



Full wwPDB EM Validation Report ⓘ

Apr 16, 2026 – 10:08 PM JST

PDB ID : 9U9H / pdb_00009u9h
EMDB ID : EMD-63964
Title : Surface Tubular Element of Vaccinia Virus
Authors : Yu, F.; Jin, G.; Liu, Y.; Sun, Z.; Lou, Z.
Deposited on : 2025-03-28
Resolution : 3.23 Å(reported)

This is a Full wwPDB EM Validation 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 : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

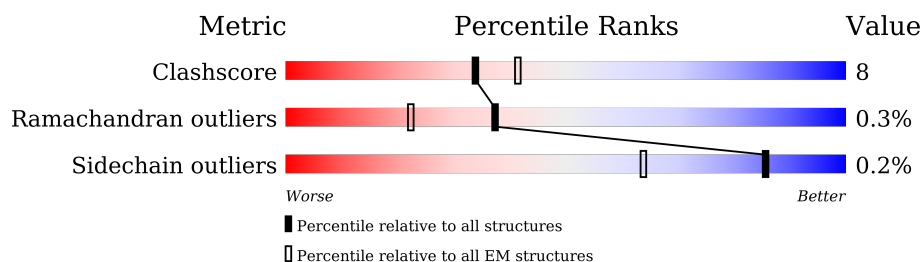
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.23 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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	90	
1	D	90	
1	G	90	
1	J	90	
2	B	169	
2	E	169	
2	H	169	
2	K	169	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5586 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.

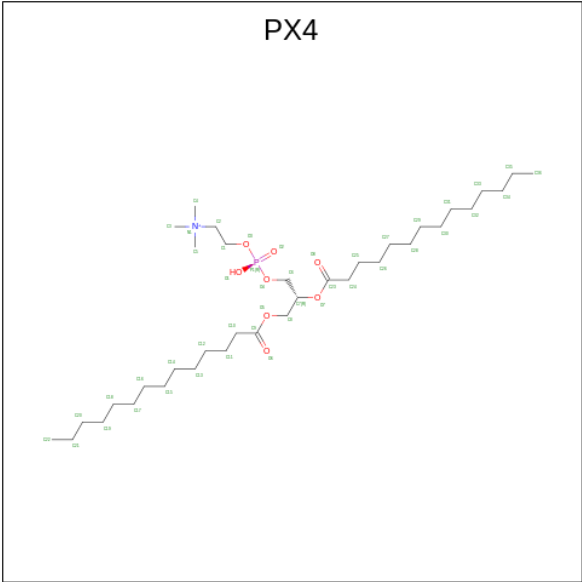
- Molecule 1 is a protein called Virion membrane protein OPG140.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	61	Total	C	N	O	S	0	0
			471	321	69	77	4		
1	D	61	Total	C	N	O	S	0	0
			471	321	69	77	4		
1	G	61	Total	C	N	O	S	0	0
			471	321	69	77	4		
1	J	61	Total	C	N	O	S	0	0
			471	321	69	77	4		

- Molecule 2 is a protein called Mature 21 kDa protein OPG144.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	105	Total	C	N	O	S	0	0
			822	557	122	136	7		
2	E	105	Total	C	N	O	S	0	0
			822	557	122	136	7		
2	H	105	Total	C	N	O	S	0	0
			822	557	122	136	7		
2	K	105	Total	C	N	O	S	0	0
			822	557	122	136	7		

- Molecule 3 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PX4) (formula: $C_{36}H_{73}NO_8P$) (labeled as "Ligand of Interest" by depositor).

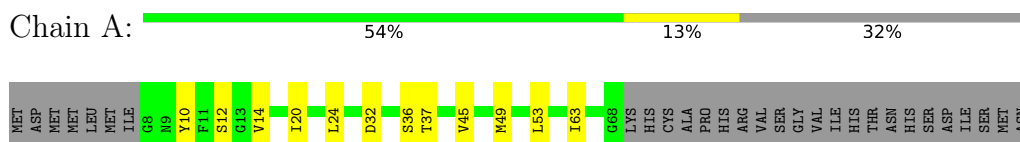


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			46	36	1	8	1	
3	A	1	Total	C	N	O	P	0
			46	36	1	8	1	
3	B	1	Total	C	N	O	P	0
			46	36	1	8	1	
3	D	1	Total	C	N	O	P	0
			46	36	1	8	1	
3	E	1	Total	C	N	O	P	0
			46	36	1	8	1	
3	G	1	Total	C	N	O	P	0
			46	36	1	8	1	
3	G	1	Total	C	N	O	P	0
			46	36	1	8	1	
3	J	1	Total	C	N	O	P	0
			46	36	1	8	1	
3	K	1	Total	C	N	O	P	0
			46	36	1	8	1	

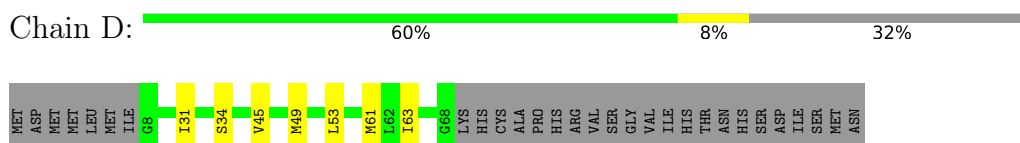
3 Residue-property plots [i](#)

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.

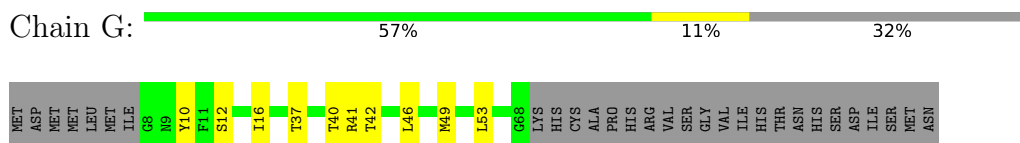
- Molecule 1: Virion membrane protein OPG140



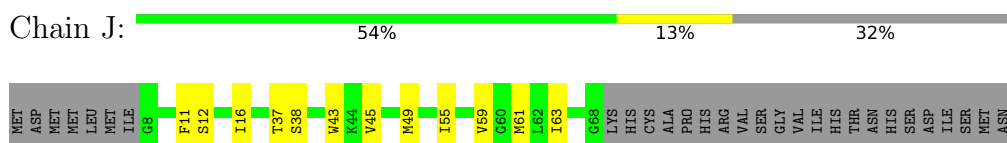
- Molecule 1: Virion membrane protein OPG140



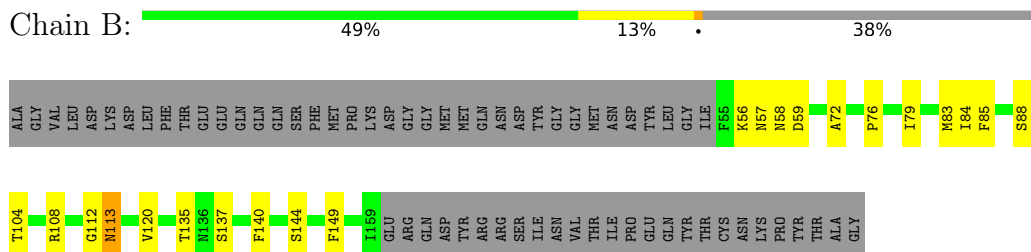
- Molecule 1: Virion membrane protein OPG140



- Molecule 1: Virion membrane protein OPG140



- Molecule 2: Mature 21 kDa protein OPG144



- Molecule 2: Mature 21 kDa protein OPG144

4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-50.00°, rise=26.58 Å, axial sym=C1	Depositor
Number of segments used	477012	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 BASE (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: PX4

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	0.16	0/482	0.36	0/653
1	D	0.16	0/482	0.31	0/653
1	G	0.15	0/482	0.31	0/653
1	J	0.16	0/482	0.31	0/653
2	B	0.19	0/838	0.38	0/1142
2	E	0.17	0/838	0.31	0/1142
2	H	0.15	0/838	0.27	0/1142
2	K	0.14	0/838	0.28	0/1142
All	All	0.16	0/5280	0.32	0/7180

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	471	0	502	10	0
1	D	471	0	502	6	0
1	G	471	0	502	6	0
1	J	471	0	502	9	0
2	B	822	0	883	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	822	0	883	16	0
2	H	822	0	883	13	0
2	K	822	0	883	15	0
3	A	92	0	144	9	0
3	B	46	0	72	0	0
3	D	46	0	72	1	0
3	E	46	0	72	1	0
3	G	92	0	144	7	0
3	J	46	0	72	2	0
3	K	46	0	72	4	0
All	All	5586	0	6188	96	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.

All (96) 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:K:113:ASN:HD22	3:K:201:PX4:H8	1.31	0.93
2:E:73:LEU:O	2:E:108:ARG:NH2	2.26	0.69
2:K:66:LEU:O	2:K:70:VAL:HG23	1.96	0.66
2:K:113:ASN:ND2	3:K:201:PX4:H8	2.10	0.66
3:A:102:PX4:H9	3:G:102:PX4:H1	1.78	0.65
2:B:104:THR:HA	2:B:108:ARG:HB2	1.80	0.64
1:A:63:ILE:HG21	2:B:135:THR:HG21	1.80	0.62
1:J:63:ILE:HG21	2:K:135:THR:HG21	1.82	0.62
1:A:14:VAL:HG23	1:J:61:MET:HE2	1.82	0.61
3:G:101:PX4:H27	2:H:120:VAL:HG22	1.83	0.61
2:K:67:ILE:O	2:K:71:LEU:HG	2.03	0.59
1:A:37:THR:HG22	3:A:101:PX4:H11	1.84	0.58
1:G:49:MET:O	1:G:53:LEU:HD12	2.03	0.57
3:A:102:PX4:H42	3:G:102:PX4:H43	1.86	0.57
3:K:201:PX4:H63	3:K:201:PX4:H29	1.86	0.57
2:H:79:ILE:O	2:H:83:MET:HG3	2.05	0.57
2:E:57:ASN:OD1	2:E:58:ASN:N	2.38	0.56
2:E:83:MET:HA	2:E:86:ILE:HG22	1.87	0.56
3:A:102:PX4:H20	1:J:43:TRP:HH2	1.69	0.56
2:H:66:LEU:O	2:H:70:VAL:HG23	2.06	0.56
2:H:73:LEU:O	2:H:108:ARG:NH2	2.39	0.55
2:B:140:PHE:O	2:B:144:SER:OG	2.22	0.55
2:K:146:ILE:O	2:K:150:ILE:HG12	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:108:ARG:HG3	2:E:108:ARG:HH11	1.72	0.54
1:D:31:ILE:O	1:D:34:SER:OG	2.24	0.54
1:A:45:VAL:O	1:A:49:MET:HG2	2.08	0.54
1:G:10:TYR:O	1:G:12:SER:N	2.42	0.53
1:G:12:SER:O	1:G:16:ILE:HG12	2.08	0.53
2:H:136:ASN:OD1	2:H:136:ASN:N	2.42	0.53
2:B:137:SER:O	2:B:137:SER:OG	2.26	0.52
1:A:20:ILE:O	1:A:24:LEU:HG	2.10	0.51
1:D:61:MET:HA	1:D:61:MET:HE3	1.93	0.51
2:H:140:PHE:O	2:H:144:SER:OG	2.24	0.51
2:E:85:PHE:HB2	2:E:149:PHE:HZ	1.75	0.51
2:K:137:SER:HB2	2:K:140:PHE:HB3	1.93	0.51
3:A:102:PX4:H24	3:A:102:PX4:H54	1.93	0.49
2:E:104:THR:HA	2:E:108:ARG:HB2	1.93	0.49
2:B:79:ILE:O	2:B:83:MET:HG3	2.13	0.49
1:G:42:THR:O	1:G:46:LEU:HD12	2.13	0.49
2:B:93:LEU:HA	2:B:96:LEU:HD12	1.95	0.49
2:E:108:ARG:HG3	2:E:108:ARG:NH1	2.28	0.49
2:K:128:ILE:HD13	2:K:144:SER:HB2	1.95	0.48
1:A:36:SER:HB3	1:J:38:SER:HB2	1.95	0.48
1:G:40:THR:OG1	1:G:41:ARG:N	2.46	0.48
1:D:49:MET:O	1:D:53:LEU:HD12	2.13	0.48
2:K:85:PHE:HB2	2:K:149:PHE:HZ	1.77	0.48
2:B:57:ASN:OD1	2:B:59:ASP:N	2.32	0.48
1:J:45:VAL:O	1:J:49:MET:HG2	2.13	0.48
2:E:137:SER:O	2:E:137:SER:OG	2.25	0.47
2:E:137:SER:OG	2:E:140:PHE:HB3	2.13	0.47
2:B:56:LYS:HA	2:B:56:LYS:HD2	1.64	0.47
2:E:93:LEU:HA	2:E:96:LEU:HD12	1.97	0.47
2:K:93:LEU:HA	2:K:96:LEU:HD12	1.96	0.47
2:H:104:THR:HA	2:H:108:ARG:HG3	1.98	0.46
3:A:102:PX4:H2	3:G:102:PX4:H1	1.98	0.46
1:D:34:SER:HB3	3:E:201:PX4:H46	1.97	0.46
1:D:45:VAL:HG22	3:D:101:PX4:H49	1.97	0.46
1:J:37:THR:HG22	3:J:101:PX4:H11	1.98	0.46
2:K:113:ASN:HB3	3:K:201:PX4:H8	1.98	0.46
2:H:69:PHE:HD1	2:H:96:LEU:HD23	1.81	0.45
2:E:123:VAL:O	2:E:127:ILE:HG13	2.16	0.45
2:B:137:SER:OG	2:B:140:PHE:HB3	2.16	0.45
2:K:84:ILE:O	2:K:88:SER:OG	2.34	0.45
2:E:158:ASN:O	2:E:158:ASN:ND2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:ILE:HG21	2:E:135:THR:HG21	1.99	0.44
2:H:157:MET:HE3	2:H:157:MET:HB3	1.81	0.44
2:B:72:ALA:HB2	2:B:83:MET:HB2	1.99	0.44
2:B:84:ILE:O	2:B:88:SER:OG	2.36	0.44
1:J:12:SER:O	1:J:16:ILE:HG12	2.17	0.44
3:A:101:PX4:H49	3:A:101:PX4:H54	1.84	0.44
1:J:55:ILE:O	1:J:59:VAL:HG23	2.18	0.44
3:G:102:PX4:H34	3:G:102:PX4:H28	1.88	0.43
1:A:32:ASP:HB2	1:J:43:TRP:HB2	1.99	0.43
1:G:49:MET:HE3	1:G:49:MET:HB3	1.83	0.43
2:B:112:GLY:C	2:B:113:ASN:OD1	2.61	0.43
3:G:102:PX4:H13	3:G:102:PX4:H14	2.01	0.43
2:H:56:LYS:HB3	2:H:61:ARG:HG2	1.99	0.43
3:J:101:PX4:H33	2:K:120:VAL:HG23	2.01	0.43
2:B:76:PRO:HD2	2:B:79:ILE:HD13	2.00	0.42
2:B:85:PHE:HB2	2:B:149:PHE:HZ	1.84	0.42
3:G:102:PX4:H18	3:G:102:PX4:H19	1.86	0.42
2:B:58:ASN:O	2:B:58:ASN:OD1	2.37	0.42
2:K:71:LEU:O	2:K:75:SER:OG	2.34	0.42
2:E:139:ILE:HD13	2:E:139:ILE:HA	1.94	0.42
2:H:85:PHE:HB2	2:H:149:PHE:HZ	1.84	0.42
1:A:49:MET:O	1:A:53:LEU:HD12	2.19	0.42
2:E:66:LEU:O	2:E:70:VAL:HG23	2.20	0.42
1:A:10:TYR:C	1:A:12:SER:H	2.29	0.41
2:E:93:LEU:HD22	2:E:145:TYR:CD1	2.56	0.41
1:A:49:MET:HE3	1:A:49:MET:HB3	1.92	0.41
2:B:108:ARG:HA	2:B:108:ARG:HD2	1.76	0.41
2:H:106:MET:HE2	2:H:106:MET:HB3	1.85	0.41
2:H:77:PRO:O	2:H:81:ILE:HG13	2.20	0.40
3:A:101:PX4:H34	2:B:120:VAL:HG23	2.04	0.40
3:A:101:PX4:H13	3:A:101:PX4:H1	1.89	0.40
2:K:139:ILE:H	2:K:139:ILE:HD12	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	59/90 (66%)	57 (97%)	2 (3%)	0	100	100
1	D	59/90 (66%)	59 (100%)	0	0	100	100
1	G	59/90 (66%)	58 (98%)	1 (2%)	0	100	100
1	J	59/90 (66%)	58 (98%)	0	1 (2%)	7	32
2	B	103/169 (61%)	96 (93%)	6 (6%)	1 (1%)	12	42
2	E	103/169 (61%)	97 (94%)	6 (6%)	0	100	100
2	H	103/169 (61%)	95 (92%)	8 (8%)	0	100	100
2	K	103/169 (61%)	94 (91%)	9 (9%)	0	100	100
All	All	648/1036 (62%)	614 (95%)	32 (5%)	2 (0%)	37	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	113	ASN
1	J	11	PHE

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	52/79 (66%)	52 (100%)	0	100	100
1	D	52/79 (66%)	52 (100%)	0	100	100
1	G	52/79 (66%)	51 (98%)	1 (2%)	50	70
1	J	52/79 (66%)	52 (100%)	0	100	100
2	B	95/150 (63%)	95 (100%)	0	100	100
2	E	95/150 (63%)	95 (100%)	0	100	100
2	H	95/150 (63%)	95 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	K	95/150 (63%)	95 (100%)	0	100	100
All	All	588/916 (64%)	587 (100%)	1 (0%)	85	88

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	37	THR

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

Mol	Chain	Res	Type
2	B	136	ASN
2	E	105	GLN
2	H	158	ASN
2	K	105	GLN
2	K	111	ASN
2	K	113	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 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	PX4	G	101	-	45,45,45	0.49	0	51,53,53	0.49	0
3	PX4	B	201	-	45,45,45	0.49	0	51,53,53	0.49	0
3	PX4	K	201	-	45,45,45	0.30	0	51,53,53	0.35	0
3	PX4	A	102	-	45,45,45	0.48	0	51,53,53	0.49	0
3	PX4	D	101	-	45,45,45	0.30	0	51,53,53	0.36	0
3	PX4	A	101	-	45,45,45	0.49	0	51,53,53	0.48	0
3	PX4	J	101	-	45,45,45	0.49	0	51,53,53	0.48	0
3	PX4	G	102	-	45,45,45	0.49	0	51,53,53	0.49	0
3	PX4	E	201	-	45,45,45	0.30	0	51,53,53	0.32	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
3	PX4	G	101	-	-	21/49/49/49	-
3	PX4	B	201	-	-	23/49/49/49	-
3	PX4	K	201	-	-	24/49/49/49	-
3	PX4	A	102	-	-	21/49/49/49	-
3	PX4	D	101	-	-	18/49/49/49	-
3	PX4	A	101	-	-	22/49/49/49	-
3	PX4	J	101	-	-	20/49/49/49	-
3	PX4	G	102	-	-	17/49/49/49	-
3	PX4	E	201	-	-	28/49/49/49	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (194) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	101	PX4	C1-O3-P1-O1
3	A	101	PX4	C6-O4-P1-O1
3	A	101	PX4	O3-C1-C2-N1

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Mol	Chain	Res	Type	Atoms
3	A	101	PX4	C24-C23-O7-C7
3	A	102	PX4	C1-O3-P1-O2
3	B	201	PX4	C6-O4-P1-O2
3	D	101	PX4	C1-O3-P1-O1
3	D	101	PX4	C6-O4-P1-O2
3	D	101	PX4	C24-C23-O7-C7
3	E	201	PX4	C1-O3-P1-O2
3	E	201	PX4	C6-O4-P1-O1
3	E	201	PX4	C6-O4-P1-O2
3	E	201	PX4	C6-O4-P1-O3
3	E	201	PX4	O3-C1-C2-N1
3	G	101	PX4	C1-O3-P1-O1
3	G	101	PX4	C1-O3-P1-O2
3	G	101	PX4	C24-C23-O7-C7
3	G	102	PX4	C1-O3-P1-O2
3	G	102	PX4	C1-O3-P1-O4
3	J	101	PX4	O3-C1-C2-N1
3	J	101	PX4	C24-C23-O7-C7
3	K	201	PX4	C1-O3-P1-O2
3	K	201	PX4	C6-O4-P1-O1
3	K	201	PX4	C6-O4-P1-O2
3	K	201	PX4	C6-O4-P1-O3
3	E	201	PX4	O6-C9-O5-C8
3	G	102	PX4	O6-C9-O5-C8
3	A	101	PX4	O8-C23-O7-C7
3	D	101	PX4	O8-C23-O7-C7
3	G	101	PX4	O8-C23-O7-C7
3	G	102	PX4	O8-C23-O7-C7
3	J	101	PX4	O8-C23-O7-C7
3	E	201	PX4	C10-C9-O5-C8
3	G	102	PX4	C10-C9-O5-C8
3	G	102	PX4	C24-C23-O7-C7
3	A	102	PX4	C10-C9-O5-C8
3	J	101	PX4	C10-C9-O5-C8
3	A	102	PX4	O6-C9-O5-C8
3	B	201	PX4	O6-C9-O5-C8
3	J	101	PX4	O6-C9-O5-C8
3	B	201	PX4	C10-C9-O5-C8
3	K	201	PX4	C7-C6-O4-P1
3	A	102	PX4	C13-C14-C15-C16
3	G	101	PX4	C10-C9-O5-C8
3	G	101	PX4	O6-C9-O5-C8

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Mol	Chain	Res	Type	Atoms
3	A	102	PX4	C23-C24-C25-C26
3	E	201	PX4	C17-C18-C19-C20
3	E	201	PX4	C14-C15-C16-C17
3	A	101	PX4	C6-O4-P1-O3
3	B	201	PX4	C6-O4-P1-O3
3	D	101	PX4	C1-O3-P1-O4
3	D	101	PX4	C6-O4-P1-O3
3	G	101	PX4	C1-O3-P1-O4
3	J	101	PX4	C1-O3-P1-O4
3	K	201	PX4	C1-O3-P1-O4
3	G	102	PX4	C13-C14-C15-C16
3	K	201	PX4	C15-C16-C17-C18
3	G	101	PX4	C12-C13-C14-C15
3	J	101	PX4	C10-C11-C12-C13
3	K	201	PX4	C10-C11-C12-C13
3	D	101	PX4	C27-C28-C29-C30
3	E	201	PX4	C23-C24-C25-C26
3	K	201	PX4	O8-C23-O7-C7
3	A	101	PX4	C14-C15-C16-C17
3	A	101	PX4	C18-C19-C20-C21
3	E	201	PX4	C1-C2-N1-C3
3	G	102	PX4	C17-C18-C19-C20
3	K	201	PX4	C32-C33-C34-C35
3	E	201	PX4	C25-C26-C27-C28
3	A	101	PX4	C32-C33-C34-C35
3	A	102	PX4	C11-C12-C13-C14
3	J	101	PX4	C13-C14-C15-C16
3	K	201	PX4	C24-C23-O7-C7
3	A	102	PX4	C32-C33-C34-C35
3	J	101	PX4	C11-C12-C13-C14
3	A	102	PX4	C25-C26-C27-C28
3	K	201	PX4	C25-C26-C27-C28
3	J	101	PX4	C16-C17-C18-C19
3	J	101	PX4	C15-C16-C17-C18
3	A	101	PX4	C1-O3-P1-O4
3	A	102	PX4	O4-C6-C7-C8
3	B	201	PX4	O4-C6-C7-C8
3	G	102	PX4	C27-C28-C29-C30
3	B	201	PX4	C11-C12-C13-C14
3	D	101	PX4	C25-C26-C27-C28
3	G	102	PX4	C12-C13-C14-C15
3	A	102	PX4	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
3	E	201	PX4	C1-C2-N1-C4
3	K	201	PX4	C27-C28-C29-C30
3	A	101	PX4	O7-C7-C8-O5
3	B	201	PX4	O7-C7-C8-O5
3	B	201	PX4	C31-C32-C33-C34
3	J	101	PX4	C12-C13-C14-C15
3	G	102	PX4	C11-C12-C13-C14
3	B	201	PX4	C7-C6-O4-P1
3	A	101	PX4	C10-C9-O5-C8
3	E	201	PX4	C6-C7-C8-O5
3	A	102	PX4	C30-C31-C32-C33
3	K	201	PX4	C26-C27-C28-C29
3	A	101	PX4	O4-C6-C7-O7
3	J	101	PX4	C14-C15-C16-C17
3	A	102	PX4	C7-C6-O4-P1
3	B	201	PX4	C27-C28-C29-C30
3	K	201	PX4	O4-C6-C7-C8
3	E	201	PX4	C30-C31-C32-C33
3	E	201	PX4	C1-C2-N1-C5
3	K	201	PX4	C8-C7-O7-C23
3	E	201	PX4	C10-C11-C12-C13
3	B	201	PX4	C6-C7-C8-O5
3	G	101	PX4	C6-C7-C8-O5
3	A	102	PX4	O4-C6-C7-O7
3	G	101	PX4	O4-C6-C7-O7
3	K	201	PX4	O4-C6-C7-O7
3	A	101	PX4	O6-C9-O5-C8
3	A	102	PX4	O7-C7-C8-O5
3	E	201	PX4	O7-C7-C8-O5
3	G	101	PX4	O7-C7-C8-O5
3	J	101	PX4	O7-C7-C8-O5
3	B	201	PX4	C33-C34-C35-C36
3	E	201	PX4	C11-C12-C13-C14
3	B	201	PX4	C15-C16-C17-C18
3	G	101	PX4	C15-C16-C17-C18
3	G	102	PX4	C14-C15-C16-C17
3	E	201	PX4	C1-O3-P1-O4
3	A	101	PX4	C1-O3-P1-O2
3	B	201	PX4	C6-O4-P1-O1
3	D	101	PX4	C1-O3-P1-O2
3	D	101	PX4	C6-O4-P1-O1
3	J	101	PX4	C1-O3-P1-O2

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Mol	Chain	Res	Type	Atoms
3	K	201	PX4	C1-O3-P1-O1
3	A	101	PX4	O4-C6-C7-C8
3	G	101	PX4	O4-C6-C7-C8
3	K	201	PX4	C2-C1-O3-P1
3	K	201	PX4	C9-C10-C11-C12
3	J	101	PX4	C28-C29-C30-C31
3	B	201	PX4	O4-C6-C7-O7
3	A	101	PX4	C28-C29-C30-C31
3	A	101	PX4	C6-C7-C8-O5
3	A	102	PX4	O3-C1-C2-N1
3	D	101	PX4	O3-C1-C2-N1
3	G	101	PX4	O3-C1-C2-N1
3	G	102	PX4	C6-C7-C8-O5
3	G	102	PX4	O7-C7-C8-O5
3	B	201	PX4	C14-C15-C16-C17
3	B	201	PX4	C32-C33-C34-C35
3	K	201	PX4	C10-C9-O5-C8
3	A	102	PX4	C1-O3-P1-O4
3	A	102	PX4	C6-O4-P1-O3
3	G	101	PX4	C6-O4-P1-O3
3	D	101	PX4	C10-C11-C12-C13
3	G	102	PX4	C18-C19-C20-C21
3	J	101	PX4	C6-C7-C8-O5
3	K	201	PX4	O6-C9-O5-C8
3	E	201	PX4	C19-C20-C21-C22
3	G	102	PX4	C10-C11-C12-C13
3	G	101	PX4	C30-C31-C32-C33
3	G	101	PX4	C17-C18-C19-C20
3	D	101	PX4	C12-C13-C14-C15
3	E	201	PX4	C15-C16-C17-C18
3	D	101	PX4	C13-C14-C15-C16
3	E	201	PX4	C12-C13-C14-C15
3	G	101	PX4	C6-C7-O7-C23
3	A	102	PX4	C14-C15-C16-C17
3	K	201	PX4	C13-C14-C15-C16
3	D	101	PX4	C7-C6-O4-P1
3	E	201	PX4	C24-C25-C26-C27
3	E	201	PX4	C28-C29-C30-C31
3	A	101	PX4	C10-C11-C12-C13
3	G	101	PX4	C14-C15-C16-C17
3	A	102	PX4	C18-C19-C20-C21
3	J	101	PX4	C1-C2-N1-C5

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Mol	Chain	Res	Type	Atoms
3	A	101	PX4	O7-C23-C24-C25
3	B	201	PX4	C1-O3-P1-O4
3	B	201	PX4	O7-C23-C24-C25
3	B	201	PX4	C10-C11-C12-C13
3	A	102	PX4	C6-C7-C8-O5
3	D	101	PX4	O4-C6-C7-O7
3	A	101	PX4	C33-C34-C35-C36
3	G	101	PX4	O7-C23-C24-C25
3	E	201	PX4	C11-C10-C9-O5
3	A	102	PX4	C27-C28-C29-C30
3	D	101	PX4	C16-C17-C18-C19
3	A	101	PX4	O8-C23-C24-C25
3	D	101	PX4	C30-C31-C32-C33
3	B	201	PX4	O8-C23-C24-C25
3	J	101	PX4	C33-C34-C35-C36
3	B	201	PX4	C1-C2-N1-C4
3	B	201	PX4	C2-C1-O3-P1
3	E	201	PX4	C2-C1-O3-P1
3	G	102	PX4	C2-C1-O3-P1
3	J	101	PX4	C2-C1-O3-P1
3	K	201	PX4	C11-C12-C13-C14
3	G	101	PX4	O8-C23-C24-C25
3	E	201	PX4	C11-C10-C9-O6

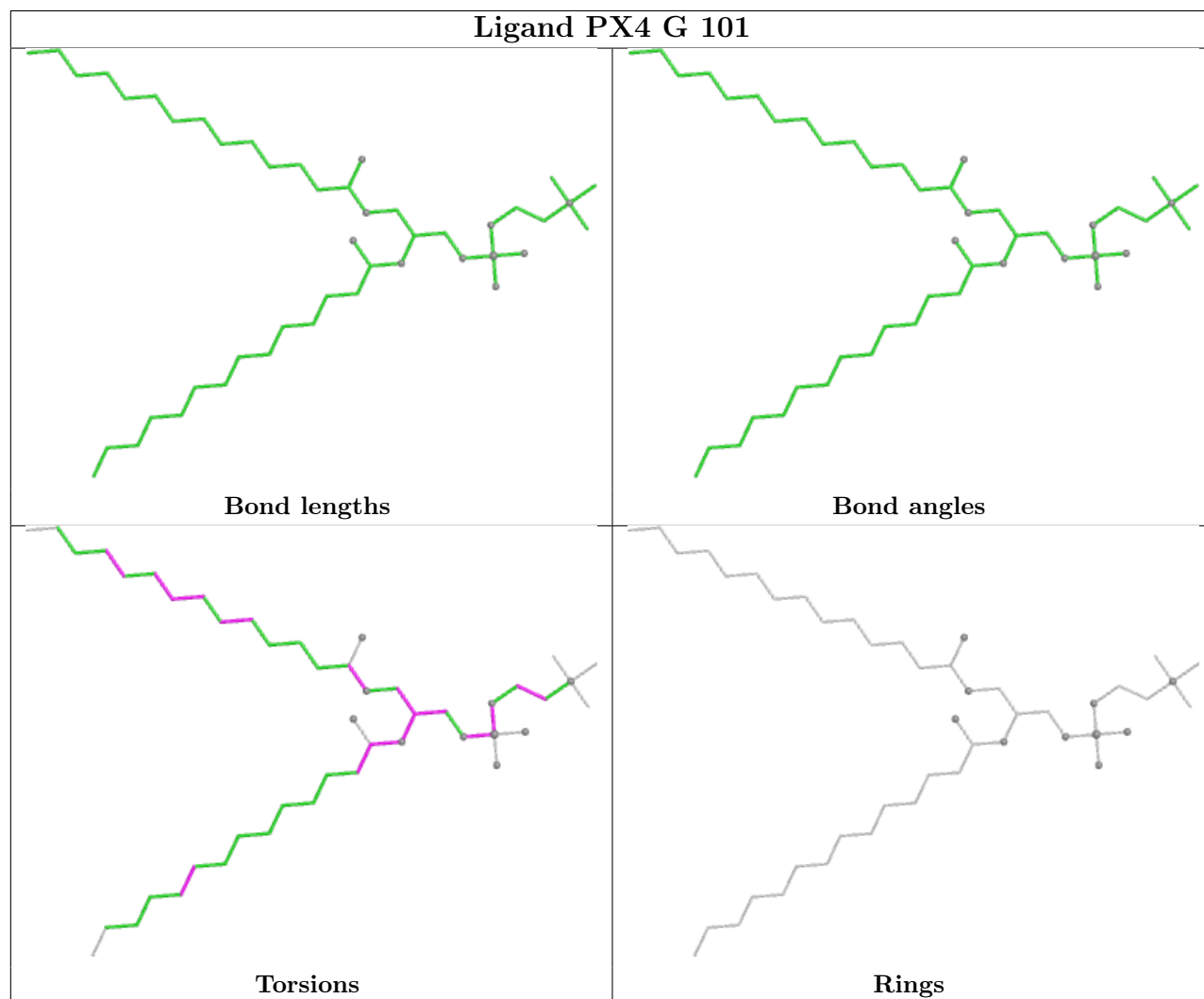
There are no ring outliers.

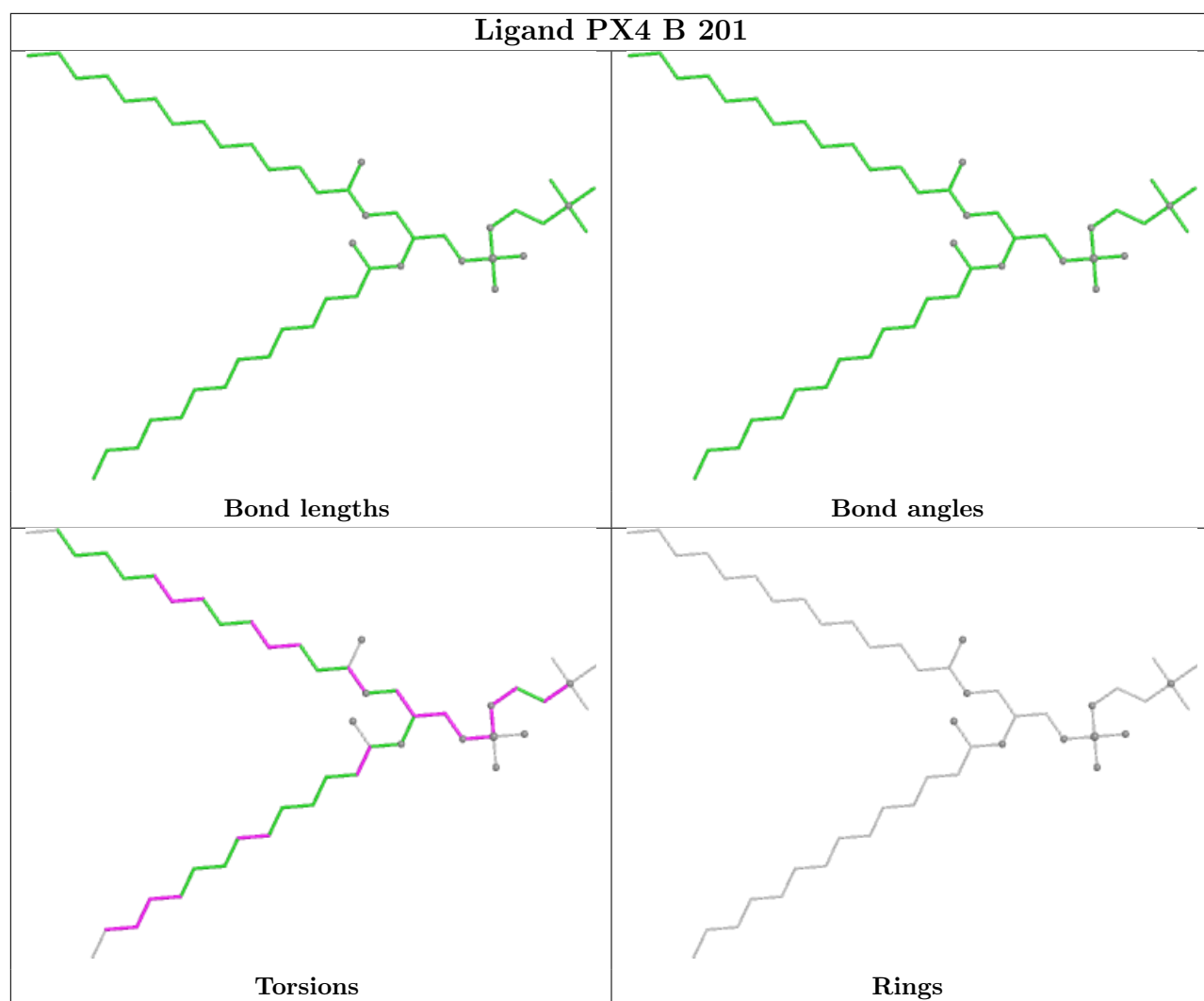
8 monomers are involved in 21 short contacts:

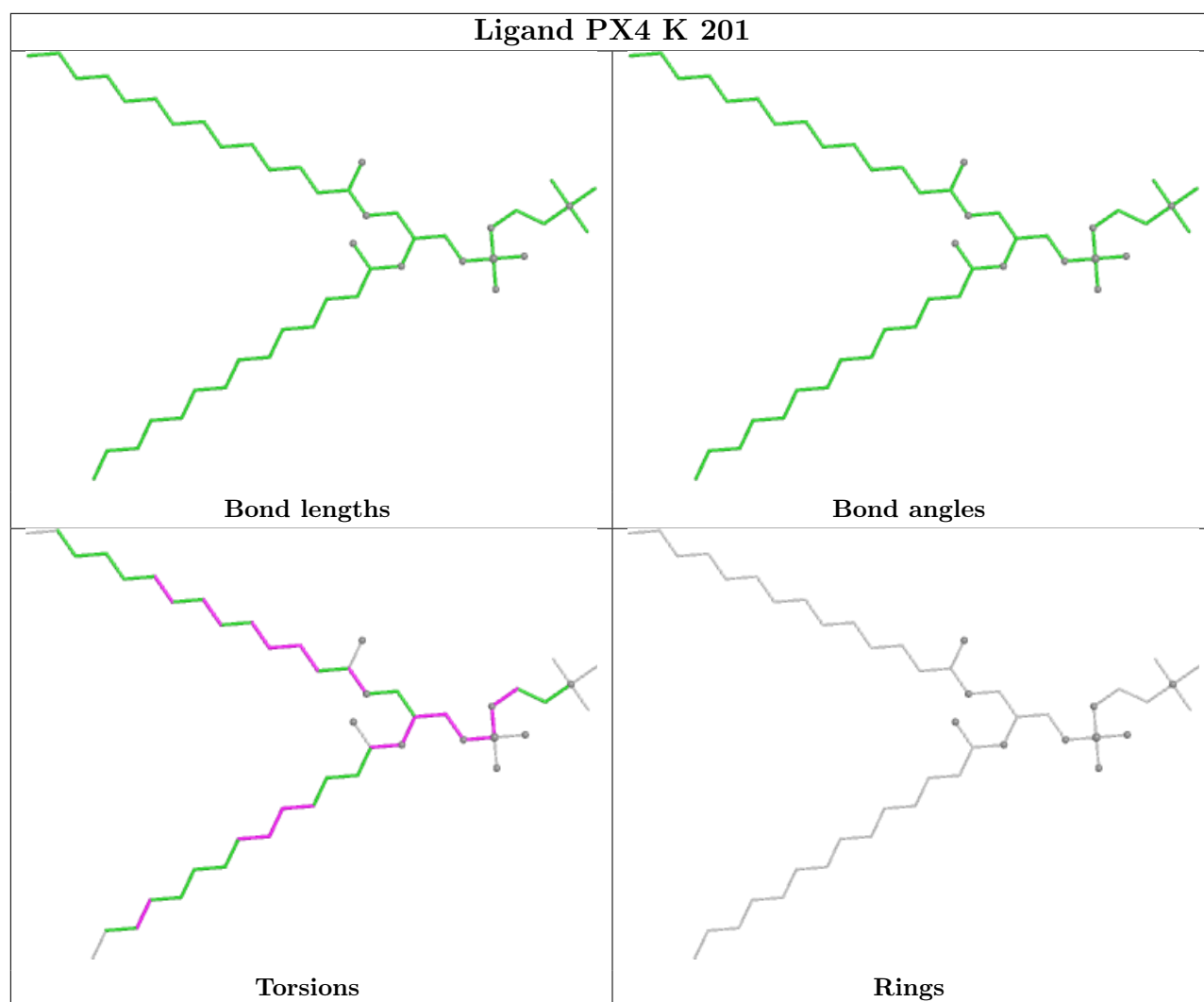
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	101	PX4	1	0
3	K	201	PX4	4	0
3	A	102	PX4	5	0
3	D	101	PX4	1	0
3	A	101	PX4	4	0
3	J	101	PX4	2	0
3	G	102	PX4	6	0
3	E	201	PX4	1	0

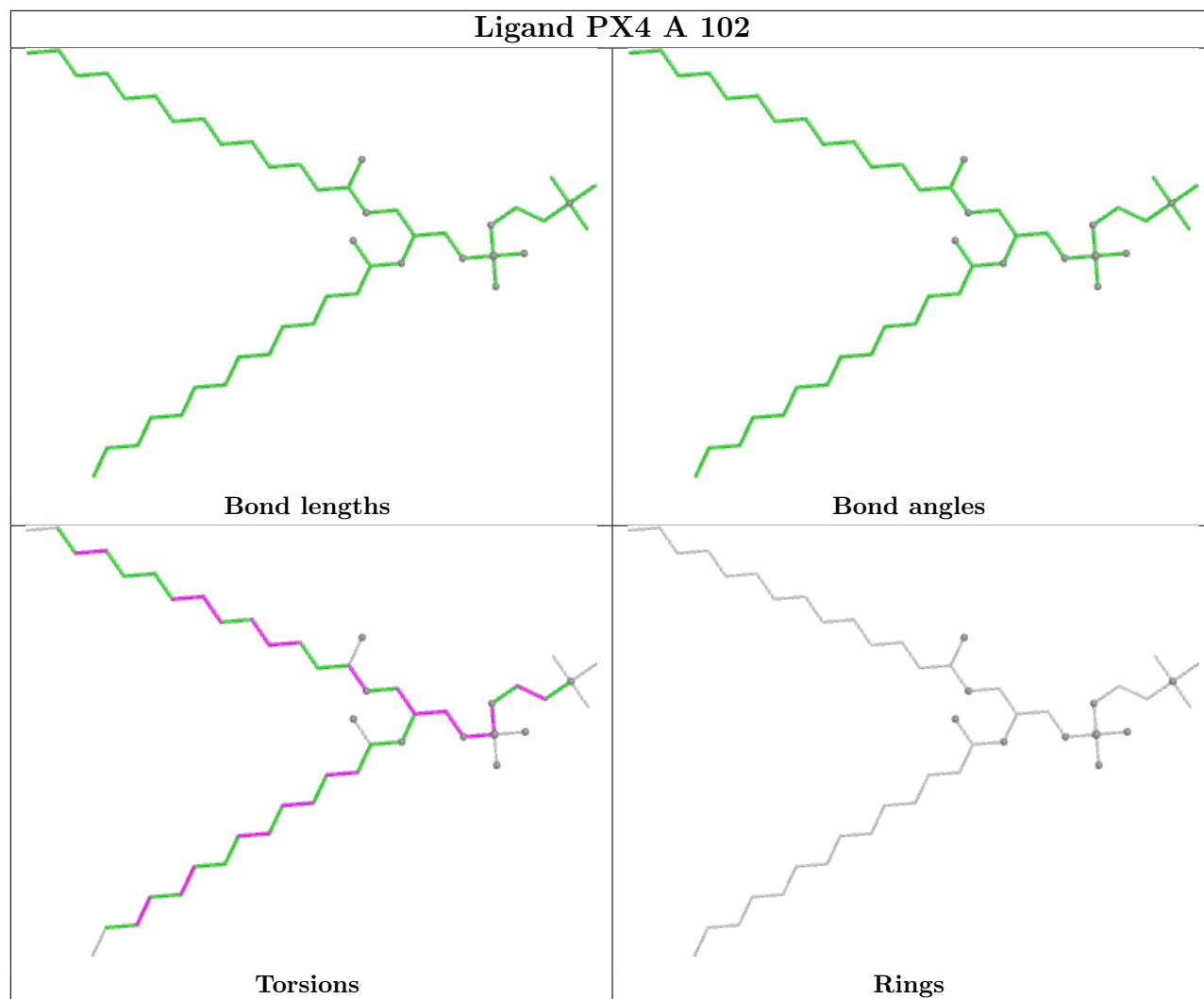
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

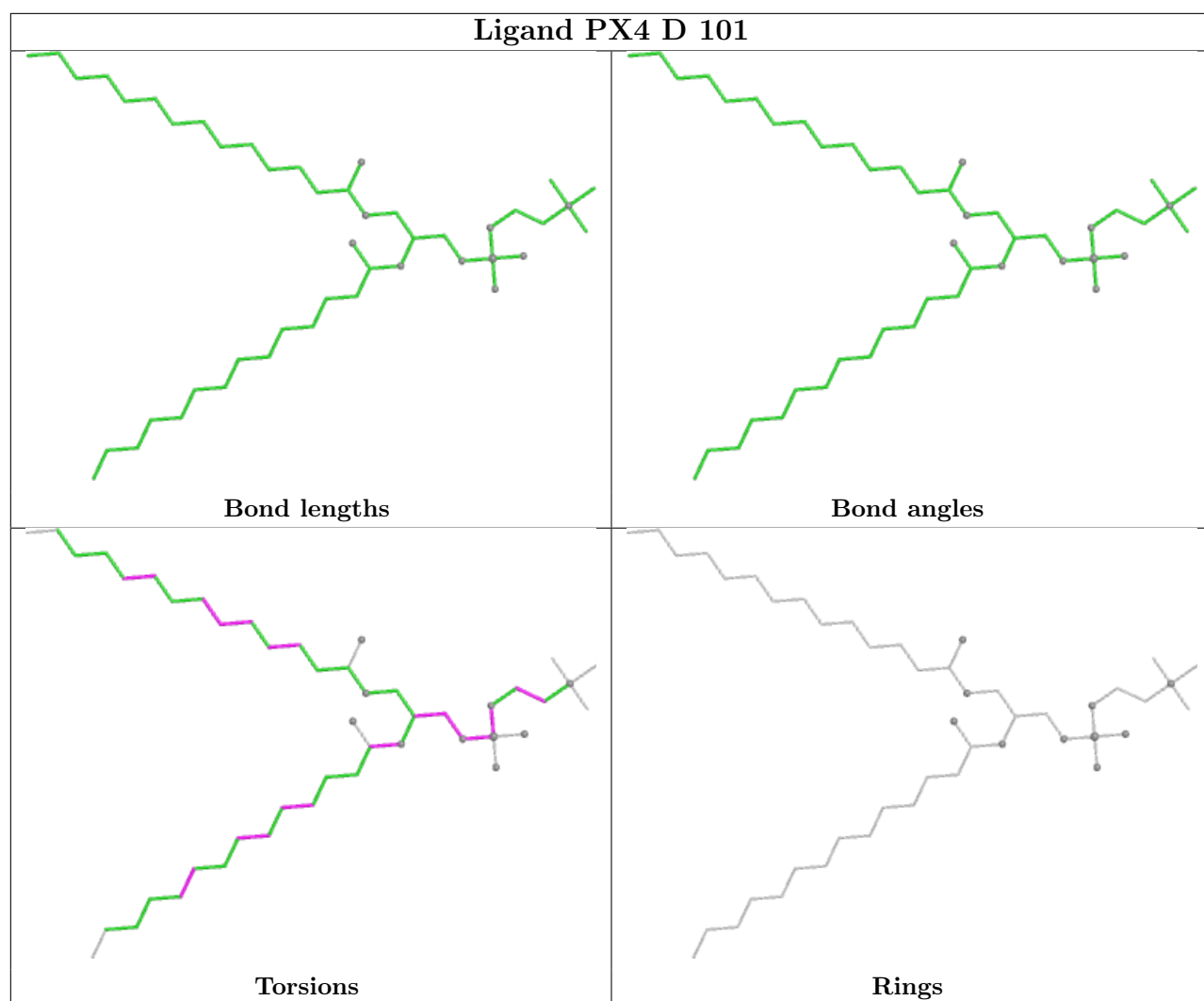
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

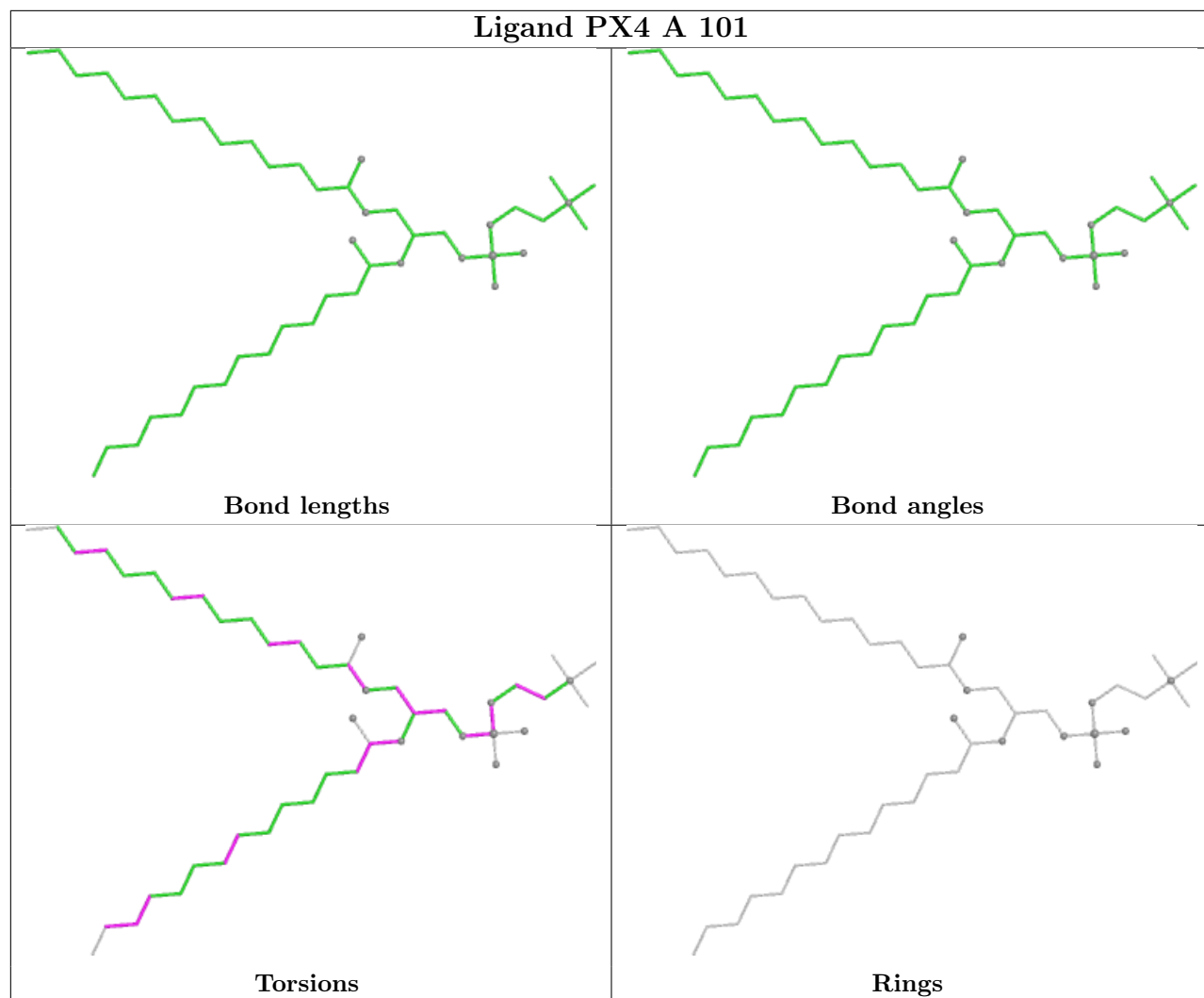


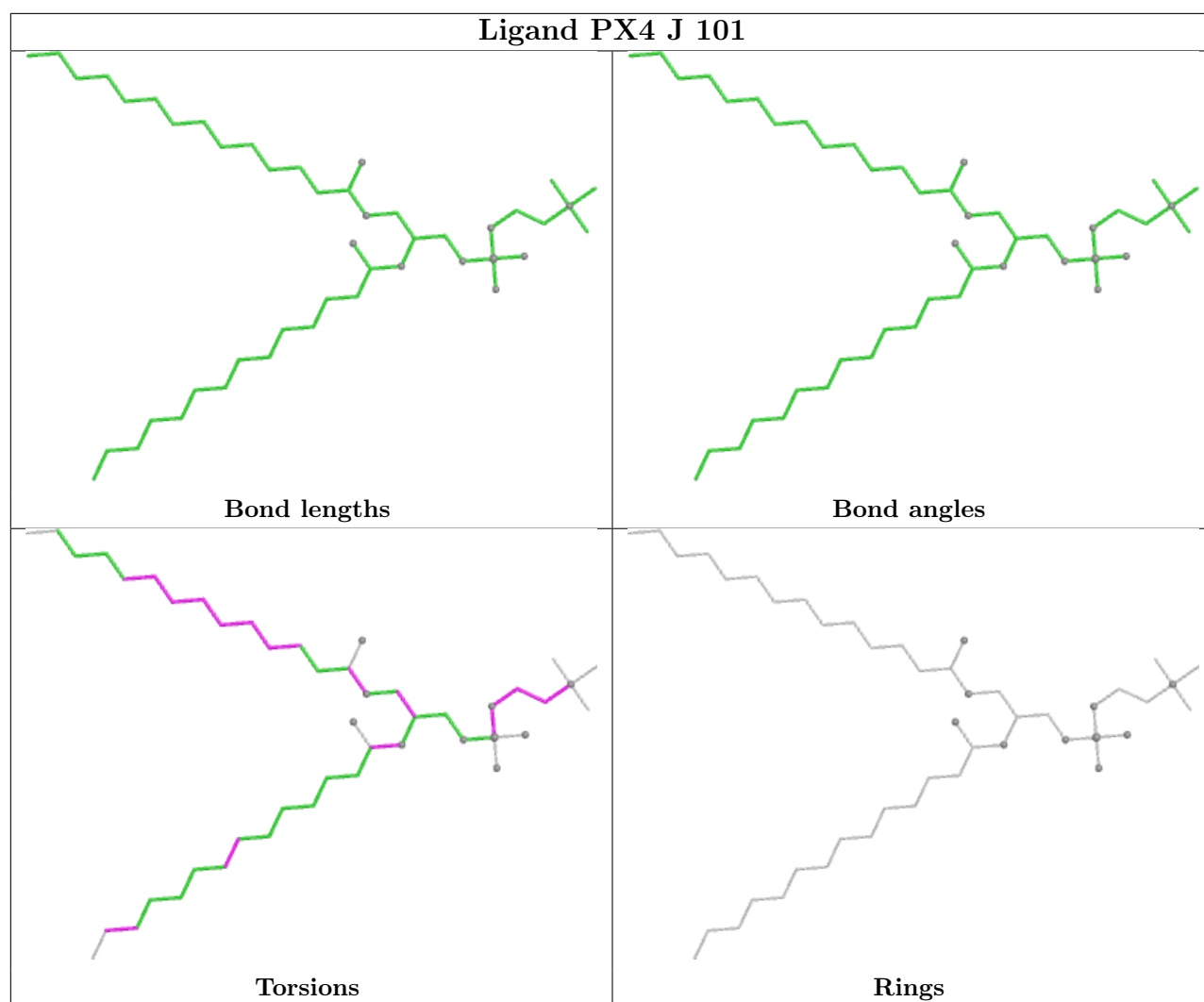


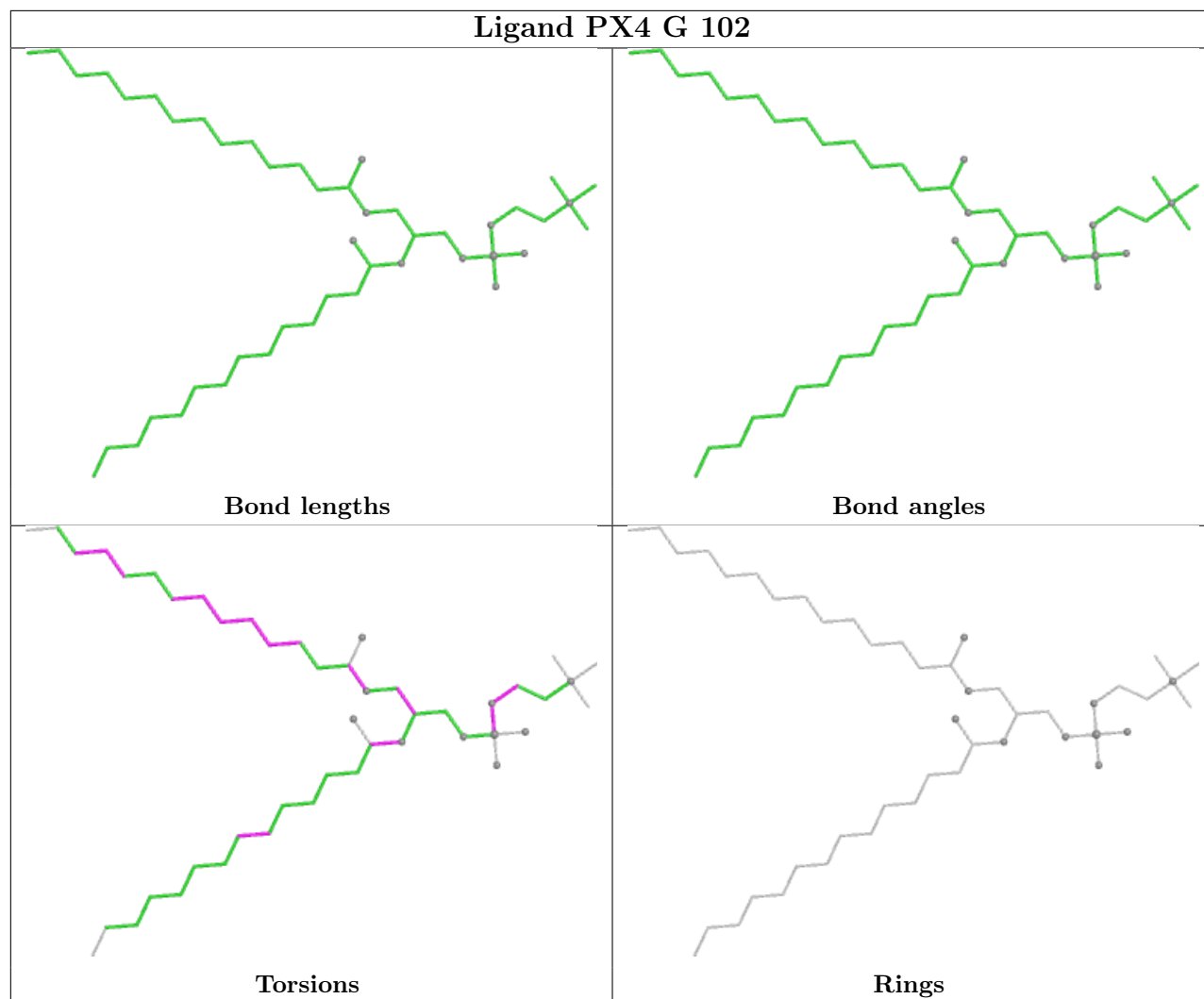


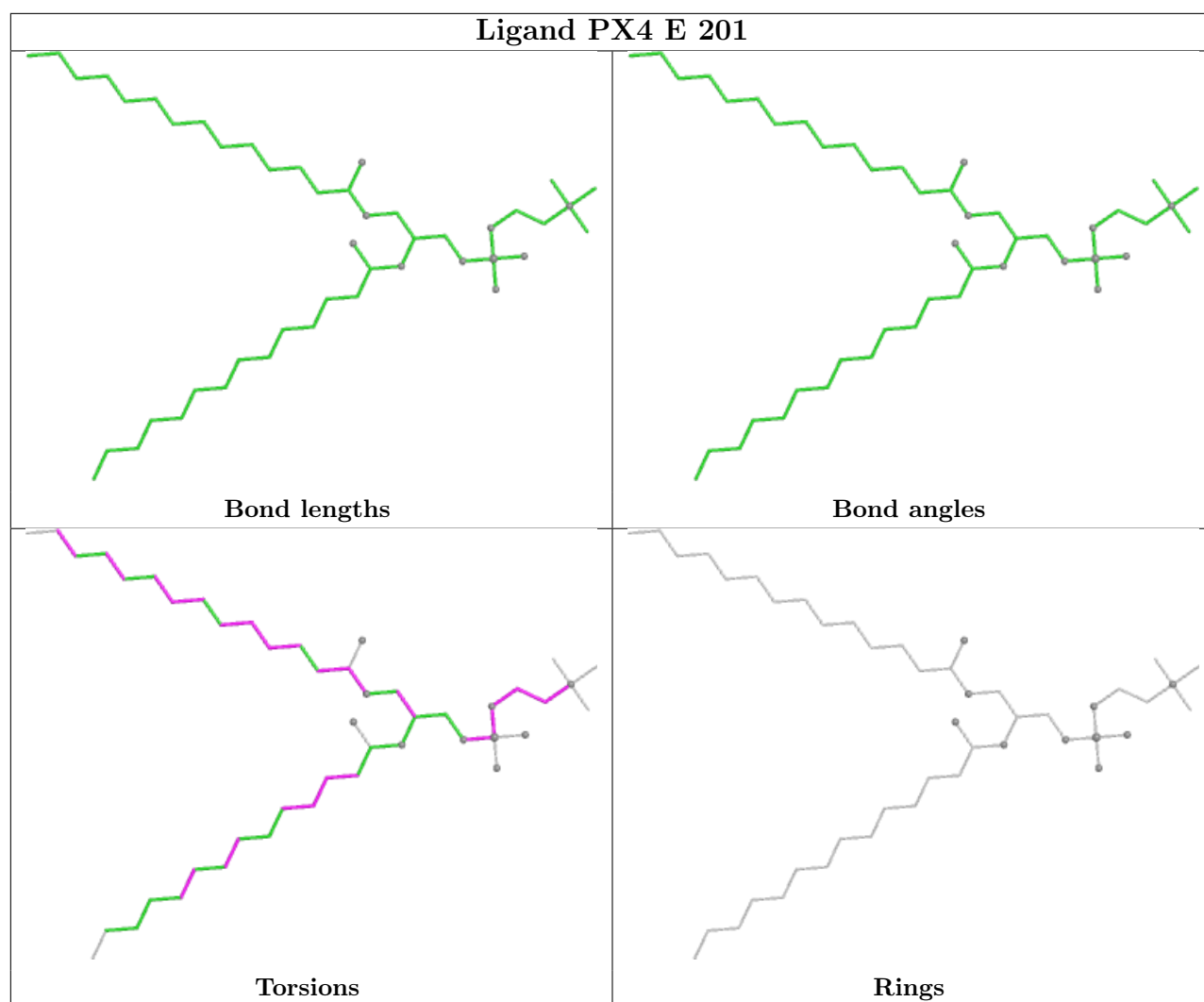












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.