



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 02:17 AM UTC

PDB ID : 8EAR / pdb_00008ear
EMDB ID : EMD-27983
Title : Structure of the full-length IP3R1 channel determined in the presence of Calcium/IP3/ATP
Authors : Fan, G.; Baker, M.R.; Terry, L.E.; Arige, V.; Chen, M.; Seryshev, A.B.; Baker, M.L.; Ludtke, S.J.; Yule, D.I.; Serysheva, I.I.
Deposited on : 2022-08-29
Resolution : 3.50 Å (reported)
Based on initial model : 7LHE

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 : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : **FAILED**
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 : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

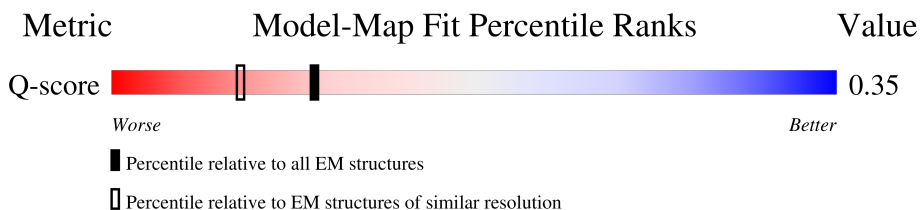
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Q-score	25397	13950 (3.00 - 4.00)

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

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 78512 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 Inositol 1,4,5-trisphosphate receptor type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2389	19296	12263	3334	3582	117	2	0
1	B	2389	19296	12263	3334	3582	117	2	0
1	C	2389	19296	12263	3334	3582	117	2	0
1	D	2389	19296	12263	3334	3582	117	2	0

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
2	A	1	1	1	0
2	B	1	1	1	0
2	C	1	1	1	0
2	D	1	1	1	0

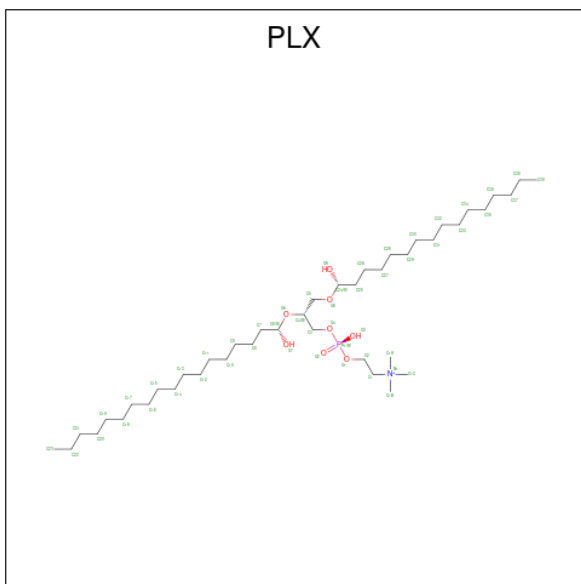
- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	O	P	0
			24	6	15	3	
4	B	1	Total	C	O	P	0
			24	6	15	3	
4	C	1	Total	C	O	P	0
			24	6	15	3	
4	D	1	Total	C	O	P	0
			24	6	15	3	

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	A	4	Total	Ca	0
			4	4	
5	B	4	Total	Ca	0
			4	4	
5	C	4	Total	Ca	0
			4	4	
5	D	4	Total	Ca	0
			4	4	

- Molecule 6 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (CCD ID: PLX) (formula: C₄₂H₈₉NO₈P).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
6	A	1	40	30	1	8	1	0
6	A	1	45	35	1	8	1	0
6	A	1	37	27	1	8	1	0
6	A	1	36	26	1	8	1	0
6	A	1	39	29	1	8	1	0
6	A	1	38	28	1	8	1	0
6	A	1	37	27	1	8	1	0
6	B	1	37	27	1	8	1	0
6	B	1	40	30	1	8	1	0
6	B	1	45	35	1	8	1	0
6	B	1	37	27	1	8	1	0
6	B	1	36	26	1	8	1	0
6	B	1	39	29	1	8	1	0
6	B	1	38	28	1	8	1	0
6	C	1	45	35	1	8	1	0
6	C	1	37	27	1	8	1	0
6	C	1	36	26	1	8	1	0
6	C	1	39	29	1	8	1	0
6	C	1	38	28	1	8	1	0
6	C	1	37	27	1	8	1	0
6	C	1	40	30	1	8	1	0
6	D	1	40	30	1	8	1	0

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Mol	Chain	Residues	Atoms					AltConf
6	D	1	Total	C	N	O	P	0
			45	35	1	8	1	
6	D	1	Total	C	N	O	P	0
			37	27	1	8	1	
6	D	1	Total	C	N	O	P	0
			36	26	1	8	1	
6	D	1	Total	C	N	O	P	0
			39	29	1	8	1	
6	D	1	Total	C	N	O	P	0
			38	28	1	8	1	
6	D	1	Total	C	N	O	P	0
			37	27	1	8	1	

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3 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	133740	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	46943	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.093	Depositor
Minimum map value	-0.049	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.011	Depositor
Map size (\AA)	359.52002, 359.52002, 359.52002	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.07, 1.07, 1.07	Depositor

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

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4.3.3 RNA [i](#)

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 56 ligands modelled in this entry, 20 are monoatomic - leaving 36 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
6	PLX	D	2802	-	39,39,51	1.22	5 (12%)	41,47,59	0.77	0
6	PLX	D	2812	-	38,38,51	1.22	5 (13%)	40,46,59	0.77	0
6	PLX	B	2802	-	36,36,51	1.22	5 (13%)	38,44,59	0.75	0
6	PLX	A	2809	-	44,44,51	1.19	5 (11%)	46,52,59	0.78	0
6	PLX	D	2811	-	35,35,51	1.26	4 (11%)	37,43,59	0.74	0
3	ATP	A	2802	-	32,33,33	0.36	0	48,52,52	0.29	0
6	PLX	B	2810	-	44,44,51	1.18	5 (11%)	46,52,59	0.79	0
6	PLX	A	2813	-	37,37,51	1.26	5 (13%)	39,45,59	0.70	0
6	PLX	C	2803	-	36,36,51	1.25	5 (13%)	38,44,59	0.77	1 (2%)
6	PLX	A	2812	-	38,38,51	1.21	5 (13%)	40,46,59	0.78	0
4	I3P	B	2804	-	24,24,24	1.33	3 (12%)	39,39,39	0.83	1 (2%)
6	PLX	C	2813	-	36,36,51	1.21	5 (13%)	38,44,59	0.75	1 (2%)
6	PLX	B	2813	-	38,38,51	1.21	5 (13%)	40,46,59	0.78	0
6	PLX	D	2813	-	37,37,51	1.26	5 (13%)	39,45,59	0.70	0
6	PLX	D	2809	-	44,44,51	1.19	5 (11%)	46,52,59	0.79	0
6	PLX	A	2814	-	36,36,51	1.22	5 (13%)	38,44,59	0.75	1 (2%)
6	PLX	A	2810	-	36,36,51	1.24	5 (13%)	38,44,59	0.77	1 (2%)
4	I3P	D	2804	-	24,24,24	1.32	3 (12%)	39,39,39	0.83	1 (2%)
6	PLX	C	2806	-	37,37,51	1.26	5 (13%)	39,45,59	0.70	0
6	PLX	C	2802	-	44,44,51	1.19	5 (11%)	46,52,59	0.79	0
6	PLX	B	2812	-	35,35,51	1.26	5 (14%)	37,43,59	0.73	0
6	PLX	B	2811	-	36,36,51	1.24	5 (13%)	38,44,59	0.77	1 (2%)
6	PLX	C	2814	-	39,39,51	1.22	4 (10%)	41,47,59	0.77	0
3	ATP	B	2803	-	32,33,33	0.35	0	48,52,52	0.29	0
6	PLX	B	2809	-	39,39,51	1.22	5 (12%)	41,47,59	0.77	0
6	PLX	B	2814	-	37,37,51	1.26	5 (13%)	39,45,59	0.70	0
3	ATP	D	2803	-	32,33,33	0.36	0	48,52,52	0.29	0
6	PLX	D	2810	-	36,36,51	1.25	5 (13%)	38,44,59	0.77	1 (2%)
6	PLX	C	2804	-	35,35,51	1.27	5 (14%)	37,43,59	0.74	0
6	PLX	D	2814	-	36,36,51	1.22	5 (13%)	38,44,59	0.75	1 (2%)
4	I3P	A	2803	-	24,24,24	1.32	3 (12%)	39,39,39	0.83	1 (2%)
4	I3P	C	2808	-	24,24,24	1.32	3 (12%)	39,39,39	0.83	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PLX	C	2805	-	38,38,51	1.21	5 (13%)	40,46,59	0.78	0
3	ATP	C	2807	-	32,33,33	0.35	0	48,52,52	0.29	0
6	PLX	A	2808	-	39,39,51	1.22	4 (10%)	41,47,59	0.77	0
6	PLX	A	2811	-	35,35,51	1.26	4 (11%)	37,43,59	0.74	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
6	PLX	D	2802	-	-	19/43/43/55	-
6	PLX	D	2812	-	-	23/42/42/55	-
6	PLX	B	2802	-	-	22/40/40/55	-
6	PLX	A	2809	-	-	28/48/48/55	-
6	PLX	D	2811	-	-	24/39/39/55	-
3	ATP	A	2802	-	-	8/22/38/38	0/3/3/3
6	PLX	B	2810	-	-	28/48/48/55	-
6	PLX	A	2813	-	-	21/41/41/55	-
6	PLX	C	2803	-	-	14/40/40/55	-
6	PLX	A	2812	-	-	23/42/42/55	-
4	I3P	B	2804	-	-	1/15/39/39	0/1/1/1
6	PLX	C	2813	-	-	22/40/40/55	-
6	PLX	B	2813	-	-	23/42/42/55	-
6	PLX	D	2813	-	-	21/41/41/55	-
6	PLX	D	2809	-	-	28/48/48/55	-
6	PLX	A	2814	-	-	22/40/40/55	-
6	PLX	A	2810	-	-	14/40/40/55	-
4	I3P	D	2804	-	-	1/15/39/39	0/1/1/1
6	PLX	C	2806	-	-	21/41/41/55	-
6	PLX	C	2802	-	-	28/48/48/55	-
6	PLX	B	2812	-	-	24/39/39/55	-
6	PLX	B	2811	-	-	14/40/40/55	-
6	PLX	C	2814	-	-	19/43/43/55	-
3	ATP	B	2803	-	-	8/22/38/38	0/3/3/3
6	PLX	B	2809	-	-	19/43/43/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PLX	B	2814	-	-	21/41/41/55	-
3	ATP	D	2803	-	-	8/22/38/38	0/3/3/3
6	PLX	D	2810	-	-	14/40/40/55	-
6	PLX	C	2804	-	-	24/39/39/55	-
6	PLX	D	2814	-	-	22/40/40/55	-
4	I3P	A	2803	-	-	1/15/39/39	0/1/1/1
4	I3P	C	2808	-	-	1/15/39/39	0/1/1/1
6	PLX	C	2805	-	-	23/42/42/55	-
3	ATP	C	2807	-	-	8/22/38/38	0/3/3/3
6	PLX	A	2808	-	-	19/43/43/55	-
6	PLX	A	2811	-	-	24/39/39/55	-

All (148) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	2804	PLX	O6-C4	-3.77	1.39	1.44
6	B	2809	PLX	O6-C4	-3.71	1.39	1.44
6	C	2814	PLX	O6-C4	-3.71	1.39	1.44
6	B	2812	PLX	O6-C4	-3.69	1.39	1.44
6	D	2809	PLX	O6-C4	-3.69	1.39	1.44
6	A	2809	PLX	O6-C4	-3.68	1.39	1.44
6	A	2811	PLX	O6-C4	-3.68	1.39	1.44
6	D	2811	PLX	O6-C4	-3.68	1.39	1.44
6	A	2808	PLX	O6-C4	-3.68	1.39	1.44
6	C	2802	PLX	O6-C4	-3.68	1.39	1.44
6	C	2803	PLX	O6-C4	-3.65	1.39	1.44
6	D	2810	PLX	O6-C4	-3.65	1.39	1.44
6	D	2802	PLX	O6-C4	-3.63	1.39	1.44
6	B	2814	PLX	O6-C4	-3.61	1.39	1.44
6	C	2806	PLX	O6-C4	-3.61	1.39	1.44
6	B	2810	PLX	O6-C4	-3.61	1.39	1.44
6	B	2811	PLX	O6-C4	-3.60	1.40	1.44
6	A	2812	PLX	O6-C4	-3.58	1.40	1.44
6	B	2813	PLX	O6-C4	-3.58	1.40	1.44
6	C	2805	PLX	O6-C4	-3.58	1.40	1.44
6	D	2812	PLX	O6-C4	-3.58	1.40	1.44
6	A	2810	PLX	O6-C4	-3.55	1.40	1.44
6	A	2813	PLX	O6-C4	-3.54	1.40	1.44
6	D	2813	PLX	O6-C4	-3.54	1.40	1.44
4	B	2804	I3P	P1-O1	3.22	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2804	I3P	P1-O1	3.20	1.65	1.59
4	B	2804	I3P	P5-O5	3.19	1.65	1.59
4	C	2808	I3P	P5-O5	3.19	1.65	1.59
4	D	2804	I3P	P5-O5	3.19	1.65	1.59
6	A	2814	PLX	O6-C4	-3.19	1.40	1.44
6	B	2802	PLX	O6-C4	-3.19	1.40	1.44
6	D	2814	PLX	O6-C4	-3.19	1.40	1.44
4	A	2803	I3P	P1-O1	3.19	1.65	1.59
4	C	2808	I3P	P1-O1	3.19	1.65	1.59
4	A	2803	I3P	P5-O5	3.19	1.65	1.59
4	B	2804	I3P	P4-O4	3.18	1.65	1.59
4	C	2808	I3P	P4-O4	3.17	1.65	1.59
4	A	2803	I3P	P4-O4	3.16	1.65	1.59
4	D	2804	I3P	P4-O4	3.14	1.65	1.59
6	C	2813	PLX	O6-C4	-3.09	1.40	1.44
6	B	2814	PLX	P1-O4	2.51	1.69	1.59
6	C	2806	PLX	P1-O4	2.51	1.69	1.59
6	A	2813	PLX	P1-O4	2.50	1.69	1.59
6	D	2813	PLX	P1-O4	2.50	1.69	1.59
6	C	2814	PLX	P1-O4	2.39	1.68	1.59
6	C	2804	PLX	P1-O4	2.39	1.68	1.59
6	A	2811	PLX	P1-O4	2.38	1.68	1.59
6	D	2811	PLX	P1-O4	2.38	1.68	1.59
6	A	2808	PLX	P1-O4	2.38	1.68	1.59
6	D	2802	PLX	P1-O4	2.38	1.68	1.59
6	A	2809	PLX	P1-O4	2.38	1.68	1.59
6	B	2810	PLX	P1-O4	2.38	1.68	1.59
6	C	2802	PLX	P1-O4	2.38	1.68	1.59
6	B	2812	PLX	P1-O4	2.37	1.68	1.59
6	D	2809	PLX	P1-O4	2.37	1.68	1.59
6	A	2810	PLX	P1-O4	2.37	1.68	1.59
6	B	2811	PLX	P1-O4	2.37	1.68	1.59
6	C	2803	PLX	P1-O4	2.37	1.68	1.59
6	D	2810	PLX	P1-O4	2.37	1.68	1.59
6	B	2809	PLX	P1-O4	2.37	1.68	1.59
6	A	2814	PLX	P1-O4	2.35	1.68	1.59
6	C	2813	PLX	P1-O4	2.35	1.68	1.59
6	D	2814	PLX	P1-O4	2.35	1.68	1.59
6	A	2812	PLX	P1-O4	2.35	1.68	1.59
6	B	2813	PLX	P1-O4	2.35	1.68	1.59
6	D	2812	PLX	P1-O4	2.35	1.68	1.59
6	C	2805	PLX	P1-O4	2.34	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	2802	PLX	P1-O4	2.33	1.68	1.59
6	A	2814	PLX	C7-C6	2.22	1.55	1.50
6	B	2802	PLX	C7-C6	2.22	1.55	1.50
6	D	2814	PLX	C7-C6	2.22	1.55	1.50
6	C	2813	PLX	C7-C6	2.18	1.55	1.50
6	D	2812	PLX	C7-C6	2.11	1.55	1.50
6	A	2813	PLX	C7-C6	2.11	1.55	1.50
6	B	2809	PLX	C1A-N1	-2.10	1.43	1.50
6	B	2810	PLX	C7-C6	2.10	1.55	1.50
6	D	2809	PLX	C7-C6	2.10	1.55	1.50
6	A	2813	PLX	C1A-N1	-2.10	1.43	1.50
6	B	2814	PLX	C1A-N1	-2.10	1.43	1.50
6	C	2806	PLX	C1A-N1	-2.10	1.43	1.50
6	A	2812	PLX	C1A-N1	-2.10	1.43	1.50
6	C	2805	PLX	C1A-N1	-2.09	1.43	1.50
6	D	2812	PLX	C1A-N1	-2.09	1.43	1.50
6	B	2813	PLX	C7-C6	2.09	1.55	1.50
6	B	2813	PLX	C1A-N1	-2.09	1.43	1.50
6	D	2802	PLX	C1A-N1	-2.09	1.43	1.50
6	C	2803	PLX	C7-C6	2.08	1.55	1.50
6	C	2803	PLX	C1A-N1	-2.08	1.44	1.50
6	D	2813	PLX	C1A-N1	-2.08	1.44	1.50
6	D	2811	PLX	C1A-N1	-2.07	1.44	1.50
6	B	2811	PLX	P1-O1	2.07	1.67	1.59
6	D	2810	PLX	C7-C6	2.07	1.55	1.50
6	A	2813	PLX	P1-O1	2.07	1.67	1.59
6	B	2814	PLX	P1-O1	2.07	1.67	1.59
6	C	2806	PLX	P1-O1	2.07	1.67	1.59
6	A	2811	PLX	C7-C6	2.07	1.55	1.50
6	D	2811	PLX	C7-C6	2.07	1.55	1.50
6	B	2814	PLX	C7-C6	2.07	1.55	1.50
6	C	2806	PLX	C7-C6	2.07	1.55	1.50
6	D	2813	PLX	C7-C6	2.07	1.55	1.50
6	D	2813	PLX	P1-O1	2.06	1.67	1.59
6	A	2808	PLX	C1A-N1	-2.06	1.44	1.50
6	C	2814	PLX	C1A-N1	-2.06	1.44	1.50
6	A	2809	PLX	C7-C6	2.06	1.55	1.50
6	C	2802	PLX	C7-C6	2.06	1.55	1.50
6	A	2814	PLX	C1A-N1	-2.06	1.44	1.50
6	B	2802	PLX	C1A-N1	-2.06	1.44	1.50
6	C	2813	PLX	C1A-N1	-2.06	1.44	1.50
6	D	2814	PLX	C1A-N1	-2.06	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	2809	PLX	P1-O1	2.06	1.67	1.59
6	A	2810	PLX	P1-O1	2.05	1.67	1.59
6	C	2803	PLX	P1-O1	2.05	1.67	1.59
6	D	2810	PLX	P1-O1	2.05	1.67	1.59
6	B	2810	PLX	C1A-N1	-2.05	1.44	1.50
6	C	2802	PLX	C1A-N1	-2.05	1.44	1.50
6	A	2812	PLX	C7-C6	2.05	1.55	1.50
6	C	2805	PLX	C7-C6	2.05	1.55	1.50
6	D	2809	PLX	C1A-N1	-2.05	1.44	1.50
6	D	2802	PLX	P1-O1	2.04	1.67	1.59
6	A	2811	PLX	C1A-N1	-2.04	1.44	1.50
6	B	2812	PLX	C1A-N1	-2.04	1.44	1.50
6	A	2809	PLX	C1A-N1	-2.04	1.44	1.50
6	C	2804	PLX	C1A-N1	-2.04	1.44	1.50
6	B	2811	PLX	C1A-N1	-2.04	1.44	1.50
6	B	2809	PLX	C7-C6	2.04	1.55	1.50
6	D	2802	PLX	C7-C6	2.04	1.55	1.50
6	B	2802	PLX	P1-O1	2.04	1.67	1.59
6	C	2813	PLX	P1-O1	2.04	1.67	1.59
6	C	2805	PLX	P1-O1	2.04	1.67	1.59
6	D	2812	PLX	P1-O1	2.04	1.67	1.59
6	B	2811	PLX	C7-C6	2.04	1.55	1.50
6	C	2804	PLX	C7-C6	2.03	1.55	1.50
6	A	2809	PLX	P1-O1	2.03	1.67	1.59
6	B	2810	PLX	P1-O1	2.03	1.67	1.59
6	A	2810	PLX	C1A-N1	-2.03	1.44	1.50
6	B	2812	PLX	P1-O1	2.03	1.67	1.59
6	A	2810	PLX	C7-C6	2.03	1.55	1.50
6	C	2802	PLX	P1-O1	2.03	1.67	1.59
6	A	2814	PLX	P1-O1	2.03	1.67	1.59
6	D	2814	PLX	P1-O1	2.03	1.67	1.59
6	C	2814	PLX	P1-O1	2.02	1.67	1.59
6	A	2808	PLX	P1-O1	2.02	1.67	1.59
6	D	2810	PLX	C1A-N1	-2.02	1.44	1.50
6	C	2804	PLX	P1-O1	2.02	1.67	1.59
6	A	2812	PLX	P1-O1	2.01	1.67	1.59
6	B	2813	PLX	P1-O1	2.01	1.67	1.59
6	B	2812	PLX	C7-C6	2.01	1.54	1.50
6	B	2809	PLX	P1-O1	2.01	1.67	1.59

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	2811	PLX	C8-C7-C6	-2.18	108.30	113.38
6	C	2803	PLX	C8-C7-C6	-2.18	108.31	113.38
6	D	2810	PLX	C8-C7-C6	-2.16	108.35	113.38
6	A	2810	PLX	C8-C7-C6	-2.15	108.38	113.38
4	A	2803	I3P	C5-C6-C1	2.04	113.25	109.11
4	D	2804	I3P	C5-C6-C1	2.04	113.25	109.11
4	B	2804	I3P	C5-C6-C1	2.03	113.22	109.11
4	C	2808	I3P	C5-C6-C1	2.01	113.19	109.11
6	A	2814	PLX	C26-C25-C24	-2.01	108.70	113.38
6	C	2813	PLX	C26-C25-C24	-2.01	108.71	113.38
6	D	2814	PLX	C26-C25-C24	-2.00	108.72	113.38

There are no chirality outliers.

All (640) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2802	ATP	C5'-O5'-PA-O1A
3	A	2802	ATP	C5'-O5'-PA-O2A
3	A	2802	ATP	C5'-O5'-PA-O3A
3	A	2802	ATP	O4'-C4'-C5'-O5'
3	B	2803	ATP	C5'-O5'-PA-O1A
3	B	2803	ATP	C5'-O5'-PA-O2A
3	B	2803	ATP	C5'-O5'-PA-O3A
3	B	2803	ATP	O4'-C4'-C5'-O5'
3	C	2807	ATP	C5'-O5'-PA-O1A
3	C	2807	ATP	C5'-O5'-PA-O2A
3	C	2807	ATP	C5'-O5'-PA-O3A
3	C	2807	ATP	O4'-C4'-C5'-O5'
3	D	2803	ATP	C5'-O5'-PA-O1A
3	D	2803	ATP	C5'-O5'-PA-O2A
3	D	2803	ATP	C5'-O5'-PA-O3A
3	D	2803	ATP	O4'-C4'-C5'-O5'
6	A	2808	PLX	O7-C6-O6-C4
6	A	2808	PLX	C3-O4-P1-O1
6	A	2808	PLX	C3-O4-P1-O2
6	A	2808	PLX	C3-O4-P1-O3
6	A	2808	PLX	C2-O1-P1-O4
6	A	2808	PLX	C2-O1-P1-O2
6	A	2808	PLX	C2-O1-P1-O3
6	A	2809	PLX	O7-C6-C7-C8
6	A	2809	PLX	O7-C6-O6-C4
6	A	2809	PLX	C2-O1-P1-O4
6	A	2809	PLX	C2-O1-P1-O2

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Mol	Chain	Res	Type	Atoms
6	A	2809	PLX	N1-C1-C2-O1
6	A	2809	PLX	O9-C24-O8-C5
6	A	2810	PLX	O7-C6-O6-C4
6	A	2810	PLX	C3-O4-P1-O1
6	A	2810	PLX	C3-O4-P1-O3
6	A	2810	PLX	N1-C1-C2-O1
6	A	2810	PLX	O9-C24-O8-C5
6	A	2810	PLX	O9-C24-C25-C26
6	A	2811	PLX	O7-C6-C7-C8
6	A	2811	PLX	C3-O4-P1-O1
6	A	2811	PLX	C3-O4-P1-O2
6	A	2811	PLX	C3-O4-P1-O3
6	A	2811	PLX	C2-O1-P1-O2
6	A	2811	PLX	C2-O1-P1-O3
6	A	2811	PLX	N1-C1-C2-O1
6	A	2812	PLX	O7-C6-C7-C8
6	A	2812	PLX	O7-C6-O6-C4
6	A	2812	PLX	O6-C4-C5-O8
6	A	2812	PLX	C3-O4-P1-O1
6	A	2812	PLX	C3-O4-P1-O2
6	A	2812	PLX	C3-O4-P1-O3
6	A	2812	PLX	C2-O1-P1-O4
6	A	2812	PLX	C2-O1-P1-O3
6	A	2812	PLX	O9-C24-C25-C26
6	A	2813	PLX	O7-C6-C7-C8
6	A	2813	PLX	O7-C6-O6-C4
6	A	2813	PLX	C4-C3-O4-P1
6	A	2813	PLX	C3-O4-P1-O1
6	A	2813	PLX	C3-O4-P1-O3
6	A	2813	PLX	O9-C24-O8-C5
6	A	2814	PLX	O7-C6-C7-C8
6	A	2814	PLX	O6-C6-C7-C8
6	A	2814	PLX	O7-C6-O6-C4
6	A	2814	PLX	C3-C4-O6-C6
6	A	2814	PLX	C3-O4-P1-O1
6	A	2814	PLX	C3-O4-P1-O2
6	A	2814	PLX	C3-O4-P1-O3
6	A	2814	PLX	C25-C24-O8-C5
6	B	2802	PLX	O7-C6-C7-C8
6	B	2802	PLX	O6-C6-C7-C8
6	B	2802	PLX	O7-C6-O6-C4
6	B	2802	PLX	C3-C4-O6-C6

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Mol	Chain	Res	Type	Atoms
6	B	2802	PLX	C3-O4-P1-O1
6	B	2802	PLX	C3-O4-P1-O2
6	B	2802	PLX	C3-O4-P1-O3
6	B	2802	PLX	C25-C24-O8-C5
6	B	2809	PLX	O7-C6-O6-C4
6	B	2809	PLX	C3-O4-P1-O1
6	B	2809	PLX	C3-O4-P1-O2
6	B	2809	PLX	C3-O4-P1-O3
6	B	2809	PLX	C2-O1-P1-O4
6	B	2809	PLX	C2-O1-P1-O2
6	B	2809	PLX	C2-O1-P1-O3
6	B	2810	PLX	O7-C6-C7-C8
6	B	2810	PLX	O7-C6-O6-C4
6	B	2810	PLX	C2-O1-P1-O4
6	B	2810	PLX	C2-O1-P1-O2
6	B	2810	PLX	N1-C1-C2-O1
6	B	2810	PLX	O9-C24-O8-C5
6	B	2811	PLX	O7-C6-O6-C4
6	B	2811	PLX	C3-O4-P1-O1
6	B	2811	PLX	C3-O4-P1-O3
6	B	2811	PLX	N1-C1-C2-O1
6	B	2811	PLX	O9-C24-O8-C5
6	B	2811	PLX	O9-C24-C25-C26
6	B	2812	PLX	O7-C6-C7-C8
6	B	2812	PLX	C3-O4-P1-O1
6	B	2812	PLX	C3-O4-P1-O2
6	B	2812	PLX	C3-O4-P1-O3
6	B	2812	PLX	C2-O1-P1-O2
6	B	2812	PLX	C2-O1-P1-O3
6	B	2812	PLX	N1-C1-C2-O1
6	B	2813	PLX	O7-C6-C7-C8
6	B	2813	PLX	O7-C6-O6-C4
6	B	2813	PLX	O6-C4-C5-O8
6	B	2813	PLX	C3-O4-P1-O1
6	B	2813	PLX	C3-O4-P1-O2
6	B	2813	PLX	C3-O4-P1-O3
6	B	2813	PLX	C2-O1-P1-O4
6	B	2813	PLX	C2-O1-P1-O3
6	B	2813	PLX	O9-C24-C25-C26
6	B	2814	PLX	O7-C6-C7-C8
6	B	2814	PLX	O7-C6-O6-C4
6	B	2814	PLX	C4-C3-O4-P1

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Mol	Chain	Res	Type	Atoms
6	B	2814	PLX	C3-O4-P1-O1
6	B	2814	PLX	C3-O4-P1-O3
6	B	2814	PLX	O9-C24-O8-C5
6	C	2802	PLX	O7-C6-C7-C8
6	C	2802	PLX	O7-C6-O6-C4
6	C	2802	PLX	C2-O1-P1-O4
6	C	2802	PLX	C2-O1-P1-O2
6	C	2802	PLX	N1-C1-C2-O1
6	C	2802	PLX	O9-C24-O8-C5
6	C	2803	PLX	O7-C6-O6-C4
6	C	2803	PLX	C3-O4-P1-O1
6	C	2803	PLX	C3-O4-P1-O3
6	C	2803	PLX	N1-C1-C2-O1
6	C	2803	PLX	O9-C24-O8-C5
6	C	2803	PLX	O9-C24-C25-C26
6	C	2804	PLX	O7-C6-C7-C8
6	C	2804	PLX	C3-O4-P1-O1
6	C	2804	PLX	C3-O4-P1-O2
6	C	2804	PLX	C3-O4-P1-O3
6	C	2804	PLX	C2-O1-P1-O2
6	C	2804	PLX	C2-O1-P1-O3
6	C	2804	PLX	N1-C1-C2-O1
6	C	2805	PLX	O7-C6-C7-C8
6	C	2805	PLX	O7-C6-O6-C4
6	C	2805	PLX	O6-C4-C5-O8
6	C	2805	PLX	C3-O4-P1-O1
6	C	2805	PLX	C3-O4-P1-O2
6	C	2805	PLX	C3-O4-P1-O3
6	C	2805	PLX	C2-O1-P1-O4
6	C	2805	PLX	C2-O1-P1-O3
6	C	2805	PLX	O9-C24-C25-C26
6	C	2806	PLX	O7-C6-C7-C8
6	C	2806	PLX	O7-C6-O6-C4
6	C	2806	PLX	C4-C3-O4-P1
6	C	2806	PLX	C3-O4-P1-O1
6	C	2806	PLX	C3-O4-P1-O3
6	C	2806	PLX	O9-C24-O8-C5
6	C	2813	PLX	O7-C6-C7-C8
6	C	2813	PLX	O6-C6-C7-C8
6	C	2813	PLX	O7-C6-O6-C4
6	C	2813	PLX	C3-C4-O6-C6
6	C	2813	PLX	C3-O4-P1-O1

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Mol	Chain	Res	Type	Atoms
6	C	2813	PLX	C3-O4-P1-O2
6	C	2813	PLX	C3-O4-P1-O3
6	C	2813	PLX	C25-C24-O8-C5
6	C	2814	PLX	O7-C6-O6-C4
6	C	2814	PLX	C3-O4-P1-O1
6	C	2814	PLX	C3-O4-P1-O2
6	C	2814	PLX	C3-O4-P1-O3
6	C	2814	PLX	C2-O1-P1-O4
6	C	2814	PLX	C2-O1-P1-O2
6	C	2814	PLX	C2-O1-P1-O3
6	D	2802	PLX	O7-C6-O6-C4
6	D	2802	PLX	C3-O4-P1-O1
6	D	2802	PLX	C3-O4-P1-O2
6	D	2802	PLX	C3-O4-P1-O3
6	D	2802	PLX	C2-O1-P1-O4
6	D	2802	PLX	C2-O1-P1-O2
6	D	2802	PLX	C2-O1-P1-O3
6	D	2809	PLX	O7-C6-C7-C8
6	D	2809	PLX	O7-C6-O6-C4
6	D	2809	PLX	C2-O1-P1-O4
6	D	2809	PLX	C2-O1-P1-O2
6	D	2809	PLX	N1-C1-C2-O1
6	D	2809	PLX	O9-C24-O8-C5
6	D	2810	PLX	O7-C6-O6-C4
6	D	2810	PLX	C3-O4-P1-O1
6	D	2810	PLX	C3-O4-P1-O3
6	D	2810	PLX	N1-C1-C2-O1
6	D	2810	PLX	O9-C24-O8-C5
6	D	2810	PLX	O9-C24-C25-C26
6	D	2811	PLX	O7-C6-C7-C8
6	D	2811	PLX	C3-O4-P1-O1
6	D	2811	PLX	C3-O4-P1-O2
6	D	2811	PLX	C3-O4-P1-O3
6	D	2811	PLX	C2-O1-P1-O2
6	D	2811	PLX	C2-O1-P1-O3
6	D	2811	PLX	N1-C1-C2-O1
6	D	2812	PLX	O7-C6-C7-C8
6	D	2812	PLX	O7-C6-O6-C4
6	D	2812	PLX	O6-C4-C5-O8
6	D	2812	PLX	C3-O4-P1-O1
6	D	2812	PLX	C3-O4-P1-O2
6	D	2812	PLX	C3-O4-P1-O3

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Mol	Chain	Res	Type	Atoms
6	D	2812	PLX	C2-O1-P1-O4
6	D	2812	PLX	C2-O1-P1-O3
6	D	2812	PLX	O9-C24-C25-C26
6	D	2813	PLX	O7-C6-C7-C8
6	D	2813	PLX	O7-C6-O6-C4
6	D	2813	PLX	C4-C3-O4-P1
6	D	2813	PLX	C3-O4-P1-O1
6	D	2813	PLX	C3-O4-P1-O3
6	D	2813	PLX	O9-C24-O8-C5
6	D	2814	PLX	O7-C6-C7-C8
6	D	2814	PLX	O6-C6-C7-C8
6	D	2814	PLX	O7-C6-O6-C4
6	D	2814	PLX	C3-C4-O6-C6
6	D	2814	PLX	C3-O4-P1-O1
6	D	2814	PLX	C3-O4-P1-O2
6	D	2814	PLX	C3-O4-P1-O3
6	D	2814	PLX	C25-C24-O8-C5
3	A	2802	ATP	C3'-C4'-C5'-O5'
3	B	2803	ATP	C3'-C4'-C5'-O5'
3	C	2807	ATP	C3'-C4'-C5'-O5'
3	D	2803	ATP	C3'-C4'-C5'-O5'
6	A	2809	PLX	O8-C24-C25-C26
6	A	2812	PLX	O8-C24-C25-C26
6	A	2813	PLX	O8-C24-C25-C26
6	B	2810	PLX	O8-C24-C25-C26
6	B	2813	PLX	O8-C24-C25-C26
6	B	2814	PLX	O8-C24-C25-C26
6	C	2802	PLX	O8-C24-C25-C26
6	C	2805	PLX	O8-C24-C25-C26
6	C	2806	PLX	O8-C24-C25-C26
6	D	2809	PLX	O6-C6-C7-C8
6	D	2809	PLX	O8-C24-C25-C26
6	D	2812	PLX	O8-C24-C25-C26
6	D	2813	PLX	O8-C24-C25-C26
6	B	2802	PLX	C28-C29-C30-C31
6	C	2813	PLX	C28-C29-C30-C31
6	D	2814	PLX	C28-C29-C30-C31
6	A	2814	PLX	C28-C29-C30-C31
6	A	2811	PLX	O9-C24-C25-C26
6	A	2813	PLX	O9-C24-C25-C26
6	A	2814	PLX	O9-C24-C25-C26
6	B	2802	PLX	O9-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
6	B	2812	PLX	O9-C24-C25-C26
6	B	2814	PLX	O9-C24-C25-C26
6	C	2804	PLX	O9-C24-C25-C26
6	C	2806	PLX	O9-C24-C25-C26
6	C	2813	PLX	O9-C24-C25-C26
6	D	2811	PLX	O9-C24-C25-C26
6	D	2813	PLX	O9-C24-C25-C26
6	D	2814	PLX	O9-C24-C25-C26
6	A	2810	PLX	C11-C10-C9-C8
6	B	2810	PLX	C12-C13-C14-C15
6	C	2803	PLX	C11-C10-C9-C8
6	D	2809	PLX	C12-C13-C14-C15
6	D	2810	PLX	C11-C10-C9-C8
6	A	2809	PLX	C12-C13-C14-C15
6	B	2811	PLX	C11-C10-C9-C8
6	C	2802	PLX	C12-C13-C14-C15
6	A	2814	PLX	C25-C26-C27-C28
6	B	2802	PLX	C25-C26-C27-C28
6	C	2813	PLX	C25-C26-C27-C28
6	D	2814	PLX	C25-C26-C27-C28
6	A	2811	PLX	C27-C28-C29-C30
6	C	2804	PLX	C27-C28-C29-C30
6	D	2811	PLX	C27-C28-C29-C30
6	B	2812	PLX	C27-C28-C29-C30
6	C	2805	PLX	C11-C10-C9-C8
6	D	2812	PLX	C11-C10-C9-C8
6	A	2812	PLX	C11-C10-C9-C8
6	B	2813	PLX	C11-C10-C9-C8
6	B	2809	PLX	C30-C31-C32-C33
6	C	2814	PLX	C30-C31-C32-C33
6	D	2802	PLX	C30-C31-C32-C33
6	A	2808	PLX	C28-C29-C30-C31
6	A	2808	PLX	C30-C31-C32-C33
6	B	2809	PLX	C28-C29-C30-C31
6	C	2814	PLX	C28-C29-C30-C31
6	D	2802	PLX	C28-C29-C30-C31
6	A	2809	PLX	C26-C27-C28-C29
6	B	2810	PLX	C26-C27-C28-C29
6	D	2809	PLX	C26-C27-C28-C29
6	C	2802	PLX	C26-C27-C28-C29
6	A	2811	PLX	C28-C29-C30-C31
6	C	2804	PLX	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
6	B	2812	PLX	C28-C29-C30-C31
6	D	2811	PLX	C28-C29-C30-C31
6	A	2809	PLX	C11-C12-C13-C14
6	D	2809	PLX	C11-C12-C13-C14
6	B	2810	PLX	C11-C12-C13-C14
6	C	2802	PLX	C11-C12-C13-C14
6	B	2811	PLX	C27-C28-C29-C30
6	A	2810	PLX	C27-C28-C29-C30
6	C	2803	PLX	C27-C28-C29-C30
6	D	2810	PLX	C27-C28-C29-C30
6	B	2802	PLX	C11-C10-C9-C8
6	C	2813	PLX	C11-C10-C9-C8
6	A	2814	PLX	C11-C10-C9-C8
6	D	2814	PLX	C11-C10-C9-C8
6	A	2811	PLX	C29-C30-C31-C32
6	A	2812	PLX	C10-C11-C12-C13
6	B	2812	PLX	C29-C30-C31-C32
6	B	2813	PLX	C10-C11-C12-C13
6	C	2804	PLX	C29-C30-C31-C32
6	C	2805	PLX	C10-C11-C12-C13
6	D	2812	PLX	C10-C11-C12-C13
6	D	2811	PLX	C29-C30-C31-C32
6	A	2808	PLX	C11-C10-C9-C8
6	B	2809	PLX	C11-C10-C9-C8
6	C	2814	PLX	C11-C10-C9-C8
6	D	2802	PLX	C11-C10-C9-C8
6	A	2809	PLX	O6-C6-C7-C8
6	A	2814	PLX	O8-C24-C25-C26
6	B	2802	PLX	O8-C24-C25-C26
6	B	2810	PLX	O6-C6-C7-C8
6	C	2802	PLX	O6-C6-C7-C8
6	C	2813	PLX	O8-C24-C25-C26
6	D	2814	PLX	O8-C24-C25-C26
6	A	2814	PLX	C3-C4-C5-O8
6	B	2802	PLX	C3-C4-C5-O8
6	C	2813	PLX	C3-C4-C5-O8
6	D	2814	PLX	C3-C4-C5-O8
6	A	2811	PLX	C26-C27-C28-C29
6	B	2812	PLX	C26-C27-C28-C29
6	C	2804	PLX	C26-C27-C28-C29
6	D	2811	PLX	C26-C27-C28-C29
6	A	2814	PLX	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
6	B	2802	PLX	C10-C11-C12-C13
6	C	2813	PLX	C10-C11-C12-C13
6	C	2802	PLX	C28-C29-C30-C31
6	D	2814	PLX	C10-C11-C12-C13
6	A	2809	PLX	C28-C29-C30-C31
6	B	2810	PLX	C28-C29-C30-C31
6	D	2809	PLX	C28-C29-C30-C31
6	C	2802	PLX	C25-C26-C27-C28
6	A	2809	PLX	C25-C26-C27-C28
6	A	2813	PLX	C10-C11-C12-C13
6	B	2810	PLX	C25-C26-C27-C28
6	D	2809	PLX	C25-C26-C27-C28
6	D	2813	PLX	C10-C11-C12-C13
6	B	2814	PLX	C10-C11-C12-C13
6	C	2806	PLX	C10-C11-C12-C13
6	C	2806	PLX	C30-C31-C32-C33
6	A	2809	PLX	C30-C31-C32-C33
6	B	2810	PLX	C30-C31-C32-C33
6	D	2809	PLX	C30-C31-C32-C33
6	A	2813	PLX	C30-C31-C32-C33
6	A	2814	PLX	C30-C31-C32-C33
6	B	2802	PLX	C30-C31-C32-C33
6	B	2814	PLX	C30-C31-C32-C33
6	C	2813	PLX	C30-C31-C32-C33
6	D	2813	PLX	C30-C31-C32-C33
6	D	2814	PLX	C30-C31-C32-C33
6	C	2802	PLX	C30-C31-C32-C33
6	C	2806	PLX	C25-C26-C27-C28
6	A	2813	PLX	C25-C26-C27-C28
6	B	2814	PLX	C25-C26-C27-C28
6	D	2813	PLX	C25-C26-C27-C28
6	A	2808	PLX	C10-C11-C12-C13
6	B	2810	PLX	C11-C10-C9-C8
6	C	2802	PLX	C11-C10-C9-C8
6	C	2814	PLX	C10-C11-C12-C13
6	D	2802	PLX	C10-C11-C12-C13
6	A	2809	PLX	C11-C10-C9-C8
6	B	2809	PLX	C10-C11-C12-C13
6	D	2809	PLX	C11-C10-C9-C8
6	A	2808	PLX	C9-C10-C11-C12
6	B	2809	PLX	C9-C10-C11-C12
6	B	2813	PLX	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
6	C	2814	PLX	C9-C10-C11-C12
6	D	2802	PLX	C9-C10-C11-C12
6	A	2812	PLX	C7-C8-C9-C10
6	C	2805	PLX	C7-C8-C9-C10
6	D	2812	PLX	C7-C8-C9-C10
6	A	2809	PLX	O9-C24-C25-C26
6	B	2810	PLX	O9-C24-C25-C26
6	C	2802	PLX	O9-C24-C25-C26
6	D	2809	PLX	O9-C24-C25-C26
6	A	2809	PLX	C10-C11-C12-C13
6	C	2802	PLX	C10-C11-C12-C13
6	D	2809	PLX	C10-C11-C12-C13
6	B	2810	PLX	C10-C11-C12-C13
6	A	2812	PLX	C29-C30-C31-C32
6	C	2805	PLX	C29-C30-C31-C32
6	D	2812	PLX	C29-C30-C31-C32
6	A	2810	PLX	C30-C31-C32-C33
6	B	2811	PLX	C30-C31-C32-C33
6	C	2803	PLX	C30-C31-C32-C33
6	D	2810	PLX	C30-C31-C32-C33
6	B	2813	PLX	C29-C30-C31-C32
6	A	2808	PLX	O4-C3-C4-C5
6	A	2813	PLX	O4-C3-C4-C5
6	B	2809	PLX	O4-C3-C4-C5
6	B	2814	PLX	O4-C3-C4-C5
6	C	2806	PLX	O4-C3-C4-C5
6	C	2814	PLX	O4-C3-C4-C5
6	D	2802	PLX	O4-C3-C4-C5
6	D	2813	PLX	O4-C3-C4-C5
6	A	2811	PLX	C3-C4-C5-O8
6	B	2812	PLX	C3-C4-C5-O8
6	C	2804	PLX	C3-C4-C5-O8
6	D	2811	PLX	C3-C4-C5-O8
6	A	2809	PLX	O4-C3-C4-O6
6	A	2812	PLX	O4-C3-C4-O6
6	B	2810	PLX	O4-C3-C4-O6
6	B	2813	PLX	O4-C3-C4-O6
6	C	2802	PLX	O4-C3-C4-O6
6	C	2805	PLX	O4-C3-C4-O6
6	D	2809	PLX	O4-C3-C4-O6
6	D	2812	PLX	O4-C3-C4-O6
6	A	2811	PLX	C4-C3-O4-P1

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Mol	Chain	Res	Type	Atoms
6	B	2812	PLX	C4-C3-O4-P1
6	C	2804	PLX	C4-C3-O4-P1
6	D	2811	PLX	C4-C3-O4-P1
6	A	2814	PLX	O6-C4-C5-O8
6	B	2802	PLX	O6-C4-C5-O8
6	C	2813	PLX	O6-C4-C5-O8
6	D	2814	PLX	O6-C4-C5-O8
6	A	2811	PLX	O6-C6-C7-C8
6	B	2812	PLX	O6-C6-C7-C8
6	C	2804	PLX	O6-C6-C7-C8
6	D	2811	PLX	O6-C6-C7-C8
6	D	2811	PLX	C25-C26-C27-C28
6	A	2811	PLX	C25-C26-C27-C28
6	B	2812	PLX	C25-C26-C27-C28
6	C	2804	PLX	C25-C26-C27-C28
6	A	2809	PLX	C27-C28-C29-C30
6	B	2810	PLX	C27-C28-C29-C30
6	D	2809	PLX	C27-C28-C29-C30
6	C	2802	PLX	C27-C28-C29-C30
6	D	2809	PLX	C33-C34-C35-C36
6	B	2810	PLX	C33-C34-C35-C36
6	C	2802	PLX	C33-C34-C35-C36
6	A	2809	PLX	C35-C36-C37-C38
6	B	2810	PLX	C35-C36-C37-C38
6	C	2802	PLX	C35-C36-C37-C38
6	D	2809	PLX	C35-C36-C37-C38
6	A	2809	PLX	C33-C34-C35-C36
6	A	2814	PLX	C4-C5-O8-C24
6	B	2802	PLX	C4-C5-O8-C24
6	C	2813	PLX	C4-C5-O8-C24
6	D	2814	PLX	C4-C5-O8-C24
6	A	2809	PLX	C24-C25-C26-C27
6	B	2810	PLX	C24-C25-C26-C27
6	C	2802	PLX	C24-C25-C26-C27
6	D	2809	PLX	C24-C25-C26-C27
6	A	2808	PLX	C25-C26-C27-C28
6	B	2809	PLX	C25-C26-C27-C28
6	C	2814	PLX	C25-C26-C27-C28
6	D	2802	PLX	C25-C26-C27-C28
6	A	2808	PLX	O4-C3-C4-O6
6	B	2809	PLX	O4-C3-C4-O6
6	C	2814	PLX	O4-C3-C4-O6

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Mol	Chain	Res	Type	Atoms
6	D	2802	PLX	O4-C3-C4-O6
6	A	2812	PLX	C3-C4-C5-O8
6	B	2813	PLX	C3-C4-C5-O8
6	C	2805	PLX	C3-C4-C5-O8
6	D	2812	PLX	C3-C4-C5-O8
6	B	2814	PLX	C7-C8-C9-C10
6	C	2806	PLX	C7-C8-C9-C10
6	D	2813	PLX	C7-C8-C9-C10
6	A	2813	PLX	C7-C8-C9-C10
6	A	2811	PLX	O6-C4-C5-O8
6	B	2812	PLX	O6-C4-C5-O8
6	C	2804	PLX	O6-C4-C5-O8
6	D	2811	PLX	O6-C4-C5-O8
3	A	2802	ATP	PG-O3B-PB-O2B
3	B	2803	ATP	PG-O3B-PB-O2B
3	C	2807	ATP	PG-O3B-PB-O2B
3	D	2803	ATP	PG-O3B-PB-O2B
6	A	2808	PLX	N1-C1-C2-O1
6	A	2812	PLX	N1-C1-C2-O1
6	B	2809	PLX	N1-C1-C2-O1
6	B	2813	PLX	N1-C1-C2-O1
6	C	2805	PLX	N1-C1-C2-O1
6	C	2814	PLX	N1-C1-C2-O1
6	D	2802	PLX	N1-C1-C2-O1
6	D	2812	PLX	N1-C1-C2-O1
6	A	2811	PLX	C25-C24-O8-C5
6	A	2812	PLX	C25-C24-O8-C5
6	B	2812	PLX	C25-C24-O8-C5
6	B	2813	PLX	C25-C24-O8-C5
6	C	2804	PLX	C25-C24-O8-C5
6	C	2805	PLX	C25-C24-O8-C5
6	D	2811	PLX	C25-C24-O8-C5
6	D	2812	PLX	C25-C24-O8-C5
6	A	2809	PLX	O4-C3-C4-C5
6	B	2810	PLX	O4-C3-C4-C5
6	C	2802	PLX	O4-C3-C4-C5
6	D	2809	PLX	O4-C3-C4-C5
6	A	2812	PLX	C4-C3-O4-P1
6	B	2813	PLX	C4-C3-O4-P1
6	C	2805	PLX	C4-C3-O4-P1
6	D	2812	PLX	C4-C3-O4-P1
6	A	2810	PLX	O8-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
6	A	2813	PLX	O6-C6-C7-C8
6	B	2811	PLX	O8-C24-C25-C26
6	B	2814	PLX	O6-C6-C7-C8
6	C	2803	PLX	O8-C24-C25-C26
6	C	2806	PLX	O6-C6-C7-C8
6	D	2810	PLX	O8-C24-C25-C26
6	D	2813	PLX	O6-C6-C7-C8
6	A	2813	PLX	O4-C3-C4-O6
6	B	2814	PLX	O4-C3-C4-O6
6	C	2806	PLX	O4-C3-C4-O6
6	D	2813	PLX	O4-C3-C4-O6
6	B	2812	PLX	C30-C31-C32-C33
6	C	2804	PLX	C30-C31-C32-C33
6	D	2811	PLX	C30-C31-C32-C33
6	A	2811	PLX	C30-C31-C32-C33
6	A	2809	PLX	C3-O4-P1-O1
6	A	2809	PLX	C3-O4-P1-O2
6	A	2809	PLX	C3-O4-P1-O3
6	A	2811	PLX	C3-C4-O6-C6
6	A	2811	PLX	C5-C4-O6-C6
6	A	2811	PLX	C2-O1-P1-O4
6	A	2813	PLX	C2-O1-P1-O4
6	A	2813	PLX	C2-O1-P1-O2
6	A	2813	PLX	C2-O1-P1-O3
6	B	2810	PLX	C3-O4-P1-O1
6	B	2810	PLX	C3-O4-P1-O2
6	B	2810	PLX	C3-O4-P1-O3
6	B	2812	PLX	C3-C4-O6-C6
6	B	2812	PLX	C5-C4-O6-C6
6	B	2812	PLX	C2-O1-P1-O4
6	B	2814	PLX	C2-O1-P1-O4
6	B	2814	PLX	C2-O1-P1-O2
6	B	2814	PLX	C2-O1-P1-O3
6	C	2802	PLX	C3-O4-P1-O1
6	C	2802	PLX	C3-O4-P1-O2
6	C	2802	PLX	C3-O4-P1-O3
6	C	2804	PLX	C3-C4-O6-C6
6	C	2804	PLX	C5-C4-O6-C6
6	C	2804	PLX	C2-O1-P1-O4
6	C	2806	PLX	C2-O1-P1-O4
6	C	2806	PLX	C2-O1-P1-O2
6	C	2806	PLX	C2-O1-P1-O3

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Mol	Chain	Res	Type	Atoms
6	D	2809	PLX	C3-O4-P1-O1
6	D	2809	PLX	C3-O4-P1-O2
6	D	2809	PLX	C3-O4-P1-O3
6	D	2811	PLX	C3-C4-O6-C6
6	D	2811	PLX	C5-C4-O6-C6
6	D	2811	PLX	C2-O1-P1-O4
6	D	2813	PLX	C2-O1-P1-O4
6	D	2813	PLX	C2-O1-P1-O2
6	D	2813	PLX	C2-O1-P1-O3
6	A	2814	PLX	C6-C7-C8-C9
6	B	2802	PLX	C6-C7-C8-C9
6	C	2813	PLX	C6-C7-C8-C9
6	D	2814	PLX	C6-C7-C8-C9
6	D	2809	PLX	C13-C14-C15-C16
6	A	2812	PLX	C27-C28-C29-C30
6	D	2812	PLX	C27-C28-C29-C30
6	A	2809	PLX	C13-C14-C15-C16
6	C	2802	PLX	C13-C14-C15-C16
6	B	2813	PLX	C27-C28-C29-C30
6	C	2805	PLX	C27-C28-C29-C30
6	B	2810	PLX	C13-C14-C15-C16
6	A	2811	PLX	C24-C25-C26-C27
6	B	2812	PLX	C24-C25-C26-C27
6	C	2804	PLX	C24-C25-C26-C27
6	D	2811	PLX	C24-C25-C26-C27
6	B	2814	PLX	C27-C28-C29-C30
6	C	2806	PLX	C27-C28-C29-C30
6	D	2813	PLX	C27-C28-C29-C30
6	A	2813	PLX	C6-C7-C8-C9
6	B	2814	PLX	C6-C7-C8-C9
6	C	2806	PLX	C6-C7-C8-C9
6	D	2813	PLX	C6-C7-C8-C9
6	A	2813	PLX	C27-C28-C29-C30
6	A	2812	PLX	O6-C6-C7-C8
6	B	2813	PLX	O6-C6-C7-C8
6	C	2805	PLX	O6-C6-C7-C8
6	D	2812	PLX	O6-C6-C7-C8
6	A	2810	PLX	C29-C30-C31-C32
6	B	2811	PLX	C29-C30-C31-C32
6	C	2803	PLX	C29-C30-C31-C32
6	D	2810	PLX	C29-C30-C31-C32
6	C	2805	PLX	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
6	D	2812	PLX	C28-C29-C30-C31
6	A	2812	PLX	C28-C29-C30-C31
6	B	2813	PLX	C28-C29-C30-C31
6	D	2810	PLX	C28-C29-C30-C31
6	A	2810	PLX	C28-C29-C30-C31
6	B	2811	PLX	C28-C29-C30-C31
6	C	2803	PLX	C28-C29-C30-C31
6	D	2802	PLX	C29-C30-C31-C32
6	A	2808	PLX	C29-C30-C31-C32
6	C	2814	PLX	C29-C30-C31-C32
6	B	2809	PLX	C29-C30-C31-C32
4	A	2803	I3P	C1-O1-P1-O11
4	B	2804	I3P	C1-O1-P1-O11
4	C	2808	I3P	C1-O1-P1-O11
4	D	2804	I3P	C1-O1-P1-O11
6	A	2813	PLX	C24-C25-C26-C27
6	B	2814	PLX	C24-C25-C26-C27
6	C	2806	PLX	C24-C25-C26-C27
6	D	2813	PLX	C24-C25-C26-C27
6	A	2808	PLX	O9-C24-C25-C26
6	B	2809	PLX	O9-C24-C25-C26
6	C	2814	PLX	O9-C24-C25-C26
6	D	2802	PLX	O9-C24-C25-C26
6	C	2814	PLX	C24-C25-C26-C27
6	D	2802	PLX	C24-C25-C26-C27
6	A	2812	PLX	O4-C3-C4-C5
6	B	2813	PLX	O4-C3-C4-C5
6	C	2805	PLX	O4-C3-C4-C5
6	D	2812	PLX	O4-C3-C4-C5
6	A	2808	PLX	C24-C25-C26-C27
6	B	2809	PLX	C24-C25-C26-C27
3	A	2802	ATP	C4'-C5'-O5'-PA
3	B	2803	ATP	C4'-C5'-O5'-PA
3	D	2803	ATP	C4'-C5'-O5'-PA
6	B	2810	PLX	C31-C32-C33-C34
6	C	2802	PLX	C31-C32-C33-C34
6	D	2809	PLX	C31-C32-C33-C34
6	A	2809	PLX	C31-C32-C33-C34
3	C	2807	ATP	C4'-C5'-O5'-PA
6	C	2813	PLX	C26-C27-C28-C29
6	D	2814	PLX	C26-C27-C28-C29
6	B	2802	PLX	C26-C27-C28-C29

Continued on next page...

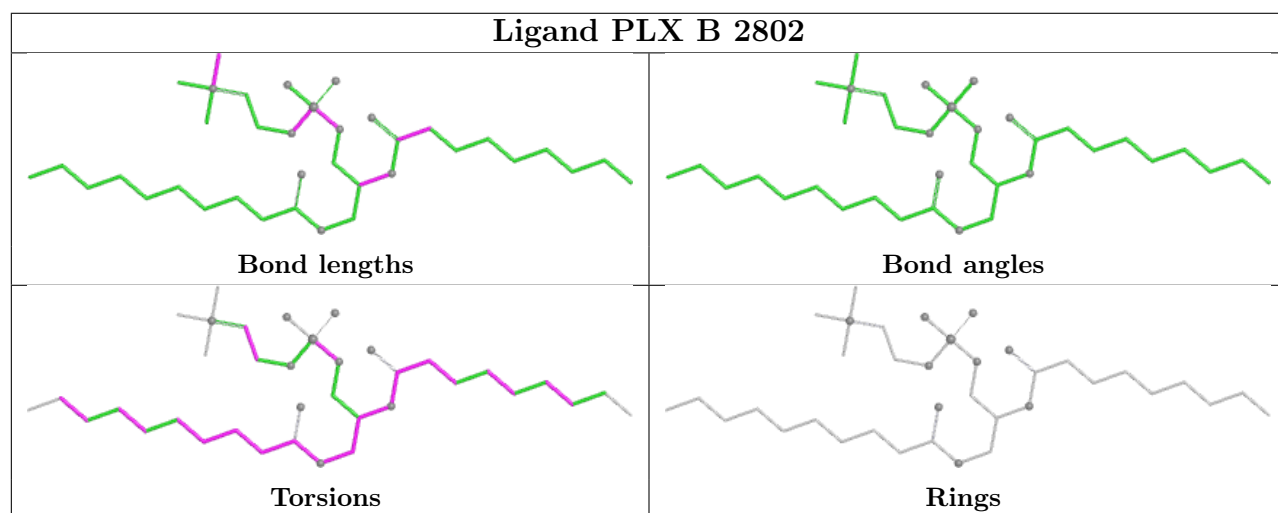
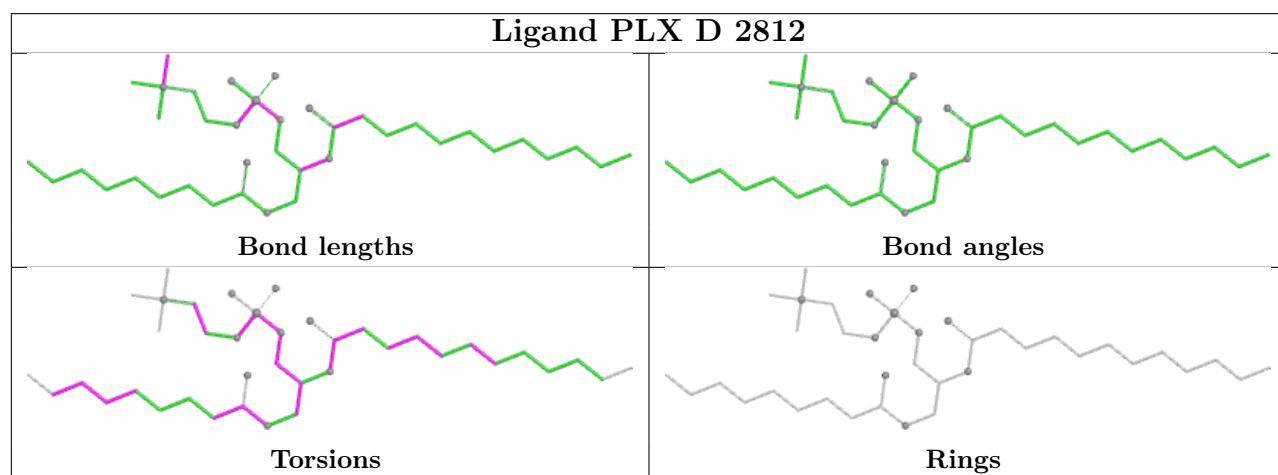
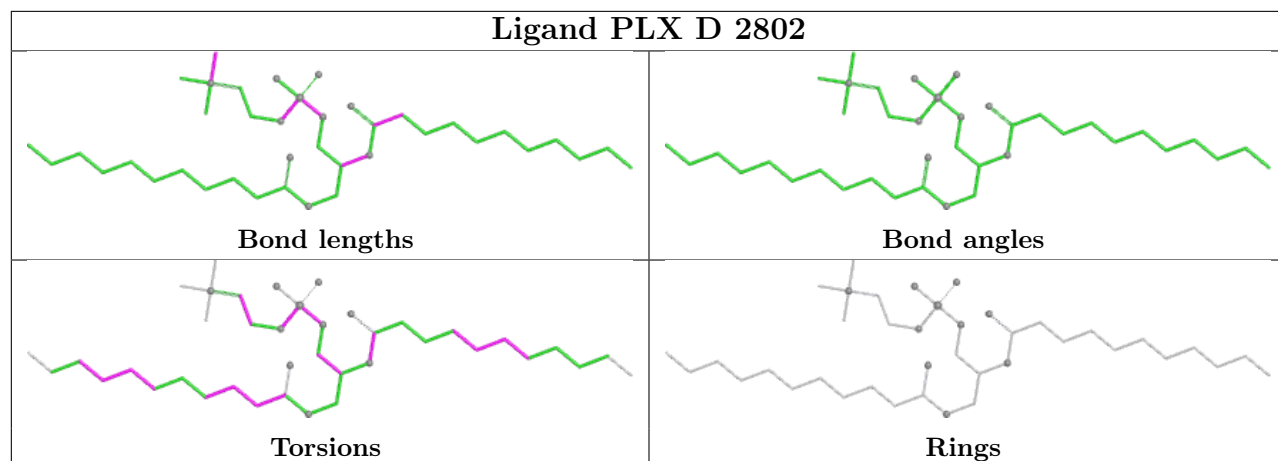
Continued from previous page...

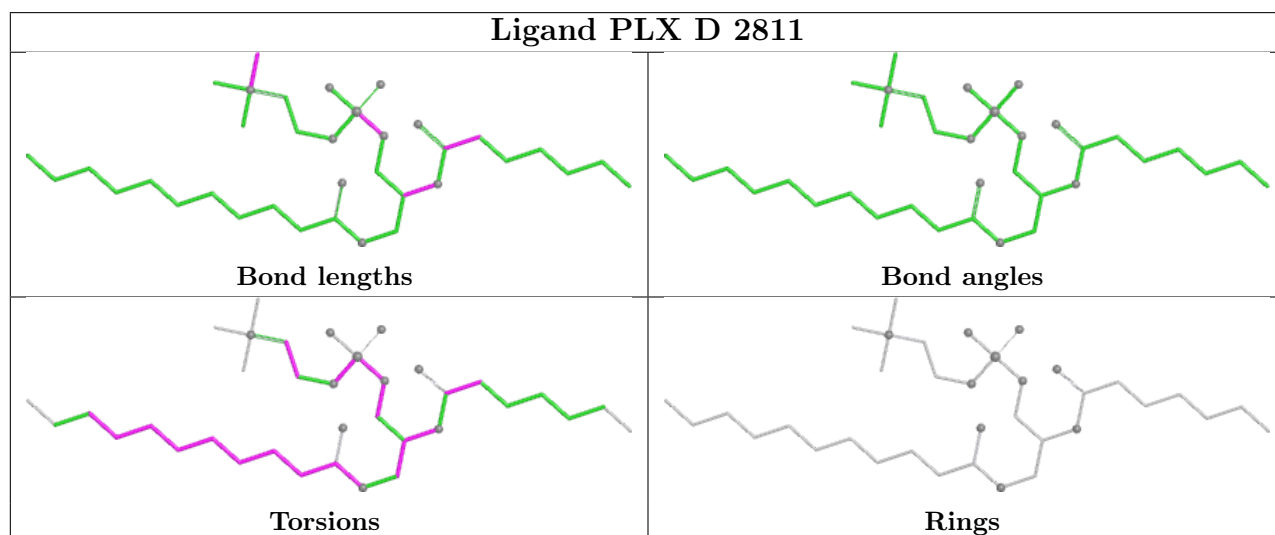
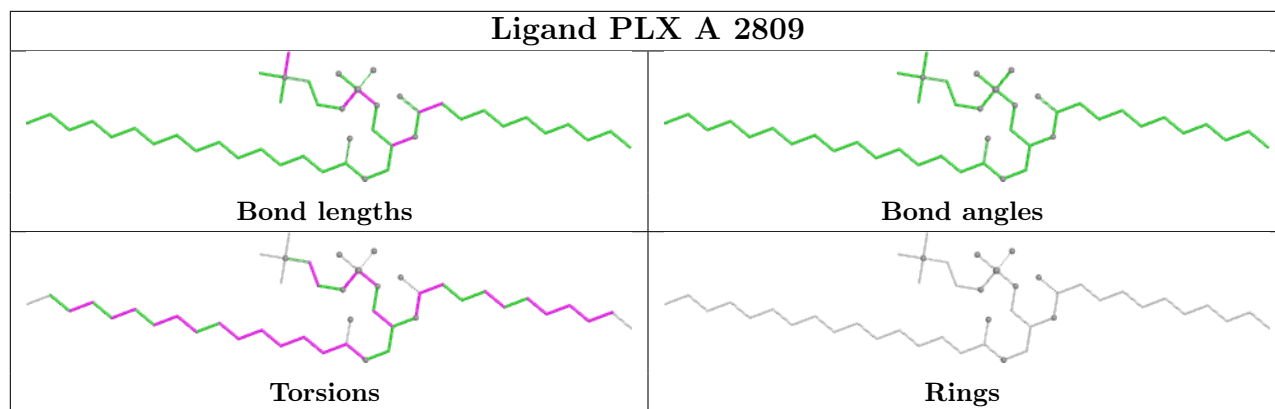
Mol	Chain	Res	Type	Atoms
3	A	2802	ATP	PG-O3B-PB-O1B
3	B	2803	ATP	PG-O3B-PB-O1B
3	C	2807	ATP	PG-O3B-PB-O1B
3	D	2803	ATP	PG-O3B-PB-O1B
6	A	2814	PLX	N1-C1-C2-O1
6	B	2802	PLX	N1-C1-C2-O1
6	C	2813	PLX	N1-C1-C2-O1
6	D	2814	PLX	N1-C1-C2-O1
6	A	2814	PLX	C26-C27-C28-C29
6	A	2810	PLX	C25-C24-O8-C5
6	B	2811	PLX	C25-C24-O8-C5
6	C	2803	PLX	C25-C24-O8-C5
6	D	2810	PLX	C25-C24-O8-C5
6	A	2814	PLX	C24-C25-C26-C27
6	B	2802	PLX	C24-C25-C26-C27
6	C	2813	PLX	C24-C25-C26-C27
6	D	2814	PLX	C24-C25-C26-C27
6	A	2811	PLX	O9-C24-O8-C5
6	B	2812	PLX	O9-C24-O8-C5
6	C	2804	PLX	O9-C24-O8-C5
6	D	2811	PLX	O9-C24-O8-C5
6	B	2811	PLX	C26-C27-C28-C29
6	D	2810	PLX	C26-C27-C28-C29
6	A	2810	PLX	C26-C27-C28-C29
6	C	2803	PLX	C26-C27-C28-C29

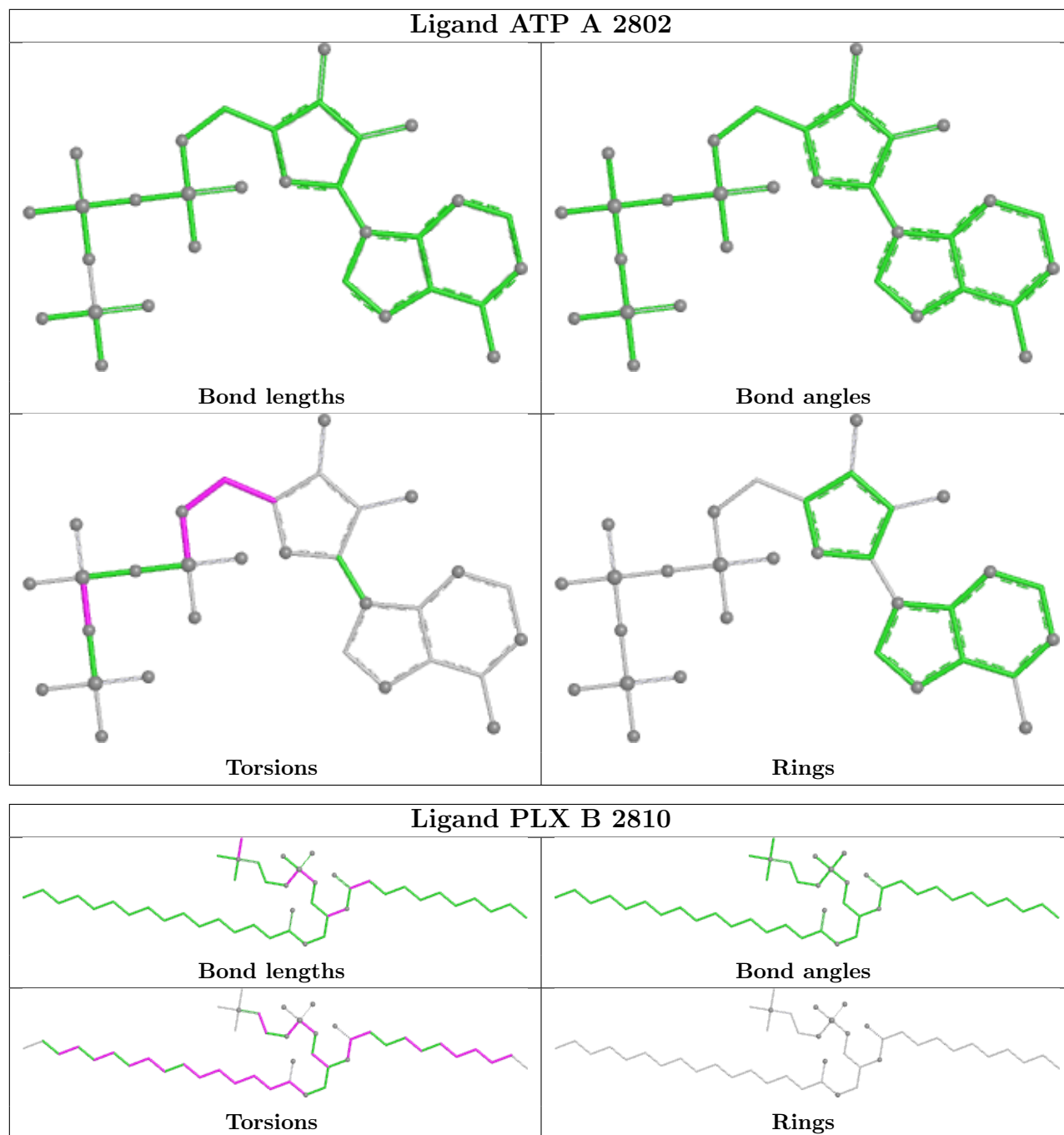
There are no ring outliers.

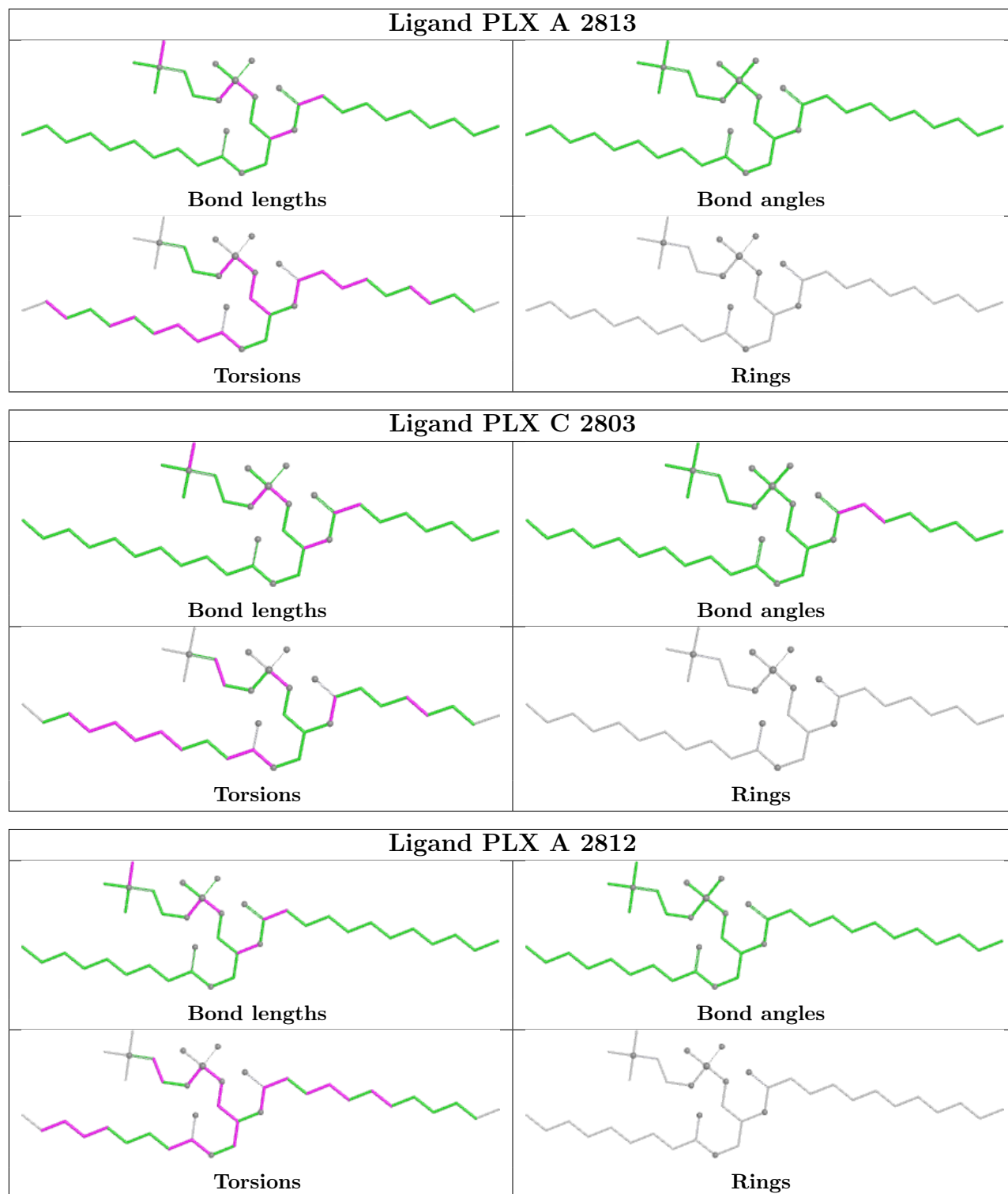
No monomer is involved in short contacts.

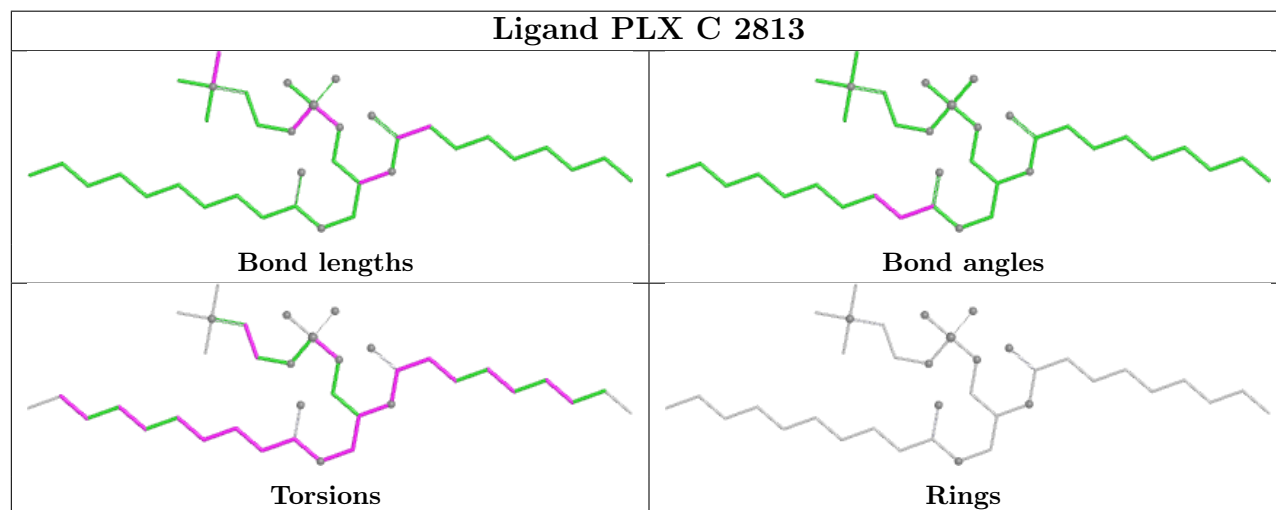
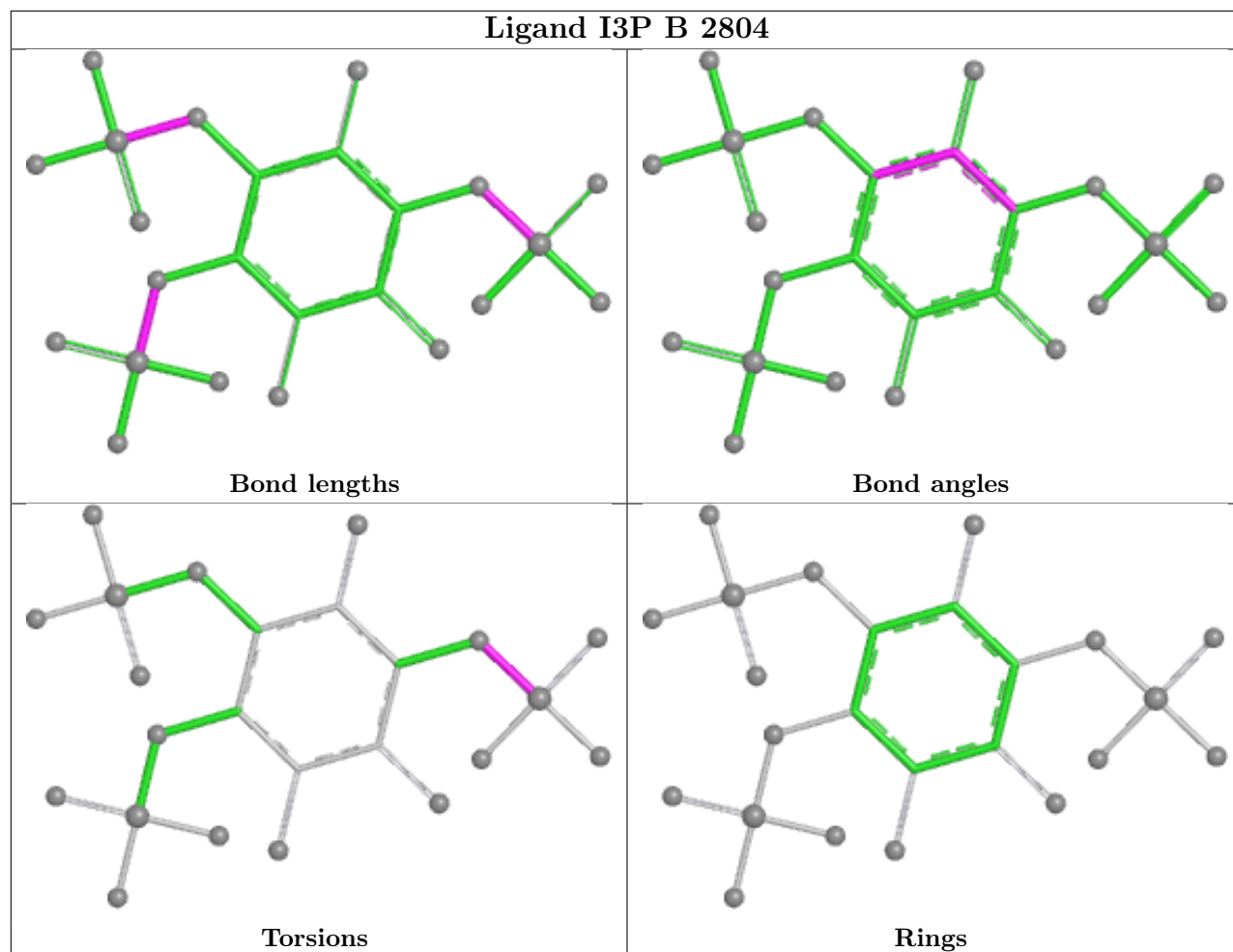
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

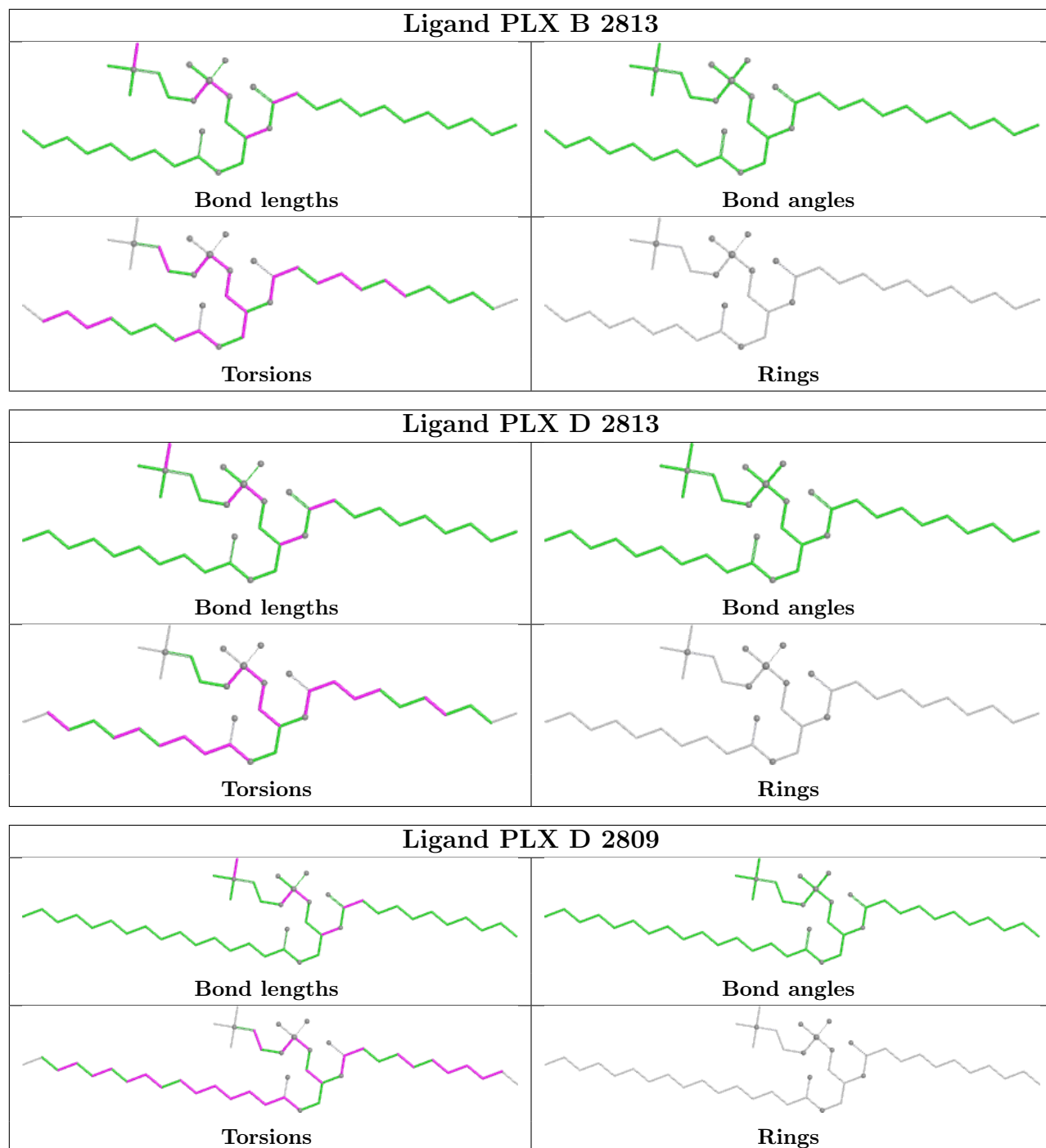


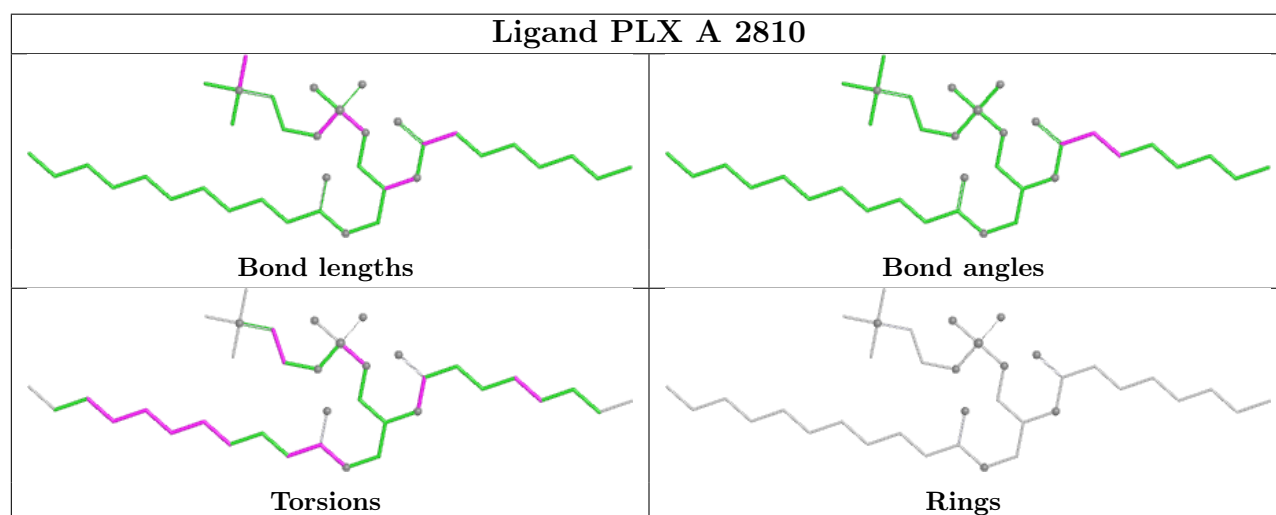
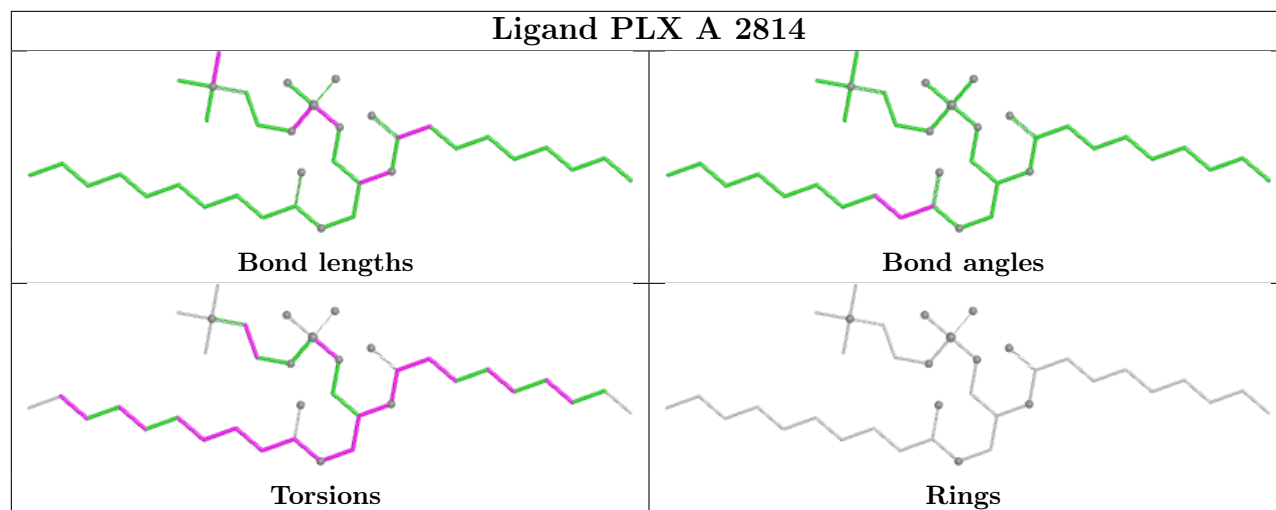


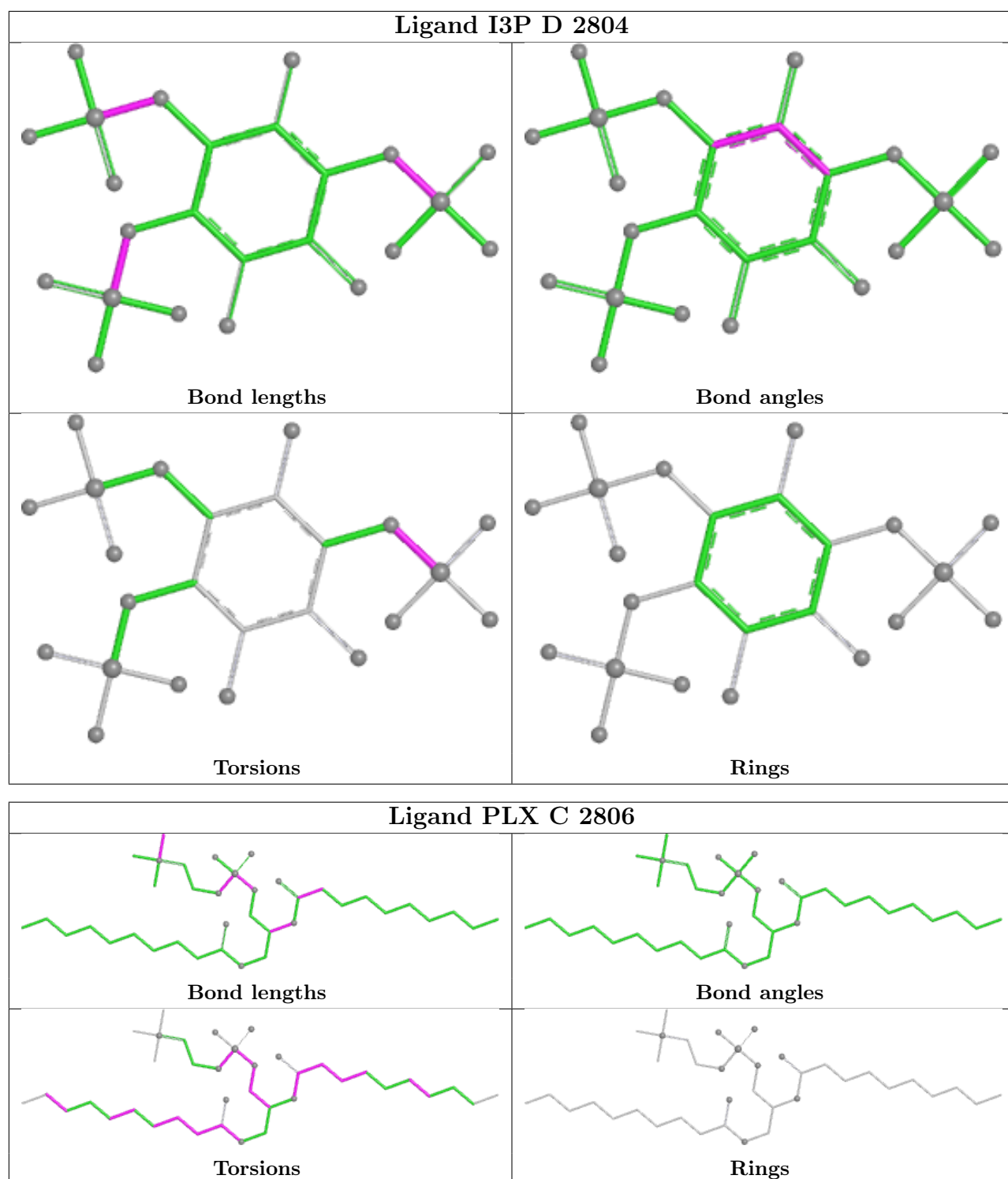


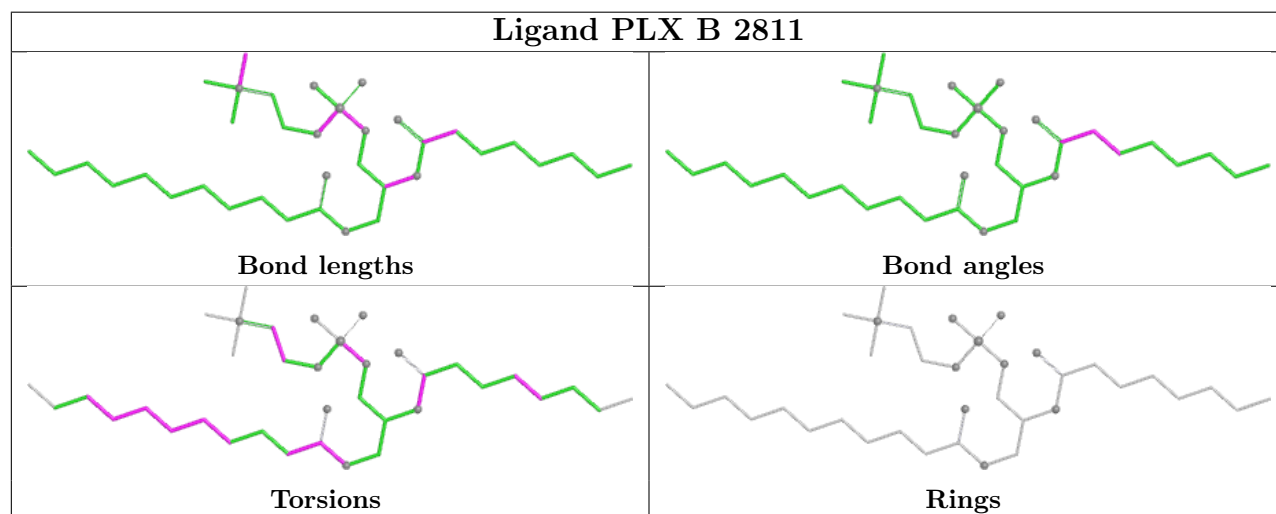
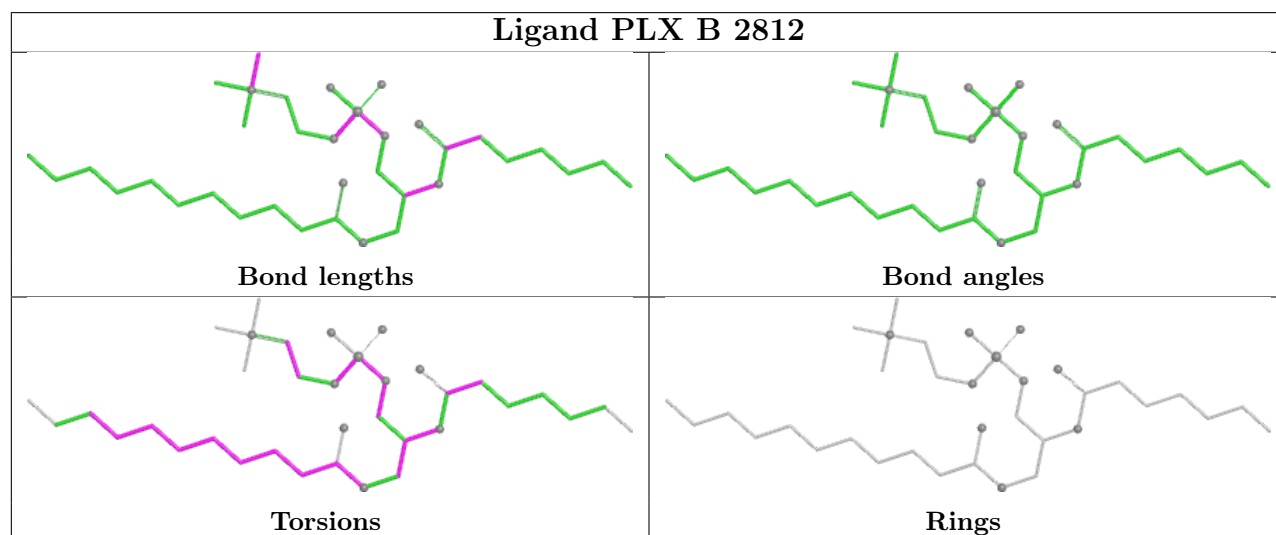
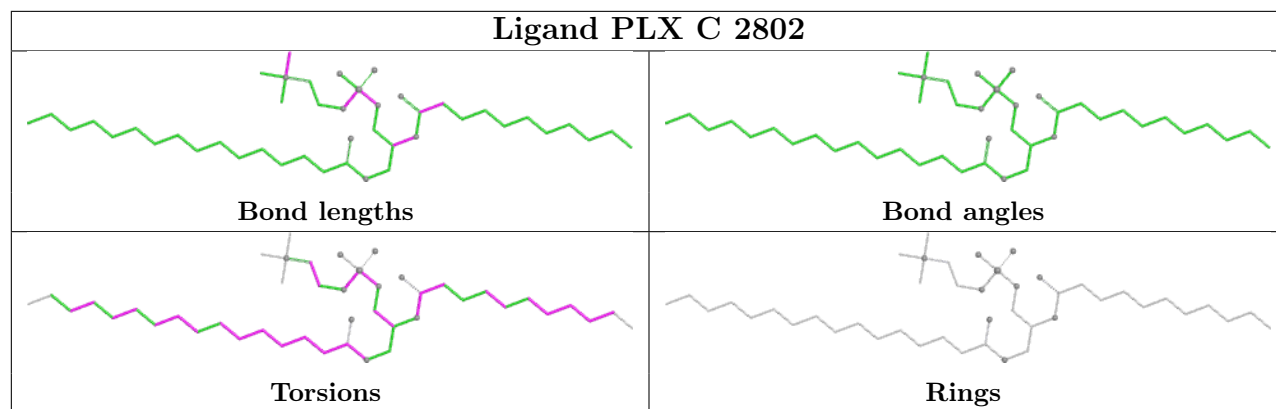


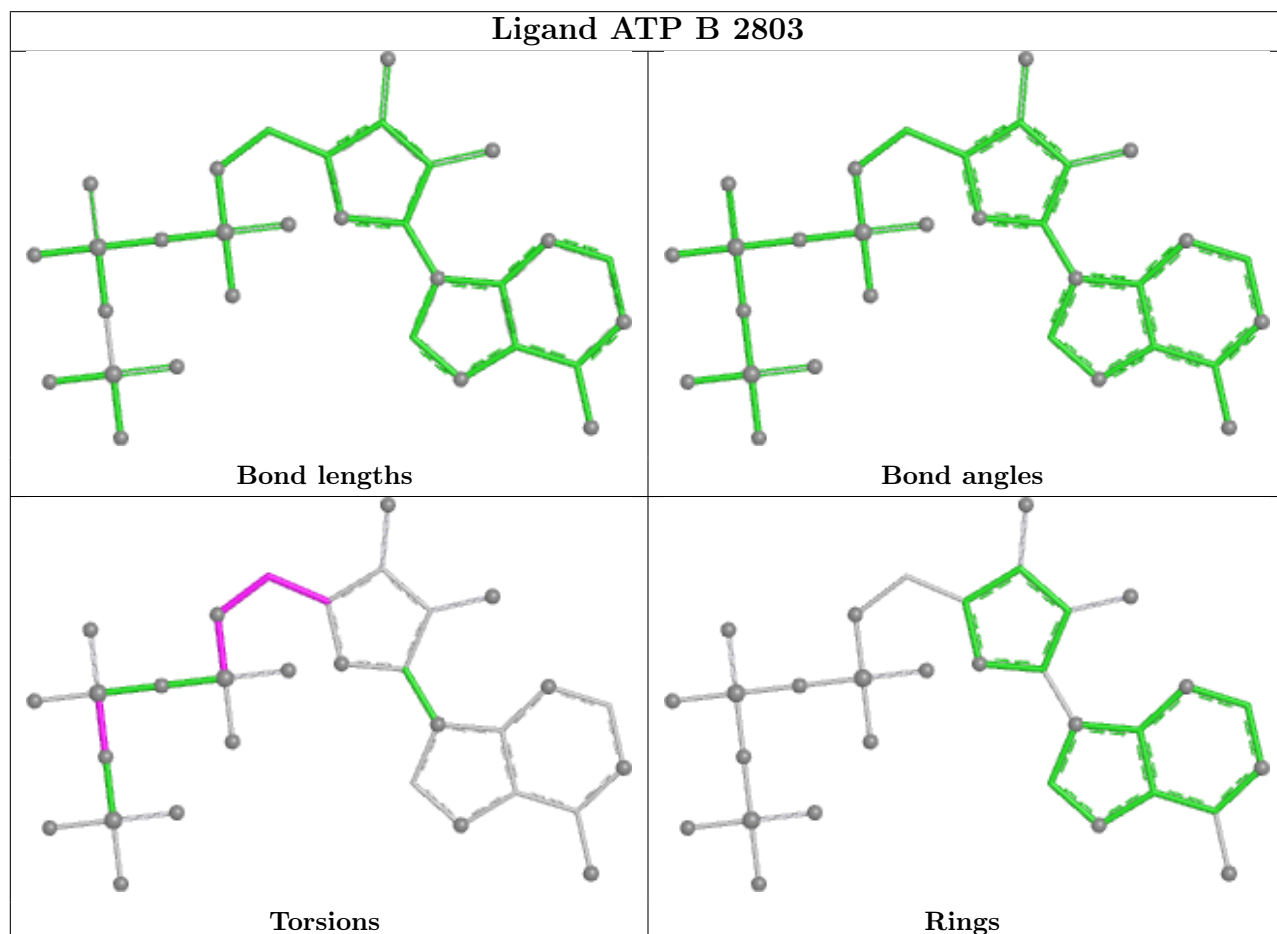
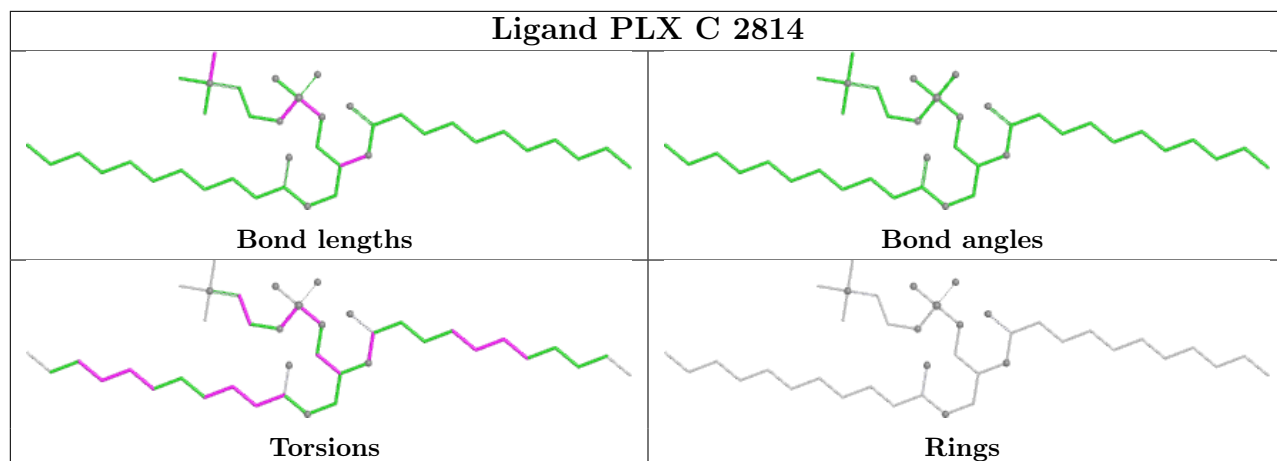


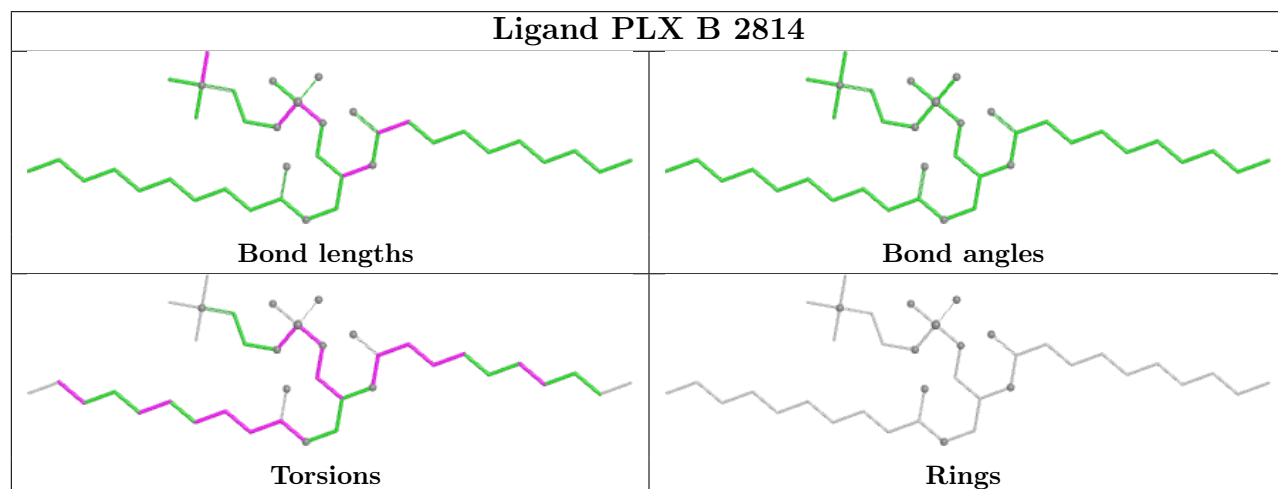
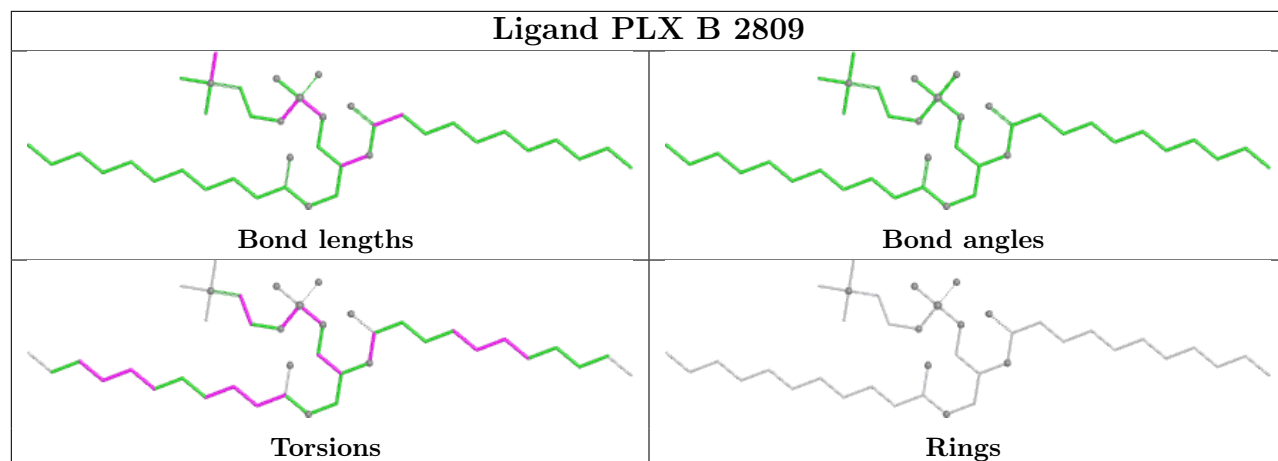


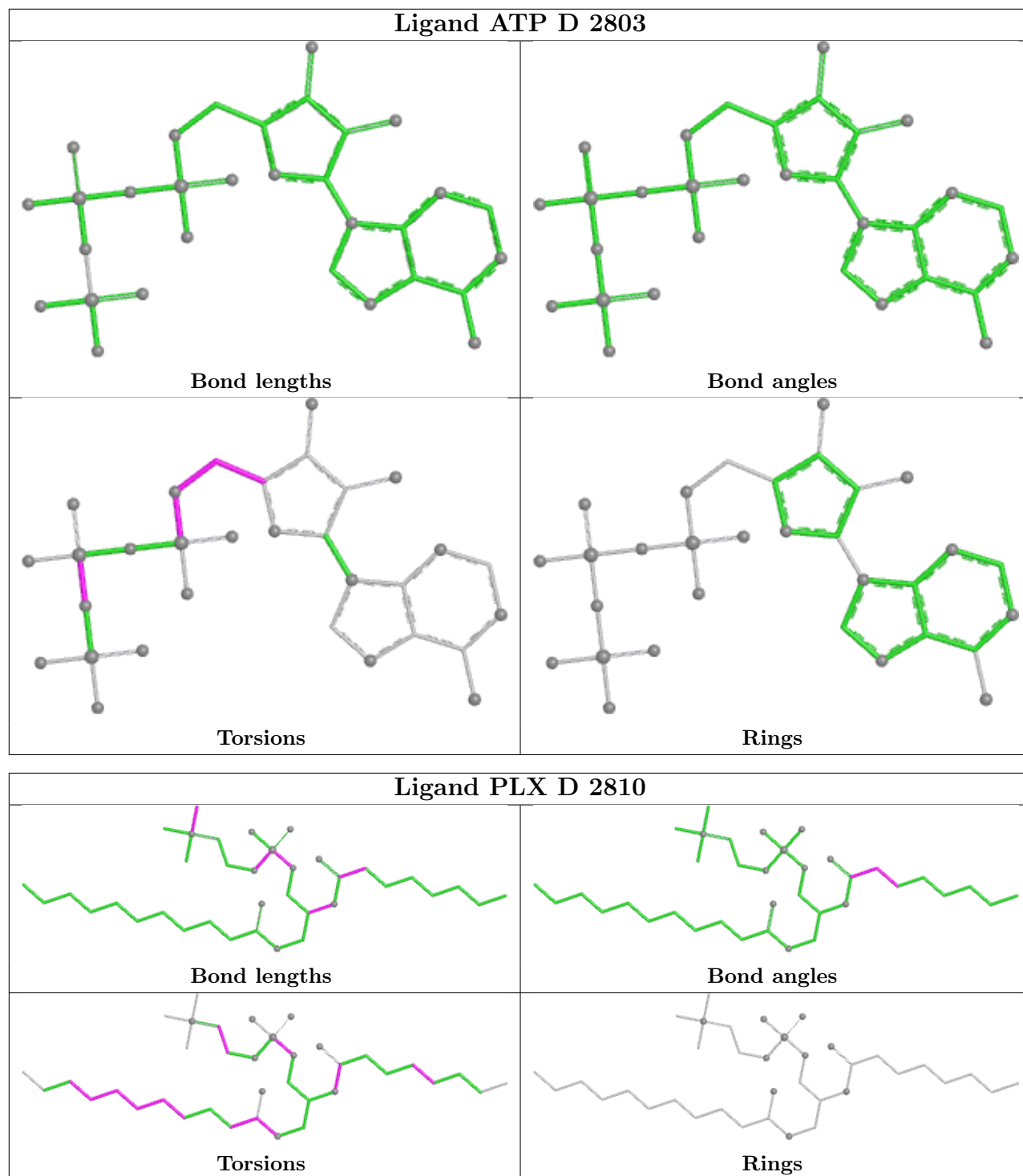


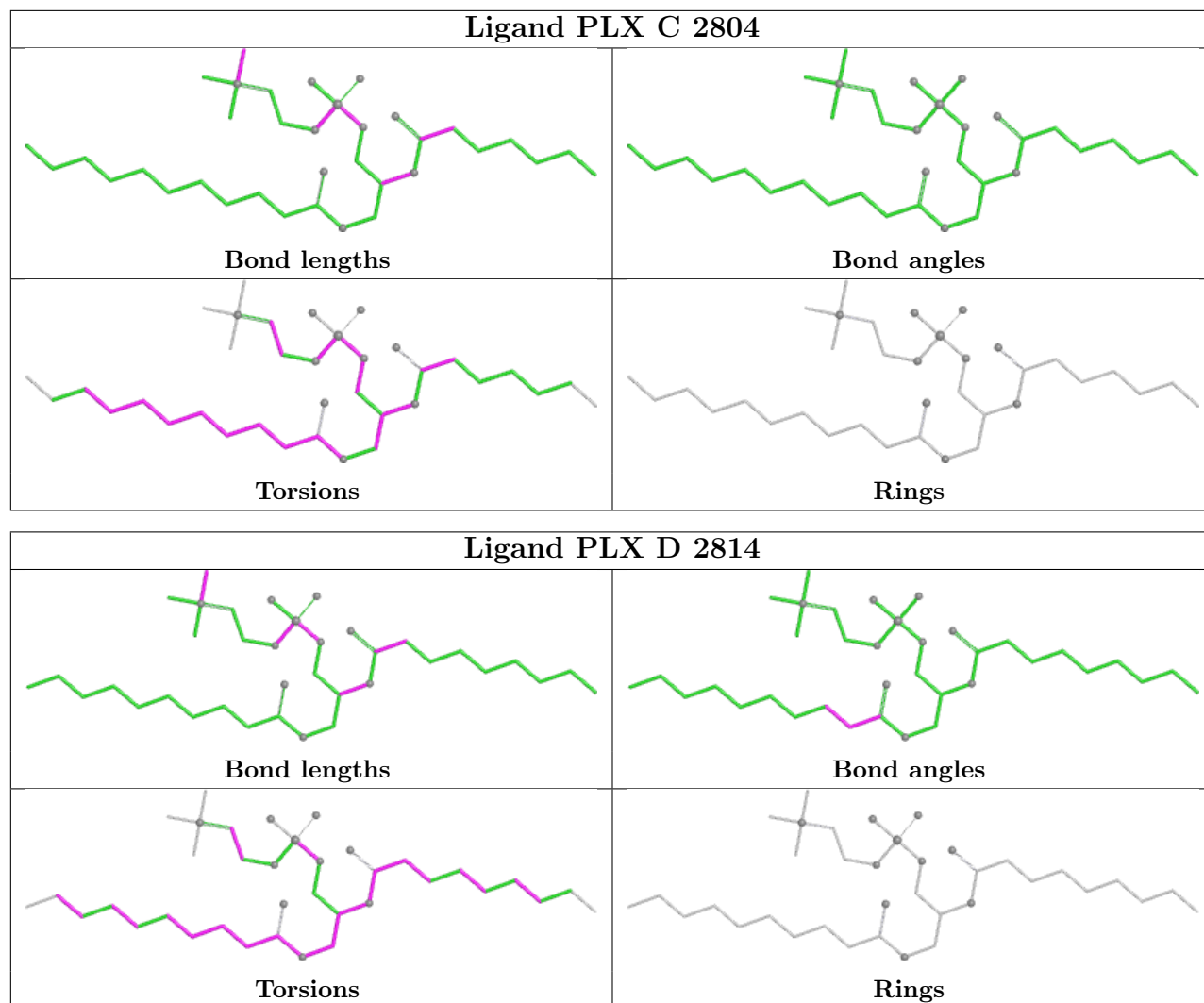


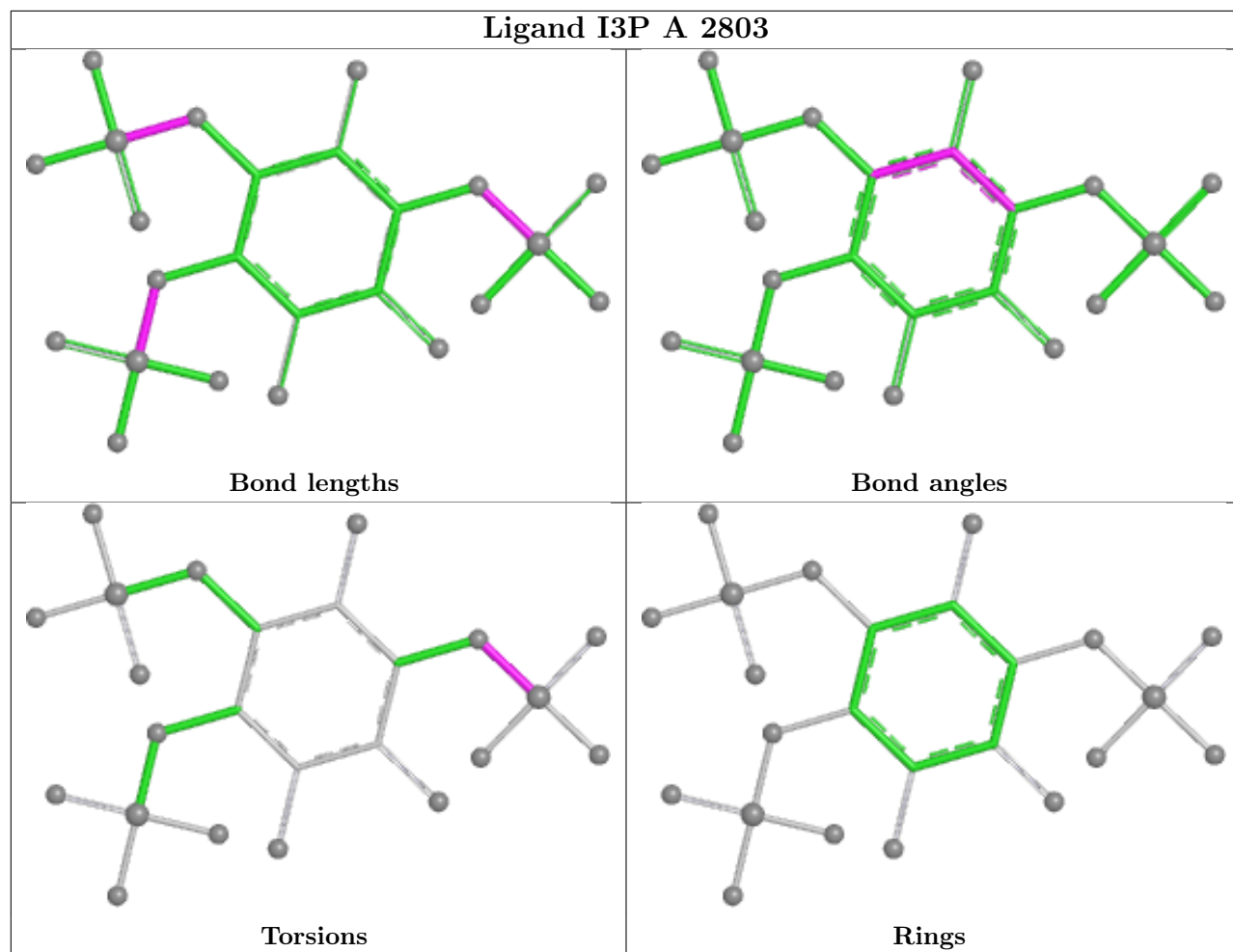


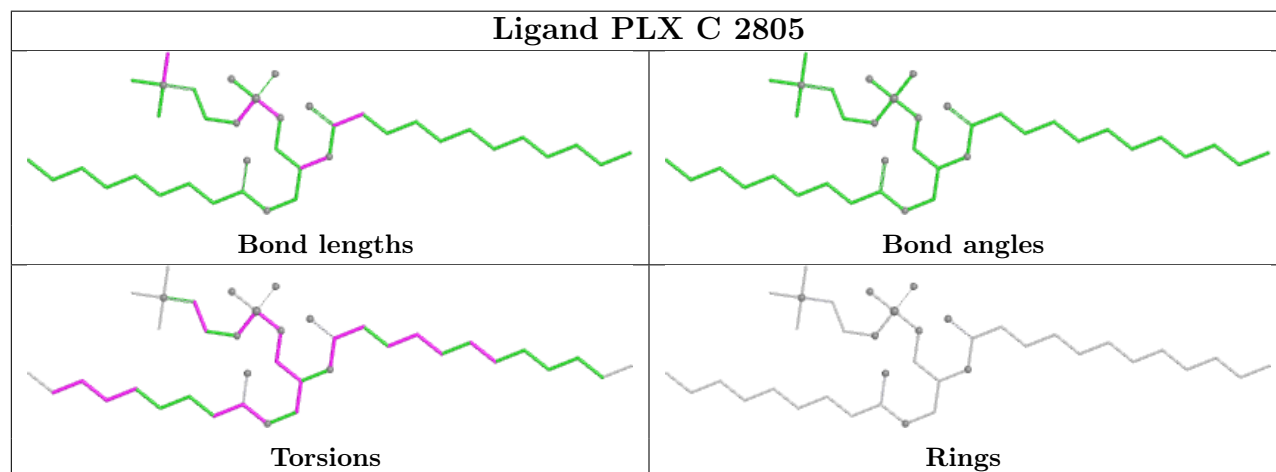
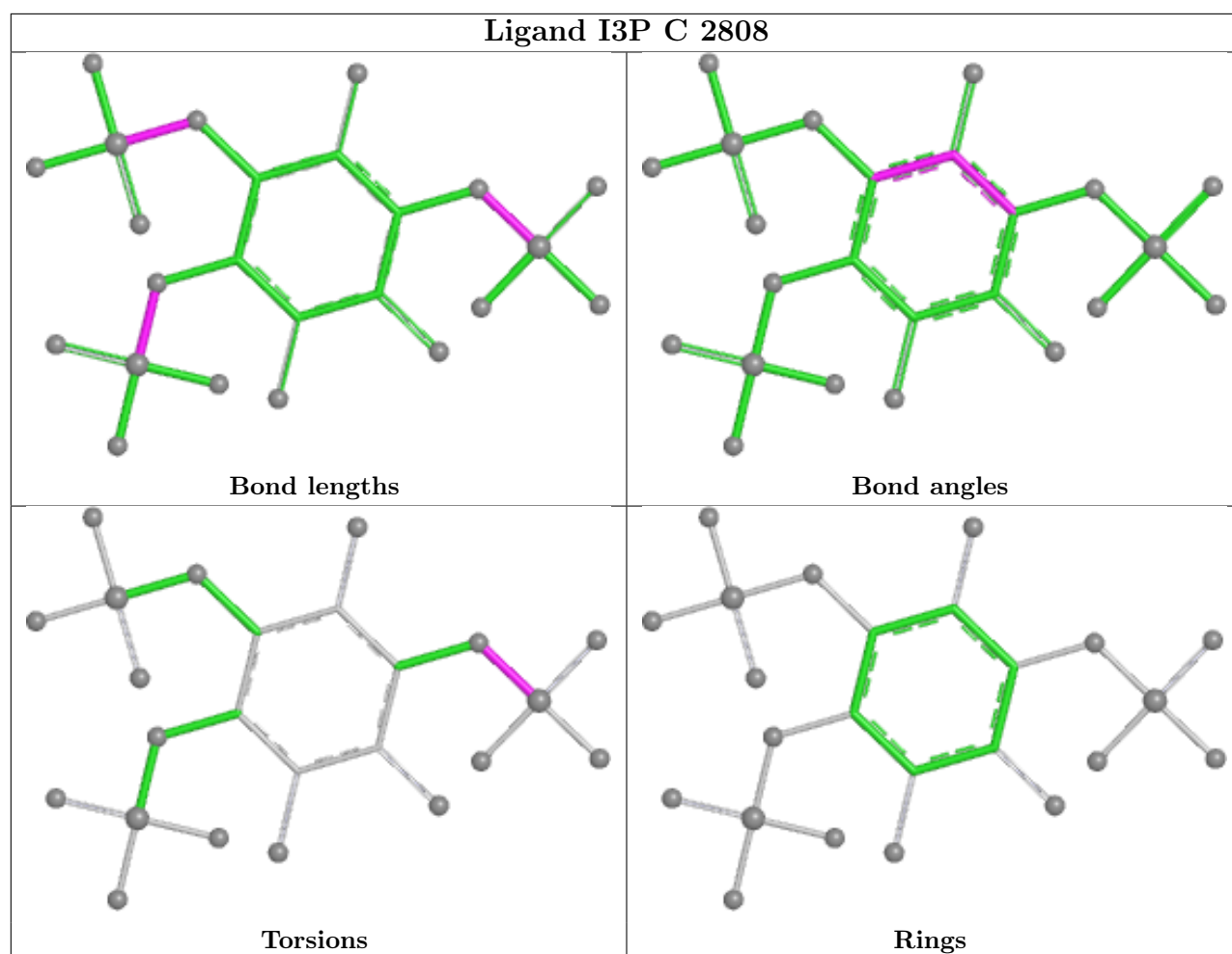


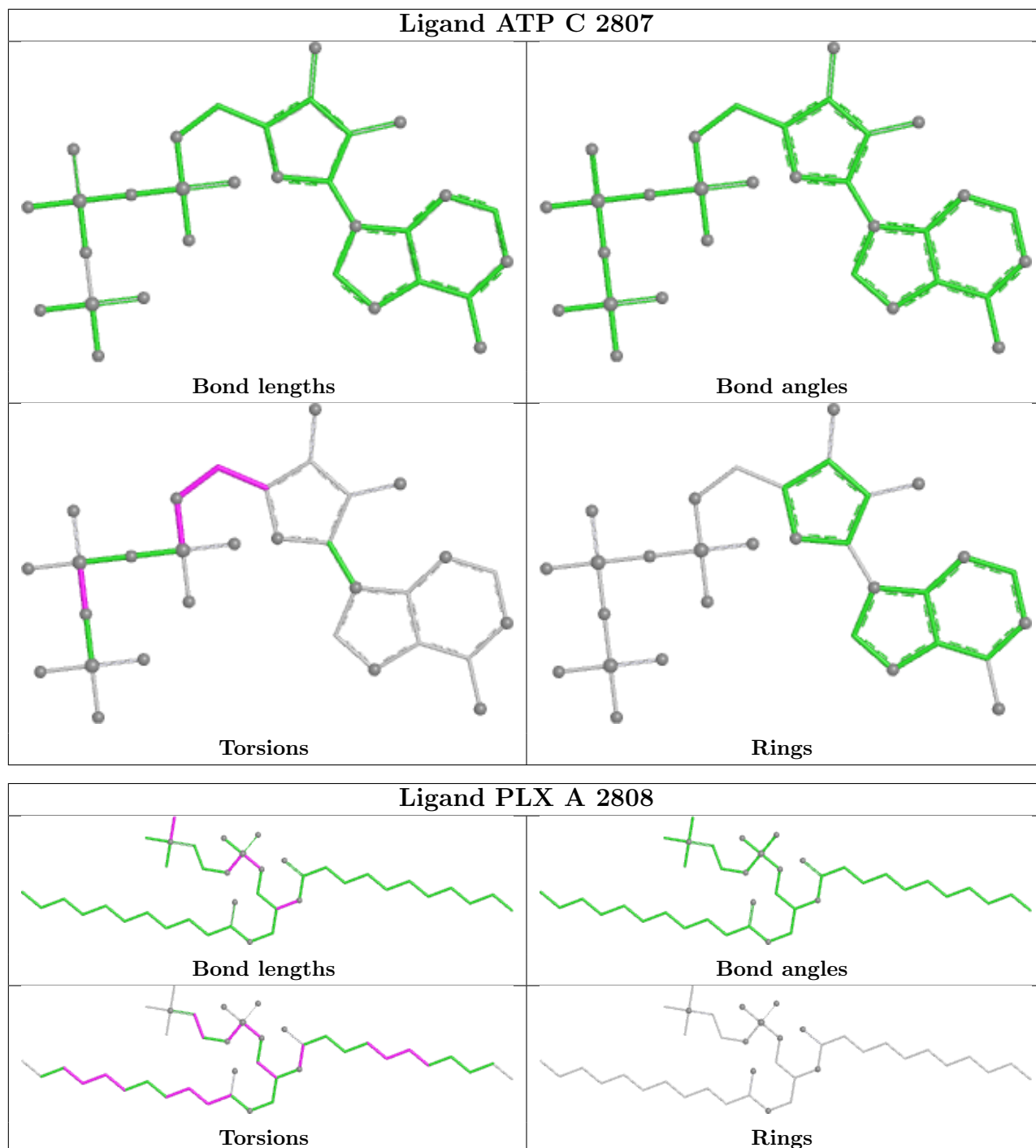


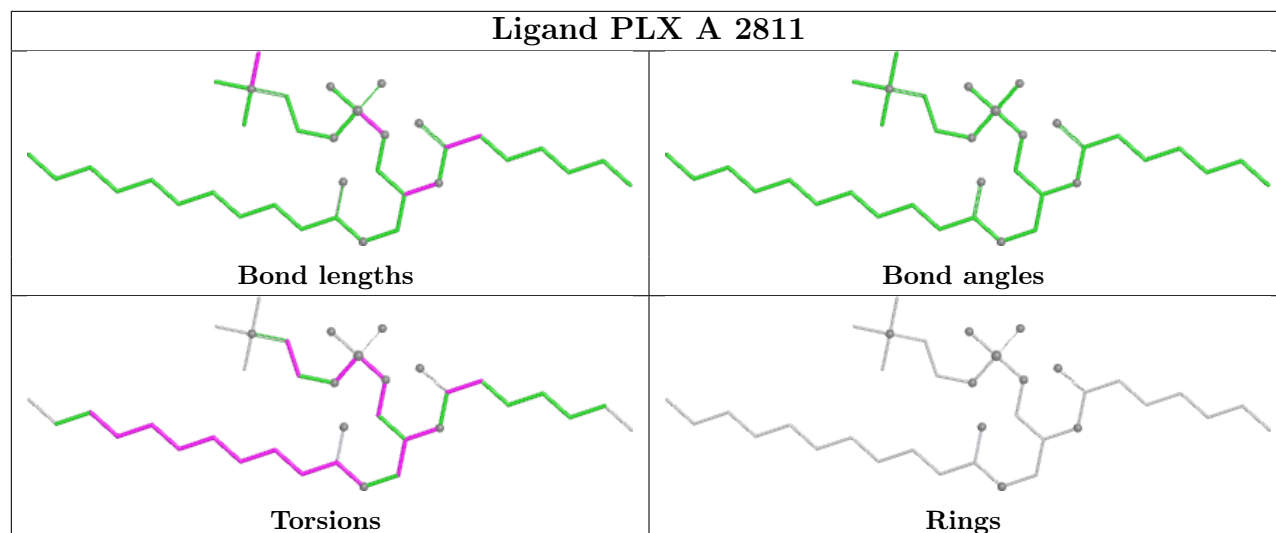












4.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

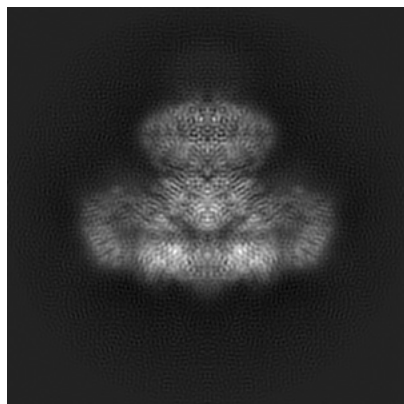
5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27983. These allow visual inspection of the internal detail of the map and identification of artifacts.

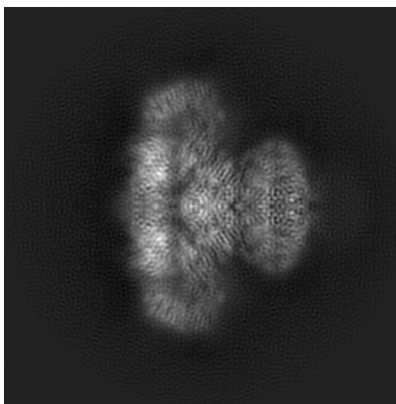
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

5.1 Orthogonal projections [i](#)

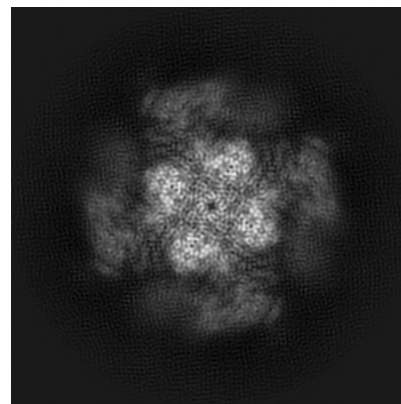
5.1.1 Primary map



X

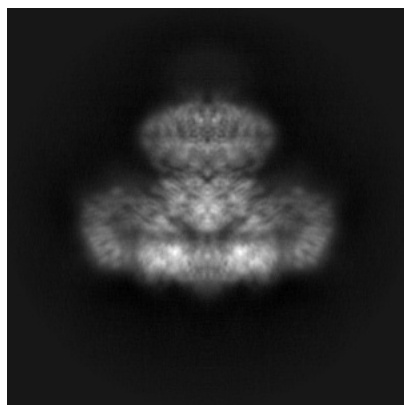


Y

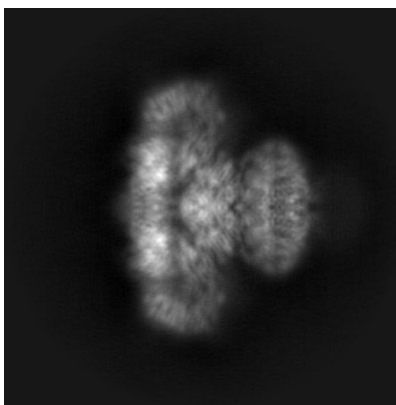


Z

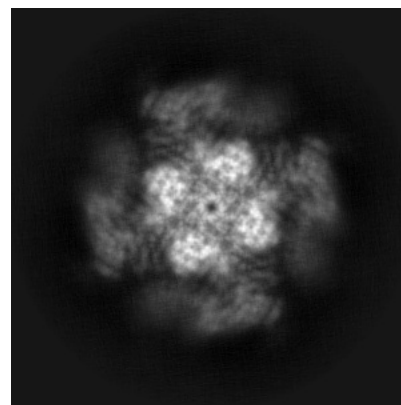
5.1.2 Raw map



X



Y

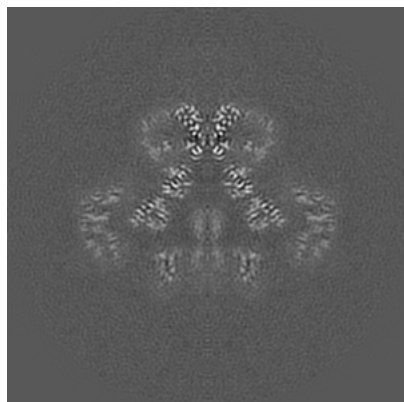


Z

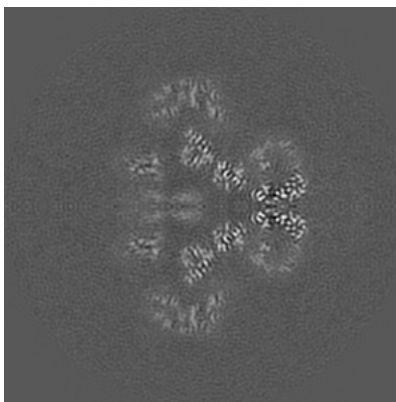
The images above show the map projected in three orthogonal directions.

5.2 Central slices [i](#)

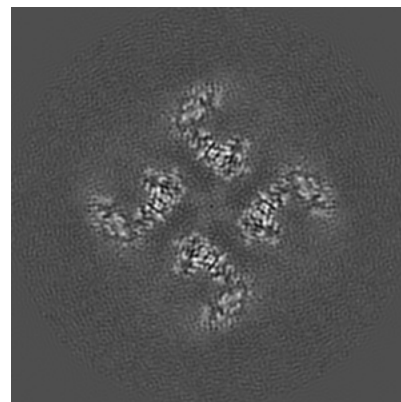
5.2.1 Primary map



X Index: 168

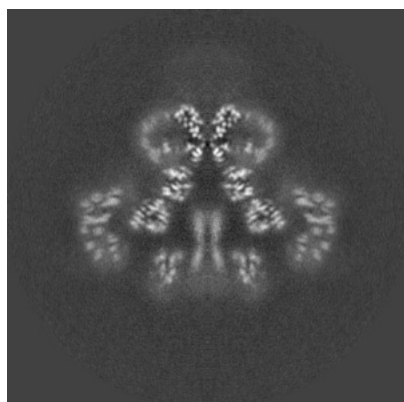


Y Index: 168

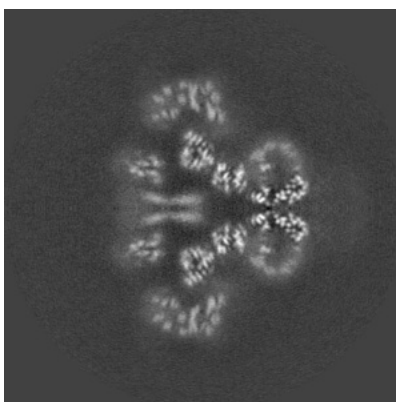


Z Index: 168

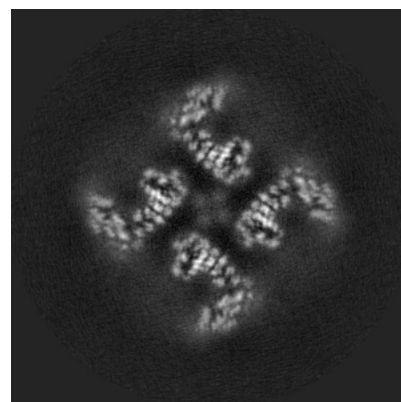
5.2.2 Raw map



X Index: 168



Y Index: 168

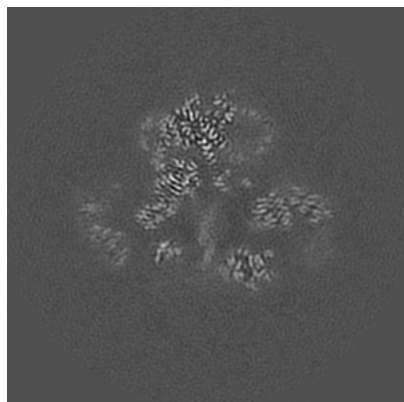


Z Index: 168

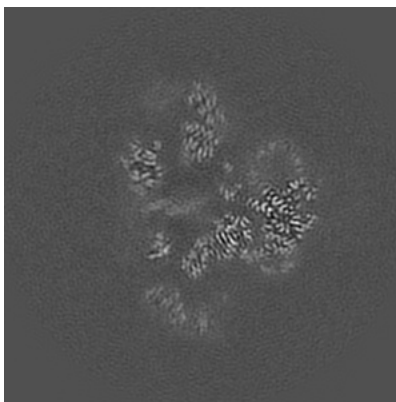
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices [i](#)

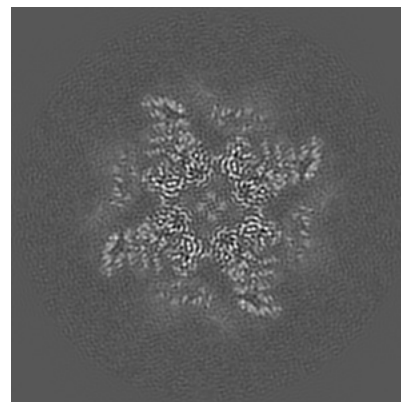
5.3.1 Primary map



X Index: 160

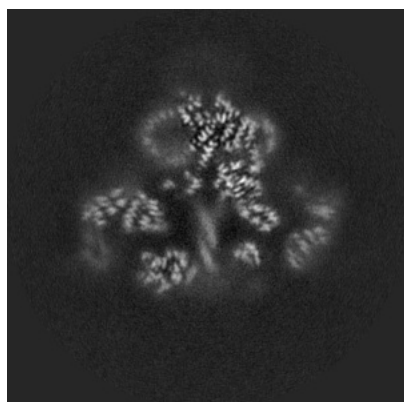


Y Index: 176

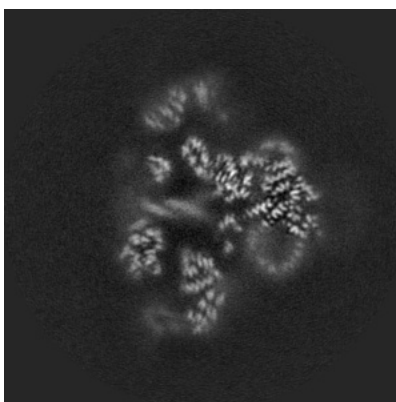


Z Index: 125

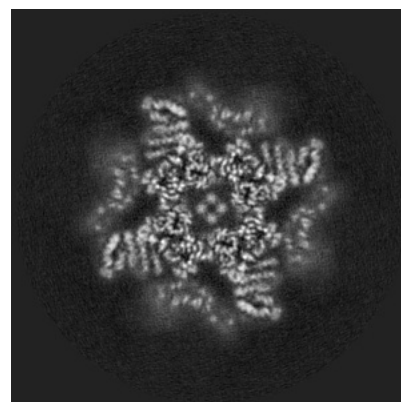
5.3.2 Raw map



X Index: 176



Y Index: 160

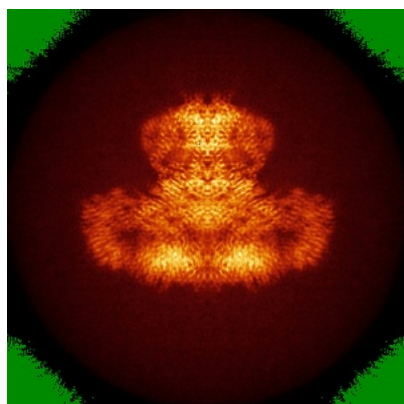


Z Index: 126

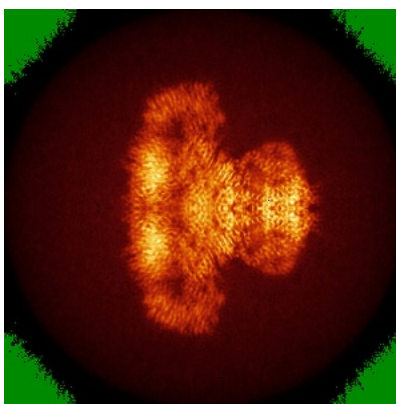
The images above show the largest variance slices of the map in three orthogonal directions.

5.4 Orthogonal standard-deviation projections (False-color) [i](#)

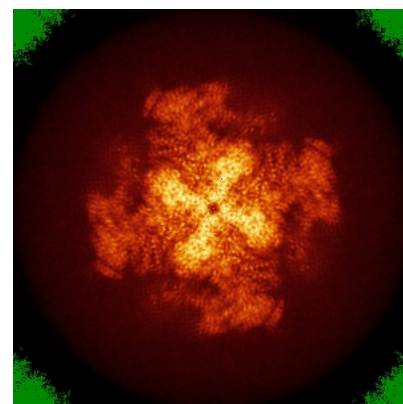
5.4.1 Primary map



X

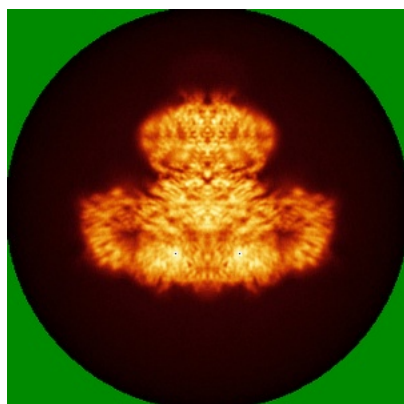


Y

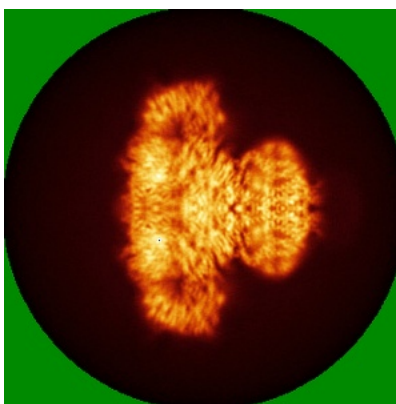


Z

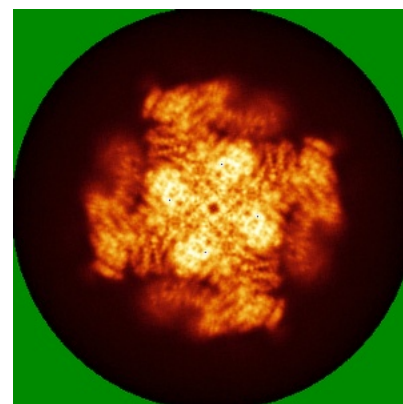
5.4.2 Raw map



X



Y

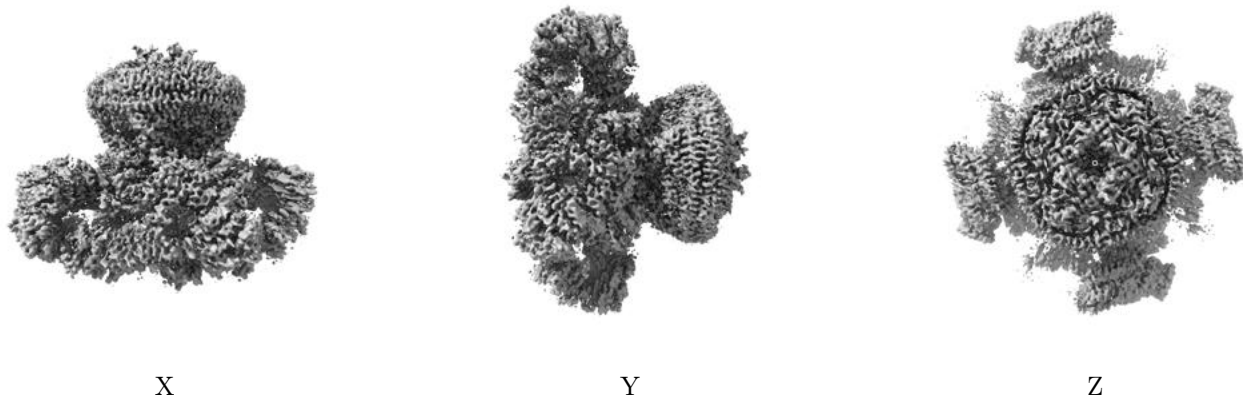


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

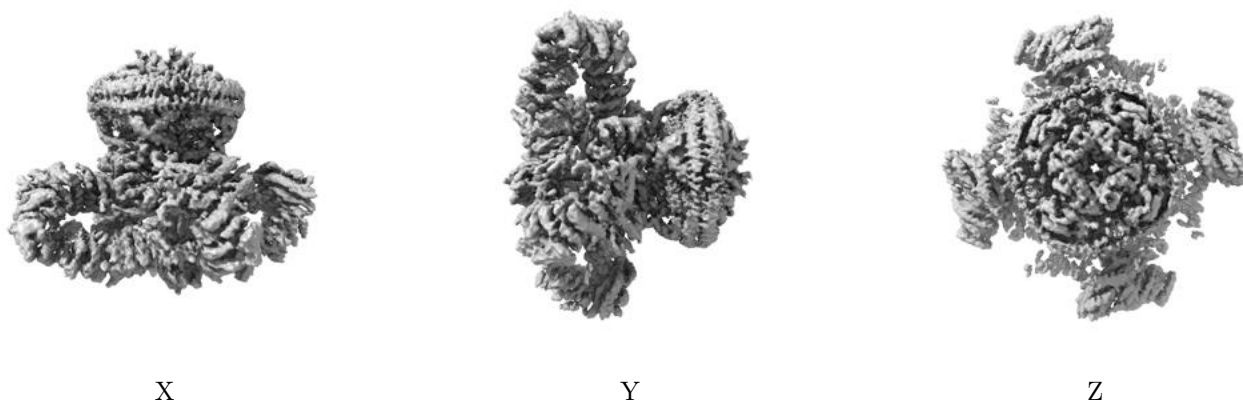
5.5 Orthogonal surface views [i](#)

5.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.011. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

5.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

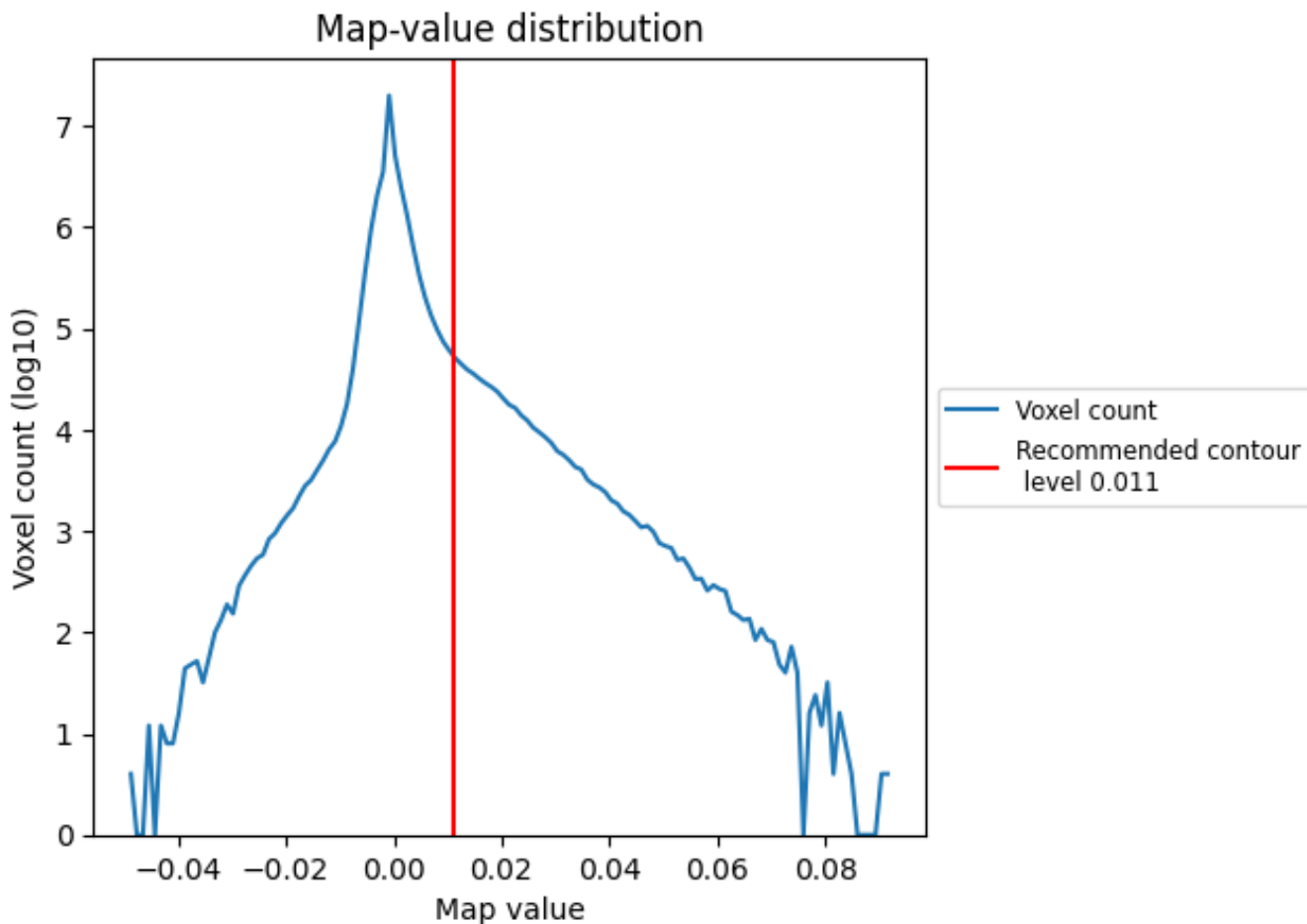
5.6 Mask visualisation [i](#)

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

6 Map analysis [i](#)

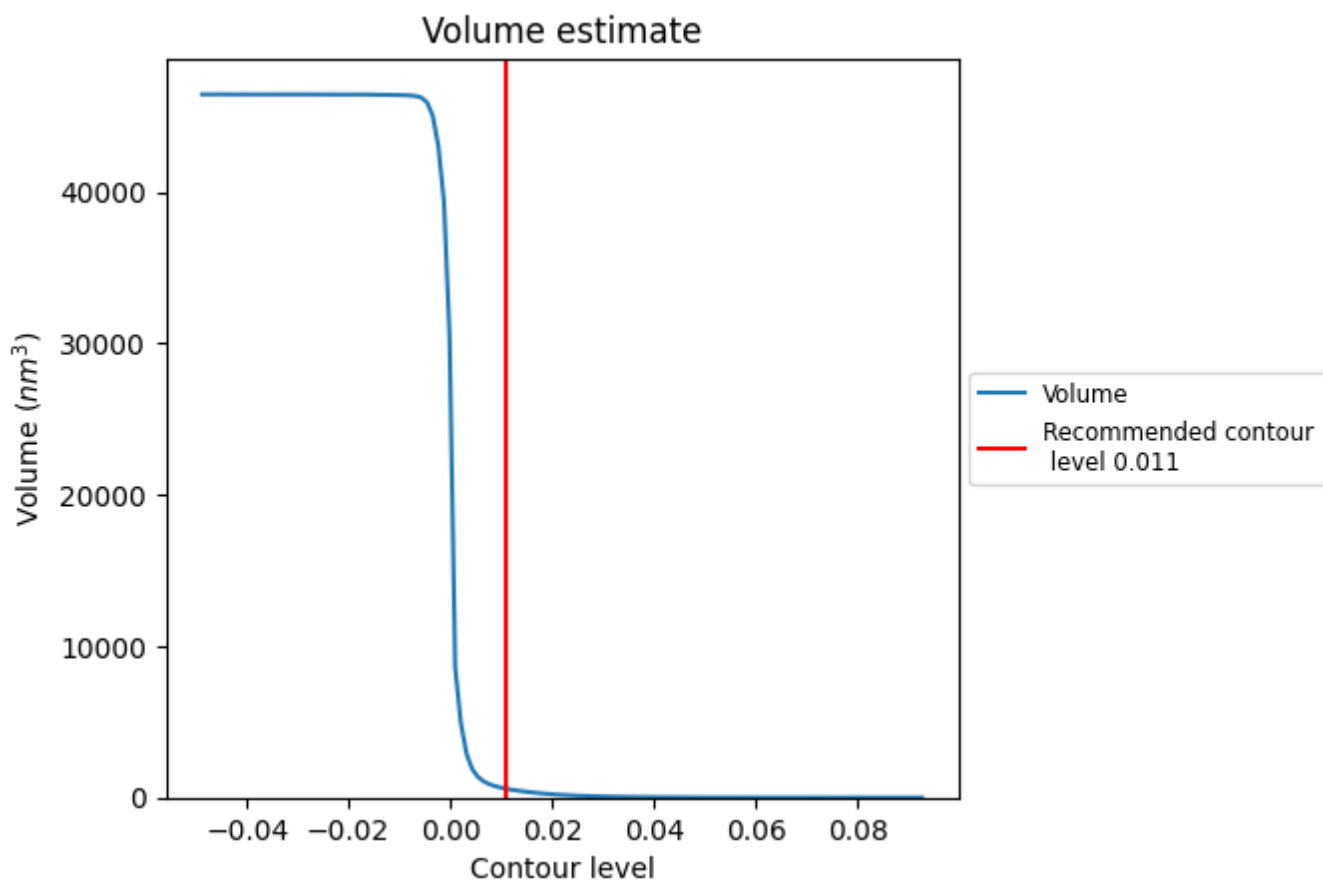
This section contains the results of statistical analysis of the map.

6.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

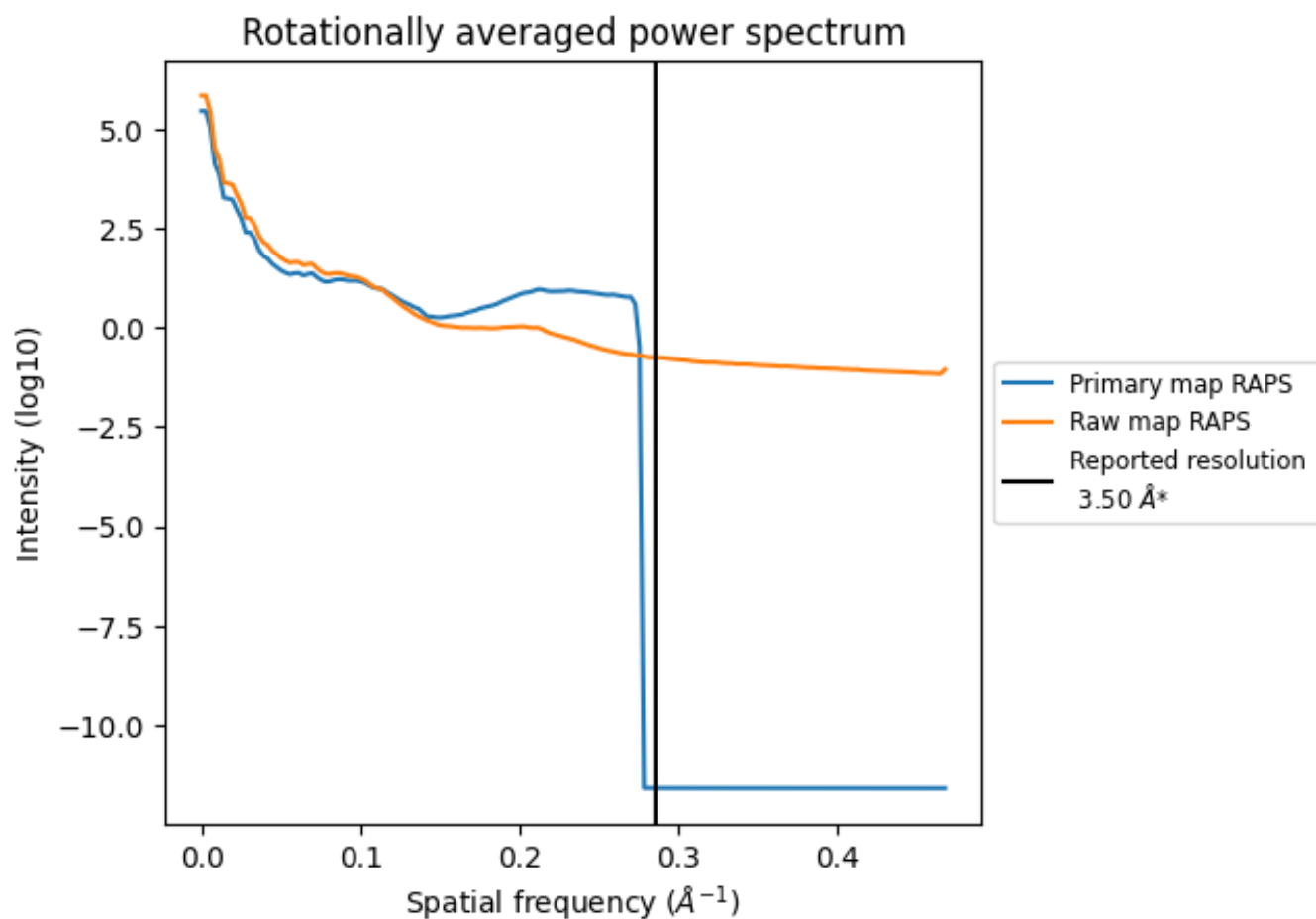
6.2 Volume estimate [i](#)



The volume at the recommended contour level is 581 nm³; this corresponds to an approximate mass of 525 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

6.3 Rotationally averaged power spectrum i

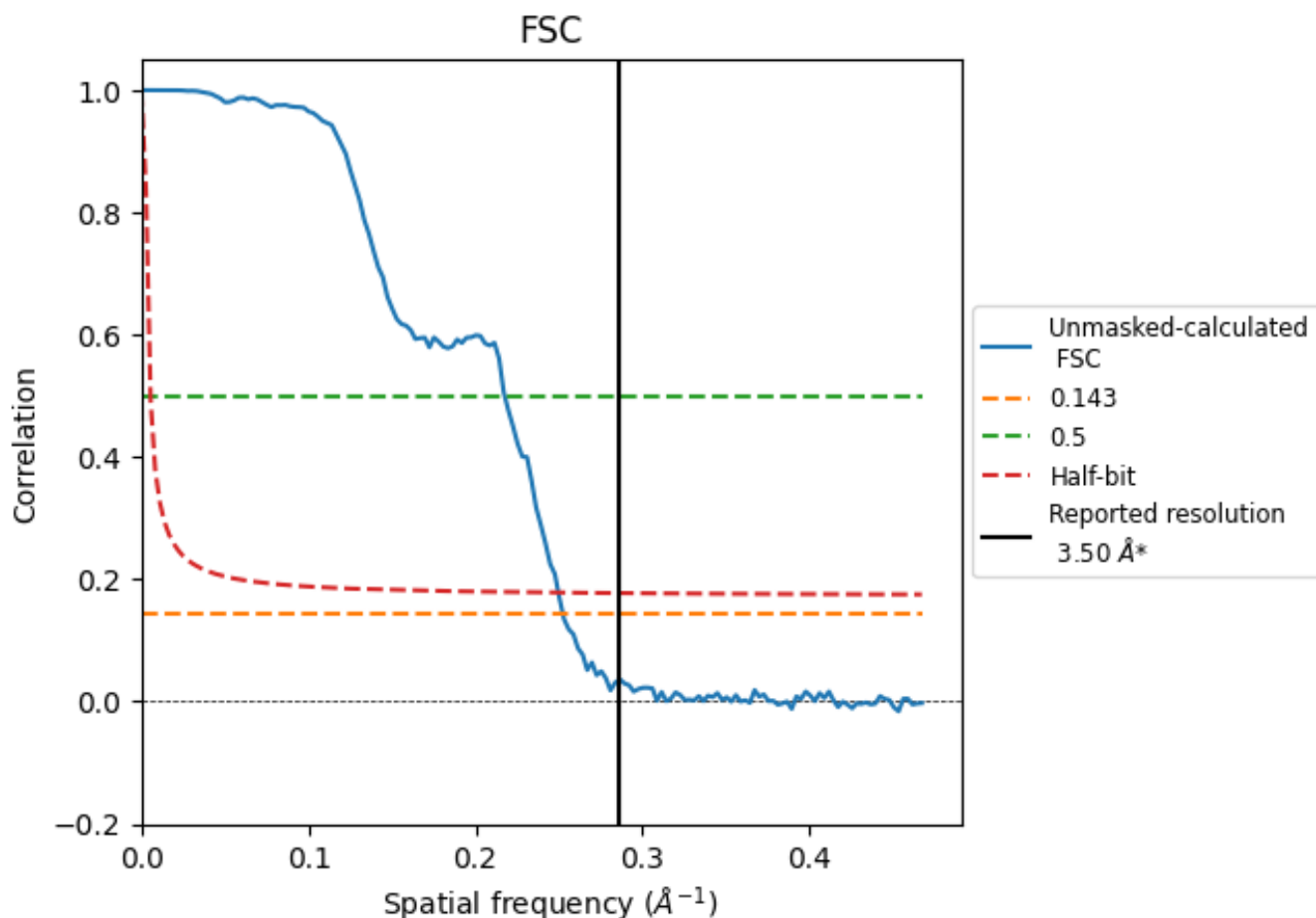


*Reported resolution corresponds to spatial frequency of 0.286 \AA^{-1}

7 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

7.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.286\AA^{-1}

7.2 Resolution estimates [i](#)

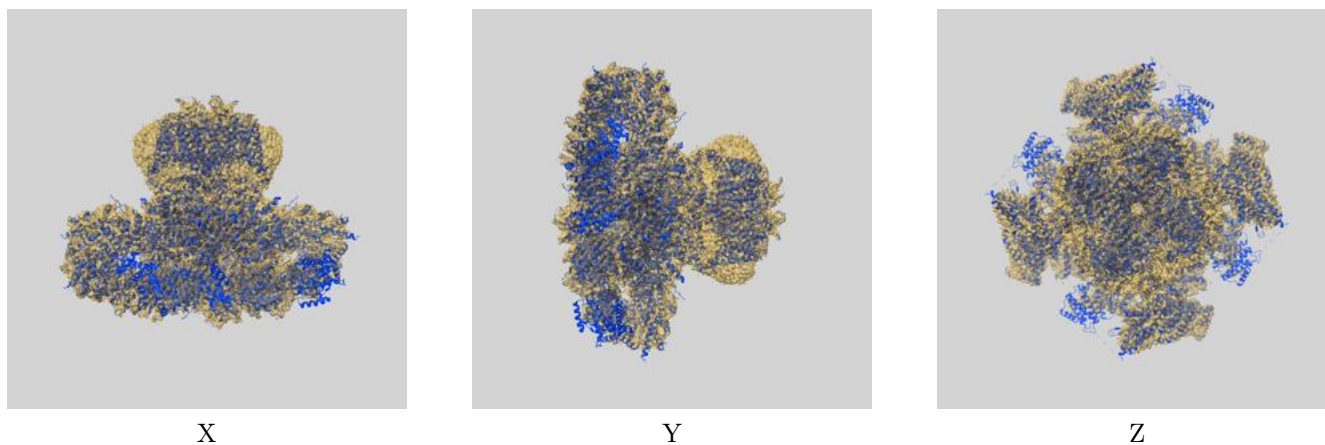
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.96	4.60	4.00

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.96 differs from the reported value 3.5 by more than 10 %

8 Map-model fit [i](#)

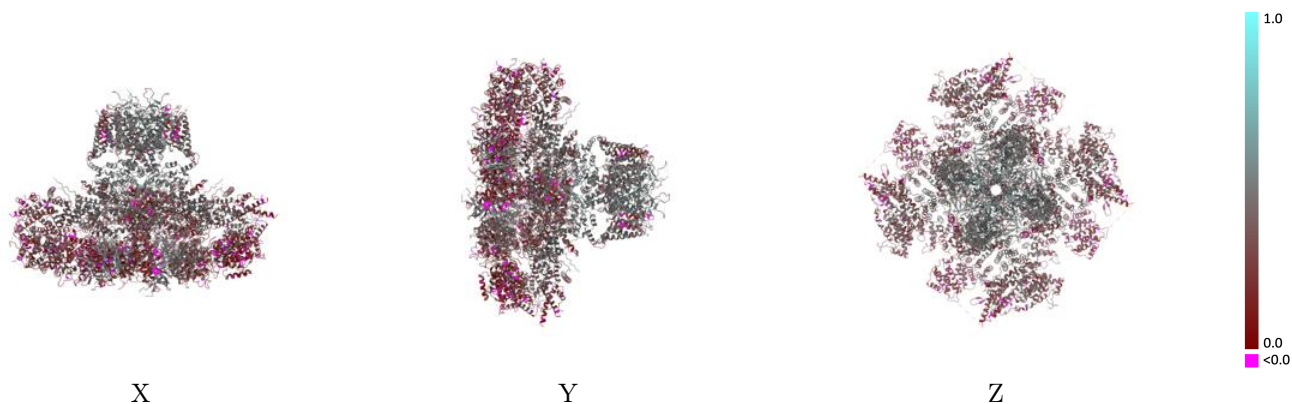
This section contains information regarding the fit between EMD map EMD-27983 and PDB model 8EAR. Per-residue inclusion information can be found in section ?? on page ??.

8.1 Map-model overlay [i](#)



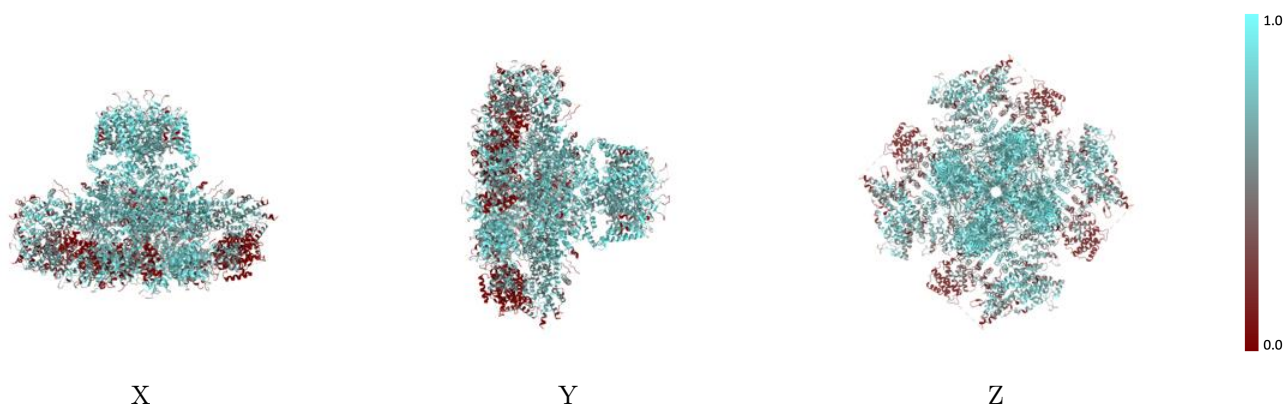
The images above show the 3D surface view of the map at the recommended contour level 0.011 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

8.2 Q-score mapped to coordinate model [i](#)



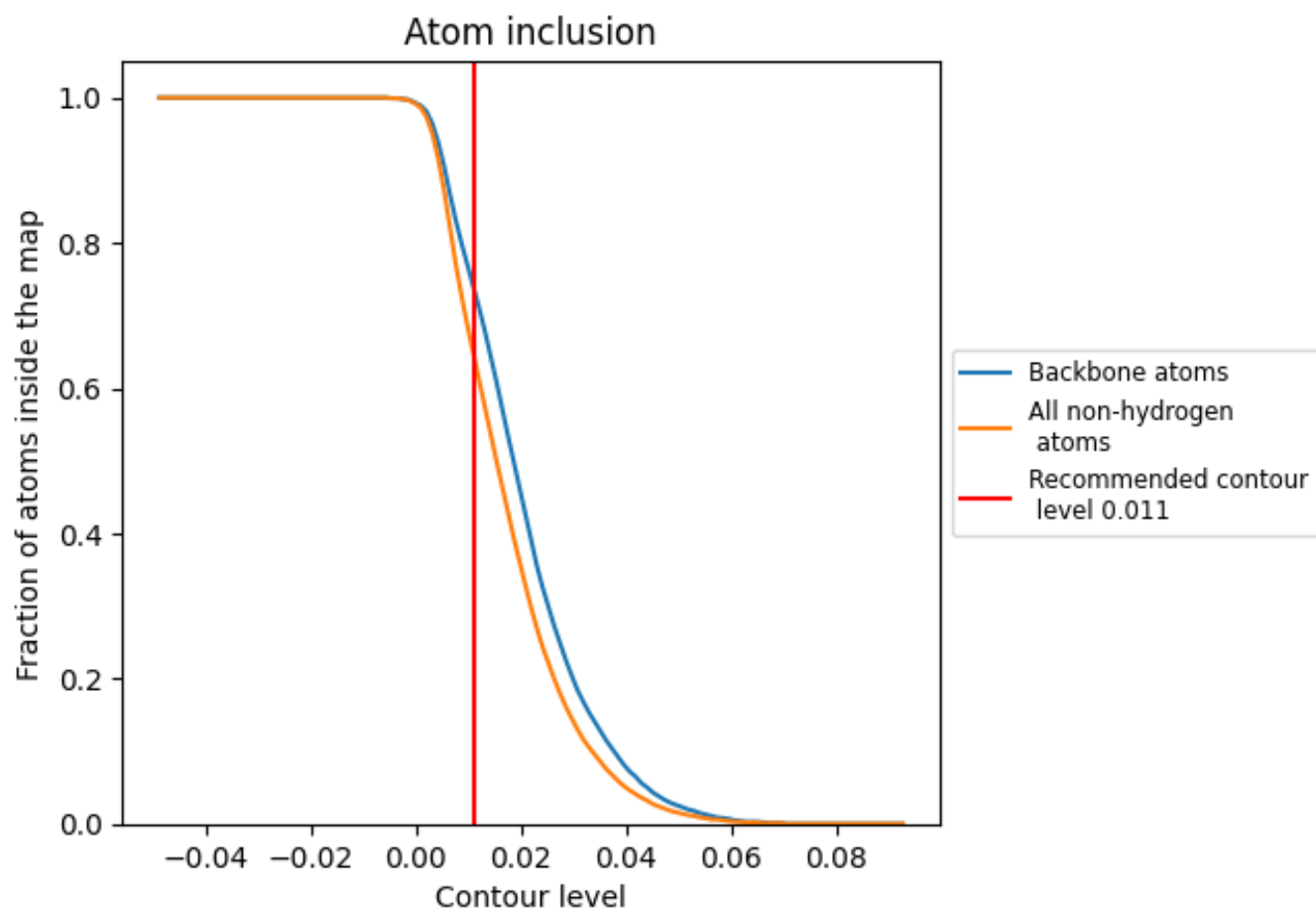
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

8.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.011).











8.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 65% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6470	 0.3500
A	 0.6470	 0.3500
B	 0.6470	 0.3500
C	 0.6470	 0.3500
D	 0.6470	 0.3500

