UNP Q9NPC2
A	263	PHE	-	expression tag	UNP Q9NPC2
A	264	GLN	-	expression tag	UNP Q9NPC2
A	265	GLY	-	expression tag	UNP Q9NPC2
A	266	VAL	-	expression tag	UNP Q9NPC2
A	267	ASP	-	expression tag	UNP Q9NPC2
A	268	ALA	-	expression tag	UNP Q9NPC2
A	269	GLY	-	expression tag	UNP Q9NPC2
A	270	LEU	-	expression tag	UNP Q9NPC2
A	271	GLU	-	expression tag	UNP Q9NPC2
A	272	VAL	-	expression tag	UNP Q9NPC2
A	273	LEU	-	expression tag	UNP Q9NPC2
A	274	PHE	-	expression tag	UNP Q9NPC2
A	275	GLN	-	expression tag	UNP Q9NPC2
B	260	ASN	-	expression tag	UNP Q9NPC2
B	261	LEU	-	expression tag	UNP Q9NPC2
B	262	TYR	-	expression tag	UNP Q9NPC2
B	263	PHE	-	expression tag	UNP Q9NPC2
B	264	GLN	-	expression tag	UNP Q9NPC2
B	265	GLY	-	expression tag	UNP Q9NPC2
B	266	VAL	-	expression tag	UNP Q9NPC2
B	267	ASP	-	expression tag	UNP Q9NPC2
B	268	ALA	-	expression tag	UNP Q9NPC2
B	269	GLY	-	expression tag	UNP Q9NPC2

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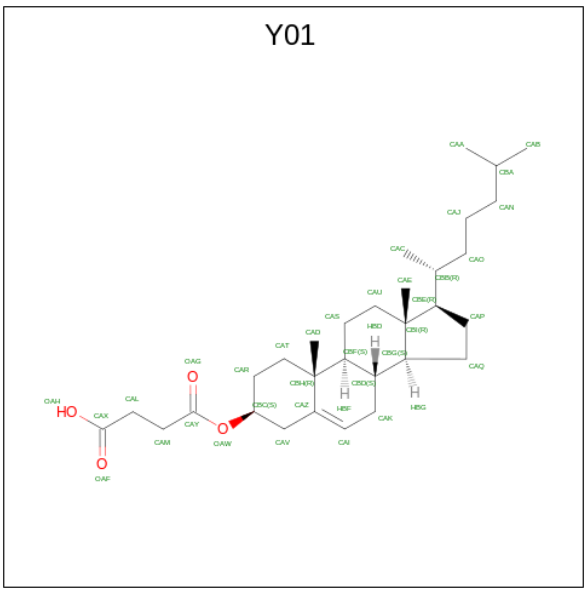
Chain	Residue	Modelled	Actual	Comment	Reference
B	270	LEU	-	expression tag	UNP Q9NPC2
B	271	GLU	-	expression tag	UNP Q9NPC2
B	272	VAL	-	expression tag	UNP Q9NPC2
B	273	LEU	-	expression tag	UNP Q9NPC2
B	274	PHE	-	expression tag	UNP Q9NPC2
B	275	GLN	-	expression tag	UNP Q9NPC2

- Molecule 2 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
2	A	1	35	31	4	0
			Total	C	O	
2	A	1	35	31	4	0
			Total	C	O	
2	A	1	35	31	4	0
			Total	C	O	
2	B	1	35	31	4	0
			Total	C	O	
2	B	1	35	31	4	0
			Total	C	O	
2	B	1	35	31	4	0

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms			AltConf
			Total	K		
3	A	5	5	5		0

- Molecule 4 is water.

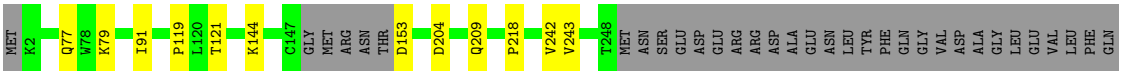
Mol	Chain	Residues	Atoms			AltConf
			Total	O		
4	A	1	1	1		0
			Total	O		
4	B	1	1	1		0

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.

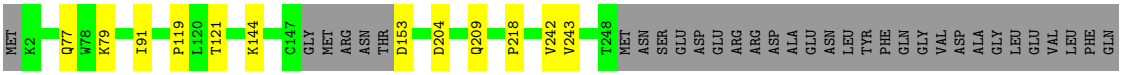
- Molecule 1: Potassium channel subfamily K member 9

Chain A:



- Molecule 1: Potassium channel subfamily K member 9

Chain B:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	451991	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
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: Y01, K

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	0.25	0/1964	0.40	0/2651
1	B	0.25	0/1964	0.40	0/2651
All	All	0.25	0/3928	0.40	0/5302

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	1921	0	1939	9	0
1	B	1921	0	1939	9	0
2	A	105	0	147	2	0
2	B	105	0	147	2	0
3	A	5	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	4059	0	4172	18	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 2.

The worst 5 of 18 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)
2:A:301:Y01:HAJ2	1:B:119:PRO:HG2	1.85	0.58
1:A:144:LYS:NZ	1:A:153:ASP:O	2.34	0.57
1:B:144:LYS:NZ	1:B:153:ASP:O	2.37	0.53
1:B:242:VAL:HG13	1:B:243:VAL:HG23	1.94	0.50
1:A:242:VAL:HG13	1:A:243:VAL:HG23	1.94	0.49

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	238/275 (86%)	236 (99%)	2 (1%)	0	100	100
1	B	238/275 (86%)	237 (100%)	1 (0%)	0	100	100
All	All	476/550 (86%)	473 (99%)	3 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	204/232 (88%)	204 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	204/232 (88%)	204 (100%)	0	100	100
All	All	408/464 (88%)	408 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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)

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)

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
2	Y01	B	302	-	38,38,38	0.54	0	57,57,57	0.54	0
2	Y01	A	302	-	38,38,38	0.54	0	57,57,57	0.54	0
2	Y01	A	303	-	38,38,38	0.54	0	57,57,57	0.54	0
2	Y01	A	301	-	38,38,38	0.54	0	57,57,57	0.53	0
2	Y01	B	301	-	38,38,38	0.54	0	57,57,57	0.54	0
2	Y01	B	303	-	38,38,38	0.54	0	57,57,57	0.53	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
2	Y01	B	302	-	-	3/19/77/77	0/4/4/4
2	Y01	A	302	-	-	5/19/77/77	0/4/4/4
2	Y01	A	303	-	-	3/19/77/77	0/4/4/4
2	Y01	A	301	-	-	2/19/77/77	0/4/4/4
2	Y01	B	301	-	-	3/19/77/77	0/4/4/4
2	Y01	B	303	-	-	5/19/77/77	0/4/4/4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	302	Y01	CAJ-CAO-CBB-CBE
2	B	303	Y01	CAJ-CAO-CBB-CBE
2	A	302	Y01	CAJ-CAO-CBB-CAC
2	B	303	Y01	CAJ-CAO-CBB-CAC
2	B	302	Y01	CAN-CAJ-CAO-CBB

There are no ring outliers.

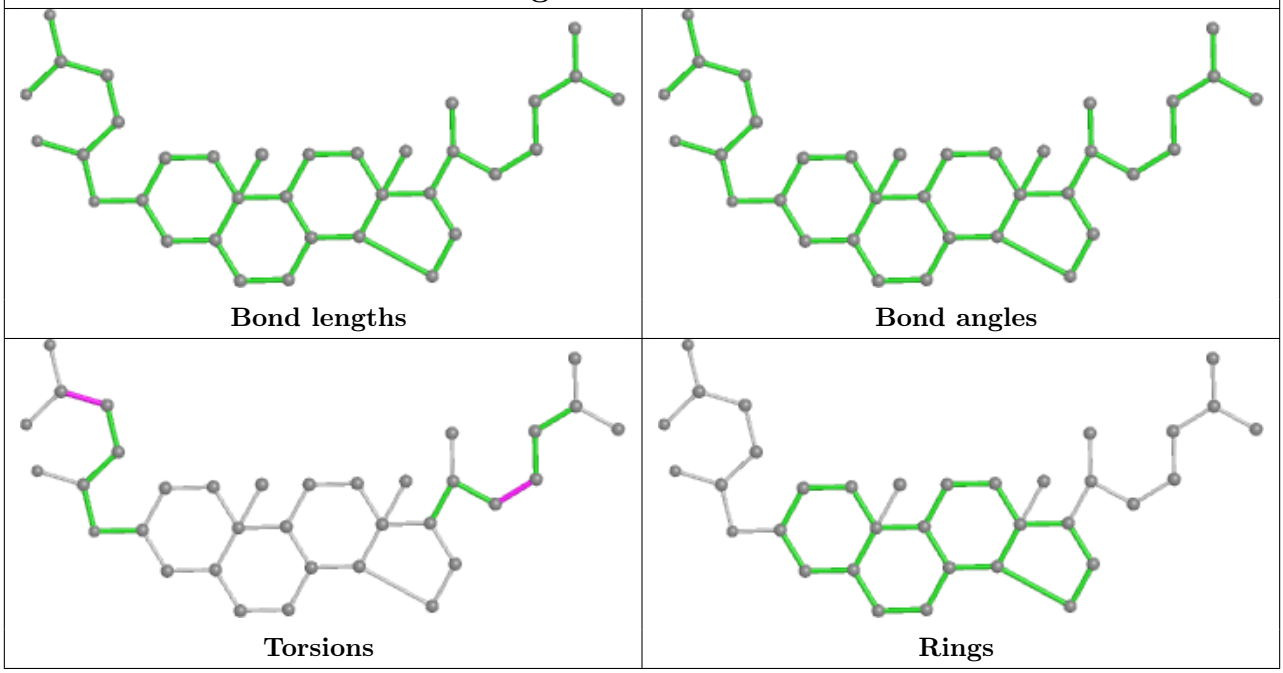
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	302	Y01	1	0
2	A	303	Y01	1	0
2	A	301	Y01	1	0
2	B	301	Y01	1	0

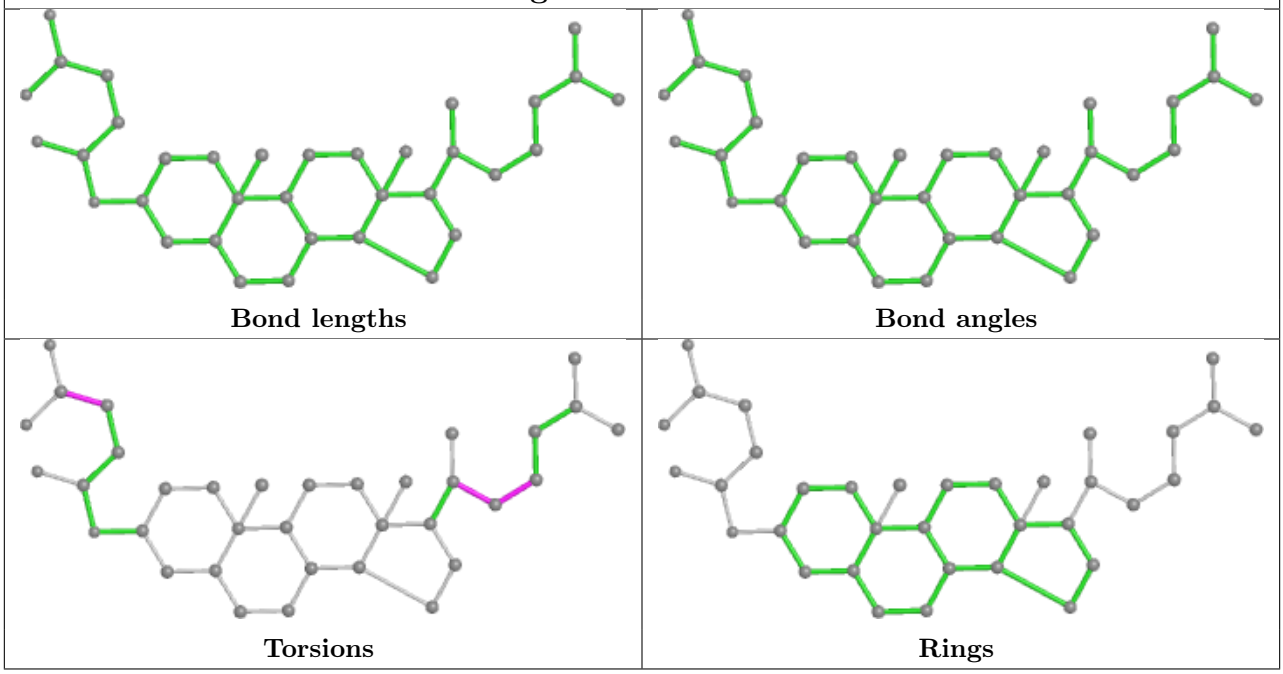
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

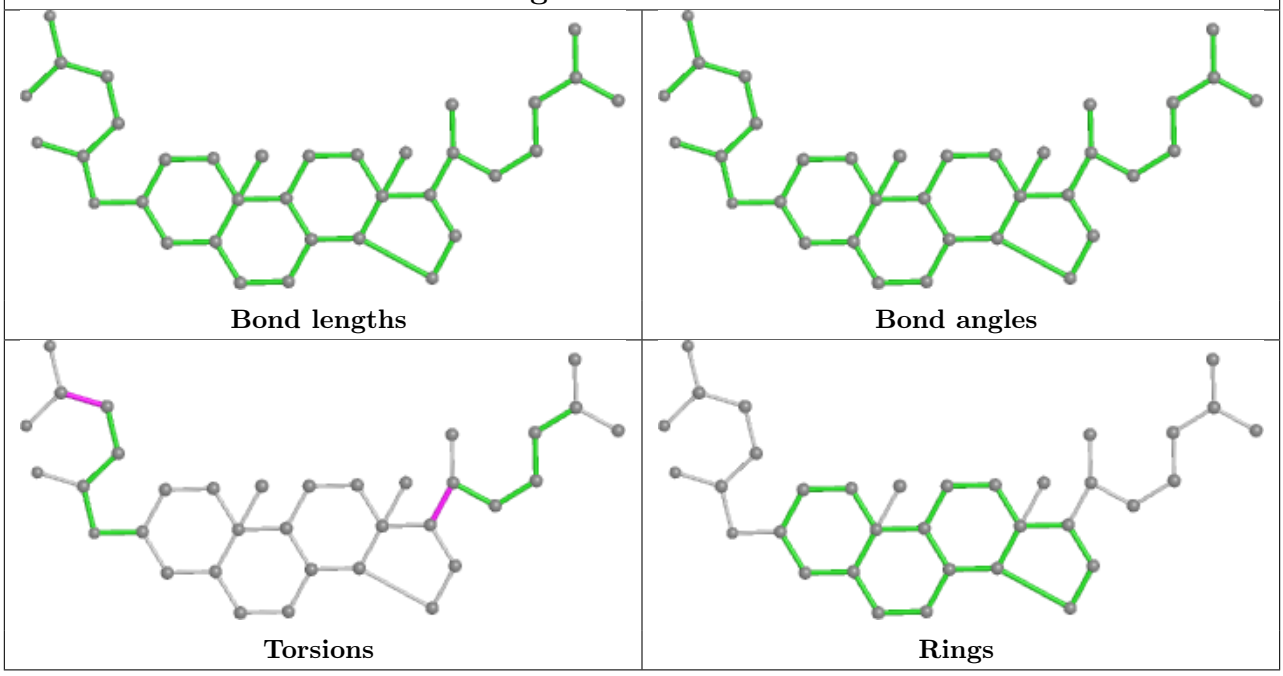
Ligand Y01 B 302



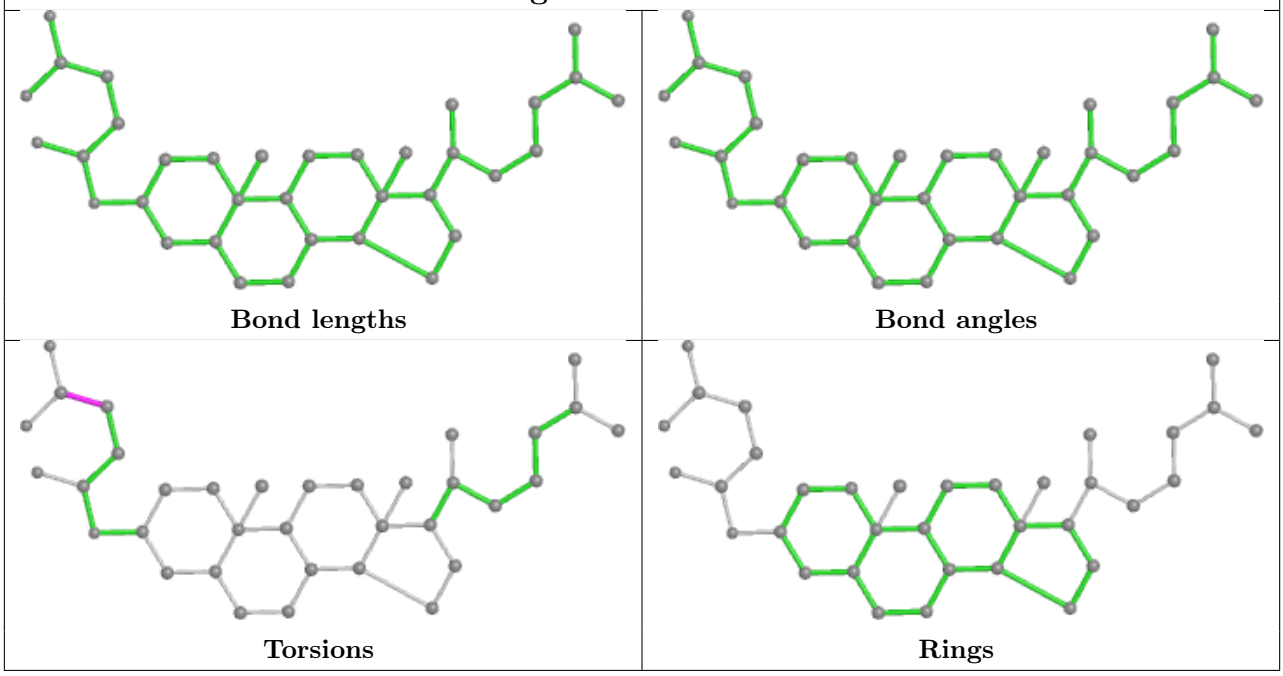
Ligand Y01 A 302



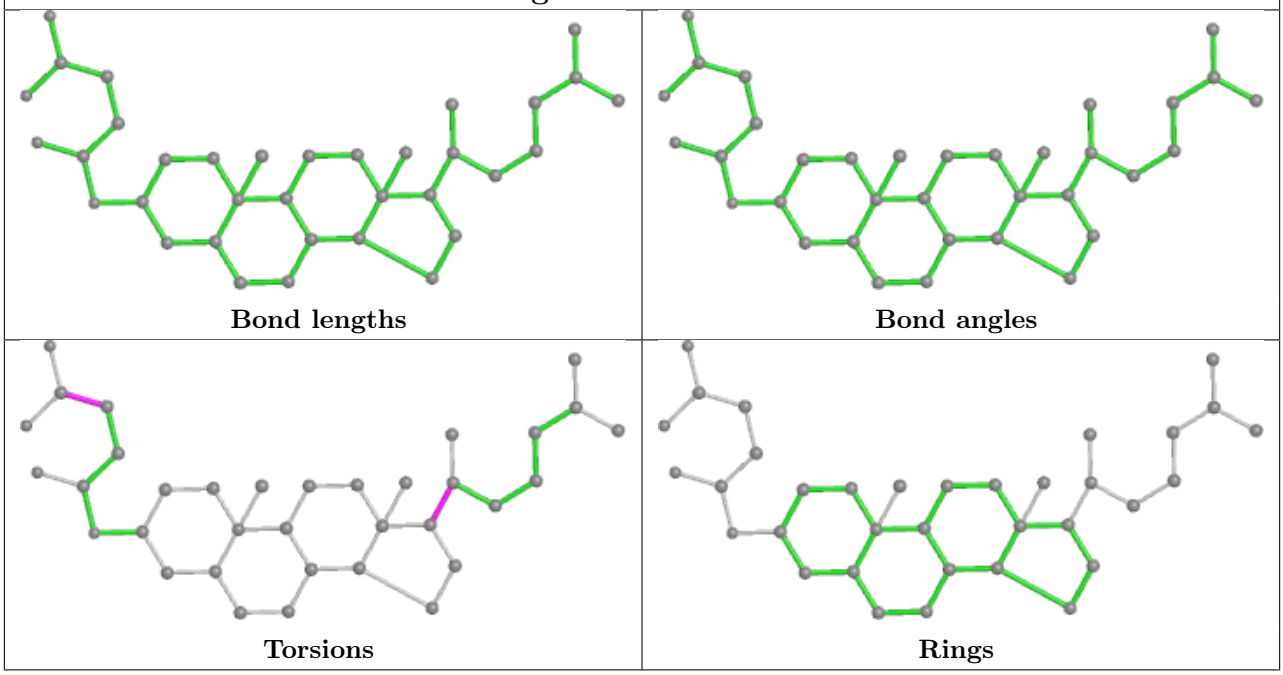
Ligand Y01 A 303



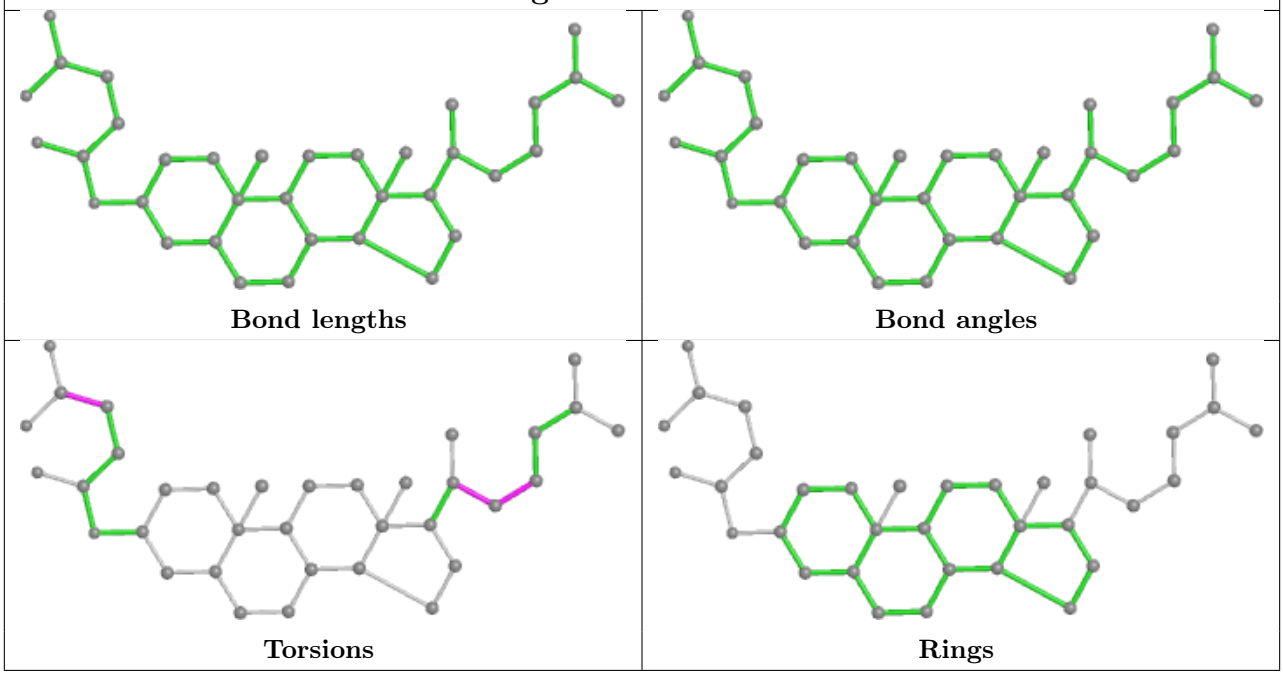
Ligand Y01 A 301



Ligand Y01 B 301



Ligand Y01 B 303



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.