



Full wwPDB EM Validation Report ⓘ

Apr 7, 2024 – 12:06 AM JST

PDB ID : 8J8J
EMDB ID : EMD-36071
Title : Membrane bound PRTase, C3 symmetry, donor bound
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Deposited on : 2023-05-01
Resolution : 2.76 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 : 4.02b-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

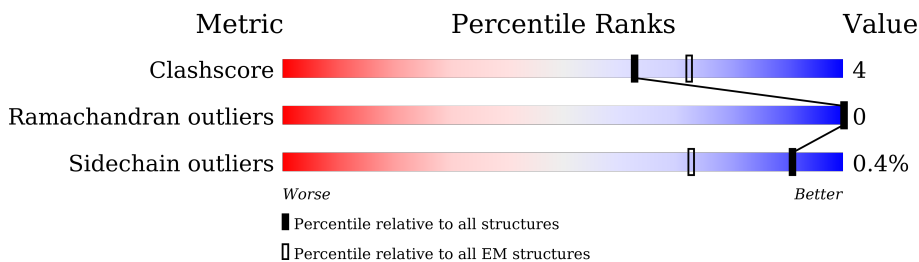
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.76 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	302	
1	B	302	
1	D	302	

2 Entry composition [i](#)

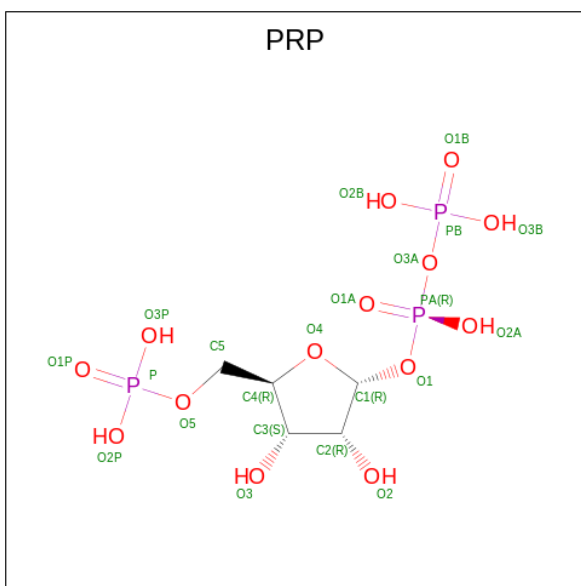
There are 4 unique types of molecules in this entry. The entry contains 6873 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Decaprenyl-phosphate phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	D	290	Total	C	N	O	S	0	0
			2217	1460	368	379	10		
1	A	290	Total	C	N	O	S	0	0
			2217	1460	368	379	10		
1	B	290	Total	C	N	O	S	0	0
			2217	1460	368	379	10		

- Molecule 2 is 1-O-pyrophosphono-5-O-phosphono-alpha-D-ribofuranose (three-letter code: PRP) (formula: $C_5H_{13}O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).

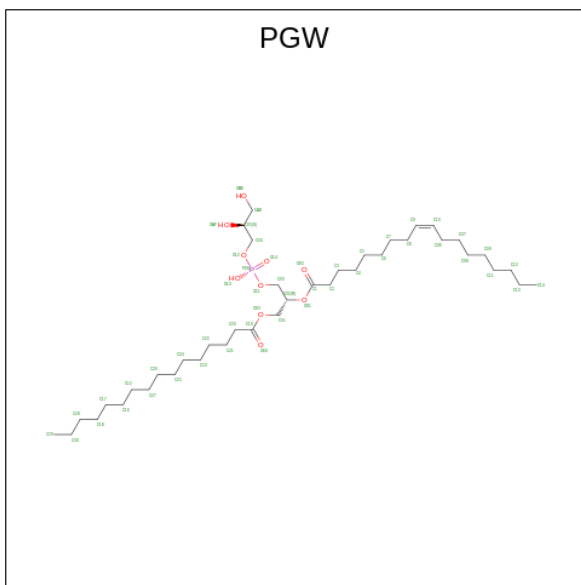


Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
2	D	1	Total	C	O	P	0
			22	5	14	3	
2	A	1	Total	C	O	P	0
			22	5	14	3	
2	B	1	Total	C	O	P	0
			22	5	14	3	

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

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

- Molecule 4 is (1R)-2-[[[(S)-{[(2S)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy]-1-[(hexadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (three-letter code: PGW) (formula: C₄₀H₇₇O₁₀P).



Mol	Chain	Residues	Atoms	AltConf
4	D	1	Total C O P 51 40 10 1	0
4	A	1	Total C O P 51 40 10 1	0
4	B	1	Total C O P 51 40 10 1	0

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	410532	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF amplitude correction was performed following 3D reconstruction	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	130000	Depositor
Image detector	FEI FALCON IV (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: PRP, MG, PGW

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	0.35	0/2269	0.52	0/3096
1	B	0.35	0/2269	0.52	0/3096
1	D	0.38	0/2269	0.53	0/3096
All	All	0.36	0/6807	0.52	0/9288

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	2217	0	2294	21	0
1	B	2217	0	2294	18	0
1	D	2217	0	2294	22	0
2	A	22	0	8	1	0
2	B	22	0	8	0	0
2	D	22	0	8	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	A	51	0	76	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	51	0	76	1	0
4	D	51	0	76	1	0
All	All	6873	0	7134	61	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 4.

All (61) 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:205:ALA:HB1	1:A:207:ARG:HG2	1.31	1.08
1:B:205:ALA:HB1	1:B:207:ARG:HG2	1.34	1.05
1:D:205:ALA:HB1	1:D:207:ARG:HG2	1.46	0.98
1:D:205:ALA:HB1	1:D:207:ARG:CG	2.18	0.73
1:B:104:THR:O	1:B:107:VAL:HG12	1.90	0.72
1:A:104:THR:O	1:A:107:VAL:HG12	1.90	0.71
1:D:104:THR:O	1:D:107:VAL:HG12	1.90	0.70
1:A:205:ALA:HB1	1:A:207:ARG:CG	2.14	0.69
1:B:191:LYS:HG3	1:B:272:GLY:HA2	1.76	0.68
1:D:191:LYS:HG3	1:D:272:GLY:HA2	1.76	0.67
1:B:205:ALA:HB1	1:B:207:ARG:CG	2.17	0.67
1:A:191:LYS:HG3	1:A:272:GLY:HA2	1.76	0.67
1:B:33:LEU:HD13	1:B:55:VAL:HG11	1.77	0.66
1:D:33:LEU:HD13	1:D:55:VAL:HG11	1.77	0.66
1:A:33:LEU:HD13	1:A:55:VAL:HG11	1.77	0.65
1:D:206:ILE:HG13	1:D:207:ARG:N	2.17	0.59
1:B:207:ARG:HD3	1:B:207:ARG:H	1.69	0.57
1:D:199:ALA:HB1	1:D:207:ARG:HE	1.70	0.54
1:A:204:ALA:O	1:A:205:ALA:HB2	2.09	0.52
1:D:104:THR:HA	1:D:107:VAL:HG12	1.92	0.52
1:A:104:THR:HA	1:A:107:VAL:HG12	1.92	0.52
1:B:104:THR:HA	1:B:107:VAL:HG12	1.91	0.51
1:D:205:ALA:CB	1:D:207:ARG:HG2	2.30	0.51
1:D:204:ALA:O	1:D:205:ALA:HB2	2.11	0.51
1:D:207:ARG:HD3	1:D:207:ARG:H	1.75	0.51
1:B:206:ILE:HG13	1:B:207:ARG:N	2.25	0.51
1:D:126:LEU:HD22	4:D:403:PGW:H4	1.93	0.50
1:A:84:HIS:O	1:A:88:ARG:HG3	2.12	0.50
1:B:84:HIS:O	1:B:88:ARG:HG3	2.12	0.50
1:D:261:ARG:O	1:D:264:VAL:HG12	2.12	0.50
1:B:261:ARG:O	1:B:264:VAL:HG12	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:LEU:HD22	4:A:403:PGW:H4	1.94	0.50
1:D:84:HIS:O	1:D:88:ARG:HG3	2.12	0.49
1:A:261:ARG:O	1:A:264:VAL:HG12	2.12	0.49
1:A:206:ILE:HG13	1:A:207:ARG:N	2.28	0.48
1:B:126:LEU:HD22	4:B:403:PGW:H4	1.95	0.48
1:A:146:ALA:O	1:A:213:TYR:OH	2.27	0.47
1:B:104:THR:O	1:B:108:VAL:HG23	2.15	0.47
1:B:271:ALA:HA	1:B:277:ILE:HD11	1.97	0.47
1:D:271:ALA:HA	1:D:277:ILE:HD11	1.97	0.47
1:A:199:ALA:HB1	1:A:207:ARG:HE	1.78	0.47
1:A:104:THR:O	1:A:108:VAL:HG23	2.15	0.47
1:A:271:ALA:HA	1:A:277:ILE:HD11	1.97	0.47
1:D:104:THR:O	1:D:108:VAL:HG23	2.15	0.46
1:B:104:THR:O	1:B:107:VAL:CG1	2.63	0.46
1:B:204:ALA:O	1:B:205:ALA:HB2	2.15	0.46
1:A:137:ALA:O	1:A:142:LEU:HD13	2.15	0.46
1:A:207:ARG:H	1:A:207:ARG:HD3	1.80	0.45
1:D:208:LYS:CG	1:D:209:SER:H	2.30	0.45
1:A:173:SER:OG	1:A:174:LYS:N	2.50	0.45
1:D:206:ILE:CG1	1:D:207:ARG:N	2.79	0.45
1:D:173:SER:OG	1:D:174:LYS:N	2.50	0.45
1:B:173:SER:OG	1:B:174:LYS:N	2.49	0.44
1:A:28:LYS:NZ	2:A:401:PRP:O1P	2.34	0.44
1:A:104:THR:O	1:A:107:VAL:CG1	2.63	0.42
1:D:81:ASP:C	1:D:83:GLU:H	2.23	0.42
1:D:210:LEU:HA	1:D:213:TYR:HD2	1.85	0.41
1:A:81:ASP:C	1:A:83:GLU:H	2.23	0.41
1:B:81:ASP:C	1:B:83:GLU:H	2.23	0.41
1:D:104:THR:O	1:D:107:VAL:CG1	2.63	0.41
1:B:199:ALA:HB1	1:B:207:ARG:HE	1.86	0.41

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	288/302 (95%)	277 (96%)	11 (4%)	0	100	100
1	B	288/302 (95%)	276 (96%)	12 (4%)	0	100	100
1	D	288/302 (95%)	276 (96%)	12 (4%)	0	100	100
All	All	864/906 (95%)	829 (96%)	35 (4%)	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	224/235 (95%)	223 (100%)	1 (0%)	91	93
1	B	224/235 (95%)	223 (100%)	1 (0%)	91	93
1	D	224/235 (95%)	223 (100%)	1 (0%)	91	93
All	All	672/705 (95%)	669 (100%)	3 (0%)	91	93

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	62	PHE
1	A	62	PHE
1	B	62	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	29	ASN
1	A	29	ASN
1	B	29	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 9 ligands modelled in this entry, 3 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
4	PGW	A	403	-	50,50,50	1.08	4 (8%)	53,56,56	1.09	5 (9%)
2	PRP	D	401	3	19,22,22	1.05	0	33,35,35	1.49	7 (21%)
4	PGW	B	403	-	50,50,50	1.08	4 (8%)	53,56,56	1.09	5 (9%)
2	PRP	B	401	3	19,22,22	1.02	0	33,35,35	1.50	6 (18%)
2	PRP	A	401	3	19,22,22	1.04	1 (5%)	33,35,35	1.53	7 (21%)
4	PGW	D	403	-	50,50,50	1.08	4 (8%)	53,56,56	1.09	5 (9%)

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	PGW	A	403	-	-	32/55/55/55	-
2	PRP	D	401	3	-	7/16/33/33	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PGW	B	403	-	-	32/55/55/55	-
2	PRP	B	401	3	-	5/16/33/33	0/1/1/1
2	PRP	A	401	3	-	6/16/33/33	0/1/1/1
4	PGW	D	403	-	-	32/55/55/55	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	403	PGW	O01-C02	-3.17	1.38	1.46
4	B	403	PGW	O01-C02	-3.17	1.38	1.46
4	A	403	PGW	O01-C02	-3.17	1.38	1.46
4	B	403	PGW	O03-C19	2.70	1.41	1.33
4	D	403	PGW	O03-C19	2.70	1.41	1.33
4	A	403	PGW	O03-C19	2.70	1.41	1.33
4	A	403	PGW	O01-C1	2.48	1.41	1.34
4	B	403	PGW	O01-C1	2.48	1.41	1.34
4	D	403	PGW	O01-C1	2.47	1.41	1.34
4	A	403	PGW	P-O11	2.13	1.67	1.59
4	B	403	PGW	P-O11	2.12	1.67	1.59
4	D	403	PGW	P-O11	2.11	1.67	1.59
2	A	401	PRP	PB-O2B	-2.01	1.47	1.54

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	PRP	O1-C1-C2	3.73	113.04	106.72
2	B	401	PRP	O3P-P-O5	-3.48	97.48	106.73
4	D	403	PGW	O01-C1-C2	3.34	118.69	111.50
4	A	403	PGW	O01-C1-C2	3.33	118.68	111.50
4	B	403	PGW	O01-C1-C2	3.33	118.68	111.50
2	D	401	PRP	O1-C1-C2	3.30	112.31	106.72
4	B	403	PGW	C03-C02-C01	-3.13	104.39	111.79
4	D	403	PGW	C03-C02-C01	-3.12	104.40	111.79
4	A	403	PGW	C03-C02-C01	-3.11	104.42	111.79
2	B	401	PRP	O1-C1-C2	2.96	111.74	106.72
2	B	401	PRP	C1-C2-C3	2.79	105.83	102.30
2	D	401	PRP	PA-O3A-PB	-2.77	123.33	132.83
2	A	401	PRP	C1-C2-C3	2.69	105.71	102.30
2	B	401	PRP	PA-O3A-PB	-2.68	123.62	132.83
2	A	401	PRP	O3P-P-O5	-2.66	99.66	106.73
2	A	401	PRP	O3P-P-O2P	2.58	117.52	107.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	403	PGW	O03-C19-C20	2.57	119.96	111.91
4	D	403	PGW	O03-C19-C20	2.57	119.96	111.91
4	B	403	PGW	O03-C19-C20	2.57	119.96	111.91
2	D	401	PRP	O3P-P-O2P	2.53	117.29	107.64
2	D	401	PRP	C1-C2-C3	2.51	105.47	102.30
2	B	401	PRP	O3P-P-O2P	2.49	117.14	107.64
2	A	401	PRP	PA-O3A-PB	-2.46	124.37	132.83
2	D	401	PRP	O3P-P-O5	-2.46	100.18	106.73
2	D	401	PRP	O2P-P-O5	-2.38	100.40	106.73
2	A	401	PRP	O2P-P-O5	-2.35	100.48	106.73
2	D	401	PRP	O3B-PB-O2B	2.28	116.35	107.64
4	A	403	PGW	O01-C02-C01	-2.27	100.17	108.40
4	B	403	PGW	O01-C02-C01	-2.27	100.20	108.40
4	D	403	PGW	O01-C02-C01	-2.26	100.21	108.40
2	A	401	PRP	O3B-PB-O2B	2.18	115.97	107.64
4	D	403	PGW	C02-O01-C1	2.17	123.12	117.79
4	A	403	PGW	C02-O01-C1	2.15	123.08	117.79
4	B	403	PGW	C02-O01-C1	2.14	123.06	117.79
2	B	401	PRP	O3B-PB-O2B	2.13	115.78	107.64

There are no chirality outliers.

All (114) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	401	PRP	C1-O1-PA-O3A
2	D	401	PRP	C5-O5-P-O1P
2	D	401	PRP	C5-O5-P-O2P
2	D	401	PRP	C5-O5-P-O3P
2	A	401	PRP	C1-O1-PA-O3A
2	A	401	PRP	C5-O5-P-O2P
2	A	401	PRP	C5-O5-P-O3P
2	B	401	PRP	C1-O1-PA-O3A
4	D	403	PGW	C04-O12-P-O14
4	A	403	PGW	C04-O12-P-O14
4	B	403	PGW	C04-O12-P-O14
4	D	403	PGW	C17-C18-C28-C30
4	A	403	PGW	C17-C18-C28-C30
4	B	403	PGW	C17-C18-C28-C30
4	D	403	PGW	O12-C04-C05-CAD
4	A	403	PGW	O12-C04-C05-CAD
4	B	403	PGW	O12-C04-C05-CAD
4	D	403	PGW	C25-C26-C27-C15

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Mol	Chain	Res	Type	Atoms
4	A	403	PGW	C25-C26-C27-C15
4	B	403	PGW	C25-C26-C27-C15
4	D	403	PGW	C19-C20-C21-C22
4	A	403	PGW	C19-C20-C21-C22
4	B	403	PGW	C19-C20-C21-C22
4	D	403	PGW	O12-C04-C05-OAF
4	A	403	PGW	O12-C04-C05-OAF
4	B	403	PGW	O12-C04-C05-OAF
4	D	403	PGW	C04-O12-P-O11
4	A	403	PGW	C04-O12-P-O11
4	B	403	PGW	C04-O12-P-O11
4	D	403	PGW	C20-C19-O03-C01
4	A	403	PGW	C20-C19-O03-C01
4	B	403	PGW	C20-C19-O03-C01
4	D	403	PGW	C2-C3-C4-C5
4	A	403	PGW	C2-C3-C4-C5
4	B	403	PGW	C2-C3-C4-C5
4	D	403	PGW	C20-C21-C22-C23
4	A	403	PGW	C20-C21-C22-C23
4	B	403	PGW	C20-C21-C22-C23
4	D	403	PGW	C04-C05-CAD-OAE
4	A	403	PGW	C04-C05-CAD-OAE
4	B	403	PGW	C04-C05-CAD-OAE
4	D	403	PGW	C06-C07-C08-C09
4	A	403	PGW	C06-C07-C08-C09
4	B	403	PGW	C06-C07-C08-C09
4	D	403	PGW	O04-C19-O03-C01
4	A	403	PGW	O04-C19-O03-C01
4	B	403	PGW	O04-C19-O03-C01
2	D	401	PRP	C3-C4-C5-O5
4	D	403	PGW	C6-C7-C8-C9
4	A	403	PGW	C6-C7-C8-C9
4	B	403	PGW	C6-C7-C8-C9
4	D	403	PGW	C1-C2-C3-C4
4	A	403	PGW	C1-C2-C3-C4
4	B	403	PGW	C1-C2-C3-C4
2	D	401	PRP	O4-C4-C5-O5
2	A	401	PRP	O4-C4-C5-O5
4	A	403	PGW	C27-C15-C16-C17
4	D	403	PGW	C27-C15-C16-C17
4	B	403	PGW	C27-C15-C16-C17
4	D	403	PGW	C09-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
4	B	403	PGW	C09-C11-C12-C13
4	A	403	PGW	C09-C11-C12-C13
2	A	401	PRP	C5-O5-P-O1P
4	D	403	PGW	C08-C09-C11-C12
4	A	403	PGW	C08-C09-C11-C12
4	B	403	PGW	C08-C09-C11-C12
4	D	403	PGW	C11-C12-C13-C14
4	A	403	PGW	C11-C12-C13-C14
4	B	403	PGW	C11-C12-C13-C14
4	A	403	PGW	C18-C28-C30-C29
4	D	403	PGW	C18-C28-C30-C29
4	B	403	PGW	C18-C28-C30-C29
2	A	401	PRP	C3-C4-C5-O5
4	D	403	PGW	C24-C25-C26-C27
4	B	403	PGW	C24-C25-C26-C27
4	A	403	PGW	C24-C25-C26-C27
4	D	403	PGW	C02-C03-O11-P
4	A	403	PGW	C02-C03-O11-P
4	B	403	PGW	C02-C03-O11-P
4	D	403	PGW	OAF-C05-CAD-OAE
4	A	403	PGW	OAF-C05-CAD-OAE
4	B	403	PGW	OAF-C05-CAD-OAE
4	D	403	PGW	C04-O12-P-O13
4	A	403	PGW	C04-O12-P-O13
4	B	403	PGW	C04-O12-P-O13
4	D	403	PGW	C21-C22-C23-C24
4	A	403	PGW	C21-C22-C23-C24
4	B	403	PGW	C21-C22-C23-C24
4	D	403	PGW	O01-C02-C03-O11
4	A	403	PGW	O01-C02-C03-O11
4	B	403	PGW	O01-C02-C03-O11
2	B	401	PRP	C5-O5-P-O1P
4	D	403	PGW	O03-C01-C02-C03
4	A	403	PGW	O03-C01-C02-C03
4	B	403	PGW	O03-C01-C02-C03
4	D	403	PGW	C23-C24-C25-C26
4	B	403	PGW	C23-C24-C25-C26
4	A	403	PGW	C23-C24-C25-C26
4	D	403	PGW	C01-C02-C03-O11
4	A	403	PGW	C01-C02-C03-O11
4	B	403	PGW	C01-C02-C03-O11
2	D	401	PRP	PB-O3A-PA-O1A

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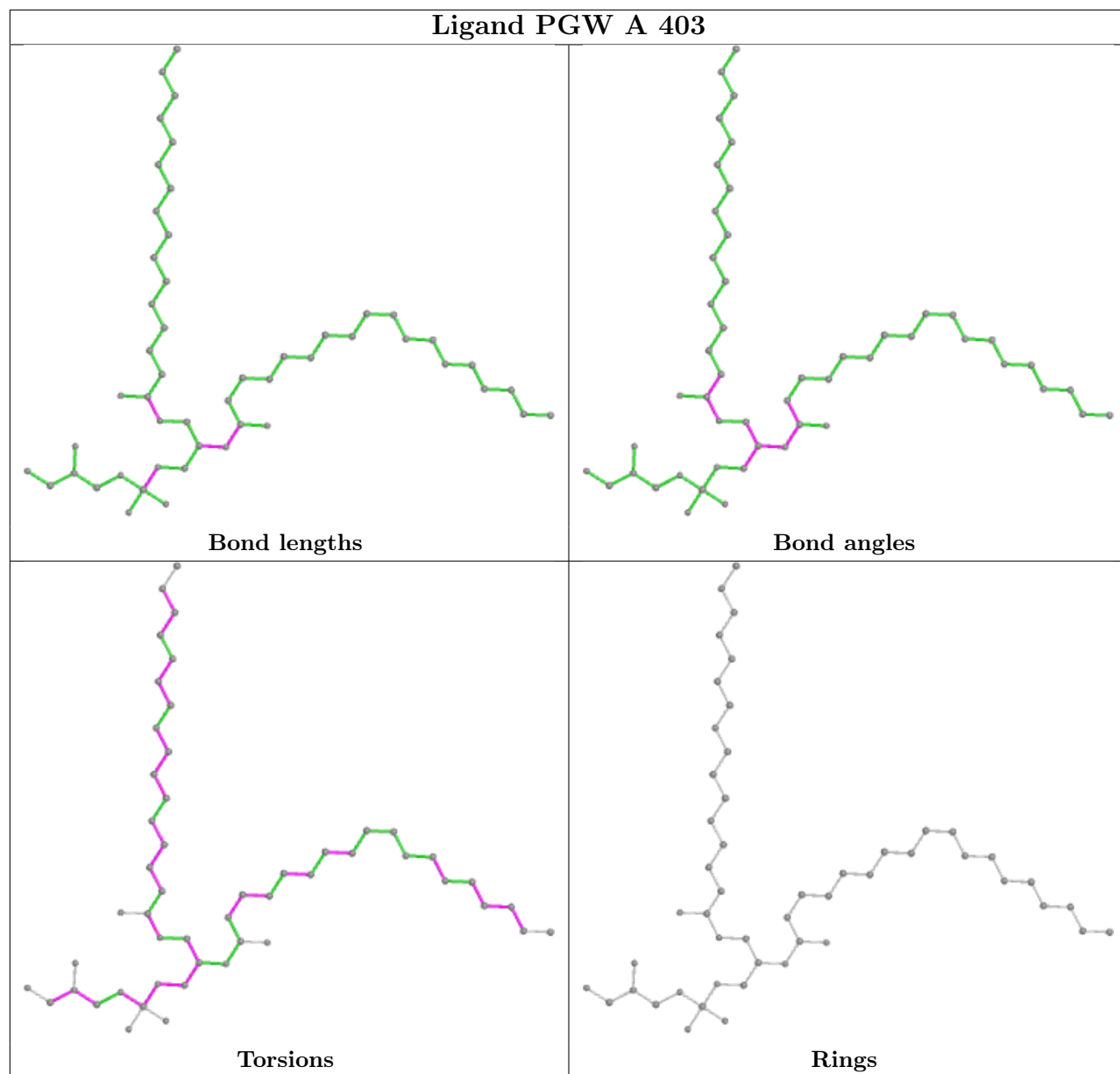
Mol	Chain	Res	Type	Atoms
2	B	401	PRP	C5-O5-P-O3P
2	B	401	PRP	C3-C4-C5-O5
2	B	401	PRP	PB-O3A-PA-O1A
4	D	403	PGW	C4-C5-C6-C7
4	A	403	PGW	C4-C5-C6-C7
4	B	403	PGW	C4-C5-C6-C7
4	D	403	PGW	C03-O11-P-O14
4	A	403	PGW	C03-O11-P-O14
4	B	403	PGW	C03-O11-P-O14
4	D	403	PGW	C15-C16-C17-C18
4	A	403	PGW	C15-C16-C17-C18
4	B	403	PGW	C15-C16-C17-C18

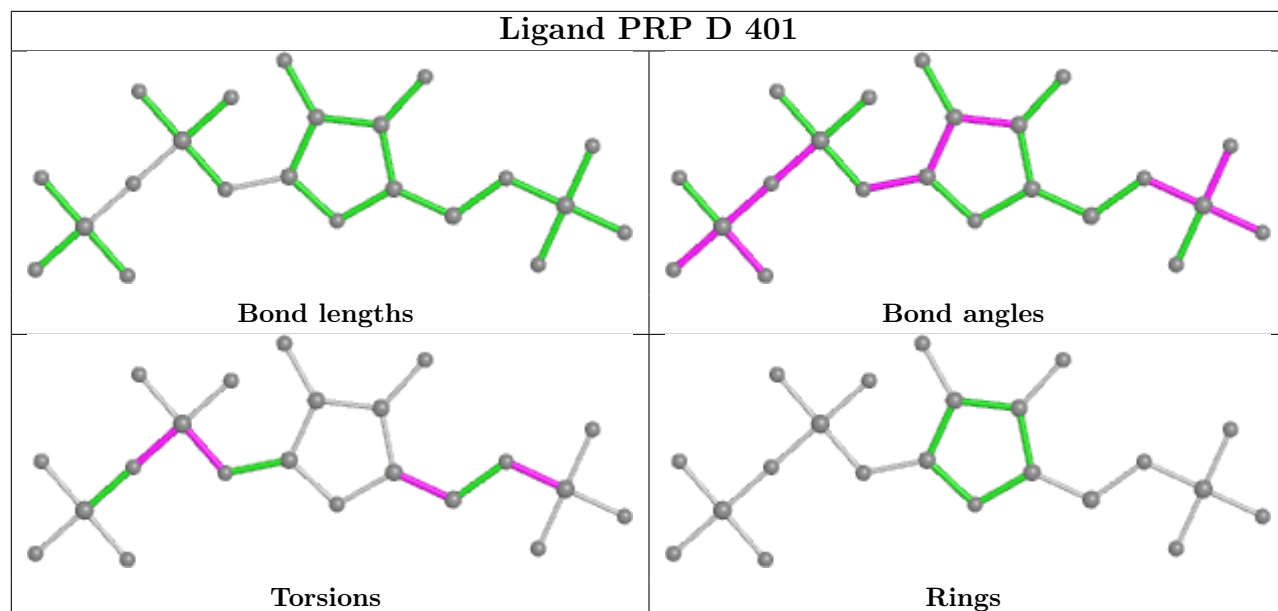
There are no ring outliers.

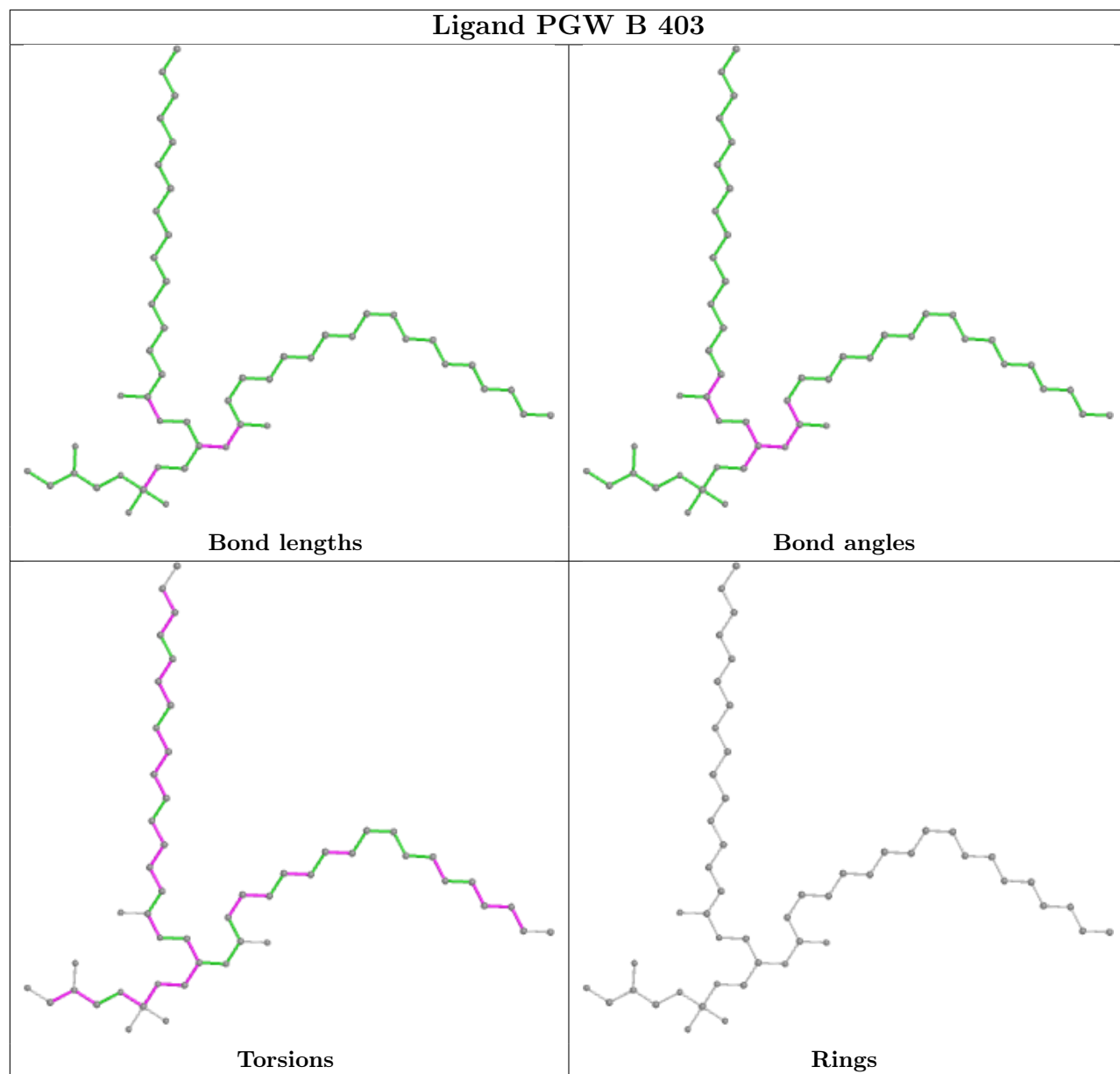
4 monomers are involved in 4 short contacts:

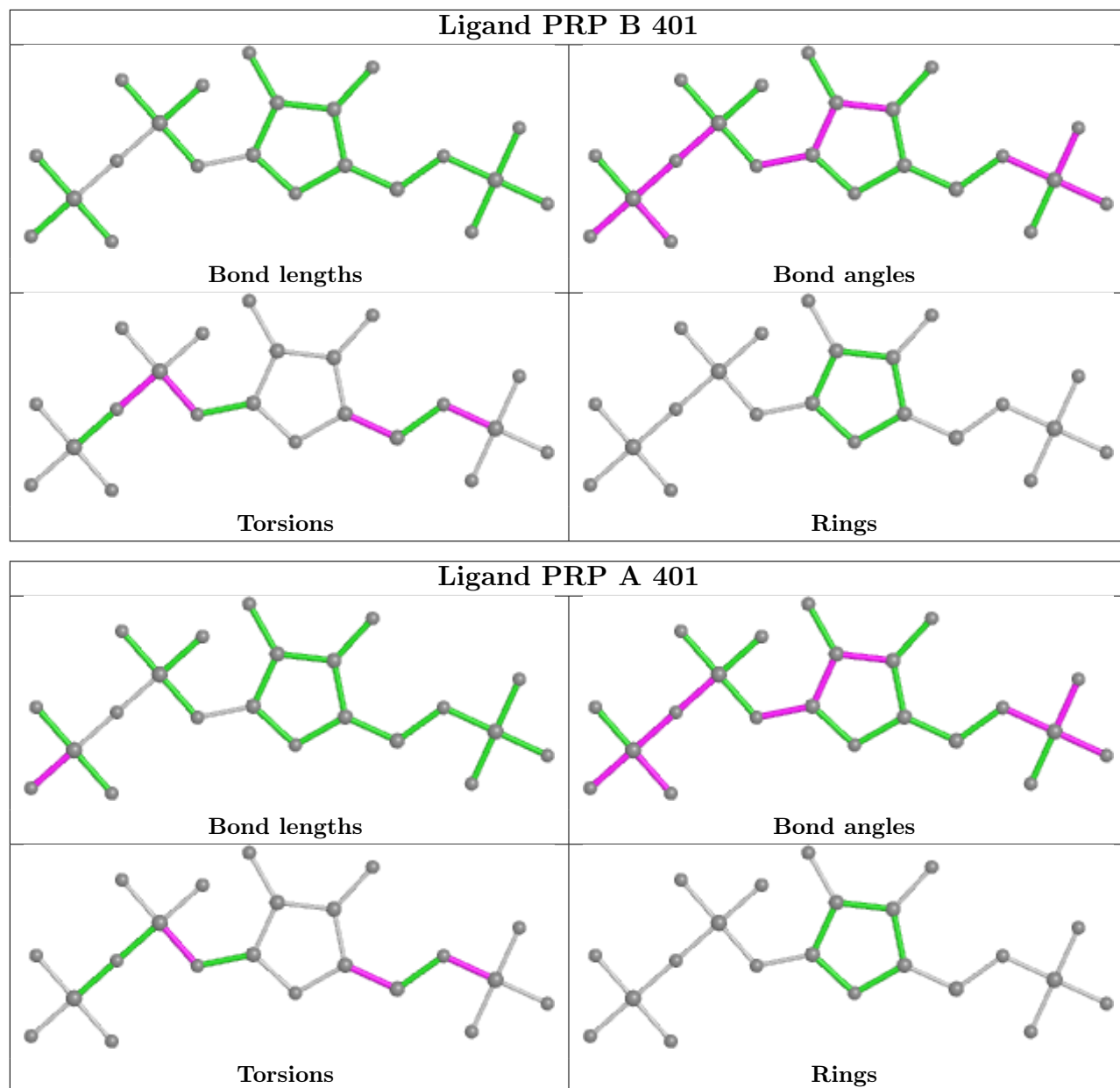
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	403	PGW	1	0
4	B	403	PGW	1	0
2	A	401	PRP	1	0
4	D	403	PGW	1	0

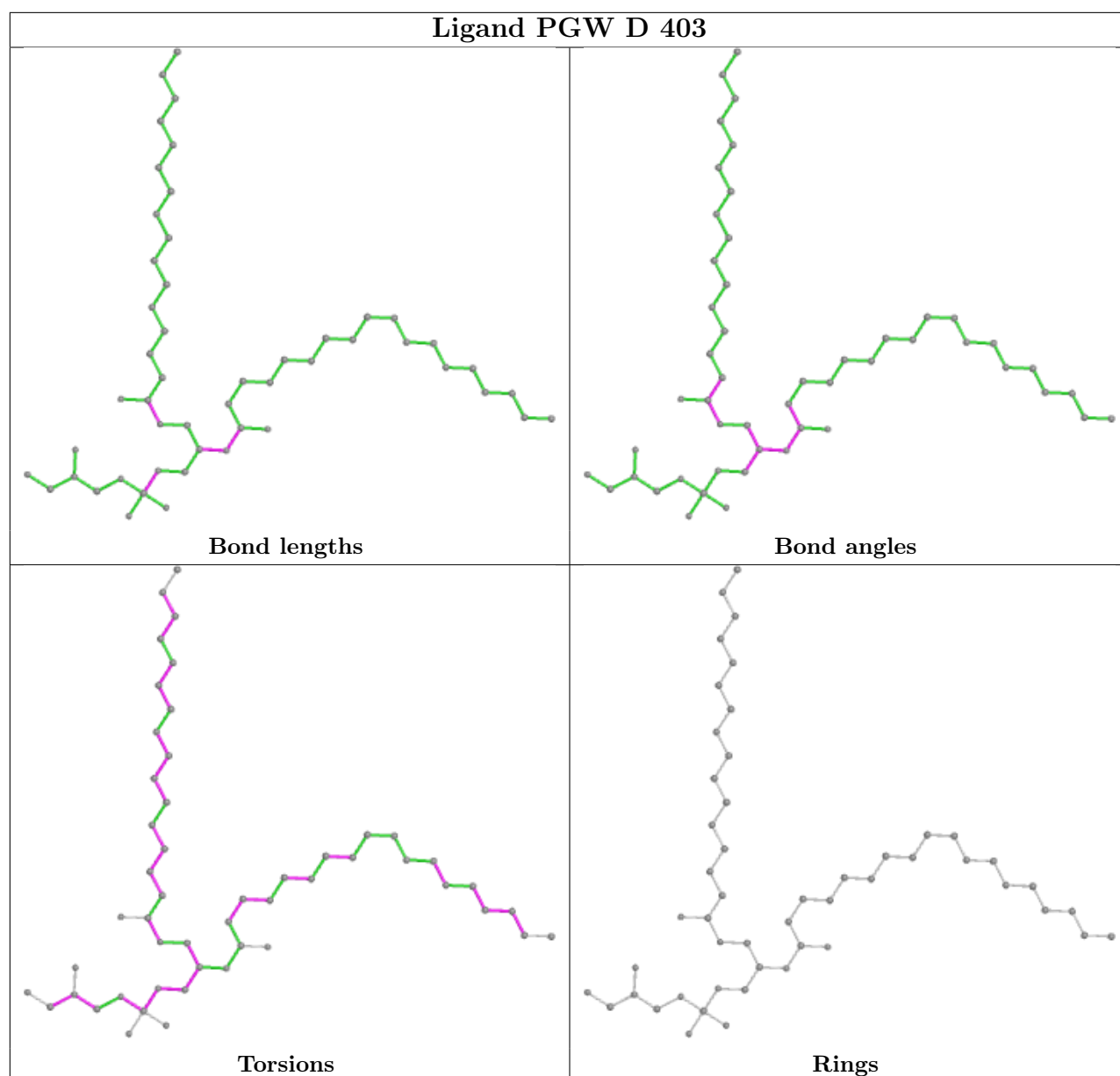
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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