



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Nov 13, 2019 – 06:52 PM EST

PDB ID : 6NSK
EMDB ID: : EMD-0499
Title : CryoEM structure of Helicobacter pylori urea channel in open state.
Authors : Cui, Y.X.; Zhou, K.; Strugatsky, D.; Wen, Y.; Sachs, G.; Munson, K.; Zhou, Z.H.
Deposited on : 2019-01-24
Resolution : 2.70 Å(reported)
Based on PDB ID : 3UX4

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB 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.

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

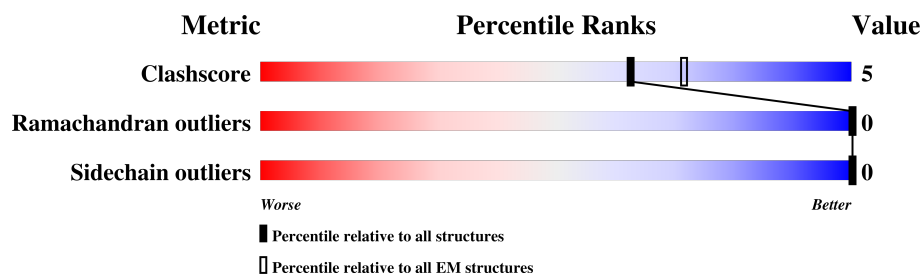
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	201	81% 10% 9%
1	B	201	82% 8% 9%
1	C	201	81% 9% 9%
1	D	201	81% 10% 9%
1	E	201	84% 6% 9%
1	F	201	83% 7% 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9096 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 Acid-activated urea channel.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	182	Total	C	N	O	S	0	0
			1449	985	222	237	5		
1	B	182	Total	C	N	O	S	0	0
			1449	985	222	237	5		
1	C	182	Total	C	N	O	S	0	0
			1449	985	222	237	5		
1	D	182	Total	C	N	O	S	0	0
			1449	985	222	237	5		
1	E	182	Total	C	N	O	S	0	0
			1449	985	222	237	5		
1	F	182	Total	C	N	O	S	0	0
			1449	985	222	237	5		

There are 36 discrepancies between the modelled and reference sequences:

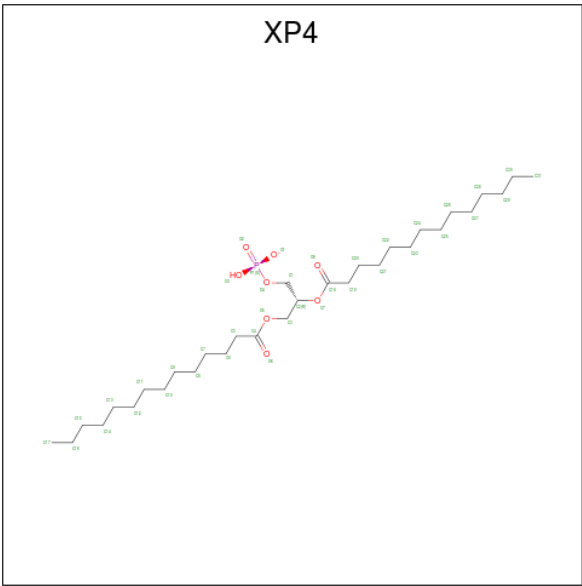
Chain	Residue	Modelled	Actual	Comment	Reference
A	55G	HIS	-	insertion	UNP P56874
A	55H	HIS	-	insertion	UNP P56874
A	55I	HIS	-	insertion	UNP P56874
A	55J	HIS	-	insertion	UNP P56874
A	55K	HIS	-	insertion	UNP P56874
A	55L	HIS	-	insertion	UNP P56874
B	55G	HIS	-	insertion	UNP P56874
B	55H	HIS	-	insertion	UNP P56874
B	55I	HIS	-	insertion	UNP P56874
B	55J	HIS	-	insertion	UNP P56874
B	55K	HIS	-	insertion	UNP P56874
B	55L	HIS	-	insertion	UNP P56874
C	55G	HIS	-	insertion	UNP P56874
C	55H	HIS	-	insertion	UNP P56874
C	55I	HIS	-	insertion	UNP P56874
C	55J	HIS	-	insertion	UNP P56874
C	55K	HIS	-	insertion	UNP P56874
C	55L	HIS	-	insertion	UNP P56874

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Chain	Residue	Modelled	Actual	Comment	Reference
D	55G	HIS	-	insertion	UNP P56874
D	55H	HIS	-	insertion	UNP P56874
D	55I	HIS	-	insertion	UNP P56874
D	55J	HIS	-	insertion	UNP P56874
D	55K	HIS	-	insertion	UNP P56874
D	55L	HIS	-	insertion	UNP P56874
E	55G	HIS	-	insertion	UNP P56874
E	55H	HIS	-	insertion	UNP P56874
E	55I	HIS	-	insertion	UNP P56874
E	55J	HIS	-	insertion	UNP P56874
E	55K	HIS	-	insertion	UNP P56874
E	55L	HIS	-	insertion	UNP P56874
F	55G	HIS	-	insertion	UNP P56874
F	55H	HIS	-	insertion	UNP P56874
F	55I	HIS	-	insertion	UNP P56874
F	55J	HIS	-	insertion	UNP P56874
F	55K	HIS	-	insertion	UNP P56874
F	55L	HIS	-	insertion	UNP P56874

- Molecule 2 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHATE (three-letter code: XP4) (formula: C₃₁H₆₀O₈P).



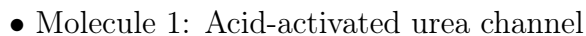
Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	C	O	0
			27	23	4	
2	A	1	Total	C	O	0
			27	23	4	

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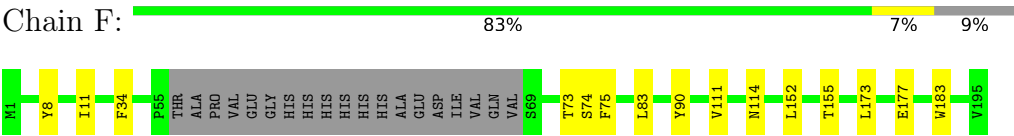
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Mol	Chain	Residues	Atoms				AltConf
2	B	1	Total	C	O	P	0
			67	54	12	1	
2	B	1	Total	C	O	P	0
			67	54	12	1	
2	B	1	Total	C	O	P	0
			67	54	12	1	
2	C	1	Total	C	O	P	0
			107	85	20	2	
2	C	1	Total	C	O	P	0
			107	85	20	2	
2	C	1	Total	C	O	P	0
			107	85	20	2	
2	C	1	Total	C	O	P	0
			107	85	20	2	
2	D	1	Total	C	O		0
			27	23	4		
2	D	1	Total	C	O		0
			27	23	4		
2	E	1	Total	C	O	P	0
			67	54	12	1	
2	E	1	Total	C	O	P	0
			67	54	12	1	
2	E	1	Total	C	O	P	0
			67	54	12	1	
2	F	1	Total	C	O	P	0
			107	85	20	2	
2	F	1	Total	C	O	P	0
			107	85	20	2	
2	F	1	Total	C	O	P	0
			107	85	20	2	
2	F	1	Total	C	O	P	0
			107	85	20	2	

- Molecule 1: Acid-activated urea channel



● Molecule 1: Acid-activated urea channel



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	279840	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 ($e^-/\text{\AA}^2$)	43	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	46730	Depositor
Image detector	GATAN K2 SUMMIT (4k 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: XP4

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 >2	RMSZ	# Z >2
1	A	0.42	0/1502	0.60	0/2065
1	B	0.41	0/1502	0.60	0/2065
1	C	0.41	0/1502	0.60	0/2065
1	D	0.42	0/1502	0.60	0/2065
1	E	0.41	0/1502	0.60	0/2065
1	F	0.41	0/1502	0.60	0/2065
All	All	0.41	0/9012	0.60	0/12390

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	1449	0	1458	15	0
1	B	1449	0	1458	16	0
1	C	1449	0	1458	17	0
1	D	1449	0	1458	16	0
1	E	1449	0	1458	12	0
1	F	1449	0	1458	13	0
2	A	27	0	37	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	67	0	97	2	0
2	C	107	0	157	5	0
2	D	27	0	37	3	0
2	E	67	0	97	2	0
2	F	107	0	157	5	0
All	All	9096	0	9330	88	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 5.

All (88) 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:F:73:THR:HG22	1:F:74:SER:N	1.86	0.90
1:C:73:THR:HG22	1:C:74:SER:N	1.86	0.88
1:C:73:THR:HG22	1:C:74:SER:H	1.38	0.88
1:F:73:THR:HG22	1:F:74:SER:H	1.38	0.86
1:D:73:THR:HG22	1:D:74:SER:N	1.91	0.85
1:B:73:THR:HG22	1:B:74:SER:N	1.93	0.84
1:E:73:THR:HG22	1:E:74:SER:N	1.93	0.84
1:D:73:THR:HG22	1:D:74:SER:H	1.45	0.79
1:D:114:ASN:HD21	1:E:183:TRP:HE1	1.29	0.77
1:A:114:ASN:HD21	1:B:183:TRP:HE1	1.29	0.76
1:C:114:ASN:HD21	1:D:183:TRP:HE1	1.33	0.75
1:E:73:THR:HG22	1:E:74:SER:H	1.52	0.74
1:F:73:THR:CG2	1:F:74:SER:H	2.02	0.73
1:A:183:TRP:HE1	1:F:114:ASN:HD21	1.34	0.73
1:B:73:THR:HG22	1:B:74:SER:H	1.52	0.73
1:E:114:ASN:HD21	1:F:183:TRP:HE1	1.35	0.73
1:A:73:THR:HG22	1:A:75:PHE:H	1.54	0.72
1:C:73:THR:CG2	1:C:74:SER:H	2.02	0.72
1:B:114:ASN:HD21	1:C:183:TRP:HE1	1.35	0.72
1:A:73:THR:HG22	1:A:74:SER:N	2.10	0.67
1:D:73:THR:CG2	1:D:74:SER:H	2.08	0.66
1:D:73:THR:CG2	1:D:74:SER:N	2.59	0.64
1:E:73:THR:CG2	1:E:74:SER:H	2.12	0.62
1:B:73:THR:CG2	1:B:74:SER:H	2.12	0.62
1:B:73:THR:CG2	1:B:74:SER:N	2.60	0.61
1:C:73:THR:CG2	1:C:74:SER:N	2.55	0.61
1:E:73:THR:CG2	1:E:74:SER:N	2.60	0.61
1:F:173:LEU:O	1:F:177:GLU:HB3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:LEU:O	1:C:177:GLU:HB3	2.04	0.57
1:A:46:VAL:HG12	2:F:202:XP4:H13	1.87	0.57
2:C:204:XP4:H13	1:D:46:VAL:HG12	1.87	0.56
1:F:73:THR:HG22	1:F:75:PHE:H	1.70	0.55
1:C:73:THR:HG22	1:C:75:PHE:H	1.70	0.55
1:A:173:LEU:O	1:A:177:GLU:HB3	2.08	0.54
1:A:118:ALA:O	1:A:122:SER:HB2	2.08	0.53
1:D:173:LEU:O	1:D:177:GLU:HB3	2.08	0.53
1:A:73:THR:CG2	1:A:74:SER:N	2.72	0.53
2:F:201:XP4:H21	2:F:201:XP4:H55	1.92	0.52
2:A:201:XP4:H58	2:B:202:XP4:H60	1.93	0.51
1:D:73:THR:HG22	1:D:75:PHE:H	1.75	0.51
1:C:177:GLU:O	1:C:181:THR:OG1	2.22	0.51
2:D:201:XP4:H58	2:E:202:XP4:H60	1.93	0.51
1:B:73:THR:HG22	1:B:75:PHE:H	1.76	0.51
2:C:203:XP4:H22	1:D:34:PHE:HB3	1.93	0.51
1:E:73:THR:HG22	1:E:75:PHE:H	1.76	0.50
1:C:34:PHE:HB3	2:C:201:XP4:H22	1.93	0.50
1:A:34:PHE:HB3	2:F:201:XP4:H22	1.93	0.50
1:F:83:LEU:HD23	1:F:111:VAL:HG13	1.94	0.50
2:C:203:XP4:H55	2:C:203:XP4:H21	1.92	0.50
1:F:34:PHE:HB3	2:F:203:XP4:H22	1.93	0.49
1:C:83:LEU:HD23	1:C:111:VAL:HG13	1.94	0.49
1:C:8:TYR:HA	1:C:11:ILE:HG22	1.94	0.48
1:F:8:TYR:HA	1:F:11:ILE:HG22	1.94	0.48
1:A:83:LEU:HD23	1:A:111:VAL:HG13	1.96	0.48
1:B:173:LEU:O	1:B:177:GLU:HB3	2.14	0.47
1:A:8:TYR:HA	1:A:11:ILE:HG22	1.97	0.47
1:E:173:LEU:O	1:E:177:GLU:HB3	2.14	0.47
1:D:86:PHE:O	1:D:90:TYR:HB2	2.15	0.47
1:E:8:TYR:HA	1:E:11:ILE:HG22	1.97	0.46
1:A:86:PHE:O	1:A:90:TYR:HB2	2.15	0.46
1:D:83:LEU:HD23	1:D:111:VAL:HG13	1.96	0.46
1:B:8:TYR:HA	1:B:11:ILE:HG22	1.97	0.46
1:B:152:LEU:O	1:B:155:THR:OG1	2.32	0.46
1:D:8:TYR:HA	1:D:11:ILE:HG22	1.97	0.45
1:B:177:GLU:O	1:B:181:THR:OG1	2.21	0.44
1:A:35:PHE:HE2	1:F:90:TYR:HB2	1.83	0.44
1:E:83:LEU:HD23	1:E:111:VAL:HG13	2.00	0.44
1:F:73:THR:CG2	1:F:74:SER:N	2.55	0.44
1:D:152:LEU:O	1:D:155:THR:OG1	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:LEU:HD23	1:B:111:VAL:HG13	2.00	0.44
1:C:152:LEU:O	1:C:155:THR:OG1	2.28	0.44
2:D:201:XP4:H51	2:D:201:XP4:H56	1.83	0.43
1:A:152:LEU:O	1:A:155:THR:OG1	2.30	0.43
1:C:90:TYR:HB2	1:D:35:PHE:HE2	1.83	0.43
1:F:152:LEU:O	1:F:155:THR:OG1	2.28	0.42
2:A:201:XP4:H51	2:A:201:XP4:H56	1.83	0.42
2:E:201:XP4:H51	2:E:201:XP4:H44	1.81	0.42
1:E:177:GLU:O	1:E:181:THR:OG1	2.21	0.41
2:B:201:XP4:H44	2:B:201:XP4:H51	1.81	0.41
2:D:202:XP4:H14	1:E:46:VAL:HG12	2.03	0.41
1:C:25:ASP:HA	1:C:26:PRO:HD3	1.88	0.41
1:D:25:ASP:HA	1:D:26:PRO:HD3	1.89	0.41
1:A:114:ASN:ND2	1:B:183:TRP:HE1	2.09	0.40
2:A:202:XP4:H14	1:B:46:VAL:HG12	2.03	0.40
2:C:202:XP4:H51	2:C:202:XP4:H56	1.94	0.40
2:F:201:XP4:H51	2:F:201:XP4:H44	1.75	0.40
1:B:110:PHE:CE1	1:C:183:TRP:CE2	3.10	0.40
1:B:53:LEU:HD13	1:C:50:TYR:HD1	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	178/201 (89%)	171 (96%)	7 (4%)	0	100	100
1	B	178/201 (89%)	171 (96%)	7 (4%)	0	100	100
1	C	178/201 (89%)	173 (97%)	5 (3%)	0	100	100
1	D	178/201 (89%)	171 (96%)	7 (4%)	0	100	100
1	E	178/201 (89%)	171 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	178/201 (89%)	173 (97%)	5 (3%)	0	100	100
All	All	1068/1206 (89%)	1030 (96%)	38 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	153/169 (90%)	153 (100%)	0	100	100
1	B	153/169 (90%)	153 (100%)	0	100	100
1	C	153/169 (90%)	153 (100%)	0	100	100
1	D	153/169 (90%)	153 (100%)	0	100	100
1	E	153/169 (90%)	153 (100%)	0	100	100
1	F	153/169 (90%)	153 (100%)	0	100	100
All	All	918/1014 (90%)	918 (100%)	0	100	100

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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	ASN
1	B	114	ASN
1	C	114	ASN
1	D	114	ASN
1	E	114	ASN
1	F	114	ASN

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

18 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	$\# Z > 2$
2	XP4	A	201	-	16,16,39	0.88	1 (6%)	16,16,44	0.67	0
2	XP4	A	202	-	9,9,39	1.19	2 (22%)	9,9,44	0.77	0
2	XP4	B	201	-	39,39,39	0.93	2 (5%)	43,44,44	0.91	2 (4%)
2	XP4	B	202	-	16,16,39	0.89	1 (6%)	16,16,44	0.66	0
2	XP4	B	203	-	9,9,39	1.17	1 (11%)	9,9,44	0.81	0
2	XP4	C	201	-	39,39,39	0.92	2 (5%)	43,44,44	0.94	2 (4%)
2	XP4	C	202	-	16,16,39	0.89	2 (12%)	16,16,44	0.67	0
2	XP4	C	203	-	39,39,39	0.93	2 (5%)	43,44,44	0.92	2 (4%)
2	XP4	C	204	-	9,9,39	1.18	2 (22%)	9,9,44	0.82	0
2	XP4	D	201	-	16,16,39	0.88	1 (6%)	16,16,44	0.67	0
2	XP4	D	202	-	9,9,39	1.18	2 (22%)	9,9,44	0.78	0
2	XP4	E	201	-	39,39,39	0.93	2 (5%)	43,44,44	0.90	2 (4%)
2	XP4	E	202	-	16,16,39	0.88	1 (6%)	16,16,44	0.66	0
2	XP4	E	203	-	9,9,39	1.17	2 (22%)	9,9,44	0.82	0
2	XP4	F	201	-	39,39,39	0.93	2 (5%)	43,44,44	0.93	2 (4%)
2	XP4	F	202	-	9,9,39	1.18	2 (22%)	9,9,44	0.81	0
2	XP4	F	203	-	39,39,39	0.92	2 (5%)	43,44,44	0.94	2 (4%)
2	XP4	F	204	-	16,16,39	0.88	1 (6%)	16,16,44	0.67	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	XP4	A	201	-	-	8/15/15/41	-
2	XP4	A	202	-	-	3/8/8/41	-
2	XP4	B	201	-	-	21/41/41/41	-
2	XP4	B	202	-	-	9/15/15/41	-
2	XP4	B	203	-	-	7/8/8/41	-
2	XP4	C	201	-	-	26/41/41/41	-
2	XP4	C	202	-	-	9/15/15/41	-
2	XP4	C	203	-	-	23/41/41/41	-
2	XP4	C	204	-	-	7/8/8/41	-
2	XP4	D	201	-	-	8/15/15/41	-
2	XP4	D	202	-	-	3/8/8/41	-
2	XP4	E	201	-	-	21/41/41/41	-
2	XP4	E	202	-	-	9/15/15/41	-
2	XP4	E	203	-	-	7/8/8/41	-
2	XP4	F	201	-	-	23/41/41/41	-
2	XP4	F	202	-	-	7/8/8/41	-
2	XP4	F	203	-	-	26/41/41/41	-
2	XP4	F	204	-	-	9/15/15/41	-

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	201	XP4	O7-C2	-2.70	1.39	1.46
2	B	201	XP4	O7-C2	-2.70	1.39	1.46
2	F	201	XP4	O7-C2	-2.66	1.39	1.46
2	C	203	XP4	O7-C2	-2.66	1.39	1.46
2	C	201	XP4	O7-C2	-2.63	1.40	1.46
2	F	203	XP4	O7-C2	-2.61	1.40	1.46
2	D	202	XP4	O5-C4	2.39	1.40	1.32
2	A	202	XP4	O5-C4	2.38	1.40	1.32
2	C	201	XP4	O5-C4	2.38	1.40	1.33
2	F	203	XP4	O5-C4	2.38	1.40	1.33
2	B	203	XP4	O5-C4	2.37	1.40	1.32
2	B	201	XP4	O5-C4	2.35	1.40	1.33
2	E	202	XP4	O7-C18	2.35	1.40	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	202	XP4	O7-C18	2.35	1.40	1.32
2	E	201	XP4	O5-C4	2.35	1.40	1.33
2	E	203	XP4	O5-C4	2.35	1.40	1.32
2	C	204	XP4	O5-C4	2.35	1.40	1.32
2	C	202	XP4	O7-C18	2.34	1.40	1.32
2	F	202	XP4	O5-C4	2.34	1.40	1.32
2	F	204	XP4	O7-C18	2.34	1.40	1.32
2	F	201	XP4	O5-C4	2.33	1.40	1.33
2	D	201	XP4	O7-C18	2.33	1.40	1.32
2	A	201	XP4	O7-C18	2.33	1.40	1.32
2	C	203	XP4	O5-C4	2.32	1.40	1.33
2	A	202	XP4	O5-C3	-2.06	1.40	1.45
2	F	202	XP4	O5-C3	-2.05	1.40	1.45
2	D	202	XP4	O5-C3	-2.03	1.40	1.45
2	C	204	XP4	O5-C3	-2.02	1.40	1.45
2	C	202	XP4	O7-C2	-2.02	1.40	1.45
2	E	203	XP4	O5-C3	-2.01	1.40	1.45

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	201	XP4	O7-C18-C19	3.72	119.64	111.51
2	F	203	XP4	O7-C18-C19	3.72	119.63	111.51
2	F	201	XP4	O7-C18-C19	3.66	119.50	111.51
2	C	203	XP4	O7-C18-C19	3.64	119.46	111.51
2	B	201	XP4	O7-C18-C19	3.53	119.22	111.51
2	E	201	XP4	O7-C18-C19	3.52	119.18	111.51
2	F	203	XP4	O5-C4-C5	2.79	120.88	111.93
2	C	201	XP4	O5-C4-C5	2.78	120.86	111.93
2	C	203	XP4	O5-C4-C5	2.74	120.73	111.93
2	F	201	XP4	O5-C4-C5	2.74	120.72	111.93
2	B	201	XP4	O5-C4-C5	2.73	120.68	111.93
2	E	201	XP4	O5-C4-C5	2.72	120.66	111.93

There are no chirality outliers.

All (226) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	201	XP4	C1-O4-P1-O1
2	F	201	XP4	C1-O4-P1-O3
2	C	203	XP4	C1-O4-P1-O1
2	C	203	XP4	C1-O4-P1-O3

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Mol	Chain	Res	Type	Atoms
2	B	201	XP4	C1-O4-P1-O1
2	B	201	XP4	C1-O4-P1-O3
2	B	201	XP4	O4-C1-C2-O7
2	E	201	XP4	C1-O4-P1-O1
2	E	201	XP4	C1-O4-P1-O3
2	E	201	XP4	O4-C1-C2-O7
2	F	203	XP4	C1-O4-P1-O1
2	F	203	XP4	C1-O4-P1-O2
2	F	203	XP4	C1-O4-P1-O3
2	C	201	XP4	C1-O4-P1-O1
2	C	201	XP4	C1-O4-P1-O2
2	C	201	XP4	C1-O4-P1-O3
2	F	201	XP4	O7-C2-C3-O5
2	C	203	XP4	O7-C2-C3-O5
2	F	201	XP4	C4-C5-C6-C7
2	C	203	XP4	C4-C5-C6-C7
2	E	202	XP4	C18-C19-C20-C21
2	B	202	XP4	C18-C19-C20-C21
2	C	202	XP4	C18-C19-C20-C21
2	D	201	XP4	C18-C19-C20-C21
2	A	201	XP4	C18-C19-C20-C21
2	C	204	XP4	C5-C4-O5-C3
2	A	202	XP4	C4-C5-C6-C7
2	E	203	XP4	C4-C5-C6-C7
2	B	201	XP4	C4-C5-C6-C7
2	F	204	XP4	C18-C19-C20-C21
2	E	201	XP4	C4-C5-C6-C7
2	B	203	XP4	C4-C5-C6-C7
2	D	202	XP4	C4-C5-C6-C7
2	F	202	XP4	C5-C4-O5-C3
2	C	204	XP4	C4-C5-C6-C7
2	F	202	XP4	C4-C5-C6-C7
2	D	201	XP4	C21-C22-C23-C24
2	A	201	XP4	C21-C22-C23-C24
2	F	201	XP4	C9-C10-C11-C12
2	C	203	XP4	C9-C10-C11-C12
2	E	202	XP4	C20-C21-C22-C23
2	B	202	XP4	C20-C21-C22-C23
2	F	201	XP4	O4-C1-C2-O7
2	C	203	XP4	O4-C1-C2-O7
2	C	201	XP4	C26-C27-C28-C29
2	F	203	XP4	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
2	F	201	XP4	C10-C11-C12-C13
2	C	203	XP4	C10-C11-C12-C13
2	E	202	XP4	C21-C22-C23-C24
2	B	202	XP4	C21-C22-C23-C24
2	F	203	XP4	C11-C12-C13-C14
2	C	201	XP4	C11-C12-C13-C14
2	F	203	XP4	C10-C11-C12-C13
2	C	201	XP4	C10-C11-C12-C13
2	F	201	XP4	C21-C22-C23-C24
2	C	203	XP4	C21-C22-C23-C24
2	F	203	XP4	C23-C24-C25-C26
2	C	201	XP4	C23-C24-C25-C26
2	D	201	XP4	C20-C21-C22-C23
2	A	201	XP4	C20-C21-C22-C23
2	E	201	XP4	C10-C11-C12-C13
2	B	201	XP4	C10-C11-C12-C13
2	C	202	XP4	C21-C22-C23-C24
2	F	204	XP4	C21-C22-C23-C24
2	F	203	XP4	C1-C2-C3-O5
2	C	201	XP4	C1-C2-C3-O5
2	F	203	XP4	C7-C8-C9-C10
2	C	201	XP4	C7-C8-C9-C10
2	C	204	XP4	C6-C7-C8-C9
2	F	202	XP4	C6-C7-C8-C9
2	F	201	XP4	C19-C18-O7-C2
2	C	203	XP4	C19-C18-O7-C2
2	B	201	XP4	C19-C18-O7-C2
2	E	201	XP4	C19-C18-O7-C2
2	F	203	XP4	C19-C18-O7-C2
2	C	201	XP4	C19-C18-O7-C2
2	C	202	XP4	C20-C21-C22-C23
2	F	204	XP4	C20-C21-C22-C23
2	F	203	XP4	C21-C22-C23-C24
2	C	201	XP4	C21-C22-C23-C24
2	C	203	XP4	C6-C7-C8-C9
2	F	201	XP4	C6-C7-C8-C9
2	C	202	XP4	C19-C20-C21-C22
2	F	201	XP4	C24-C25-C26-C27
2	C	203	XP4	C24-C25-C26-C27
2	F	204	XP4	C19-C20-C21-C22
2	F	201	XP4	C23-C24-C25-C26
2	C	203	XP4	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
2	F	203	XP4	C4-C5-C6-C7
2	C	201	XP4	C4-C5-C6-C7
2	F	203	XP4	O4-C1-C2-O7
2	C	201	XP4	O4-C1-C2-O7
2	F	203	XP4	C6-C7-C8-C9
2	C	201	XP4	C6-C7-C8-C9
2	E	202	XP4	C24-C25-C26-C27
2	B	202	XP4	C24-C25-C26-C27
2	B	201	XP4	O7-C2-C3-O5
2	E	201	XP4	O7-C2-C3-O5
2	F	203	XP4	O7-C2-C3-O5
2	C	201	XP4	O7-C2-C3-O5
2	F	203	XP4	O8-C18-O7-C2
2	E	203	XP4	C6-C7-C8-C9
2	A	202	XP4	C5-C6-C7-C8
2	B	203	XP4	C6-C7-C8-C9
2	D	202	XP4	C5-C6-C7-C8
2	F	201	XP4	O4-C1-C2-C3
2	C	203	XP4	O4-C1-C2-C3
2	F	203	XP4	O4-C1-C2-C3
2	C	201	XP4	O4-C1-C2-C3
2	F	201	XP4	C26-C27-C28-C29
2	C	203	XP4	C26-C27-C28-C29
2	C	201	XP4	C9-C10-C11-C12
2	D	201	XP4	C19-C20-C21-C22
2	A	201	XP4	C19-C20-C21-C22
2	D	201	XP4	C24-C25-C26-C27
2	F	203	XP4	C9-C10-C11-C12
2	A	201	XP4	C24-C25-C26-C27
2	B	201	XP4	C5-C6-C7-C8
2	B	201	XP4	C21-C22-C23-C24
2	E	201	XP4	C5-C6-C7-C8
2	E	201	XP4	C21-C22-C23-C24
2	F	201	XP4	C1-C2-C3-O5
2	C	203	XP4	C1-C2-C3-O5
2	B	201	XP4	C1-C2-C3-O5
2	E	201	XP4	C1-C2-C3-O5
2	C	202	XP4	C24-C25-C26-C27
2	F	204	XP4	C24-C25-C26-C27
2	C	202	XP4	O7-C18-C19-C20
2	F	204	XP4	O7-C18-C19-C20
2	F	201	XP4	O8-C18-O7-C2

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Mol	Chain	Res	Type	Atoms
2	C	203	XP4	O8-C18-O7-C2
2	C	201	XP4	O8-C18-O7-C2
2	F	201	XP4	C1-O4-P1-O2
2	C	203	XP4	C1-O4-P1-O2
2	B	201	XP4	C1-O4-P1-O2
2	E	201	XP4	C1-O4-P1-O2
2	B	201	XP4	O8-C18-O7-C2
2	D	201	XP4	O7-C18-C19-C20
2	A	201	XP4	O7-C18-C19-C20
2	C	204	XP4	O6-C4-O5-C3
2	F	202	XP4	O6-C4-O5-C3
2	B	203	XP4	C5-C4-O5-C3
2	E	201	XP4	O8-C18-O7-C2
2	E	202	XP4	O7-C18-C19-C20
2	B	202	XP4	O7-C18-C19-C20
2	B	201	XP4	C7-C8-C9-C10
2	E	203	XP4	C5-C4-O5-C3
2	E	201	XP4	C7-C8-C9-C10
2	B	201	XP4	O4-C1-C2-C3
2	E	201	XP4	O4-C1-C2-C3
2	B	201	XP4	C24-C25-C26-C27
2	E	201	XP4	C24-C25-C26-C27
2	B	201	XP4	C6-C7-C8-C9
2	E	201	XP4	C6-C7-C8-C9
2	B	201	XP4	C9-C10-C11-C12
2	E	201	XP4	C9-C10-C11-C12
2	E	202	XP4	C19-C20-C21-C22
2	B	202	XP4	C19-C20-C21-C22
2	C	201	XP4	C20-C21-C22-C23
2	F	203	XP4	C20-C21-C22-C23
2	F	203	XP4	C2-C1-O4-P1
2	C	201	XP4	C2-C1-O4-P1
2	F	201	XP4	C11-C12-C13-C14
2	C	203	XP4	C11-C12-C13-C14
2	C	203	XP4	C7-C8-C9-C10
2	F	201	XP4	C7-C8-C9-C10
2	B	202	XP4	C23-C24-C25-C26
2	E	202	XP4	C23-C24-C25-C26
2	A	202	XP4	C7-C8-C9-C10
2	D	202	XP4	C7-C8-C9-C10
2	F	203	XP4	O5-C4-C5-C6
2	C	201	XP4	O5-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
2	C	203	XP4	O5-C4-C5-C6
2	F	201	XP4	O5-C4-C5-C6
2	B	201	XP4	C23-C24-C25-C26
2	E	201	XP4	C23-C24-C25-C26
2	C	202	XP4	C26-C27-C28-C29
2	F	204	XP4	C26-C27-C28-C29
2	C	201	XP4	C12-C13-C14-C15
2	F	203	XP4	C12-C13-C14-C15
2	B	201	XP4	O5-C4-C5-C6
2	E	201	XP4	O5-C4-C5-C6
2	C	202	XP4	C23-C24-C25-C26
2	F	201	XP4	C2-C1-O4-P1
2	C	203	XP4	C2-C1-O4-P1
2	B	201	XP4	C2-C1-O4-P1
2	E	201	XP4	C2-C1-O4-P1
2	F	204	XP4	C23-C24-C25-C26
2	F	201	XP4	C20-C21-C22-C23
2	C	201	XP4	C19-C20-C21-C22
2	C	203	XP4	C20-C21-C22-C23
2	F	201	XP4	C5-C6-C7-C8
2	C	203	XP4	C5-C6-C7-C8
2	C	201	XP4	C5-C6-C7-C8
2	F	203	XP4	C5-C6-C7-C8
2	F	203	XP4	C19-C20-C21-C22
2	F	204	XP4	O8-C18-C19-C20
2	B	203	XP4	O6-C4-O5-C3
2	C	202	XP4	O8-C18-C19-C20
2	E	203	XP4	O6-C4-O5-C3
2	D	201	XP4	O8-C18-C19-C20
2	A	201	XP4	O8-C18-C19-C20
2	C	201	XP4	C24-C25-C26-C27
2	F	203	XP4	C24-C25-C26-C27
2	D	201	XP4	C26-C27-C28-C29
2	A	201	XP4	C26-C27-C28-C29
2	B	201	XP4	C22-C23-C24-C25
2	E	201	XP4	C22-C23-C24-C25
2	C	201	XP4	C28-C29-C30-C31
2	E	202	XP4	O8-C18-C19-C20
2	B	202	XP4	O8-C18-C19-C20
2	F	203	XP4	C28-C29-C30-C31
2	B	203	XP4	O5-C4-C5-C6
2	E	203	XP4	O5-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
2	B	202	XP4	C26-C27-C28-C29
2	E	202	XP4	C26-C27-C28-C29
2	B	203	XP4	O6-C4-C5-C6
2	E	203	XP4	O6-C4-C5-C6
2	C	204	XP4	C5-C6-C7-C8
2	F	202	XP4	C5-C6-C7-C8
2	C	204	XP4	O5-C4-C5-C6
2	F	202	XP4	O5-C4-C5-C6
2	F	202	XP4	O6-C4-C5-C6
2	E	203	XP4	C5-C6-C7-C8
2	B	203	XP4	C5-C6-C7-C8
2	C	204	XP4	O6-C4-C5-C6

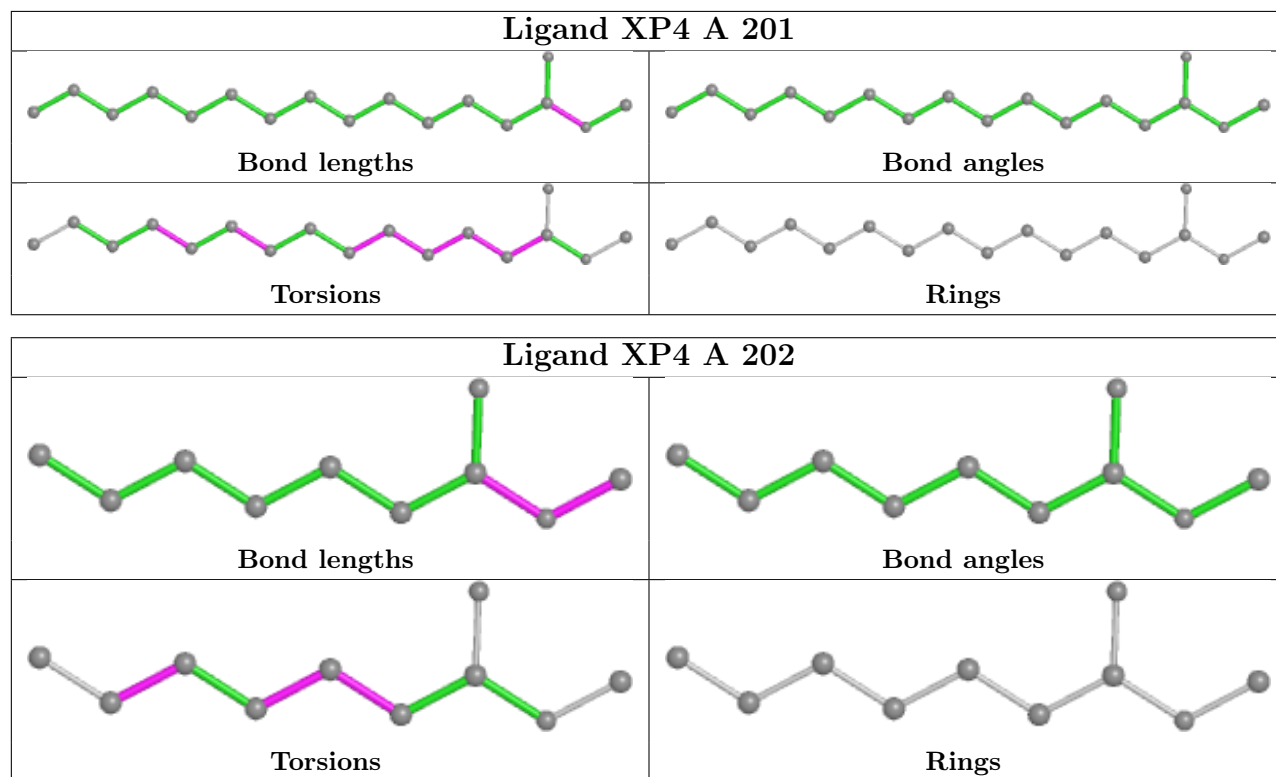
There are no ring outliers.

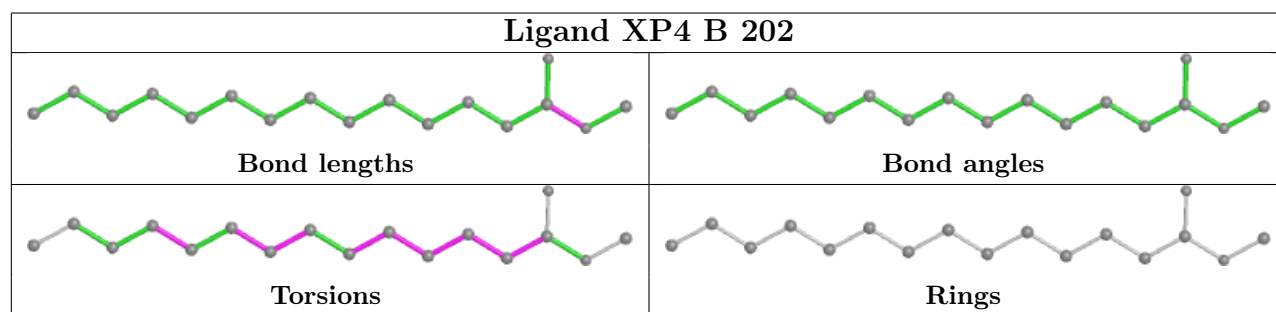
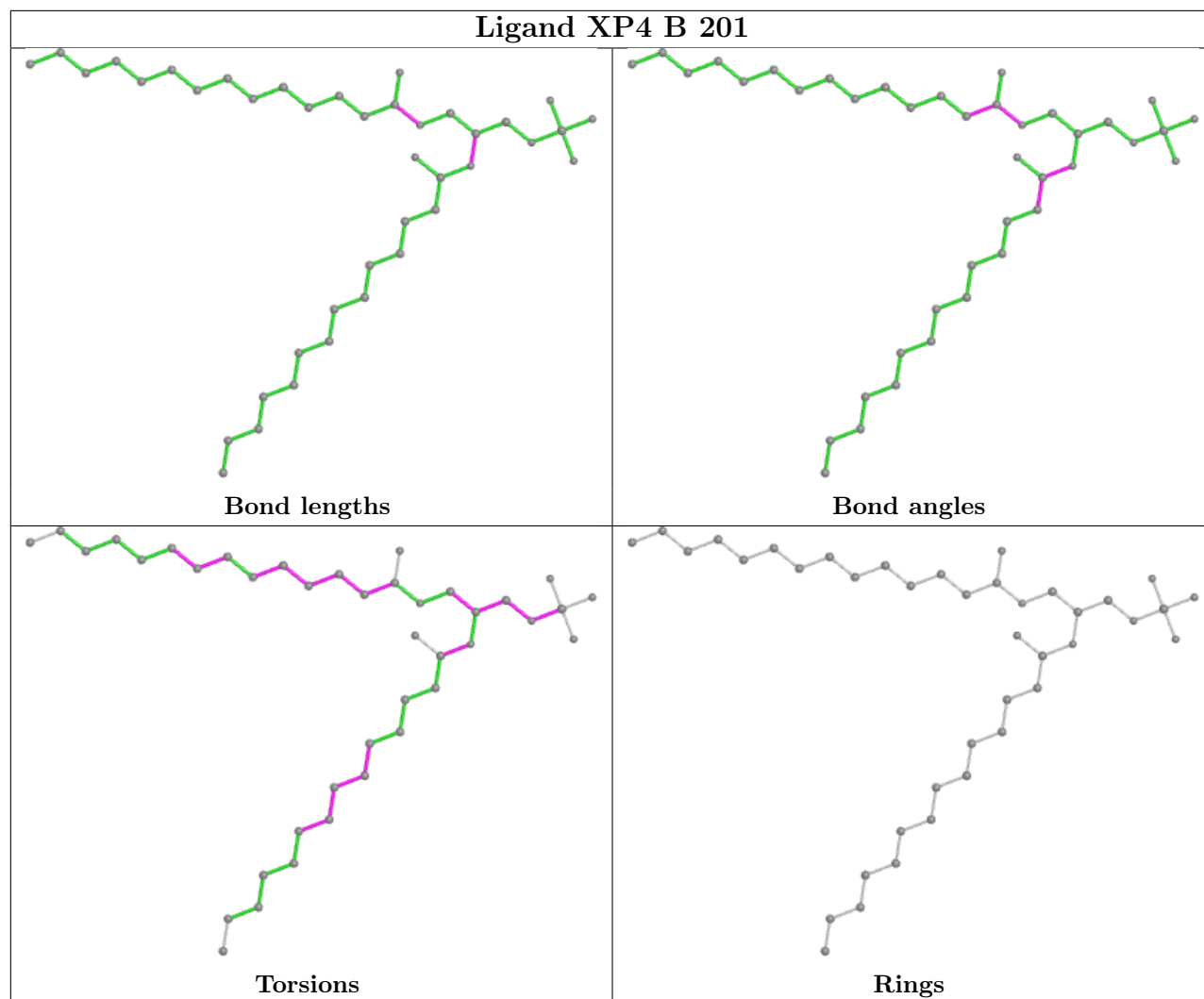
15 monomers are involved in 18 short contacts:

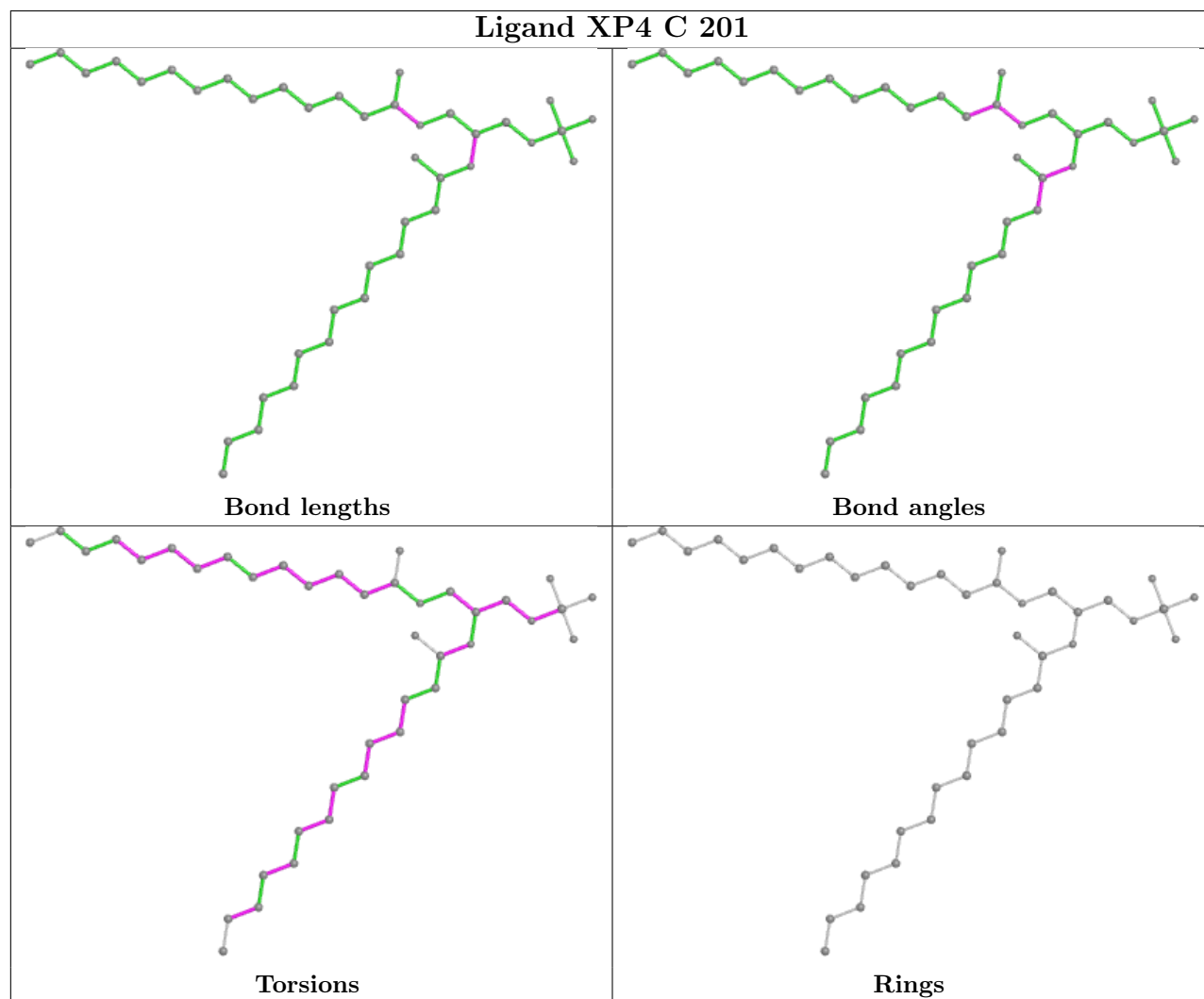
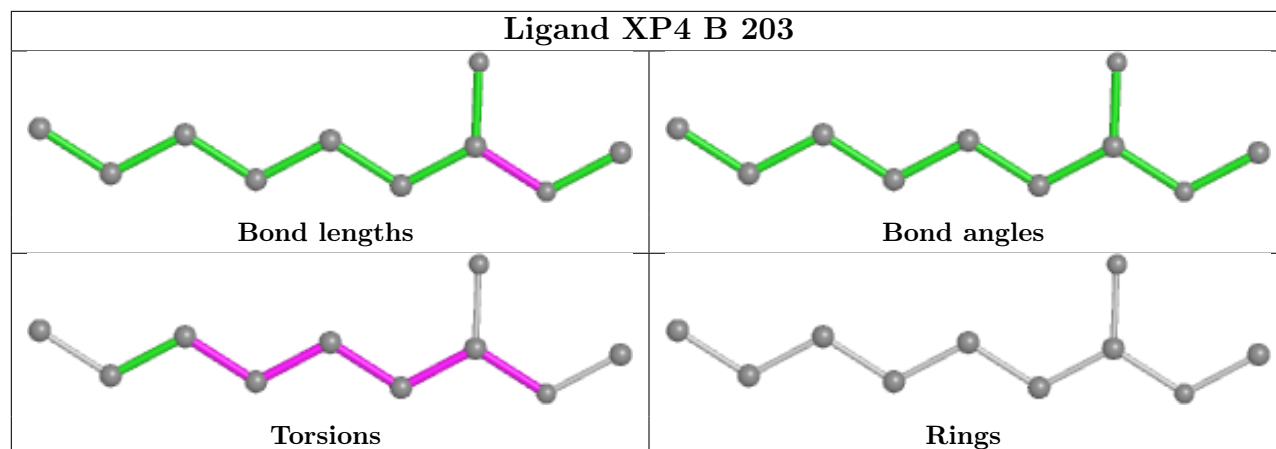
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	XP4	2	0
2	A	202	XP4	1	0
2	B	201	XP4	1	0
2	B	202	XP4	1	0
2	C	201	XP4	1	0
2	C	202	XP4	1	0
2	C	203	XP4	2	0
2	C	204	XP4	1	0
2	D	201	XP4	2	0
2	D	202	XP4	1	0
2	E	201	XP4	1	0
2	E	202	XP4	1	0
2	F	201	XP4	3	0
2	F	202	XP4	1	0
2	F	203	XP4	1	0

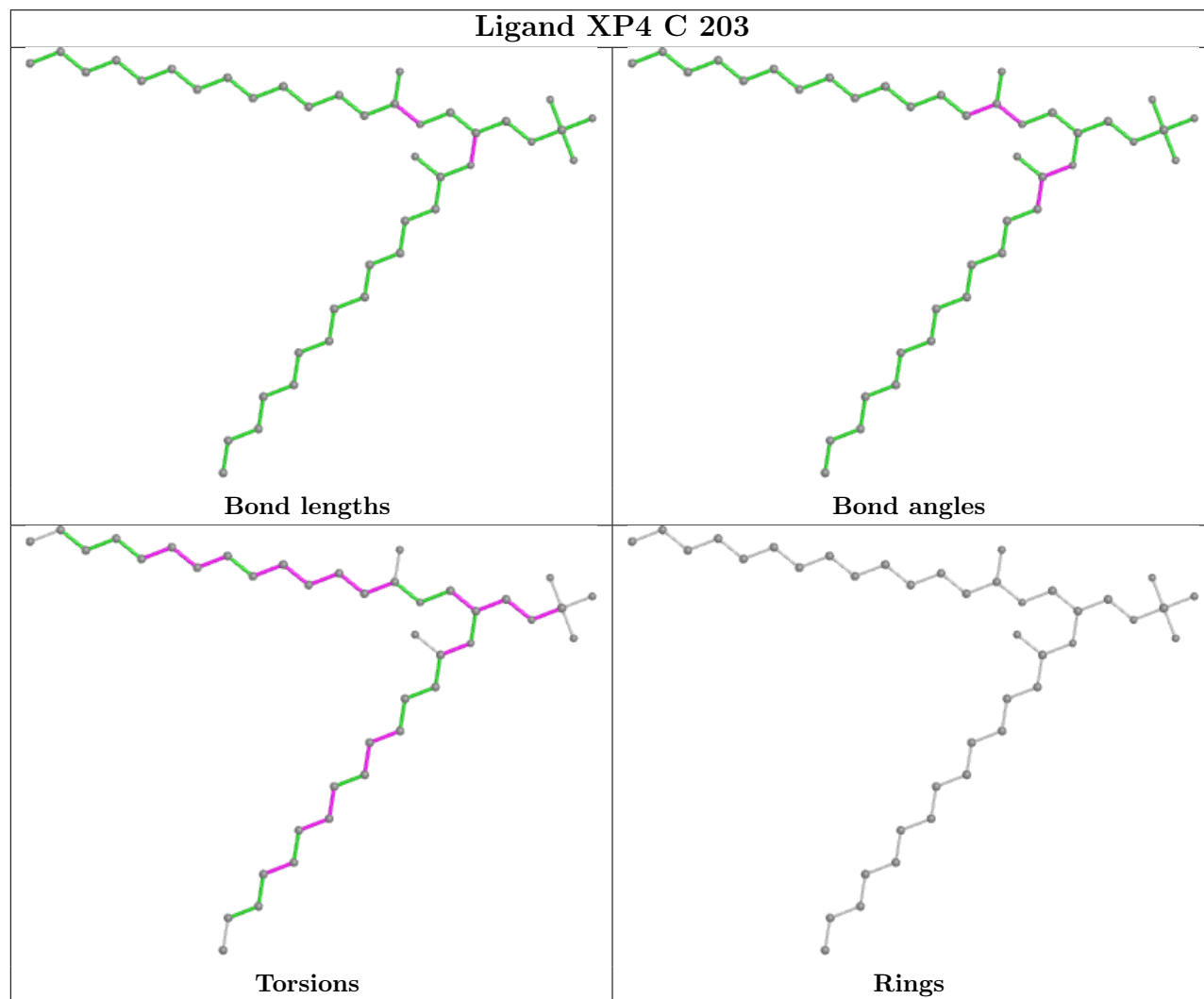
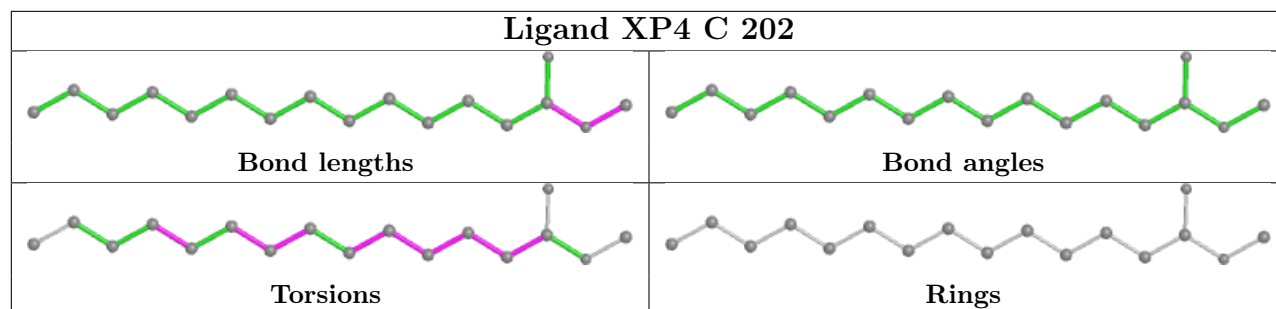
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

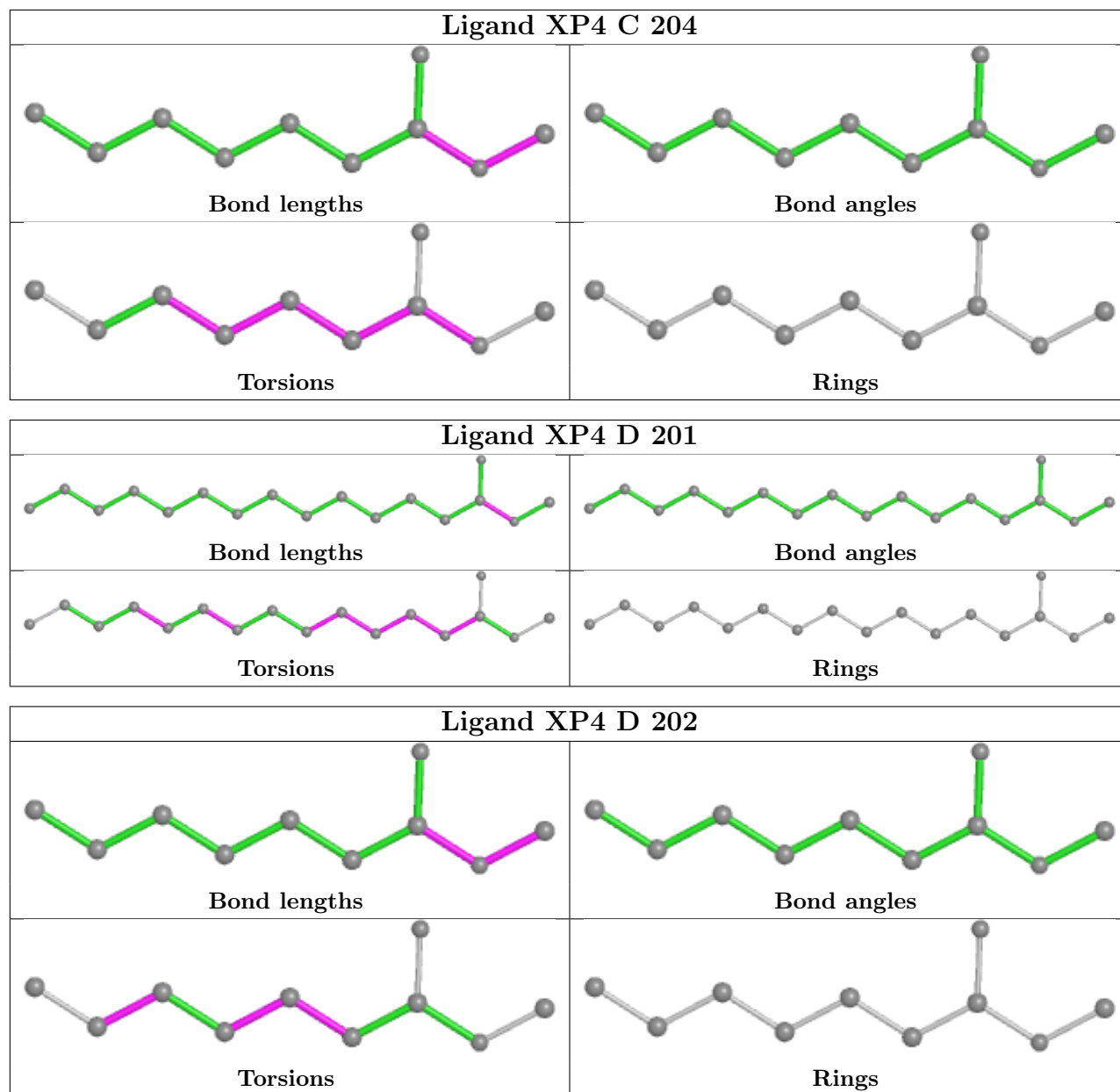
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

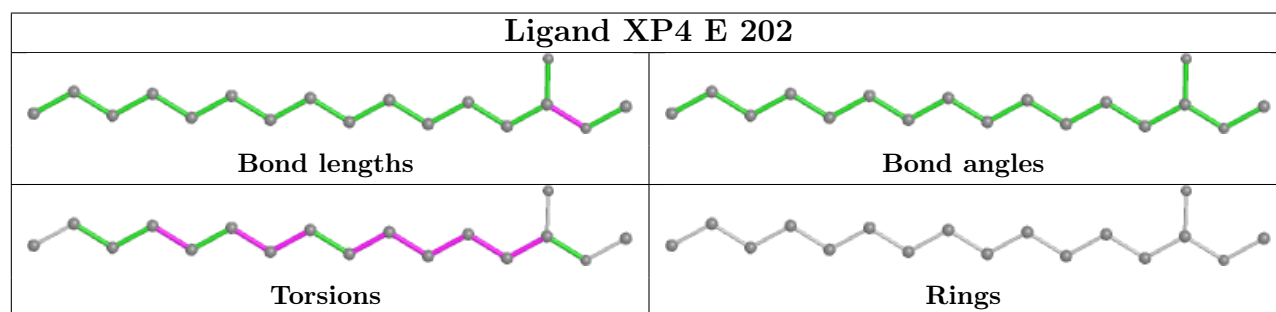
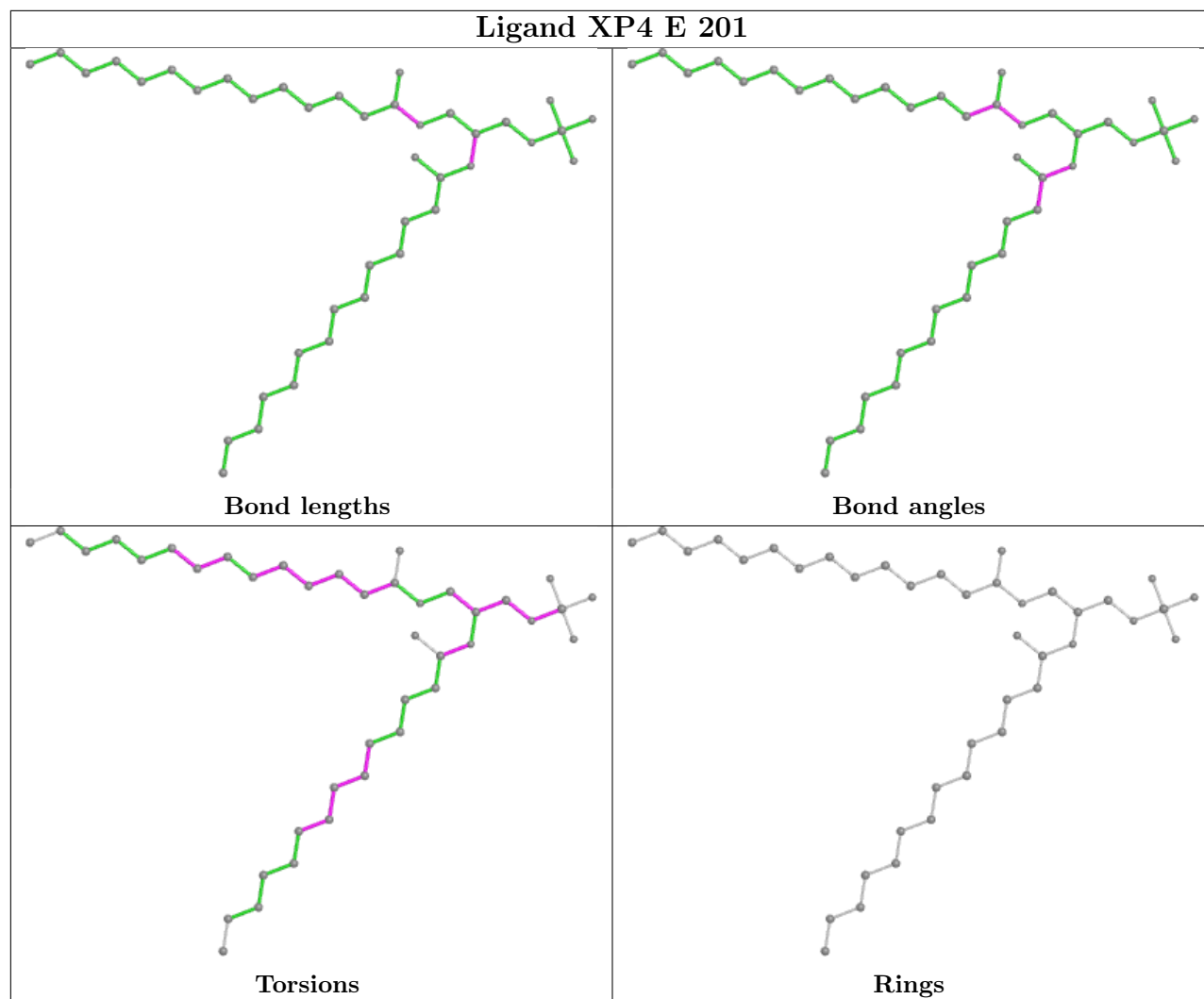


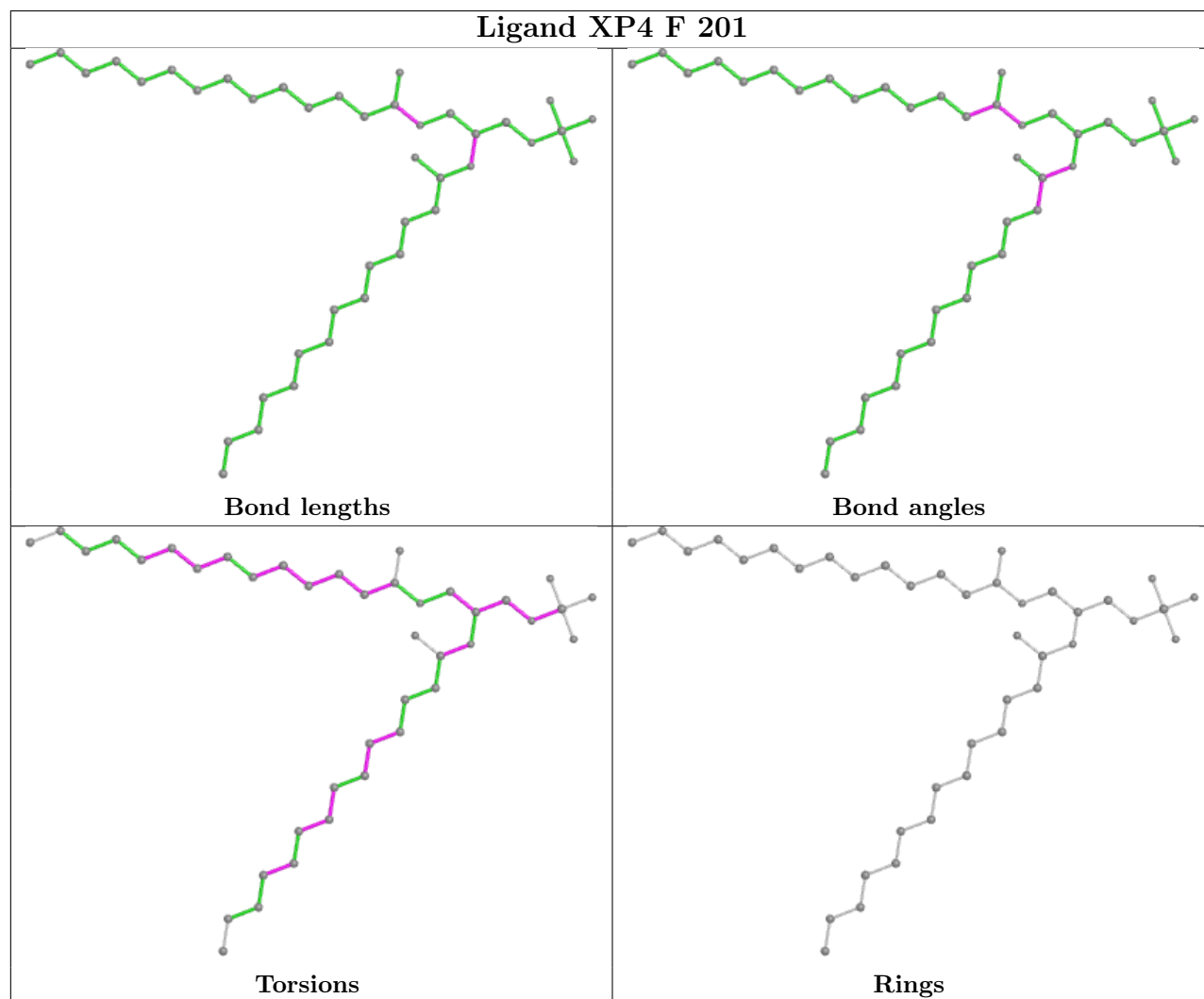
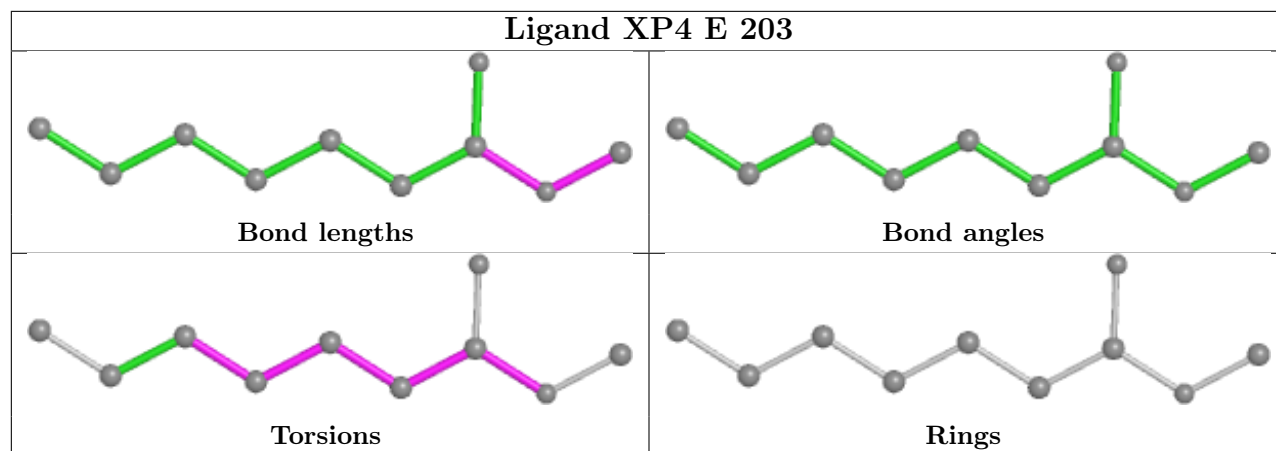


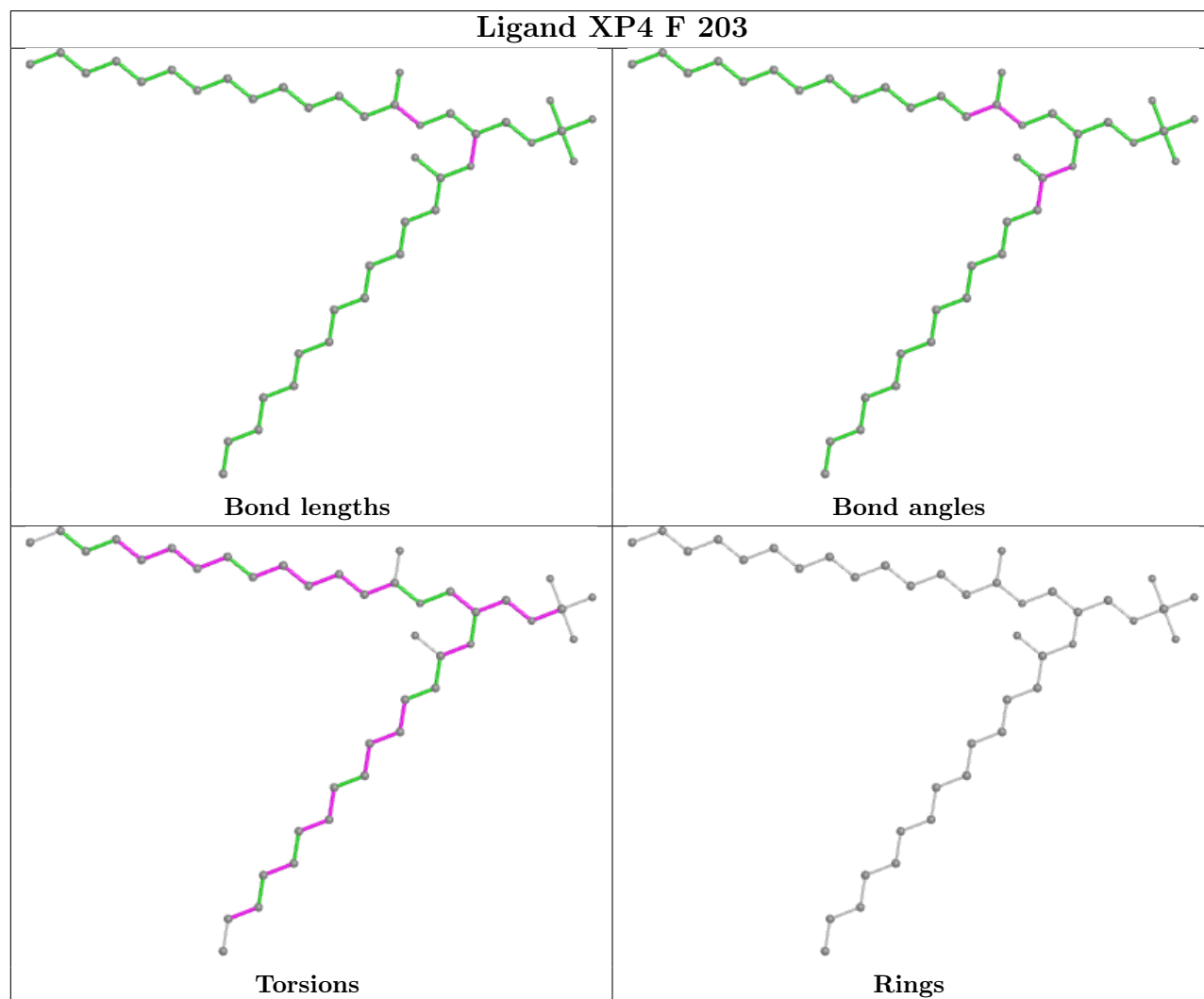
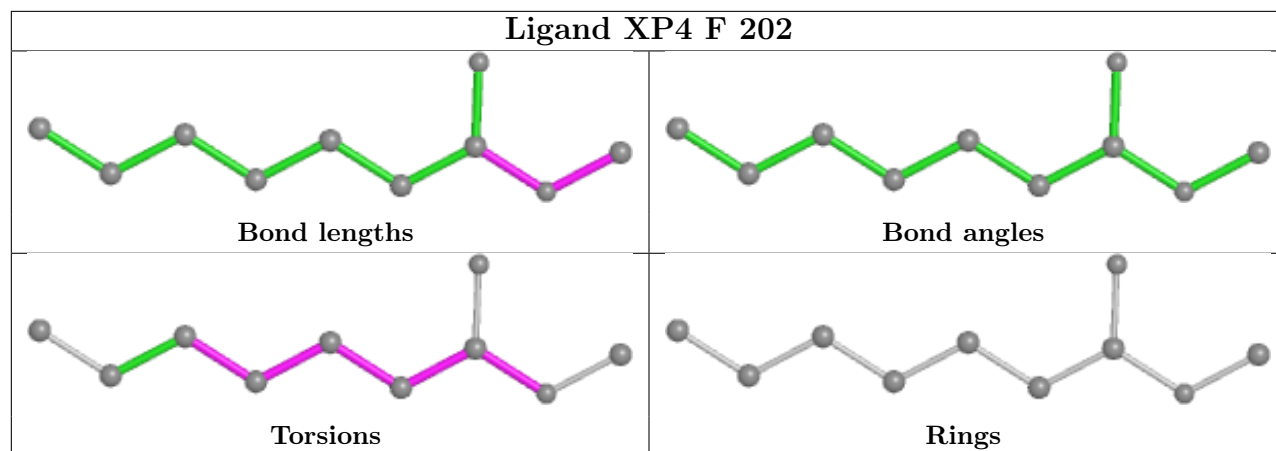


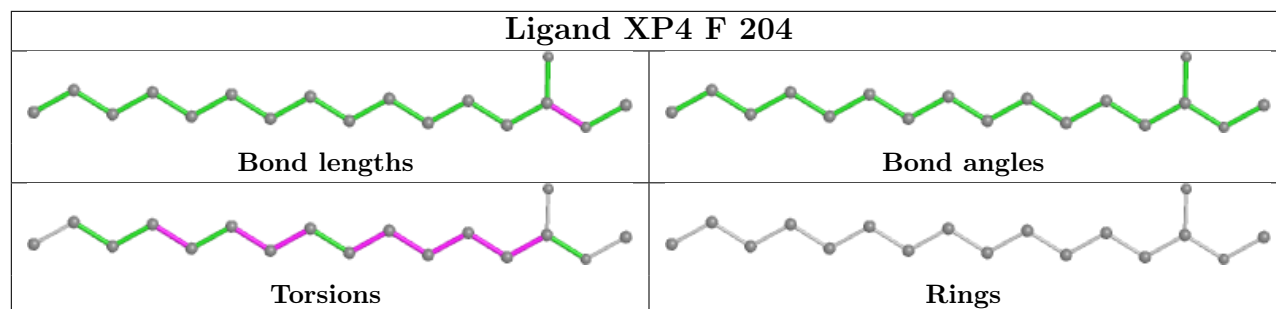












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.