



## wwPDB EM Validation Summary Report ⓘ

Sep 22, 2025 – 10:13 AM JST

PDB ID : 9VJ1 / pdb\_00009vj1  
EMDB ID : EMD-65101  
Title : Cryo-EM structure of Na<sup>+</sup>,K<sup>+</sup>-ATPase that forms a cation channel with palytoxin (ADP form)  
Authors : Kanai, R.; Cornelius, F.; Vilsen, B.; Toyoshima, C.  
Deposited on : 2025-06-19  
Resolution : 3.40 Å(reported)  
Based on initial model : 8jtz

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

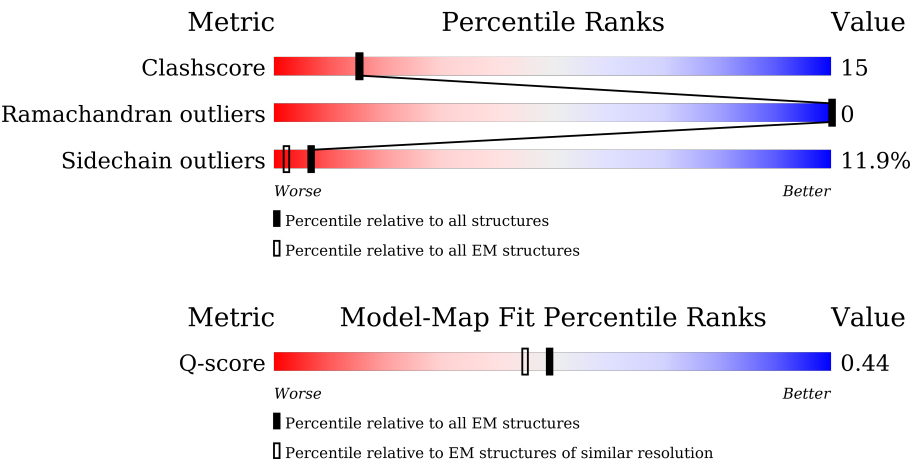
EMDB validation analysis : 0.0.1.dev129  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : 202505.v01 (Using data in the 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) : 2.46

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.40 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.






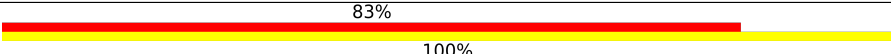
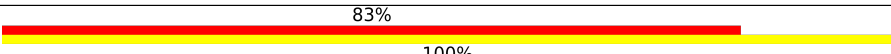
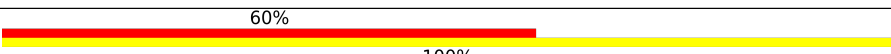
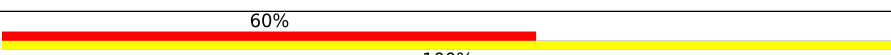
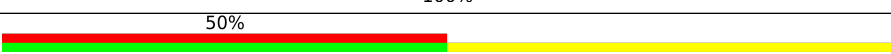

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	14717 ( 2.90 - 3.90 )

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	305	<div><div></div><div><div></div><div>67%</div><div>26%</div><div></div><div></div></div><div></div></div>
1	D	305	<div><div></div><div><div></div><div>66%</div><div>26%</div><div></div><div></div></div><div></div></div>
2	A	1028	<div><div>10%</div><div><div></div><div>62%</div><div>30%</div><div></div><div></div></div><div></div></div>
2	C	1028	<div><div>9%</div><div><div></div><div>61%</div><div>30%</div><div></div><div></div></div><div></div></div>
3	E	94	<div><div></div><div><div></div><div>27%</div><div>16%</div><div>57%</div><div></div></div><div></div></div>

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Mol	Chain	Length	Quality of chain
3	G	94	 27% 16% 57%
4	F	6	 33% 83% 17%
4	K	6	 33% 83% 17%
5	H	6	 83% 100%
5	L	6	 83% 100%
6	I	5	 60% 100%
6	M	5	 60% 100%
7	J	2	 50% 50%
7	N	2	 50% 50%

## 2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 22636 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 Na<sup>+</sup>,K<sup>+</sup>-ATPase beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	294	Total	C	N	O	S	0	0
			2399	1551	394	443	11		
1	B	294	Total	C	N	O	S	0	0
			2399	1551	394	443	11		

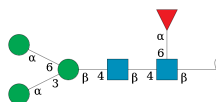
- Molecule 2 is a protein called Na, K-ATPase alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	982	Total	C	N	O	S	0	0
			7594	4835	1278	1436	45		
2	A	982	Total	C	N	O	S	0	0
			7594	4835	1278	1436	45		

- Molecule 3 is a protein called FXYD domain-containing ion transport regulator.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	40	Total	C	N	O	S	0	0
			311	203	51	55	2		
3	G	40	Total	C	N	O	S	0	0
			311	203	51	55	2		

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



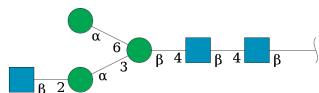
Mol	Chain	Residues	Atoms				AltConf	Trace
4	F	6	Total	C	N	O	0	0
			71	40	2	29		

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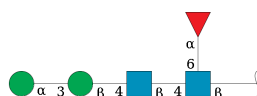
Mol	Chain	Residues	Atoms				AltConf	Trace
4	K	6	Total	C	N	O	0	0
			71	40	2	29		

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
5	H	6	Total	C	N	O	0	0
			75	42	3	30		
5	L	6	Total	C	N	O	0	0
			75	42	3	30		

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
6	I	5	Total	C	N	O	0	0
			60	34	2	24		
6	M	5	Total	C	N	O	0	0
			60	34	2	24		

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
7	J	2	Total	C	N	O	0	0
			28	16	2	10		

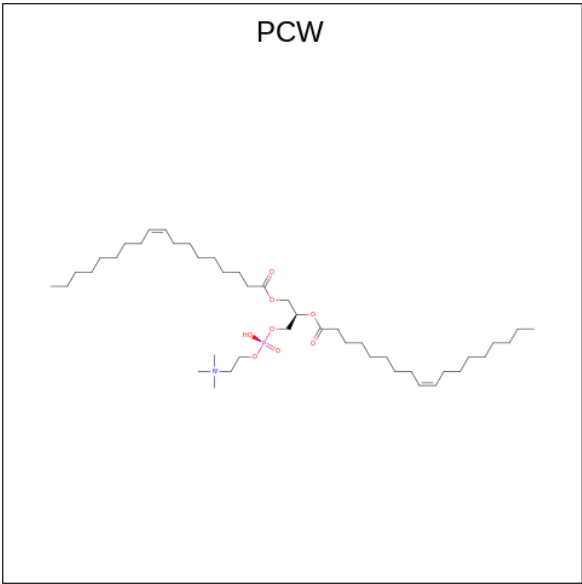
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Mol	Chain	Residues	Atoms				AltConf	Trace
7	N	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms			AltConf
8	D	1	Total 28	C 27	O 1	0
8	D	1	Total 28	C 27	O 1	0
8	C	1	Total 28	C 27	O 1	0
8	C	1	Total 28	C 27	O 1	0
8	C	1	Total 28	C 27	O 1	0
8	B	1	Total 28	C 27	O 1	0
8	B	1	Total 28	C 27	O 1	0
8	A	1	Total 28	C 27	O 1	0
8	A	1	Total 28	C 27	O 1	0
8	A	1	Total 28	C 27	O 1	0

- Molecule 9 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula: C<sub>44</sub>H<sub>85</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					AltConf
9	C	1	Total	C	N	O	P	0
			22	12	1	8	1	
9	C	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	C	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	C	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	C	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	C	1	Total	C	N	O	P	0
			22	12	1	8	1	
9	E	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	E	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	B	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	A	1	Total	C	N	O	P	0
			22	12	1	8	1	
9	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	A	1	Total	C	N	O	P	0
			54	44	1	8	1	

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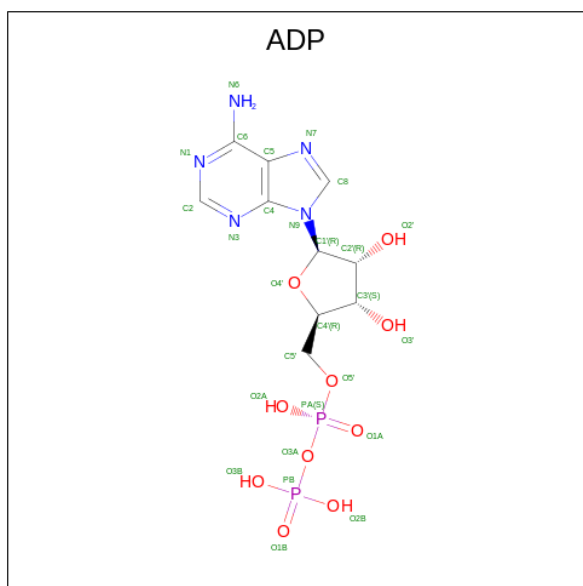
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Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	A	1	Total	C	N	O	P	0
			22	12	1	8	1	
9	G	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	G	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
10	C	1	Total	Mg	0
			1	1	
10	A	1	Total	Mg	0
			1	1	

- Molecule 11 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					AltConf
11	C	1	Total	C	N	O	P	0
			27	10	5	10	2	

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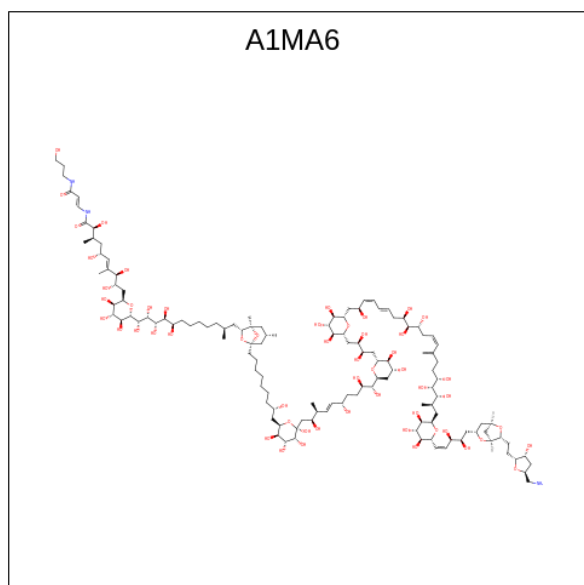
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Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 12 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
12	C	4	Total	Na	0
			4	4	
12	A	4	Total	Na	0
			4	4	

- Molecule 13 is palytoxin (CCD ID: A1MA6) (formula: C<sub>129</sub>H<sub>223</sub>N<sub>3</sub>O<sub>54</sub>) (labeled as "Ligand of Interest" by depositor).

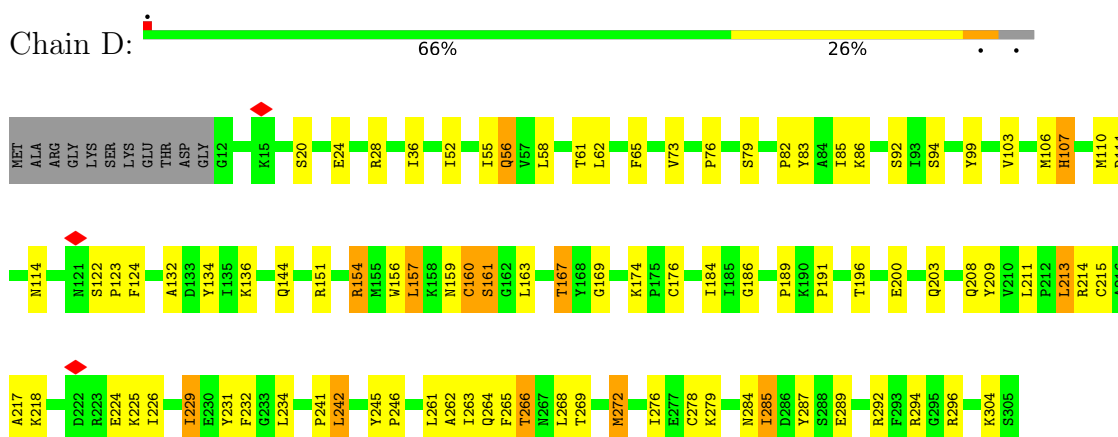


Mol	Chain	Residues	Atoms				AltConf
13	C	1	Total	C	N	O	0
			186	129	3	54	
13	A	1	Total	C	N	O	0
			186	129	3	54	

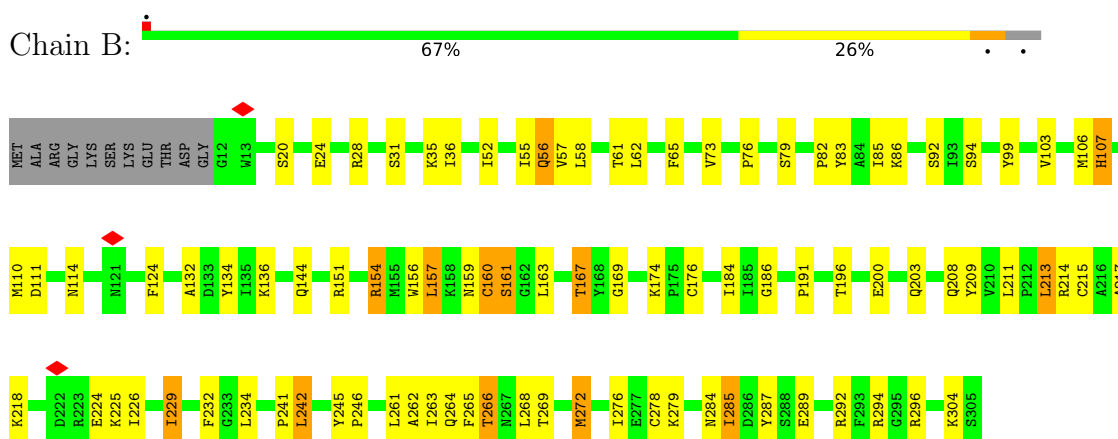
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

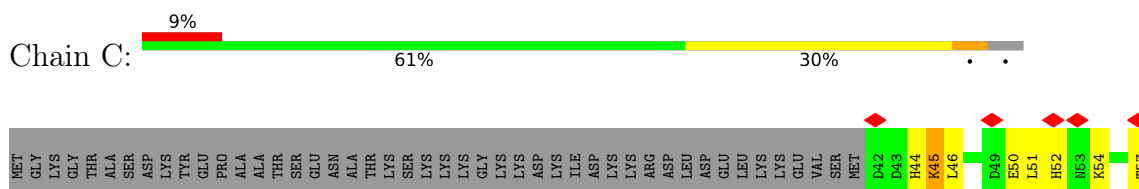
- Molecule 1: Na<sup>+</sup>,K<sup>+</sup>-ATPase beta subunit

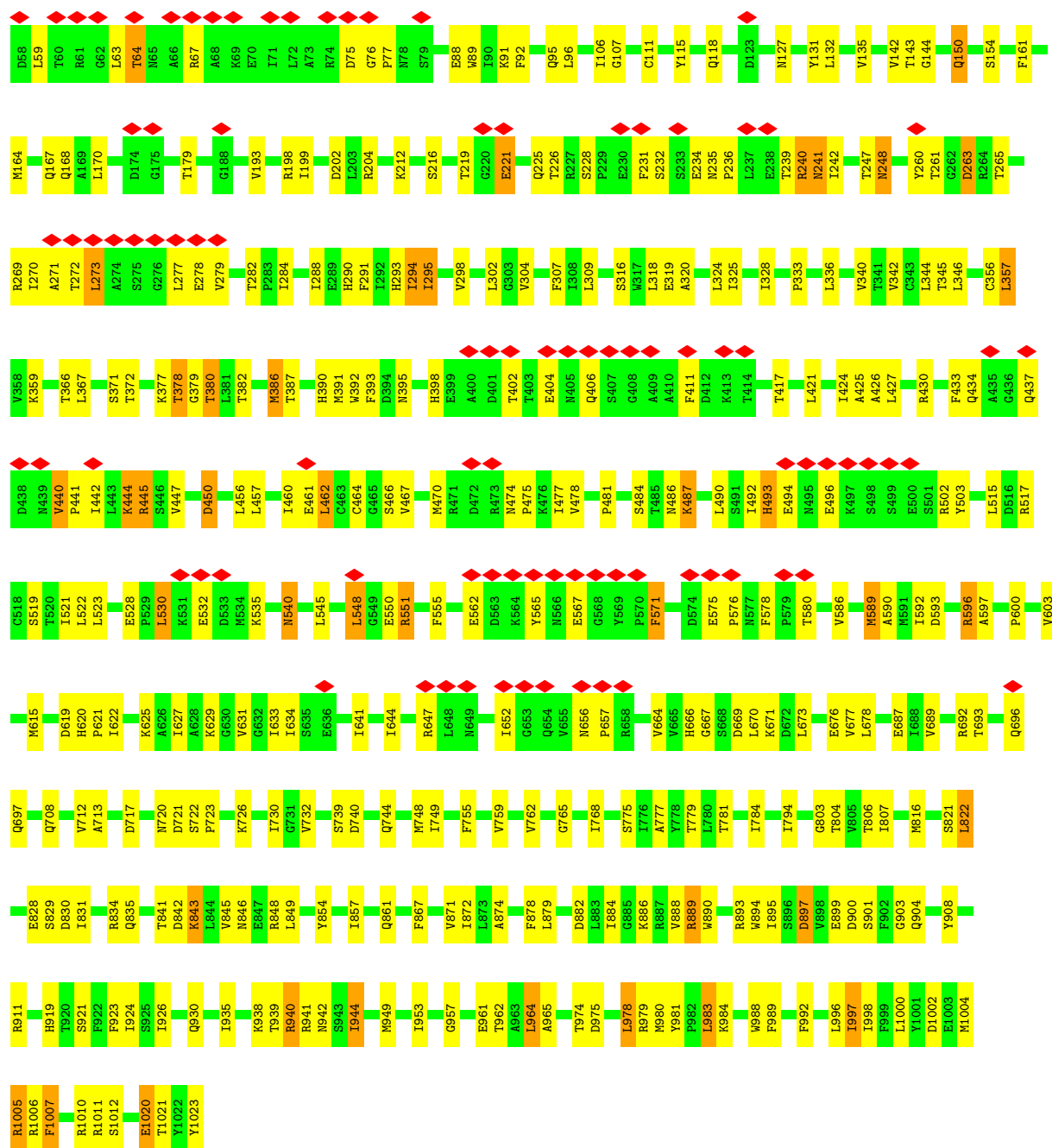


- Molecule 1: Na<sup>+</sup>,K<sup>+</sup>-ATPase beta subunit

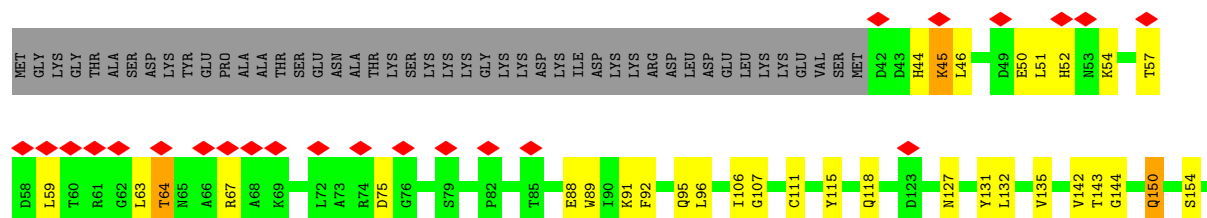


- Molecule 2: Na, K-ATPase alpha subunit

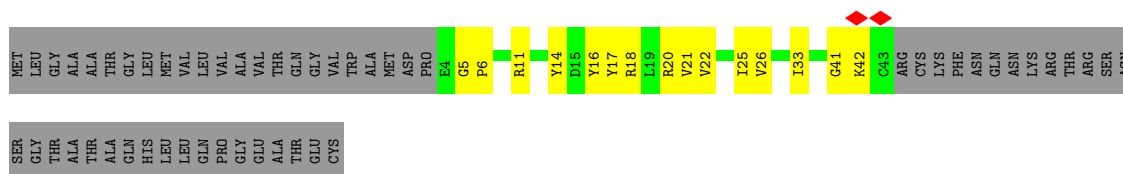




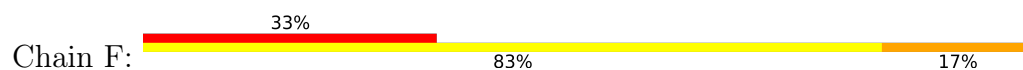
• Molecule 2: Na, K-ATPase alpha subunit



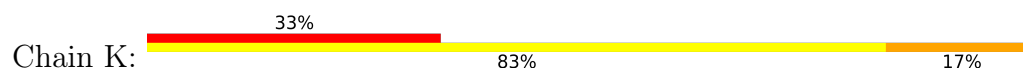
Chain G:  27% 16% 57%



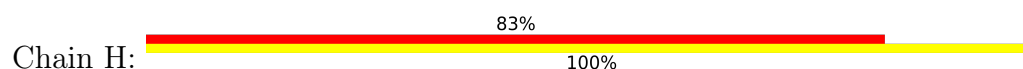
- Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



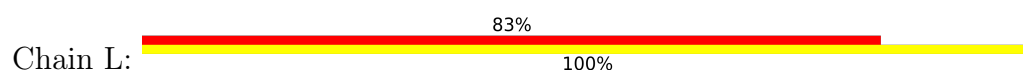
- Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 6: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	28472	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.068	Depositor
Minimum map value	-0.028	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	258.24, 258.24, 258.24	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.076, 1.076, 1.076	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: A1MA6, BMA, NAG, PCW, FUC, MAN, NA, MG, ADP, CLR

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	B	0.21	0/2462	0.65	0/3317
1	D	0.21	0/2462	0.65	0/3317
2	A	0.32	0/7744	0.73	2/10509 (0.0%)
2	C	0.32	0/7744	0.73	2/10509 (0.0%)
3	E	0.20	0/315	0.50	0/427
3	G	0.20	0/315	0.50	0/427
All	All	0.30	0/21042	0.71	4/28506 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	444	LYS	CA-C-N	-5.21	112.17	122.02
2	C	444	LYS	C-N-CA	-5.21	112.17	122.02
2	A	444	LYS	CA-C-N	-5.21	112.17	122.02
2	A	444	LYS	C-N-CA	-5.21	112.17	122.02

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	B	2399	0	2354	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2399	0	2354	56	0
2	A	7594	0	7612	232	0
2	C	7594	0	7612	240	0
3	E	311	0	323	15	0
3	G	311	0	323	15	0
4	F	71	0	61	1	0
4	K	71	0	61	1	0
5	H	75	0	64	0	0
5	L	75	0	64	0	0
6	I	60	0	52	0	0
6	M	60	0	52	0	0
7	J	28	0	25	0	0
7	N	28	0	25	0	0
8	A	84	0	138	18	0
8	B	56	0	92	4	0
8	C	84	0	138	20	0
8	D	56	0	92	9	0
9	A	314	0	456	56	0
9	B	54	0	84	11	0
9	C	260	0	372	46	0
9	E	108	0	168	6	0
9	G	108	0	168	6	0
10	A	1	0	0	0	0
10	C	1	0	0	0	0
11	A	27	0	12	1	0
11	C	27	0	12	1	0
12	A	4	0	0	0	0
12	C	4	0	0	0	0
13	A	186	0	0	5	0
13	C	186	0	0	5	0
All	All	22636	0	22714	661	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 15.

The worst 5 of 661 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)
9:C:1305:PCW:H452	9:A:1305:PCW:H272	1.33	1.11
9:B:401:PCW:H252	8:A:1302:CLR:H263	1.32	1.10
9:C:1305:PCW:H472	9:A:1305:PCW:H271	1.32	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:1302:CLR:H263	9:A:1304:PCW:H252	1.36	1.03
9:C:1305:PCW:H472	9:A:1305:PCW:C27	1.90	1.00

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	B	292/305 (96%)	268 (92%)	24 (8%)	0	100	100
1	D	292/305 (96%)	268 (92%)	24 (8%)	0	100	100
2	A	980/1028 (95%)	893 (91%)	87 (9%)	0	100	100
2	C	980/1028 (95%)	893 (91%)	87 (9%)	0	100	100
3	E	38/94 (40%)	36 (95%)	2 (5%)	0	100	100
3	G	38/94 (40%)	36 (95%)	2 (5%)	0	100	100
All	All	2620/2854 (92%)	2394 (91%)	226 (9%)	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	B	258/266 (97%)	225 (87%)	33 (13%)	3	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	258/266 (97%)	225 (87%)	33 (13%)	3	13
2	A	830/869 (96%)	731 (88%)	99 (12%)	4	16
2	C	830/869 (96%)	731 (88%)	99 (12%)	4	16
3	E	33/75 (44%)	32 (97%)	1 (3%)	36	61
3	G	33/75 (44%)	32 (97%)	1 (3%)	36	61
All	All	2242/2420 (93%)	1976 (88%)	266 (12%)	7	16

5 of 266 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	720	ASN
2	A	822	LEU
2	A	1007	PHE
2	C	708	GLN
2	C	676	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	203	GLN
2	A	248	ASN
2	A	946	GLN
2	A	826	GLN
1	B	258	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

38 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	NAG	F	1	4,1	14,14,15	0.63	0	17,19,21	1.32	2 (11%)
4	NAG	F	2	4	14,14,15	0.65	0	17,19,21	1.05	1 (5%)
4	BMA	F	3	4	11,11,12	0.86	0	15,15,17	1.44	2 (13%)
4	MAN	F	4	4	11,11,12	0.79	0	15,15,17	1.06	1 (6%)
4	MAN	F	5	4	11,11,12	0.76	0	15,15,17	1.00	1 (6%)
4	FUC	F	6	4	10,10,11	0.93	1 (10%)	14,14,16	0.80	0
5	NAG	H	1	5,1	14,14,15	0.77	0	17,19,21	1.69	2 (11%)
5	NAG	H	2	5	14,14,15	0.60	0	17,19,21	2.14	3 (17%)
5	BMA	H	3	5	11,11,12	0.93	1 (9%)	15,15,17	1.64	3 (20%)
5	MAN	H	4	5	11,11,12	0.78	0	15,15,17	1.61	3 (20%)
5	NAG	H	5	5	14,14,15	0.76	0	17,19,21	1.10	1 (5%)
5	MAN	H	6	5	11,11,12	0.70	0	15,15,17	1.17	1 (6%)
6	NAG	I	1	6,1	14,14,15	0.71	0	17,19,21	1.68	2 (11%)
6	NAG	I	2	6	14,14,15	0.68	0	17,19,21	0.93	1 (5%)
6	BMA	I	3	6	11,11,12	0.85	0	15,15,17	1.36	2 (13%)
6	MAN	I	4	6	11,11,12	0.78	0	15,15,17	1.08	1 (6%)
6	FUC	I	5	6	10,10,11	0.92	1 (10%)	14,14,16	0.80	0
7	NAG	J	1	7,1	14,14,15	0.74	0	17,19,21	0.99	1 (5%)
7	NAG	J	2	7	14,14,15	0.70	0	17,19,21	0.79	0
4	NAG	K	1	4,1	14,14,15	0.63	0	17,19,21	1.32	2 (11%)
4	NAG	K	2	4	14,14,15	0.65	0	17,19,21	1.05	1 (5%)
4	BMA	K	3	4	11,11,12	0.86	0	15,15,17	1.44	2 (13%)
4	MAN	K	4	4	11,11,12	0.79	0	15,15,17	1.06	1 (6%)
4	MAN	K	5	4	11,11,12	0.76	0	15,15,17	1.00	1 (6%)
4	FUC	K	6	4	10,10,11	0.93	1 (10%)	14,14,16	0.80	0
5	NAG	L	1	5,1	14,14,15	0.77	0	17,19,21	1.69	2 (11%)
5	NAG	L	2	5	14,14,15	0.60	0	17,19,21	2.14	3 (17%)
5	BMA	L	3	5	11,11,12	0.93	1 (9%)	15,15,17	1.64	3 (20%)
5	MAN	L	4	5	11,11,12	0.78	0	15,15,17	1.61	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	L	5	5	14,14,15	0.77	0	17,19,21	1.10	1 (5%)
5	MAN	L	6	5	11,11,12	0.70	0	15,15,17	1.17	1 (6%)
6	NAG	M	1	6,1	14,14,15	0.71	0	17,19,21	1.67	2 (11%)
6	NAG	M	2	6	14,14,15	0.68	0	17,19,21	0.93	1 (5%)
6	BMA	M	3	6	11,11,12	0.85	0	15,15,17	1.36	2 (13%)
6	MAN	M	4	6	11,11,12	0.78	0	15,15,17	1.08	1 (6%)
6	FUC	M	5	6	10,10,11	0.92	1 (10%)	14,14,16	0.80	0
7	NAG	N	1	7,1	14,14,15	0.74	0	17,19,21	0.99	1 (5%)
7	NAG	N	2	7	14,14,15	0.70	0	17,19,21	0.80	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
4	NAG	F	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	BMA	F	3	4	-	1/2/19/22	0/1/1/1
4	MAN	F	4	4	-	0/2/19/22	0/1/1/1
4	MAN	F	5	4	-	0/2/19/22	0/1/1/1
4	FUC	F	6	4	-	-	0/1/1/1
5	NAG	H	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	H	2	5	-	3/6/23/26	0/1/1/1
5	BMA	H	3	5	-	2/2/19/22	0/1/1/1
5	MAN	H	4	5	-	0/2/19/22	0/1/1/1
5	NAG	H	5	5	-	4/6/23/26	0/1/1/1
5	MAN	H	6	5	-	2/2/19/22	0/1/1/1
6	NAG	I	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	I	2	6	-	0/6/23/26	0/1/1/1
6	BMA	I	3	6	-	1/2/19/22	0/1/1/1
6	MAN	I	4	6	-	0/2/19/22	0/1/1/1
6	FUC	I	5	6	-	-	0/1/1/1
7	NAG	J	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	J	2	7	-	0/6/23/26	0/1/1/1
4	NAG	K	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1
4	BMA	K	3	4	-	1/2/19/22	0/1/1/1
4	MAN	K	4	4	-	0/2/19/22	0/1/1/1
4	MAN	K	5	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FUC	K	6	4	-	-	0/1/1/1
5	NAG	L	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	L	2	5	-	3/6/23/26	0/1/1/1
5	BMA	L	3	5	-	2/2/19/22	0/1/1/1
5	MAN	L	4	5	-	0/2/19/22	0/1/1/1
5	NAG	L	5	5	-	4/6/23/26	0/1/1/1
5	MAN	L	6	5	-	2/2/19/22	0/1/1/1
6	NAG	M	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	M	2	6	-	0/6/23/26	0/1/1/1
6	BMA	M	3	6	-	1/2/19/22	0/1/1/1
6	MAN	M	4	6	-	0/2/19/22	0/1/1/1
6	FUC	M	5	6	-	-	0/1/1/1
7	NAG	N	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	N	2	7	-	0/6/23/26	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	6	FUC	O5-C1	-2.28	1.40	1.43
4	F	6	FUC	O5-C1	-2.28	1.40	1.43
5	L	3	BMA	C2-C3	2.26	1.55	1.52
5	H	3	BMA	C2-C3	2.25	1.55	1.52
6	M	5	FUC	O5-C1	-2.20	1.40	1.43

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	2	NAG	C1-O5-C5	5.68	119.89	112.19
5	H	2	NAG	C1-O5-C5	5.68	119.89	112.19
6	I	1	NAG	C1-O5-C5	5.49	119.64	112.19
6	M	1	NAG	C1-O5-C5	5.49	119.64	112.19
5	H	2	NAG	C2-N2-C7	5.10	130.16	122.90

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	2	NAG	C3-C2-N2-C7
5	L	2	NAG	C3-C2-N2-C7
5	H	6	MAN	O5-C5-C6-O6
5	L	6	MAN	O5-C5-C6-O6

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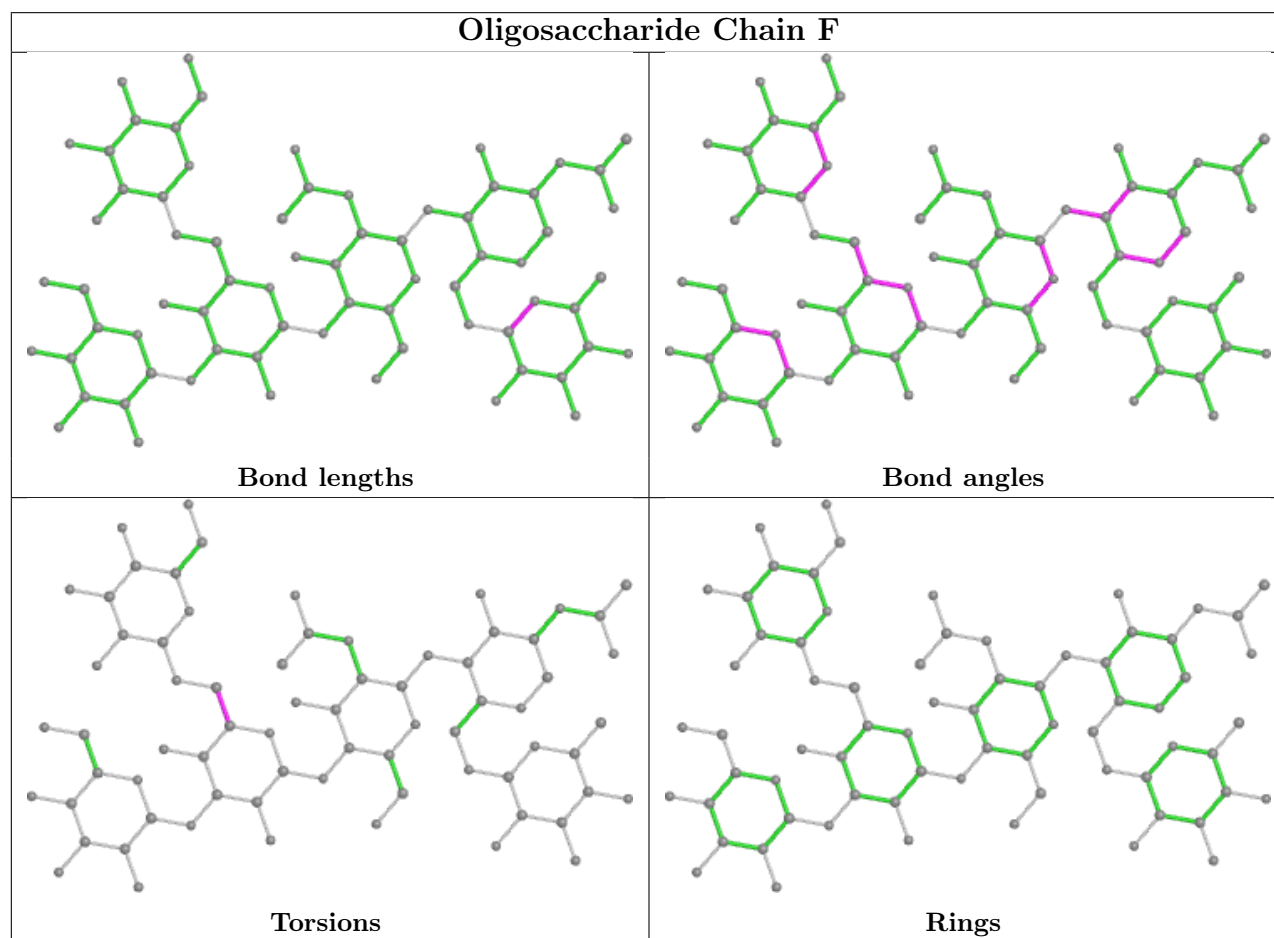
Mol	Chain	Res	Type	Atoms
5	H	5	NAG	O5-C5-C6-O6

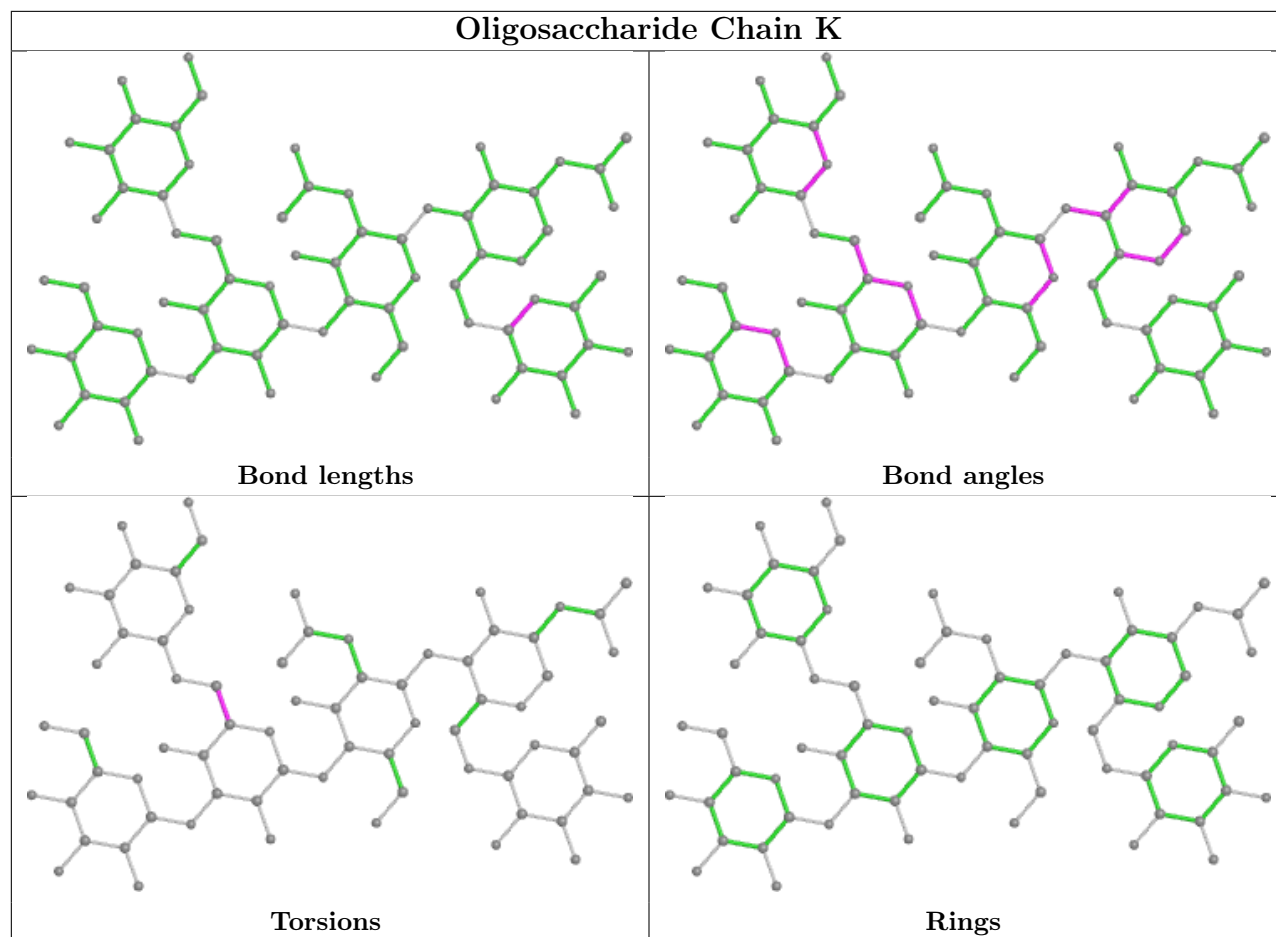
There are no ring outliers.

2 monomers are involved in 2 short contacts:

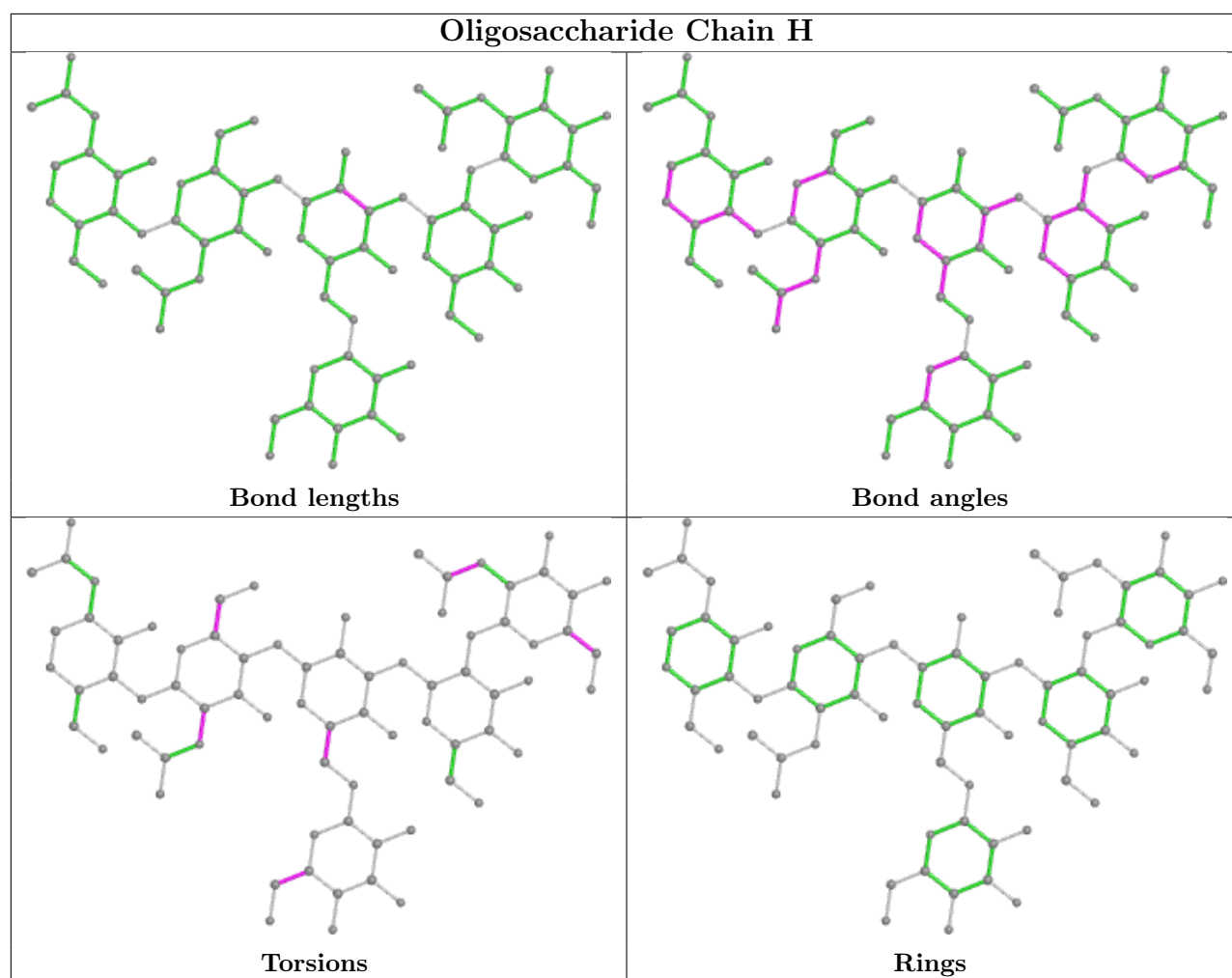
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	6	FUC	1	0
4	K	6	FUC	1	0

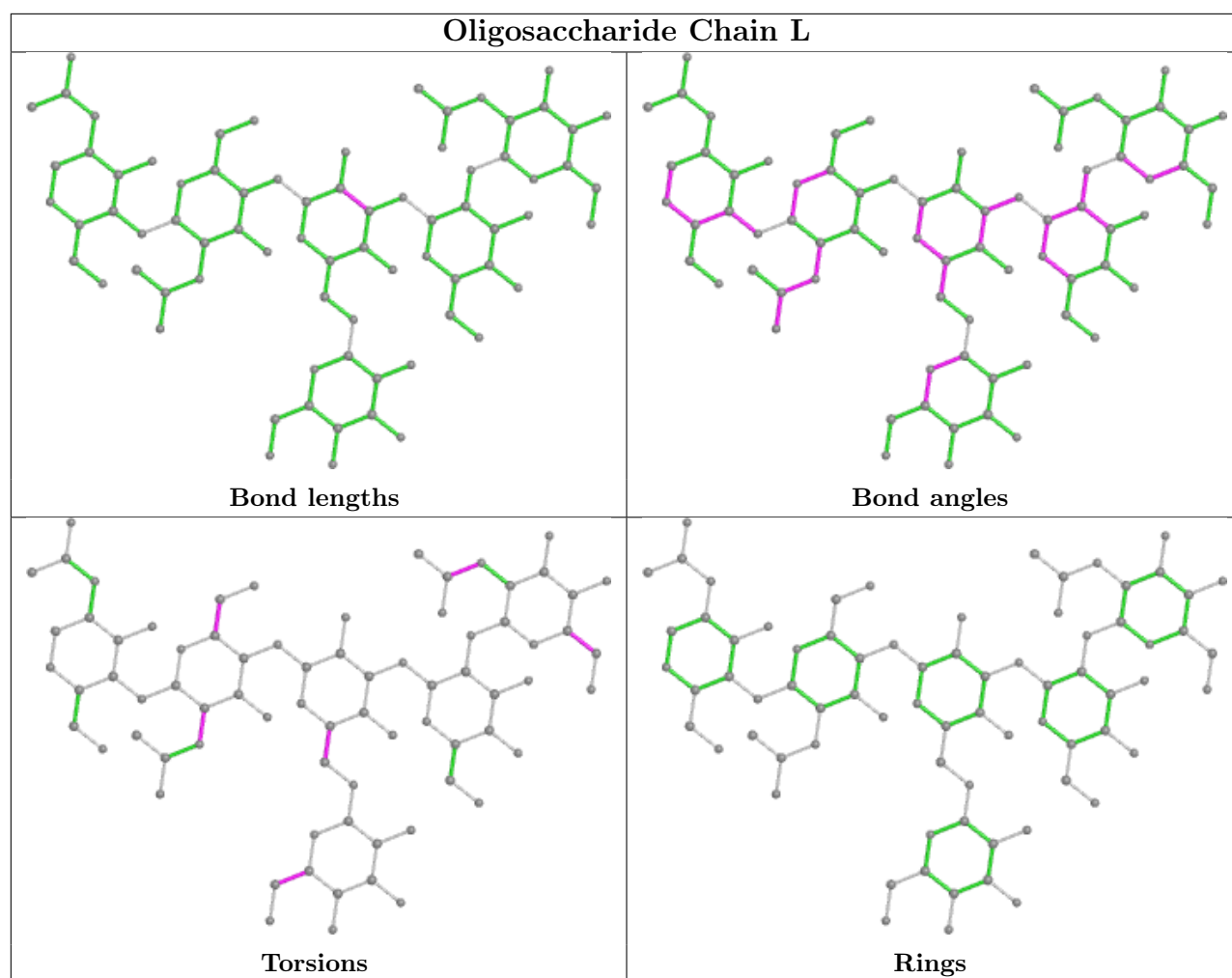
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

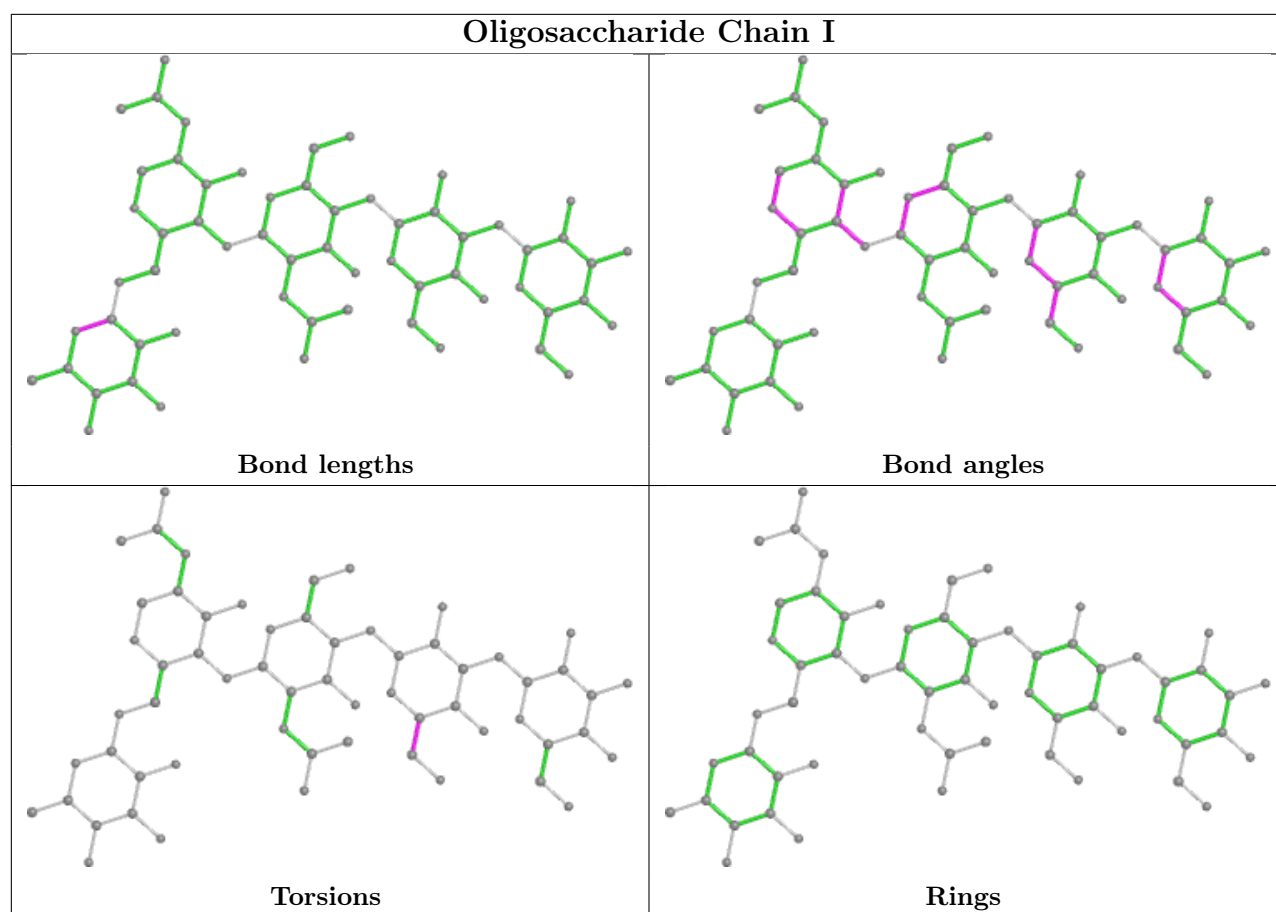


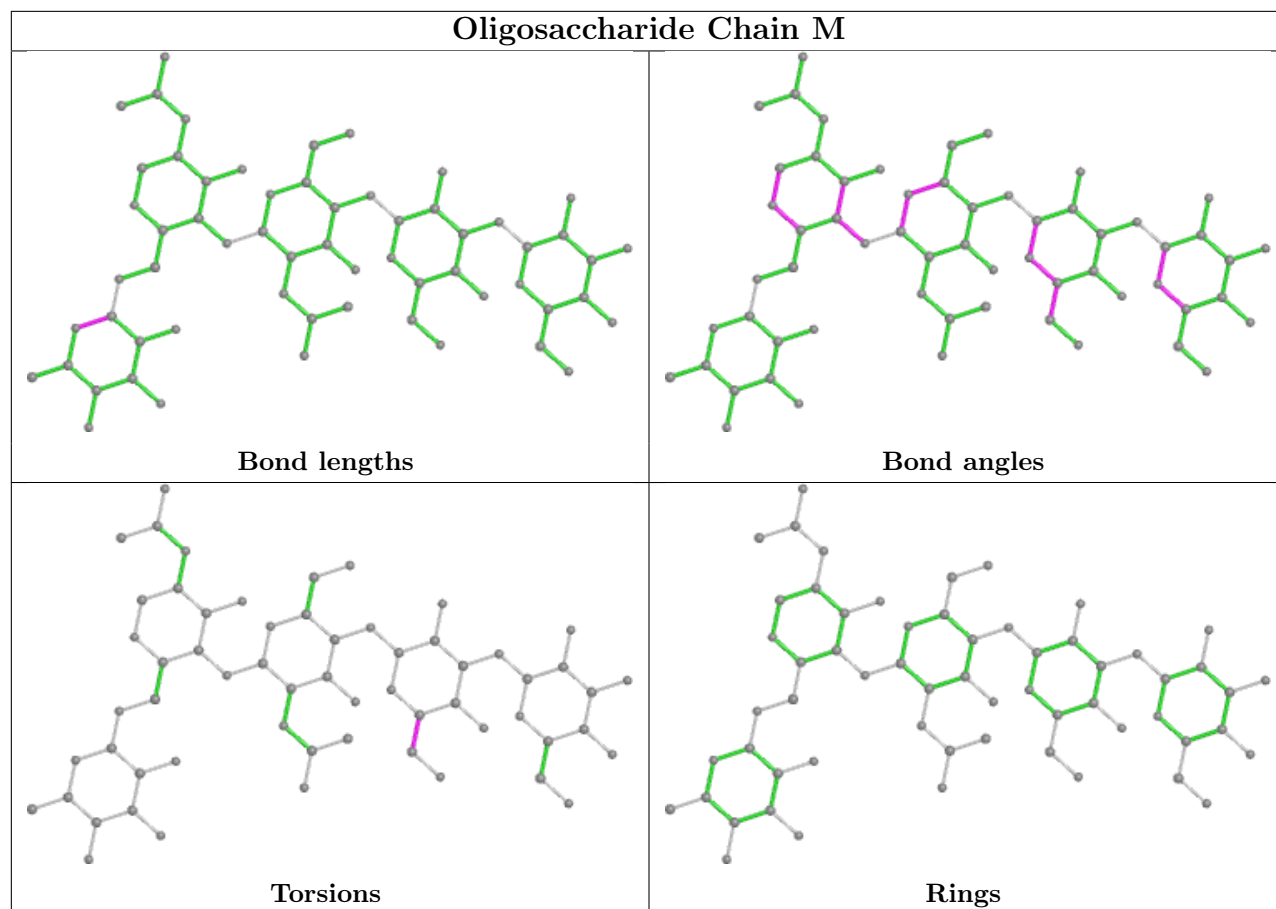


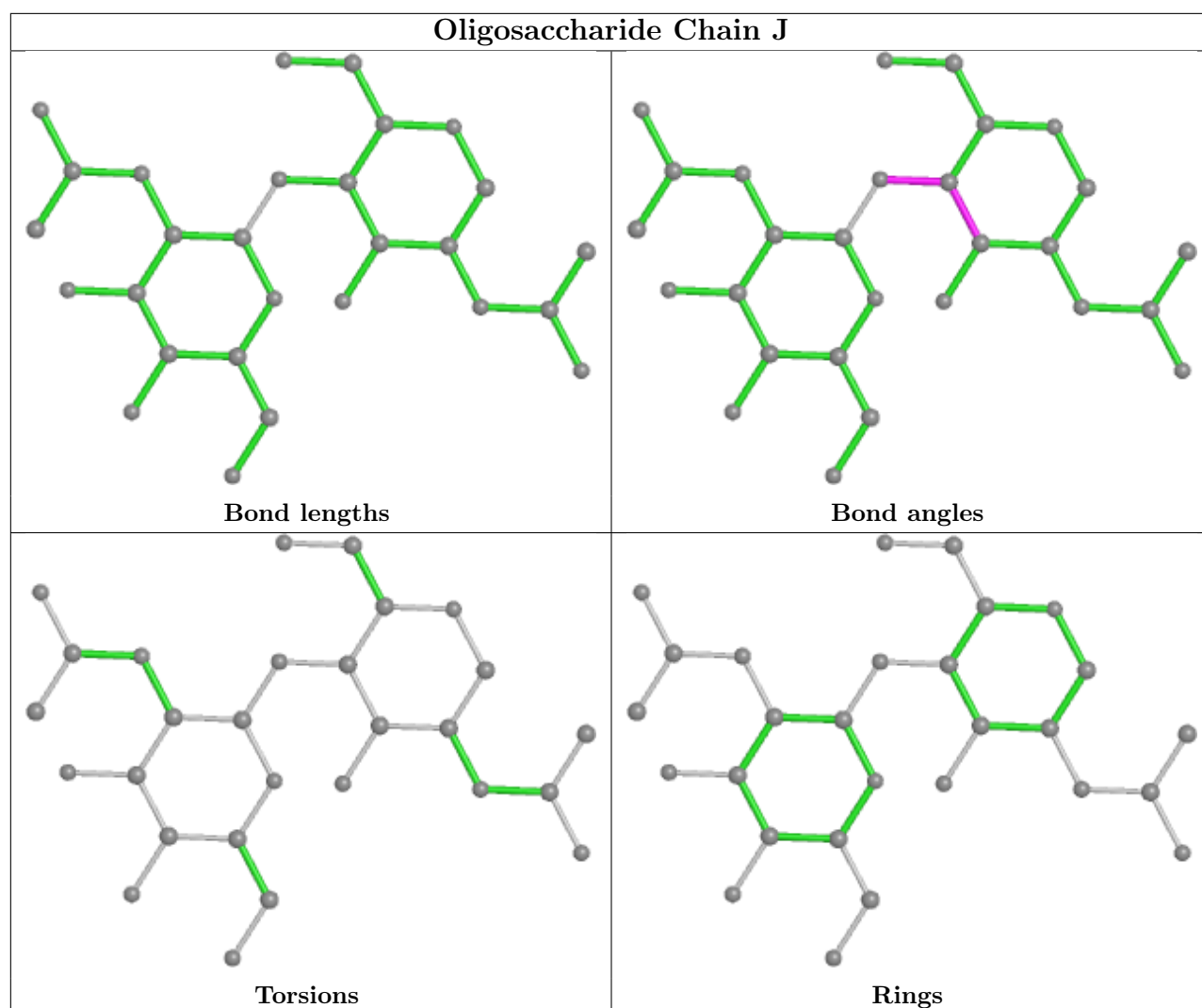


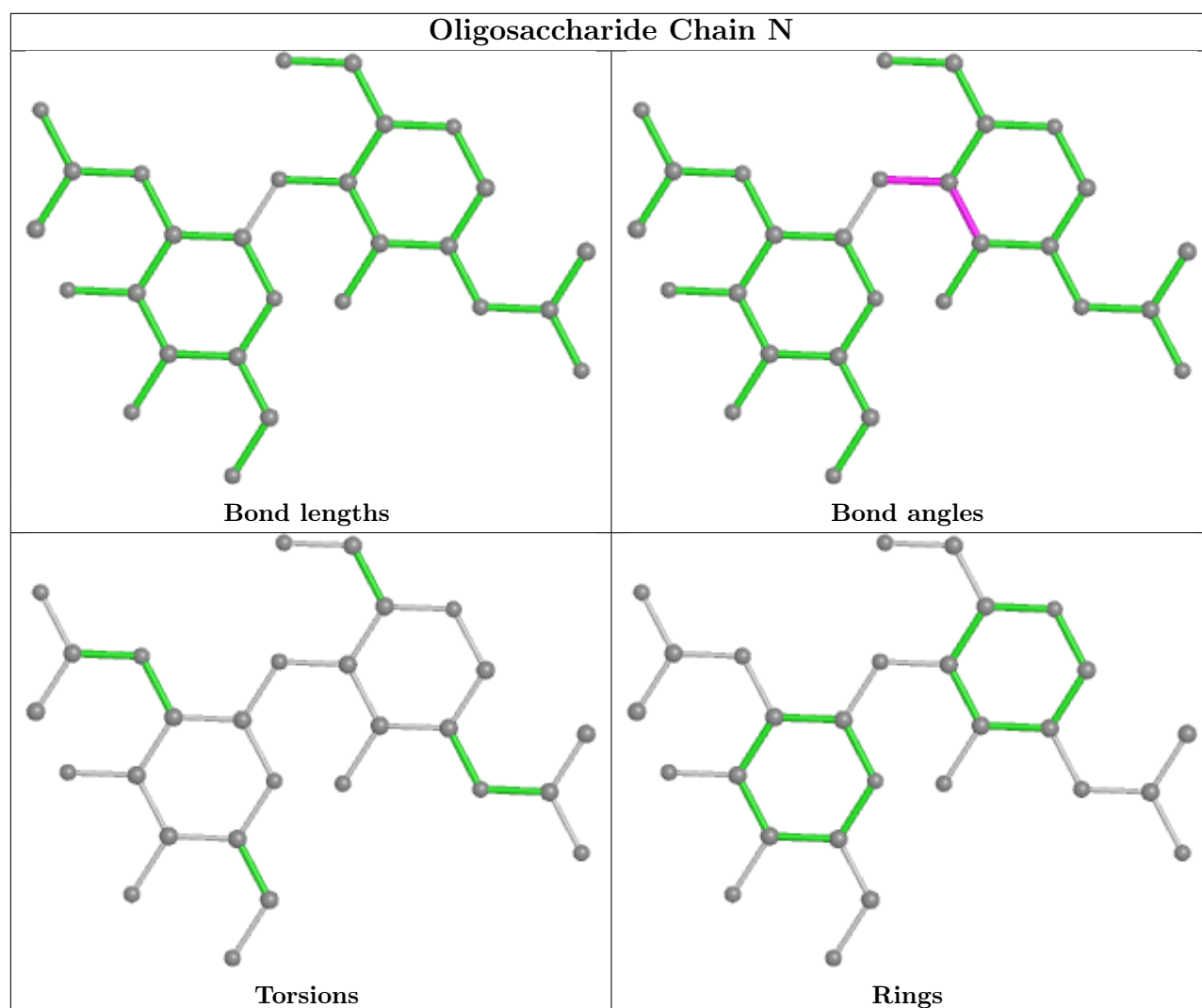












## 5.6 Ligand geometry [i](#)

Of 42 ligands modelled in this entry, 10 are monoatomic - leaving 32 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	$\# Z  > 2$
9	PCW	A	1303	-	21,21,53	0.88	0	27,29,61	1.08	2 (7%)
8	CLR	A	1301	-	31,31,31	1.15	1 (3%)	48,48,48	1.38	4 (8%)
8	CLR	C	1309	-	31,31,31	1.15	1 (3%)	48,48,48	1.40	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  >
9	PCW	A	1306	-	53,53,53	0.96	2 (3%)	59,61,61	0.90	1 (1%)
9	PCW	A	1308	-	53,53,53	0.94	2 (3%)	59,61,61	0.88	1 (1%)
9	PCW	E	101	-	53,53,53	0.98	2 (3%)	59,61,61	0.74	0
9	PCW	B	401	-	53,53,53	0.94	2 (3%)	59,61,61	0.88	1 (1%)
9	PCW	G	101	-	53,53,53	0.98	2 (3%)	59,61,61	0.74	0
8	CLR	B	403	-	31,31,31	1.13	1 (3%)	48,48,48	1.38	6 (12%)
13	A1MA6	C	1316	-	190,195,195	1.34	20 (10%)	219,278,278	1.68	36 (16%)
9	PCW	C	1308	-	21,21,53	0.87	0	27,29,61	1.27	4 (14%)
13	A1MA6	A	1317	-	190,195,195	1.34	20 (10%)	219,278,278	1.68	36 (16%)
9	PCW	A	1305	-	53,53,53	0.97	2 (3%)	59,61,61	0.90	2 (3%)
9	PCW	A	1304	-	53,53,53	0.94	2 (3%)	59,61,61	0.88	1 (1%)
9	PCW	G	102	-	53,53,53	0.98	2 (3%)	59,61,61	0.75	1 (1%)
8	CLR	B	402	-	31,31,31	1.15	1 (3%)	48,48,48	1.39	6 (12%)
11	ADP	A	1312	10	24,29,29	0.95	1 (4%)	29,45,45	1.29	3 (10%)
8	CLR	A	1310	-	31,31,31	1.15	1 (3%)	48,48,48	1.40	6 (12%)
9	PCW	C	1304	-	53,53,53	0.97	2 (3%)	59,61,61	0.90	2 (3%)
8	CLR	C	1301	-	31,31,31	1.15	1 (3%)	48,48,48	1.38	4 (8%)
8	CLR	A	1302	-	31,31,31	1.13	1 (3%)	48,48,48	1.38	5 (10%)
9	PCW	C	1305	-	53,53,53	0.96	2 (3%)	59,61,61	0.90	1 (1%)
8	CLR	D	502	-	31,31,31	1.13	1 (3%)	48,48,48	1.38	6 (12%)
8	CLR	C	1302	-	31,31,31	1.13	1 (3%)	48,48,48	1.38	5 (10%)
9	PCW	A	1307	-	53,53,53	0.96	2 (3%)	59,61,61	0.75	0
9	PCW	C	1303	-	21,21,53	0.88	0	27,29,61	1.08	2 (7%)
9	PCW	C	1306	-	53,53,53	0.96	2 (3%)	59,61,61	0.75	0
8	CLR	D	501	-	31,31,31	1.15	1 (3%)	48,48,48	1.39	6 (12%)
11	ADP	C	1311	10	24,29,29	0.95	1 (4%)	29,45,45	1.29	3 (10%)
9	PCW	A	1309	-	21,21,53	0.87	0	27,29,61	1.27	4 (14%)
9	PCW	E	102	-	53,53,53	0.98	2 (3%)	59,61,61	0.75	1 (1%)
9	PCW	C	1307	-	53,53,53	0.94	2 (3%)	59,61,61	0.88	1 (1%)

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
9	PCW	A	1303	-	-	9/23/23/57	-
8	CLR	A	1301	-	-	0/10/68/68	0/4/4/4
8	CLR	C	1309	-	-	0/10/68/68	0/4/4/4
9	PCW	A	1306	-	-	19/57/57/57	-
9	PCW	A	1308	-	-	28/57/57/57	-
9	PCW	E	101	-	-	23/57/57/57	-
9	PCW	B	401	-	-	23/57/57/57	-
9	PCW	G	101	-	-	23/57/57/57	-
8	CLR	B	403	-	-	1/10/68/68	0/4/4/4
13	A1MA6	C	1316	-	-	101/192/350/350	1/12/10/10
9	PCW	C	1308	-	-	5/23/23/57	-
13	A1MA6	A	1317	-	-	101/192/350/350	1/12/10/10
9	PCW	A	1305	-	-	17/57/57/57	-
9	PCW	A	1304	-	-	23/57/57/57	-
9	PCW	G	102	-	-	18/57/57/57	-
8	CLR	B	402	-	-	1/10/68/68	0/4/4/4
11	ADP	A	1312	10	-	7/12/32/32	0/3/3/3
8	CLR	A	1310	-	-	0/10/68/68	0/4/4/4
9	PCW	C	1304	-	-	17/57/57/57	-
8	CLR	C	1301	-	-	0/10/68/68	0/4/4/4
8	CLR	A	1302	-	-	2/10/68/68	0/4/4/4
9	PCW	C	1305	-	-	19/57/57/57	-
8	CLR	D	502	-	-	1/10/68/68	0/4/4/4
8	CLR	C	1302	-	-	2/10/68/68	0/4/4/4
9	PCW	A	1307	-	-	28/57/57/57	-
9	PCW	C	1303	-	-	9/23/23/57	-
9	PCW	C	1306	-	-	28/57/57/57	-
8	CLR	D	501	-	-	1/10/68/68	0/4/4/4
11	ADP	C	1311	10	-	7/12/32/32	0/3/3/3
9	PCW	A	1309	-	-	5/23/23/57	-
9	PCW	E	102	-	-	18/57/57/57	-
9	PCW	C	1307	-	-	28/57/57/57	-

The worst 5 of 80 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	1316	A1MA6	OC2-C43	5.47	1.54	1.43
13	A	1317	A1MA6	OC2-C43	5.47	1.54	1.43

*Continued on next page...*



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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1317	A1MA6	OA0-CAP	5.35	1.57	1.45
13	C	1316	A1MA6	OA0-CAP	5.35	1.57	1.45
13	A	1317	A1MA6	CBL-CBM	-5.23	1.43	1.52

The worst 5 of 156 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	1316	A1MA6	C97-C96-C95	-7.97	115.12	125.41
13	A	1317	A1MA6	C97-C96-C95	-7.97	115.12	125.41
13	A	1317	A1MA6	C44-O46-C47	-7.14	101.65	111.08
13	C	1316	A1MA6	C44-O46-C47	-7.13	101.65	111.08
13	C	1316	A1MA6	CA2-CA3-CA4	-6.71	115.34	125.92

There are no chirality outliers.

5 of 564 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	1304	PCW	O3P-C1-C2-O2
9	C	1305	PCW	C1-O3P-P-O1P
9	C	1305	PCW	C1-O3P-P-O2P
9	C	1305	PCW	C1-O3P-P-O4P
9	C	1306	PCW	C1-O3P-P-O1P

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	C	1316	A1MA6	C75-C77-CBL-CBM-CBO-O76
13	A	1317	A1MA6	C75-C77-CBL-CBM-CBO-O76

30 monomers are involved in 141 short contacts:

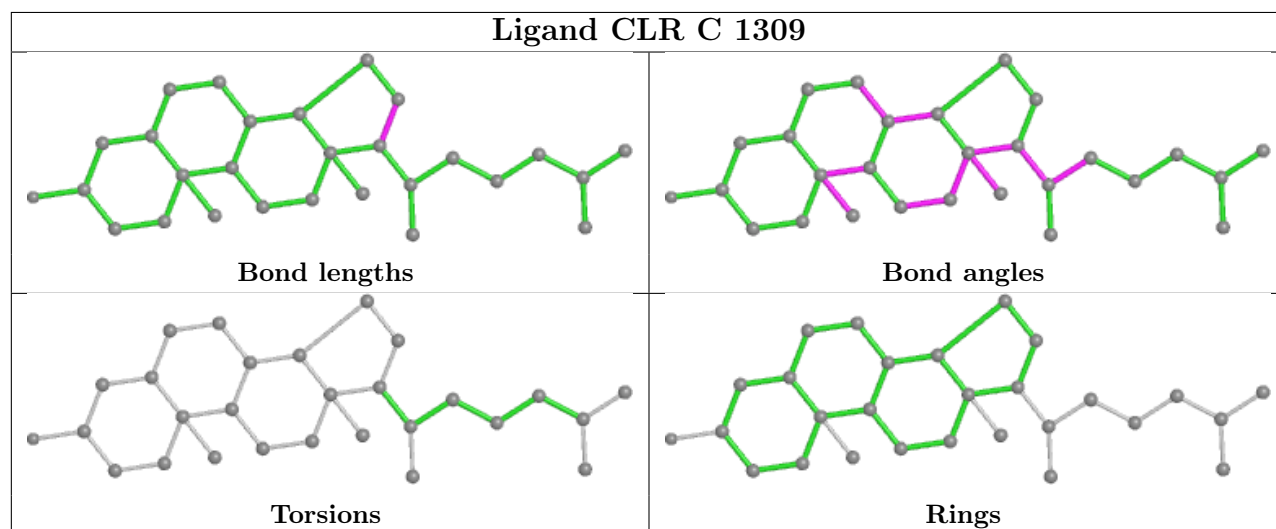
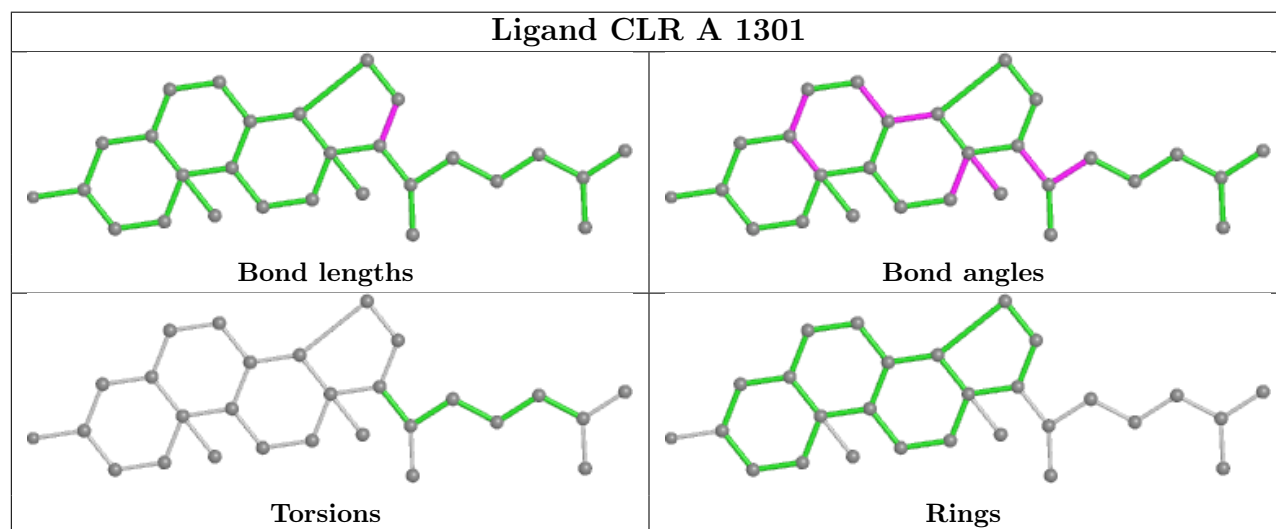
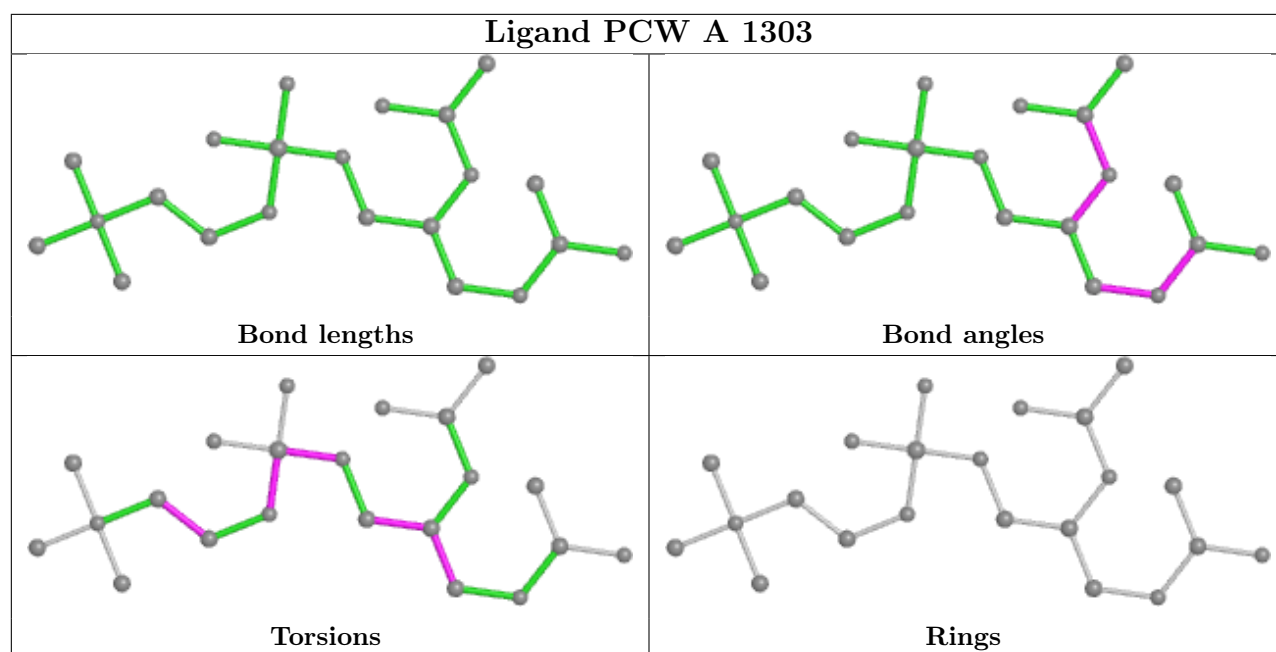
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1301	CLR	6	0
8	C	1309	CLR	5	0
9	A	1306	PCW	16	0
9	A	1308	PCW	4	0
9	E	101	PCW	5	0
9	B	401	PCW	11	0
9	G	101	PCW	5	0
8	B	403	CLR	3	0
13	C	1316	A1MA6	5	0

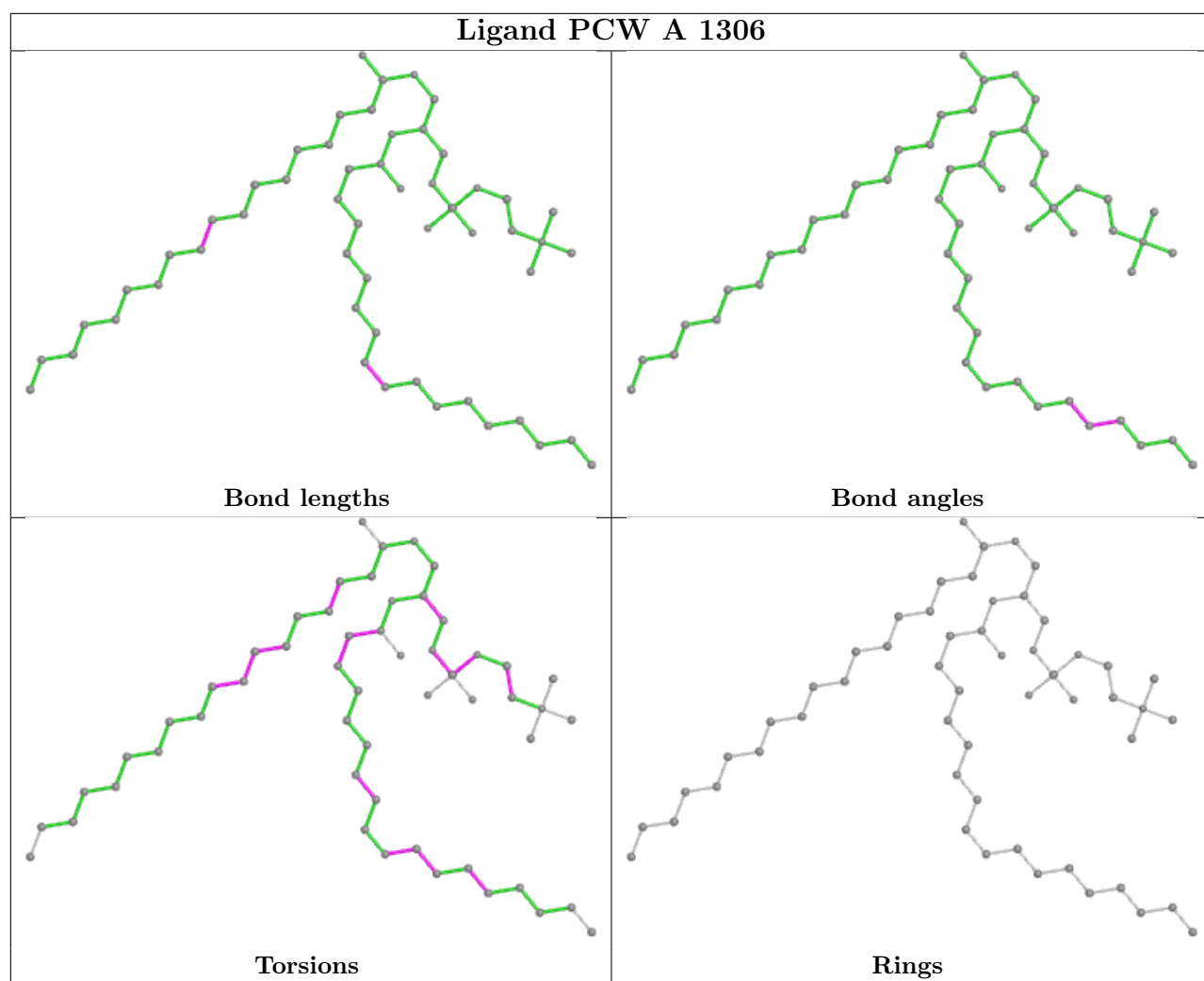
*Continued on next page...*

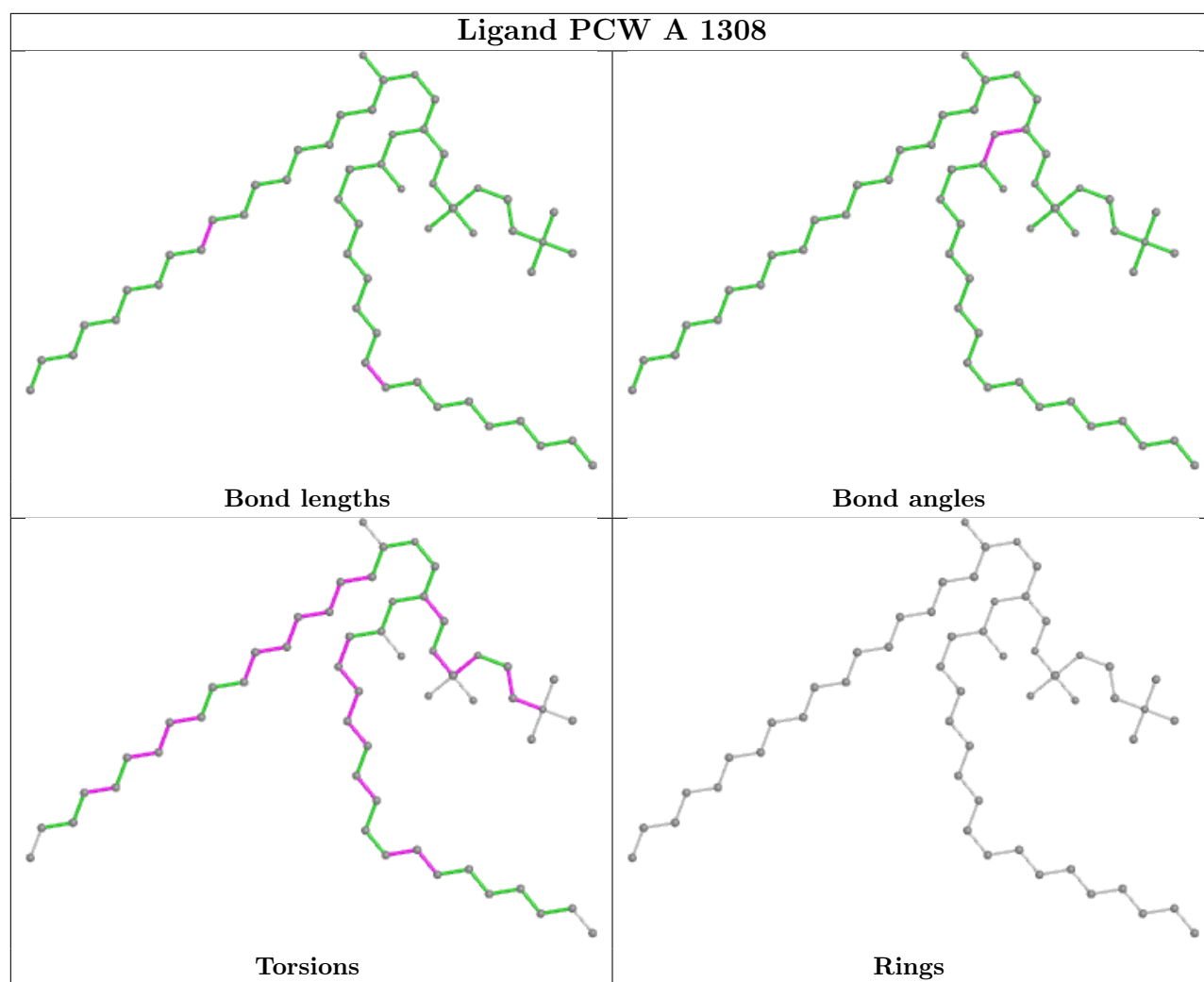
*Continued from previous page...*

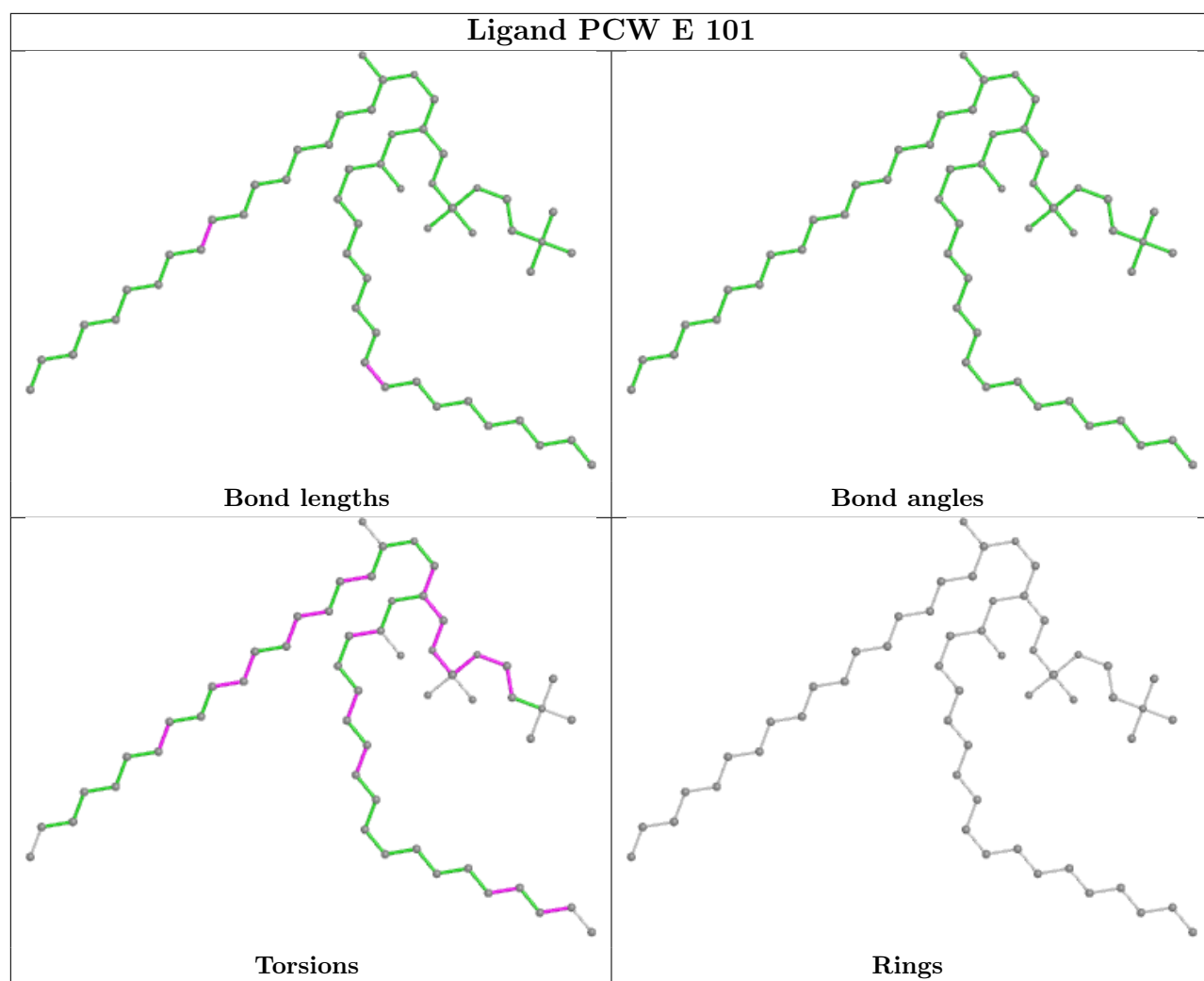
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	1308	PCW	6	0
13	A	1317	A1MA6	5	0
9	A	1305	PCW	15	0
9	A	1304	PCW	14	0
9	G	102	PCW	1	0
8	B	402	CLR	1	0
11	A	1312	ADP	1	0
8	A	1310	CLR	5	0
9	C	1304	PCW	15	0
8	C	1301	CLR	7	0
8	A	1302	CLR	7	0
9	C	1305	PCW	16	0
8	D	502	CLR	8	0
8	C	1302	CLR	8	0
9	A	1307	PCW	3	0
9	C	1306	PCW	5	0
8	D	501	CLR	1	0
11	C	1311	ADP	1	0
9	A	1309	PCW	6	0
9	E	102	PCW	1	0
9	C	1307	PCW	6	0

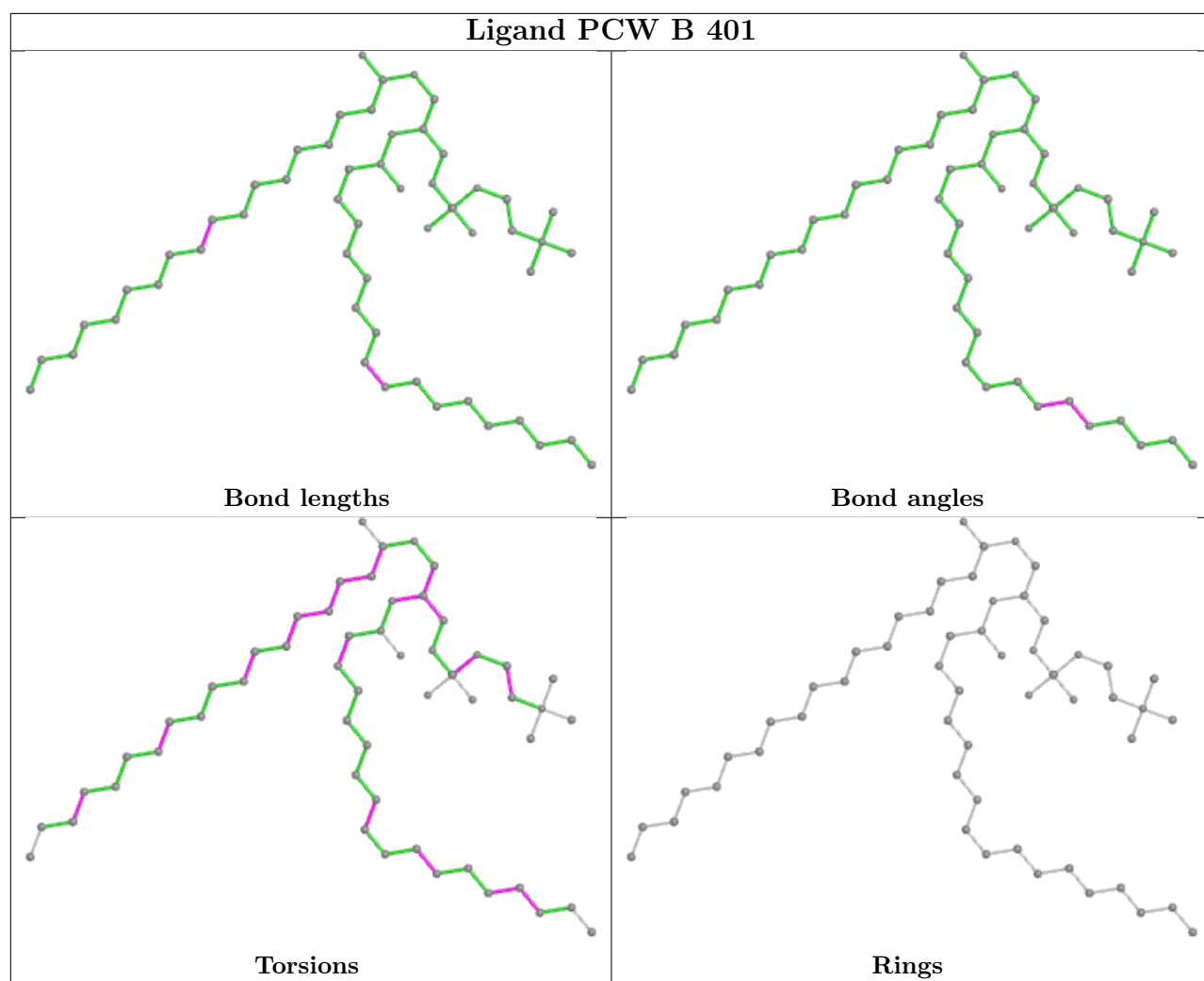
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

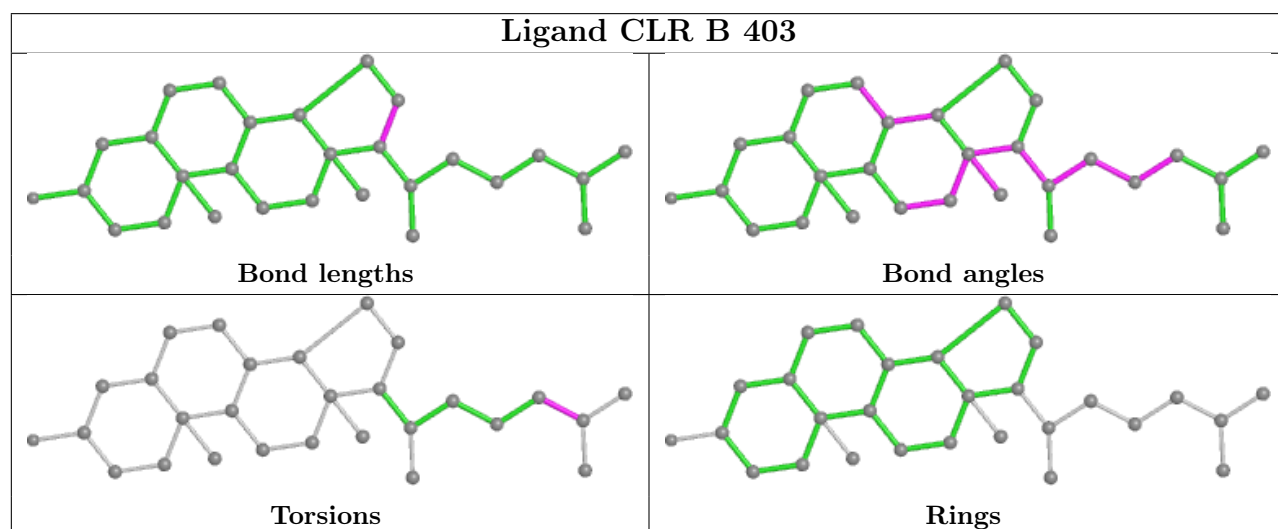
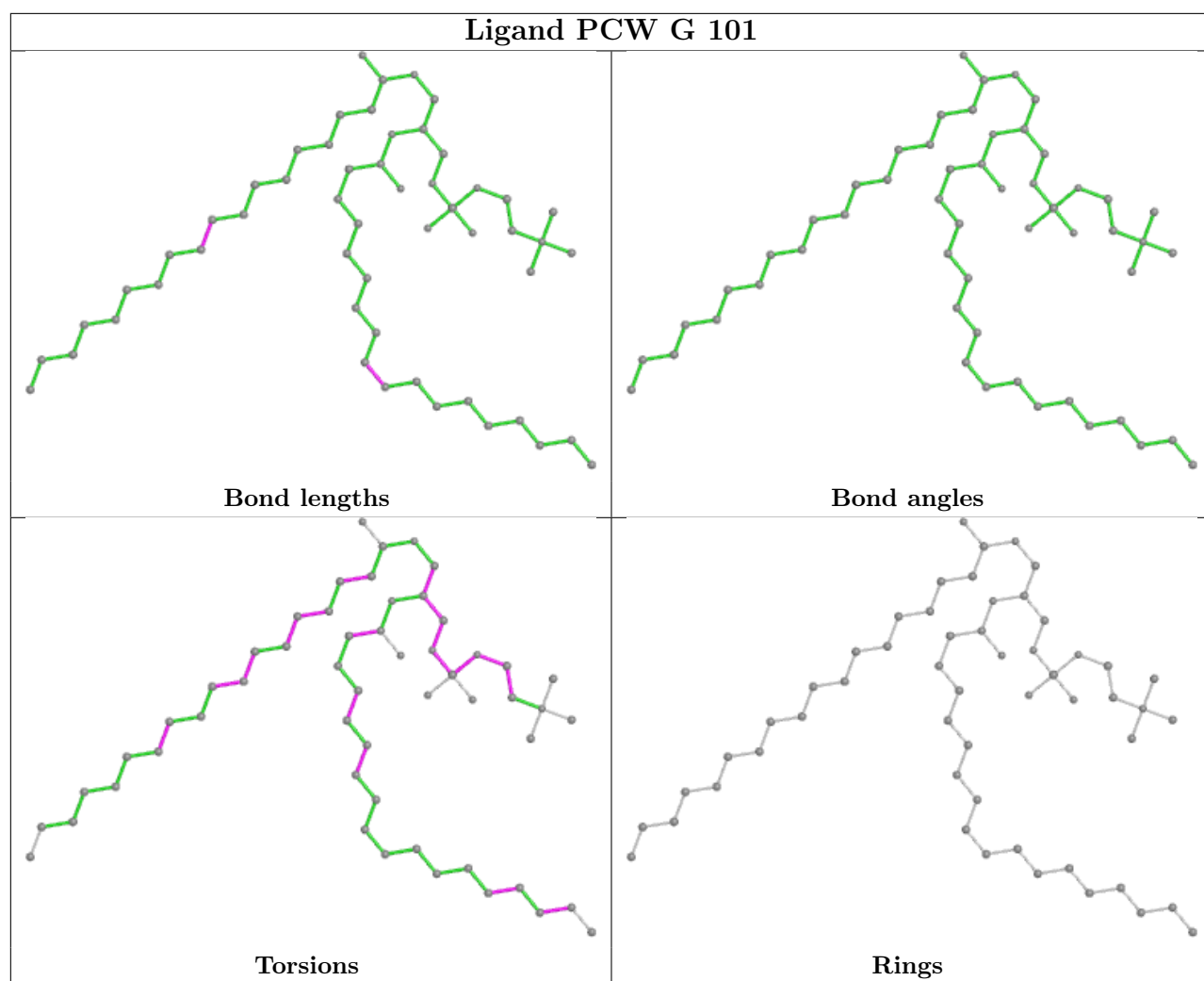




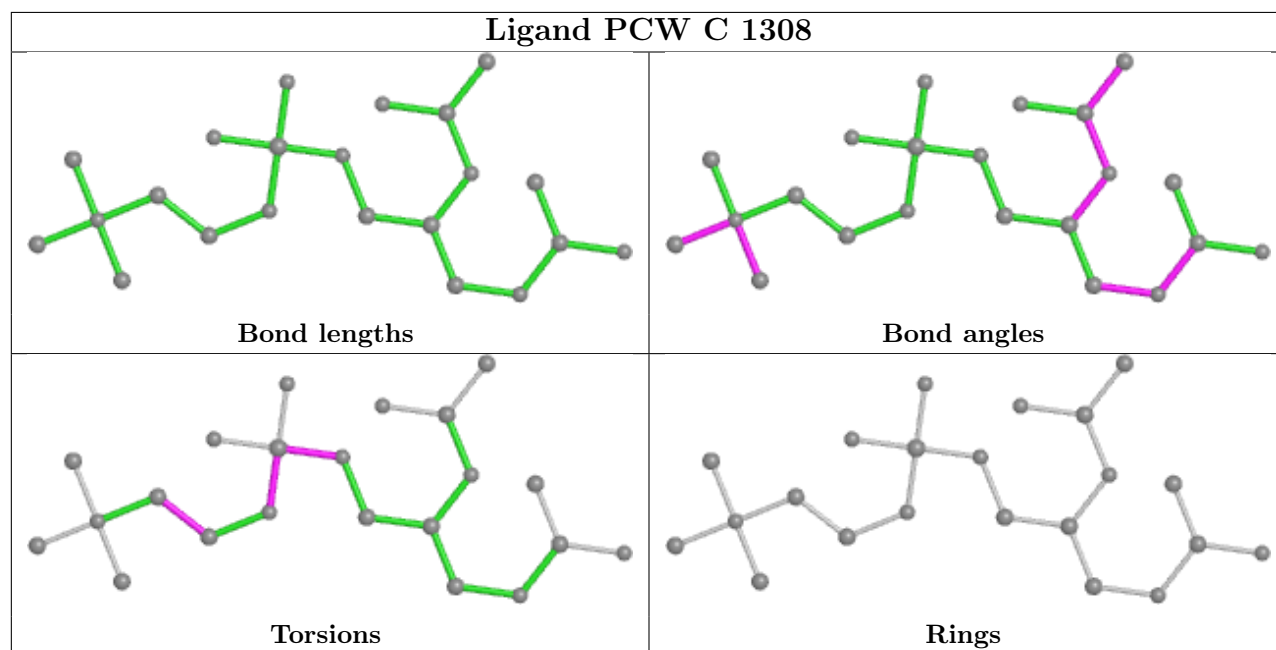
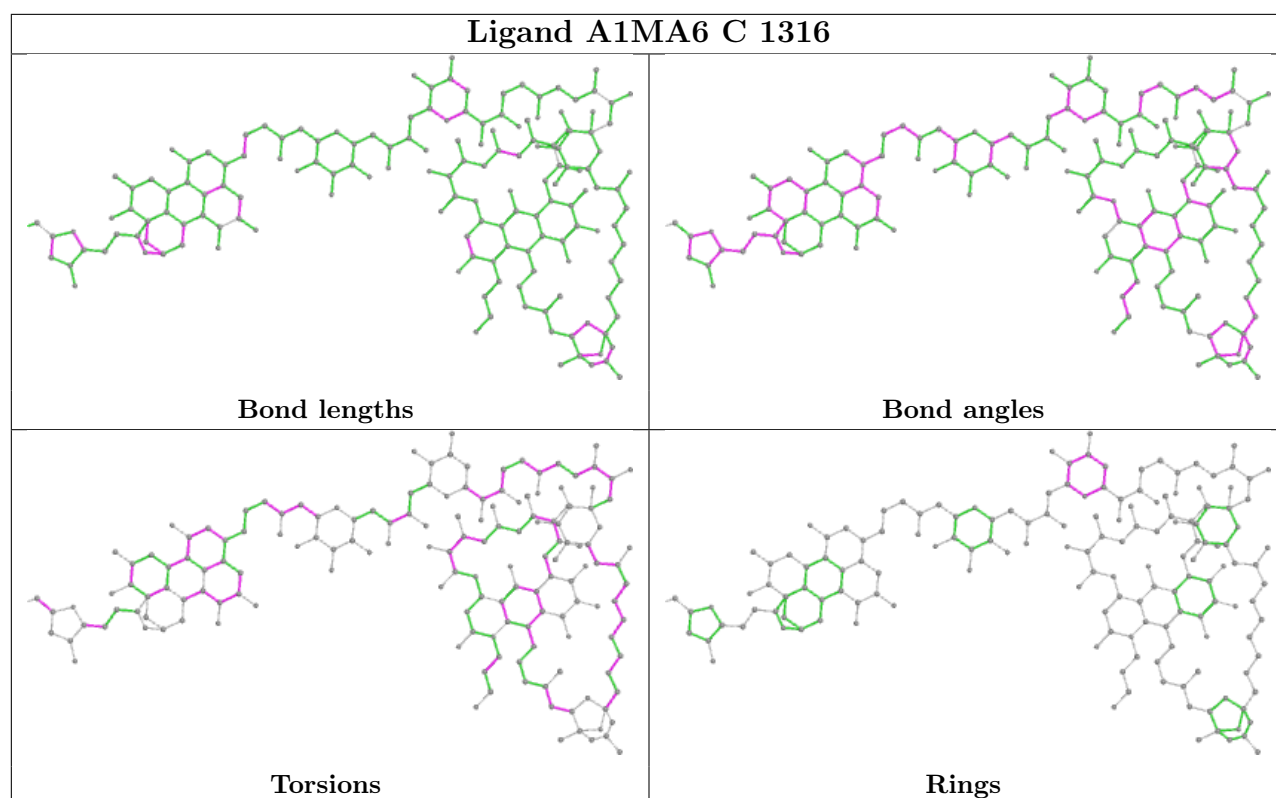


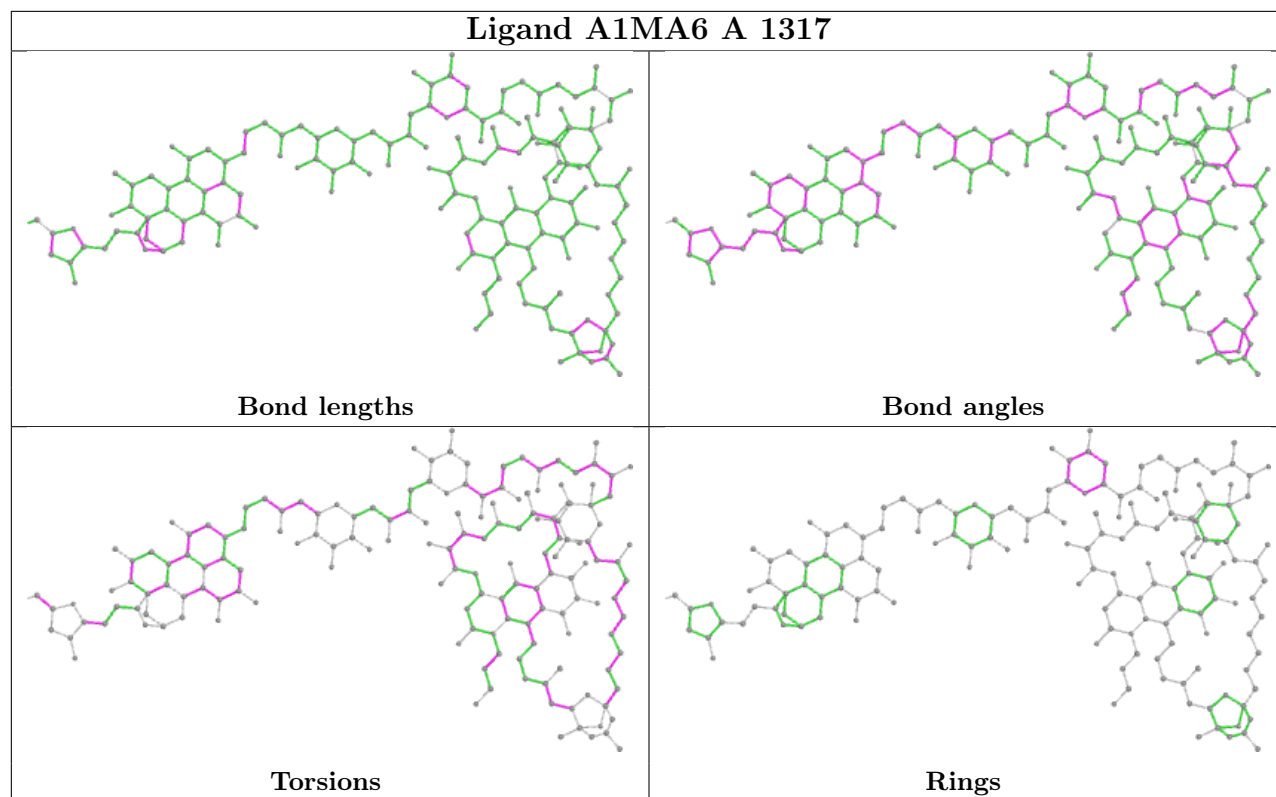


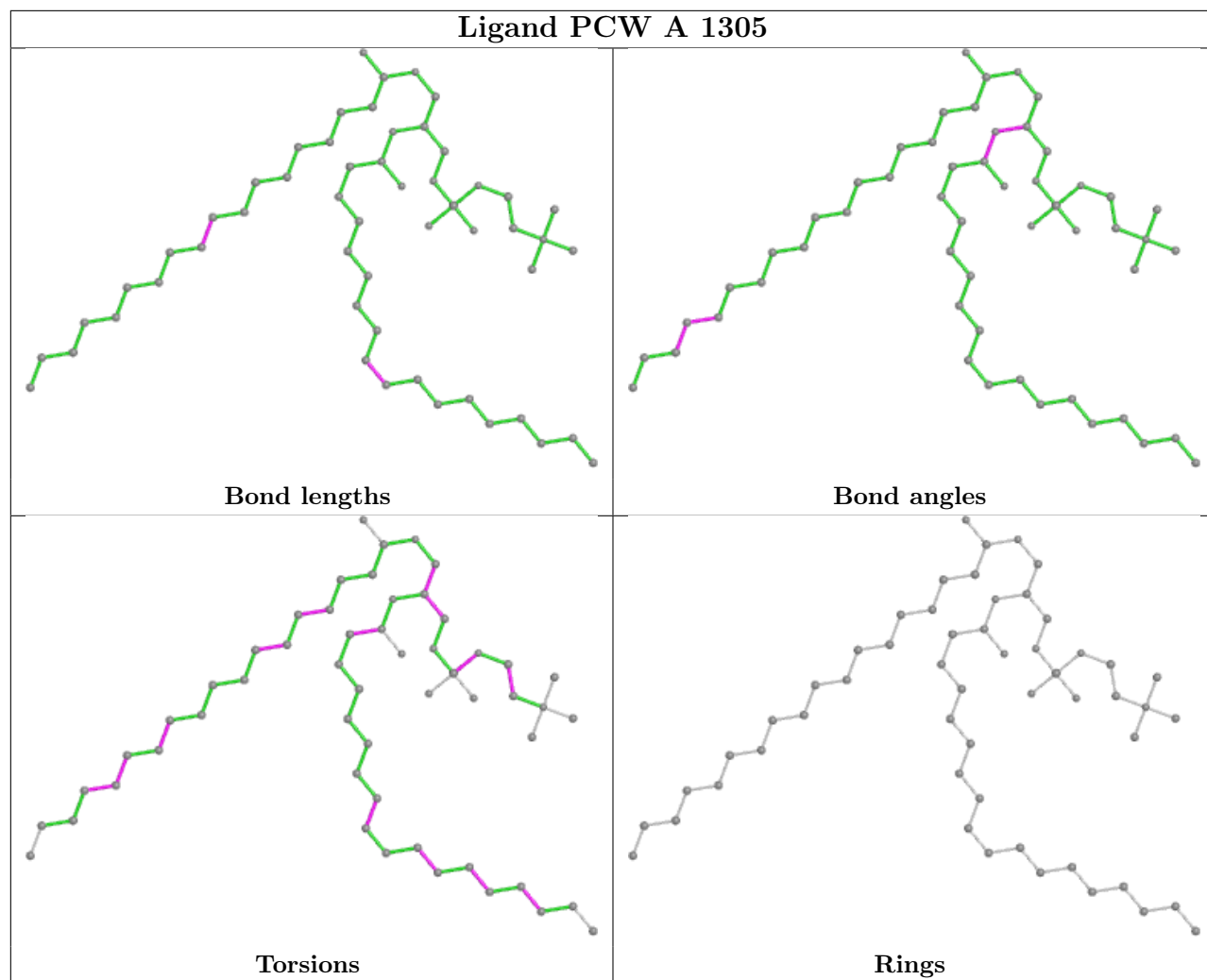


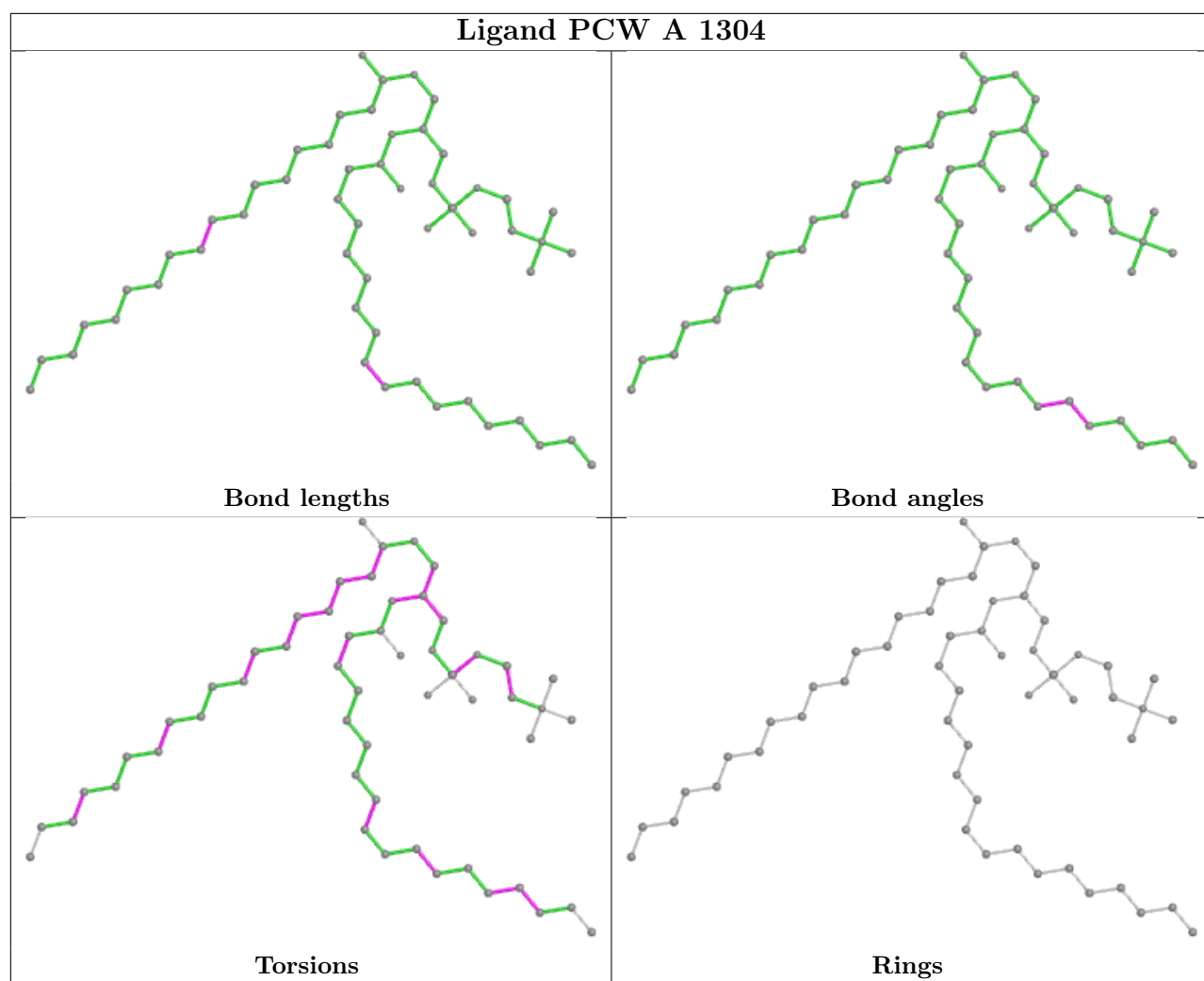


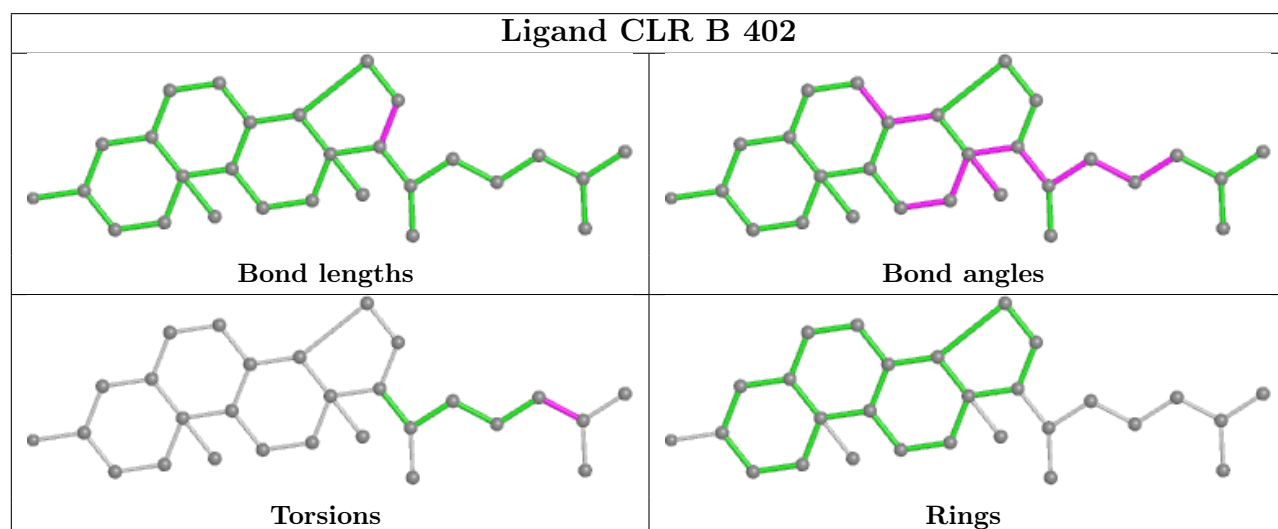
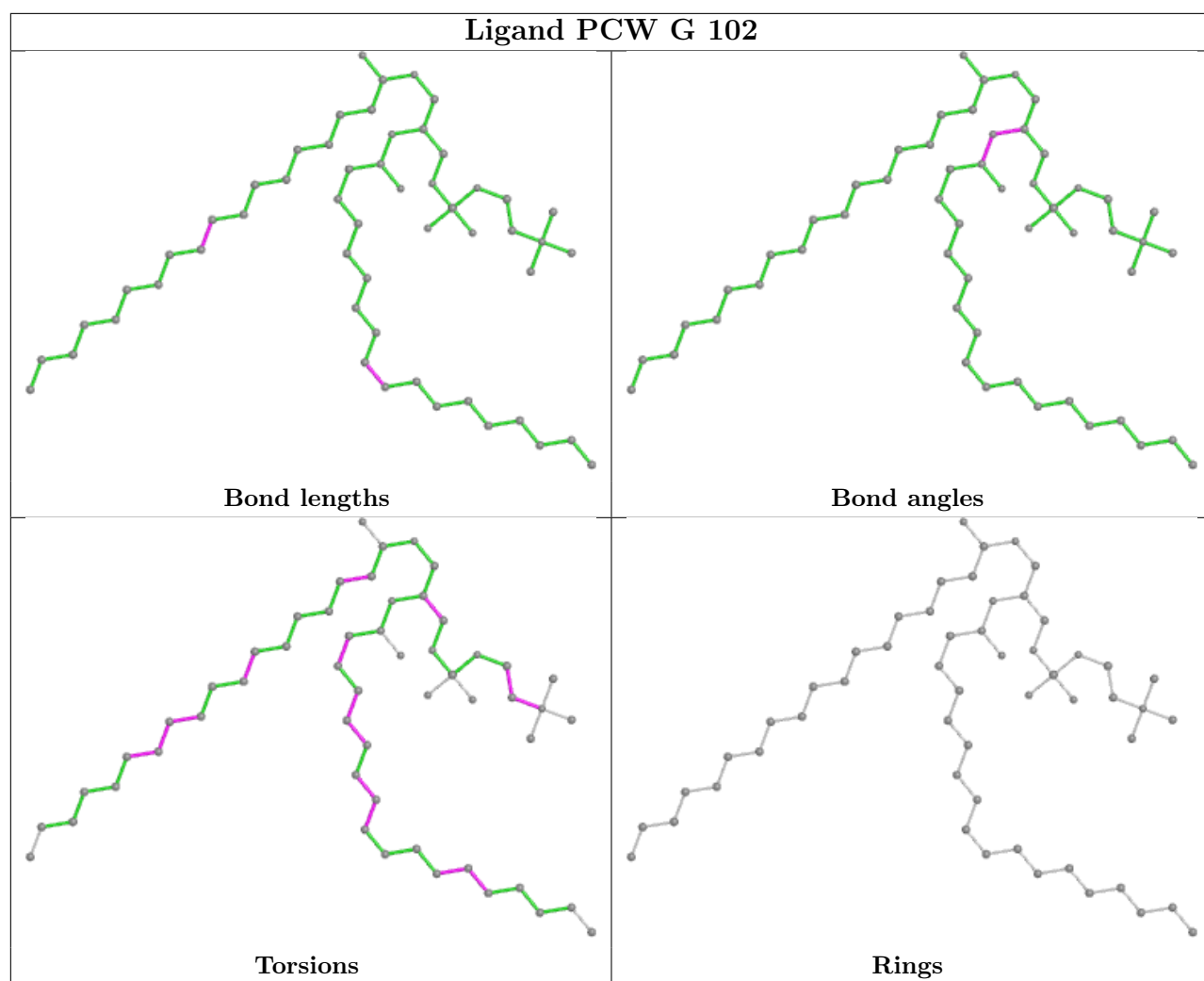


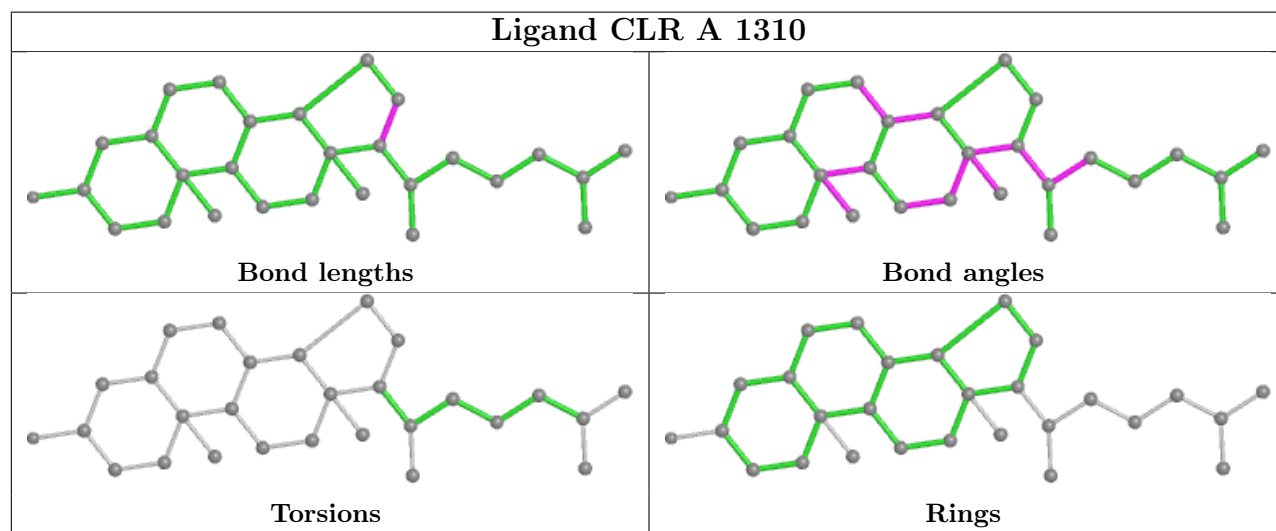
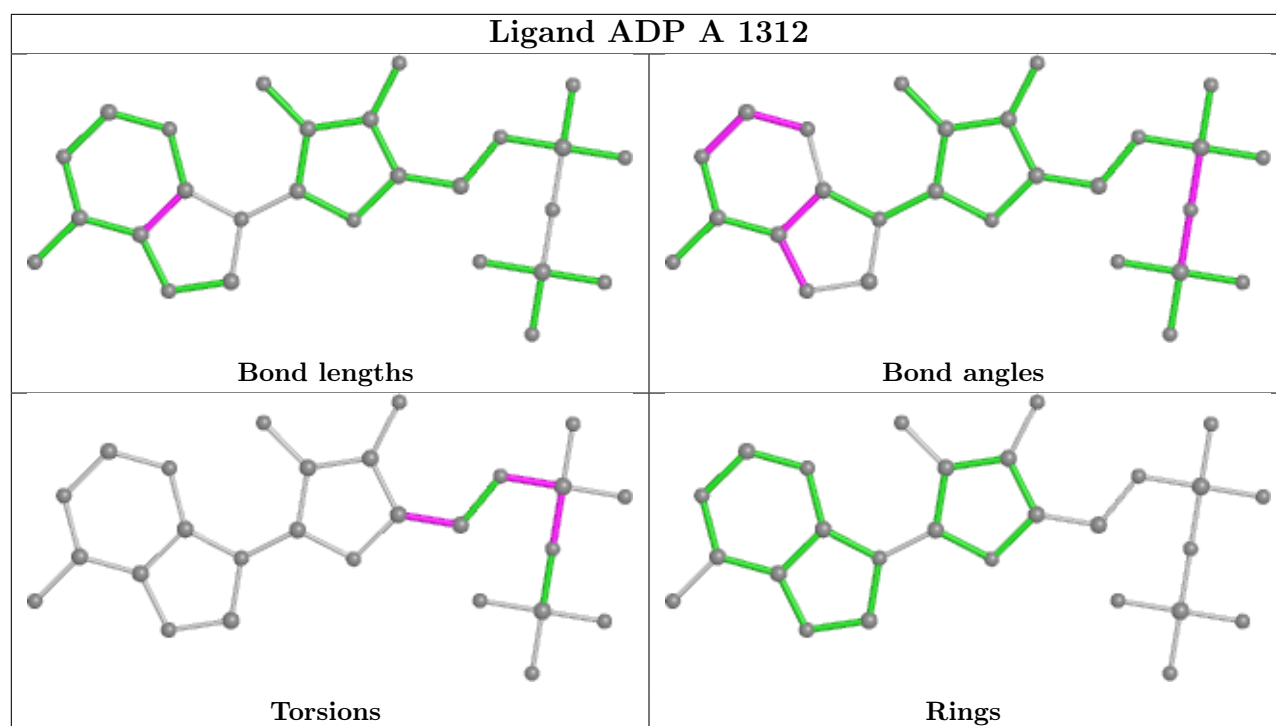


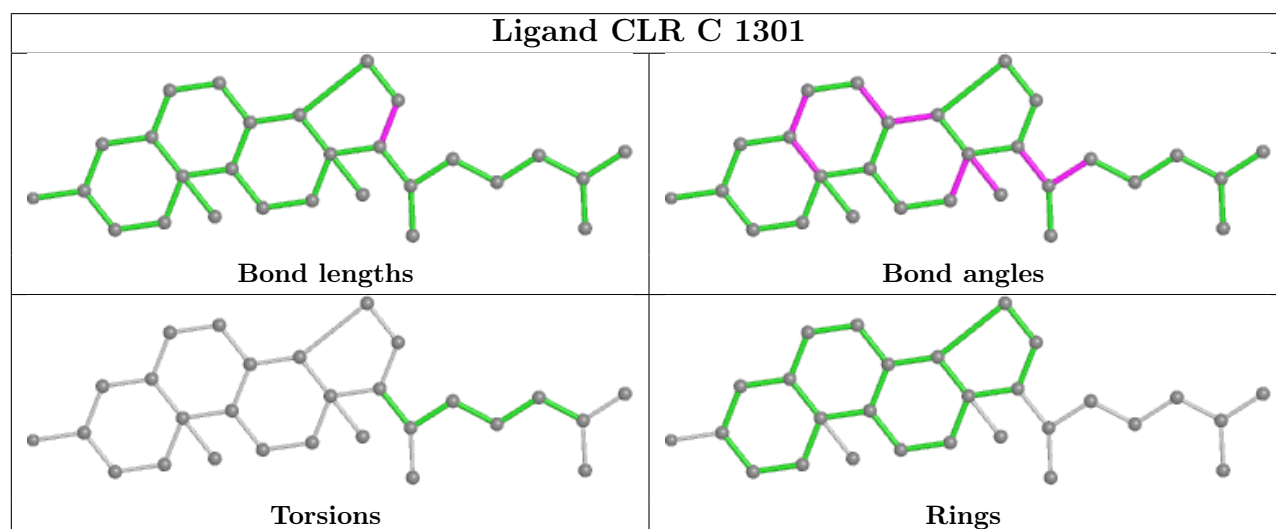
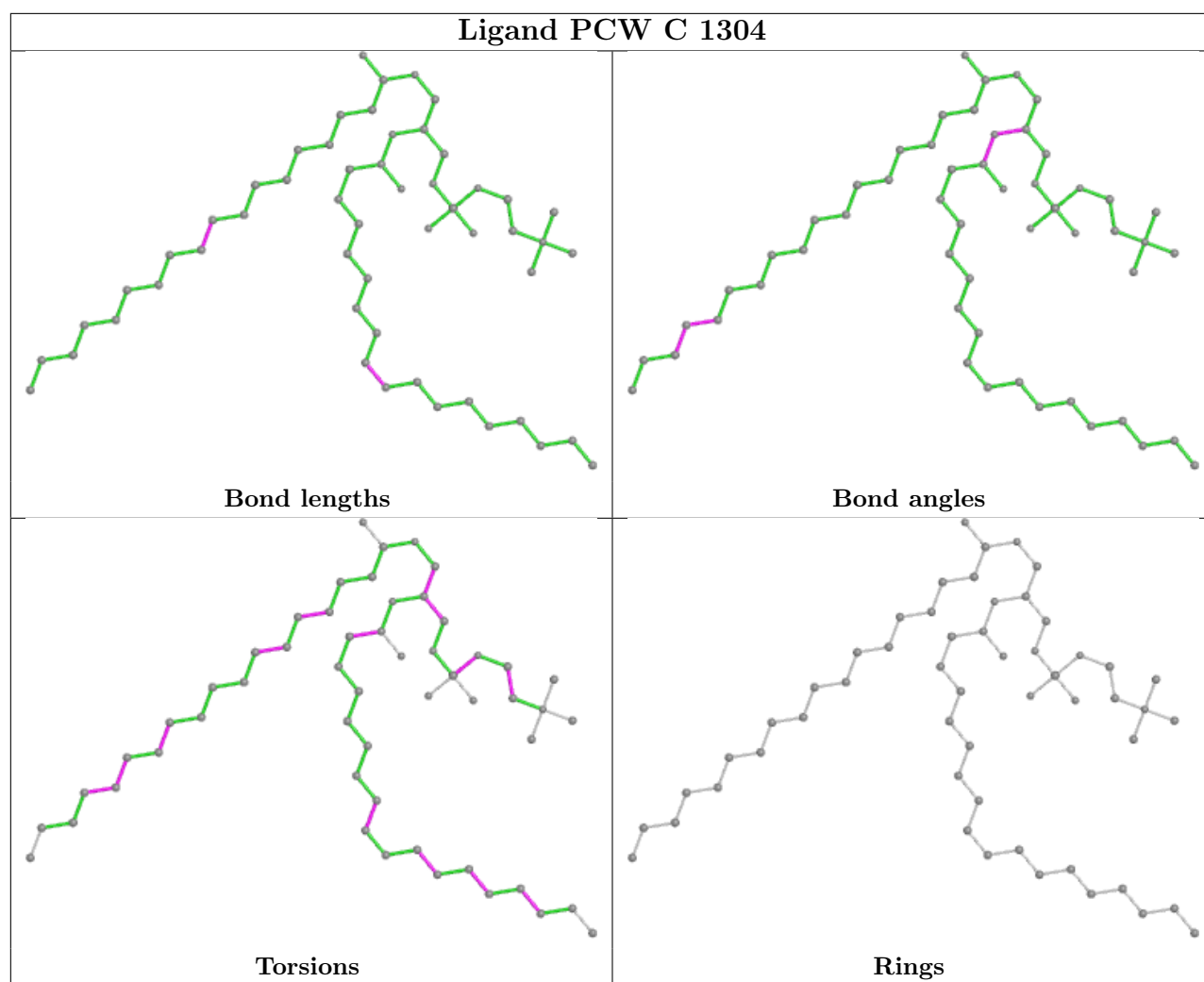


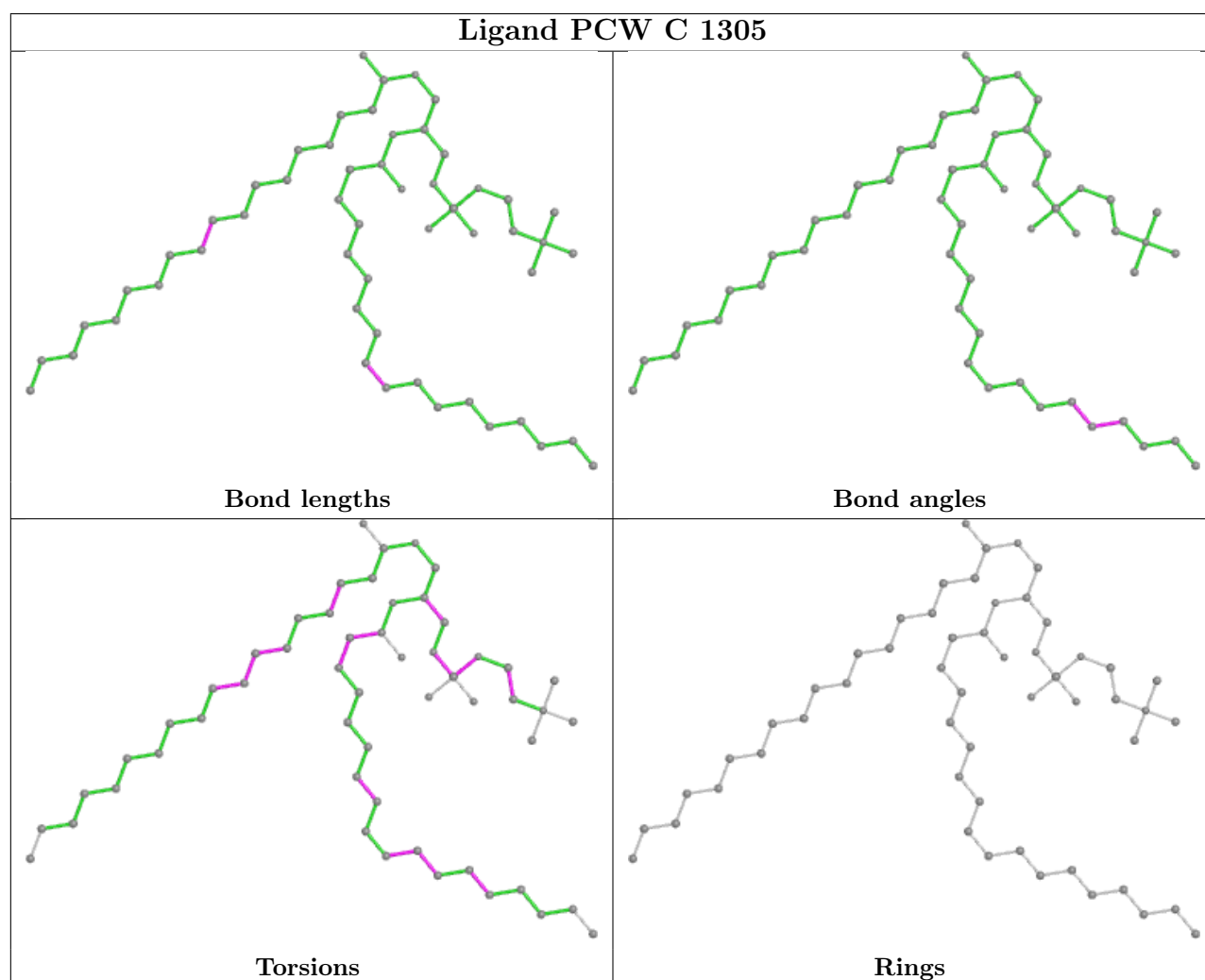
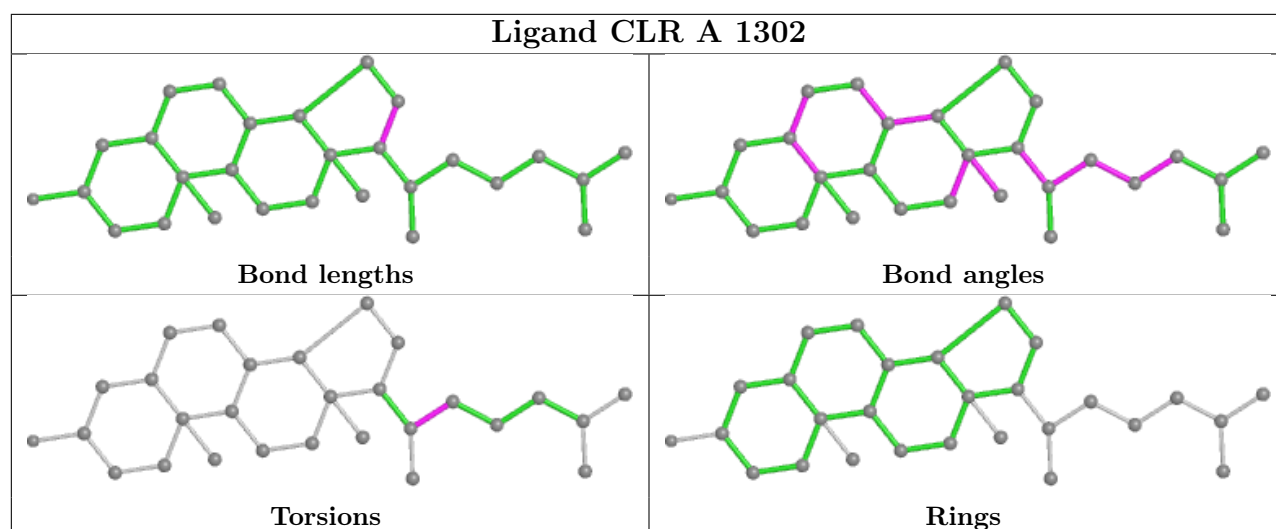




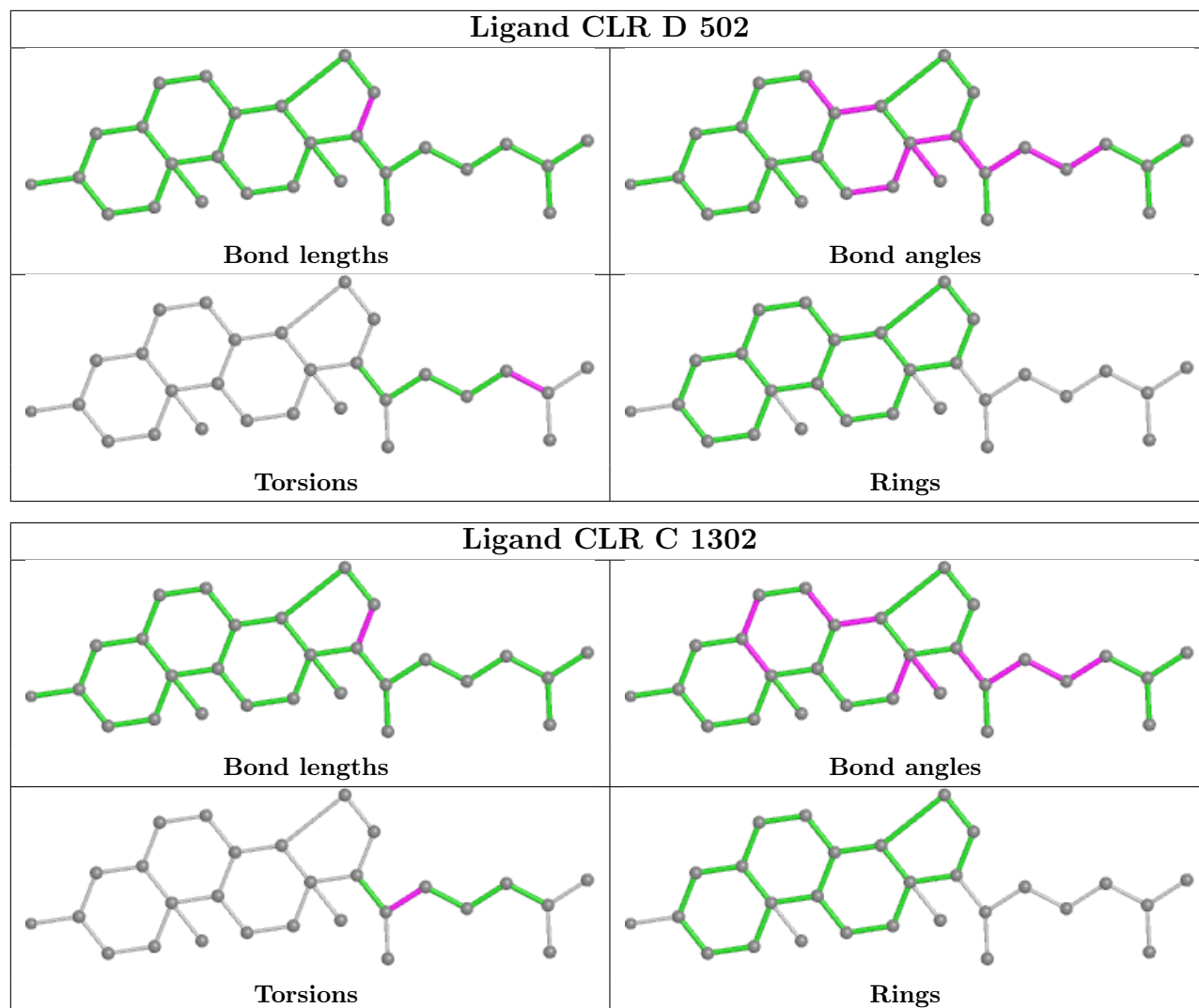


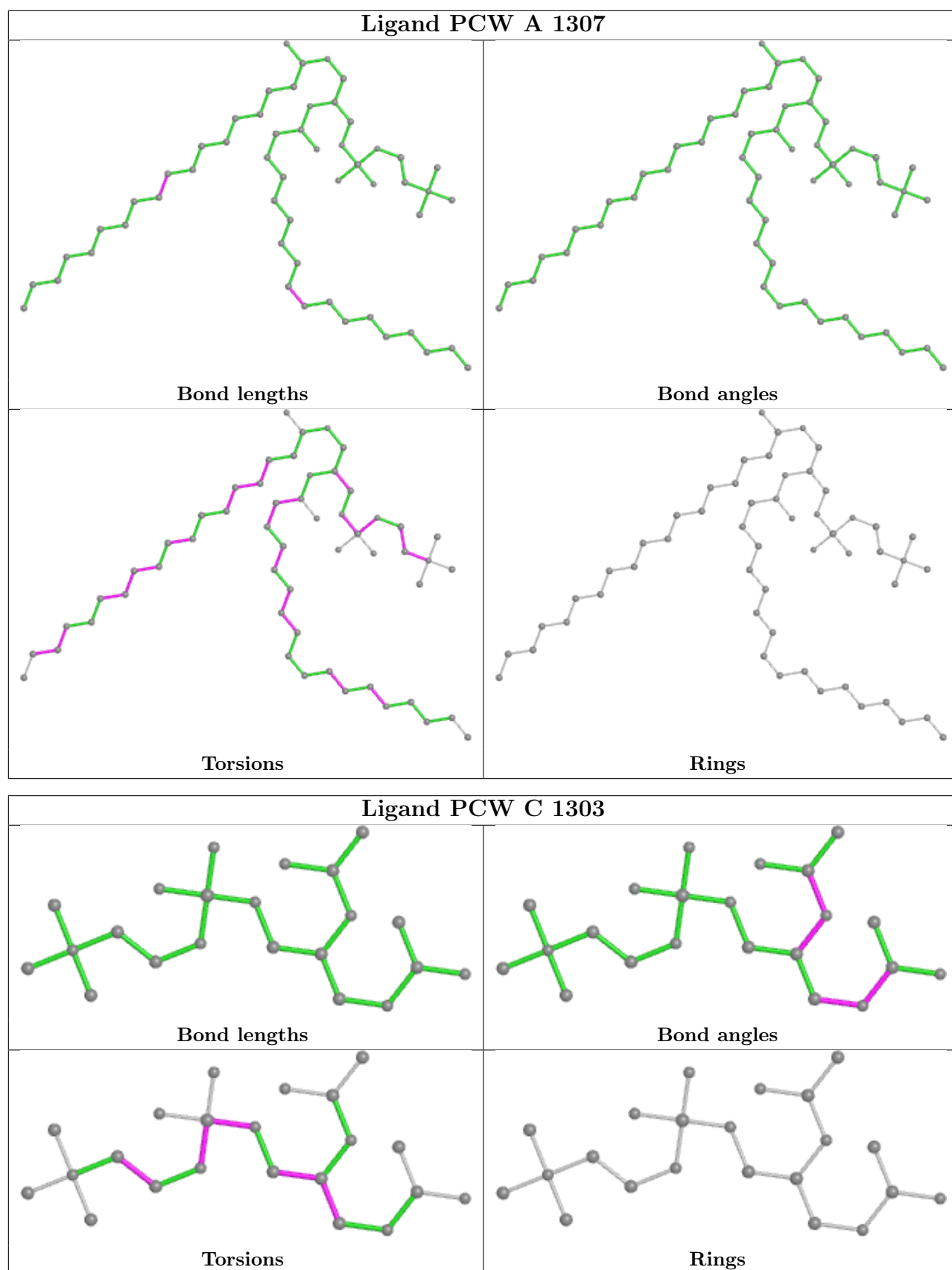




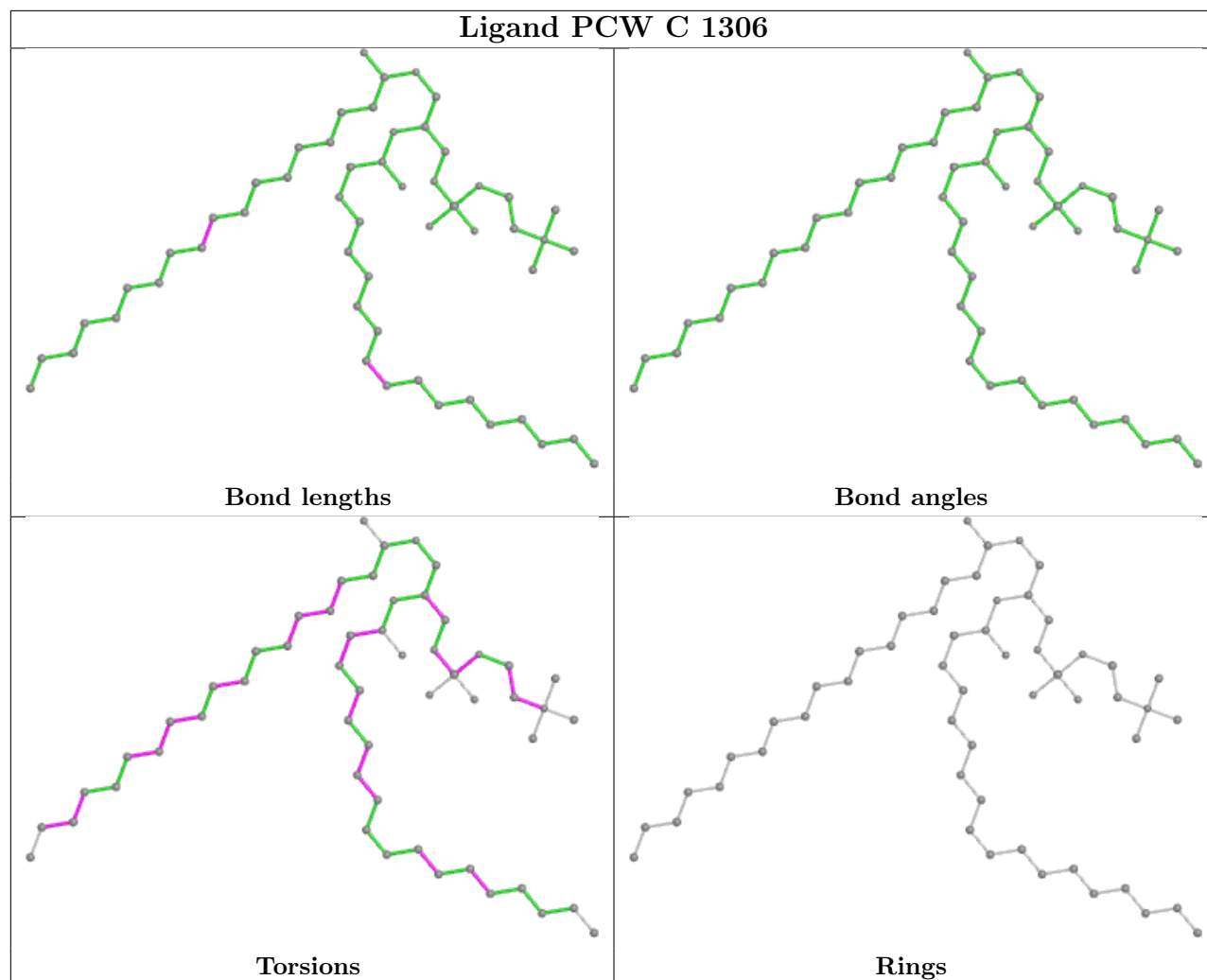




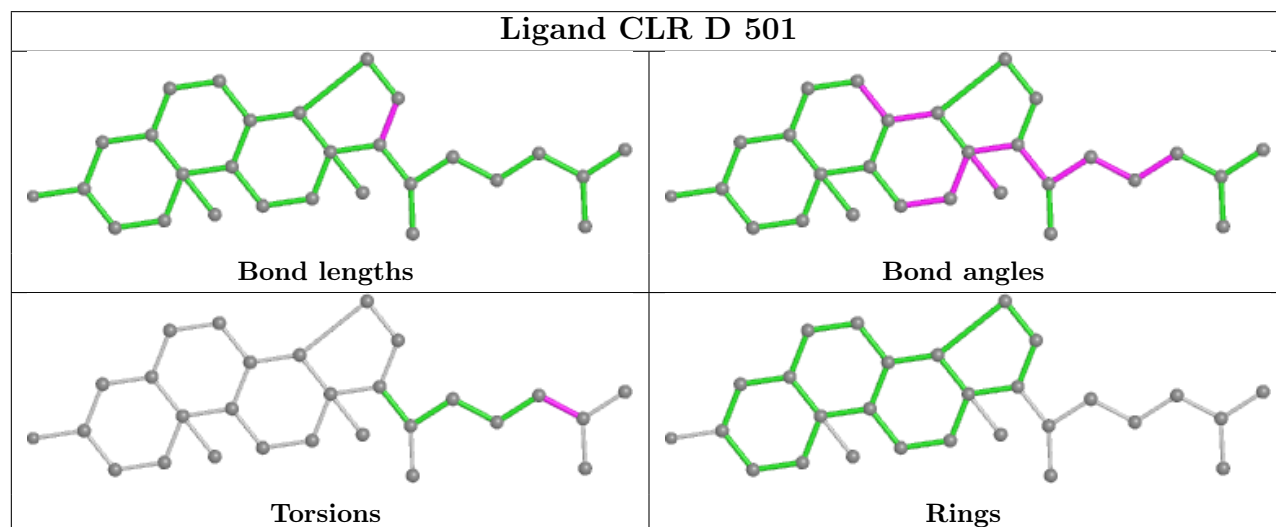


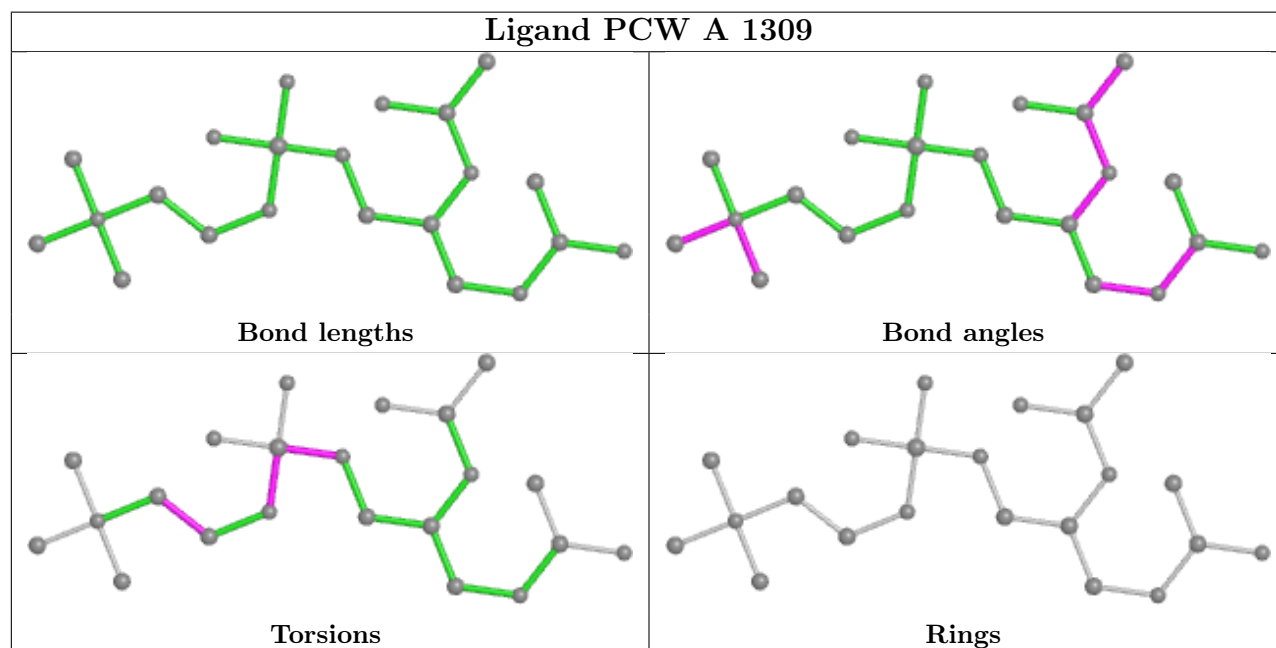
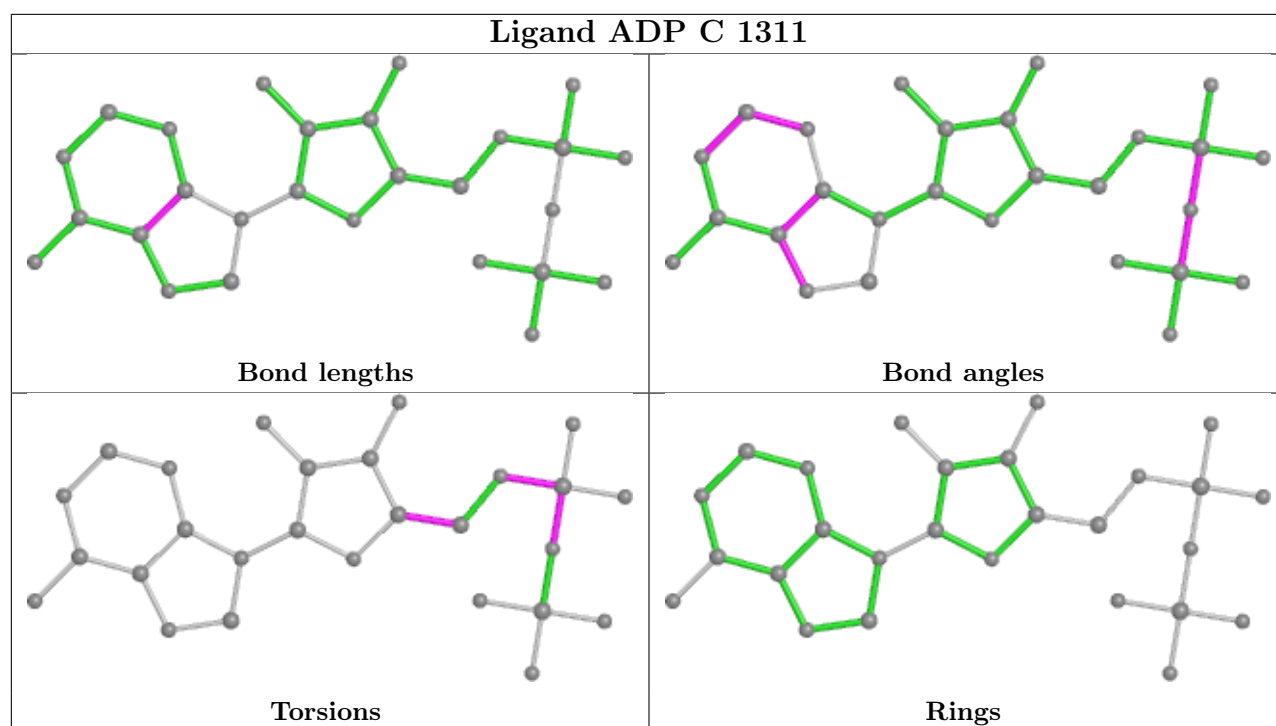


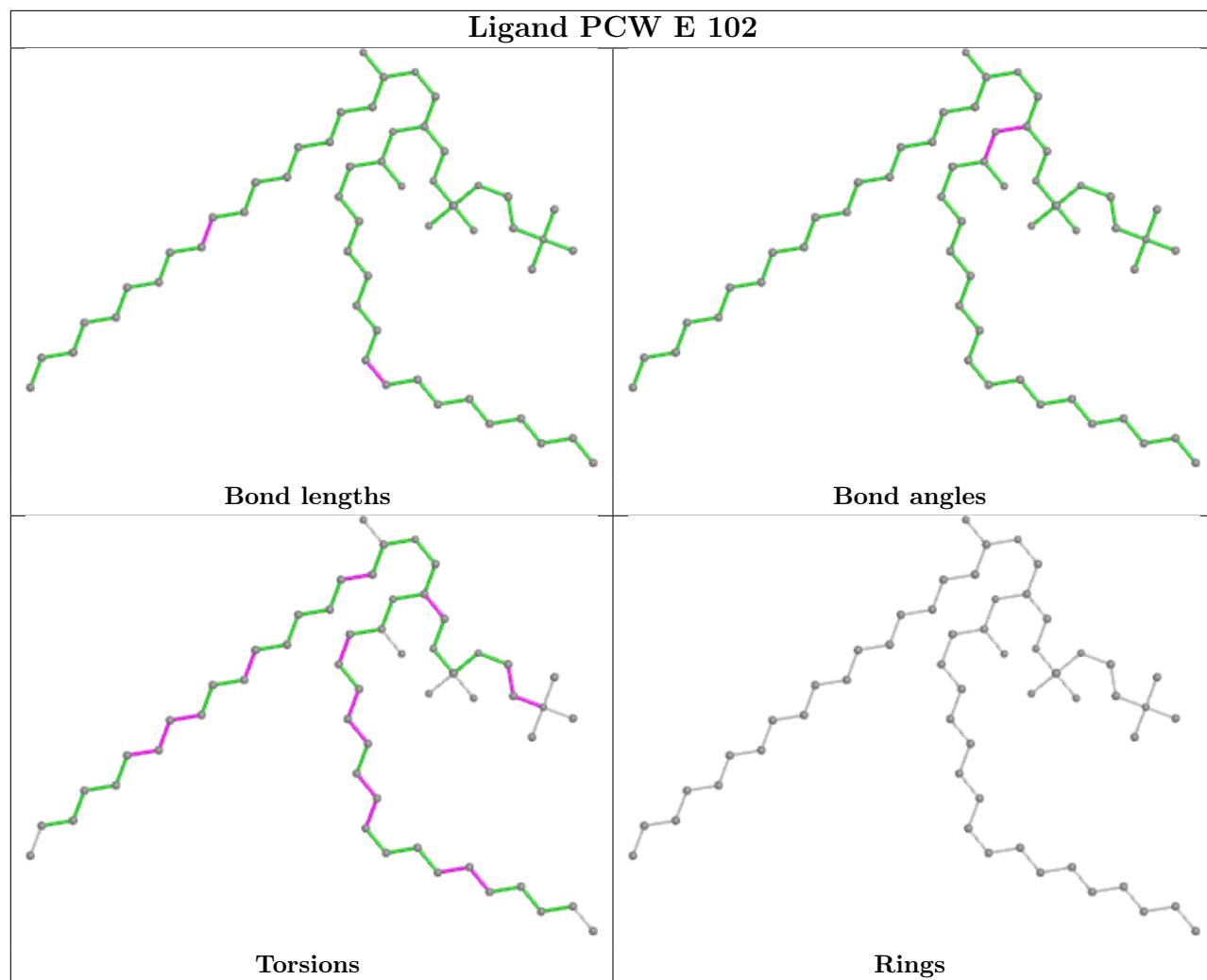
## Ligand PCW C 1306

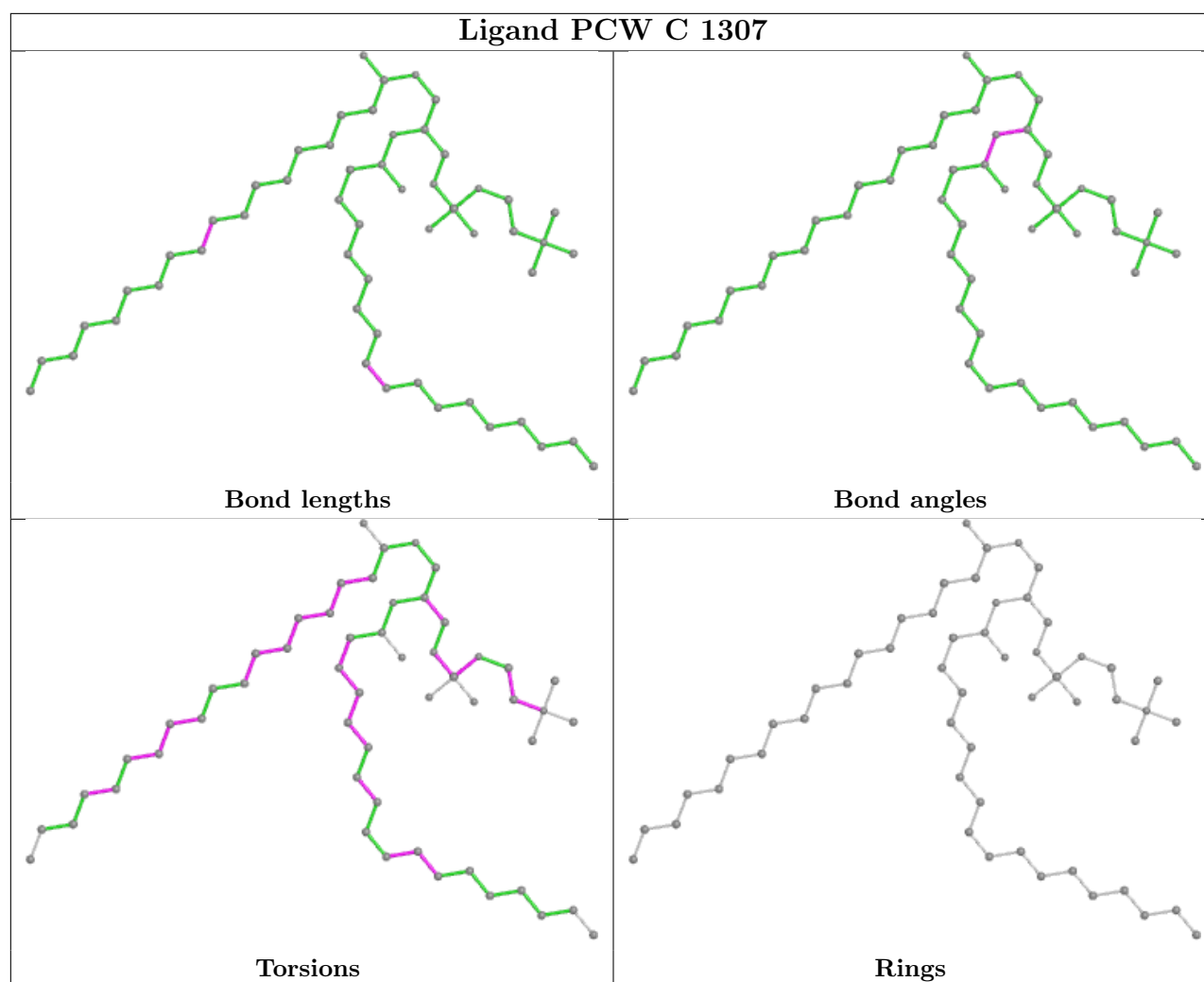


## Ligand CLR D 501









## 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.

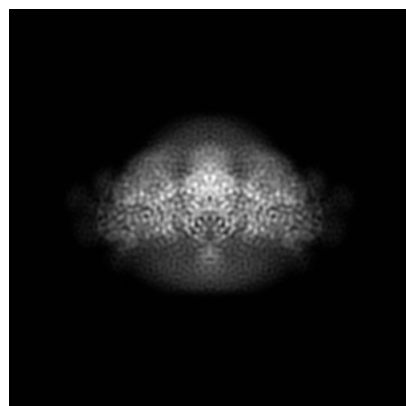
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65101. These allow visual inspection of the internal detail of the map and identification of artifacts.

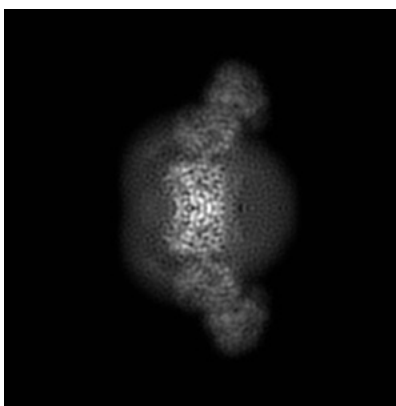
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

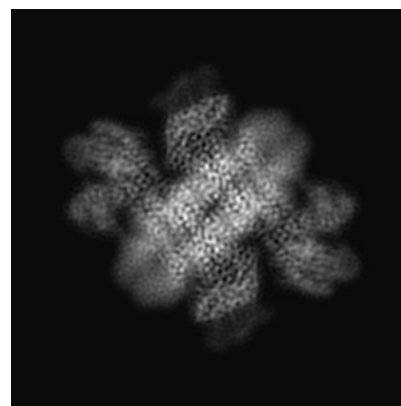
#### 6.1.1 Primary map



X

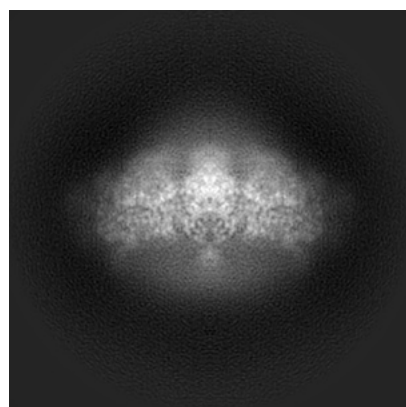


Y

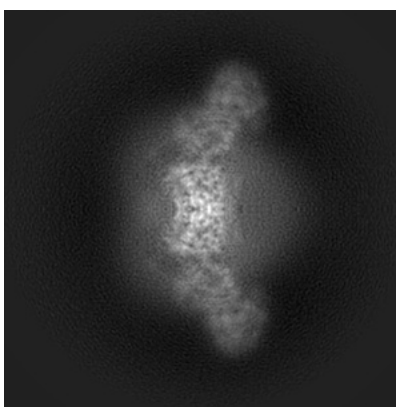


Z

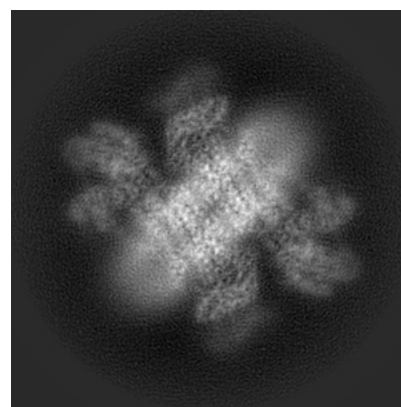
#### 6.1.2 Raw map



X



Y

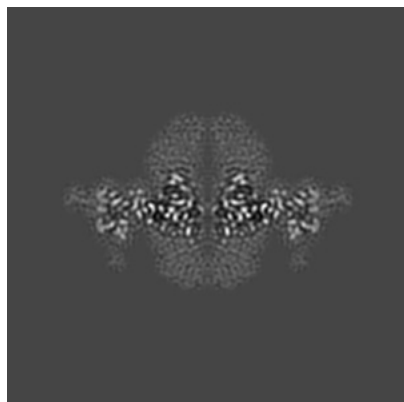


Z

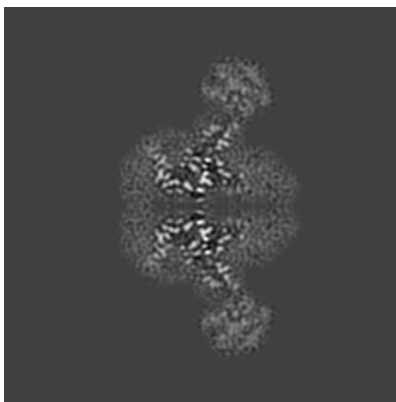
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

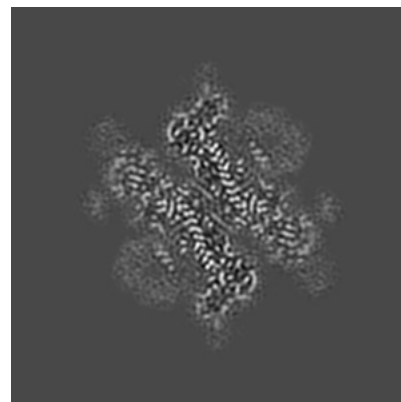
### 6.2.1 Primary map



X Index: 120

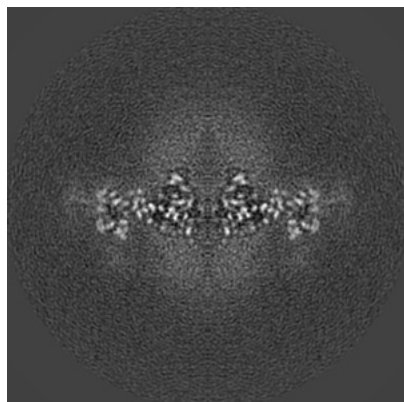


Y Index: 120

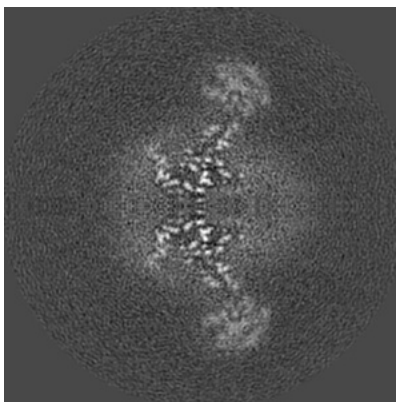


Z Index: 120

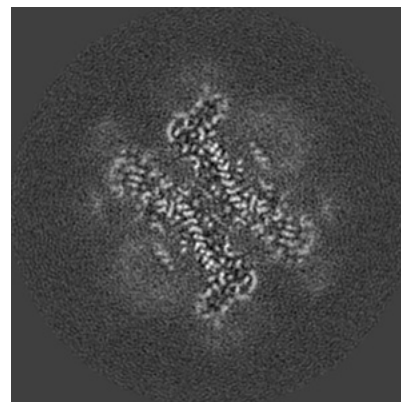
### 6.2.2 Raw map



X Index: 120



Y Index: 120



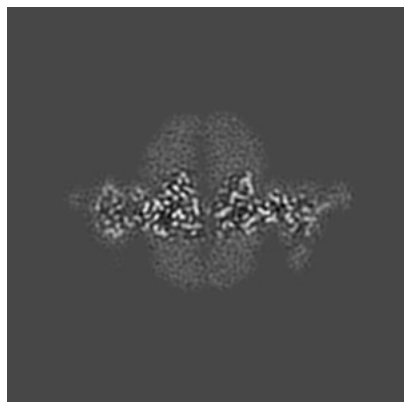
Z Index: 120

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

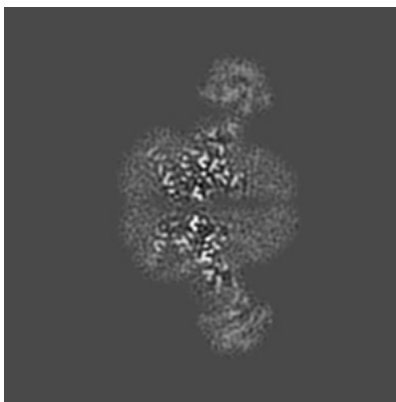


## 6.3 Largest variance slices [i](#)

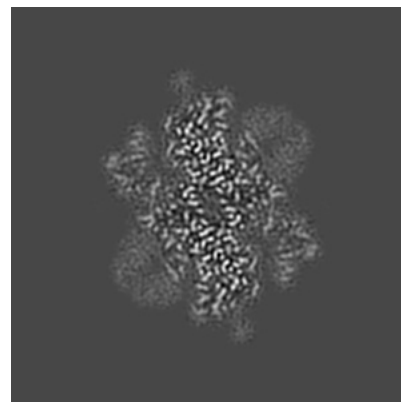
### 6.3.1 Primary map



X Index: 117

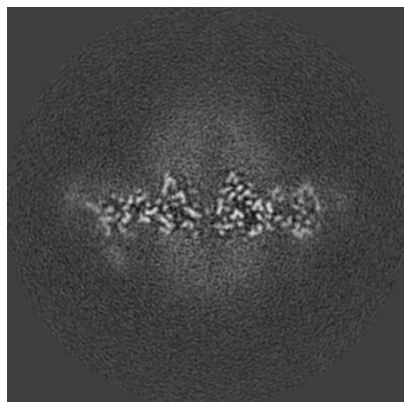


Y Index: 122

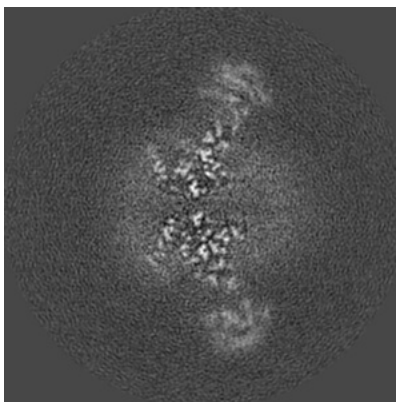


Z Index: 113

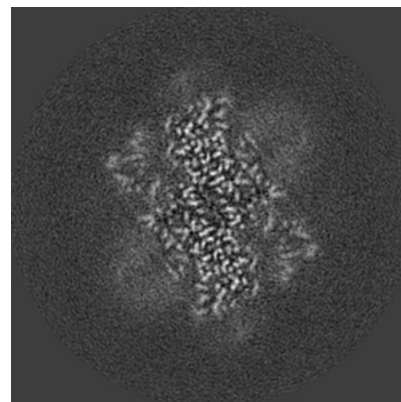
### 6.3.2 Raw map



X Index: 123



Y Index: 118

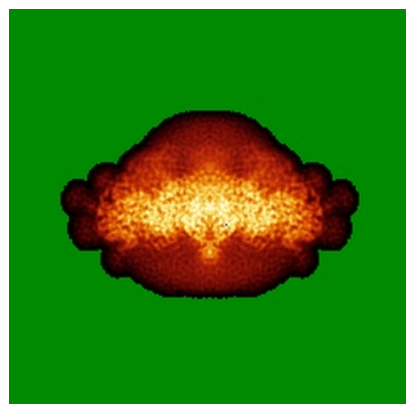


Z Index: 113

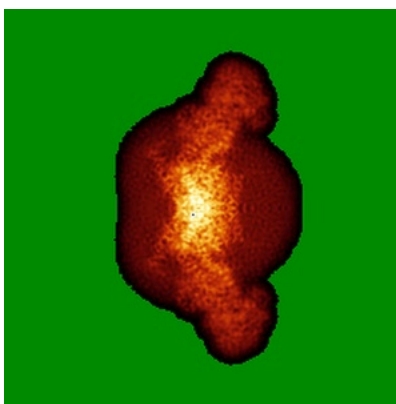
The images above show the largest variance slices of the map in three orthogonal directions.

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

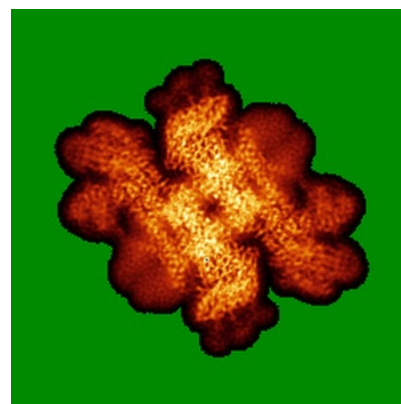
### 6.4.1 Primary map



X

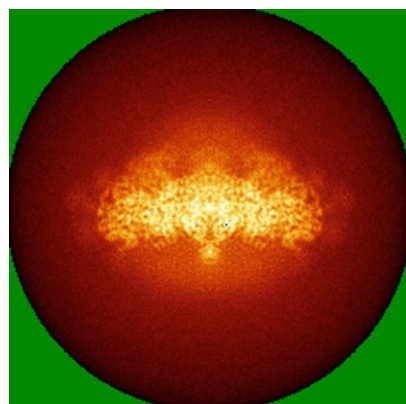


Y

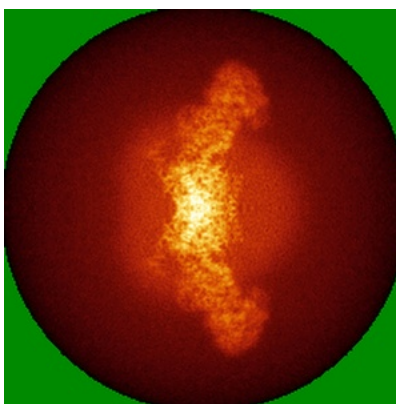


Z

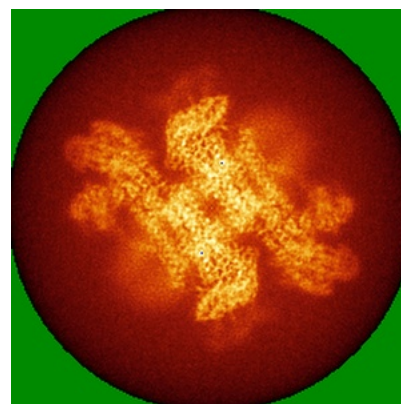
### 6.4.2 Raw map



X



Y

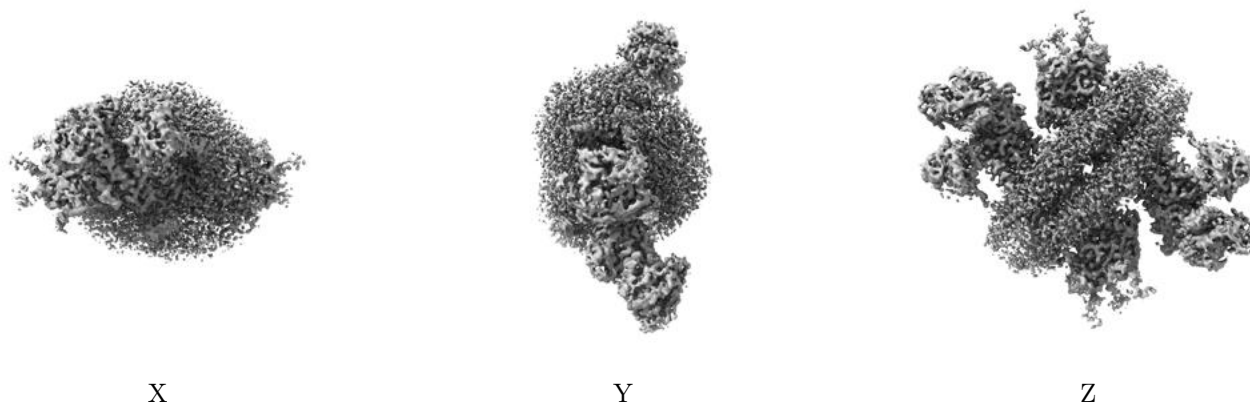


Z

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.

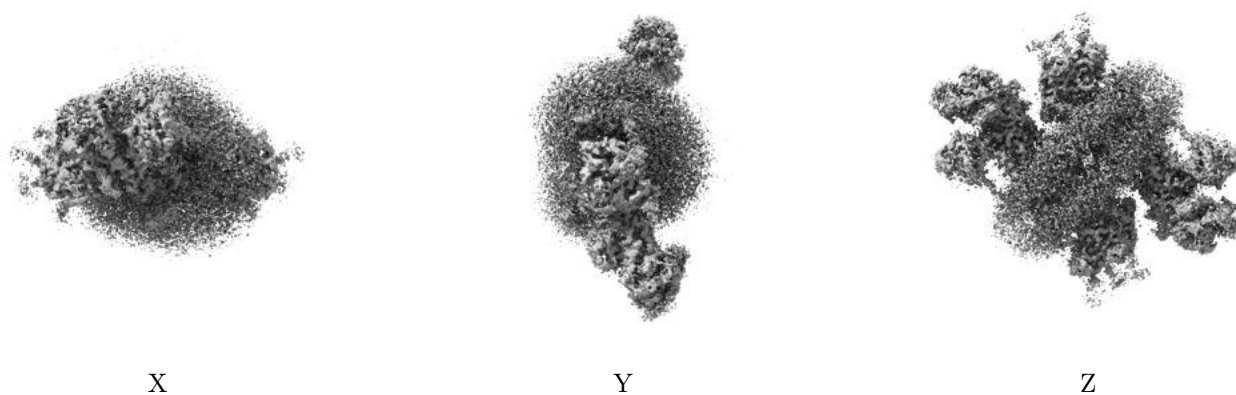
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 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.

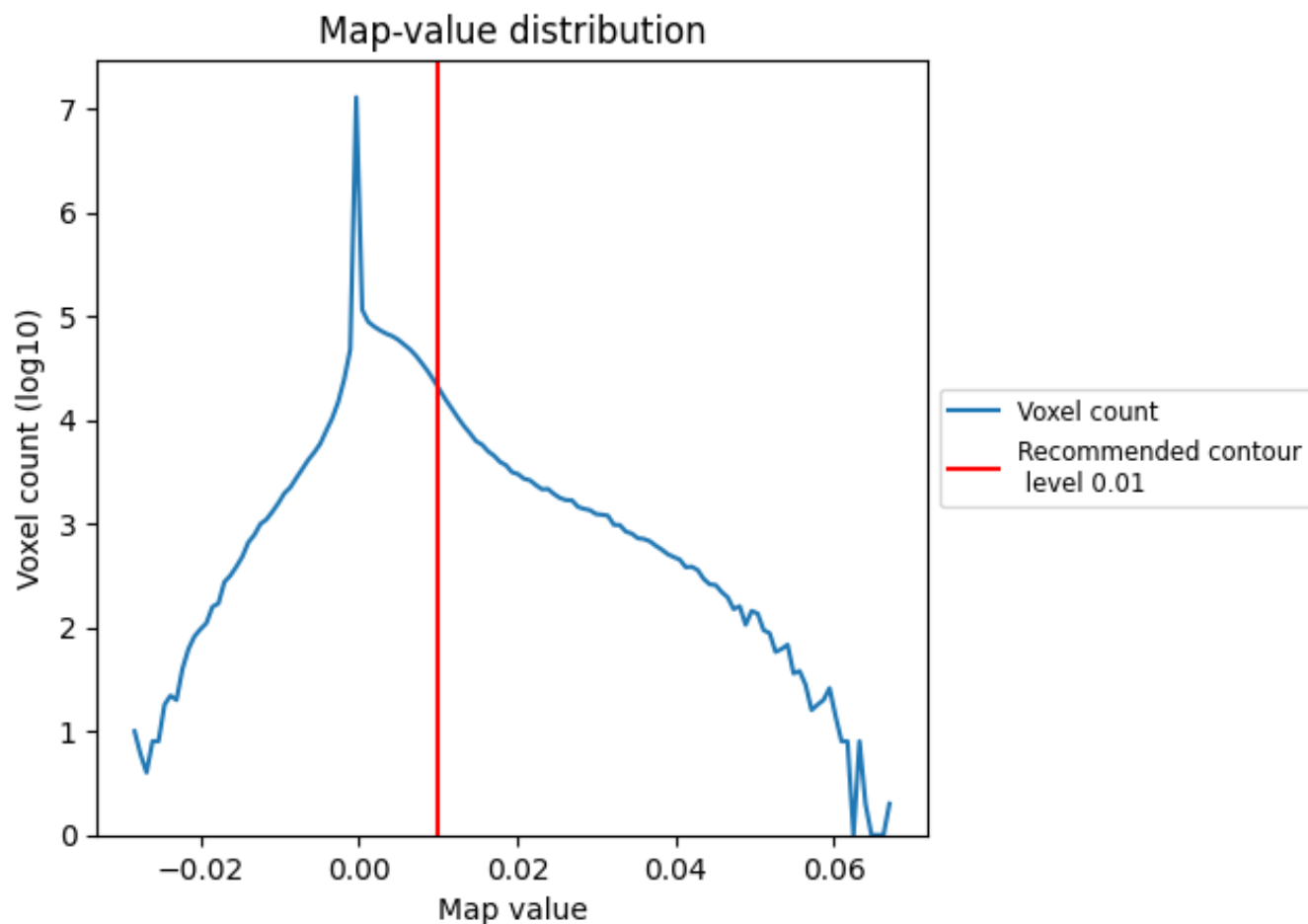
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

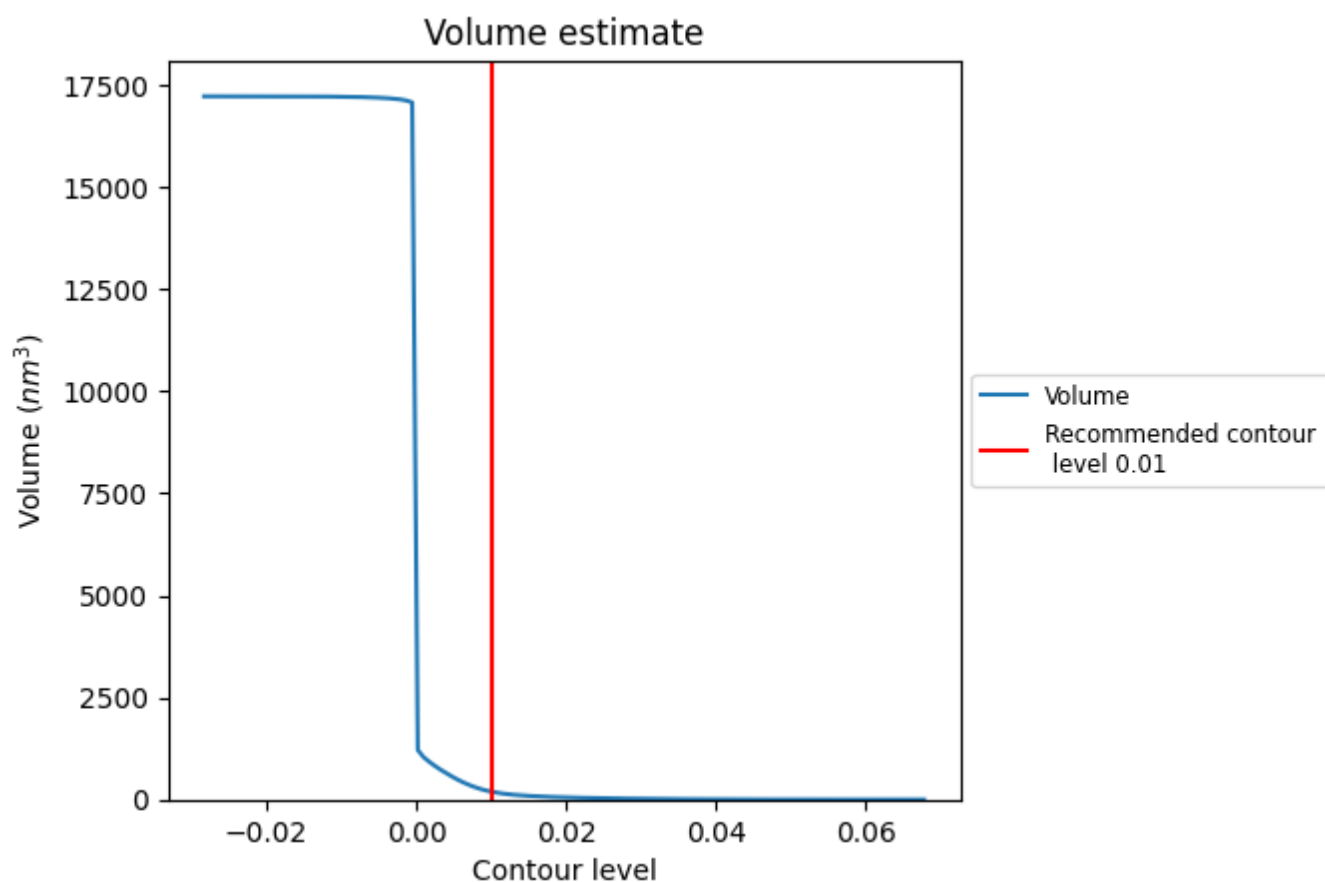
This section contains the results of statistical analysis of the map.

### 7.1 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.

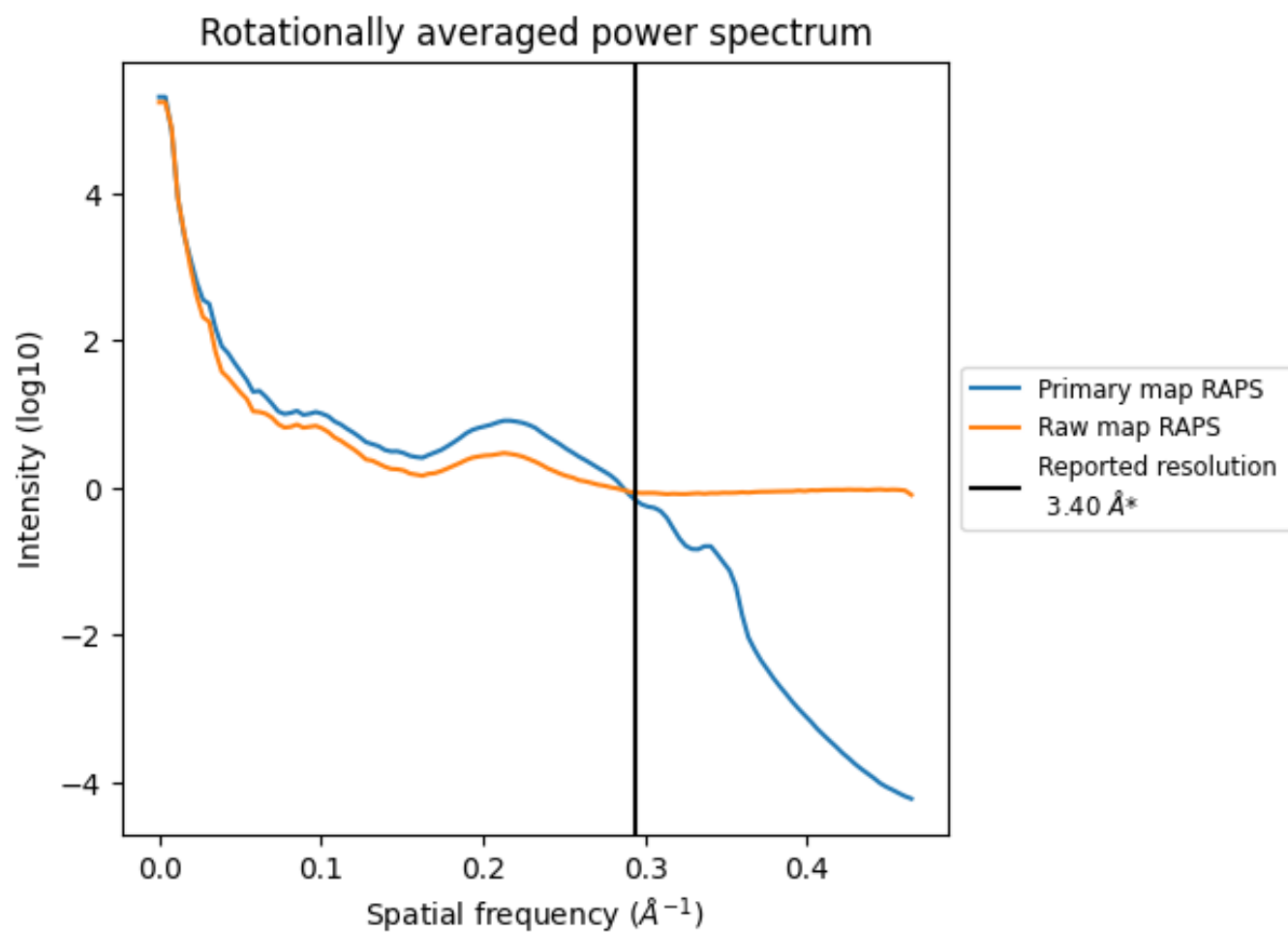
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 193 nm<sup>3</sup>; this corresponds to an approximate mass of 175 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.

### 7.3 Rotationally averaged power spectrum ⓘ

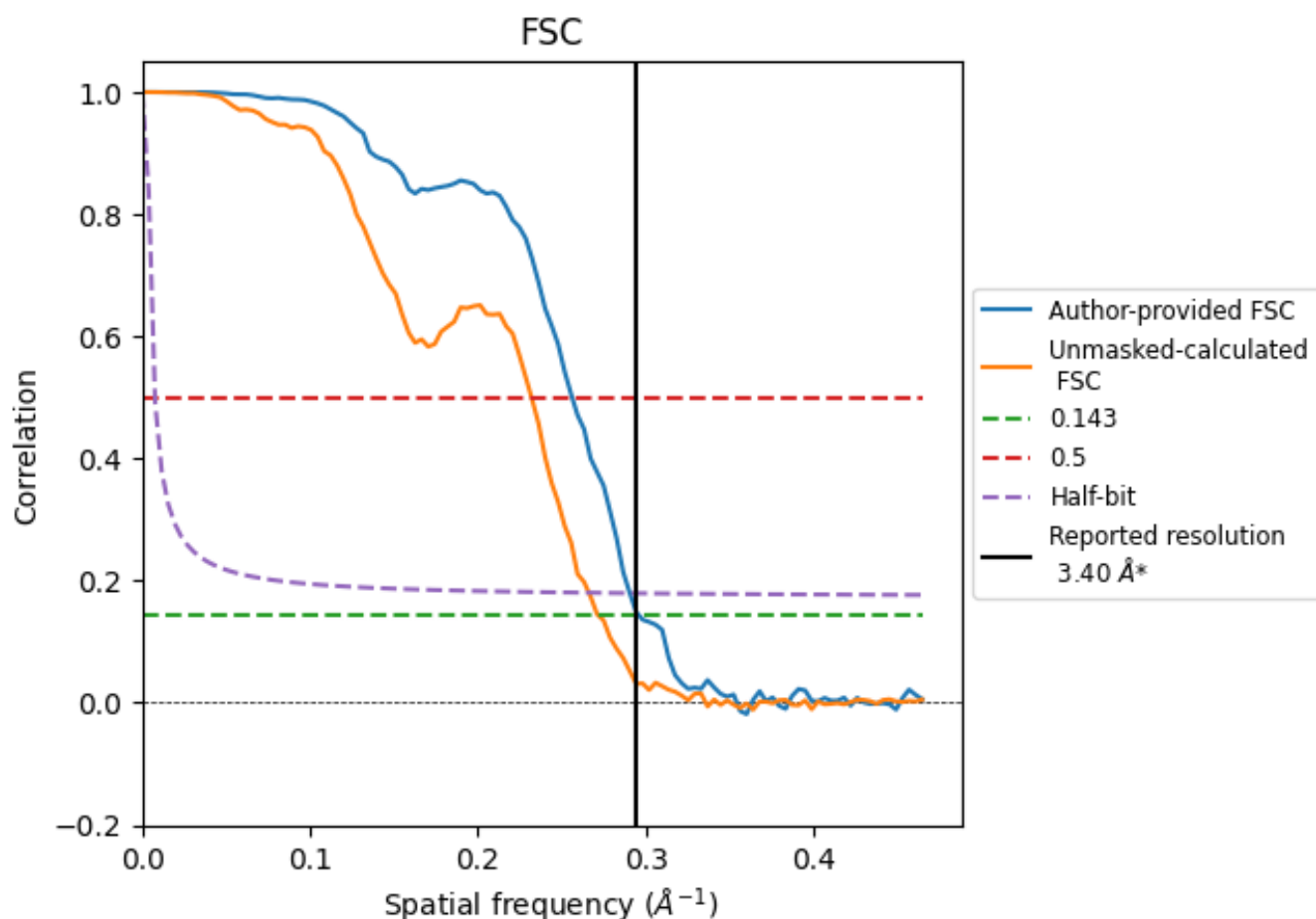


\*Reported resolution corresponds to spatial frequency of 0.294 Å<sup>-1</sup>

## 8 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.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.294 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.38	3.90	3.44
Unmasked-calculated*	3.68	4.31	3.76

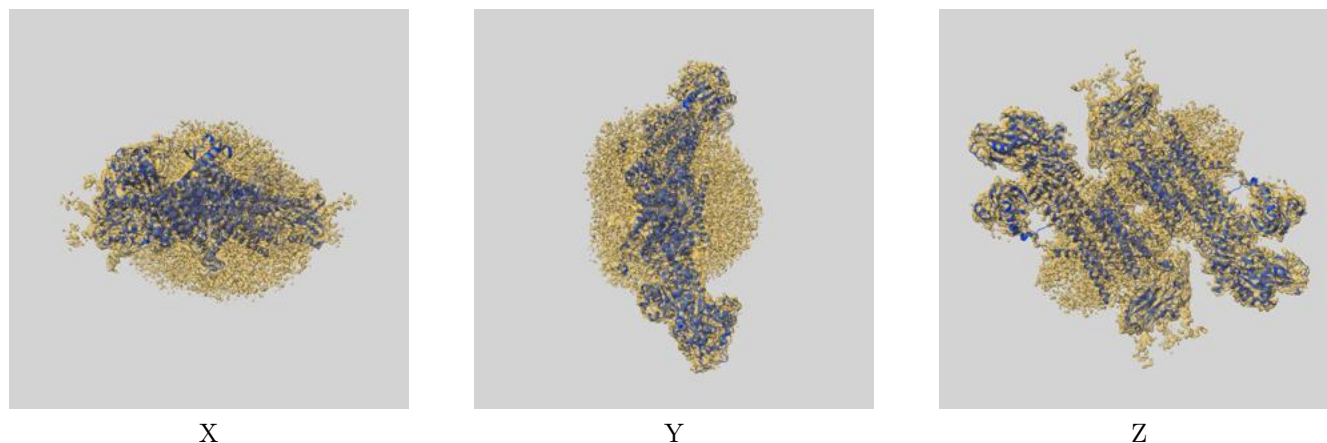
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.



## 9 Map-model fit [i](#)

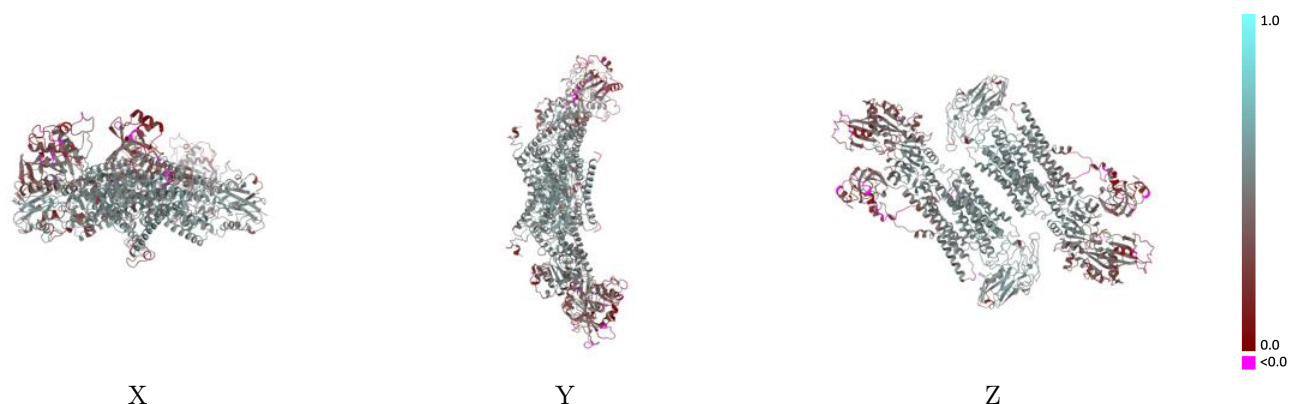
This section contains information regarding the fit between EMDB map EMD-65101 and PDB model 9VJ1. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

### 9.1 Map-model overlay [i](#)



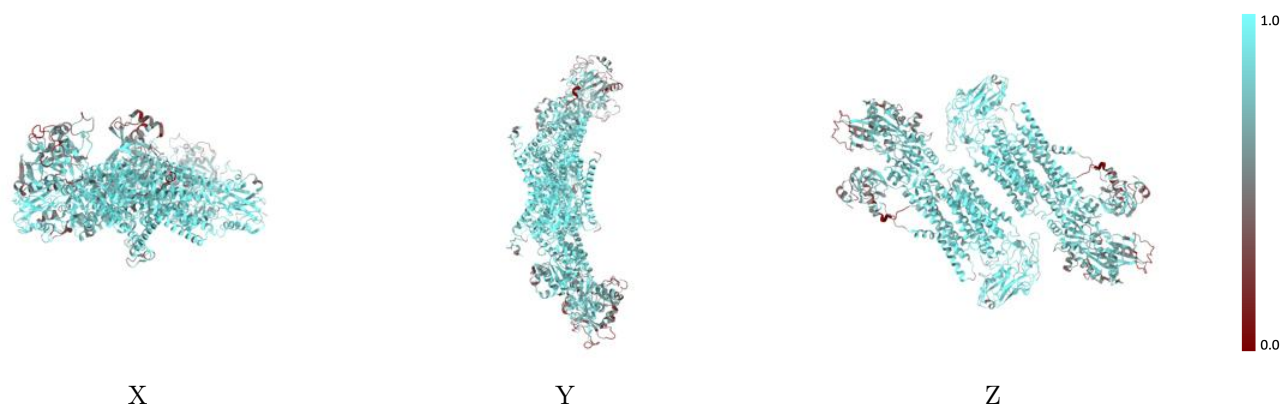
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



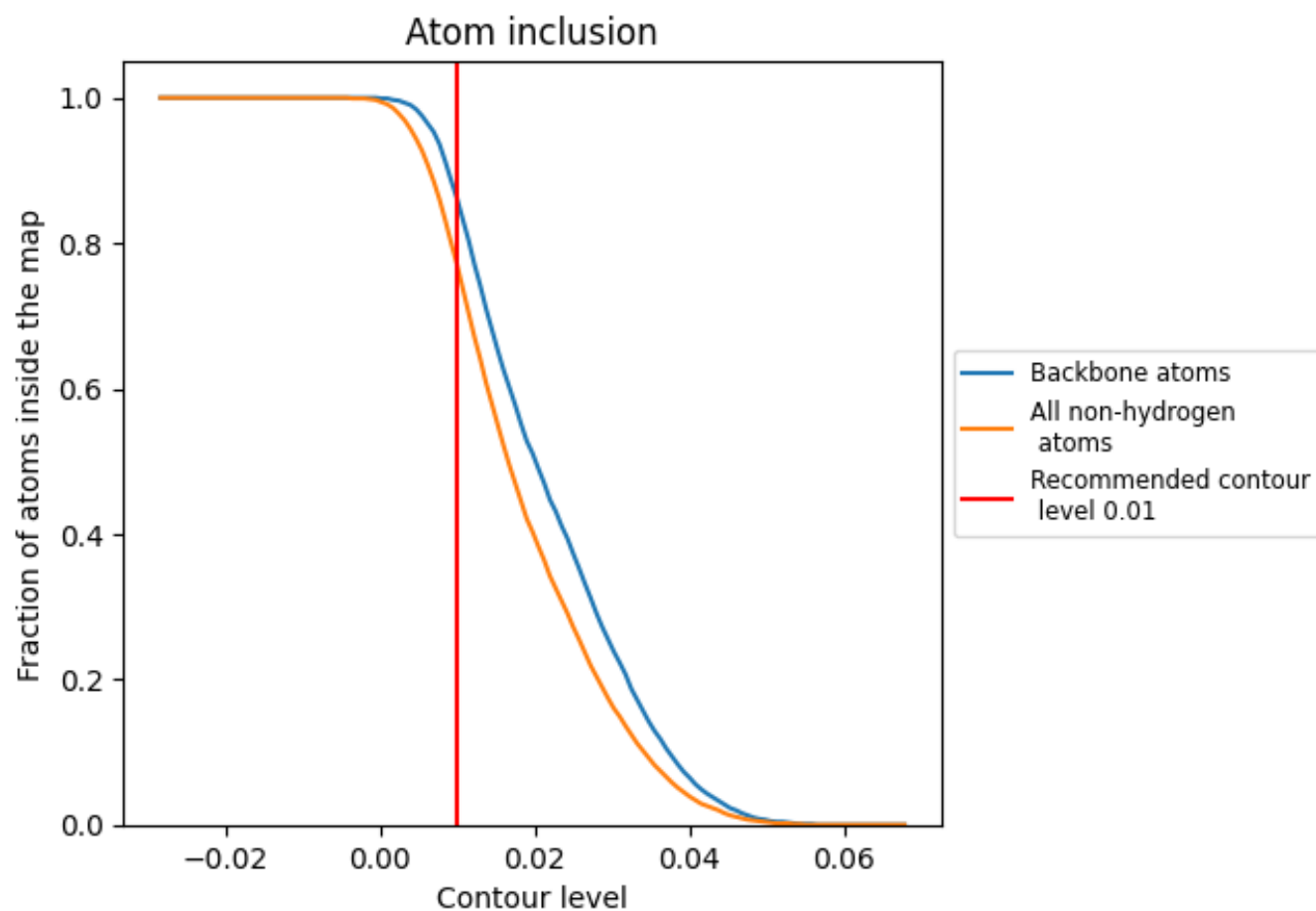
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

## 9.3 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 (0.01).































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7690	 0.4400
A	 0.7510	 0.4270
B	 0.8610	 0.4990
C	 0.7540	 0.4300
D	 0.8640	 0.4990
E	 0.7440	 0.4500
F	 0.5070	 0.3010
G	 0.7580	 0.4510
H	 0.2000	 0.1230
I	 0.4500	 0.2520
J	 0.4290	 0.2410
K	 0.4930	 0.2960
L	 0.2130	 0.1250
M	 0.4330	 0.2120
N	 0.3930	 0.2320

