



wwPDB EM Validation Summary Report ⓘ

Mar 7, 2026 – 02:01 AM UTC

PDB ID : 6WLW / pdb_00006wlw
EMDB ID : EMD-21844
Title : The Vo region of human V-ATPase in state 1 (focused refinement)
Authors : Wang, L.; Wu, H.; Fu, T.-M.
Deposited on : 2020-04-20
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

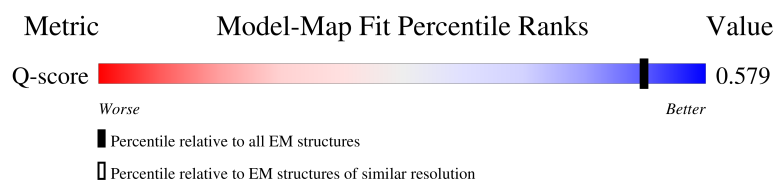
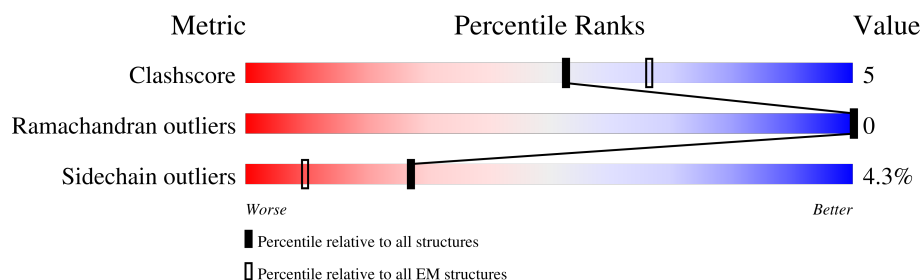
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.00 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.



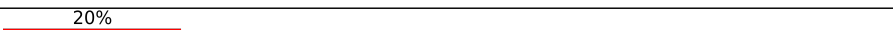
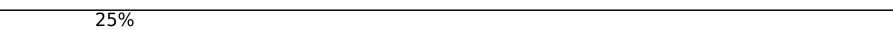
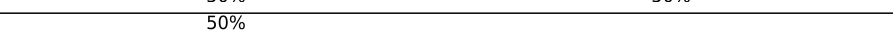
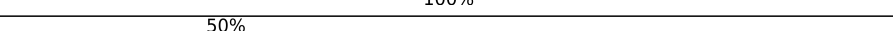
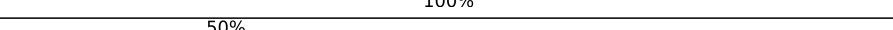
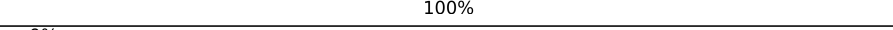
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	0	205	 88% 12%
2	1	155	 83% 12% . .
2	2	155	 87% 10% .
2	3	155	 85% 12% .

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Mol	Chain	Length	Quality of chain
2	4	155	 88% 8% . .
2	5	155	 86% 11% .
2	6	155	 91% 6% .
2	7	155	 88% 7% . .
2	8	155	 92% 5% . .
2	9	155	 89% 8% .
3	Q	351	 83% 16% .
4	R	837	 45% 6% 49%
5	S	81	 80% 14% . 5%
6	T	137	 53% 9% 38%
7	U	470	 32% 11% . 56%
8	V	350	 11% . 86%
9	W	5	 20% 60% 40%
10	A	4	 25% 50% 50%
11	B	2	 50% 100%
11	C	2	 50% 100%
11	D	2	 50% 50%
11	s	2	 50% 50%
11	u	2	 50% 100%
12	r	11	 9% 55% 36% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	NGA	A	2	X	-	-	-
12	MAN	r	11	X	-	-	-
14	PTY	0	306	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	PTY	R	903	X	-	-	-

2 Entry composition [i](#)

There are 19 unique types of molecules in this entry. The entry contains 22145 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 V-type proton ATPase 21 kDa proteolipid subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	204	Total	C	N	O	S	0	0
			1495	988	238	259	10		

- Molecule 2 is a protein called V-type proton ATPase 16 kDa proteolipid subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
2	2	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
2	3	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
2	4	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
2	5	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
2	6	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
2	7	150	Total	C	N	O	S	0	0
			1059	695	166	191	7		
2	8	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
2	9	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		

- Molecule 3 is a protein called V-type proton ATPase subunit d 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Q	350	Total	C	N	O	S	0	0
			2829	1825	461	530	13		

- Molecule 4 is a protein called V-type proton ATPase 116 kDa subunit a isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	R	428	Total	C	N	O	S	0	0
			3477	2335	542	578	22		

- Molecule 5 is a protein called V-type proton ATPase subunit e 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	S	77	Total	C	N	O	S	0	0
			631	436	97	93	5		

- Molecule 6 is a protein called Ribonuclease kappa.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	85	Total	C	N	O	S	0	0
			654	431	101	115	7		

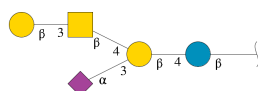
- Molecule 7 is a protein called V-type proton ATPase subunit S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	205	Total	C	N	O	S	0	0
			1664	1089	265	300	10		

- Molecule 8 is a protein called Renin receptor.

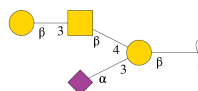
Mol	Chain	Residues	Atoms					AltConf	Trace
8	V	50	Total	C	N	O	S	0	0
			417	283	58	73	3		

- Molecule 9 is an oligosaccharide called beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[N-acetyl-alpha-neuraminic acid-(2-3)]beta-D-galactopyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					AltConf	Trace
9	W	5	Total	C	N	O		0	0
			68	37	2	29			

- Molecule 10 is an oligosaccharide called beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[N-acetyl-alpha-neuraminic acid-(2-3)]beta-D-galactopyranose.



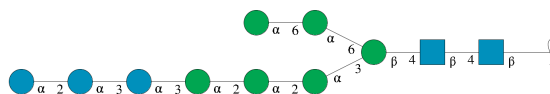
Mol	Chain	Residues	Atoms				AltConf	Trace
10	A	4	Total	C	N	O	0	0
			56	31	2	23		

- Molecule 11 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
11	s	2	Total	C	N	O	0	0
			28	16	2	10		
11	u	2	Total	C	N	O	0	0
			28	16	2	10		
11	B	2	Total	C	N	O	0	0
			28	16	2	10		
11	C	2	Total	C	N	O	0	0
			28	16	2	10		
11	D	2	Total	C	N	O	0	0
			28	16	2	10		

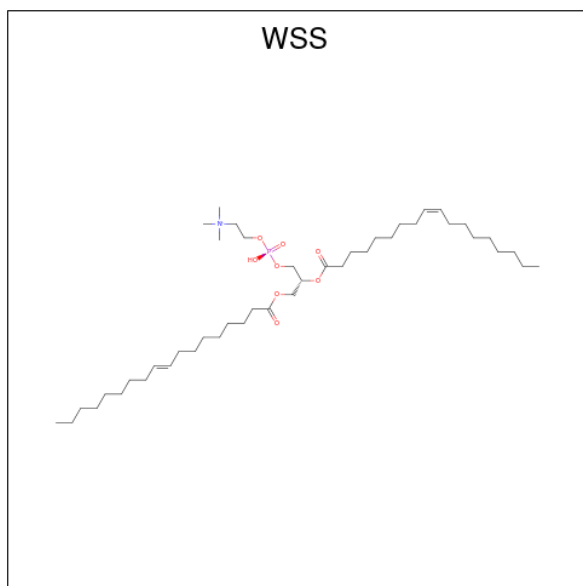
- Molecule 12 is an oligosaccharide called alpha-D-glucopyranose-(1-2)-alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
12	r	11	Total	C	N	O	0	0
			127	70	2	55		

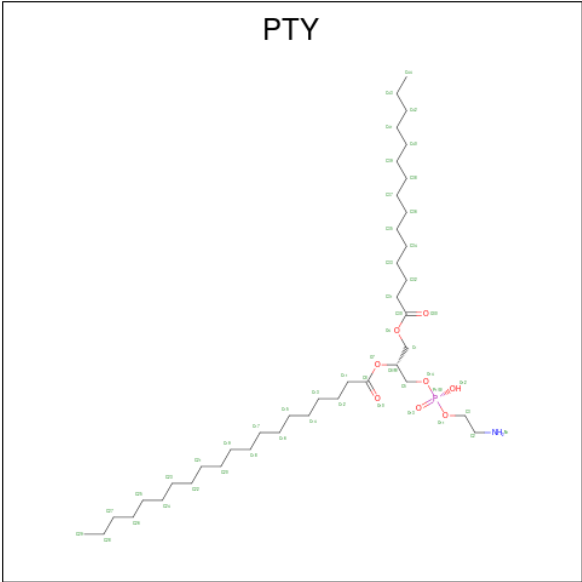
- Molecule 13 is tri(methyl)-[2-[[[(2 {R})-2-[({Z})-octadec-9-enoyl]oxy-3-[({E})-1-oxidanylideneoctadec-9-enoyl]propoxy]-oxidanyl-phosphoryl]oxyethyl]azanum (CCD ID: WSS)

(formula: $C_{44}H_{85}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
13	0	1	Total	C	N	O	P	0
			41	31	1	8	1	
13	0	1	Total	C	N	O	P	0
			37	27	1	8	1	
13	0	1	Total	C	N	O	P	0
			26	16	1	8	1	
13	0	1	Total	C	O	P		0
			31	22	8	1		
13	1	1	Total	C	N	O	P	0
			34	24	1	8	1	
13	3	1	Total	C	O	P		0
			41	32	8	1		
13	R	1	Total	C	N	O	P	0
			40	30	1	8	1	
13	U	1	Total	C	N	O	P	0
			44	34	1	8	1	
13	U	1	Total	C	N	O	P	0
			39	29	1	8	1	
13	V	1	Total	C	N	O	P	0
			37	27	1	8	1	

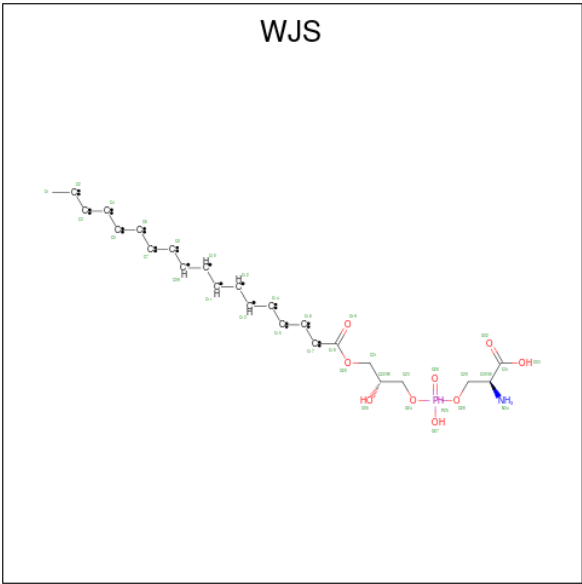
- Molecule 14 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
14	0	1	Total	C	O	P		0
			17	9	7	1		
14	0	1	Total	C	N	O	P	0
			48	38	1	8	1	
14	2	1	Total	C	N	O	P	0
			29	20	1	7	1	
14	5	1	Total	C	N	O	P	0
			35	25	1	8	1	
14	6	1	Total	C	O	P		0
			21	13	7	1		
14	6	1	Total	C	N	O	P	0
			42	32	1	8	1	
14	8	1	Total	C	N	O	P	0
			50	40	1	8	1	
14	8	1	Total	C	O			0
			33	28	5			
14	R	1	Total	C	N	O	P	0
			29	20	1	7	1	
14	S	1	Total	C	O			0
			32	27	5			
14	U	1	Total	C	N	O	P	0
			30	20	1	8	1	
14	U	1	Total	C	O			0
			26	21	5			
14	V	1	Total	C	N	O	P	0
			29	20	1	7	1	

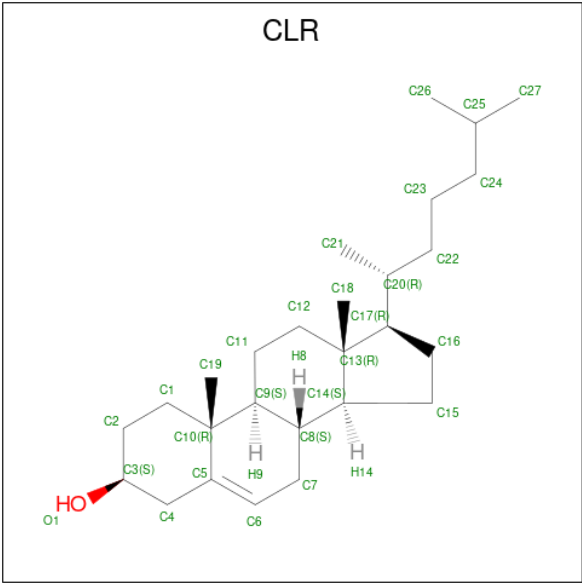
- Molecule 15 is (2 {S})-2-\$l^{\{4\}}\$-azanyl-3-[[(2 {R})-3-octadecanoyloxy-2-oxidanyl-propoxy]

-oxidanyl-oxidanylidene-\$l^{\wedge}\{6\}\$-phosphanyl]oxy-propanoic acid (CCD ID: WJS) (formula: C₂₄H₂₀NO₉P).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
15	3	1	27	16	1	9	1	0

- Molecule 16 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O).



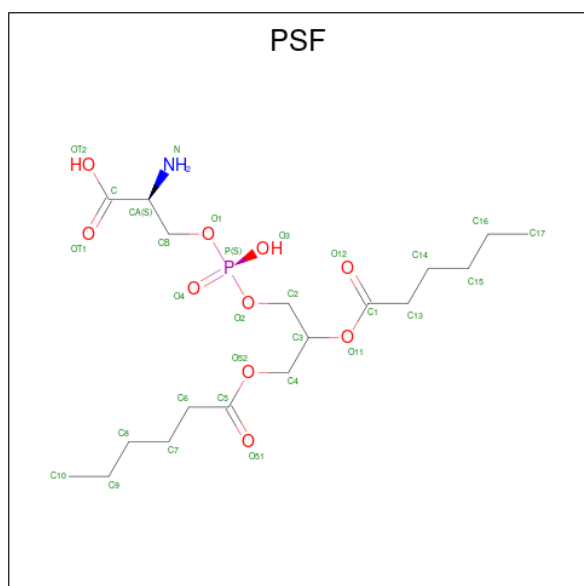
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
16	5	1	28	27	1	0

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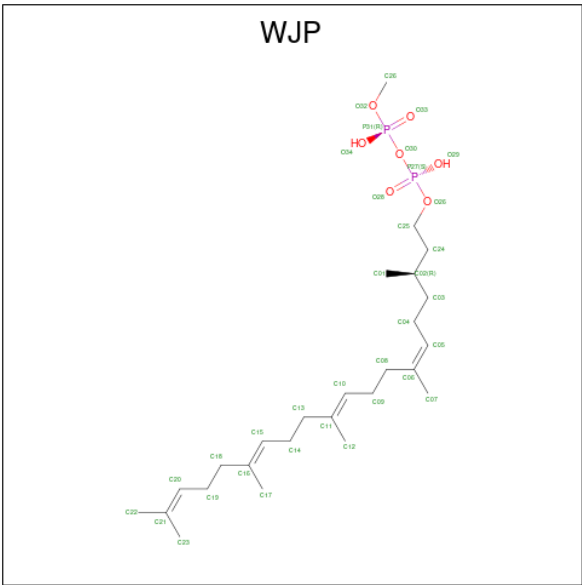
Mol	Chain	Residues	Atoms			AltConf
16	R	1	Total	C	O	0
			28	27	1	
16	V	1	Total	C	O	0
			28	27	1	
16	V	1	Total	C	O	0
			28	27	1	

- Molecule 17 is 1,2-DICAPROYL-SN-PHOSPHATIDYL-L-SERINE (CCD ID: PSF) (formula: $C_{18}H_{34}NO_{10}P$).



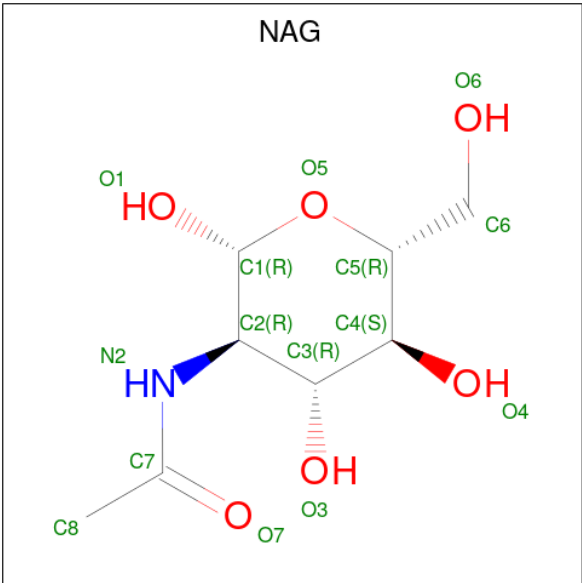
Mol	Chain	Residues	Atoms					AltConf
17	R	1	Total	C	N	O	P	0
			30	18	1	10	1	

- Molecule 18 is methyl (3R,6Z,10E,14E)-3,7,11,15,19-pentamethylicos-6,10,14,18-tetraen-1-yl dihydrogen diphosphate (CCD ID: WJP) (formula: $C_{26}H_{48}O_7P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
18	R	1	Total	C	O	P	0
			34	25	7	2	

- Molecule 19 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

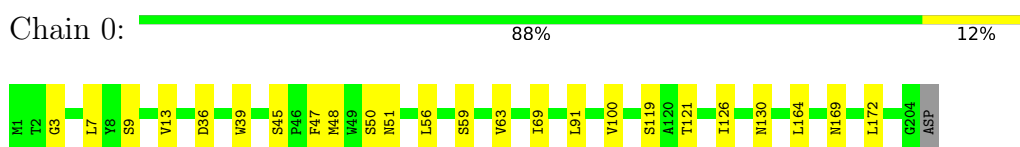


Mol	Chain	Residues	Atoms				AltConf
19	U	1	Total	C	N	O	0
			14	8	1	5	

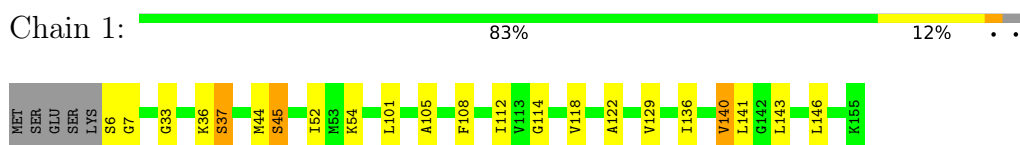
3 Residue-property plots

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.

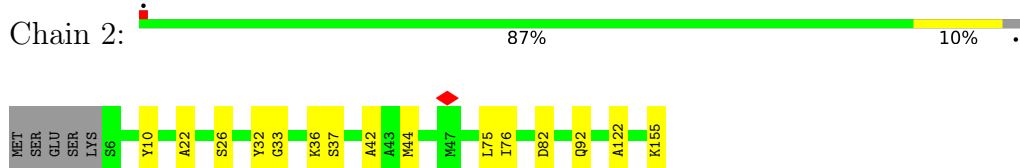
- Molecule 1: V-type proton ATPase 21 kDa proteolipid subunit



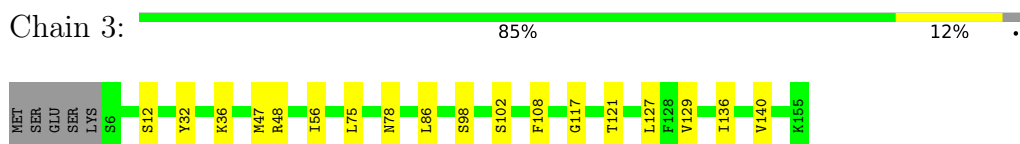
- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit



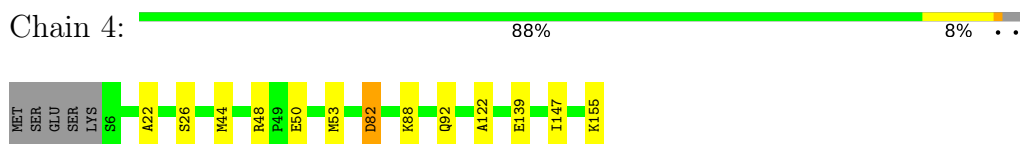
- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit



- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit



- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit



- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit

Chain 5:  86% 11%



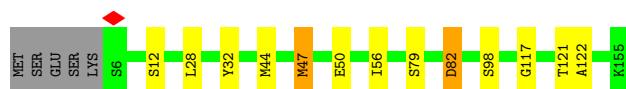
- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit

Chain 6:  91% 6%



- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit

Chain 7:  88% 7%



- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit

Chain 8:  92% 5%



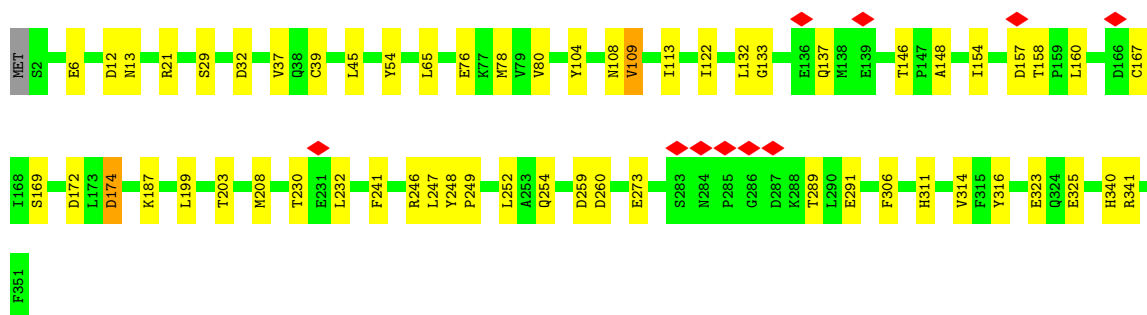
- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit

Chain 9:  89% 8%



- Molecule 3: V-type proton ATPase subunit d 1

Chain Q:  83% 16%



- Molecule 4: V-type proton ATPase 116 kDa subunit a isoform 1

- Molecule 10: beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[N-acetyl-alpha-neuraminic acid-(2-3)]beta-D-galactopyranose



- Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

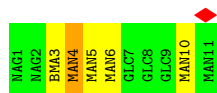


- Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 12: alpha-D-glucopyranose-(1-2)-alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-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

Chain r: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1000000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.1	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.470	Depositor
Minimum map value	-1.625	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.068	Depositor
Recommended contour level	0.6	Depositor
Map size ($\text{\AA}$)	388.80002, 388.80002, 388.80002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.08, 1.08, 1.08	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: SIA, WSS, GAL, WJS, PSF, BGC, WJP, MAN, BMA, NGA, GLC, NAG, PTY, 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	0	0.18	0/1529	0.31	0/2079
2	1	0.18	0/1080	0.31	0/1461
2	2	0.17	0/1080	0.29	0/1461
2	3	0.17	0/1080	0.33	1/1461 (0.1%)
2	4	0.17	0/1080	0.27	0/1461
2	5	0.17	0/1080	0.31	0/1461
2	6	0.17	0/1080	0.30	0/1461
2	7	0.17	0/1074	0.31	1/1454 (0.1%)
2	8	0.18	0/1080	0.33	0/1461
2	9	0.18	0/1080	0.30	0/1461
3	Q	0.20	0/2895	0.34	0/3922
4	R	0.17	0/3591	0.32	0/4876
5	S	0.17	0/657	0.33	0/902
6	T	0.13	0/670	0.29	0/911
7	U	0.16	0/1718	0.35	0/2337
8	V	0.16	0/431	0.26	0/591
All	All	0.17	0/21205	0.32	2/28760 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	56	ILE	N-CA-C	-5.91	106.65	111.91
2	7	56	ILE	N-CA-C	-5.07	107.40	111.91

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	0	1495	0	1537	15	0
2	1	1065	0	1131	12	0
2	2	1065	0	1131	11	0
2	3	1065	0	1131	11	0
2	4	1065	0	1131	7	0
2	5	1065	0	1131	8	0
2	6	1065	0	1131	4	0
2	7	1059	0	1120	8	0
2	8	1065	0	1131	7	0
2	9	1065	0	1131	4	0
3	Q	2829	0	2757	26	0
4	R	3477	0	3478	34	0
5	S	631	0	646	8	0
6	T	654	0	641	4	0
7	U	1664	0	1583	43	0
8	V	417	0	405	8	0
9	W	68	0	58	6	0
10	A	56	0	47	5	0
11	B	28	0	25	0	0
11	C	28	0	25	0	0
11	D	28	0	25	2	0
11	s	28	0	25	0	0
11	u	28	0	25	0	0
12	r	127	0	106	1	0
13	0	135	0	0	1	0
13	1	34	0	0	0	0
13	3	41	0	0	0	0
13	R	40	0	0	6	0
13	U	83	0	0	3	0
13	V	37	0	0	0	0
14	0	65	0	85	4	0
14	2	29	0	40	4	0
14	5	35	0	46	7	0
14	6	63	0	79	10	0
14	8	83	0	129	11	0
14	R	29	0	37	1	0
14	S	32	0	48	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	U	56	0	66	18	0
14	V	29	0	40	9	0
15	3	27	0	0	5	0
16	5	28	0	46	16	0
16	R	28	0	46	2	0
16	V	56	0	92	12	0
17	R	30	0	32	0	0
18	R	34	0	0	1	0
19	U	14	0	13	0	0
All	All	22145	0	22350	237	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 5.

The worst 5 of 237 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)
7:U:273:ASN:ND2	11:D:1:NAG:C1	1.72	1.50
4:R:473:ASN:ND2	13:R:904:WSS:C4	1.80	1.45
4:R:473:ASN:HD22	13:R:904:WSS:C4	1.43	1.23
14:6:201:PTY:O13	14:6:202:PTY:C2	1.95	1.14
7:U:438:PHE:CE2	14:U:504:PTY:H181	1.86	1.10

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	0	202/205 (98%)	202 (100%)	0	0	100	100
2	1	148/155 (96%)	147 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	2	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
2	3	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
2	4	148/155 (96%)	148 (100%)	0	0	100	100
2	5	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
2	6	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
2	7	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
2	8	148/155 (96%)	145 (98%)	3 (2%)	0	100	100
2	9	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
3	Q	348/351 (99%)	338 (97%)	10 (3%)	0	100	100
4	R	424/837 (51%)	409 (96%)	15 (4%)	0	100	100
5	S	75/81 (93%)	72 (96%)	3 (4%)	0	100	100
6	T	83/137 (61%)	80 (96%)	3 (4%)	0	100	100
7	U	203/470 (43%)	192 (95%)	11 (5%)	0	100	100
8	V	48/350 (14%)	45 (94%)	3 (6%)	0	100	100
All	All	2715/3826 (71%)	2659 (98%)	56 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	153/155 (99%)	147 (96%)	6 (4%)	28	62
2	1	107/112 (96%)	102 (95%)	5 (5%)	23	58
2	2	107/112 (96%)	106 (99%)	1 (1%)	70	85
2	3	107/112 (96%)	103 (96%)	4 (4%)	30	64
2	4	107/112 (96%)	104 (97%)	3 (3%)	38	70
2	5	107/112 (96%)	101 (94%)	6 (6%)	19	52
2	6	107/112 (96%)	103 (96%)	4 (4%)	30	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	7	106/112 (95%)	100 (94%)	6 (6%)	18	52
2	8	107/112 (96%)	105 (98%)	2 (2%)	50	76
2	9	107/112 (96%)	103 (96%)	4 (4%)	30	64
3	Q	303/306 (99%)	287 (95%)	16 (5%)	20	54
4	R	376/746 (50%)	363 (96%)	13 (4%)	32	65
5	S	69/72 (96%)	68 (99%)	1 (1%)	59	80
6	T	70/116 (60%)	64 (91%)	6 (9%)	10	36
7	U	182/397 (46%)	169 (93%)	13 (7%)	13	43
8	V	45/308 (15%)	43 (96%)	2 (4%)	25	60
All	All	2160/3108 (70%)	2068 (96%)	92 (4%)	27	60

5 of 92 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	R	452	LEU
6	T	74	VAL
4	R	469	SER
4	R	718	VAL
6	T	124	CYS

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

Mol	Chain	Res	Type
6	T	107	ASN
7	U	398	GLN
7	U	272	GLN
7	U	338	HIS
7	U	411	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 ⓘ

30 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
10	GAL	A	1	10	11,11,12	0.57	0	15,15,17	1.31	2 (13%)
10	NGA	A	2	10	14,14,15	0.71	0	17,19,21	1.91	4 (23%)
10	GAL	A	3	10	11,11,12	0.58	0	15,15,17	1.64	2 (13%)
10	SIA	A	4	10	20,20,21	0.75	1 (5%)	21,28,31	1.15	2 (9%)
11	NAG	B	1	7,11	14,14,15	0.18	0	17,19,21	0.49	0
11	NAG	B	2	11	14,14,15	0.27	0	17,19,21	0.46	0
11	NAG	C	1	7,11	14,14,15	0.33	0	17,19,21	0.80	1 (5%)
11	NAG	C	2	11	14,14,15	0.19	0	17,19,21	0.60	1 (5%)
11	NAG	D	1	11	14,14,15	0.33	0	17,19,21	0.39	0
11	NAG	D	2	11	14,14,15	0.24	0	17,19,21	0.41	0
9	BGC	W	1	9	12,12,12	0.55	0	17,17,17	1.39	3 (17%)
9	GAL	W	2	9	11,11,12	0.75	0	15,15,17	1.34	1 (6%)
9	NGA	W	3	9	14,14,15	0.42	0	17,19,21	1.99	6 (35%)
9	GAL	W	4	9	11,11,12	0.32	0	15,15,17	0.73	1 (6%)
9	SIA	W	5	9	20,20,21	0.60	0	21,28,31	1.45	2 (9%)
12	NAG	r	1	12	14,14,15	0.18	0	17,19,21	0.47	0
12	MAN	r	10	12	11,11,12	0.54	0	15,15,17	1.00	2 (13%)
12	MAN	r	11	12	11,11,12	0.35	0	15,15,17	0.70	0
12	NAG	r	2	12	14,14,15	0.21	0	17,19,21	0.46	0
12	BMA	r	3	12	11,11,12	0.52	0	15,15,17	0.85	1 (6%)
12	MAN	r	4	12	11,11,12	0.58	0	15,15,17	0.99	2 (13%)
12	MAN	r	5	12	11,11,12	0.60	0	15,15,17	1.12	2 (13%)
12	MAN	r	6	12	11,11,12	0.70	0	15,15,17	0.89	1 (6%)
12	GLC	r	7	12	11,11,12	0.65	0	15,15,17	0.57	0
12	GLC	r	8	12	11,11,12	0.60	0	15,15,17	0.74	0
12	GLC	r	9	12	11,11,12	0.61	0	15,15,17	0.69	0
11	NAG	s	1	5,11	14,14,15	0.33	0	17,19,21	0.70	1 (5%)
11	NAG	s	2	11	14,14,15	0.30	0	17,19,21	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	NAG	u	1	7,11	14,14,15	0.26	0	17,19,21	0.50	0
11	NAG	u	2	11	14,14,15	0.34	0	17,19,21	0.51	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
10	GAL	A	1	10	-	0/2/19/22	0/1/1/1
10	NGA	A	2	10	1/1/5/7	3/6/23/26	0/1/1/1
10	GAL	A	3	10	-	1/2/19/22	0/1/1/1
10	SIA	A	4	10	-	13/18/34/38	0/1/1/1
11	NAG	B	1	7,11	-	1/6/23/26	0/1/1/1
11	NAG	B	2	11	-	4/6/23/26	0/1/1/1
11	NAG	C	1	7,11	-	3/6/23/26	0/1/1/1
11	NAG	C	2	11	-	2/6/23/26	0/1/1/1
11	NAG	D	1	11	-	2/6/23/26	0/1/1/1
11	NAG	D	2	11	-	3/6/23/26	0/1/1/1
9	BGC	W	1	9	-	1/2/22/22	0/1/1/1
9	GAL	W	2	9	-	0/2/19/22	0/1/1/1
9	NGA	W	3	9	-	2/6/23/26	0/1/1/1
9	GAL	W	4	9	-	1/2/19/22	0/1/1/1
9	SIA	W	5	9	-	2/18/34/38	0/1/1/1
12	NAG	r	1	12	-	2/6/23/26	0/1/1/1
12	MAN	r	10	12	-	2/2/19/22	0/1/1/1
12	MAN	r	11	12	1/1/4/5	0/2/19/22	0/1/1/1
12	NAG	r	2	12	-	0/6/23/26	0/1/1/1
12	BMA	r	3	12	-	0/2/19/22	0/1/1/1
12	MAN	r	4	12	-	2/2/19/22	0/1/1/1
12	MAN	r	5	12	-	2/2/19/22	0/1/1/1
12	MAN	r	6	12	-	2/2/19/22	0/1/1/1
12	GLC	r	7	12	-	1/2/19/22	0/1/1/1
12	GLC	r	8	12	-	0/2/19/22	0/1/1/1
12	GLC	r	9	12	-	0/2/19/22	0/1/1/1
11	NAG	s	1	5,11	-	2/6/23/26	0/1/1/1
11	NAG	s	2	11	-	4/6/23/26	0/1/1/1
11	NAG	u	1	7,11	-	2/6/23/26	0/1/1/1
11	NAG	u	2	11	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	4	SIA	O1B-C1	-2.95	1.21	1.30

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	2	NGA	C1-O5-C5	4.89	118.74	112.19
10	A	3	GAL	C1-O5-C5	4.09	117.67	112.19
9	W	3	NGA	C1-C2-N2	4.03	116.78	110.43
10	A	2	NGA	C2-N2-C7	-3.94	117.61	122.90
10	A	3	GAL	C1-C2-C3	3.78	115.15	109.64

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	A	2	NGA	C1
12	r	11	MAN	C1

5 of 60 torsion outliers are listed below:

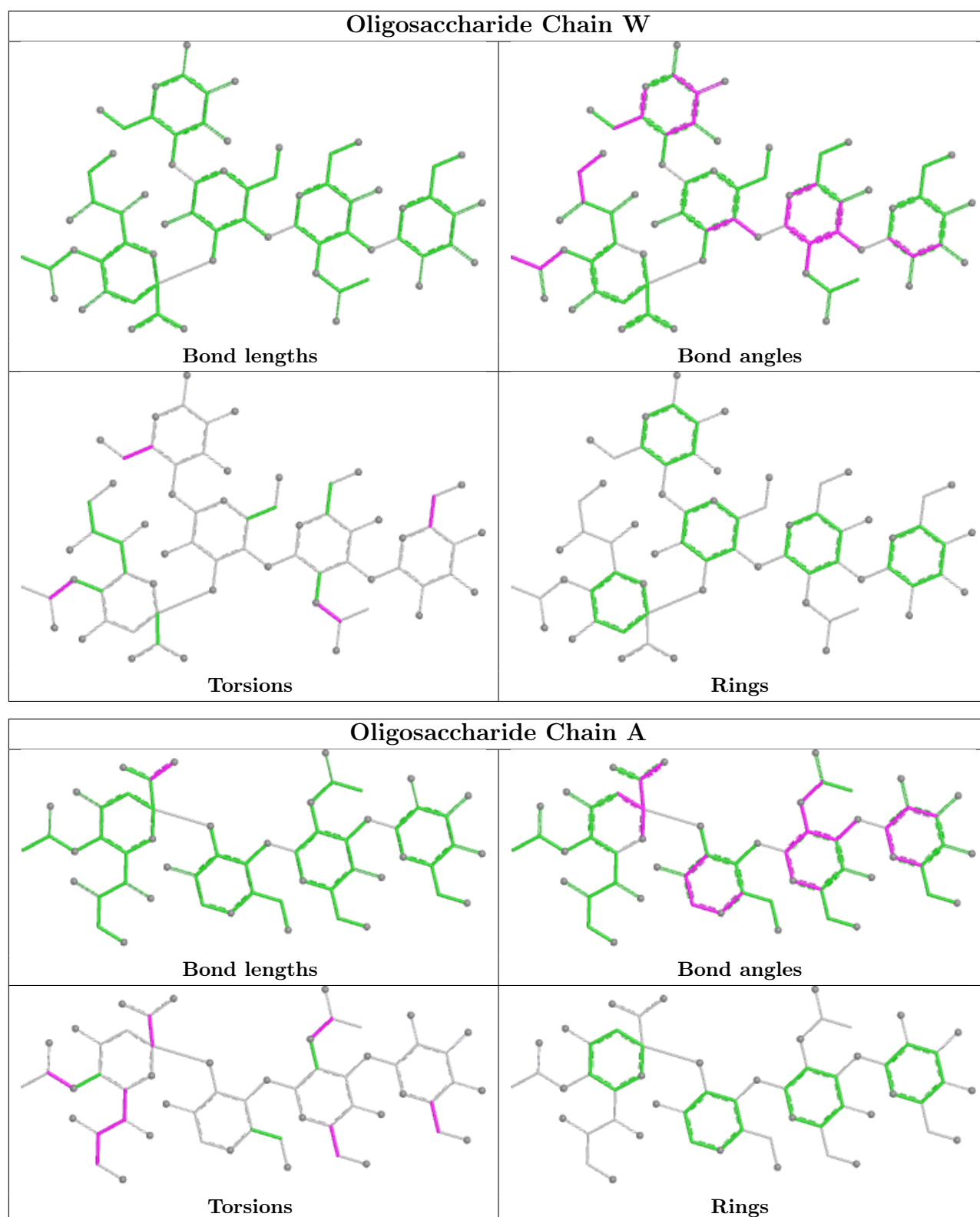
Mol	Chain	Res	Type	Atoms
9	W	3	NGA	C8-C7-N2-C2
9	W	3	NGA	O7-C7-N2-C2
10	A	4	SIA	C5-C6-C7-C8
10	A	4	SIA	C5-C6-C7-O7
10	A	4	SIA	O6-C6-C7-C8

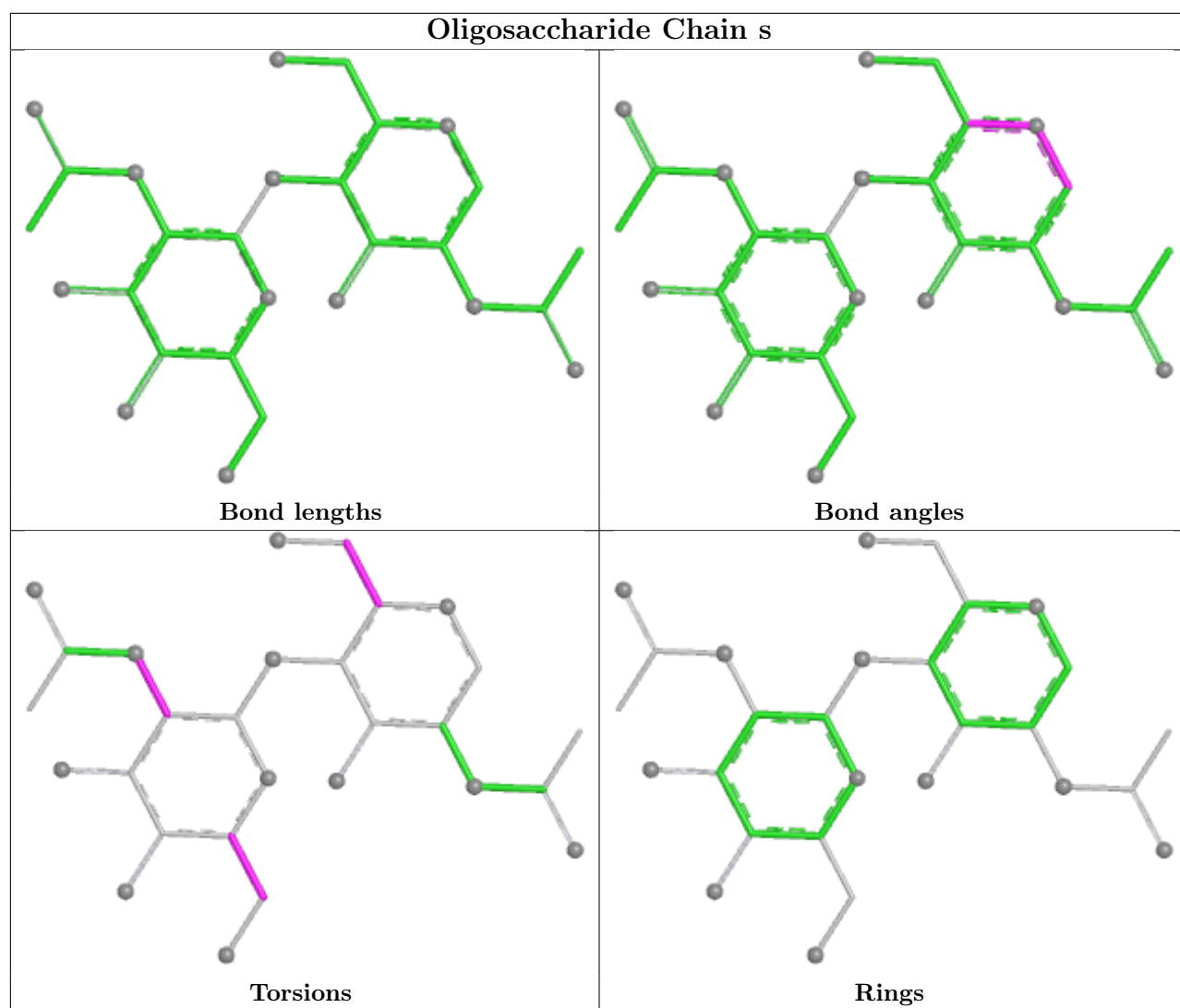
There are no ring outliers.

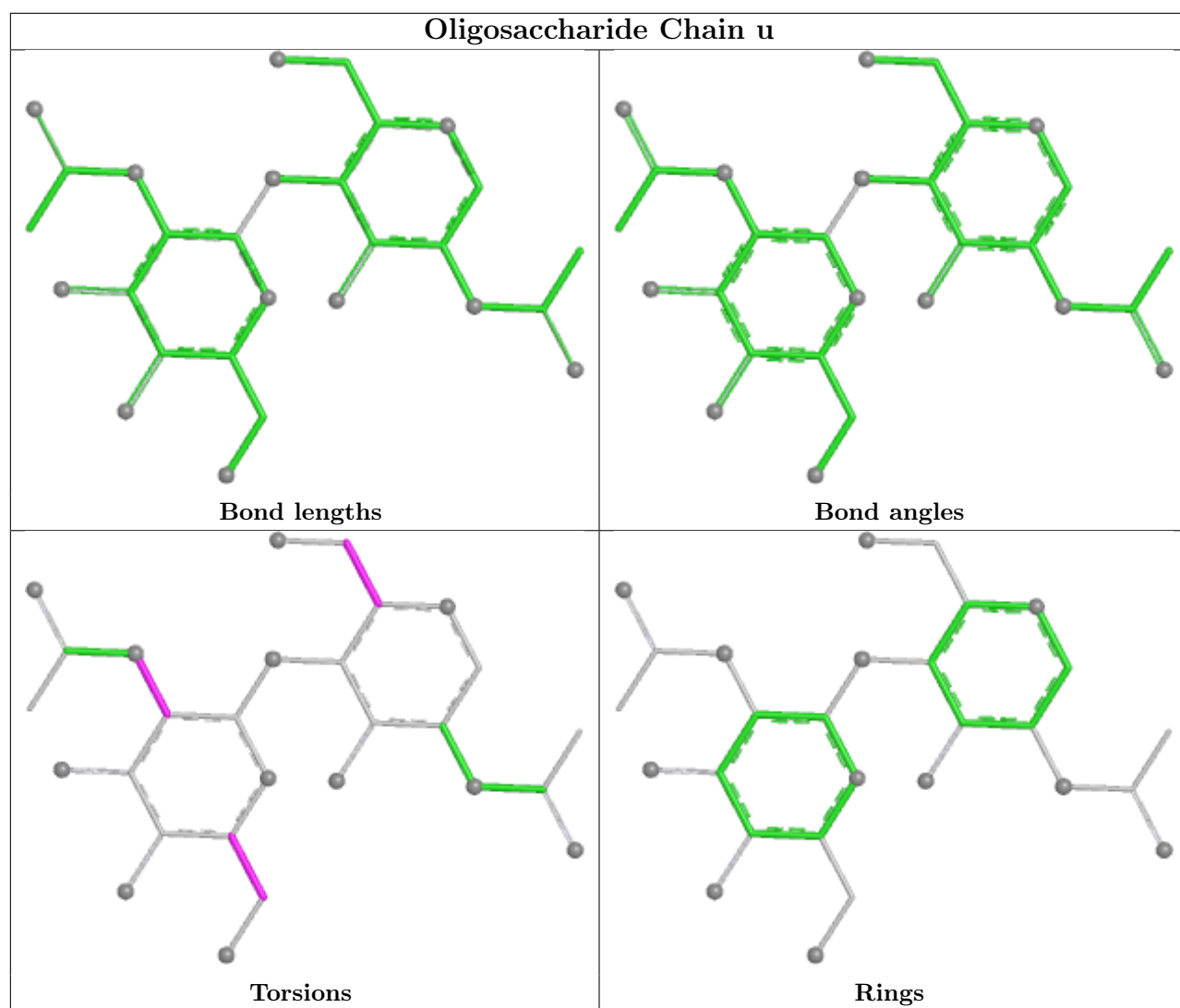
6 monomers are involved in 12 short contacts:

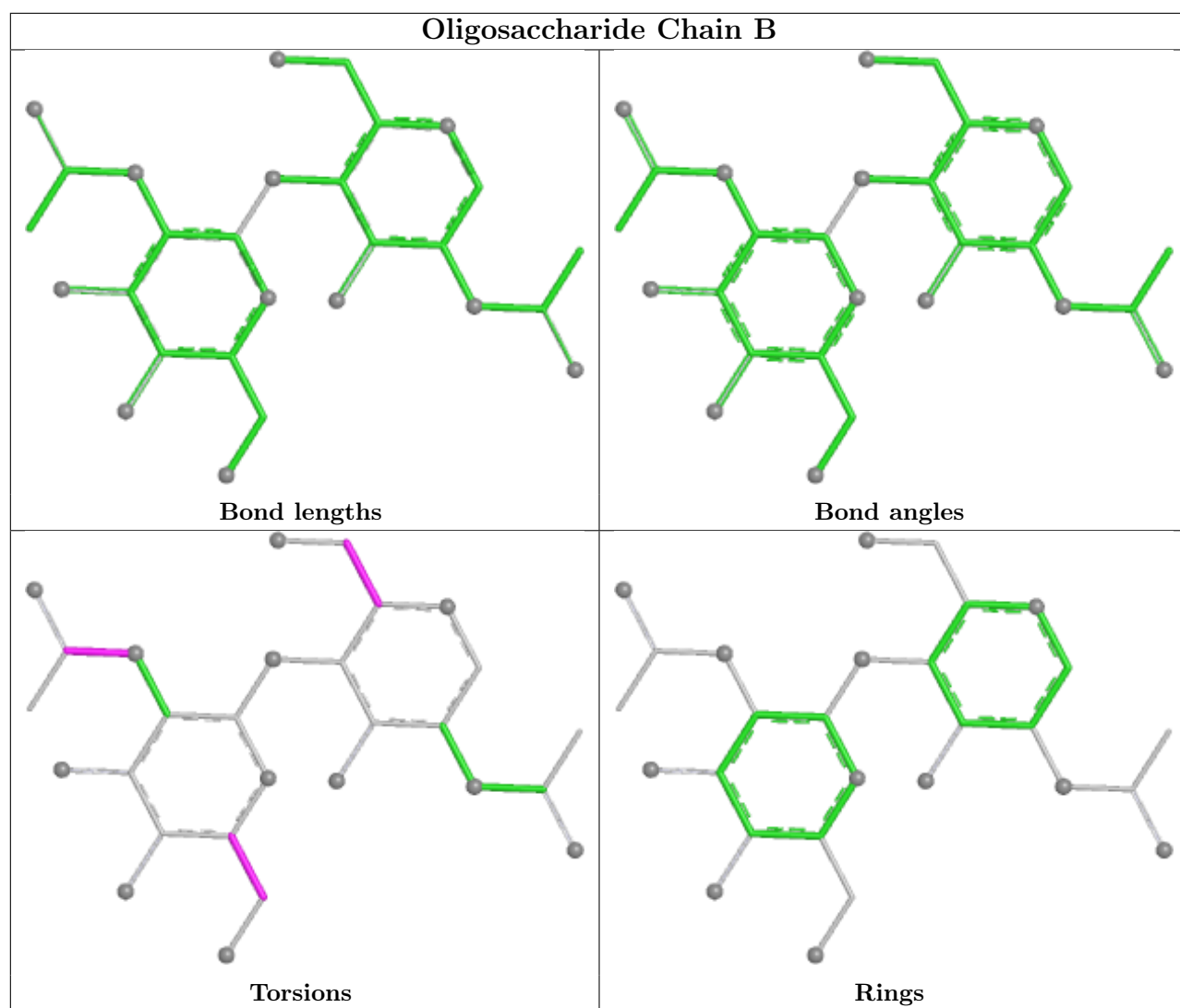
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	W	1	BGC	1	0
10	A	2	NGA	1	0
11	D	1	NAG	2	0
9	W	5	SIA	5	0
12	r	4	MAN	1	0
10	A	4	SIA	4	0

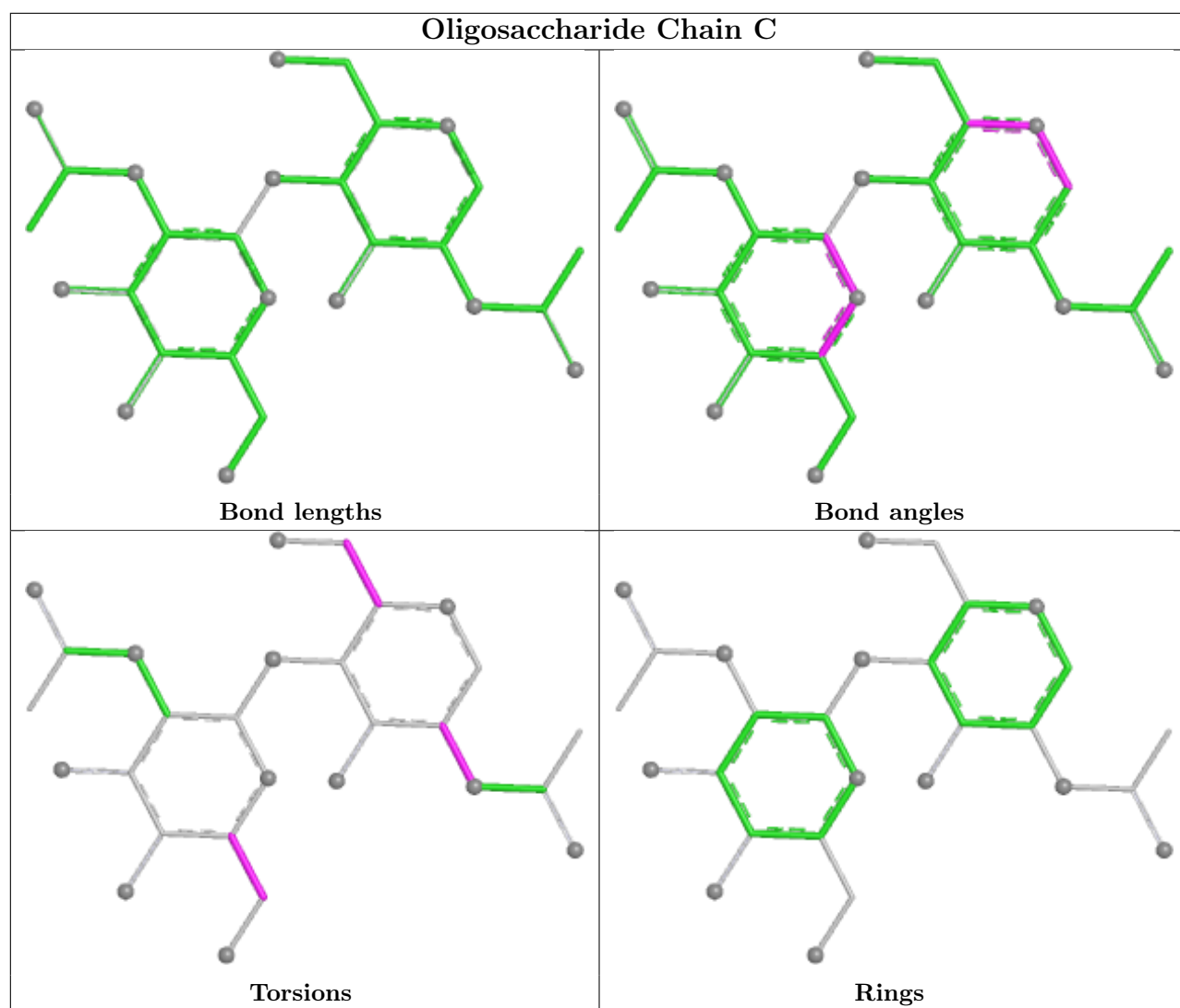
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

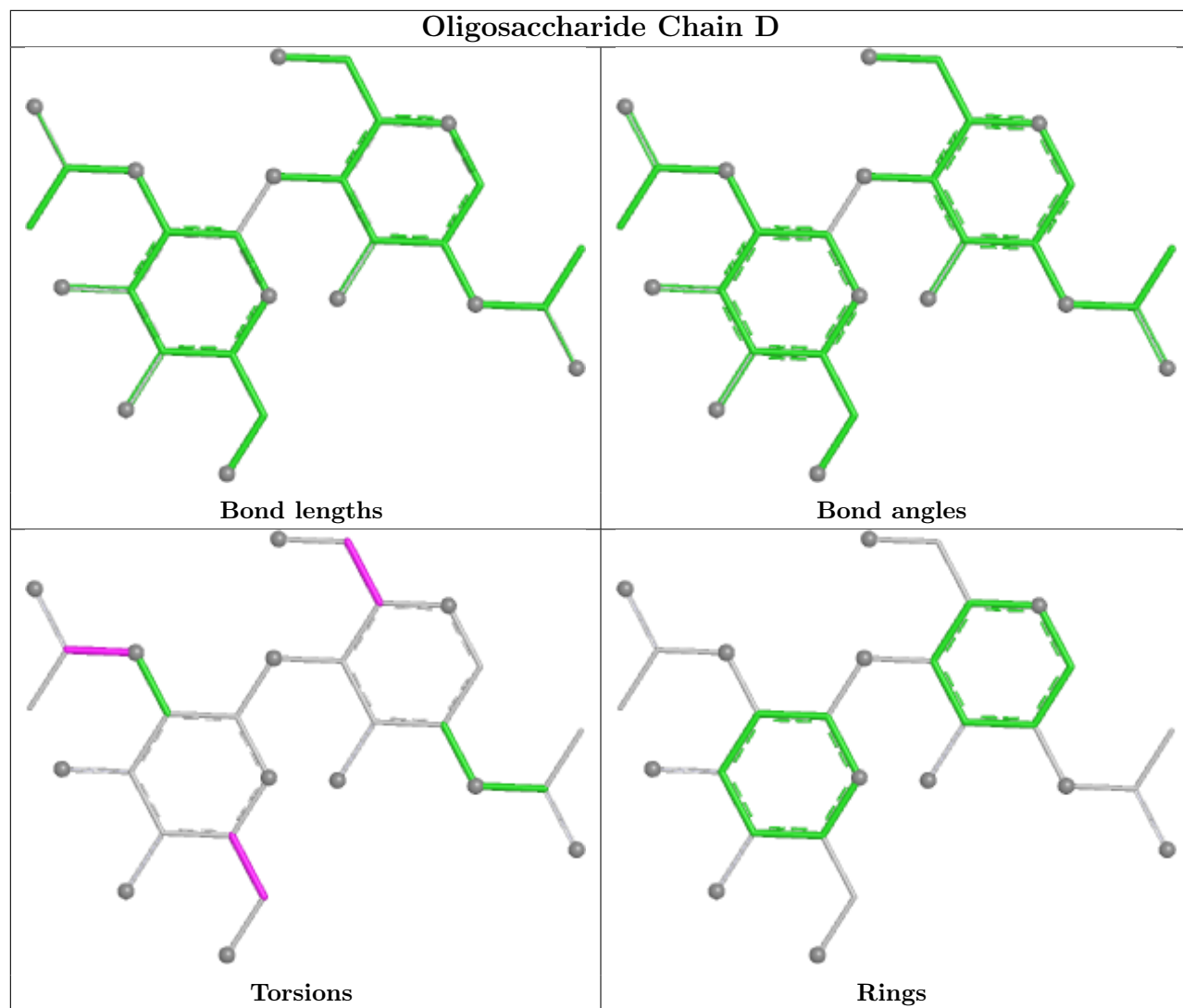


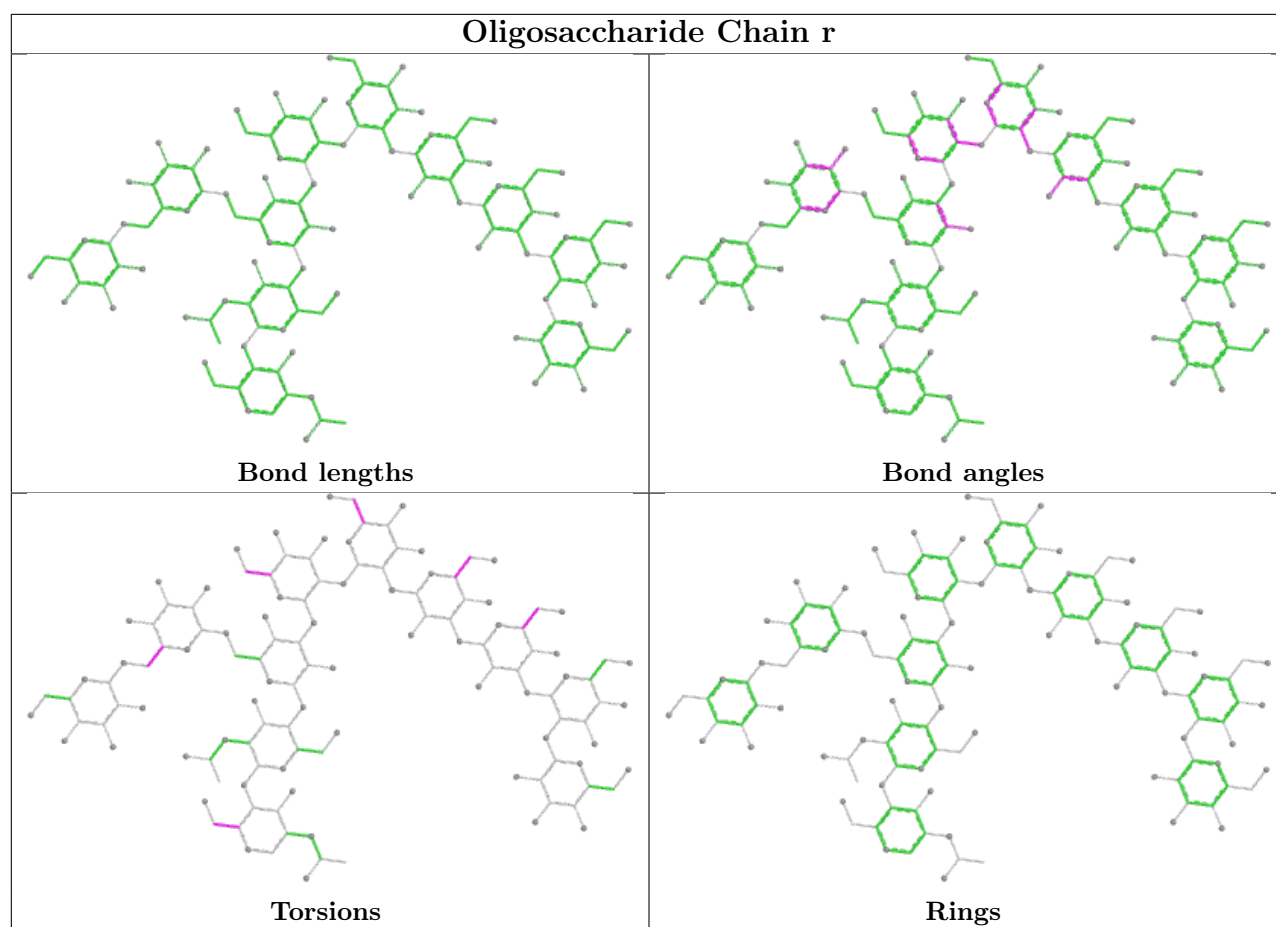












5.6 Ligand geometry [i](#)

31 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
14	PTY	S	101	-	31,31,49	0.31	0	33,33,54	0.32	0
16	CLR	V	402	-	31,31,31	0.31	0	48,48,48	0.41	0
13	WSS	U	502	-	38,38,53	0.37	0	44,46,61	0.35	0
19	NAG	U	505	7	14,14,15	0.19	0	17,19,21	0.45	0
14	PTY	8	201	-	49,49,49	0.31	0	52,54,54	0.31	0
14	PTY	5	202	-	34,34,49	0.36	0	37,39,54	0.44	0
16	CLR	5	201	-	31,31,31	0.30	0	48,48,48	0.66	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	PTY	6	202	-	41,41,49	0.31	0	44,46,54	0.38	0
13	WSS	V	401	-	36,36,53	0.35	0	42,44,61	0.48	0
17	PSF	R	902	-	28,29,29	0.52	0	30,36,36	0.49	0
13	WSS	R	904	-	39,39,53	0.35	0	45,47,61	0.39	0
13	WSS	0	302	-	36,36,53	0.39	0	42,44,61	0.54	0
13	WSS	3	201	-	40,40,53	0.46	0	43,45,61	0.69	1 (2%)
14	PTY	8	202	-	32,32,49	0.29	0	34,34,54	0.44	0
14	PTY	R	903	-	28,28,49	0.33	0	30,32,54	0.46	0
14	PTY	V	404	-	28,28,49	0.36	0	30,32,54	0.41	0
13	WSS	0	303	-	25,25,53	0.39	0	31,33,61	0.82	1 (3%)
15	WJS	3	202	-	25,26,34	1.45	2 (8%)	26,32,40	1.53	2 (7%)
14	PTY	U	503	-	29,29,49	0.36	0	32,34,54	0.46	0
18	WJP	R	905	-	32,33,34	1.69	6 (18%)	39,43,44	1.93	10 (25%)
14	PTY	0	305	-	16,16,49	0.59	0	18,20,54	0.73	1 (5%)
14	PTY	U	504	-	25,25,49	0.34	0	27,27,54	0.33	0
14	PTY	2	201	-	28,28,49	0.35	0	30,32,54	0.48	0
13	WSS	0	304	-	30,30,53	0.47	0	33,35,61	0.63	1 (3%)
16	CLR	V	403	-	31,31,31	0.53	0	48,48,48	0.62	0
13	WSS	0	301	-	40,40,53	0.34	0	46,48,61	0.40	0
14	PTY	6	201	-	20,20,49	0.44	0	22,24,54	0.44	0
13	WSS	1	201	-	33,33,53	0.38	0	39,41,61	0.67	1 (2%)
13	WSS	U	501	-	43,43,53	0.35	0	49,51,61	0.81	2 (4%)
16	CLR	R	901	-	31,31,31	0.27	0	48,48,48	0.50	0
14	PTY	0	306	-	47,47,49	0.29	0	50,52,54	0.35	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
14	PTY	S	101	-	-	19/33/33/53	-
16	CLR	V	402	-	-	0/10/68/68	0/4/4/4
13	WSS	U	502	-	-	3/42/42/57	-
19	NAG	U	505	7	-	2/6/23/26	0/1/1/1
14	PTY	8	201	-	-	28/53/53/53	-
14	PTY	5	202	-	-	23/38/38/53	-
16	CLR	5	201	-	-	0/10/68/68	0/4/4/4
14	PTY	6	202	-	-	22/45/45/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	WSS	V	401	-	-	6/40/40/57	-
17	PSF	R	902	-	-	15/35/35/35	-
13	WSS	R	904	-	-	18/43/43/57	-
13	WSS	0	302	-	-	4/40/40/57	-
13	WSS	3	201	-	-	9/44/44/57	-
14	PTY	8	202	-	-	17/34/34/53	-
14	PTY	R	903	-	1/1/3/4	19/31/31/53	-
14	PTY	V	404	-	-	18/30/30/53	-
13	WSS	0	303	-	-	6/29/29/57	-
15	WJS	3	202	-	-	10/30/30/38	-
14	PTY	U	503	-	-	15/33/33/53	-
18	WJP	R	905	-	-	12/37/37/40	-
14	PTY	0	305	-	-	6/16/16/53	-
14	PTY	U	504	-	-	10/27/27/53	-
14	PTY	2	201	-	-	11/30/30/53	-
13	WSS	0	304	-	-	8/32/32/57	-
16	CLR	V	403	-	-	0/10/68/68	0/4/4/4
13	WSS	0	301	-	-	12/44/44/57	-
14	PTY	6	201	-	-	11/22/22/53	-
13	WSS	1	201	-	-	3/37/37/57	-
13	WSS	U	501	-	-	15/47/47/57	-
16	CLR	R	901	-	-	6/10/68/68	0/4/4/4
14	PTY	0	306	-	1/1/4/4	34/51/51/53	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	905	WJP	P31-O34	5.27	1.74	1.54
15	3	202	WJS	P25-O24	4.43	1.76	1.59
18	R	905	WJP	P27-O26	4.07	1.75	1.59
18	R	905	WJP	C15-C16	3.22	1.40	1.33
18	R	905	WJP	C10-C11	3.14	1.40	1.33

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	3	202	WJS	O28-C29-C30	6.17	113.44	108.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	905	WJP	C12-C11-C13	5.29	124.42	115.23
18	R	905	WJP	C04-C05-C06	-4.98	116.23	127.62
18	R	905	WJP	C17-C16-C18	4.08	122.31	115.23
13	U	501	WSS	O2-C31-C32	4.05	120.25	111.48

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	0	306	PTY	C6
14	R	903	PTY	C6

5 of 362 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	0	301	WSS	C5-C4-O4P-P
13	0	301	WSS	C1-O3P-P-O2P
13	0	301	WSS	C1-O3P-P-O4P
13	0	301	WSS	C4-O4P-P-O2P
13	0	301	WSS	C4-O4P-P-O3P

There are no ring outliers.

20 monomers are involved in 84 short contacts:

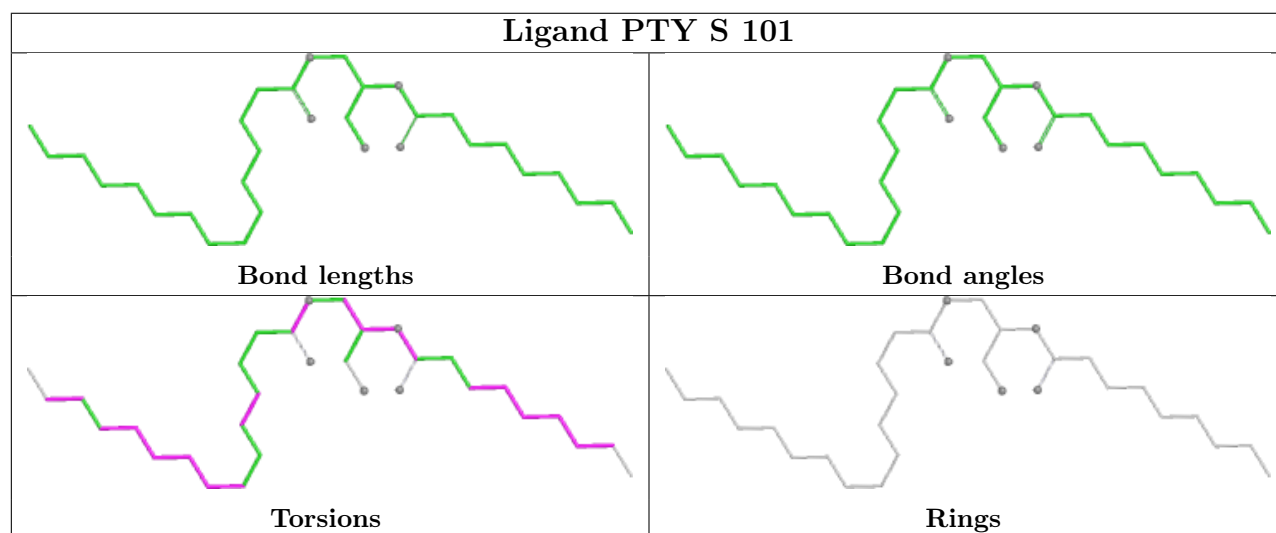
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	U	502	WSS	3	0
14	8	201	PTY	7	0
14	5	202	PTY	7	0
16	5	201	CLR	16	0
14	6	202	PTY	6	0
13	R	904	WSS	6	0
14	8	202	PTY	4	0
14	R	903	PTY	1	0
14	V	404	PTY	9	0
15	3	202	WJS	5	0
14	U	503	PTY	6	0
18	R	905	WJP	1	0
14	0	305	PTY	1	0
14	U	504	PTY	17	0
14	2	201	PTY	4	0
13	0	304	WSS	1	0
16	V	403	CLR	12	0
14	6	201	PTY	7	0

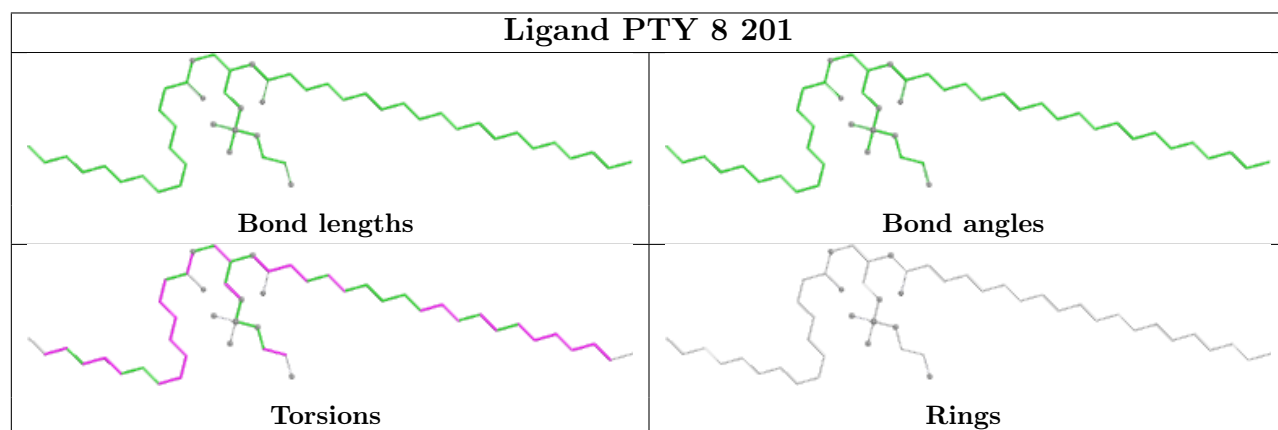
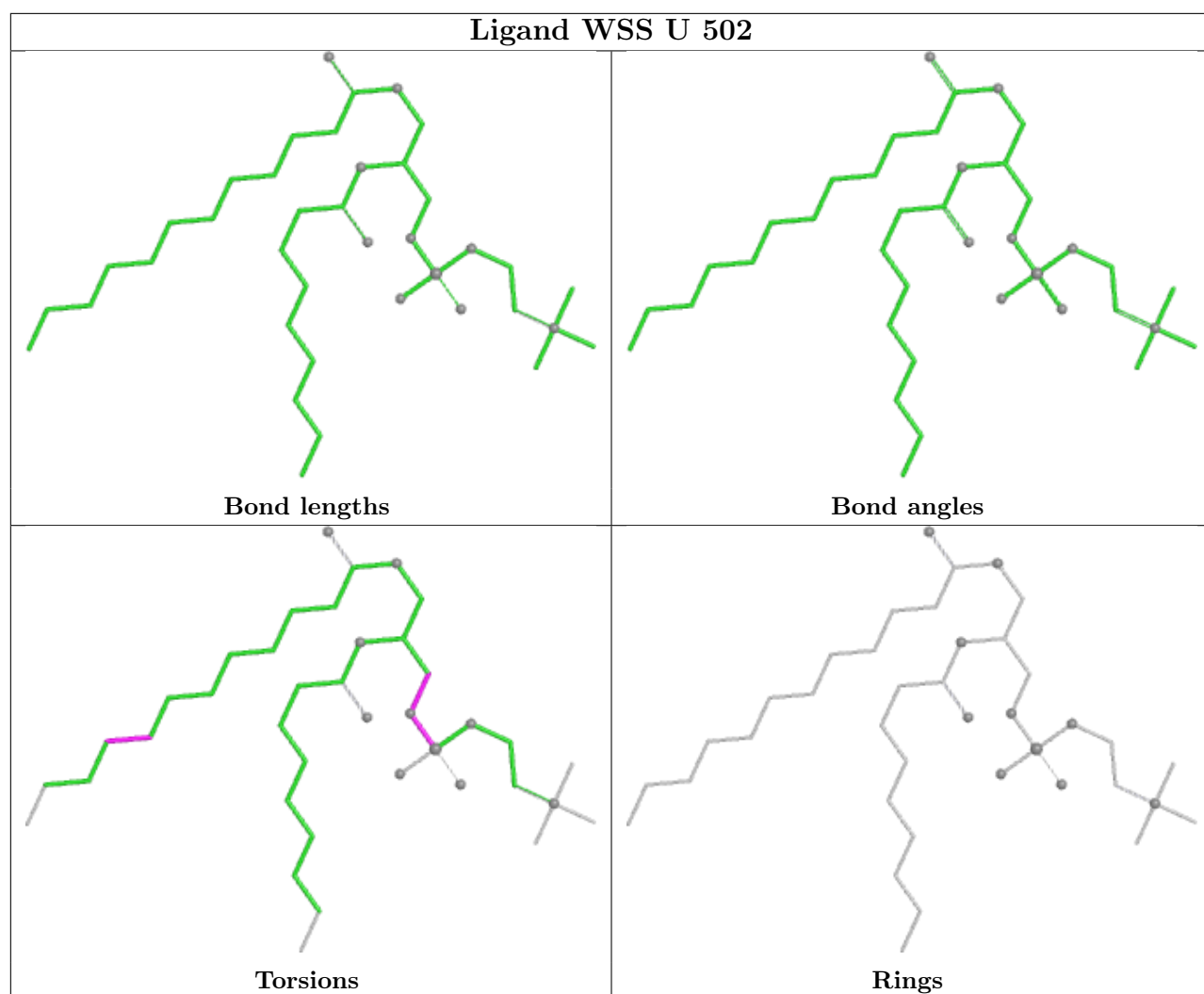
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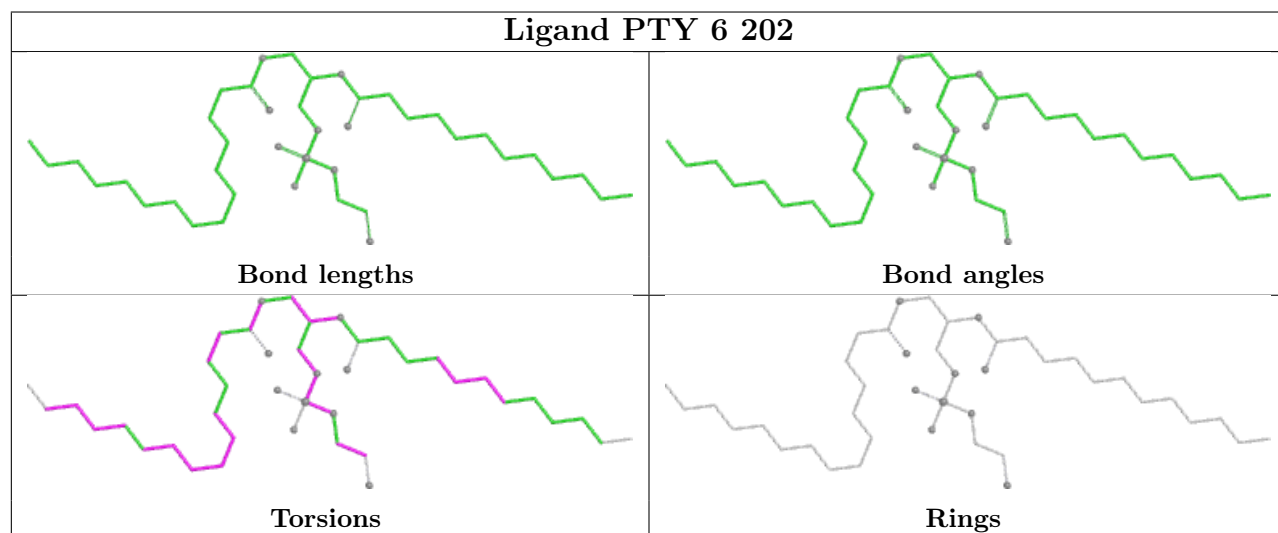
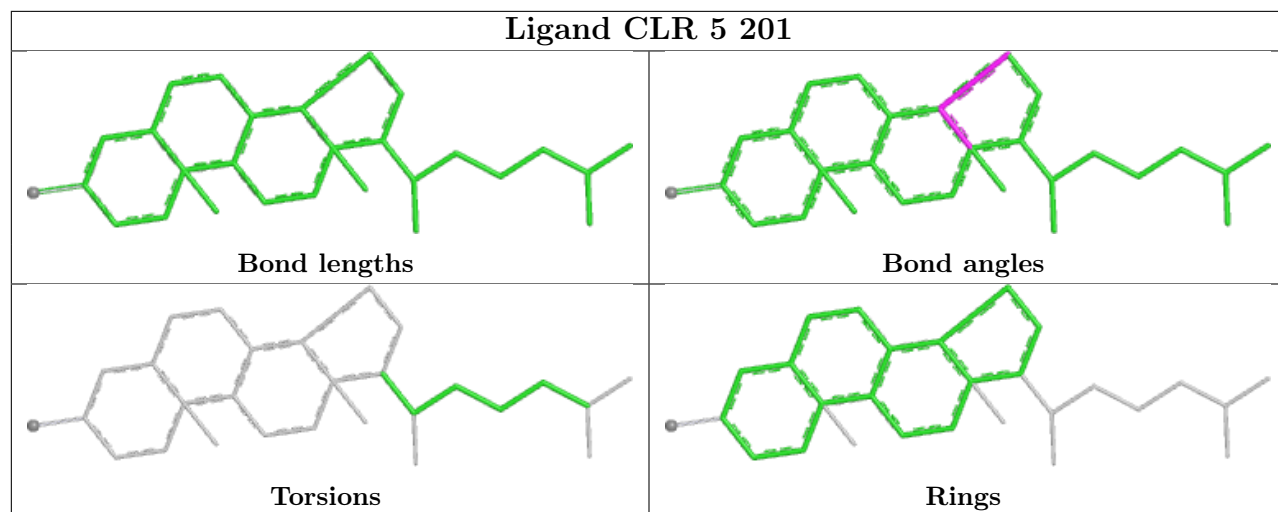
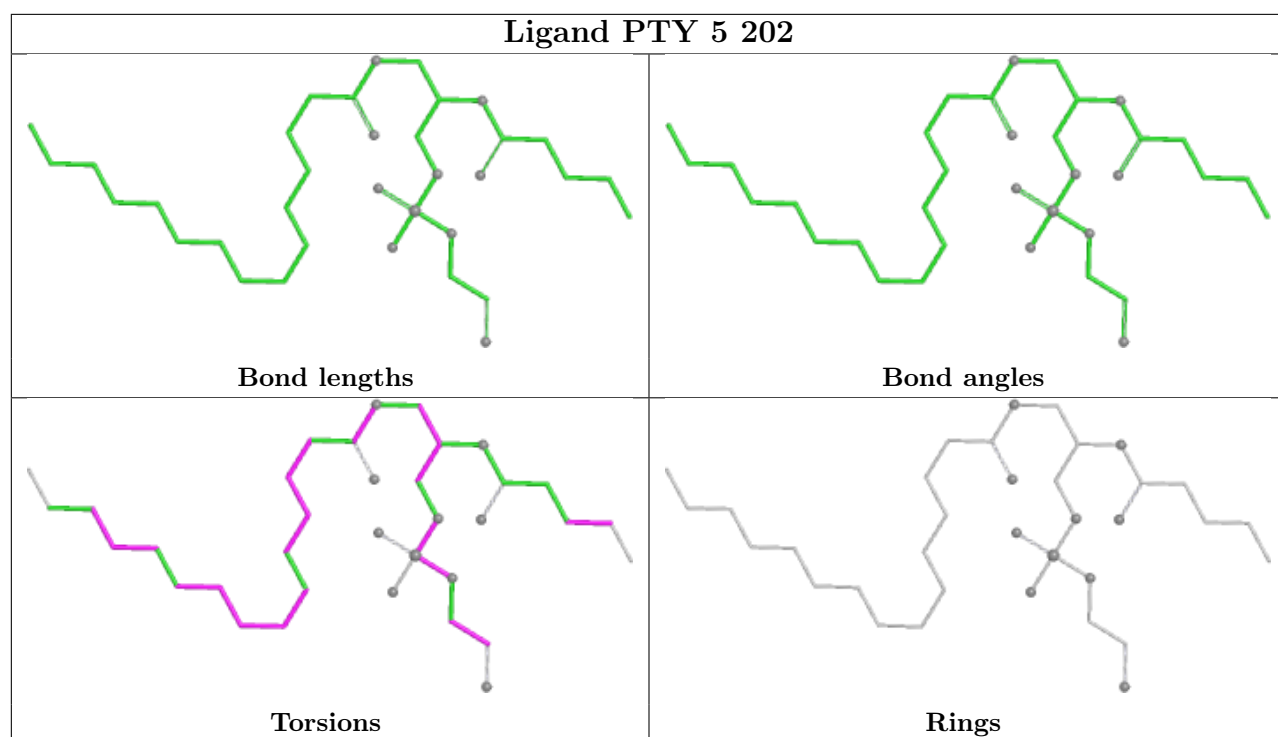
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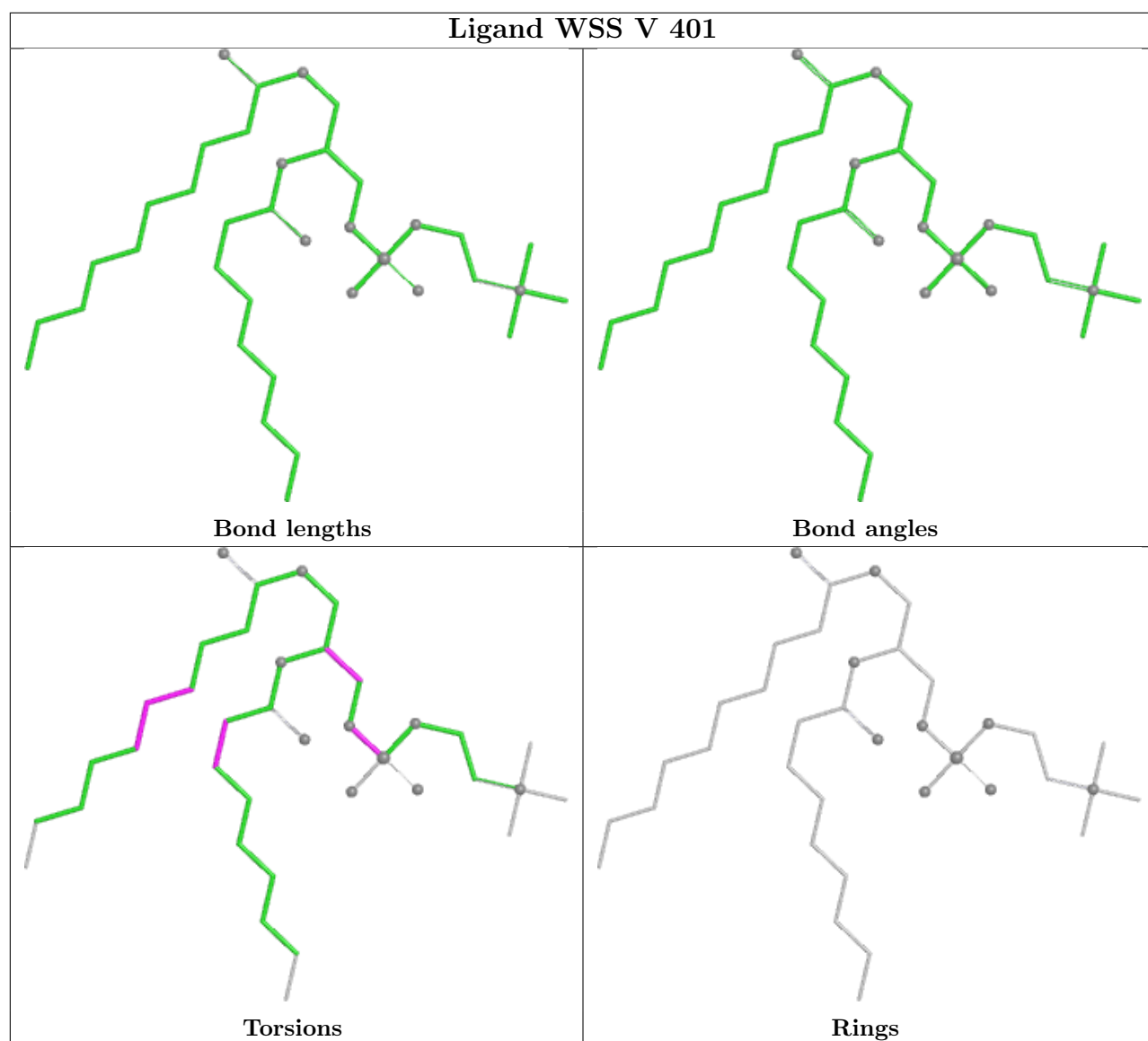
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	R	901	CLR	2	0
14	0	306	PTY	3	0

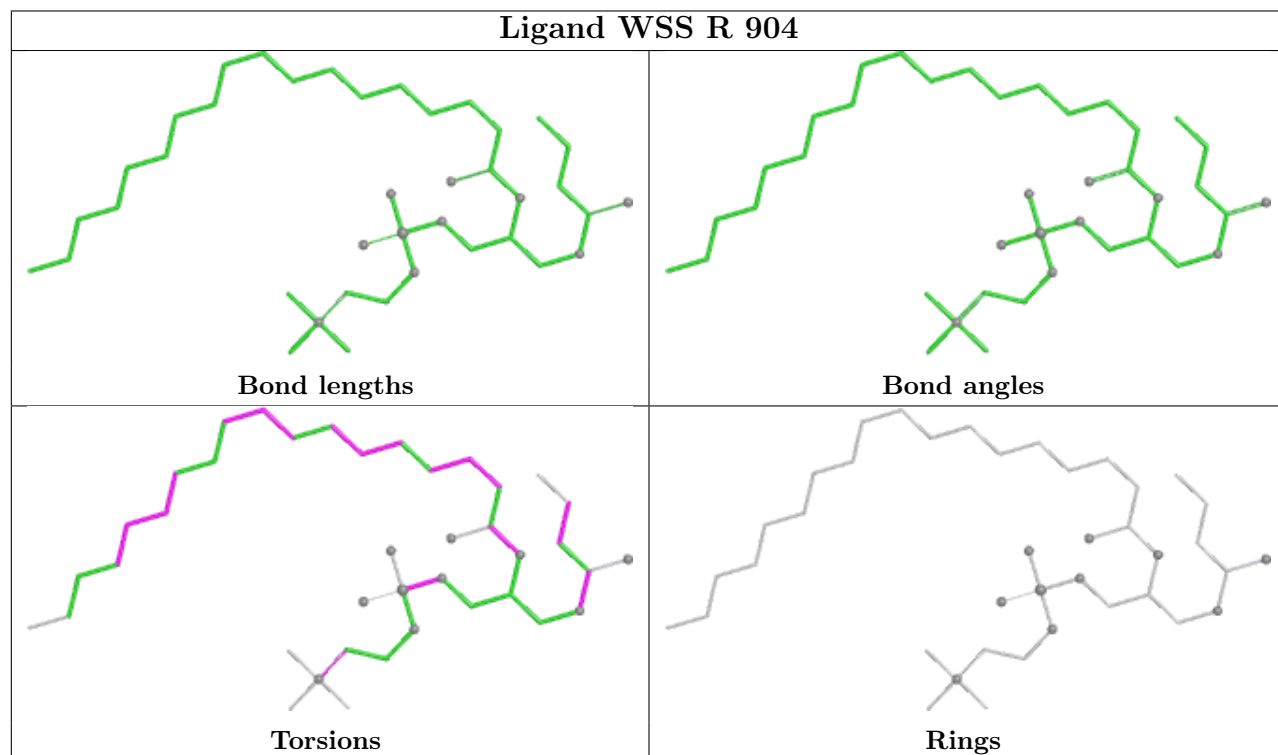
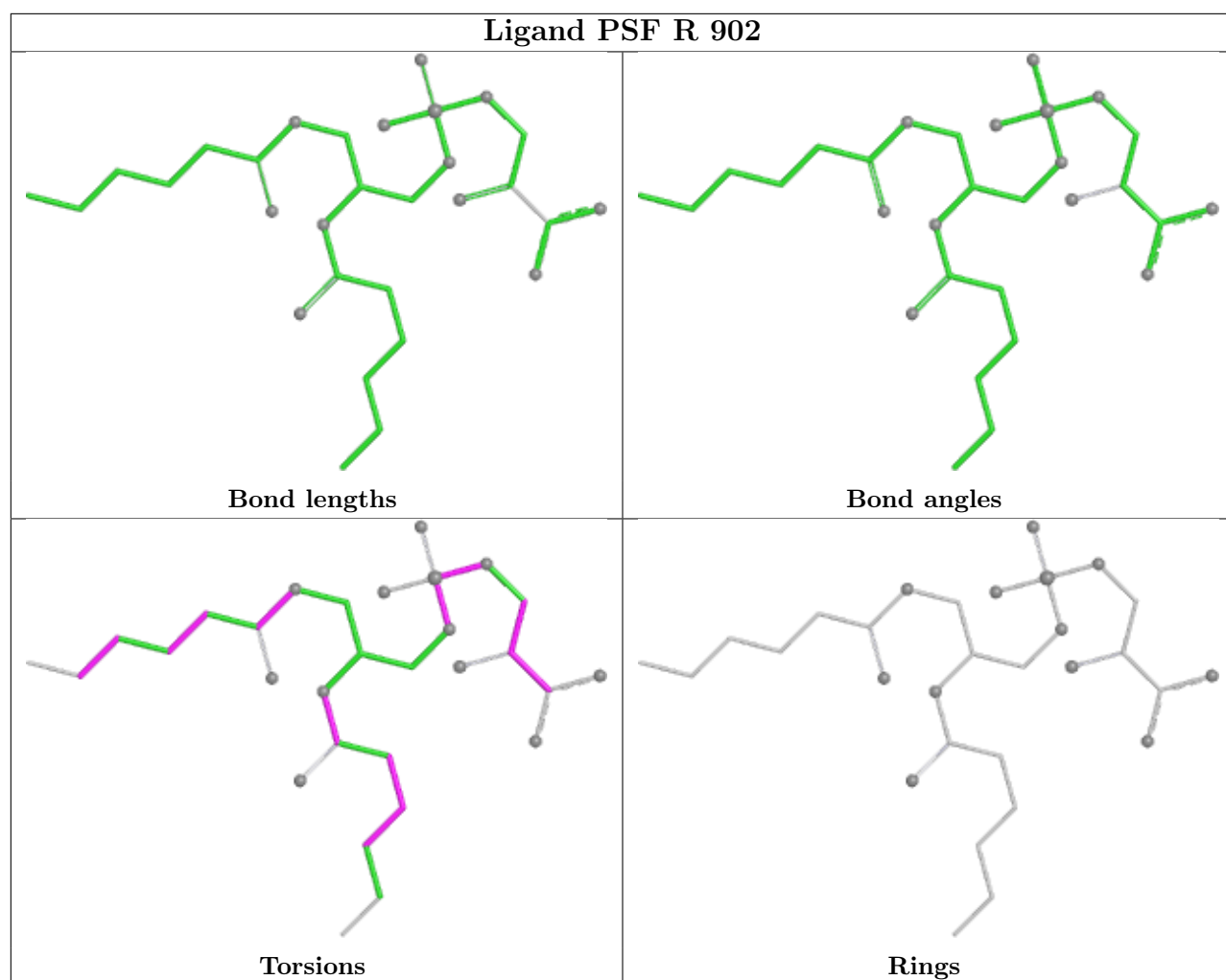
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

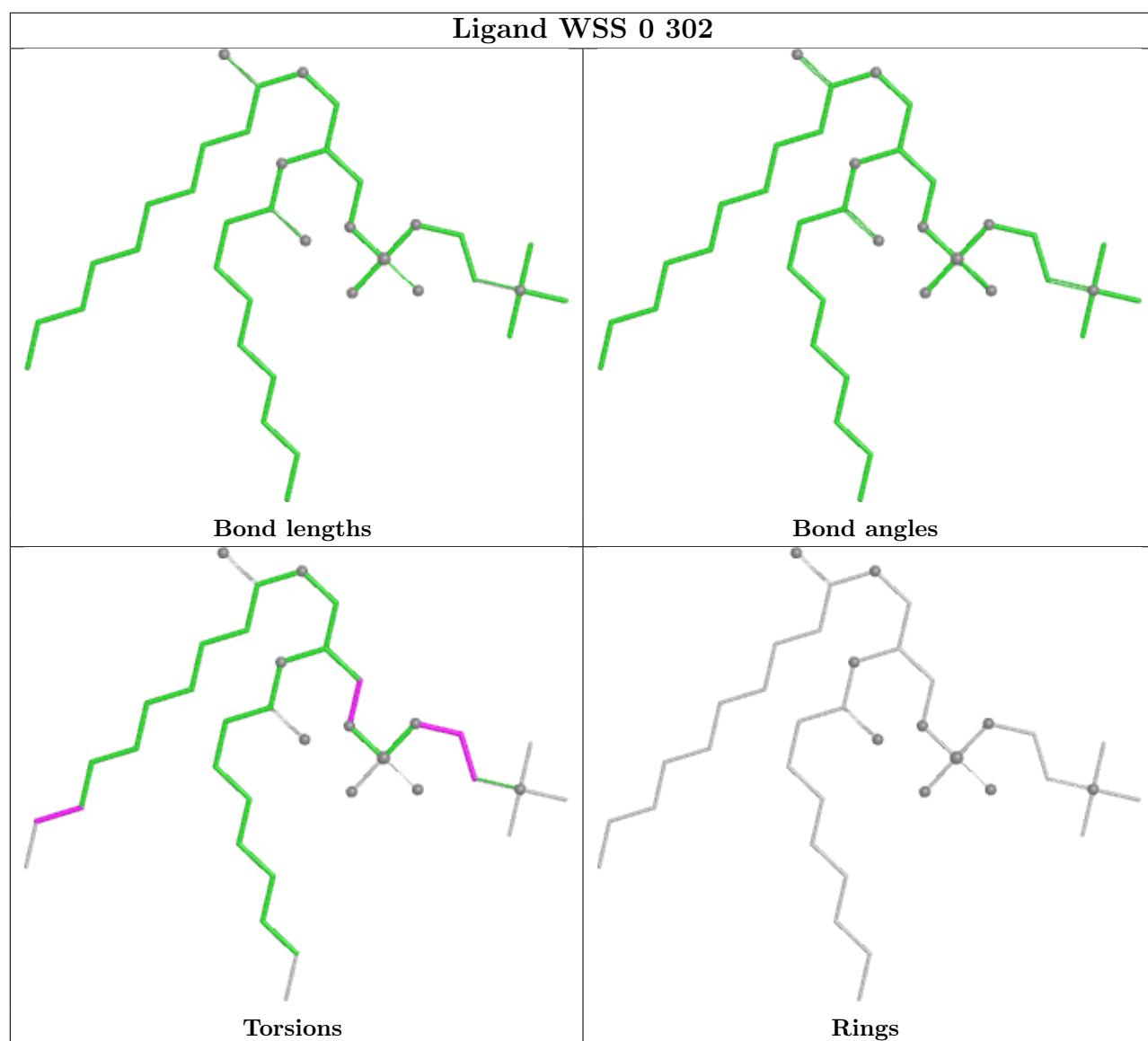


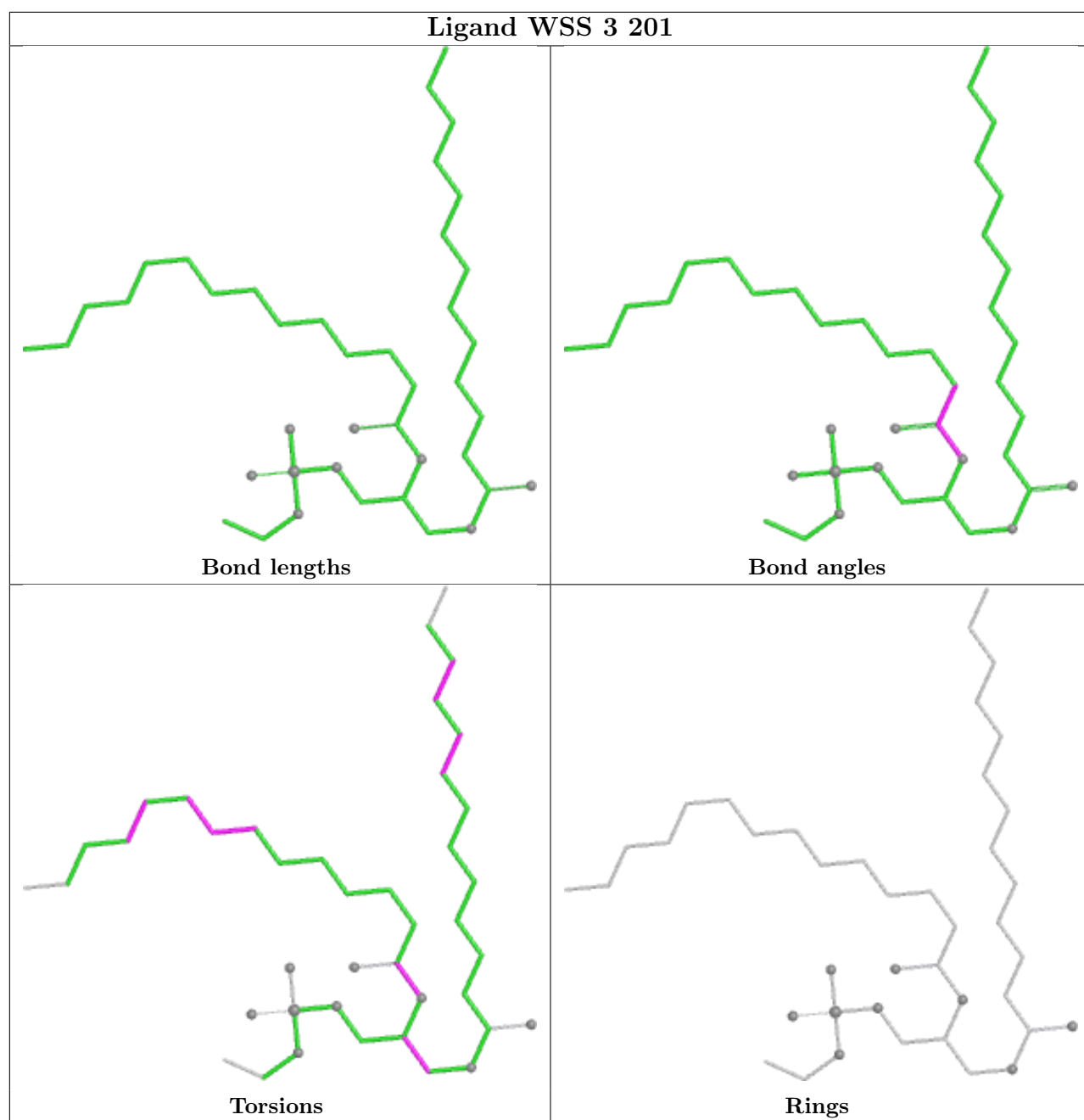


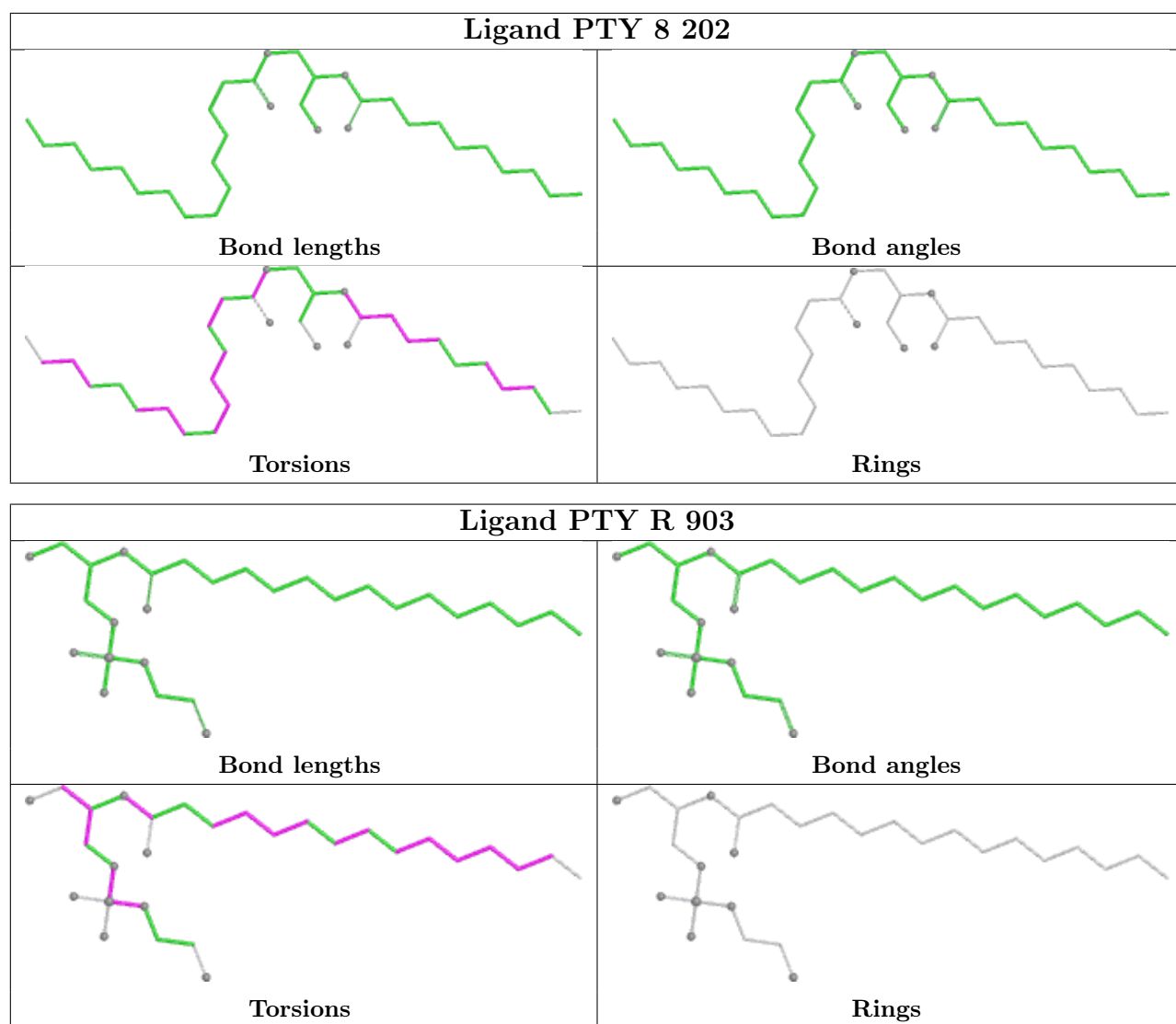


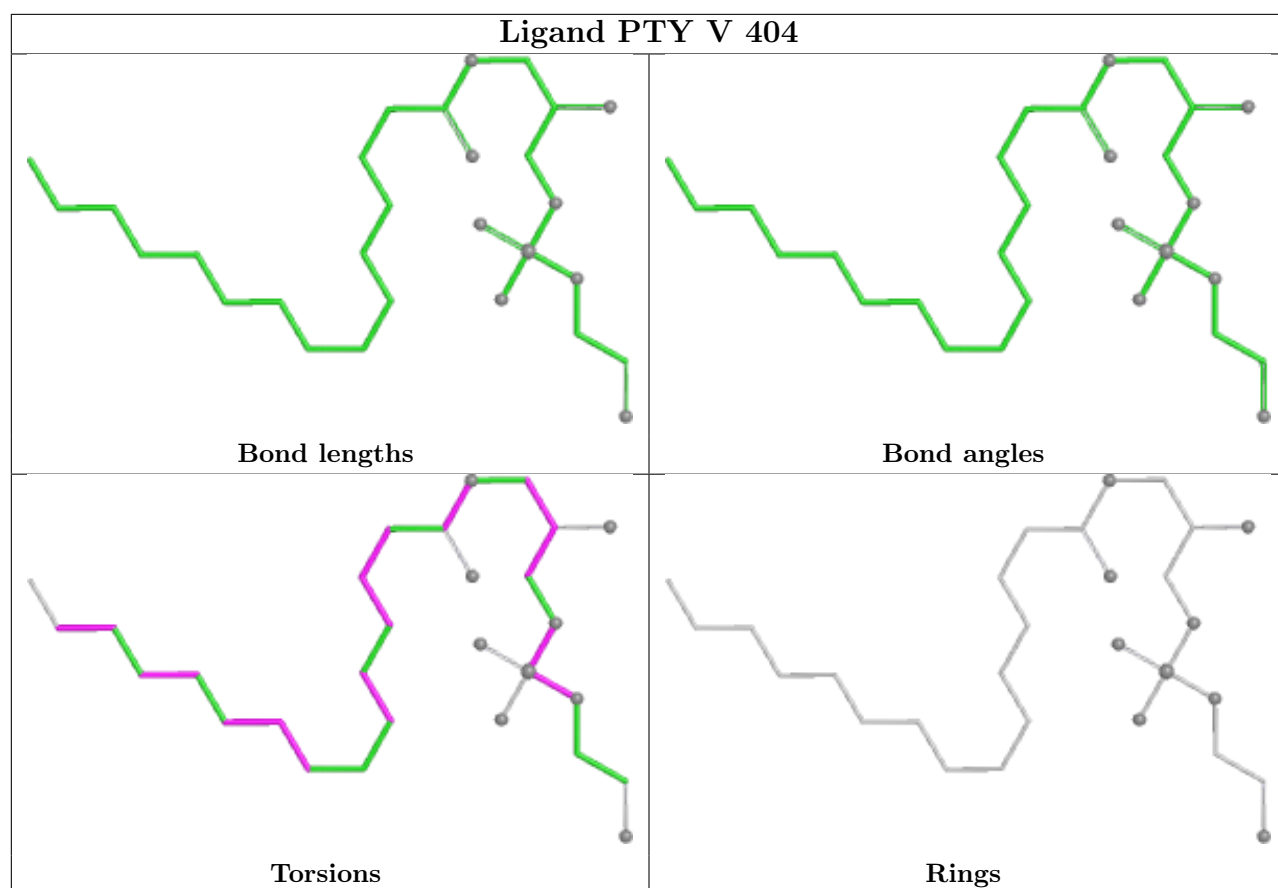


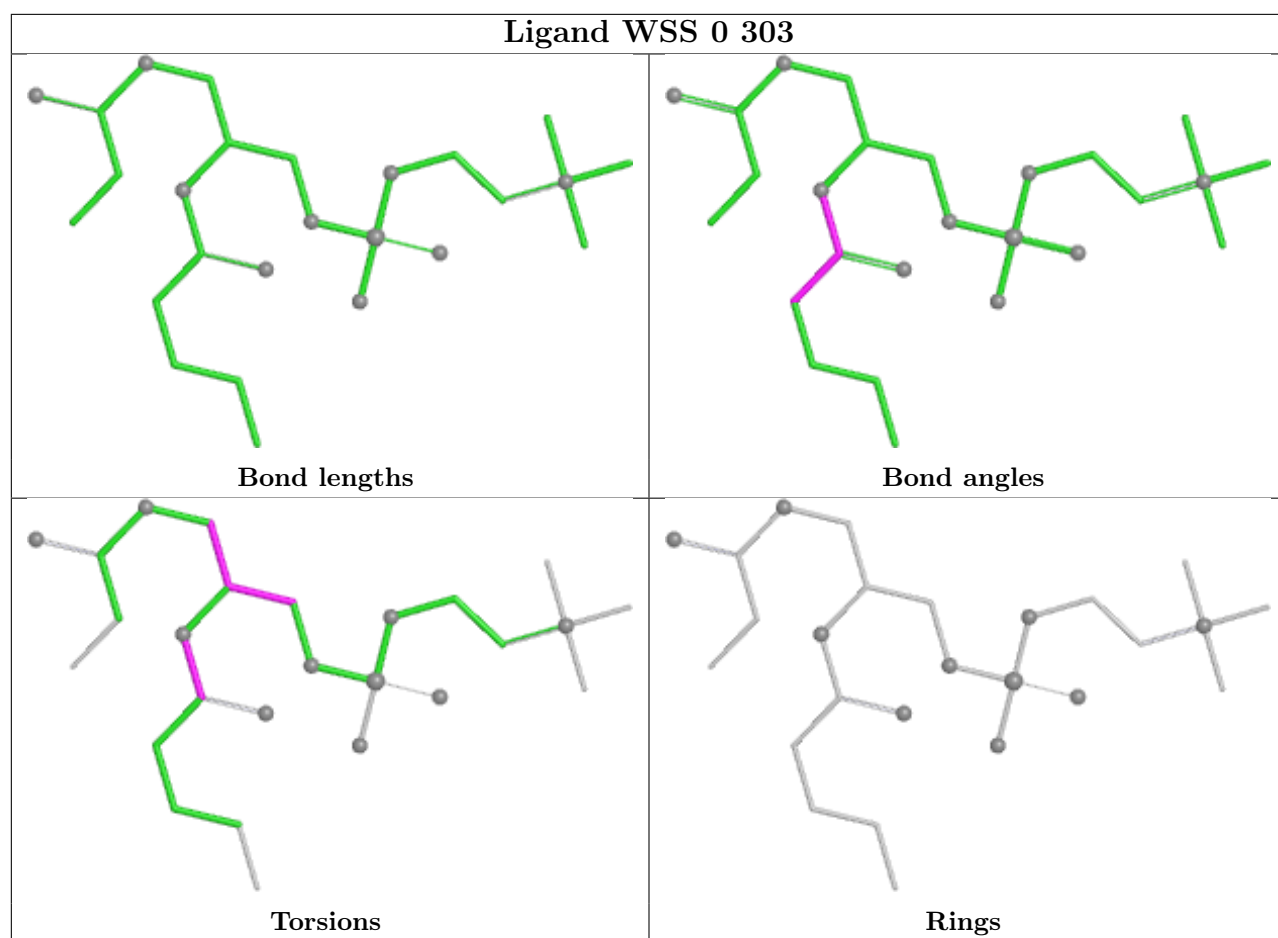


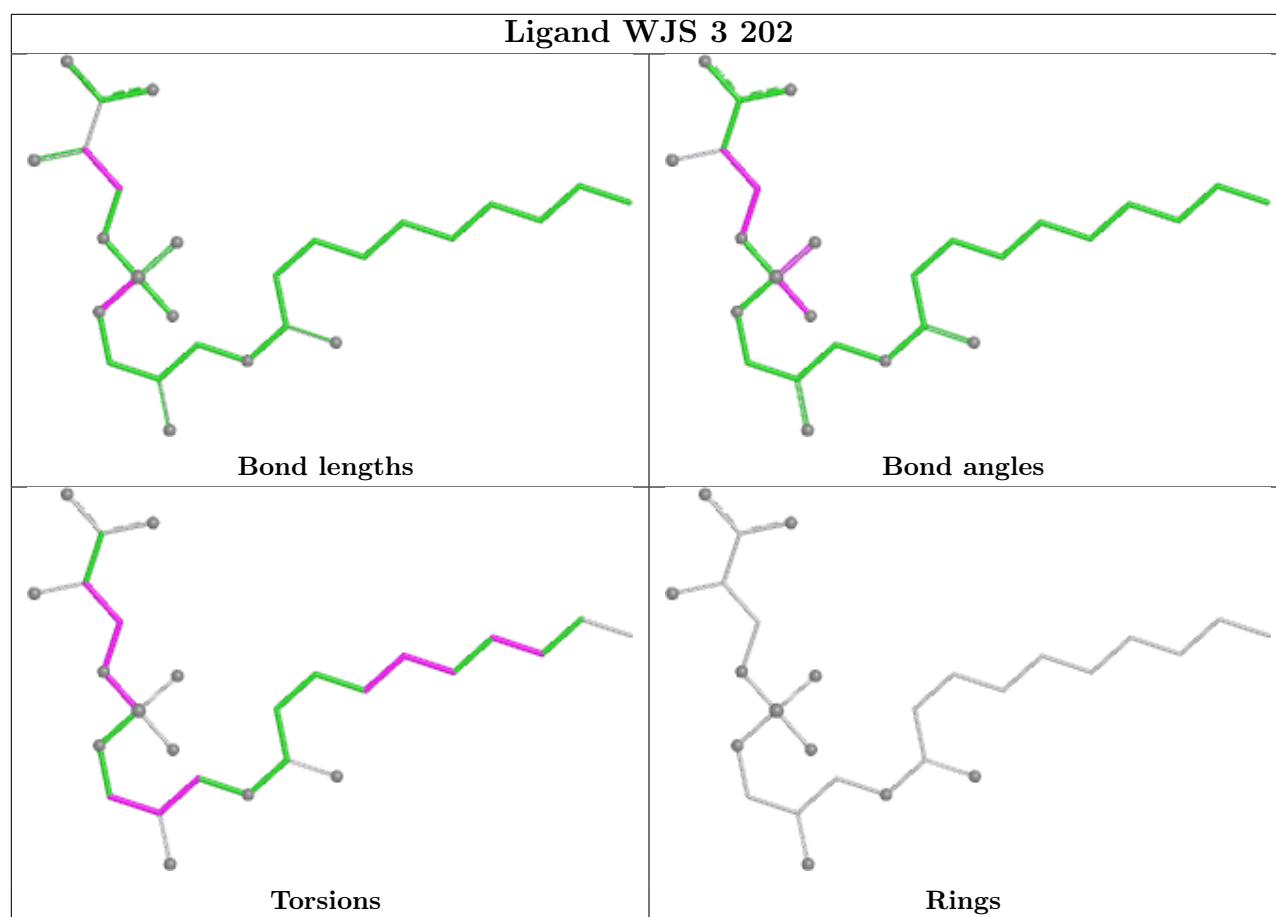


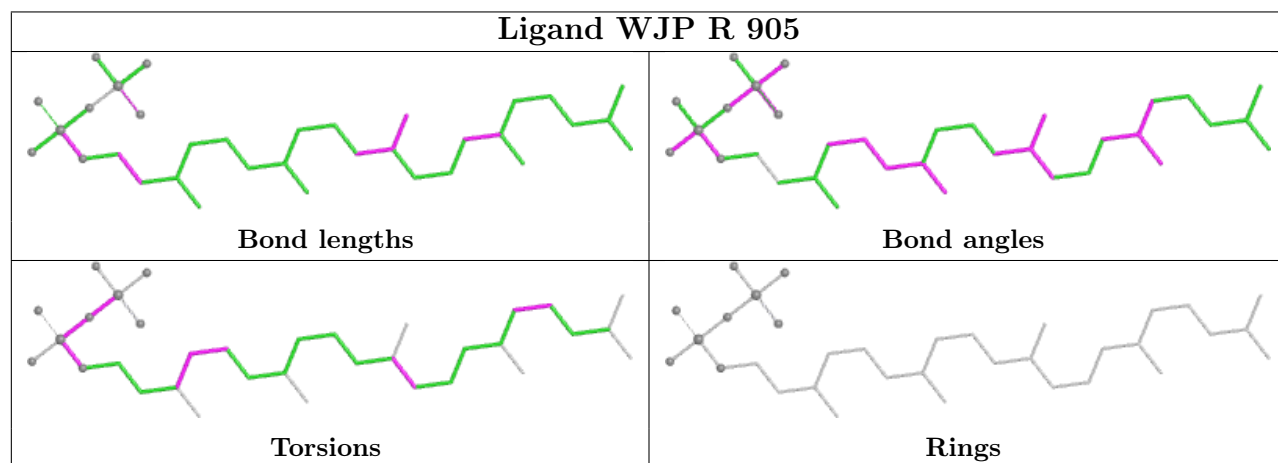
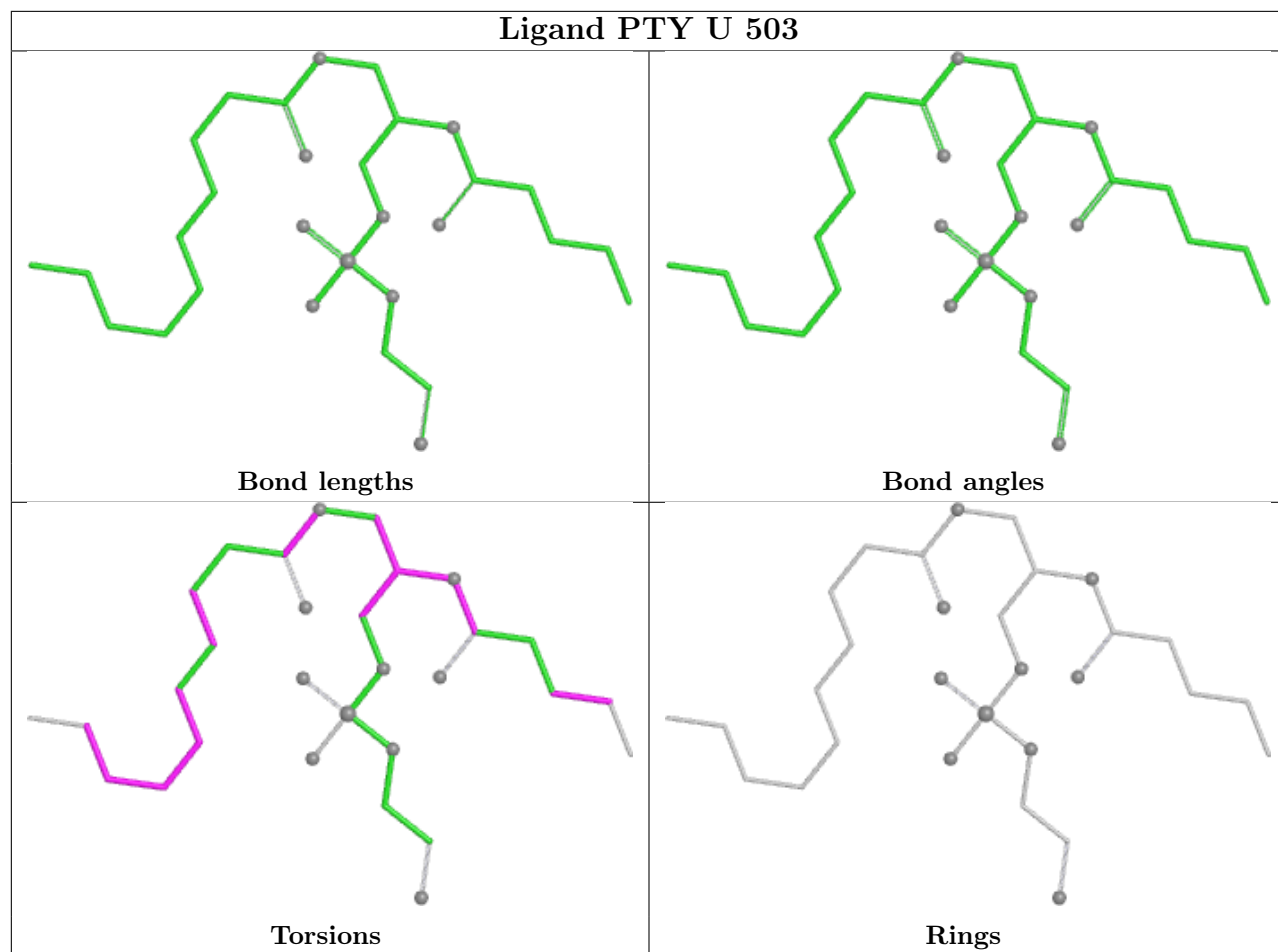


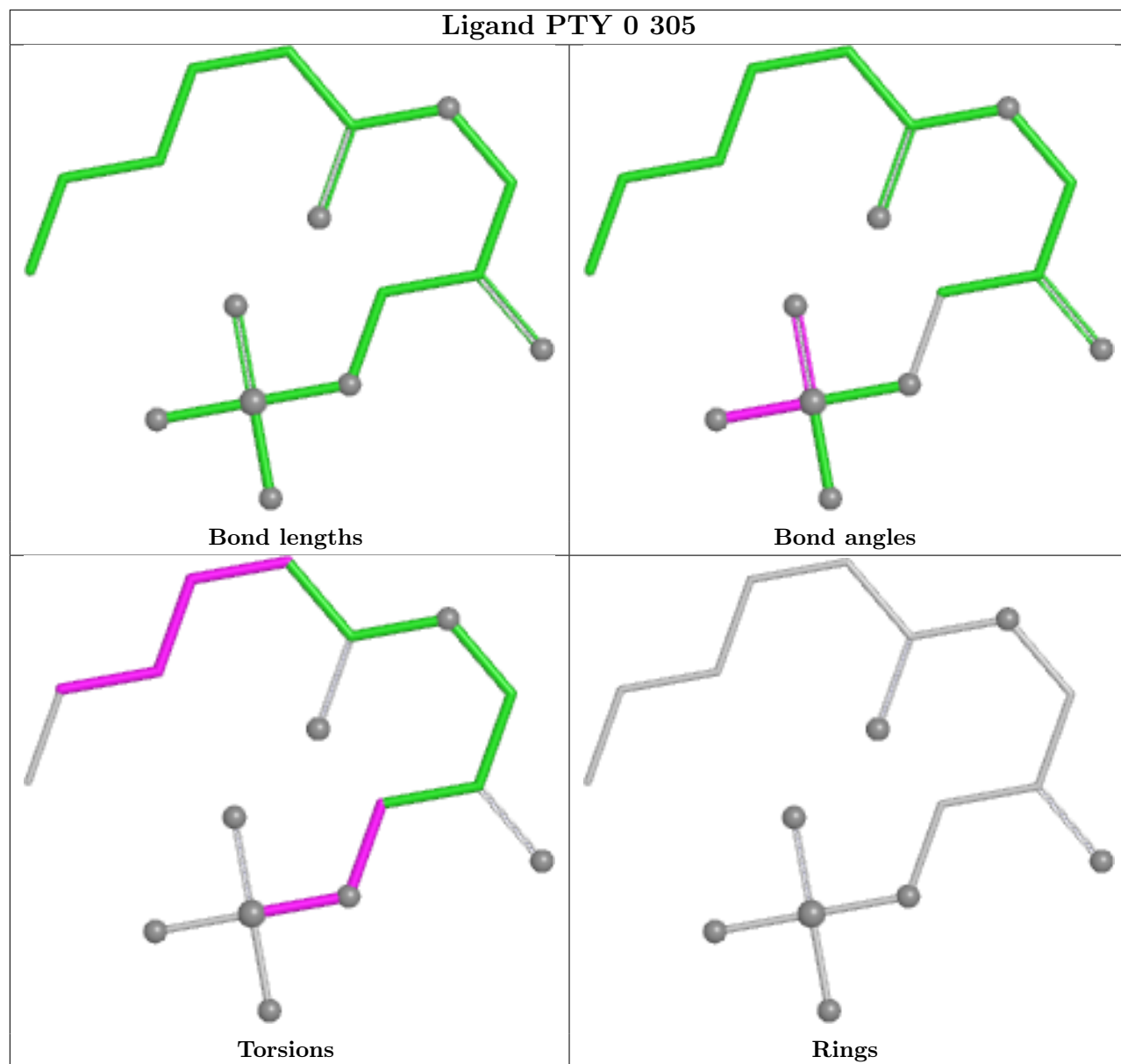


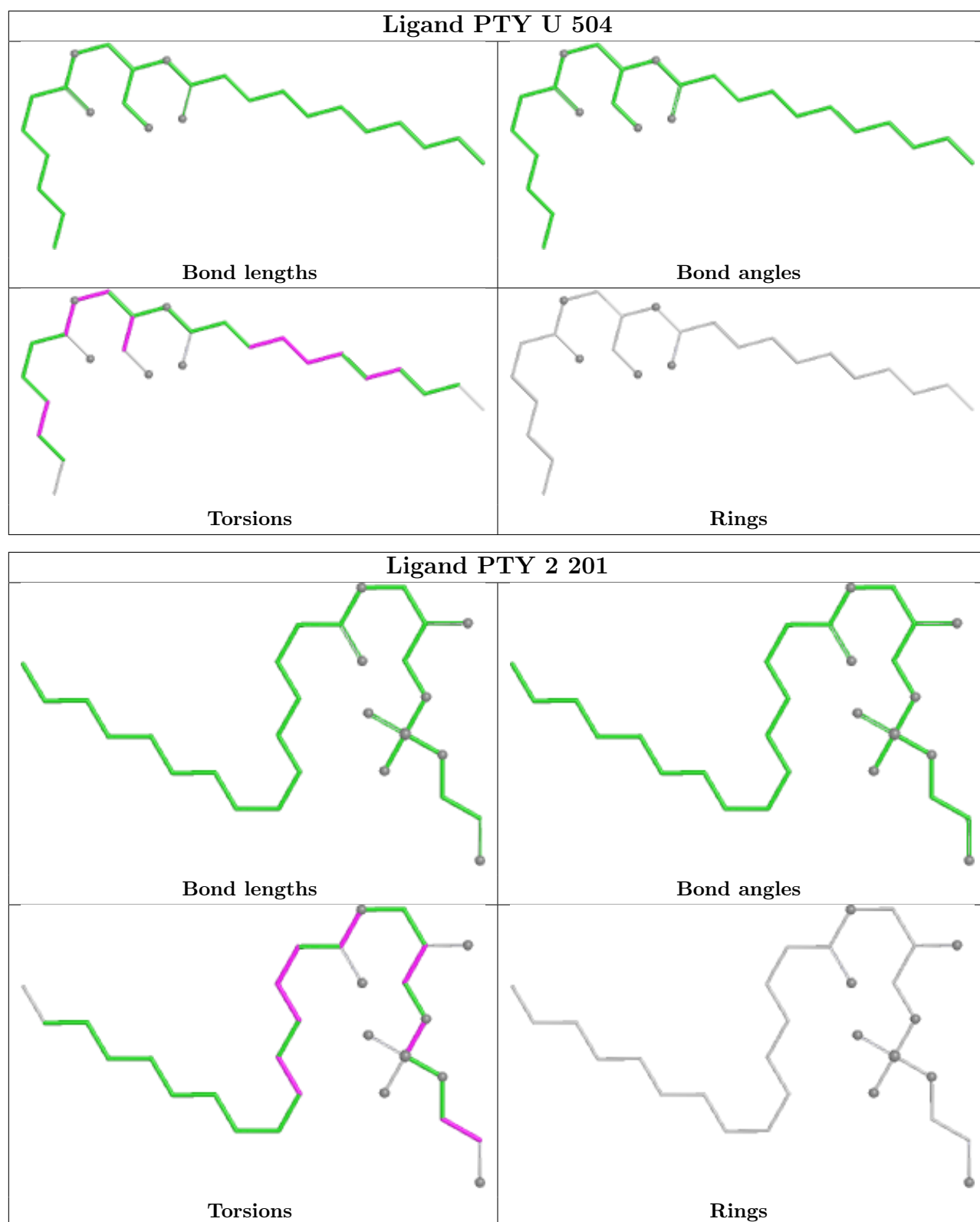


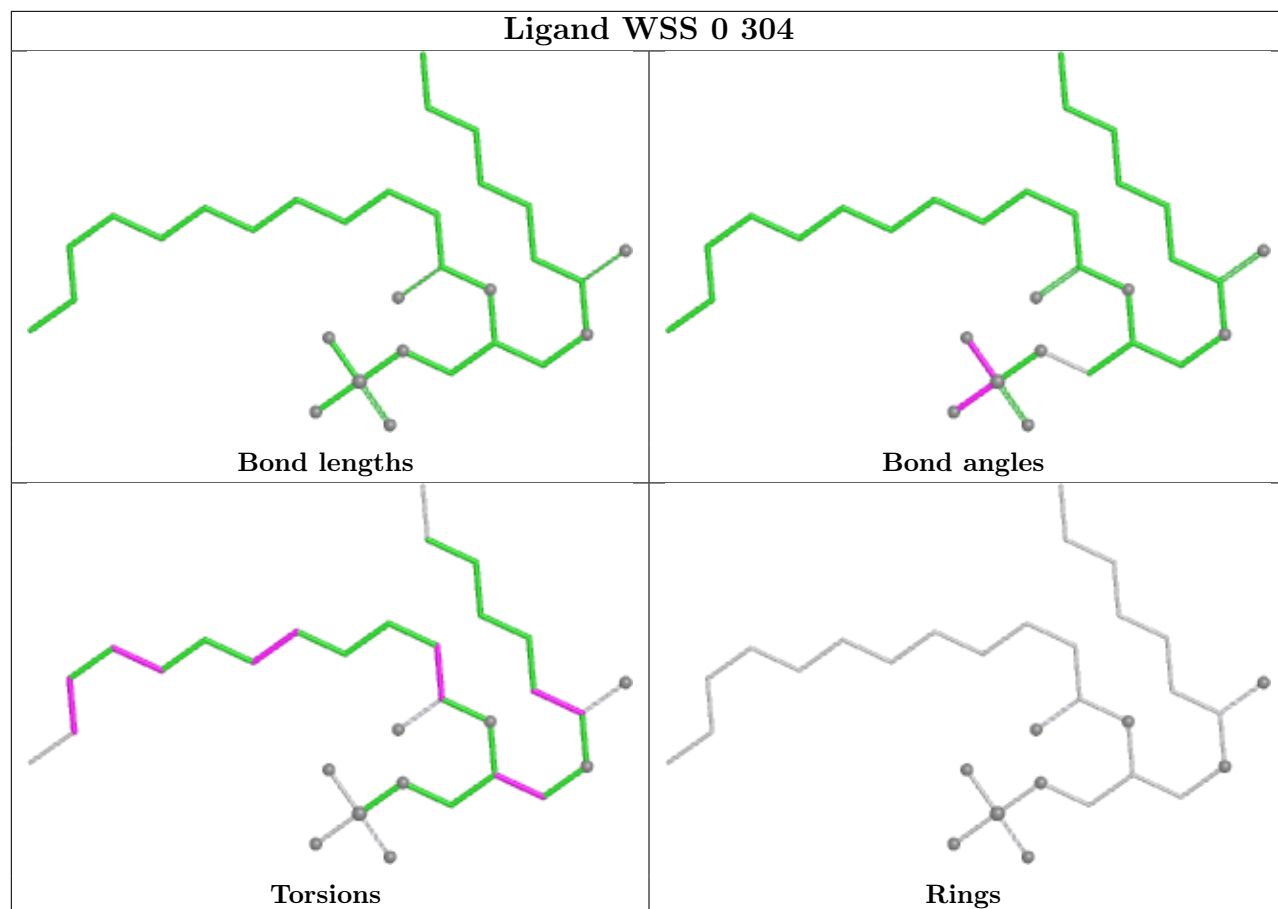


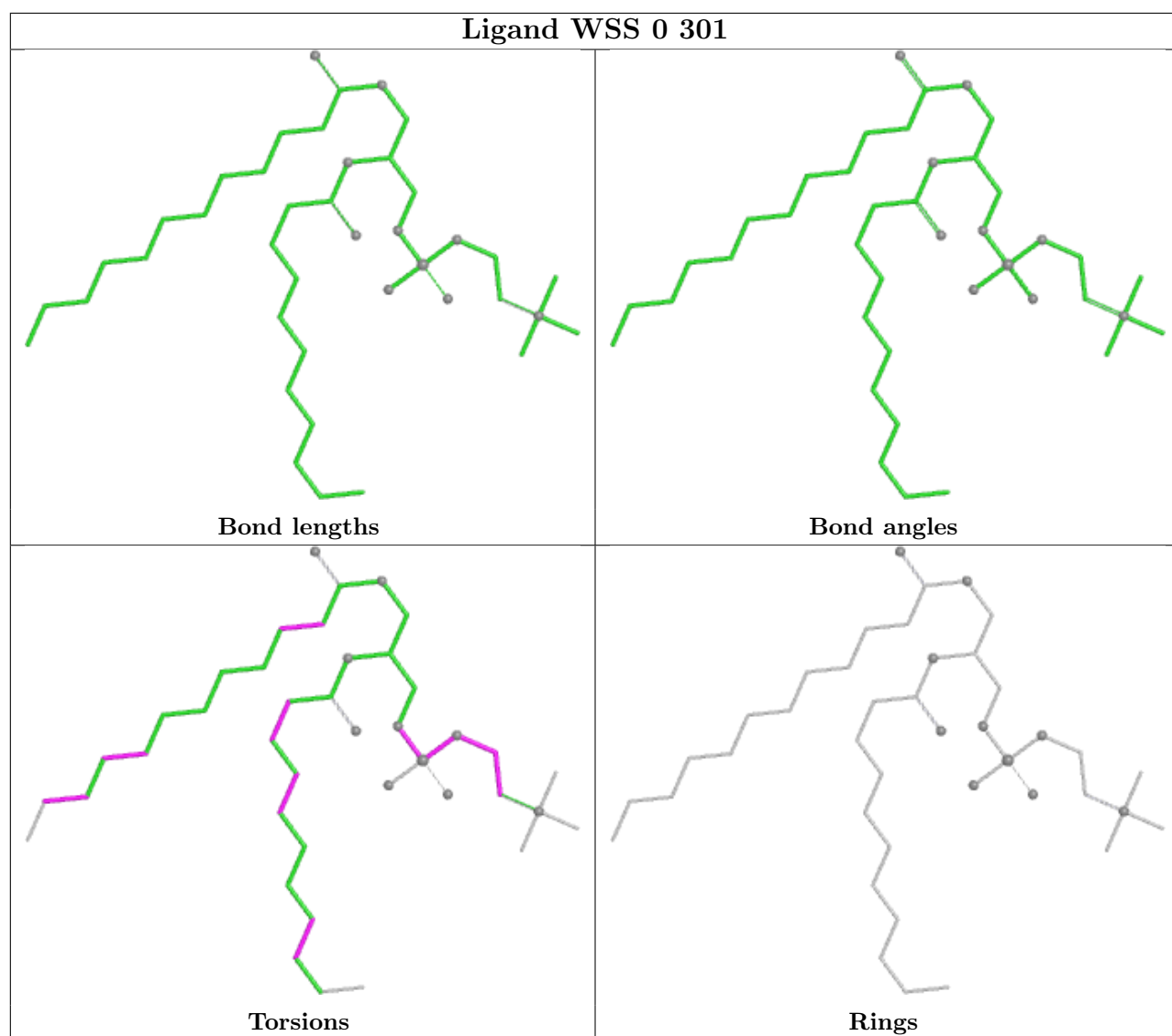




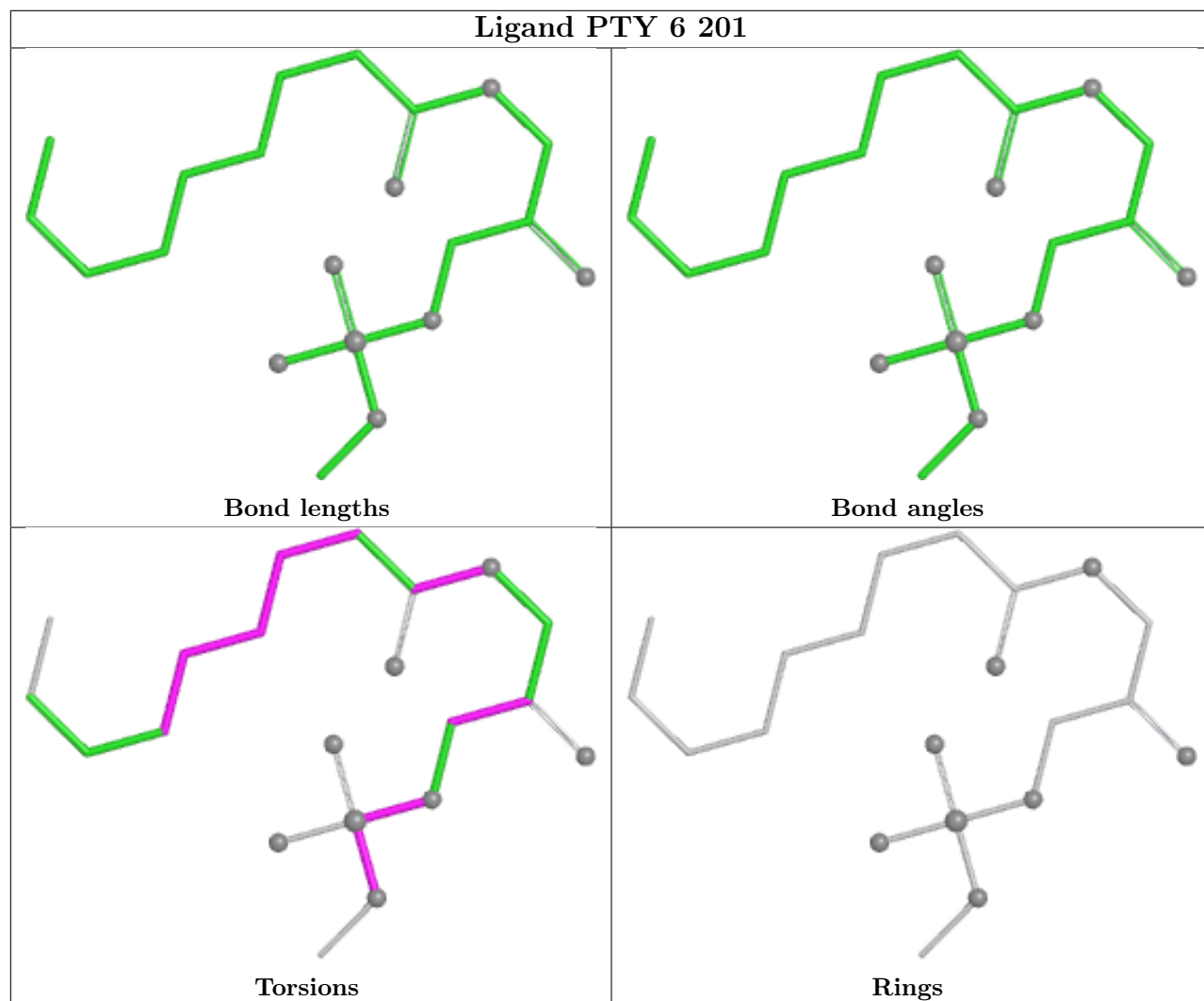


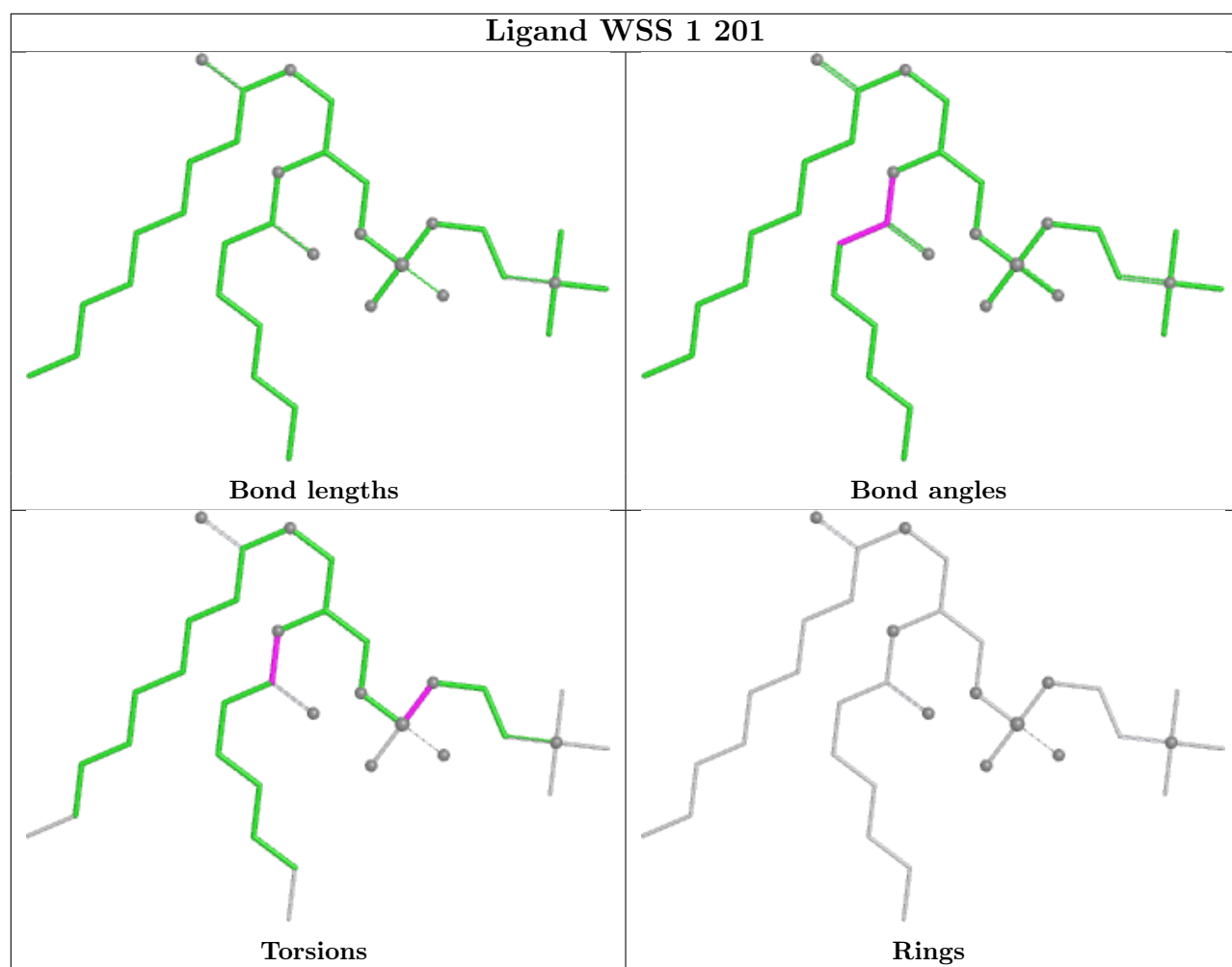


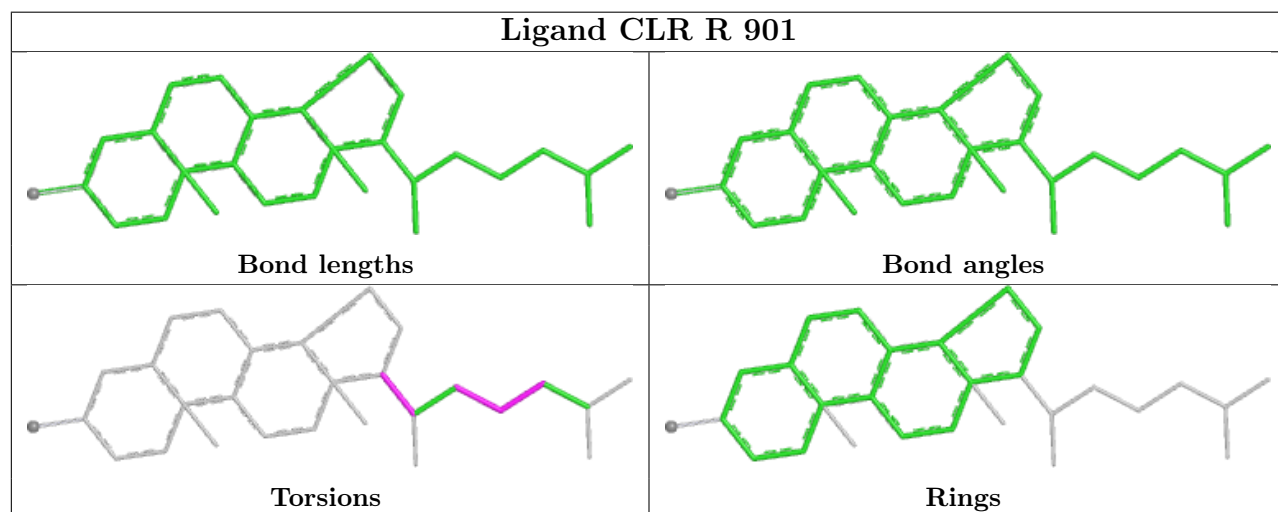
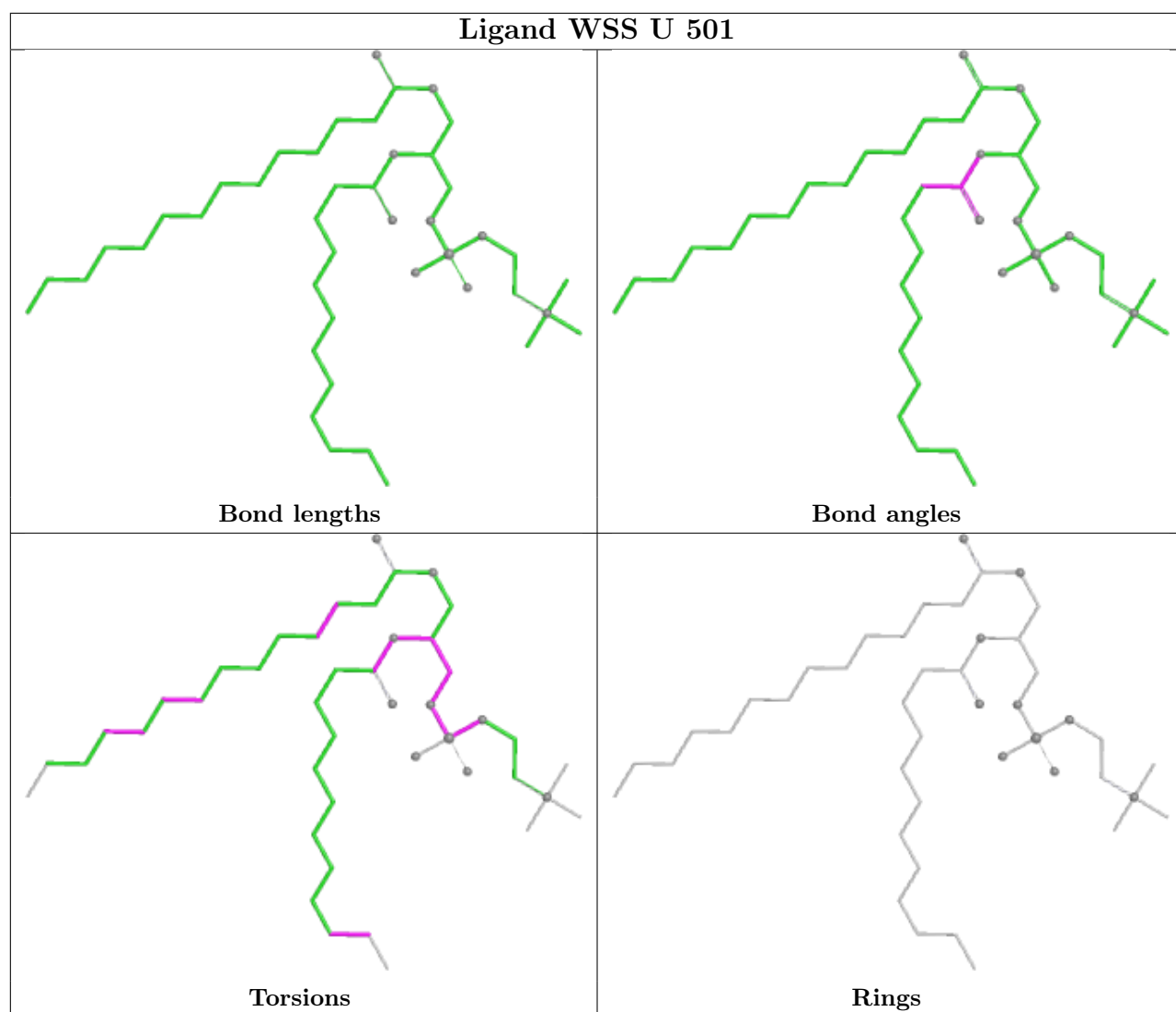


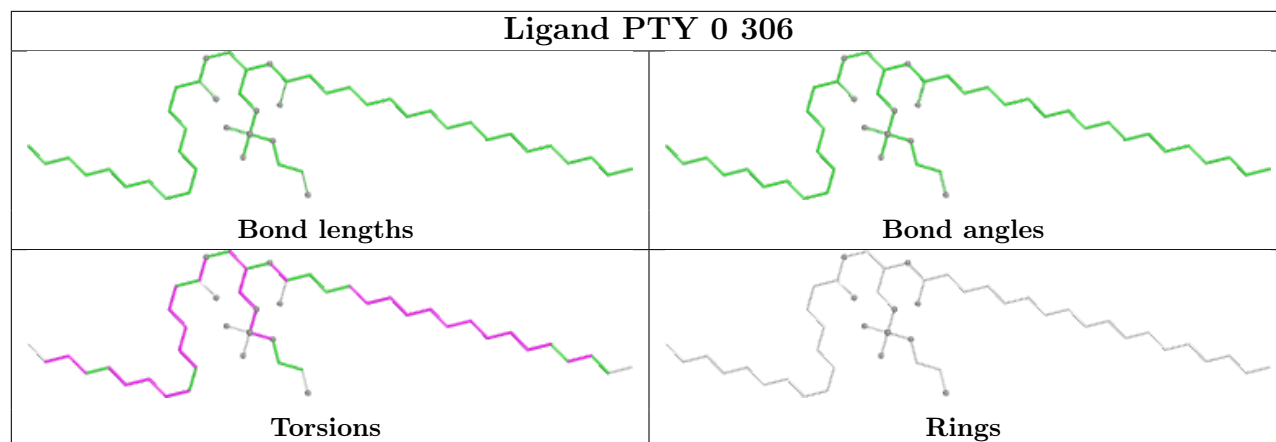


Ligand PTY 6 201









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.

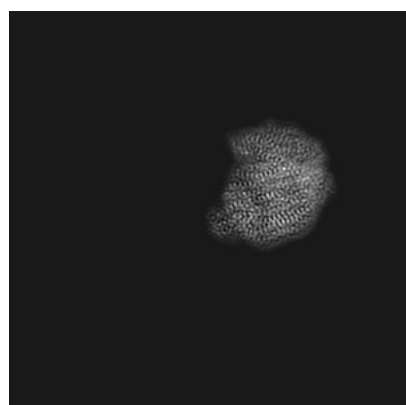
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21844. These allow visual inspection of the internal detail of the map and identification of artifacts.

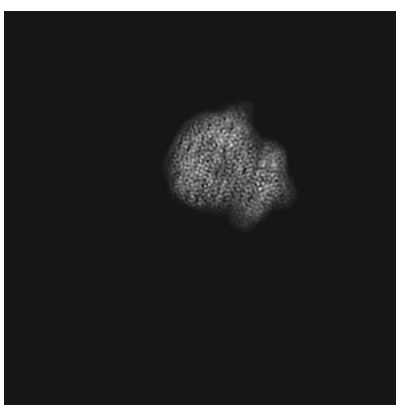
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

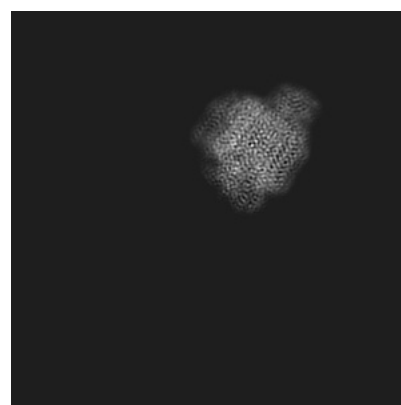
6.1.1 Primary map



X



Y

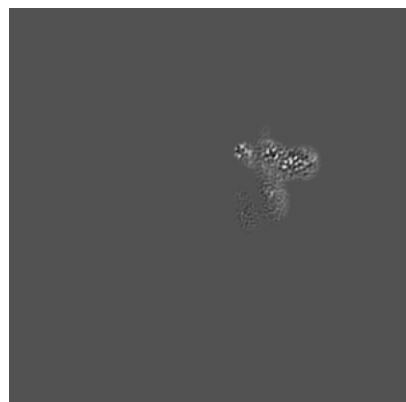


Z

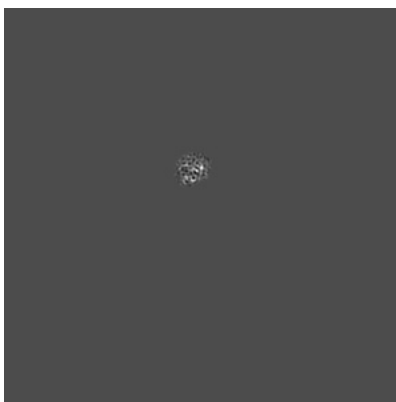
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

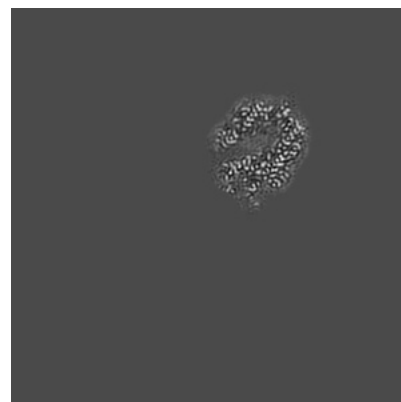
6.2.1 Primary map



X Index: 180



Y Index: 180

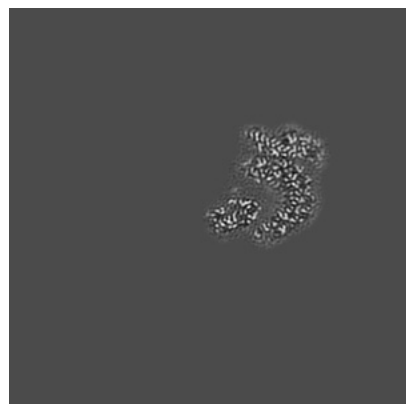


Z Index: 180

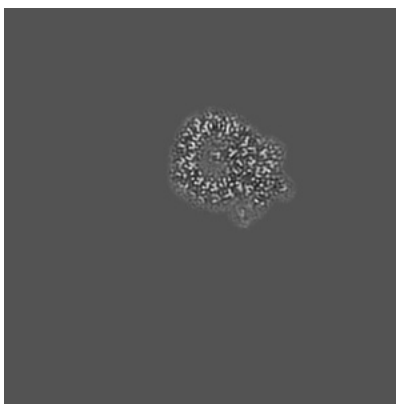
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

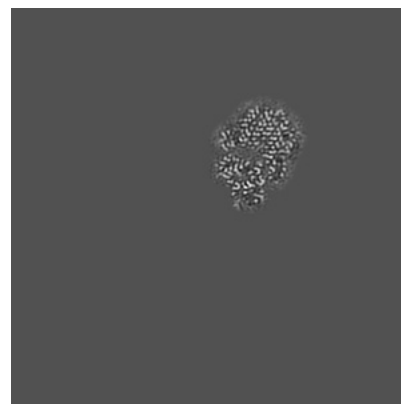
6.3.1 Primary map



X Index: 212



Y Index: 242

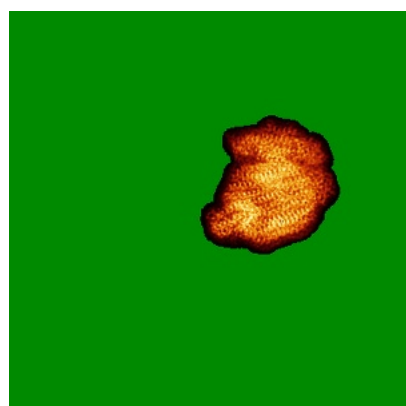


Z Index: 170

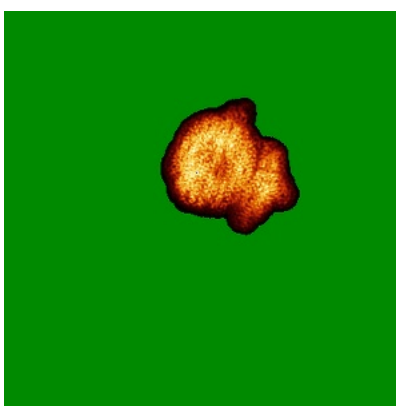
The images above show the largest variance slices of the map in three orthogonal directions.

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

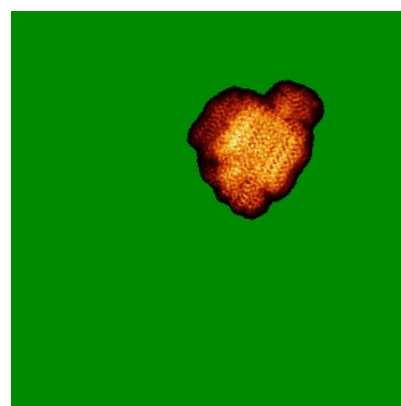
6.4.1 Primary map



X



Y

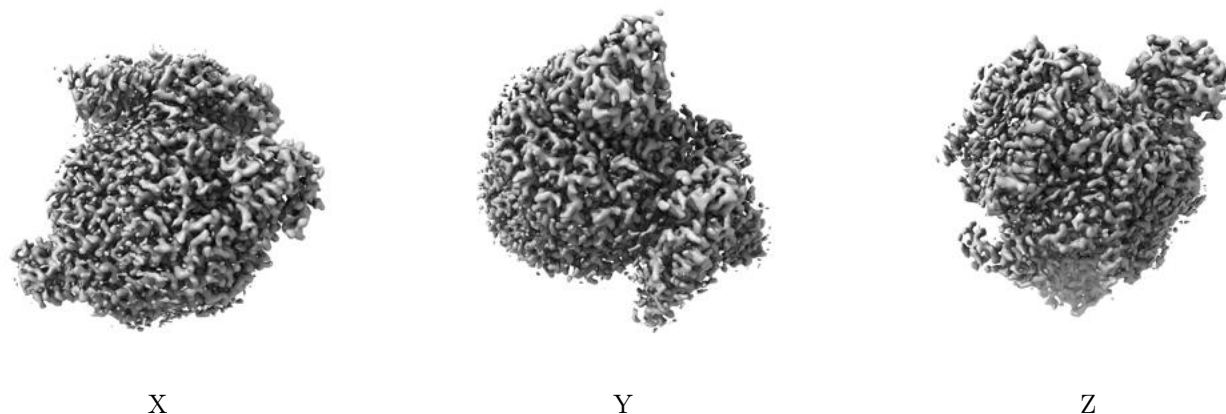


Z

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 0.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

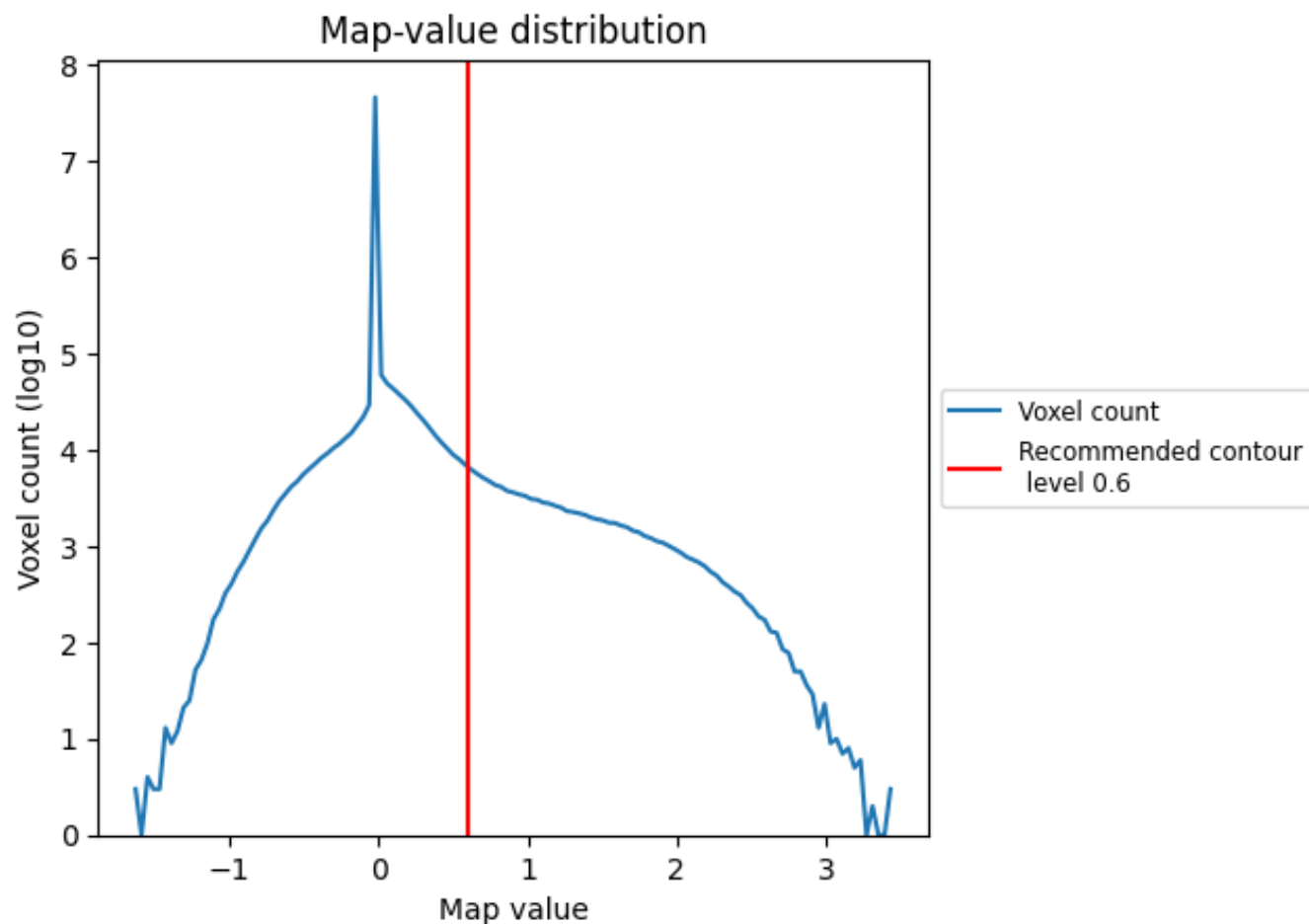
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

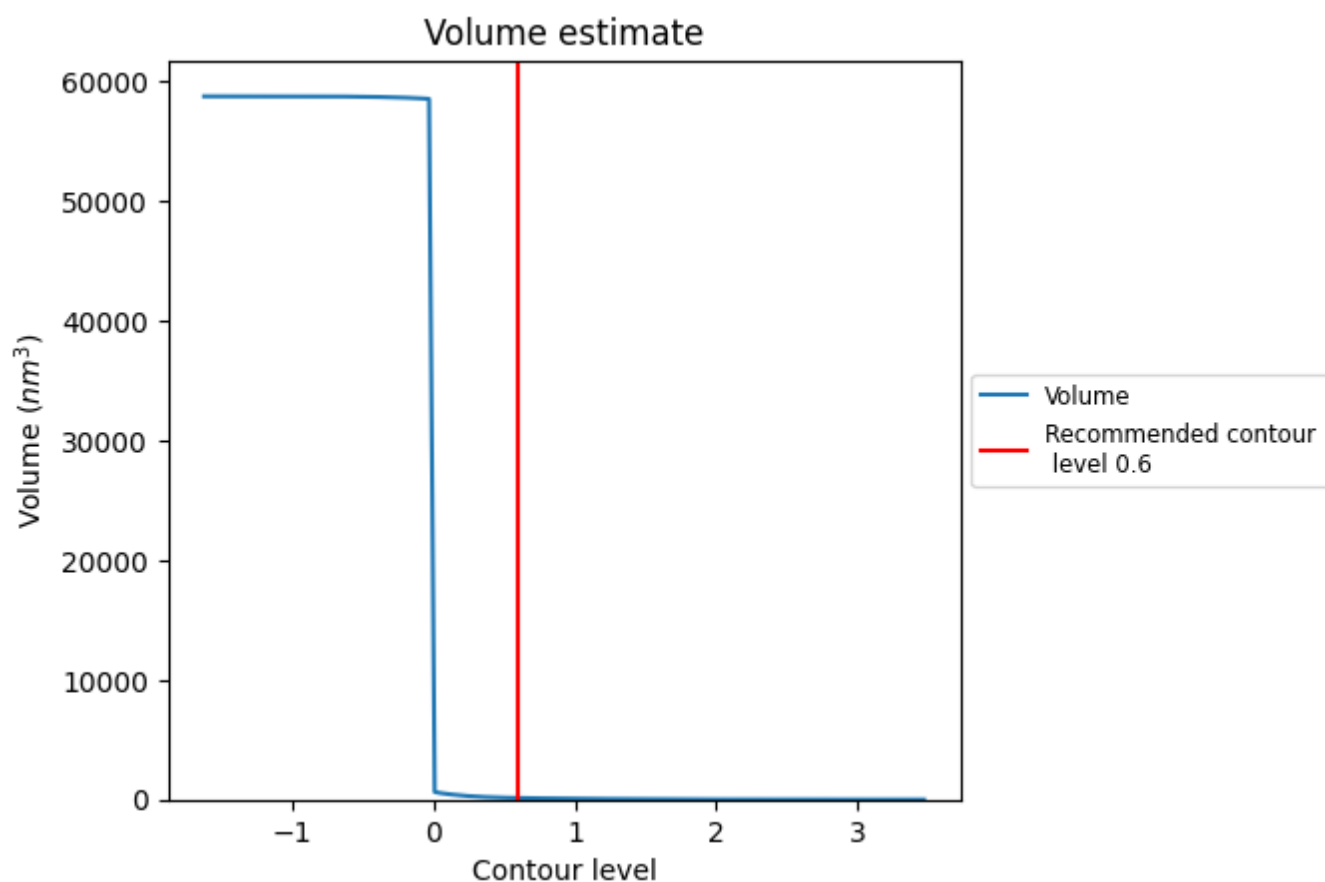
This section contains the results of statistical analysis of the map.

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.

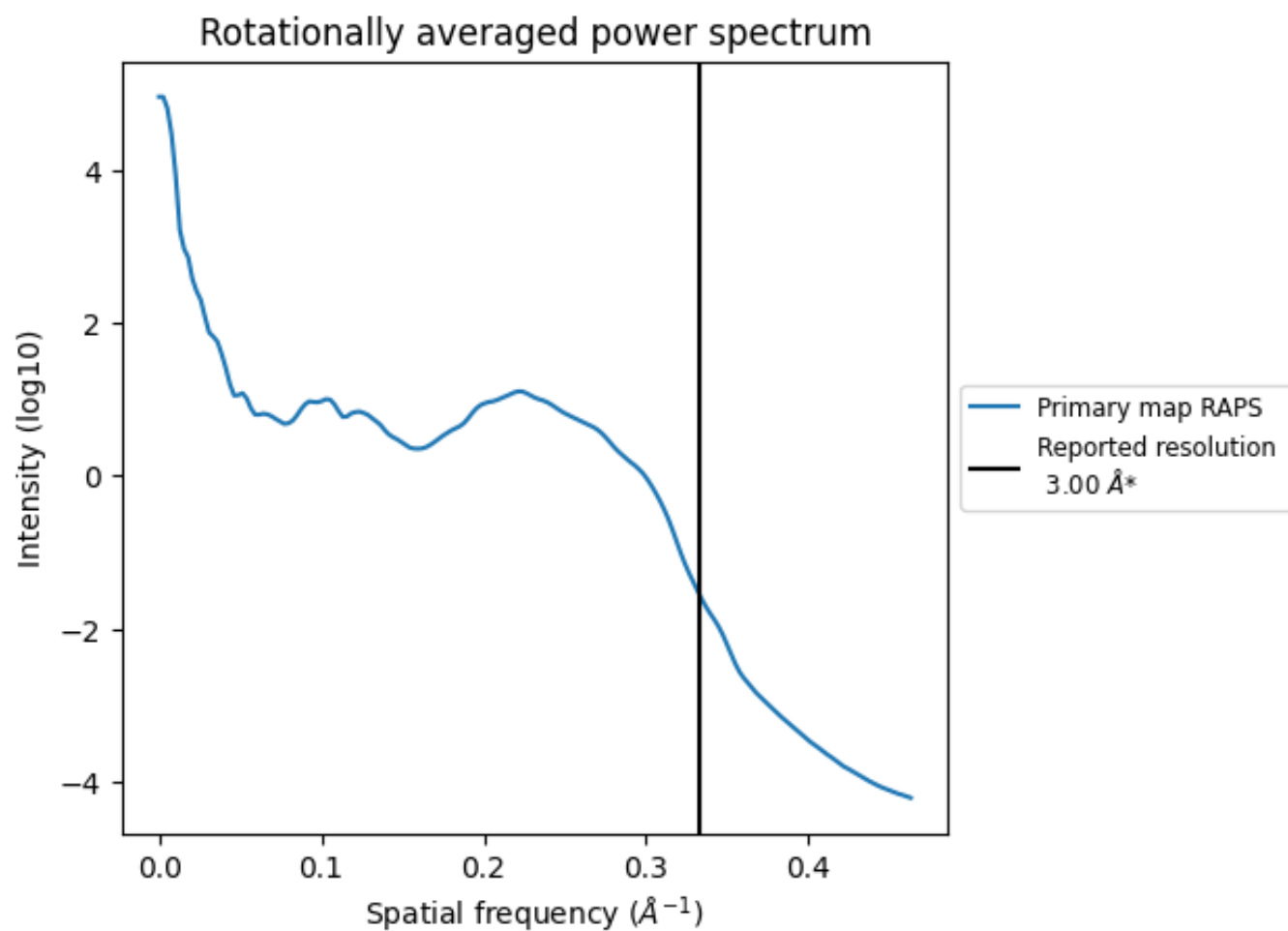
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 130 nm^3 ; this corresponds to an approximate mass of 118 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 0.333 Å⁻¹

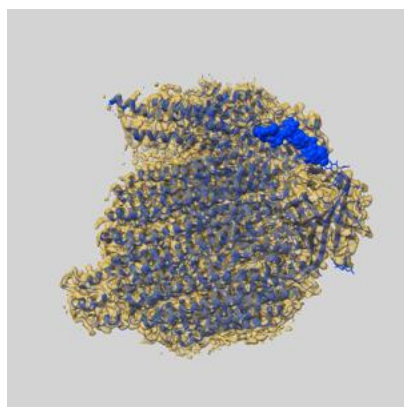
8 Fourier-Shell correlation ⓘ

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

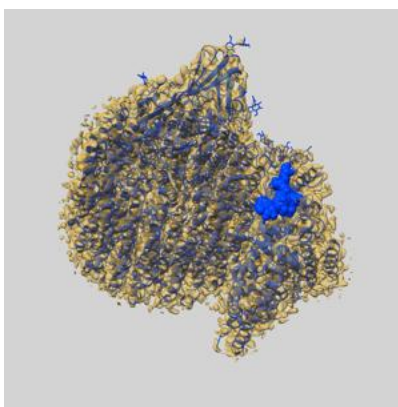
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21844 and PDB model 6WLW. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

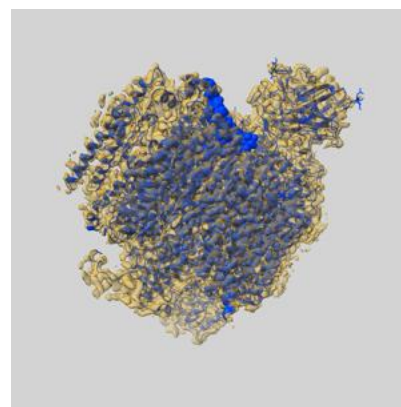
9.1 Map-model overlay [i](#)



X



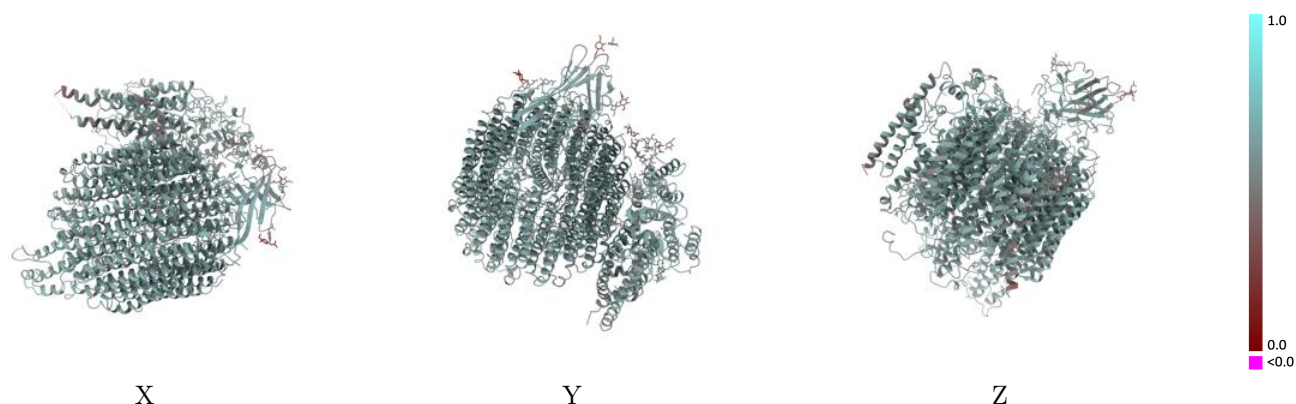
Y



Z

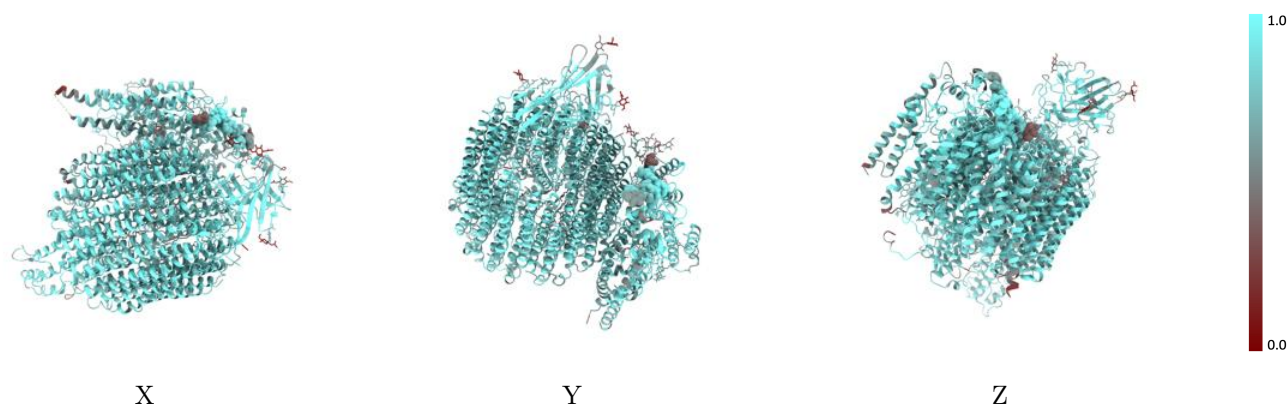
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



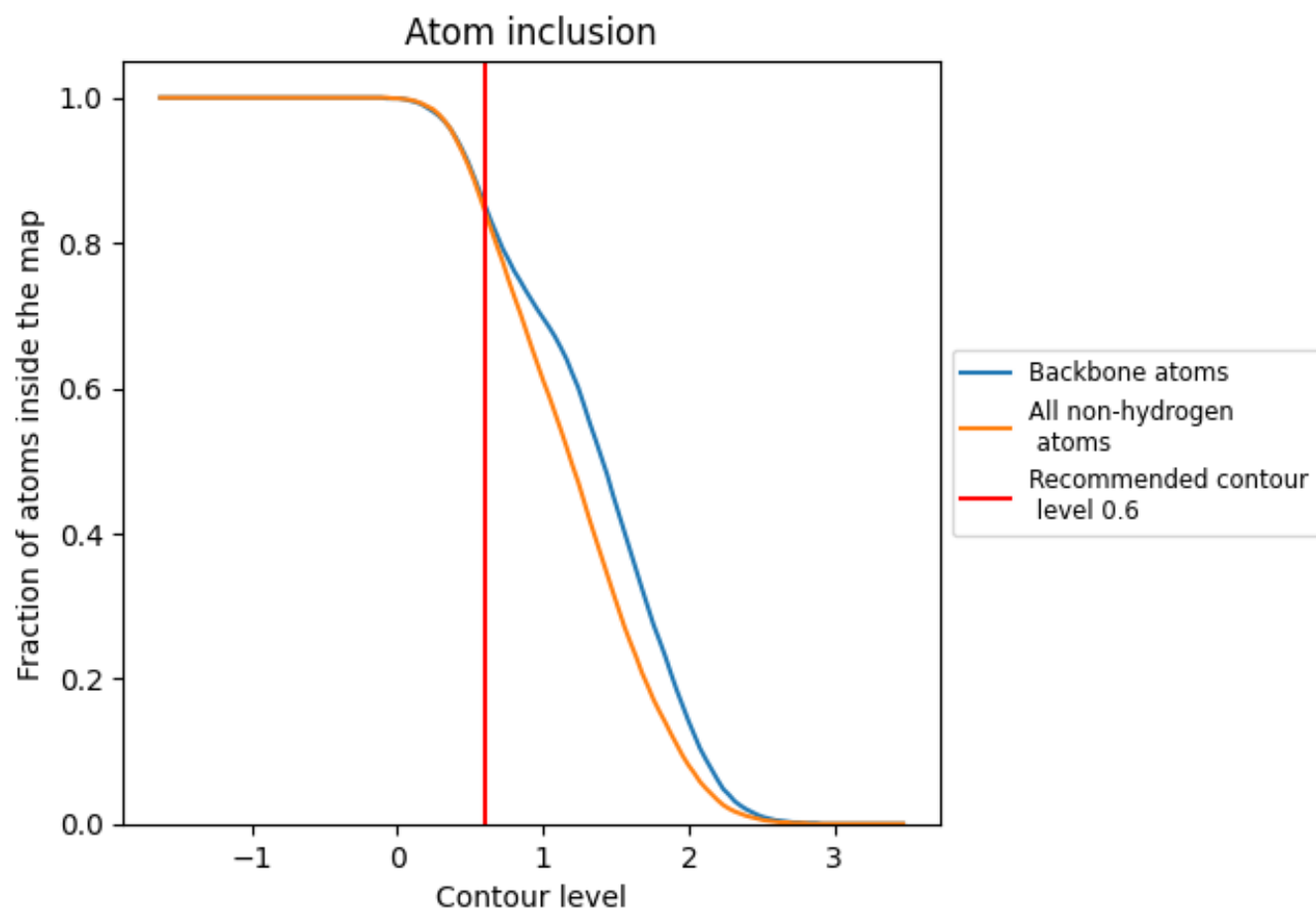
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 84% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8440	 0.5790
0	 0.8880	 0.5940
1	 0.8870	 0.5900
2	 0.8660	 0.5850
3	 0.8620	 0.5920
4	 0.8630	 0.5860
5	 0.8380	 0.5830
6	 0.8430	 0.5860
7	 0.8540	 0.5860
8	 0.8430	 0.5850
9	 0.8780	 0.5880
A	 0.5360	 0.4410
B	 0.5000	 0.4410
C	 0.3930	 0.2610
D	 0.3570	 0.4090
Q	 0.8450	 0.5860
R	 0.8320	 0.5700
S	 0.8290	 0.5660
T	 0.7500	 0.5380
U	 0.8400	 0.5770
V	 0.8450	 0.5810
W	 0.5000	 0.4060
r	 0.8030	 0.5450
s	 0.6790	 0.4850
u	 0.2500	 0.3750

