



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 2, 2023 – 06:35 AM EDT

PDB ID : 6N95
Title : Methylmalonyl-CoA decarboxylase in complex with 2-sulfonate-propionyl-CoA
Authors : Stunkard, L.M.; Dixon, A.D.; Huth, T.J.; Lohman, J.R.
Deposited on : 2018-11-30
Resolution : 1.80 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : **FAILED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 15205 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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.

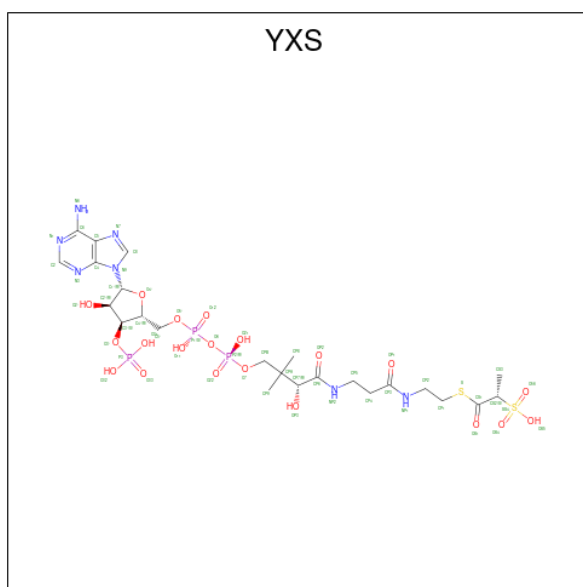
- Molecule 1 is a protein called Methylmalonyl-CoA decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	260	2149	1382	366	388	13	0	20	0
1	B	260	2111	1357	359	383	12	0	11	0
1	C	260	2114	1354	359	389	12	0	13	0
1	D	260	2103	1348	354	388	13	0	13	0
1	E	260	2120	1363	359	386	12	0	15	0
1	F	260	2117	1362	356	387	12	0	15	0

There are 6 discrepancies between the modelled and reference sequences:

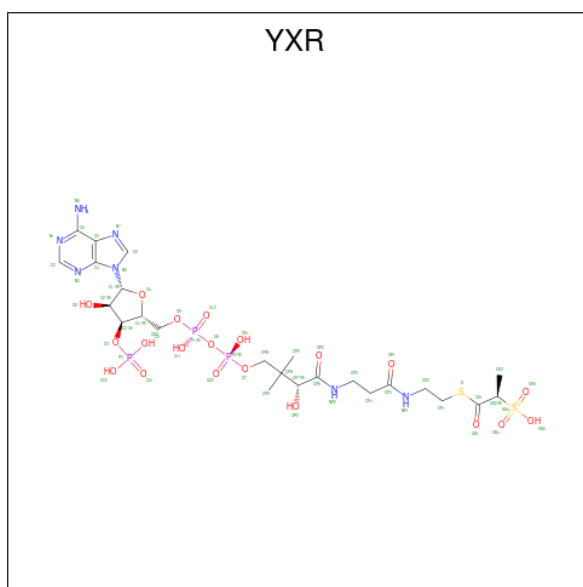
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	SER	engineered mutation	UNP P52045
B	2	ALA	SER	engineered mutation	UNP P52045
C	2	ALA	SER	engineered mutation	UNP P52045
D	2	ALA	SER	engineered mutation	UNP P52045
E	2	ALA	SER	engineered mutation	UNP P52045
F	2	ALA	SER	engineered mutation	UNP P52045

- Molecule 2 is (2S)-sulfonatepropionyl-CoA (three-letter code: YXS) (formula: C₂₄H₄₀N₇O₂₀P₃S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf		
			Total	C	N	O	P			S	
2	A	1	Total	56	24	7	20	3	2	0	1
2	B	1	Total	56	24	7	20	3	2	0	1
2	C	1	Total	56	24	7	20	3	2	0	1
2	D	1	Total	56	24	7	20	3	2	0	1
2	E	1	Total	56	24	7	20	3	2	0	1
2	F	1	Total	56	24	7	20	3	2	0	1

- Molecule 3 is (2R)-sulfonatepropionyl-CoA (three-letter code: YXR) (formula: $C_{24}H_{40}N_7O_{20}P_3S_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
3	A	1	56	24	7	20	3	2	0	1
3	B	1	56	24	7	20	3	2	0	1
3	C	1	56	24	7	20	3	2	0	1
3	D	1	56	24	7	20	3	2	0	1
3	E	1	56	24	7	20	3	2	0	1
3	F	1	56	24	7	20	3	2	0	1

- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ni		
4	A	1	1	1	0	0
4	D	1	1	1	0	0

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

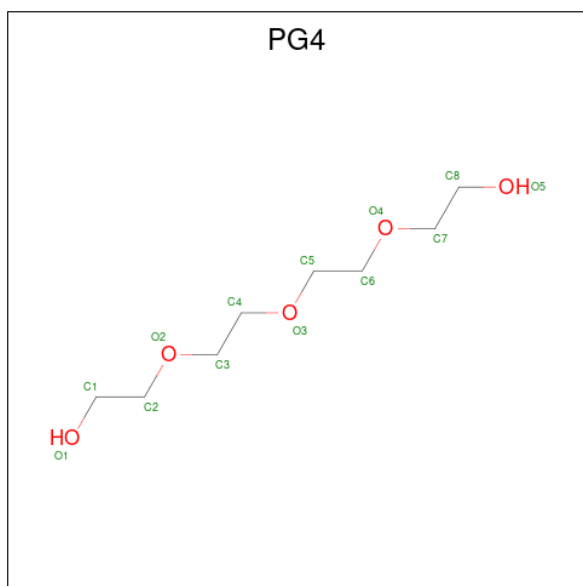
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
5	C	1	1	1	0	0

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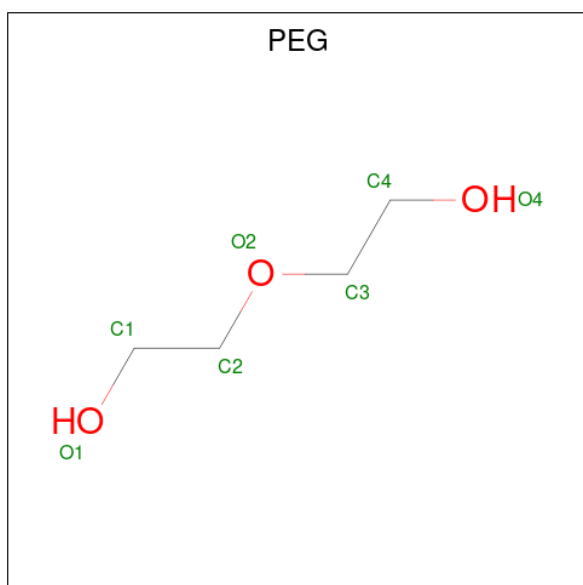
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	1	Total K 1 1	0	0

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



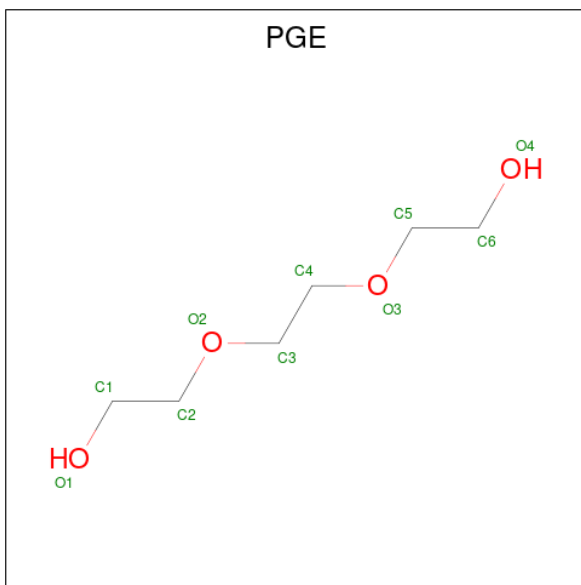
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 13 8 5	0	0

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			7	4	3		
7	F	1	Total	C	O	0	0
			7	4	3		

- Molecule 8 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	F	1	Total	C	O	0	0
			10	6	4		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	305	Total	O	1	19
			322	322		
9	B	265	Total	O	0	9
			274	274		
9	C	283	Total	O	0	19
			301	301		
9	D	282	Total	O	0	14
			295	295		
9	E	271	Total	O	0	14
			285	285		
9	F	288	Total	O	0	13
			301	301		

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.93Å 114.42Å 193.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80	Depositor
% Data completeness (in resolution range)	99.7 (20.00-1.80)	Depositor
R_{merge}	0.17	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 1.79Å)	Xtrriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.159 , 0.192	Depositor
Wilson B-factor (Å ²)	22.7	Xtrriage
Anisotropy	0.067	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	15205	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 4 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
2	YXS	E	301[B]	-	48,58,58	0.91	2 (4%)	60,88,88	1.74	13 (21%)
3	YXR	F	302[A]	-	48,58,58	1.01	3 (6%)	60,88,88	1.75	10 (16%)
6	PG4	C	304	5	12,12,12	0.26	0	11,11,11	0.25	0
2	YXS	A	301[B]	-	48,58,58	1.21	3 (6%)	60,88,88	1.72	10 (16%)
7	PEG	F	305	-	6,6,6	0.29	0	5,5,5	0.26	0
2	YXS	F	301[B]	-	48,58,58	1.12	3 (6%)	60,88,88	3.34	16 (26%)
2	YXS	C	301[B]	-	48,58,58	0.96	2 (4%)	60,88,88	1.55	6 (10%)
7	PEG	C	305	-	6,6,6	0.33	0	5,5,5	0.19	0
2	YXS	B	301[B]	-	48,58,58	0.94	4 (8%)	60,88,88	1.57	13 (21%)
8	PGE	F	304	5	9,9,9	0.35	0	8,8,8	0.20	0
2	YXS	D	302[B]	-	48,58,58	1.00	3 (6%)	60,88,88	3.28	17 (28%)
3	YXR	C	302[A]	-	48,58,58	0.96	3 (6%)	60,88,88	1.70	8 (13%)
3	YXR	A	302[A]	-	48,58,58	1.13	3 (6%)	60,88,88	1.62	9 (15%)
3	YXR	D	303[A]	-	48,58,58	1.01	2 (4%)	60,88,88	3.26	16 (26%)
3	YXR	B	302[A]	-	48,58,58	0.87	1 (2%)	60,88,88	3.54	17 (28%)
3	YXR	E	302[A]	-	48,58,58	0.93	2 (4%)	60,88,88	3.25	18 (30%)

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	YXS	E	301[B]	-	-	8/54/77/77	0/3/3/3
3	YXR	F	302[A]	-	-	7/54/77/77	0/3/3/3
6	PG4	C	304	5	-	2/10/10/10	-
2	YXS	A	301[B]	-	-	4/54/77/77	0/3/3/3
7	PEG	F	305	-	-	1/4/4/4	-
2	YXS	F	301[B]	-	-	15/54/77/77	0/3/3/3
2	YXS	C	301[B]	-	-	4/54/77/77	0/3/3/3
7	PEG	C	305	-	-	0/4/4/4	-
2	YXS	B	301[B]	-	-	7/54/77/77	0/3/3/3
8	PGE	F	304	5	-	0/7/7/7	-
2	YXS	D	302[B]	-	-	7/54/77/77	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	YXR	C	302[A]	-	-	2/54/77/77	0/3/3/3
3	YXR	A	302[A]	-	-	2/54/77/77	0/3/3/3
3	YXR	D	303[A]	-	-	6/54/77/77	0/3/3/3
3	YXR	B	302[A]	-	-	10/54/77/77	0/3/3/3
3	YXR	E	302[A]	-	-	15/54/77/77	0/3/3/3

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301[B]	YXS	CS2-CS1	-4.47	1.47	1.52
2	F	301[B]	YXS	CS2-CS1	-3.66	1.48	1.52
3	A	302[A]	YXR	CS2-CS1	-3.60	1.48	1.52
3	D	303[A]	YXR	OS1-CS1	3.21	1.25	1.20
2	A	301[B]	YXS	O4'-C1'	3.19	1.45	1.41

The worst 5 of 153 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302[A]	YXR	CP8-CPA-CPB	-14.66	84.33	108.23
3	E	302[A]	YXR	CP8-CPA-CPB	-14.09	85.25	108.23
2	D	302[B]	YXS	CP8-CPA-CPB	-13.80	85.72	108.23
3	D	303[A]	YXR	CP8-CPA-CPB	-13.71	85.87	108.23
3	B	302[A]	YXR	CP8-CPA-CP7	-13.40	85.59	108.82

There are no chirality outliers.

5 of 90 torsion outliers are listed below:

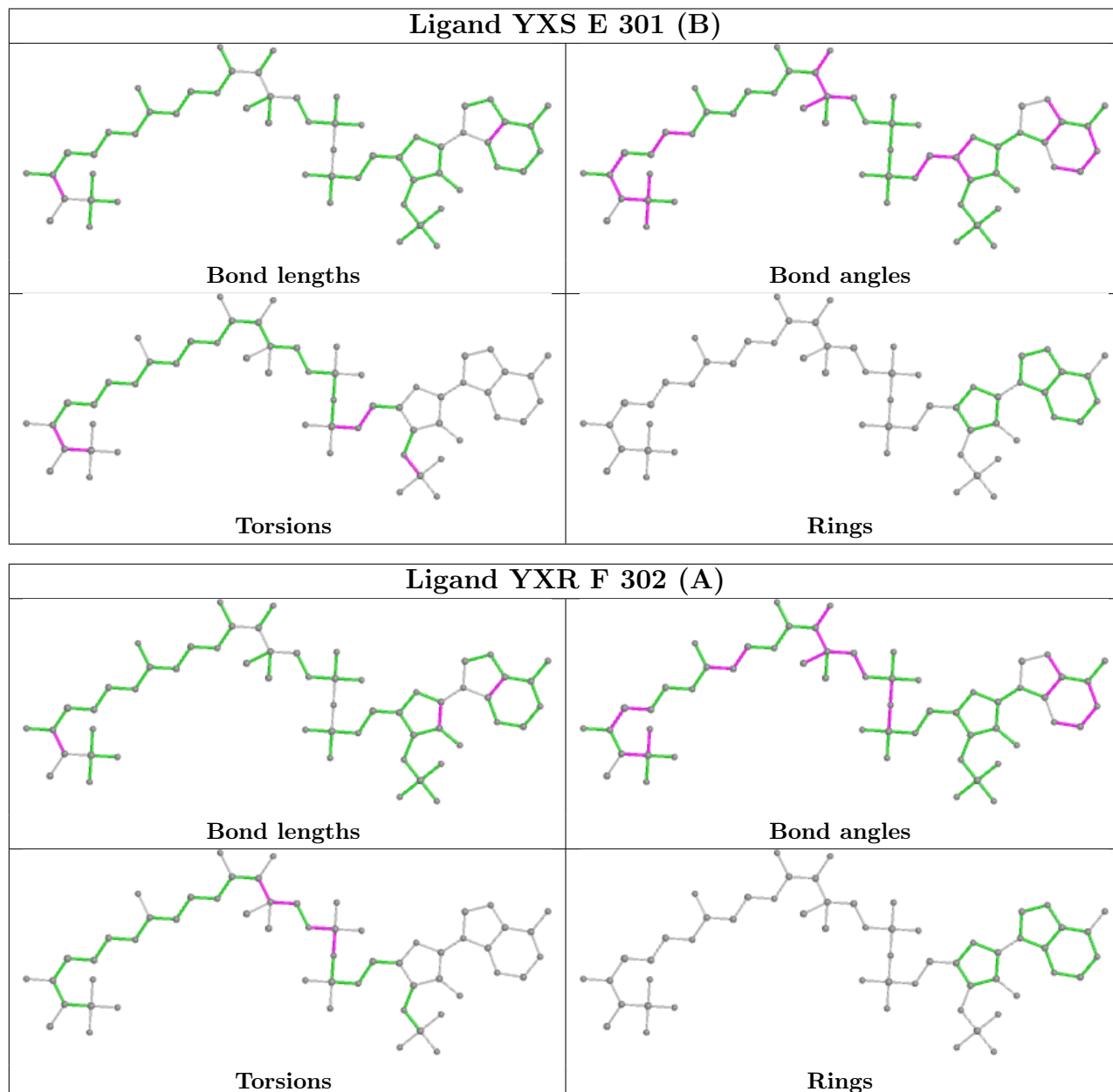
Mol	Chain	Res	Type	Atoms
2	A	301[B]	YXS	OS1-CS1-CS2-CS3
2	C	301[B]	YXS	CS3-CS2-SS4-OS5
2	D	302[B]	YXS	CP7-CPA-CPB-O7
2	D	302[B]	YXS	OP3-CP7-CPA-CP9
2	D	302[B]	YXS	CP6-CP7-CPA-CP9

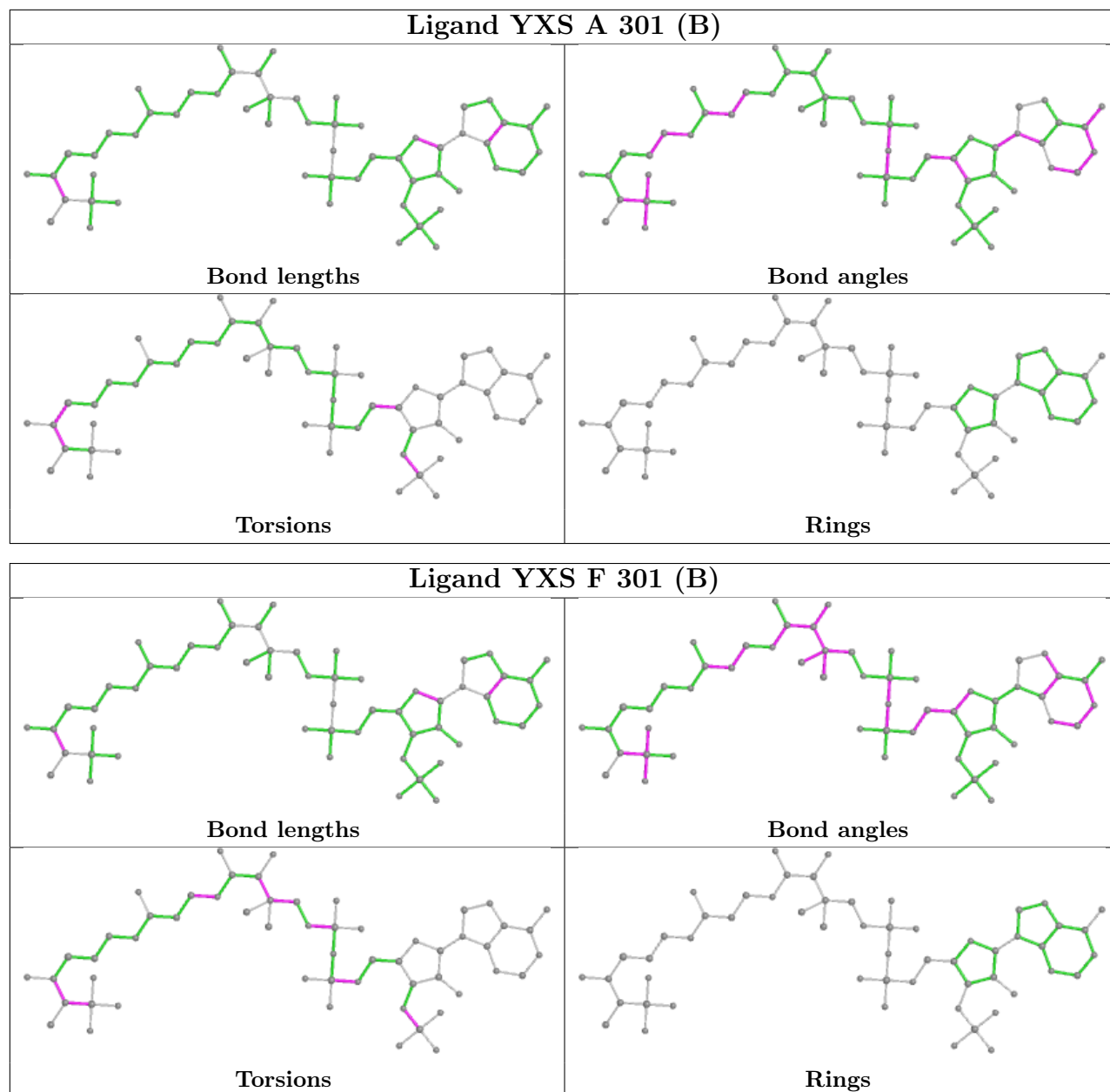
There are no ring outliers.

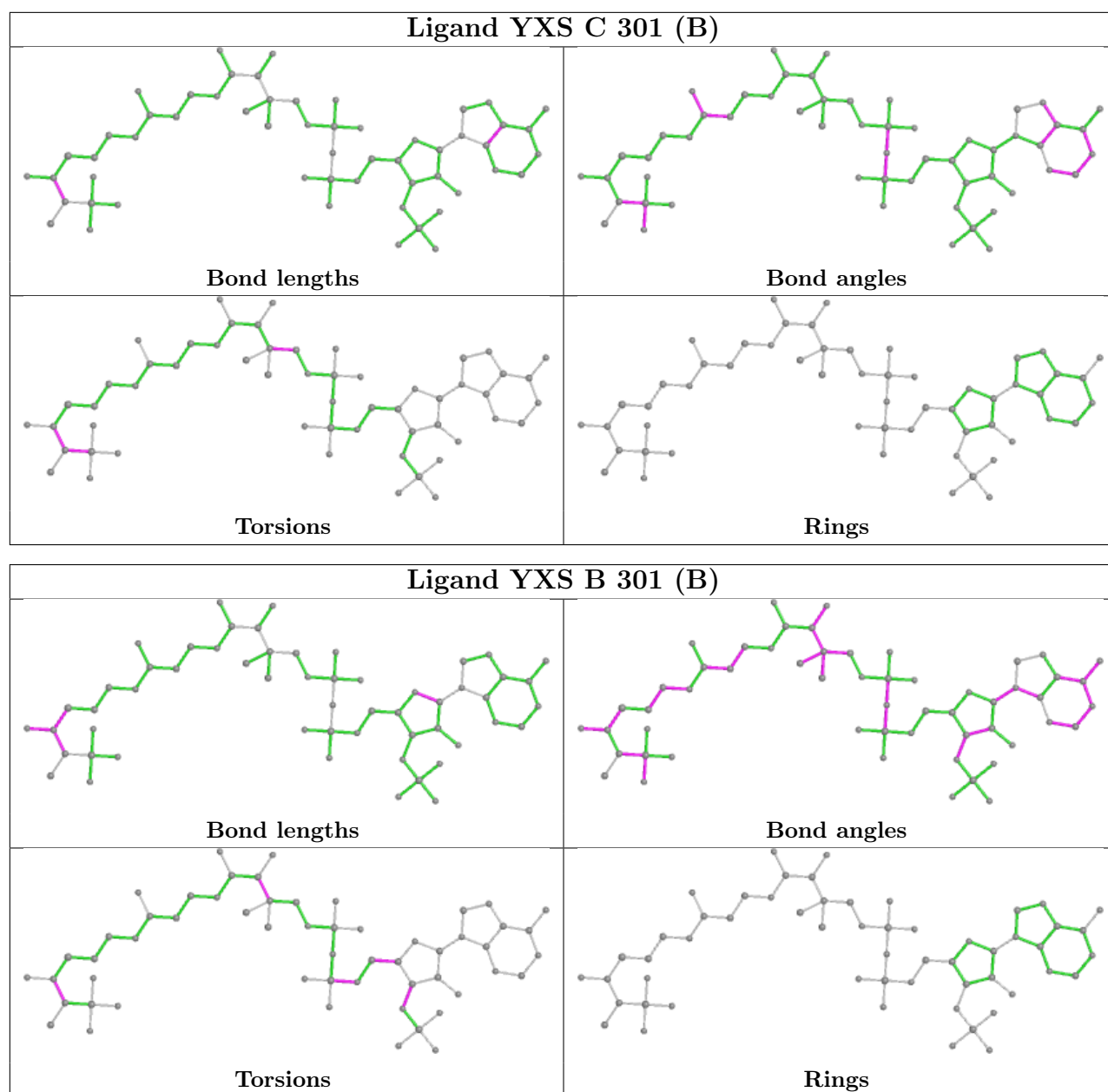
No monomer is involved in short contacts.

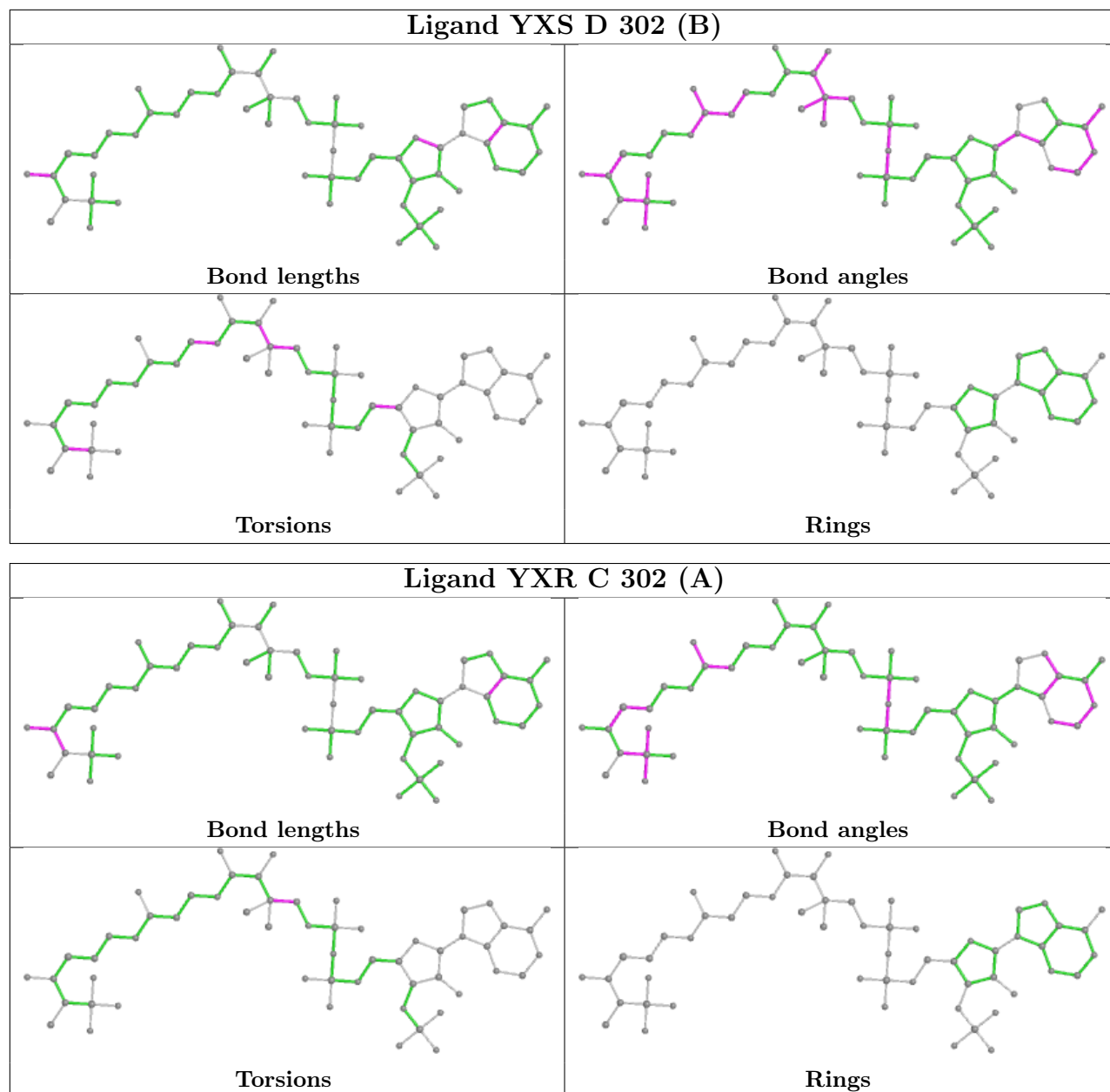
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

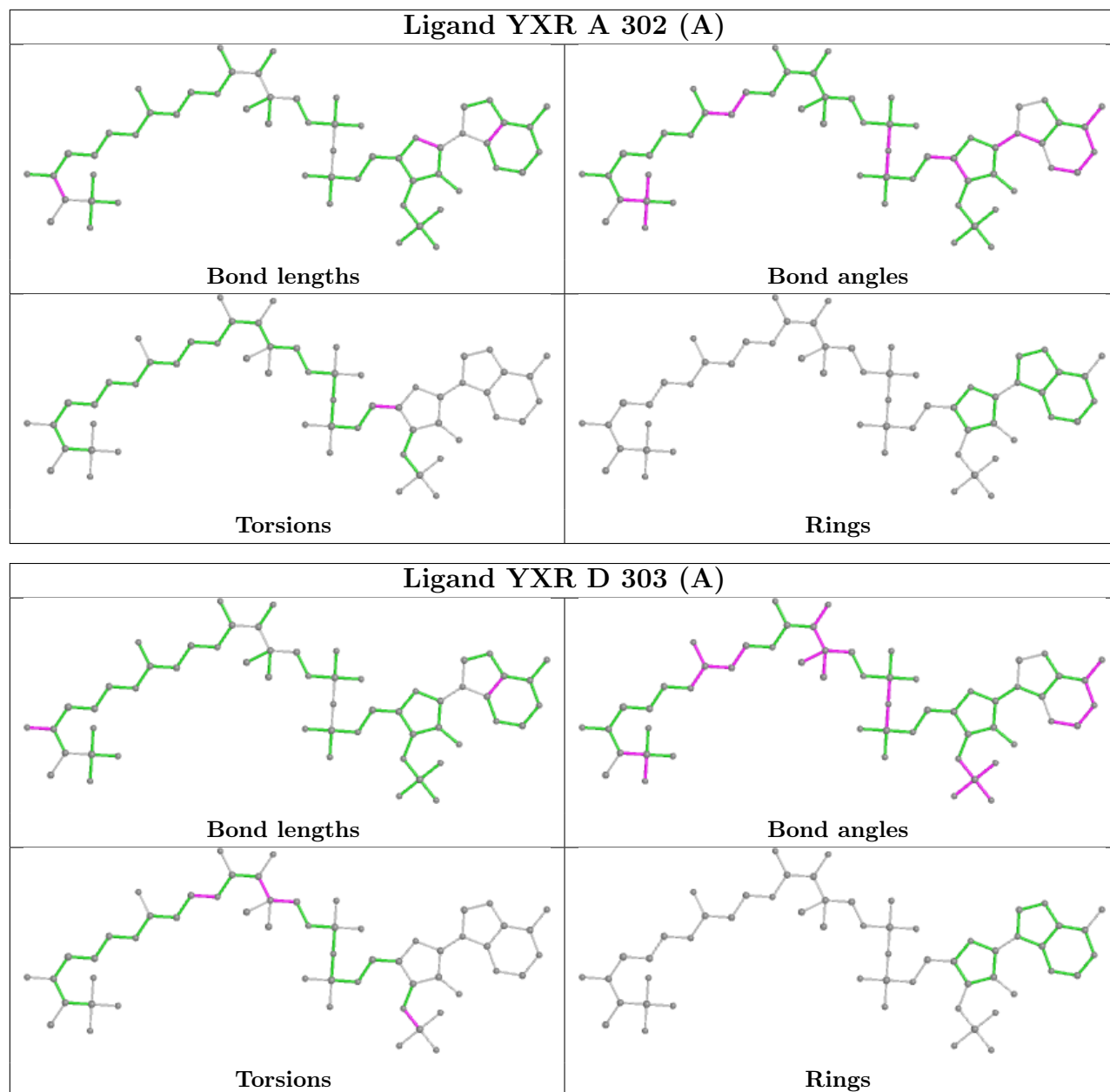
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

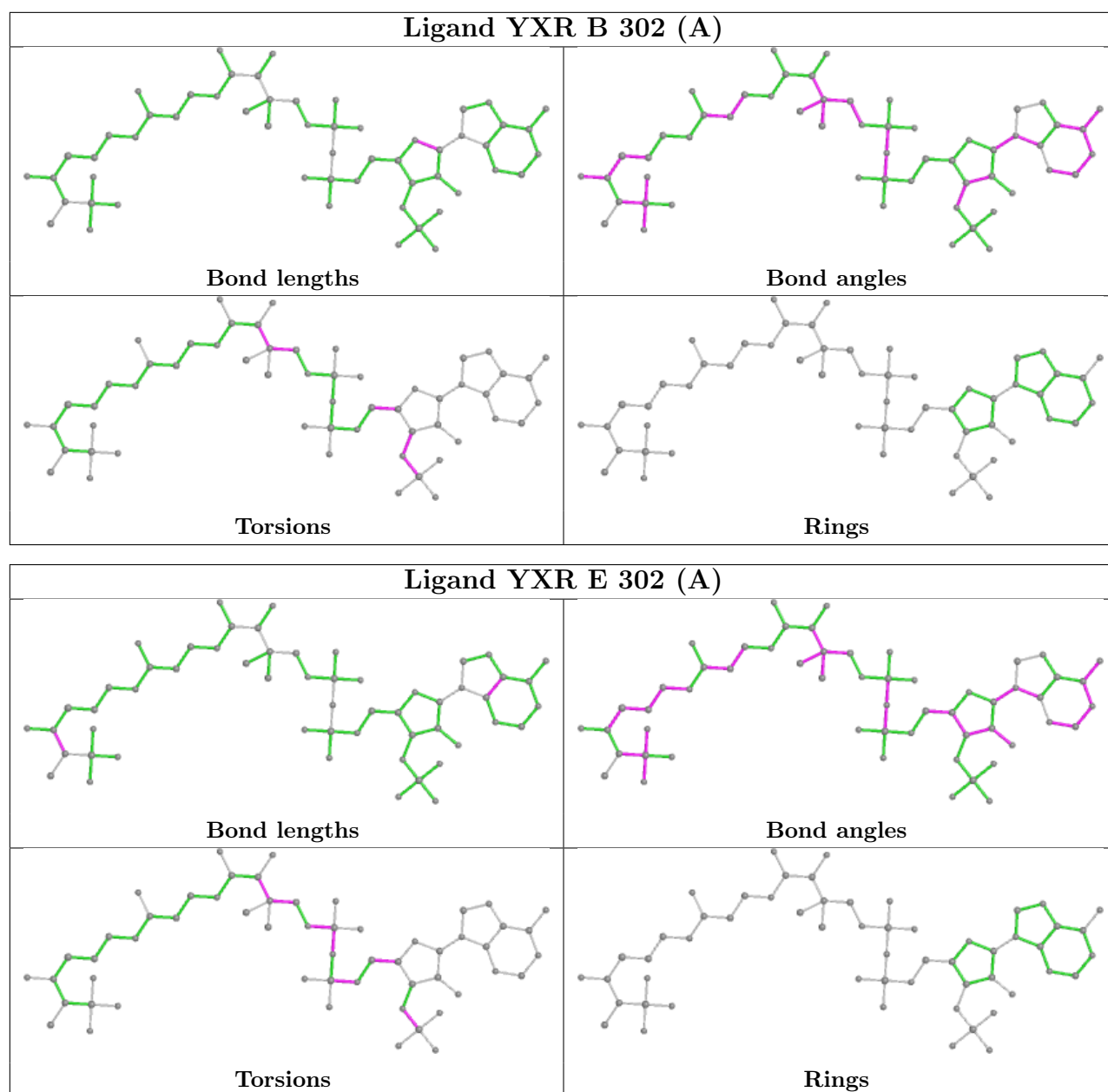












4.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

5 Fit of model and data [i](#)

5.1 Protein, DNA and RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

5.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.