



## Full wwPDB EM Validation Report ⓘ

Sep 22, 2025 – 10:14 AM JST

PDB ID : 9VJ0 / pdb\_00009vj0  
EMDB ID : EMD-65100  
Title : Cryo-EM structure of Na<sup>+</sup>,K<sup>+</sup>-ATPase that forms a cation channel with palytoxin (ATP form)  
Authors : Kanai, R.; Vilsen, B.; Cornelius, F.; Toyoshima, C.  
Deposited on : 2025-06-19  
Resolution : 3.70 Å(reported)  
Based on initial model : 8jtz

This is a Full wwPDB EM Validation 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:

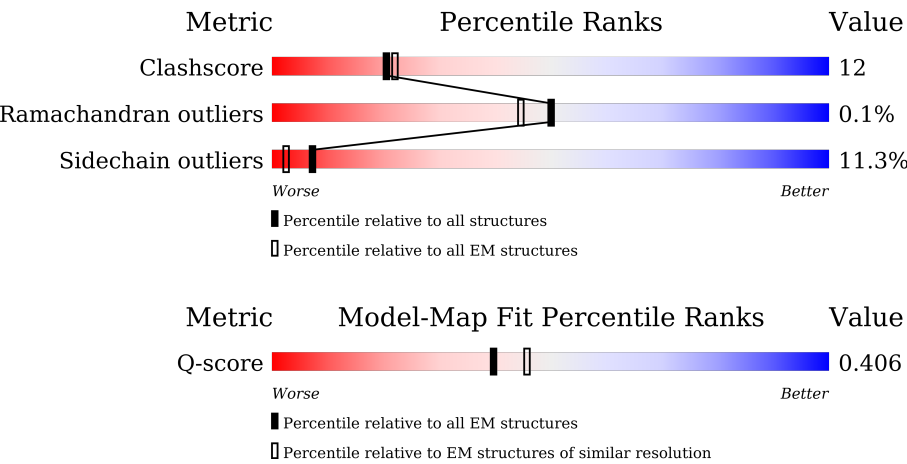
EMDB validation analysis : 0.0.1.dev129  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : 202505.v01 (Using data in the 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 3.70 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	11569 ( 3.20 - 4.20 )

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>70%23%</div><div></div></div>
1	D	305	<div><div></div><div>69%24%</div><div></div></div>
2	A	1028	<div><div>10%</div><div>65%27%</div><div></div></div>
2	C	1028	<div><div>10%</div><div>65%28%</div><div></div></div>
3	E	94	<div><div></div><div>29%14%57%</div><div></div></div>

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Mol	Chain	Length	Quality of chain
3	G	94	 29% 14% 57%
4	F	6	 50% 100%
4	K	6	 50% 83% 17%
5	H	6	 83% 100%
5	L	6	 83% 100%
6	I	5	 80% 100%
6	M	5	 80% 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 22600 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		

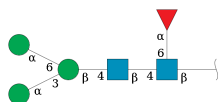
- Molecule 2 is a protein called Na, K-ATPase alpha subunit.

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.



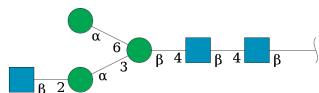
Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	6	Total	C	N	O		0	0
			71	40	2	29			

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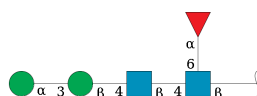
Mol	Chain	Residues	Atoms				AltConf	Trace
4	K	6	Total	C	N	O	0	0
			71	40	2	29		

- 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.



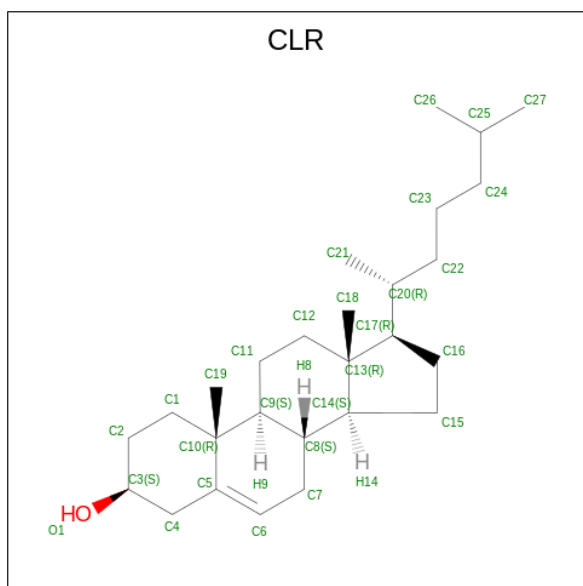
Mol	Chain	Residues	Atoms				AltConf	Trace
7	J	2	Total	C	N	O	0	0
			28	16	2	10		

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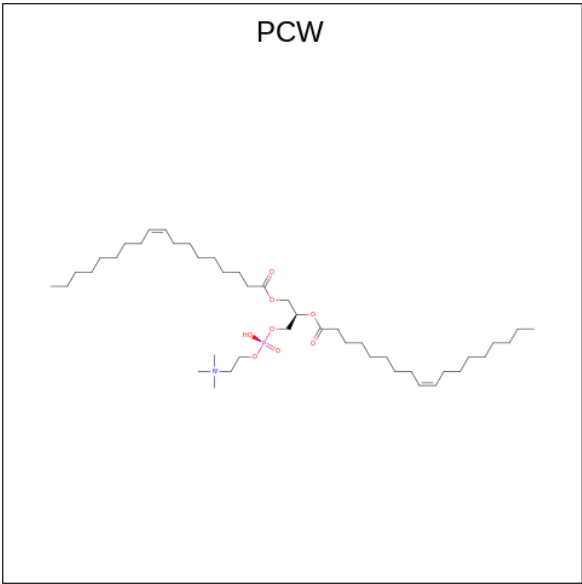
Mol	Chain	Residues	Atoms				AltConf	Trace
7	N	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 8 is CHOLESTEROL (CCD ID: CLR) (formula:  $C_{27}H_{46}O$ ).



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

- 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
			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
			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
			54	44	1	8	1	

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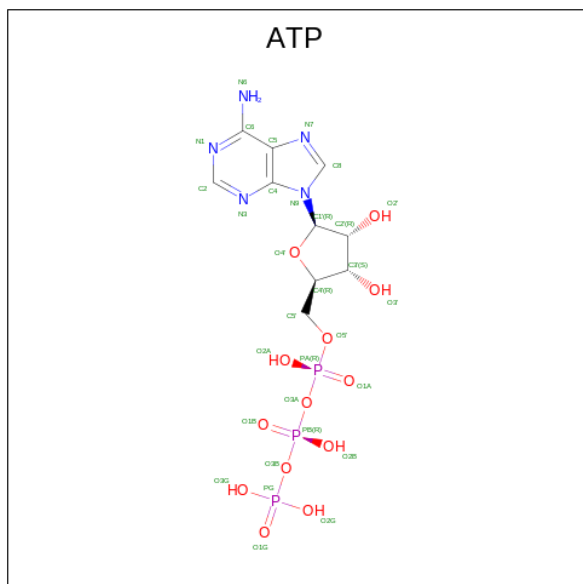
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Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	A	1	Total	C	N	O	P	0
			22	12	1	8	1	
9	G	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	G	1	Total	C	N	O	P	0
			54	44	1	8	1	

- 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	

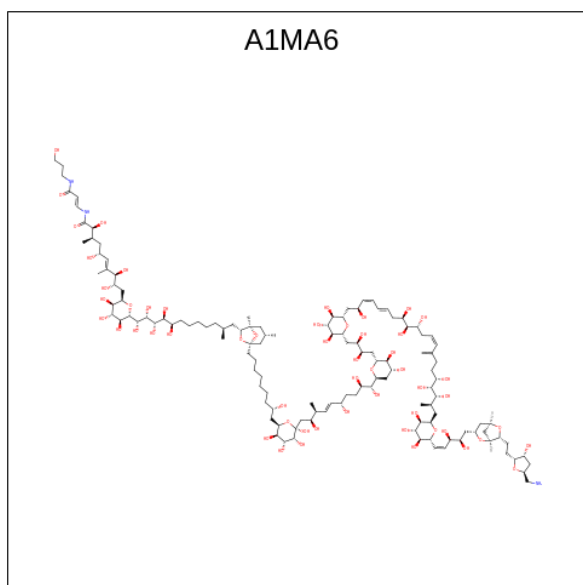
- Molecule 11 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).





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).

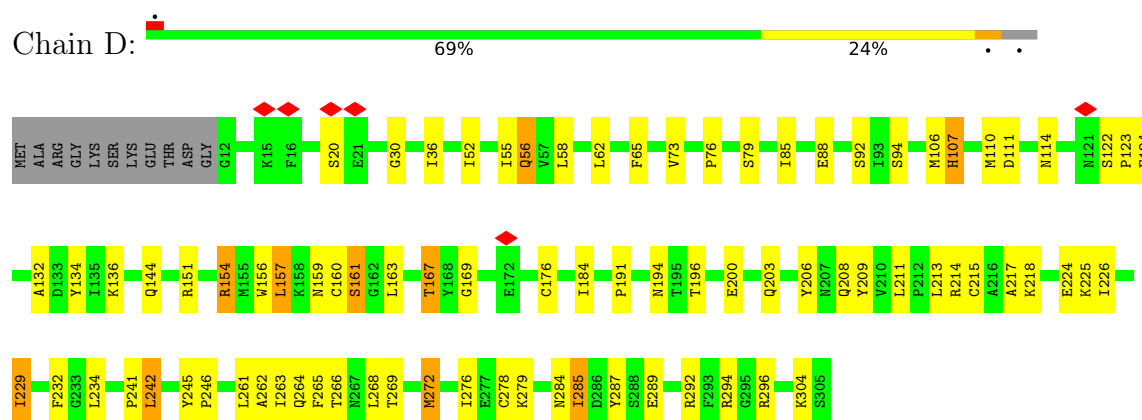


Mol	Chain	Residues	Atoms				AltConf
13	C	1	Total	C	N	O	0
			186	129	3	54	
13	A	1	Total	C	N	O	0
			186	129	3	54	

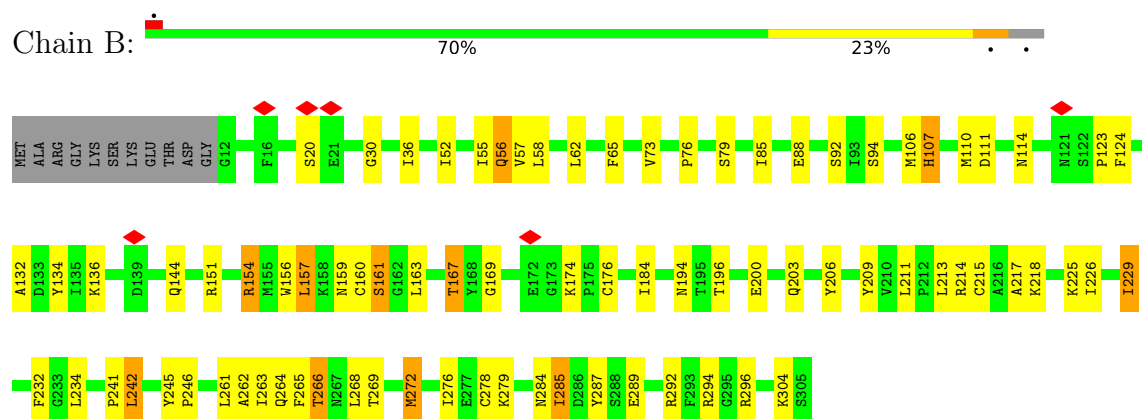
### 3 Residue-property plots

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.

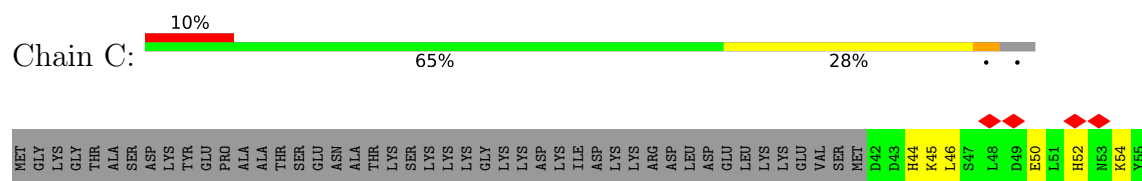
- Molecule 1: Na<sup>+</sup>,K<sup>+</sup>-ATPase beta subunit

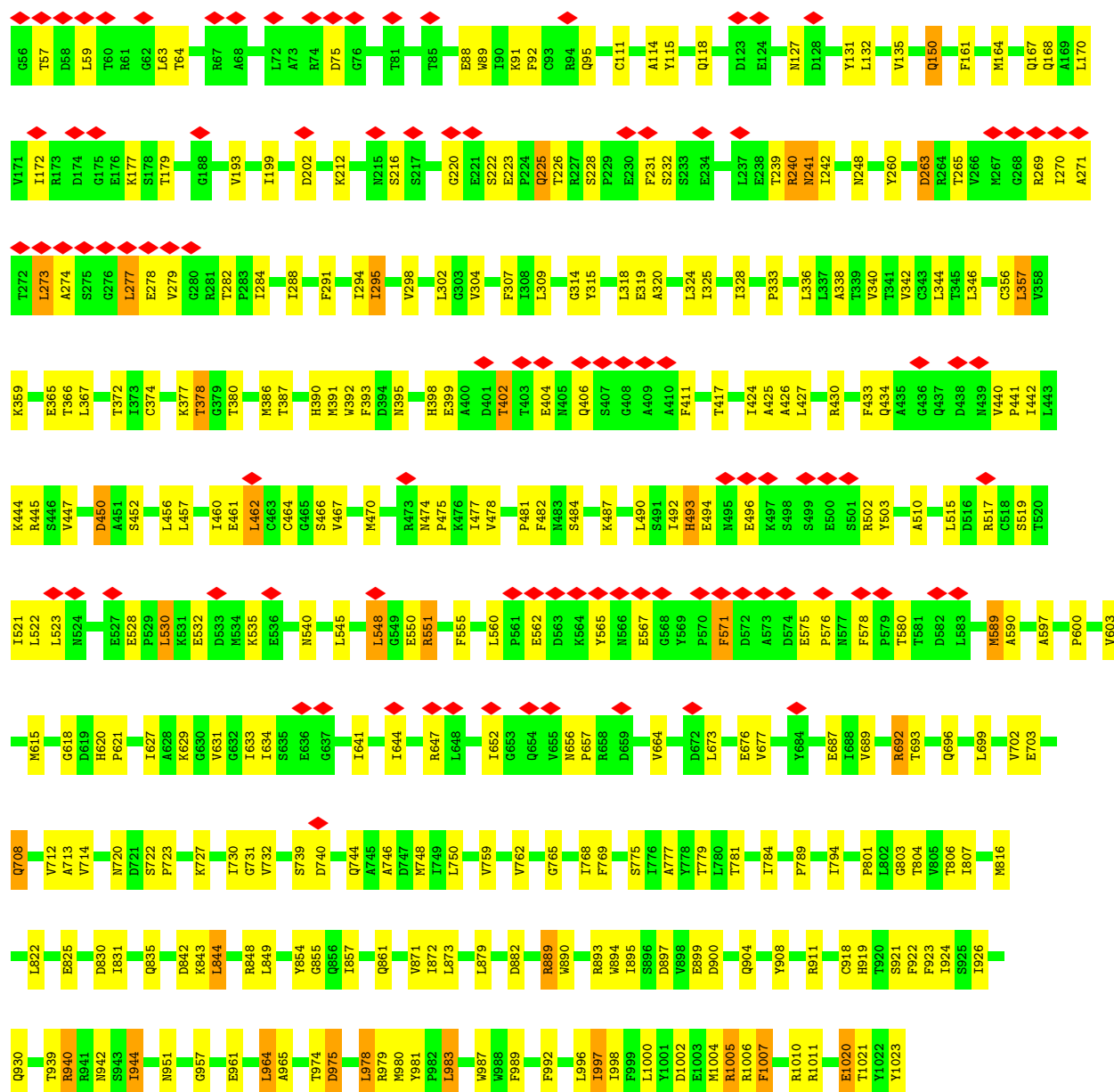


- Molecule 1: Na<sup>+</sup>,K<sup>+</sup>-ATPase beta subunit

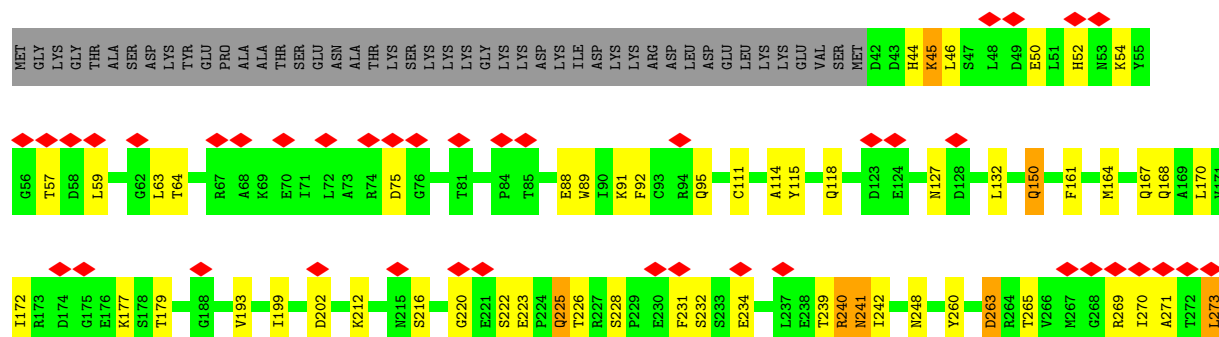


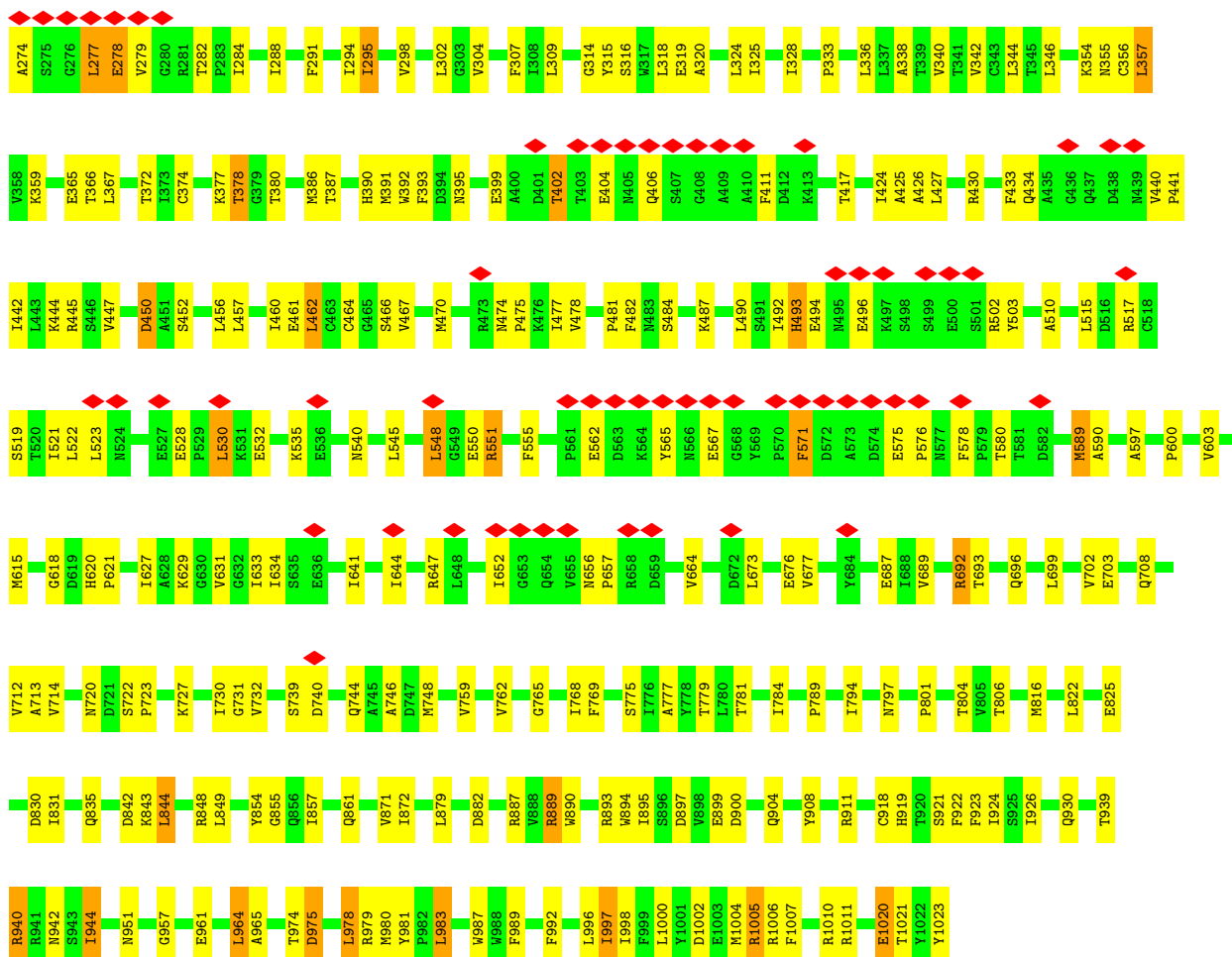
- Molecule 2: Na, K-ATPase alpha subunit



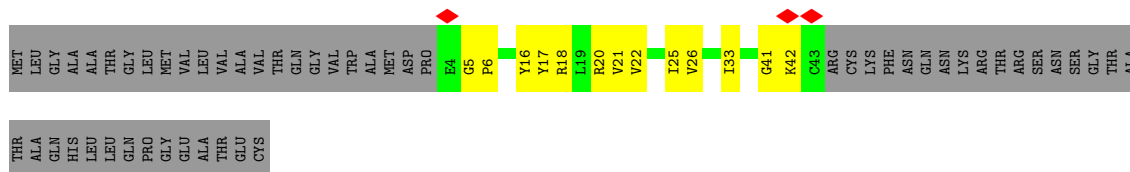


• Molecule 2: Na, K-ATPase alpha subunit

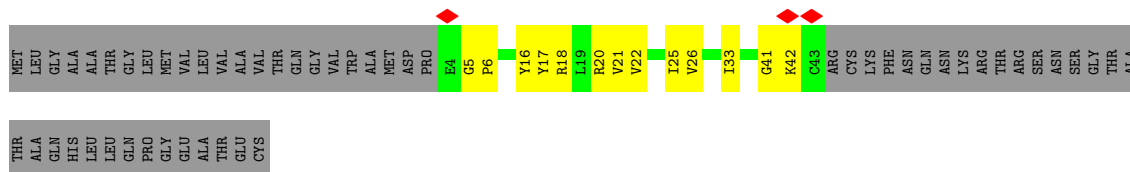




• Molecule 3: FXYD domain-containing ion transport regulator



• Molecule 3: FXYD domain-containing ion transport regulator

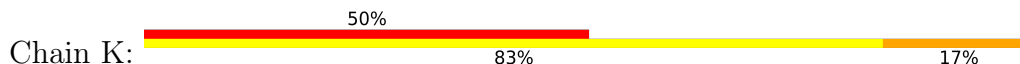


• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamid

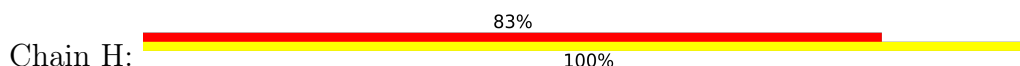
o-2-deoxy-beta-D-glucopyranose



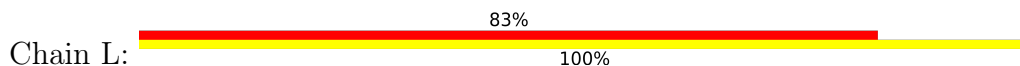
• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



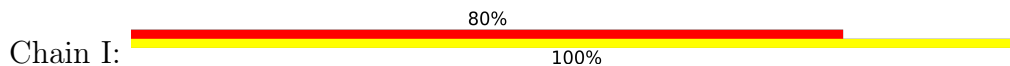
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



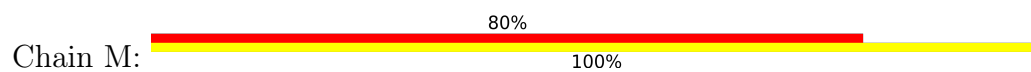
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• 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	31891	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	0.047	Depositor
Minimum map value	-0.023	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0095	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, NA, PCW, BMA, ATP, MG, MAN, CLR, NAG, FUC

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	0.19	0/2462	0.61	0/3317
1	D	0.19	0/2462	0.61	0/3317
2	A	0.28	0/7744	0.65	1/10509 (0.0%)
2	C	0.28	0/7744	0.65	1/10509 (0.0%)
3	E	0.18	0/315	0.40	0/427
3	G	0.18	0/315	0.40	0/427
All	All	0.26	0/21042	0.64	2/28506 (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	C	855	GLY	N-CA-C	9.33	123.32	112.50
2	A	855	GLY	N-CA-C	9.33	123.32	112.50

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	44	0
1	D	2399	0	2354	44	0
2	A	7594	0	7612	185	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	7594	0	7612	189	0
3	E	311	0	323	12	0
3	G	311	0	323	12	0
4	F	71	0	61	0	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	112	0	184	13	0
8	B	28	0	46	3	0
8	C	112	0	184	11	0
8	D	28	0	46	5	0
9	A	292	0	438	49	0
9	B	54	0	84	11	0
9	C	238	0	354	37	0
9	E	108	0	168	5	0
9	G	108	0	168	6	0
10	A	1	0	0	0	0
10	C	1	0	0	0	0
11	A	31	0	12	1	0
11	C	31	0	12	1	0
12	A	4	0	0	0	0
12	C	4	0	0	0	0
13	A	186	0	0	4	0
13	C	186	0	0	4	0
All	All	22600	0	22678	538	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 12.

All (538) 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:B:401:PCW:H252	8:A:1103:CLR:H263	1.41	0.99
8:C:1103:CLR:H263	9:A:1104:PCW:H252	1.44	0.98
9:A:1107:PCW:H372	9:G:101:PCW:H39	1.49	0.92
9:C:1106:PCW:H372	9:E:101:PCW:H39	1.49	0.92
9:A:1105:PCW:H262	9:A:1106:PCW:H271	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:1104:PCW:H262	9:C:1105:PCW:H271	1.53	0.88
2:A:325:ILE:HD13	8:A:1110:CLR:H273	1.61	0.83
2:A:1000:LEU:HD23	9:A:1104:PCW:H251	1.60	0.82
2:C:1000:LEU:HD23	9:B:401:PCW:H251	1.60	0.82
2:C:325:ILE:HD13	8:C:1109:CLR:H273	1.61	0.81
2:C:996:LEU:HD13	9:A:1106:PCW:H461	1.61	0.81
9:C:1105:PCW:H472	9:A:1105:PCW:C27	2.11	0.80
9:C:1105:PCW:H461	2:A:996:LEU:HD13	1.62	0.80
9:C:1105:PCW:H452	9:A:1105:PCW:H272	1.62	0.80
9:C:1105:PCW:H472	9:A:1105:PCW:H271	1.64	0.79
2:A:806:THR:HG21	2:A:919:HIS:HB3	1.64	0.79
2:C:964:LEU:HD11	9:C:1106:PCW:H262	1.65	0.78
2:C:475:PRO:HD2	2:C:494:GLU:HB2	1.65	0.78
8:A:1102:CLR:H71	3:G:26:VAL:HG11	1.66	0.78
2:C:806:THR:HG21	2:C:919:HIS:HB3	1.64	0.77
2:A:964:LEU:HD11	9:A:1107:PCW:H262	1.65	0.77
2:A:52:HIS:HE1	2:A:59:LEU:HD12	1.49	0.77
2:A:475:PRO:HD2	2:A:494:GLU:HB2	1.65	0.77
2:C:202:ASP:HB2	2:C:260:TYR:HB2	1.67	0.77
8:C:1102:CLR:H71	3:E:26:VAL:HG11	1.66	0.76
2:C:52:HIS:HE1	2:C:59:LEU:HD12	1.49	0.76
1:D:76:PRO:HG3	1:D:184:ILE:HD12	1.67	0.76
1:B:76:PRO:HG3	1:B:184:ILE:HD12	1.67	0.75
2:C:228:SER:H	2:C:240:ARG:HB2	1.52	0.74
2:A:202:ASP:HB2	2:A:260:TYR:HB2	1.67	0.74
9:C:1104:PCW:C27	9:A:1106:PCW:H472	2.18	0.74
2:A:228:SER:H	2:A:240:ARG:HB2	1.52	0.74
2:A:924:ILE:HD12	2:A:983:LEU:HD22	1.68	0.74
2:C:924:ILE:HD12	2:C:983:LEU:HD22	1.68	0.73
8:C:1102:CLR:H161	9:C:1104:PCW:H482	1.70	0.73
2:A:1004:MET:HE2	9:A:1104:PCW:H39	1.70	0.73
2:C:1004:MET:HE2	9:B:401:PCW:H39	1.70	0.73
2:A:223:GLU:O	2:A:225:GLN:NE2	2.23	0.72
2:C:223:GLU:O	2:C:225:GLN:NE2	2.23	0.71
2:A:992:PHE:CD2	9:A:1105:PCW:H261	2.25	0.71
8:A:1102:CLR:H161	9:A:1105:PCW:H482	1.70	0.71
2:A:212:LYS:HG2	2:A:226:THR:HG22	1.72	0.71
2:C:212:LYS:HG2	2:C:226:THR:HG22	1.72	0.71
2:A:372:THR:HB	2:A:712:VAL:HG12	1.74	0.70
1:B:161:SER:HB3	1:B:163:LEU:HD12	1.74	0.70
2:C:372:THR:HB	2:C:712:VAL:HG12	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:992:PHE:CD2	9:C:1104:PCW:H261	2.25	0.70
2:A:318:LEU:HD21	8:A:1110:CLR:H151	1.72	0.70
1:D:213:LEU:HD23	1:D:261:LEU:HD13	1.74	0.69
1:D:161:SER:HB3	1:D:163:LEU:HD12	1.74	0.69
2:C:318:LEU:HD21	8:C:1109:CLR:H151	1.72	0.69
1:B:213:LEU:HD23	1:B:261:LEU:HD13	1.74	0.69
2:A:503:TYR:HE2	2:A:567:GLU:HA	1.59	0.68
9:C:1104:PCW:H271	9:A:1106:PCW:H472	1.75	0.68
9:B:401:PCW:H452	8:A:1103:CLR:H262	1.74	0.68
2:C:889:ARG:HH11	2:C:889:ARG:HA	1.59	0.67
9:C:1104:PCW:H272	9:A:1106:PCW:H452	1.74	0.67
2:C:503:TYR:HE2	2:C:567:GLU:HA	1.59	0.67
8:C:1102:CLR:H25	9:C:1105:PCW:H272	1.76	0.67
2:A:889:ARG:HH11	2:A:889:ARG:HA	1.59	0.67
2:C:889:ARG:HA	2:C:889:ARG:NH1	2.10	0.66
8:A:1102:CLR:H25	9:A:1106:PCW:H272	1.76	0.66
2:A:889:ARG:HA	2:A:889:ARG:NH1	2.10	0.66
2:C:366:THR:HG22	2:C:730:ILE:HD11	1.77	0.66
1:D:136:LYS:HZ1	3:E:6:PRO:HD3	1.60	0.66
2:A:366:THR:HG22	2:A:730:ILE:HD11	1.77	0.66
2:C:393:PHE:HB2	2:C:417:THR:HG21	1.79	0.65
2:A:641:ILE:HG12	2:A:652:ILE:HG13	1.77	0.65
1:B:136:LYS:HZ1	3:G:6:PRO:HD3	1.61	0.65
3:G:20:ARG:HH12	9:G:101:PCW:H52	1.61	0.65
3:E:20:ARG:HH12	9:E:101:PCW:H52	1.61	0.65
2:A:393:PHE:HB2	2:A:417:THR:HG21	1.79	0.64
2:C:641:ILE:HG12	2:C:652:ILE:HG13	1.77	0.64
9:C:1105:PCW:H39	2:A:989:PHE:HB3	1.79	0.64
2:C:426:ALA:HB2	2:C:460:ILE:HG21	1.80	0.64
9:B:401:PCW:H472	8:A:1103:CLR:H261	1.81	0.63
2:C:503:TYR:CE2	2:C:567:GLU:HA	2.34	0.63
9:C:1105:PCW:H471	9:A:1106:PCW:H471	1.81	0.63
2:A:161:PHE:HB3	2:A:357:LEU:HD11	1.81	0.63
2:A:503:TYR:CE2	2:A:567:GLU:HA	2.34	0.63
9:C:1105:PCW:H472	9:A:1105:PCW:H272	1.81	0.62
2:A:404:GLU:HA	2:A:462:LEU:HD11	1.80	0.62
2:A:426:ALA:HB2	2:A:460:ILE:HG21	1.80	0.62
2:C:404:GLU:HA	2:C:462:LEU:HD11	1.80	0.62
2:A:872:ILE:HD11	2:A:921:SER:OG	2.00	0.62
2:C:872:ILE:HD11	2:C:921:SER:OG	2.00	0.62
8:C:1103:CLR:H262	9:A:1104:PCW:H452	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:241:ASN:HD22	2:A:241:ASN:H	1.48	0.61
2:C:161:PHE:HB3	2:C:357:LEU:HD11	1.81	0.61
1:B:36:ILE:HD13	2:A:1020:GLU:HG2	1.83	0.61
2:C:241:ASN:H	2:C:241:ASN:HD22	1.48	0.60
2:C:46:LEU:HD22	2:C:50:GLU:HG2	1.83	0.60
2:A:46:LEU:HD22	2:A:50:GLU:HG2	1.83	0.60
2:A:523:LEU:HD12	2:A:528:GLU:HB2	1.84	0.60
3:G:21:VAL:O	3:G:25:ILE:HG12	2.02	0.60
2:C:523:LEU:HD12	2:C:528:GLU:HB2	1.84	0.60
3:E:21:VAL:O	3:E:25:ILE:HG12	2.02	0.60
1:D:217:ALA:HB2	1:D:226:ILE:HD12	1.84	0.59
2:C:989:PHE:HB3	9:A:1106:PCW:H39	1.83	0.59
9:C:1104:PCW:H272	9:A:1106:PCW:H472	1.83	0.59
3:G:20:ARG:NH1	9:G:101:PCW:H52	2.17	0.59
1:D:36:ILE:HD13	2:C:1020:GLU:HG2	1.83	0.59
2:C:456:LEU:HD11	2:C:555:PHE:HZ	1.68	0.59
2:A:482:PHE:HZ	11:A:1112:ATP:H5'1	1.68	0.59
3:E:20:ARG:NH1	9:E:101:PCW:H52	2.17	0.59
2:A:115:TYR:HE2	2:A:127:ASN:HD22	1.51	0.59
2:C:456:LEU:HD11	2:C:555:PHE:CZ	2.38	0.59
2:A:456:LEU:HD11	2:A:555:PHE:CZ	2.38	0.59
2:C:477:ILE:HG22	2:C:478:VAL:HG23	1.85	0.59
2:C:115:TYR:HE2	2:C:127:ASN:HD22	1.51	0.58
2:C:482:PHE:HZ	11:C:1111:ATP:H5'1	1.68	0.58
1:B:217:ALA:HB2	1:B:226:ILE:HD12	1.84	0.58
2:A:456:LEU:HD11	2:A:555:PHE:HZ	1.67	0.58
1:D:55:ILE:HG21	9:C:1107:PCW:H341	1.85	0.58
2:A:232:SER:OG	2:A:240:ARG:HD3	2.04	0.58
2:A:530:LEU:HD22	2:A:535:LYS:HG3	1.86	0.58
8:D:401:CLR:C21	9:A:1104:PCW:H422	2.34	0.57
2:A:477:ILE:HG22	2:A:478:VAL:HG23	1.85	0.57
1:B:55:ILE:HG21	9:A:1108:PCW:H341	1.85	0.57
2:A:402:THR:O	2:A:402:THR:OG1	2.19	0.57
1:D:209:TYR:HA	1:D:242:LEU:HD22	1.87	0.57
1:D:279:LYS:HG3	1:D:296:ARG:HB3	1.87	0.57
2:C:232:SER:OG	2:C:240:ARG:HD3	2.04	0.57
2:A:391:MET:HE1	2:A:411:PHE:HE2	1.70	0.57
2:C:997:ILE:HG13	9:B:401:PCW:H261	1.87	0.57
2:A:992:PHE:HD2	9:A:1105:PCW:H261	1.70	0.57
2:C:391:MET:HE1	2:C:411:PHE:HE2	1.70	0.56
2:A:44:HIS:HB3	2:A:242:ILE:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:530:LEU:HD22	2:C:535:LYS:HG3	1.86	0.56
1:B:279:LYS:HG3	1:B:296:ARG:HB3	1.87	0.56
1:D:136:LYS:NZ	3:E:6:PRO:HD3	2.20	0.56
1:B:209:TYR:HA	1:B:242:LEU:HD22	1.87	0.56
2:A:974:THR:HG23	2:A:978:LEU:HB2	1.87	0.56
2:C:44:HIS:HB3	2:C:242:ILE:HD11	1.88	0.56
2:C:430:ARG:NH2	2:C:481:PRO:HB3	2.21	0.56
1:B:136:LYS:NZ	3:G:6:PRO:HD3	2.20	0.56
2:A:442:ILE:HB	2:A:462:LEU:HD12	1.88	0.56
2:A:997:ILE:HG13	9:A:1104:PCW:H261	1.87	0.55
2:C:974:THR:HG23	2:C:978:LEU:HB2	1.87	0.55
2:A:575:GLU:HB3	2:A:576:PRO:HD2	1.88	0.55
2:C:442:ILE:HB	2:C:462:LEU:HD12	1.88	0.55
2:A:430:ARG:NH2	2:A:481:PRO:HB3	2.21	0.55
1:D:176:CYS:SG	1:D:264:GLN:HG3	2.47	0.55
2:C:575:GLU:HB3	2:C:576:PRO:HD2	1.88	0.55
8:C:1102:CLR:H242	9:C:1104:PCW:H472	1.89	0.55
2:A:170:LEU:HG	2:A:179:THR:HG22	1.89	0.55
2:C:170:LEU:HG	2:C:179:THR:HG22	1.89	0.54
2:A:656:ASN:HD22	2:A:657:PRO:HD2	1.72	0.54
1:D:58:LEU:HD22	2:C:871:VAL:HG22	1.89	0.54
2:C:52:HIS:CE1	2:C:59:LEU:HD12	2.38	0.54
2:A:265:THR:O	2:A:269:ARG:HD3	2.07	0.54
1:B:176:CYS:SG	1:B:264:GLN:HG3	2.47	0.54
2:C:861:GLN:OE1	2:C:930:GLN:NE2	2.41	0.54
2:A:241:ASN:HD22	2:A:241:ASN:N	2.06	0.54
2:C:656:ASN:HD22	2:C:657:PRO:HD2	1.73	0.54
2:C:298:VAL:O	2:C:302:LEU:HG	2.07	0.54
8:A:1102:CLR:H242	9:A:1105:PCW:H472	1.89	0.53
2:C:88:GLU:HA	2:C:91:LYS:HB2	1.90	0.53
2:C:265:THR:O	2:C:269:ARG:HD3	2.07	0.53
2:A:861:GLN:OE1	2:A:930:GLN:NE2	2.41	0.53
2:A:193:VAL:HG11	2:A:199:ILE:HD13	1.91	0.53
2:A:298:VAL:O	2:A:302:LEU:HG	2.07	0.53
2:C:992:PHE:HD2	9:C:1104:PCW:H261	1.70	0.53
1:B:58:LEU:HD22	2:A:871:VAL:HG22	1.89	0.53
2:A:957:GLY:O	2:A:961:GLU:HG2	2.09	0.53
2:A:893:ARG:HA	2:A:908:TYR:CD1	2.44	0.53
2:C:241:ASN:HD22	2:C:241:ASN:N	2.06	0.53
2:C:957:GLY:O	2:C:961:GLU:HG2	2.09	0.53
2:C:284:ILE:O	2:C:288:ILE:HG12	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:1105:PCW:C48	9:A:1106:PCW:H471	2.40	0.52
2:C:893:ARG:HA	2:C:908:TYR:CD1	2.44	0.52
2:A:517:ARG:HG2	2:A:517:ARG:HH11	1.75	0.52
2:C:502:ARG:HG2	2:C:562:GLU:HB3	1.91	0.52
8:A:1102:CLR:H222	9:A:1105:PCW:H482	1.92	0.52
2:A:304:VAL:O	2:A:307:PHE:HB3	2.10	0.52
2:A:759:VAL:O	2:A:762:VAL:HG22	2.10	0.52
3:G:18:ARG:O	3:G:22:VAL:HG23	2.09	0.52
2:A:88:GLU:HA	2:A:91:LYS:HB2	1.90	0.52
2:C:517:ARG:HG2	2:C:517:ARG:HH11	1.75	0.52
2:C:939:THR:O	2:C:1006:ARG:NH2	2.43	0.52
2:C:193:VAL:HG11	2:C:199:ILE:HD13	1.91	0.51
2:A:284:ILE:O	2:A:288:ILE:HG12	2.09	0.51
8:C:1103:CLR:H261	9:A:1104:PCW:H472	1.91	0.51
9:C:1105:PCW:H481	9:A:1106:PCW:H242	1.91	0.51
3:E:18:ARG:O	3:E:22:VAL:HG23	2.10	0.51
2:A:942:ASN:HA	2:A:1010:ARG:HH11	1.75	0.51
8:C:1102:CLR:H222	9:C:1104:PCW:H482	1.91	0.51
1:D:136:LYS:HZ1	3:E:5:GLY:HA2	1.76	0.51
9:C:1105:PCW:H471	9:A:1106:PCW:C48	2.39	0.51
2:C:270:ILE:O	2:C:273:LEU:HG	2.11	0.51
2:A:216:SER:O	2:A:220:GLY:HA2	2.10	0.51
2:A:939:THR:O	2:A:1006:ARG:NH2	2.43	0.51
2:C:759:VAL:O	2:C:762:VAL:HG22	2.10	0.51
13:C:1116:A1MA6:CBE	13:C:1116:A1MA6:CA1	2.89	0.51
2:A:502:ARG:HG2	2:A:562:GLU:HB3	1.91	0.51
2:A:944:ILE:HD11	9:A:1105:PCW:H142	1.92	0.51
2:C:344:LEU:HA	2:C:768:ILE:HD11	1.93	0.51
2:C:216:SER:O	2:C:220:GLY:HA2	2.10	0.50
2:C:304:VAL:O	2:C:307:PHE:HB3	2.10	0.50
2:C:565:TYR:HB3	2:C:571:PHE:HE2	1.75	0.50
1:B:136:LYS:HZ1	3:G:5:GLY:HA2	1.75	0.50
2:A:270:ILE:O	2:A:273:LEU:HG	2.11	0.50
2:A:872:ILE:HD11	2:A:921:SER:CB	2.41	0.50
2:A:765:GLY:O	2:A:768:ILE:HG22	2.11	0.50
2:C:510:ALA:HB1	2:C:692:ARG:HH12	1.76	0.50
2:C:944:ILE:HD11	9:C:1104:PCW:H142	1.92	0.50
2:A:510:ALA:HB1	2:A:692:ARG:HH12	1.76	0.50
2:A:565:TYR:HB3	2:A:571:PHE:HE2	1.75	0.50
2:C:942:ASN:HA	2:C:1010:ARG:HH11	1.75	0.50
2:A:430:ARG:HH22	2:A:481:PRO:HB3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:732:VAL:HG22	2:A:748:MET:HE2	1.93	0.50
1:D:110:MET:HE1	1:D:157:LEU:HD13	1.94	0.50
2:A:615:MET:HE3	2:A:633:ILE:HD12	1.93	0.50
2:C:615:MET:HE3	2:C:633:ILE:HD12	1.93	0.50
2:A:150:GLN:OE1	2:A:150:GLN:HA	2.11	0.50
2:A:545:LEU:HD13	2:A:590:ALA:HB2	1.93	0.50
1:B:56:GLN:HG3	8:B:402:CLR:H12	1.94	0.50
9:B:401:PCW:C45	8:A:1103:CLR:H262	2.40	0.50
2:A:713:ALA:HA	2:A:730:ILE:O	2.11	0.50
2:C:732:VAL:HG22	2:C:748:MET:HE2	1.93	0.50
2:C:872:ILE:HD11	2:C:921:SER:CB	2.41	0.50
1:B:110:MET:HE1	1:B:157:LEU:HD13	1.94	0.50
2:A:450:ASP:OD1	2:A:450:ASP:N	2.39	0.50
2:C:890:TRP:O	2:C:911:ARG:NH1	2.45	0.49
3:E:17:TYR:O	3:E:21:VAL:HG23	2.11	0.49
2:C:713:ALA:HA	2:C:730:ILE:O	2.11	0.49
2:C:548:LEU:HB3	2:C:550:GLU:HG3	1.94	0.49
9:C:1105:PCW:C47	9:A:1106:PCW:H471	2.41	0.49
2:A:890:TRP:O	2:A:911:ARG:NH1	2.45	0.49
2:A:926:ILE:O	2:A:930:GLN:HG2	2.11	0.49
2:C:765:GLY:O	2:C:768:ILE:HG22	2.11	0.49
9:C:1105:PCW:H471	9:A:1106:PCW:C47	2.42	0.49
2:A:979:ARG:NH1	2:A:981:TYR:OH	2.46	0.49
3:G:17:TYR:O	3:G:21:VAL:HG23	2.11	0.49
2:C:150:GLN:OE1	2:C:150:GLN:HA	2.11	0.49
2:A:344:LEU:HA	2:A:768:ILE:HD11	1.93	0.49
1:B:232:PHE:HB2	1:B:262:ALA:HB3	1.95	0.49
2:A:324:LEU:O	2:A:328:ILE:HG13	2.13	0.49
2:A:548:LEU:HB3	2:A:550:GLU:HG3	1.94	0.49
2:C:545:LEU:HD13	2:C:590:ALA:HB2	1.93	0.48
2:C:926:ILE:O	2:C:930:GLN:HG2	2.12	0.48
2:C:979:ARG:NH1	2:C:981:TYR:OH	2.46	0.48
2:C:430:ARG:HH22	2:C:481:PRO:HB3	1.76	0.48
2:C:474:ASN:OD1	2:C:496:GLU:N	2.46	0.48
2:C:702:VAL:HG13	2:C:712:VAL:HG21	1.95	0.48
2:A:784:ILE:HD11	2:A:854:TYR:CD2	2.48	0.48
2:C:784:ILE:HD11	2:C:854:TYR:CD2	2.48	0.48
2:A:634:ILE:HA	2:A:687:GLU:OE1	2.14	0.48
2:C:597:ALA:O	2:C:600:PRO:HD2	2.14	0.48
2:C:940:ARG:NH1	2:C:1023:TYR:O	2.47	0.48
9:A:1105:PCW:H212	9:A:1105:PCW:H182	1.55	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:216:SER:HB3	2:C:222:SER:HA	1.94	0.48
2:A:699:LEU:O	2:A:703:GLU:HG2	2.13	0.48
2:A:702:VAL:HG13	2:A:712:VAL:HG21	1.95	0.48
2:A:777:ALA:O	2:A:781:THR:HG23	2.13	0.48
2:A:940:ARG:NH1	2:A:1023:TYR:O	2.47	0.48
13:C:1116:A1MA6:OCD	13:C:1116:A1MA6:CCC	2.59	0.48
2:A:52:HIS:CE1	2:A:59:LEU:HD12	2.38	0.48
2:C:777:ALA:O	2:C:781:THR:HG23	2.13	0.48
2:A:216:SER:HB3	2:A:222:SER:HA	1.94	0.48
2:C:699:LEU:O	2:C:703:GLU:HG2	2.13	0.48
2:A:474:ASN:OD1	2:A:496:GLU:N	2.46	0.48
1:D:56:GLN:HG3	8:D:401:CLR:H12	1.94	0.48
1:D:232:PHE:HB2	1:D:262:ALA:HB3	1.95	0.48
2:C:692:ARG:HA	2:C:692:ARG:HD3	1.64	0.48
2:A:441:PRO:HG2	2:A:444:LYS:HE3	1.95	0.48
13:A:1117:A1MA6:CBE	13:A:1117:A1MA6:CA1	2.89	0.47
2:C:441:PRO:HG2	2:C:444:LYS:HE3	1.95	0.47
1:B:167:THR:HG22	1:B:169:GLY:H	1.78	0.47
2:A:825:GLU:OE1	2:A:951:ASN:ND2	2.44	0.47
2:C:324:LEU:O	2:C:328:ILE:HG13	2.13	0.47
9:B:401:PCW:H422	8:B:402:CLR:C21	2.44	0.47
1:D:167:THR:HG22	1:D:169:GLY:H	1.78	0.47
2:C:634:ILE:HA	2:C:687:GLU:OE1	2.14	0.47
2:C:656:ASN:HD22	2:C:657:PRO:CD	2.27	0.47
2:C:722:SER:OG	2:C:723:PRO:HD3	2.15	0.47
2:A:271:ALA:HA	2:A:274:ALA:HB3	1.97	0.47
2:A:597:ALA:O	2:A:600:PRO:HD2	2.14	0.47
2:A:722:SER:OG	2:A:723:PRO:HD3	2.15	0.47
2:A:978:LEU:O	2:A:979:ARG:HB2	2.14	0.47
2:C:664:VAL:HG22	2:C:689:VAL:HB	1.97	0.47
9:C:1106:PCW:H381	9:C:1106:PCW:H411	1.68	0.47
1:B:215:CYS:HA	1:B:278:CYS:HA	1.96	0.47
2:A:656:ASN:HD22	2:A:657:PRO:CD	2.27	0.47
2:C:271:ALA:HA	2:C:274:ALA:HB3	1.97	0.47
1:B:52:ILE:HD11	9:A:1108:PCW:H39	1.97	0.47
2:A:664:VAL:HG22	2:A:689:VAL:HB	1.97	0.47
2:C:150:GLN:HG3	2:C:342:VAL:CG2	2.45	0.47
9:A:1105:PCW:H251	9:A:1106:PCW:H251	1.97	0.47
2:C:239:THR:OG1	2:C:241:ASN:ND2	2.48	0.46
1:B:92:SER:HA	1:B:304:LYS:O	2.15	0.46
1:D:92:SER:HA	1:D:304:LYS:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:978:LEU:O	2:C:979:ARG:HB2	2.14	0.46
2:C:452:SER:OG	2:C:551:ARG:NH2	2.49	0.46
2:A:239:THR:OG1	2:A:241:ASN:ND2	2.48	0.46
2:A:433:PHE:HD1	2:A:447:VAL:HG22	1.81	0.46
1:D:52:ILE:HD11	9:C:1107:PCW:H39	1.97	0.46
1:D:215:CYS:HA	1:D:278:CYS:HA	1.96	0.46
2:C:621:PRO:HB3	2:C:664:VAL:HG11	1.98	0.46
2:C:872:ILE:HD12	2:C:918:CYS:HA	1.98	0.46
9:B:401:PCW:H211	9:B:401:PCW:H181	1.63	0.46
2:C:274:ALA:O	2:C:277:LEU:HD22	2.15	0.46
2:C:457:LEU:CD1	2:C:467:VAL:HG21	2.46	0.46
2:C:618:GLY:O	2:C:692:ARG:NE	2.48	0.46
2:A:618:GLY:O	2:A:692:ARG:NE	2.48	0.46
2:A:895:ILE:O	2:A:911:ARG:NH2	2.49	0.46
2:C:314:GLY:HA2	13:C:1116:A1MA6:C13	2.46	0.46
1:B:284:ASN:O	1:B:285:ILE:HD12	2.16	0.46
2:A:274:ALA:O	2:A:277:LEU:HD22	2.15	0.46
2:A:872:ILE:HD12	2:A:918:CYS:HA	1.98	0.46
9:A:1107:PCW:H241	9:A:1107:PCW:H271	1.66	0.46
2:C:433:PHE:HD1	2:C:447:VAL:HG22	1.81	0.46
2:C:540:ASN:H	2:C:540:ASN:HD22	1.64	0.46
2:C:740:ASP:O	2:C:744:GLN:HG3	2.16	0.46
2:A:740:ASP:O	2:A:744:GLN:HG3	2.16	0.46
2:A:784:ILE:HD11	2:A:854:TYR:HD2	1.80	0.46
9:G:101:PCW:H411	9:G:101:PCW:H382	1.70	0.46
2:A:315:TYR:HD1	2:A:319:GLU:OE1	1.99	0.45
2:A:452:SER:OG	2:A:551:ARG:NH2	2.49	0.45
2:A:532:GLU:HA	2:A:535:LYS:HB2	1.98	0.45
1:D:56:GLN:HG3	8:D:401:CLR:C1	2.46	0.45
9:C:1107:PCW:H451	9:C:1107:PCW:H483	1.79	0.45
1:B:56:GLN:HG3	8:B:402:CLR:C1	2.46	0.45
2:A:150:GLN:HG3	2:A:342:VAL:CG2	2.45	0.45
2:A:555:PHE:CE1	2:A:589:MET:HB2	2.51	0.45
2:C:241:ASN:H	2:C:241:ASN:ND2	2.14	0.45
2:C:315:TYR:HD1	2:C:319:GLU:OE1	1.99	0.45
2:C:532:GLU:HA	2:C:535:LYS:HB2	1.98	0.45
2:A:91:LYS:O	2:A:95:GLN:HG2	2.16	0.45
8:D:401:CLR:C26	9:A:1104:PCW:H483	2.46	0.45
2:A:621:PRO:HB3	2:A:664:VAL:HG11	1.98	0.45
2:C:450:ASP:OD1	2:C:450:ASP:N	2.39	0.45
2:A:314:GLY:HA2	13:A:1117:A1MA6:C13	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:540:ASN:HD22	2:A:540:ASN:H	1.64	0.45
1:D:284:ASN:O	1:D:285:ILE:HD12	2.16	0.45
2:C:784:ILE:HD11	2:C:854:TYR:HD2	1.80	0.45
2:A:52:HIS:CD2	2:A:57:THR:HG23	2.52	0.45
2:A:641:ILE:HG23	2:A:652:ILE:HD11	1.98	0.45
1:D:107:HIS:O	1:D:111:ASP:HB2	2.16	0.45
2:C:111:CYS:SG	2:C:132:LEU:HD23	2.57	0.45
1:B:107:HIS:O	1:B:111:ASP:HB2	2.16	0.45
1:B:225:LYS:HD2	1:B:272:MET:SD	2.57	0.45
2:A:457:LEU:CD1	2:A:467:VAL:HG21	2.46	0.45
1:D:215:CYS:SG	1:D:263:ILE:HD13	2.57	0.45
2:C:291:PHE:CZ	2:C:295:ILE:HD12	2.52	0.45
2:C:461:GLU:OE1	2:C:466:SER:HA	2.17	0.45
2:C:555:PHE:CE1	2:C:589:MET:HB2	2.51	0.45
2:C:460:ILE:O	2:C:464:CYS:HB3	2.17	0.45
2:C:492:ILE:HD12	2:C:578:PHE:CE1	2.52	0.45
2:C:895:ILE:O	2:C:911:ARG:NH2	2.49	0.45
2:A:545:LEU:HD23	2:A:545:LEU:HA	1.70	0.45
9:A:1107:PCW:H152	9:A:1107:PCW:H122	1.64	0.45
2:C:52:HIS:CD2	2:C:57:THR:HG23	2.52	0.44
9:C:1104:PCW:H251	9:C:1105:PCW:H251	1.97	0.44
1:B:132:ALA:O	1:B:209:TYR:HB3	2.17	0.44
2:A:492:ILE:HD12	2:A:578:PHE:CE1	2.52	0.44
1:D:124:PHE:HB3	1:D:151:ARG:HG2	1.98	0.44
2:C:641:ILE:HG23	2:C:652:ILE:HD11	1.98	0.44
2:A:377:LYS:HE3	2:A:378:THR:HG23	2.00	0.44
1:D:134:TYR:HE1	1:D:242:LEU:HG	1.83	0.44
2:C:91:LYS:O	2:C:95:GLN:HG2	2.16	0.44
2:A:461:GLU:OE1	2:A:466:SER:HA	2.17	0.44
2:A:114:ALA:HA	13:A:1117:A1MA6:OBI	2.18	0.44
9:A:1104:PCW:H181	9:A:1104:PCW:H211	1.63	0.44
1:D:225:LYS:HD2	1:D:272:MET:SD	2.57	0.44
2:C:377:LYS:HE3	2:C:378:THR:HG23	2.00	0.44
2:C:644:ILE:O	2:C:647:ARG:HG2	2.18	0.44
1:B:215:CYS:SG	1:B:263:ILE:HD13	2.57	0.44
2:A:291:PHE:CZ	2:A:295:ILE:HD12	2.52	0.44
2:A:391:MET:HE3	2:A:391:MET:HB2	1.90	0.44
1:D:132:ALA:O	1:D:209:TYR:HB3	2.17	0.44
1:B:234:LEU:HG	1:B:241:PRO:HG3	2.00	0.44
2:A:111:CYS:SG	2:A:132:LEU:HD23	2.57	0.44
2:C:857:ILE:HD12	2:C:998:ILE:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:517:ARG:NH1	2:A:580:THR:HB	2.33	0.44
8:A:1103:CLR:H161	8:A:1103:CLR:H222	1.94	0.44
2:C:114:ALA:HA	13:C:1116:A1MA6:OBI	2.18	0.44
1:B:124:PHE:HB3	1:B:151:ARG:HG2	1.98	0.44
9:A:1107:PCW:H411	9:A:1107:PCW:H381	1.68	0.44
2:C:517:ARG:NH1	2:C:580:THR:HB	2.33	0.43
2:C:889:ARG:NH1	2:C:895:ILE:HD12	2.33	0.43
2:A:644:ILE:O	2:A:647:ARG:HG2	2.18	0.43
2:A:392:TRP:CZ2	2:A:395:ASN:HA	2.53	0.43
13:A:1117:A1MA6:OCD	13:A:1117:A1MA6:CCC	2.59	0.43
1:D:265:PHE:CZ	1:D:276:ILE:HD12	2.54	0.43
2:C:392:TRP:CZ2	2:C:395:ASN:HA	2.53	0.43
1:B:245:TYR:HB3	1:B:246:PRO:HA	1.99	0.43
2:A:273:LEU:HG	2:A:273:LEU:H	1.58	0.43
2:A:460:ILE:O	2:A:464:CYS:HB3	2.17	0.43
1:D:245:TYR:HB3	1:D:246:PRO:HA	1.99	0.43
2:C:390:HIS:CD2	2:C:399:GLU:HG2	2.54	0.43
9:C:1107:PCW:H361	9:C:1107:PCW:H332	1.35	0.43
2:A:857:ILE:HD12	2:A:998:ILE:HG23	2.00	0.43
2:A:893:ARG:HG2	2:A:908:TYR:CZ	2.53	0.43
2:C:551:ARG:O	2:C:590:ALA:HA	2.19	0.43
2:C:825:GLU:OE1	2:C:951:ASN:ND2	2.44	0.43
2:C:893:ARG:HG2	2:C:908:TYR:CZ	2.53	0.43
2:C:1007:PHE:HD1	2:C:1007:PHE:HA	1.69	0.43
1:B:134:TYR:HE1	1:B:242:LEU:HG	1.83	0.43
9:C:1104:PCW:H382	9:C:1104:PCW:H412	1.89	0.43
1:B:229:ILE:H	1:B:229:ILE:HG13	1.40	0.43
2:A:720:ASN:O	2:A:723:PRO:HD2	2.19	0.43
2:C:922:PHE:O	2:C:926:ILE:HG12	2.19	0.43
2:A:172:ILE:HG12	2:A:177:LYS:HG2	2.01	0.43
2:A:241:ASN:H	2:A:241:ASN:ND2	2.14	0.43
2:A:374:CYS:HB2	2:A:714:VAL:HG22	2.00	0.43
1:D:122:SER:HA	1:D:123:PRO:HA	1.62	0.43
2:C:374:CYS:HB2	2:C:714:VAL:HG22	2.00	0.43
2:C:620:HIS:CD2	2:C:621:PRO:HD2	2.54	0.43
2:C:336:LEU:O	2:C:340:VAL:HG23	2.19	0.42
2:C:402:THR:O	2:C:402:THR:OG1	2.19	0.42
2:C:720:ASN:O	2:C:723:PRO:HD2	2.19	0.42
2:A:889:ARG:NH1	2:A:895:ILE:HD12	2.33	0.42
1:D:52:ILE:O	1:D:55:ILE:HG22	2.19	0.42
1:D:224:GLU:H	1:D:224:GLU:HG3	1.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:924:ILE:HG12	2:C:965:ALA:HB1	2.01	0.42
2:C:983:LEU:HG	2:C:987:TRP:HE3	1.85	0.42
2:A:284:ILE:HG13	2:A:365:GLU:OE2	2.19	0.42
2:A:521:ILE:HD11	2:A:530:LEU:HG	2.01	0.42
1:D:279:LYS:HD3	1:D:287:TYR:CZ	2.54	0.42
2:A:924:ILE:HG12	2:A:965:ALA:HB1	2.01	0.42
2:C:338:ALA:O	2:C:342:VAL:HG23	2.20	0.42
2:C:750:LEU:HD12	2:C:750:LEU:HA	1.87	0.42
9:C:1105:PCW:H242	9:A:1106:PCW:H481	2.01	0.42
9:C:1105:PCW:H483	9:A:1106:PCW:H471	2.01	0.42
2:A:551:ARG:O	2:A:590:ALA:HA	2.19	0.42
2:A:620:HIS:CD2	2:A:621:PRO:HD2	2.54	0.42
2:A:983:LEU:HG	2:A:987:TRP:HE3	1.85	0.42
1:D:234:LEU:HG	1:D:241:PRO:HG3	2.00	0.42
2:C:521:ILE:HD11	2:C:530:LEU:HG	2.01	0.42
8:A:1102:CLR:H231	8:A:1102:CLR:H273	1.81	0.42
1:B:57:VAL:HG22	9:B:401:PCW:H39	2.00	0.42
2:A:307:PHE:CD1	2:A:320:ALA:HB1	2.55	0.42
2:C:673:LEU:HD22	2:C:677:VAL:HG11	2.01	0.42
3:E:41:GLY:O	3:E:42:LYS:HB2	2.20	0.42
1:B:52:ILE:O	1:B:55:ILE:HG22	2.19	0.42
1:B:279:LYS:HD3	1:B:287:TYR:CZ	2.54	0.42
2:A:922:PHE:O	2:A:926:ILE:HG12	2.19	0.42
2:C:274:ALA:O	2:C:277:LEU:HD13	2.20	0.42
2:A:390:HIS:CD2	2:A:399:GLU:HG2	2.54	0.42
2:A:975:ASP:OD1	2:A:975:ASP:N	2.52	0.42
2:C:540:ASN:HD22	2:C:540:ASN:N	2.18	0.42
2:C:900:ASP:OD2	2:C:904:GLN:HB2	2.20	0.42
1:B:265:PHE:CZ	1:B:276:ILE:HD12	2.53	0.42
2:A:336:LEU:O	2:A:340:VAL:HG23	2.19	0.42
2:C:225:GLN:H	2:C:225:GLN:HE21	1.68	0.42
2:C:263:ASP:C	2:C:265:THR:H	2.27	0.42
2:A:731:GLY:O	2:A:746:ALA:HB1	2.20	0.42
1:D:85:ILE:HG23	2:C:894:TRP:NE1	2.35	0.41
1:D:229:ILE:H	1:D:229:ILE:HG13	1.40	0.41
2:C:284:ILE:HG13	2:C:365:GLU:OE2	2.19	0.41
8:C:1103:CLR:H262	9:A:1104:PCW:C45	2.50	0.41
1:B:85:ILE:HG23	2:A:894:TRP:NE1	2.35	0.41
1:B:114:ASN:OD1	1:B:154:ARG:NH1	2.53	0.41
2:A:673:LEU:HD22	2:A:677:VAL:HG11	2.01	0.41
3:G:16:TYR:CD2	9:G:101:PCW:H62	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:150:GLN:HG3	2:C:342:VAL:HG21	2.02	0.41
2:C:307:PHE:CD1	2:C:320:ALA:HB1	2.55	0.41
2:C:545:LEU:HA	2:C:545:LEU:HD23	1.70	0.41
2:C:899:GLU:HA	2:C:904:GLN:O	2.20	0.41
9:C:1106:PCW:H271	9:C:1106:PCW:H241	1.66	0.41
1:B:85:ILE:O	1:B:88:GLU:HG2	2.20	0.41
9:B:401:PCW:H412	9:B:401:PCW:H20	2.02	0.41
2:A:540:ASN:HD22	2:A:540:ASN:N	2.17	0.41
2:C:172:ILE:HG12	2:C:177:LYS:HG2	2.01	0.41
2:C:425:ALA:HB1	2:C:456:LEU:HD22	2.01	0.41
2:A:263:ASP:C	2:A:265:THR:H	2.27	0.41
2:A:899:GLU:HA	2:A:904:GLN:O	2.20	0.41
9:A:1104:PCW:H412	9:A:1104:PCW:H20	2.02	0.41
1:D:106:MET:O	1:D:110:MET:HG2	2.21	0.41
2:C:975:ASP:OD1	2:C:975:ASP:N	2.52	0.41
2:A:225:GLN:HE21	2:A:225:GLN:H	1.68	0.41
2:A:900:ASP:OD2	2:A:904:GLN:HB2	2.20	0.41
1:D:85:ILE:O	1:D:88:GLU:HG2	2.20	0.41
8:D:401:CLR:H161	8:D:401:CLR:H222	1.94	0.41
3:E:16:TYR:CD2	9:E:101:PCW:H62	2.55	0.41
2:A:338:ALA:O	2:A:342:VAL:HG23	2.20	0.41
2:A:427:LEU:HG	2:A:493:HIS:CE1	2.55	0.41
2:A:433:PHE:CD1	2:A:447:VAL:HG22	2.55	0.41
2:A:692:ARG:HA	2:A:692:ARG:HD3	1.65	0.41
2:A:1002:ASP:OD1	2:A:1005:ARG:NH1	2.54	0.41
2:C:708:GLN:HE21	2:C:708:GLN:N	2.19	0.41
2:A:789:PRO:HB3	2:A:801:PRO:HD2	2.02	0.41
2:A:797:ASN:OD1	2:A:887:ARG:NE	2.46	0.41
2:A:942:ASN:HA	2:A:1010:ARG:NH1	2.35	0.41
1:D:114:ASN:OD1	1:D:154:ARG:NH1	2.53	0.41
2:C:731:GLY:O	2:C:746:ALA:HB1	2.20	0.41
3:G:41:GLY:O	3:G:42:LYS:HB2	2.20	0.41
1:D:123:PRO:HD2	1:D:124:PHE:CE2	2.56	0.41
2:C:390:HIS:CE1	2:C:548:LEU:HD23	2.56	0.41
2:C:427:LEU:HG	2:C:493:HIS:CE1	2.56	0.41
2:C:433:PHE:CD1	2:C:447:VAL:HG22	2.55	0.41
2:C:523:LEU:HA	2:C:523:LEU:HD23	1.82	0.41
2:C:996:LEU:HD12	9:A:1106:PCW:H482	2.03	0.41
2:C:996:LEU:CD1	9:A:1106:PCW:H482	2.51	0.41
2:C:1002:ASP:OD1	2:C:1005:ARG:NH1	2.54	0.41
1:B:106:MET:O	1:B:110:MET:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:150:GLN:HG3	2:A:342:VAL:HG21	2.02	0.41
2:A:603:VAL:HG21	2:A:631:VAL:O	2.21	0.41
2:A:627:ILE:O	2:A:631:VAL:HG22	2.21	0.41
2:A:923:PHE:CD2	2:A:980:MET:HE1	2.56	0.41
9:A:1106:PCW:H182	9:A:1106:PCW:H412	2.03	0.41
1:D:56:GLN:OE1	1:D:56:GLN:HA	2.20	0.41
1:D:191:PRO:HG3	1:D:208:GLN:O	2.21	0.41
2:C:803:GLY:O	2:C:807:ILE:HG13	2.21	0.41
1:B:56:GLN:OE1	1:B:56:GLN:HA	2.20	0.41
2:A:132:LEU:HD12	2:A:132:LEU:HA	1.92	0.41
2:C:560:LEU:HD23	2:C:560:LEU:HA	1.91	0.40
3:E:25:ILE:HD13	9:E:101:PCW:H172	2.03	0.40
1:B:174:LYS:HD3	1:B:266:THR:HG23	2.03	0.40
1:B:194:ASN:HB2	1:B:206:TYR:CE2	2.57	0.40
2:A:295:ILE:HD13	2:A:333:PRO:HD3	2.03	0.40
2:A:390:HIS:CE1	2:A:548:LEU:HD23	2.56	0.40
2:A:425:ALA:HB1	2:A:456:LEU:HD22	2.01	0.40
2:A:979:ARG:HA	2:A:979:ARG:HD2	1.80	0.40
2:C:603:VAL:HG21	2:C:631:VAL:O	2.21	0.40
2:C:979:ARG:HD2	2:C:979:ARG:HA	1.80	0.40
9:C:1104:PCW:H182	9:C:1104:PCW:H212	1.55	0.40
2:A:274:ALA:O	2:A:277:LEU:HD13	2.20	0.40
2:A:769:PHE:CZ	2:A:844:LEU:HD12	2.56	0.40
3:G:25:ILE:HD13	9:G:101:PCW:H172	2.03	0.40
2:C:131:TYR:O	2:C:135:VAL:HG23	2.21	0.40
2:C:295:ILE:HD13	2:C:333:PRO:HD3	2.03	0.40
2:C:398:HIS:ND1	2:C:411:PHE:HB3	2.37	0.40
2:C:769:PHE:CZ	2:C:844:LEU:HD12	2.56	0.40
2:C:789:PRO:HB3	2:C:801:PRO:HD2	2.02	0.40
2:C:942:ASN:HA	2:C:1010:ARG:NH1	2.35	0.40
1:B:163:LEU:HD23	4:K:6:FUC:H61	2.04	0.40
2:A:277:LEU:HB3	2:A:278:GLU:H	1.72	0.40
1:D:194:ASN:HB2	1:D:206:TYR:CE2	2.57	0.40
2:C:295:ILE:HG21	2:C:333:PRO:HD2	2.04	0.40
2:C:873:LEU:HD23	2:C:873:LEU:HA	1.87	0.40
2:C:923:PHE:CD2	2:C:980:MET:HE1	2.56	0.40
1:B:123:PRO:HD2	1:B:124:PHE:CE2	2.56	0.40
2:A:45:LYS:NZ	2:A:234:GLU:OE1	2.44	0.40
2:A:316:SER:O	2:A:319:GLU:N	2.53	0.40
2:A:354:LYS:O	2:A:355:ASN:HB2	2.21	0.40
2:C:627:ILE:O	2:C:631:VAL:HG22	2.21	0.40

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%)	270 (92%)	21 (7%)	1 (0%)	37	67
1	D	292/305 (96%)	270 (92%)	21 (7%)	1 (0%)	37	67
2	A	980/1028 (95%)	895 (91%)	85 (9%)	0	100	100
2	C	980/1028 (95%)	895 (91%)	85 (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%)	2402 (92%)	216 (8%)	2 (0%)	50	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	30	GLY
1	B	30	GLY

### 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%)	226 (88%)	32 (12%)	4	20
1	D	258/266 (97%)	226 (88%)	32 (12%)	4	20
2	A	830/869 (96%)	736 (89%)	94 (11%)	4	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	830/869 (96%)	736 (89%)	94 (11%)	4	23
3	E	33/75 (44%)	32 (97%)	1 (3%)	36	58
3	G	33/75 (44%)	32 (97%)	1 (3%)	36	58
All	All	2242/2420 (93%)	1988 (89%)	254 (11%)	7	23

All (254) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	20	SER
1	D	56	GLN
1	D	62	LEU
1	D	65	PHE
1	D	73	VAL
1	D	79	SER
1	D	94	SER
1	D	107	HIS
1	D	144	GLN
1	D	154	ARG
1	D	156	TRP
1	D	157	LEU
1	D	159	ASN
1	D	160	CYS
1	D	161	SER
1	D	167	THR
1	D	196	THR
1	D	200	GLU
1	D	203	GLN
1	D	211	LEU
1	D	214	ARG
1	D	218	LYS
1	D	229	ILE
1	D	242	LEU
1	D	266	THR
1	D	268	LEU
1	D	269	THR
1	D	272	MET
1	D	285	ILE
1	D	289	GLU
1	D	292	ARG
1	D	294	ARG
2	C	45	LYS

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Mol	Chain	Res	Type
2	C	54	LYS
2	C	63	LEU
2	C	64	THR
2	C	75	ASP
2	C	89	TRP
2	C	92	PHE
2	C	118	GLN
2	C	150	GLN
2	C	164	MET
2	C	167	GLN
2	C	168	GLN
2	C	225	GLN
2	C	231	PHE
2	C	240	ARG
2	C	241	ASN
2	C	248	ASN
2	C	263	ASP
2	C	273	LEU
2	C	277	LEU
2	C	278	GLU
2	C	279	VAL
2	C	282	THR
2	C	294	ILE
2	C	295	ILE
2	C	309	LEU
2	C	346	LEU
2	C	356	CYS
2	C	357	LEU
2	C	359	LYS
2	C	367	LEU
2	C	378	THR
2	C	380	THR
2	C	386	MET
2	C	387	THR
2	C	402	THR
2	C	406	GLN
2	C	424	ILE
2	C	434	GLN
2	C	440	VAL
2	C	445	ARG
2	C	450	ASP
2	C	462	LEU

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Mol	Chain	Res	Type
2	C	470	MET
2	C	484	SER
2	C	487	LYS
2	C	490	LEU
2	C	493	HIS
2	C	515	LEU
2	C	519	SER
2	C	522	LEU
2	C	530	LEU
2	C	548	LEU
2	C	551	ARG
2	C	571	PHE
2	C	589	MET
2	C	629	LYS
2	C	676	GLU
2	C	692	ARG
2	C	693	THR
2	C	696	GLN
2	C	708	GLN
2	C	727	LYS
2	C	739	SER
2	C	775	SER
2	C	779	THR
2	C	794	ILE
2	C	804	THR
2	C	816	MET
2	C	822	LEU
2	C	830	ASP
2	C	831	ILE
2	C	835	GLN
2	C	842	ASP
2	C	843	LYS
2	C	844	LEU
2	C	848	ARG
2	C	849	LEU
2	C	879	LEU
2	C	882	ASP
2	C	889	ARG
2	C	897	ASP
2	C	940	ARG
2	C	944	ILE
2	C	964	LEU

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Mol	Chain	Res	Type
2	C	975	ASP
2	C	978	LEU
2	C	983	LEU
2	C	997	ILE
2	C	1005	ARG
2	C	1007	PHE
2	C	1011	ARG
2	C	1020	GLU
2	C	1021	THR
3	E	33	ILE
1	B	20	SER
1	B	56	GLN
1	B	62	LEU
1	B	65	PHE
1	B	73	VAL
1	B	79	SER
1	B	94	SER
1	B	107	HIS
1	B	144	GLN
1	B	154	ARG
1	B	156	TRP
1	B	157	LEU
1	B	159	ASN
1	B	160	CYS
1	B	161	SER
1	B	167	THR
1	B	196	THR
1	B	200	GLU
1	B	203	GLN
1	B	211	LEU
1	B	214	ARG
1	B	218	LYS
1	B	229	ILE
1	B	242	LEU
1	B	266	THR
1	B	268	LEU
1	B	269	THR
1	B	272	MET
1	B	285	ILE
1	B	289	GLU
1	B	292	ARG
1	B	294	ARG

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Mol	Chain	Res	Type
2	A	45	LYS
2	A	54	LYS
2	A	63	LEU
2	A	64	THR
2	A	75	ASP
2	A	89	TRP
2	A	92	PHE
2	A	118	GLN
2	A	150	GLN
2	A	164	MET
2	A	167	GLN
2	A	168	GLN
2	A	225	GLN
2	A	231	PHE
2	A	240	ARG
2	A	241	ASN
2	A	248	ASN
2	A	263	ASP
2	A	273	LEU
2	A	277	LEU
2	A	278	GLU
2	A	279	VAL
2	A	282	THR
2	A	294	ILE
2	A	295	ILE
2	A	309	LEU
2	A	346	LEU
2	A	356	CYS
2	A	357	LEU
2	A	359	LYS
2	A	367	LEU
2	A	378	THR
2	A	380	THR
2	A	386	MET
2	A	387	THR
2	A	402	THR
2	A	406	GLN
2	A	424	ILE
2	A	434	GLN
2	A	440	VAL
2	A	445	ARG
2	A	450	ASP

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Mol	Chain	Res	Type
2	A	462	LEU
2	A	470	MET
2	A	484	SER
2	A	487	LYS
2	A	490	LEU
2	A	493	HIS
2	A	515	LEU
2	A	519	SER
2	A	522	LEU
2	A	530	LEU
2	A	548	LEU
2	A	551	ARG
2	A	571	PHE
2	A	589	MET
2	A	629	LYS
2	A	676	GLU
2	A	692	ARG
2	A	693	THR
2	A	696	GLN
2	A	708	GLN
2	A	727	LYS
2	A	739	SER
2	A	775	SER
2	A	779	THR
2	A	794	ILE
2	A	804	THR
2	A	816	MET
2	A	822	LEU
2	A	830	ASP
2	A	831	ILE
2	A	835	GLN
2	A	842	ASP
2	A	843	LYS
2	A	844	LEU
2	A	848	ARG
2	A	849	LEU
2	A	879	LEU
2	A	882	ASP
2	A	889	ARG
2	A	897	ASP
2	A	940	ARG
2	A	944	ILE

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Mol	Chain	Res	Type
2	A	964	LEU
2	A	975	ASP
2	A	978	LEU
2	A	983	LEU
2	A	997	ILE
2	A	1005	ARG
2	A	1007	PHE
2	A	1011	ARG
2	A	1020	GLU
2	A	1021	THR
3	G	33	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	121	ASN
1	D	203	GLN
1	D	258	GLN
2	C	52	HIS
2	C	127	ASN
2	C	225	GLN
2	C	241	ASN
2	C	248	ASN
2	C	360	ASN
2	C	383	GLN
2	C	390	HIS
2	C	434	GLN
2	C	539	GLN
2	C	540	ASN
2	C	620	HIS
2	C	654	GLN
2	C	656	ASN
2	C	708	GLN
2	C	744	GLN
2	C	826	GLN
2	C	835	GLN
2	C	861	GLN
2	C	930	GLN
2	C	942	ASN
2	C	946	GLN
1	B	203	GLN
1	B	258	GLN

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Mol	Chain	Res	Type
2	A	52	HIS
2	A	127	ASN
2	A	225	GLN
2	A	241	ASN
2	A	248	ASN
2	A	360	ASN
2	A	383	GLN
2	A	390	HIS
2	A	434	GLN
2	A	540	ASN
2	A	557	HIS
2	A	620	HIS
2	A	654	GLN
2	A	656	ASN
2	A	696	GLN
2	A	708	GLN
2	A	720	ASN
2	A	744	GLN
2	A	826	GLN
2	A	835	GLN
2	A	861	GLN
2	A	930	GLN
2	A	942	ASN
2	A	946	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

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	0.66	0	17,19,21	1.45	4 (23%)
4	NAG	F	2	4	14,14,15	0.66	0	17,19,21	1.22	2 (11%)
4	BMA	F	3	4	11,11,12	0.82	0	15,15,17	1.76	2 (13%)
4	MAN	F	4	4	11,11,12	0.82	0	15,15,17	1.06	1 (6%)
4	MAN	F	5	4	11,11,12	0.77	0	15,15,17	1.01	1 (6%)
4	FUC	F	6	4	10,10,11	0.95	1 (10%)	14,14,16	1.11	0
5	NAG	H	1	5,1	14,14,15	0.76	0	17,19,21	1.89	2 (11%)
5	NAG	H	2	5	14,14,15	0.67	0	17,19,21	2.54	6 (35%)
5	BMA	H	3	5	11,11,12	1.41	1 (9%)	15,15,17	1.90	5 (33%)
5	MAN	H	4	5	11,11,12	0.79	0	15,15,17	1.47	3 (20%)
5	NAG	H	5	5	14,14,15	0.75	0	17,19,21	1.15	1 (5%)
5	MAN	H	6	5	11,11,12	0.68	0	15,15,17	1.14	1 (6%)
6	NAG	I	1	6,1	14,14,15	0.72	0	17,19,21	1.69	3 (17%)
6	NAG	I	2	6	14,14,15	0.67	0	17,19,21	1.05	1 (5%)
6	BMA	I	3	6	11,11,12	0.80	0	15,15,17	1.66	2 (13%)
6	MAN	I	4	6	11,11,12	0.82	0	15,15,17	1.08	1 (6%)
6	FUC	I	5	6	10,10,11	0.93	1 (10%)	14,14,16	1.09	0
7	NAG	J	1	7,1	14,14,15	0.73	0	17,19,21	1.18	2 (11%)
7	NAG	J	2	7	14,14,15	0.69	0	17,19,21	0.95	0
4	NAG	K	1	4,1	14,14,15	0.66	0	17,19,21	1.45	4 (23%)
4	NAG	K	2	4	14,14,15	0.66	0	17,19,21	1.22	2 (11%)
4	BMA	K	3	4	11,11,12	0.82	0	15,15,17	1.76	2 (13%)
4	MAN	K	4	4	11,11,12	0.82	0	15,15,17	1.06	1 (6%)
4	MAN	K	5	4	11,11,12	0.77	0	15,15,17	1.01	1 (6%)
4	FUC	K	6	4	10,10,11	0.95	1 (10%)	14,14,16	1.11	0
5	NAG	L	1	5,1	14,14,15	0.76	0	17,19,21	1.89	2 (11%)
5	NAG	L	2	5	14,14,15	0.67	0	17,19,21	2.54	6 (35%)
5	BMA	L	3	5	11,11,12	1.41	1 (9%)	15,15,17	1.90	5 (33%)
5	MAN	L	4	5	11,11,12	0.79	0	15,15,17	1.47	3 (20%)
5	NAG	L	5	5	14,14,15	0.74	0	17,19,21	1.15	1 (5%)
5	MAN	L	6	5	11,11,12	0.68	0	15,15,17	1.14	1 (6%)
6	NAG	M	1	6,1	14,14,15	0.72	0	17,19,21	1.69	3 (17%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	M	2	6	14,14,15	0.67	0	17,19,21	1.06	1 (5%)
6	BMA	M	3	6	11,11,12	0.80	0	15,15,17	1.66	2 (13%)
6	MAN	M	4	6	11,11,12	0.82	0	15,15,17	1.08	1 (6%)
6	FUC	M	5	6	10,10,11	0.93	1 (10%)	14,14,16	1.09	0
7	NAG	N	1	7,1	14,14,15	0.73	0	17,19,21	1.18	2 (11%)
7	NAG	N	2	7	14,14,15	0.69	0	17,19,21	0.95	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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	3	BMA	O5-C1	-3.76	1.37	1.43
5	H	3	BMA	O5-C1	-3.75	1.37	1.43
4	F	6	FUC	O5-C1	-2.39	1.39	1.43
4	K	6	FUC	O5-C1	-2.39	1.39	1.43
6	I	5	FUC	O5-C1	-2.28	1.40	1.43
6	M	5	FUC	O5-C1	-2.28	1.40	1.43

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	2	NAG	C1-O5-C5	6.12	120.48	112.19
5	L	2	NAG	C1-O5-C5	6.11	120.48	112.19
5	H	2	NAG	C2-N2-C7	5.09	130.15	122.90
5	L	2	NAG	C2-N2-C7	5.09	130.15	122.90
5	L	1	NAG	O4-C4-C5	4.79	121.19	109.30
5	H	1	NAG	O4-C4-C5	4.79	121.19	109.30
5	H	1	NAG	C1-O5-C5	4.78	118.66	112.19
5	L	1	NAG	C1-O5-C5	4.78	118.66	112.19
6	M	1	NAG	C1-O5-C5	4.59	118.41	112.19
5	L	3	BMA	O5-C5-C6	4.59	114.40	107.20
5	H	3	BMA	O5-C5-C6	4.59	114.40	107.20
6	I	1	NAG	C1-O5-C5	4.59	118.41	112.19
4	K	3	BMA	O5-C5-C6	4.32	113.98	107.20
4	F	3	BMA	O5-C5-C6	4.32	113.97	107.20
4	K	3	BMA	C1-O5-C5	3.89	117.46	112.19
4	F	3	BMA	C1-O5-C5	3.89	117.46	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	3	BMA	O5-C5-C6	3.80	113.16	107.20
6	I	3	BMA	O5-C5-C6	3.79	113.15	107.20
6	M	3	BMA	C1-O5-C5	3.32	116.69	112.19
6	I	3	BMA	C1-O5-C5	3.32	116.69	112.19
5	L	2	NAG	O4-C4-C3	-3.25	102.84	110.35
5	H	2	NAG	O4-C4-C3	-3.25	102.84	110.35
5	L	4	MAN	C1-O5-C5	3.19	116.51	112.19
5	H	4	MAN	C1-O5-C5	3.19	116.51	112.19
5	L	6	MAN	C1-O5-C5	3.18	116.50	112.19
5	H	6	MAN	C1-O5-C5	3.18	116.50	112.19
7	J	1	NAG	O4-C4-C3	-3.08	103.23	110.35
7	N	1	NAG	O4-C4-C3	-3.08	103.24	110.35
4	K	2	NAG	C1-O5-C5	3.00	116.26	112.19
4	F	2	NAG	C1-O5-C5	3.00	116.25	112.19
4	K	1	NAG	C1-O5-C5	2.96	116.20	112.19
4	F	1	NAG	C1-O5-C5	2.95	116.19	112.19
5	H	2	NAG	C3-C4-C5	-2.90	105.07	110.24
5	L	2	NAG	C3-C4-C5	-2.90	105.07	110.24
5	H	5	NAG	C1-O5-C5	2.79	115.98	112.19
5	L	5	NAG	C1-O5-C5	2.79	115.97	112.19
5	L	4	MAN	O2-C2-C3	2.70	115.55	110.14
4	K	1	NAG	O4-C4-C3	-2.70	104.10	110.35
4	F	1	NAG	O4-C4-C3	-2.70	104.11	110.35
5	H	4	MAN	O2-C2-C3	2.70	115.54	110.14
6	I	1	NAG	O4-C4-C3	-2.64	104.25	110.35
6	M	1	NAG	O4-C4-C3	-2.64	104.25	110.35
5	H	4	MAN	O2-C2-C1	2.64	114.55	109.15
5	L	4	MAN	O2-C2-C1	2.63	114.54	109.15
5	L	3	BMA	C1-O5-C5	2.62	115.75	112.19
5	H	3	BMA	C1-O5-C5	2.62	115.75	112.19
4	F	5	MAN	C1-O5-C5	2.51	115.59	112.19
4	K	5	MAN	C1-O5-C5	2.51	115.59	112.19
5	L	3	BMA	O3-C3-C4	2.50	116.12	110.35
5	H	3	BMA	O3-C3-C4	2.49	116.11	110.35
6	M	2	NAG	C1-O5-C5	2.48	115.55	112.19
6	I	2	NAG	C1-O5-C5	2.48	115.55	112.19
4	F	1	NAG	O5-C1-C2	-2.39	107.51	111.29
4	K	1	NAG	O5-C1-C2	-2.39	107.51	111.29
6	I	4	MAN	C1-O5-C5	2.32	115.34	112.19
6	M	4	MAN	C1-O5-C5	2.32	115.34	112.19
7	N	1	NAG	O5-C1-C2	-2.26	107.71	111.29
4	F	4	MAN	C1-O5-C5	2.26	115.26	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	4	MAN	C1-O5-C5	2.26	115.26	112.19
7	J	1	NAG	O5-C1-C2	-2.26	107.72	111.29
5	L	3	BMA	O4-C4-C5	2.26	114.90	109.30
5	H	3	BMA	O4-C4-C5	2.25	114.89	109.30
5	H	2	NAG	O4-C4-C5	2.23	114.84	109.30
5	L	2	NAG	O4-C4-C5	2.23	114.84	109.30
4	K	2	NAG	O5-C1-C2	-2.17	107.86	111.29
4	F	2	NAG	O5-C1-C2	-2.17	107.87	111.29
5	H	3	BMA	O3-C3-C2	2.16	114.13	109.99
5	L	3	BMA	O3-C3-C2	2.16	114.13	109.99
6	M	1	NAG	O4-C4-C5	2.10	114.51	109.30
6	I	1	NAG	O4-C4-C5	2.10	114.50	109.30
5	L	2	NAG	O5-C1-C2	-2.08	108.01	111.29
5	H	2	NAG	O5-C1-C2	-2.08	108.01	111.29
4	K	1	NAG	O4-C4-C5	2.01	114.30	109.30
4	F	1	NAG	O4-C4-C5	2.01	114.30	109.30

There are no chirality outliers.

All (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	3	BMA	O5-C5-C6-O6
5	L	3	BMA	O5-C5-C6-O6
5	H	6	MAN	O5-C5-C6-O6
5	L	6	MAN	O5-C5-C6-O6
5	H	5	NAG	C4-C5-C6-O6
5	L	5	NAG	C4-C5-C6-O6
5	H	5	NAG	O5-C5-C6-O6
5	L	5	NAG	O5-C5-C6-O6
5	H	6	MAN	C4-C5-C6-O6
5	L	6	MAN	C4-C5-C6-O6
5	H	3	BMA	C4-C5-C6-O6
5	L	3	BMA	C4-C5-C6-O6
5	H	5	NAG	C8-C7-N2-C2
5	H	5	NAG	O7-C7-N2-C2
5	L	5	NAG	C8-C7-N2-C2
5	L	5	NAG	O7-C7-N2-C2
5	H	2	NAG	C4-C5-C6-O6
5	L	2	NAG	C4-C5-C6-O6
5	H	2	NAG	O5-C5-C6-O6

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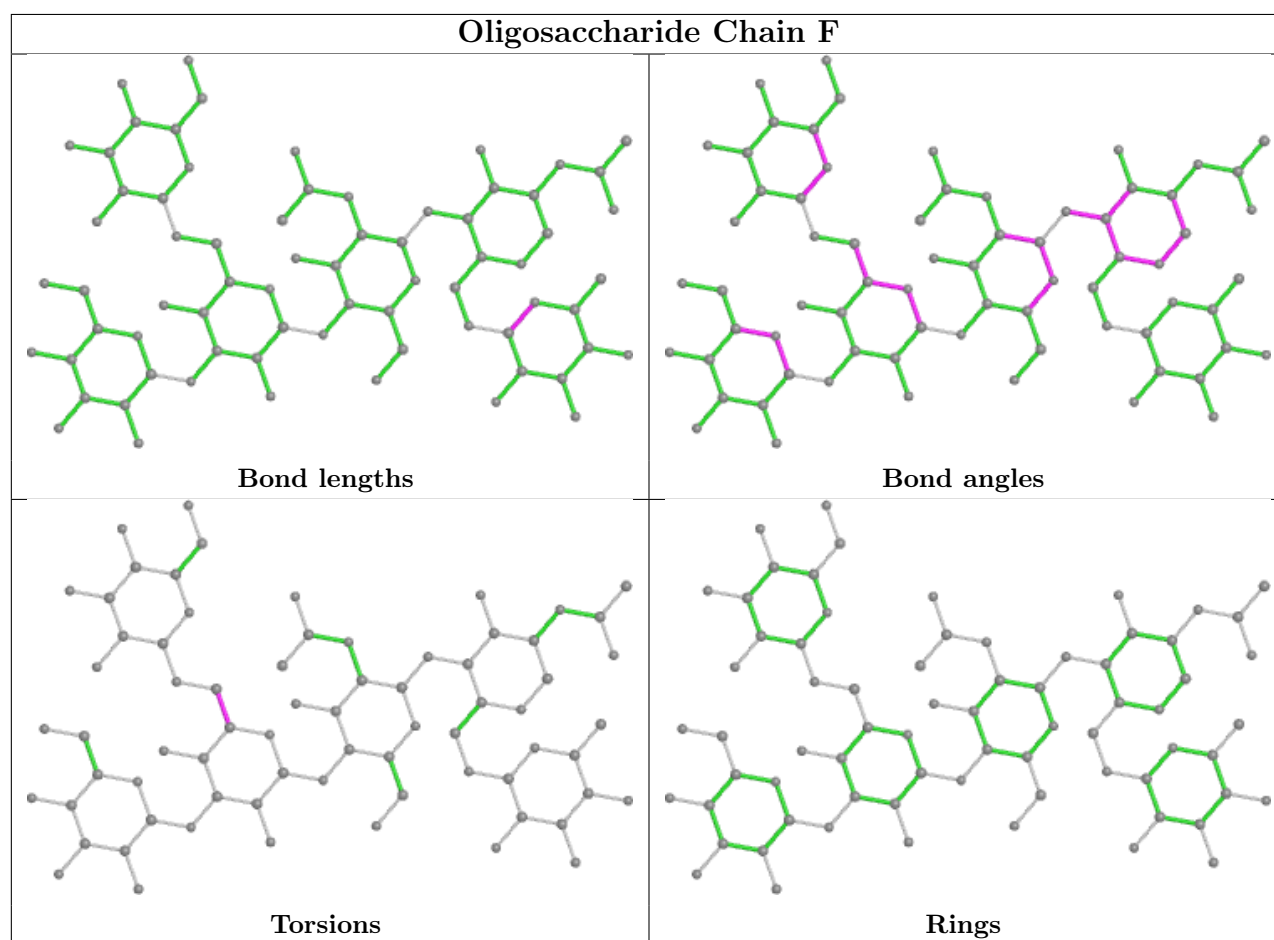
Mol	Chain	Res	Type	Atoms
5	L	2	NAG	O5-C5-C6-O6
6	I	3	BMA	O5-C5-C6-O6
6	M	3	BMA	O5-C5-C6-O6
4	F	3	BMA	O5-C5-C6-O6
4	K	3	BMA	O5-C5-C6-O6

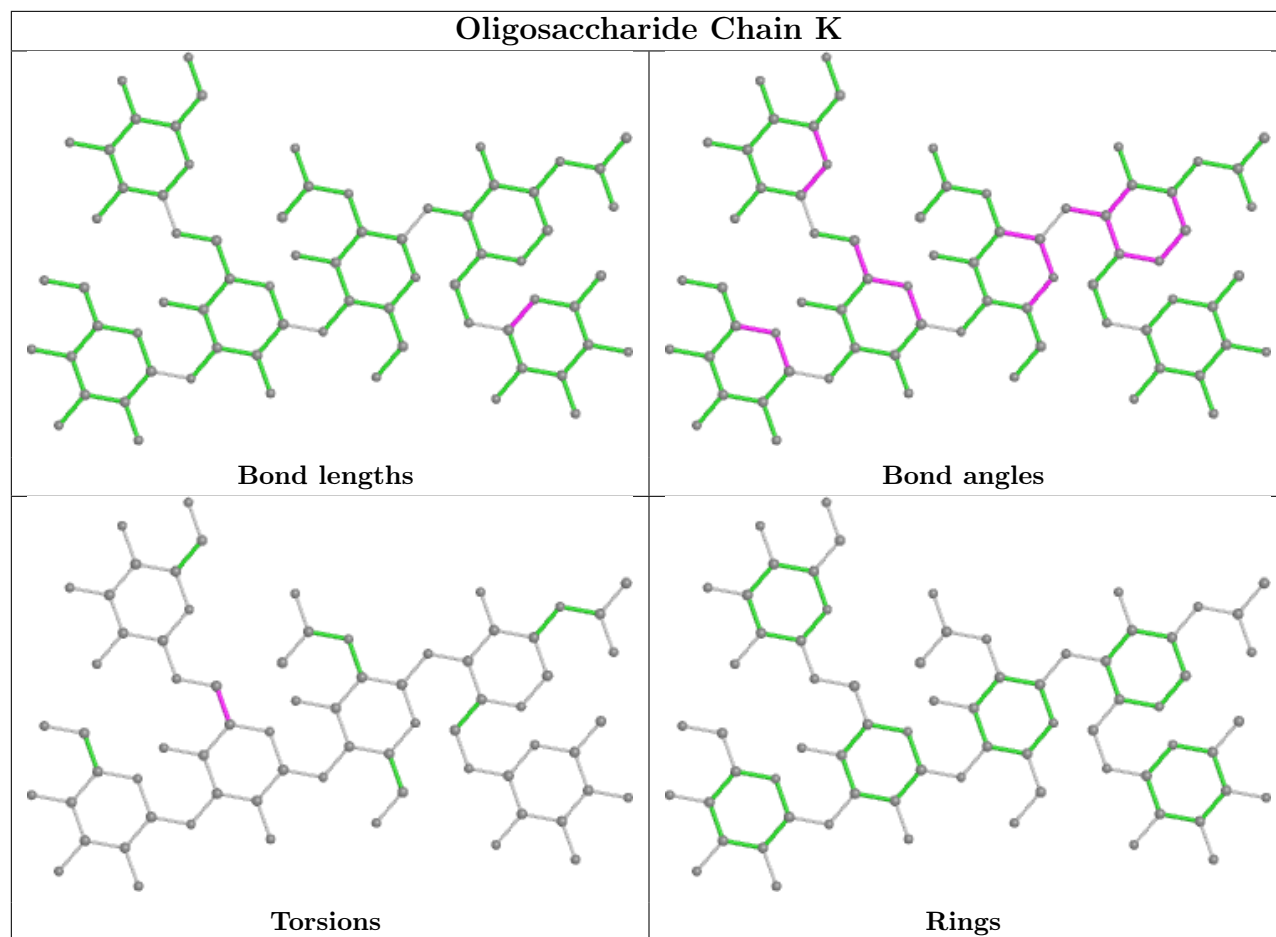
There are no ring outliers.

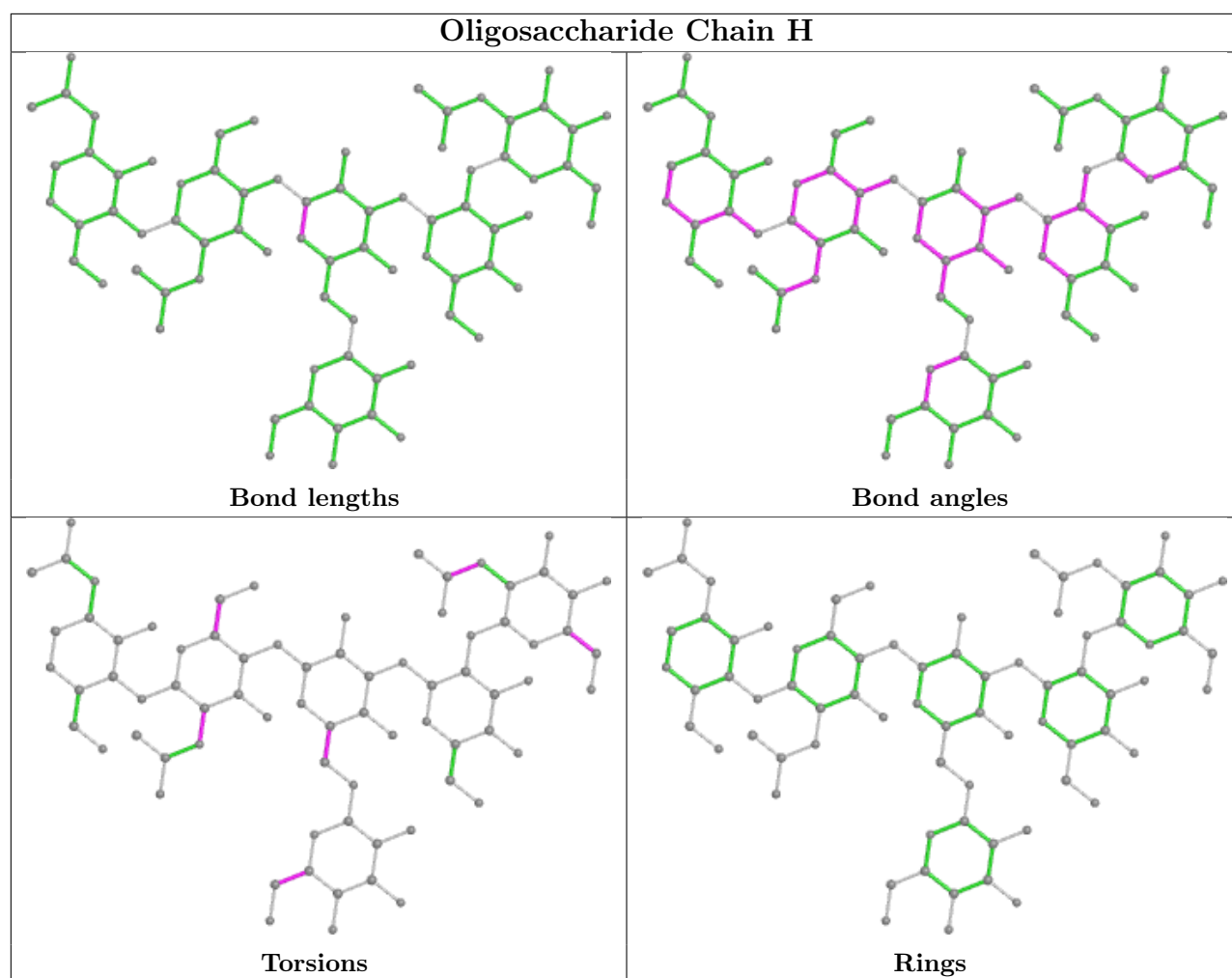
1 monomer is involved in 1 short contact:

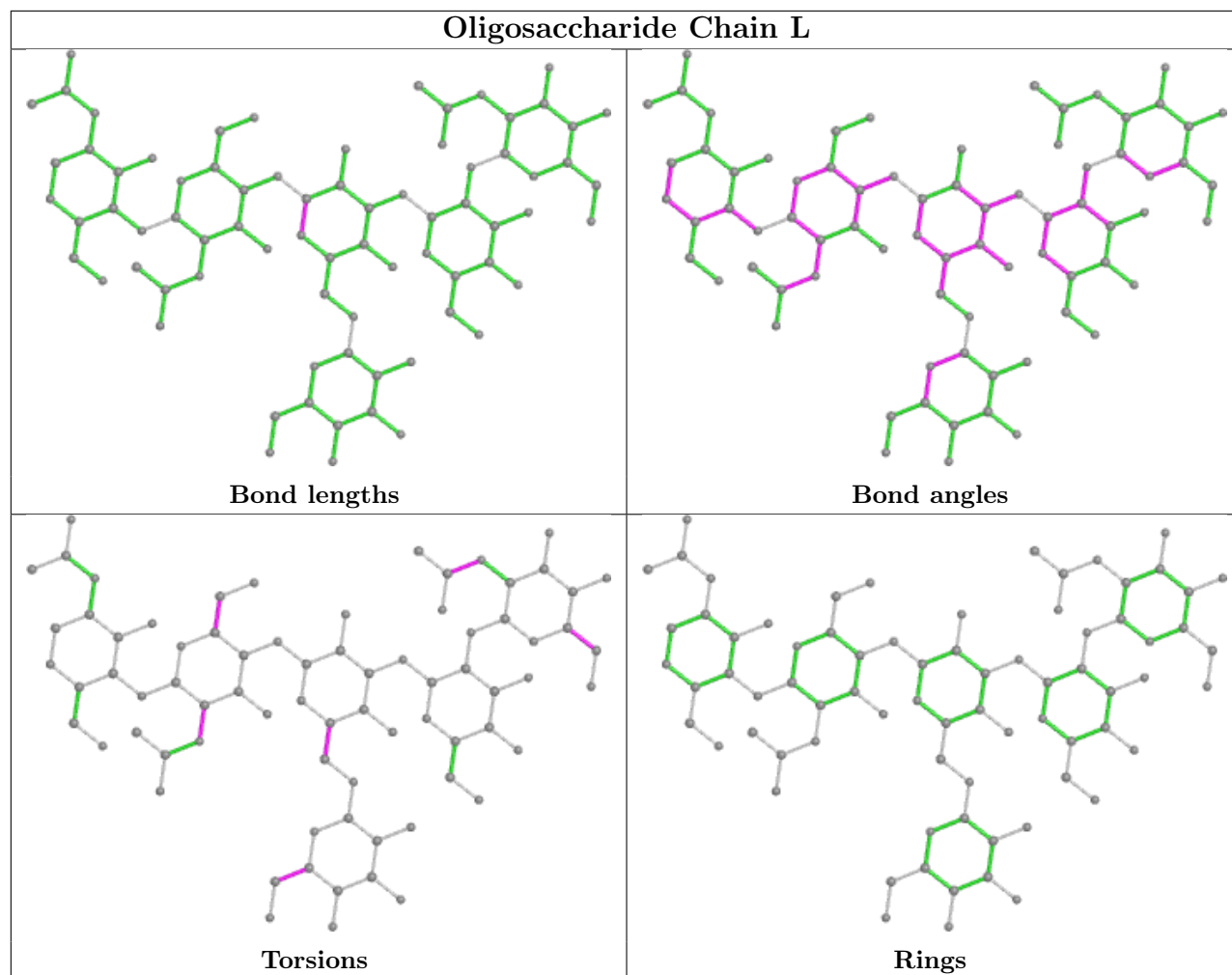
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	6	FUC	1	0

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

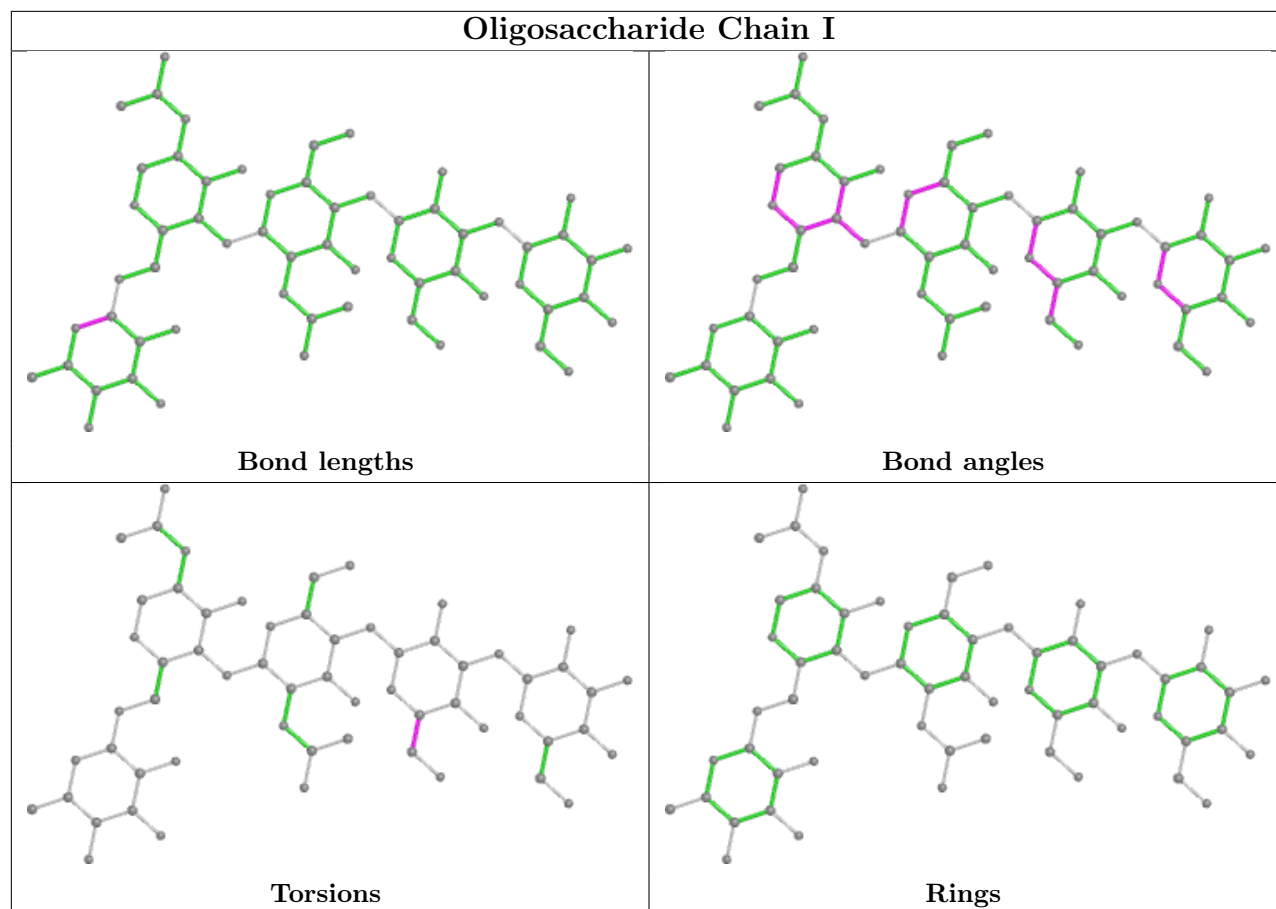


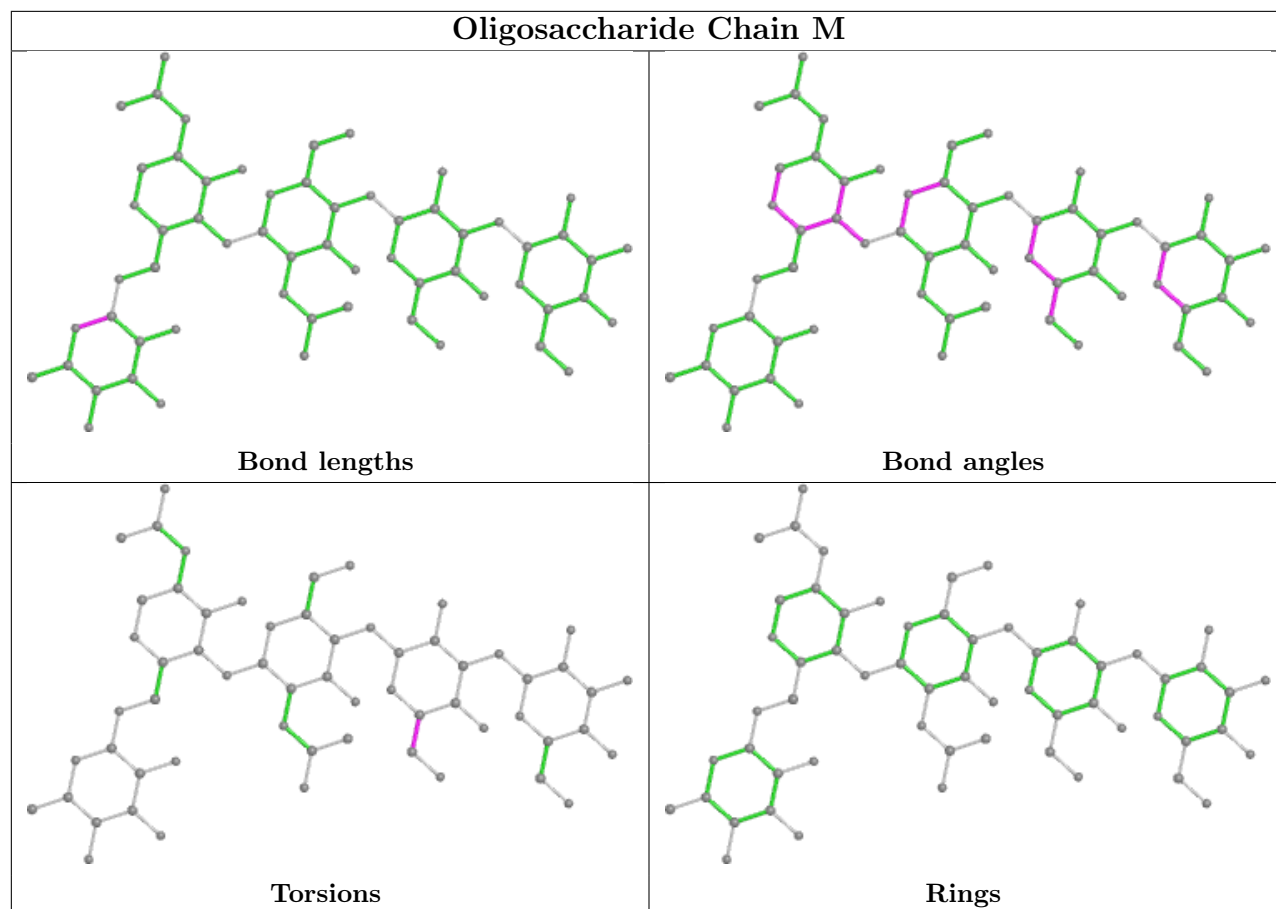


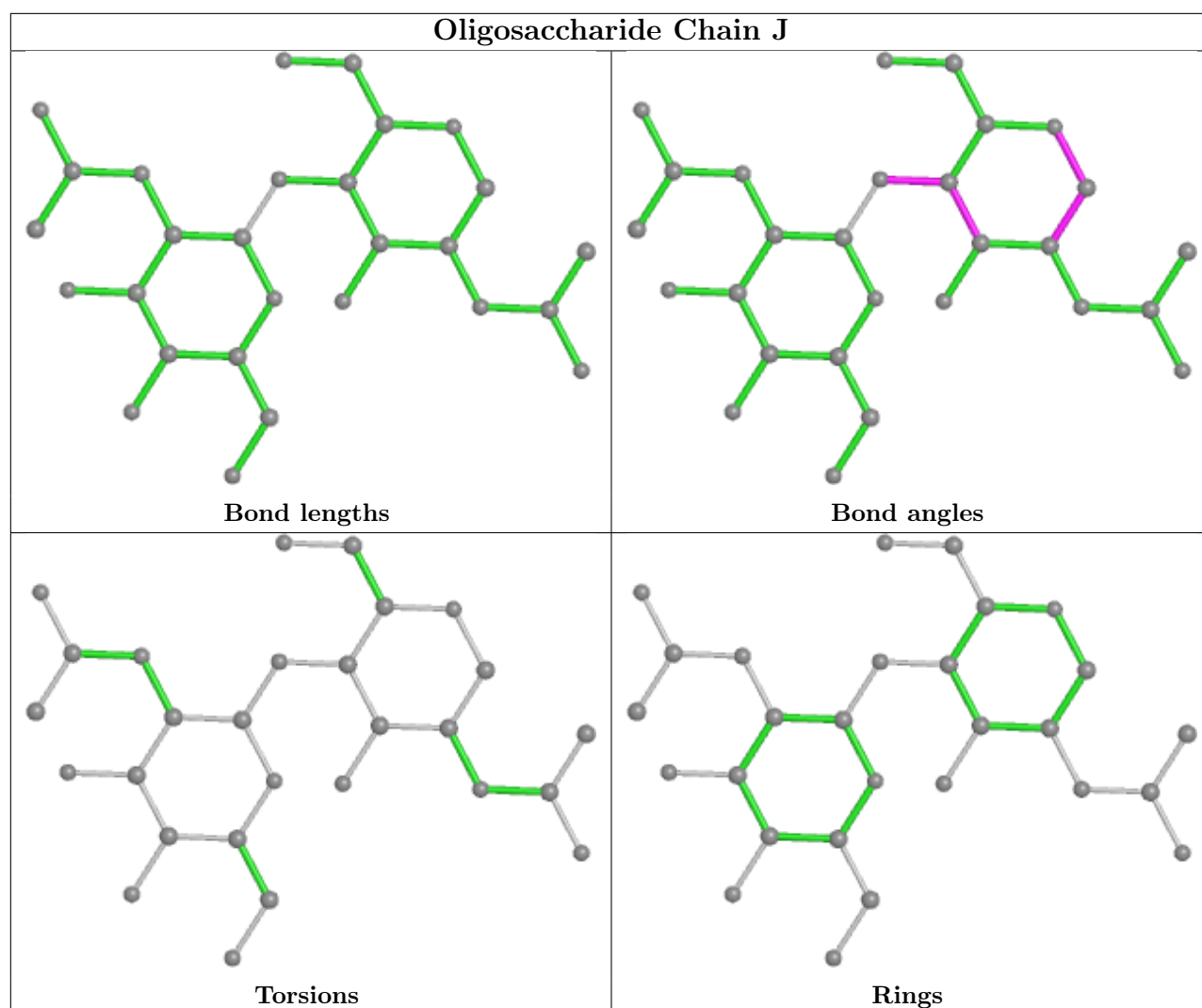


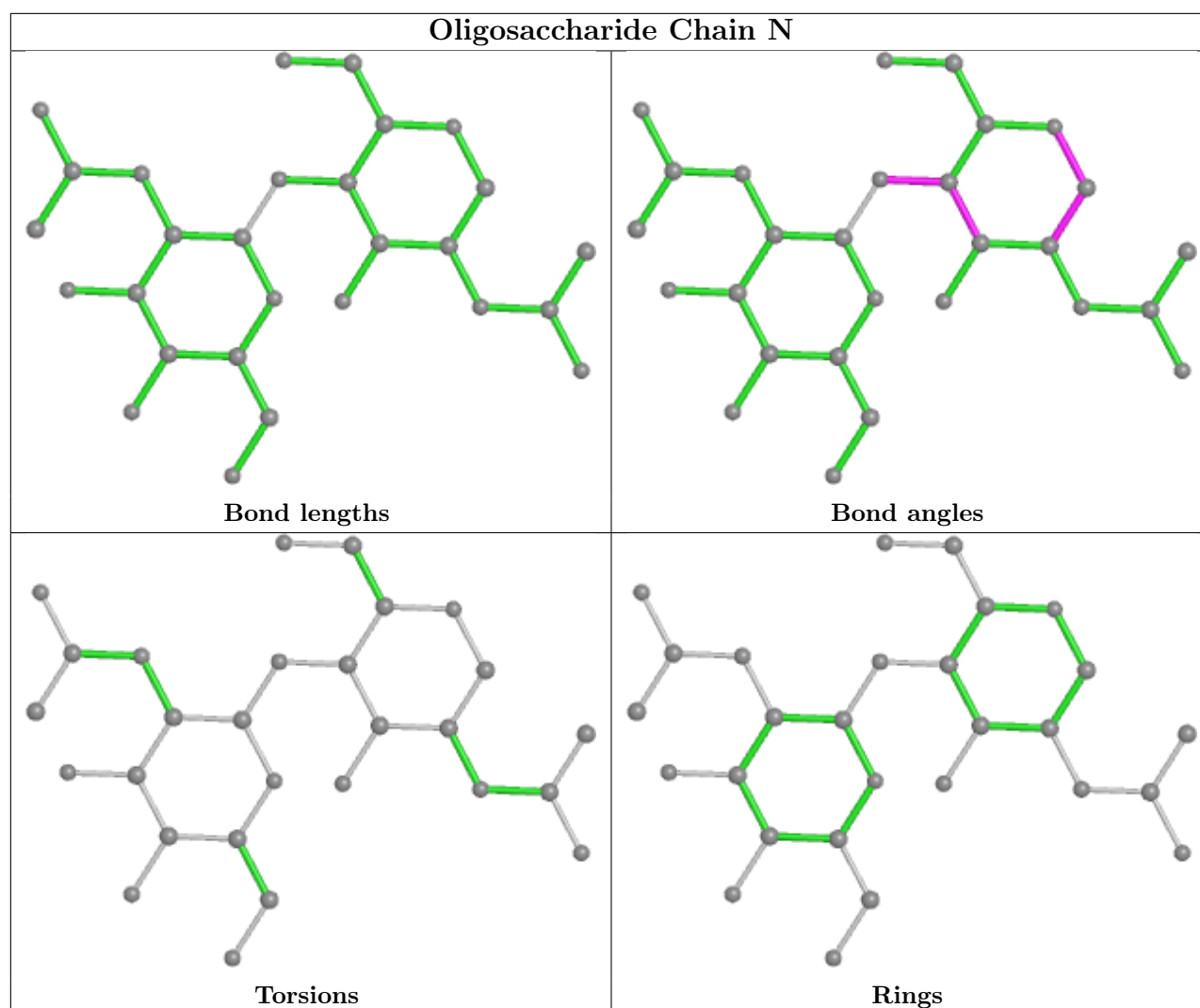












## 5.6 Ligand geometry [i](#)

Of 40 ligands modelled in this entry, 10 are monoatomic - leaving 30 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	C	1107	-	53,53,53	0.95	2 (3%)	59,61,61	0.89	1 (1%)
9	PCW	C	1106	-	53,53,53	0.96	2 (3%)	59,61,61	0.77	0
8	CLR	A	1103	-	31,31,31	1.16	3 (9%)	48,48,48	1.33	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  >
8	CLR	A	1102	-	31,31,31	1.15	3 (9%)	48,48,48	1.35	6 (12%)
11	ATP	C	1111	10	26,33,33	0.59	0	31,52,52	0.74	2 (6%)
9	PCW	B	401	-	53,53,53	0.95	2 (3%)	59,61,61	0.85	0
8	CLR	C	1101	-	31,31,31	1.15	2 (6%)	48,48,48	1.35	7 (14%)
9	PCW	E	101	-	53,53,53	0.97	2 (3%)	59,61,61	0.75	0
8	CLR	B	402	-	31,31,31	1.15	3 (9%)	48,48,48	1.34	5 (10%)
8	CLR	C	1109	-	31,31,31	1.16	3 (9%)	48,48,48	1.35	6 (12%)
8	CLR	C	1103	-	31,31,31	1.16	3 (9%)	48,48,48	1.33	4 (8%)
9	PCW	G	102	-	53,53,53	0.98	2 (3%)	59,61,61	0.78	1 (1%)
8	CLR	C	1102	-	31,31,31	1.15	3 (9%)	48,48,48	1.35	6 (12%)
8	CLR	A	1101	-	31,31,31	1.15	2 (6%)	48,48,48	1.35	7 (14%)
9	PCW	A	1106	-	53,53,53	0.96	2 (3%)	59,61,61	0.87	1 (1%)
9	PCW	A	1109	-	21,21,53	0.86	0	27,29,61	1.13	3 (11%)
13	A1MA6	C	1116	-	190,195,195	1.31	21 (11%)	219,278,278	1.69	35 (15%)
11	ATP	A	1112	10	26,33,33	0.59	0	31,52,52	0.74	2 (6%)
9	PCW	E	102	-	53,53,53	0.98	2 (3%)	59,61,61	0.78	1 (1%)
9	PCW	A	1108	-	53,53,53	0.95	2 (3%)	59,61,61	0.89	1 (1%)
9	PCW	C	1108	-	21,21,53	0.86	0	27,29,61	1.13	3 (11%)
9	PCW	A	1107	-	53,53,53	0.96	2 (3%)	59,61,61	0.77	0
13	A1MA6	A	1117	-	190,195,195	1.31	21 (11%)	219,278,278	1.69	35 (15%)
8	CLR	D	401	-	31,31,31	1.15	3 (9%)	48,48,48	1.34	5 (10%)
9	PCW	C	1104	-	53,53,53	0.97	2 (3%)	59,61,61	0.89	1 (1%)
9	PCW	C	1105	-	53,53,53	0.96	2 (3%)	59,61,61	0.87	1 (1%)
9	PCW	A	1105	-	53,53,53	0.97	2 (3%)	59,61,61	0.89	1 (1%)
8	CLR	A	1110	-	31,31,31	1.16	3 (9%)	48,48,48	1.35	6 (12%)
9	PCW	G	101	-	53,53,53	0.97	2 (3%)	59,61,61	0.75	0
9	PCW	A	1104	-	53,53,53	0.95	2 (3%)	59,61,61	0.85	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
9	PCW	C	1107	-	-	27/57/57/57	-
9	PCW	C	1106	-	-	28/57/57/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	CLR	A	1103	-	-	2/10/68/68	0/4/4/4
8	CLR	A	1102	-	-	0/10/68/68	0/4/4/4
11	ATP	C	1111	10	-	5/18/38/38	0/3/3/3
9	PCW	B	401	-	-	23/57/57/57	-
8	CLR	C	1101	-	-	1/10/68/68	0/4/4/4
9	PCW	E	101	-	-	21/57/57/57	-
8	CLR	B	402	-	-	0/10/68/68	0/4/4/4
8	CLR	C	1109	-	-	0/10/68/68	0/4/4/4
8	CLR	C	1103	-	-	2/10/68/68	0/4/4/4
9	PCW	G	102	-	-	20/57/57/57	-
8	CLR	C	1102	-	-	0/10/68/68	0/4/4/4
8	CLR	A	1101	-	-	1/10/68/68	0/4/4/4
9	PCW	A	1106	-	-	19/57/57/57	-
9	PCW	A	1109	-	-	5/23/23/57	-
13	A1MA6	C	1116	-	-	102/192/350/350	1/12/10/10
11	ATP	A	1112	10	-	5/18/38/38	0/3/3/3
9	PCW	E	102	-	-	20/57/57/57	-
9	PCW	A	1108	-	-	27/57/57/57	-
9	PCW	C	1108	-	-	5/23/23/57	-
9	PCW	A	1107	-	-	28/57/57/57	-
13	A1MA6	A	1117	-	-	102/192/350/350	1/12/10/10
8	CLR	D	401	-	-	0/10/68/68	0/4/4/4
9	PCW	C	1104	-	-	16/57/57/57	-
9	PCW	C	1105	-	-	19/57/57/57	-
9	PCW	A	1105	-	-	16/57/57/57	-
8	CLR	A	1110	-	-	0/10/68/68	0/4/4/4
9	PCW	G	101	-	-	21/57/57/57	-
9	PCW	A	1104	-	-	23/57/57/57	-

All (98) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	1116	A1MA6	OC2-C43	5.44	1.54	1.43
13	A	1117	A1MA6	OC2-C43	5.44	1.54	1.43
13	C	1116	A1MA6	OAO-CAP	5.38	1.57	1.45
13	A	1117	A1MA6	OAO-CAP	5.38	1.57	1.45
13	A	1117	A1MA6	CBL-CBM	-5.16	1.43	1.52
13	C	1116	A1MA6	CBL-CBM	-5.15	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	1116	A1MA6	CA3-CA4	4.50	1.54	1.45
13	A	1117	A1MA6	CA3-CA4	4.50	1.54	1.45
13	C	1116	A1MA6	OC2-C47	4.01	1.49	1.43
13	A	1117	A1MA6	OC2-C47	4.00	1.49	1.43
9	G	102	PCW	C20-C19	3.87	1.54	1.31
9	E	102	PCW	C20-C19	3.87	1.54	1.31
9	E	102	PCW	C40-C39	3.86	1.54	1.31
9	G	102	PCW	C40-C39	3.85	1.54	1.31
9	C	1106	PCW	C40-C39	3.85	1.54	1.31
9	A	1107	PCW	C40-C39	3.85	1.54	1.31
9	A	1106	PCW	C20-C19	3.83	1.54	1.31
9	C	1105	PCW	C20-C19	3.83	1.54	1.31
9	A	1105	PCW	C40-C39	3.83	1.54	1.31
9	C	1104	PCW	C40-C39	3.82	1.53	1.31
13	C	1116	A1MA6	C48-C49	-3.82	1.46	1.53
13	A	1117	A1MA6	C48-C49	-3.82	1.46	1.53
9	G	101	PCW	C40-C39	3.81	1.53	1.31
9	C	1107	PCW	C40-C39	3.81	1.53	1.31
9	A	1108	PCW	C40-C39	3.81	1.53	1.31
9	E	101	PCW	C40-C39	3.81	1.53	1.31
9	G	101	PCW	C20-C19	3.80	1.53	1.31
9	E	101	PCW	C20-C19	3.80	1.53	1.31
9	A	1104	PCW	C20-C19	3.77	1.53	1.31
9	B	401	PCW	C20-C19	3.77	1.53	1.31
9	C	1104	PCW	C20-C19	3.77	1.53	1.31
9	A	1105	PCW	C20-C19	3.77	1.53	1.31
9	A	1107	PCW	C20-C19	3.75	1.53	1.31
9	C	1106	PCW	C20-C19	3.75	1.53	1.31
9	C	1107	PCW	C20-C19	3.75	1.53	1.31
9	A	1108	PCW	C20-C19	3.75	1.53	1.31
9	B	401	PCW	C40-C39	3.72	1.53	1.31
9	A	1104	PCW	C40-C39	3.72	1.53	1.31
9	A	1106	PCW	C40-C39	3.71	1.53	1.31
9	C	1105	PCW	C40-C39	3.71	1.53	1.31
13	C	1116	A1MA6	C51-C49	-3.61	1.46	1.53
13	A	1117	A1MA6	C51-C49	-3.61	1.46	1.53
13	A	1117	A1MA6	CAN-CAM	-3.37	1.45	1.52
13	C	1116	A1MA6	CAN-CAM	-3.37	1.45	1.52
13	A	1117	A1MA6	C95-C94	3.36	1.53	1.44
13	C	1116	A1MA6	C95-C94	3.36	1.53	1.44
13	A	1117	A1MA6	CAV-CAW	-3.13	1.45	1.52
13	C	1116	A1MA6	CAV-CAW	-3.13	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	1103	CLR	C16-C17	3.06	1.60	1.54
8	A	1103	CLR	C16-C17	3.05	1.60	1.54
8	C	1109	CLR	C16-C17	2.96	1.60	1.54
8	A	1110	CLR	C16-C17	2.96	1.60	1.54
8	D	401	CLR	C16-C17	2.96	1.60	1.54
8	B	402	CLR	C16-C17	2.96	1.60	1.54
8	C	1101	CLR	C16-C17	2.90	1.60	1.54
8	A	1101	CLR	C16-C17	2.89	1.60	1.54
13	C	1116	A1MA6	O46-C44	-2.88	1.40	1.45
13	A	1117	A1MA6	O46-C44	-2.88	1.40	1.45
8	A	1102	CLR	C16-C17	2.84	1.60	1.54
8	C	1102	CLR	C16-C17	2.84	1.60	1.54
13	C	1116	A1MA6	C07-C06	2.67	1.53	1.48
13	A	1117	A1MA6	C07-C06	2.67	1.53	1.48
13	C	1116	A1MA6	CAN-CB0	-2.60	1.47	1.52
13	A	1117	A1MA6	CAN-CB0	-2.60	1.47	1.52
13	C	1116	A1MA6	C15-C17	2.42	1.53	1.50
13	A	1117	A1MA6	C15-C17	2.41	1.53	1.50
13	C	1116	A1MA6	CAL-CAK	-2.31	1.46	1.52
13	A	1117	A1MA6	CAL-CAK	-2.31	1.46	1.52
13	A	1117	A1MA6	O76-C77	-2.29	1.38	1.44
13	C	1116	A1MA6	O76-C77	-2.29	1.38	1.44
13	C	1116	A1MA6	O76-C75	2.24	1.49	1.44
13	A	1117	A1MA6	O76-C75	2.24	1.49	1.44
8	A	1110	CLR	C7-C6	2.20	1.54	1.50
8	C	1109	CLR	C7-C6	2.20	1.54	1.50
13	C	1116	A1MA6	CAH-CAG	2.18	1.53	1.50
13	A	1117	A1MA6	CAH-CAG	2.18	1.53	1.50
13	C	1116	A1MA6	OAO-CAM	2.17	1.49	1.44
13	A	1117	A1MA6	OAO-CAM	2.17	1.49	1.44
8	D	401	CLR	C7-C6	2.14	1.54	1.50
8	B	402	CLR	C7-C6	2.14	1.54	1.50
8	A	1103	CLR	C7-C6	2.10	1.54	1.50
8	C	1103	CLR	C7-C6	2.10	1.54	1.50
8	C	1101	CLR	C7-C6	2.08	1.54	1.50
8	A	1102	CLR	C7-C6	2.08	1.54	1.50
8	A	1101	CLR	C7-C6	2.08	1.54	1.50
8	C	1102	CLR	C7-C6	2.08	1.54	1.50
13	A	1117	A1MA6	CAT-CAS	2.06	1.58	1.53
13	C	1116	A1MA6	CAT-CAS	2.06	1.58	1.53
8	A	1110	CLR	C16-C15	2.05	1.59	1.54
8	C	1109	CLR	C16-C15	2.05	1.59	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	401	CLR	C16-C15	2.01	1.59	1.54
8	B	402	CLR	C16-C15	2.01	1.59	1.54
13	A	1117	A1MA6	CBL-C75	2.01	1.55	1.52
8	C	1102	CLR	C16-C15	2.01	1.59	1.54
13	C	1116	A1MA6	CBL-C75	2.01	1.55	1.52
8	A	1102	CLR	C16-C15	2.01	1.59	1.54
8	A	1103	CLR	C16-C15	2.01	1.59	1.54
8	C	1103	CLR	C16-C15	2.01	1.59	1.54

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	1116	A1MA6	C97-C96-C95	-8.04	115.03	125.41
13	A	1117	A1MA6	C97-C96-C95	-8.04	115.03	125.41
13	A	1117	A1MA6	C44-O46-C47	-6.96	101.88	111.08
13	C	1116	A1MA6	C44-O46-C47	-6.96	101.88	111.08
13	C	1116	A1MA6	CA2-CA3-CA4	-6.68	115.40	125.92
13	A	1117	A1MA6	CA2-CA3-CA4	-6.67	115.41	125.92
13	C	1116	A1MA6	CAH-CAG-CAF	-6.22	115.17	124.93
13	A	1117	A1MA6	CAH-CAG-CAF	-6.22	115.17	124.93
13	A	1117	A1MA6	CA1-CA2-CA3	-4.84	115.17	126.00
13	C	1116	A1MA6	CA1-CA2-CA3	-4.84	115.17	126.00
13	A	1117	A1MA6	CAE-CAF-CAG	-4.75	115.28	124.61
13	C	1116	A1MA6	CAE-CAF-CAG	-4.75	115.28	124.61
13	C	1116	A1MA6	C92-C93-C94	-4.09	115.18	125.14
13	A	1117	A1MA6	C92-C93-C94	-4.09	115.18	125.14
13	A	1117	A1MA6	CAR-CAS-CAT	-3.99	107.91	116.29
13	C	1116	A1MA6	CAR-CAS-CAT	-3.99	107.91	116.29
13	A	1117	A1MA6	C70-C69-C68	-3.84	115.07	125.09
13	C	1116	A1MA6	C70-C69-C68	-3.84	115.08	125.09
13	A	1117	A1MA6	CAQ-CAP-CB0	-3.72	108.23	116.25
13	C	1116	A1MA6	CAQ-CAP-CB0	-3.71	108.23	116.25
13	C	1116	A1MA6	C63-O62-C61	-3.68	109.92	114.61
13	A	1117	A1MA6	C63-O62-C61	-3.68	109.92	114.61
13	A	1117	A1MA6	C53-C52-C47	-3.45	109.53	114.64
13	C	1116	A1MA6	C53-C52-C47	-3.44	109.53	114.64
13	A	1117	A1MA6	C67-C68-C69	-3.42	115.05	125.67
13	C	1116	A1MA6	C67-C68-C69	-3.42	115.05	125.67
13	A	1117	A1MA6	OAZ-CAW-CAV	-3.38	100.71	105.07
13	C	1116	A1MA6	OAZ-CAW-CAV	-3.38	100.71	105.07
13	C	1116	A1MA6	C08-N09-C10	-3.25	116.93	123.51
13	A	1117	A1MA6	C08-N09-C10	-3.25	116.94	123.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	1108	PCW	C2-O2-C31	-3.24	111.85	117.90
9	A	1109	PCW	C2-O2-C31	-3.24	111.86	117.90
8	C	1103	CLR	C22-C20-C17	-3.15	103.78	110.28
8	A	1103	CLR	C22-C20-C17	-3.15	103.78	110.28
8	C	1101	CLR	C22-C20-C17	-3.10	103.88	110.28
8	A	1101	CLR	C22-C20-C17	-3.10	103.88	110.28
8	C	1102	CLR	C22-C20-C17	-3.09	103.90	110.28
8	A	1102	CLR	C22-C20-C17	-3.09	103.91	110.28
8	B	402	CLR	C22-C20-C17	-3.05	103.98	110.28
8	D	401	CLR	C22-C20-C17	-3.05	103.98	110.28
8	A	1110	CLR	C22-C20-C17	-2.94	104.21	110.28
8	C	1109	CLR	C22-C20-C17	-2.94	104.21	110.28
9	C	1104	PCW	C2-O2-C31	-2.91	110.62	117.79
9	A	1105	PCW	C2-O2-C31	-2.91	110.63	117.79
9	C	1108	PCW	C3-O3-C11	-2.91	109.80	117.10
9	A	1109	PCW	C3-O3-C11	-2.91	109.80	117.10
13	C	1116	A1MA6	CAA-CAB-CAC	-2.89	109.51	115.47
13	A	1117	A1MA6	CAA-CAB-CAC	-2.89	109.51	115.47
13	C	1116	A1MA6	C37-C36-C34	-2.85	109.50	114.18
13	A	1117	A1MA6	C37-C36-C34	-2.85	109.50	114.18
13	C	1116	A1MA6	C32-C30-C28	-2.73	109.48	113.26
13	A	1117	A1MA6	C32-C30-C28	-2.73	109.48	113.26
13	C	1116	A1MA6	CAS-OAZ-CAW	-2.72	102.53	108.92
13	A	1117	A1MA6	CAS-OAZ-CAW	-2.72	102.54	108.92
13	C	1116	A1MA6	C30-C28-C26	-2.72	109.50	113.26
9	C	1107	PCW	C2-O2-C31	-2.72	111.10	117.79
9	A	1108	PCW	C2-O2-C31	-2.72	111.10	117.79
13	A	1117	A1MA6	C30-C28-C26	-2.71	109.50	113.26
13	A	1117	A1MA6	O62-C61-C60	2.71	109.41	105.95
13	C	1116	A1MA6	O62-C61-C60	2.71	109.40	105.95
13	A	1117	A1MA6	C78-C77-CBO	-2.61	109.17	113.47
13	C	1116	A1MA6	C78-C77-CBO	-2.60	109.18	113.47
13	C	1116	A1MA6	CAA-CA9-CA8	-2.59	109.45	114.66
13	A	1117	A1MA6	CAA-CA9-CA8	-2.59	109.46	114.66
13	A	1117	A1MA6	C60-C61-CBV	-2.52	109.32	113.47
13	C	1116	A1MA6	C60-C61-CBV	-2.52	109.32	113.47
13	A	1117	A1MA6	C81-C82-C83	-2.51	109.33	113.47
13	C	1116	A1MA6	C81-C82-C83	-2.51	109.34	113.47
13	A	1117	A1MA6	C91-C90-C85	-2.50	109.34	113.47
13	C	1116	A1MA6	C91-C90-C85	-2.50	109.35	113.47
9	C	1105	PCW	C2-O2-C31	-2.50	111.63	117.79
9	A	1106	PCW	C2-O2-C31	-2.50	111.63	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	1117	A1MA6	CAB-CAC-CB8	-2.41	109.49	113.47
13	C	1116	A1MA6	CAB-CAC-CB8	-2.41	109.50	113.47
9	E	102	PCW	C2-O2-C31	-2.41	111.86	117.79
9	G	102	PCW	C2-O2-C31	-2.41	111.86	117.79
8	A	1102	CLR	C18-C13-C12	2.36	114.32	110.59
8	C	1102	CLR	C18-C13-C12	2.36	114.32	110.59
13	A	1117	A1MA6	C71-C72-C73	-2.32	109.52	113.51
13	C	1116	A1MA6	C71-C72-C73	-2.32	109.52	113.51
8	A	1101	CLR	C18-C13-C12	2.31	114.24	110.59
8	C	1101	CLR	C18-C13-C12	2.31	114.24	110.59
8	A	1102	CLR	C7-C8-C14	-2.30	107.57	110.91
8	C	1102	CLR	C7-C8-C14	-2.30	107.57	110.91
13	A	1117	A1MA6	C22-C23-CC7	-2.30	109.68	113.47
13	C	1116	A1MA6	C22-C23-CC7	-2.30	109.69	113.47
8	A	1101	CLR	C7-C8-C14	-2.29	107.58	110.91
8	C	1101	CLR	C7-C8-C14	-2.29	107.58	110.91
11	A	1112	ATP	C5-C6-N6	2.29	123.83	120.35
11	C	1111	ATP	C5-C6-N6	2.29	123.83	120.35
8	A	1110	CLR	C13-C17-C20	-2.29	115.90	119.49
8	C	1109	CLR	C13-C17-C20	-2.29	115.91	119.49
8	B	402	CLR	C7-C8-C14	-2.28	107.59	110.91
8	D	401	CLR	C7-C8-C14	-2.28	107.60	110.91
8	A	1103	CLR	C7-C8-C14	-2.28	107.60	110.91
13	C	1116	A1MA6	C61-C60-C59	-2.28	109.50	114.61
8	C	1103	CLR	C7-C8-C14	-2.28	107.61	110.91
13	A	1117	A1MA6	C61-C60-C59	-2.28	109.51	114.61
8	C	1109	CLR	C7-C8-C14	-2.27	107.62	110.91
8	A	1110	CLR	C7-C8-C14	-2.26	107.62	110.91
13	C	1116	A1MA6	C77-O76-C75	-2.26	109.20	113.16
13	A	1117	A1MA6	C77-O76-C75	-2.26	109.20	113.16
13	A	1117	A1MA6	C04-C03-C02	-2.23	109.50	112.99
13	C	1116	A1MA6	C04-C03-C02	-2.23	109.51	112.99
8	C	1103	CLR	C18-C13-C12	2.20	114.06	110.59
8	A	1103	CLR	C18-C13-C12	2.20	114.06	110.59
8	A	1110	CLR	C18-C13-C12	2.20	114.06	110.59
8	C	1109	CLR	C18-C13-C12	2.20	114.06	110.59
8	B	402	CLR	C18-C13-C12	2.17	114.02	110.59
8	D	401	CLR	C18-C13-C12	2.17	114.02	110.59
8	A	1110	CLR	C11-C12-C13	-2.16	109.08	112.78
8	C	1109	CLR	C11-C12-C13	-2.16	109.08	112.78
13	C	1116	A1MA6	CAP-OAO-CAM	-2.13	103.92	108.92
13	A	1117	A1MA6	CAP-OAO-CAM	-2.13	103.92	108.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	1102	CLR	C21-C20-C17	2.13	116.18	112.92
8	A	1102	CLR	C21-C20-C17	2.13	116.18	112.92
9	C	1108	PCW	O2-C31-C32	2.09	114.94	111.09
9	A	1109	PCW	O2-C31-C32	2.09	114.94	111.09
13	A	1117	A1MA6	C47-C48-C49	-2.09	108.76	112.79
8	D	401	CLR	C13-C17-C20	-2.09	116.22	119.49
8	B	402	CLR	C13-C17-C20	-2.09	116.22	119.49
13	C	1116	A1MA6	C47-C48-C49	-2.09	108.77	112.79
8	A	1101	CLR	C21-C20-C17	2.08	116.11	112.92
8	C	1101	CLR	C21-C20-C17	2.08	116.11	112.92
11	C	1111	ATP	PB-O3B-PG	2.05	139.87	132.83
8	C	1102	CLR	C11-C12-C13	-2.05	109.26	112.78
11	A	1112	ATP	PB-O3B-PG	2.05	139.87	132.83
8	A	1102	CLR	C11-C12-C13	-2.05	109.26	112.78
8	A	1101	CLR	C13-C17-C20	-2.04	116.29	119.49
8	C	1101	CLR	C13-C17-C20	-2.04	116.29	119.49
8	B	402	CLR	C11-C12-C13	-2.03	109.29	112.78
8	D	401	CLR	C11-C12-C13	-2.03	109.29	112.78
8	C	1101	CLR	C24-C23-C22	-2.03	103.93	113.24
8	A	1101	CLR	C24-C23-C22	-2.03	103.93	113.24
8	A	1110	CLR	C21-C20-C17	2.02	116.01	112.92
8	C	1109	CLR	C21-C20-C17	2.02	116.01	112.92
8	A	1101	CLR	C11-C12-C13	-2.01	109.33	112.78
8	C	1101	CLR	C11-C12-C13	-2.01	109.33	112.78
8	C	1103	CLR	C24-C23-C22	-2.01	104.00	113.24
8	A	1103	CLR	C24-C23-C22	-2.01	104.00	113.24
8	C	1102	CLR	C24-C23-C22	-2.01	104.02	113.24
8	A	1102	CLR	C24-C23-C22	-2.01	104.02	113.24
13	A	1117	A1MA6	CAQ-CAR-CAS	-2.00	109.45	113.88
13	C	1116	A1MA6	CAQ-CAR-CAS	-2.00	109.45	113.88

There are no chirality outliers.

All (538) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	1104	PCW	O3P-C1-C2-O2
9	C	1105	PCW	C1-O3P-P-O1P
9	C	1105	PCW	C1-O3P-P-O2P
9	C	1105	PCW	C1-O3P-P-O4P
9	C	1106	PCW	C1-O3P-P-O1P
9	C	1106	PCW	C1-O3P-P-O2P
9	C	1106	PCW	C1-O3P-P-O4P

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Mol	Chain	Res	Type	Atoms
9	C	1107	PCW	C1-O3P-P-O1P
9	C	1107	PCW	C1-O3P-P-O2P
9	C	1107	PCW	C1-O3P-P-O4P
9	C	1108	PCW	C4-O4P-P-O2P
9	E	101	PCW	O2-C2-C3-O3
9	E	101	PCW	O4P-C4-C5-N
9	E	101	PCW	C1-O3P-P-O2P
9	A	1105	PCW	O3P-C1-C2-O2
9	A	1106	PCW	C1-O3P-P-O1P
9	A	1106	PCW	C1-O3P-P-O2P
9	A	1106	PCW	C1-O3P-P-O4P
9	A	1107	PCW	C1-O3P-P-O1P
9	A	1107	PCW	C1-O3P-P-O2P
9	A	1107	PCW	C1-O3P-P-O4P
9	A	1108	PCW	C1-O3P-P-O1P
9	A	1108	PCW	C1-O3P-P-O2P
9	A	1108	PCW	C1-O3P-P-O4P
9	A	1109	PCW	C4-O4P-P-O2P
9	G	101	PCW	O2-C2-C3-O3
9	G	101	PCW	O4P-C4-C5-N
9	G	101	PCW	C1-O3P-P-O2P
11	C	1111	ATP	C5'-O5'-PA-O1A
11	A	1112	ATP	C5'-O5'-PA-O1A
13	C	1116	A1MA6	N09-C10-C11-O12
13	C	1116	A1MA6	C10-C11-C13-C14
13	C	1116	A1MA6	C10-C11-C13-CCC
13	C	1116	A1MA6	O12-C11-C13-C14
13	C	1116	A1MA6	O12-C11-C13-CCC
13	C	1116	A1MA6	CCB-C18-C19-C21
13	C	1116	A1MA6	O20-C19-C21-OCA
13	C	1116	A1MA6	C21-C22-C23-O24
13	C	1116	A1MA6	O24-C25-C26-O27
13	C	1116	A1MA6	O24-C25-C26-C28
13	C	1116	A1MA6	CC4-C25-C26-O27
13	C	1116	A1MA6	CC4-C25-C26-C28
13	C	1116	A1MA6	C26-C28-C30-O31
13	C	1116	A1MA6	C26-C28-C30-C32
13	C	1116	A1MA6	O29-C28-C30-O31
13	C	1116	A1MA6	O29-C28-C30-C32
13	C	1116	A1MA6	C30-C32-C34-O35
13	C	1116	A1MA6	C30-C32-C34-C36
13	C	1116	A1MA6	O33-C32-C34-O35

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Mol	Chain	Res	Type	Atoms
13	C	1116	A1MA6	O33-C32-C34-C36
13	C	1116	A1MA6	O35-C34-C36-C37
13	C	1116	A1MA6	C40-C41-C42-C43
13	C	1116	A1MA6	CC3-C41-C42-C43
13	C	1116	A1MA6	C41-C42-C43-OC2
13	C	1116	A1MA6	C59-C60-C61-O62
13	C	1116	A1MA6	C59-C60-C61-CBV
13	C	1116	A1MA6	C63-C65-C66-C67
13	C	1116	A1MA6	C68-C69-C70-OBS
13	C	1116	A1MA6	C69-C70-C71-C72
13	C	1116	A1MA6	OBS-C70-C71-C72
13	C	1116	A1MA6	C71-C72-C73-OBK
13	C	1116	A1MA6	C72-C73-C74-OBQ
13	C	1116	A1MA6	OBK-C73-C74-C75
13	C	1116	A1MA6	OBK-C73-C74-OBQ
13	C	1116	A1MA6	C73-C74-C75-O76
13	C	1116	A1MA6	C78-C79-C80-C81
13	C	1116	A1MA6	C78-C79-C80-OBK
13	C	1116	A1MA6	OBK-C79-C80-C81
13	C	1116	A1MA6	OBK-C79-C80-OBK
13	C	1116	A1MA6	C85-C90-C91-C92
13	C	1116	A1MA6	O89-C90-C91-C92
13	C	1116	A1MA6	C90-C91-C92-C93
13	C	1116	A1MA6	C90-C91-C92-OBK
13	C	1116	A1MA6	OBK-C92-C93-C94
13	C	1116	A1MA6	C96-C97-C98-C99
13	C	1116	A1MA6	C96-C97-C98-OBK
13	C	1116	A1MA6	C98-C99-CA0-OBK
13	C	1116	A1MA6	OBK-C99-CA0-CA1
13	C	1116	A1MA6	OBK-C99-CA0-OBK
13	C	1116	A1MA6	C99-CA0-CA1-CA2
13	C	1116	A1MA6	OBK-CA0-CA1-CA2
13	C	1116	A1MA6	CA4-CA5-CA6-CA7
13	C	1116	A1MA6	OAD-CAE-CAF-CAG
13	C	1116	A1MA6	CB4-CAE-CAF-CAG
13	C	1116	A1MA6	CAG-CAH-CAI-CAJ
13	C	1116	A1MA6	CAG-CAH-CAI-OB2
13	C	1116	A1MA6	OB3-CAH-CAI-CAJ
13	C	1116	A1MA6	OB3-CAH-CAI-OB2
13	C	1116	A1MA6	CAI-CAJ-CAK-CAL
13	C	1116	A1MA6	CAI-CAJ-CAK-OB1
13	C	1116	A1MA6	CAQ-CAR-CAS-OAZ

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Mol	Chain	Res	Type	Atoms
13	C	1116	A1MA6	OAZ-CAW-CAX-NAY
13	A	1117	A1MA6	N09-C10-C11-O12
13	A	1117	A1MA6	C10-C11-C13-C14
13	A	1117	A1MA6	C10-C11-C13-CCC
13	A	1117	A1MA6	O12-C11-C13-C14
13	A	1117	A1MA6	O12-C11-C13-CCC
13	A	1117	A1MA6	CCB-C18-C19-C21
13	A	1117	A1MA6	O20-C19-C21-OCA
13	A	1117	A1MA6	C21-C22-C23-O24
13	A	1117	A1MA6	O24-C25-C26-O27
13	A	1117	A1MA6	O24-C25-C26-C28
13	A	1117	A1MA6	CC4-C25-C26-O27
13	A	1117	A1MA6	CC4-C25-C26-C28
13	A	1117	A1MA6	C26-C28-C30-O31
13	A	1117	A1MA6	C26-C28-C30-C32
13	A	1117	A1MA6	O29-C28-C30-O31
13	A	1117	A1MA6	O29-C28-C30-C32
13	A	1117	A1MA6	C30-C32-C34-O35
13	A	1117	A1MA6	C30-C32-C34-C36
13	A	1117	A1MA6	O33-C32-C34-O35
13	A	1117	A1MA6	O33-C32-C34-C36
13	A	1117	A1MA6	O35-C34-C36-C37
13	A	1117	A1MA6	C40-C41-C42-C43
13	A	1117	A1MA6	CC3-C41-C42-C43
13	A	1117	A1MA6	C41-C42-C43-OC2
13	A	1117	A1MA6	C59-C60-C61-O62
13	A	1117	A1MA6	C59-C60-C61-CBV
13	A	1117	A1MA6	C63-C65-C66-C67
13	A	1117	A1MA6	C68-C69-C70-OBS
13	A	1117	A1MA6	C69-C70-C71-C72
13	A	1117	A1MA6	OBS-C70-C71-C72
13	A	1117	A1MA6	C71-C72-C73-OBR
13	A	1117	A1MA6	C72-C73-C74-OBQ
13	A	1117	A1MA6	OBR-C73-C74-C75
13	A	1117	A1MA6	OBR-C73-C74-OBQ
13	A	1117	A1MA6	C73-C74-C75-O76
13	A	1117	A1MA6	C78-C79-C80-C81
13	A	1117	A1MA6	C78-C79-C80-OBJ
13	A	1117	A1MA6	OBK-C79-C80-C81
13	A	1117	A1MA6	OBK-C79-C80-OBJ
13	A	1117	A1MA6	C85-C90-C91-C92
13	A	1117	A1MA6	O89-C90-C91-C92

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Mol	Chain	Res	Type	Atoms
13	A	1117	A1MA6	C90-C91-C92-C93
13	A	1117	A1MA6	C90-C91-C92-OB1
13	A	1117	A1MA6	OB1-C92-C93-C94
13	A	1117	A1MA6	C96-C97-C98-C99
13	A	1117	A1MA6	C96-C97-C98-OBH
13	A	1117	A1MA6	C98-C99-CA0-OBF
13	A	1117	A1MA6	OBG-C99-CA0-CA1
13	A	1117	A1MA6	OBG-C99-CA0-OBF
13	A	1117	A1MA6	C99-CA0-CA1-CA2
13	A	1117	A1MA6	OBF-CA0-CA1-CA2
13	A	1117	A1MA6	CA4-CA5-CA6-CA7
13	A	1117	A1MA6	OAD-CAE-CAF-CAG
13	A	1117	A1MA6	CB4-CAE-CAF-CAG
13	A	1117	A1MA6	CAG-CAH-CAI-CAJ
13	A	1117	A1MA6	CAG-CAH-CAI-OB2
13	A	1117	A1MA6	OB3-CAH-CAI-CAJ
13	A	1117	A1MA6	OB3-CAH-CAI-OB2
13	A	1117	A1MA6	CAI-CAJ-CAK-CAL
13	A	1117	A1MA6	CAI-CAJ-CAK-OB1
13	A	1117	A1MA6	CAQ-CAR-CAS-OAZ
13	A	1117	A1MA6	OAZ-CAW-CAX-NAY
9	C	1106	PCW	C4-C5-N-C8
9	A	1107	PCW	C4-C5-N-C8
9	C	1105	PCW	C42-C43-C44-C45
9	C	1107	PCW	C23-C24-C25-C26
9	A	1106	PCW	C42-C43-C44-C45
9	A	1108	PCW	C23-C24-C25-C26
11	C	1111	ATP	C3'-C4'-C5'-O5'
11	A	1112	ATP	C3'-C4'-C5'-O5'
13	C	1116	A1MA6	C72-C73-C74-C75
13	C	1116	A1MA6	C98-C99-CA0-CA1
13	C	1116	A1MA6	CA6-CA7-CA8-CA9
13	A	1117	A1MA6	C72-C73-C74-C75
13	A	1117	A1MA6	C98-C99-CA0-CA1
13	A	1117	A1MA6	CA6-CA7-CA8-CA9
9	C	1107	PCW	C4-C5-N-C8
9	E	102	PCW	C4-C5-N-C8
9	A	1108	PCW	C4-C5-N-C8
9	G	102	PCW	C4-C5-N-C8
9	C	1106	PCW	C24-C25-C26-C27
9	A	1107	PCW	C24-C25-C26-C27
9	C	1107	PCW	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
9	A	1108	PCW	C33-C34-C35-C36
9	C	1105	PCW	C31-C32-C33-C34
9	E	101	PCW	C11-C12-C13-C14
9	A	1106	PCW	C31-C32-C33-C34
9	G	101	PCW	C11-C12-C13-C14
11	C	1111	ATP	O4'-C4'-C5'-O5'
11	A	1112	ATP	O4'-C4'-C5'-O5'
9	C	1107	PCW	C4-C5-N-C7
9	A	1108	PCW	C4-C5-N-C7
9	C	1106	PCW	C31-C32-C33-C34
9	A	1107	PCW	C31-C32-C33-C34
13	C	1116	A1MA6	C02-C03-C04-N05
13	A	1117	A1MA6	C02-C03-C04-N05
9	C	1107	PCW	C4-O4P-P-O3P
9	C	1108	PCW	C1-O3P-P-O4P
9	E	101	PCW	C1-O3P-P-O4P
9	A	1108	PCW	C4-O4P-P-O3P
9	A	1109	PCW	C1-O3P-P-O4P
9	G	101	PCW	C1-O3P-P-O4P
13	C	1116	A1MA6	OBQ-C74-C75-CBL
13	A	1117	A1MA6	OBQ-C74-C75-CBL
9	C	1107	PCW	C31-C32-C33-C34
9	A	1108	PCW	C31-C32-C33-C34
13	C	1116	A1MA6	OC1-C59-C60-C61
13	A	1117	A1MA6	OC1-C59-C60-C61
9	C	1106	PCW	C4-C5-N-C6
9	E	102	PCW	C4-C5-N-C6
9	E	102	PCW	C4-C5-N-C7
9	A	1107	PCW	C4-C5-N-C6
9	G	102	PCW	C4-C5-N-C6
9	G	102	PCW	C4-C5-N-C7
13	C	1116	A1MA6	C58-C59-C60-C61
13	A	1117	A1MA6	C58-C59-C60-C61
9	E	102	PCW	C41-C42-C43-C44
9	G	102	PCW	C41-C42-C43-C44
13	C	1116	A1MA6	C52-C53-C54-C55
13	A	1117	A1MA6	C52-C53-C54-C55
9	C	1106	PCW	C42-C43-C44-C45
9	A	1107	PCW	C42-C43-C44-C45
9	C	1107	PCW	C13-C14-C15-C16
9	E	102	PCW	C34-C35-C36-C37
9	A	1108	PCW	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
9	G	102	PCW	C34-C35-C36-C37
13	C	1116	A1MA6	OCD-C10-C11-O12
13	A	1117	A1MA6	OCD-C10-C11-O12
13	C	1116	A1MA6	C32-C34-C36-C37
13	C	1116	A1MA6	C71-C72-C73-C74
13	A	1117	A1MA6	C32-C34-C36-C37
13	A	1117	A1MA6	C71-C72-C73-C74
9	B	401	PCW	C13-C14-C15-C16
9	A	1104	PCW	C13-C14-C15-C16
9	C	1106	PCW	C4-C5-N-C7
9	C	1107	PCW	C4-C5-N-C6
9	A	1107	PCW	C4-C5-N-C7
9	A	1108	PCW	C4-C5-N-C6
9	C	1106	PCW	C13-C14-C15-C16
9	A	1107	PCW	C13-C14-C15-C16
9	E	102	PCW	C21-C22-C23-C24
9	G	102	PCW	C21-C22-C23-C24
9	C	1104	PCW	C44-C45-C46-C47
9	A	1105	PCW	C44-C45-C46-C47
9	C	1106	PCW	C35-C36-C37-C38
9	A	1107	PCW	C35-C36-C37-C38
9	E	101	PCW	C13-C14-C15-C16
9	G	101	PCW	C13-C14-C15-C16
9	C	1107	PCW	C11-C12-C13-C14
9	A	1108	PCW	C11-C12-C13-C14
9	E	102	PCW	C11-C12-C13-C14
9	G	102	PCW	C11-C12-C13-C14
9	C	1106	PCW	C12-C13-C14-C15
9	C	1107	PCW	C15-C16-C17-C18
9	A	1107	PCW	C12-C13-C14-C15
9	A	1108	PCW	C15-C16-C17-C18
9	C	1105	PCW	C36-C37-C38-C39
9	C	1106	PCW	C36-C37-C38-C39
9	C	1106	PCW	C40-C41-C42-C43
9	A	1106	PCW	C36-C37-C38-C39
9	A	1107	PCW	C36-C37-C38-C39
9	A	1107	PCW	C40-C41-C42-C43
9	C	1104	PCW	C42-C43-C44-C45
9	A	1105	PCW	C42-C43-C44-C45
9	C	1106	PCW	C33-C34-C35-C36
9	A	1107	PCW	C33-C34-C35-C36
9	E	102	PCW	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
9	G	102	PCW	C33-C34-C35-C36
9	E	102	PCW	C42-C43-C44-C45
9	G	102	PCW	C42-C43-C44-C45
9	C	1104	PCW	C40-C41-C42-C43
9	A	1105	PCW	C40-C41-C42-C43
9	B	401	PCW	C11-C12-C13-C14
13	C	1116	A1MA6	C36-C37-C38-C39
13	A	1117	A1MA6	C36-C37-C38-C39
13	C	1116	A1MA6	OBD-CA7-CA8-CA9
13	A	1117	A1MA6	OBD-CA7-CA8-CA9
9	A	1104	PCW	C11-C12-C13-C14
9	C	1105	PCW	O3P-C1-C2-C3
9	C	1106	PCW	O3P-C1-C2-C3
9	C	1107	PCW	O3P-C1-C2-C3
9	E	102	PCW	O3P-C1-C2-C3
9	B	401	PCW	O3P-C1-C2-C3
9	A	1104	PCW	O3P-C1-C2-C3
9	A	1106	PCW	O3P-C1-C2-C3
9	A	1107	PCW	O3P-C1-C2-C3
9	A	1108	PCW	O3P-C1-C2-C3
9	G	102	PCW	O3P-C1-C2-C3
9	B	401	PCW	C16-C17-C18-C19
9	A	1104	PCW	C16-C17-C18-C19
13	C	1116	A1MA6	O46-C47-C52-C53
13	C	1116	A1MA6	C68-C69-C70-C71
13	C	1116	A1MA6	C91-C92-C93-C94
13	A	1117	A1MA6	O46-C47-C52-C53
13	A	1117	A1MA6	C68-C69-C70-C71
13	A	1117	A1MA6	C91-C92-C93-C94
9	C	1104	PCW	C1-C2-C3-O3
9	A	1105	PCW	C1-C2-C3-O3
9	C	1104	PCW	C22-C23-C24-C25
9	A	1105	PCW	C22-C23-C24-C25
9	C	1105	PCW	C40-C41-C42-C43
9	A	1106	PCW	C40-C41-C42-C43
9	B	401	PCW	C12-C13-C14-C15
9	A	1104	PCW	C12-C13-C14-C15
9	C	1107	PCW	C12-C13-C14-C15
9	A	1108	PCW	C12-C13-C14-C15
9	B	401	PCW	C43-C44-C45-C46
9	A	1104	PCW	C43-C44-C45-C46
9	C	1107	PCW	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
9	A	1108	PCW	C32-C33-C34-C35
9	E	101	PCW	C35-C36-C37-C38
9	G	101	PCW	C35-C36-C37-C38
13	C	1116	A1MA6	C73-C74-C75-CBL
13	A	1117	A1MA6	C73-C74-C75-CBL
9	C	1106	PCW	C25-C26-C27-C28
9	A	1107	PCW	C25-C26-C27-C28
13	C	1116	A1MA6	CAQ-CAR-CAS-CAT
13	A	1117	A1MA6	CAQ-CAR-CAS-CAT
9	E	101	PCW	C45-C46-C47-C48
9	G	101	PCW	C45-C46-C47-C48
9	C	1104	PCW	C20-C21-C22-C23
9	C	1107	PCW	C16-C17-C18-C19
9	A	1105	PCW	C20-C21-C22-C23
9	A	1108	PCW	C16-C17-C18-C19
9	C	1104	PCW	O3P-C1-C2-C3
9	E	101	PCW	O3P-C1-C2-C3
9	A	1105	PCW	O3P-C1-C2-C3
9	G	101	PCW	O3P-C1-C2-C3
13	C	1116	A1MA6	C54-C55-C56-C57
13	A	1117	A1MA6	C54-C55-C56-C57
13	C	1116	A1MA6	C21-C22-C23-CC7
13	A	1117	A1MA6	C21-C22-C23-CC7
9	B	401	PCW	C1-C2-C3-O3
9	A	1104	PCW	C1-C2-C3-O3
13	C	1116	A1MA6	C17-C18-C19-C21
13	A	1117	A1MA6	C17-C18-C19-C21
9	E	101	PCW	O3P-C1-C2-O2
9	G	101	PCW	O3P-C1-C2-O2
9	C	1105	PCW	C12-C13-C14-C15
9	A	1106	PCW	C12-C13-C14-C15
9	C	1106	PCW	C14-C15-C16-C17
9	B	401	PCW	C14-C15-C16-C17
9	A	1104	PCW	C14-C15-C16-C17
9	A	1107	PCW	C14-C15-C16-C17
9	C	1106	PCW	C20-C21-C22-C23
9	A	1107	PCW	C20-C21-C22-C23
13	C	1116	A1MA6	OBQ-C74-C75-O76
13	A	1117	A1MA6	OBQ-C74-C75-O76
13	C	1116	A1MA6	OBD-CA7-CA8-OBC
13	A	1117	A1MA6	OBD-CA7-CA8-OBC
9	E	101	PCW	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
9	G	101	PCW	C1-C2-C3-O3
9	C	1105	PCW	O3P-C1-C2-O2
9	B	401	PCW	O3P-C1-C2-O2
9	A	1104	PCW	O3P-C1-C2-O2
9	A	1106	PCW	O3P-C1-C2-O2
13	C	1116	A1MA6	C11-C13-C14-C15
13	A	1117	A1MA6	C11-C13-C14-C15
9	B	401	PCW	O2-C2-C3-O3
9	A	1104	PCW	O2-C2-C3-O3
13	C	1116	A1MA6	OB2-CAI-CAJ-CAK
13	A	1117	A1MA6	OB2-CAI-CAJ-CAK
13	C	1116	A1MA6	OBB-CA9-CAA-CBA
13	A	1117	A1MA6	OBB-CA9-CAA-CBA
11	C	1111	ATP	PA-O3A-PB-O1B
11	A	1112	ATP	PA-O3A-PB-O1B
13	C	1116	A1MA6	C48-C47-C52-C53
13	A	1117	A1MA6	C48-C47-C52-C53
9	C	1107	PCW	C4-O4P-P-O1P
9	C	1108	PCW	C1-O3P-P-O2P
9	E	101	PCW	C1-O3P-P-O1P
9	A	1108	PCW	C4-O4P-P-O1P
9	A	1109	PCW	C1-O3P-P-O2P
9	G	101	PCW	C1-O3P-P-O1P
13	C	1116	A1MA6	C56-C57-C58-C59
13	A	1117	A1MA6	C56-C57-C58-C59
9	E	102	PCW	C31-C32-C33-C34
9	G	102	PCW	C31-C32-C33-C34
9	C	1105	PCW	C15-C16-C17-C18
9	A	1106	PCW	C15-C16-C17-C18
9	C	1107	PCW	O3P-C1-C2-O2
9	A	1108	PCW	O3P-C1-C2-O2
9	C	1104	PCW	C23-C24-C25-C26
9	A	1105	PCW	C23-C24-C25-C26
9	C	1104	PCW	O4P-C4-C5-N
9	C	1105	PCW	O4P-C4-C5-N
9	C	1106	PCW	O4P-C4-C5-N
9	C	1107	PCW	O4P-C4-C5-N
9	C	1108	PCW	O4P-C4-C5-N
9	E	102	PCW	O4P-C4-C5-N
9	B	401	PCW	O4P-C4-C5-N
9	A	1104	PCW	O4P-C4-C5-N
9	A	1105	PCW	O4P-C4-C5-N

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Mol	Chain	Res	Type	Atoms
9	A	1106	PCW	O4P-C4-C5-N
9	A	1107	PCW	O4P-C4-C5-N
9	A	1108	PCW	O4P-C4-C5-N
9	A	1109	PCW	O4P-C4-C5-N
9	G	102	PCW	O4P-C4-C5-N
9	B	401	PCW	C40-C41-C42-C43
9	A	1104	PCW	C40-C41-C42-C43
9	E	101	PCW	C2-C1-O3P-P
9	G	101	PCW	C2-C1-O3P-P
9	C	1107	PCW	C14-C15-C16-C17
9	A	1108	PCW	C14-C15-C16-C17
13	C	1116	A1MA6	CCC-C13-C14-C15
13	A	1117	A1MA6	CCC-C13-C14-C15
13	C	1116	A1MA6	CAF-CAG-CAH-OB3
13	A	1117	A1MA6	CAF-CAG-CAH-OB3
9	C	1105	PCW	C16-C17-C18-C19
9	A	1106	PCW	C16-C17-C18-C19
13	C	1116	A1MA6	CAF-CAG-CAH-CAI
13	A	1117	A1MA6	CAF-CAG-CAH-CAI
13	C	1116	A1MA6	CBT-C67-C68-C69
13	A	1117	A1MA6	CBT-C67-C68-C69
9	C	1106	PCW	O3P-C1-C2-O2
9	E	102	PCW	O3P-C1-C2-O2
9	A	1107	PCW	O3P-C1-C2-O2
9	G	102	PCW	O3P-C1-C2-O2
9	B	401	PCW	C24-C25-C26-C27
9	A	1104	PCW	C24-C25-C26-C27
8	C	1101	CLR	C23-C24-C25-C27
8	A	1101	CLR	C23-C24-C25-C27
9	C	1104	PCW	O2-C2-C3-O3
9	A	1105	PCW	O2-C2-C3-O3
9	C	1104	PCW	C4-O4P-P-O3P
9	C	1105	PCW	C4-O4P-P-O3P
9	C	1106	PCW	C4-O4P-P-O3P
9	C	1108	PCW	C4-O4P-P-O3P
9	E	101	PCW	C4-O4P-P-O3P
9	B	401	PCW	C4-O4P-P-O3P
9	A	1104	PCW	C4-O4P-P-O3P
9	A	1105	PCW	C4-O4P-P-O3P
9	A	1106	PCW	C4-O4P-P-O3P
9	A	1107	PCW	C4-O4P-P-O3P
9	A	1109	PCW	C4-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
9	G	101	PCW	C4-O4P-P-O3P
9	C	1107	PCW	C40-C41-C42-C43
9	A	1108	PCW	C40-C41-C42-C43
9	E	101	PCW	C43-C44-C45-C46
9	G	101	PCW	C43-C44-C45-C46
9	C	1105	PCW	C39-C40-C41-C42
9	A	1106	PCW	C39-C40-C41-C42
13	C	1116	A1MA6	CA0-CA1-CA2-CA3
13	A	1117	A1MA6	CA0-CA1-CA2-CA3
9	B	401	PCW	C44-C45-C46-C47
9	A	1104	PCW	C44-C45-C46-C47
9	C	1107	PCW	C36-C37-C38-C39
9	E	102	PCW	C20-C21-C22-C23
9	A	1108	PCW	C36-C37-C38-C39
9	G	102	PCW	C20-C21-C22-C23
8	C	1103	CLR	C21-C20-C22-C23
8	A	1103	CLR	C21-C20-C22-C23
9	C	1105	PCW	C17-C18-C19-C20
9	A	1106	PCW	C17-C18-C19-C20
8	C	1103	CLR	C17-C20-C22-C23
9	B	401	PCW	C1-C2-O2-C31
9	A	1104	PCW	C1-C2-O2-C31
8	A	1103	CLR	C17-C20-C22-C23
9	C	1107	PCW	C21-C22-C23-C24
9	A	1108	PCW	C21-C22-C23-C24
13	C	1116	A1MA6	C55-C56-C57-C58
13	A	1117	A1MA6	C55-C56-C57-C58
9	B	401	PCW	C31-C32-C33-C34
9	A	1104	PCW	C31-C32-C33-C34
9	E	102	PCW	C36-C37-C38-C39
9	G	102	PCW	C36-C37-C38-C39
9	C	1104	PCW	O2-C31-C32-C33
9	A	1105	PCW	O2-C31-C32-C33
9	C	1107	PCW	C20-C21-C22-C23
9	B	401	PCW	C20-C21-C22-C23
9	A	1104	PCW	C20-C21-C22-C23
9	A	1108	PCW	C20-C21-C22-C23
9	C	1104	PCW	C37-C38-C39-C40
9	C	1107	PCW	C39-C40-C41-C42
9	E	101	PCW	C17-C18-C19-C20
9	A	1105	PCW	C37-C38-C39-C40
9	A	1108	PCW	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
9	G	101	PCW	C17-C18-C19-C20
9	E	101	PCW	C14-C15-C16-C17
9	G	101	PCW	C14-C15-C16-C17
9	E	101	PCW	O2-C31-C32-C33
9	G	101	PCW	O2-C31-C32-C33
9	C	1106	PCW	C19-C20-C21-C22
9	C	1107	PCW	C19-C20-C21-C22
9	A	1107	PCW	C19-C20-C21-C22
9	A	1108	PCW	C19-C20-C21-C22
9	C	1106	PCW	C17-C18-C19-C20
9	E	102	PCW	C19-C20-C21-C22
9	A	1107	PCW	C17-C18-C19-C20
9	G	102	PCW	C19-C20-C21-C22
9	E	101	PCW	C16-C17-C18-C19
9	G	101	PCW	C16-C17-C18-C19
9	C	1106	PCW	O2-C31-C32-C33
9	B	401	PCW	O3-C11-C12-C13
9	A	1104	PCW	O3-C11-C12-C13
9	A	1107	PCW	O2-C31-C32-C33
11	C	1111	ATP	C5'-O5'-PA-O3A
11	A	1112	ATP	C5'-O5'-PA-O3A
9	E	102	PCW	C16-C17-C18-C19
9	G	102	PCW	C16-C17-C18-C19
9	E	102	PCW	C37-C38-C39-C40
9	G	102	PCW	C37-C38-C39-C40
9	C	1106	PCW	C21-C22-C23-C24
9	A	1107	PCW	C21-C22-C23-C24
9	C	1104	PCW	O31-C31-C32-C33
9	A	1105	PCW	O31-C31-C32-C33
13	C	1116	A1MA6	CCB-C18-C19-O20
13	A	1117	A1MA6	CCB-C18-C19-O20
9	C	1106	PCW	O31-C31-C32-C33
9	A	1107	PCW	O31-C31-C32-C33
9	C	1105	PCW	C4-O4P-P-O2P
9	C	1106	PCW	C4-O4P-P-O2P
9	E	101	PCW	C4-O4P-P-O2P
9	E	102	PCW	C1-O3P-P-O1P
9	E	102	PCW	C1-O3P-P-O2P
9	B	401	PCW	C4-O4P-P-O2P
9	A	1104	PCW	C4-O4P-P-O2P
9	A	1106	PCW	C4-O4P-P-O2P
9	A	1107	PCW	C4-O4P-P-O2P

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Mol	Chain	Res	Type	Atoms
9	G	101	PCW	C4-O4P-P-O2P
9	G	102	PCW	C1-O3P-P-O1P
9	G	102	PCW	C1-O3P-P-O2P
13	C	1116	A1MA6	O20-C19-C21-C22
13	C	1116	A1MA6	C41-C42-C43-C44
13	C	1116	A1MA6	CA6-CA7-CA8-OBC
13	A	1117	A1MA6	O20-C19-C21-C22
13	A	1117	A1MA6	C41-C42-C43-C44
13	A	1117	A1MA6	CA6-CA7-CA8-OBC
9	E	101	PCW	C5-C4-O4P-P
9	B	401	PCW	C3-C2-O2-C31
9	A	1104	PCW	C3-C2-O2-C31
9	G	101	PCW	C5-C4-O4P-P
9	B	401	PCW	O11-C11-C12-C13
9	A	1104	PCW	O11-C11-C12-C13
9	B	401	PCW	C37-C38-C39-C40
9	A	1104	PCW	C37-C38-C39-C40
9	C	1105	PCW	O2-C31-C32-C33
9	A	1106	PCW	O2-C31-C32-C33
9	C	1104	PCW	C13-C14-C15-C16
9	A	1105	PCW	C13-C14-C15-C16
13	C	1116	A1MA6	CA2-CA3-CA4-CBE
13	A	1117	A1MA6	CA2-CA3-CA4-CBE
13	C	1116	A1MA6	OBUC66-C67-CBT
13	A	1117	A1MA6	OBUC66-C67-CBT
9	C	1105	PCW	O31-C31-C32-C33
9	A	1106	PCW	O31-C31-C32-C33

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	C	1116	A1MA6	C75-C77-CBL-CBM-CBO-O76
13	A	1117	A1MA6	C75-C77-CBL-CBM-CBO-O76

24 monomers are involved in 113 short contacts:

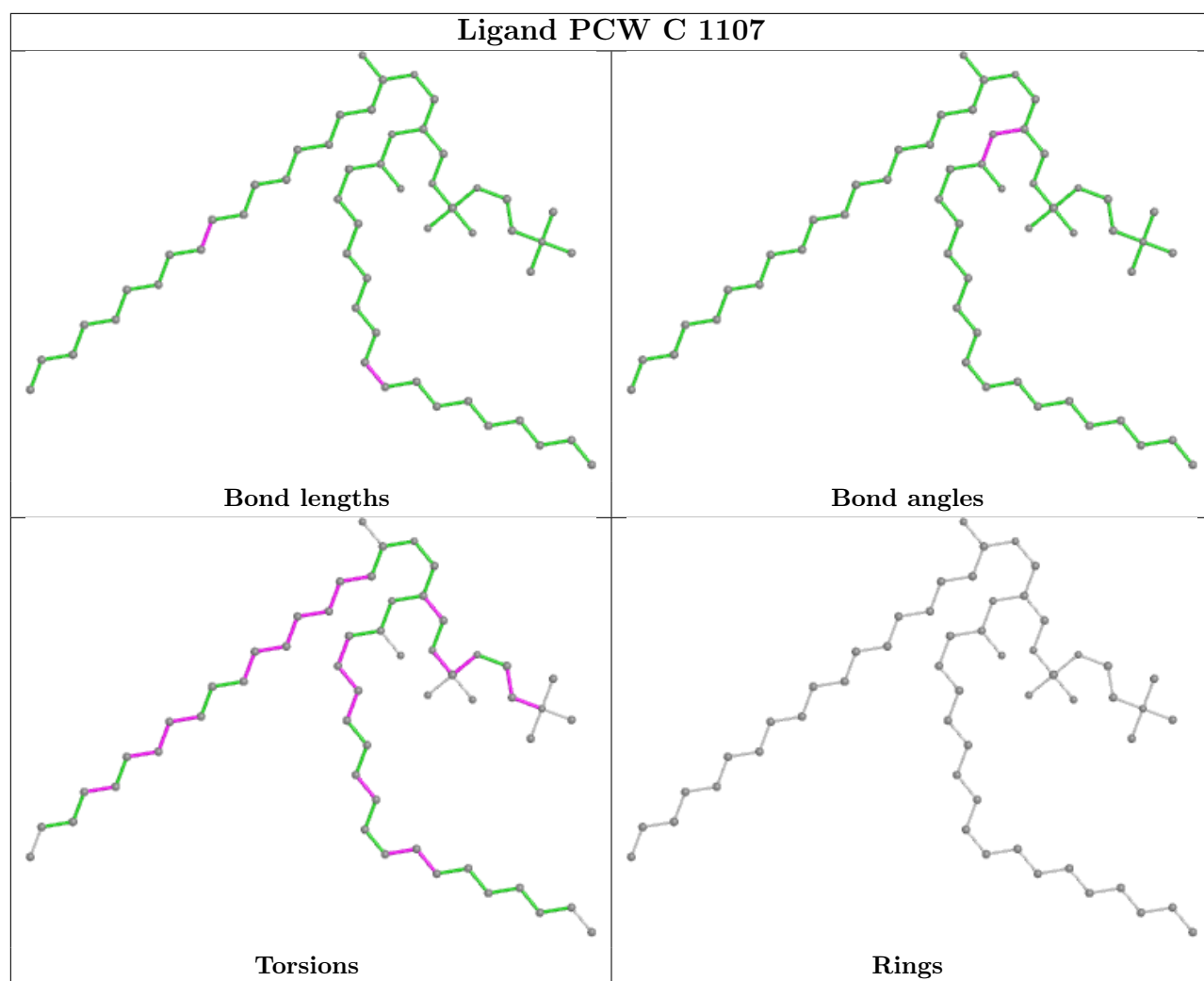
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	1107	PCW	4	0
9	C	1106	PCW	4	0
8	A	1103	CLR	5	0
8	A	1102	CLR	6	0
11	C	1111	ATP	1	0

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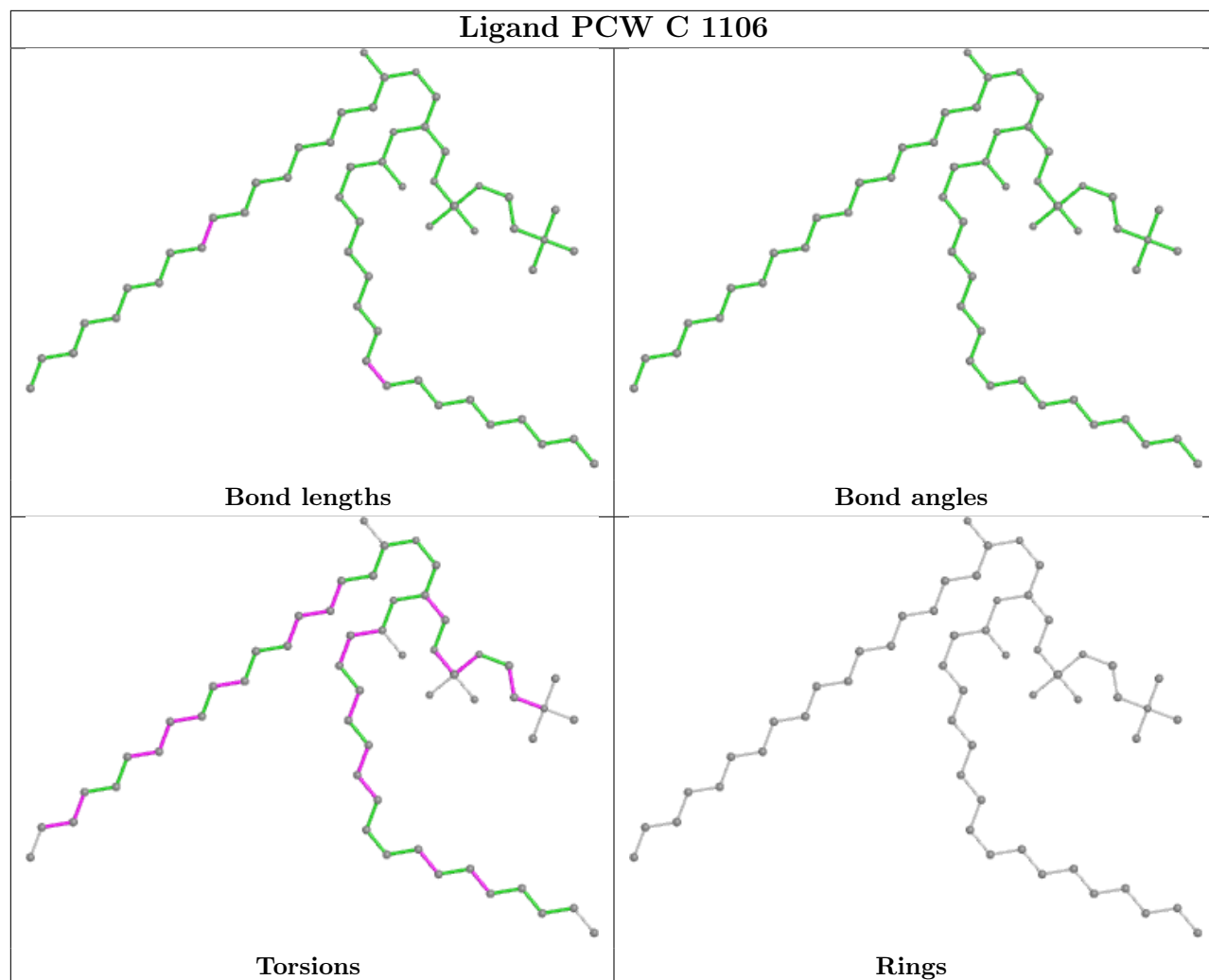
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	401	PCW	11	0
9	E	101	PCW	5	0
8	B	402	CLR	3	0
8	C	1109	CLR	2	0
8	C	1103	CLR	4	0
8	C	1102	CLR	5	0
9	A	1106	PCW	20	0
13	C	1116	A1MA6	4	0
11	A	1112	ATP	1	0
9	A	1108	PCW	2	0
9	A	1107	PCW	5	0
13	A	1117	A1MA6	4	0
8	D	401	CLR	5	0
9	C	1104	PCW	14	0
9	C	1105	PCW	17	0
9	A	1105	PCW	13	0
8	A	1110	CLR	2	0
9	G	101	PCW	6	0
9	A	1104	PCW	11	0

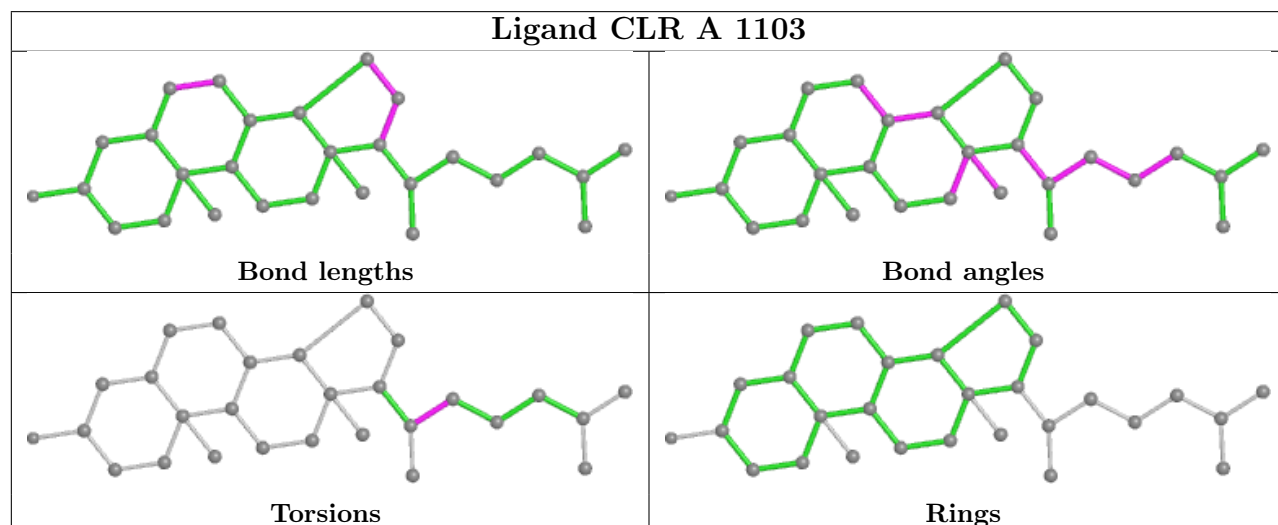
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

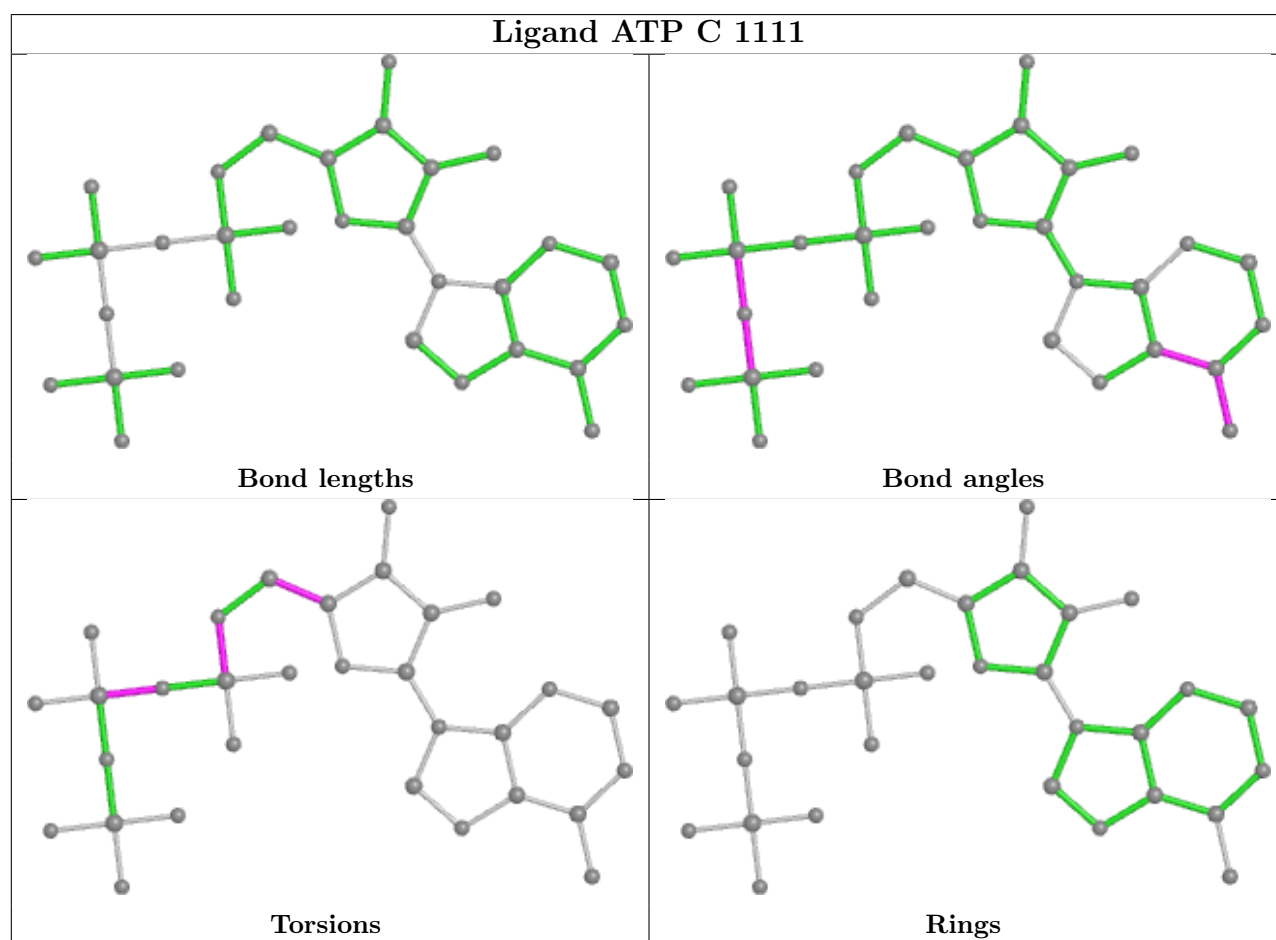
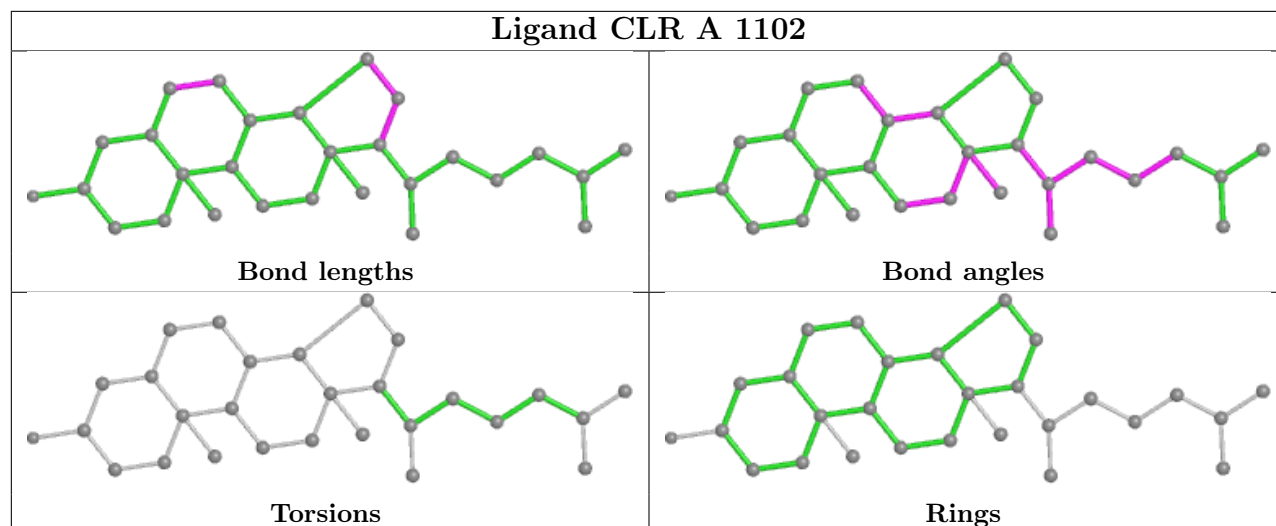


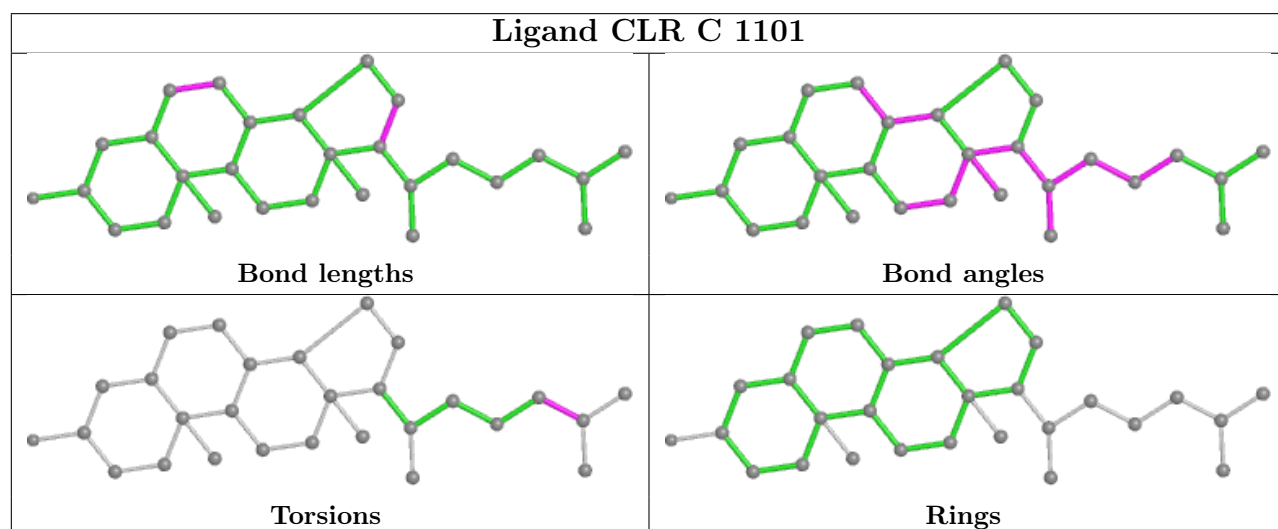
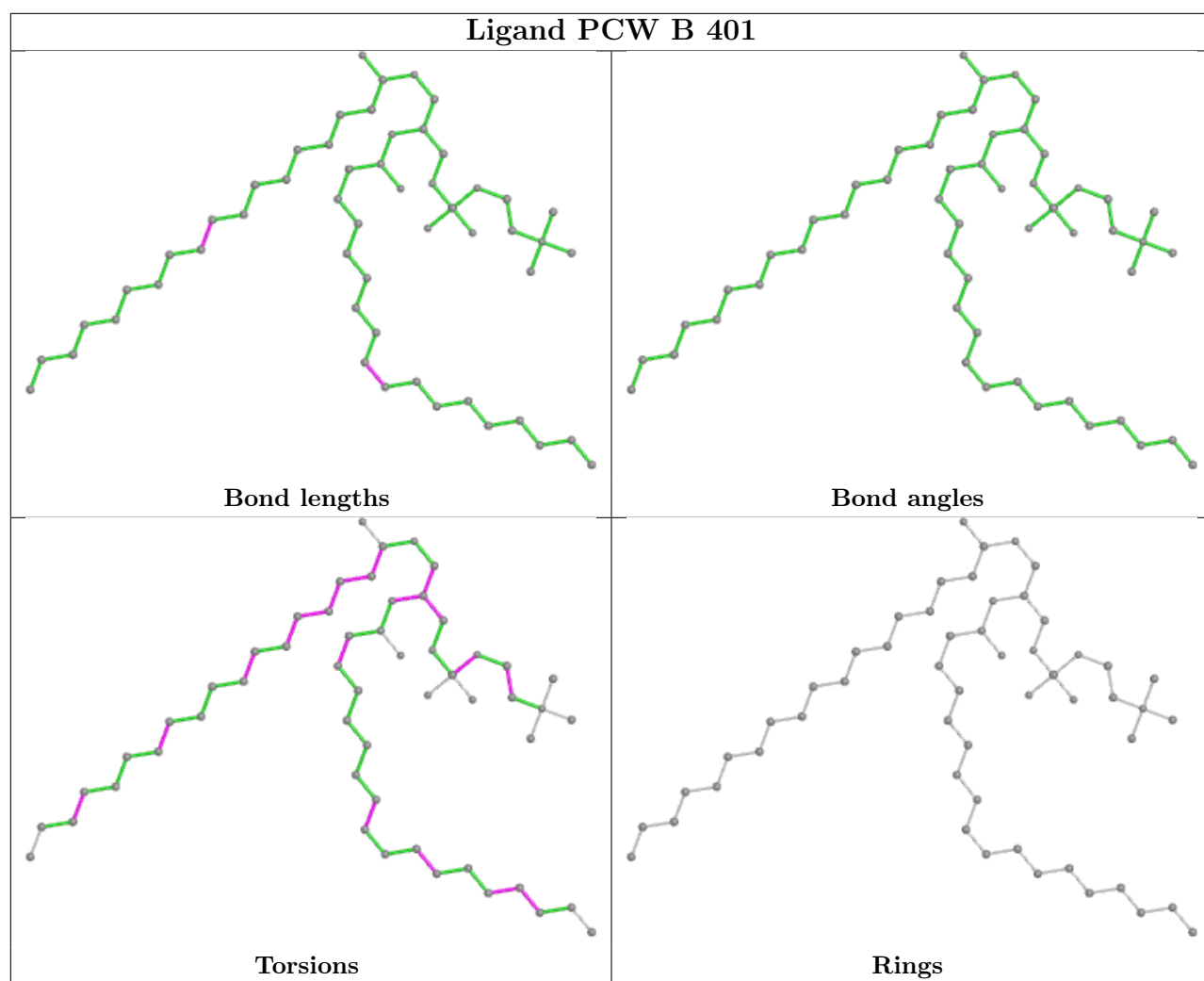
## Ligand PCW C 1106

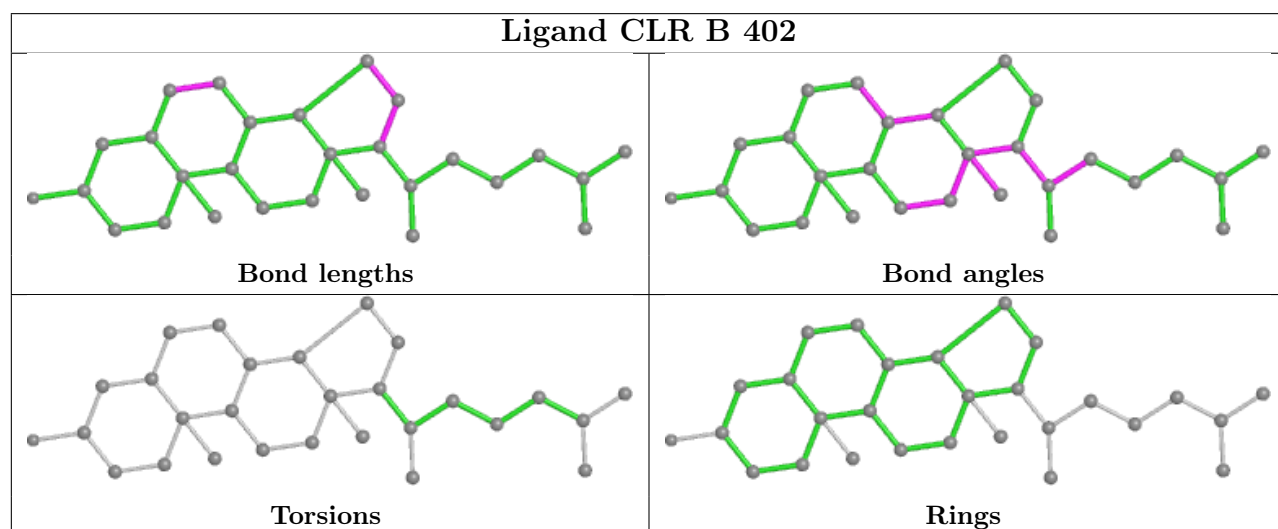
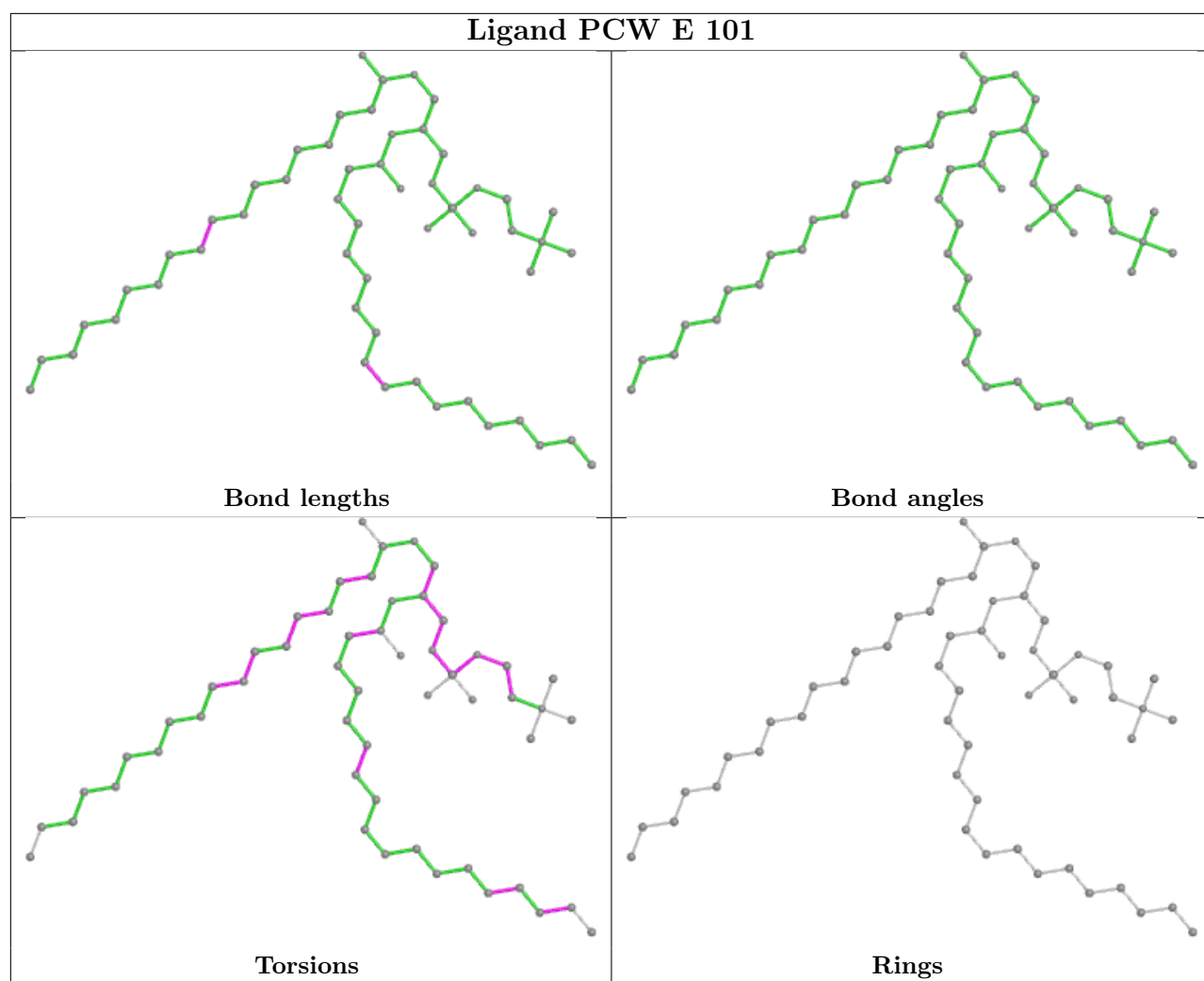


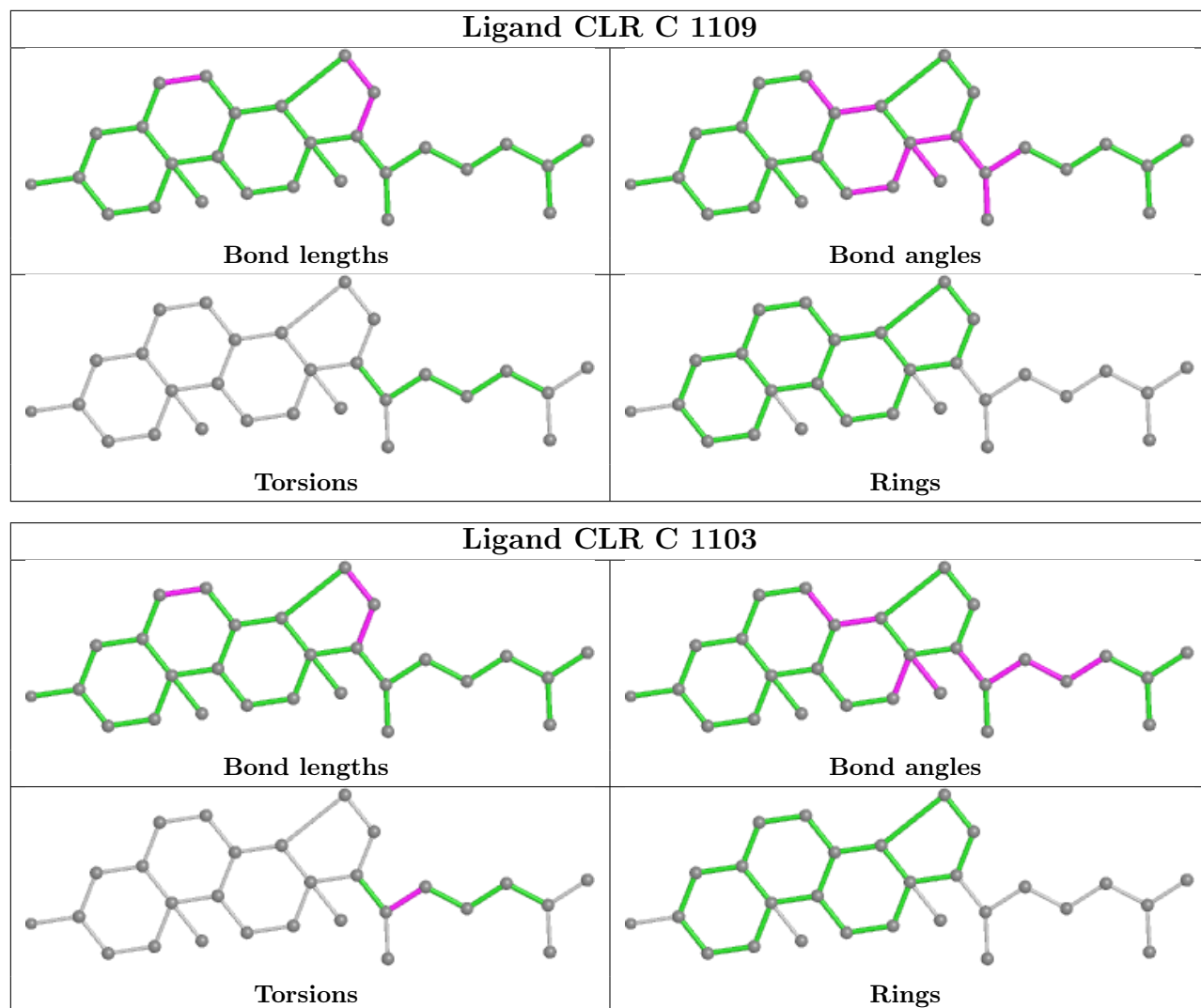
## Ligand CLR A 1103



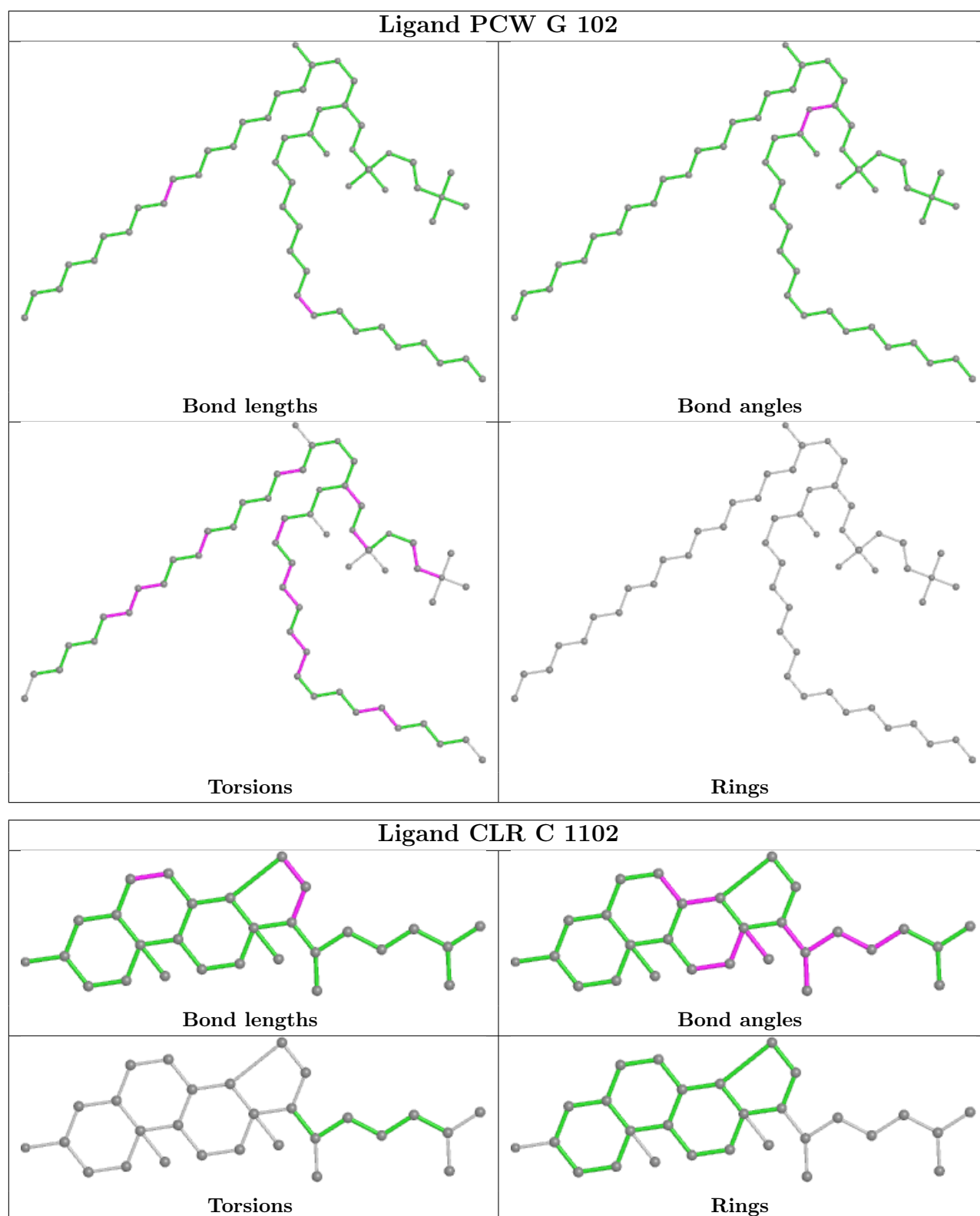


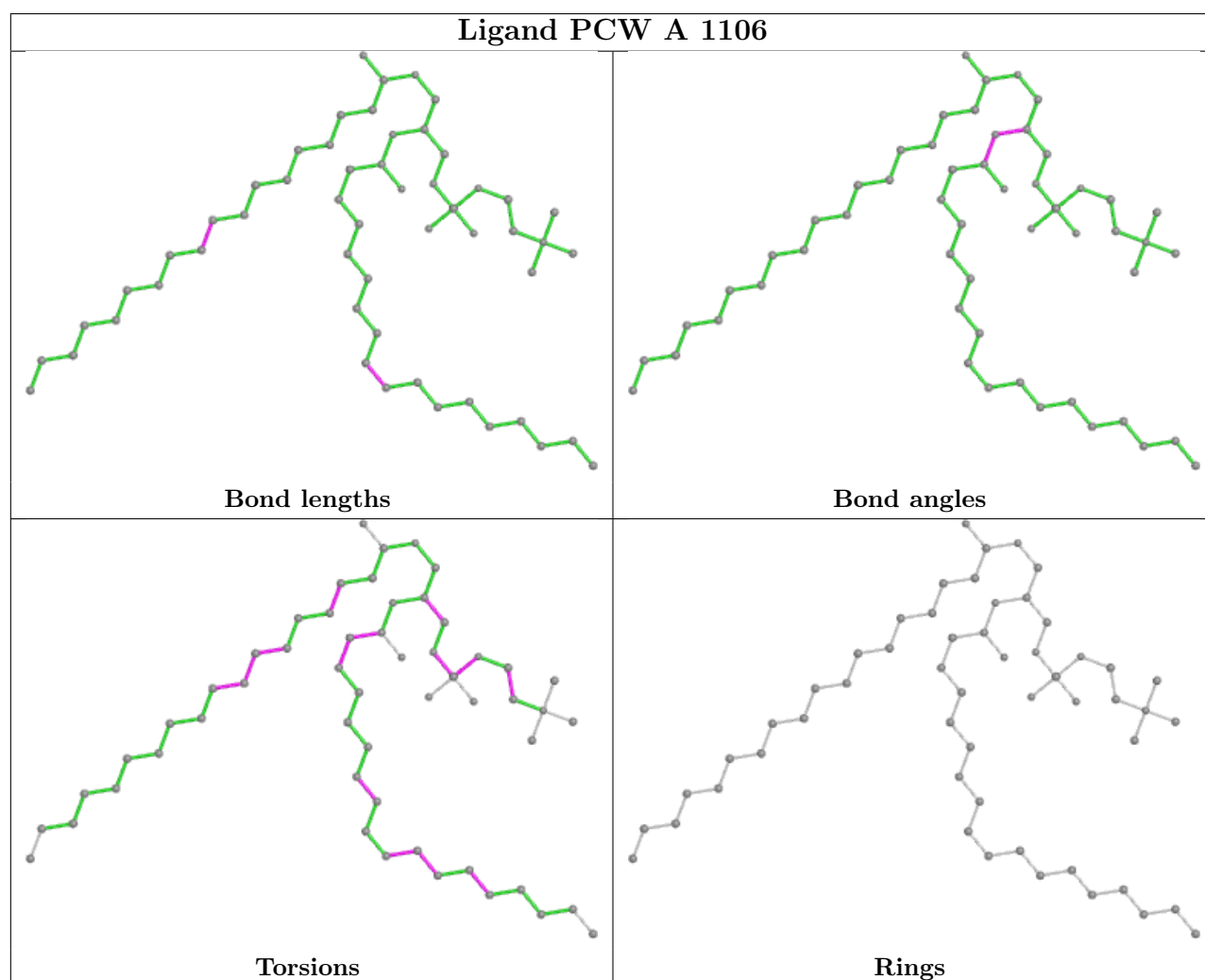
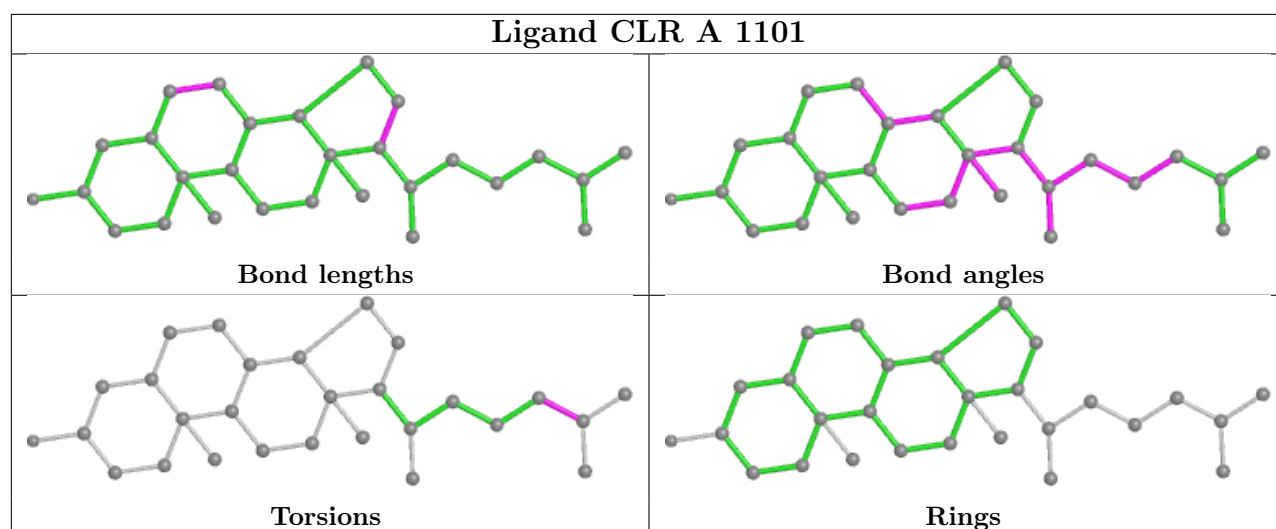


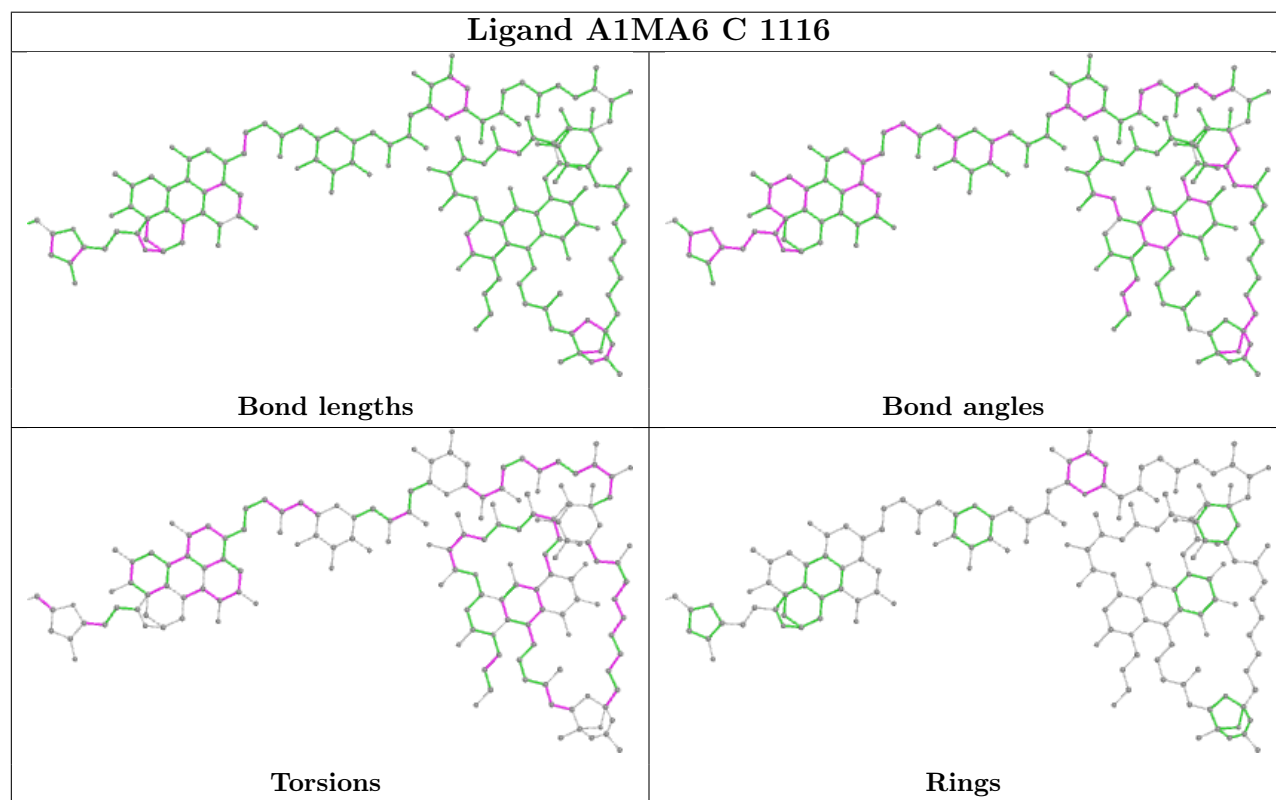
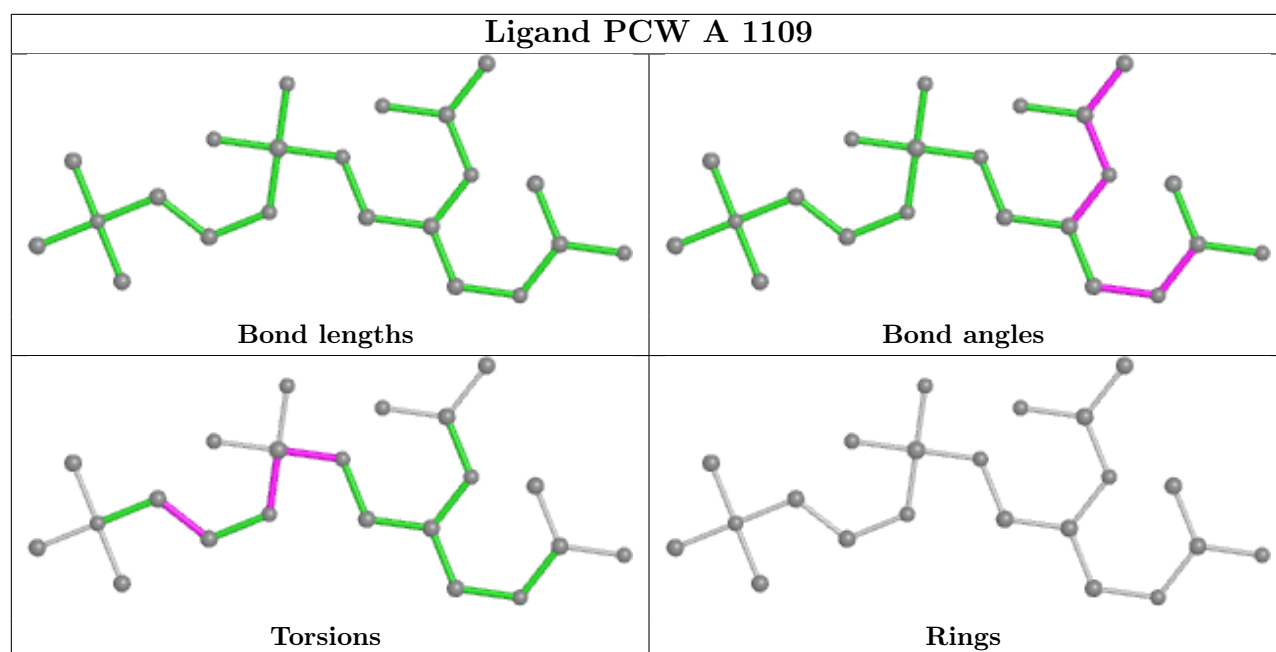


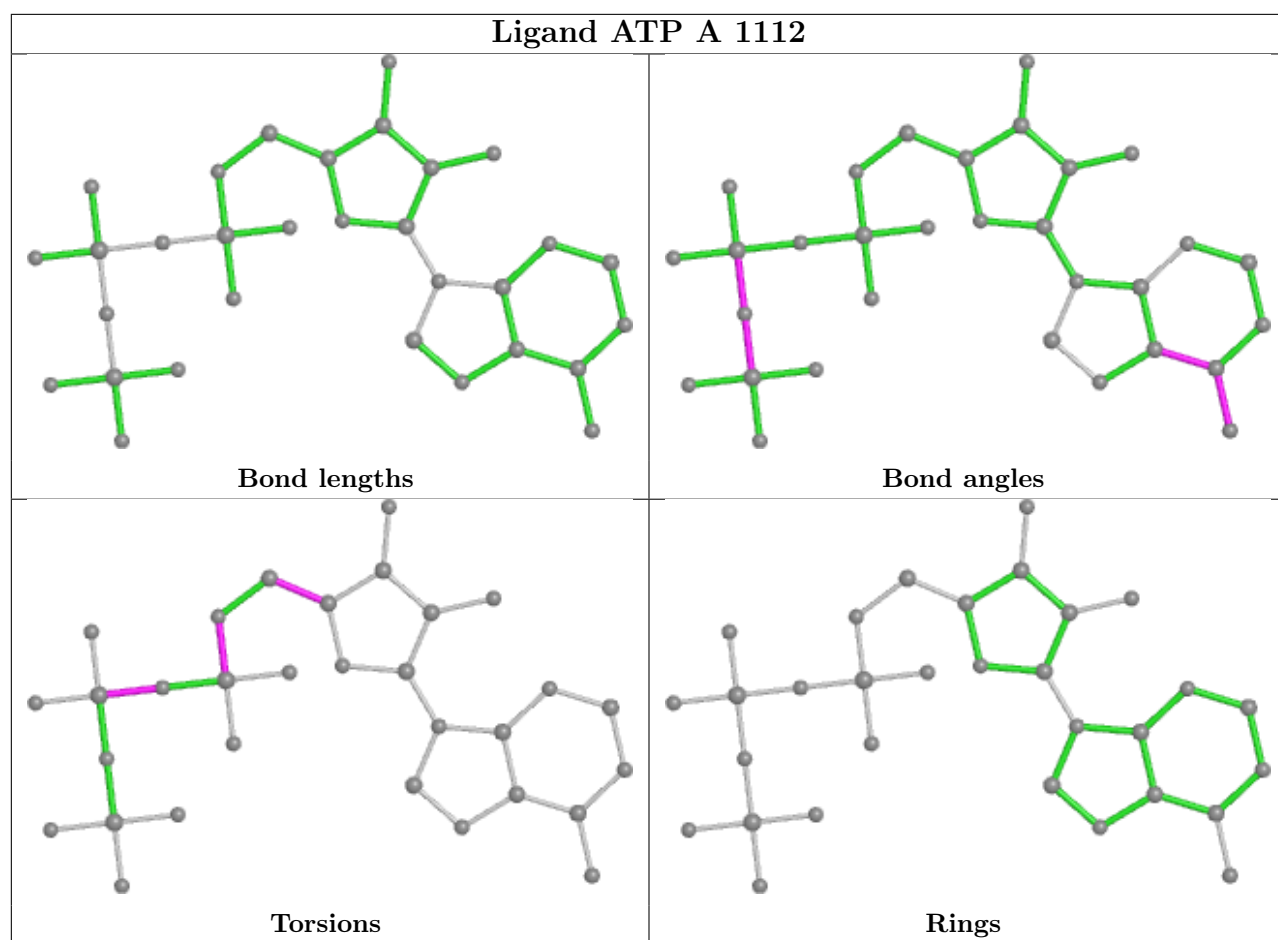


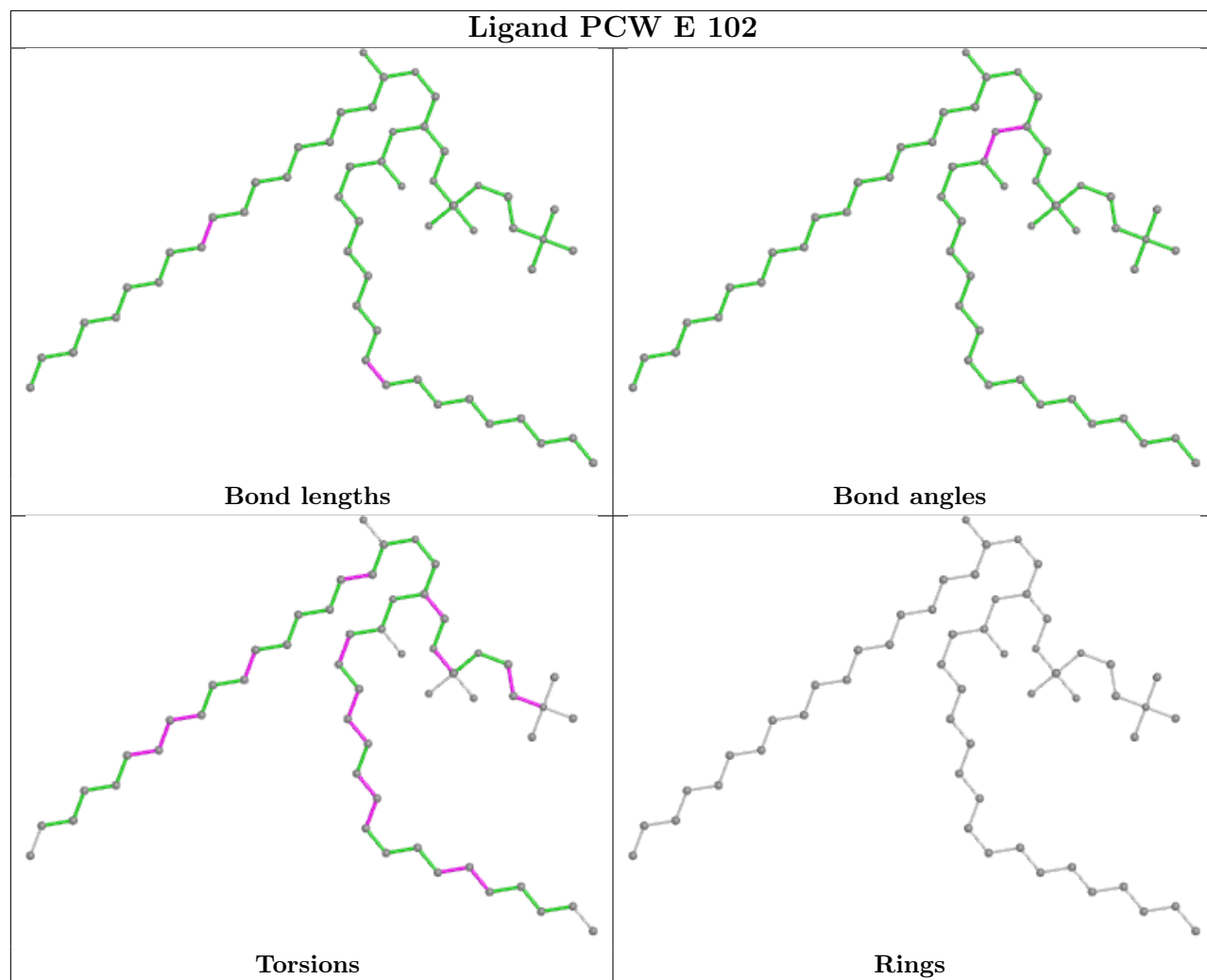


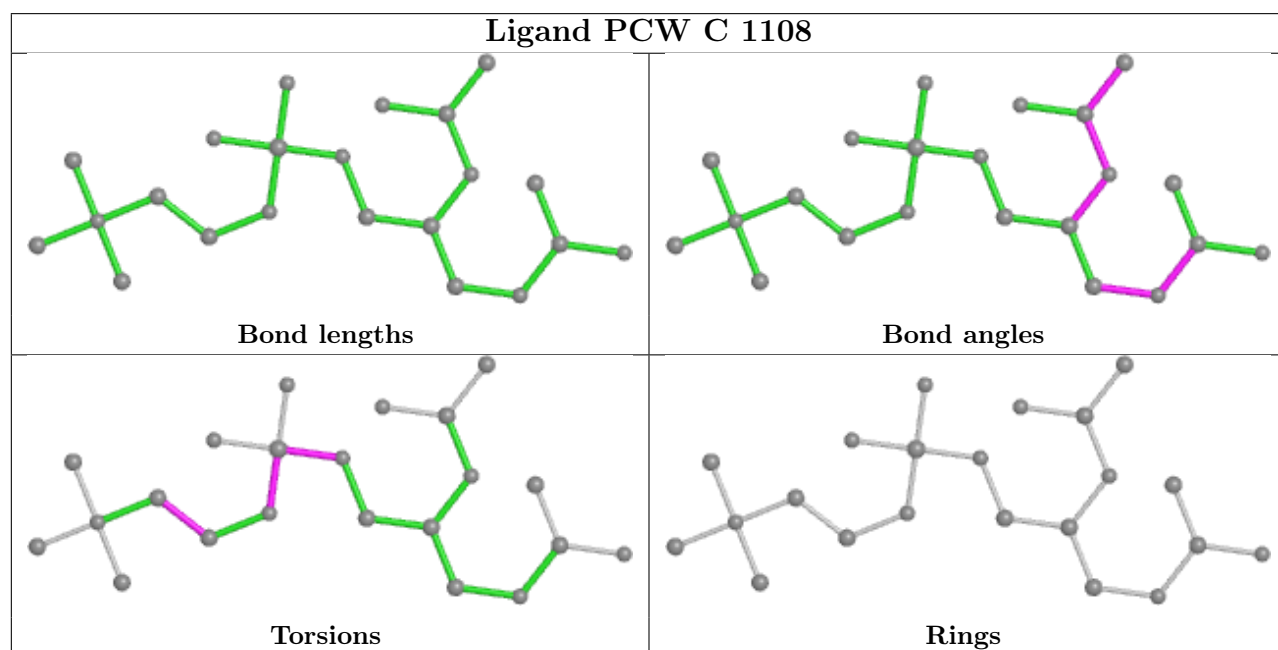
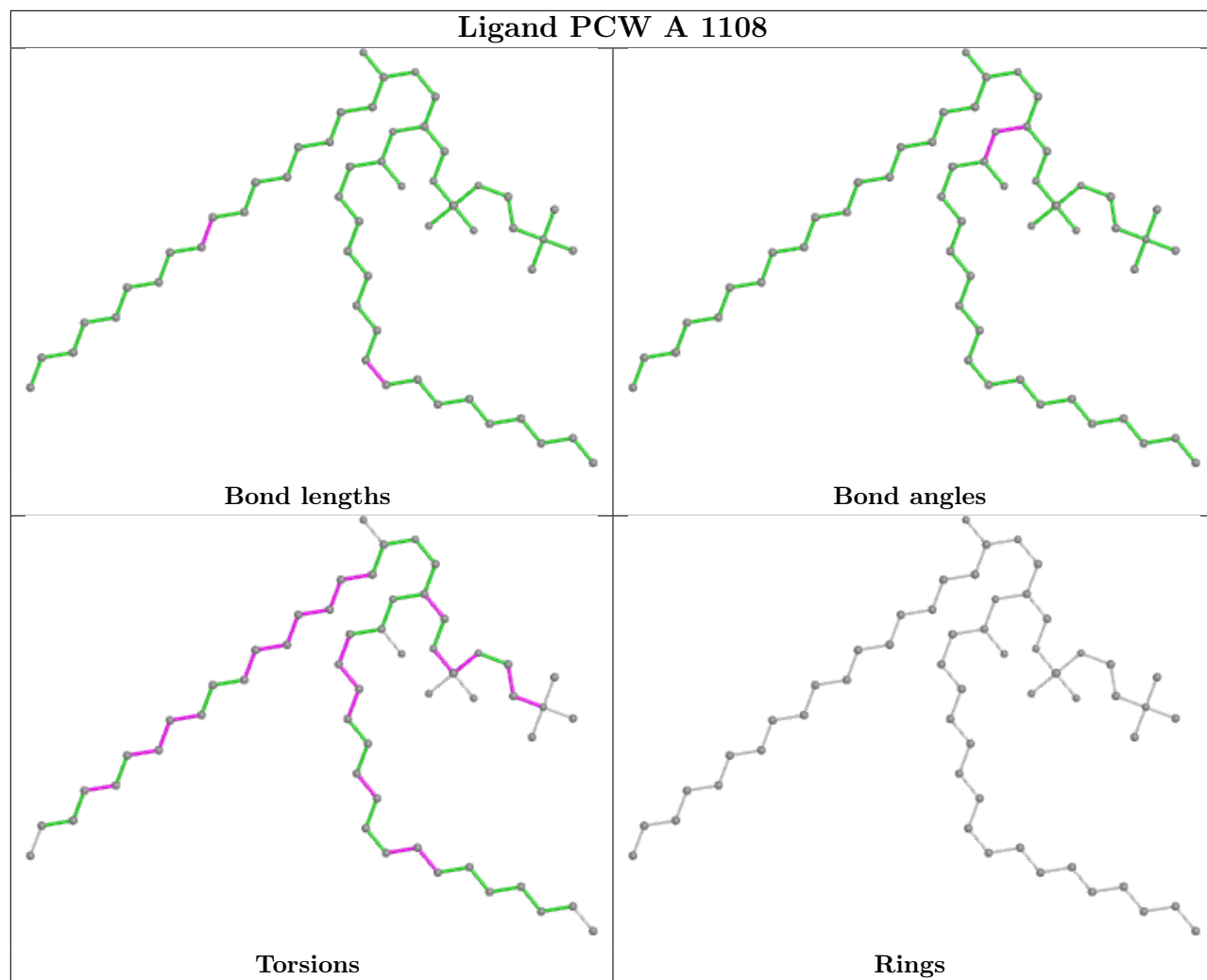


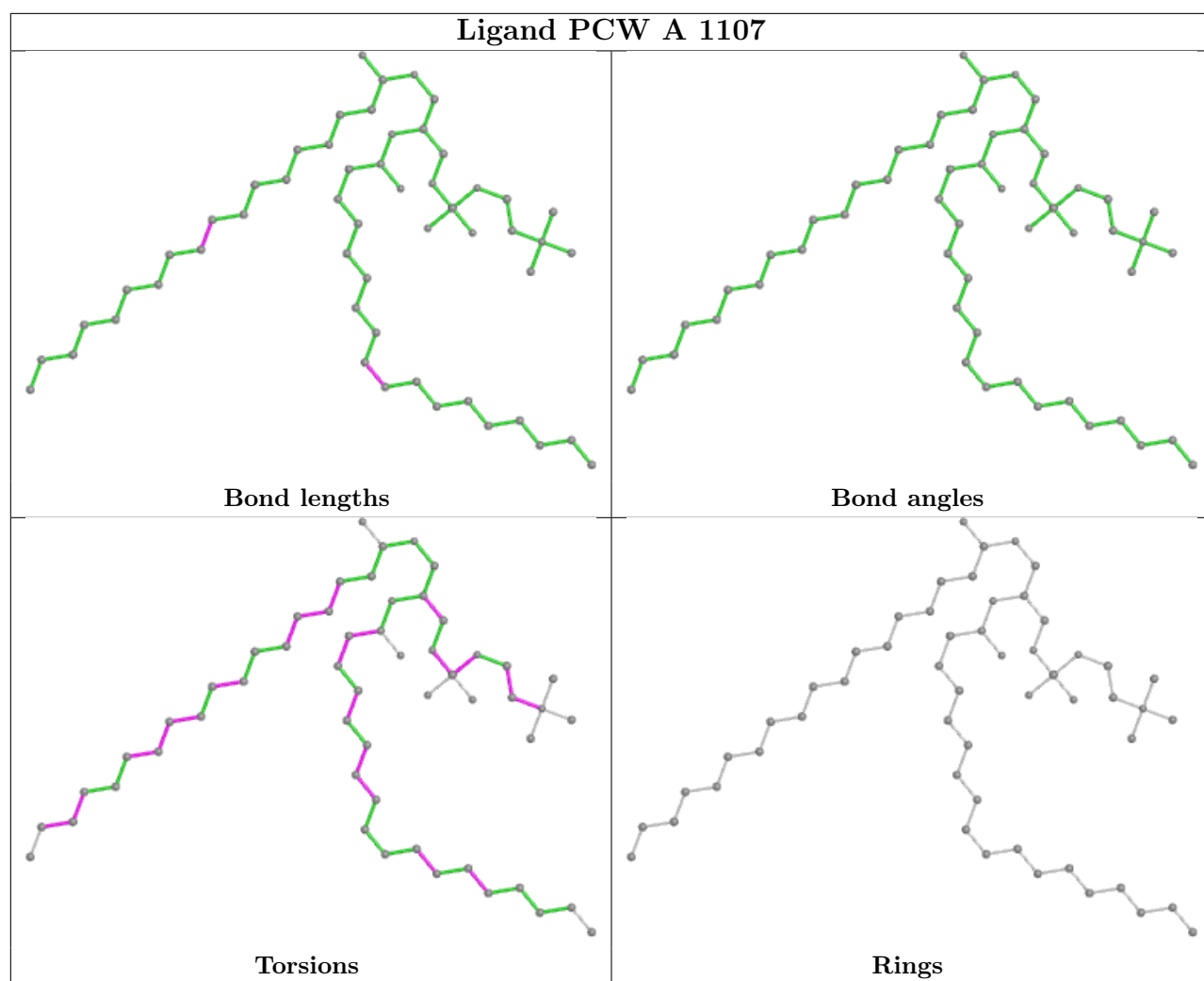


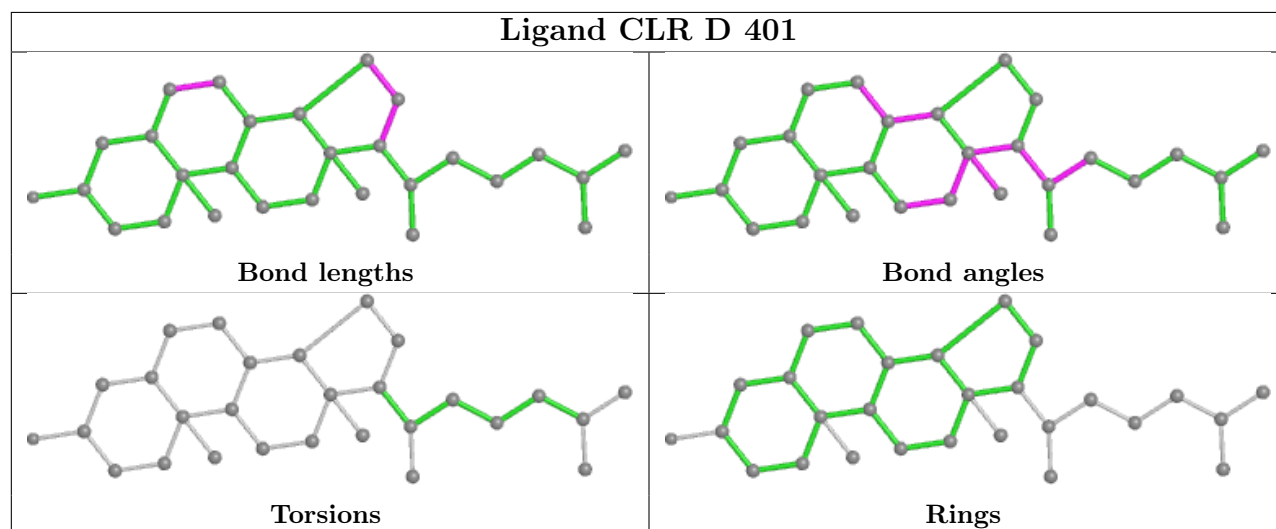
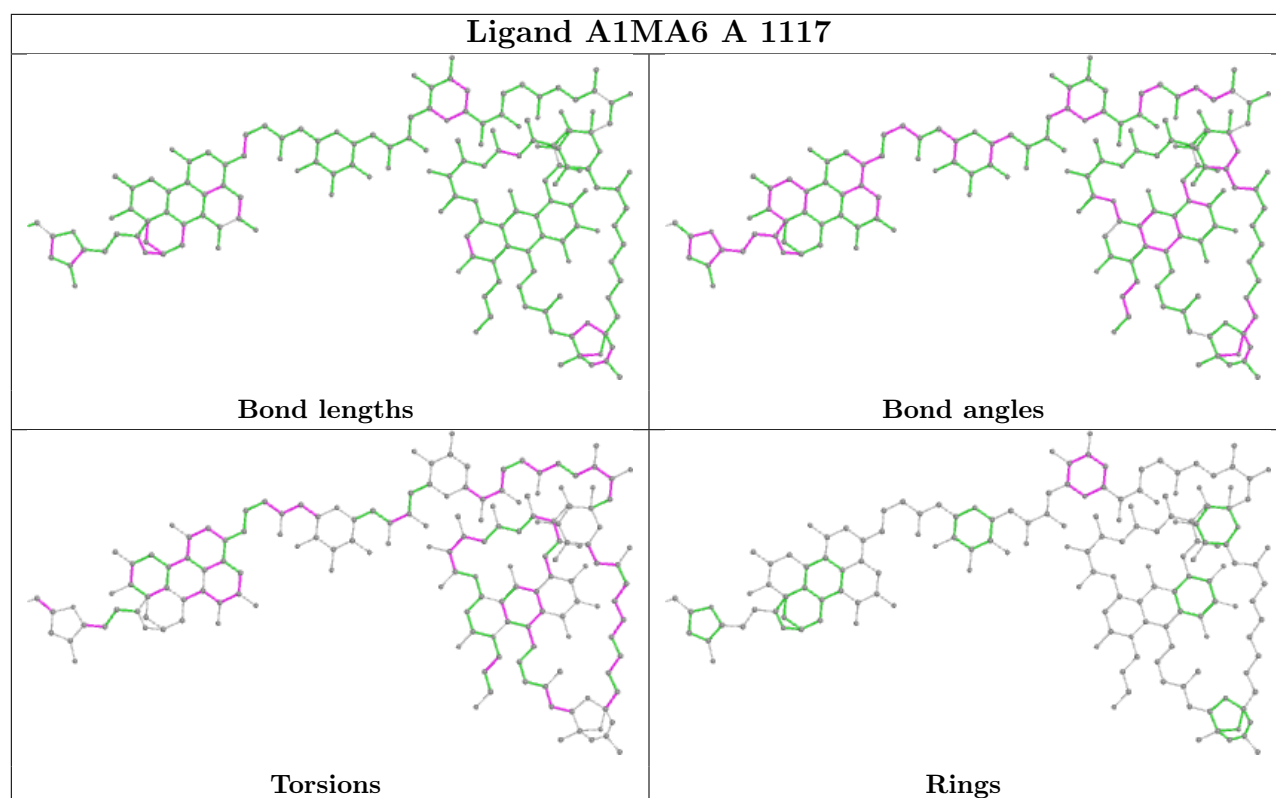




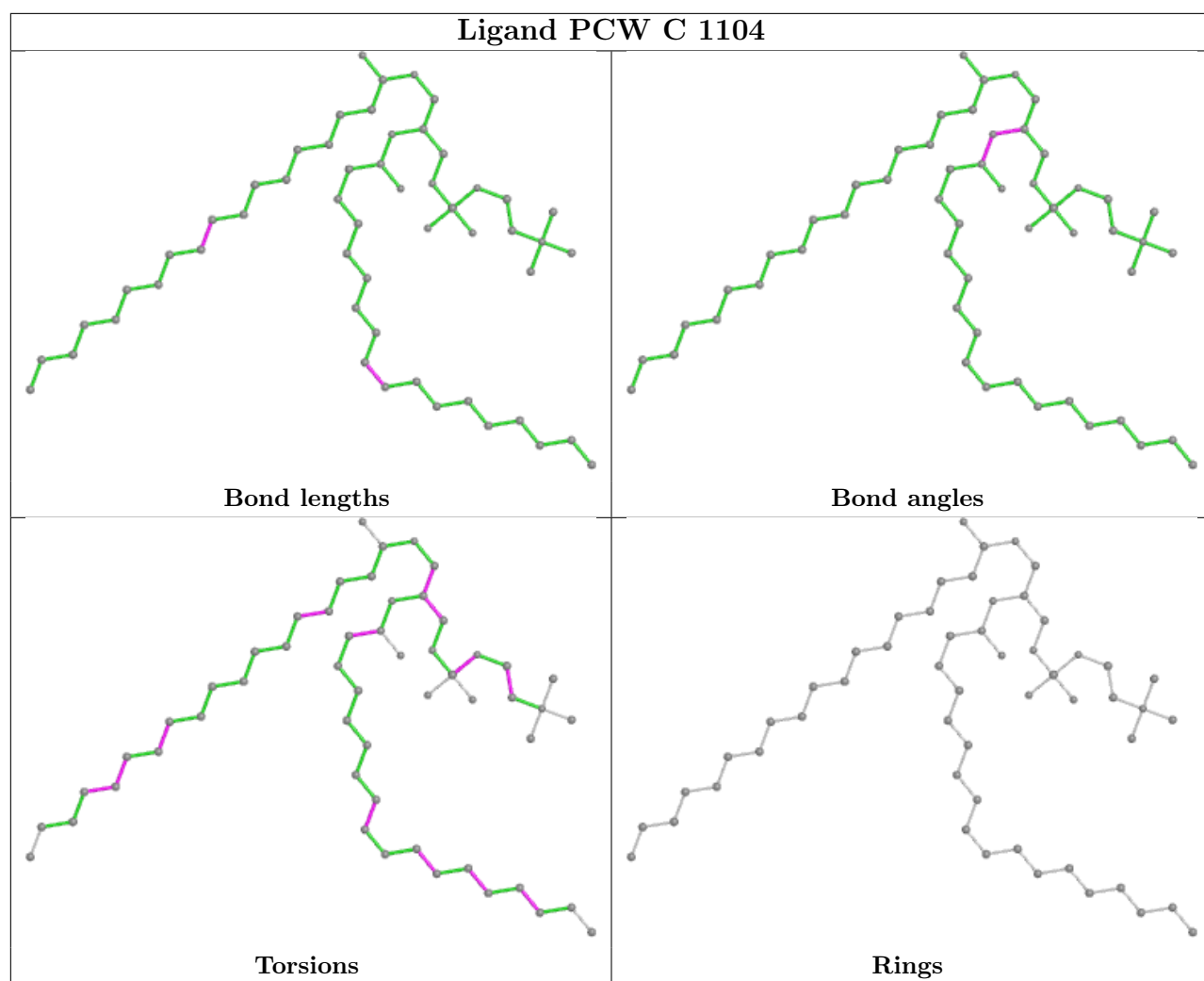


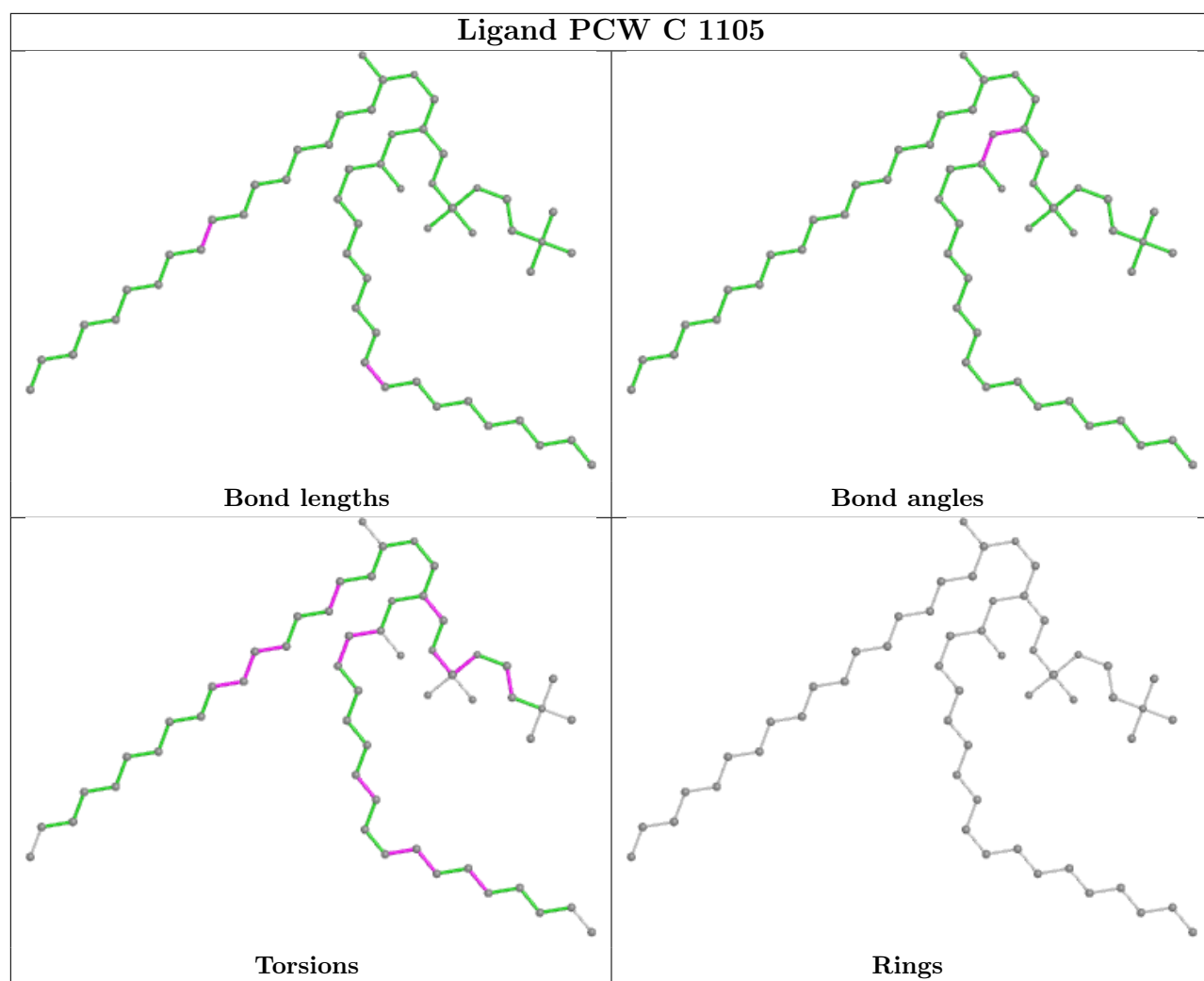




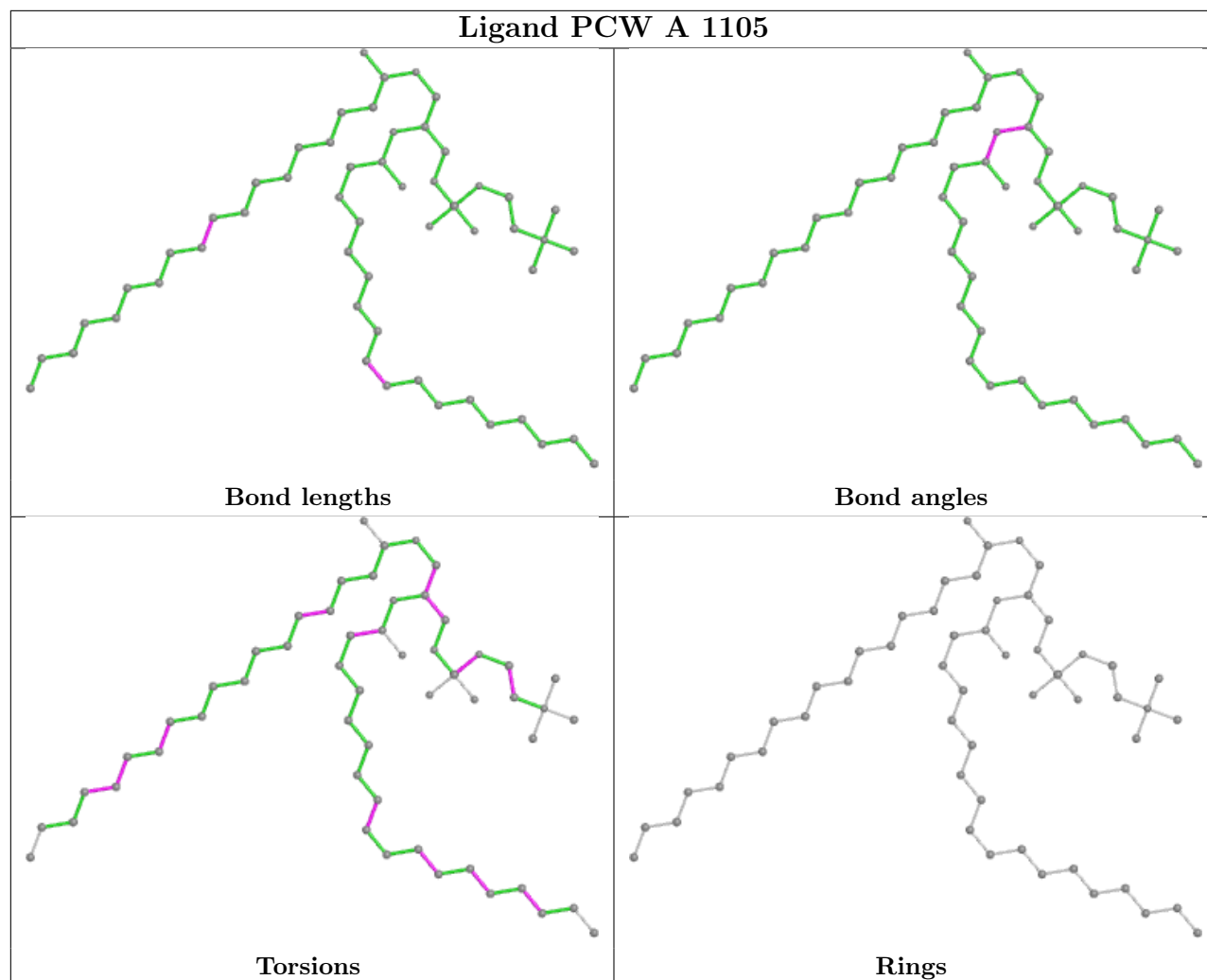




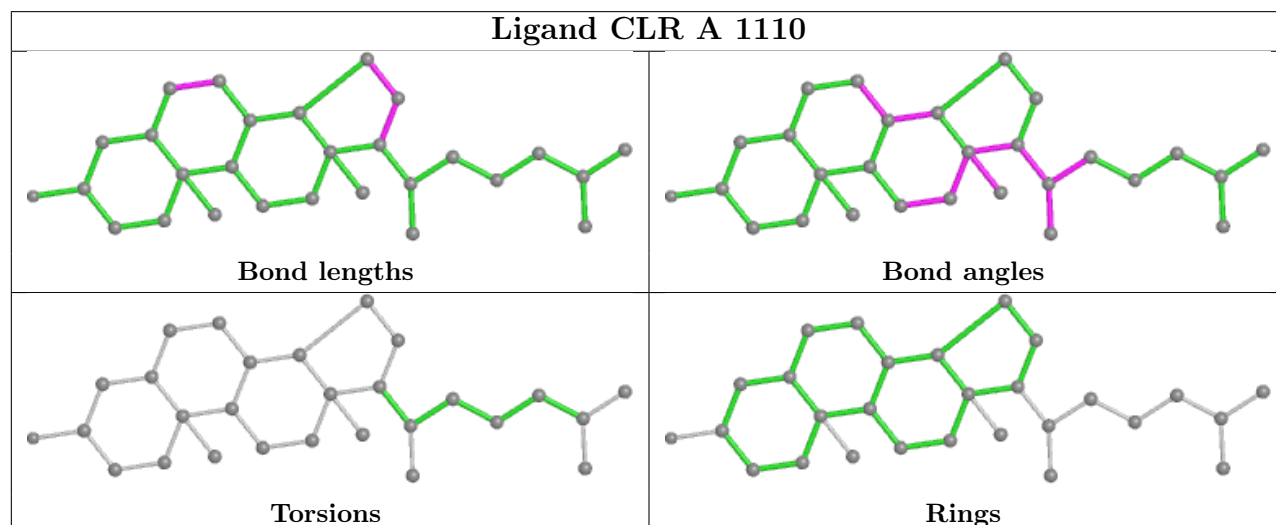


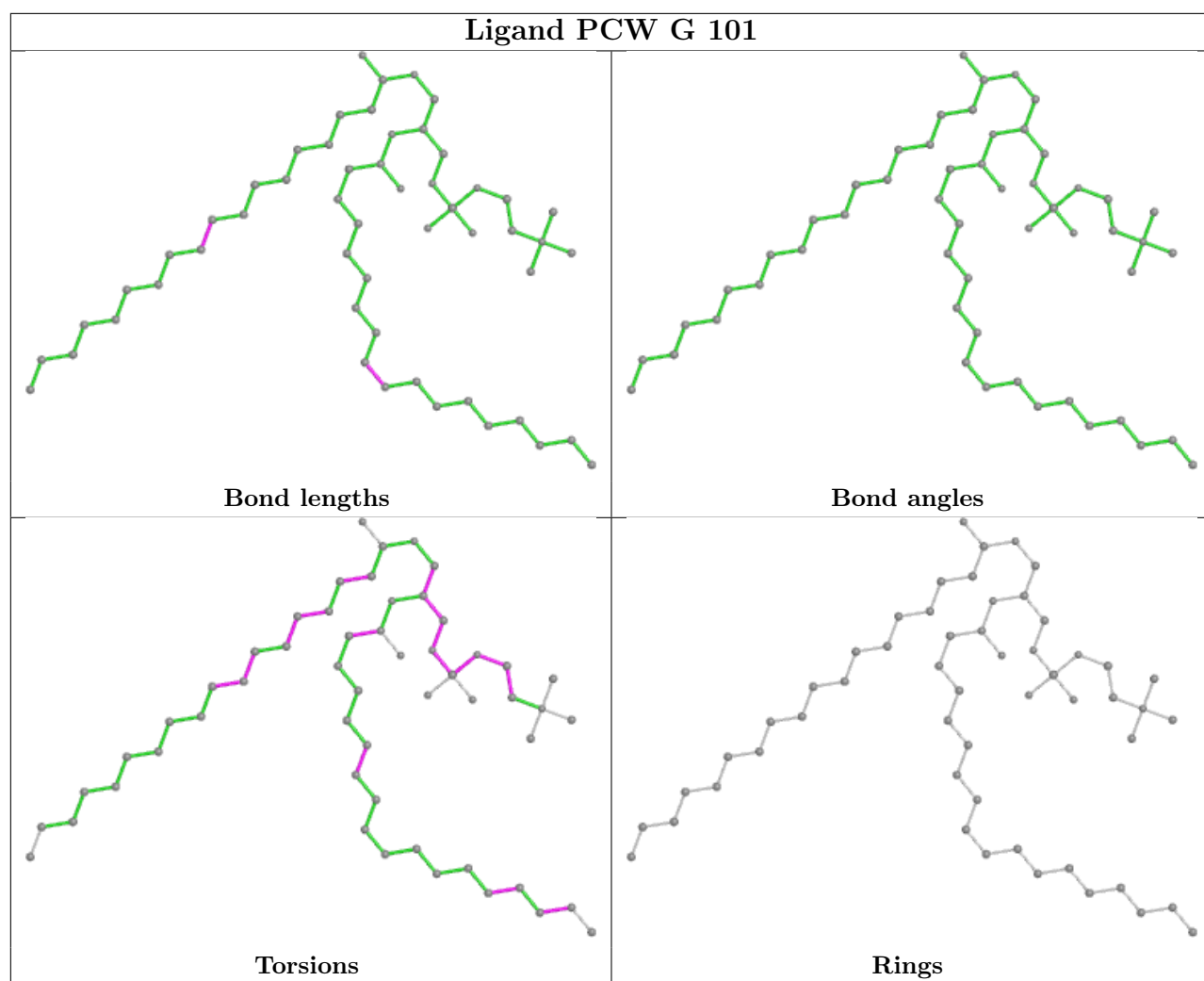


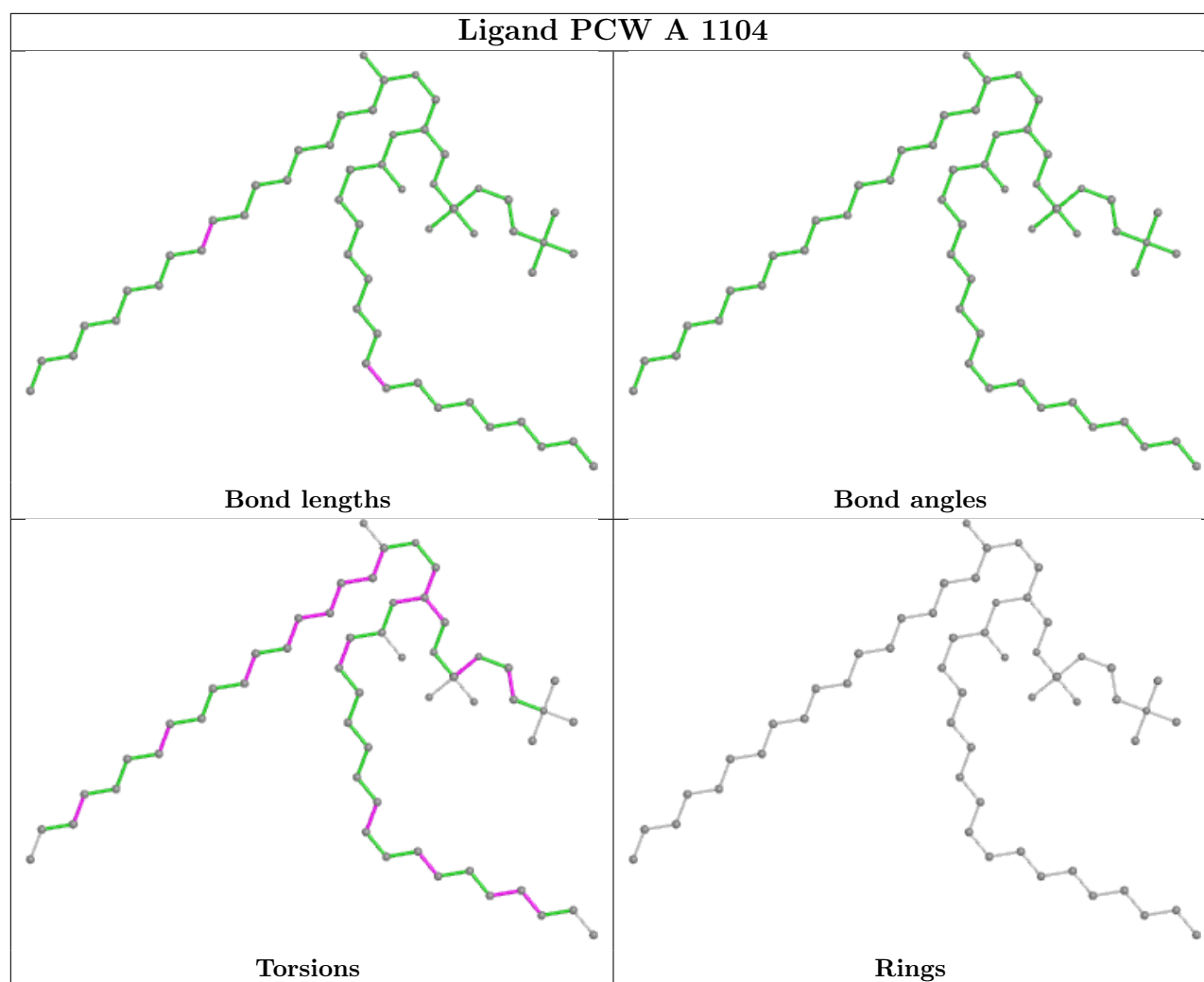
## Ligand PCW A 1105



## Ligand CLR A 1110







## 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.

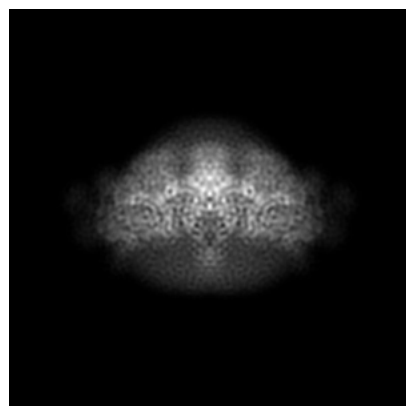
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65100. These allow visual inspection of the internal detail of the map and identification of artifacts.

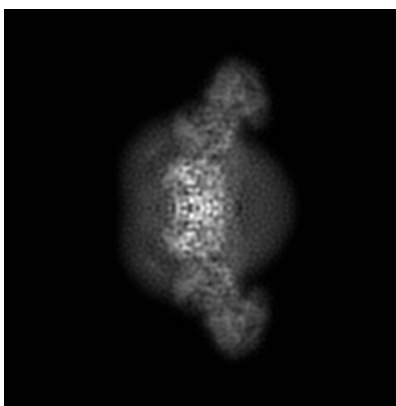
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

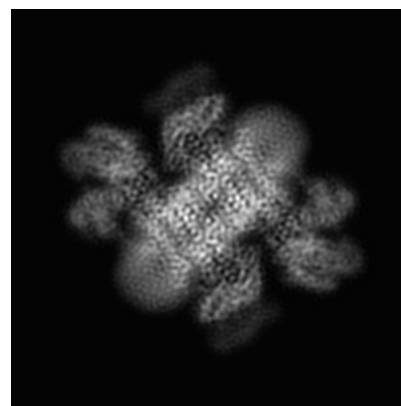
#### 6.1.1 Primary map



X

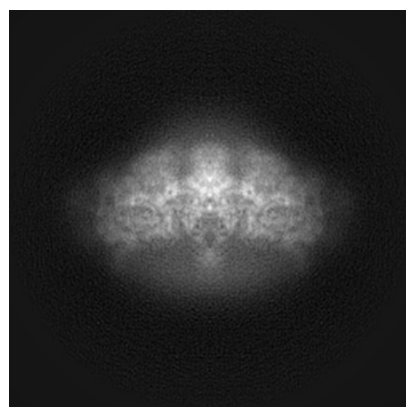


Y

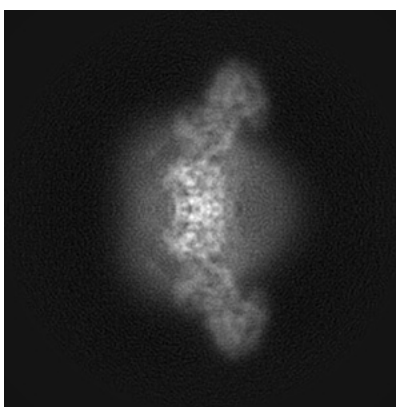


Z

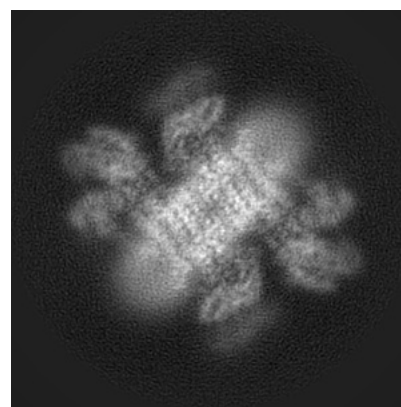
#### 6.1.2 Raw map



X



Y

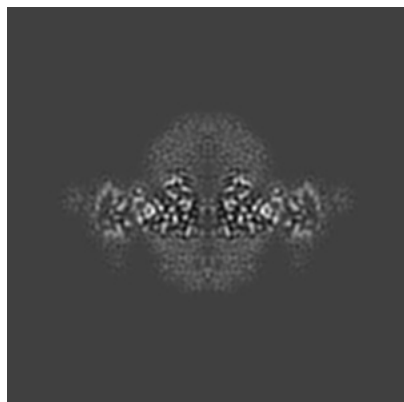


Z

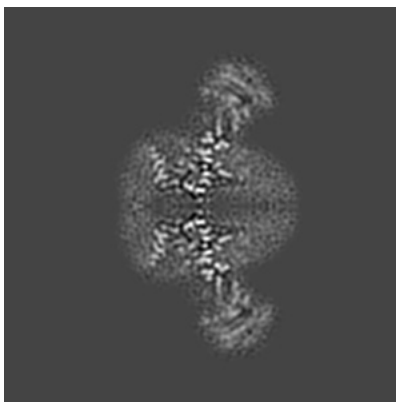
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

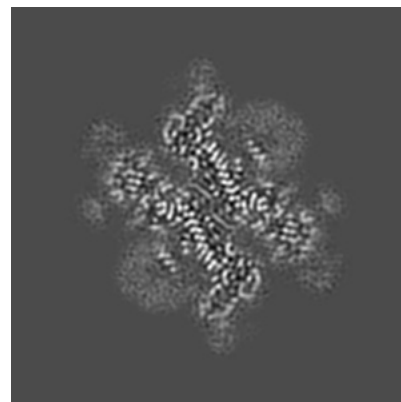
### 6.2.1 Primary map



X Index: 120

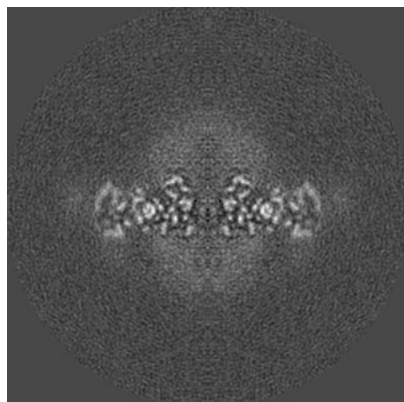


Y Index: 120

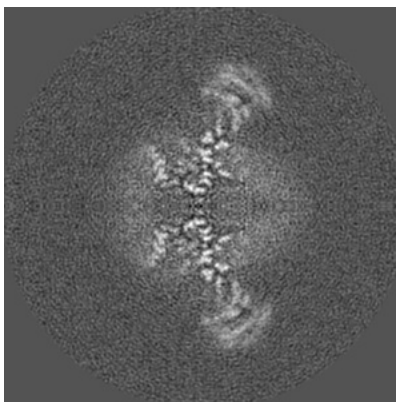


Z Index: 120

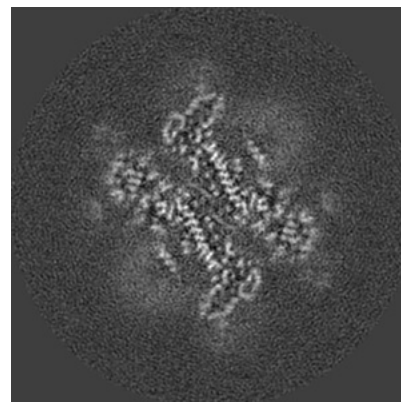
### 6.2.2 Raw map



X Index: 120



Y Index: 120

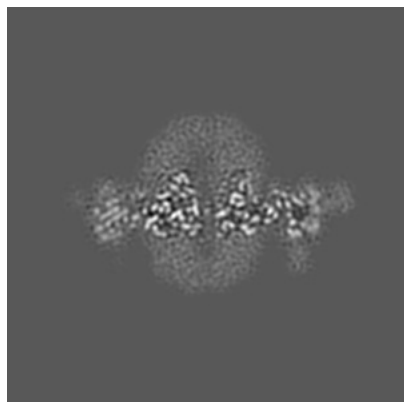


Z Index: 120

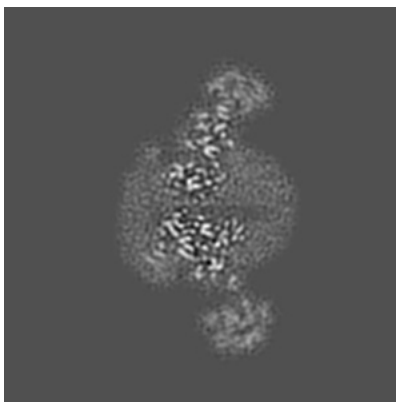
The images above show central slices of the map in three orthogonal directions.

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

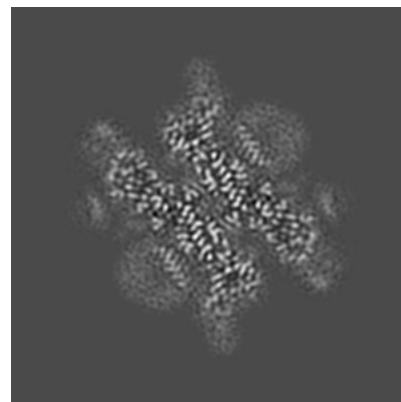
### 6.3.1 Primary map



X Index: 117

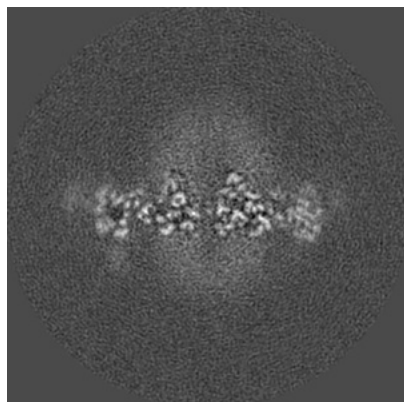


Y Index: 115

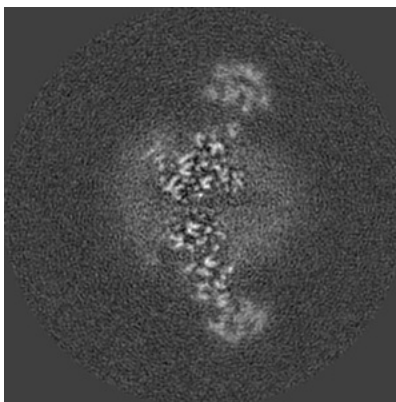


Z Index: 122

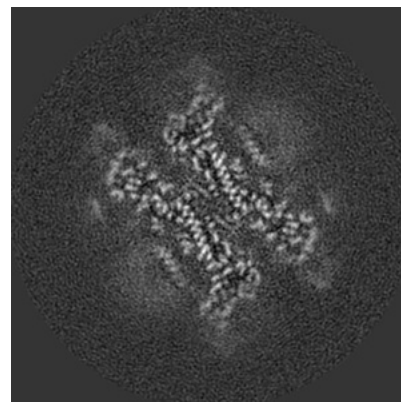
### 6.3.2 Raw map



X Index: 123



Y Index: 125



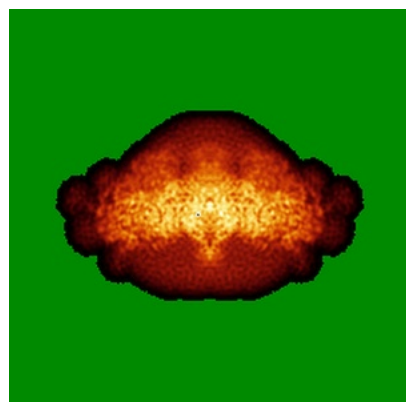
Z Index: 121

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

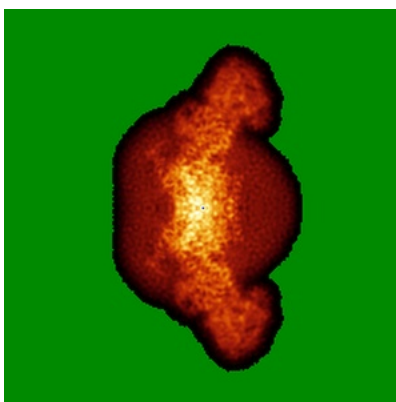


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

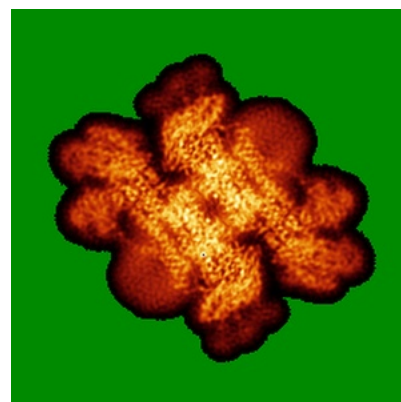
### 6.4.1 Primary map



X

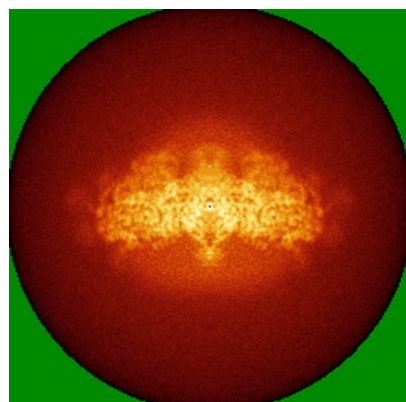


Y

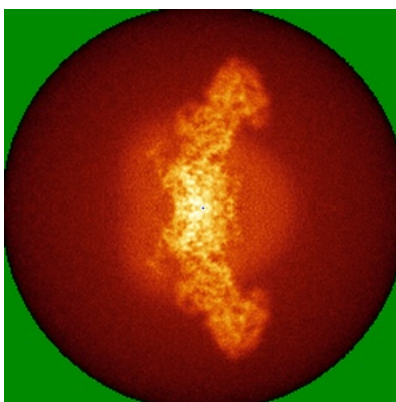


Z

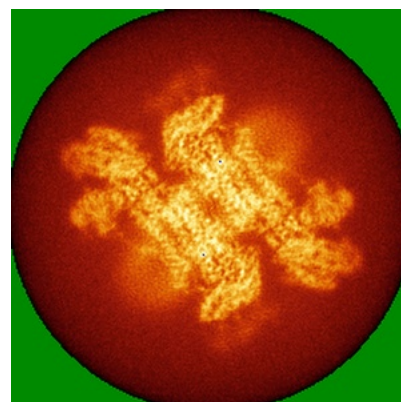
### 6.4.2 Raw map



X



Y

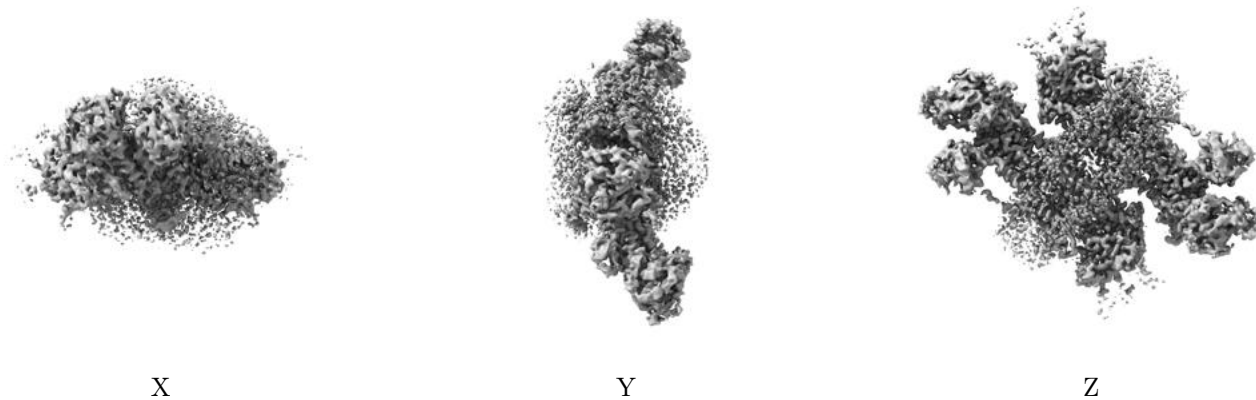


Z

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.

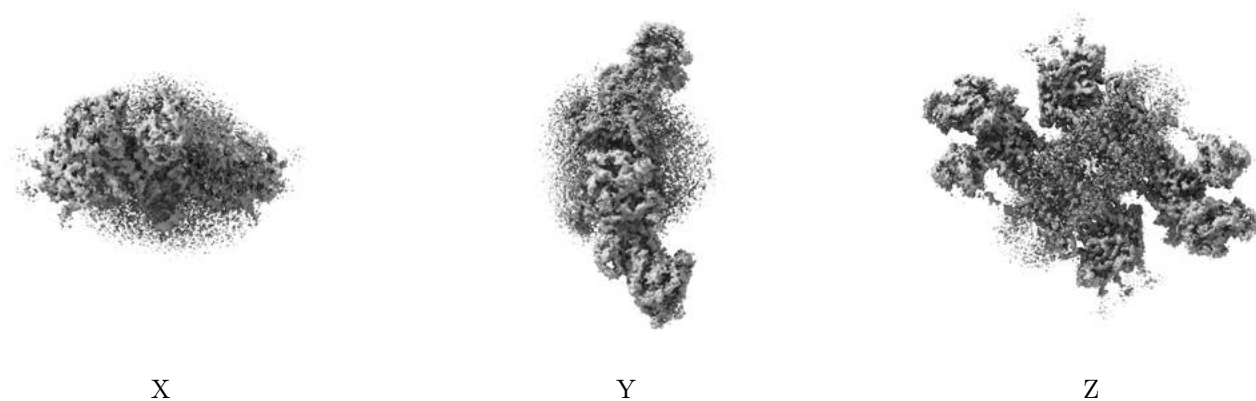
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0095. 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.

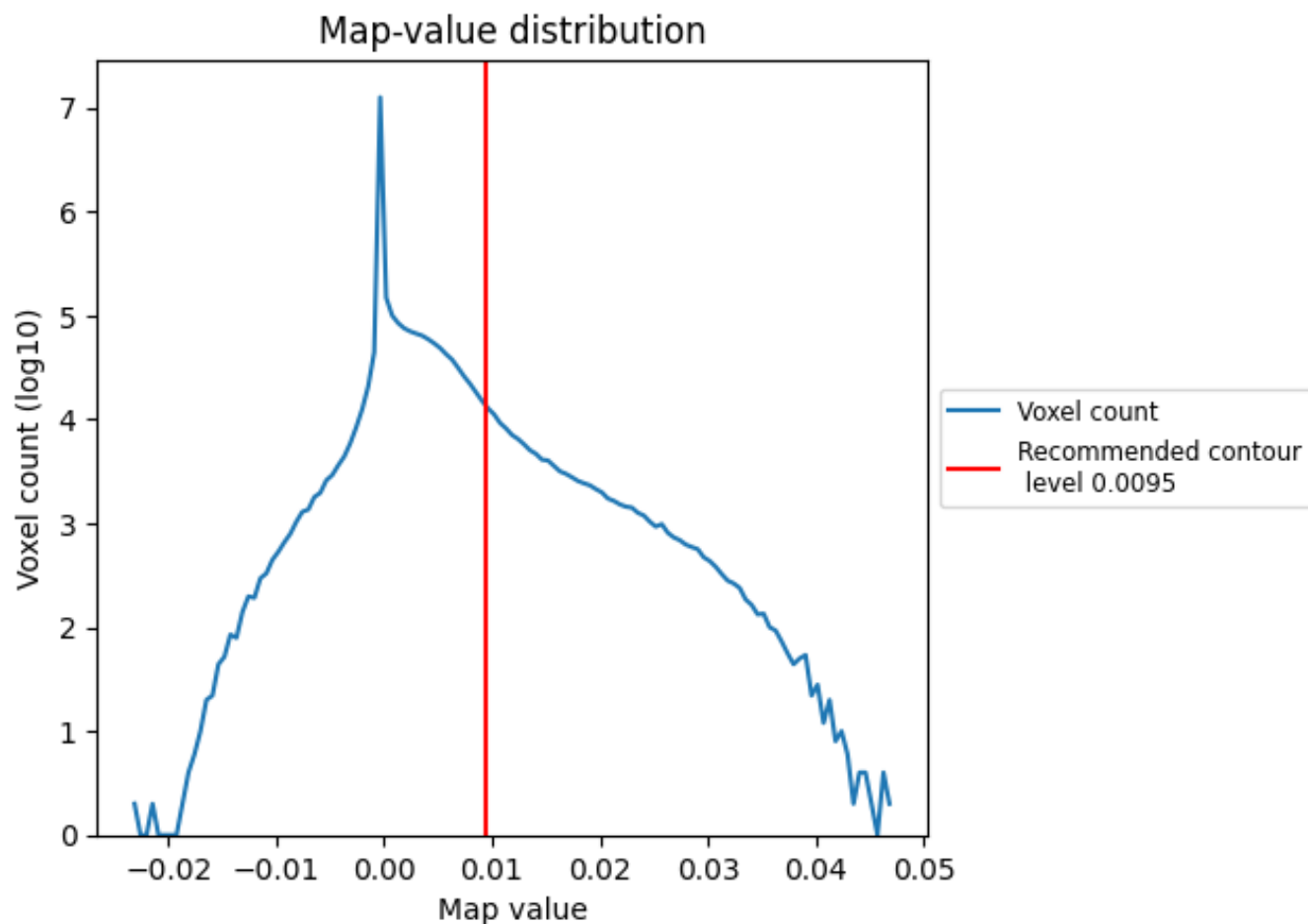
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

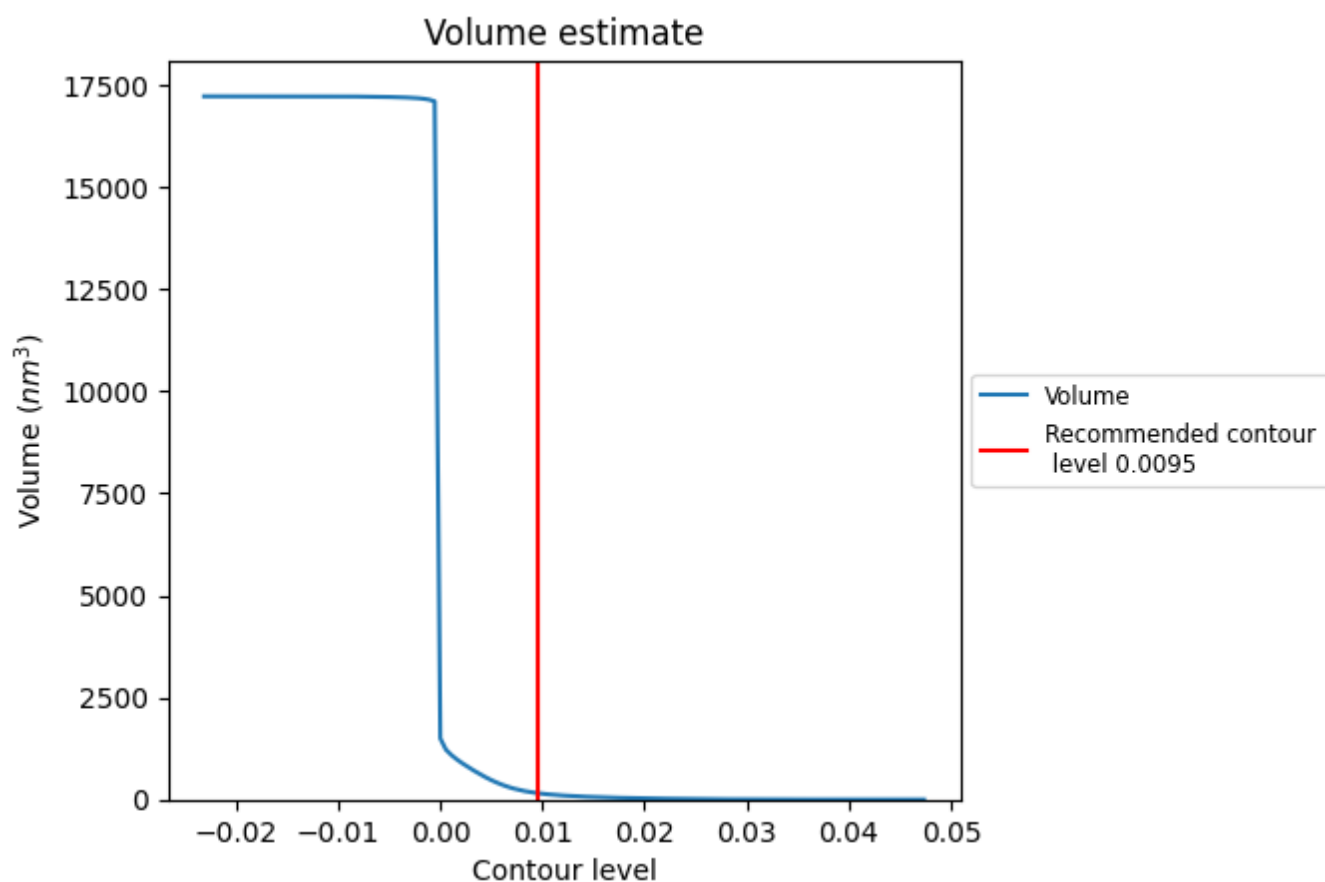
This section contains the results of statistical analysis of the map.

### 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.

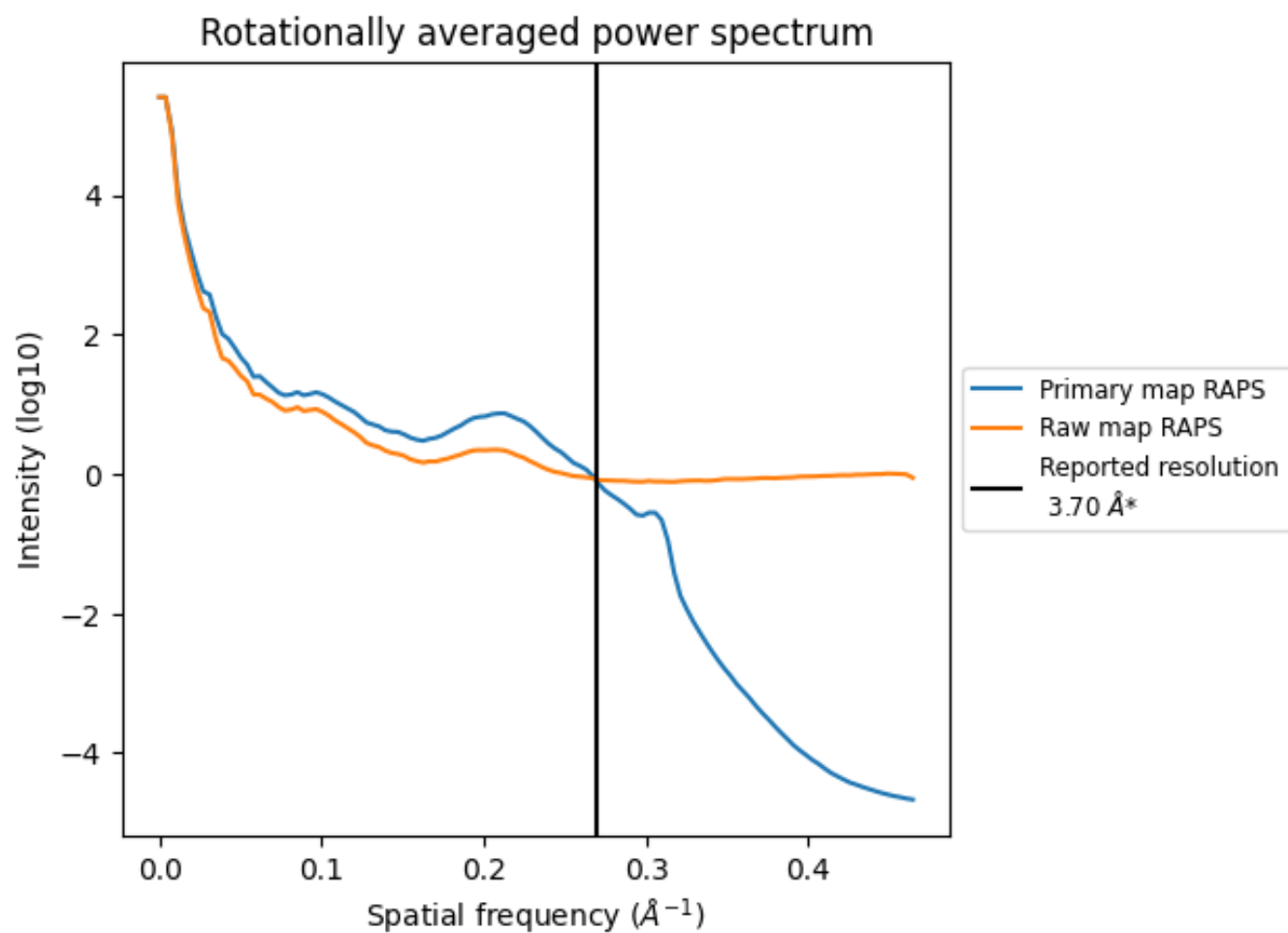
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 158 nm<sup>3</sup>; this corresponds to an approximate mass of 143 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 ⓘ

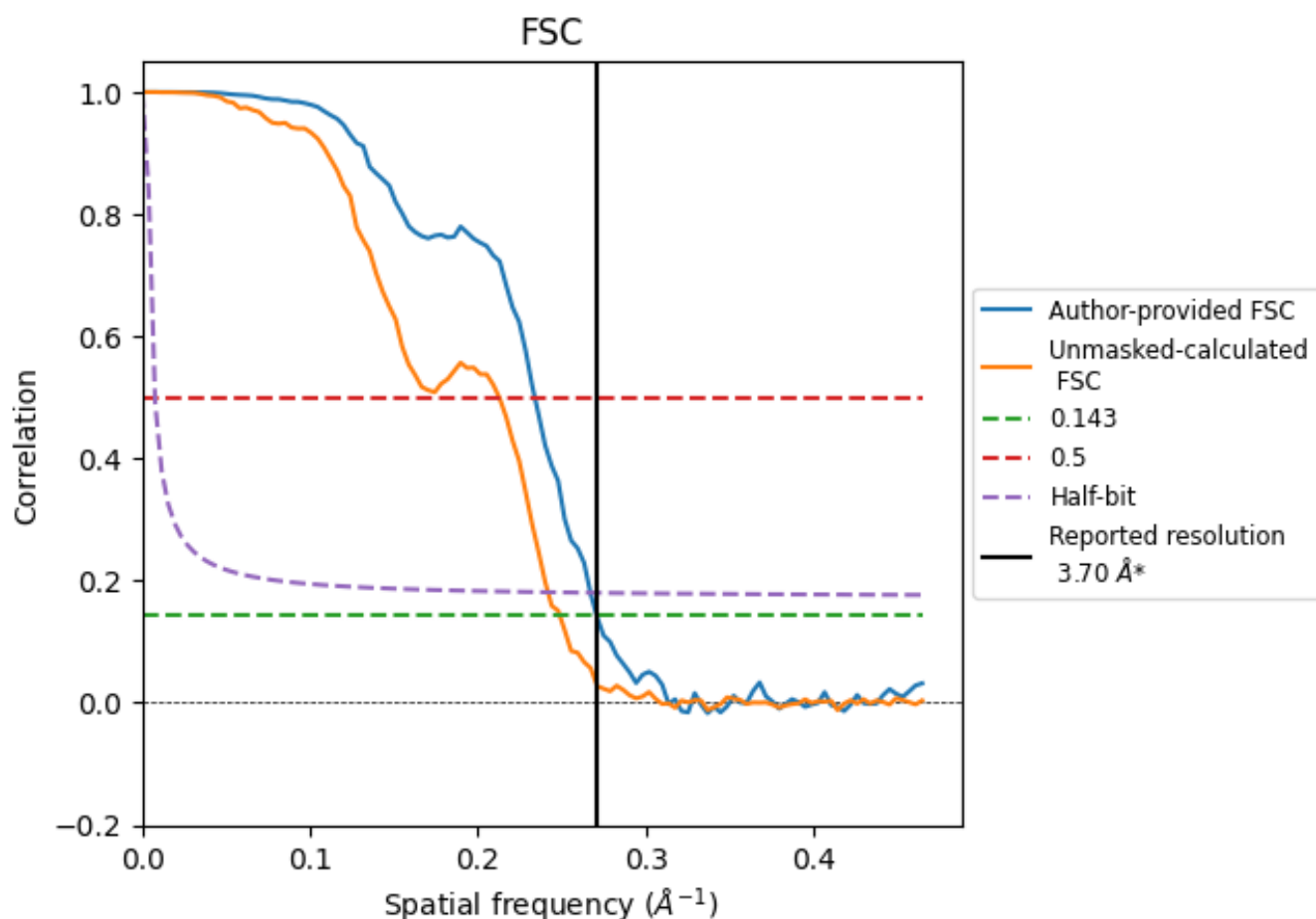


\*Reported resolution corresponds to spatial frequency of 0.270 Å<sup>-1</sup>

## 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 0.270  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

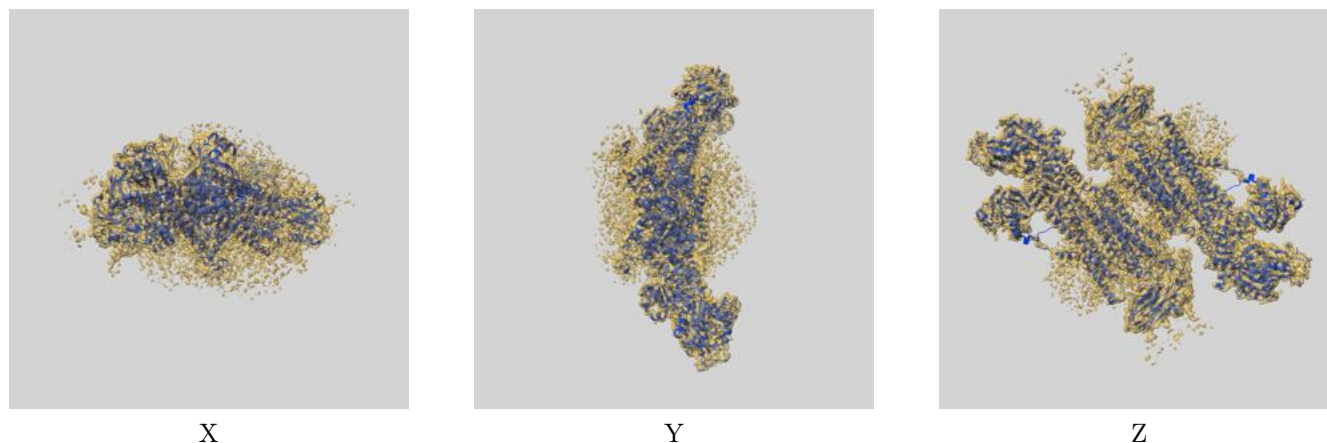
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.69	4.28	3.74
Unmasked-calculated*	4.02	4.70	4.14

\*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-65100 and PDB model 9VJ0. Per-residue inclusion information can be found in section [3](#) on page [10](#).

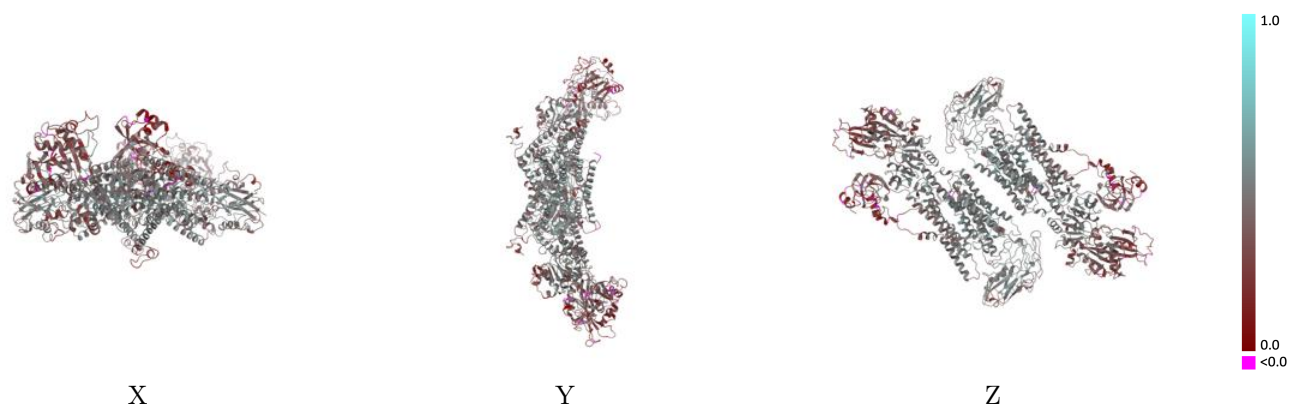
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0095 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.

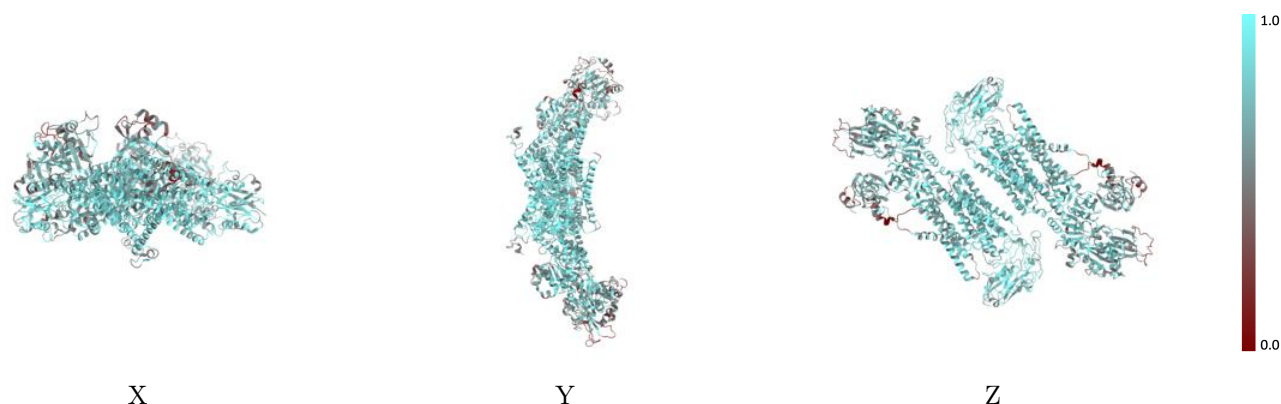


## 9.2 Q-score mapped to coordinate model [i](#)



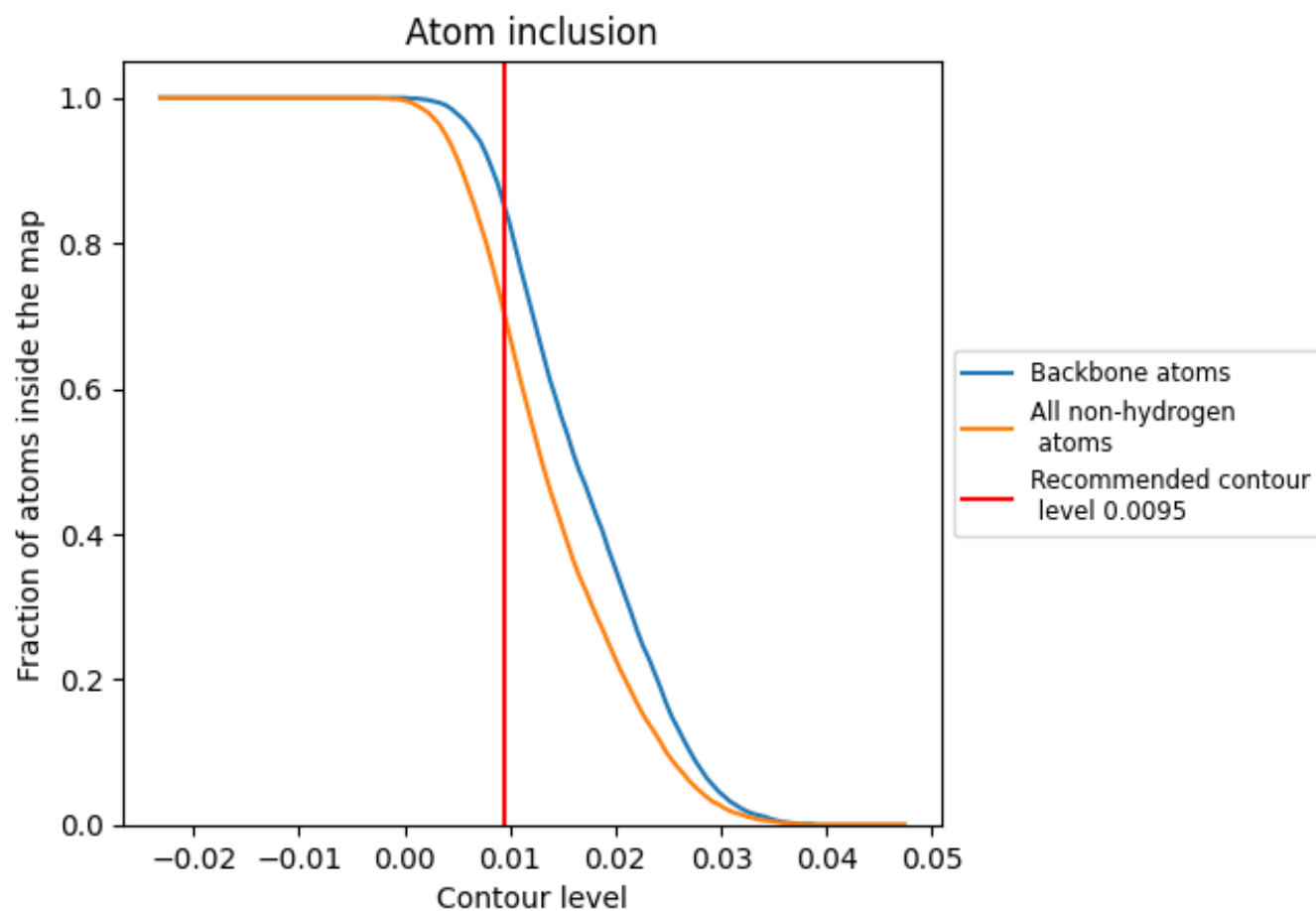
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0095).































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 70% 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 (0.0095) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7010	 0.4060
A	 0.6920	 0.4000
B	 0.7780	 0.4460
C	 0.6940	 0.3990
D	 0.7810	 0.4440
E	 0.6220	 0.4110
F	 0.4510	 0.3110
G	 0.6100	 0.4070
H	 0.1330	 0.1750
I	 0.3500	 0.2850
J	 0.2860	 0.0940
K	 0.4510	 0.3040
L	 0.1600	 0.1680
M	 0.3330	 0.2900
N	 0.2860	 0.0680

