



Full wwPDB EM Validation Report ⓘ

Sep 22, 2025 – 10:14 AM JST

PDB ID : 9VIY / pdb_00009viy
EMDB ID : EMD-65098
Title : Cryo-EM structure of palytoxin-bound Na⁺,K⁺-ATPase in the E2P state
Authors : Kanai, R.; Vilsen, B.; Cornelius, F.; Toyoshima, C.
Deposited on : 2025-06-19
Resolution : 3.30 Å(reported)
Based on initial model : 7wz0

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

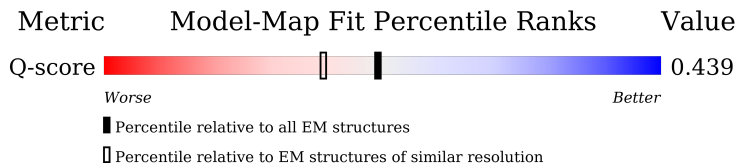
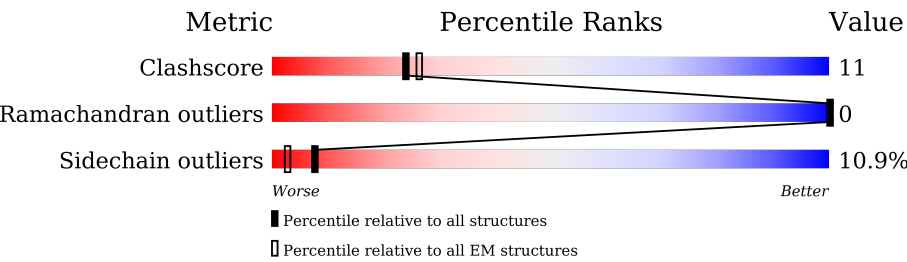
EMDB validation analysis : 0.0.1.dev129
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive 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 3.30 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.






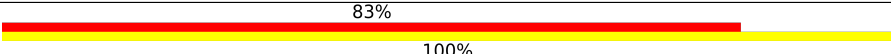
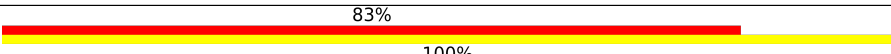
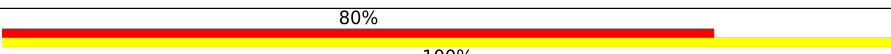
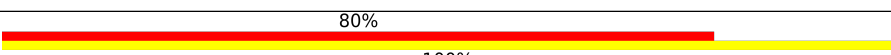
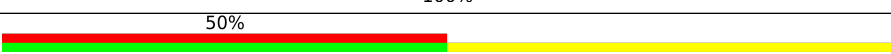

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	15087 (2.80 - 3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1028	<div><div>8%</div><div><div></div><div>71%</div><div>22%</div><div></div><div></div></div><div></div></div>
1	C	1028	<div><div>8%</div><div><div></div><div>71%</div><div>22%</div><div></div><div></div></div><div></div></div>
2	B	305	<div><div></div><div><div></div><div>66%</div><div>24%</div><div>6%</div><div></div></div><div></div></div>
2	D	305	<div><div></div><div><div></div><div>65%</div><div>26%</div><div>5%</div><div></div></div><div></div></div>
3	E	94	<div><div></div><div><div></div><div>30%</div><div>13%</div><div>57%</div><div></div></div><div></div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	G	94	 29% 14% 57%
4	F	6	 50% 83% 17%
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 11 unique types of molecules in this entry. The entry contains 22878 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 Sodium/potassium-transporting ATPase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	993	Total	C	N	O	P	S	
			7687	4890	1291	1459	1	46	0
1	C	993	Total	C	N	O	P	S	
			7687	4890	1291	1459	1	46	0

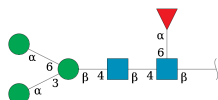
- Molecule 2 is a protein called Na⁺,K⁺-ATPase beta subunit.

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

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

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

- 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.



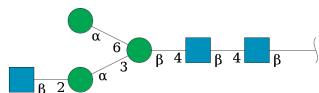
Mol	Chain	Residues	Atoms				AltConf	Trace
4	F	6	Total	C	N	O		
			71	40	2	29	0	0

Continued on next page...

Continued from previous page...

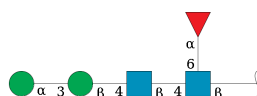
Mol	Chain	Residues	Atoms				AltConf	Trace
4	K	6	Total	C	N	O	0	0
			71	40	2	29		

- 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.



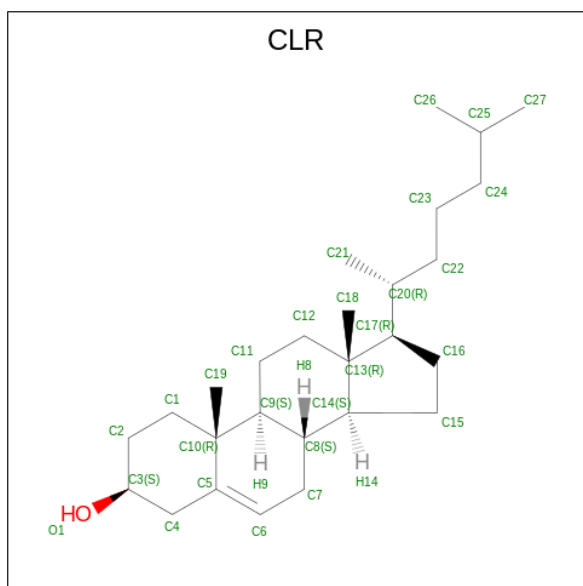
Mol	Chain	Residues	Atoms				AltConf	Trace
7	J	2	Total	C	N	O	0	0
			28	16	2	10		

Continued on next page...

Continued from previous page...

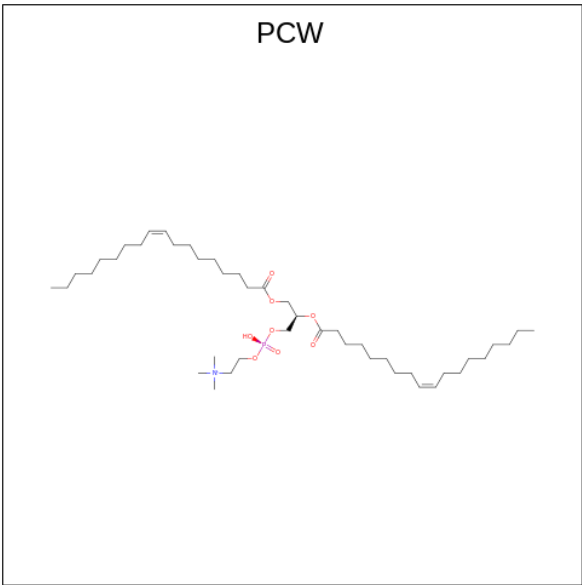
Mol	Chain	Residues	Atoms				AltConf	Trace
7	N	2	Total	C	N	O	0	0
			28	16	2	10		

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



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

- Molecule 9 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula: $C_{44}H_{85}NO_8P$).



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

Continued on next page...

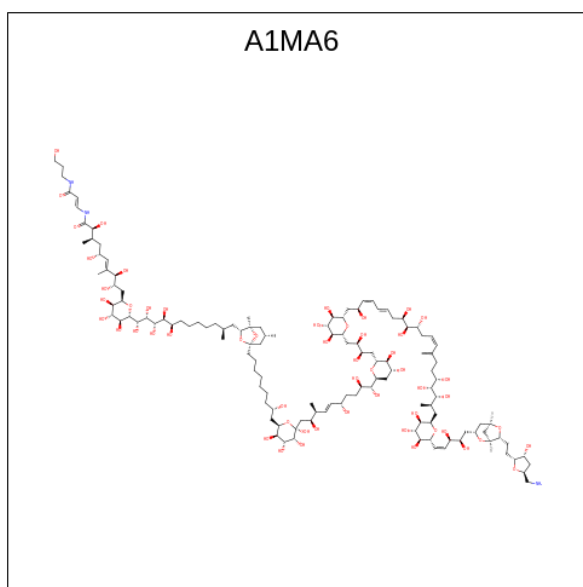
Continued from previous page...

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	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	E	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	A	2	Total	Mg	0
			2	2	
10	C	2	Total	Mg	0
			2	2	

- Molecule 11 is palytoxin (CCD ID: A1MA6) (formula: C₁₂₉H₂₂₃N₃O₅₄) (labeled as "Ligand of Interest" by depositor).



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

Continued on next page...

Continued from previous page...

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

3 Residue-property plots

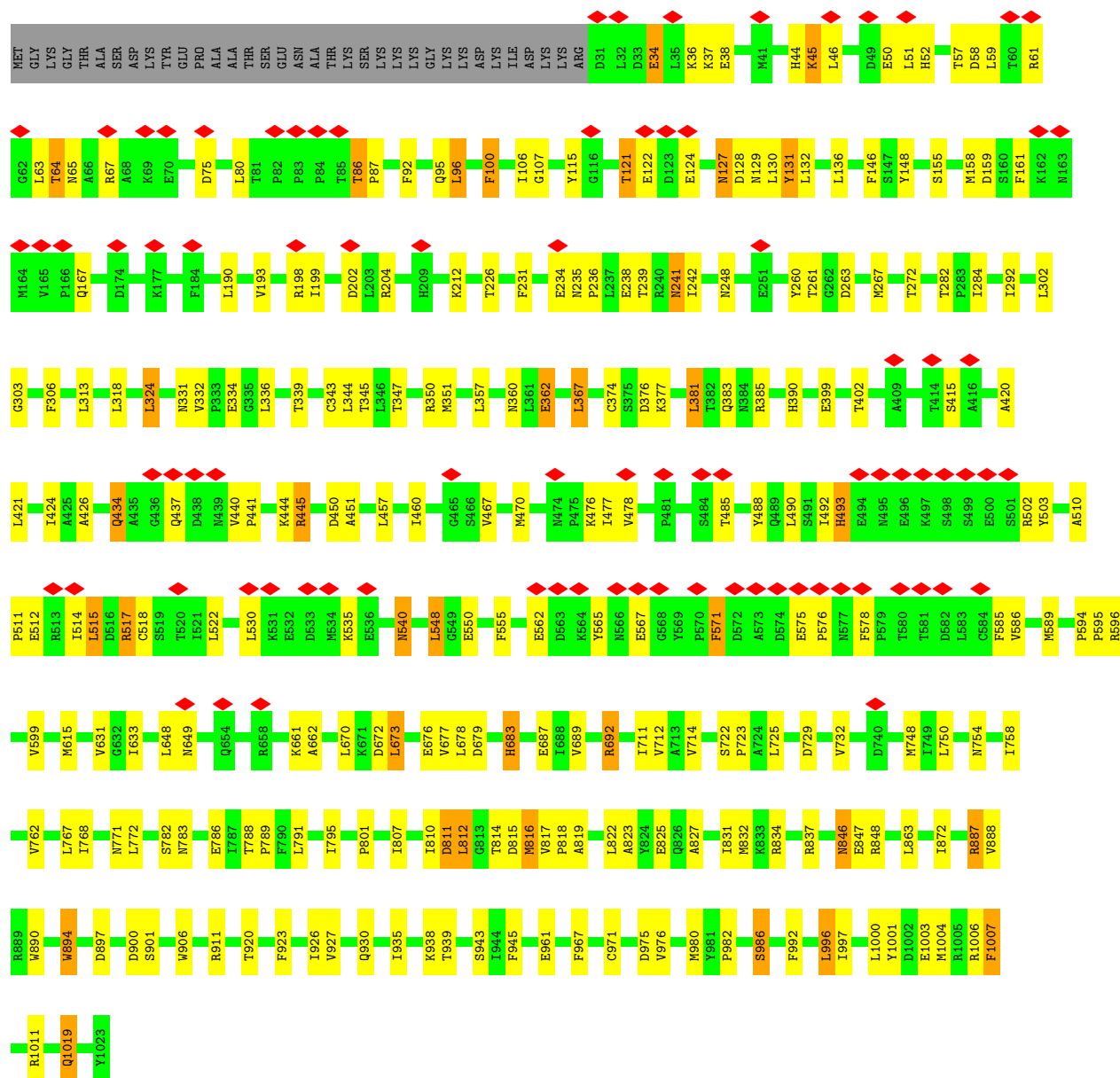
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Sodium/potassium-transporting ATPase subunit alpha



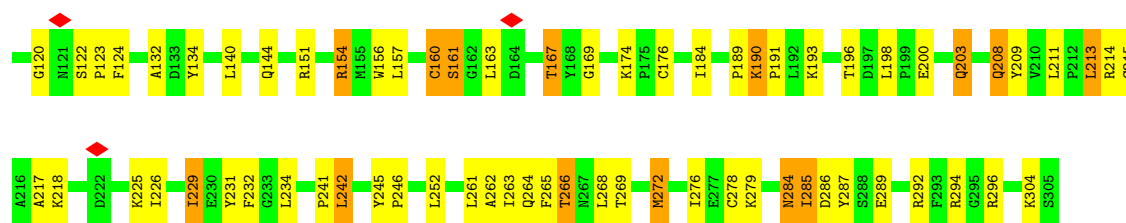


• Molecule 1: Sodium/potassium-transporting ATPase subunit alpha

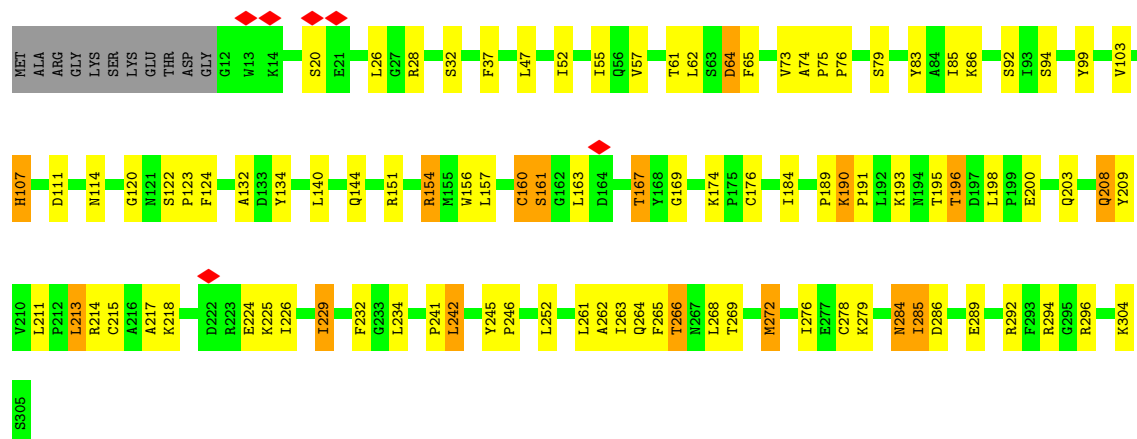


• Molecule 2: Na⁺,K⁺-ATPase beta subunit

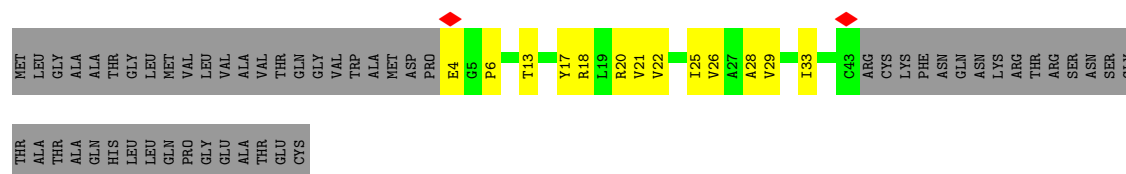




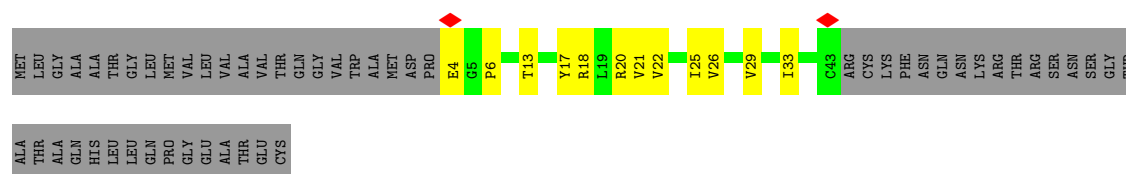
• Molecule 2: Na⁺,K⁺-ATPase beta subunit



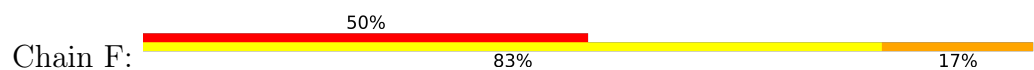
• Molecule 3: FXYP domain-containing ion transport regulator



• Molecule 3: FXYP domain-containing ion transport regulator

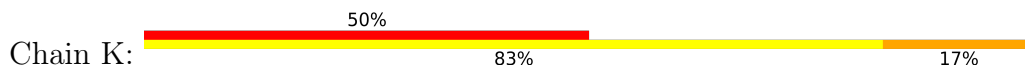


• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

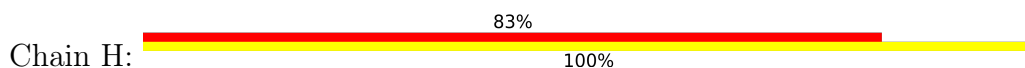




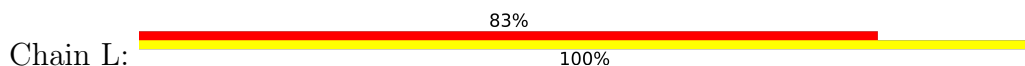
- Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



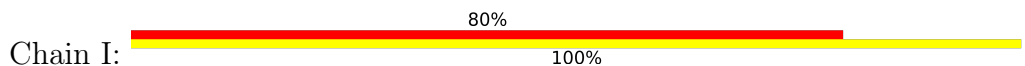
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



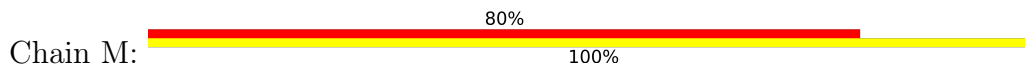
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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





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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	24807	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	0.063	Depositor
Minimum map value	-0.029	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: PCW, BMA, FUC, CLR, MAN, MG, A1MA6, NAG, PHD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.29	0/7824	0.74	0/10613
1	C	0.29	0/7824	0.74	0/10613
2	B	0.24	0/2462	0.76	0/3317
2	D	0.24	0/2462	0.76	0/3317
3	E	0.22	0/315	0.53	0/427
3	G	0.22	0/315	0.53	0/427
All	All	0.27	0/21202	0.74	0/28714

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7687	0	7703	174	0
1	C	7687	0	7703	168	0
2	B	2399	0	2354	47	0
2	D	2399	0	2354	49	0
3	E	311	0	323	8	0
3	G	311	0	323	9	0
4	F	71	0	61	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	28	0	46	5	0
8	B	56	0	92	2	0
8	C	28	0	46	4	0
8	D	56	0	92	2	0
8	E	28	0	46	3	0
8	G	28	0	46	7	0
9	A	346	0	522	28	0
9	C	346	0	522	31	0
9	E	162	0	252	22	0
9	G	162	0	252	17	0
10	A	2	0	0	0	0
10	C	2	0	0	0	0
11	A	186	0	0	4	0
11	C	186	0	0	4	0
All	All	22878	0	23080	485	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 11.

All (485) 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:G:1304:PCW:H382	9:E:1304:PCW:H482	1.46	0.95
1:C:303:GLY:HA3	1:C:324:LEU:HD13	1.54	0.89
1:A:967:PHE:HZ	9:A:1107:PCW:H172	1.38	0.88
1:A:121:THR:HG22	1:A:122:GLU:HG3	1.55	0.88
1:A:303:GLY:HA3	1:A:324:LEU:HD13	1.54	0.88
3:G:29:VAL:HG11	9:G:1303:PCW:H261	1.56	0.88
1:C:121:THR:HG22	1:C:122:GLU:HG3	1.55	0.88
1:C:967:PHE:HZ	9:C:1107:PCW:H172	1.38	0.86
9:C:1104:PCW:H442	8:E:1301:CLR:H273	1.57	0.86
9:A:1104:PCW:H442	8:G:1301:CLR:H273	1.57	0.86
3:E:29:VAL:HG11	9:E:1303:PCW:H261	1.56	0.84
1:C:421:LEU:HG	1:C:589:MET:HE2	1.61	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:THR:HG21	11:A:1111:A1MA6:C97	2.09	0.82
1:A:421:LEU:HG	1:A:589:MET:HE2	1.60	0.81
2:B:124:PHE:HB3	2:B:151:ARG:HG2	1.62	0.81
1:C:121:THR:HG21	11:C:1111:A1MA6:C97	2.09	0.81
2:D:124:PHE:HB3	2:D:151:ARG:HG2	1.62	0.79
2:D:76:PRO:HG3	2:D:184:ILE:HD12	1.65	0.79
9:G:1304:PCW:H482	9:E:1304:PCW:H382	1.65	0.79
1:C:52:HIS:HE1	1:C:59:LEU:HD12	1.48	0.79
2:B:76:PRO:HG3	2:B:184:ILE:HD12	1.65	0.78
1:A:967:PHE:CZ	9:A:1107:PCW:H172	2.18	0.78
1:A:52:HIS:HE1	1:A:59:LEU:HD12	1.48	0.78
1:C:967:PHE:CZ	9:C:1107:PCW:H172	2.18	0.78
1:C:503:TYR:HE2	1:C:567:GLU:HA	1.50	0.77
1:A:36:LYS:HZ1	1:A:272:THR:HB	1.50	0.77
9:G:1304:PCW:H432	9:E:1304:PCW:H432	1.66	0.77
1:A:503:TYR:HE2	1:A:567:GLU:HA	1.50	0.76
1:A:202:ASP:HB2	1:A:260:TYR:HB2	1.69	0.74
1:A:894:TRP:HB2	2:B:83:TYR:HE1	1.52	0.74
1:C:202:ASP:HB2	1:C:260:TYR:HB2	1.69	0.73
1:A:996:LEU:HD22	9:C:1105:PCW:H283	1.70	0.72
1:C:894:TRP:HB2	2:D:83:TYR:HE1	1.52	0.72
1:A:426:ALA:HB2	1:A:460:ILE:HG21	1.71	0.72
8:G:1301:CLR:H272	9:G:1304:PCW:H272	1.70	0.72
8:E:1301:CLR:H272	9:E:1304:PCW:H272	1.70	0.72
1:C:426:ALA:HB2	1:C:460:ILE:HG21	1.71	0.72
1:C:241:ASN:H	1:C:241:ASN:HD22	1.39	0.71
2:D:161:SER:HB3	2:D:163:LEU:HD12	1.72	0.71
1:C:575:GLU:HB3	1:C:576:PRO:HD2	1.73	0.71
9:E:1303:PCW:H262	9:E:1304:PCW:H20	1.73	0.70
2:B:161:SER:HB3	2:B:163:LEU:HD12	1.72	0.69
1:C:477:ILE:HG22	1:C:478:VAL:HG23	1.75	0.69
1:A:575:GLU:HB3	1:A:576:PRO:HD2	1.73	0.69
2:B:176:CYS:SG	2:B:264:GLN:HG3	2.34	0.68
9:G:1303:PCW:H262	9:G:1304:PCW:H20	1.73	0.68
1:A:241:ASN:HD22	1:A:241:ASN:H	1.39	0.68
1:A:477:ILE:HG22	1:A:478:VAL:HG23	1.75	0.68
1:C:982:PRO:HD3	3:E:20:ARG:HH21	1.58	0.68
2:D:176:CYS:SG	2:D:264:GLN:HG3	2.34	0.68
1:A:441:PRO:O	1:A:445:ARG:HG2	1.94	0.68
9:G:1304:PCW:H412	9:E:1304:PCW:H461	1.76	0.67
1:A:982:PRO:HD3	3:G:20:ARG:HH21	1.58	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:GLN:HE22	1:A:148:TYR:HA	1.59	0.66
1:C:95:GLN:HE22	1:C:148:TYR:HA	1.59	0.66
1:C:441:PRO:O	1:C:445:ARG:HG2	1.94	0.66
1:A:1001:TYR:HD1	9:A:1103:PCW:H40	1.61	0.65
8:G:1301:CLR:H263	9:E:1304:PCW:H441	1.77	0.65
9:G:1304:PCW:H481	9:E:1304:PCW:H182	1.78	0.65
1:C:303:GLY:CA	1:C:324:LEU:HD13	2.26	0.65
2:B:213:LEU:HD23	2:B:261:LEU:HD13	1.78	0.65
2:D:213:LEU:HD23	2:D:261:LEU:HD13	1.78	0.65
1:C:1001:TYR:HD1	9:C:1103:PCW:H40	1.61	0.64
3:G:26:VAL:HG11	8:G:1301:CLR:H71	1.79	0.64
1:C:324:LEU:HD12	1:C:324:LEU:O	1.98	0.64
1:A:303:GLY:CA	1:A:324:LEU:HD13	2.26	0.64
11:C:1111:A1MA6:CBE	11:C:1111:A1MA6:CA1	2.76	0.64
1:C:212:LYS:HG2	1:C:226:THR:HG22	1.80	0.64
1:C:530:LEU:HD22	1:C:535:LYS:HE3	1.79	0.64
3:E:26:VAL:HG11	8:E:1301:CLR:H71	1.79	0.64
1:A:503:TYR:CE2	1:A:567:GLU:HA	2.32	0.63
1:A:324:LEU:HD12	1:A:324:LEU:O	1.98	0.63
1:A:212:LYS:HG2	1:A:226:THR:HG22	1.80	0.63
1:A:992:PHE:CD2	9:A:1104:PCW:H271	2.34	0.63
11:A:1111:A1MA6:CBE	11:A:1111:A1MA6:CA1	2.76	0.63
8:G:1301:CLR:H213	9:E:1304:PCW:H483	1.80	0.63
1:C:100:PHE:HB3	1:C:292:ILE:HD11	1.80	0.63
1:A:530:LEU:HD22	1:A:535:LYS:HE3	1.79	0.62
1:C:36:LYS:HZ1	1:C:272:THR:HB	1.64	0.62
1:A:146:PHE:CZ	1:A:345:THR:HG21	2.34	0.62
1:C:503:TYR:CE2	1:C:567:GLU:HA	2.32	0.62
1:A:100:PHE:HB3	1:A:292:ILE:HD11	1.80	0.62
1:C:992:PHE:CD2	9:C:1104:PCW:H271	2.34	0.62
11:A:1111:A1MA6:OCD	11:A:1111:A1MA6:CCC	2.47	0.62
3:G:18:ARG:O	3:G:22:VAL:HG23	2.00	0.62
1:C:146:PHE:CZ	1:C:345:THR:HG21	2.34	0.62
11:C:1111:A1MA6:OCD	11:C:1111:A1MA6:CCC	2.47	0.62
2:B:217:ALA:HB2	2:B:226:ILE:HD12	1.82	0.62
1:C:812:LEU:HD12	1:C:816:MET:HE2	1.82	0.61
2:B:209:TYR:HA	2:B:242:LEU:HD22	1.82	0.61
1:C:306:PHE:CZ	1:C:791:LEU:HD13	2.36	0.61
1:A:80:LEU:HD11	1:A:267:MET:SD	2.41	0.60
1:C:80:LEU:HD11	1:C:267:MET:SD	2.41	0.60
1:C:127:ASN:HB2	1:C:131:TYR:CZ	2.36	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:18:ARG:O	3:E:22:VAL:HG23	2.00	0.60
2:D:217:ALA:HB2	2:D:226:ILE:HD12	1.82	0.60
2:D:209:TYR:HA	2:D:242:LEU:HD22	1.82	0.60
1:A:127:ASN:HB2	1:A:131:TYR:CZ	2.36	0.60
1:C:992:PHE:HD2	9:C:1104:PCW:H271	1.66	0.60
1:A:306:PHE:CZ	1:A:791:LEU:HD13	2.36	0.59
9:A:1105:PCW:H283	1:C:996:LEU:HD22	1.84	0.59
1:A:992:PHE:HD2	9:A:1104:PCW:H271	1.67	0.59
1:A:722:SER:HB2	1:A:723:PRO:HD3	1.84	0.59
9:G:1304:PCW:C41	9:E:1304:PCW:H461	2.32	0.59
1:A:812:LEU:HD12	1:A:816:MET:HE2	1.82	0.59
3:G:21:VAL:O	3:G:25:ILE:HG12	2.02	0.59
3:E:21:VAL:O	3:E:25:ILE:HG12	2.02	0.58
1:C:722:SER:HB2	1:C:723:PRO:HD3	1.84	0.58
1:C:241:ASN:HD22	1:C:241:ASN:N	1.99	0.58
1:C:424:ILE:HG21	1:C:555:PHE:HB3	1.87	0.57
3:E:17:TYR:O	3:E:21:VAL:HG23	2.04	0.57
3:G:17:TYR:O	3:G:21:VAL:HG23	2.04	0.57
1:A:44:HIS:HB3	1:A:242:ILE:HD11	1.87	0.57
1:A:46:LEU:HD22	1:A:50:GLU:HG2	1.87	0.57
1:C:115:TYR:CD2	1:C:130:LEU:HB2	2.40	0.57
1:A:241:ASN:HD22	1:A:241:ASN:N	1.99	0.56
1:A:441:PRO:HG2	1:A:444:LYS:HE3	1.87	0.56
2:B:64:ASP:N	2:B:64:ASP:OD1	2.38	0.56
1:A:115:TYR:CD2	1:A:130:LEU:HB2	2.40	0.56
1:A:377:LYS:HA	1:A:381:LEU:HB2	1.88	0.56
1:C:44:HIS:HB3	1:C:242:ILE:HD11	1.87	0.56
1:A:424:ILE:HG21	1:A:555:PHE:HB3	1.87	0.56
2:B:279:LYS:HG3	2:B:296:ARG:HB3	1.88	0.56
1:C:46:LEU:HD22	1:C:50:GLU:HG2	1.87	0.56
1:C:306:PHE:CE2	1:C:791:LEU:HD22	2.41	0.56
1:C:303:GLY:HA3	1:C:324:LEU:CD1	2.31	0.55
1:C:377:LYS:HA	1:C:381:LEU:HB2	1.87	0.55
1:C:441:PRO:HG2	1:C:444:LYS:HE3	1.87	0.55
1:A:306:PHE:CE2	1:A:791:LEU:HD22	2.41	0.55
2:B:61:THR:HA	1:C:1007:PHE:HZ	1.71	0.55
2:D:64:ASP:N	2:D:64:ASP:OD1	2.38	0.55
2:D:279:LYS:HG3	2:D:296:ARG:HB3	1.88	0.55
1:A:92:PHE:CE1	1:A:96:LEU:HD13	2.42	0.55
1:C:92:PHE:CE1	1:C:96:LEU:HD13	2.42	0.54
1:C:1000:LEU:HD11	9:C:1105:PCW:H39	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:GLY:HA3	1:A:324:LEU:CD1	2.31	0.54
2:B:190:LYS:NZ	3:G:6:PRO:O	2.40	0.54
2:D:190:LYS:NZ	3:E:6:PRO:O	2.40	0.54
1:C:106:ILE:HG13	1:C:107:GLY:N	2.23	0.54
1:C:488:TYR:CE1	1:C:490:LEU:HD23	2.43	0.54
1:A:863:LEU:HD12	2:B:47:LEU:HD22	1.90	0.54
1:C:193:VAL:HG11	1:C:199:ILE:HD13	1.89	0.54
9:A:1108:PCW:H19	8:B:501:CLR:H151	1.90	0.53
1:C:515:LEU:HD11	1:C:535:LYS:HE2	1.90	0.53
1:A:193:VAL:HG11	1:A:199:ILE:HD13	1.89	0.53
9:G:1304:PCW:H451	9:E:1304:PCW:H261	1.90	0.53
1:A:488:TYR:CE1	1:A:490:LEU:HD23	2.43	0.53
1:C:863:LEU:HD12	2:D:47:LEU:HD22	1.90	0.53
9:G:1304:PCW:H461	9:E:1304:PCW:H412	1.90	0.53
1:C:95:GLN:NE2	1:C:148:TYR:HA	2.23	0.53
1:A:106:ILE:HG13	1:A:107:GLY:N	2.23	0.53
1:A:1000:LEU:HD11	9:A:1105:PCW:H39	1.90	0.53
1:C:36:LYS:NZ	1:C:272:THR:HB	2.22	0.53
1:C:492:ILE:HD12	1:C:578:PHE:CE1	2.44	0.53
1:A:515:LEU:HD11	1:A:535:LYS:HE2	1.90	0.53
1:A:36:LYS:NZ	1:A:272:THR:HB	2.23	0.53
1:A:890:TRP:CZ2	1:A:911:ARG:HB2	2.44	0.53
1:C:241:ASN:H	1:C:241:ASN:ND2	2.06	0.53
1:C:810:ILE:HD13	1:C:926:ILE:HG21	1.91	0.53
9:C:1108:PCW:H19	8:D:501:CLR:H151	1.90	0.53
1:A:95:GLN:NE2	1:A:148:TYR:HA	2.23	0.52
1:A:492:ILE:HD12	1:A:578:PHE:CE1	2.44	0.52
1:C:450:ASP:OD1	1:C:451:ALA:N	2.42	0.52
9:G:1303:PCW:H283	9:G:1304:PCW:H222	1.91	0.52
2:D:75:PRO:HG2	2:D:286:ASP:N	2.25	0.52
1:A:52:HIS:CE1	1:A:59:LEU:HD12	2.38	0.52
1:C:825:GLU:OE2	1:C:938:LYS:NZ	2.42	0.52
1:C:762:VAL:HG13	1:C:832:MET:HE1	1.92	0.52
1:A:810:ILE:HD13	1:A:926:ILE:HG21	1.91	0.52
1:A:825:GLU:OE2	1:A:938:LYS:NZ	2.42	0.52
9:E:1303:PCW:H283	9:E:1304:PCW:H222	1.91	0.52
1:C:502:ARG:HG2	1:C:562:GLU:HB3	1.92	0.52
2:B:75:PRO:HG2	2:B:286:ASP:N	2.25	0.52
1:C:887:ARG:HG3	1:C:888:VAL:N	2.24	0.52
1:C:890:TRP:CZ2	1:C:911:ARG:HB2	2.44	0.52
1:A:782:SER:HB3	1:A:930:GLN:NE2	2.26	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:306:PHE:CD2	1:C:791:LEU:HD22	2.46	0.51
1:C:817:VAL:HB	1:C:818:PRO:HD3	1.93	0.51
1:A:502:ARG:HG2	1:A:562:GLU:HB3	1.92	0.51
1:A:450:ASP:OD1	1:A:451:ALA:N	2.42	0.51
1:A:783:ASN:O	1:A:786:GLU:HB2	2.10	0.51
9:E:1303:PCW:H262	9:E:1304:PCW:C20	2.40	0.51
1:A:920:THR:HG23	1:A:980:MET:HE2	1.93	0.51
1:C:52:HIS:CE1	1:C:59:LEU:HB2	2.45	0.51
1:A:810:ILE:HG13	1:A:923:PHE:HD2	1.75	0.51
1:A:846:ASN:OD1	1:A:846:ASN:N	2.44	0.51
1:C:34:GLU:O	1:C:38:GLU:HG3	2.10	0.51
1:A:52:HIS:CE1	1:A:59:LEU:HB2	2.45	0.51
1:A:517:ARG:HG2	1:A:517:ARG:HH11	1.76	0.51
9:A:1103:PCW:H462	8:C:1101:CLR:H263	1.91	0.51
1:C:782:SER:HB3	1:C:930:GLN:NE2	2.26	0.51
1:C:920:THR:HG23	1:C:980:MET:HE2	1.93	0.51
1:A:817:VAL:HB	1:A:818:PRO:HD3	1.93	0.51
1:A:306:PHE:CD2	1:A:791:LEU:HD22	2.46	0.51
1:A:762:VAL:HG13	1:A:832:MET:HE1	1.92	0.51
1:A:887:ARG:HG3	1:A:888:VAL:N	2.24	0.51
1:C:517:ARG:HG2	1:C:517:ARG:HH11	1.76	0.51
1:C:783:ASN:O	1:C:786:GLU:HB2	2.10	0.50
1:C:565:TYR:HB3	1:C:571:PHE:HE2	1.77	0.50
1:A:672:ASP:O	1:A:673:LEU:HD23	2.12	0.50
1:A:34:GLU:O	1:A:38:GLU:HG3	2.10	0.50
1:C:52:HIS:CE1	1:C:59:LEU:HD12	2.38	0.50
3:E:21:VAL:HG22	9:E:1302:PCW:O11	2.12	0.50
1:A:565:TYR:HB3	1:A:571:PHE:HE2	1.77	0.50
1:C:711:ILE:HA	1:C:729:ASP:OD2	2.12	0.50
1:A:711:ILE:HA	1:A:729:ASP:OD2	2.12	0.50
9:G:1303:PCW:H262	9:G:1304:PCW:C20	2.40	0.50
1:C:810:ILE:HG13	1:C:923:PHE:HD2	1.76	0.50
1:A:997:ILE:HG21	9:A:1103:PCW:H261	1.94	0.50
2:B:120:GLY:O	2:B:151:ARG:NH2	2.45	0.50
3:G:21:VAL:HG22	9:G:1302:PCW:O11	2.12	0.50
1:A:1004:MET:SD	9:A:1103:PCW:H422	2.51	0.50
1:A:1007:PHE:HZ	2:D:61:THR:HA	1.76	0.50
9:A:1105:PCW:C28	1:C:996:LEU:HD22	2.41	0.50
1:C:121:THR:CG2	1:C:122:GLU:HG3	2.36	0.50
2:D:92:SER:HA	2:D:304:LYS:O	2.12	0.49
2:D:174:LYS:HD3	2:D:266:THR:HG23	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1007:PHE:CZ	2:D:61:THR:HA	2.48	0.49
8:A:1101:CLR:H242	9:C:1105:PCW:H272	1.93	0.49
2:D:120:GLY:O	2:D:151:ARG:NH2	2.45	0.49
2:B:174:LYS:HD3	2:B:266:THR:HG23	1.94	0.49
2:B:92:SER:HA	2:B:304:LYS:O	2.12	0.49
9:G:1304:PCW:H451	9:E:1304:PCW:H241	1.93	0.49
1:C:239:THR:OG1	1:C:241:ASN:ND2	2.45	0.49
1:C:897:ASP:OD1	1:C:897:ASP:N	2.44	0.49
1:C:1004:MET:SD	9:C:1103:PCW:H422	2.51	0.49
1:A:239:THR:OG1	1:A:241:ASN:ND2	2.45	0.49
1:A:897:ASP:OD1	1:A:897:ASP:N	2.44	0.49
8:G:1301:CLR:H241	9:E:1304:PCW:H462	1.95	0.49
1:C:672:ASP:O	1:C:673:LEU:HD23	2.12	0.49
1:C:714:VAL:HG12	1:C:725:LEU:HD23	1.95	0.49
1:C:997:ILE:HG21	9:C:1103:PCW:H261	1.94	0.49
1:A:128:ASP:O	1:A:132:LEU:HB2	2.13	0.49
1:C:476:LYS:HE2	1:C:493:HIS:CE1	2.48	0.49
1:A:476:LYS:HE2	1:A:493:HIS:CE1	2.48	0.48
1:C:771:ASN:ND2	1:C:823:ALA:O	2.46	0.48
1:A:1000:LEU:CD1	9:A:1105:PCW:H39	2.43	0.48
1:C:1000:LEU:CD1	9:C:1105:PCW:H39	2.43	0.48
2:D:191:PRO:HG3	2:D:208:GLN:O	2.13	0.48
1:C:827:ALA:HB2	1:C:831:ILE:HD11	1.95	0.48
1:A:827:ALA:HB2	1:A:831:ILE:HD11	1.95	0.48
1:A:997:ILE:HD13	9:A:1103:PCW:H261	1.95	0.48
8:G:1301:CLR:H263	9:E:1304:PCW:C44	2.43	0.48
2:D:225:LYS:HD2	2:D:272:MET:SD	2.54	0.48
1:C:128:ASP:O	1:C:132:LEU:HB2	2.13	0.48
1:C:997:ILE:HD13	9:C:1103:PCW:H261	1.95	0.48
1:A:517:ARG:HH11	1:A:517:ARG:CG	2.27	0.48
1:C:517:ARG:HH11	1:C:517:ARG:CG	2.27	0.48
2:B:191:PRO:HG3	2:B:208:GLN:O	2.13	0.48
2:B:225:LYS:HD2	2:B:272:MET:SD	2.54	0.48
1:C:235:ASN:OD1	1:C:236:PRO:HD2	2.14	0.48
1:C:540:ASN:N	1:C:540:ASN:HD22	2.12	0.48
1:A:241:ASN:H	1:A:241:ASN:ND2	2.06	0.48
1:C:814:THR:O	1:C:818:PRO:HD2	2.14	0.48
2:D:74:ALA:HA	2:D:75:PRO:C	2.39	0.47
1:A:45:LYS:NZ	1:A:234:GLU:OE1	2.43	0.47
1:A:52:HIS:CD2	1:A:57:THR:HG23	2.49	0.47
1:A:648:LEU:O	1:A:649:ASN:HB2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:306:PHE:CE2	1:C:795:ILE:HD11	2.49	0.47
1:C:679:ASP:O	1:C:683:HIS:HB2	2.14	0.47
1:A:714:VAL:HG12	1:A:725:LEU:HD23	1.95	0.47
1:A:383:GLN:OE1	1:A:385:ARG:NH2	2.48	0.47
1:A:768:ILE:O	1:A:768:ILE:HG13	2.14	0.47
1:A:814:THR:O	1:A:818:PRO:HD2	2.14	0.47
1:C:45:LYS:NZ	1:C:234:GLU:OE1	2.43	0.47
1:A:235:ASN:OD1	1:A:236:PRO:HD2	2.14	0.47
1:A:771:ASN:ND2	1:A:823:ALA:O	2.46	0.47
2:B:74:ALA:HA	2:B:75:PRO:C	2.39	0.47
1:C:339:THR:HG21	1:C:819:ALA:HB1	1.96	0.47
1:A:339:THR:HG21	1:A:819:ALA:HB1	1.96	0.47
1:A:540:ASN:N	1:A:540:ASN:HD22	2.12	0.47
1:C:420:ALA:O	1:C:424:ILE:HG13	2.14	0.47
1:C:548:LEU:HB3	1:C:550:GLU:HG3	1.97	0.47
2:D:232:PHE:HB2	2:D:262:ALA:HB3	1.97	0.47
1:A:390:HIS:CD2	1:A:399:GLU:HG2	2.50	0.47
1:A:791:LEU:HB3	9:A:1108:PCW:H282	1.97	0.47
1:A:986:SER:OG	8:A:1101:CLR:H41	2.15	0.47
1:A:420:ALA:O	1:A:424:ILE:HG13	2.14	0.47
1:A:945:PHE:HD1	9:A:1104:PCW:H121	1.80	0.47
1:C:52:HIS:CD2	1:C:57:THR:HG23	2.49	0.47
2:D:132:ALA:O	2:D:209:TYR:HB3	2.15	0.47
2:B:203:GLN:HE21	2:B:203:GLN:HB2	1.56	0.47
1:C:900:ASP:OD2	1:C:906:TRP:NE1	2.46	0.47
2:D:215:CYS:HA	2:D:278:CYS:HA	1.97	0.47
1:A:306:PHE:CE2	1:A:795:ILE:HD11	2.49	0.46
9:A:1103:PCW:H72	9:A:1103:PCW:H41	1.70	0.46
1:C:424:ILE:HG22	1:C:555:PHE:HD2	1.79	0.46
1:C:768:ILE:HG13	1:C:768:ILE:O	2.14	0.46
2:B:134:TYR:HE1	2:B:242:LEU:HG	1.80	0.46
1:A:424:ILE:HG22	1:A:555:PHE:HD2	1.79	0.46
1:A:679:ASP:O	1:A:683:HIS:HB2	2.14	0.46
2:B:132:ALA:O	2:B:209:TYR:HB3	2.15	0.46
2:B:232:PHE:HB2	2:B:262:ALA:HB3	1.97	0.46
1:C:390:HIS:CD2	1:C:399:GLU:HG2	2.50	0.46
1:A:318:LEU:HD23	11:A:1111:A1MA6:OBR	2.16	0.46
1:A:548:LEU:HB3	1:A:550:GLU:HG3	1.97	0.46
1:C:648:LEU:O	1:C:649:ASN:HB2	2.14	0.46
1:C:673:LEU:HD13	1:C:677:VAL:CG1	2.46	0.46
1:C:615:MET:HB3	1:C:689:VAL:HG22	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:986:SER:OG	8:C:1101:CLR:H41	2.15	0.46
2:D:134:TYR:HE1	2:D:242:LEU:HG	1.80	0.46
1:C:318:LEU:HD23	11:C:1111:A1MA6:OBR	2.16	0.46
2:D:167:THR:HG22	2:D:169:GLY:H	1.80	0.46
2:B:215:CYS:HA	2:B:278:CYS:HA	1.97	0.46
1:C:383:GLN:OE1	1:C:385:ARG:NH2	2.48	0.46
1:A:712:VAL:O	1:A:729:ASP:HB2	2.16	0.45
1:A:807:ILE:O	1:A:811:ASP:HB2	2.16	0.45
1:A:159:ASP:C	1:A:161:PHE:H	2.24	0.45
1:A:997:ILE:HG21	9:A:1103:PCW:C26	2.46	0.45
9:A:1103:PCW:H483	8:C:1101:CLR:H272	1.98	0.45
2:B:265:PHE:CZ	2:B:276:ILE:HD12	2.52	0.45
1:C:791:LEU:HB3	9:C:1108:PCW:H282	1.97	0.45
2:D:163:LEU:HD23	4:K:6:FUC:H61	1.98	0.45
1:A:673:LEU:HD13	1:A:677:VAL:CG1	2.46	0.45
1:A:732:VAL:HG11	1:A:758:ILE:HD11	1.99	0.45
1:C:997:ILE:HG12	9:C:1103:PCW:H472	1.99	0.45
1:C:347:THR:OG1	1:C:768:ILE:HD13	2.16	0.45
1:A:347:THR:OG1	1:A:768:ILE:HD13	2.16	0.45
1:A:421:LEU:HD13	1:A:586:VAL:HG12	1.99	0.45
1:C:807:ILE:O	1:C:811:ASP:HB2	2.16	0.45
1:C:997:ILE:HG21	9:C:1103:PCW:C26	2.46	0.45
2:B:167:THR:HG22	2:B:169:GLY:H	1.80	0.45
1:A:615:MET:HB3	1:A:689:VAL:HG22	1.98	0.45
1:A:997:ILE:HG12	9:A:1103:PCW:H472	1.99	0.45
9:A:1103:PCW:C40	9:A:1103:PCW:H20	2.47	0.45
1:C:284:ILE:HG21	1:C:362:GLU:HB2	1.99	0.45
1:C:712:VAL:O	1:C:729:ASP:HB2	2.16	0.45
1:C:945:PHE:HD1	9:C:1104:PCW:H121	1.80	0.45
9:C:1103:PCW:C40	9:C:1103:PCW:H20	2.47	0.45
1:A:789:PRO:HB3	1:A:801:PRO:HB2	1.99	0.44
1:A:997:ILE:HG21	9:A:1103:PCW:H272	1.99	0.44
9:G:1304:PCW:H461	9:E:1304:PCW:C41	2.47	0.44
1:C:402:THR:HB	1:C:594:PRO:HG3	2.00	0.44
2:D:122:SER:HA	2:D:123:PRO:HA	1.69	0.44
1:A:615:MET:HB2	1:A:633:ILE:HD13	1.99	0.44
1:C:789:PRO:HB3	1:C:801:PRO:HB2	1.99	0.44
1:C:515:LEU:CD1	1:C:535:LYS:HE2	2.47	0.44
1:C:939:THR:OG1	1:C:1006:ARG:NH1	2.51	0.44
1:A:510:ALA:O	1:A:514:ILE:HG12	2.18	0.44
1:A:996:LEU:HD22	9:C:1105:PCW:C28	2.41	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:215:CYS:SG	2:B:263:ILE:HD13	2.58	0.44
2:D:265:PHE:CZ	2:D:276:ILE:HD12	2.52	0.44
1:A:336:LEU:HD12	1:A:336:LEU:HA	1.73	0.44
1:C:159:ASP:C	1:C:161:PHE:H	2.24	0.44
1:C:596:ARG:HB2	1:C:599:VAL:HG23	1.99	0.44
1:A:284:ILE:HG21	1:A:362:GLU:HB2	1.99	0.44
1:A:894:TRP:CE2	2:B:85:ILE:HG23	2.53	0.44
2:D:229:ILE:H	2:D:229:ILE:HG13	1.46	0.44
1:A:150:GLN:HG3	1:A:151:GLU:N	2.32	0.44
1:A:515:LEU:CD1	1:A:535:LYS:HE2	2.47	0.44
1:C:615:MET:HB2	1:C:633:ILE:HD13	1.99	0.44
1:C:732:VAL:HG11	1:C:758:ILE:HD11	1.99	0.44
1:A:402:THR:HB	1:A:594:PRO:HG3	2.00	0.44
1:A:662:ALA:HB2	1:A:687:GLU:HB2	2.00	0.44
1:C:1003:GLU:HG2	9:C:1105:PCW:H352	2.00	0.44
1:A:939:THR:OG1	1:A:1006:ARG:NH1	2.51	0.43
1:A:1011:ARG:NH2	2:D:64:ASP:OD1	2.51	0.43
1:A:596:ARG:HB2	1:A:599:VAL:HG23	1.99	0.43
8:A:1101:CLR:H273	9:C:1105:PCW:H281	1.99	0.43
1:C:510:ALA:O	1:C:514:ILE:HG12	2.18	0.43
2:D:215:CYS:SG	2:D:263:ILE:HD13	2.58	0.43
1:A:575:GLU:HB3	1:A:576:PRO:CD	2.44	0.43
1:C:846:ASN:OD1	1:C:846:ASN:N	2.44	0.43
1:C:894:TRP:CE2	2:D:85:ILE:HG23	2.53	0.43
2:D:140:LEU:HD23	2:D:252:LEU:HD12	2.00	0.43
2:B:163:LEU:HD23	4:F:6:FUC:H61	1.98	0.43
1:C:421:LEU:HD13	1:C:586:VAL:HG12	1.99	0.43
1:C:662:ALA:HB2	1:C:687:GLU:HB2	2.00	0.43
8:A:1101:CLR:H161	8:A:1101:CLR:H222	1.93	0.43
8:C:1101:CLR:H161	8:C:1101:CLR:H222	1.93	0.43
2:D:229:ILE:HD12	2:D:229:ILE:O	2.19	0.43
2:D:224:GLU:H	2:D:224:GLU:HG3	1.47	0.43
2:B:229:ILE:HD12	2:B:229:ILE:O	2.19	0.42
8:B:502:CLR:H161	8:B:502:CLR:H222	1.96	0.42
1:C:434:GLN:O	1:C:437:GLN:HG2	2.19	0.42
1:C:997:ILE:HG21	9:C:1103:PCW:H272	1.99	0.42
1:A:1003:GLU:HG2	9:A:1105:PCW:H352	2.00	0.42
2:B:140:LEU:HD23	2:B:252:LEU:HD12	2.00	0.42
2:D:160:CYS:SG	2:D:262:ALA:HB1	2.60	0.42
1:A:344:LEU:HD12	1:A:344:LEU:HA	1.89	0.42
1:A:1004:MET:HE3	2:D:57:VAL:HG22	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1101:CLR:H273	9:C:1105:PCW:C27	2.49	0.42
1:C:374:CYS:HB2	1:C:714:VAL:HG22	2.02	0.42
1:C:927:VAL:HG13	1:C:961:GLU:HG2	2.01	0.42
1:A:443:LEU:O	1:A:458:LYS:NZ	2.44	0.42
2:B:107:HIS:O	2:B:111:ASP:HB2	2.20	0.42
1:C:1019:GLN:OE1	9:C:1103:PCW:H61	2.20	0.42
1:C:127:ASN:C	1:C:129:ASN:H	2.27	0.42
2:D:107:HIS:O	2:D:111:ASP:HB2	2.20	0.42
1:A:548:LEU:HD12	1:A:548:LEU:HA	1.90	0.42
1:A:1019:GLN:OE1	9:A:1103:PCW:H61	2.20	0.42
2:D:234:LEU:HG	2:D:241:PRO:HG3	2.02	0.42
1:A:434:GLN:O	1:A:437:GLN:HG2	2.19	0.42
1:A:518:CYS:SG	1:A:585:PHE:HB2	2.59	0.42
1:A:772:LEU:HD23	1:A:772:LEU:HA	1.95	0.42
1:A:927:VAL:HG13	1:A:961:GLU:HG2	2.01	0.42
1:C:190:LEU:HD12	1:C:190:LEU:HA	1.91	0.42
1:A:631:VAL:HG23	1:A:633:ILE:HG13	2.02	0.42
1:A:800:LEU:HA	1:A:801:PRO:HD3	1.91	0.42
1:A:900:ASP:OD2	1:A:906:TRP:NE1	2.46	0.42
2:B:122:SER:HA	2:B:123:PRO:HA	1.69	0.42
2:B:160:CYS:SG	2:B:262:ALA:HB1	2.59	0.42
1:C:518:CYS:SG	1:C:585:PHE:HB2	2.59	0.42
1:A:127:ASN:C	1:A:129:ASN:N	2.78	0.41
1:A:127:ASN:C	1:A:129:ASN:H	2.27	0.41
9:C:1108:PCW:C19	8:D:501:CLR:H151	2.50	0.41
2:D:52:ILE:O	2:D:55:ILE:HG22	2.20	0.41
9:E:1302:PCW:H382	9:E:1302:PCW:H411	1.85	0.41
1:C:381:LEU:HD12	1:C:381:LEU:HA	1.88	0.41
1:C:511:PRO:O	1:C:515:LEU:HB2	2.21	0.41
2:D:114:ASN:OD1	2:D:154:ARG:NH1	2.53	0.41
1:A:374:CYS:HB2	1:A:714:VAL:HG22	2.02	0.41
1:A:510:ALA:HB1	1:A:512:GLU:OE2	2.21	0.41
1:C:86:THR:HA	1:C:87:PRO:HD3	1.92	0.41
1:C:238:GLU:OE2	1:C:692:ARG:NH2	2.53	0.41
1:C:676:GLU:OE1	1:C:676:GLU:N	2.45	0.41
1:C:926:ILE:O	1:C:930:GLN:HG2	2.21	0.41
2:D:189:PRO:HG2	2:D:245:TYR:CD2	2.56	0.41
1:A:121:THR:CG2	1:A:122:GLU:HG3	2.36	0.41
1:C:127:ASN:C	1:C:129:ASN:N	2.78	0.41
1:C:457:LEU:HD12	1:C:467:VAL:HG21	2.02	0.41
2:D:99:TYR:O	2:D:103:VAL:HG23	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:GLU:OE2	1:A:692:ARG:NH2	2.53	0.41
1:A:367:LEU:HD21	1:A:748:MET:HE1	2.02	0.41
1:A:750:LEU:HD13	1:A:754:ASN:O	2.21	0.41
9:A:1106:PCW:H221	9:A:1106:PCW:H471	2.01	0.41
2:B:99:TYR:O	2:B:103:VAL:HG23	2.20	0.41
1:C:575:GLU:HB3	1:C:576:PRO:CD	2.44	0.41
1:C:594:PRO:HA	1:C:595:PRO:HD3	1.88	0.41
2:D:85:ILE:O	2:D:86:LYS:HB2	2.20	0.41
1:A:926:ILE:O	1:A:930:GLN:HG2	2.20	0.41
2:B:28:ARG:HD3	2:B:32:SER:HB3	2.03	0.41
2:B:189:PRO:HG2	2:B:245:TYR:CD2	2.56	0.41
1:A:51:LEU:HD22	1:A:204:ARG:HD2	2.02	0.41
1:A:457:LEU:HD12	1:A:467:VAL:HG21	2.02	0.41
1:C:51:LEU:HD22	1:C:204:ARG:HD2	2.02	0.41
1:A:332:VAL:O	1:A:332:VAL:HG12	2.20	0.41
2:B:61:THR:HA	1:C:1007:PHE:CZ	2.54	0.41
1:C:64:THR:HG23	1:C:67:ARG:HB3	2.03	0.41
1:A:64:THR:HG23	1:A:67:ARG:HB3	2.03	0.41
1:A:100:PHE:C	1:A:102:ILE:N	2.79	0.41
1:A:312:ILE:HD13	1:A:312:ILE:HA	1.92	0.41
1:A:930:GLN:HA	1:A:930:GLN:OE1	2.21	0.41
2:B:75:PRO:HG2	2:B:286:ASP:H	1.86	0.41
2:B:114:ASN:OD1	2:B:154:ARG:NH1	2.53	0.41
1:C:336:LEU:HA	1:C:336:LEU:HD12	1.73	0.41
1:C:367:LEU:HD21	1:C:748:MET:HE1	2.02	0.41
1:C:383:GLN:OE1	1:C:385:ARG:NH1	2.54	0.41
1:C:750:LEU:HD13	1:C:754:ASN:O	2.21	0.41
1:C:930:GLN:OE1	1:C:930:GLN:HA	2.21	0.41
1:C:997:ILE:HG21	9:C:1103:PCW:C27	2.51	0.41
2:D:245:TYR:HB3	2:D:246:PRO:HA	2.03	0.41
9:E:1303:PCW:H242	9:E:1304:PCW:H19	2.02	0.41
1:A:203:LEU:HB2	1:A:243:ALA:HB3	2.03	0.41
1:A:306:PHE:HZ	9:A:1108:PCW:H282	1.86	0.41
1:A:383:GLN:OE1	1:A:385:ARG:NH1	2.54	0.41
2:B:193:LYS:O	2:B:198:LEU:HD13	2.21	0.41
2:B:229:ILE:HD13	2:B:231:TYR:OH	2.21	0.41
1:C:146:PHE:HZ	1:C:345:THR:HG21	1.84	0.41
1:C:976:VAL:HG21	9:C:1107:PCW:H51	2.03	0.41
9:C:1106:PCW:H221	9:C:1106:PCW:H471	2.01	0.41
1:A:540:ASN:HD22	1:A:540:ASN:H	1.69	0.40
1:A:814:THR:OG1	1:A:815:ASP:N	2.53	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:976:VAL:HG21	9:A:1107:PCW:H51	2.03	0.40
2:B:284:ASN:O	2:B:285:ILE:HD12	2.21	0.40
1:C:58:ASP:CG	1:C:61:ARG:HB2	2.47	0.40
2:D:193:LYS:O	2:D:198:LEU:HD13	2.21	0.40
1:A:492:ILE:HG13	1:A:505:LEU:HD13	2.04	0.40
2:B:279:LYS:HD3	2:B:287:TYR:CZ	2.57	0.40
1:C:302:LEU:HD21	9:C:1108:PCW:C21	2.51	0.40
1:C:306:PHE:HZ	9:C:1108:PCW:H282	1.86	0.40
1:C:510:ALA:HB1	1:C:512:GLU:OE2	2.21	0.40
2:B:234:LEU:HG	2:B:241:PRO:HG3	2.02	0.40
1:C:313:LEU:HD11	1:C:795:ILE:HG23	2.03	0.40
2:D:195:THR:HG22	2:D:196:THR:N	2.36	0.40
1:A:404:GLU:H	1:A:404:GLU:HG3	1.57	0.40
1:A:411:PHE:HZ	1:A:418:TRP:CZ2	2.39	0.40
1:A:511:PRO:O	1:A:515:LEU:HB2	2.20	0.40
2:B:245:TYR:HB3	2:B:246:PRO:HA	2.03	0.40
3:G:28:ALA:HB1	9:G:1302:PCW:H20	2.03	0.40
1:C:772:LEU:HD23	1:C:772:LEU:HA	1.95	0.40
1:C:814:THR:OG1	1:C:815:ASP:N	2.53	0.40
1:A:461:GLU:OE1	1:A:466:SER:HA	2.21	0.40
1:C:631:VAL:HG23	1:C:633:ILE:HG13	2.02	0.40
2:D:284:ASN:O	2:D:285:ILE:HD12	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	A	990/1028 (96%)	918 (93%)	72 (7%)	0	100	100
1	C	990/1028 (96%)	917 (93%)	73 (7%)	0	100	100
2	B	292/305 (96%)	259 (89%)	33 (11%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	292/305 (96%)	259 (89%)	33 (11%)	0	100	100
3	E	38/94 (40%)	33 (87%)	5 (13%)	0	100	100
3	G	38/94 (40%)	33 (87%)	5 (13%)	0	100	100
All	All	2640/2854 (92%)	2419 (92%)	221 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	840/868 (97%)	759 (90%)	81 (10%)	7	25
1	C	840/868 (97%)	759 (90%)	81 (10%)	7	25
2	B	258/266 (97%)	219 (85%)	39 (15%)	2	10
2	D	258/266 (97%)	219 (85%)	39 (15%)	2	10
3	E	33/75 (44%)	30 (91%)	3 (9%)	7	27
3	G	33/75 (44%)	30 (91%)	3 (9%)	7	27
All	All	2262/2418 (94%)	2016 (89%)	246 (11%)	8	20

All (246) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	GLU
1	A	37	LYS
1	A	45	LYS
1	A	63	LEU
1	A	64	THR
1	A	65	ASN
1	A	75	ASP
1	A	86	THR
1	A	96	LEU
1	A	100	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	121	THR
1	A	124	GLU
1	A	127	ASN
1	A	131	TYR
1	A	136	LEU
1	A	155	SER
1	A	158	MET
1	A	167	GLN
1	A	198	ARG
1	A	231	PHE
1	A	241	ASN
1	A	248	ASN
1	A	261	THR
1	A	263	ASP
1	A	282	THR
1	A	324	LEU
1	A	331	ASN
1	A	332	VAL
1	A	334	GLU
1	A	343	CYS
1	A	344	LEU
1	A	350	ARG
1	A	351	MET
1	A	357	LEU
1	A	360	ASN
1	A	362	GLU
1	A	367	LEU
1	A	381	LEU
1	A	415	SER
1	A	434	GLN
1	A	440	VAL
1	A	445	ARG
1	A	470	MET
1	A	485	THR
1	A	493	HIS
1	A	515	LEU
1	A	517	ARG
1	A	522	LEU
1	A	540	ASN
1	A	548	LEU
1	A	571	PHE
1	A	661	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	670	LEU
1	A	673	LEU
1	A	678	LEU
1	A	683	HIS
1	A	692	ARG
1	A	767	LEU
1	A	788	THR
1	A	811	ASP
1	A	812	LEU
1	A	816	MET
1	A	822	LEU
1	A	834	ARG
1	A	837	ARG
1	A	846	ASN
1	A	847	GLU
1	A	848	ARG
1	A	872	ILE
1	A	887	ARG
1	A	894	TRP
1	A	901	SER
1	A	935	ILE
1	A	943	SER
1	A	971	CYS
1	A	975	ASP
1	A	986	SER
1	A	996	LEU
1	A	1007	PHE
1	A	1011	ARG
1	A	1019	GLN
2	B	20	SER
2	B	26	LEU
2	B	28	ARG
2	B	32	SER
2	B	37	PHE
2	B	62	LEU
2	B	64	ASP
2	B	65	PHE
2	B	73	VAL
2	B	79	SER
2	B	94	SER
2	B	107	HIS
2	B	144	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	154	ARG
2	B	156	TRP
2	B	157	LEU
2	B	160	CYS
2	B	161	SER
2	B	167	THR
2	B	190	LYS
2	B	196	THR
2	B	200	GLU
2	B	203	GLN
2	B	208	GLN
2	B	211	LEU
2	B	213	LEU
2	B	214	ARG
2	B	218	LYS
2	B	229	ILE
2	B	242	LEU
2	B	266	THR
2	B	268	LEU
2	B	269	THR
2	B	272	MET
2	B	284	ASN
2	B	285	ILE
2	B	289	GLU
2	B	292	ARG
2	B	294	ARG
3	G	4	GLU
3	G	13	THR
3	G	33	ILE
1	C	34	GLU
1	C	37	LYS
1	C	45	LYS
1	C	63	LEU
1	C	64	THR
1	C	65	ASN
1	C	75	ASP
1	C	86	THR
1	C	96	LEU
1	C	100	PHE
1	C	121	THR
1	C	124	GLU
1	C	127	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	131	TYR
1	C	136	LEU
1	C	155	SER
1	C	158	MET
1	C	167	GLN
1	C	198	ARG
1	C	231	PHE
1	C	241	ASN
1	C	248	ASN
1	C	261	THR
1	C	263	ASP
1	C	282	THR
1	C	324	LEU
1	C	331	ASN
1	C	332	VAL
1	C	334	GLU
1	C	343	CYS
1	C	344	LEU
1	C	350	ARG
1	C	351	MET
1	C	357	LEU
1	C	360	ASN
1	C	362	GLU
1	C	367	LEU
1	C	381	LEU
1	C	415	SER
1	C	434	GLN
1	C	440	VAL
1	C	445	ARG
1	C	470	MET
1	C	485	THR
1	C	493	HIS
1	C	515	LEU
1	C	517	ARG
1	C	522	LEU
1	C	540	ASN
1	C	548	LEU
1	C	571	PHE
1	C	661	LYS
1	C	670	LEU
1	C	673	LEU
1	C	678	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	683	HIS
1	C	692	ARG
1	C	767	LEU
1	C	788	THR
1	C	811	ASP
1	C	812	LEU
1	C	816	MET
1	C	822	LEU
1	C	834	ARG
1	C	837	ARG
1	C	846	ASN
1	C	847	GLU
1	C	848	ARG
1	C	872	ILE
1	C	887	ARG
1	C	894	TRP
1	C	901	SER
1	C	935	ILE
1	C	943	SER
1	C	971	CYS
1	C	975	ASP
1	C	986	SER
1	C	996	LEU
1	C	1007	PHE
1	C	1011	ARG
1	C	1019	GLN
2	D	20	SER
2	D	26	LEU
2	D	28	ARG
2	D	32	SER
2	D	37	PHE
2	D	62	LEU
2	D	64	ASP
2	D	65	PHE
2	D	73	VAL
2	D	79	SER
2	D	94	SER
2	D	107	HIS
2	D	144	GLN
2	D	154	ARG
2	D	156	TRP
2	D	157	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	160	CYS
2	D	161	SER
2	D	167	THR
2	D	190	LYS
2	D	196	THR
2	D	200	GLU
2	D	203	GLN
2	D	208	GLN
2	D	211	LEU
2	D	213	LEU
2	D	214	ARG
2	D	218	LYS
2	D	229	ILE
2	D	242	LEU
2	D	266	THR
2	D	268	LEU
2	D	269	THR
2	D	272	MET
2	D	284	ASN
2	D	285	ILE
2	D	289	GLU
2	D	292	ARG
2	D	294	ARG
3	E	4	GLU
3	E	13	THR
3	E	33	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	HIS
1	A	118	GLN
1	A	129	ASN
1	A	241	ASN
1	A	293	HIS
1	A	360	ASN
1	A	434	GLN
1	A	474	ASN
1	A	489	GLN
1	A	539	GLN
1	A	540	ASN
1	A	904	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	56	GLN
2	B	144	GLN
2	B	203	GLN
2	B	207	ASN
1	C	52	HIS
1	C	241	ASN
1	C	293	HIS
1	C	360	ASN
1	C	434	GLN
1	C	474	ASN
1	C	489	GLN
1	C	540	ASN
1	C	649	ASN
1	C	904	GLN
2	D	56	GLN
2	D	144	GLN
2	D	203	GLN
2	D	207	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	PHD	C	376	1,10	9,11,12	1.87	1 (11%)	10,15,17	1.37	2 (20%)
1	PHD	A	376	1,10	9,11,12	1.87	1 (11%)	10,15,17	1.37	2 (20%)

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
1	PHD	C	376	1,10	-	2/8/11/13	-
1	PHD	A	376	1,10	-	2/8/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	376	PHD	P-OD1	-4.93	1.51	1.59
1	C	376	PHD	P-OD1	-4.92	1.51	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	376	PHD	OD1-CG-CB	2.99	119.32	111.11
1	A	376	PHD	OD1-CG-CB	2.99	119.32	111.11
1	A	376	PHD	OP3-P-OD1	2.04	111.48	105.25
1	C	376	PHD	OP3-P-OD1	2.04	111.48	105.25

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	376	PHD	CA-CB-CG-OD1
1	C	376	PHD	CA-CB-CG-OD1
1	A	376	PHD	CA-CB-CG-OD2
1	C	376	PHD	CA-CB-CG-OD2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

38 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	F	1	4,2	14,14,15	0.64	0	17,19,21	1.30	2 (11%)
4	NAG	F	2	4	14,14,15	0.68	0	17,19,21	0.82	1 (5%)
4	BMA	F	3	4	11,11,12	0.91	1 (9%)	15,15,17	1.34	1 (6%)
4	MAN	F	4	4	11,11,12	0.76	0	15,15,17	1.10	1 (6%)
4	MAN	F	5	4	11,11,12	0.76	0	15,15,17	1.02	1 (6%)
4	FUC	F	6	4	10,10,11	0.98	1 (10%)	14,14,16	0.68	0
5	NAG	H	1	5,2	14,14,15	0.79	0	17,19,21	1.41	2 (11%)
5	NAG	H	2	5	14,14,15	0.58	0	17,19,21	2.02	3 (17%)
5	BMA	H	3	5	11,11,12	0.97	1 (9%)	15,15,17	1.22	2 (13%)
5	MAN	H	4	5	11,11,12	0.81	0	15,15,17	1.62	3 (20%)
5	NAG	H	5	5	14,14,15	0.78	0	17,19,21	1.03	1 (5%)
5	MAN	H	6	5	11,11,12	0.70	0	15,15,17	1.21	1 (6%)
6	NAG	I	1	2,6	14,14,15	0.69	0	17,19,21	1.64	2 (11%)
6	NAG	I	2	6	14,14,15	0.68	0	17,19,21	0.75	1 (5%)
6	BMA	I	3	6	11,11,12	0.90	0	15,15,17	1.26	1 (6%)
6	MAN	I	4	6	11,11,12	0.74	0	15,15,17	1.09	1 (6%)
6	FUC	I	5	6	10,10,11	0.95	1 (10%)	14,14,16	0.71	0
7	NAG	J	1	2,7	14,14,15	0.69	0	17,19,21	0.79	1 (5%)
7	NAG	J	2	7	14,14,15	0.68	0	17,19,21	0.59	0
4	NAG	K	1	4,2	14,14,15	0.64	0	17,19,21	1.30	2 (11%)
4	NAG	K	2	4	14,14,15	0.68	0	17,19,21	0.82	1 (5%)
4	BMA	K	3	4	11,11,12	0.92	1 (9%)	15,15,17	1.34	1 (6%)
4	MAN	K	4	4	11,11,12	0.76	0	15,15,17	1.10	1 (6%)
4	MAN	K	5	4	11,11,12	0.76	0	15,15,17	1.02	1 (6%)
4	FUC	K	6	4	10,10,11	0.98	1 (10%)	14,14,16	0.68	0
5	NAG	L	1	5,2	14,14,15	0.79	0	17,19,21	1.41	2 (11%)
5	NAG	L	2	5	14,14,15	0.58	0	17,19,21	2.02	3 (17%)
5	BMA	L	3	5	11,11,12	0.97	1 (9%)	15,15,17	1.22	2 (13%)
5	MAN	L	4	5	11,11,12	0.81	0	15,15,17	1.62	3 (20%)
5	NAG	L	5	5	14,14,15	0.77	0	17,19,21	1.03	1 (5%)
5	MAN	L	6	5	11,11,12	0.70	0	15,15,17	1.21	1 (6%)
6	NAG	M	1	2,6	14,14,15	0.69	0	17,19,21	1.64	2 (11%)
6	NAG	M	2	6	14,14,15	0.68	0	17,19,21	0.75	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	BMA	M	3	6	11,11,12	0.90	1 (9%)	15,15,17	1.26	1 (6%)
6	MAN	M	4	6	11,11,12	0.74	0	15,15,17	1.09	1 (6%)
6	FUC	M	5	6	10,10,11	0.95	1 (10%)	14,14,16	0.71	0
7	NAG	N	1	2,7	14,14,15	0.69	0	17,19,21	0.79	1 (5%)
7	NAG	N	2	7	14,14,15	0.68	0	17,19,21	0.59	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	4,2	-	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	5,2	-	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	2,6	-	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	2,7	-	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	4,2	-	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	5,2	-	0/6/23/26	0/1/1/1
5	NAG	L	2	5	-	3/6/23/26	0/1/1/1
5	BMA	L	3	5	-	2/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	2,6	-	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	2,7	-	0/6/23/26	0/1/1/1
7	NAG	N	2	7	-	0/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	6	FUC	O5-C1	-2.38	1.39	1.43
4	K	6	FUC	O5-C1	-2.38	1.39	1.43
5	H	3	BMA	C2-C3	2.34	1.56	1.52
5	L	3	BMA	C2-C3	2.34	1.56	1.52
6	M	5	FUC	O5-C1	-2.27	1.40	1.43
6	I	5	FUC	O5-C1	-2.27	1.40	1.43
4	K	3	BMA	C2-C3	2.05	1.55	1.52
4	F	3	BMA	C2-C3	2.05	1.55	1.52
6	M	3	BMA	C2-C3	2.00	1.55	1.52

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	1	NAG	C1-O5-C5	5.64	119.84	112.19
6	I	1	NAG	C1-O5-C5	5.64	119.84	112.19
5	H	2	NAG	C2-N2-C7	5.40	130.59	122.90
5	L	2	NAG	C2-N2-C7	5.40	130.59	122.90
5	L	2	NAG	C1-O5-C5	4.89	118.81	112.19
5	H	2	NAG	C1-O5-C5	4.89	118.81	112.19
4	F	1	NAG	C1-O5-C5	4.19	117.86	112.19
4	K	1	NAG	C1-O5-C5	4.18	117.86	112.19
5	L	4	MAN	C1-O5-C5	4.01	117.62	112.19
5	H	4	MAN	C1-O5-C5	4.01	117.62	112.19
5	L	1	NAG	O4-C4-C5	4.00	119.22	109.30
5	H	1	NAG	O4-C4-C5	4.00	119.22	109.30
5	L	5	NAG	C1-O5-C5	3.53	116.98	112.19
5	H	5	NAG	C1-O5-C5	3.53	116.97	112.19
5	L	6	MAN	C1-O5-C5	3.51	116.95	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	6	MAN	C1-O5-C5	3.51	116.95	112.19
4	F	3	BMA	O5-C5-C6	3.17	112.17	107.20
4	K	3	BMA	O5-C5-C6	3.17	112.17	107.20
5	H	1	NAG	C1-O5-C5	3.12	116.42	112.19
5	L	1	NAG	C1-O5-C5	3.12	116.41	112.19
5	H	4	MAN	O2-C2-C3	2.88	115.92	110.14
5	L	4	MAN	O2-C2-C3	2.88	115.91	110.14
6	I	3	BMA	O5-C5-C6	2.68	111.41	107.20
6	M	3	BMA	O5-C5-C6	2.68	111.41	107.20
5	L	2	NAG	O7-C7-N2	2.66	126.84	121.95
5	H	2	NAG	O7-C7-N2	2.66	126.83	121.95
4	F	2	NAG	C1-O5-C5	2.65	115.79	112.19
4	K	2	NAG	C1-O5-C5	2.65	115.79	112.19
5	H	3	BMA	O3-C3-C2	2.60	114.96	109.99
5	L	3	BMA	O3-C3-C2	2.59	114.96	109.99
5	L	4	MAN	O2-C2-C1	2.55	114.36	109.15
5	H	4	MAN	O2-C2-C1	2.54	114.36	109.15
4	F	5	MAN	C1-O5-C5	2.52	115.61	112.19
4	K	5	MAN	C1-O5-C5	2.52	115.61	112.19
4	F	4	MAN	C1-O5-C5	2.52	115.60	112.19
4	K	4	MAN	C1-O5-C5	2.51	115.60	112.19
6	M	4	MAN	C1-O5-C5	2.50	115.58	112.19
6	I	4	MAN	C1-O5-C5	2.50	115.58	112.19
7	J	1	NAG	O4-C4-C3	-2.44	104.71	110.35
7	N	1	NAG	O4-C4-C3	-2.43	104.72	110.35
6	M	2	NAG	C1-O5-C5	2.38	115.42	112.19
6	I	2	NAG	C1-O5-C5	2.38	115.42	112.19
6	I	1	NAG	O4-C4-C3	-2.22	105.21	110.35
6	M	1	NAG	O4-C4-C3	-2.22	105.21	110.35
4	F	1	NAG	O4-C4-C3	-2.07	105.57	110.35
4	K	1	NAG	O4-C4-C3	-2.06	105.58	110.35
5	H	3	BMA	O5-C5-C6	2.01	110.36	107.20
5	L	3	BMA	O5-C5-C6	2.01	110.36	107.20

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	5	NAG	O5-C5-C6-O6
5	L	5	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

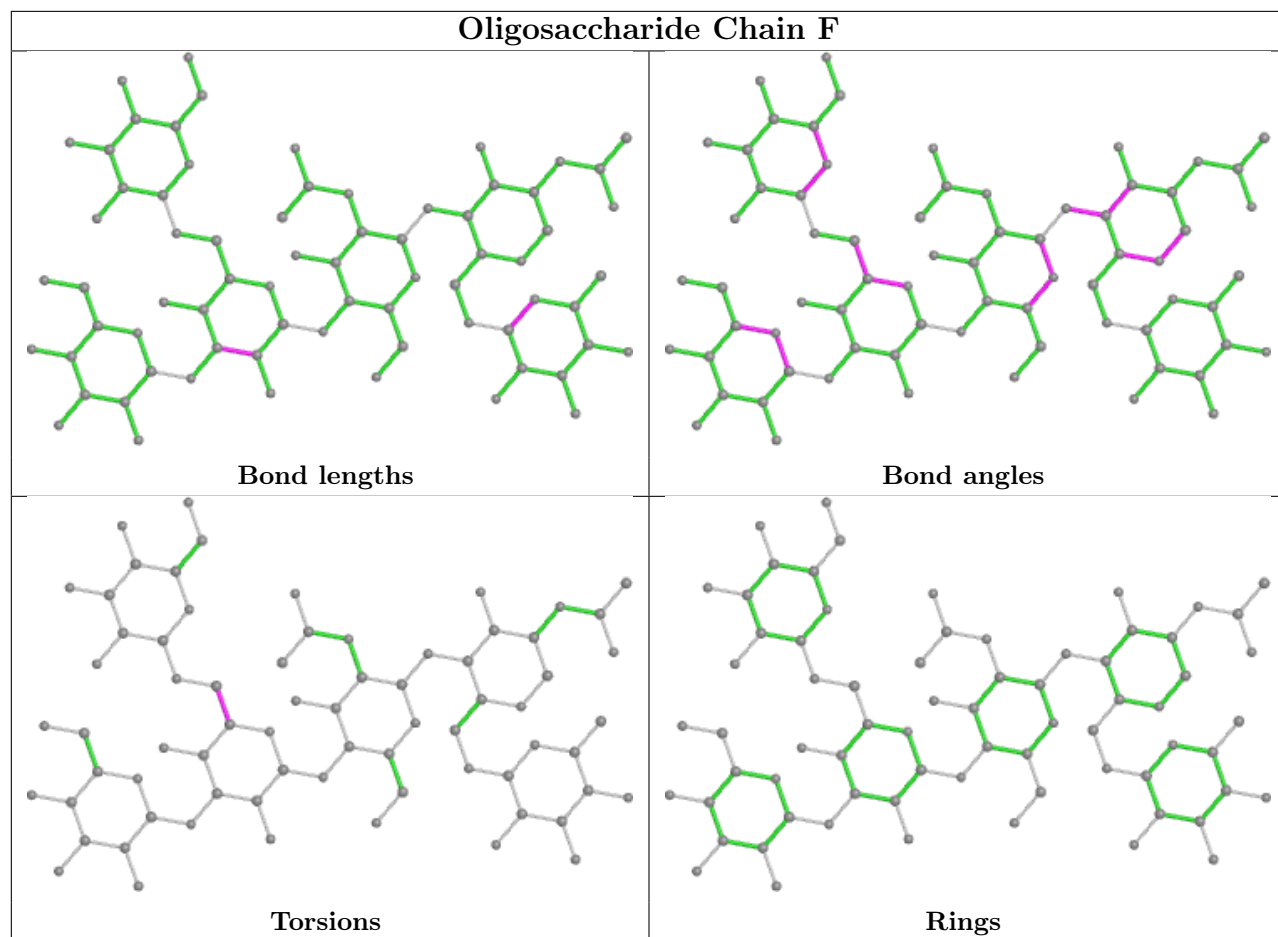
Mol	Chain	Res	Type	Atoms
5	H	6	MAN	O5-C5-C6-O6
5	L	6	MAN	O5-C5-C6-O6
5	H	2	NAG	O5-C5-C6-O6
5	L	2	NAG	O5-C5-C6-O6
5	H	3	BMA	O5-C5-C6-O6
5	L	3	BMA	O5-C5-C6-O6
5	H	6	MAN	C4-C5-C6-O6
5	L	6	MAN	C4-C5-C6-O6
5	H	5	NAG	C4-C5-C6-O6
5	L	5	NAG	C4-C5-C6-O6
5	H	2	NAG	C4-C5-C6-O6
5	L	2	NAG	C4-C5-C6-O6
5	H	5	NAG	C8-C7-N2-C2
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	3	BMA	C4-C5-C6-O6
5	L	3	BMA	C4-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

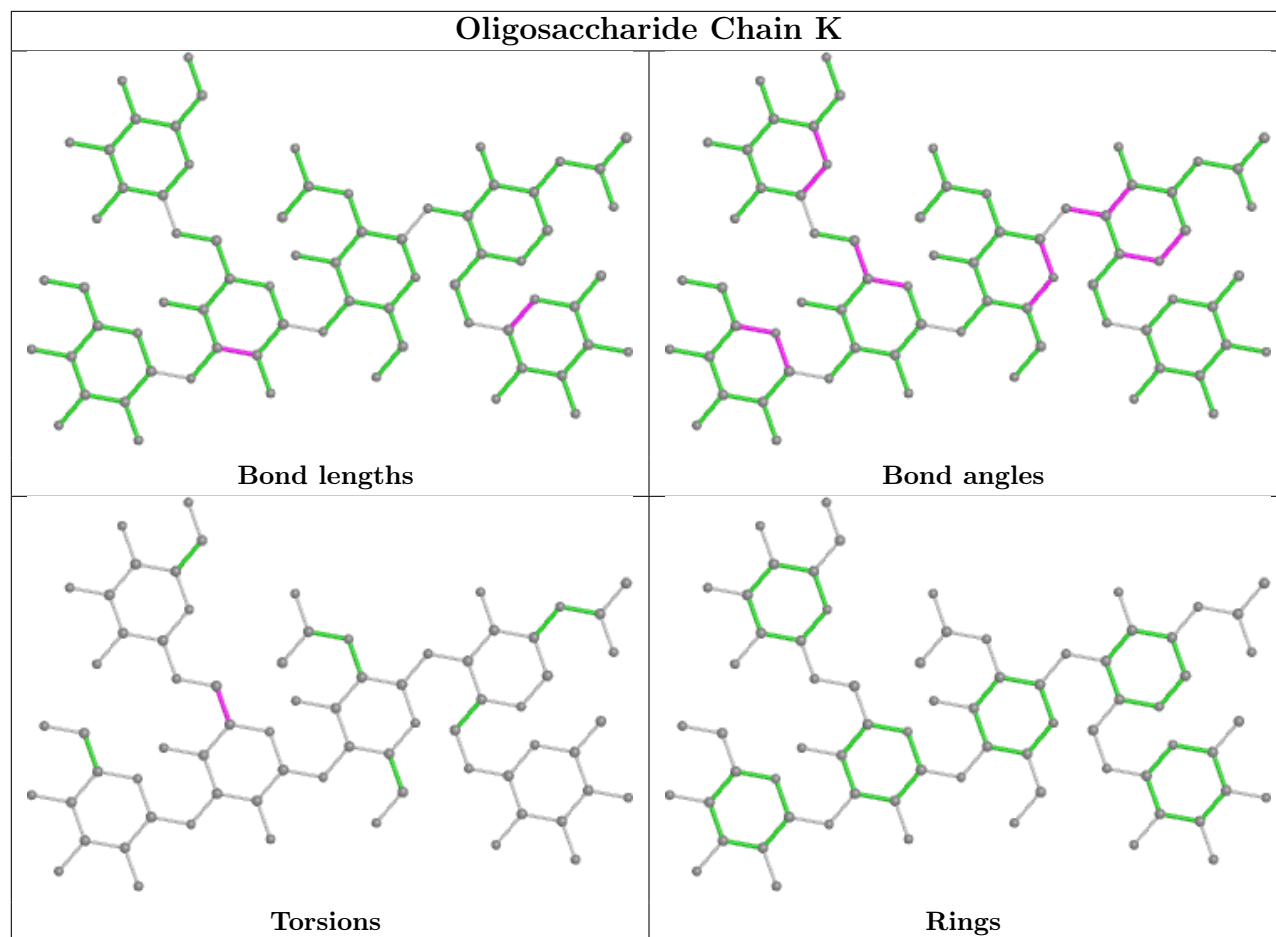
There are no ring outliers.

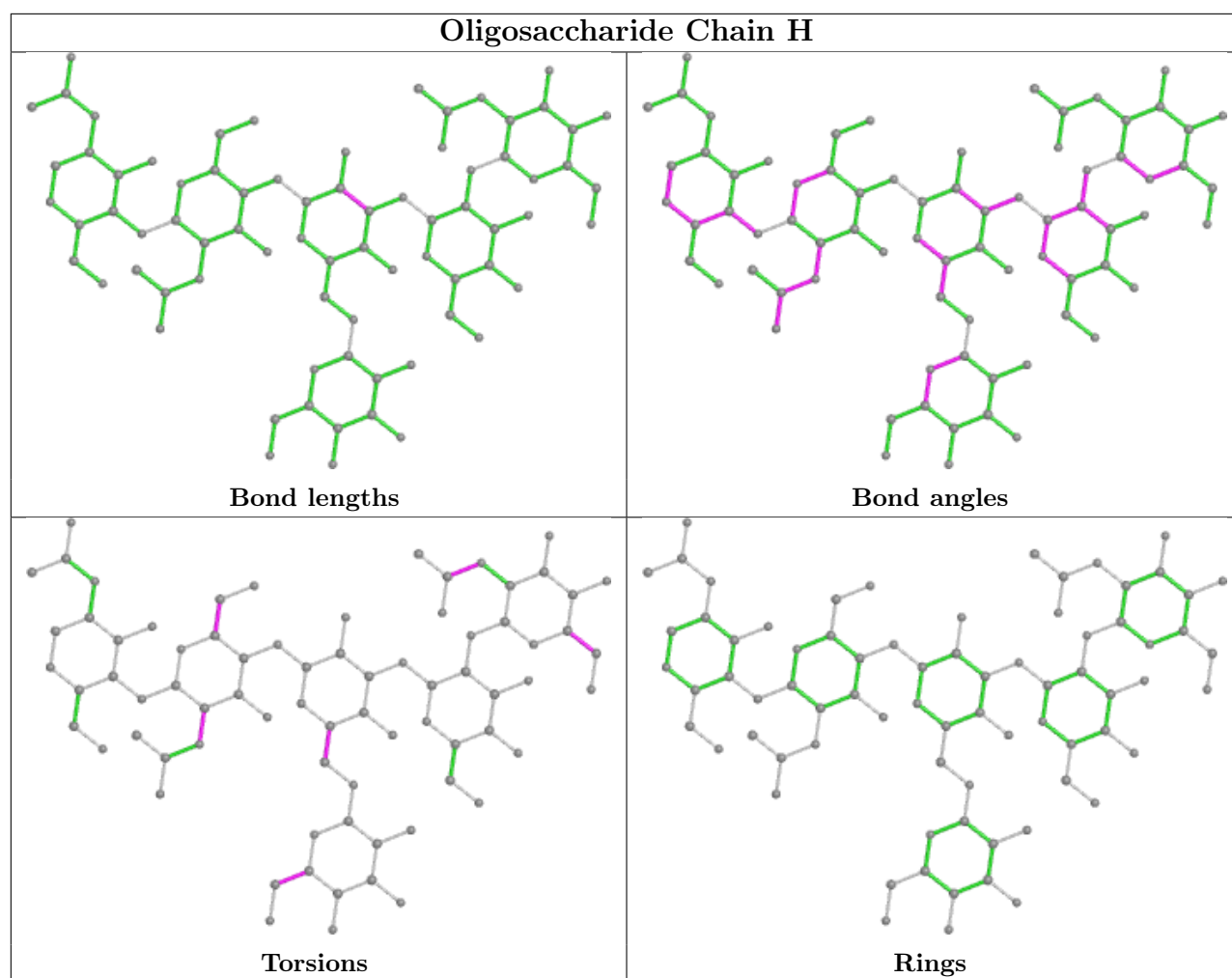
2 monomers are involved in 2 short contacts:

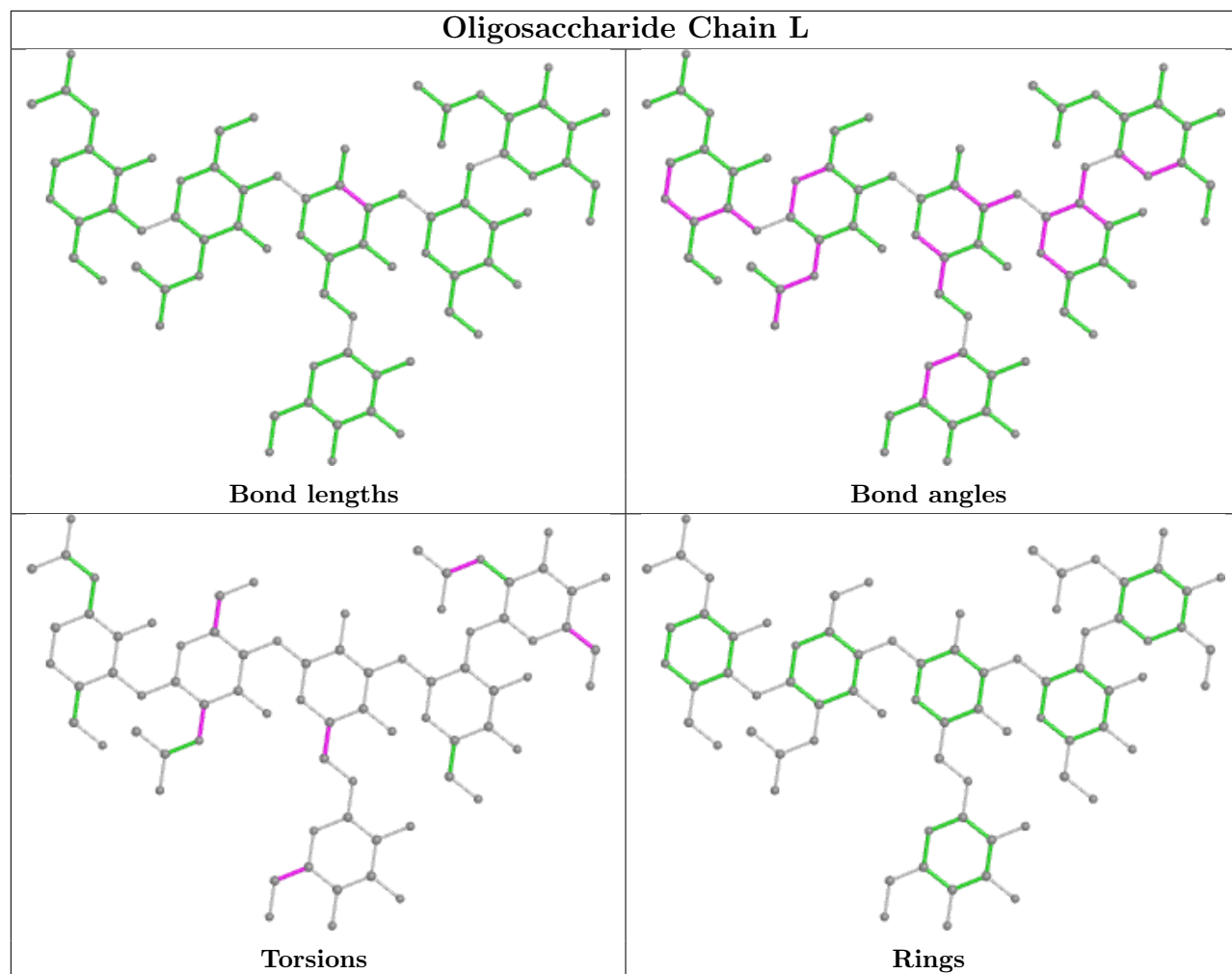
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	6	FUC	1	0
4	K	6	FUC	1	0

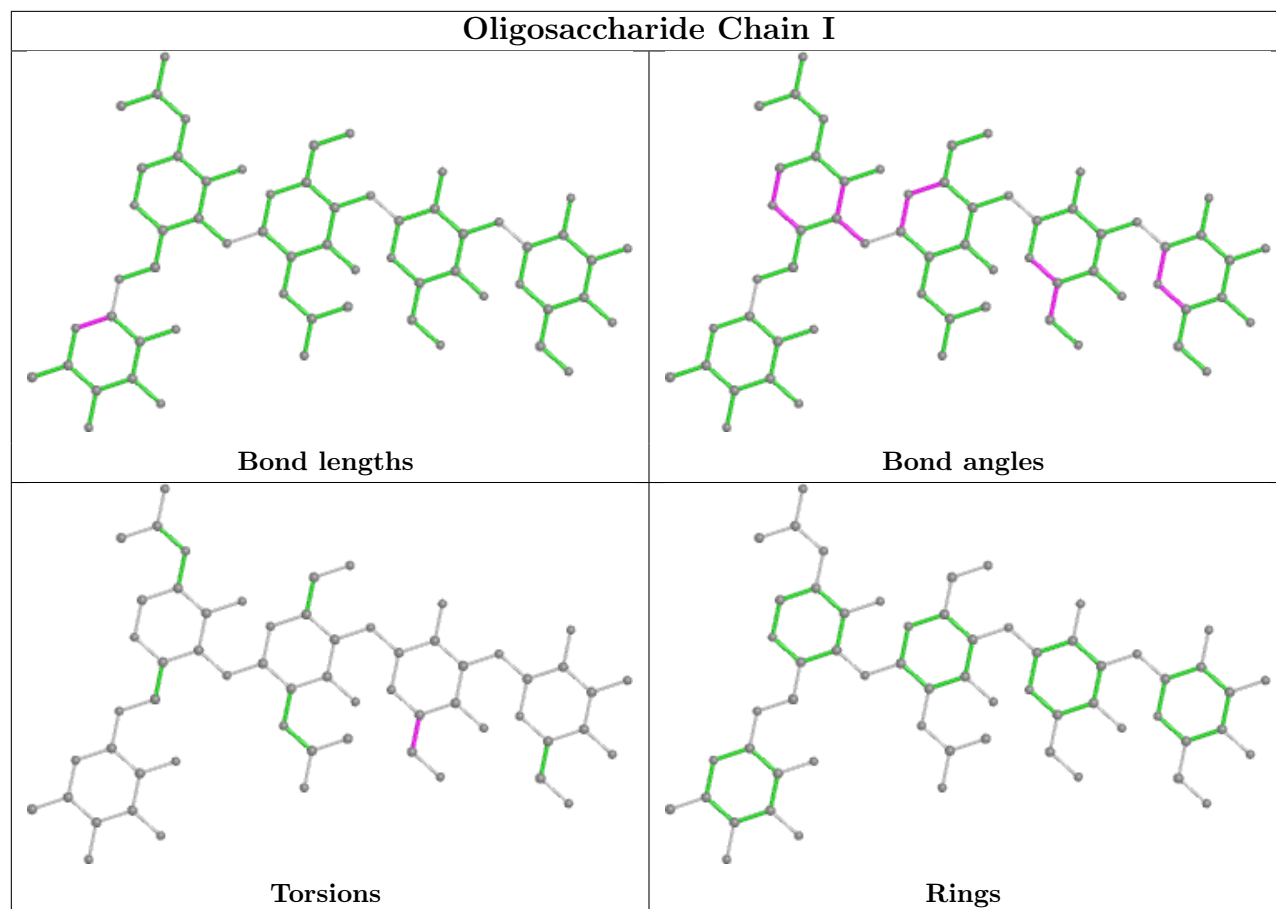
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

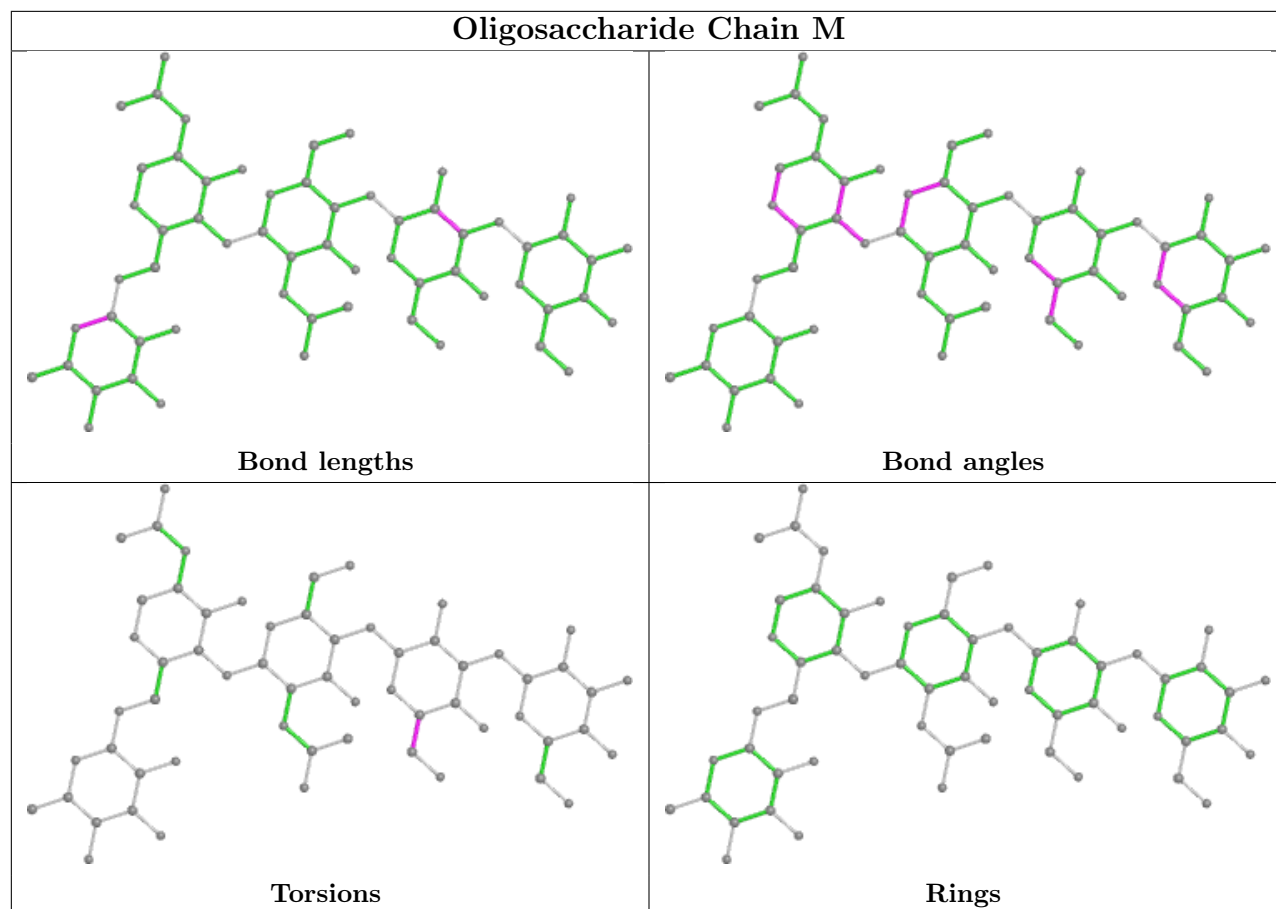


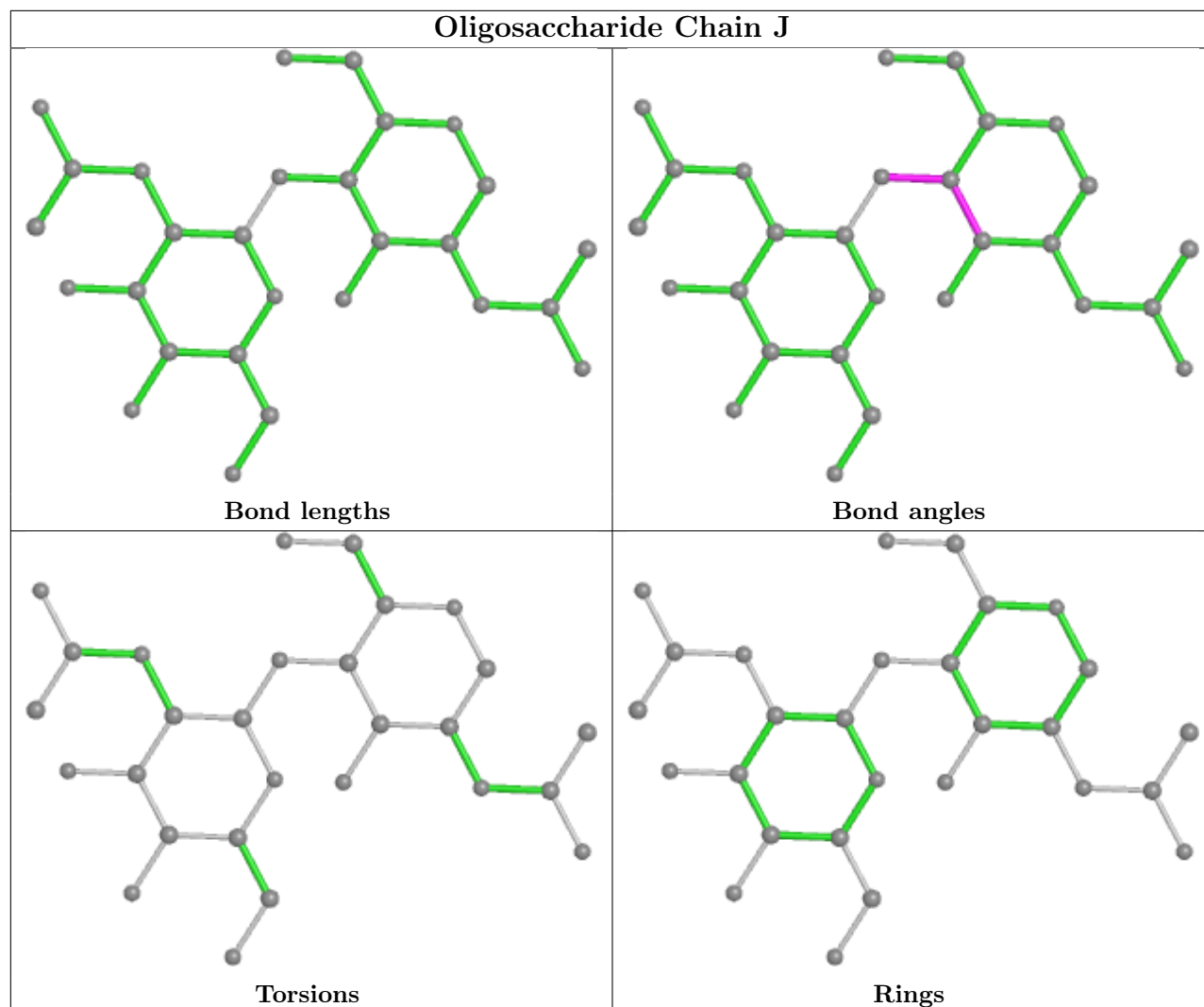


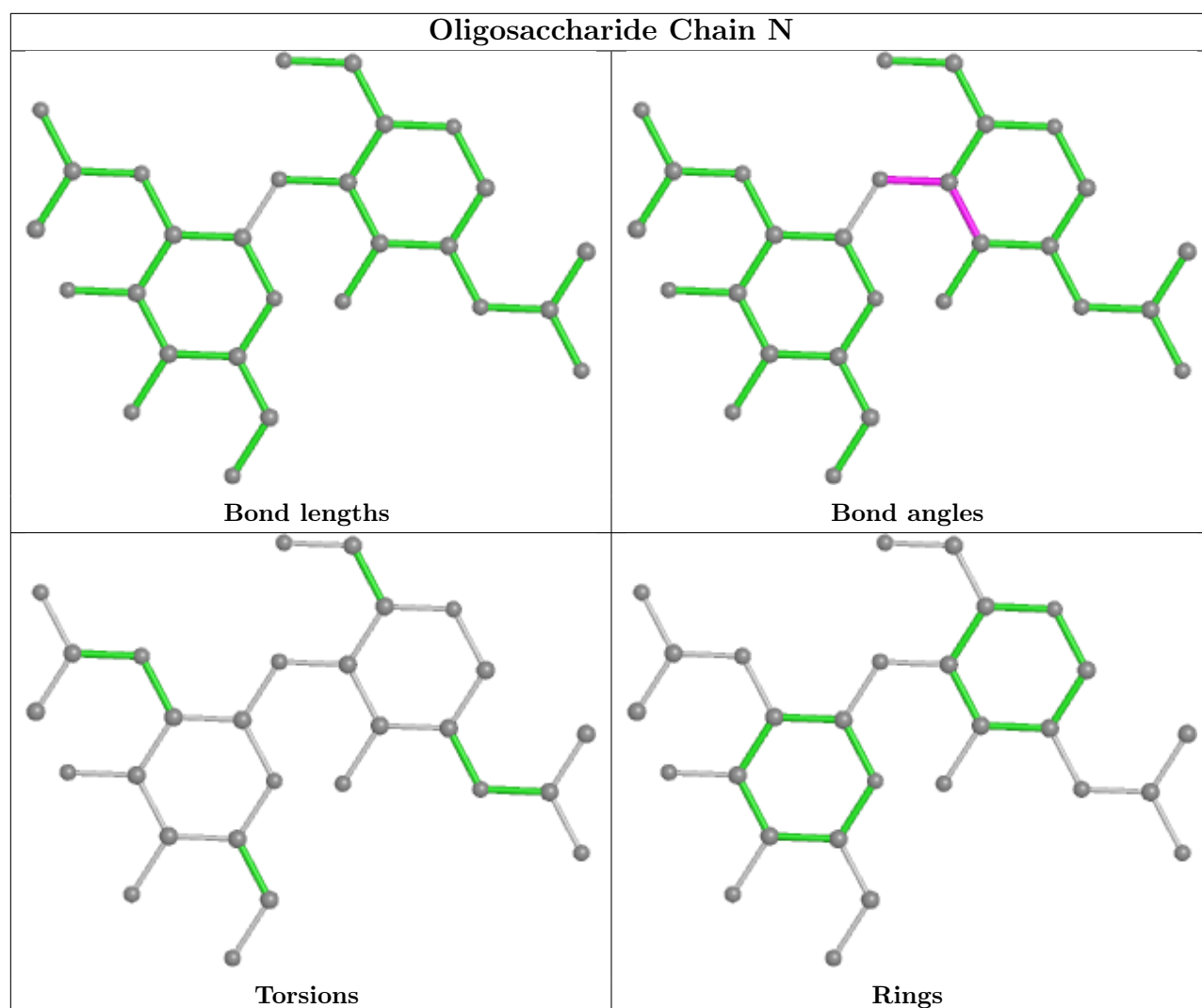












5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 4 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	A	1105	-	53,53,53	0.95	2 (3%)	59,61,61	0.78	0
8	CLR	B	501	-	31,31,31	1.21	4 (12%)	48,48,48	1.37	6 (12%)
8	CLR	E	1301	-	31,31,31	1.23	4 (12%)	48,48,48	1.36	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >
8	CLR	A	1101	-	31,31,31	1.24	4 (12%)	48,48,48	1.36	6 (12%)
8	CLR	C	1101	-	31,31,31	1.24	4 (12%)	48,48,48	1.36	6 (12%)
9	PCW	A	1102	-	21,21,53	0.87	0	27,29,61	1.15	3 (11%)
9	PCW	G	1302	-	53,53,53	0.98	2 (3%)	59,61,61	0.77	0
9	PCW	G	1303	-	53,53,53	0.98	2 (3%)	59,61,61	0.75	0
9	PCW	A	1108	-	53,53,53	0.99	2 (3%)	59,61,61	0.62	0
9	PCW	A	1104	-	53,53,53	0.99	2 (3%)	59,61,61	0.70	0
9	PCW	C	1105	-	53,53,53	0.95	2 (3%)	59,61,61	0.78	0
8	CLR	G	1301	-	31,31,31	1.23	4 (12%)	48,48,48	1.36	6 (12%)
9	PCW	E	1302	-	53,53,53	0.98	2 (3%)	59,61,61	0.77	0
9	PCW	A	1103	-	53,53,53	0.97	2 (3%)	59,61,61	0.72	0
9	PCW	C	1103	-	53,53,53	0.97	2 (3%)	59,61,61	0.72	0
8	CLR	D	502	-	31,31,31	1.24	4 (12%)	48,48,48	1.36	6 (12%)
9	PCW	E	1303	-	53,53,53	0.98	2 (3%)	59,61,61	0.75	0
11	A1MA6	C	1111	-	190,195,195	1.35	21 (11%)	219,278,278	1.68	36 (16%)
9	PCW	C	1108	-	53,53,53	0.99	2 (3%)	59,61,61	0.62	0
11	A1MA6	A	1111	-	190,195,195	1.35	21 (11%)	219,278,278	1.68	36 (16%)
9	PCW	C	1104	-	53,53,53	0.99	2 (3%)	59,61,61	0.70	0
9	PCW	E	1304	-	53,53,53	0.99	2 (3%)	59,61,61	0.65	0
8	CLR	B	502	-	31,31,31	1.24	4 (12%)	48,48,48	1.36	6 (12%)
9	PCW	C	1106	-	53,53,53	0.99	2 (3%)	59,61,61	0.67	0
8	CLR	D	501	-	31,31,31	1.21	4 (12%)	48,48,48	1.37	6 (12%)
9	PCW	A	1107	-	53,53,53	0.98	2 (3%)	59,61,61	0.72	0
9	PCW	C	1107	-	53,53,53	0.98	2 (3%)	59,61,61	0.72	0
9	PCW	A	1106	-	53,53,53	0.99	2 (3%)	59,61,61	0.67	0
9	PCW	C	1102	-	21,21,53	0.87	0	27,29,61	1.15	3 (11%)
9	PCW	G	1304	-	53,53,53	0.99	2 (3%)	59,61,61	0.65	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	A	1105	-	-	14/57/57/57	-
8	CLR	B	501	-	-	1/10/68/68	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	CLR	E	1301	-	-	0/10/68/68	0/4/4/4
8	CLR	A	1101	-	-	0/10/68/68	0/4/4/4
8	CLR	C	1101	-	-	0/10/68/68	0/4/4/4
9	PCW	A	1102	-	-	9/23/23/57	-
9	PCW	G	1302	-	-	18/57/57/57	-
9	PCW	G	1303	-	-	22/57/57/57	-
9	PCW	A	1108	-	-	24/57/57/57	-
9	PCW	A	1104	-	-	18/57/57/57	-
9	PCW	C	1105	-	-	14/57/57/57	-
8	CLR	G	1301	-	-	0/10/68/68	0/4/4/4
9	PCW	E	1302	-	-	18/57/57/57	-
9	PCW	A	1103	-	-	21/57/57/57	-
9	PCW	C	1103	-	-	21/57/57/57	-
8	CLR	D	502	-	-	0/10/68/68	0/4/4/4
9	PCW	E	1303	-	-	22/57/57/57	-
11	A1MA6	C	1111	-	-	101/192/350/350	1/12/10/10
9	PCW	C	1108	-	-	24/57/57/57	-
11	A1MA6	A	1111	-	-	101/192/350/350	1/12/10/10
9	PCW	C	1104	-	-	18/57/57/57	-
9	PCW	E	1304	-	-	18/57/57/57	-
8	CLR	B	502	-	-	0/10/68/68	0/4/4/4
9	PCW	C	1106	-	-	22/57/57/57	-
8	CLR	D	501	-	-	1/10/68/68	0/4/4/4
9	PCW	A	1107	-	-	19/57/57/57	-
9	PCW	C	1107	-	-	19/57/57/57	-
9	PCW	A	1106	-	-	22/57/57/57	-
9	PCW	C	1102	-	-	9/23/23/57	-
9	PCW	G	1304	-	-	18/57/57/57	-

All (110) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	1111	A1MA6	OC2-C43	5.63	1.54	1.43
11	A	1111	A1MA6	OC2-C43	5.63	1.54	1.43
11	C	1111	A1MA6	OAO-CAP	5.41	1.57	1.45
11	A	1111	A1MA6	OAO-CAP	5.41	1.57	1.45
11	C	1111	A1MA6	CBL-CBM	-5.07	1.44	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1111	A1MA6	CBL-CBM	-5.06	1.44	1.52
11	A	1111	A1MA6	CA3-CA4	4.50	1.54	1.45
11	C	1111	A1MA6	CA3-CA4	4.50	1.54	1.45
9	G	1304	PCW	C40-C39	4.03	1.55	1.31
9	E	1304	PCW	C40-C39	4.03	1.55	1.31
11	A	1111	A1MA6	OC2-C47	3.99	1.49	1.43
11	C	1111	A1MA6	OC2-C47	3.99	1.49	1.43
9	C	1108	PCW	C20-C19	3.93	1.54	1.31
9	A	1108	PCW	C20-C19	3.92	1.54	1.31
11	A	1111	A1MA6	C48-C49	-3.90	1.46	1.53
11	C	1111	A1MA6	C48-C49	-3.90	1.46	1.53
9	G	1302	PCW	C20-C19	3.90	1.54	1.31
9	E	1302	PCW	C20-C19	3.90	1.54	1.31
9	C	1107	PCW	C40-C39	3.90	1.54	1.31
9	A	1107	PCW	C40-C39	3.89	1.54	1.31
9	C	1104	PCW	C20-C19	3.89	1.54	1.31
9	C	1106	PCW	C20-C19	3.89	1.54	1.31
9	A	1104	PCW	C20-C19	3.89	1.54	1.31
9	A	1106	PCW	C20-C19	3.89	1.54	1.31
9	E	1303	PCW	C40-C39	3.89	1.54	1.31
9	G	1303	PCW	C40-C39	3.89	1.54	1.31
9	E	1302	PCW	C40-C39	3.88	1.54	1.31
9	G	1302	PCW	C40-C39	3.88	1.54	1.31
9	C	1104	PCW	C40-C39	3.88	1.54	1.31
9	A	1104	PCW	C40-C39	3.88	1.54	1.31
9	C	1107	PCW	C20-C19	3.87	1.54	1.31
9	A	1107	PCW	C20-C19	3.86	1.54	1.31
9	A	1106	PCW	C40-C39	3.86	1.54	1.31
9	C	1106	PCW	C40-C39	3.86	1.54	1.31
9	A	1108	PCW	C40-C39	3.83	1.54	1.31
9	C	1108	PCW	C40-C39	3.83	1.54	1.31
9	G	1304	PCW	C20-C19	3.82	1.53	1.31
9	C	1103	PCW	C20-C19	3.82	1.53	1.31
9	E	1304	PCW	C20-C19	3.82	1.53	1.31
9	A	1103	PCW	C20-C19	3.82	1.53	1.31
9	C	1105	PCW	C40-C39	3.79	1.53	1.31
9	A	1105	PCW	C40-C39	3.79	1.53	1.31
9	A	1105	PCW	C20-C19	3.78	1.53	1.31
9	C	1105	PCW	C20-C19	3.78	1.53	1.31
9	C	1103	PCW	C40-C39	3.73	1.53	1.31
9	A	1103	PCW	C40-C39	3.72	1.53	1.31
9	G	1303	PCW	C20-C19	3.70	1.53	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	1303	PCW	C20-C19	3.70	1.53	1.31
11	C	1111	A1MA6	C51-C49	-3.65	1.46	1.53
11	A	1111	A1MA6	C51-C49	-3.65	1.46	1.53
11	C	1111	A1MA6	CAN-CAM	-3.44	1.45	1.52
11	A	1111	A1MA6	CAN-CAM	-3.43	1.45	1.52
11	C	1111	A1MA6	C95-C94	3.25	1.53	1.44
11	A	1111	A1MA6	C95-C94	3.25	1.53	1.44
8	C	1101	CLR	C16-C17	3.17	1.61	1.54
8	A	1101	CLR	C16-C17	3.16	1.60	1.54
8	D	502	CLR	C16-C17	3.15	1.60	1.54
8	B	502	CLR	C16-C17	3.14	1.60	1.54
8	E	1301	CLR	C16-C17	3.12	1.60	1.54
8	G	1301	CLR	C16-C17	3.12	1.60	1.54
8	D	501	CLR	C16-C17	3.09	1.60	1.54
8	B	501	CLR	C16-C17	3.09	1.60	1.54
11	A	1111	A1MA6	CAV-CAW	-3.03	1.46	1.52
11	C	1111	A1MA6	CAV-CAW	-3.02	1.46	1.52
11	C	1111	A1MA6	O46-C44	-2.79	1.40	1.45
11	A	1111	A1MA6	O46-C44	-2.79	1.41	1.45
11	A	1111	A1MA6	CAN-CB0	-2.56	1.47	1.52
11	C	1111	A1MA6	CAN-CB0	-2.56	1.47	1.52
11	A	1111	A1MA6	OAZ-CAS	2.49	1.50	1.45
11	C	1111	A1MA6	OAZ-CAS	2.49	1.50	1.45
11	A	1111	A1MA6	CAL-CAK	-2.45	1.46	1.52
11	C	1111	A1MA6	CAL-CAK	-2.45	1.46	1.52
11	C	1111	A1MA6	O76-C77	-2.37	1.38	1.44
11	A	1111	A1MA6	O76-C77	-2.37	1.38	1.44
8	C	1101	CLR	C7-C8	2.34	1.57	1.53
8	A	1101	CLR	C7-C8	2.34	1.57	1.53
11	C	1111	A1MA6	C15-C17	2.31	1.53	1.50
11	A	1111	A1MA6	C15-C17	2.31	1.53	1.50
8	D	501	CLR	C7-C6	2.27	1.55	1.50
8	B	501	CLR	C7-C6	2.27	1.55	1.50
8	B	502	CLR	C7-C8	2.27	1.57	1.53
8	D	502	CLR	C7-C8	2.27	1.57	1.53
11	A	1111	A1MA6	C63-CBZ	-2.25	1.52	1.53
11	C	1111	A1MA6	C63-CBZ	-2.25	1.52	1.53
8	E	1301	CLR	C7-C8	2.24	1.56	1.53
8	G	1301	CLR	C7-C8	2.24	1.56	1.53
11	A	1111	A1MA6	O76-C75	2.18	1.49	1.44
11	C	1111	A1MA6	O76-C75	2.18	1.49	1.44
8	G	1301	CLR	C7-C6	2.15	1.54	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	502	CLR	C7-C6	2.15	1.54	1.50
8	B	502	CLR	C7-C6	2.15	1.54	1.50
8	E	1301	CLR	C7-C6	2.15	1.54	1.50
8	B	501	CLR	C4-C3	2.15	1.55	1.52
8	D	501	CLR	C4-C3	2.15	1.55	1.52
8	D	501	CLR	C7-C8	2.14	1.56	1.53
8	B	501	CLR	C7-C8	2.14	1.56	1.53
11	A	1111	A1MA6	CAH-CAG	2.12	1.53	1.50
8	E	1301	CLR	C4-C3	2.12	1.55	1.52
8	G	1301	CLR	C4-C3	2.12	1.55	1.52
8	D	502	CLR	C4-C3	2.12	1.55	1.52
11	C	1111	A1MA6	CAH-CAG	2.11	1.53	1.50
8	B	502	CLR	C4-C3	2.11	1.55	1.52
11	C	1111	A1MA6	OAO-CAM	2.07	1.48	1.44
11	A	1111	A1MA6	OAO-CAM	2.07	1.48	1.44
8	A	1101	CLR	C4-C3	2.07	1.55	1.52
8	C	1101	CLR	C4-C3	2.06	1.55	1.52
11	C	1111	A1MA6	CBL-C75	2.02	1.55	1.52
11	A	1111	A1MA6	CBL-C75	2.02	1.55	1.52
8	C	1101	CLR	C7-C6	2.02	1.54	1.50
8	A	1101	CLR	C7-C6	2.02	1.54	1.50

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	1111	A1MA6	C97-C96-C95	-8.06	115.01	125.41
11	A	1111	A1MA6	C97-C96-C95	-8.05	115.01	125.41
11	C	1111	A1MA6	C44-O46-C47	-7.11	101.68	111.08
11	A	1111	A1MA6	C44-O46-C47	-7.11	101.69	111.08
11	C	1111	A1MA6	CA2-CA3-CA4	-6.72	115.33	125.92
11	A	1111	A1MA6	CA2-CA3-CA4	-6.72	115.33	125.92
11	C	1111	A1MA6	CAH-CAG-CAF	-6.04	115.46	124.93
11	A	1111	A1MA6	CAH-CAG-CAF	-6.04	115.46	124.93
11	A	1111	A1MA6	CA1-CA2-CA3	-4.78	115.31	126.00
11	C	1111	A1MA6	CA1-CA2-CA3	-4.78	115.32	126.00
11	C	1111	A1MA6	CAE-CAF-CAG	-4.64	115.50	124.61
11	A	1111	A1MA6	CAE-CAF-CAG	-4.64	115.51	124.61
9	C	1102	PCW	C2-O2-C31	-4.26	109.95	117.90
9	A	1102	PCW	C2-O2-C31	-4.26	109.95	117.90
11	A	1111	A1MA6	C92-C93-C94	-4.03	115.31	125.14
11	C	1111	A1MA6	C92-C93-C94	-4.03	115.32	125.14
11	A	1111	A1MA6	CAR-CAS-CAT	-3.95	108.00	116.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	1111	A1MA6	CAR-CAS-CAT	-3.95	108.00	116.29
11	A	1111	A1MA6	C63-O62-C61	-3.88	109.67	114.61
11	C	1111	A1MA6	C63-O62-C61	-3.87	109.68	114.61
11	A	1111	A1MA6	C70-C69-C68	-3.79	115.20	125.09
11	C	1111	A1MA6	C70-C69-C68	-3.79	115.20	125.09
11	A	1111	A1MA6	CAQ-CAP-CB0	-3.71	108.24	116.25
11	C	1111	A1MA6	CAQ-CAP-CB0	-3.71	108.25	116.25
11	C	1111	A1MA6	C67-C68-C69	-3.53	114.70	125.67
11	A	1111	A1MA6	C67-C68-C69	-3.53	114.71	125.67
11	C	1111	A1MA6	C53-C52-C47	-3.37	109.65	114.64
11	A	1111	A1MA6	C53-C52-C47	-3.36	109.66	114.64
11	A	1111	A1MA6	C08-N09-C10	-3.28	116.88	123.51
11	C	1111	A1MA6	C08-N09-C10	-3.27	116.88	123.51
11	C	1111	A1MA6	OAZ-CAW-CAV	-3.24	100.89	105.07
11	A	1111	A1MA6	OAZ-CAW-CAV	-3.24	100.90	105.07
8	B	502	CLR	C22-C20-C17	-3.12	103.84	110.28
8	D	502	CLR	C22-C20-C17	-3.12	103.84	110.28
8	A	1101	CLR	C22-C20-C17	-3.03	104.03	110.28
8	C	1101	CLR	C22-C20-C17	-3.03	104.03	110.28
11	C	1111	A1MA6	C30-C28-C26	-2.88	109.28	113.26
8	G	1301	CLR	C22-C20-C17	-2.88	104.34	110.28
8	E	1301	CLR	C22-C20-C17	-2.88	104.34	110.28
11	A	1111	A1MA6	C30-C28-C26	-2.88	109.28	113.26
11	C	1111	A1MA6	CAA-CAB-CAC	-2.83	109.66	115.47
11	A	1111	A1MA6	CAA-CAB-CAC	-2.82	109.66	115.47
11	C	1111	A1MA6	O62-C61-C60	2.82	109.55	105.95
11	A	1111	A1MA6	O62-C61-C60	2.82	109.54	105.95
8	B	501	CLR	C22-C20-C17	-2.80	104.51	110.28
8	D	501	CLR	C22-C20-C17	-2.79	104.51	110.28
11	C	1111	A1MA6	C37-C36-C34	-2.77	109.63	114.18
11	A	1111	A1MA6	C37-C36-C34	-2.76	109.63	114.18
11	A	1111	A1MA6	CAS-OAZ-CAW	-2.62	102.77	108.92
11	C	1111	A1MA6	CAS-OAZ-CAW	-2.62	102.77	108.92
11	C	1111	A1MA6	C32-C30-C28	-2.58	109.68	113.26
11	A	1111	A1MA6	C32-C30-C28	-2.58	109.69	113.26
11	A	1111	A1MA6	C78-C77-CBO	-2.56	109.25	113.47
11	C	1111	A1MA6	C78-C77-CBO	-2.56	109.25	113.47
11	C	1111	A1MA6	CAA-CA9-CA8	-2.55	109.53	114.66
11	A	1111	A1MA6	CAA-CA9-CA8	-2.55	109.54	114.66
11	C	1111	A1MA6	C91-C90-C85	-2.49	109.36	113.47
11	A	1111	A1MA6	C91-C90-C85	-2.49	109.36	113.47
11	A	1111	A1MA6	C81-C82-C83	-2.49	109.37	113.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	1111	A1MA6	C81-C82-C83	-2.49	109.37	113.47
11	A	1111	A1MA6	C60-C61-CBV	-2.43	109.47	113.47
11	C	1111	A1MA6	C60-C61-CBV	-2.43	109.47	113.47
11	C	1111	A1MA6	CAB-CAC-CB8	-2.42	109.49	113.47
11	A	1111	A1MA6	CAB-CAC-CB8	-2.42	109.49	113.47
8	B	501	CLR	C13-C17-C20	-2.41	115.71	119.49
8	D	501	CLR	C13-C17-C20	-2.41	115.71	119.49
8	E	1301	CLR	C18-C13-C12	2.37	114.32	110.59
8	G	1301	CLR	C18-C13-C12	2.36	114.32	110.59
9	A	1102	PCW	O2-C31-C32	2.35	115.41	111.09
9	C	1102	PCW	O2-C31-C32	2.35	115.41	111.09
11	C	1111	A1MA6	C71-C72-C73	-2.34	109.48	113.51
8	D	502	CLR	C18-C13-C12	2.34	114.29	110.59
8	B	502	CLR	C18-C13-C12	2.34	114.29	110.59
8	E	1301	CLR	C7-C8-C14	-2.34	107.51	110.91
11	A	1111	A1MA6	C71-C72-C73	-2.34	109.48	113.51
8	G	1301	CLR	C7-C8-C14	-2.34	107.52	110.91
8	B	502	CLR	C7-C8-C14	-2.33	107.53	110.91
8	D	502	CLR	C7-C8-C14	-2.33	107.53	110.91
8	C	1101	CLR	C18-C13-C12	2.32	114.25	110.59
11	A	1111	A1MA6	C61-C60-C59	-2.32	109.42	114.61
11	C	1111	A1MA6	C61-C60-C59	-2.32	109.42	114.61
8	A	1101	CLR	C18-C13-C12	2.32	114.25	110.59
11	C	1111	A1MA6	C22-C23-CC7	-2.31	109.66	113.47
11	A	1111	A1MA6	C22-C23-CC7	-2.31	109.66	113.47
8	B	501	CLR	C7-C8-C14	-2.30	107.57	110.91
8	D	501	CLR	C7-C8-C14	-2.30	107.57	110.91
8	B	501	CLR	C18-C13-C12	2.27	114.18	110.59
8	D	501	CLR	C18-C13-C12	2.27	114.17	110.59
8	A	1101	CLR	C7-C8-C14	-2.25	107.64	110.91
8	C	1101	CLR	C7-C8-C14	-2.25	107.64	110.91
11	A	1111	A1MA6	C77-O76-C75	-2.25	109.23	113.16
8	E	1301	CLR	C13-C17-C20	-2.25	115.97	119.49
11	C	1111	A1MA6	C77-O76-C75	-2.24	109.23	113.16
8	G	1301	CLR	C13-C17-C20	-2.24	115.97	119.49
8	E	1301	CLR	C21-C20-C17	2.24	116.34	112.92
8	G	1301	CLR	C21-C20-C17	2.23	116.34	112.92
8	A	1101	CLR	C13-C17-C20	-2.23	115.99	119.49
8	C	1101	CLR	C13-C17-C20	-2.23	115.99	119.49
8	D	501	CLR	C21-C20-C17	2.20	116.29	112.92
8	B	501	CLR	C21-C20-C17	2.20	116.29	112.92
9	A	1102	PCW	C3-O3-C11	-2.15	111.69	117.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	1102	PCW	C3-O3-C11	-2.15	111.70	117.10
8	D	502	CLR	C21-C20-C17	2.14	116.19	112.92
8	B	502	CLR	C21-C20-C17	2.13	116.19	112.92
11	A	1111	A1MA6	CAP-OAO-CAM	-2.13	103.92	108.92
11	C	1111	A1MA6	CAP-OAO-CAM	-2.13	103.93	108.92
8	B	502	CLR	C13-C17-C20	-2.11	116.18	119.49
8	D	502	CLR	C13-C17-C20	-2.11	116.19	119.49
11	A	1111	A1MA6	C04-C03-C02	-2.10	109.71	112.99
11	A	1111	A1MA6	C47-C48-C49	-2.10	108.75	112.79
11	C	1111	A1MA6	C04-C03-C02	-2.10	109.71	112.99
11	C	1111	A1MA6	C47-C48-C49	-2.10	108.75	112.79
8	A	1101	CLR	C19-C10-C9	-2.10	109.18	111.68
8	C	1101	CLR	C19-C10-C9	-2.09	109.19	111.68
8	E	1301	CLR	C19-C10-C9	-2.07	109.22	111.68
8	G	1301	CLR	C19-C10-C9	-2.07	109.22	111.68
8	A	1101	CLR	C21-C20-C17	2.05	116.06	112.92
8	C	1101	CLR	C21-C20-C17	2.05	116.06	112.92
11	A	1111	A1MA6	C34-C32-C30	-2.04	109.27	112.47
11	C	1111	A1MA6	OC2-C43-C44	-2.04	101.66	104.70
11	A	1111	A1MA6	OC2-C43-C44	-2.04	101.67	104.70
8	B	502	CLR	C19-C10-C9	-2.04	109.25	111.68
11	C	1111	A1MA6	C34-C32-C30	-2.04	109.28	112.47
8	D	502	CLR	C19-C10-C9	-2.03	109.26	111.68
8	B	501	CLR	C19-C10-C9	-2.03	109.26	111.68
8	D	501	CLR	C19-C10-C9	-2.03	109.26	111.68

There are no chirality outliers.

All (574) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	1102	PCW	C4-O4P-P-O1P
9	A	1103	PCW	O4P-C4-C5-N
9	A	1103	PCW	C4-O4P-P-O1P
9	A	1104	PCW	O3P-C1-C2-O2
9	A	1104	PCW	C1-O3P-P-O2P
9	A	1107	PCW	O2-C2-C3-O3
9	A	1108	PCW	C1-O3P-P-O2P
9	G	1302	PCW	O2-C2-C3-O3
9	G	1302	PCW	C1-O3P-P-O1P
9	G	1302	PCW	C1-O3P-P-O2P
9	G	1302	PCW	C4-O4P-P-O2P
9	G	1302	PCW	C4-O4P-P-O3P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	G	1303	PCW	C4-O4P-P-O3P
9	C	1102	PCW	C4-O4P-P-O1P
9	C	1103	PCW	O4P-C4-C5-N
9	C	1103	PCW	C4-O4P-P-O1P
9	C	1104	PCW	O3P-C1-C2-O2
9	C	1104	PCW	C1-O3P-P-O2P
9	C	1107	PCW	O2-C2-C3-O3
9	C	1108	PCW	C1-O3P-P-O2P
9	E	1302	PCW	O2-C2-C3-O3
9	E	1302	PCW	C1-O3P-P-O1P
9	E	1302	PCW	C1-O3P-P-O2P
9	E	1302	PCW	C4-O4P-P-O2P
9	E	1302	PCW	C4-O4P-P-O3P
9	E	1303	PCW	C4-O4P-P-O3P
11	A	1111	A1MA6	N09-C10-C11-O12
11	A	1111	A1MA6	C10-C11-C13-C14
11	A	1111	A1MA6	C10-C11-C13-CCC
11	A	1111	A1MA6	O12-C11-C13-C14
11	A	1111	A1MA6	O12-C11-C13-CCC
11	A	1111	A1MA6	C18-C19-C21-C22
11	A	1111	A1MA6	C18-C19-C21-OCA
11	A	1111	A1MA6	O20-C19-C21-OCA
11	A	1111	A1MA6	C21-C22-C23-O24
11	A	1111	A1MA6	C21-C22-C23-CC7
11	A	1111	A1MA6	O24-C25-C26-O27
11	A	1111	A1MA6	O24-C25-C26-C28
11	A	1111	A1MA6	CC4-C25-C26-O27
11	A	1111	A1MA6	CC4-C25-C26-C28
11	A	1111	A1MA6	C26-C28-C30-O31
11	A	1111	A1MA6	C26-C28-C30-C32
11	A	1111	A1MA6	O29-C28-C30-O31
11	A	1111	A1MA6	O29-C28-C30-C32
11	A	1111	A1MA6	C30-C32-C34-O35
11	A	1111	A1MA6	O33-C32-C34-O35
11	A	1111	A1MA6	O33-C32-C34-C36
11	A	1111	A1MA6	O35-C34-C36-C37
11	A	1111	A1MA6	C40-C41-C42-C43
11	A	1111	A1MA6	CC3-C41-C42-C43
11	A	1111	A1MA6	C41-C42-C43-OC2
11	A	1111	A1MA6	C58-C59-C60-C61
11	A	1111	A1MA6	OC1-C59-C60-C61
11	A	1111	A1MA6	C59-C60-C61-O62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	A	1111	A1MA6	C59-C60-C61-CBV
11	A	1111	A1MA6	C65-C66-C67-C68
11	A	1111	A1MA6	C65-C66-C67-CBT
11	A	1111	A1MA6	OBU-C66-C67-C68
11	A	1111	A1MA6	OBU-C66-C67-CBT
11	A	1111	A1MA6	C69-C70-C71-C72
11	A	1111	A1MA6	OBS-C70-C71-C72
11	A	1111	A1MA6	C71-C72-C73-C74
11	A	1111	A1MA6	C71-C72-C73-OBK
11	A	1111	A1MA6	C72-C73-C74-OBQ
11	A	1111	A1MA6	C73-C74-C75-O76
11	A	1111	A1MA6	C73-C74-C75-CBL
11	A	1111	A1MA6	OBQ-C74-C75-O76
11	A	1111	A1MA6	OBQ-C74-C75-CBL
11	A	1111	A1MA6	C78-C79-C80-OBK
11	A	1111	A1MA6	OBK-C79-C80-C81
11	A	1111	A1MA6	OBK-C79-C80-OBK
11	A	1111	A1MA6	C90-C91-C92-C93
11	A	1111	A1MA6	C90-C91-C92-OBK
11	A	1111	A1MA6	C96-C97-C98-C99
11	A	1111	A1MA6	C96-C97-C98-OBK
11	A	1111	A1MA6	C98-C99-CA0-OBK
11	A	1111	A1MA6	OBK-C99-CA0-CA1
11	A	1111	A1MA6	OBK-C99-CA0-OBK
11	A	1111	A1MA6	C99-CA0-CA1-CA2
11	A	1111	A1MA6	OBK-CA0-CA1-CA2
11	A	1111	A1MA6	OAD-CAE-CAF-CAG
11	A	1111	A1MA6	CB4-CAE-CAF-CAG
11	A	1111	A1MA6	CAG-CAH-CAI-CAJ
11	A	1111	A1MA6	CAG-CAH-CAI-OB2
11	A	1111	A1MA6	OB3-CAH-CAI-CAJ
11	A	1111	A1MA6	OB3-CAH-CAI-OB2
11	A	1111	A1MA6	OAO-CAP-CAQ-CAR
11	A	1111	A1MA6	CB0-CAP-CAQ-CAR
11	C	1111	A1MA6	N09-C10-C11-O12
11	C	1111	A1MA6	C10-C11-C13-C14
11	C	1111	A1MA6	C10-C11-C13-CCC
11	C	1111	A1MA6	O12-C11-C13-C14
11	C	1111	A1MA6	O12-C11-C13-CCC
11	C	1111	A1MA6	C18-C19-C21-C22
11	C	1111	A1MA6	C18-C19-C21-OCA
11	C	1111	A1MA6	O20-C19-C21-OCA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	C	1111	A1MA6	C21-C22-C23-O24
11	C	1111	A1MA6	C21-C22-C23-CC7
11	C	1111	A1MA6	O24-C25-C26-O27
11	C	1111	A1MA6	O24-C25-C26-C28
11	C	1111	A1MA6	CC4-C25-C26-O27
11	C	1111	A1MA6	CC4-C25-C26-C28
11	C	1111	A1MA6	C26-C28-C30-O31
11	C	1111	A1MA6	C26-C28-C30-C32
11	C	1111	A1MA6	O29-C28-C30-O31
11	C	1111	A1MA6	O29-C28-C30-C32
11	C	1111	A1MA6	C30-C32-C34-O35
11	C	1111	A1MA6	O33-C32-C34-O35
11	C	1111	A1MA6	O33-C32-C34-C36
11	C	1111	A1MA6	O35-C34-C36-C37
11	C	1111	A1MA6	C40-C41-C42-C43
11	C	1111	A1MA6	CC3-C41-C42-C43
11	C	1111	A1MA6	C41-C42-C43-OC2
11	C	1111	A1MA6	C58-C59-C60-C61
11	C	1111	A1MA6	OC1-C59-C60-C61
11	C	1111	A1MA6	C59-C60-C61-O62
11	C	1111	A1MA6	C59-C60-C61-CBV
11	C	1111	A1MA6	C65-C66-C67-C68
11	C	1111	A1MA6	C65-C66-C67-CBT
11	C	1111	A1MA6	OBU-C66-C67-C68
11	C	1111	A1MA6	OBU-C66-C67-CBT
11	C	1111	A1MA6	C69-C70-C71-C72
11	C	1111	A1MA6	OBS-C70-C71-C72
11	C	1111	A1MA6	C71-C72-C73-C74
11	C	1111	A1MA6	C71-C72-C73-OBK
11	C	1111	A1MA6	C72-C73-C74-OBQ
11	C	1111	A1MA6	C73-C74-C75-O76
11	C	1111	A1MA6	C73-C74-C75-CBL
11	C	1111	A1MA6	OBQ-C74-C75-O76
11	C	1111	A1MA6	OBQ-C74-C75-CBL
11	C	1111	A1MA6	C78-C79-C80-OBK
11	C	1111	A1MA6	OBK-C79-C80-C81
11	C	1111	A1MA6	OBK-C79-C80-OBK
11	C	1111	A1MA6	C90-C91-C92-C93
11	C	1111	A1MA6	C90-C91-C92-OBK
11	C	1111	A1MA6	C96-C97-C98-C99
11	C	1111	A1MA6	C96-C97-C98-OBK
11	C	1111	A1MA6	C98-C99-CA0-OBK

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	C	1111	A1MA6	OBG-C99-CA0-CA1
11	C	1111	A1MA6	OBG-C99-CA0-OBF
11	C	1111	A1MA6	C99-CA0-CA1-CA2
11	C	1111	A1MA6	OBF-CA0-CA1-CA2
11	C	1111	A1MA6	OAD-CAE-CAF-CAG
11	C	1111	A1MA6	CB4-CAE-CAF-CAG
11	C	1111	A1MA6	CAG-CAH-CAI-CAJ
11	C	1111	A1MA6	CAG-CAH-CAI-OB2
11	C	1111	A1MA6	OB3-CAH-CAI-CAJ
11	C	1111	A1MA6	OB3-CAH-CAI-OB2
11	C	1111	A1MA6	OAO-CAP-CAQ-CAR
11	C	1111	A1MA6	CB0-CAP-CAQ-CAR
9	A	1102	PCW	C32-C31-O2-C2
9	C	1102	PCW	C32-C31-O2-C2
9	A	1102	PCW	C12-C11-O3-C3
9	C	1102	PCW	C12-C11-O3-C3
11	A	1111	A1MA6	OBR-C73-C74-C75
11	C	1111	A1MA6	OBR-C73-C74-C75
11	A	1111	A1MA6	C98-C99-CA0-CA1
11	C	1111	A1MA6	C98-C99-CA0-CA1
9	A	1102	PCW	O31-C31-O2-C2
9	C	1102	PCW	O31-C31-O2-C2
9	A	1106	PCW	C4-C5-N-C8
9	A	1107	PCW	C4-C5-N-C8
9	A	1108	PCW	C4-C5-N-C8
9	G	1302	PCW	C4-C5-N-C8
9	G	1303	PCW	C4-C5-N-C8
9	C	1106	PCW	C4-C5-N-C8
9	C	1107	PCW	C4-C5-N-C8
9	C	1108	PCW	C4-C5-N-C8
9	E	1302	PCW	C4-C5-N-C8
9	E	1303	PCW	C4-C5-N-C8
9	A	1102	PCW	O11-C11-O3-C3
9	C	1102	PCW	O11-C11-O3-C3
9	A	1103	PCW	C11-C12-C13-C14
9	A	1103	PCW	C31-C32-C33-C34
9	A	1105	PCW	C31-C32-C33-C34
9	A	1107	PCW	C31-C32-C33-C34
9	A	1108	PCW	C11-C12-C13-C14
9	C	1103	PCW	C11-C12-C13-C14
9	C	1103	PCW	C31-C32-C33-C34
9	C	1105	PCW	C31-C32-C33-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	C	1107	PCW	C31-C32-C33-C34
9	C	1108	PCW	C11-C12-C13-C14
9	G	1303	PCW	C11-C12-C13-C14
9	E	1303	PCW	C11-C12-C13-C14
11	A	1111	A1MA6	C30-C32-C34-C36
11	C	1111	A1MA6	C30-C32-C34-C36
9	A	1106	PCW	C16-C17-C18-C19
9	C	1106	PCW	C16-C17-C18-C19
11	A	1111	A1MA6	C02-C03-C04-N05
11	C	1111	A1MA6	C02-C03-C04-N05
9	A	1102	PCW	C4-O4P-P-O3P
9	A	1103	PCW	C4-O4P-P-O3P
9	G	1302	PCW	C1-O3P-P-O4P
9	C	1102	PCW	C4-O4P-P-O3P
9	C	1103	PCW	C4-O4P-P-O3P
9	E	1302	PCW	C1-O3P-P-O4P
9	A	1106	PCW	C4-C5-N-C6
9	A	1106	PCW	C4-C5-N-C7
9	A	1107	PCW	C4-C5-N-C6
9	A	1107	PCW	C4-C5-N-C7
9	A	1108	PCW	C4-C5-N-C6
9	A	1108	PCW	C4-C5-N-C7
9	G	1302	PCW	C4-C5-N-C6
9	G	1302	PCW	C4-C5-N-C7
9	G	1303	PCW	C4-C5-N-C6
9	G	1303	PCW	C4-C5-N-C7
9	G	1304	PCW	C4-C5-N-C6
9	G	1304	PCW	C4-C5-N-C7
9	G	1304	PCW	C4-C5-N-C8
9	C	1106	PCW	C4-C5-N-C6
9	C	1106	PCW	C4-C5-N-C7
9	C	1107	PCW	C4-C5-N-C6
9	C	1107	PCW	C4-C5-N-C7
9	C	1108	PCW	C4-C5-N-C6
9	C	1108	PCW	C4-C5-N-C7
9	E	1302	PCW	C4-C5-N-C6
9	E	1302	PCW	C4-C5-N-C7
9	E	1303	PCW	C4-C5-N-C6
9	E	1303	PCW	C4-C5-N-C7
9	E	1304	PCW	C4-C5-N-C6
9	E	1304	PCW	C4-C5-N-C7
9	E	1304	PCW	C4-C5-N-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	A	1111	A1MA6	OBR-C73-C74-OBQ
11	C	1111	A1MA6	OBR-C73-C74-OBQ
9	A	1105	PCW	C34-C35-C36-C37
9	G	1304	PCW	C21-C22-C23-C24
9	E	1304	PCW	C21-C22-C23-C24
9	A	1106	PCW	C22-C23-C24-C25
9	G	1303	PCW	C13-C14-C15-C16
9	G	1304	PCW	C43-C44-C45-C46
9	C	1105	PCW	C34-C35-C36-C37
9	C	1106	PCW	C22-C23-C24-C25
9	E	1303	PCW	C13-C14-C15-C16
9	E	1304	PCW	C43-C44-C45-C46
11	A	1111	A1MA6	CAF-CAG-CAH-OB3
11	C	1111	A1MA6	CAF-CAG-CAH-OB3
9	A	1106	PCW	C43-C44-C45-C46
9	C	1106	PCW	C43-C44-C45-C46
9	G	1304	PCW	C34-C35-C36-C37
9	E	1304	PCW	C34-C35-C36-C37
9	A	1107	PCW	C42-C43-C44-C45
9	C	1107	PCW	C42-C43-C44-C45
11	A	1111	A1MA6	C52-C53-C54-C55
11	C	1111	A1MA6	C52-C53-C54-C55
9	A	1104	PCW	C44-C45-C46-C47
9	C	1104	PCW	C44-C45-C46-C47
11	A	1111	A1MA6	OCD-C10-C11-O12
11	A	1111	A1MA6	CAI-CAJ-CAK-CAL
11	A	1111	A1MA6	CAI-CAJ-CAK-OB1
11	C	1111	A1MA6	OCD-C10-C11-O12
11	C	1111	A1MA6	CAI-CAJ-CAK-CAL
11	C	1111	A1MA6	CAI-CAJ-CAK-OB1
9	A	1104	PCW	C20-C21-C22-C23
9	A	1107	PCW	C40-C41-C42-C43
9	C	1104	PCW	C20-C21-C22-C23
9	C	1107	PCW	C40-C41-C42-C43
9	A	1106	PCW	C21-C22-C23-C24
9	A	1106	PCW	C23-C24-C25-C26
9	A	1107	PCW	C35-C36-C37-C38
9	C	1106	PCW	C21-C22-C23-C24
9	C	1106	PCW	C23-C24-C25-C26
9	C	1107	PCW	C35-C36-C37-C38
11	A	1111	A1MA6	C72-C73-C74-C75
11	C	1111	A1MA6	C72-C73-C74-C75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	A	1103	PCW	C33-C34-C35-C36
9	C	1103	PCW	C33-C34-C35-C36
9	A	1105	PCW	C15-C16-C17-C18
9	C	1105	PCW	C15-C16-C17-C18
9	G	1304	PCW	C33-C34-C35-C36
9	E	1304	PCW	C33-C34-C35-C36
9	A	1107	PCW	C33-C34-C35-C36
9	C	1107	PCW	C33-C34-C35-C36
9	A	1108	PCW	C20-C21-C22-C23
9	C	1108	PCW	C20-C21-C22-C23
11	A	1111	A1MA6	C66-C67-C68-C69
11	C	1111	A1MA6	C66-C67-C68-C69
9	G	1303	PCW	C34-C35-C36-C37
9	E	1303	PCW	C34-C35-C36-C37
9	A	1105	PCW	C41-C42-C43-C44
9	C	1105	PCW	C41-C42-C43-C44
9	A	1103	PCW	C16-C17-C18-C19
9	A	1103	PCW	C40-C41-C42-C43
9	C	1103	PCW	C16-C17-C18-C19
9	C	1103	PCW	C40-C41-C42-C43
11	A	1111	A1MA6	CA4-CA5-CA6-CA7
11	C	1111	A1MA6	CA4-CA5-CA6-CA7
9	A	1103	PCW	C20-C21-C22-C23
9	A	1104	PCW	C40-C41-C42-C43
9	A	1107	PCW	C36-C37-C38-C39
9	G	1302	PCW	C40-C41-C42-C43
9	C	1103	PCW	C20-C21-C22-C23
9	C	1104	PCW	C40-C41-C42-C43
9	C	1107	PCW	C36-C37-C38-C39
9	E	1302	PCW	C40-C41-C42-C43
9	A	1108	PCW	C31-C32-C33-C34
9	C	1108	PCW	C31-C32-C33-C34
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	1304	PCW	O3P-C1-C2-C3
9	C	1104	PCW	O3P-C1-C2-C3
9	C	1106	PCW	O3P-C1-C2-C3
9	C	1107	PCW	O3P-C1-C2-C3
9	C	1108	PCW	O3P-C1-C2-C3
9	E	1304	PCW	O3P-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	A	1105	PCW	C40-C41-C42-C43
9	C	1105	PCW	C40-C41-C42-C43
9	G	1304	PCW	C11-C12-C13-C14
9	E	1304	PCW	C11-C12-C13-C14
9	A	1106	PCW	C32-C33-C34-C35
9	C	1106	PCW	C32-C33-C34-C35
9	G	1302	PCW	C35-C36-C37-C38
9	E	1302	PCW	C35-C36-C37-C38
11	A	1111	A1MA6	O46-C47-C52-C53
11	A	1111	A1MA6	C68-C69-C70-C71
11	A	1111	A1MA6	C91-C92-C93-C94
11	C	1111	A1MA6	O46-C47-C52-C53
11	C	1111	A1MA6	C68-C69-C70-C71
11	C	1111	A1MA6	C91-C92-C93-C94
9	A	1107	PCW	C14-C15-C16-C17
9	C	1107	PCW	C14-C15-C16-C17
9	A	1104	PCW	C1-C2-C3-O3
9	A	1107	PCW	C1-C2-C3-O3
9	C	1104	PCW	C1-C2-C3-O3
9	C	1107	PCW	C1-C2-C3-O3
9	G	1302	PCW	C43-C44-C45-C46
9	E	1302	PCW	C43-C44-C45-C46
9	G	1303	PCW	C31-C32-C33-C34
9	E	1303	PCW	C31-C32-C33-C34
9	A	1106	PCW	C14-C15-C16-C17
9	C	1106	PCW	C14-C15-C16-C17
9	G	1304	PCW	C16-C17-C18-C19
9	E	1304	PCW	C16-C17-C18-C19
11	A	1111	A1MA6	C36-C37-C38-C39
11	C	1111	A1MA6	C36-C37-C38-C39
9	A	1104	PCW	C14-C15-C16-C17
9	C	1104	PCW	C14-C15-C16-C17
11	A	1111	A1MA6	CAF-CAG-CAH-CAI
11	C	1111	A1MA6	CAF-CAG-CAH-CAI
9	G	1304	PCW	C31-C32-C33-C34
9	E	1304	PCW	C31-C32-C33-C34
9	A	1106	PCW	O2-C2-C3-O3
9	G	1303	PCW	O2-C2-C3-O3
9	C	1106	PCW	O2-C2-C3-O3
9	E	1303	PCW	O2-C2-C3-O3
11	A	1111	A1MA6	C54-C55-C56-C57
11	C	1111	A1MA6	C54-C55-C56-C57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	A	1111	A1MA6	CCB-C18-C19-C21
11	C	1111	A1MA6	CCB-C18-C19-C21
9	G	1303	PCW	C23-C24-C25-C26
9	E	1303	PCW	C23-C24-C25-C26
9	A	1108	PCW	C25-C26-C27-C28
9	C	1108	PCW	C25-C26-C27-C28
9	A	1102	PCW	C1-C2-C3-O3
9	A	1106	PCW	C1-C2-C3-O3
9	A	1108	PCW	C1-C2-C3-O3
9	C	1102	PCW	C1-C2-C3-O3
9	C	1106	PCW	C1-C2-C3-O3
9	C	1108	PCW	C1-C2-C3-O3
11	A	1111	A1MA6	C17-C18-C19-C21
11	C	1111	A1MA6	C17-C18-C19-C21
9	A	1108	PCW	C1-O3P-P-O4P
9	C	1108	PCW	C1-O3P-P-O4P
9	A	1106	PCW	O3P-C1-C2-O2
9	A	1108	PCW	O3P-C1-C2-O2
9	C	1106	PCW	O3P-C1-C2-O2
9	C	1108	PCW	O3P-C1-C2-O2
9	A	1102	PCW	O2-C2-C3-O3
9	A	1104	PCW	O2-C2-C3-O3
9	C	1102	PCW	O2-C2-C3-O3
9	C	1104	PCW	O2-C2-C3-O3
9	A	1105	PCW	C43-C44-C45-C46
9	G	1303	PCW	C35-C36-C37-C38
9	C	1105	PCW	C43-C44-C45-C46
9	E	1303	PCW	C35-C36-C37-C38
9	A	1108	PCW	C45-C46-C47-C48
9	C	1108	PCW	C45-C46-C47-C48
9	A	1108	PCW	C15-C16-C17-C18
9	C	1108	PCW	C15-C16-C17-C18
9	A	1103	PCW	C1-C2-C3-O3
9	G	1302	PCW	C1-C2-C3-O3
9	C	1103	PCW	C1-C2-C3-O3
9	E	1302	PCW	C1-C2-C3-O3
9	G	1303	PCW	O3P-C1-C2-O2
9	E	1303	PCW	O3P-C1-C2-O2
11	A	1111	A1MA6	C11-C13-C14-C15
11	C	1111	A1MA6	C11-C13-C14-C15
9	A	1106	PCW	C15-C16-C17-C18
9	C	1106	PCW	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	A	1103	PCW	O2-C2-C3-O3
9	C	1103	PCW	O2-C2-C3-O3
11	A	1111	A1MA6	C56-C57-C58-C59
11	C	1111	A1MA6	C56-C57-C58-C59
11	A	1111	A1MA6	OB2-CAI-CAJ-CAK
11	C	1111	A1MA6	OB2-CAI-CAJ-CAK
11	A	1111	A1MA6	OBB-CA9-CAA-CBA
11	C	1111	A1MA6	OBB-CA9-CAA-CBA
11	A	1111	A1MA6	C55-C56-C57-C58
11	C	1111	A1MA6	C55-C56-C57-C58
11	A	1111	A1MA6	C32-C34-C36-C37
11	A	1111	A1MA6	C48-C47-C52-C53
11	C	1111	A1MA6	C32-C34-C36-C37
11	C	1111	A1MA6	C48-C47-C52-C53
9	A	1104	PCW	C1-O3P-P-O4P
9	C	1104	PCW	C1-O3P-P-O4P
11	A	1111	A1MA6	CA6-CA7-CA8-CA9
11	C	1111	A1MA6	CA6-CA7-CA8-CA9
9	G	1303	PCW	C4-O4P-P-O1P
9	E	1303	PCW	C4-O4P-P-O1P
9	G	1303	PCW	O3P-C1-C2-C3
9	E	1303	PCW	O3P-C1-C2-C3
11	A	1111	A1MA6	C68-C69-C70-OBS
11	A	1111	A1MA6	OBI-C92-C93-C94
11	C	1111	A1MA6	C68-C69-C70-OBS
11	C	1111	A1MA6	OBI-C92-C93-C94
9	C	1105	PCW	C32-C33-C34-C35
11	A	1111	A1MA6	C78-C79-C80-C81
11	C	1111	A1MA6	C78-C79-C80-C81
9	A	1105	PCW	C32-C33-C34-C35
9	A	1107	PCW	O3P-C1-C2-O2
9	C	1107	PCW	O3P-C1-C2-O2
9	G	1303	PCW	O2-C31-C32-C33
9	E	1303	PCW	O2-C31-C32-C33
9	A	1102	PCW	O4P-C4-C5-N
9	A	1104	PCW	O4P-C4-C5-N
9	A	1105	PCW	O4P-C4-C5-N
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	G	1302	PCW	O4P-C4-C5-N
9	G	1303	PCW	O4P-C4-C5-N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	G	1304	PCW	O4P-C4-C5-N
9	C	1102	PCW	O4P-C4-C5-N
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	1302	PCW	O4P-C4-C5-N
9	E	1303	PCW	O4P-C4-C5-N
9	E	1304	PCW	O4P-C4-C5-N
9	A	1108	PCW	O2-C2-C3-O3
9	C	1108	PCW	O2-C2-C3-O3
9	A	1105	PCW	C14-C15-C16-C17
9	C	1105	PCW	C14-C15-C16-C17
11	A	1111	A1MA6	CA0-CA1-CA2-CA3
11	C	1111	A1MA6	CA0-CA1-CA2-CA3
11	A	1111	A1MA6	CCC-C13-C14-C15
11	C	1111	A1MA6	CCC-C13-C14-C15
9	A	1103	PCW	C35-C36-C37-C38
9	C	1103	PCW	C35-C36-C37-C38
9	A	1108	PCW	C39-C40-C41-C42
9	C	1108	PCW	C39-C40-C41-C42
11	A	1111	A1MA6	CBT-C67-C68-C69
11	C	1111	A1MA6	CBT-C67-C68-C69
9	G	1304	PCW	O3P-C1-C2-O2
9	E	1304	PCW	O3P-C1-C2-O2
9	A	1103	PCW	C1-O3P-P-O4P
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	1108	PCW	C4-O4P-P-O3P
9	C	1103	PCW	C1-O3P-P-O4P
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	1107	PCW	C4-O4P-P-O3P
9	C	1108	PCW	C4-O4P-P-O3P
9	A	1106	PCW	C41-C42-C43-C44
9	C	1106	PCW	C41-C42-C43-C44
9	G	1303	PCW	C1-C2-C3-O3
9	E	1303	PCW	C1-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	A	1106	PCW	C42-C43-C44-C45
9	C	1106	PCW	C42-C43-C44-C45
9	A	1104	PCW	C17-C18-C19-C20
9	A	1108	PCW	C19-C20-C21-C22
9	C	1104	PCW	C17-C18-C19-C20
9	C	1108	PCW	C19-C20-C21-C22
9	G	1304	PCW	C20-C21-C22-C23
9	E	1304	PCW	C20-C21-C22-C23
9	A	1108	PCW	C41-C42-C43-C44
9	C	1108	PCW	C41-C42-C43-C44
9	A	1105	PCW	O2-C2-C3-O3
9	C	1105	PCW	O2-C2-C3-O3
11	A	1111	A1MA6	C37-C38-C39-C40
11	C	1111	A1MA6	C37-C38-C39-C40
9	A	1103	PCW	C2-C1-O3P-P
9	C	1103	PCW	C2-C1-O3P-P
9	G	1302	PCW	C17-C18-C19-C20
9	E	1302	PCW	C17-C18-C19-C20
9	A	1108	PCW	C43-C44-C45-C46
9	C	1108	PCW	C43-C44-C45-C46
9	A	1106	PCW	C19-C20-C21-C22
9	C	1106	PCW	C19-C20-C21-C22
9	G	1302	PCW	C36-C37-C38-C39
9	G	1303	PCW	C36-C37-C38-C39
9	E	1302	PCW	C36-C37-C38-C39
9	E	1303	PCW	C36-C37-C38-C39
9	G	1302	PCW	C41-C42-C43-C44
9	E	1302	PCW	C41-C42-C43-C44
11	A	1111	A1MA6	CA2-CA3-CA4-CA5
11	C	1111	A1MA6	CA2-CA3-CA4-CA5
9	A	1105	PCW	C1-C2-C3-O3
9	C	1105	PCW	C1-C2-C3-O3
9	A	1105	PCW	C39-C40-C41-C42
9	C	1105	PCW	C39-C40-C41-C42
9	A	1103	PCW	O3P-C1-C2-O2
9	C	1103	PCW	O3P-C1-C2-O2
9	A	1103	PCW	O3P-C1-C2-C3
9	C	1103	PCW	O3P-C1-C2-C3
9	A	1104	PCW	C22-C23-C24-C25
9	C	1104	PCW	C22-C23-C24-C25
9	A	1104	PCW	C36-C37-C38-C39
9	C	1104	PCW	C36-C37-C38-C39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	A	1108	PCW	O2-C31-C32-C33
9	C	1108	PCW	O2-C31-C32-C33
9	A	1104	PCW	O2-C31-C32-C33
9	C	1104	PCW	O2-C31-C32-C33
9	A	1103	PCW	C19-C20-C21-C22
9	G	1303	PCW	C17-C18-C19-C20
9	G	1303	PCW	C19-C20-C21-C22
9	C	1103	PCW	C19-C20-C21-C22
9	E	1303	PCW	C17-C18-C19-C20
9	E	1303	PCW	C19-C20-C21-C22
9	A	1103	PCW	O2-C31-C32-C33
9	C	1103	PCW	O2-C31-C32-C33
9	G	1304	PCW	C19-C20-C21-C22
9	G	1304	PCW	C37-C38-C39-C40
9	E	1304	PCW	C19-C20-C21-C22
9	E	1304	PCW	C37-C38-C39-C40
9	G	1303	PCW	C20-C21-C22-C23
9	E	1303	PCW	C20-C21-C22-C23
8	B	501	CLR	C23-C24-C25-C27
8	D	501	CLR	C23-C24-C25-C27
9	G	1303	PCW	C32-C33-C34-C35
9	E	1303	PCW	C32-C33-C34-C35
9	A	1103	PCW	C37-C38-C39-C40
9	A	1104	PCW	C37-C38-C39-C40
9	A	1107	PCW	C19-C20-C21-C22
9	C	1103	PCW	C37-C38-C39-C40
9	C	1104	PCW	C37-C38-C39-C40
9	C	1107	PCW	C19-C20-C21-C22
9	A	1107	PCW	O2-C31-C32-C33
9	C	1107	PCW	O2-C31-C32-C33
9	A	1103	PCW	O31-C31-C32-C33
9	C	1103	PCW	O31-C31-C32-C33
9	A	1106	PCW	C37-C38-C39-C40
9	C	1106	PCW	C37-C38-C39-C40
9	A	1108	PCW	O31-C31-C32-C33
9	C	1108	PCW	O31-C31-C32-C33
9	A	1104	PCW	O31-C31-C32-C33
9	C	1104	PCW	O31-C31-C32-C33
9	A	1103	PCW	C1-O3P-P-O2P
9	A	1106	PCW	C4-O4P-P-O2P
9	A	1107	PCW	C4-O4P-P-O2P
9	A	1108	PCW	C4-O4P-P-O2P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	G	1304	PCW	C1-O3P-P-O2P
9	C	1103	PCW	C1-O3P-P-O2P
9	C	1106	PCW	C4-O4P-P-O2P
9	C	1107	PCW	C4-O4P-P-O2P
9	C	1108	PCW	C4-O4P-P-O2P
9	E	1304	PCW	C1-O3P-P-O2P
11	A	1111	A1MA6	O20-C19-C21-C22
11	A	1111	A1MA6	C41-C42-C43-C44
11	C	1111	A1MA6	O20-C19-C21-C22
11	C	1111	A1MA6	C41-C42-C43-C44
9	G	1302	PCW	C5-C4-O4P-P
9	E	1302	PCW	C5-C4-O4P-P
9	A	1105	PCW	O3-C11-C12-C13
9	C	1105	PCW	O3-C11-C12-C13
9	G	1304	PCW	C32-C33-C34-C35
9	E	1304	PCW	C32-C33-C34-C35

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	C	1111	A1MA6	C75-C77-CBL-CBM-CBO-O76
11	A	1111	A1MA6	C75-C77-CBL-CBM-CBO-O76

27 monomers are involved in 103 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1105	PCW	5	0
8	B	501	CLR	1	0
8	E	1301	CLR	3	0
8	A	1101	CLR	5	0
8	C	1101	CLR	4	0
9	G	1302	PCW	2	0
9	G	1303	PCW	4	0
9	A	1108	PCW	3	0
9	A	1104	PCW	4	0
9	C	1105	PCW	8	0
8	G	1301	CLR	7	0
9	E	1302	PCW	2	0
9	A	1103	PCW	12	0
9	C	1103	PCW	10	0
9	E	1303	PCW	5	0
11	C	1111	A1MA6	4	0

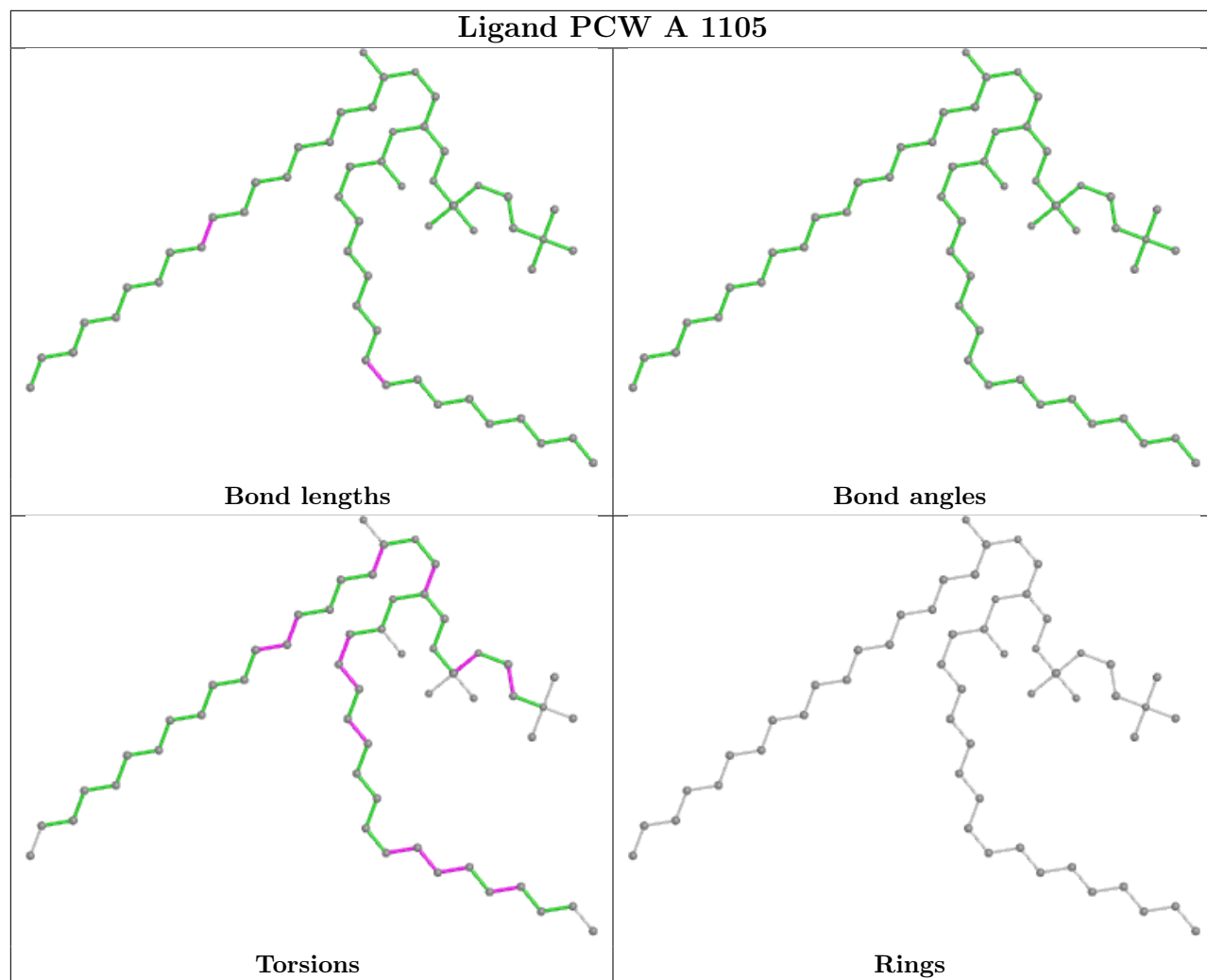
Continued on next page...

Continued from previous page...

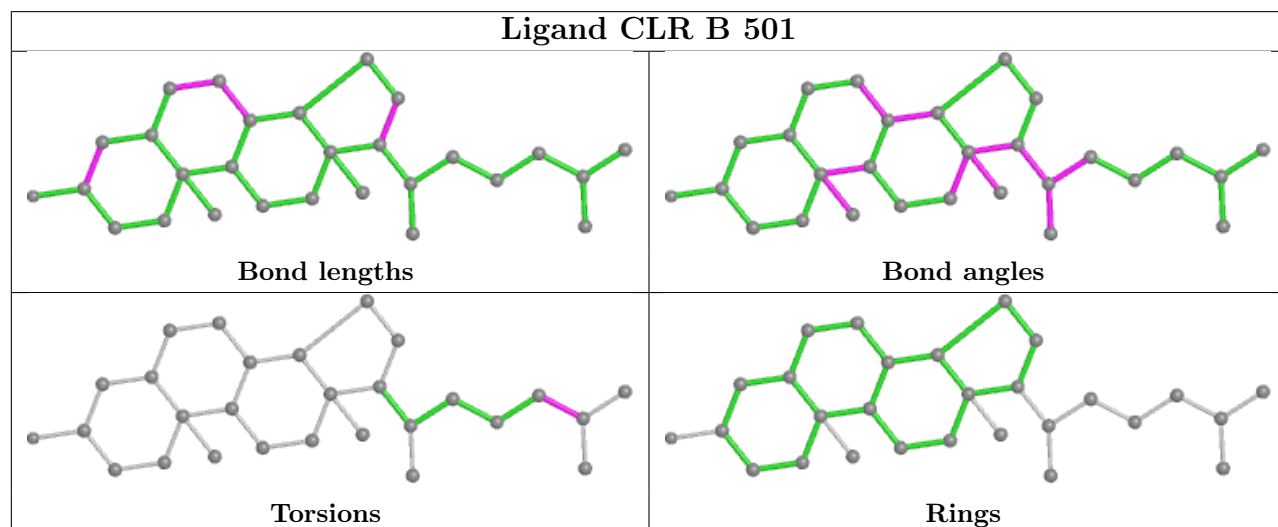
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	1108	PCW	5	0
11	A	1111	A1MA6	4	0
9	C	1104	PCW	4	0
9	E	1304	PCW	19	0
8	B	502	CLR	1	0
9	C	1106	PCW	1	0
8	D	501	CLR	2	0
9	A	1107	PCW	3	0
9	C	1107	PCW	3	0
9	A	1106	PCW	1	0
9	G	1304	PCW	14	0

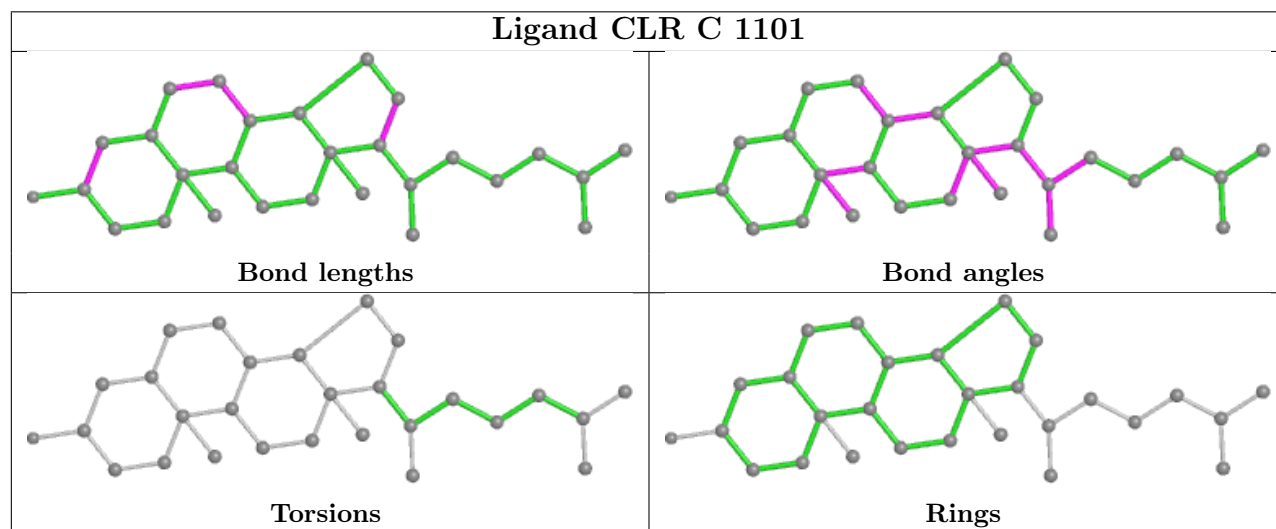
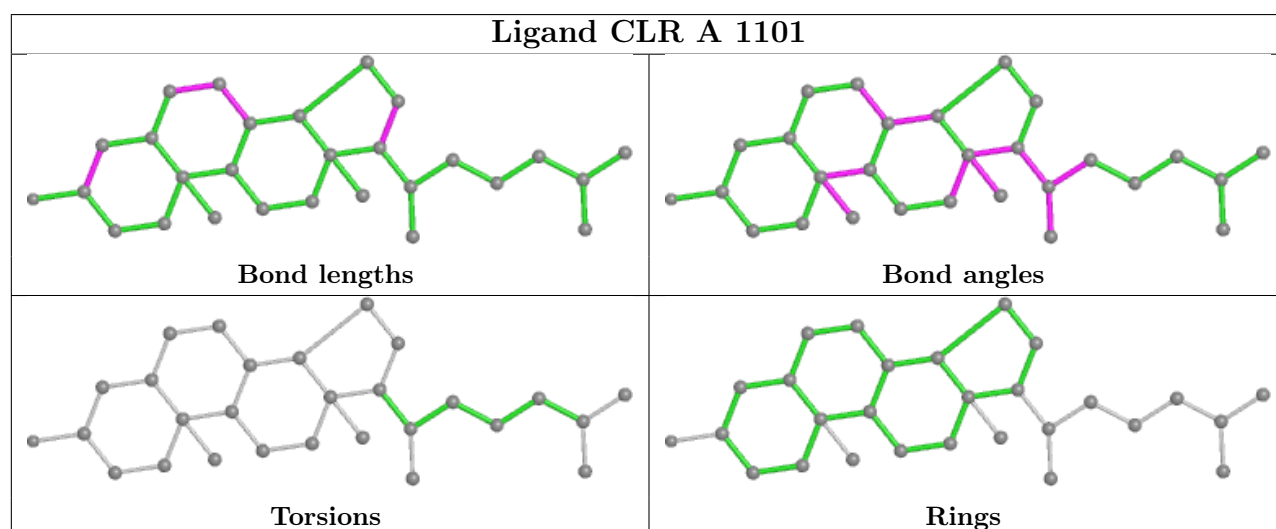
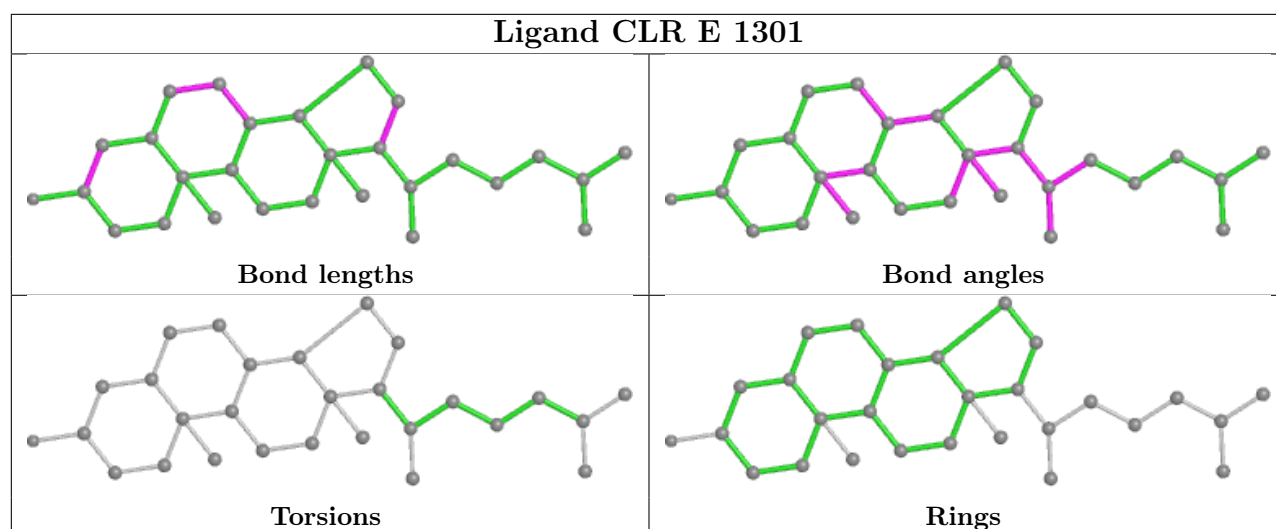
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

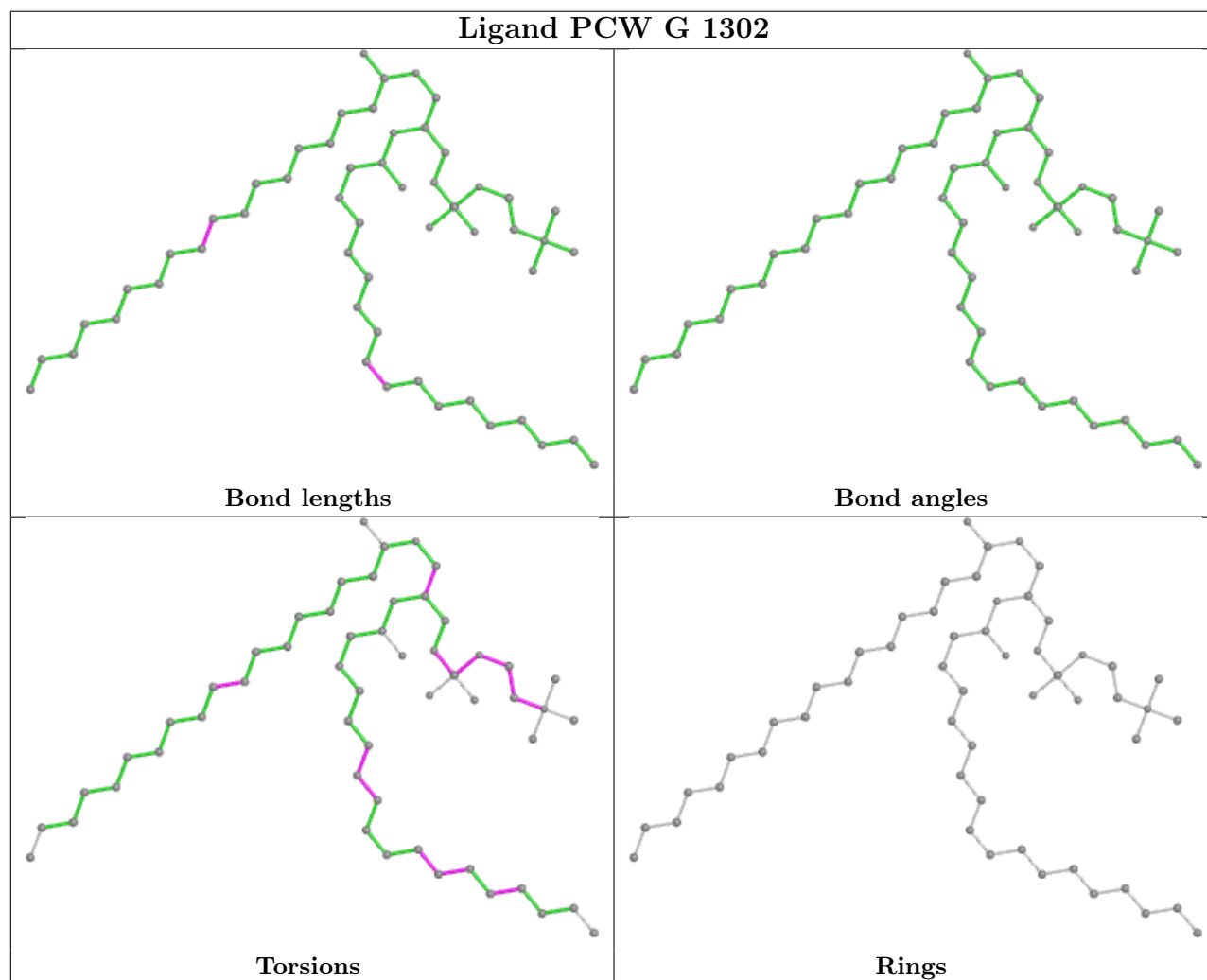
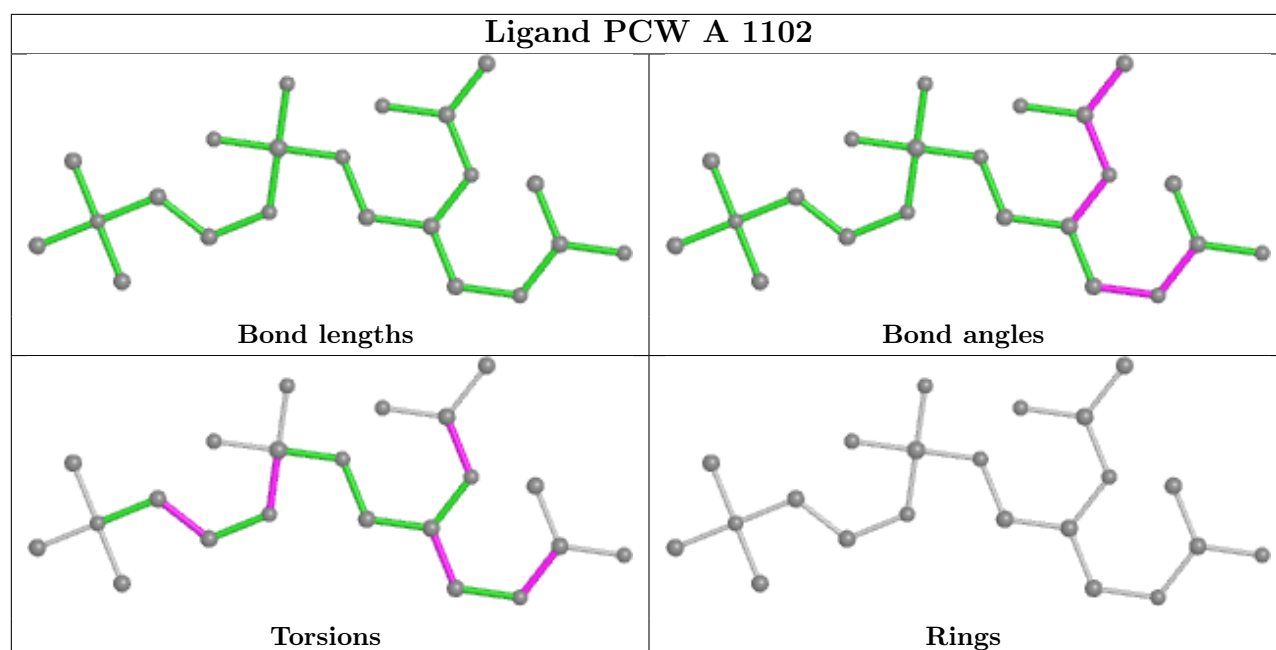
Ligand PCW A 1105

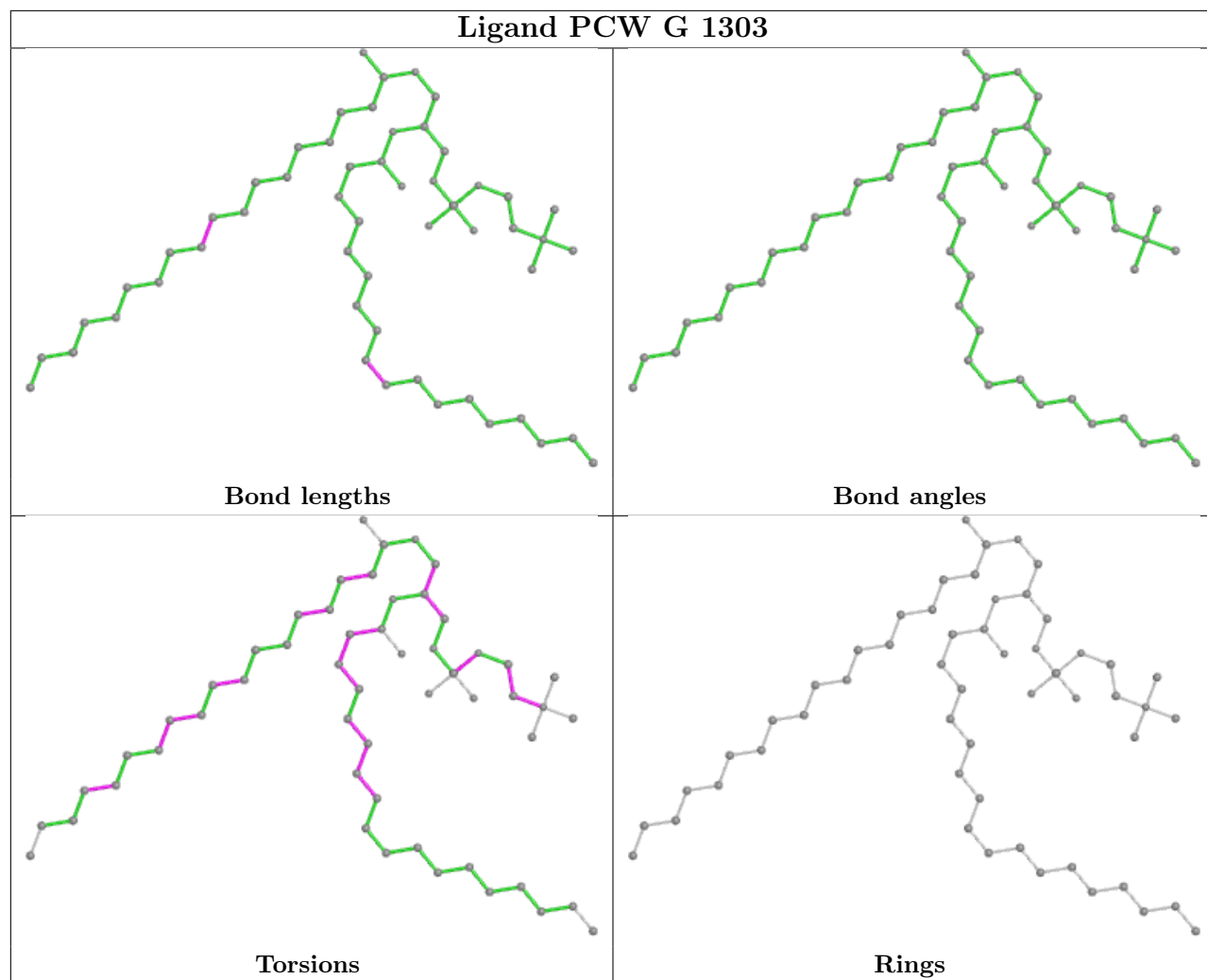


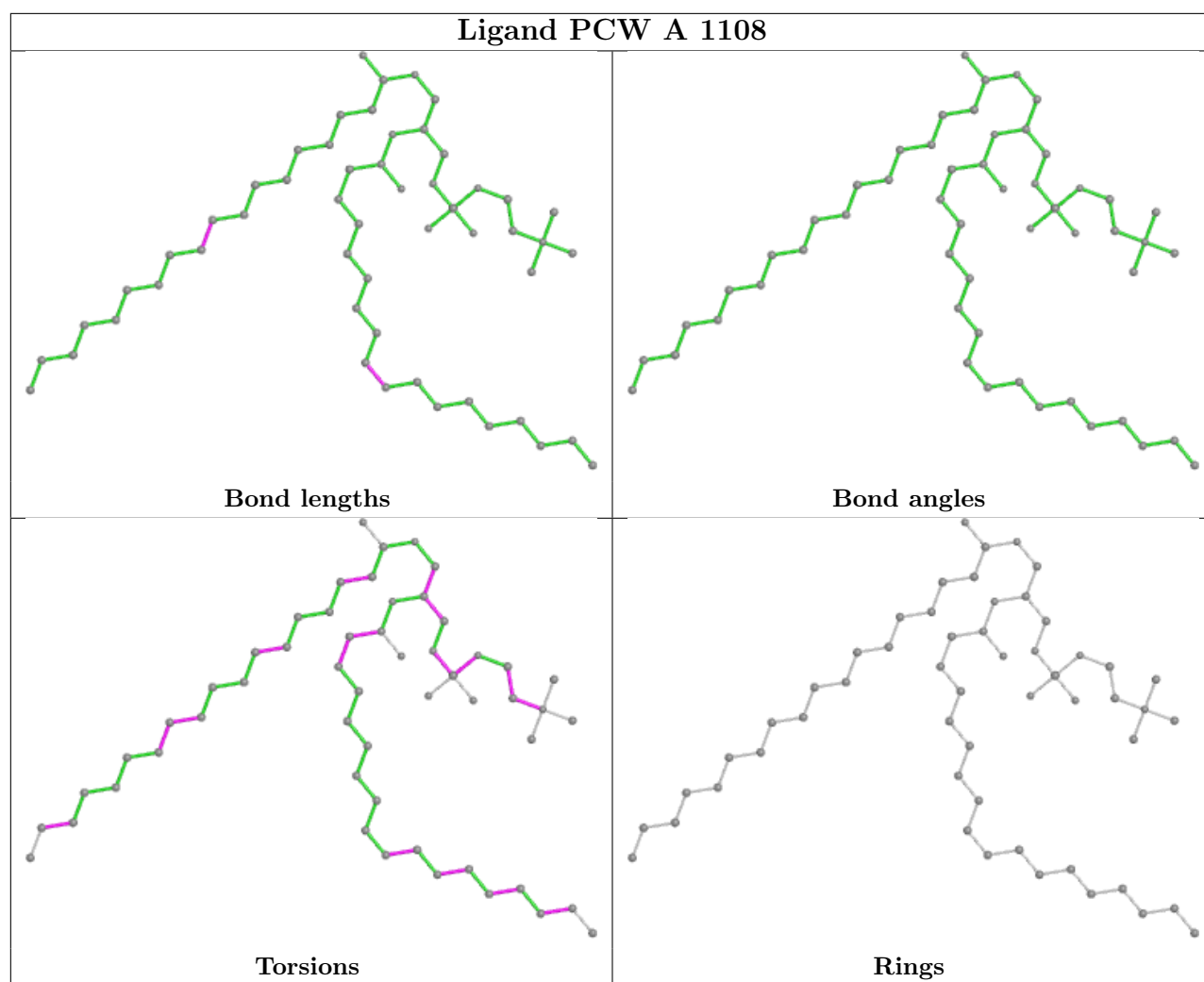
Ligand CLR B 501

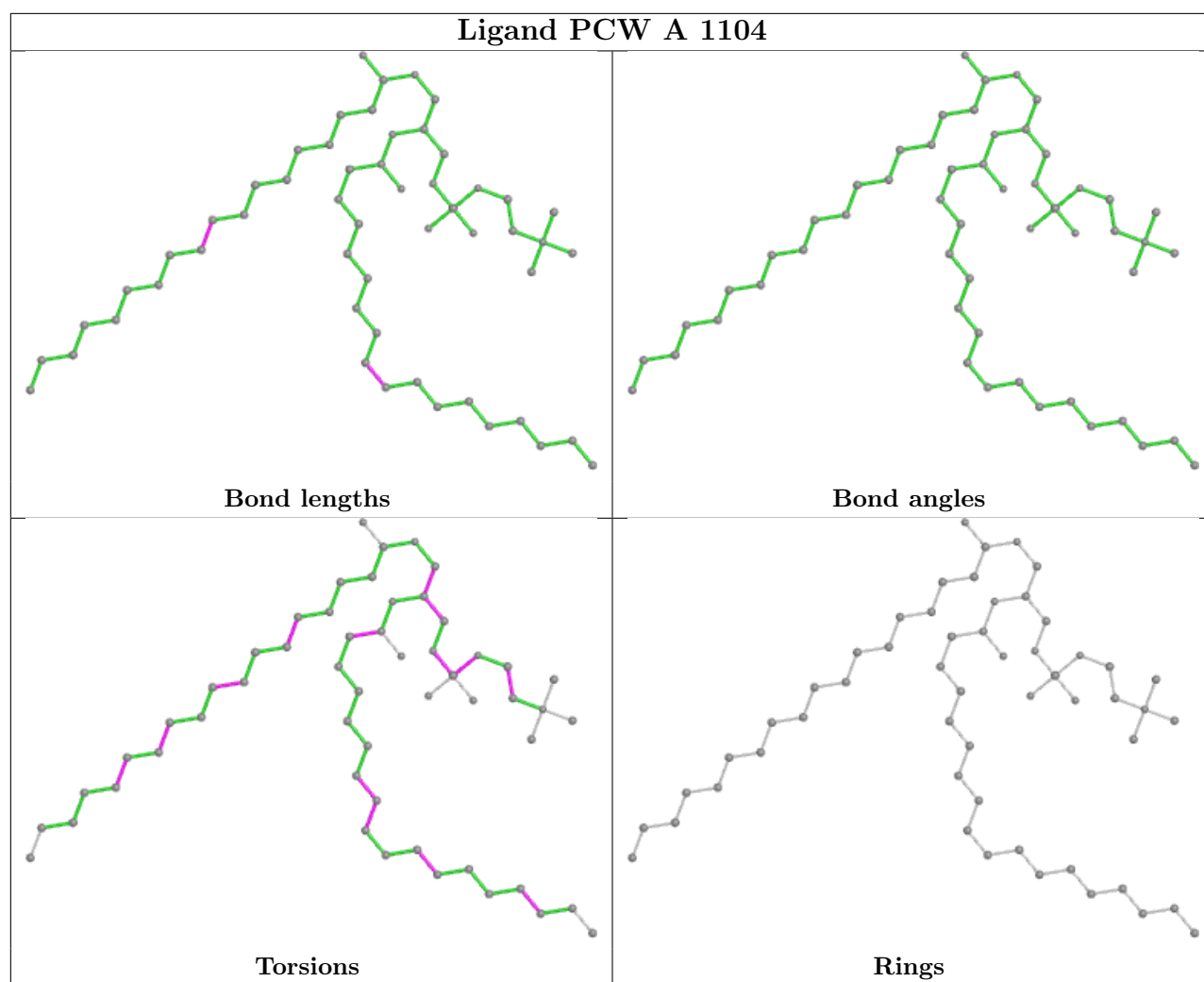


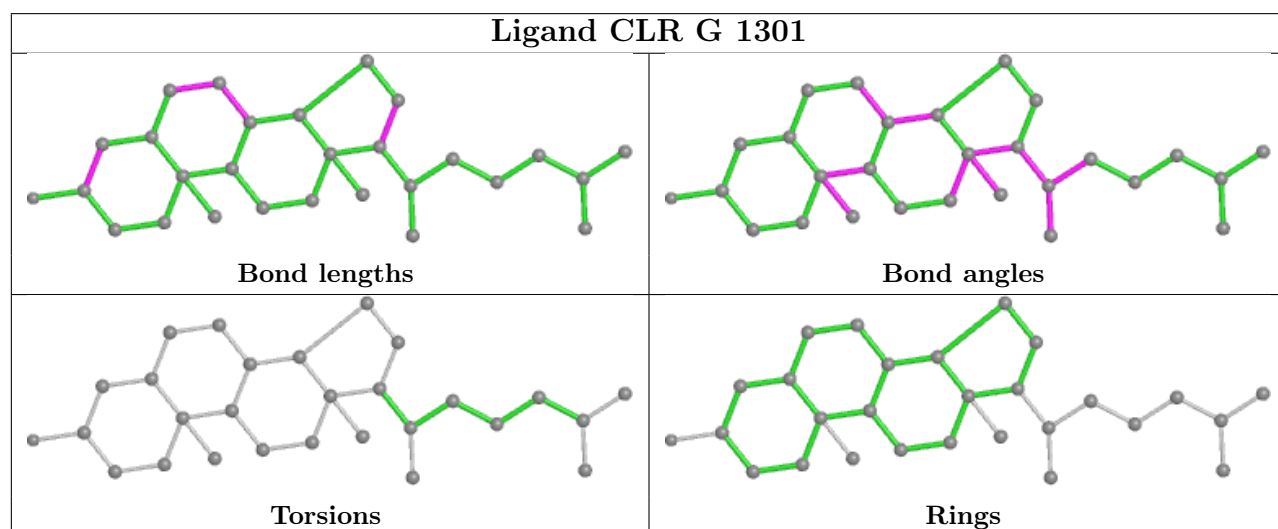
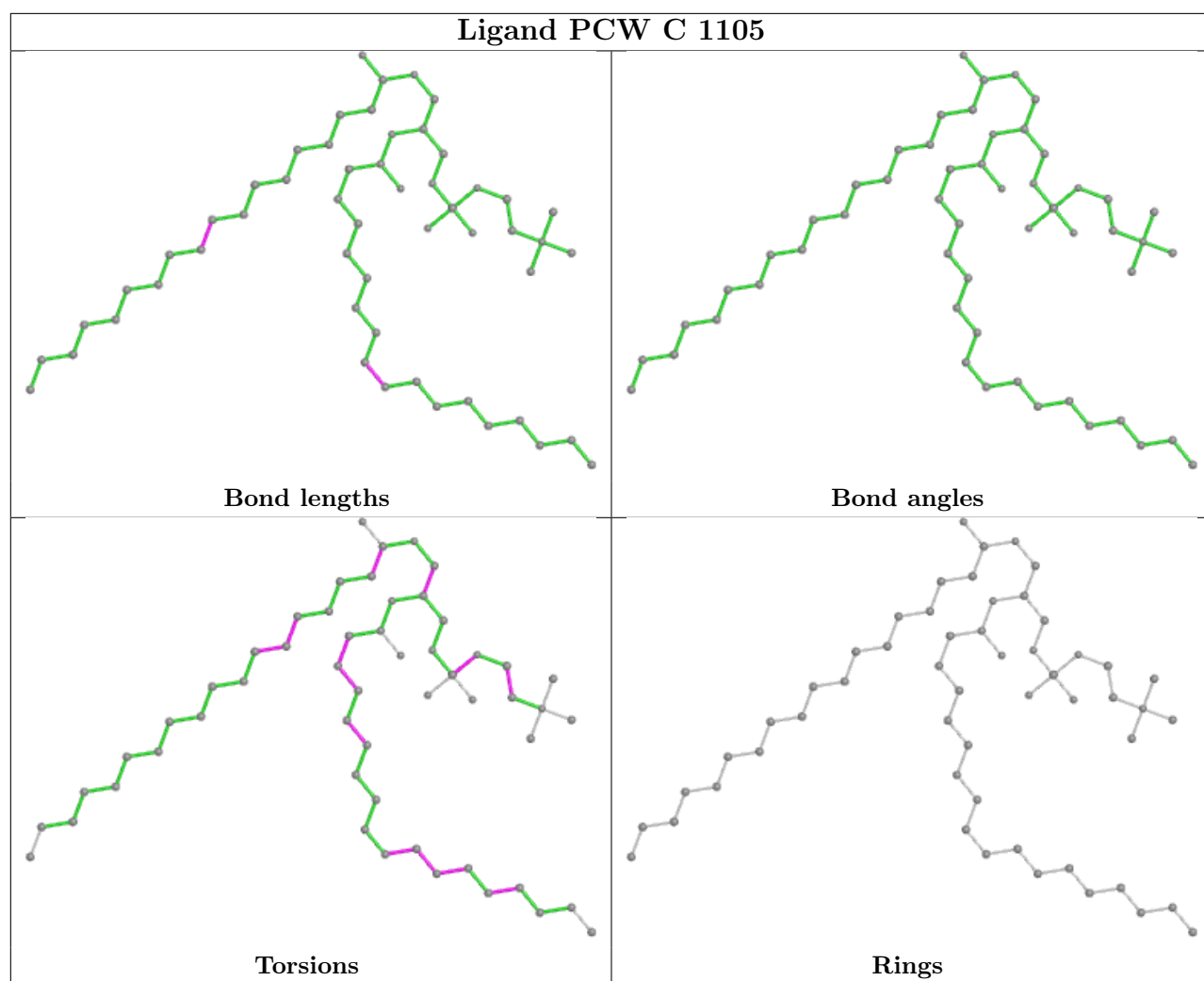


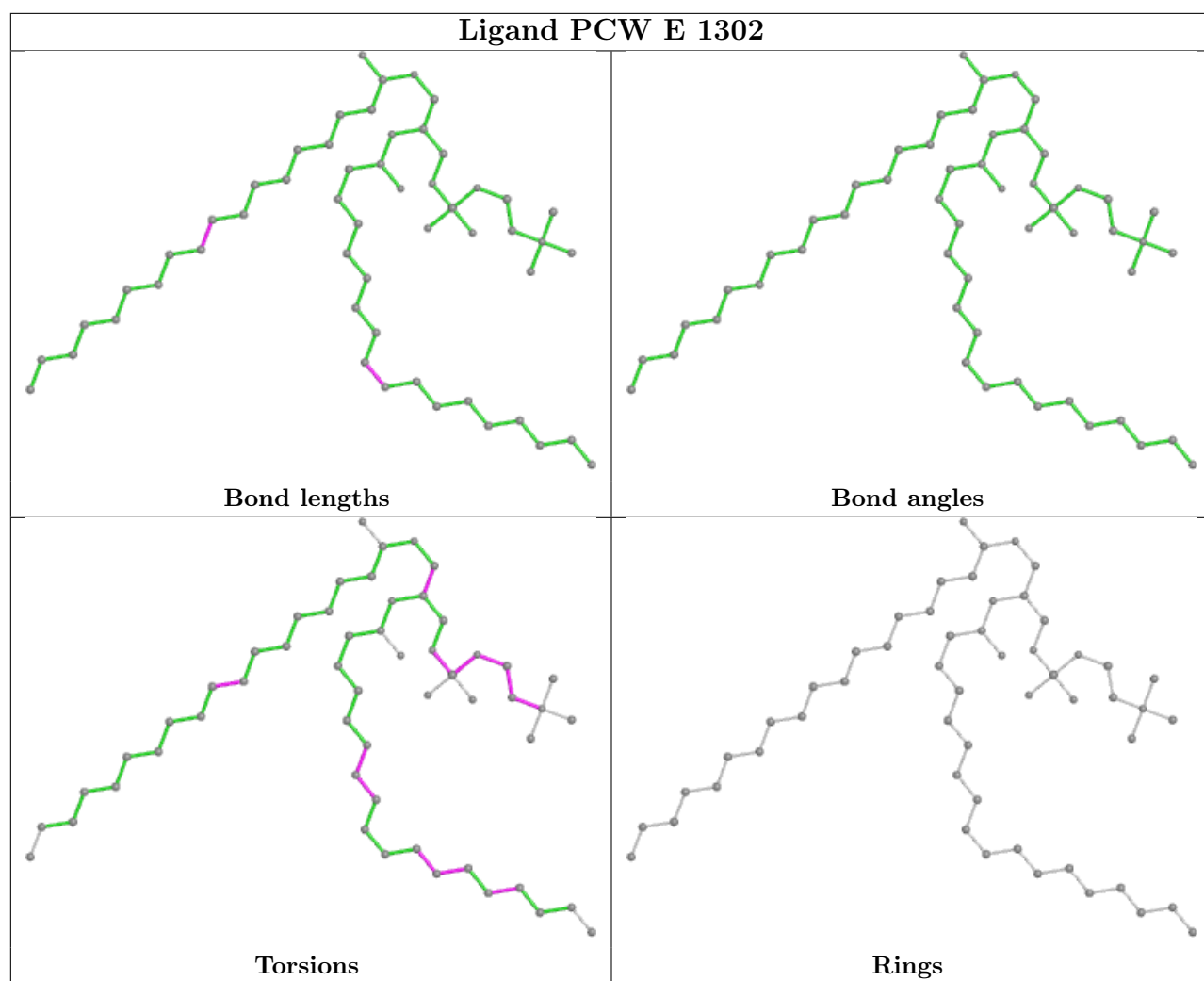


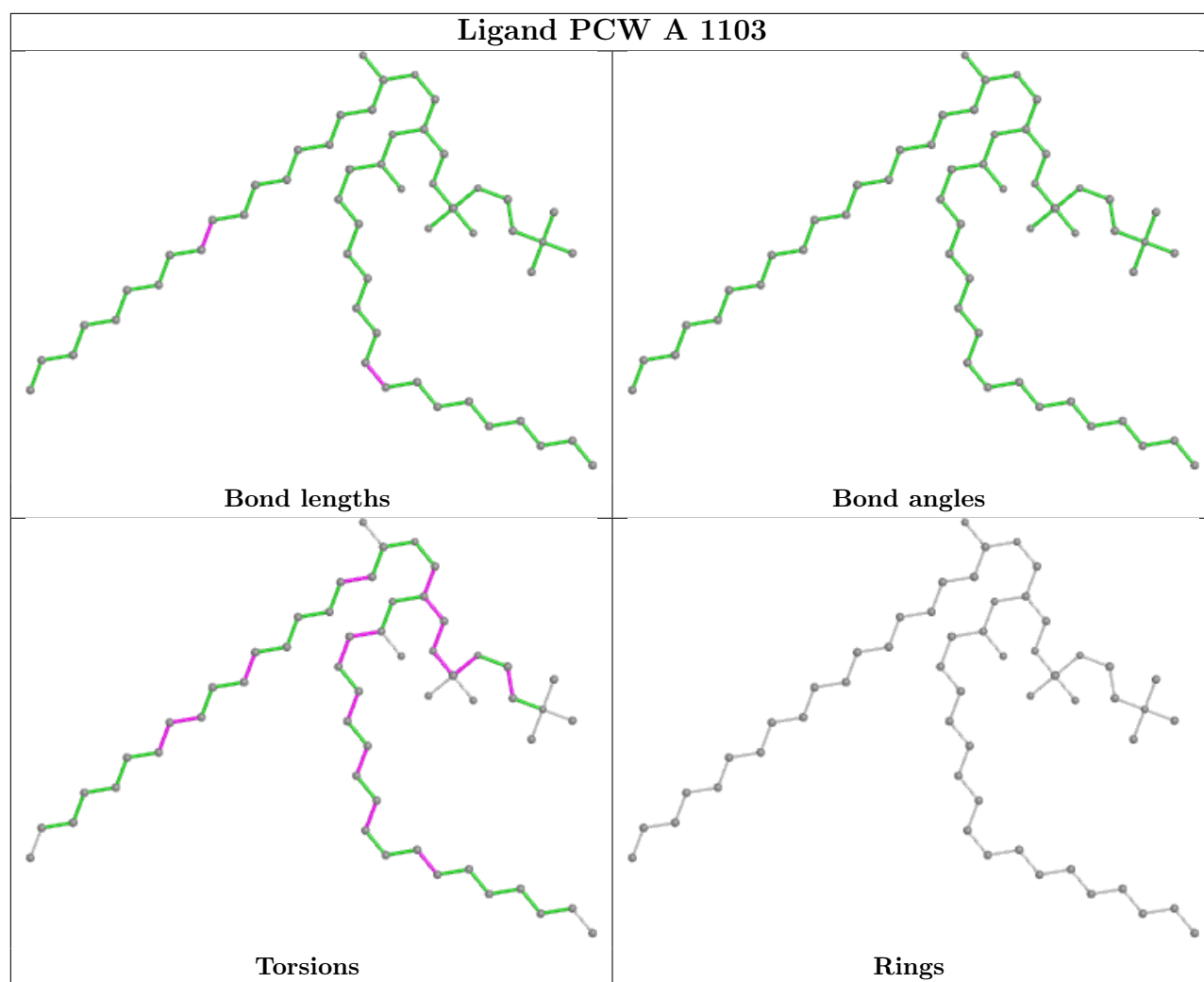




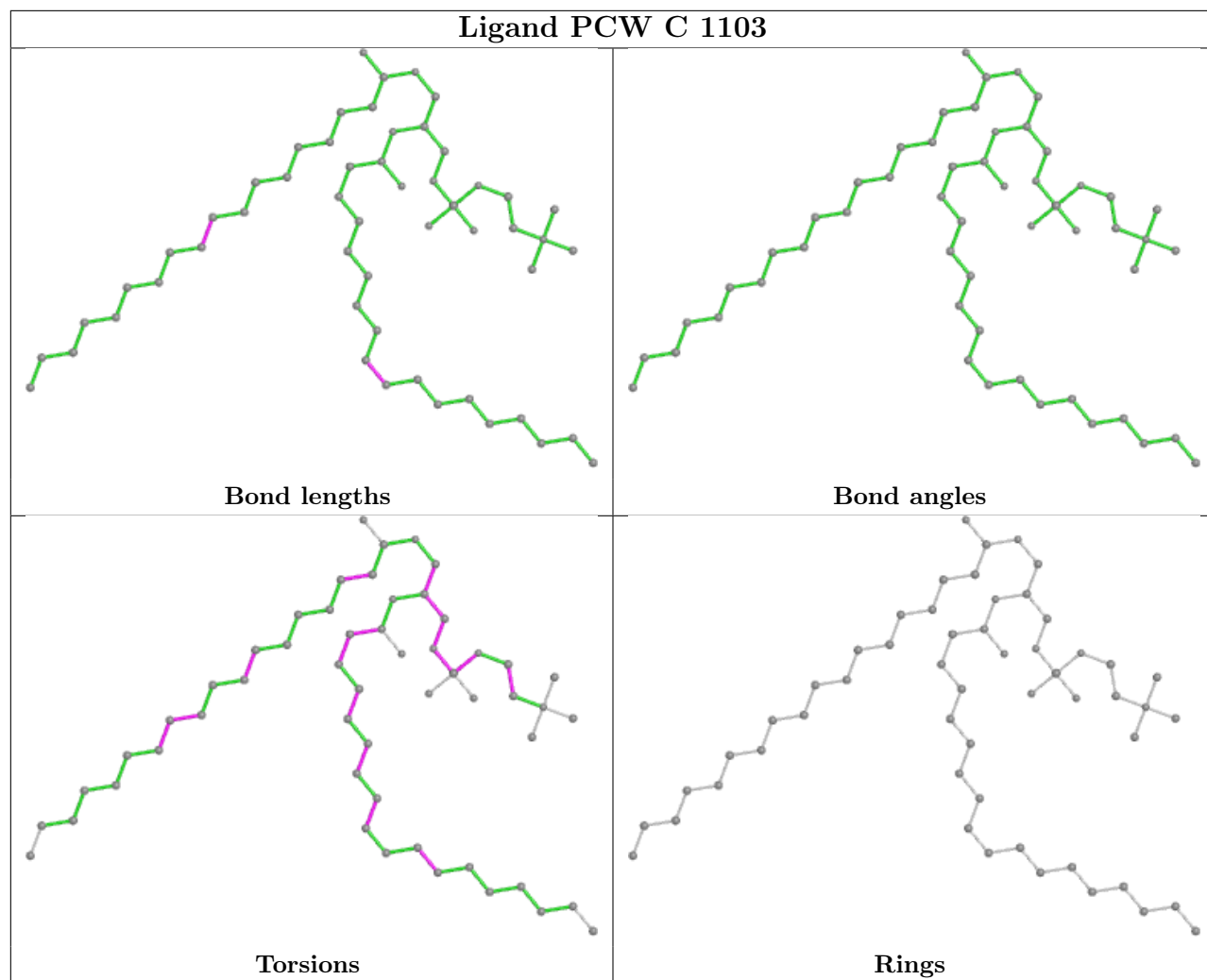




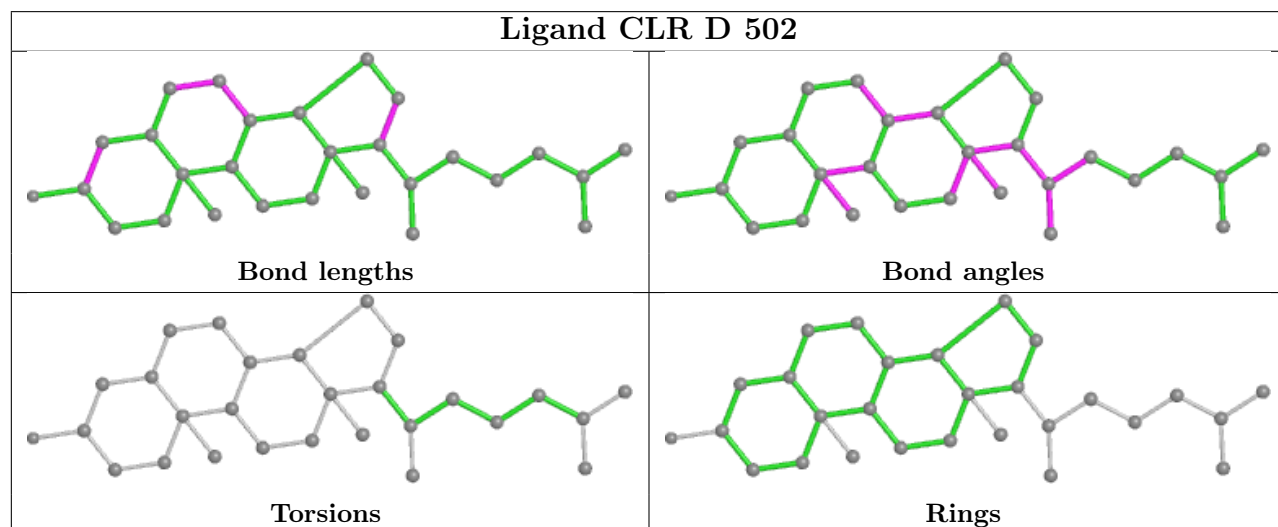


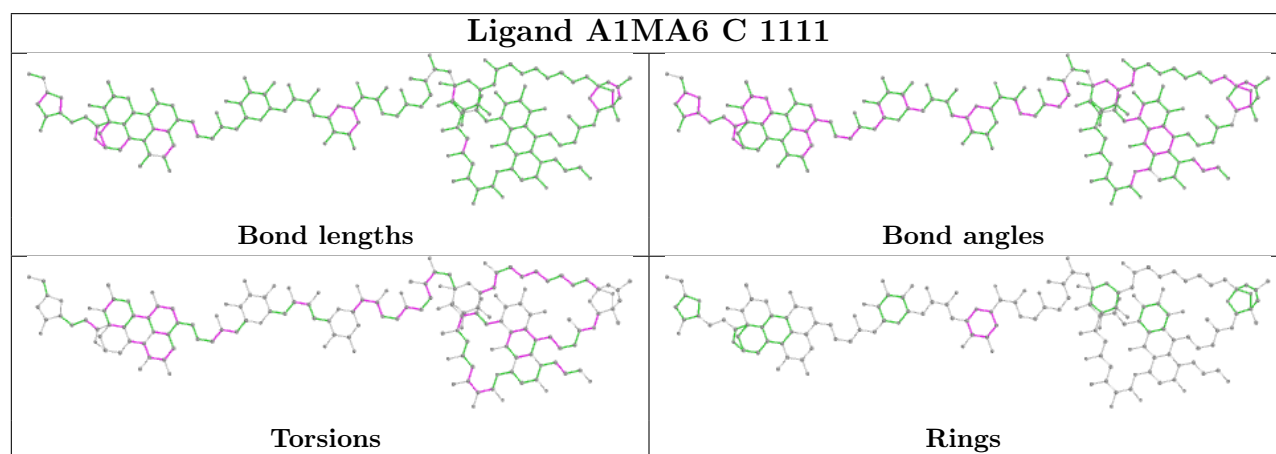
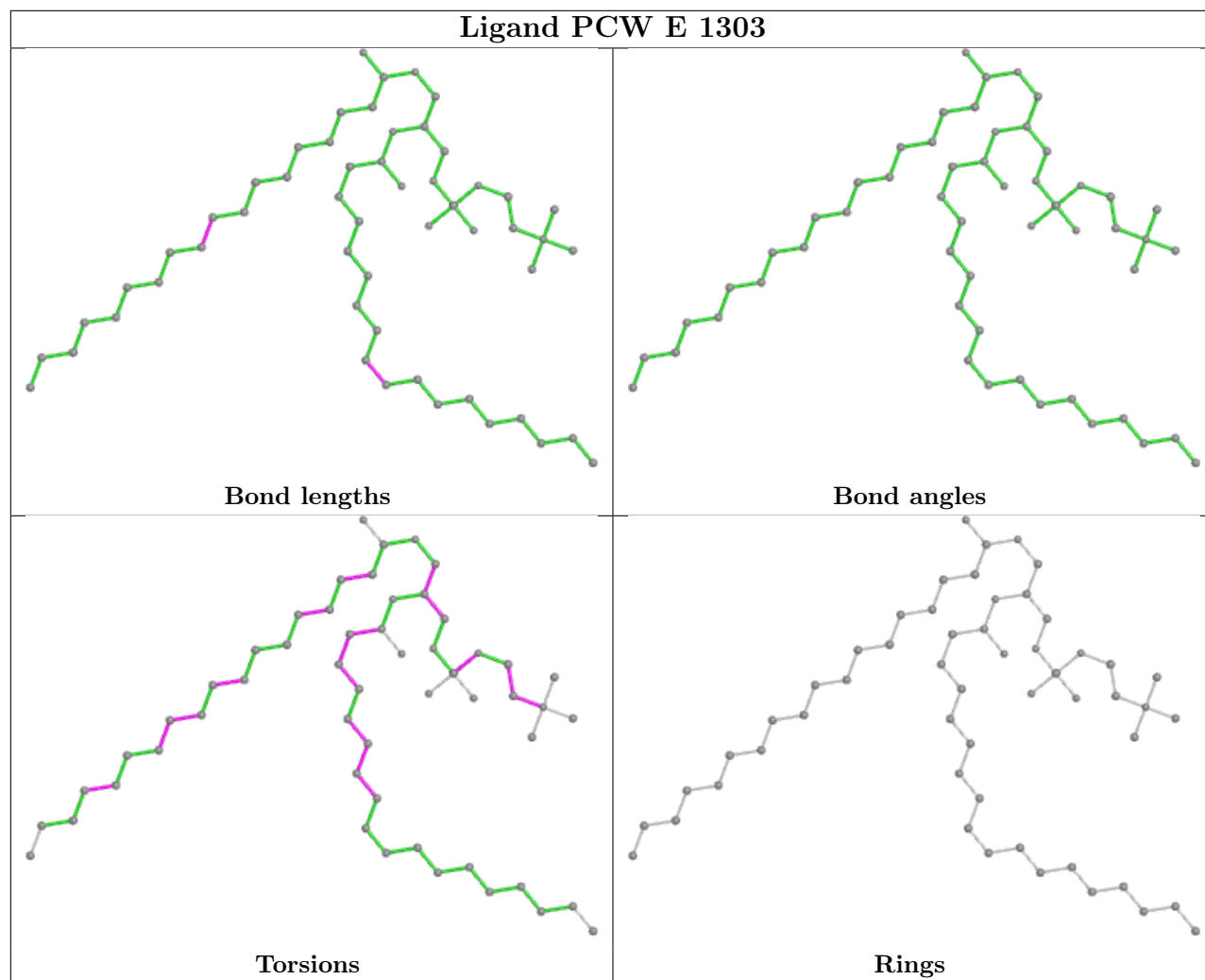


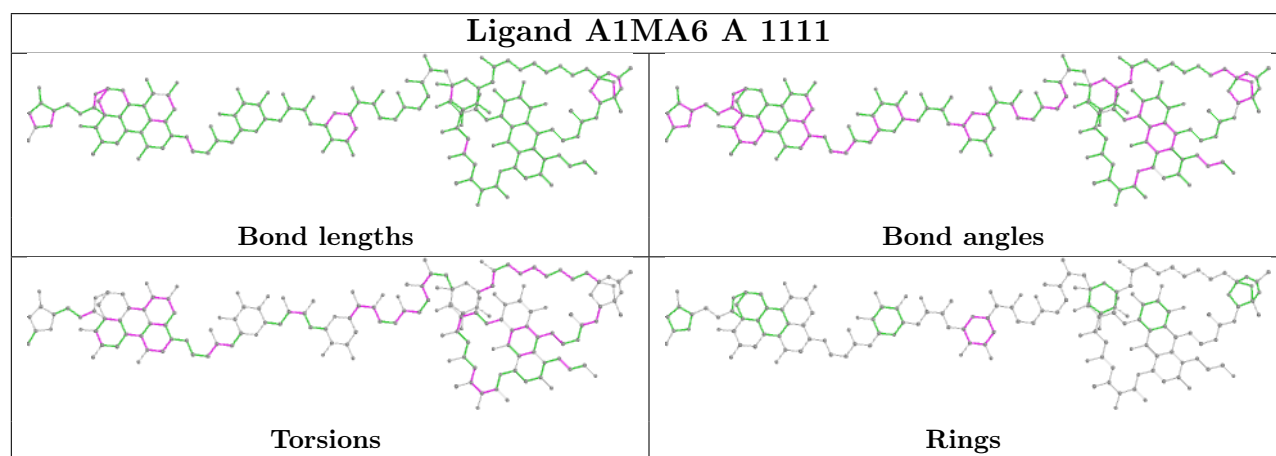
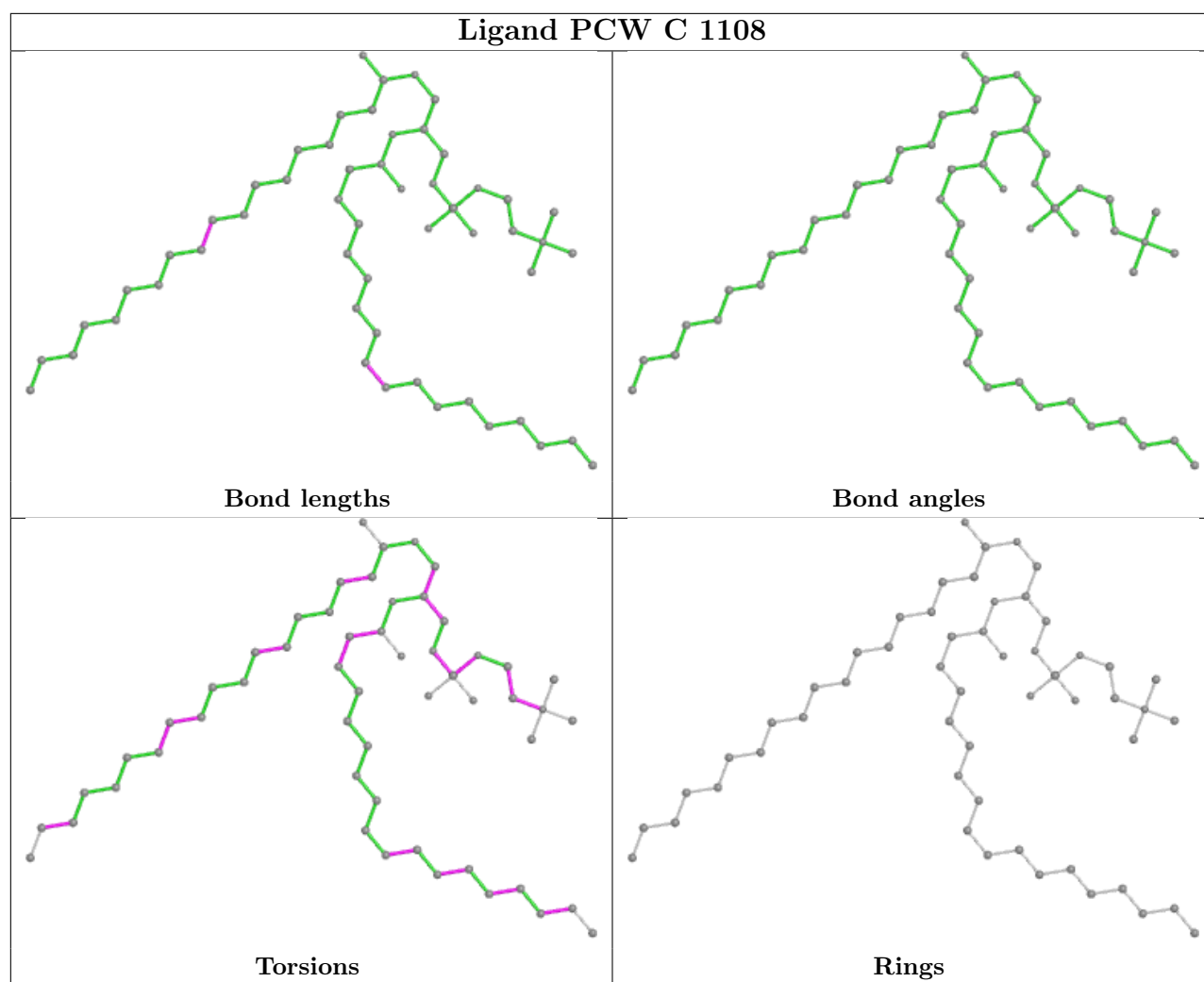
Ligand PCW C 1103

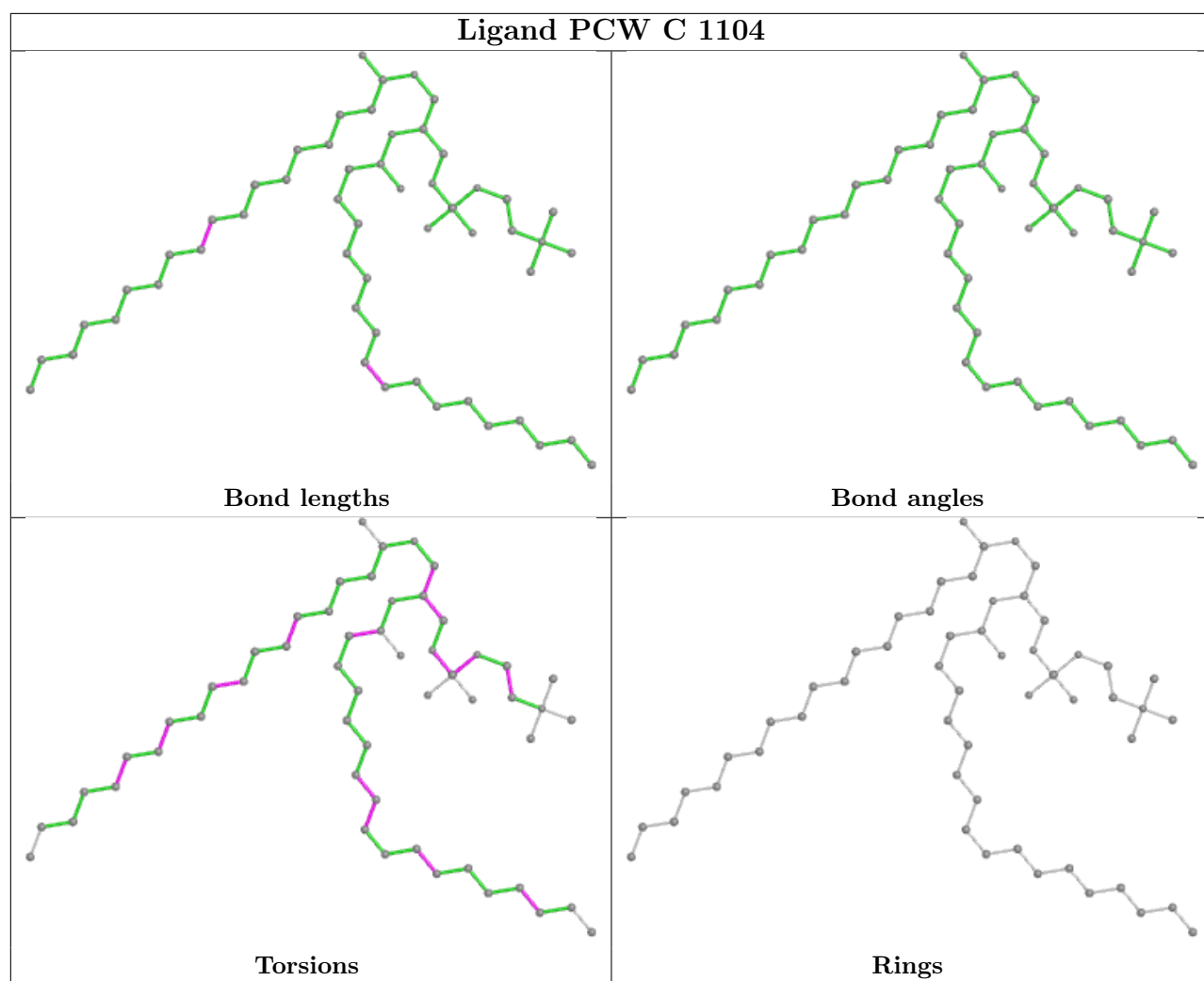


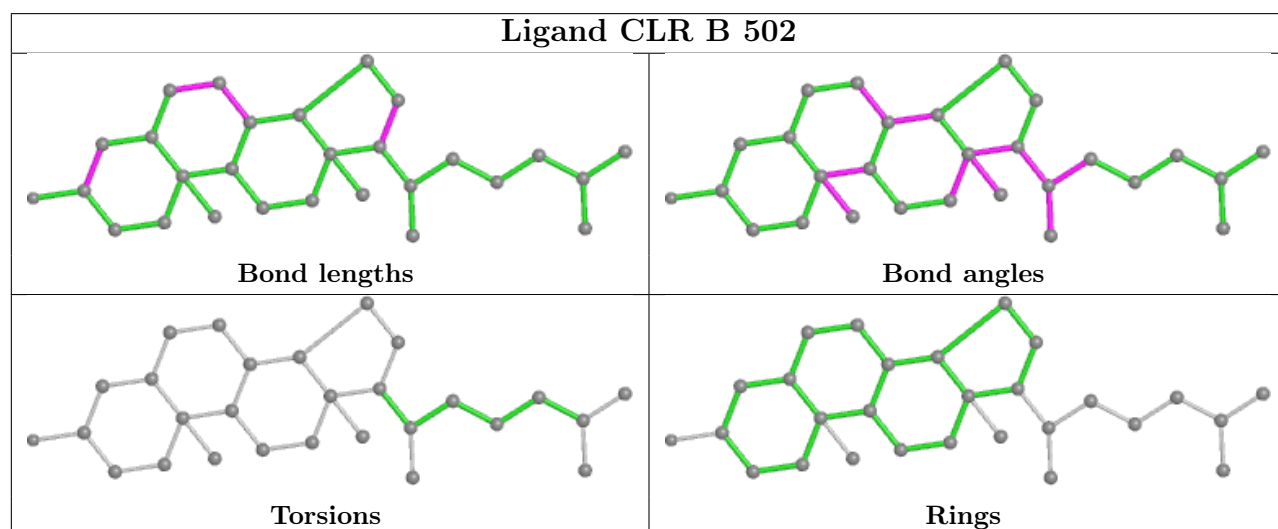
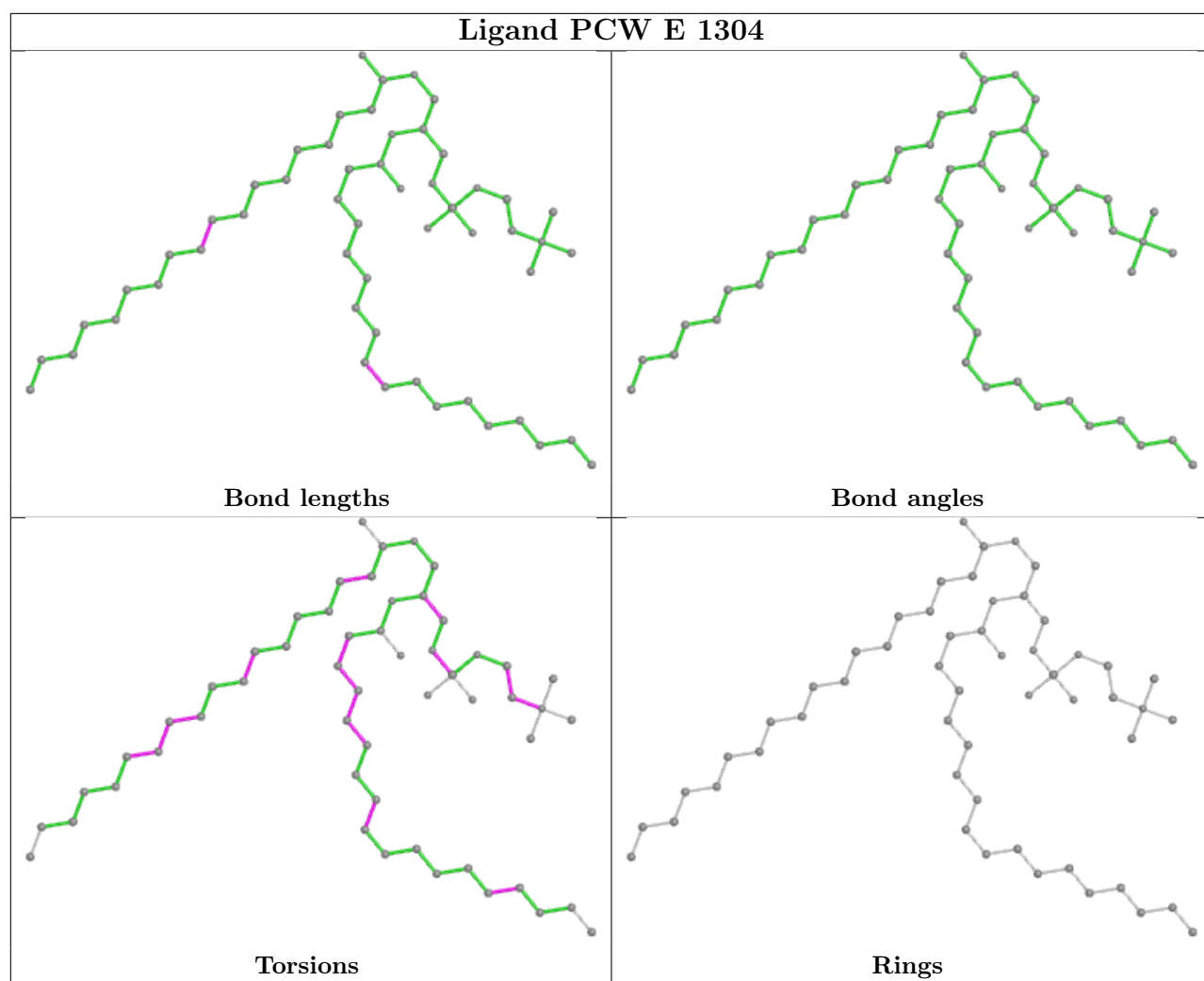
Ligand CLR D 502



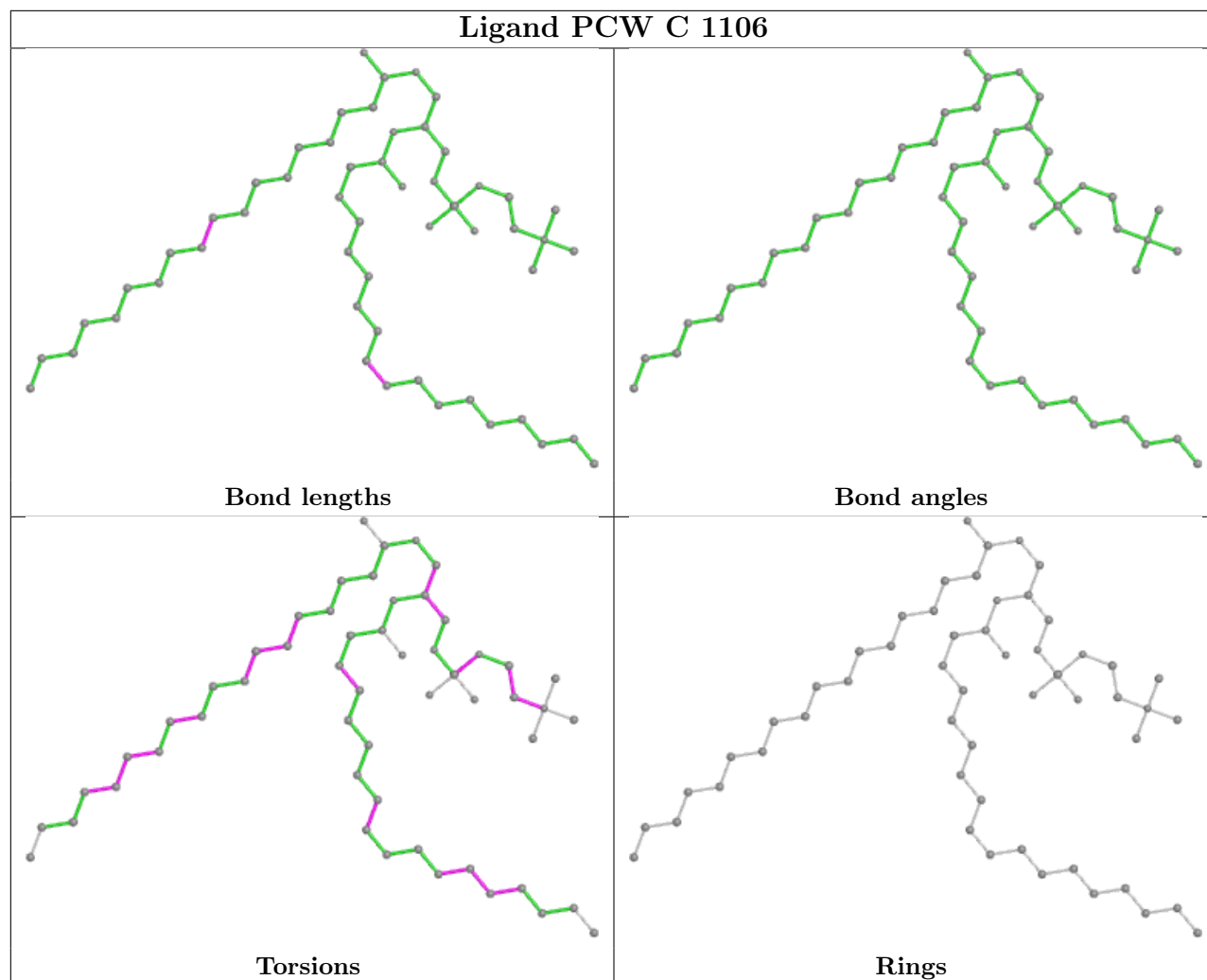




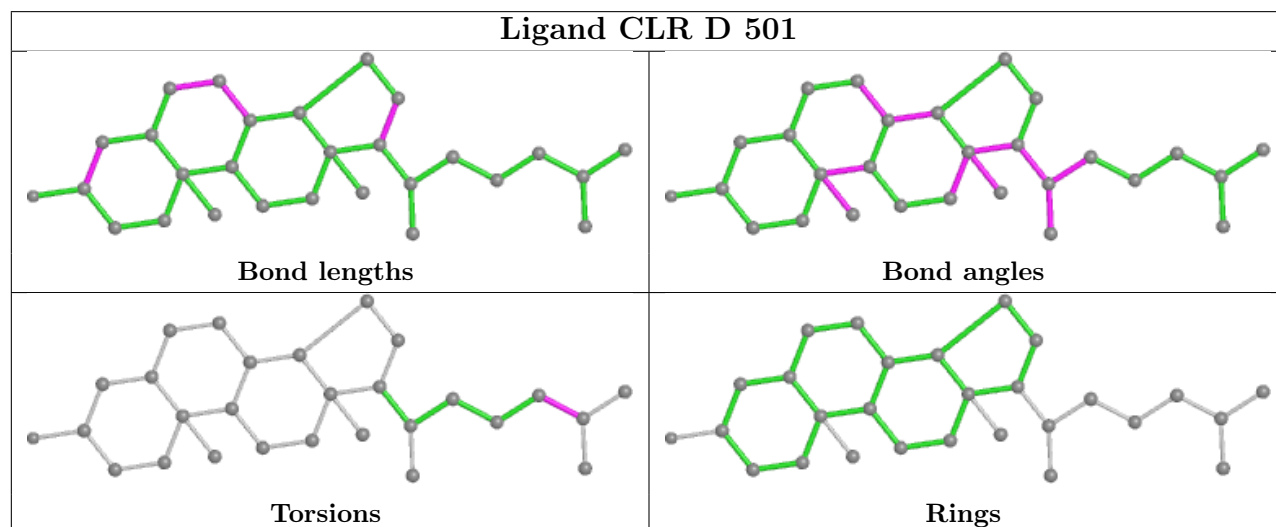


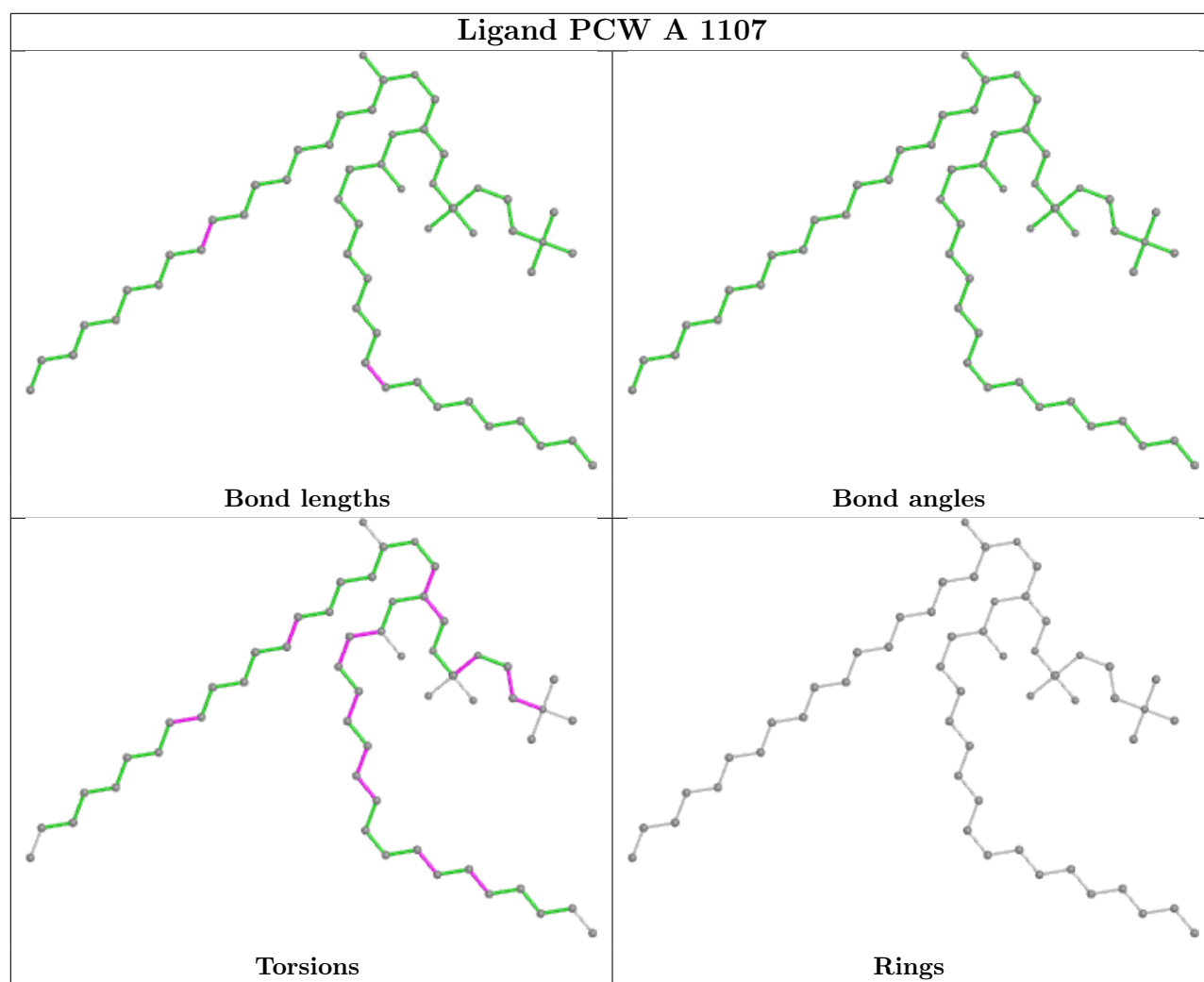


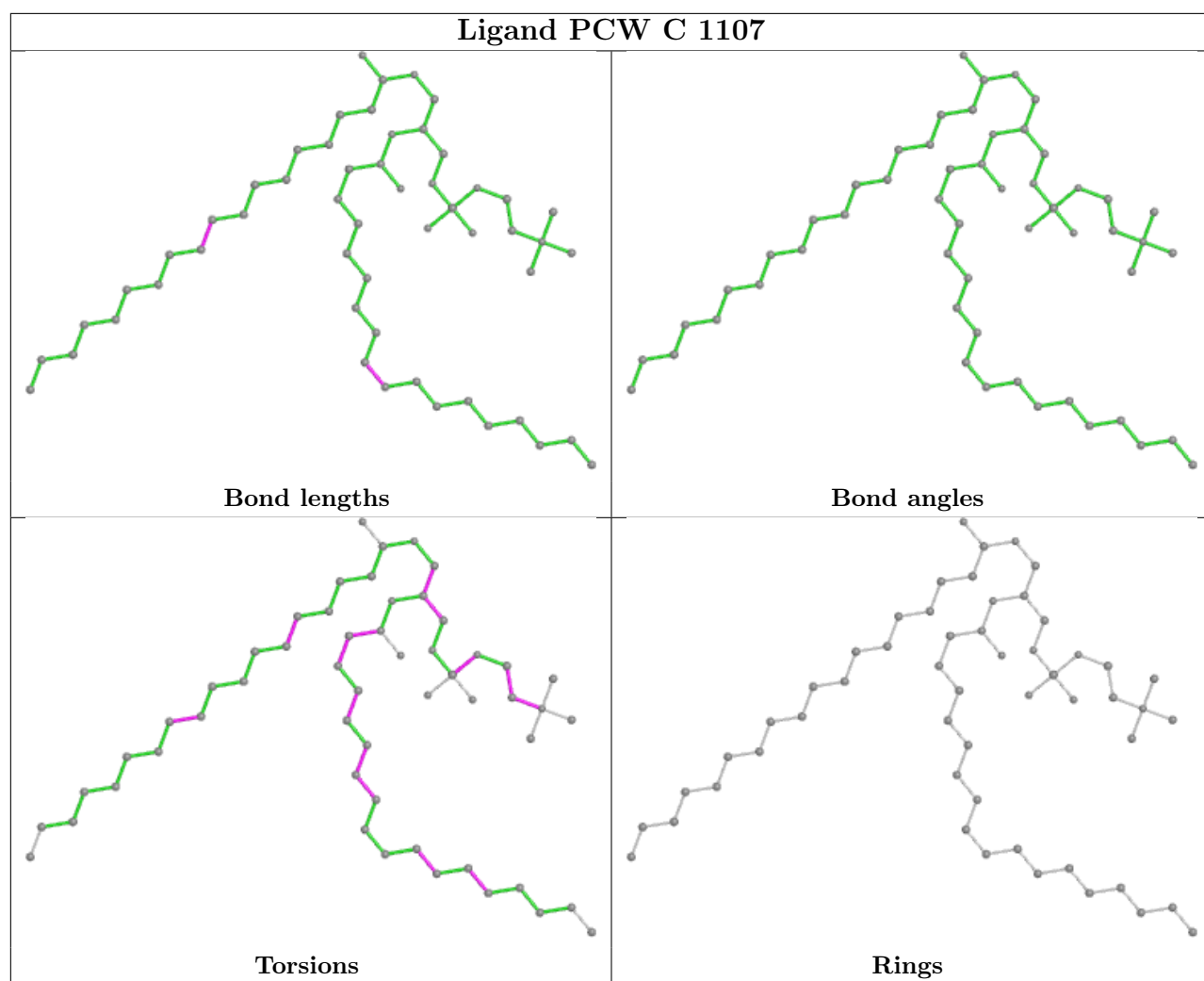
Ligand PCW C 1106

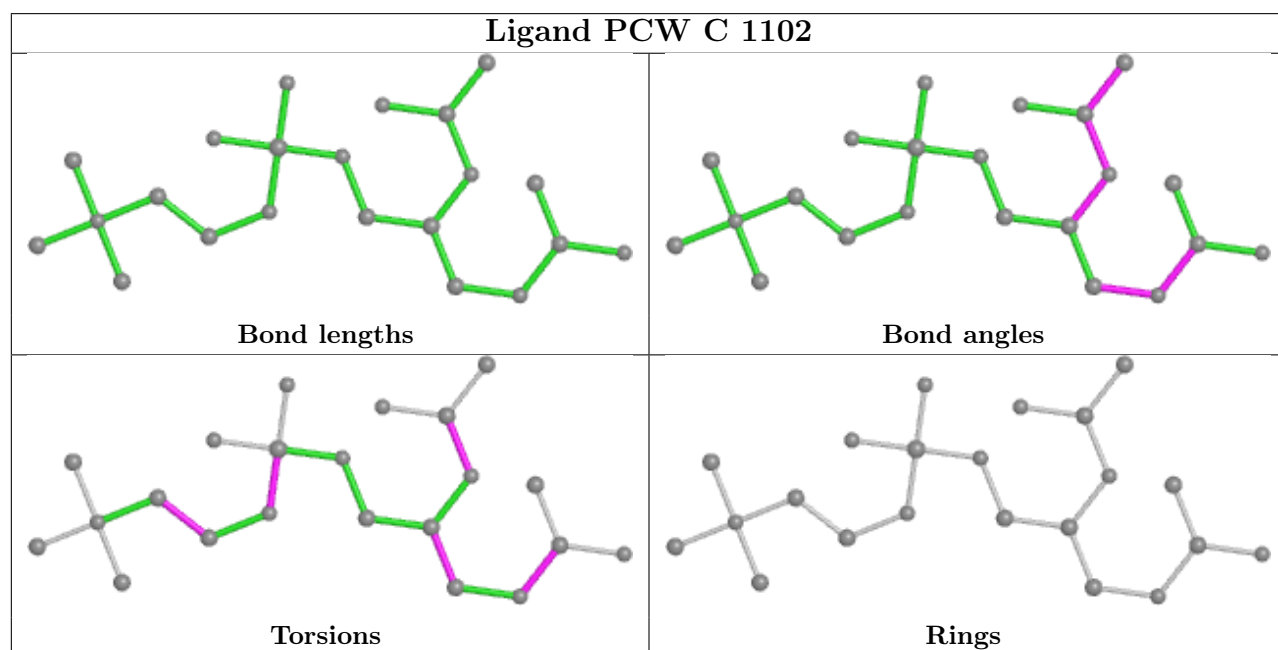
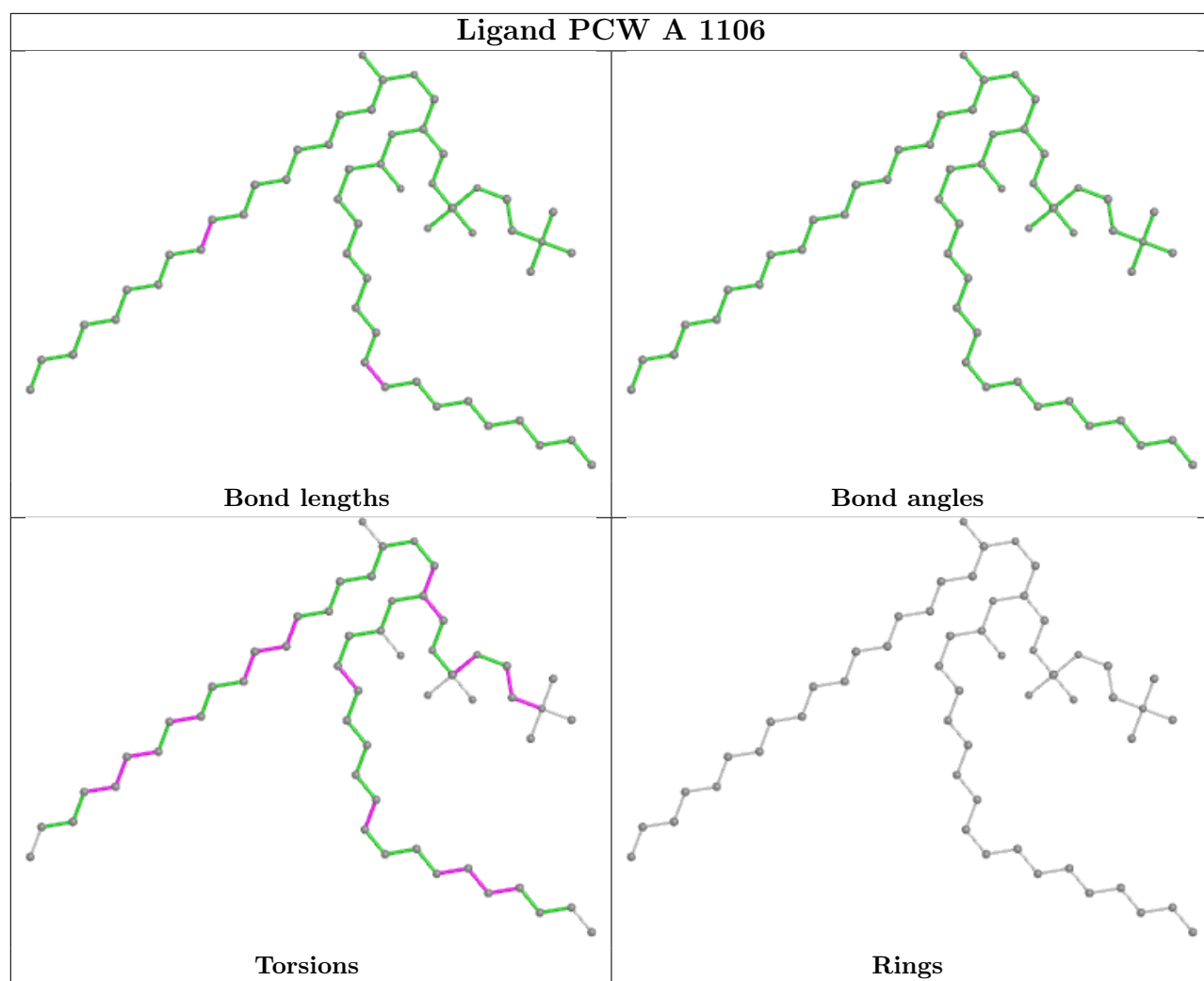


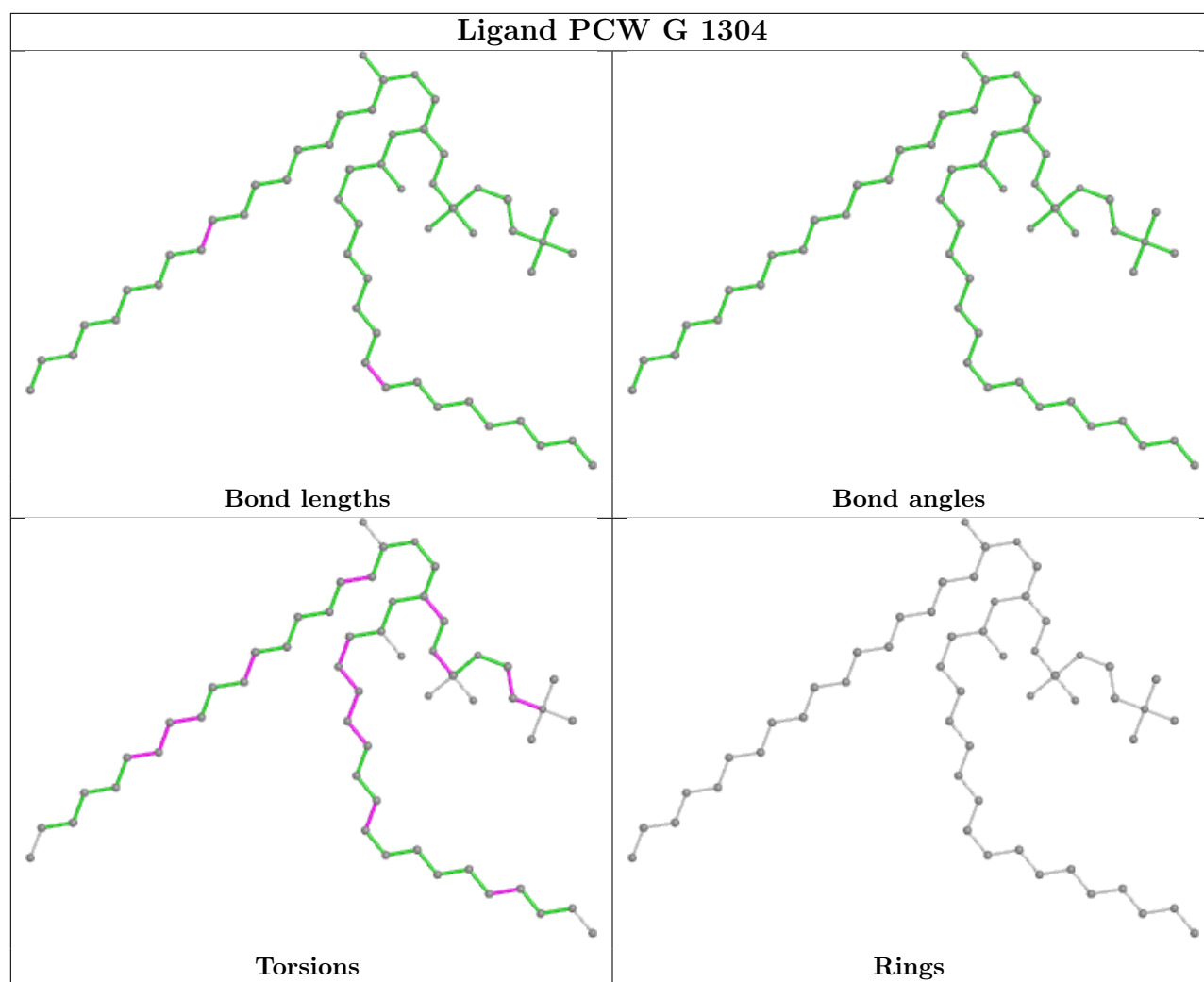
Ligand CLR D 501











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

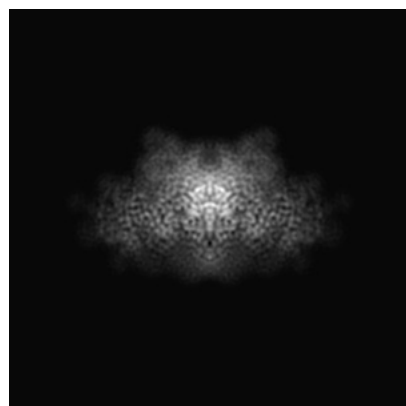
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65098. These allow visual inspection of the internal detail of the map and identification of artifacts.

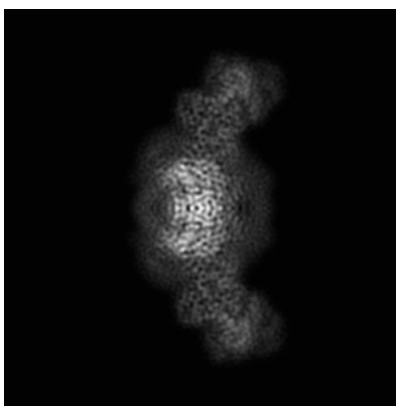
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

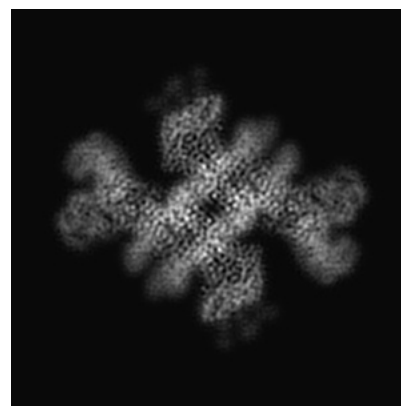
6.1.1 Primary map



X

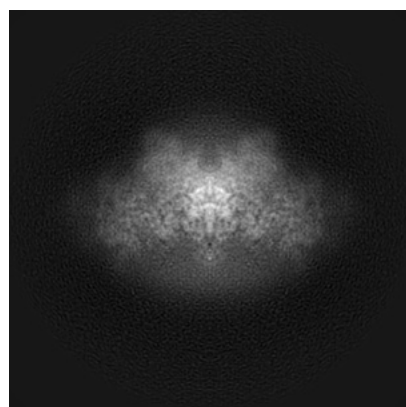


Y

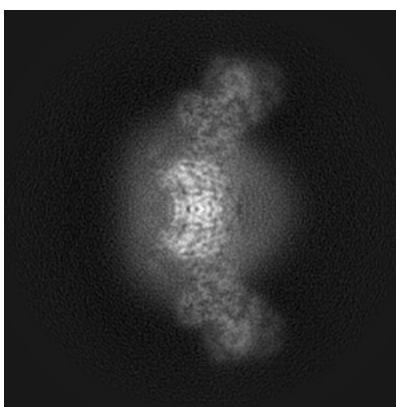


Z

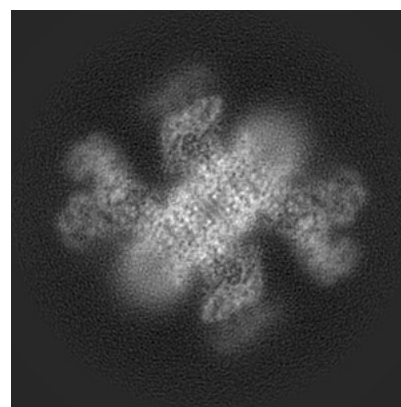
6.1.2 Raw map



X



Y

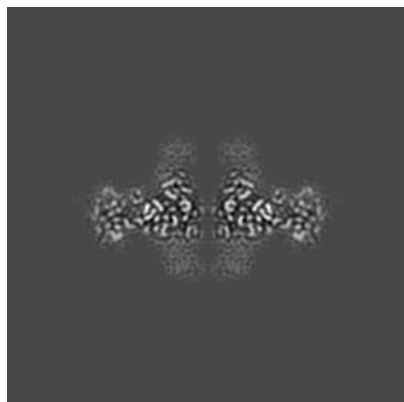


Z

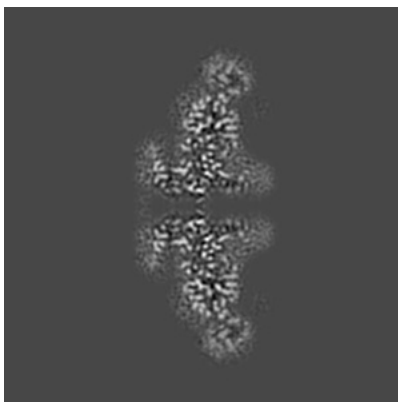
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

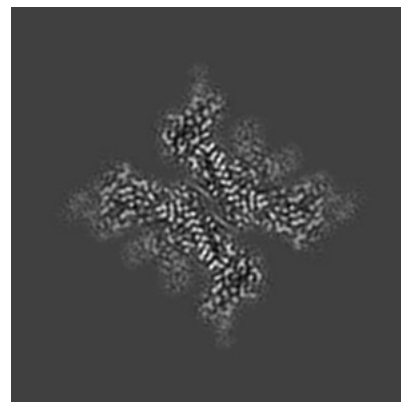
6.2.1 Primary map



X Index: 120

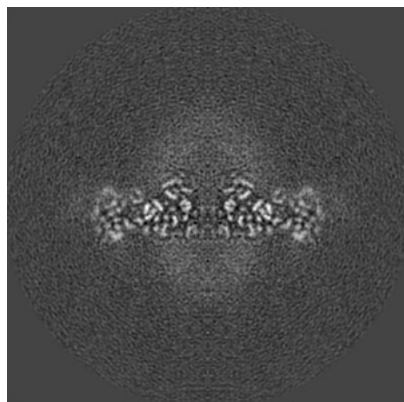


Y Index: 120

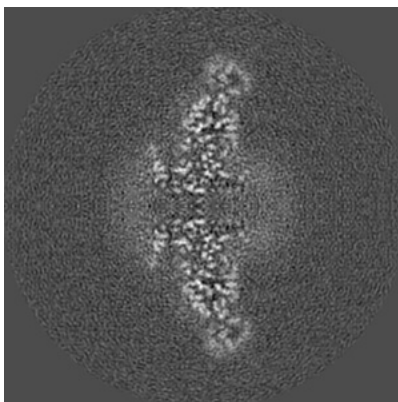


Z Index: 120

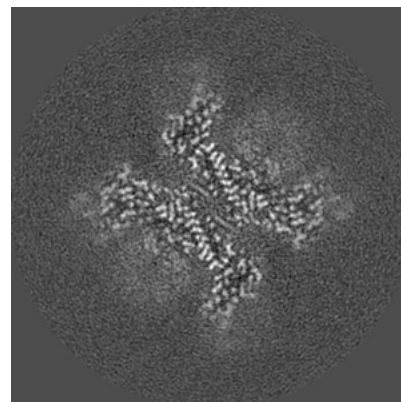
6.2.2 Raw map



X Index: 120



Y Index: 120

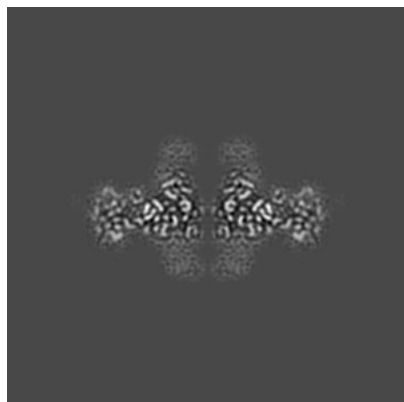


Z Index: 120

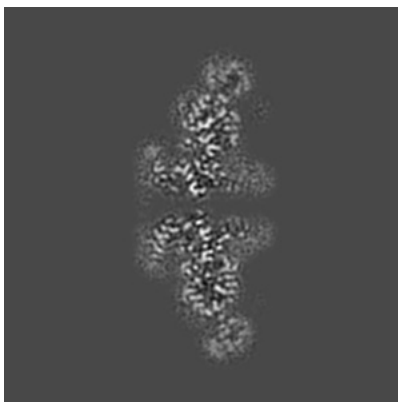
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

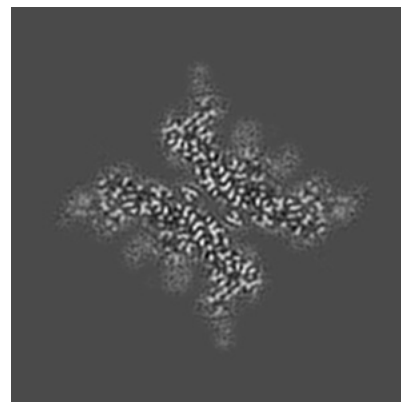
6.3.1 Primary map



X Index: 120

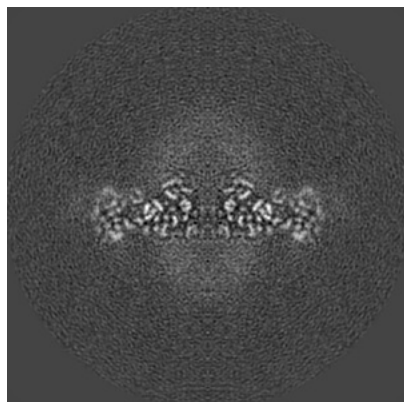


Y Index: 119

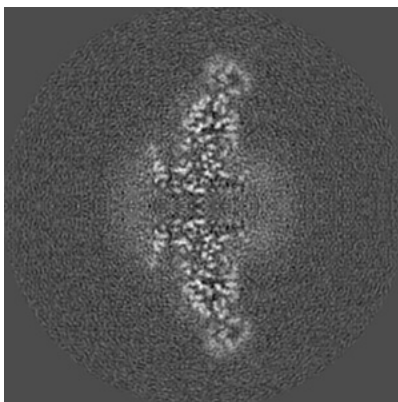


Z Index: 122

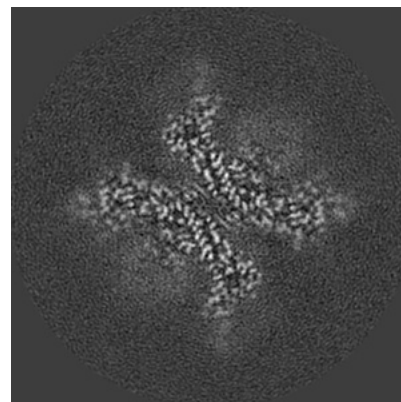
6.3.2 Raw map



X Index: 120



Y Index: 120

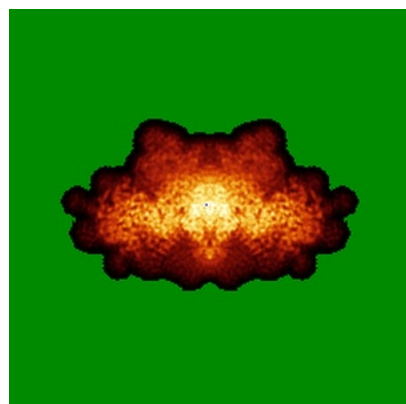


Z Index: 121

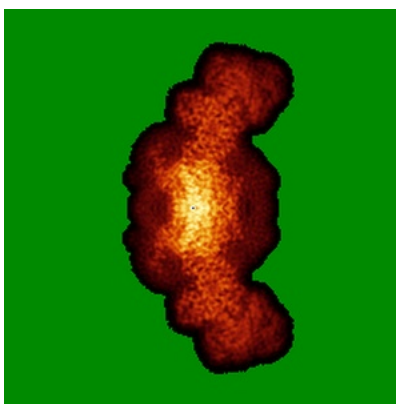
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

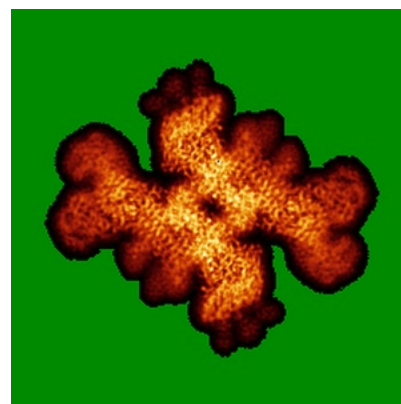
6.4.1 Primary map



X

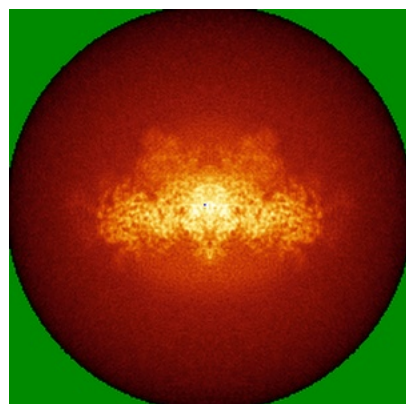


Y

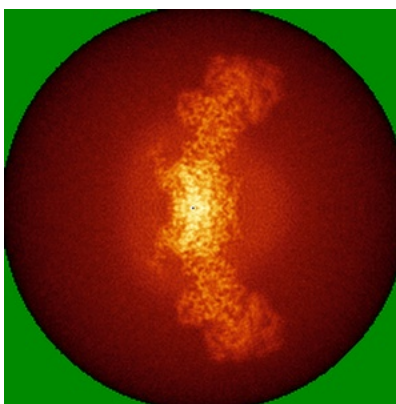


Z

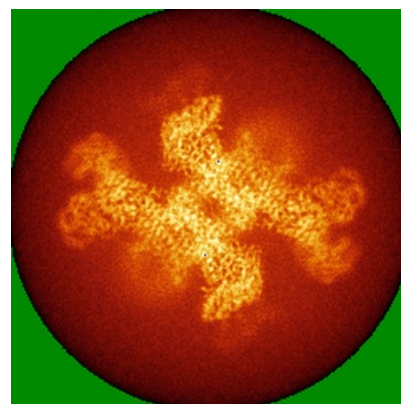
6.4.2 Raw map



X



Y

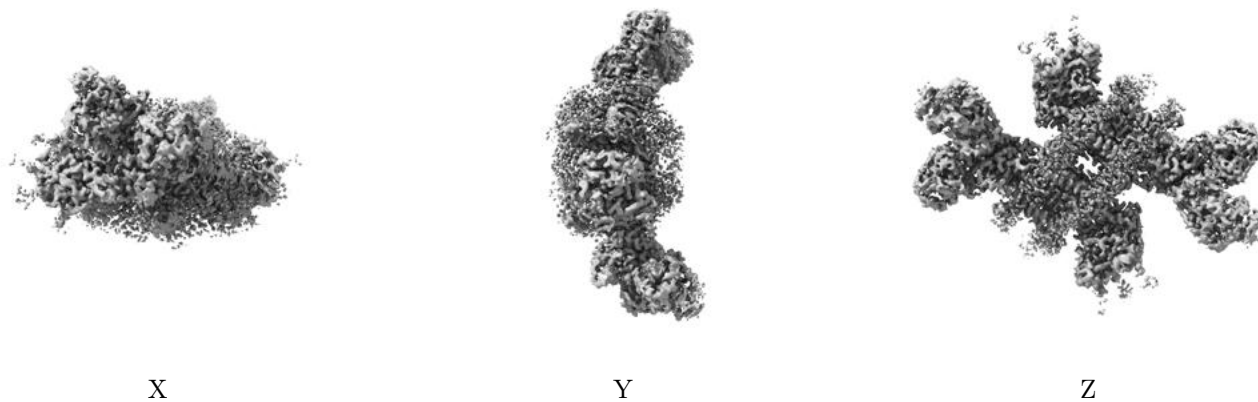


Z

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.

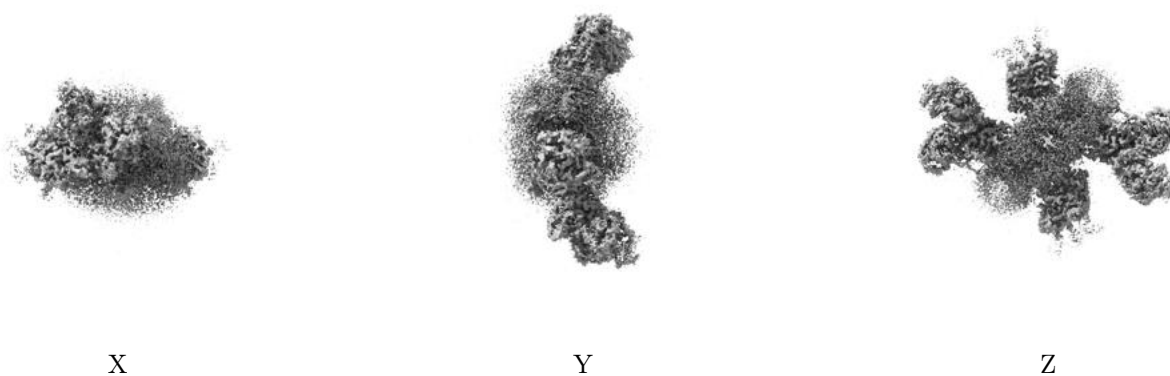
6.5 Orthogonal surface views [i](#)

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.

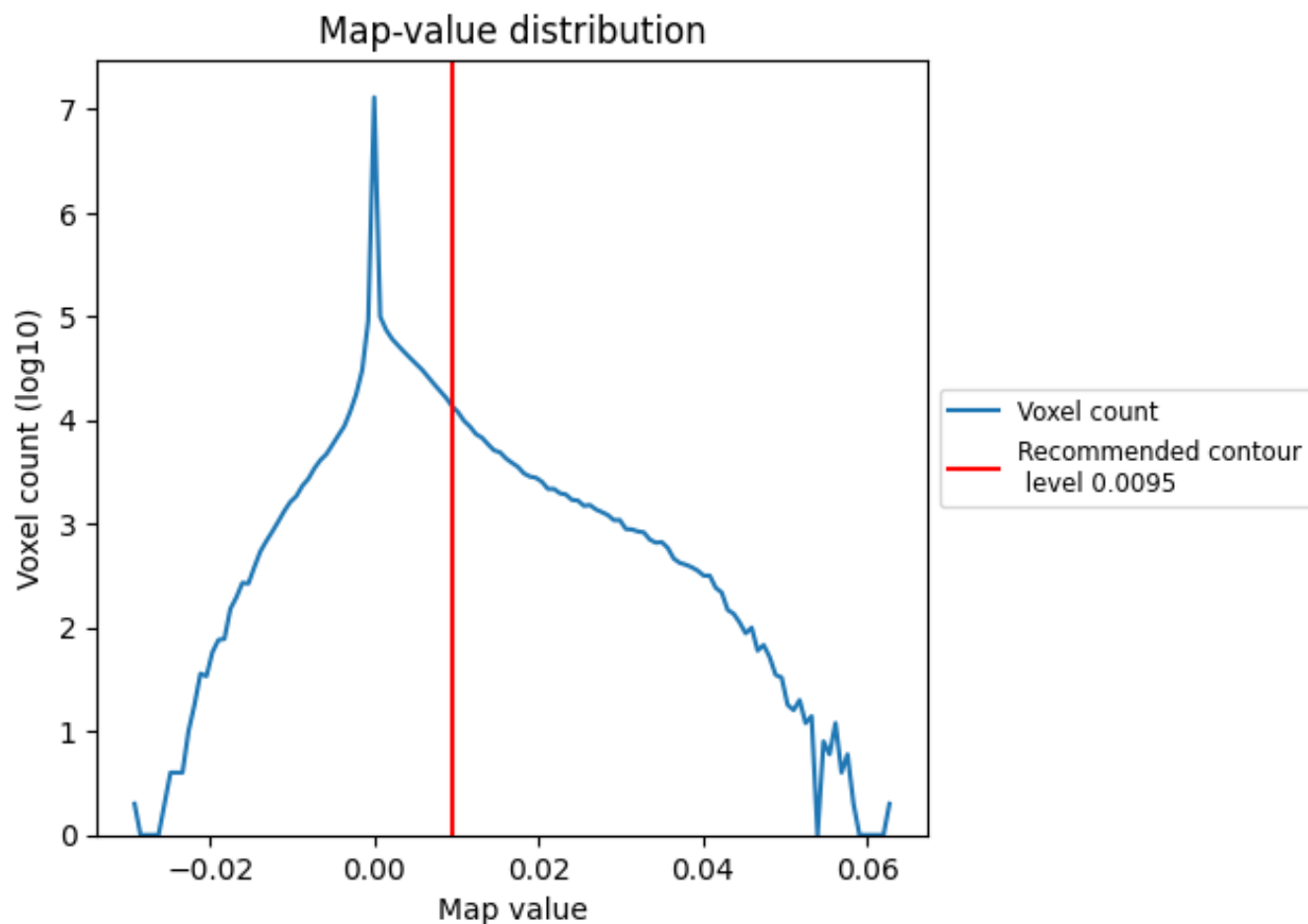
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

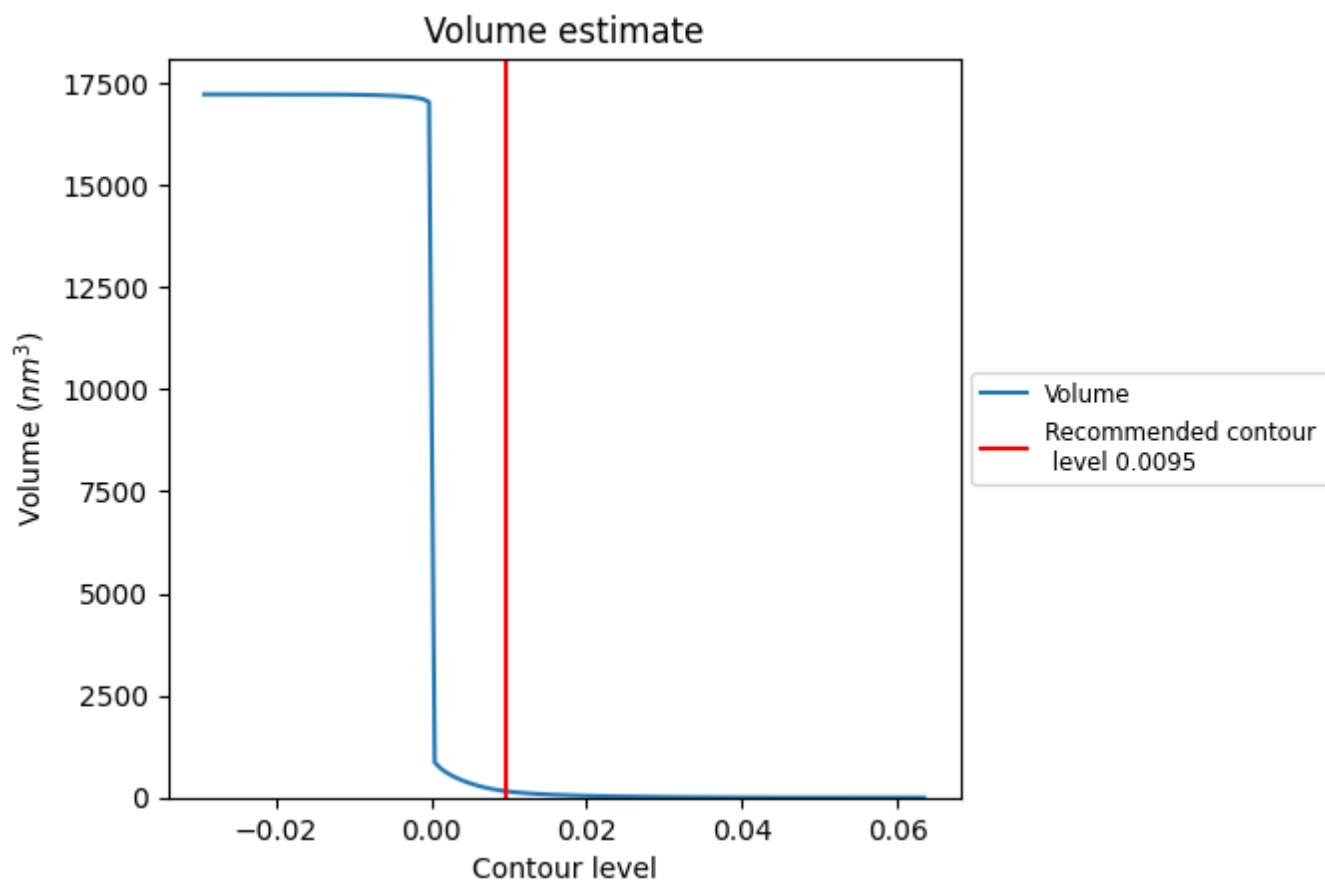
This section contains the results of statistical analysis of the map.

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.

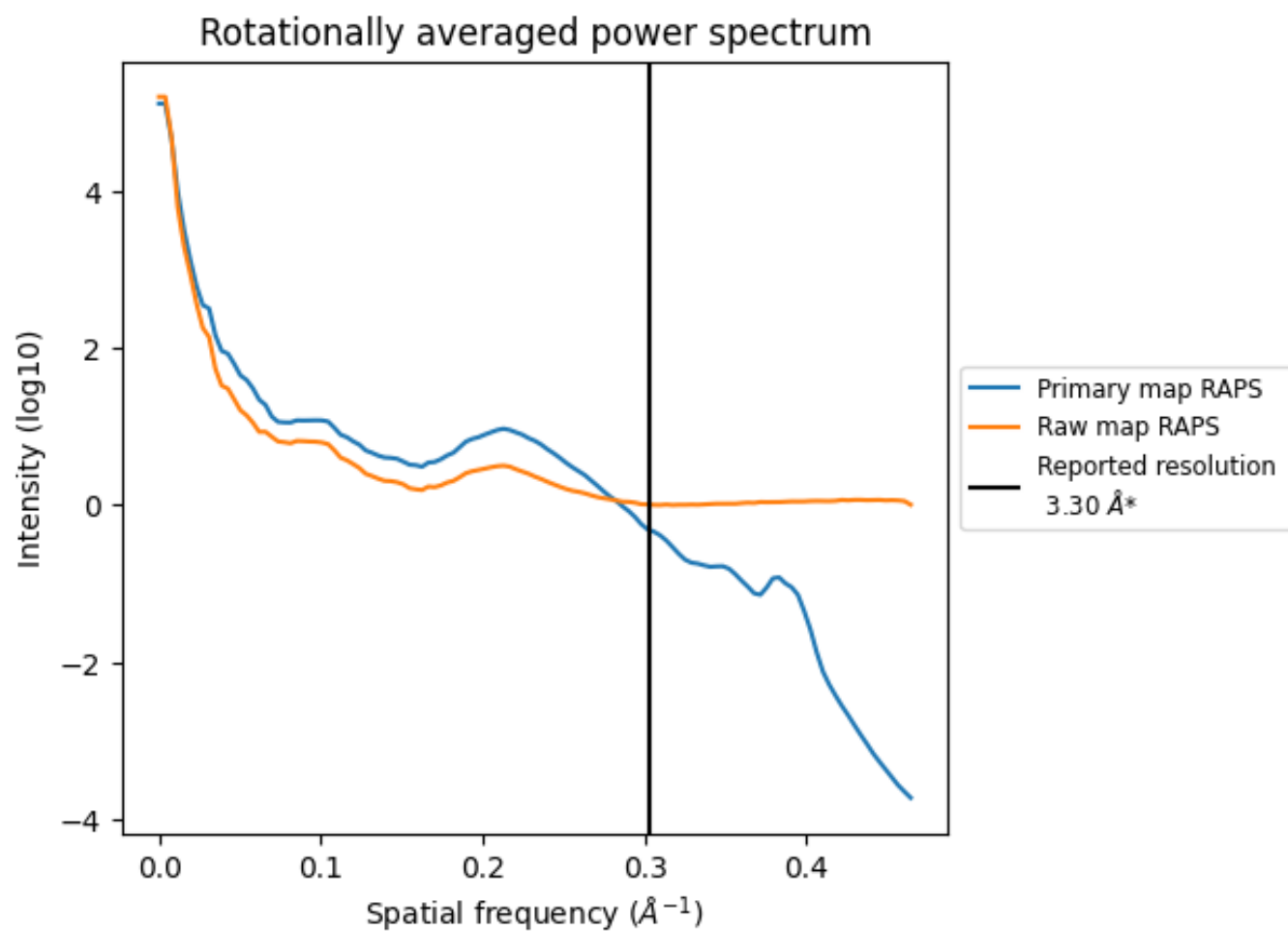
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 158 nm^3 ; 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 ⓘ

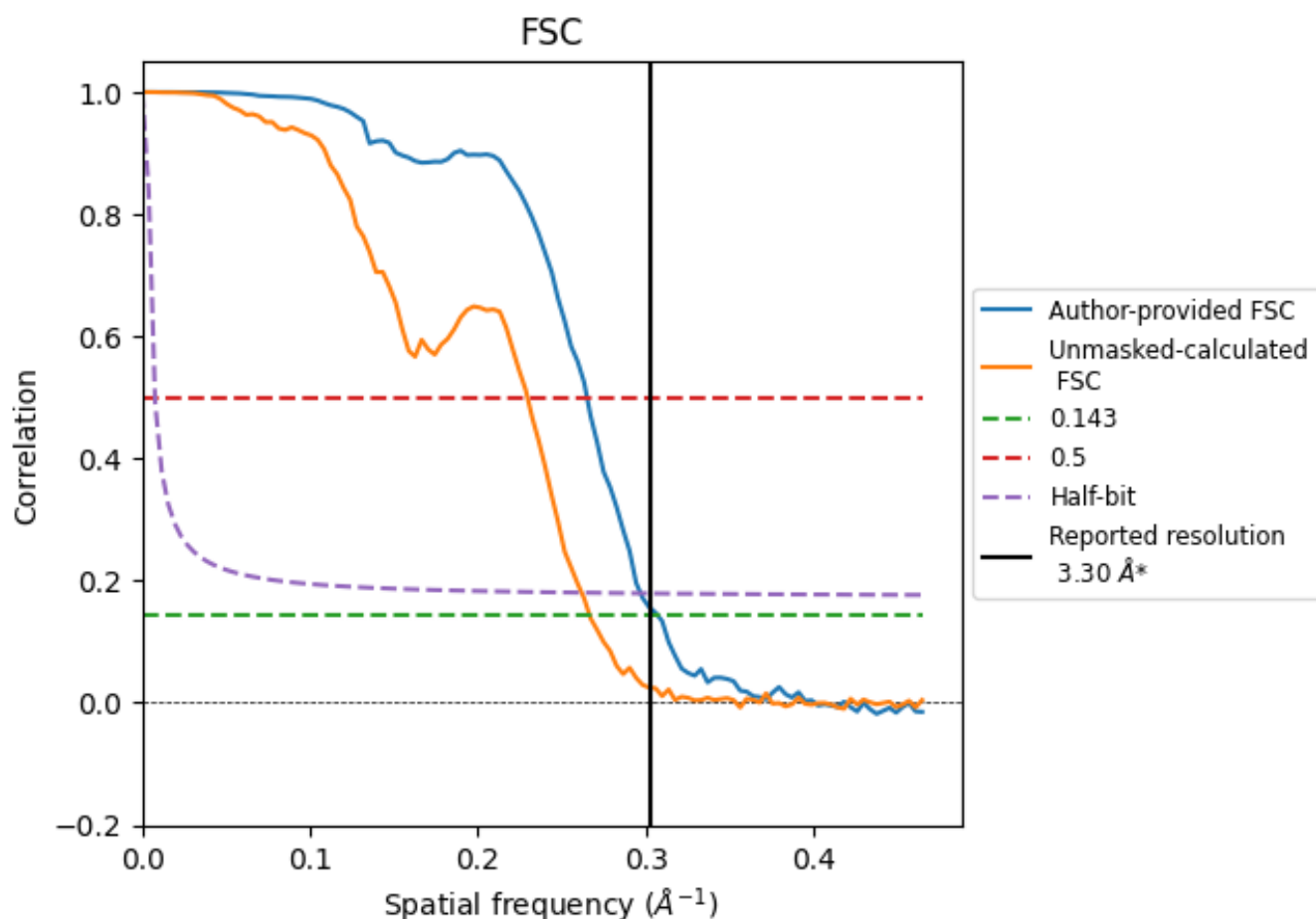


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 \AA^{-1}

8.2 Resolution estimates [i](#)

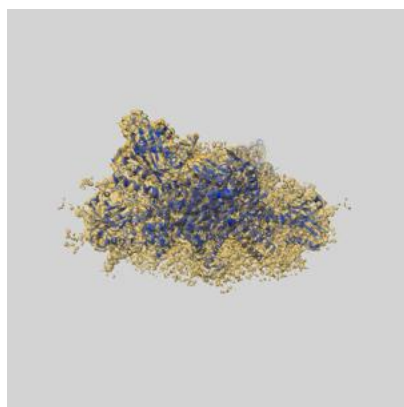
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.26	3.77	3.37
Unmasked-calculated*	3.75	4.36	3.82

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.75 differs from the reported value 3.3 by more than 10 %

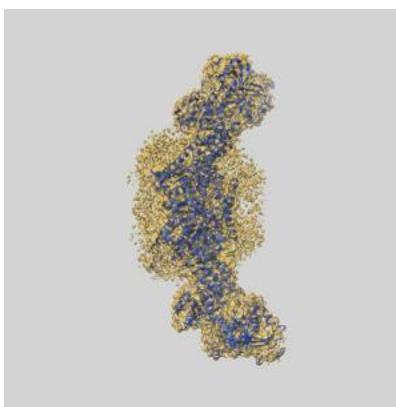
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-65098 and PDB model 9VIY. Per-residue inclusion information can be found in section [3](#) on page [10](#).

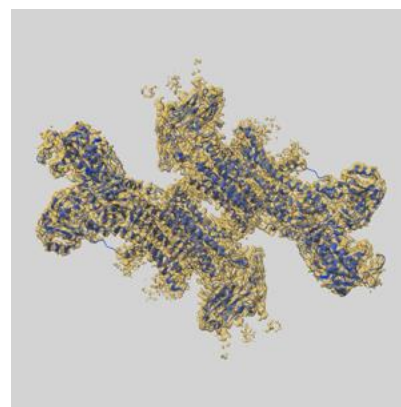
9.1 Map-model overlay [i](#)



X



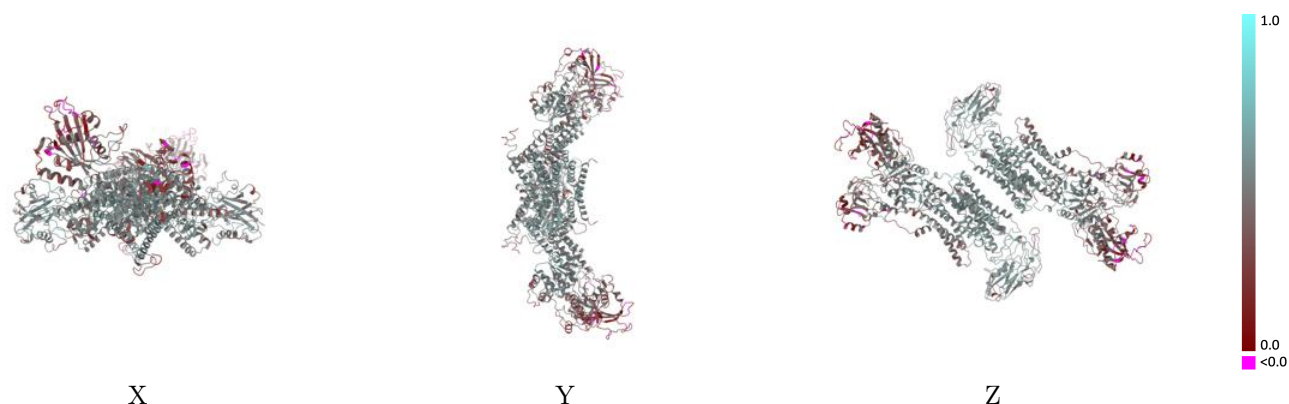
Y



Z

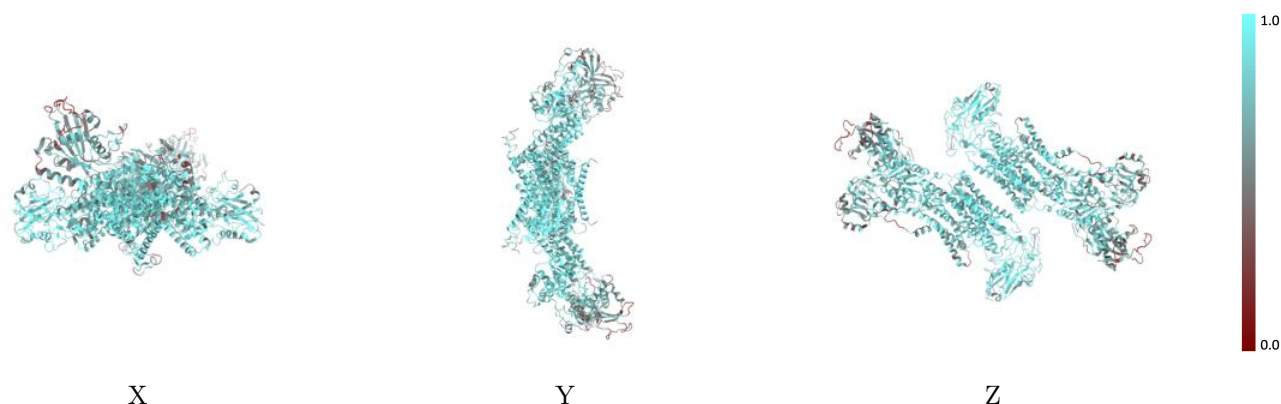
The images above show the 3D surface view of the map at the recommended contour level 0.0095 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



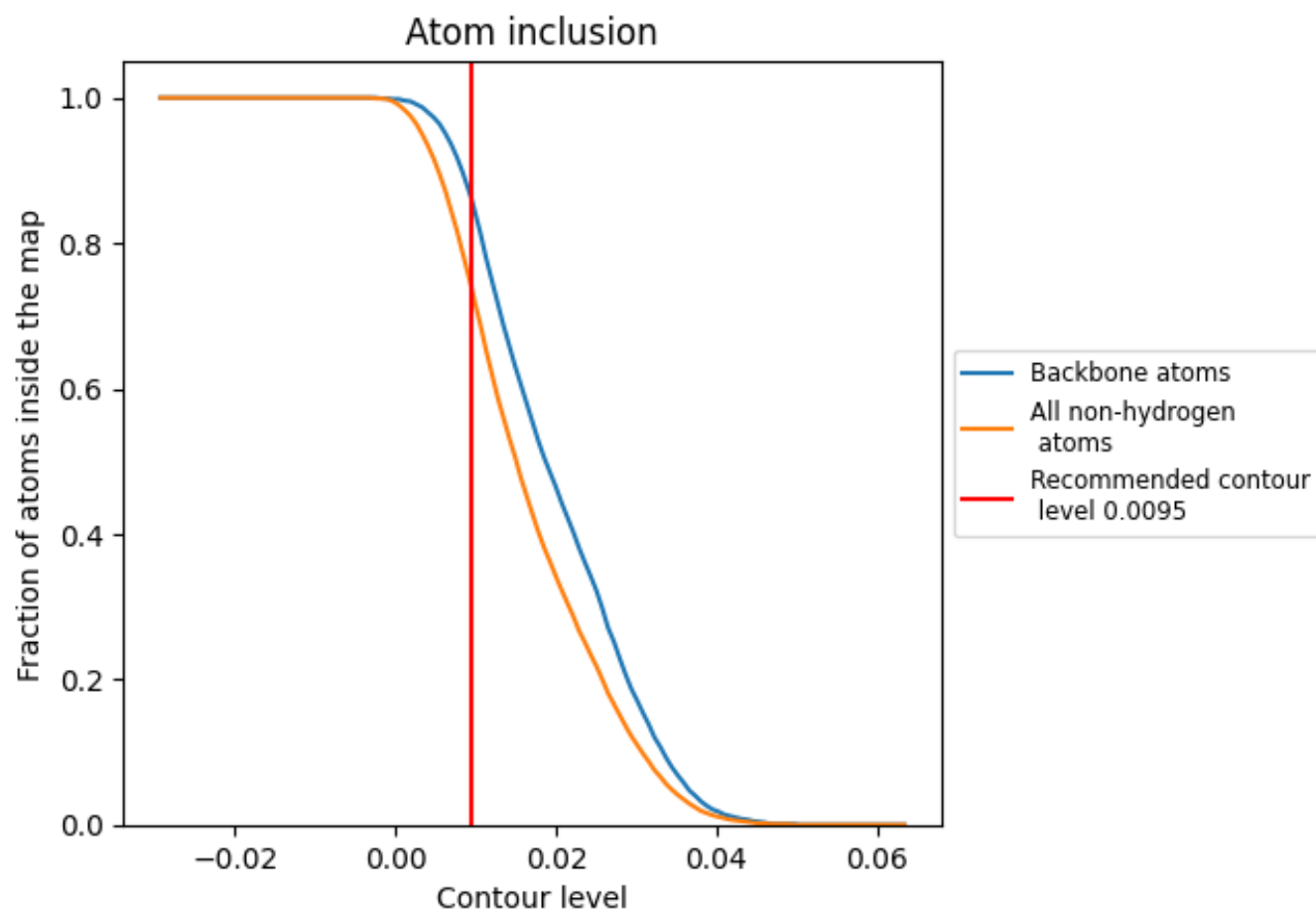
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 86% of all backbone atoms, 74% 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	<div></div> 0.7390	<div></div> 0.4390
A	<div></div> 0.7290	<div></div> 0.4320
B	<div></div> 0.8350	<div></div> 0.4930
C	<div></div> 0.7300	<div></div> 0.4330
D	<div></div> 0.8360	<div></div> 0.4910
E	<div></div> 0.6320	<div></div> 0.4210
F	<div></div> 0.4650	<div></div> 0.2640
G	<div></div> 0.6280	<div></div> 0.4160
H	<div></div> 0.1600	<div></div> 0.1120
I	<div></div> 0.3170	<div></div> 0.1900
J	<div></div> 0.2500	<div></div> 0.1590
K	<div></div> 0.4510	<div></div> 0.2700
L	<div></div> 0.1600	<div></div> 0.0990
M	<div></div> 0.3170	<div></div> 0.1900
N	<div></div> 0.2140	<div></div> 0.1330

1.0

0.0

<0.0