



wwPDB EM Validation Summary Report ⓘ

Apr 15, 2026 – 02:58 AM UTC

PDB ID : 7JPW / pdb_00007jpw
EMDB ID : EMD-22425
Title : Rabbit Cav1.1 in the presence of 100 micromolar (R)-(+)-Bay K8644 in nanodiscs at 3.2 Angstrom resolution
Authors : Yan, N.; Gao, S.
Deposited on : 2020-08-10
Resolution : 3.20 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at
<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
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

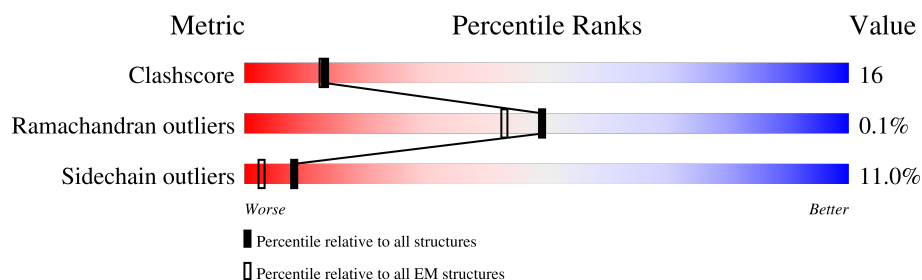
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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	1873	
2	E	222	
3	F	1105	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18583 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 Voltage-dependent L-type calcium channel subunit alpha-1S.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1115	Total	C	N	O	S	0	0
			9009	5976	1437	1537	59		

- Molecule 2 is a protein called Voltage-dependent calcium channel gamma-1 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	169	Total	C	N	O	S	0	0
			1326	872	216	220	18		

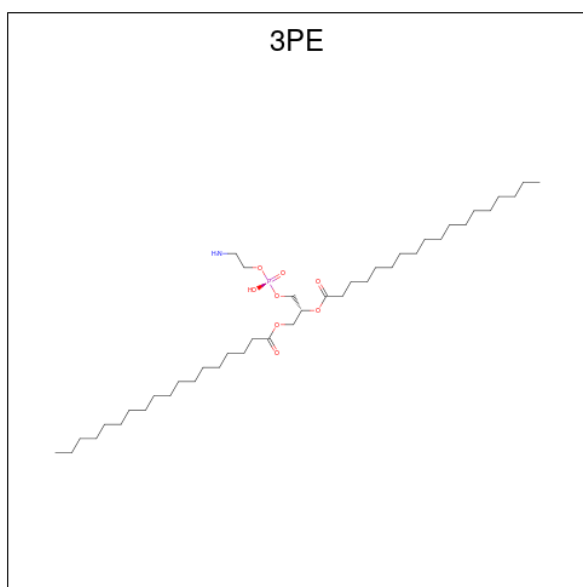
- Molecule 3 is a protein called Voltage-dependent calcium channel subunit alpha-2/delta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	973	Total	C	N	O	S	1	0
			7804	4942	1320	1510	32		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

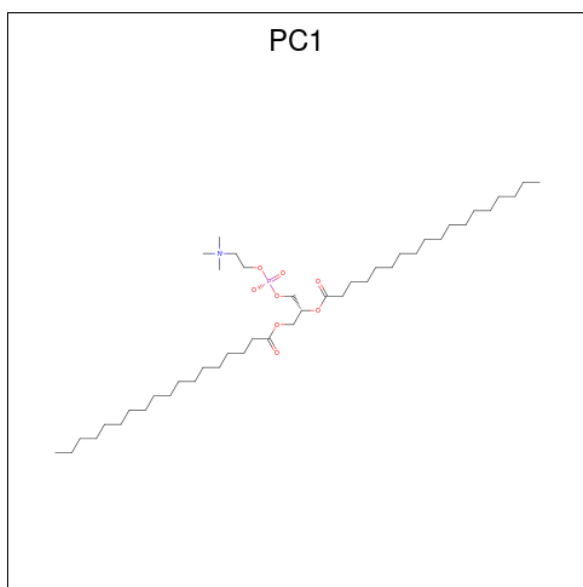
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Ca	0
			1	1	

- Molecule 5 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P).



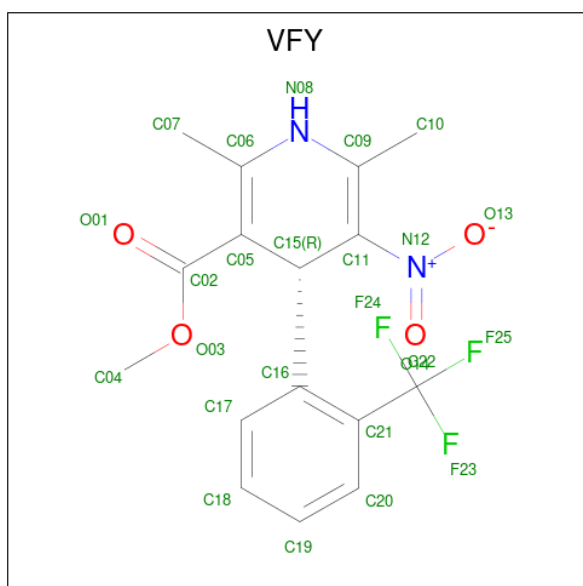
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			33	23	1	8	1	
5	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
5	A	1	Total	C	N	O	P	0
			43	33	1	8	1	
5	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
5	A	1	Total	C	N	O	P	0
			44	34	1	8	1	
5	A	1	Total	C	N	O	P	0
			38	28	1	8	1	
5	A	1	Total	C	N	O	P	0
			21	13	1	6	1	
5	A	1	Total	C	N	O	P	0
			32	22	1	8	1	
5	A	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 6 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 7 is methyl (4R)-2,6-dimethyl-5-nitro-4-[2-(trifluoromethyl)phenyl]-1,4-dihydropyridine-3-carboxylate (CCD ID: VFY) (formula: $C_{16}H_{15}F_3N_2O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	F	N	O	0
			25	16	3	2	4	



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	94695	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
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: PC1, CA, VFY, 3PE

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	0.55	0/9233	0.56	4/12534 (0.0%)
2	E	0.30	0/1358	0.54	2/1832 (0.1%)
3	F	0.70	0/7974	0.57	0/10816
All	All	0.60	0/18565	0.56	6/25182 (0.0%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	81	SER	CA-C-N	6.28	132.21	121.29
2	E	81	SER	C-N-CA	6.28	132.21	121.29
1	A	661	VAL	N-CA-C	-6.16	107.85	113.71
1	A	541	TYR	CA-C-N	5.30	131.66	121.54
1	A	541	TYR	C-N-CA	5.30	131.66	121.54

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	9009	0	9145	322	0
2	E	1326	0	1345	50	0
3	F	7804	0	7617	181	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
5	A	364	0	524	87	0
6	A	54	0	88	20	0
7	A	25	0	0	5	0
All	All	18583	0	18719	603	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 16.

The worst 5 of 603 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:502:PHE:HA	1:A:505:CYS:SG	1.35	1.65
1:A:647:CYS:SG	5:A:1905:3PE:C3I	2.04	1.43
1:A:502:PHE:CA	1:A:505:CYS:SG	2.14	1.33
5:A:1904:3PE:H2I1	7:A:1912:VFY:C04	1.64	1.25
1:A:1366:MET:CE	5:A:1904:3PE:H2A1	1.77	1.13

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	1095/1873 (58%)	993 (91%)	101 (9%)	1 (0%)	48	79
2	E	159/222 (72%)	142 (89%)	17 (11%)	0	100	100
3	F	968/1105 (88%)	871 (90%)	96 (10%)	1 (0%)	48	79
All	All	2222/3200 (69%)	2006 (90%)	214 (10%)	2 (0%)	49	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	542	TRP
3	F	871	THR

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	981/1628 (60%)	853 (87%)	128 (13%)	4	20
2	E	143/192 (74%)	128 (90%)	15 (10%)	6	28
3	F	868/973 (89%)	791 (91%)	77 (9%)	9	34
All	All	1992/2793 (71%)	1772 (89%)	220 (11%)	8	26

5 of 220 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1295	VAL
3	F	31	VAL
3	F	1068	LEU
3	F	798	SER
1	A	1342	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
3	F	348	ASN
3	F	847	ASN
3	F	470	ASN
3	F	556	GLN
3	F	1039	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 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$
5	3PE	A	1905	-	50,50,50	0.92	2 (4%)	53,55,55	1.06	3 (5%)
5	3PE	A	1908	-	20,20,50	1.05	1 (5%)	22,23,55	1.00	1 (4%)
6	PC1	A	1909	-	53,53,53	0.94	2 (3%)	59,61,61	1.02	3 (5%)
5	3PE	A	1910	-	31,31,50	1.17	2 (6%)	34,36,55	1.17	2 (5%)
5	3PE	A	1902	-	32,32,50	1.15	2 (6%)	35,37,55	1.20	4 (11%)
5	3PE	A	1907	-	37,37,50	1.07	2 (5%)	40,42,55	1.11	3 (7%)
5	3PE	A	1911	-	50,50,50	0.92	2 (4%)	53,55,55	1.06	3 (5%)
5	3PE	A	1903	-	50,50,50	0.92	2 (4%)	53,55,55	1.07	3 (5%)
5	3PE	A	1904	-	42,42,50	1.00	2 (4%)	45,47,55	1.12	3 (6%)
7	VFY	A	1912	-	24,26,26	3.75	7 (29%)	32,39,39	2.63	8 (25%)
5	3PE	A	1906	-	43,43,50	1.00	2 (4%)	46,48,55	1.10	3 (6%)

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
5	3PE	A	1905	-	-	29/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	3PE	A	1908	-	-	11/21/21/54	-
6	PC1	A	1909	-	-	35/57/57/57	-
5	3PE	A	1910	-	-	18/35/35/54	-
5	3PE	A	1902	-	-	12/36/36/54	-
5	3PE	A	1907	-	-	25/41/41/54	-
5	3PE	A	1911	-	-	25/54/54/54	-
5	3PE	A	1903	-	-	22/54/54/54	-
5	3PE	A	1904	-	-	25/46/46/54	-
7	VFY	A	1912	-	-	6/18/40/40	0/2/2/2
5	3PE	A	1906	-	-	31/47/47/54	-

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1912	VFY	C06-C05	15.28	1.53	1.35
7	A	1912	VFY	C06-N08	5.13	1.45	1.38
7	A	1912	VFY	C09-N08	4.82	1.44	1.38
5	A	1906	3PE	O31-C31	4.36	1.46	1.33
5	A	1907	3PE	O31-C31	4.30	1.45	1.33

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1912	VFY	C07-C06-C05	-8.40	119.26	127.61
7	A	1912	VFY	C10-C09-N08	5.46	119.76	113.42
7	A	1912	VFY	C07-C06-N08	5.04	119.28	113.42
5	A	1905	3PE	O21-C21-C22	4.42	121.05	111.48
5	A	1904	3PE	O21-C21-C22	4.41	121.02	111.48

There are no chirality outliers.

5 of 239 torsion outliers are listed below:

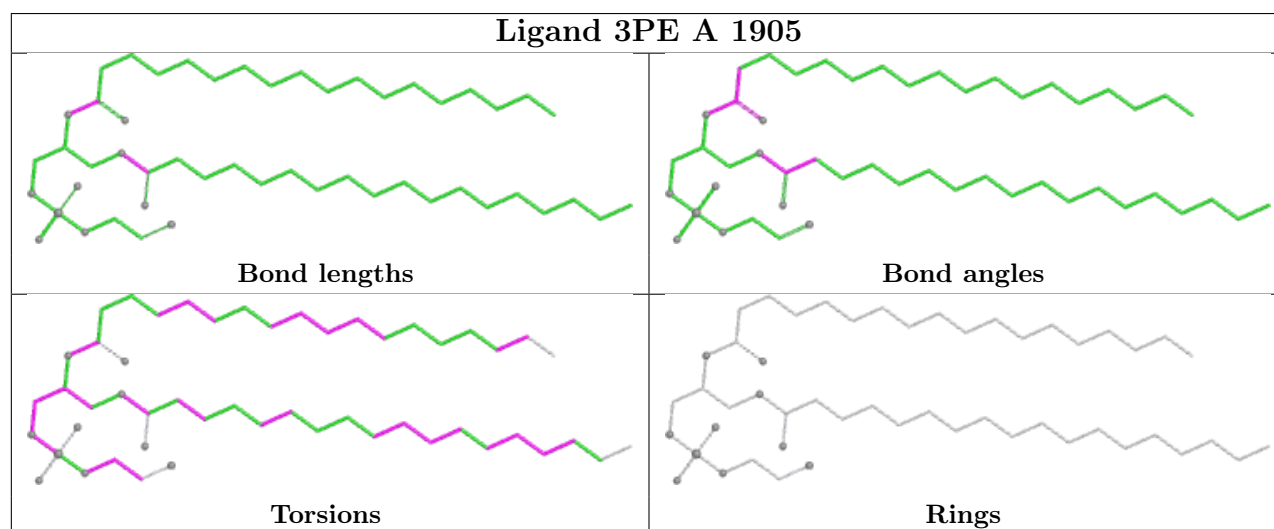
Mol	Chain	Res	Type	Atoms
5	A	1902	3PE	O22-C21-O21-C2
5	A	1902	3PE	C22-C21-O21-C2
5	A	1903	3PE	C22-C21-O21-C2
5	A	1904	3PE	C1-O11-P-O12
5	A	1904	3PE	C1-O11-P-O14

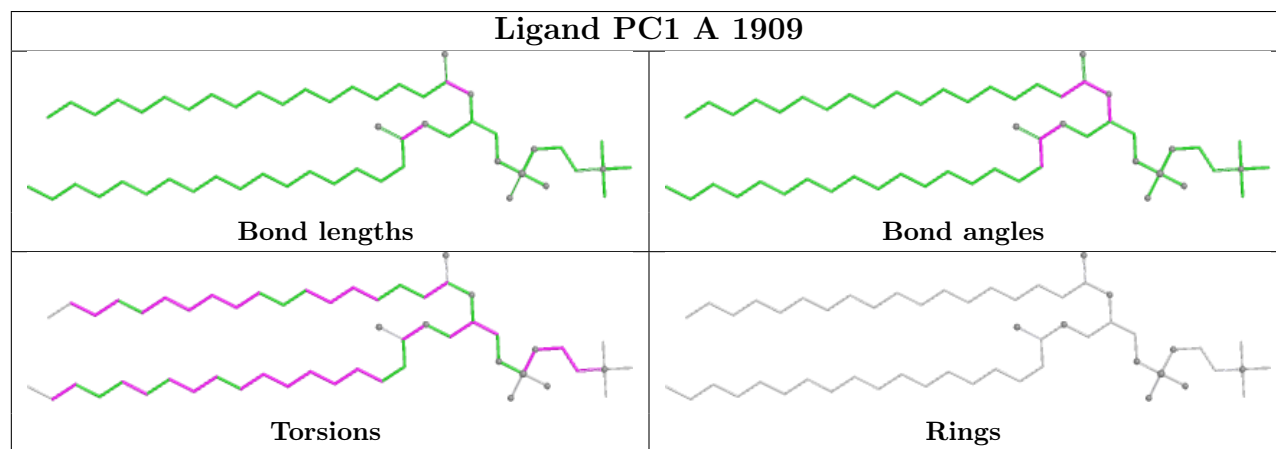
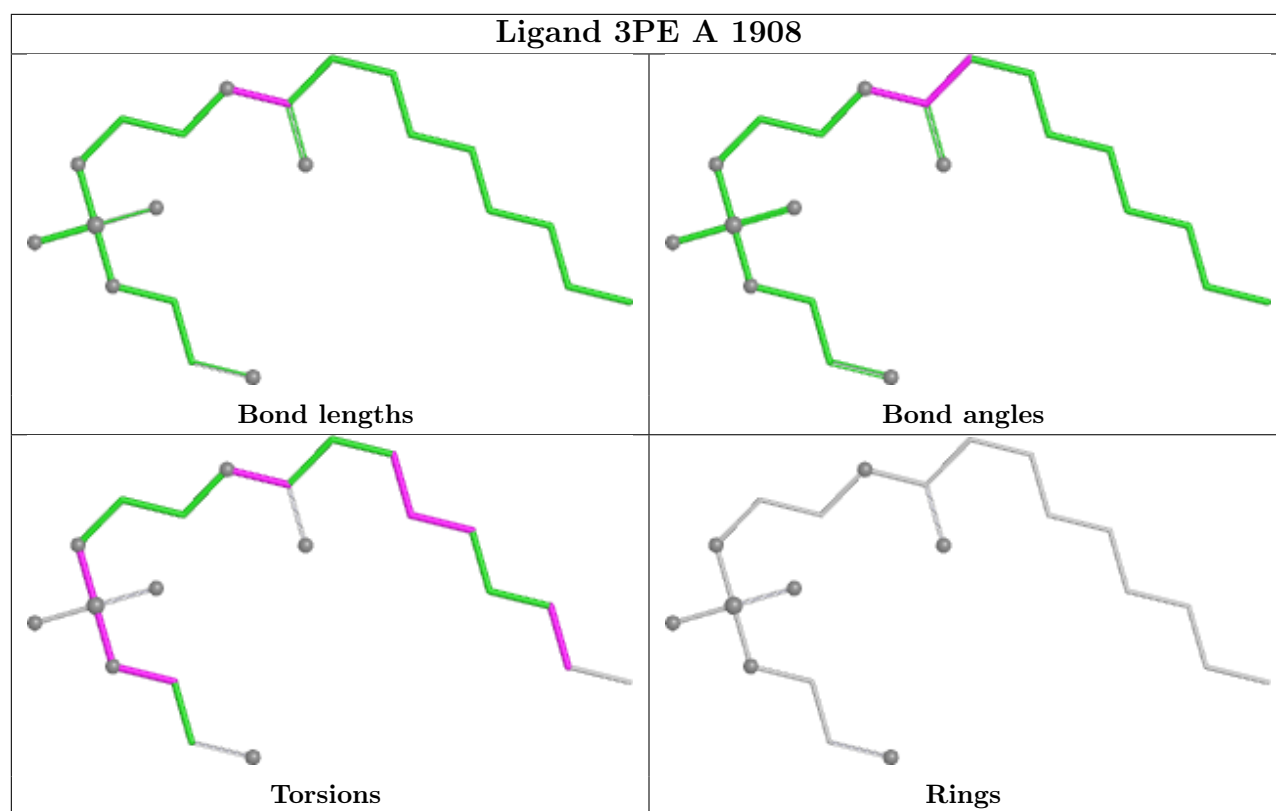
There are no ring outliers.

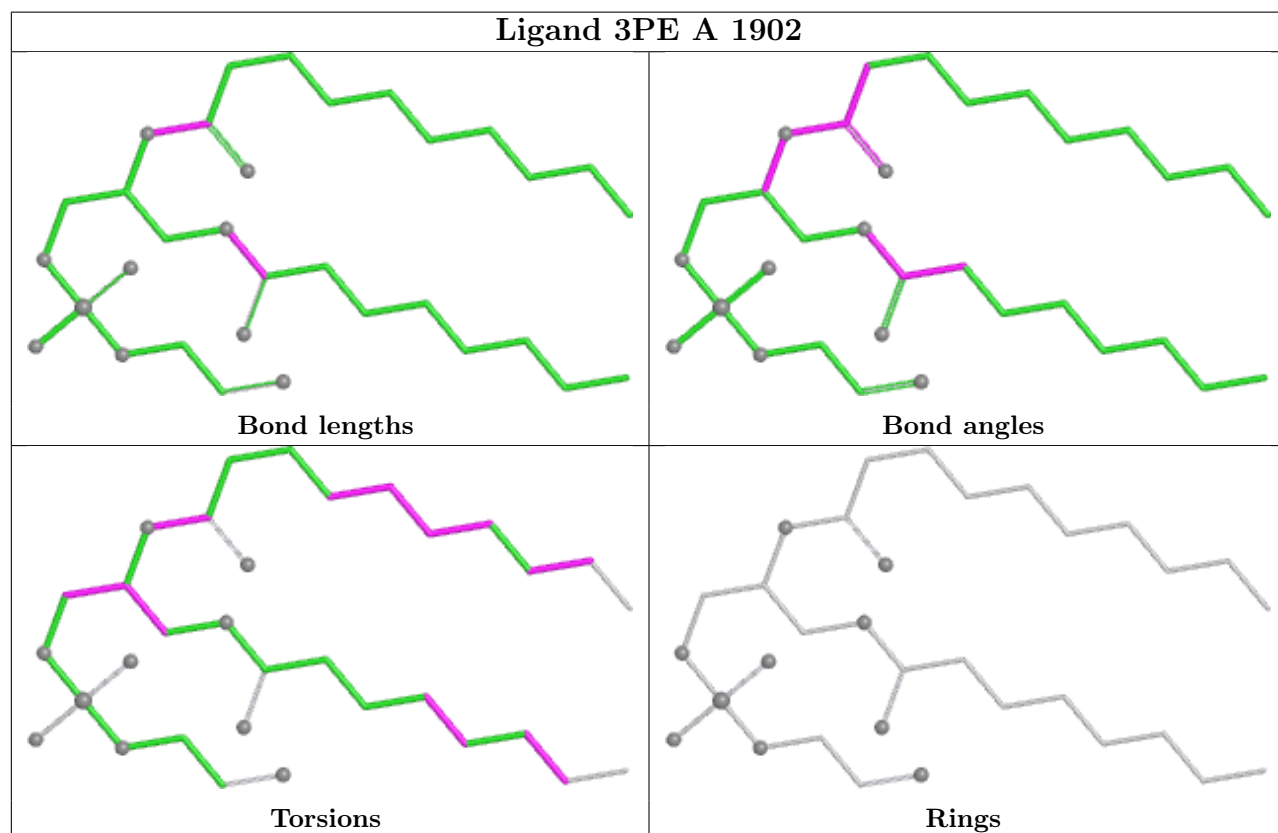
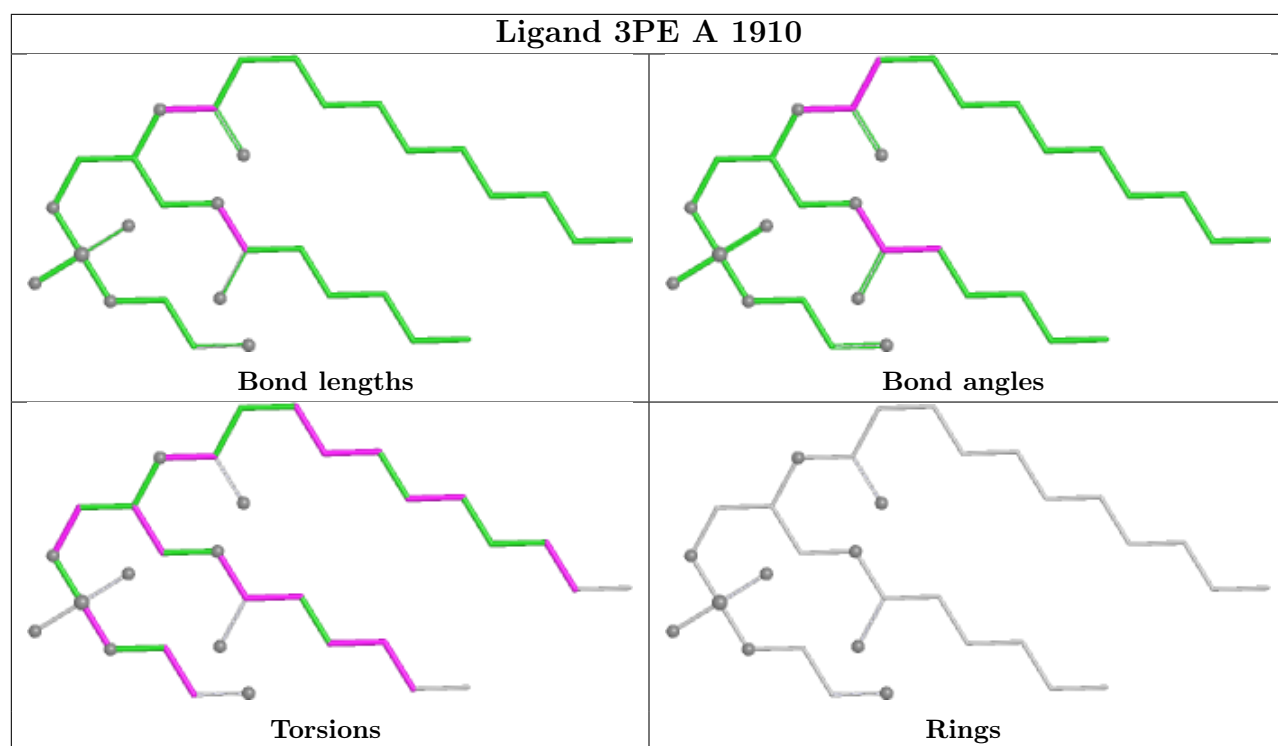
11 monomers are involved in 110 short contacts:

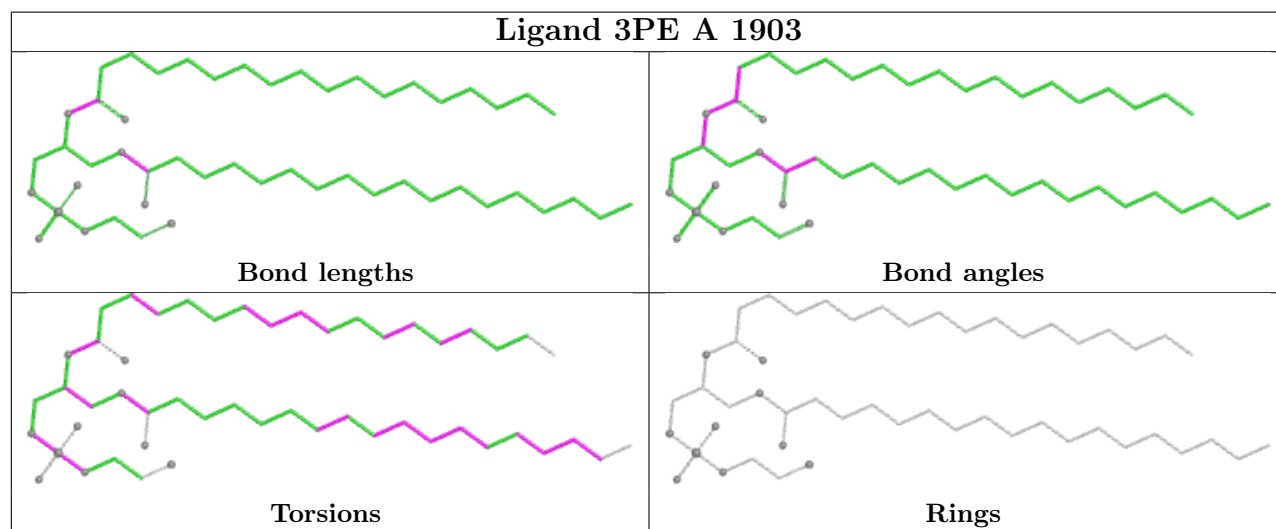
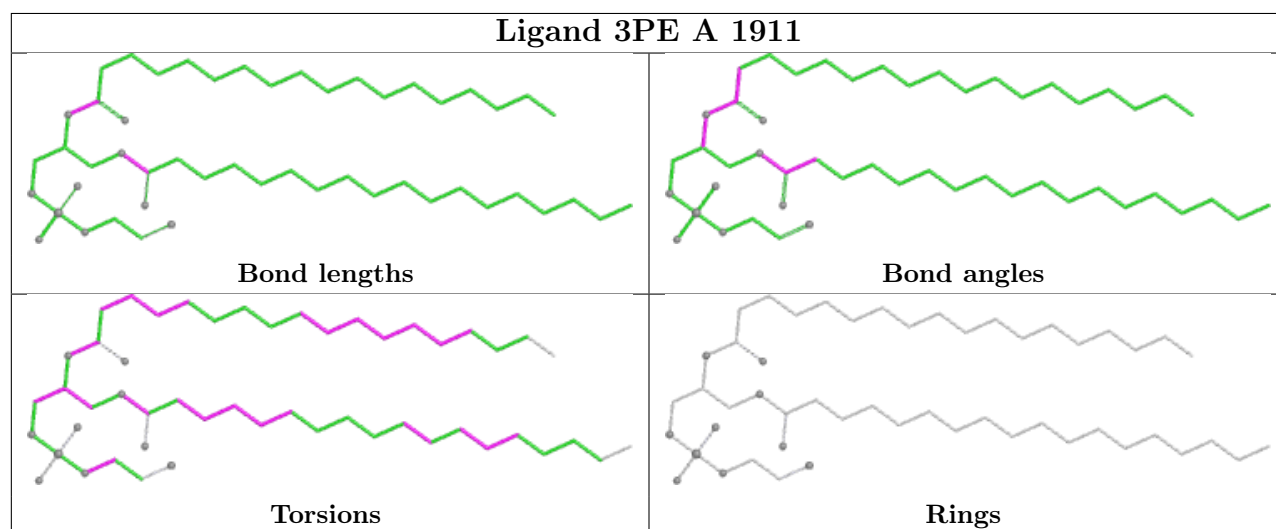
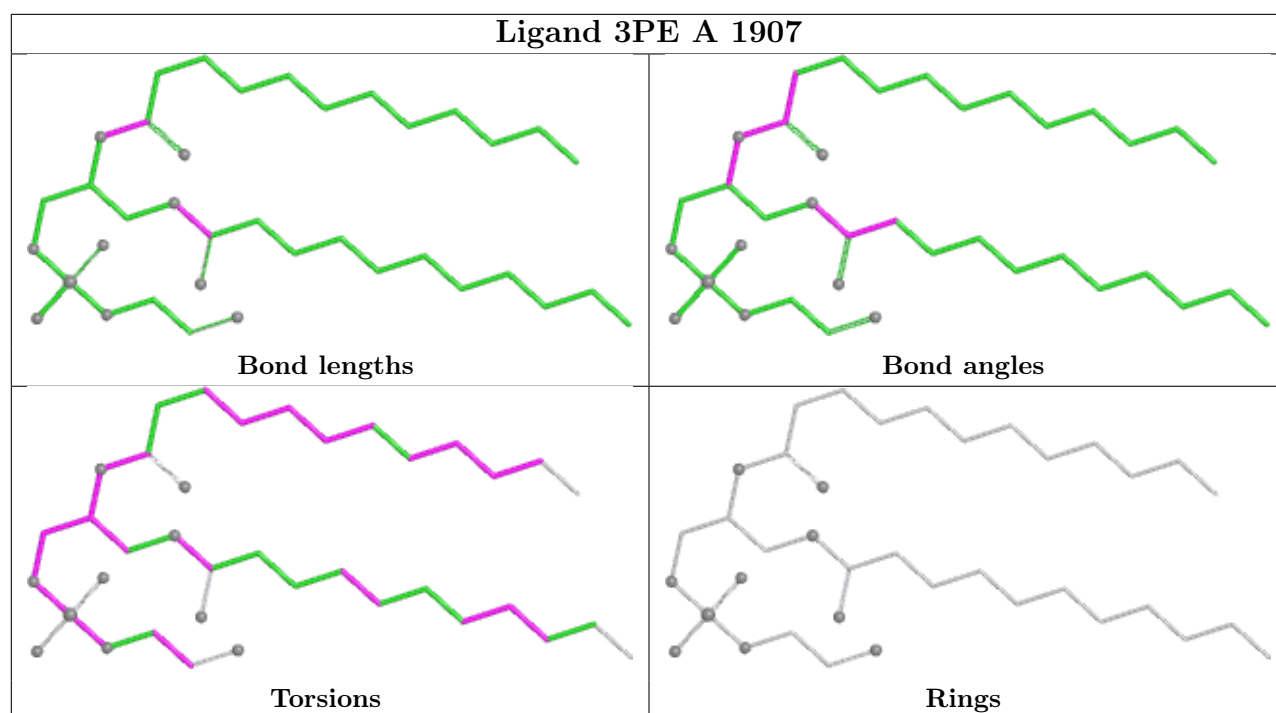
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1905	3PE	9	0
5	A	1908	3PE	10	0
6	A	1909	PC1	20	0
5	A	1910	3PE	4	0
5	A	1902	3PE	2	0
5	A	1907	3PE	11	0
5	A	1911	3PE	15	0
5	A	1903	3PE	12	0
5	A	1904	3PE	14	0
7	A	1912	VFY	5	0
5	A	1906	3PE	12	0

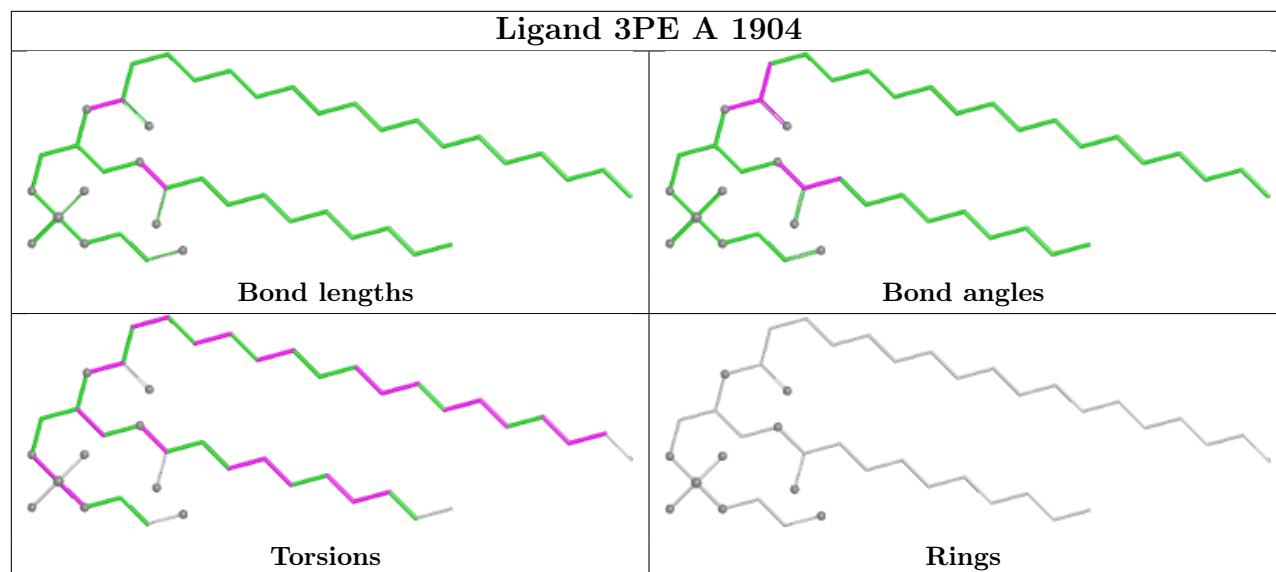
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

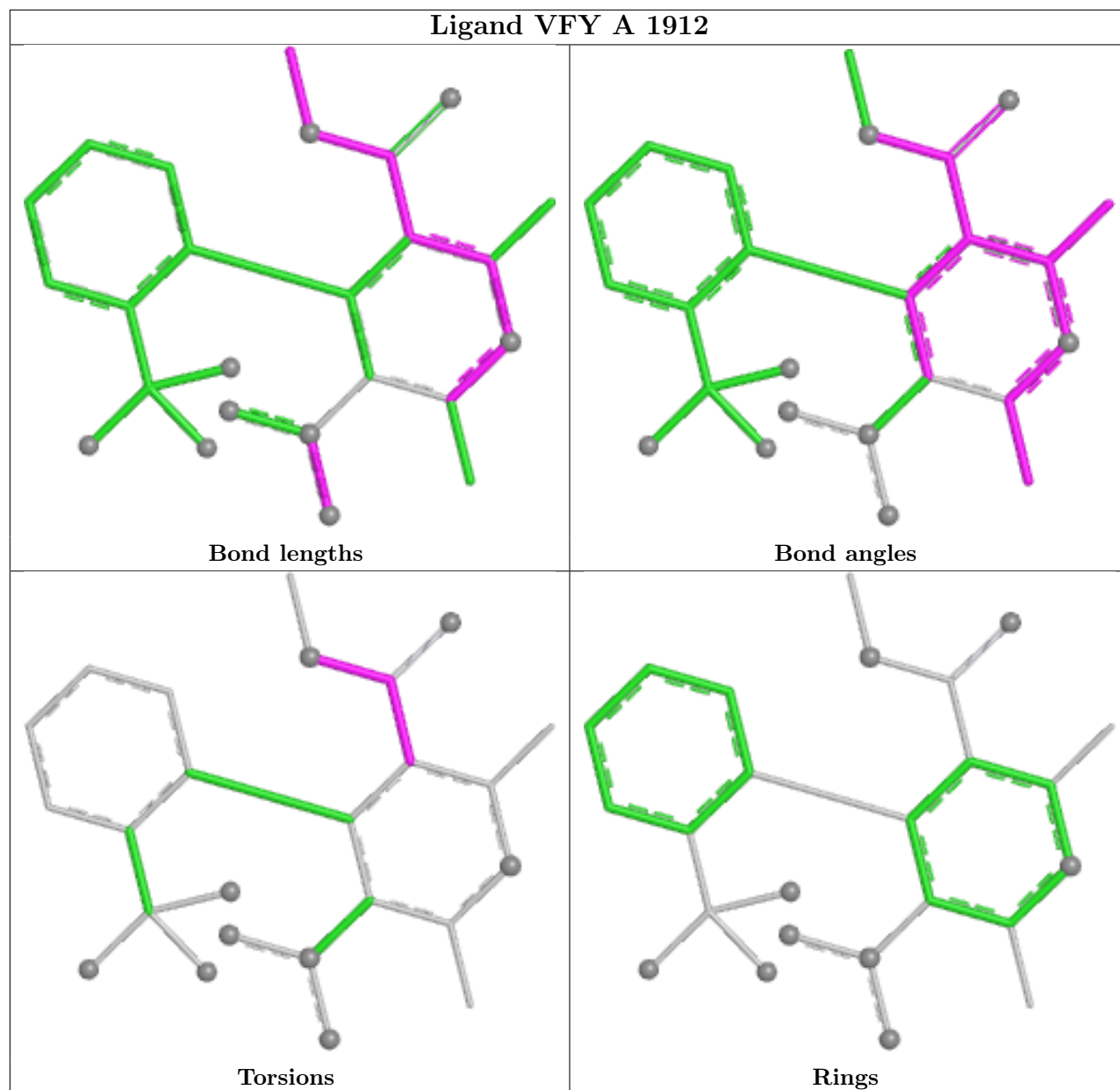


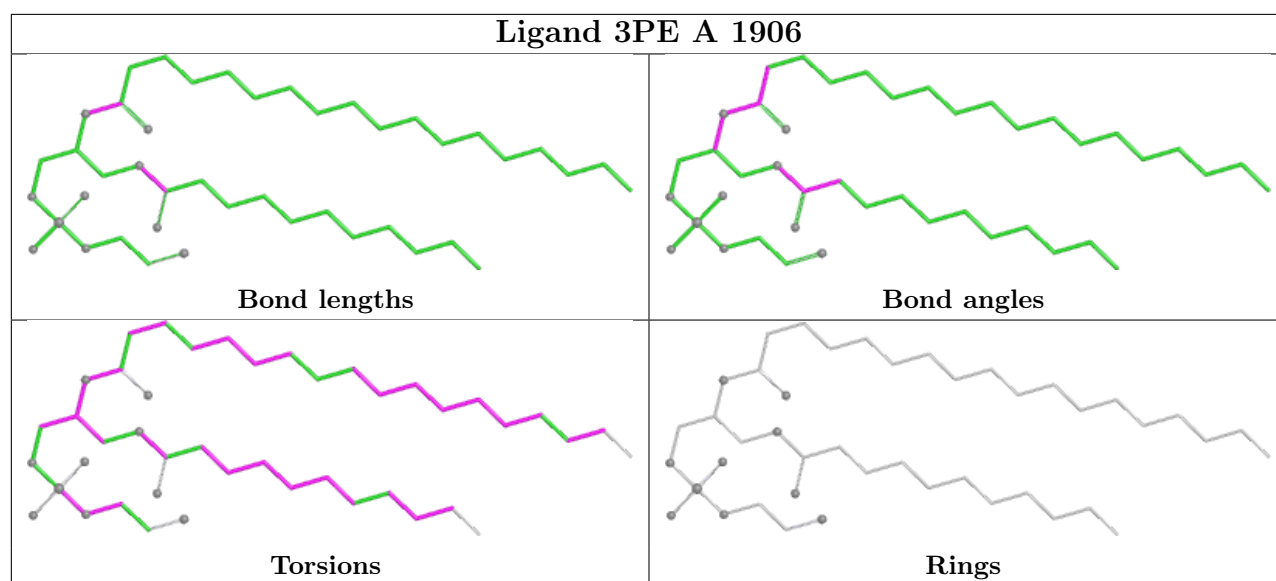












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-22425. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

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

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.