



wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 09:09 AM EST

PDB ID : 7MBU
EMDB ID : EMD-23747
Title : Cryo-EM structure of zebrafish TRPM5 E337A mutant in the presence of 5 mM calcium (high calcium occupancy in the transmembrane domain)
Authors : Ruan, Z.; Lu, W.; Du, J.; Haley, E.
Deposited on : 2021-04-01
Resolution : Not provided

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.dev43
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) : 2.31.2

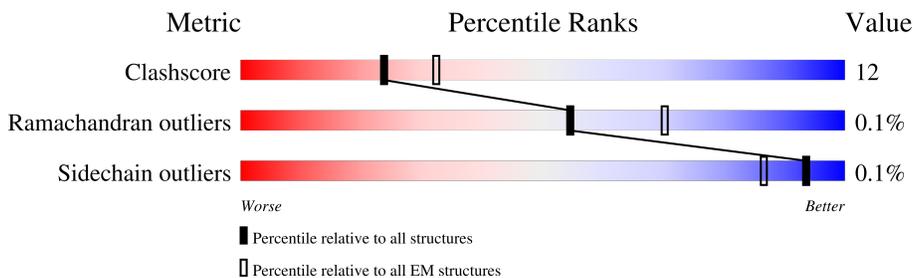
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is unknown.

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	1165	67% 18% 15%
1	B	1165	67% 18% 15%
1	C	1165	67% 18% 15%
1	D	1165	67% 18% 15%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 30780 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.

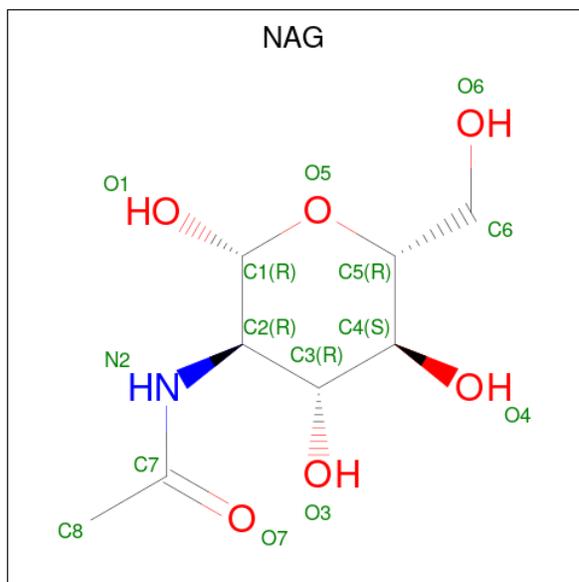
- Molecule 1 is a protein called Transient receptor potential melastatin 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	996	7591	4976	1299	1272	44	1	0
1	B	996	7591	4976	1299	1272	44	1	0
1	C	996	7591	4976	1299	1272	44	1	0
1	D	996	7591	4976	1299	1272	44	1	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	337	ALA	GLU	engineered mutation	UNP S5UH55
B	337	ALA	GLU	engineered mutation	UNP S5UH55
C	337	ALA	GLU	engineered mutation	UNP S5UH55
D	337	ALA	GLU	engineered mutation	UNP S5UH55

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).

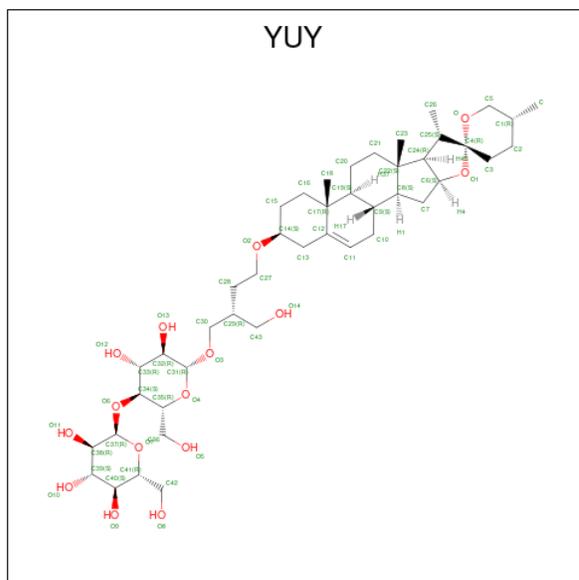


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
2	A	1	14	8	1	5	0
2	B	1	14	8	1	5	0
2	C	1	14	8	1	5	0
2	D	1	14	8	1	5	0

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

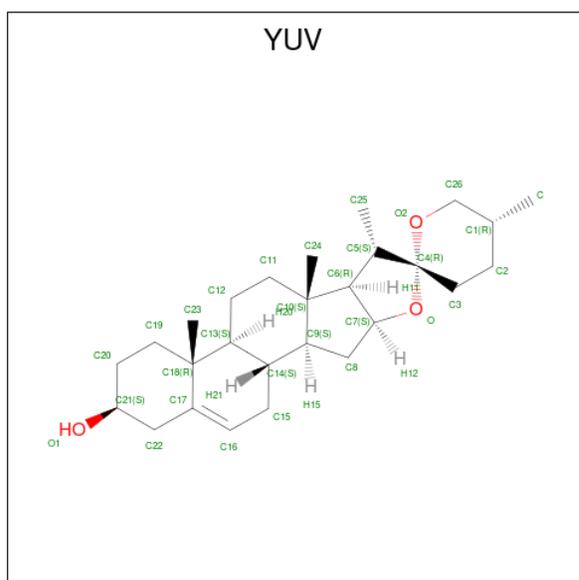
Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
3	A	1	1	1	0
3	B	1	1	1	0
3	C	1	1	1	0
3	D	1	1	1	0

- Molecule 4 is (2R)-2-(hydroxymethyl)-4-{[(25R)-10alpha,14beta,17beta-spirost-5-en-3beta-yloxy]butyl 4-O-alpha-D-glucopyranosyl-beta-D-glucopyranoside (three-letter code: YUY) (formula: C₄₄H₇₂O₁₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			118	88	30	
4	A	1	Total	C	O	0
			118	88	30	
4	B	1	Total	C	O	0
			59	44	15	
4	C	1	Total	C	O	0
			59	44	15	

- Molecule 5 is (25R)-14beta,17beta-spirost-5-en-3beta-ol (three-letter code: YUV) (formula: $C_{27}H_{42}O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total 30	C 27	O 3	0
5	B	1	Total 30	C 27	O 3	0
5	C	1	Total 30	C 27	O 3	0
5	D	1	Total 30	C 27	O 3	0

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	139000	Depositor
Resolution determination method	Not provided	
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	47	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (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: YUV, CA, NAG, YUY

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	0.33	0/7784	0.47	0/10616
1	B	0.33	0/7784	0.47	0/10616
1	C	0.33	0/7784	0.47	0/10616
1	D	0.33	0/7784	0.47	0/10616
All	All	0.33	0/31136	0.47	0/42464

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	7591	0	7422	250	0
1	B	7591	0	7422	250	0
1	C	7591	0	7422	247	0
1	D	7591	0	7422	250	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
2	C	14	0	13	0	0
2	D	14	0	13	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	118	0	0	9	0
4	B	59	0	0	4	0
4	C	59	0	0	4	0
5	A	30	0	0	0	0
5	B	30	0	0	0	0
5	C	30	0	0	0	0
5	D	30	0	0	0	0
All	All	30780	0	29740	734	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 12.

The worst 5 of 734 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:1078:LEU:HD11	1:D:1078:LEU:CD2	1.58	1.34
1:C:1078:LEU:CD2	1:D:1078:LEU:HD11	1.58	1.34
1:A:1078:LEU:CD2	1:B:1078:LEU:HD11	1.58	1.32
1:B:1078:LEU:CD2	1:C:1078:LEU:HD11	1.60	1.29
1:A:1083:GLY:HA2	1:B:1081:MET:CE	1.63	1.28

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	987/1165 (85%)	948 (96%)	38 (4%)	1 (0%)	51	51
1	B	987/1165 (85%)	949 (96%)	37 (4%)	1 (0%)	51	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	987/1165 (85%)	948 (96%)	38 (4%)	1 (0%)	51	51
1	D	987/1165 (85%)	948 (96%)	38 (4%)	1 (0%)	51	51
All	All	3948/4660 (85%)	3793 (96%)	151 (4%)	4 (0%)	54	51

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1006	ILE
1	B	1006	ILE
1	C	1006	ILE
1	D	1006	ILE

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	747/1017 (74%)	746 (100%)	1 (0%)	93	93
1	B	747/1017 (74%)	746 (100%)	1 (0%)	93	93
1	C	747/1017 (74%)	746 (100%)	1 (0%)	93	93
1	D	747/1017 (74%)	746 (100%)	1 (0%)	93	93
All	All	2988/4068 (74%)	2984 (100%)	4 (0%)	93	93

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	811	ARG
1	B	811	ARG
1	C	811	ARG
1	D	811	ARG

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	D	943	ASN
1	D	974	GLN
1	B	943	ASN
1	B	842	HIS
1	D	990	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](#)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	$\# Z > 2$
4	YUY	A	1503	-	66,66,66	0.12	0	100,102,102	0.18	0
4	YUY	B	1504	-	66,66,66	0.12	0	100,102,102	0.18	0
2	NAG	D	1501	1	14,14,15	0.28	0	17,19,21	0.62	0
5	YUV	C	1503	-	35,35,35	0.11	0	58,58,58	0.18	0
2	NAG	B	1501	1	14,14,15	0.29	0	17,19,21	0.60	0
2	NAG	C	1501	1	14,14,15	0.27	0	17,19,21	0.61	0
5	YUV	B	1503	-	35,35,35	0.11	0	58,58,58	0.18	0
4	YUY	A	1505	-	66,66,66	0.12	0	100,102,102	0.18	0
5	YUV	A	1504	-	35,35,35	0.11	0	58,58,58	0.18	0
5	YUV	D	1503	-	35,35,35	0.11	0	58,58,58	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	1501	1	14,14,15	0.28	0	17,19,21	0.61	0
4	YUY	C	1504	-	66,66,66	0.13	0	100,102,102	0.18	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
4	YUY	A	1503	-	-	11/21/149/149	0/8/8/8
4	YUY	B	1504	-	-	11/21/149/149	0/8/8/8
2	NAG	D	1501	1	-	3/6/23/26	0/1/1/1
5	YUV	C	1503	-	-	-	0/6/6/6
2	NAG	B	1501	1	-	3/6/23/26	0/1/1/1
2	NAG	C	1501	1	-	3/6/23/26	0/1/1/1
5	YUV	B	1503	-	-	-	0/6/6/6
4	YUY	A	1505	-	-	11/21/149/149	0/8/8/8
5	YUV	A	1504	-	-	-	0/6/6/6
5	YUV	D	1503	-	-	-	0/6/6/6
2	NAG	A	1501	1	-	3/6/23/26	0/1/1/1
4	YUY	C	1504	-	-	11/21/149/149	0/8/8/8

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 56 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1501	NAG	O7-C7-N2-C2
2	B	1501	NAG	O7-C7-N2-C2
2	C	1501	NAG	O7-C7-N2-C2
2	D	1501	NAG	O7-C7-N2-C2
4	A	1503	YUY	C43-C29-C30-O3

There are no ring outliers.

4 monomers are involved in 17 short contacts:

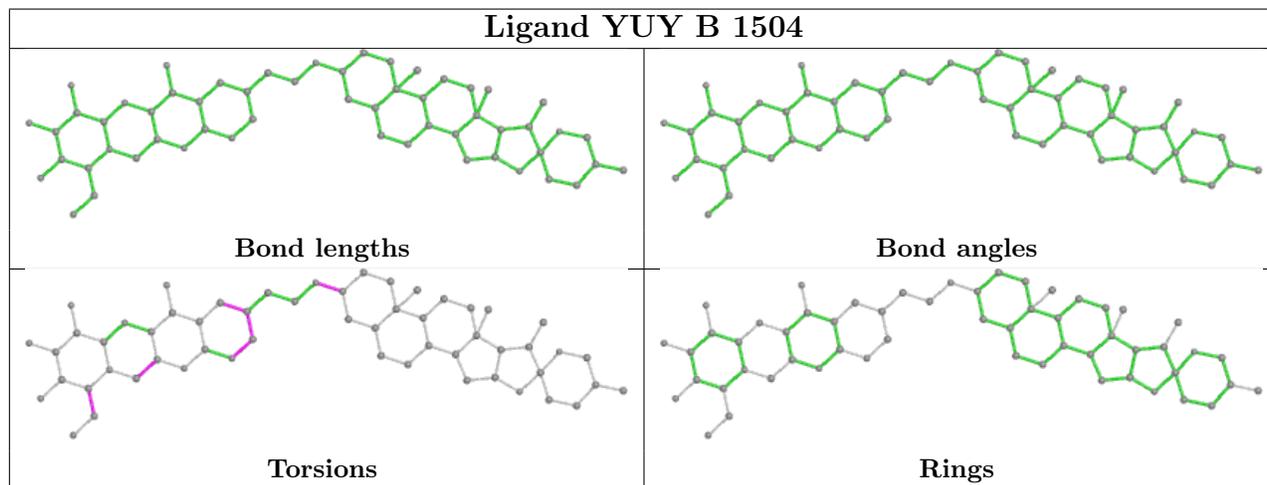
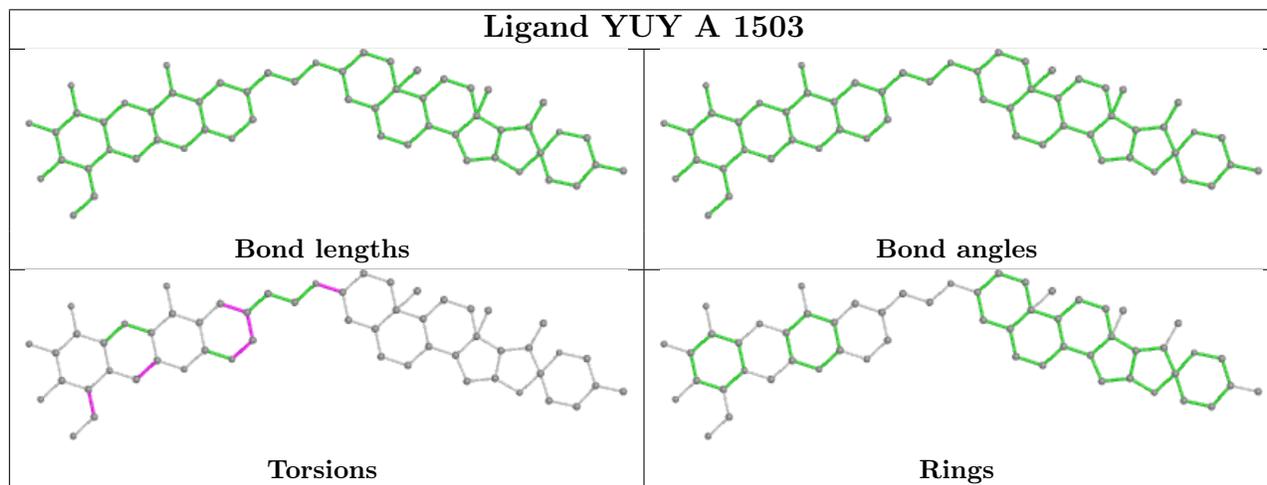
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1503	YUY	4	0

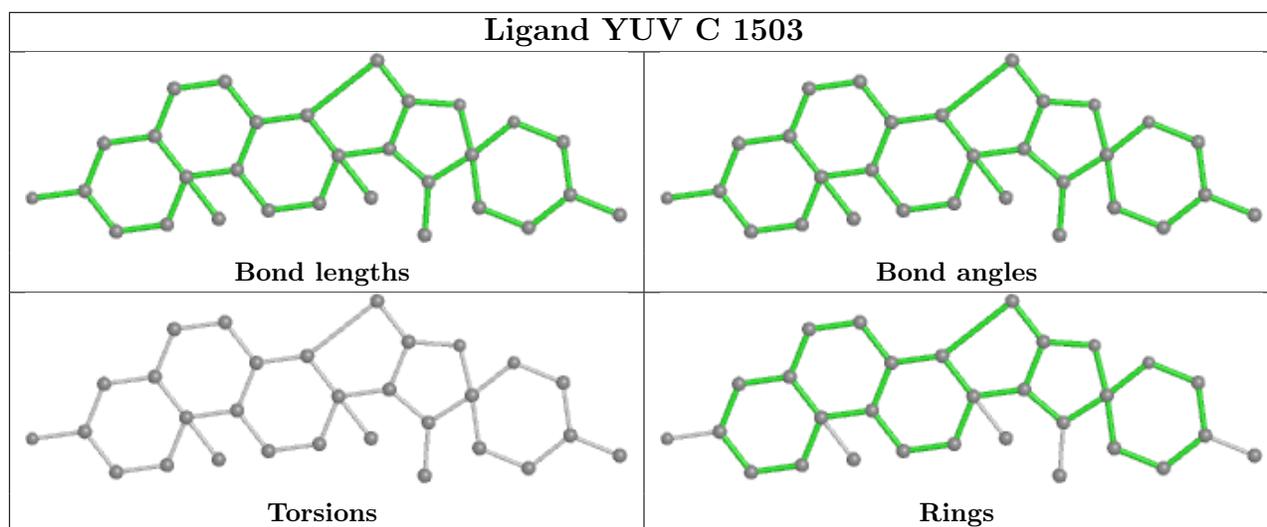
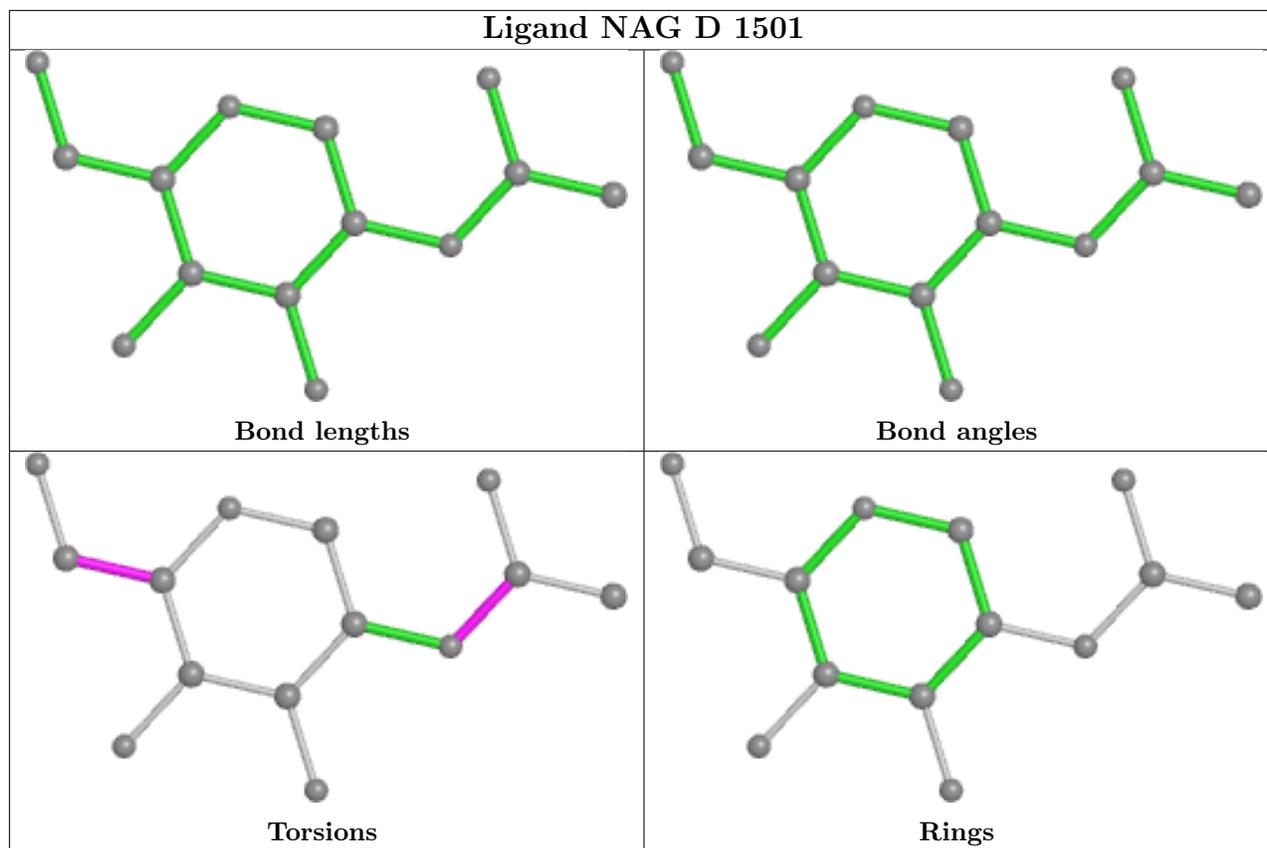
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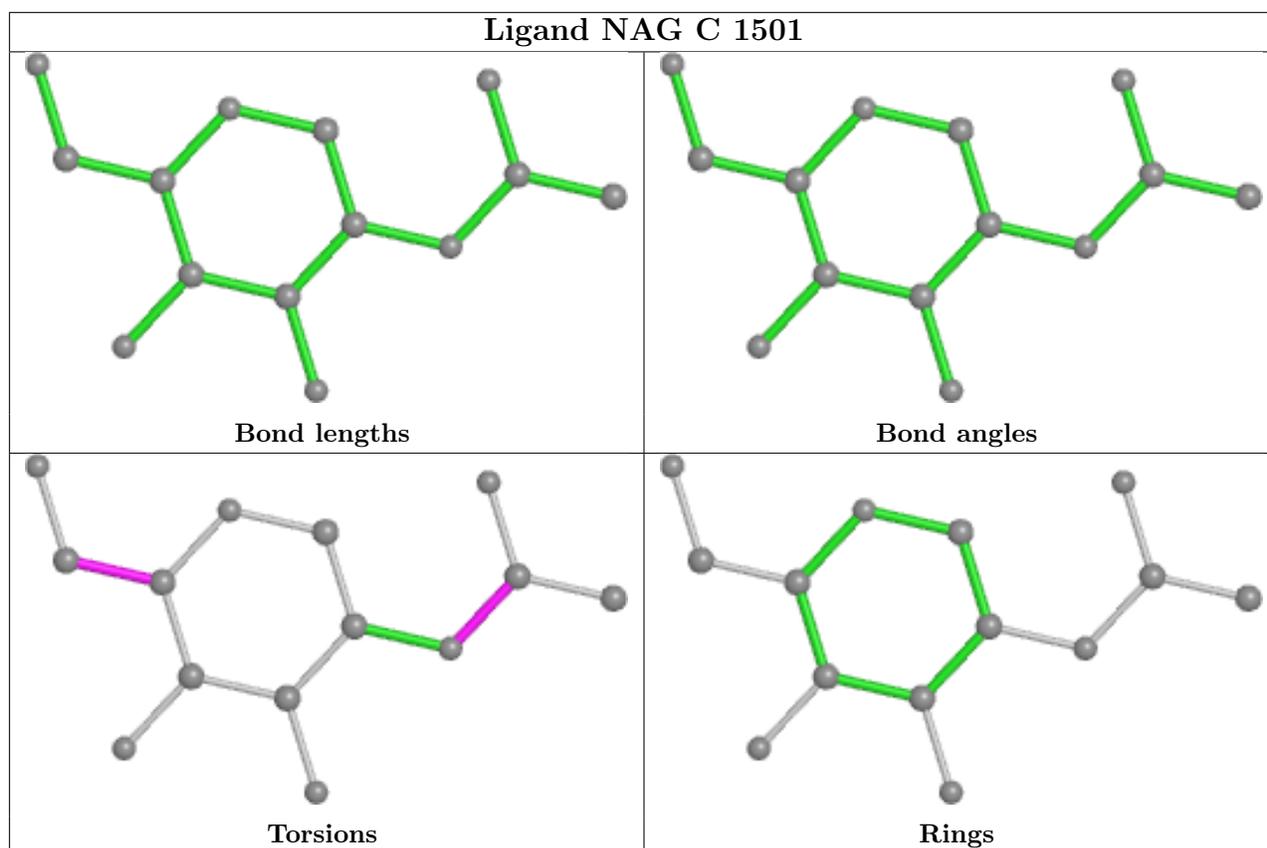
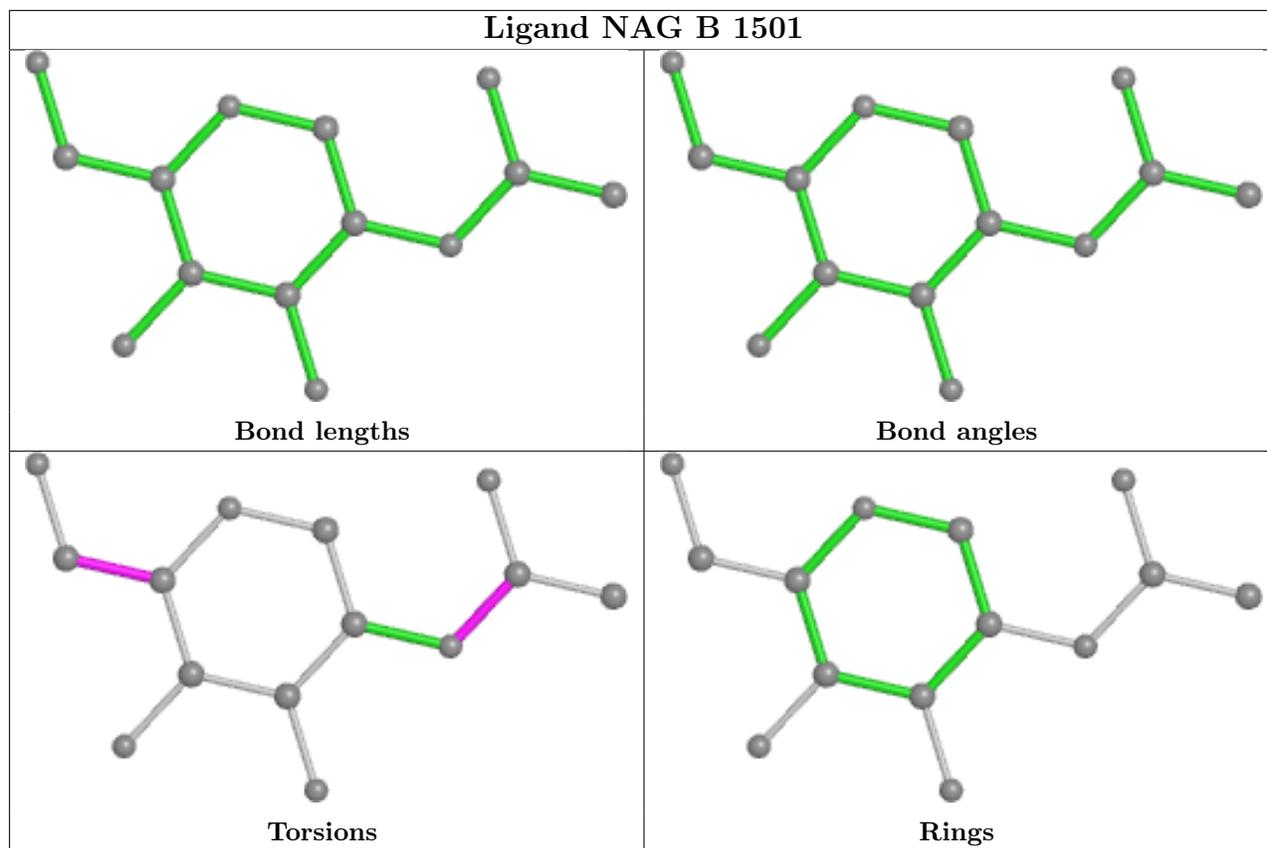
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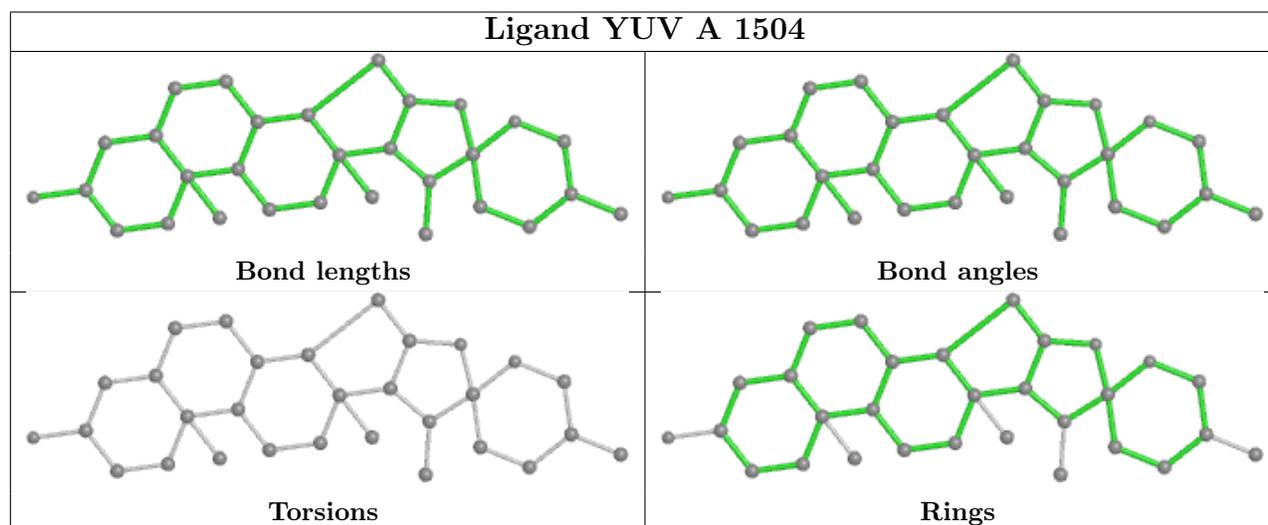
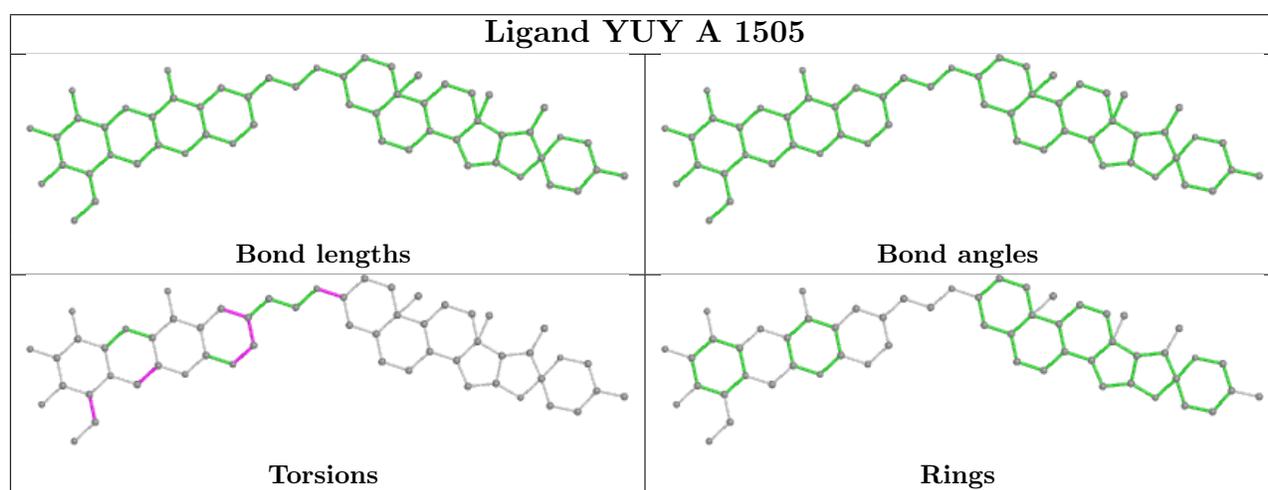
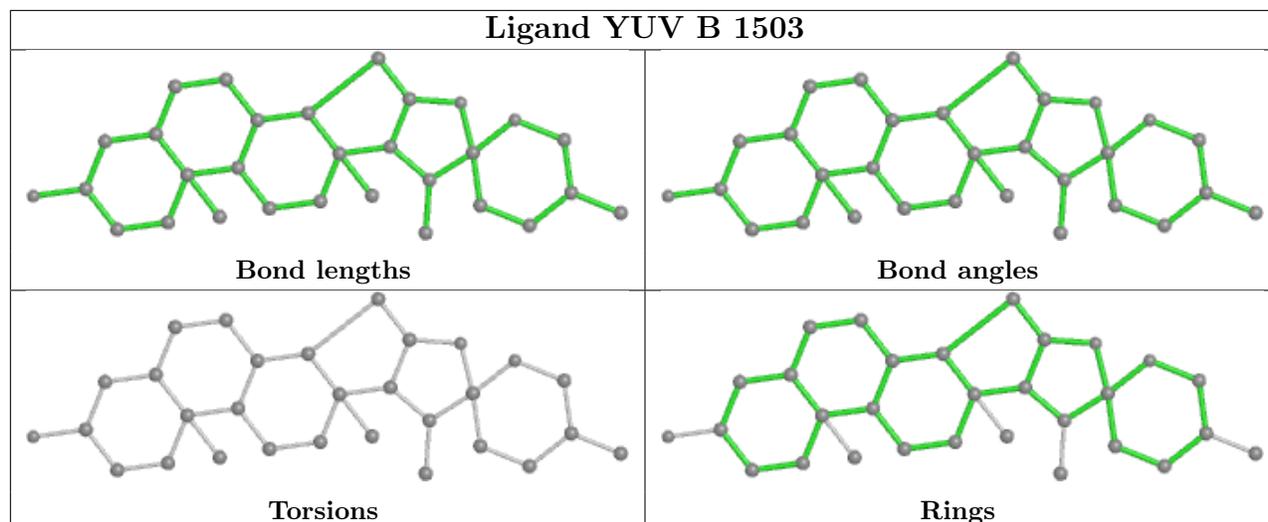
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1504	YUY	4	0
4	A	1505	YUY	5	0
4	C	1504	YUY	4	0

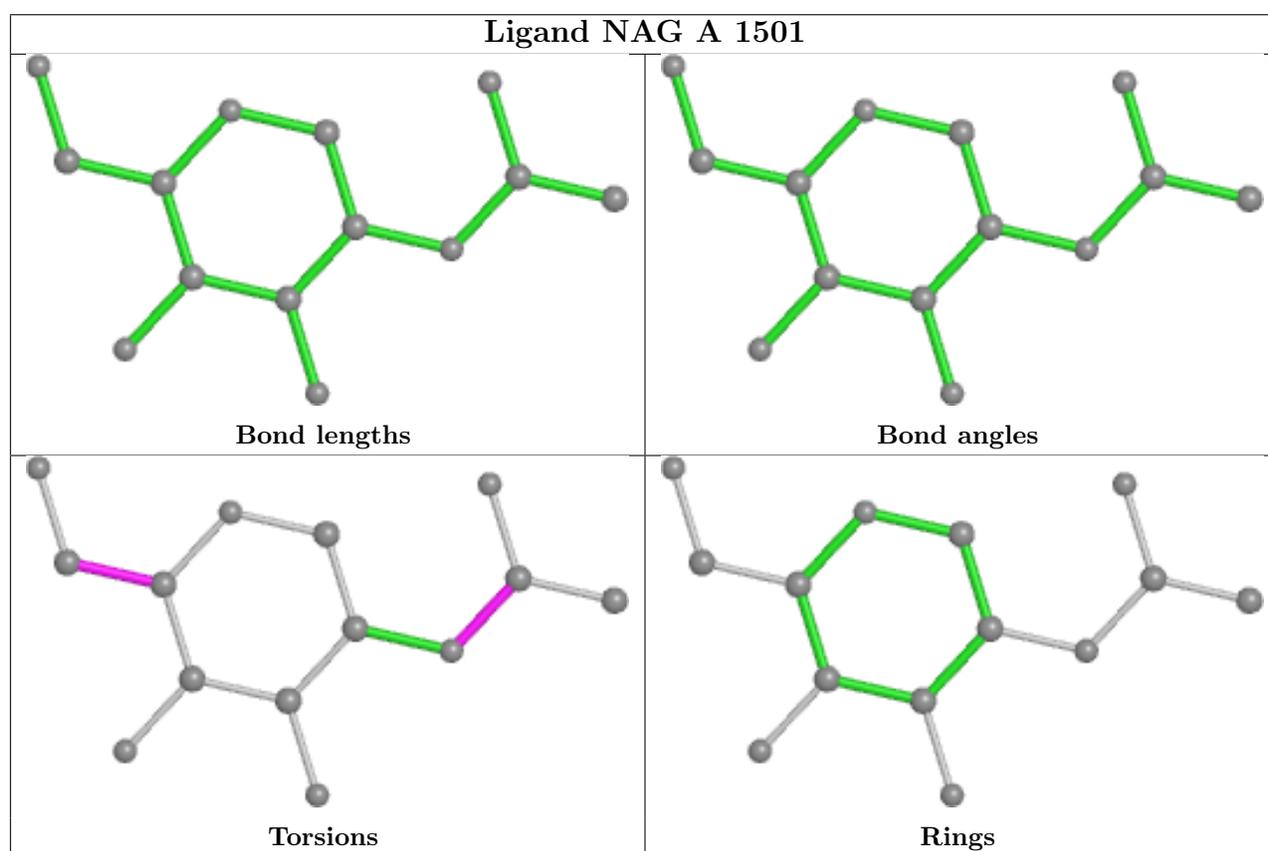
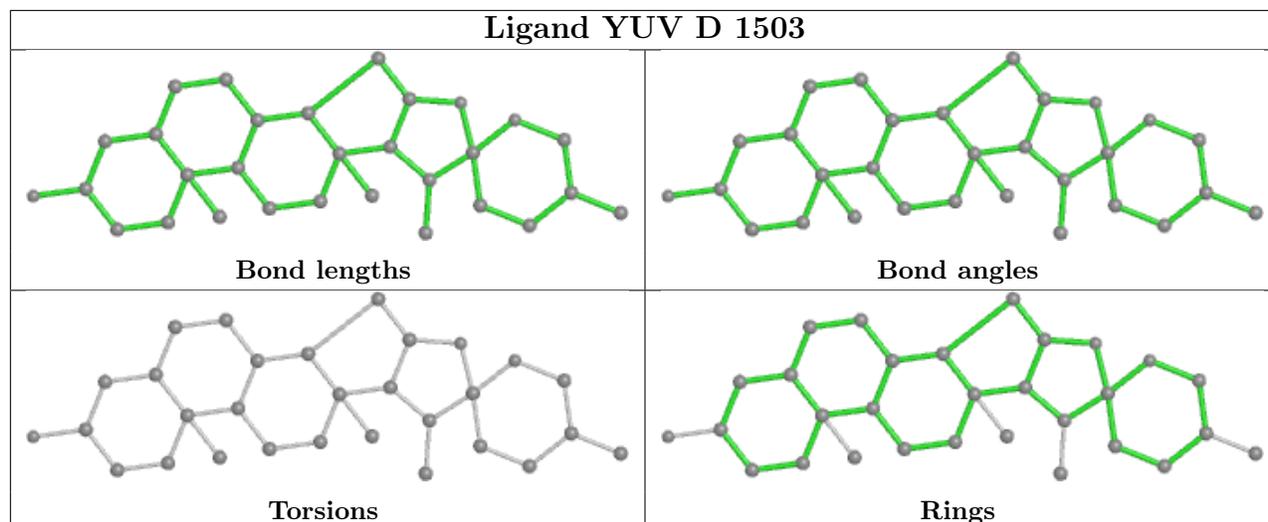
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

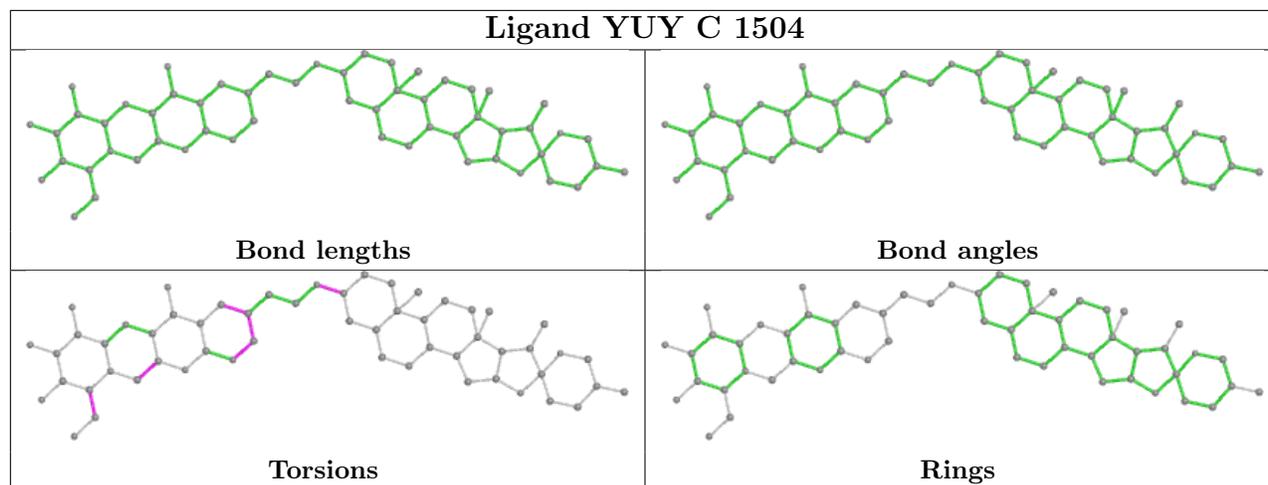












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23747. 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 surface views

This section was not generated.

6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.