



Full wwPDB EM Validation Report ⓘ

Oct 21, 2024 – 09:33 PM JST

PDB ID : 7Y45
EMDB ID : EMD-33601
Title : Cryo-EM structure of the Na⁺,K⁺-ATPase in the E2.2K⁺ state
Authors : Kanai, R.; Cornelius, F.; Vilsen, B.; Toyoshima, C.
Deposited on : 2022-06-14
Resolution : 3.30 Å (reported)
Based on initial model : 2ZXE

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.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

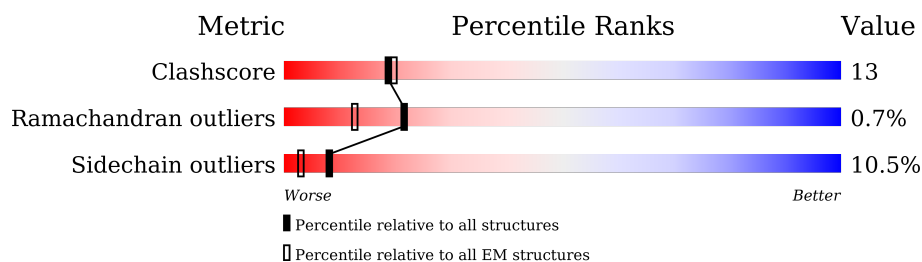
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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>27%</div> <div>68%</div> <div>26%</div> <div>• •</div> </div>
1	C	1028	<div> <div>28%</div> <div>68%</div> <div>26%</div> <div>• •</div> </div>
2	B	305	<div> <div>60%</div> <div>31%</div> <div>6%</div> <div>•</div> </div>
2	D	305	<div> <div>61%</div> <div>30%</div> <div>5%</div> <div>•</div> </div>
3	E	94	<div> <div>32%</div> <div>11%</div> <div>57%</div> </div>
3	G	94	<div> <div>30%</div> <div>13%</div> <div>57%</div> </div>
4	F	6	<div> <div>67%</div> <div>83%</div> <div>17%</div> </div>
4	K	6	<div> <div>50%</div> <div>83%</div> <div>17%</div> </div>

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Mol	Chain	Length	Quality of chain
5	H	6	<div><div></div><div>83%</div><div>17%</div></div>
5	L	6	<div><div></div><div>83%</div><div>17%</div></div>
6	I	5	<div><div></div><div>80%</div><div>100%</div></div>
6	M	5	<div><div></div><div>80%</div><div>100%</div></div>
7	J	2	<div><div></div><div>100%</div><div>100%</div></div>
7	N	2	<div><div></div><div>100%</div><div>100%</div></div>

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 22638 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Na, K-ATPase alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	993	Total	C	N	O	S	0	0
			7683	4890	1291	1456	46		
1	A	993	Total	C	N	O	S	0	0
			7683	4890	1291	1456	46		

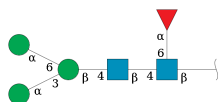
- Molecule 2 is a protein called Na⁺,K⁺-ATPase beta subunit.

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

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

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

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



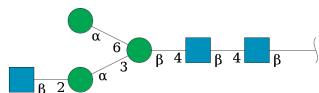
Mol	Chain	Residues	Atoms				AltConf	Trace
4	F	6	Total	C	N	O	0	0
			71	40	2	29		

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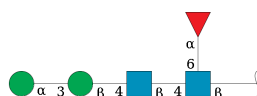
Mol	Chain	Residues	Atoms				AltConf	Trace
4	K	6	Total	C	N	O	0	0
			71	40	2	29		

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



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

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



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

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



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

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

- | Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|----------------|---------|
| 8 | C | 3 | Total K
3 3 | 0 |
| 8 | A | 3 | Total K
3 3 | 0 |

- # CLR

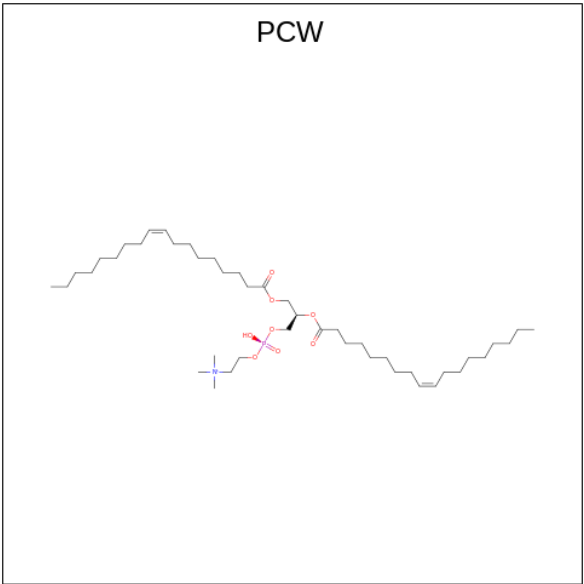
Mol	Chain	Residues	Atoms			AltConf
9	C	1	Total 28	C 27	O 1	0
9	C	1	Total 28	C 27	O 1	0
9	D	1	Total 28	C 27	O 1	0
9	D	1	Total 28	C 27	O 1	0
9	A	1	Total 28	C 27	O 1	0
9	A	1	Total 28	C 27	O 1	0



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Mol	Chain	Residues	Atoms			AltConf
9	B	1	Total	C	O	0
			28	27	1	
9	B	1	Total	C	O	0
			28	27	1	

- Molecule 10 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: C₄₄H₈₅NO₈P).



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

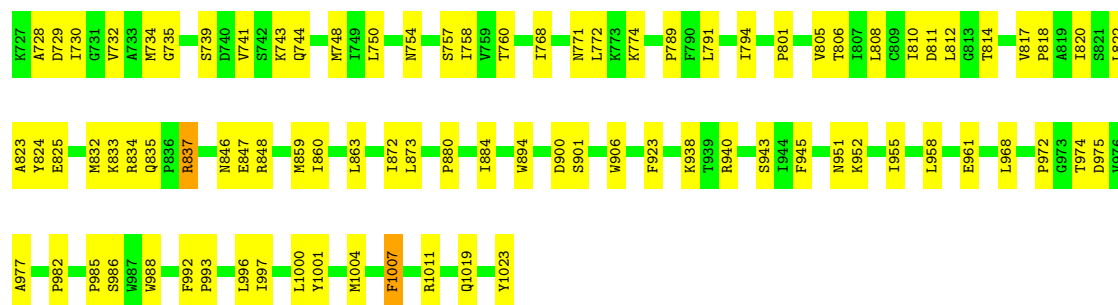
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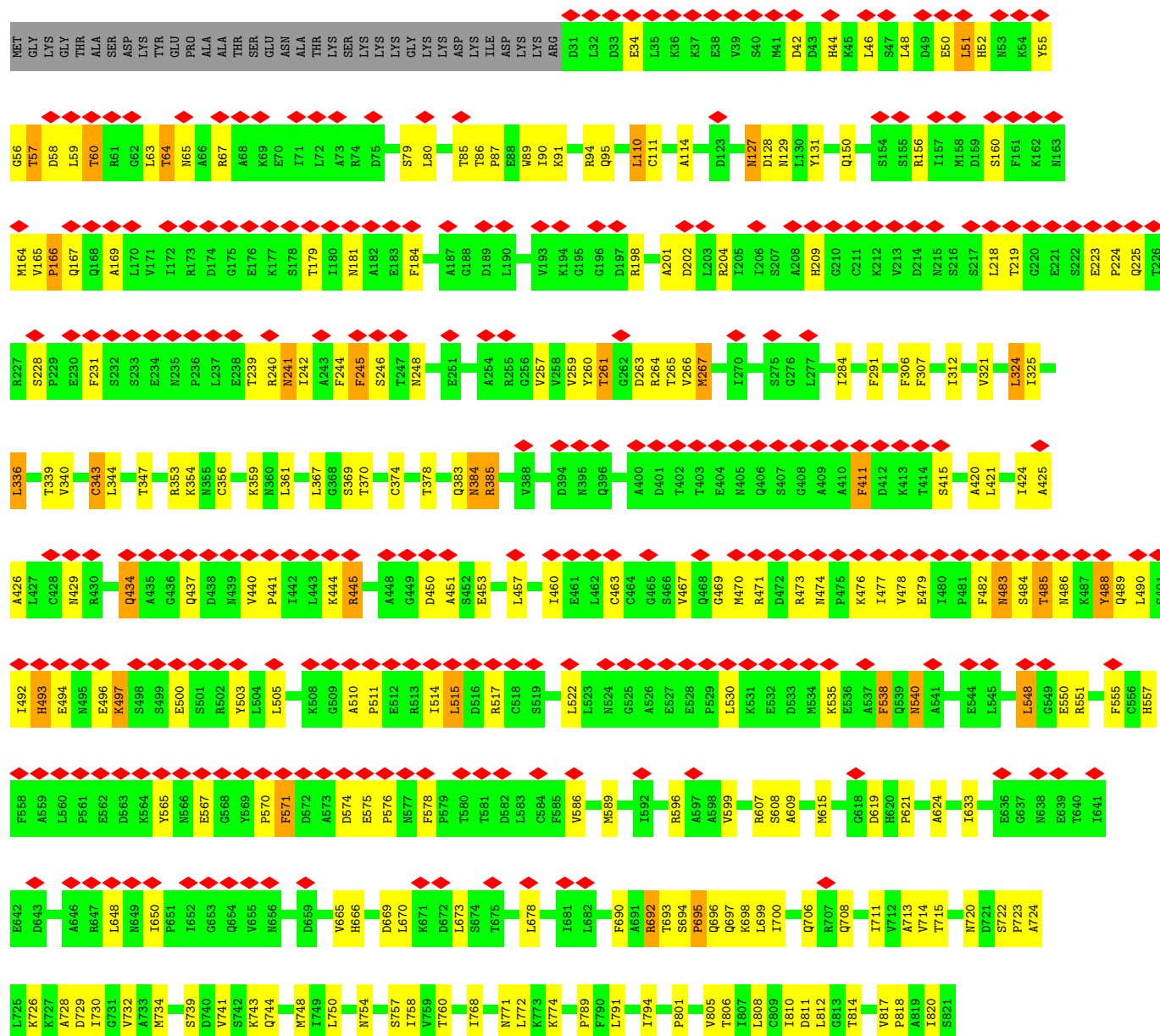
Mol	Chain	Residues	Atoms					AltConf
10	C	1	Total	C	N	O	P	0
			54	44	1	8	1	
10	C	1	Total	C	N	O	P	0
			22	12	1	8	1	
10	E	1	Total	C	N	O	P	0
			22	12	1	8	1	
10	E	1	Total	C	N	O	P	0
			54	44	1	8	1	
10	A	1	Total	C	N	O	P	0
			22	12	1	8	1	
10	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
10	A	1	Total	C	N	O	P	0
			54	44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

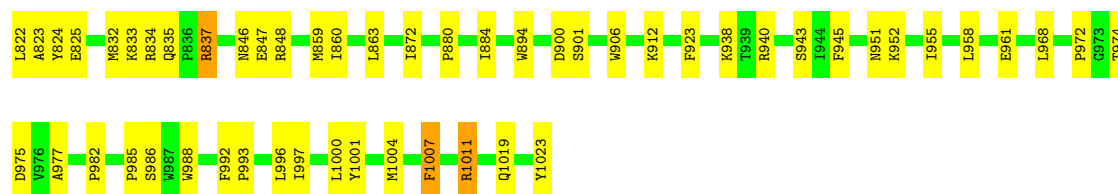
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		AltConf
11	C	3	Total	O	0
			3	3	
11	A	3	Total	O	0
			3	3	

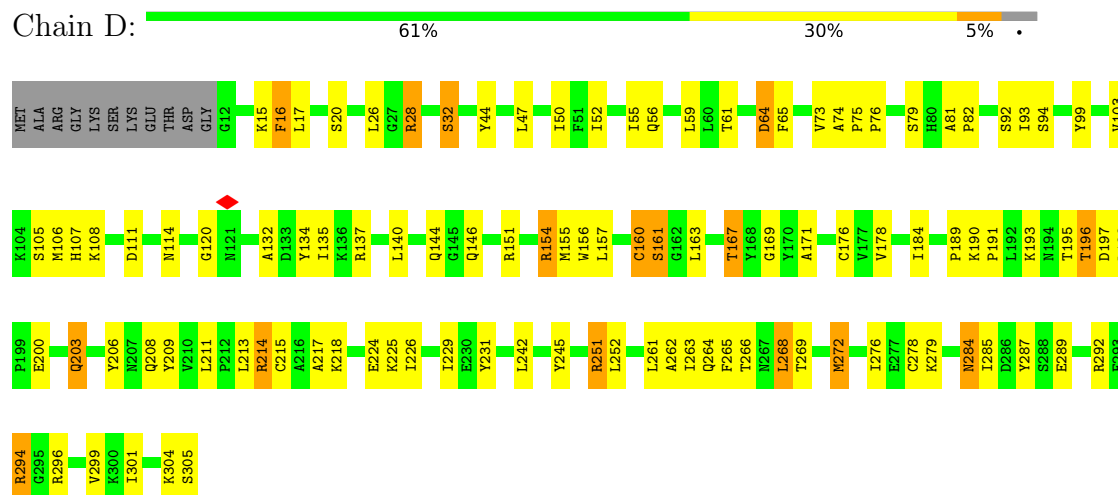


• Molecule 1: Na, K-ATPase alpha subunit

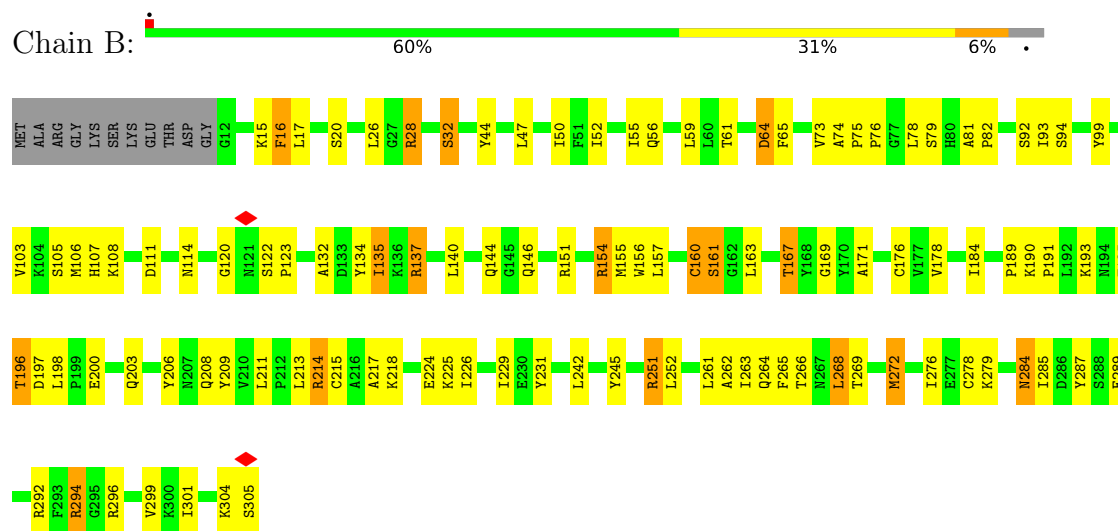




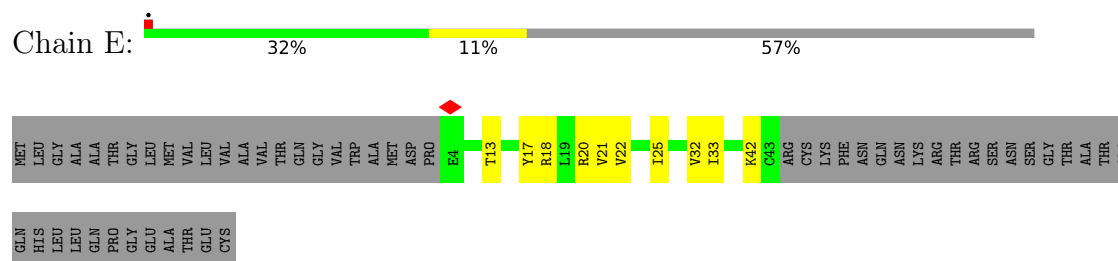
• Molecule 2: Na⁺,K⁺-ATPase beta subunit




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

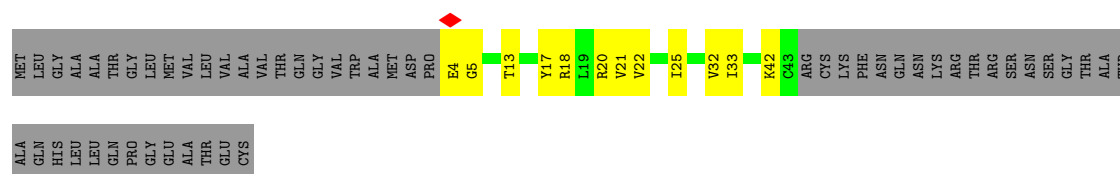


• Molecule 3: FXYP domain-containing ion transport regulator




- Molecule 3: FXYD domain-containing ion transport regulator

Chain G: 




- 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

Chain F: 




- 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

Chain K: 




- 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

Chain H: 

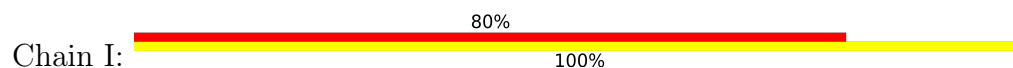


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

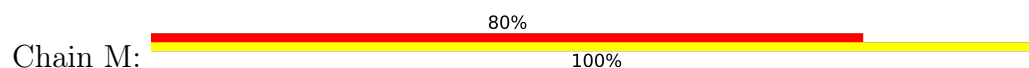
Chain L: 



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



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



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	47461	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN 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	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.121	Depositor
Minimum map value	-0.057	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0199	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: FUC, K, NAG, CLR, PCW, MAN, BMA

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	0.31	0/7833	0.67	0/10627
1	C	0.31	0/7833	0.67	0/10627
2	B	0.31	0/2462	0.68	0/3317
2	D	0.31	0/2462	0.68	0/3317
3	E	0.27	0/315	0.52	0/427
3	G	0.27	0/315	0.53	0/427
All	All	0.30	0/21220	0.66	0/28742

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	7683	0	7703	198	0
1	C	7683	0	7703	185	0
2	B	2399	0	2354	71	0
2	D	2399	0	2354	72	0
3	E	311	0	323	6	0
3	G	311	0	323	7	0
4	F	71	0	61	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	71	0	61	1	0
5	H	75	0	64	1	0
5	L	75	0	64	1	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	3	0	0	0	0
8	C	3	0	0	0	0
9	A	56	0	92	8	0
9	B	56	0	92	8	0
9	C	56	0	92	7	0
9	D	56	0	92	8	0
10	A	498	0	726	45	0
10	C	498	0	726	50	0
10	E	76	0	102	16	0
10	G	76	0	102	16	0
11	A	3	0	0	0	0
11	C	3	0	0	0	0
All	All	22638	0	23188	580	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 13.

All (580) 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)
1:C:996:LEU:HD23	10:A:1109:PCW:H283	1.36	1.04
10:E:102:PCW:H461	10:G:102:PCW:H412	1.53	0.91
10:E:102:PCW:H462	9:A:1104:CLR:H241	1.54	0.88
1:C:791:LEU:HD13	10:C:1115:PCW:H261	1.55	0.88
1:A:791:LEU:HD13	10:A:1115:PCW:H261	1.55	0.86
9:C:1104:CLR:H273	10:C:1108:PCW:H442	1.60	0.83
9:A:1104:CLR:H273	10:A:1108:PCW:H442	1.60	0.83
1:A:245:PHE:HD1	1:A:246:SER:H	1.28	0.82
9:C:1104:CLR:H241	10:G:102:PCW:H462	1.63	0.81
10:C:1109:PCW:H283	1:A:996:LEU:HD23	1.63	0.81
1:C:245:PHE:HD1	1:C:246:SER:H	1.28	0.80
10:E:102:PCW:H261	10:G:102:PCW:H451	1.65	0.77
10:E:102:PCW:H412	10:G:102:PCW:H461	1.65	0.76
1:C:202:ASP:HB2	1:C:260:TYR:HB2	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ASP:HB2	1:A:260:TYR:HB2	1.68	0.75
1:C:165:VAL:HB	1:C:245:PHE:HZ	1.53	0.74
1:A:165:VAL:HB	1:A:245:PHE:HZ	1.53	0.74
2:D:176:CYS:SG	2:D:264:GLN:HG3	2.28	0.73
2:D:161:SER:HB3	2:D:163:LEU:HD12	1.69	0.73
1:C:165:VAL:HB	1:C:245:PHE:CZ	2.23	0.73
2:B:176:CYS:SG	2:B:264:GLN:HG3	2.28	0.73
10:C:1115:PCW:H262	9:D:501:CLR:H272	1.71	0.73
2:B:161:SER:HB3	2:B:163:LEU:HD12	1.69	0.72
1:A:165:VAL:HB	1:A:245:PHE:CZ	2.23	0.72
2:B:74:ALA:HB3	2:B:75:PRO:HD3	1.72	0.72
1:C:87:PRO:HD2	1:C:90:ILE:HD12	1.72	0.72
10:A:1115:PCW:H262	9:B:501:CLR:H272	1.71	0.71
1:C:426:ALA:HB2	1:C:460:ILE:HG21	1.72	0.71
1:A:339:THR:HG23	1:A:820:ILE:HD13	1.73	0.71
2:D:74:ALA:HB3	2:D:75:PRO:HD3	1.72	0.71
1:A:87:PRO:HD2	1:A:90:ILE:HD12	1.72	0.71
1:C:339:THR:HG23	1:C:820:ILE:HD13	1.73	0.71
10:E:102:PCW:H482	10:G:102:PCW:H382	1.73	0.70
1:A:411:PHE:HZ	1:A:463:CYS:HG	1.39	0.70
1:C:246:SER:HB3	1:C:267:MET:CB	2.22	0.70
1:A:246:SER:HB3	1:A:267:MET:CB	2.22	0.69
1:A:690:PHE:HB3	1:A:693:THR:HG21	1.75	0.69
1:A:426:ALA:HB2	1:A:460:ILE:HG21	1.73	0.69
10:A:1113:PCW:H472	10:A:1113:PCW:H283	1.75	0.69
1:C:1001:TYR:HD1	10:C:1107:PCW:H40	1.59	0.68
10:C:1113:PCW:H472	10:C:1113:PCW:H283	1.75	0.68
10:E:102:PCW:H483	9:A:1104:CLR:H221	1.74	0.68
1:C:690:PHE:HB3	1:C:693:THR:HG21	1.75	0.68
9:C:1105:CLR:H272	10:A:1107:PCW:H483	1.76	0.68
1:A:1001:TYR:HD1	10:A:1107:PCW:H40	1.58	0.68
1:C:713:ALA:HA	1:C:730:ILE:O	1.94	0.68
1:C:441:PRO:O	1:C:445:ARG:HG2	1.94	0.68
1:A:441:PRO:O	1:A:445:ARG:HG2	1.94	0.68
10:A:1110:PCW:H451	10:A:1110:PCW:H241	1.77	0.67
1:A:713:ALA:HA	1:A:730:ILE:O	1.94	0.67
1:C:343:CYS:SG	1:C:823:ALA:HB2	2.35	0.67
1:C:354:LYS:HD3	1:C:760:THR:HG21	1.77	0.67
1:A:354:LYS:HD3	1:A:760:THR:HG21	1.77	0.67
1:C:884:ILE:HD11	10:C:1113:PCW:H162	1.77	0.67
1:A:884:ILE:HD11	10:A:1113:PCW:H162	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1104:CLR:H272	10:G:102:PCW:H272	1.76	0.66
1:A:343:CYS:SG	1:A:823:ALA:HB2	2.35	0.66
10:C:1110:PCW:H241	10:C:1110:PCW:H451	1.77	0.66
1:C:789:PRO:HB3	1:C:801:PRO:HB2	1.78	0.65
9:C:1104:CLR:H272	10:E:102:PCW:H272	1.76	0.65
1:A:789:PRO:HB3	1:A:801:PRO:HB2	1.78	0.65
1:A:219:THR:O	1:A:695:PRO:HD2	1.96	0.65
1:C:860:ILE:HG12	2:D:47:LEU:HD21	1.79	0.65
1:C:127:ASN:OD1	1:C:127:ASN:N	2.27	0.65
1:A:860:ILE:HG12	2:B:47:LEU:HD21	1.79	0.65
1:C:411:PHE:HZ	1:C:463:CYS:HG	1.45	0.65
1:C:46:LEU:HD22	1:C:50:GLU:HG2	1.80	0.64
10:A:1111:PCW:H19	10:A:1112:PCW:H40	1.79	0.64
2:B:206:TYR:O	2:B:206:TYR:CD1	2.51	0.64
2:D:217:ALA:HB2	2:D:226:ILE:HD12	1.79	0.64
1:C:219:THR:O	1:C:695:PRO:HD2	1.96	0.64
1:C:575:GLU:HB3	1:C:576:PRO:HD2	1.80	0.64
10:C:1115:PCW:H262	9:D:501:CLR:C27	2.27	0.64
2:B:217:ALA:HB2	2:B:226:ILE:HD12	1.79	0.64
2:B:76:PRO:HG3	2:B:184:ILE:HD12	1.80	0.64
3:G:18:ARG:O	3:G:22:VAL:HG23	1.98	0.64
1:A:575:GLU:HB3	1:A:576:PRO:HD2	1.80	0.63
1:A:46:LEU:HD22	1:A:50:GLU:HG2	1.80	0.63
10:A:1115:PCW:H262	9:B:501:CLR:C27	2.28	0.63
1:A:90:ILE:O	1:A:94:ARG:HG2	1.99	0.63
2:D:206:TYR:O	2:D:206:TYR:CD1	2.51	0.63
10:A:1112:PCW:H282	3:G:32:VAL:HG11	1.81	0.63
1:C:90:ILE:O	1:C:94:ARG:HG2	1.98	0.63
10:C:1112:PCW:H282	3:E:32:VAL:HG11	1.81	0.63
10:E:102:PCW:H241	10:G:102:PCW:H471	1.80	0.63
1:C:241:ASN:H	1:C:241:ASN:HD22	1.47	0.63
10:C:1111:PCW:H19	10:C:1112:PCW:H40	1.79	0.63
2:D:231:TYR:HD1	2:D:263:ILE:HG12	1.64	0.63
3:E:18:ARG:O	3:E:22:VAL:HG23	1.98	0.62
2:D:213:LEU:HD23	2:D:261:LEU:HD13	1.81	0.62
1:A:127:ASN:OD1	1:A:127:ASN:N	2.27	0.62
1:A:241:ASN:HD22	1:A:241:ASN:H	1.47	0.62
1:A:246:SER:HB3	1:A:267:MET:HB2	1.82	0.62
2:B:213:LEU:HD23	2:B:261:LEU:HD13	1.81	0.62
2:B:231:TYR:HD1	2:B:263:ILE:HG12	1.64	0.62
1:C:241:ASN:HD22	1:C:241:ASN:N	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:648:LEU:O	1:A:650:ILE:HG23	2.00	0.62
2:D:209:TYR:HA	2:D:242:LEU:HD22	1.81	0.61
9:C:1105:CLR:H11	2:D:61:THR:HG21	1.82	0.61
2:B:209:TYR:HA	2:B:242:LEU:HD22	1.81	0.61
1:C:347:THR:OG1	1:C:768:ILE:HD13	2.00	0.61
2:D:76:PRO:HG3	2:D:184:ILE:HD12	1.80	0.61
1:A:44:HIS:HB3	1:A:242:ILE:HD11	1.83	0.61
1:A:241:ASN:HD22	1:A:241:ASN:N	1.98	0.61
9:D:502:CLR:H272	9:B:502:CLR:H272	1.83	0.61
2:B:56:GLN:HE22	2:B:59:LEU:HD12	1.66	0.61
1:C:59:LEU:HD12	1:C:60:THR:HG23	1.83	0.61
10:C:1109:PCW:H272	9:A:1105:CLR:H273	1.83	0.61
2:D:56:GLN:HE22	2:D:59:LEU:HD12	1.66	0.61
1:A:347:THR:OG1	1:A:768:ILE:HD13	2.00	0.61
1:C:44:HIS:HB3	1:C:242:ILE:HD11	1.83	0.61
1:C:225:GLN:HG2	1:C:484:SER:HB3	1.83	0.61
1:C:648:LEU:O	1:C:650:ILE:HG23	2.00	0.61
1:C:245:PHE:HD1	1:C:246:SER:N	1.98	0.60
1:A:225:GLN:HG2	1:A:484:SER:HB3	1.83	0.60
1:C:805:VAL:HG13	10:C:1110:PCW:H141	1.84	0.60
1:C:246:SER:HB3	1:C:267:MET:HB2	1.82	0.60
9:A:1105:CLR:H11	2:B:61:THR:HG21	1.83	0.60
1:C:863:LEU:HD12	2:D:47:LEU:HD22	1.83	0.60
1:A:59:LEU:HD12	1:A:60:THR:HG23	1.83	0.60
1:A:245:PHE:HD1	1:A:246:SER:N	1.98	0.60
1:C:244:PHE:CD1	1:C:266:VAL:HG21	2.37	0.59
1:A:863:LEU:HD12	2:B:47:LEU:HD22	1.83	0.59
1:C:992:PHE:HD2	10:C:1108:PCW:H271	1.67	0.59
3:E:21:VAL:O	3:E:25:ILE:HG12	2.02	0.59
1:A:992:PHE:HD2	10:A:1108:PCW:H271	1.67	0.59
1:A:244:PHE:CD1	1:A:266:VAL:HG21	2.37	0.59
10:E:102:PCW:C26	10:G:102:PCW:H451	2.32	0.59
1:A:774:LYS:HE2	1:A:940:ARG:HG3	1.85	0.59
1:A:805:VAL:HG13	10:A:1110:PCW:H141	1.84	0.59
1:A:982:PRO:HD3	3:G:20:ARG:HH21	1.68	0.59
1:A:722:SER:HB2	1:A:723:PRO:HD3	1.85	0.59
1:A:483:ASN:HB3	1:A:486:ASN:HB2	1.85	0.59
1:A:992:PHE:CD2	10:A:1108:PCW:H271	2.38	0.59
1:C:64:THR:HG23	1:C:67:ARG:HB2	1.85	0.58
1:C:982:PRO:HD3	3:E:20:ARG:HH21	1.68	0.58
1:C:483:ASN:HB3	1:C:486:ASN:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:SER:H	1:A:240:ARG:HB3	1.69	0.58
1:C:228:SER:H	1:C:240:ARG:HB3	1.68	0.58
2:B:64:ASP:N	2:B:64:ASP:OD1	2.36	0.58
2:B:75:PRO:HB2	2:B:294:ARG:HD3	1.86	0.58
1:C:421:LEU:HG	1:C:589:MET:HE2	1.84	0.58
3:G:21:VAL:O	3:G:25:ILE:HG12	2.02	0.58
1:C:722:SER:HB2	1:C:723:PRO:HD3	1.85	0.58
1:C:774:LYS:HE2	1:C:940:ARG:HG3	1.85	0.58
1:A:244:PHE:HD1	1:A:266:VAL:HG21	1.67	0.58
1:C:791:LEU:CD1	10:C:1115:PCW:H261	2.32	0.58
1:C:244:PHE:HD1	1:C:266:VAL:HG21	1.67	0.57
1:C:992:PHE:CD2	10:C:1108:PCW:H271	2.38	0.57
1:A:706:GLN:NE2	1:A:728:ALA:HA	2.19	0.57
2:D:64:ASP:N	2:D:64:ASP:OD1	2.36	0.57
10:E:102:PCW:H382	10:G:102:PCW:H482	1.86	0.57
1:C:441:PRO:HG2	1:C:444:LYS:HE3	1.87	0.57
1:C:492:ILE:HD12	1:C:578:PHE:CE1	2.40	0.57
1:A:64:THR:HG23	1:A:67:ARG:HB2	1.85	0.57
1:A:441:PRO:HG2	1:A:444:LYS:HE3	1.87	0.57
1:C:706:GLN:NE2	1:C:728:ALA:HA	2.19	0.57
9:C:1105:CLR:C27	10:A:1107:PCW:H483	2.34	0.57
2:D:75:PRO:HB2	2:D:294:ARG:HD3	1.86	0.57
10:A:1113:PCW:H341	2:B:55:ILE:HG21	1.87	0.57
1:A:492:ILE:HD12	1:A:578:PHE:CE1	2.40	0.56
1:A:114:ALA:HB2	1:A:321:VAL:HG11	1.87	0.56
1:A:246:SER:HB3	1:A:267:MET:HB3	1.87	0.56
1:C:246:SER:HB3	1:C:267:MET:HB3	1.87	0.56
1:A:739:SER:O	1:A:743:LYS:HG2	2.06	0.56
1:C:239:THR:OG1	1:C:241:ASN:ND2	2.39	0.56
1:A:421:LEU:HG	1:A:589:MET:HE2	1.87	0.56
1:C:880:PRO:HB2	10:C:1113:PCW:H141	1.87	0.56
1:A:880:PRO:HB2	10:A:1113:PCW:H141	1.87	0.56
1:A:791:LEU:CD1	10:A:1115:PCW:H261	2.31	0.55
1:C:715:THR:HA	1:C:732:VAL:O	2.06	0.55
1:A:239:THR:OG1	1:A:241:ASN:ND2	2.39	0.55
1:C:114:ALA:HB2	1:C:321:VAL:HG11	1.87	0.55
10:C:1113:PCW:H341	2:D:55:ILE:HG21	1.87	0.55
1:A:715:THR:HA	1:A:732:VAL:O	2.06	0.55
1:C:739:SER:O	1:C:743:LYS:HG2	2.06	0.55
1:A:424:ILE:HG21	1:A:555:PHE:HB3	1.89	0.55
1:C:621:PRO:HA	1:C:624:ALA:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:SER:OG	1:A:837:ARG:NH1	2.40	0.55
9:C:1104:CLR:H221	10:G:102:PCW:H483	1.89	0.55
2:D:92:SER:HA	2:D:304:LYS:O	2.07	0.55
1:C:369:SER:OG	1:C:837:ARG:NH1	2.40	0.54
1:C:848:ARG:HD2	1:C:1023:TYR:O	2.07	0.54
1:A:621:PRO:HA	1:A:624:ALA:HB3	1.89	0.54
1:C:694:SER:O	1:C:696:GLN:N	2.39	0.54
1:C:424:ILE:HG21	1:C:555:PHE:HB3	1.89	0.54
2:B:92:SER:HA	2:B:304:LYS:O	2.07	0.54
1:A:694:SER:O	1:A:696:GLN:N	2.39	0.54
1:A:474:ASN:HD21	1:A:496:GLU:CD	2.11	0.54
1:A:848:ARG:HD2	1:A:1023:TYR:O	2.07	0.54
1:C:474:ASN:HD21	1:C:496:GLU:CD	2.11	0.54
1:C:615:MET:HB2	1:C:633:ILE:CD1	2.38	0.54
1:C:615:MET:HB2	1:C:633:ILE:HD13	1.90	0.54
1:C:476:LYS:HD3	1:C:479:GLU:HB3	1.91	0.53
1:A:450:ASP:OD1	1:A:451:ALA:N	2.41	0.53
1:A:615:MET:HB2	1:A:633:ILE:CD1	2.38	0.53
1:A:131:TYR:CD2	10:A:1110:PCW:H31	2.44	0.53
1:C:515:LEU:HG	1:C:538:PHE:CE2	2.43	0.53
1:C:968:LEU:O	1:C:974:THR:HG21	2.08	0.53
3:E:17:TYR:O	3:E:21:VAL:HG23	2.09	0.53
1:A:997:ILE:HG12	10:A:1107:PCW:H472	1.90	0.53
1:A:515:LEU:HG	1:A:538:PHE:CE2	2.43	0.53
1:C:411:PHE:HZ	1:C:463:CYS:SG	2.32	0.53
1:A:218:LEU:HD12	1:A:266:VAL:HG11	1.91	0.53
1:A:968:LEU:O	1:A:974:THR:HG21	2.08	0.53
1:C:450:ASP:OD1	1:C:451:ALA:N	2.40	0.53
1:C:997:ILE:HG12	10:C:1107:PCW:H472	1.90	0.53
1:A:771:ASN:ND2	1:A:823:ALA:O	2.42	0.53
1:A:615:MET:HB2	1:A:633:ILE:HD13	1.90	0.52
1:C:515:LEU:HD11	1:C:535:LYS:HE2	1.91	0.52
1:C:218:LEU:HD12	1:C:266:VAL:HG11	1.91	0.52
10:C:1107:PCW:H271	2:D:47:LEU:CD2	2.38	0.52
1:A:429:ASN:O	1:A:471:ARG:NH2	2.42	0.52
10:A:1107:PCW:H271	2:B:47:LEU:CD2	2.38	0.52
1:A:245:PHE:HD2	1:A:265:THR:HG21	1.75	0.52
1:C:492:ILE:HG12	1:C:505:LEU:HB2	1.92	0.52
1:C:771:ASN:ND2	1:C:823:ALA:O	2.42	0.52
1:C:209:HIS:ND1	1:C:574:ASP:OD1	2.41	0.52
1:A:476:LYS:HD3	1:A:479:GLU:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:429:ASN:O	1:C:471:ARG:NH2	2.42	0.52
2:D:64:ASP:OD1	1:A:1011:ARG:NH2	2.43	0.52
1:A:57:THR:OG1	1:A:58:ASP:N	2.43	0.52
10:C:1115:PCW:H251	9:D:501:CLR:H242	1.92	0.52
1:C:245:PHE:HD2	1:C:265:THR:HG21	1.75	0.51
3:G:17:TYR:O	3:G:21:VAL:HG23	2.09	0.51
1:A:825:GLU:OE2	1:A:938:LYS:NZ	2.43	0.51
1:C:477:ILE:HG22	1:C:478:VAL:HG23	1.91	0.51
1:A:411:PHE:HZ	1:A:463:CYS:SG	2.32	0.51
10:A:1115:PCW:H251	9:B:501:CLR:H242	1.92	0.51
2:B:190:LYS:HB2	2:B:284:ASN:OD1	2.11	0.51
1:C:492:ILE:HD12	1:C:578:PHE:CD1	2.46	0.51
2:D:81:ALA:HB3	2:D:82:PRO:HD3	1.92	0.51
1:A:52:HIS:O	1:A:56:GLY:N	2.43	0.51
1:C:52:HIS:O	1:C:56:GLY:N	2.43	0.51
1:A:477:ILE:HG22	1:A:478:VAL:HG23	1.91	0.51
1:A:492:ILE:HD12	1:A:578:PHE:CD1	2.46	0.51
2:B:56:GLN:HG3	9:B:502:CLR:H6	1.93	0.51
1:A:515:LEU:HD11	1:A:535:LYS:HE2	1.92	0.51
1:C:131:TYR:CD2	10:C:1110:PCW:H31	2.44	0.51
2:D:190:LYS:HB2	2:D:284:ASN:OD1	2.11	0.51
1:A:411:PHE:N	1:A:411:PHE:CD1	2.79	0.51
1:A:209:HIS:ND1	1:A:574:ASP:OD1	2.41	0.50
1:A:492:ILE:HG12	1:A:505:LEU:HB2	1.92	0.50
1:C:1007:PHE:HZ	2:B:61:THR:HA	1.76	0.50
1:C:411:PHE:CD1	1:C:411:PHE:N	2.79	0.50
2:D:56:GLN:HG3	9:D:502:CLR:H6	1.93	0.50
1:C:997:ILE:HG21	10:C:1107:PCW:H261	1.93	0.50
1:C:57:THR:OG1	1:C:58:ASP:N	2.43	0.50
1:C:669:ASP:O	1:C:673:LEU:HG	2.11	0.50
1:C:732:VAL:HG11	1:C:758:ILE:HD11	1.94	0.50
2:D:279:LYS:HG3	2:D:296:ARG:HB3	1.94	0.50
1:A:732:VAL:HG11	1:A:758:ILE:HD11	1.94	0.50
10:C:1109:PCW:H251	1:A:993:PRO:HB3	1.94	0.50
1:A:240:ARG:NH2	1:A:485:THR:OG1	2.45	0.50
1:A:669:ASP:O	1:A:673:LEU:HG	2.12	0.50
1:A:997:ILE:HG21	10:A:1107:PCW:H261	1.93	0.50
2:B:81:ALA:HB3	2:B:82:PRO:HD3	1.93	0.50
1:C:240:ARG:NH2	1:C:485:THR:OG1	2.45	0.49
1:A:353:ARG:NH1	10:G:101:PCW:H52	2.27	0.49
1:C:565:TYR:HB3	1:C:571:PHE:HE2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1004:MET:SD	10:C:1107:PCW:H422	2.51	0.49
10:A:1113:PCW:H471	2:B:44:TYR:CE2	2.47	0.49
1:C:825:GLU:OE2	1:C:938:LYS:NZ	2.43	0.49
10:C:1107:PCW:H271	2:D:47:LEU:HD23	1.94	0.49
2:D:163:LEU:HD23	4:F:6:FUC:H61	1.94	0.49
1:C:85:THR:OG1	1:C:86:THR:N	2.46	0.49
1:A:80:LEU:HD11	1:A:267:MET:SD	2.52	0.49
1:A:1004:MET:SD	10:A:1107:PCW:H422	2.51	0.49
1:C:80:LEU:HD11	1:C:267:MET:SD	2.52	0.49
2:B:163:LEU:HD23	4:K:6:FUC:H61	1.94	0.49
10:A:1107:PCW:H271	2:B:47:LEU:HD23	1.94	0.49
10:E:102:PCW:H432	10:G:102:PCW:H432	1.95	0.49
2:B:279:LYS:HG3	2:B:296:ARG:HB3	1.94	0.49
1:A:565:TYR:HB3	1:A:571:PHE:HE2	1.77	0.49
10:C:1109:PCW:C28	9:A:1105:CLR:H273	2.43	0.48
10:C:1113:PCW:H471	2:D:44:TYR:CE2	2.47	0.48
1:A:972:PRO:HB3	10:A:1112:PCW:H11	1.96	0.48
1:C:476:LYS:HE2	1:C:493:HIS:CE1	2.49	0.48
2:D:28:ARG:HD3	2:D:32:SER:HB3	1.95	0.48
1:C:540:ASN:N	1:C:540:ASN:HD22	2.11	0.48
1:A:340:VAL:HG22	1:A:772:LEU:HD22	1.96	0.48
2:D:56:GLN:HG3	9:D:502:CLR:C6	2.44	0.48
2:D:61:THR:HA	1:A:1007:PHE:CZ	2.48	0.48
1:A:356:CYS:SG	1:A:757:SER:HB3	2.53	0.48
2:B:28:ARG:HD3	2:B:32:SER:HB3	1.95	0.48
2:B:56:GLN:HG3	9:B:502:CLR:C6	2.44	0.48
1:C:340:VAL:HG22	1:C:772:LEU:HD22	1.96	0.48
1:C:370:THR:HA	1:C:711:ILE:HB	1.96	0.48
1:A:476:LYS:HE2	1:A:493:HIS:CE1	2.49	0.48
1:A:517:ARG:HG2	1:A:517:ARG:HH11	1.79	0.48
10:C:1115:PCW:C26	9:D:501:CLR:H272	2.43	0.48
2:B:134:TYR:HE1	2:B:242:LEU:HG	1.79	0.48
1:C:517:ARG:HG2	1:C:517:ARG:HH11	1.79	0.48
1:C:768:ILE:HG13	1:C:768:ILE:O	2.13	0.48
2:B:215:CYS:SG	2:B:263:ILE:HD13	2.54	0.48
1:A:85:THR:OG1	1:A:86:THR:N	2.46	0.48
2:B:206:TYR:O	2:B:206:TYR:HD1	1.96	0.48
1:C:356:CYS:SG	1:C:757:SER:HB3	2.53	0.47
1:A:241:ASN:H	1:A:241:ASN:ND2	2.11	0.47
2:B:191:PRO:HG3	2:B:208:GLN:O	2.14	0.47
1:A:336:LEU:O	1:A:339:THR:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:768:ILE:O	1:A:768:ILE:HG13	2.13	0.47
1:C:353:ARG:NH1	10:E:101:PCW:H52	2.27	0.47
1:C:808:LEU:O	1:C:812:LEU:HB2	2.15	0.47
1:C:900:ASP:OD2	1:C:906:TRP:NE1	2.46	0.47
2:D:134:TYR:HE1	2:D:242:LEU:HG	1.79	0.47
2:D:203:GLN:HE21	2:D:203:GLN:HB2	1.57	0.47
1:A:218:LEU:O	1:A:720:ASN:ND2	2.47	0.47
1:A:540:ASN:N	1:A:540:ASN:HD22	2.11	0.47
2:D:265:PHE:HB3	2:D:268:LEU:CD1	2.45	0.47
1:A:492:ILE:HG13	1:A:505:LEU:HD13	1.96	0.47
2:D:81:ALA:HB2	2:D:178:VAL:HB	1.96	0.47
1:C:166:PRO:HD3	1:C:198:ARG:CB	2.45	0.47
1:C:972:PRO:HB3	10:C:1112:PCW:H11	1.95	0.47
1:A:166:PRO:HD3	1:A:198:ARG:CB	2.44	0.47
1:A:420:ALA:O	1:A:424:ILE:HG13	2.15	0.47
2:B:52:ILE:O	2:B:55:ILE:HG22	2.15	0.47
1:C:241:ASN:H	1:C:241:ASN:ND2	2.11	0.47
2:D:52:ILE:O	2:D:55:ILE:HG22	2.15	0.47
2:D:61:THR:HG22	1:A:1007:PHE:CZ	2.50	0.47
2:D:191:PRO:HG3	2:D:208:GLN:O	2.14	0.47
2:D:229:ILE:HD12	2:D:229:ILE:O	2.15	0.47
10:E:102:PCW:H261	10:G:102:PCW:C45	2.39	0.47
1:A:224:PRO:O	1:A:483:ASN:ND2	2.47	0.47
2:B:229:ILE:HD12	2:B:229:ILE:O	2.15	0.47
1:C:218:LEU:O	1:C:720:ASN:ND2	2.47	0.47
1:C:488:TYR:CE1	1:C:490:LEU:HD23	2.50	0.47
2:D:215:CYS:SG	2:D:263:ILE:HD13	2.54	0.47
10:E:102:PCW:H451	10:G:102:PCW:H261	1.97	0.47
1:A:370:THR:HA	1:A:711:ILE:HB	1.96	0.47
1:A:488:TYR:CE1	1:A:490:LEU:HD23	2.50	0.47
3:G:4:GLU:HB2	3:G:5:GLY:H	1.60	0.47
1:C:420:ALA:O	1:C:424:ILE:HG13	2.15	0.47
2:D:189:PRO:HG2	2:D:245:TYR:CD2	2.50	0.47
1:A:421:LEU:HD13	1:A:586:VAL:HG12	1.97	0.46
1:C:306:PHE:CZ	1:C:791:LEU:HD22	2.50	0.46
1:A:808:LEU:O	1:A:812:LEU:HB2	2.15	0.46
2:B:132:ALA:O	2:B:209:TYR:HB3	2.16	0.46
1:C:201:ALA:HB1	1:C:260:TYR:O	2.15	0.46
10:E:102:PCW:H461	10:G:102:PCW:C41	2.36	0.46
1:A:354:LYS:HD3	1:A:760:THR:CG2	2.46	0.46
2:B:122:SER:HA	2:B:123:PRO:HA	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:215:CYS:HA	2:B:278:CYS:HA	1.98	0.46
1:C:732:VAL:HG13	1:C:748:MET:HE2	1.97	0.46
2:D:215:CYS:HA	2:D:278:CYS:HA	1.98	0.46
1:A:218:LEU:O	1:A:696:GLN:HB2	2.16	0.46
1:A:425:ALA:HB2	1:A:589:MET:HE3	1.97	0.46
1:A:517:ARG:HH11	1:A:517:ARG:CG	2.28	0.46
2:B:265:PHE:HB3	2:B:268:LEU:CD1	2.45	0.46
1:A:48:LEU:HD21	1:A:59:LEU:HD22	1.98	0.46
1:A:111:CYS:SG	1:A:325:ILE:HD13	2.56	0.46
2:B:81:ALA:HB2	2:B:178:VAL:HB	1.96	0.46
1:C:510:ALA:O	1:C:514:ILE:HG12	2.16	0.46
1:C:997:ILE:HG21	10:C:1107:PCW:C26	2.46	0.46
2:D:132:ALA:O	2:D:209:TYR:HB3	2.16	0.46
1:C:596:ARG:HD2	1:C:754:ASN:OD1	2.16	0.46
1:A:201:ALA:HB1	1:A:260:TYR:O	2.15	0.46
1:C:336:LEU:O	1:C:339:THR:N	2.45	0.46
2:D:140:LEU:HD23	2:D:252:LEU:HD12	1.98	0.46
1:C:111:CYS:SG	1:C:325:ILE:HD13	2.56	0.46
1:C:424:ILE:HG22	1:C:555:PHE:HD2	1.81	0.46
2:B:140:LEU:HD23	2:B:252:LEU:HD12	1.98	0.46
1:C:224:PRO:O	1:C:483:ASN:ND2	2.47	0.45
1:C:517:ARG:HH11	1:C:517:ARG:CG	2.28	0.45
1:C:955:ILE:HA	1:C:958:LEU:HD12	1.98	0.45
1:A:51:LEU:HD13	1:A:204:ARG:HG3	1.98	0.45
1:A:306:PHE:CZ	1:A:791:LEU:HD22	2.50	0.45
1:A:955:ILE:HA	1:A:958:LEU:HD12	1.99	0.45
10:A:1107:PCW:H262	2:B:50:ILE:HD12	1.98	0.45
1:C:503:TYR:CE2	1:C:567:GLU:HA	2.52	0.45
1:C:945:PHE:HD1	10:C:1108:PCW:H121	1.81	0.45
2:D:61:THR:HA	1:A:1007:PHE:HZ	1.81	0.45
1:A:596:ARG:HD2	1:A:754:ASN:OD1	2.16	0.45
1:C:218:LEU:O	1:C:696:GLN:HB2	2.16	0.45
1:C:492:ILE:HG13	1:C:505:LEU:HD13	1.96	0.45
10:C:1115:PCW:H322	2:D:16:PHE:HE2	1.81	0.45
1:A:261:THR:O	1:A:264:ARG:NE	2.47	0.45
1:A:945:PHE:HD1	10:A:1108:PCW:H121	1.80	0.45
1:A:424:ILE:HG22	1:A:555:PHE:HD2	1.81	0.45
1:C:421:LEU:HD13	1:C:586:VAL:HG12	1.97	0.45
1:C:425:ALA:HB2	1:C:589:MET:HE3	1.99	0.45
10:C:1107:PCW:H262	2:D:50:ILE:HD12	1.98	0.45
2:D:99:TYR:O	2:D:103:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:699:LEU:HD13	1:A:724:ALA:HA	1.98	0.45
10:A:1113:PCW:H481	9:B:501:CLR:H25	1.99	0.45
2:B:189:PRO:HG2	2:B:245:TYR:CD2	2.50	0.45
2:B:299:VAL:HG12	2:B:301:ILE:HG13	1.99	0.45
1:A:732:VAL:HG13	1:A:748:MET:HE2	1.98	0.45
2:B:99:TYR:O	2:B:103:VAL:HG23	2.16	0.45
1:C:48:LEU:HD21	1:C:59:LEU:HD22	1.98	0.45
1:C:354:LYS:HD3	1:C:760:THR:CG2	2.46	0.45
10:C:1113:PCW:H481	9:D:501:CLR:H25	1.99	0.45
2:D:299:VAL:HG12	2:D:301:ILE:HG13	1.99	0.45
2:B:265:PHE:HB3	2:B:268:LEU:HD12	1.99	0.45
1:C:164:MET:HG2	1:C:267:MET:CE	2.47	0.45
1:C:166:PRO:HD3	1:C:198:ARG:HB2	1.99	0.45
1:A:503:TYR:CE2	1:A:567:GLU:HA	2.52	0.45
1:C:609:ALA:O	1:C:835:GLN:HA	2.17	0.45
1:A:166:PRO:HD3	1:A:198:ARG:HB2	1.99	0.45
1:A:711:ILE:HA	1:A:729:ASP:OD2	2.17	0.45
1:C:863:LEU:HD23	1:C:863:LEU:HA	1.83	0.44
2:D:114:ASN:OD1	2:D:154:ARG:NH1	2.50	0.44
1:A:530:LEU:O	1:A:530:LEU:HG	2.17	0.44
1:A:900:ASP:OD2	1:A:906:TRP:NE1	2.46	0.44
1:A:997:ILE:HG21	10:A:1107:PCW:C26	2.46	0.44
1:C:55:TYR:OH	1:C:259:VAL:HG13	2.17	0.44
1:C:530:LEU:O	1:C:530:LEU:HG	2.18	0.44
1:A:510:ALA:O	1:A:514:ILE:HG12	2.16	0.44
1:C:51:LEU:HD13	1:C:204:ARG:HG3	1.98	0.44
1:A:181:ASN:HB3	1:A:184:PHE:CD2	2.53	0.44
2:D:265:PHE:HB3	2:D:268:LEU:HD12	1.99	0.44
1:A:164:MET:HG2	1:A:267:MET:CE	2.47	0.44
1:A:488:TYR:C	1:A:488:TYR:HD1	2.21	0.44
10:A:1115:PCW:H322	2:B:16:PHE:HE2	1.81	0.44
10:C:1113:PCW:H262	10:C:1113:PCW:H452	2.00	0.44
1:A:245:PHE:CD1	1:A:246:SER:N	2.82	0.44
1:A:609:ALA:O	1:A:835:GLN:HA	2.17	0.44
1:C:711:ILE:HA	1:C:729:ASP:OD2	2.17	0.44
2:D:120:GLY:O	2:D:151:ARG:NH2	2.51	0.44
2:D:224:GLU:H	2:D:224:GLU:HG3	1.45	0.44
1:A:488:TYR:C	1:A:488:TYR:CD1	2.91	0.44
10:A:1113:PCW:H452	10:A:1113:PCW:H262	2.00	0.44
1:C:181:ASN:HB3	1:C:184:PHE:CD2	2.53	0.44
1:C:488:TYR:HD1	1:C:488:TYR:C	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:1113:PCW:O2P	10:C:1113:PCW:H52	2.18	0.44
2:B:120:GLY:O	2:B:151:ARG:NH2	2.50	0.44
1:C:488:TYR:C	1:C:488:TYR:CD1	2.91	0.43
2:D:107:HIS:O	2:D:111:ASP:HB2	2.18	0.43
1:A:55:TYR:OH	1:A:259:VAL:HG13	2.17	0.43
10:A:1107:PCW:C40	10:A:1107:PCW:H20	2.48	0.43
2:B:15:LYS:C	2:B:17:LEU:H	2.22	0.43
1:C:699:LEU:HD13	1:C:724:ALA:HA	1.98	0.43
2:D:265:PHE:CZ	2:D:276:ILE:HD12	2.53	0.43
1:A:697:GLN:O	1:A:700:ILE:HB	2.19	0.43
1:C:160:SER:HB3	1:C:741:VAL:HG22	2.00	0.43
1:C:824:TYR:HB2	1:C:951:ASN:HD21	1.83	0.43
2:D:15:LYS:C	2:D:17:LEU:H	2.22	0.43
1:A:596:ARG:HB2	1:A:599:VAL:HG23	2.00	0.43
1:C:469:GLY:O	1:C:473:ARG:HB2	2.18	0.43
1:A:673:LEU:HD23	1:A:673:LEU:HA	1.85	0.43
2:B:114:ASN:OD1	2:B:154:ARG:NH1	2.50	0.43
2:B:265:PHE:CZ	2:B:276:ILE:HD12	2.53	0.43
1:C:810:ILE:HD13	1:C:810:ILE:HA	1.86	0.43
10:C:1107:PCW:H20	10:C:1107:PCW:C40	2.48	0.43
1:A:160:SER:HB3	1:A:741:VAL:HG22	2.00	0.43
1:A:824:TYR:HB2	1:A:951:ASN:HD21	1.83	0.43
1:C:697:GLN:O	1:C:700:ILE:HB	2.19	0.43
1:C:1000:LEU:HD11	10:C:1109:PCW:H39	2.01	0.43
10:C:1109:PCW:C27	9:A:1105:CLR:H273	2.46	0.43
1:A:1000:LEU:HD11	10:A:1109:PCW:H39	2.01	0.43
2:B:78:LEU:HD12	2:B:78:LEU:HA	1.93	0.43
1:A:110:LEU:HD12	1:A:110:LEU:HA	1.85	0.43
10:A:1115:PCW:C26	9:B:501:CLR:H272	2.43	0.43
1:C:374:CYS:HB2	1:C:714:VAL:HG22	1.99	0.43
1:A:511:PRO:O	1:A:515:LEU:HB2	2.19	0.43
1:C:814:THR:HB	1:C:961:GLU:HG3	2.01	0.43
1:A:863:LEU:HD23	1:A:863:LEU:HA	1.82	0.43
1:A:977:ALA:HA	10:A:1110:PCW:O31	2.19	0.43
2:B:107:HIS:O	2:B:111:ASP:HB2	2.18	0.43
1:A:374:CYS:HB2	1:A:714:VAL:HG22	2.00	0.42
1:A:469:GLY:O	1:A:473:ARG:HB2	2.18	0.42
1:A:997:ILE:HG21	10:A:1107:PCW:H272	2.00	0.42
10:A:1113:PCW:O31	2:B:56:GLN:NE2	2.52	0.42
10:C:1112:PCW:H261	3:E:32:VAL:HG21	2.01	0.42
1:A:814:THR:HB	1:A:961:GLU:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:93:ILE:HB	2:B:305:SER:OG	2.19	0.42
2:B:225:LYS:HD2	2:B:272:MET:SD	2.59	0.42
2:D:93:ILE:HB	2:D:305:SER:OG	2.19	0.42
1:C:997:ILE:HG21	10:C:1107:PCW:H272	2.00	0.42
2:D:206:TYR:O	2:D:206:TYR:HD1	1.96	0.42
2:B:74:ALA:CB	2:B:75:PRO:HD3	2.45	0.42
2:B:193:LYS:O	2:B:198:LEU:HD13	2.19	0.42
1:C:324:LEU:HD22	1:C:324:LEU:HA	1.90	0.42
1:C:501:SER:O	1:C:501:SER:OG	2.35	0.42
1:C:665:VAL:HB	1:C:690:PHE:CD1	2.55	0.42
1:A:378:THR:HG22	1:A:384:ASN:HD21	1.84	0.42
1:C:596:ARG:HB2	1:C:599:VAL:HG23	2.01	0.42
2:D:160:CYS:SG	2:D:262:ALA:HB1	2.60	0.42
1:A:353:ARG:HH12	10:G:101:PCW:H52	1.84	0.42
1:A:810:ILE:HD13	1:A:810:ILE:HA	1.86	0.42
10:A:1112:PCW:H261	3:G:32:VAL:HG21	2.01	0.42
10:A:1113:PCW:O2P	10:A:1113:PCW:H52	2.18	0.42
1:C:482:PHE:HB2	1:C:489:GLN:HG3	2.01	0.42
2:D:225:LYS:HD2	2:D:272:MET:SD	2.59	0.42
1:A:482:PHE:HB2	1:A:489:GLN:HG3	2.02	0.42
1:A:665:VAL:HB	1:A:690:PHE:CD1	2.55	0.42
2:B:167:THR:HG22	2:B:169:GLY:H	1.84	0.42
2:D:74:ALA:CB	2:D:75:PRO:HD3	2.45	0.42
2:D:146:GLN:NE2	2:D:251:ARG:O	2.53	0.42
1:C:223:GLU:HB3	1:C:484:SER:HB2	2.02	0.42
1:A:46:LEU:HD23	1:A:46:LEU:HA	1.80	0.42
1:A:383:GLN:C	1:A:385:ARG:H	2.24	0.42
1:C:150:GLN:HG3	1:C:361:LEU:HD23	2.02	0.41
1:C:383:GLN:C	1:C:385:ARG:H	2.24	0.41
1:C:666:HIS:CD2	1:C:692:ARG:HB2	2.55	0.41
2:D:193:LYS:O	2:D:198:LEU:HD13	2.19	0.41
10:C:1113:PCW:O31	2:D:56:GLN:NE2	2.52	0.41
2:D:167:THR:HG21	2:D:171:ALA:HB2	2.02	0.41
1:A:494:GLU:HG2	1:A:503:TYR:HE1	1.85	0.41
1:A:666:HIS:CD2	1:A:692:ARG:HB2	2.55	0.41
1:A:750:LEU:HD11	1:A:758:ILE:CD1	2.50	0.41
2:B:160:CYS:SG	2:B:262:ALA:HB1	2.60	0.41
1:C:241:ASN:N	1:C:241:ASN:ND2	2.67	0.41
1:C:261:THR:O	1:C:264:ARG:NE	2.47	0.41
2:D:167:THR:HG22	2:D:169:GLY:H	1.85	0.41
1:A:457:LEU:HD12	1:A:467:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:TYR:HD1	1:A:488:TYR:O	2.04	0.41
1:A:540:ASN:HD22	1:A:540:ASN:H	1.68	0.41
1:C:494:GLU:HG2	1:C:503:TYR:HE1	1.85	0.41
1:C:540:ASN:HD22	1:C:540:ASN:H	1.68	0.41
1:A:515:LEU:CD1	1:A:535:LYS:HE2	2.51	0.41
1:A:575:GLU:HB3	1:A:576:PRO:CD	2.49	0.41
2:B:154:ARG:HB3	2:B:163:LEU:HD11	2.03	0.41
1:C:750:LEU:HD11	1:C:758:ILE:CD1	2.50	0.41
1:C:993:PRO:HA	10:A:1109:PCW:H271	2.01	0.41
10:C:1113:PCW:H411	10:C:1113:PCW:H381	1.80	0.41
2:D:213:LEU:HD12	2:D:214:ARG:N	2.34	0.41
2:D:284:ASN:OD1	2:D:284:ASN:N	2.53	0.41
1:A:312:ILE:HD13	1:A:312:ILE:HA	1.89	0.41
1:A:497:LYS:HD3	1:A:497:LYS:HA	1.77	0.41
1:A:551:ARG:NE	1:A:619:ASP:OD2	2.39	0.41
2:B:167:THR:HG21	2:B:171:ALA:HB2	2.02	0.41
2:B:213:LEU:HD12	2:B:214:ARG:N	2.34	0.41
1:C:378:THR:HG22	1:C:384:ASN:HD21	1.84	0.41
1:C:457:LEU:HD12	1:C:467:VAL:HG21	2.02	0.41
10:C:1113:PCW:H471	2:D:44:TYR:CD2	2.56	0.41
1:A:150:GLN:HG3	1:A:361:LEU:HD23	2.02	0.41
1:A:359:LYS:NZ	1:A:744:GLN:HA	2.35	0.41
1:A:1019:GLN:HE21	1:A:1019:GLN:HB3	1.69	0.41
1:C:515:LEU:CD1	1:C:535:LYS:HE2	2.50	0.41
1:C:548:LEU:HB3	1:C:550:GLU:HG3	2.03	0.41
1:A:307:PHE:CD1	1:A:324:LEU:HD23	2.55	0.41
1:A:817:VAL:HB	1:A:818:PRO:HD3	2.03	0.41
2:B:146:GLN:NE2	2:B:251:ARG:O	2.53	0.41
2:B:195:THR:HG22	2:B:196:THR:N	2.36	0.41
2:B:224:GLU:H	2:B:224:GLU:HG3	1.45	0.41
1:C:245:PHE:CD1	1:C:246:SER:N	2.82	0.41
1:C:353:ARG:HH12	10:E:101:PCW:H52	1.84	0.41
1:C:511:PRO:O	1:C:515:LEU:HB2	2.19	0.41
2:D:154:ARG:HB3	2:D:163:LEU:HD11	2.03	0.41
1:A:772:LEU:HD23	1:A:772:LEU:HA	1.94	0.41
1:A:912:LYS:HD3	1:A:912:LYS:HA	1.88	0.41
5:L:2:NAG:O7	5:L:2:NAG:C3	2.69	0.41
1:C:307:PHE:CD1	1:C:324:LEU:HD23	2.55	0.41
1:C:817:VAL:HB	1:C:818:PRO:HD3	2.03	0.41
1:C:873:LEU:HD23	1:C:873:LEU:HA	1.94	0.41
10:C:1113:PCW:H181	10:C:1113:PCW:H211	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:195:THR:HG22	2:D:196:THR:N	2.36	0.41
2:B:284:ASN:OD1	2:B:284:ASN:N	2.54	0.41
1:C:977:ALA:HA	10:C:1110:PCW:O31	2.20	0.41
10:C:1111:PCW:H381	10:C:1111:PCW:H411	1.89	0.41
1:A:52:HIS:CE1	1:A:257:VAL:HG21	2.56	0.41
1:A:483:ASN:HD22	1:A:483:ASN:HA	1.60	0.41
10:A:1113:PCW:H471	2:B:44:TYR:CD2	2.56	0.41
2:B:105:SER:O	2:B:106:MET:C	2.58	0.41
2:B:276:ILE:HG13	2:B:276:ILE:O	2.21	0.41
5:H:2:NAG:O7	5:H:2:NAG:C3	2.69	0.41
1:C:52:HIS:CE1	1:C:257:VAL:HG21	2.56	0.40
1:C:1019:GLN:HE21	1:C:1019:GLN:HB3	1.69	0.40
1:C:359:LYS:NZ	1:C:744:GLN:HA	2.35	0.40
1:C:699:LEU:HD22	1:C:723:PRO:HB2	2.03	0.40
1:A:218:LEU:O	1:A:218:LEU:HD23	2.21	0.40
1:A:223:GLU:HB3	1:A:484:SER:HB2	2.02	0.40
1:A:434:GLN:O	1:A:437:GLN:HG2	2.22	0.40
1:C:1001:TYR:CD1	10:C:1107:PCW:H40	2.48	0.40
2:D:105:SER:O	2:D:106:MET:C	2.58	0.40
1:A:997:ILE:HG21	10:A:1107:PCW:C27	2.52	0.40
1:C:169:ALA:O	1:C:179:THR:HA	2.21	0.40
1:C:735:GLY:HA3	1:C:750:LEU:O	2.21	0.40
2:D:105:SER:O	2:D:108:LYS:N	2.54	0.40
2:D:276:ILE:HG13	2:D:276:ILE:O	2.21	0.40
1:A:169:ALA:O	1:A:179:THR:HA	2.21	0.40
1:A:548:LEU:HB3	1:A:550:GLU:HG3	2.03	0.40
1:C:997:ILE:HG21	10:C:1107:PCW:C27	2.51	0.40
1:A:91:LYS:O	1:A:95:GLN:HG2	2.21	0.40
1:A:473:ARG:O	1:A:474:ASN:ND2	2.55	0.40
1:A:699:LEU:HD22	1:A:723:PRO:HB2	2.03	0.40
1:A:974:THR:HG22	1:A:974:THR:O	2.22	0.40
2:B:105:SER:O	2:B:108:LYS:N	2.54	0.40
2:B:135:ILE:HD11	2:B:137:ARG:HD3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	991/1028 (96%)	894 (90%)	90 (9%)	7 (1%)	19	50
1	C	991/1028 (96%)	894 (90%)	90 (9%)	7 (1%)	19	50
2	B	292/305 (96%)	254 (87%)	36 (12%)	2 (1%)	19	50
2	D	292/305 (96%)	254 (87%)	36 (12%)	2 (1%)	19	50
3	E	38/94 (40%)	32 (84%)	6 (16%)	0	100	100
3	G	38/94 (40%)	32 (84%)	6 (16%)	0	100	100
All	All	2642/2854 (93%)	2360 (89%)	264 (10%)	18 (1%)	21	50

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	695	PRO
1	A	695	PRO
1	C	988	TRP
2	D	155	MET
1	A	384	ASN
1	A	988	TRP
2	B	155	MET
1	C	384	ASN
1	C	985	PRO
2	D	16	PHE
1	A	985	PRO
2	B	16	PHE
1	C	336	LEU
1	A	336	LEU
1	C	166	PRO
1	C	570	PRO
1	A	166	PRO
1	A	570	PRO

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	841/869 (97%)	761 (90%)	80 (10%)	7	25
1	C	841/869 (97%)	761 (90%)	80 (10%)	7	25
2	B	258/266 (97%)	222 (86%)	36 (14%)	3	13
2	D	258/266 (97%)	222 (86%)	36 (14%)	3	13
3	E	33/75 (44%)	30 (91%)	3 (9%)	7	27
3	G	33/75 (44%)	30 (91%)	3 (9%)	7	27
All	All	2264/2420 (94%)	2026 (90%)	238 (10%)	8	21

All (238) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	34	GLU
1	C	42	ASP
1	C	51	LEU
1	C	57	THR
1	C	60	THR
1	C	63	LEU
1	C	64	THR
1	C	65	ASN
1	C	79	SER
1	C	89	TRP
1	C	110	LEU
1	C	127	ASN
1	C	128	ASP
1	C	129	ASN
1	C	156	ARG
1	C	167	GLN
1	C	231	PHE
1	C	241	ASN
1	C	245	PHE
1	C	248	ASN
1	C	261	THR
1	C	263	ASP

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Mol	Chain	Res	Type
1	C	267	MET
1	C	284	ILE
1	C	291	PHE
1	C	324	LEU
1	C	343	CYS
1	C	344	LEU
1	C	367	LEU
1	C	385	ARG
1	C	411	PHE
1	C	415	SER
1	C	434	GLN
1	C	440	VAL
1	C	445	ARG
1	C	453	GLU
1	C	470	MET
1	C	483	ASN
1	C	485	THR
1	C	488	TYR
1	C	493	HIS
1	C	497	LYS
1	C	500	GLU
1	C	515	LEU
1	C	522	LEU
1	C	538	PHE
1	C	540	ASN
1	C	548	LEU
1	C	557	HIS
1	C	571	PHE
1	C	607	ARG
1	C	608	SER
1	C	670	LEU
1	C	678	LEU
1	C	692	ARG
1	C	698	LYS
1	C	708	GLN
1	C	726	LYS
1	C	734	MET
1	C	794	ILE
1	C	806	THR
1	C	811	ASP
1	C	822	LEU
1	C	832	MET

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Mol	Chain	Res	Type
1	C	833	LYS
1	C	834	ARG
1	C	837	ARG
1	C	846	ASN
1	C	847	GLU
1	C	859	MET
1	C	872	ILE
1	C	894	TRP
1	C	901	SER
1	C	923	PHE
1	C	943	SER
1	C	952	LYS
1	C	975	ASP
1	C	986	SER
1	C	1007	PHE
1	C	1011	ARG
2	D	20	SER
2	D	26	LEU
2	D	28	ARG
2	D	32	SER
2	D	64	ASP
2	D	65	PHE
2	D	73	VAL
2	D	79	SER
2	D	94	SER
2	D	135	ILE
2	D	137	ARG
2	D	144	GLN
2	D	154	ARG
2	D	156	TRP
2	D	157	LEU
2	D	160	CYS
2	D	161	SER
2	D	167	THR
2	D	196	THR
2	D	197	ASP
2	D	200	GLU
2	D	203	GLN
2	D	211	LEU
2	D	214	ARG
2	D	218	LYS
2	D	251	ARG

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Mol	Chain	Res	Type
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	287	TYR
2	D	289	GLU
2	D	292	ARG
2	D	294	ARG
3	E	13	THR
3	E	33	ILE
3	E	42	LYS
1	A	34	GLU
1	A	42	ASP
1	A	51	LEU
1	A	57	THR
1	A	60	THR
1	A	63	LEU
1	A	64	THR
1	A	65	ASN
1	A	79	SER
1	A	89	TRP
1	A	110	LEU
1	A	127	ASN
1	A	128	ASP
1	A	129	ASN
1	A	156	ARG
1	A	167	GLN
1	A	231	PHE
1	A	241	ASN
1	A	245	PHE
1	A	248	ASN
1	A	261	THR
1	A	263	ASP
1	A	267	MET
1	A	284	ILE
1	A	291	PHE
1	A	324	LEU
1	A	343	CYS
1	A	344	LEU
1	A	367	LEU

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Mol	Chain	Res	Type
1	A	385	ARG
1	A	411	PHE
1	A	415	SER
1	A	434	GLN
1	A	440	VAL
1	A	445	ARG
1	A	453	GLU
1	A	470	MET
1	A	483	ASN
1	A	485	THR
1	A	488	TYR
1	A	493	HIS
1	A	497	LYS
1	A	500	GLU
1	A	515	LEU
1	A	522	LEU
1	A	538	PHE
1	A	540	ASN
1	A	548	LEU
1	A	557	HIS
1	A	571	PHE
1	A	607	ARG
1	A	608	SER
1	A	670	LEU
1	A	678	LEU
1	A	692	ARG
1	A	698	LYS
1	A	708	GLN
1	A	726	LYS
1	A	734	MET
1	A	794	ILE
1	A	806	THR
1	A	811	ASP
1	A	822	LEU
1	A	832	MET
1	A	833	LYS
1	A	834	ARG
1	A	837	ARG
1	A	846	ASN
1	A	847	GLU
1	A	859	MET
1	A	872	ILE

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Mol	Chain	Res	Type
1	A	894	TRP
1	A	901	SER
1	A	923	PHE
1	A	943	SER
1	A	952	LYS
1	A	975	ASP
1	A	986	SER
1	A	1007	PHE
1	A	1011	ARG
2	B	20	SER
2	B	26	LEU
2	B	28	ARG
2	B	32	SER
2	B	64	ASP
2	B	65	PHE
2	B	73	VAL
2	B	79	SER
2	B	94	SER
2	B	135	ILE
2	B	137	ARG
2	B	144	GLN
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	196	THR
2	B	197	ASP
2	B	200	GLU
2	B	203	GLN
2	B	211	LEU
2	B	214	ARG
2	B	218	LYS
2	B	251	ARG
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	287	TYR

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Mol	Chain	Res	Type
2	B	289	GLU
2	B	292	ARG
2	B	294	ARG
3	G	13	THR
3	G	33	ILE
3	G	42	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	129	ASN
1	C	241	ASN
1	C	434	GLN
1	C	474	ASN
1	C	483	ASN
1	C	486	ASN
1	C	489	GLN
1	C	540	ASN
1	C	557	HIS
1	C	566	ASN
1	C	620	HIS
1	C	696	GLN
1	C	720	ASN
1	C	744	GLN
1	C	904	GLN
2	D	56	GLN
2	D	203	GLN
1	A	129	ASN
1	A	241	ASN
1	A	434	GLN
1	A	474	ASN
1	A	483	ASN
1	A	486	ASN
1	A	489	GLN
1	A	540	ASN
1	A	557	HIS
1	A	566	ASN
1	A	620	HIS
1	A	696	GLN
1	A	720	ASN
1	A	744	GLN
1	A	904	GLN

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Mol	Chain	Res	Type
1	A	1019	GLN
2	B	56	GLN
2	B	203	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

38 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	F	1	4,2	14,14,15	1.25	2 (14%)	17,19,21	1.32	1 (5%)
4	NAG	F	2	4	14,14,15	0.21	0	17,19,21	0.63	1 (5%)
4	BMA	F	3	4	11,11,12	0.80	0	15,15,17	1.41	2 (13%)
4	MAN	F	4	4	11,11,12	0.75	0	15,15,17	0.98	2 (13%)
4	MAN	F	5	4	11,11,12	0.71	0	15,15,17	0.93	2 (13%)
4	FUC	F	6	4	10,10,11	1.06	1 (10%)	14,14,16	0.75	0
5	NAG	H	1	2,5	14,14,15	0.62	1 (7%)	17,19,21	1.17	2 (11%)
5	NAG	H	2	5	14,14,15	0.35	0	17,19,21	1.55	2 (11%)
5	BMA	H	3	5	11,11,12	1.25	1 (9%)	15,15,17	1.05	1 (6%)
5	MAN	H	4	5	11,11,12	1.47	2 (18%)	15,15,17	1.38	2 (13%)
5	NAG	H	5	5	14,14,15	0.67	0	17,19,21	0.91	1 (5%)
5	MAN	H	6	5	11,11,12	0.75	0	15,15,17	0.95	2 (13%)
6	NAG	I	1	2,6	14,14,15	0.87	1 (7%)	17,19,21	1.64	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	I	2	6	14,14,15	0.19	0	17,19,21	0.65	1 (5%)
6	BMA	I	3	6	11,11,12	0.61	0	15,15,17	1.35	2 (13%)
6	MAN	I	4	6	11,11,12	0.67	0	15,15,17	0.97	2 (13%)
6	FUC	I	5	6	10,10,11	1.01	1 (10%)	14,14,16	0.74	0
7	NAG	J	1	7,2	14,14,15	0.50	0	17,19,21	0.63	0
7	NAG	J	2	7	14,14,15	0.19	0	17,19,21	0.38	0
4	NAG	K	1	4,2	14,14,15	1.26	2 (14%)	17,19,21	1.31	1 (5%)
4	NAG	K	2	4	14,14,15	0.22	0	17,19,21	0.63	1 (5%)
4	BMA	K	3	4	11,11,12	0.80	0	15,15,17	1.41	2 (13%)
4	MAN	K	4	4	11,11,12	0.74	0	15,15,17	0.98	2 (13%)
4	MAN	K	5	4	11,11,12	0.71	0	15,15,17	0.93	1 (6%)
4	FUC	K	6	4	10,10,11	1.05	1 (10%)	14,14,16	0.75	0
5	NAG	L	1	2,5	14,14,15	0.62	1 (7%)	17,19,21	1.16	2 (11%)
5	NAG	L	2	5	14,14,15	0.35	0	17,19,21	1.55	2 (11%)
5	BMA	L	3	5	11,11,12	1.26	1 (9%)	15,15,17	1.06	1 (6%)
5	MAN	L	4	5	11,11,12	1.47	2 (18%)	15,15,17	1.38	2 (13%)
5	NAG	L	5	5	14,14,15	0.65	0	17,19,21	0.90	1 (5%)
5	MAN	L	6	5	11,11,12	0.74	0	15,15,17	0.96	2 (13%)
6	NAG	M	1	2,6	14,14,15	0.87	1 (7%)	17,19,21	1.63	1 (5%)
6	NAG	M	2	6	14,14,15	0.20	0	17,19,21	0.64	1 (5%)
6	BMA	M	3	6	11,11,12	0.61	0	15,15,17	1.35	2 (13%)
6	MAN	M	4	6	11,11,12	0.66	0	15,15,17	0.98	2 (13%)
6	FUC	M	5	6	10,10,11	1.01	1 (10%)	14,14,16	0.74	0
7	NAG	N	1	7,2	14,14,15	0.49	0	17,19,21	0.63	0
7	NAG	N	2	7	14,14,15	0.20	0	17,19,21	0.38	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

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

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	1	NAG	O5-C1	4.20	1.50	1.43
4	F	1	NAG	O5-C1	4.18	1.50	1.43
5	L	4	MAN	O2-C2	3.13	1.50	1.43
5	H	4	MAN	O2-C2	3.12	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	6	FUC	O5-C1	-2.79	1.39	1.43
4	K	6	FUC	O5-C1	-2.75	1.39	1.43
6	I	1	NAG	O5-C1	2.65	1.48	1.43
6	M	1	NAG	O5-C1	2.63	1.47	1.43
6	I	5	FUC	O5-C1	-2.39	1.39	1.43
6	M	5	FUC	O5-C1	-2.37	1.39	1.43
5	L	4	MAN	C1-C2	2.29	1.57	1.52
5	H	4	MAN	C1-C2	2.27	1.57	1.52
5	L	3	BMA	C2-C3	2.25	1.55	1.52
5	H	3	BMA	C2-C3	2.22	1.55	1.52
5	H	1	NAG	C1-C2	2.05	1.55	1.52
4	K	1	NAG	C1-C2	2.04	1.55	1.52
5	L	1	NAG	C1-C2	2.04	1.55	1.52
4	F	1	NAG	C1-C2	2.02	1.55	1.52

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	1	NAG	C1-O5-C5	6.24	120.65	112.19
6	M	1	NAG	C1-O5-C5	6.19	120.58	112.19
4	F	1	NAG	C1-O5-C5	4.98	118.94	112.19
4	K	1	NAG	C1-O5-C5	4.96	118.92	112.19
5	H	2	NAG	C1-O5-C5	4.37	118.11	112.19
5	L	2	NAG	C1-O5-C5	4.35	118.08	112.19
5	H	4	MAN	O2-C2-C1	4.26	117.88	109.15
5	L	4	MAN	O2-C2-C1	4.25	117.85	109.15
5	L	2	NAG	C2-N2-C7	3.98	128.57	122.90
5	H	2	NAG	C2-N2-C7	3.97	128.56	122.90
5	H	5	NAG	C1-O5-C5	3.57	117.03	112.19
5	L	5	NAG	C1-O5-C5	3.56	117.02	112.19
5	L	3	BMA	O3-C3-C2	3.22	116.17	109.99
5	H	3	BMA	O3-C3-C2	3.21	116.14	109.99
5	H	1	NAG	O4-C4-C5	3.10	116.98	109.30
5	L	1	NAG	O4-C4-C5	3.07	116.92	109.30
4	K	3	BMA	O5-C5-C6	2.94	111.81	107.20
4	F	3	BMA	O5-C5-C6	2.93	111.79	107.20
5	H	1	NAG	C1-O5-C5	2.80	115.98	112.19
5	L	1	NAG	C1-O5-C5	2.78	115.97	112.19
6	I	3	BMA	O5-C5-C6	2.63	111.33	107.20
6	M	3	BMA	O5-C5-C6	2.62	111.31	107.20
5	H	4	MAN	C1-O5-C5	2.59	115.70	112.19
5	L	4	MAN	C1-O5-C5	2.56	115.66	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	3	BMA	C3-C4-C5	-2.41	105.94	110.24
6	I	3	BMA	C3-C4-C5	-2.39	105.97	110.24
6	I	2	NAG	C1-O5-C5	2.33	115.34	112.19
6	M	2	NAG	C1-O5-C5	2.31	115.32	112.19
4	K	5	MAN	O2-C2-C3	-2.27	105.60	110.14
4	F	3	BMA	C3-C4-C5	-2.26	106.21	110.24
4	F	5	MAN	O2-C2-C3	-2.26	105.61	110.14
4	F	2	NAG	C1-O5-C5	2.25	115.24	112.19
4	K	2	NAG	C1-O5-C5	2.25	115.24	112.19
4	K	3	BMA	C3-C4-C5	-2.25	106.23	110.24
4	K	4	MAN	O2-C2-C3	-2.25	105.64	110.14
4	F	4	MAN	O2-C2-C3	-2.24	105.64	110.14
5	H	6	MAN	O2-C2-C3	-2.24	105.65	110.14
5	L	6	MAN	O2-C2-C3	-2.23	105.67	110.14
6	M	4	MAN	C1-O5-C5	2.21	115.19	112.19
5	H	6	MAN	C1-O5-C5	2.20	115.17	112.19
6	M	4	MAN	O2-C2-C3	-2.19	105.74	110.14
5	L	6	MAN	C1-O5-C5	2.19	115.16	112.19
6	I	4	MAN	O2-C2-C3	-2.19	105.76	110.14
6	I	4	MAN	C1-O5-C5	2.18	115.15	112.19
4	K	4	MAN	C1-O5-C5	2.16	115.11	112.19
4	F	4	MAN	C1-O5-C5	2.15	115.11	112.19
4	F	5	MAN	C1-O5-C5	2.02	114.93	112.19

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	2	NAG	O5-C5-C6-O6
5	H	5	NAG	O5-C5-C6-O6
5	L	2	NAG	O5-C5-C6-O6
5	L	5	NAG	O5-C5-C6-O6
5	H	6	MAN	O5-C5-C6-O6
5	L	6	MAN	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

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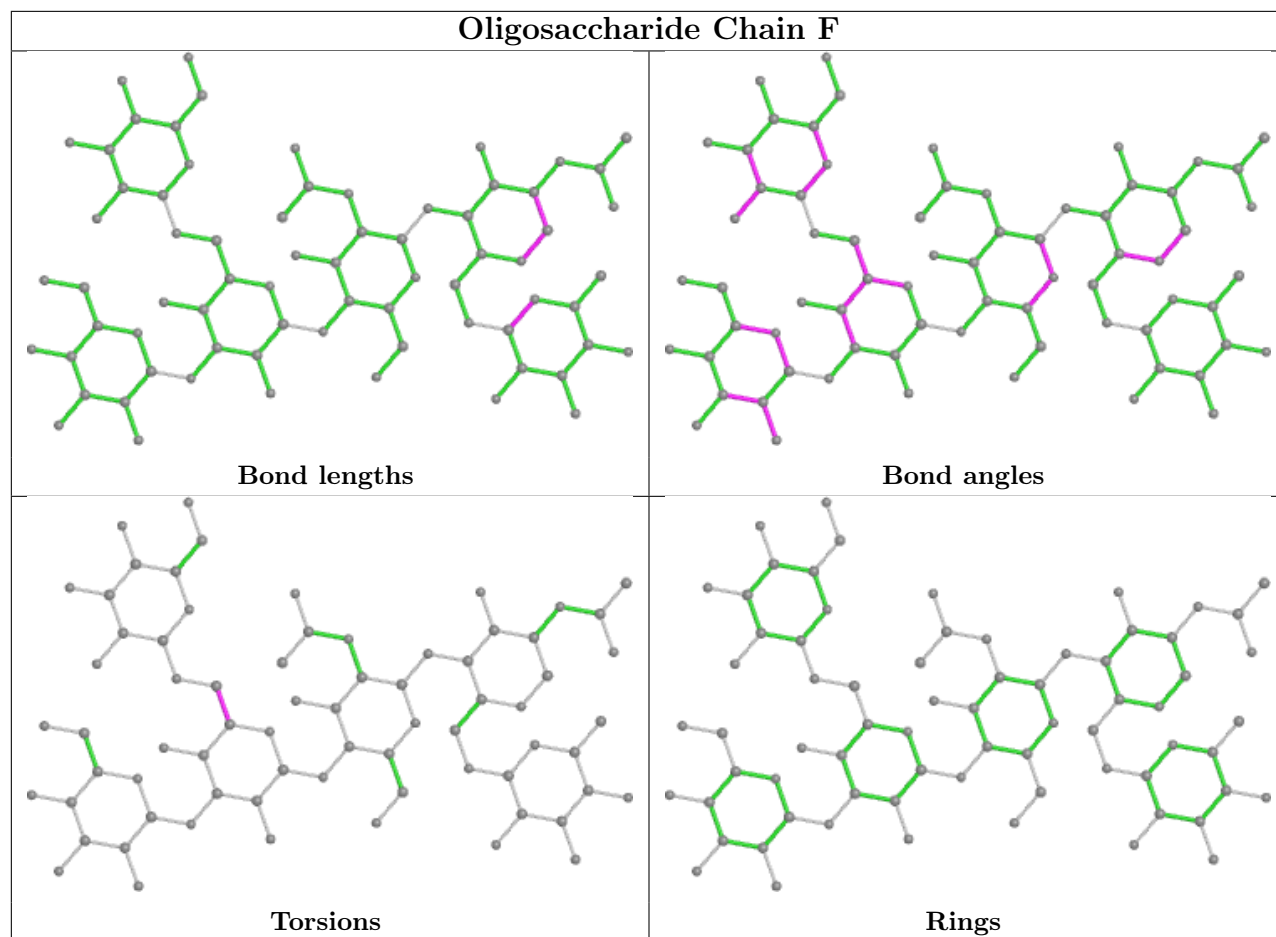
Mol	Chain	Res	Type	Atoms
5	H	5	NAG	C8-C7-N2-C2
5	H	5	NAG	O7-C7-N2-C2
5	L	5	NAG	C8-C7-N2-C2
5	L	5	NAG	O7-C7-N2-C2
5	H	3	BMA	C4-C5-C6-O6
5	L	3	BMA	C4-C5-C6-O6
5	H	2	NAG	C4-C5-C6-O6
5	L	2	NAG	C4-C5-C6-O6
6	M	3	BMA	O5-C5-C6-O6
6	I	3	BMA	O5-C5-C6-O6
4	F	3	BMA	O5-C5-C6-O6
4	K	3	BMA	O5-C5-C6-O6

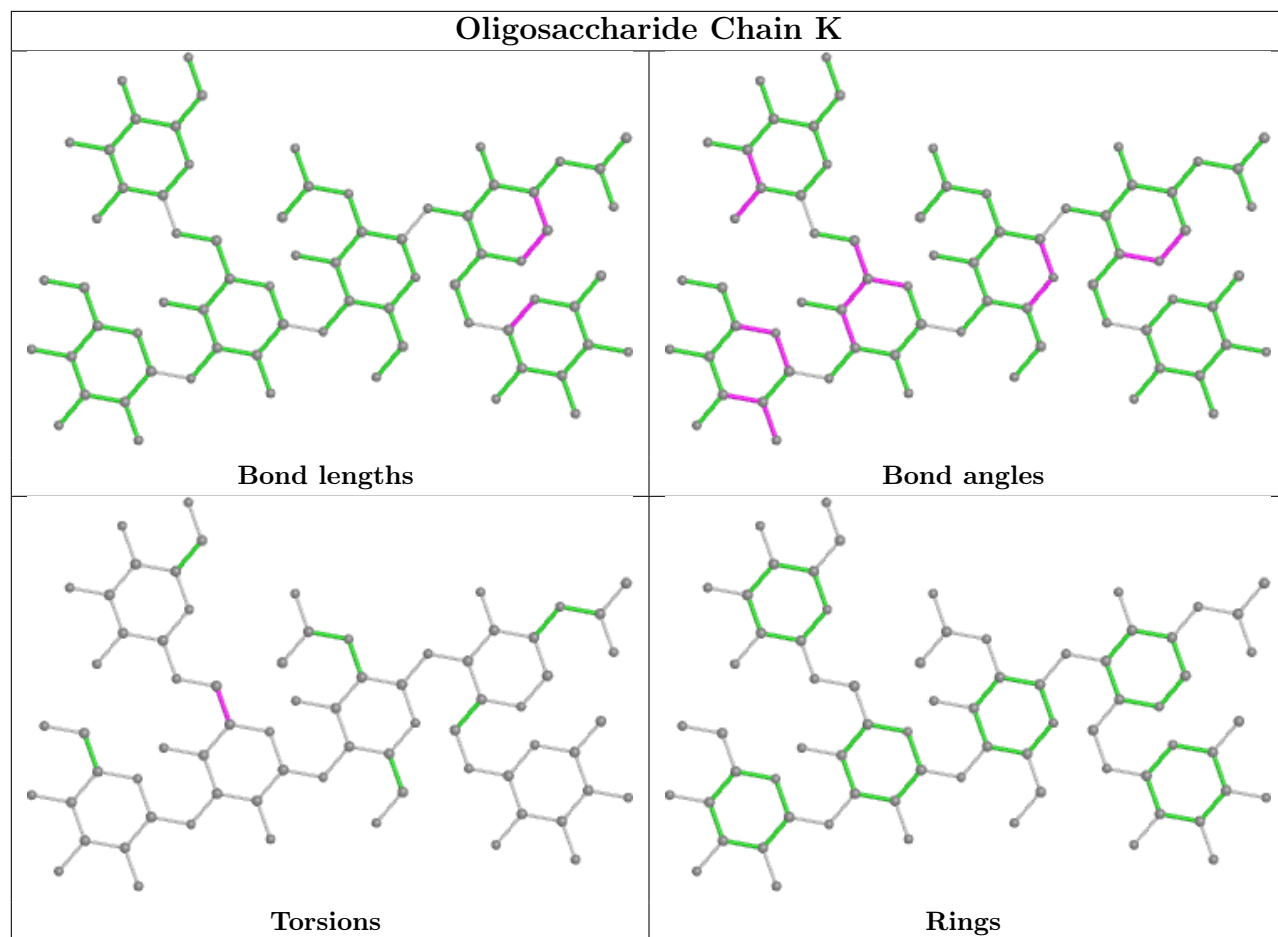
There are no ring outliers.

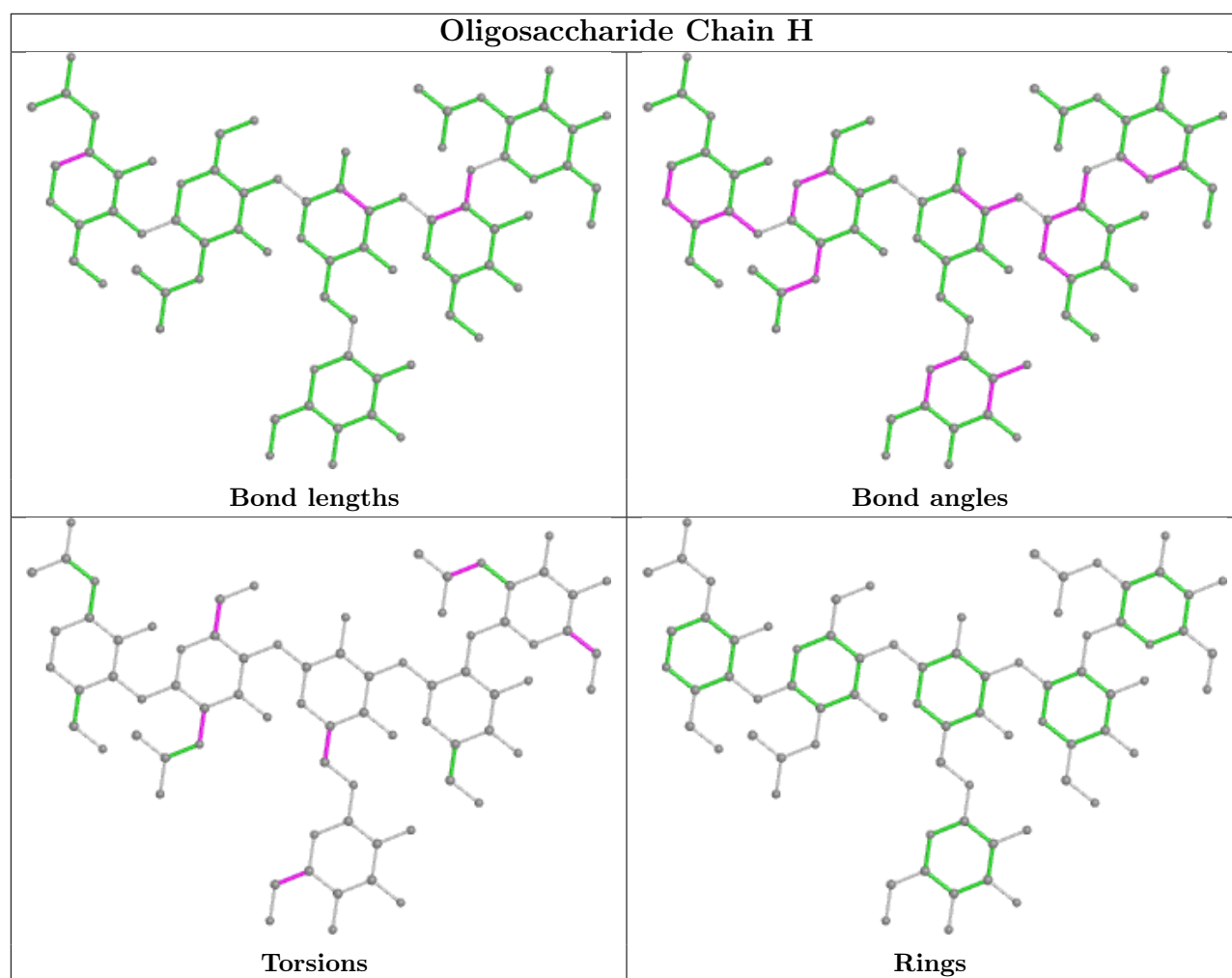
4 monomers are involved in 4 short contacts:

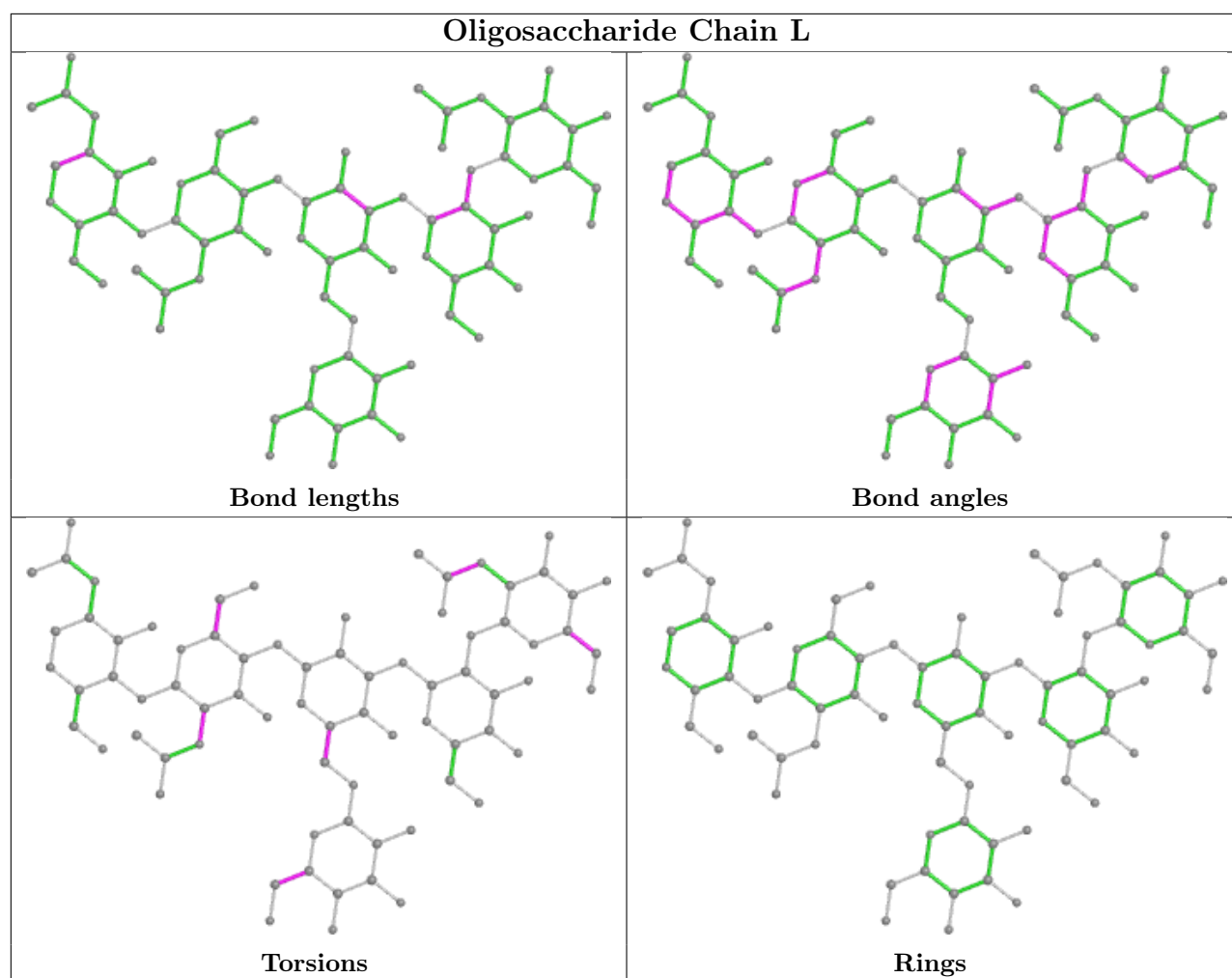
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	6	FUC	1	0
4	K	6	FUC	1	0
5	H	2	NAG	1	0
5	L	2	NAG	1	0

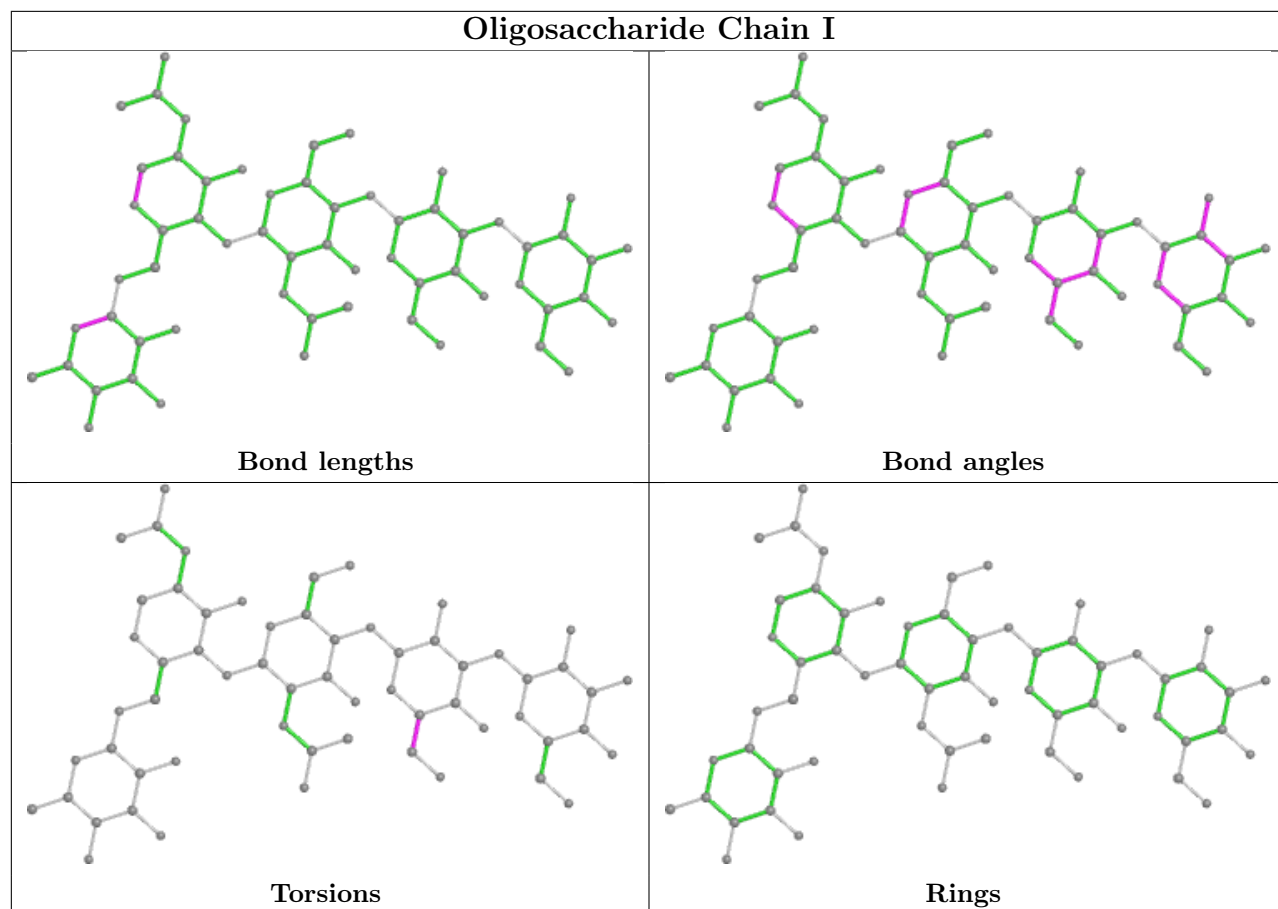
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

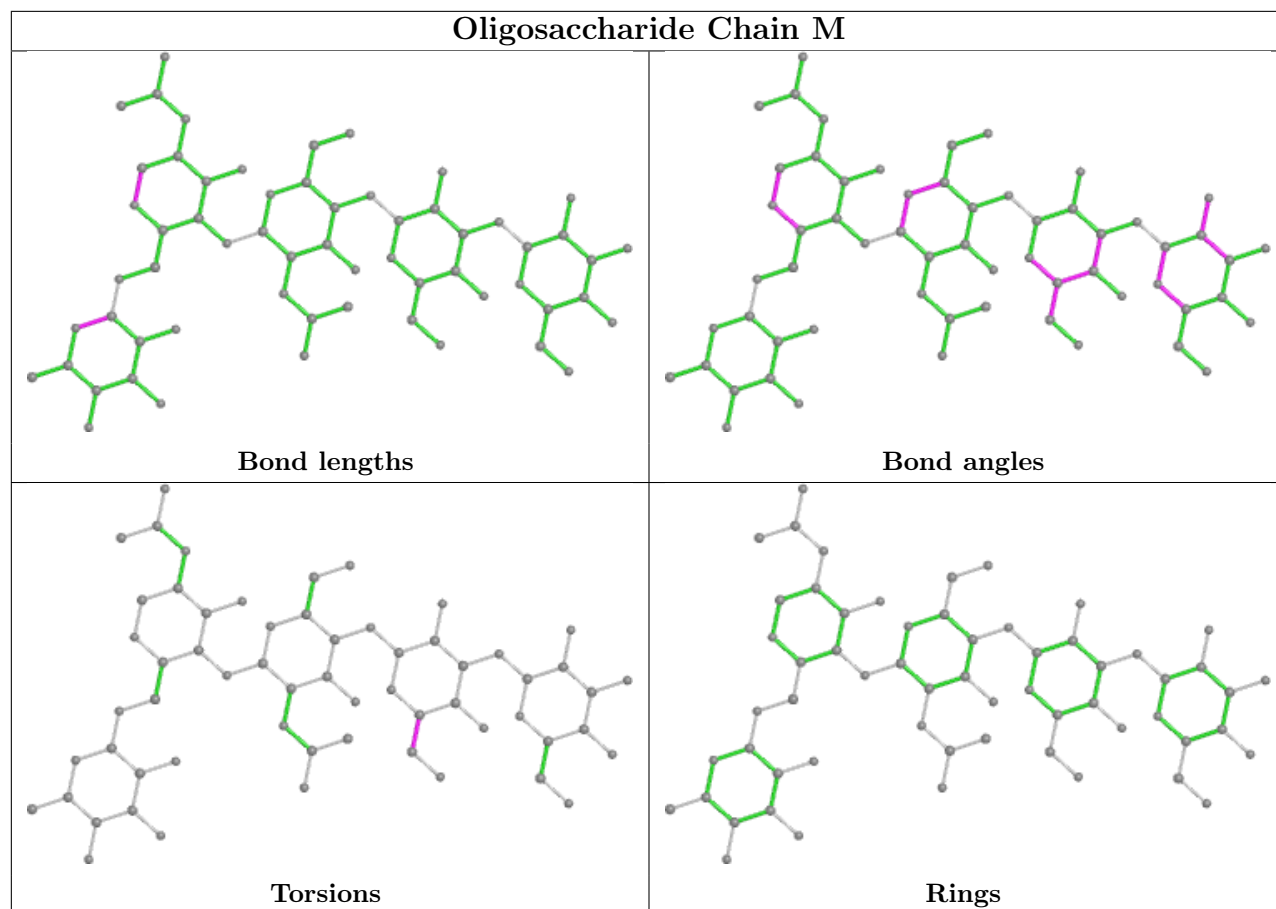


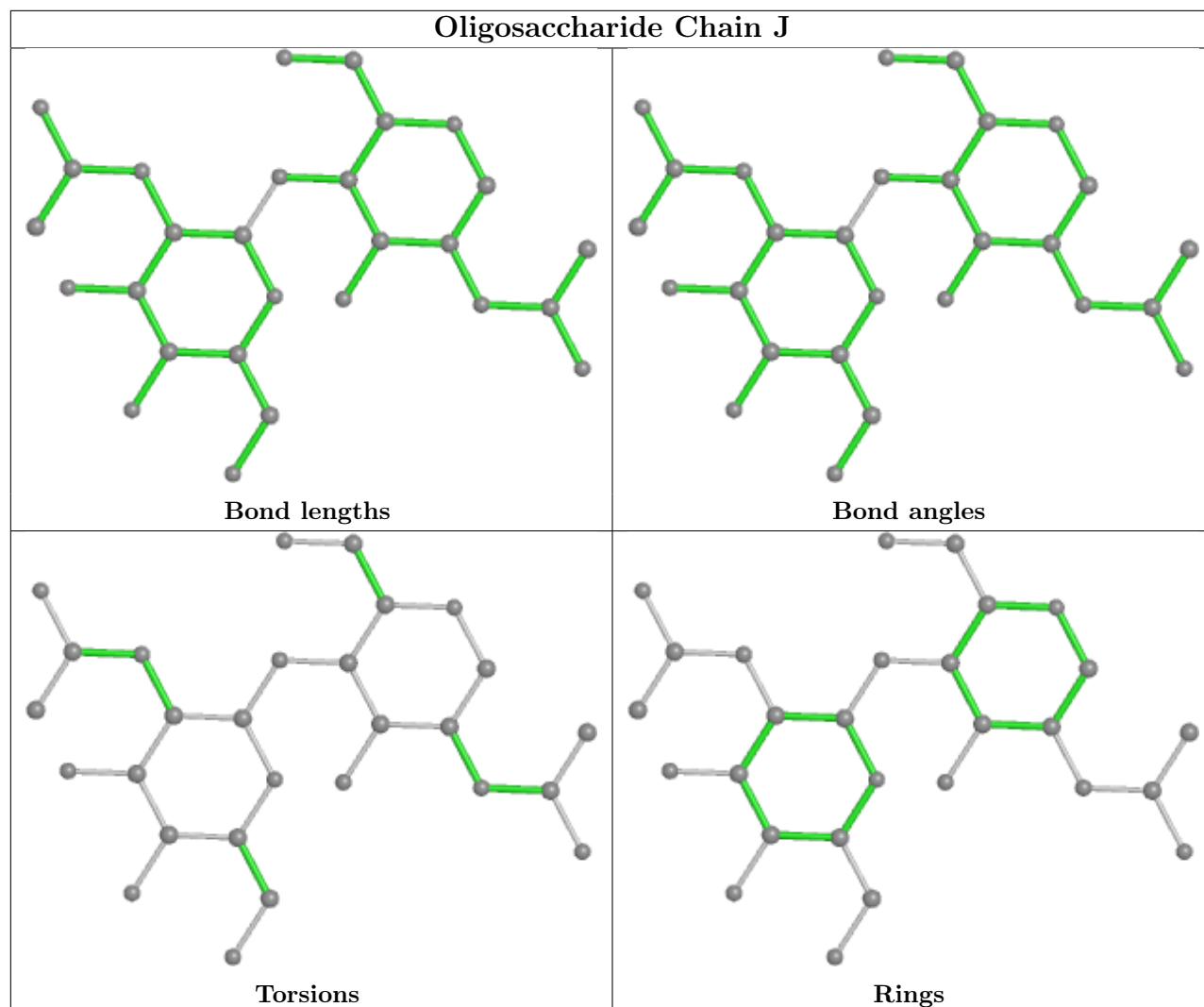


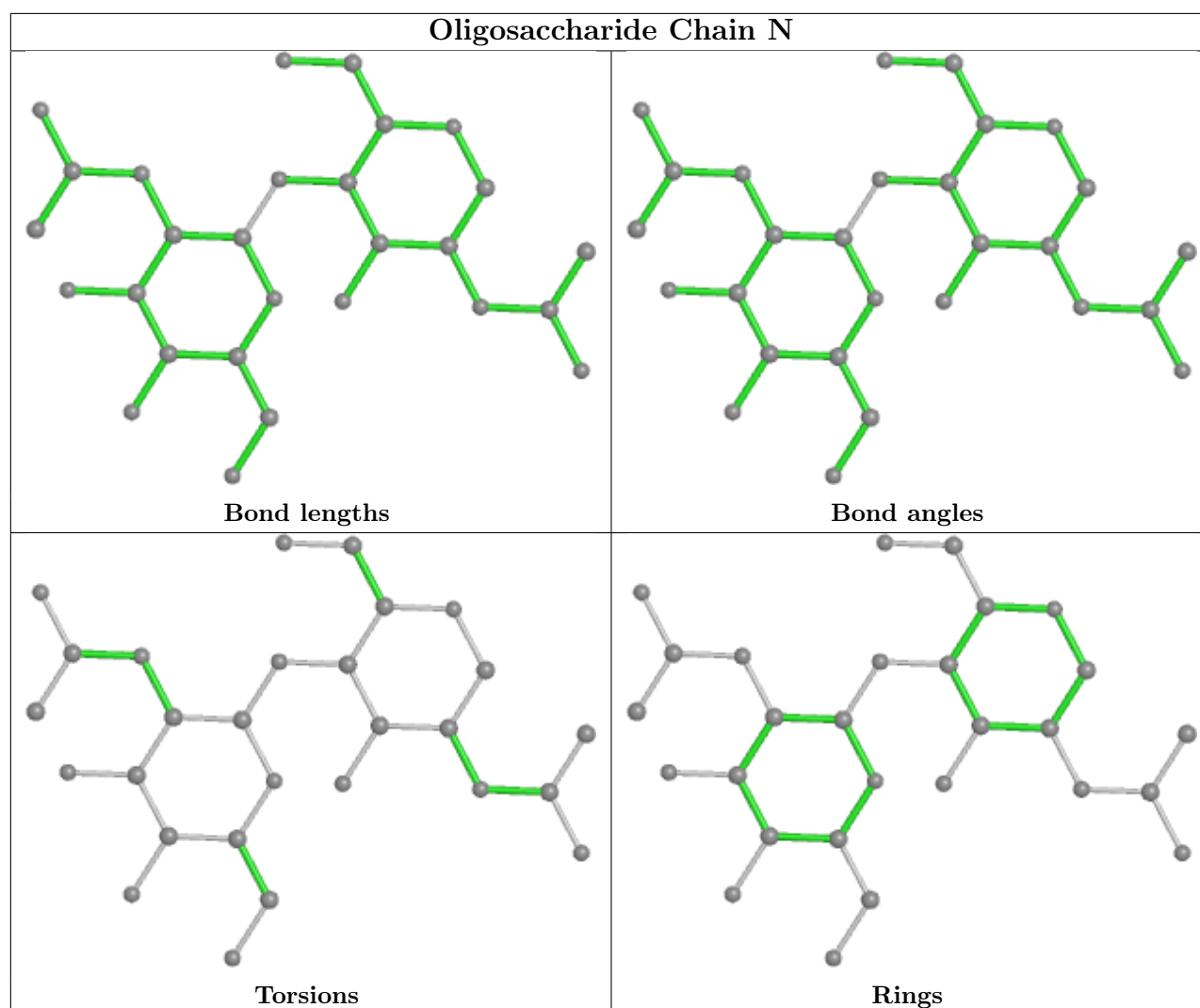












5.6 Ligand geometry [i](#)

Of 40 ligands modelled in this entry, 6 are monoatomic - leaving 34 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	$\# Z > 2$
10	PCW	C	1113	-	53,53,53	0.95	2 (3%)	59,61,61	0.93	1 (1%)
9	CLR	C	1105	-	31,31,31	1.56	7 (22%)	48,48,48	1.60	8 (16%)
10	PCW	A	1108	-	53,53,53	0.98	2 (3%)	59,61,61	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	PCW	A	1114	-	21,21,53	0.87	0	27,29,61	1.22	3 (11%)
10	PCW	E	101	-	21,21,53	0.87	0	27,29,61	1.24	3 (11%)
9	CLR	A	1104	-	31,31,31	1.55	8 (25%)	48,48,48	1.53	8 (16%)
10	PCW	C	1115	-	53,53,53	0.98	2 (3%)	59,61,61	0.68	0
10	PCW	A	1113	-	53,53,53	0.95	2 (3%)	59,61,61	0.93	1 (1%)
10	PCW	A	1116	-	21,21,53	0.86	0	27,29,61	1.06	2 (7%)
10	PCW	C	1114	-	21,21,53	0.87	0	27,29,61	1.22	3 (11%)
9	CLR	C	1104	-	31,31,31	1.55	8 (25%)	48,48,48	1.53	8 (16%)
10	PCW	A	1115	-	53,53,53	0.98	2 (3%)	59,61,61	0.68	0
10	PCW	C	1108	-	53,53,53	0.98	2 (3%)	59,61,61	0.73	0
10	PCW	A	1111	-	53,53,53	0.97	2 (3%)	59,61,61	0.75	0
10	PCW	C	1110	-	53,53,53	0.96	2 (3%)	59,61,61	0.73	0
10	PCW	A	1110	-	53,53,53	0.96	2 (3%)	59,61,61	0.73	0
10	PCW	G	102	-	53,53,53	1.00	2 (3%)	59,61,61	0.68	0
10	PCW	C	1112	-	53,53,53	0.98	2 (3%)	59,61,61	0.73	0
10	PCW	C	1107	-	53,53,53	0.95	2 (3%)	59,61,61	0.75	0
9	CLR	B	501	-	31,31,31	1.52	5 (16%)	48,48,48	1.55	10 (20%)
10	PCW	C	1111	-	53,53,53	0.97	2 (3%)	59,61,61	0.75	0
10	PCW	A	1112	-	53,53,53	0.99	2 (3%)	59,61,61	0.73	0
10	PCW	C	1106	-	21,21,53	0.87	0	27,29,61	1.08	3 (11%)
9	CLR	A	1105	-	31,31,31	1.56	7 (22%)	48,48,48	1.60	8 (16%)
10	PCW	A	1107	-	53,53,53	0.95	2 (3%)	59,61,61	0.75	0
10	PCW	C	1116	-	21,21,53	0.87	0	27,29,61	1.06	2 (7%)
10	PCW	E	102	-	53,53,53	0.99	2 (3%)	59,61,61	0.68	0
10	PCW	C	1109	-	53,53,53	0.96	2 (3%)	59,61,61	0.77	0
10	PCW	A	1109	-	53,53,53	0.96	2 (3%)	59,61,61	0.77	0
9	CLR	B	502	-	31,31,31	1.59	9 (29%)	48,48,48	1.79	15 (31%)
9	CLR	D	501	-	31,31,31	1.52	5 (16%)	48,48,48	1.55	10 (20%)
9	CLR	D	502	-	31,31,31	1.59	9 (29%)	48,48,48	1.79	15 (31%)
10	PCW	A	1106	-	21,21,53	0.88	0	27,29,61	1.08	3 (11%)
10	PCW	G	101	-	21,21,53	0.88	0	27,29,61	1.23	3 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	PCW	C	1113	-	-	26/57/57/57	-
9	CLR	C	1105	-	-	0/10/68/68	0/4/4/4
10	PCW	A	1108	-	-	18/57/57/57	-
10	PCW	A	1114	-	-	4/23/23/57	-
10	PCW	E	101	-	-	5/23/23/57	-
9	CLR	A	1104	-	-	0/10/68/68	0/4/4/4
10	PCW	C	1115	-	-	21/57/57/57	-
10	PCW	A	1113	-	-	26/57/57/57	-
10	PCW	A	1116	-	-	7/23/23/57	-
10	PCW	C	1114	-	-	4/23/23/57	-
9	CLR	C	1104	-	-	0/10/68/68	0/4/4/4
10	PCW	A	1115	-	-	21/57/57/57	-
10	PCW	C	1108	-	-	18/57/57/57	-
10	PCW	A	1111	-	-	20/57/57/57	-
10	PCW	C	1110	-	-	27/57/57/57	-
10	PCW	A	1110	-	-	27/57/57/57	-
10	PCW	G	102	-	-	18/57/57/57	-
10	PCW	C	1112	-	-	21/57/57/57	-
10	PCW	C	1107	-	-	21/57/57/57	-
9	CLR	B	501	-	-	1/10/68/68	0/4/4/4
10	PCW	C	1111	-	-	20/57/57/57	-
10	PCW	A	1112	-	-	21/57/57/57	-
10	PCW	C	1106	-	-	16/23/23/57	-
9	CLR	A	1105	-	-	0/10/68/68	0/4/4/4
10	PCW	A	1107	-	-	21/57/57/57	-
10	PCW	C	1116	-	-	7/23/23/57	-
10	PCW	E	102	-	-	18/57/57/57	-
10	PCW	C	1109	-	-	14/57/57/57	-
10	PCW	A	1109	-	-	14/57/57/57	-
9	CLR	B	502	-	-	0/10/68/68	0/4/4/4
9	CLR	D	501	-	-	1/10/68/68	0/4/4/4
9	CLR	D	502	-	-	0/10/68/68	0/4/4/4
10	PCW	A	1106	-	-	16/23/23/57	-
10	PCW	G	101	-	-	5/23/23/57	-

All (94) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	501	CLR	C12-C13	4.53	1.62	1.54
9	D	501	CLR	C12-C13	4.49	1.62	1.54
9	A	1104	CLR	C12-C13	4.17	1.61	1.54
9	C	1104	CLR	C12-C13	4.15	1.61	1.54
9	C	1105	CLR	C12-C13	4.14	1.61	1.54
9	A	1105	CLR	C12-C13	4.09	1.61	1.54
10	G	102	PCW	C40-C39	3.96	1.54	1.31
10	E	102	PCW	C40-C39	3.95	1.54	1.31
10	A	1108	PCW	C20-C19	3.91	1.54	1.31
10	C	1108	PCW	C20-C19	3.90	1.54	1.31
10	E	102	PCW	C20-C19	3.87	1.54	1.31
10	C	1111	PCW	C20-C19	3.87	1.54	1.31
10	A	1110	PCW	C40-C39	3.87	1.54	1.31
10	C	1112	PCW	C40-C39	3.86	1.54	1.31
10	A	1112	PCW	C40-C39	3.86	1.54	1.31
10	A	1111	PCW	C20-C19	3.86	1.54	1.31
10	G	102	PCW	C20-C19	3.86	1.54	1.31
10	A	1112	PCW	C20-C19	3.85	1.54	1.31
10	C	1115	PCW	C20-C19	3.85	1.54	1.31
10	C	1110	PCW	C40-C39	3.85	1.54	1.31
10	A	1115	PCW	C20-C19	3.85	1.54	1.31
10	C	1112	PCW	C20-C19	3.83	1.54	1.31
10	C	1110	PCW	C20-C19	3.83	1.54	1.31
10	A	1110	PCW	C20-C19	3.83	1.53	1.31
10	A	1111	PCW	C40-C39	3.82	1.53	1.31
10	C	1111	PCW	C40-C39	3.82	1.53	1.31
10	C	1108	PCW	C40-C39	3.81	1.53	1.31
10	C	1115	PCW	C40-C39	3.81	1.53	1.31
10	A	1108	PCW	C40-C39	3.81	1.53	1.31
10	C	1109	PCW	C40-C39	3.81	1.53	1.31
10	A	1107	PCW	C20-C19	3.80	1.53	1.31
10	A	1115	PCW	C40-C39	3.80	1.53	1.31
10	A	1109	PCW	C40-C39	3.79	1.53	1.31
10	C	1107	PCW	C20-C19	3.79	1.53	1.31
10	C	1109	PCW	C20-C19	3.78	1.53	1.31
10	A	1109	PCW	C20-C19	3.78	1.53	1.31
10	A	1107	PCW	C40-C39	3.74	1.53	1.31
10	C	1107	PCW	C40-C39	3.74	1.53	1.31
10	A	1113	PCW	C40-C39	3.73	1.53	1.31
10	C	1113	PCW	C40-C39	3.71	1.53	1.31
10	C	1113	PCW	C20-C19	3.70	1.53	1.31
10	A	1113	PCW	C20-C19	3.69	1.53	1.31
9	B	502	CLR	C11-C9	3.19	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	502	CLR	C11-C9	3.17	1.59	1.53
9	A	1104	CLR	C10-C5	3.10	1.59	1.52
9	C	1104	CLR	C10-C5	3.09	1.59	1.52
9	D	502	CLR	C10-C5	3.03	1.58	1.52
9	B	502	CLR	C10-C5	3.00	1.58	1.52
9	D	502	CLR	C12-C13	2.96	1.59	1.54
9	B	502	CLR	C12-C13	2.93	1.59	1.54
9	D	501	CLR	C4-C3	2.82	1.57	1.52
9	A	1105	CLR	C10-C5	2.81	1.58	1.52
9	A	1105	CLR	C16-C17	2.80	1.60	1.54
9	C	1105	CLR	C16-C17	2.80	1.60	1.54
9	C	1105	CLR	C10-C5	2.79	1.58	1.52
9	C	1104	CLR	C16-C17	2.79	1.60	1.54
9	B	501	CLR	C4-C3	2.78	1.57	1.52
9	A	1104	CLR	C16-C17	2.77	1.60	1.54
9	D	502	CLR	C12-C11	2.73	1.59	1.53
9	B	502	CLR	C12-C11	2.73	1.59	1.53
9	D	501	CLR	C16-C17	2.68	1.59	1.54
9	B	501	CLR	C16-C17	2.64	1.59	1.54
9	B	502	CLR	C8-C14	-2.53	1.48	1.53
9	A	1104	CLR	C4-C3	2.52	1.56	1.52
9	C	1105	CLR	C8-C14	-2.51	1.48	1.53
9	D	502	CLR	C8-C14	-2.51	1.48	1.53
9	A	1105	CLR	C8-C14	-2.50	1.48	1.53
9	A	1105	CLR	C4-C3	2.50	1.56	1.52
9	C	1104	CLR	C4-C3	2.49	1.56	1.52
9	C	1105	CLR	C4-C3	2.47	1.56	1.52
9	C	1105	CLR	C12-C11	2.44	1.58	1.53
9	B	502	CLR	C16-C17	2.44	1.59	1.54
9	A	1105	CLR	C12-C11	2.44	1.58	1.53
9	D	502	CLR	C16-C17	2.43	1.59	1.54
9	C	1104	CLR	C8-C14	-2.38	1.49	1.53
9	A	1104	CLR	C8-C14	-2.37	1.49	1.53
9	D	501	CLR	C10-C5	2.34	1.57	1.52
9	C	1105	CLR	C11-C9	2.30	1.57	1.53
9	A	1105	CLR	C11-C9	2.28	1.57	1.53
9	B	502	CLR	C2-C3	2.27	1.57	1.51
9	C	1104	CLR	C12-C11	2.27	1.58	1.53
9	D	502	CLR	C4-C5	2.27	1.56	1.51
9	B	501	CLR	C10-C5	2.27	1.57	1.52
9	D	502	CLR	C2-C3	2.26	1.57	1.51
9	A	1104	CLR	C12-C11	2.26	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	502	CLR	C4-C5	2.23	1.56	1.51
9	C	1104	CLR	C11-C9	2.16	1.57	1.53
9	A	1104	CLR	C11-C9	2.15	1.57	1.53
9	D	502	CLR	C4-C3	2.13	1.55	1.52
9	B	502	CLR	C4-C3	2.13	1.55	1.52
9	B	501	CLR	C4-C5	2.06	1.56	1.51
9	A	1104	CLR	C2-C3	2.05	1.56	1.51
9	C	1104	CLR	C2-C3	2.05	1.56	1.51
9	D	501	CLR	C4-C5	2.03	1.56	1.51

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1105	CLR	C7-C8-C9	4.46	115.11	109.71
9	C	1105	CLR	C7-C8-C9	4.45	115.10	109.71
9	A	1104	CLR	C7-C8-C9	4.36	114.99	109.71
9	C	1104	CLR	C7-C8-C9	4.33	114.96	109.71
10	C	1114	PCW	C2-O2-C31	-4.33	109.83	117.90
10	A	1114	PCW	C2-O2-C31	-4.31	109.87	117.90
10	G	101	PCW	C2-O2-C31	-4.27	109.93	117.90
10	E	101	PCW	C2-O2-C31	-4.26	109.95	117.90
9	D	502	CLR	C10-C5-C6	4.22	129.36	122.90
9	B	502	CLR	C10-C5-C6	4.20	129.34	122.90
10	C	1106	PCW	C2-O2-C31	-3.83	110.77	117.90
10	A	1106	PCW	C2-O2-C31	-3.81	110.80	117.90
9	D	502	CLR	C7-C8-C9	3.71	114.21	109.71
9	B	502	CLR	C7-C8-C9	3.68	114.17	109.71
9	D	501	CLR	C7-C8-C9	3.60	114.08	109.71
9	B	501	CLR	C7-C8-C9	3.56	114.03	109.71
9	D	502	CLR	C18-C13-C12	3.35	115.89	110.59
9	B	502	CLR	C18-C13-C12	3.32	115.83	110.59
9	D	502	CLR	C15-C14-C13	3.15	107.64	103.84
9	B	502	CLR	C15-C14-C13	3.12	107.60	103.84
10	C	1116	PCW	C3-O3-C11	-3.08	109.37	117.10
10	A	1116	PCW	C3-O3-C11	-3.08	109.37	117.10
10	G	101	PCW	C3-O3-C11	-2.99	109.59	117.10
10	E	101	PCW	C3-O3-C11	-2.98	109.61	117.10
9	D	501	CLR	C18-C13-C12	2.97	115.28	110.59
9	B	501	CLR	C18-C13-C12	2.95	115.25	110.59
9	A	1105	CLR	C15-C14-C13	2.77	107.19	103.84
9	C	1105	CLR	C15-C14-C13	2.77	107.18	103.84
10	A	1113	PCW	C2-O2-C31	-2.76	110.99	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	501	CLR	C15-C14-C13	2.75	107.16	103.84
10	C	1113	PCW	C2-O2-C31	-2.75	111.03	117.79
9	B	502	CLR	C22-C20-C17	-2.72	104.67	110.28
9	B	501	CLR	C15-C14-C13	2.71	107.11	103.84
9	D	502	CLR	C22-C20-C17	-2.70	104.70	110.28
10	C	1114	PCW	C3-O3-C11	-2.68	110.36	117.10
9	C	1104	CLR	C15-C14-C13	2.67	107.06	103.84
10	A	1114	PCW	C3-O3-C11	-2.67	110.39	117.10
9	A	1104	CLR	C15-C14-C13	2.67	107.06	103.84
9	B	502	CLR	C13-C17-C20	-2.66	115.31	119.49
9	A	1105	CLR	C18-C13-C12	2.66	114.79	110.59
9	C	1105	CLR	C10-C5-C6	2.66	126.97	122.90
10	C	1116	PCW	C2-O2-C31	-2.66	112.94	117.90
9	A	1105	CLR	C10-C5-C6	2.65	126.97	122.90
9	D	502	CLR	C13-C17-C20	-2.65	115.33	119.49
10	A	1116	PCW	C2-O2-C31	-2.65	112.96	117.90
9	A	1104	CLR	C18-C13-C12	2.64	114.76	110.59
9	C	1104	CLR	C18-C13-C12	2.64	114.76	110.59
9	C	1105	CLR	C18-C13-C12	2.64	114.75	110.59
9	B	502	CLR	C10-C9-C8	2.50	116.49	112.73
9	D	502	CLR	C10-C9-C8	2.48	116.46	112.73
9	D	501	CLR	C10-C5-C6	2.44	126.64	122.90
9	B	501	CLR	C10-C5-C6	2.44	126.63	122.90
9	A	1105	CLR	C13-C17-C20	-2.43	115.67	119.49
9	B	502	CLR	C4-C5-C6	-2.43	117.10	120.61
9	D	502	CLR	C4-C5-C6	-2.43	117.10	120.61
9	A	1104	CLR	C22-C20-C17	-2.43	105.26	110.28
9	C	1105	CLR	C13-C17-C20	-2.43	115.68	119.49
9	D	501	CLR	C13-C17-C20	-2.42	115.69	119.49
9	C	1104	CLR	C22-C20-C17	-2.42	105.29	110.28
9	D	502	CLR	C21-C20-C17	2.42	116.62	112.92
9	A	1105	CLR	C22-C20-C17	-2.42	105.30	110.28
9	C	1105	CLR	C22-C20-C17	-2.41	105.31	110.28
9	B	501	CLR	C13-C17-C20	-2.41	115.72	119.49
9	B	502	CLR	C21-C20-C17	2.40	116.59	112.92
9	C	1105	CLR	C16-C17-C20	-2.39	108.44	112.15
9	A	1105	CLR	C16-C17-C20	-2.39	108.45	112.15
9	B	502	CLR	C13-C14-C8	-2.38	110.85	114.38
9	A	1104	CLR	C13-C17-C20	-2.38	115.76	119.49
9	D	502	CLR	C13-C14-C8	-2.37	110.87	114.38
9	C	1104	CLR	C13-C17-C20	-2.35	115.81	119.49
9	D	501	CLR	C3-C4-C5	2.33	115.98	112.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1104	CLR	C16-C17-C20	-2.32	108.56	112.15
9	B	501	CLR	C3-C4-C5	2.32	115.95	112.03
9	C	1104	CLR	C16-C17-C20	-2.32	108.56	112.15
10	A	1106	PCW	C3-O3-C11	-2.30	111.33	117.10
10	C	1106	PCW	C3-O3-C11	-2.28	111.37	117.10
9	D	502	CLR	C4-C5-C10	-2.25	113.43	116.42
9	B	502	CLR	C4-C5-C10	-2.23	113.45	116.42
9	B	502	CLR	C16-C17-C20	-2.19	108.75	112.15
9	D	501	CLR	C1-C2-C3	2.19	113.27	110.47
9	D	501	CLR	C16-C17-C20	-2.18	108.76	112.15
9	B	502	CLR	C19-C10-C5	2.18	111.88	108.34
9	D	502	CLR	C19-C10-C5	2.17	111.86	108.34
9	B	501	CLR	C1-C2-C3	2.16	113.25	110.47
9	D	502	CLR	C16-C17-C20	-2.15	108.82	112.15
9	B	501	CLR	C16-C17-C20	-2.15	108.82	112.15
9	C	1105	CLR	C1-C2-C3	2.13	113.20	110.47
9	C	1104	CLR	C3-C4-C5	2.12	115.61	112.03
9	A	1105	CLR	C1-C2-C3	2.11	113.17	110.47
10	A	1114	PCW	O2-C31-C32	2.10	114.96	111.09
9	D	501	CLR	C22-C20-C17	-2.10	105.94	110.28
10	E	101	PCW	O2-C31-C32	2.10	114.95	111.09
9	C	1104	CLR	C1-C2-C3	2.10	113.16	110.47
9	B	501	CLR	C19-C10-C9	-2.09	109.18	111.68
10	C	1114	PCW	O2-C31-C32	2.09	114.94	111.09
9	B	501	CLR	C22-C20-C17	-2.09	105.97	110.28
9	A	1104	CLR	C3-C4-C5	2.09	115.56	112.03
10	G	101	PCW	O2-C31-C32	2.07	114.90	111.09
9	D	501	CLR	C19-C10-C9	-2.07	109.21	111.68
9	D	502	CLR	C1-C2-C3	2.07	113.12	110.47
9	A	1104	CLR	C1-C2-C3	2.07	113.12	110.47
10	A	1106	PCW	O2-C31-C32	2.07	114.89	111.09
10	C	1106	PCW	O2-C31-C32	2.06	114.88	111.09
9	B	502	CLR	C1-C2-C3	2.04	113.08	110.47
9	B	502	CLR	C3-C4-C5	2.03	115.46	112.03
9	D	502	CLR	C3-C4-C5	2.02	115.45	112.03

There are no chirality outliers.

All (438) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	C	1106	PCW	C1-O3P-P-O1P
10	C	1106	PCW	C1-O3P-P-O2P

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Mol	Chain	Res	Type	Atoms
10	C	1107	PCW	C4-O4P-P-O1P
10	C	1108	PCW	O3P-C1-C2-O2
10	C	1108	PCW	C1-O3P-P-O2P
10	C	1110	PCW	C1-O3P-P-O2P
10	C	1111	PCW	O2-C2-C3-O3
10	C	1112	PCW	O2-C2-C3-O3
10	C	1112	PCW	C1-O3P-P-O1P
10	C	1112	PCW	C1-O3P-P-O2P
10	C	1112	PCW	C4-O4P-P-O2P
10	C	1112	PCW	C4-O4P-P-O3P
10	C	1113	PCW	C5-C4-O4P-P
10	C	1113	PCW	C1-O3P-P-O1P
10	C	1113	PCW	C1-O3P-P-O4P
10	C	1113	PCW	C4-O4P-P-O3P
10	C	1114	PCW	C4-O4P-P-O2P
10	C	1114	PCW	C4-O4P-P-O3P
10	C	1116	PCW	C4-O4P-P-O2P
10	E	101	PCW	C1-O3P-P-O1P
10	A	1106	PCW	C1-O3P-P-O1P
10	A	1106	PCW	C1-O3P-P-O2P
10	A	1107	PCW	C4-O4P-P-O1P
10	A	1108	PCW	O3P-C1-C2-O2
10	A	1108	PCW	C1-O3P-P-O2P
10	A	1110	PCW	C1-O3P-P-O2P
10	A	1111	PCW	O2-C2-C3-O3
10	A	1112	PCW	O2-C2-C3-O3
10	A	1112	PCW	C1-O3P-P-O1P
10	A	1112	PCW	C1-O3P-P-O2P
10	A	1112	PCW	C4-O4P-P-O2P
10	A	1112	PCW	C4-O4P-P-O3P
10	A	1113	PCW	C5-C4-O4P-P
10	A	1113	PCW	C1-O3P-P-O1P
10	A	1113	PCW	C1-O3P-P-O4P
10	A	1113	PCW	C4-O4P-P-O3P
10	A	1114	PCW	C4-O4P-P-O2P
10	A	1114	PCW	C4-O4P-P-O3P
10	A	1116	PCW	C4-O4P-P-O2P
10	G	101	PCW	C1-O3P-P-O1P
10	C	1106	PCW	C12-C11-O3-C3
10	A	1106	PCW	C12-C11-O3-C3
10	C	1110	PCW	C4-C5-N-C8
10	C	1111	PCW	C4-C5-N-C8

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Mol	Chain	Res	Type	Atoms
10	C	1112	PCW	C4-C5-N-C8
10	C	1113	PCW	C4-C5-N-C8
10	C	1115	PCW	C4-C5-N-C8
10	A	1110	PCW	C4-C5-N-C8
10	A	1111	PCW	C4-C5-N-C8
10	A	1112	PCW	C4-C5-N-C8
10	A	1113	PCW	C4-C5-N-C8
10	A	1115	PCW	C4-C5-N-C8
10	C	1106	PCW	O11-C11-O3-C3
10	A	1106	PCW	O11-C11-O3-C3
10	C	1107	PCW	C11-C12-C13-C14
10	C	1107	PCW	C31-C32-C33-C34
10	C	1109	PCW	C31-C32-C33-C34
10	C	1111	PCW	C31-C32-C33-C34
10	C	1113	PCW	C31-C32-C33-C34
10	A	1107	PCW	C11-C12-C13-C14
10	A	1107	PCW	C31-C32-C33-C34
10	A	1109	PCW	C31-C32-C33-C34
10	A	1111	PCW	C31-C32-C33-C34
10	A	1113	PCW	C31-C32-C33-C34
10	C	1115	PCW	C11-C12-C13-C14
10	A	1115	PCW	C11-C12-C13-C14
10	C	1106	PCW	C1-O3P-P-O4P
10	C	1106	PCW	C4-O4P-P-O3P
10	C	1107	PCW	C4-O4P-P-O3P
10	C	1112	PCW	C1-O3P-P-O4P
10	C	1116	PCW	C1-O3P-P-O4P
10	E	101	PCW	C1-O3P-P-O4P
10	E	101	PCW	C4-O4P-P-O3P
10	A	1106	PCW	C1-O3P-P-O4P
10	A	1106	PCW	C4-O4P-P-O3P
10	A	1107	PCW	C4-O4P-P-O3P
10	A	1112	PCW	C1-O3P-P-O4P
10	A	1116	PCW	C1-O3P-P-O4P
10	G	101	PCW	C1-O3P-P-O4P
10	G	101	PCW	C4-O4P-P-O3P
10	C	1113	PCW	C11-C12-C13-C14
10	A	1113	PCW	C11-C12-C13-C14
10	C	1110	PCW	C4-C5-N-C6
10	C	1110	PCW	C4-C5-N-C7
10	C	1111	PCW	C4-C5-N-C6
10	C	1111	PCW	C4-C5-N-C7

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Mol	Chain	Res	Type	Atoms
10	C	1112	PCW	C4-C5-N-C6
10	C	1112	PCW	C4-C5-N-C7
10	C	1113	PCW	C4-C5-N-C6
10	C	1115	PCW	C4-C5-N-C6
10	C	1115	PCW	C4-C5-N-C7
10	E	102	PCW	C4-C5-N-C6
10	E	102	PCW	C4-C5-N-C7
10	E	102	PCW	C4-C5-N-C8
10	A	1110	PCW	C4-C5-N-C6
10	A	1110	PCW	C4-C5-N-C7
10	A	1111	PCW	C4-C5-N-C6
10	A	1111	PCW	C4-C5-N-C7
10	A	1112	PCW	C4-C5-N-C6
10	A	1112	PCW	C4-C5-N-C7
10	A	1113	PCW	C4-C5-N-C6
10	A	1115	PCW	C4-C5-N-C6
10	A	1115	PCW	C4-C5-N-C7
10	G	102	PCW	C4-C5-N-C6
10	G	102	PCW	C4-C5-N-C7
10	G	102	PCW	C4-C5-N-C8
10	G	102	PCW	C43-C44-C45-C46
10	C	1110	PCW	C22-C23-C24-C25
10	C	1113	PCW	C13-C14-C15-C16
10	E	102	PCW	C43-C44-C45-C46
10	E	102	PCW	C21-C22-C23-C24
10	A	1110	PCW	C22-C23-C24-C25
10	A	1113	PCW	C13-C14-C15-C16
10	G	102	PCW	C21-C22-C23-C24
10	C	1110	PCW	C43-C44-C45-C46
10	E	102	PCW	C34-C35-C36-C37
10	A	1110	PCW	C43-C44-C45-C46
10	G	102	PCW	C34-C35-C36-C37
10	C	1111	PCW	C42-C43-C44-C45
10	A	1111	PCW	C42-C43-C44-C45
10	C	1108	PCW	C44-C45-C46-C47
10	C	1113	PCW	C33-C34-C35-C36
10	A	1113	PCW	C33-C34-C35-C36
10	A	1108	PCW	C44-C45-C46-C47
10	C	1110	PCW	C21-C22-C23-C24
10	A	1110	PCW	C21-C22-C23-C24
10	C	1111	PCW	C40-C41-C42-C43
10	C	1112	PCW	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
10	A	1111	PCW	C40-C41-C42-C43
10	A	1112	PCW	C16-C17-C18-C19
10	C	1110	PCW	C23-C24-C25-C26
10	C	1111	PCW	C14-C15-C16-C17
10	C	1111	PCW	C35-C36-C37-C38
10	A	1111	PCW	C14-C15-C16-C17
10	A	1111	PCW	C35-C36-C37-C38
10	C	1113	PCW	C4-C5-N-C7
10	A	1113	PCW	C4-C5-N-C7
10	A	1110	PCW	C23-C24-C25-C26
10	C	1107	PCW	C33-C34-C35-C36
10	A	1107	PCW	C33-C34-C35-C36
10	C	1109	PCW	C15-C16-C17-C18
10	C	1109	PCW	C34-C35-C36-C37
10	A	1109	PCW	C15-C16-C17-C18
10	A	1109	PCW	C34-C35-C36-C37
10	E	102	PCW	C33-C34-C35-C36
10	G	102	PCW	C33-C34-C35-C36
10	C	1111	PCW	C33-C34-C35-C36
10	A	1111	PCW	C33-C34-C35-C36
10	C	1108	PCW	C20-C21-C22-C23
10	A	1108	PCW	C20-C21-C22-C23
10	C	1109	PCW	C41-C42-C43-C44
10	A	1109	PCW	C41-C42-C43-C44
10	C	1107	PCW	C16-C17-C18-C19
10	C	1107	PCW	C40-C41-C42-C43
10	C	1112	PCW	C40-C41-C42-C43
10	C	1113	PCW	C40-C41-C42-C43
10	A	1107	PCW	C16-C17-C18-C19
10	A	1107	PCW	C40-C41-C42-C43
10	A	1112	PCW	C40-C41-C42-C43
10	A	1113	PCW	C40-C41-C42-C43
10	C	1111	PCW	C15-C16-C17-C18
10	A	1111	PCW	C15-C16-C17-C18
10	C	1112	PCW	C15-C16-C17-C18
10	A	1112	PCW	C15-C16-C17-C18
10	C	1107	PCW	C20-C21-C22-C23
10	C	1108	PCW	C40-C41-C42-C43
10	C	1111	PCW	C36-C37-C38-C39
10	A	1107	PCW	C20-C21-C22-C23
10	A	1108	PCW	C40-C41-C42-C43
10	A	1111	PCW	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
10	C	1110	PCW	C1-O3P-P-O4P
10	A	1110	PCW	C1-O3P-P-O4P
10	C	1115	PCW	C31-C32-C33-C34
10	C	1108	PCW	O3P-C1-C2-C3
10	C	1111	PCW	O3P-C1-C2-C3
10	C	1115	PCW	O3P-C1-C2-C3
10	C	1116	PCW	O3P-C1-C2-C3
10	E	102	PCW	O3P-C1-C2-C3
10	A	1108	PCW	O3P-C1-C2-C3
10	A	1111	PCW	O3P-C1-C2-C3
10	A	1115	PCW	O3P-C1-C2-C3
10	A	1116	PCW	O3P-C1-C2-C3
10	G	102	PCW	O3P-C1-C2-C3
10	A	1115	PCW	C31-C32-C33-C34
10	C	1110	PCW	C32-C33-C34-C35
10	C	1112	PCW	C35-C36-C37-C38
10	A	1110	PCW	C32-C33-C34-C35
10	A	1112	PCW	C35-C36-C37-C38
10	C	1109	PCW	C40-C41-C42-C43
10	A	1109	PCW	C40-C41-C42-C43
10	C	1110	PCW	C24-C25-C26-C27
10	A	1110	PCW	C24-C25-C26-C27
10	E	102	PCW	C11-C12-C13-C14
10	C	1115	PCW	C21-C22-C23-C24
10	A	1115	PCW	C21-C22-C23-C24
10	C	1108	PCW	C1-C2-C3-O3
10	C	1111	PCW	C1-C2-C3-O3
10	A	1108	PCW	C1-C2-C3-O3
10	A	1111	PCW	C1-C2-C3-O3
10	G	102	PCW	C11-C12-C13-C14
10	C	1110	PCW	C14-C15-C16-C17
10	C	1112	PCW	C43-C44-C45-C46
10	A	1110	PCW	C14-C15-C16-C17
10	A	1112	PCW	C43-C44-C45-C46
10	E	102	PCW	C16-C17-C18-C19
10	G	102	PCW	C16-C17-C18-C19
10	C	1108	PCW	C14-C15-C16-C17
10	A	1108	PCW	C14-C15-C16-C17
10	C	1113	PCW	O3P-C1-C2-O2
10	A	1113	PCW	O3P-C1-C2-O2
10	C	1110	PCW	C15-C16-C17-C18
10	A	1110	PCW	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
10	E	102	PCW	C31-C32-C33-C34
10	G	102	PCW	C31-C32-C33-C34
10	C	1113	PCW	O3P-C1-C2-C3
10	A	1113	PCW	O3P-C1-C2-C3
10	C	1113	PCW	C43-C44-C45-C46
10	A	1113	PCW	C43-C44-C45-C46
10	C	1106	PCW	C1-C2-C3-O3
10	C	1110	PCW	C1-C2-C3-O3
10	C	1115	PCW	C1-C2-C3-O3
10	A	1106	PCW	C1-C2-C3-O3
10	A	1110	PCW	C1-C2-C3-O3
10	A	1115	PCW	C1-C2-C3-O3
10	C	1113	PCW	C14-C15-C16-C17
10	A	1113	PCW	C14-C15-C16-C17
10	C	1113	PCW	C23-C24-C25-C26
10	A	1113	PCW	C23-C24-C25-C26
10	C	1110	PCW	O3P-C1-C2-O2
10	C	1115	PCW	O3P-C1-C2-O2
10	C	1116	PCW	O3P-C1-C2-O2
10	A	1110	PCW	O3P-C1-C2-O2
10	A	1115	PCW	O3P-C1-C2-O2
10	A	1116	PCW	O3P-C1-C2-O2
10	C	1113	PCW	C35-C36-C37-C38
10	C	1115	PCW	C22-C23-C24-C25
10	A	1113	PCW	C35-C36-C37-C38
10	C	1106	PCW	O2-C2-C3-O3
10	C	1108	PCW	O2-C2-C3-O3
10	A	1106	PCW	O2-C2-C3-O3
10	A	1108	PCW	O2-C2-C3-O3
10	A	1115	PCW	C22-C23-C24-C25
10	C	1115	PCW	C45-C46-C47-C48
10	A	1115	PCW	C45-C46-C47-C48
10	C	1110	PCW	C33-C34-C35-C36
10	C	1113	PCW	C21-C22-C23-C24
10	A	1110	PCW	C33-C34-C35-C36
10	A	1113	PCW	C21-C22-C23-C24
10	C	1107	PCW	C1-C2-C3-O3
10	C	1112	PCW	C1-C2-C3-O3
10	A	1107	PCW	C1-C2-C3-O3
10	A	1112	PCW	C1-C2-C3-O3
10	C	1107	PCW	O2-C2-C3-O3
10	A	1107	PCW	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
10	C	1109	PCW	C36-C37-C38-C39
10	A	1109	PCW	C36-C37-C38-C39
10	C	1108	PCW	C1-O3P-P-O4P
10	A	1108	PCW	C1-O3P-P-O4P
10	C	1106	PCW	C4-C5-N-C6
10	C	1106	PCW	C4-O4P-P-O1P
10	C	1106	PCW	C4-O4P-P-O2P
10	C	1113	PCW	C1-O3P-P-O2P
10	C	1113	PCW	C4-O4P-P-O1P
10	C	1116	PCW	C1-O3P-P-O2P
10	E	101	PCW	C4-O4P-P-O1P
10	A	1106	PCW	C4-C5-N-C6
10	A	1106	PCW	C4-O4P-P-O1P
10	A	1106	PCW	C4-O4P-P-O2P
10	A	1113	PCW	C1-O3P-P-O2P
10	A	1113	PCW	C4-O4P-P-O1P
10	A	1116	PCW	C1-O3P-P-O2P
10	G	101	PCW	C4-O4P-P-O1P
10	A	1109	PCW	C32-C33-C34-C35
10	C	1109	PCW	C32-C33-C34-C35
10	C	1106	PCW	O4P-C4-C5-N
10	C	1107	PCW	O4P-C4-C5-N
10	C	1108	PCW	O4P-C4-C5-N
10	C	1109	PCW	O4P-C4-C5-N
10	C	1110	PCW	O4P-C4-C5-N
10	C	1111	PCW	O4P-C4-C5-N
10	C	1112	PCW	O4P-C4-C5-N
10	C	1113	PCW	O4P-C4-C5-N
10	C	1114	PCW	O4P-C4-C5-N
10	C	1115	PCW	O4P-C4-C5-N
10	C	1116	PCW	O4P-C4-C5-N
10	E	101	PCW	O4P-C4-C5-N
10	E	102	PCW	O4P-C4-C5-N
10	A	1106	PCW	O4P-C4-C5-N
10	A	1107	PCW	O4P-C4-C5-N
10	A	1108	PCW	O4P-C4-C5-N
10	A	1109	PCW	O4P-C4-C5-N
10	A	1110	PCW	O4P-C4-C5-N
10	A	1111	PCW	O4P-C4-C5-N
10	A	1112	PCW	O4P-C4-C5-N
10	A	1113	PCW	O4P-C4-C5-N
10	A	1114	PCW	O4P-C4-C5-N

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Mol	Chain	Res	Type	Atoms
10	A	1115	PCW	O4P-C4-C5-N
10	A	1116	PCW	O4P-C4-C5-N
10	G	101	PCW	O4P-C4-C5-N
10	G	102	PCW	O4P-C4-C5-N
10	C	1110	PCW	O2-C2-C3-O3
10	C	1115	PCW	O2-C2-C3-O3
10	A	1110	PCW	O2-C2-C3-O3
10	A	1115	PCW	O2-C2-C3-O3
10	C	1109	PCW	C14-C15-C16-C17
10	A	1109	PCW	C14-C15-C16-C17
10	C	1107	PCW	C35-C36-C37-C38
10	A	1107	PCW	C35-C36-C37-C38
10	C	1115	PCW	C39-C40-C41-C42
10	A	1115	PCW	C39-C40-C41-C42
10	C	1106	PCW	O3P-C1-C2-C3
10	A	1106	PCW	O3P-C1-C2-C3
10	C	1111	PCW	O3P-C1-C2-O2
10	E	102	PCW	O3P-C1-C2-O2
10	A	1111	PCW	O3P-C1-C2-O2
10	G	102	PCW	O3P-C1-C2-O2
10	C	1106	PCW	C4-C5-N-C8
10	A	1106	PCW	C4-C5-N-C8
10	C	1107	PCW	C1-O3P-P-O4P
10	C	1108	PCW	C4-O4P-P-O3P
10	C	1109	PCW	C4-O4P-P-O3P
10	C	1110	PCW	C4-O4P-P-O3P
10	C	1111	PCW	C4-O4P-P-O3P
10	C	1115	PCW	C4-O4P-P-O3P
10	C	1116	PCW	C4-O4P-P-O3P
10	A	1107	PCW	C1-O3P-P-O4P
10	A	1108	PCW	C4-O4P-P-O3P
10	A	1109	PCW	C4-O4P-P-O3P
10	A	1110	PCW	C4-O4P-P-O3P
10	A	1111	PCW	C4-O4P-P-O3P
10	A	1115	PCW	C4-O4P-P-O3P
10	A	1116	PCW	C4-O4P-P-O3P
10	C	1110	PCW	C41-C42-C43-C44
10	A	1110	PCW	C41-C42-C43-C44
10	C	1113	PCW	C34-C35-C36-C37
10	A	1113	PCW	C34-C35-C36-C37
10	C	1110	PCW	C42-C43-C44-C45
10	A	1110	PCW	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
10	C	1108	PCW	C17-C18-C19-C20
10	A	1108	PCW	C17-C18-C19-C20
10	C	1115	PCW	C41-C42-C43-C44
10	A	1115	PCW	C41-C42-C43-C44
10	C	1106	PCW	O3P-C1-C2-O2
10	A	1106	PCW	O3P-C1-C2-O2
10	E	102	PCW	C20-C21-C22-C23
10	G	102	PCW	C20-C21-C22-C23
10	C	1109	PCW	O2-C2-C3-O3
10	A	1109	PCW	O2-C2-C3-O3
10	C	1107	PCW	C2-C1-O3P-P
10	A	1107	PCW	C2-C1-O3P-P
10	C	1109	PCW	C1-C2-C3-O3
10	A	1109	PCW	C1-C2-C3-O3
10	C	1106	PCW	C4-C5-N-C7
10	A	1106	PCW	C4-C5-N-C7
9	D	501	CLR	C23-C24-C25-C27
9	B	501	CLR	C23-C24-C25-C27
10	C	1115	PCW	C43-C44-C45-C46
10	A	1115	PCW	C43-C44-C45-C46
10	C	1107	PCW	O3P-C1-C2-C3
10	C	1110	PCW	O3P-C1-C2-C3
10	C	1114	PCW	O3P-C1-C2-C3
10	A	1107	PCW	O3P-C1-C2-C3
10	A	1110	PCW	O3P-C1-C2-C3
10	A	1114	PCW	O3P-C1-C2-C3
10	C	1110	PCW	C19-C20-C21-C22
10	A	1110	PCW	C19-C20-C21-C22
10	C	1112	PCW	C36-C37-C38-C39
10	A	1112	PCW	C36-C37-C38-C39
10	C	1112	PCW	C41-C42-C43-C44
10	A	1112	PCW	C41-C42-C43-C44
10	C	1112	PCW	C14-C15-C16-C17
10	A	1112	PCW	C14-C15-C16-C17
10	C	1108	PCW	C22-C23-C24-C25
10	A	1108	PCW	C22-C23-C24-C25
10	C	1115	PCW	C19-C20-C21-C22
10	A	1115	PCW	C19-C20-C21-C22
10	C	1107	PCW	O3P-C1-C2-O2
10	A	1107	PCW	O3P-C1-C2-O2
10	C	1109	PCW	C39-C40-C41-C42
10	A	1109	PCW	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
10	G	102	PCW	C19-C20-C21-C22
10	C	1108	PCW	C36-C37-C38-C39
10	A	1108	PCW	C36-C37-C38-C39
10	C	1113	PCW	C17-C18-C19-C20
10	E	102	PCW	C19-C20-C21-C22
10	A	1113	PCW	C17-C18-C19-C20
10	C	1115	PCW	O2-C31-C32-C33
10	A	1115	PCW	O2-C31-C32-C33
10	C	1108	PCW	O2-C31-C32-C33
10	A	1108	PCW	O2-C31-C32-C33
10	C	1107	PCW	C19-C20-C21-C22
10	C	1110	PCW	C17-C18-C19-C20
10	C	1112	PCW	C17-C18-C19-C20
10	A	1107	PCW	C19-C20-C21-C22
10	A	1112	PCW	C17-C18-C19-C20
10	C	1107	PCW	O2-C31-C32-C33
10	A	1107	PCW	O2-C31-C32-C33
10	A	1110	PCW	C17-C18-C19-C20
10	G	102	PCW	C37-C38-C39-C40
10	C	1110	PCW	C16-C17-C18-C19
10	A	1110	PCW	C16-C17-C18-C19
10	C	1109	PCW	C19-C20-C21-C22
10	C	1111	PCW	C19-C20-C21-C22
10	C	1113	PCW	C19-C20-C21-C22
10	E	102	PCW	C37-C38-C39-C40
10	A	1109	PCW	C19-C20-C21-C22
10	A	1111	PCW	C19-C20-C21-C22
10	A	1113	PCW	C19-C20-C21-C22
10	C	1107	PCW	C37-C38-C39-C40
10	A	1107	PCW	C37-C38-C39-C40
10	C	1108	PCW	C37-C38-C39-C40
10	A	1108	PCW	C37-C38-C39-C40
10	C	1111	PCW	O2-C31-C32-C33
10	A	1111	PCW	O2-C31-C32-C33
10	C	1110	PCW	C37-C38-C39-C40
10	A	1110	PCW	C37-C38-C39-C40
10	A	1108	PCW	O31-C31-C32-C33
10	C	1108	PCW	O31-C31-C32-C33
10	C	1115	PCW	O31-C31-C32-C33
10	A	1107	PCW	O31-C31-C32-C33
10	C	1107	PCW	O31-C31-C32-C33
10	A	1115	PCW	O31-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
10	C	1113	PCW	C37-C38-C39-C40
10	A	1113	PCW	C37-C38-C39-C40
10	C	1107	PCW	C1-O3P-P-O2P
10	C	1110	PCW	C4-O4P-P-O2P
10	C	1111	PCW	C4-O4P-P-O2P
10	C	1115	PCW	C4-O4P-P-O2P
10	E	102	PCW	C1-O3P-P-O2P
10	A	1107	PCW	C1-O3P-P-O2P
10	A	1110	PCW	C4-O4P-P-O2P
10	A	1111	PCW	C4-O4P-P-O2P
10	A	1115	PCW	C4-O4P-P-O2P
10	G	102	PCW	C1-O3P-P-O2P
10	C	1112	PCW	C5-C4-O4P-P
10	A	1112	PCW	C5-C4-O4P-P
10	E	102	PCW	C32-C33-C34-C35
10	G	102	PCW	C32-C33-C34-C35

There are no ring outliers.

28 monomers are involved in 123 short contacts:

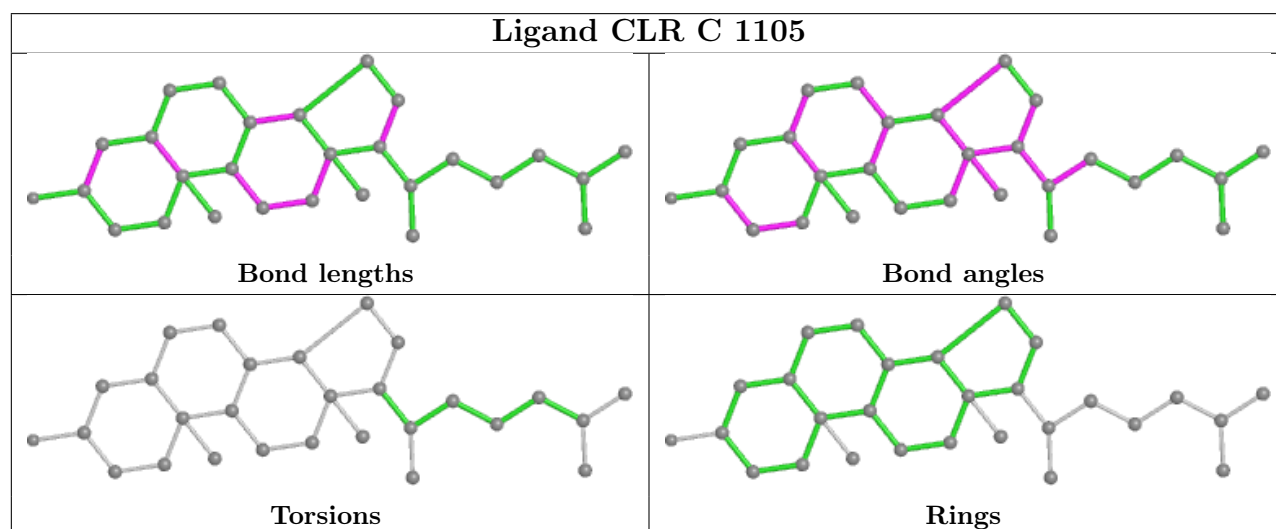
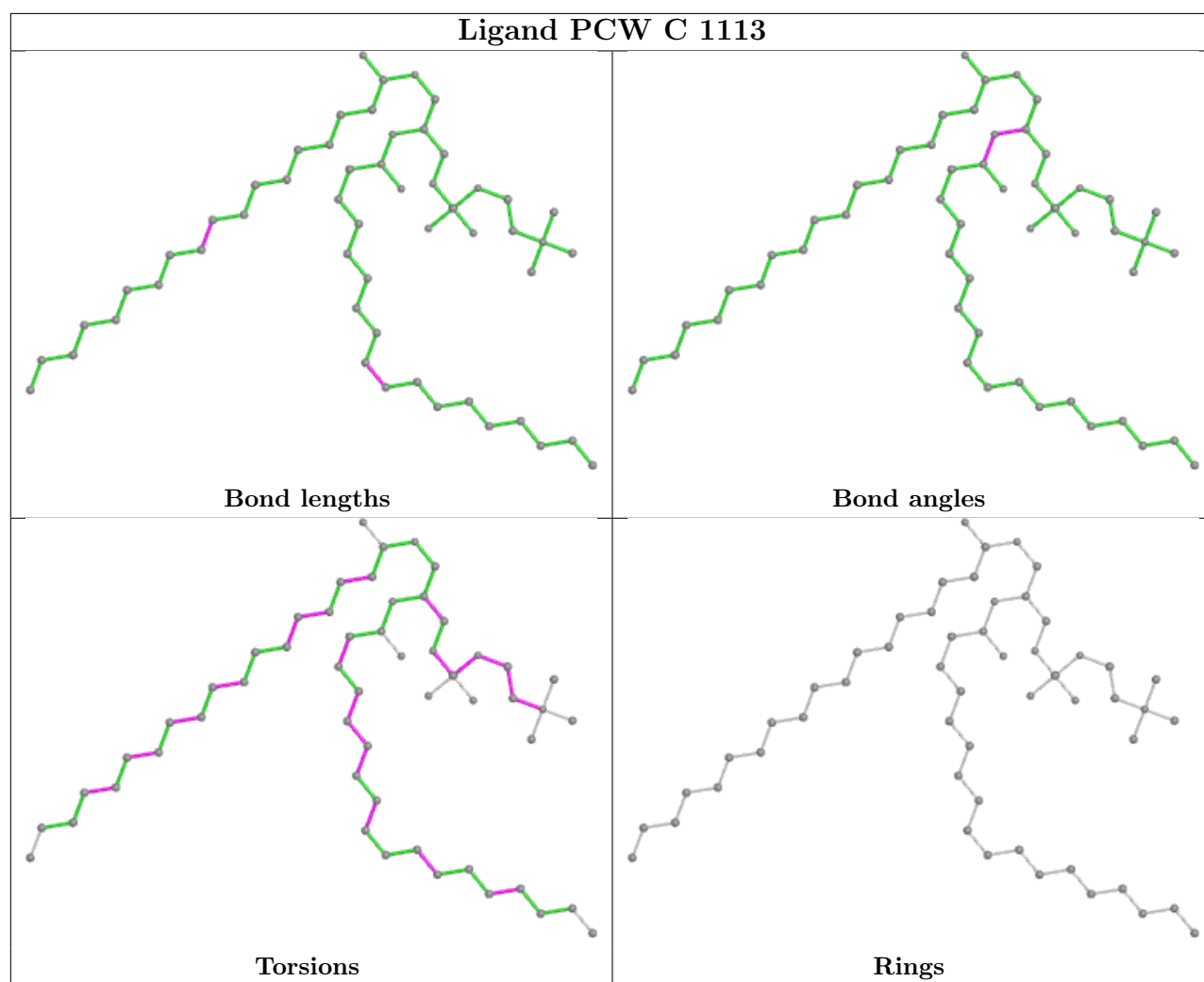
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	1113	PCW	12	0
9	C	1105	CLR	3	0
10	A	1108	PCW	4	0
10	E	101	PCW	2	0
9	A	1104	CLR	4	0
10	C	1115	PCW	7	0
10	A	1113	PCW	10	0
9	C	1104	CLR	4	0
10	A	1115	PCW	7	0
10	C	1108	PCW	4	0
10	A	1111	PCW	1	0
10	C	1110	PCW	4	0
10	A	1110	PCW	4	0
10	G	102	PCW	14	0
10	C	1112	PCW	4	0
10	C	1107	PCW	12	0
9	B	501	CLR	5	0
10	C	1111	PCW	2	0
10	A	1112	PCW	4	0
9	A	1105	CLR	4	0
10	A	1107	PCW	13	0

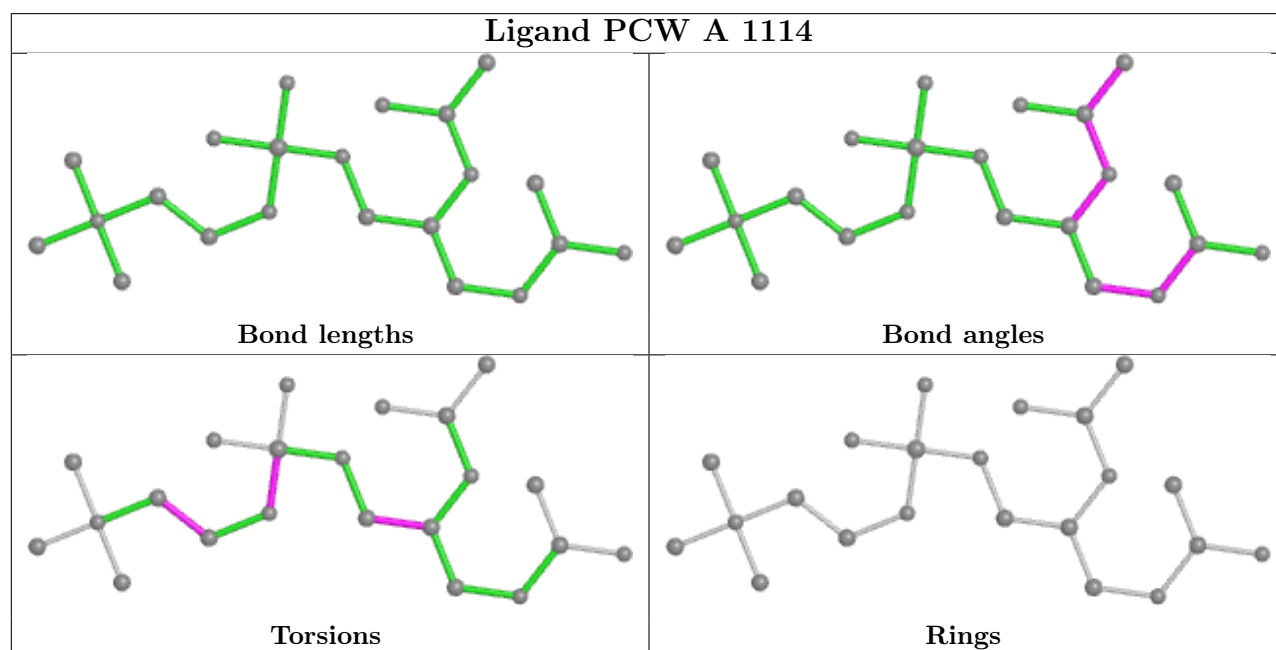
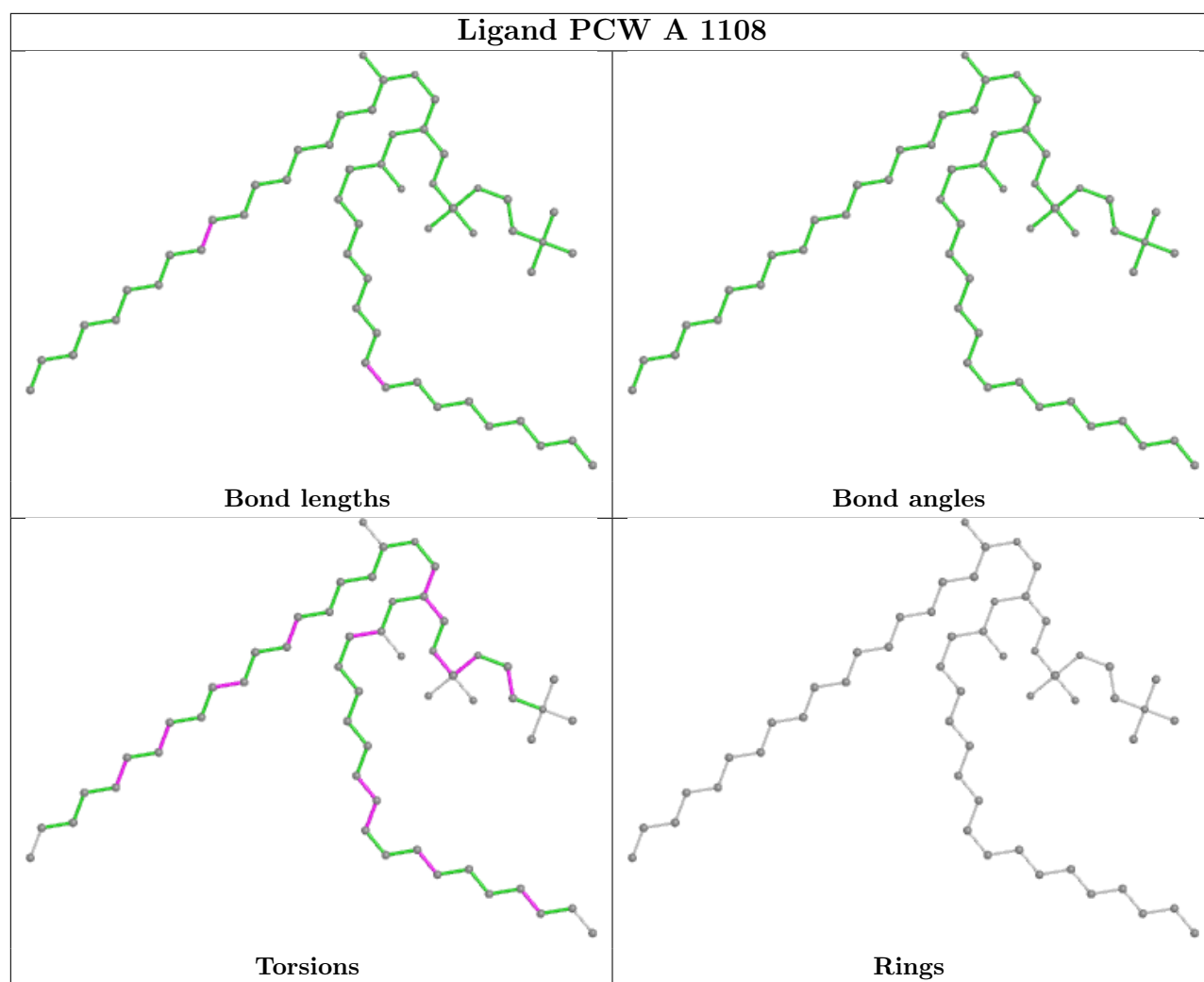
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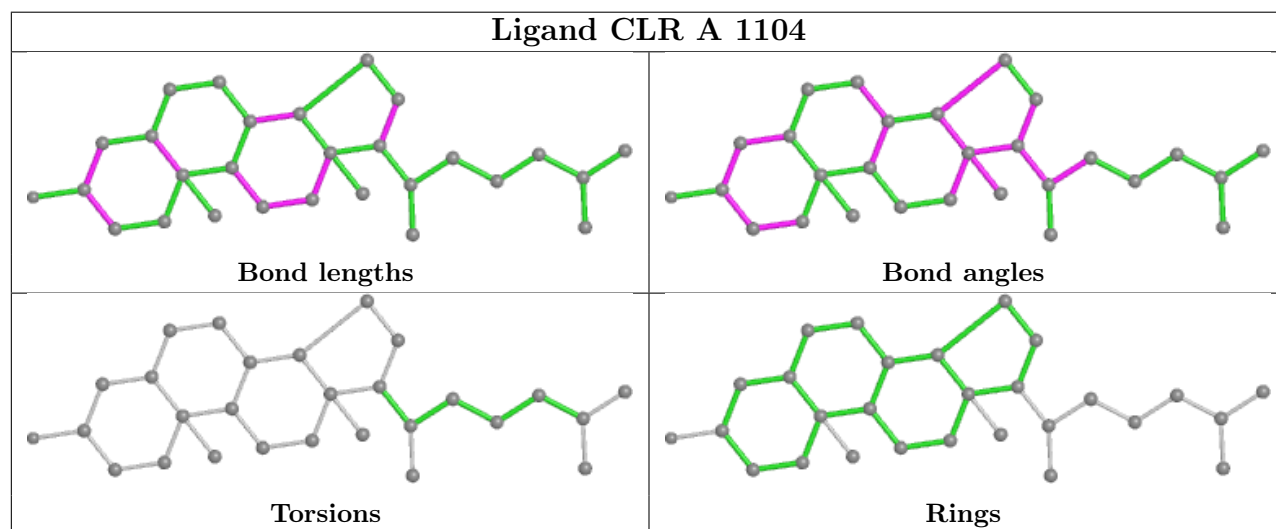
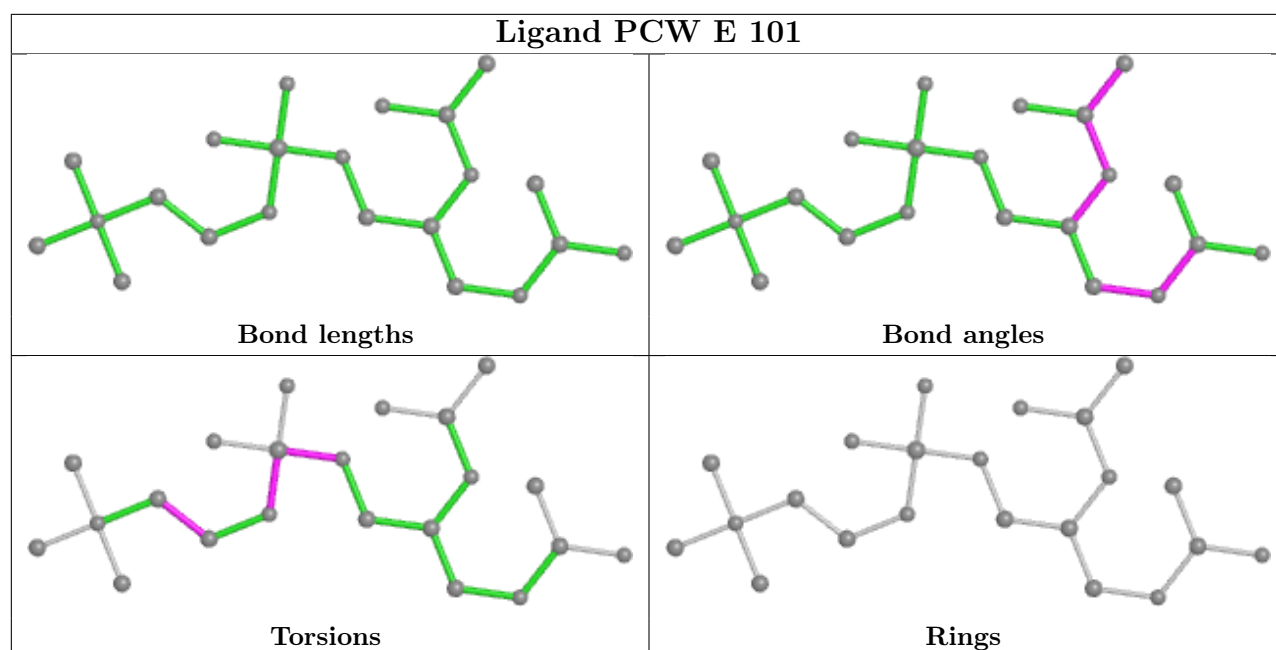
Continued from previous page...

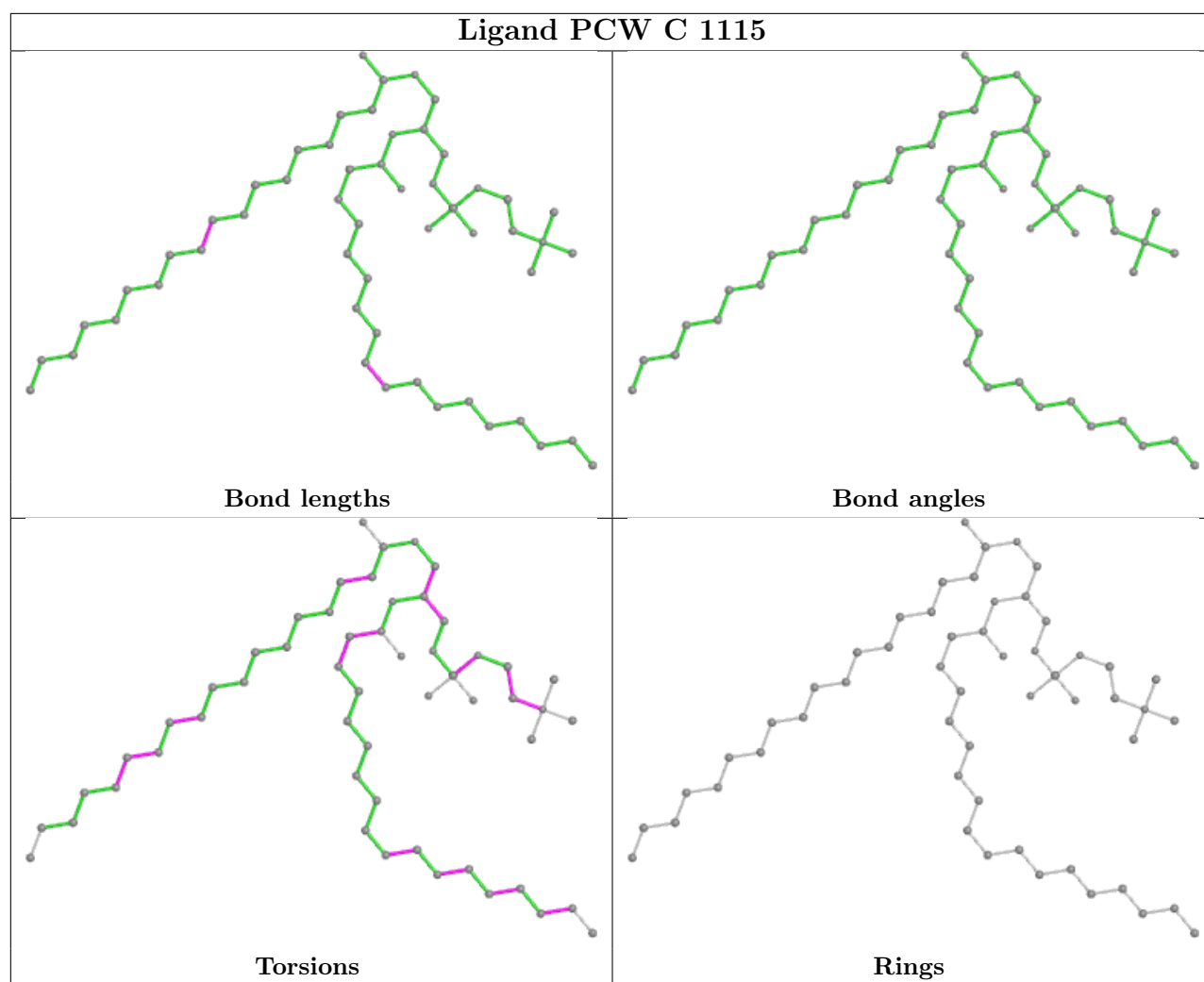
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	E	102	PCW	14	0
10	C	1109	PCW	6	0
10	A	1109	PCW	3	0
9	B	502	CLR	3	0
9	D	501	CLR	5	0
9	D	502	CLR	3	0
10	G	101	PCW	2	0

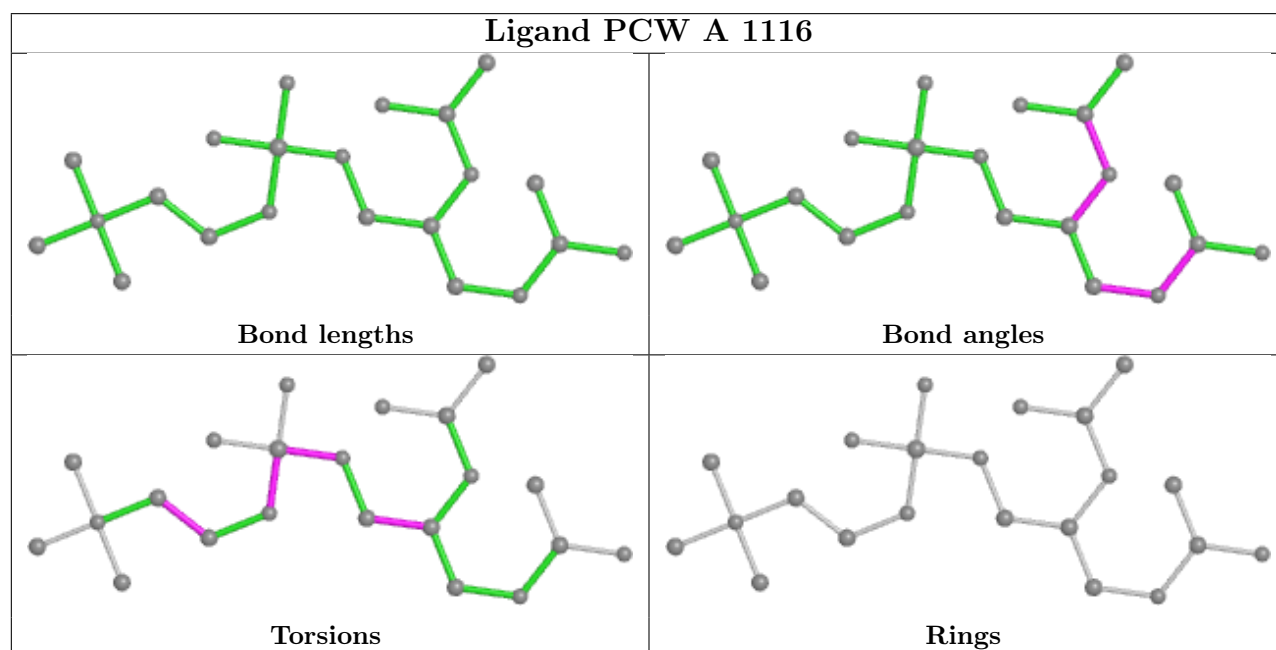
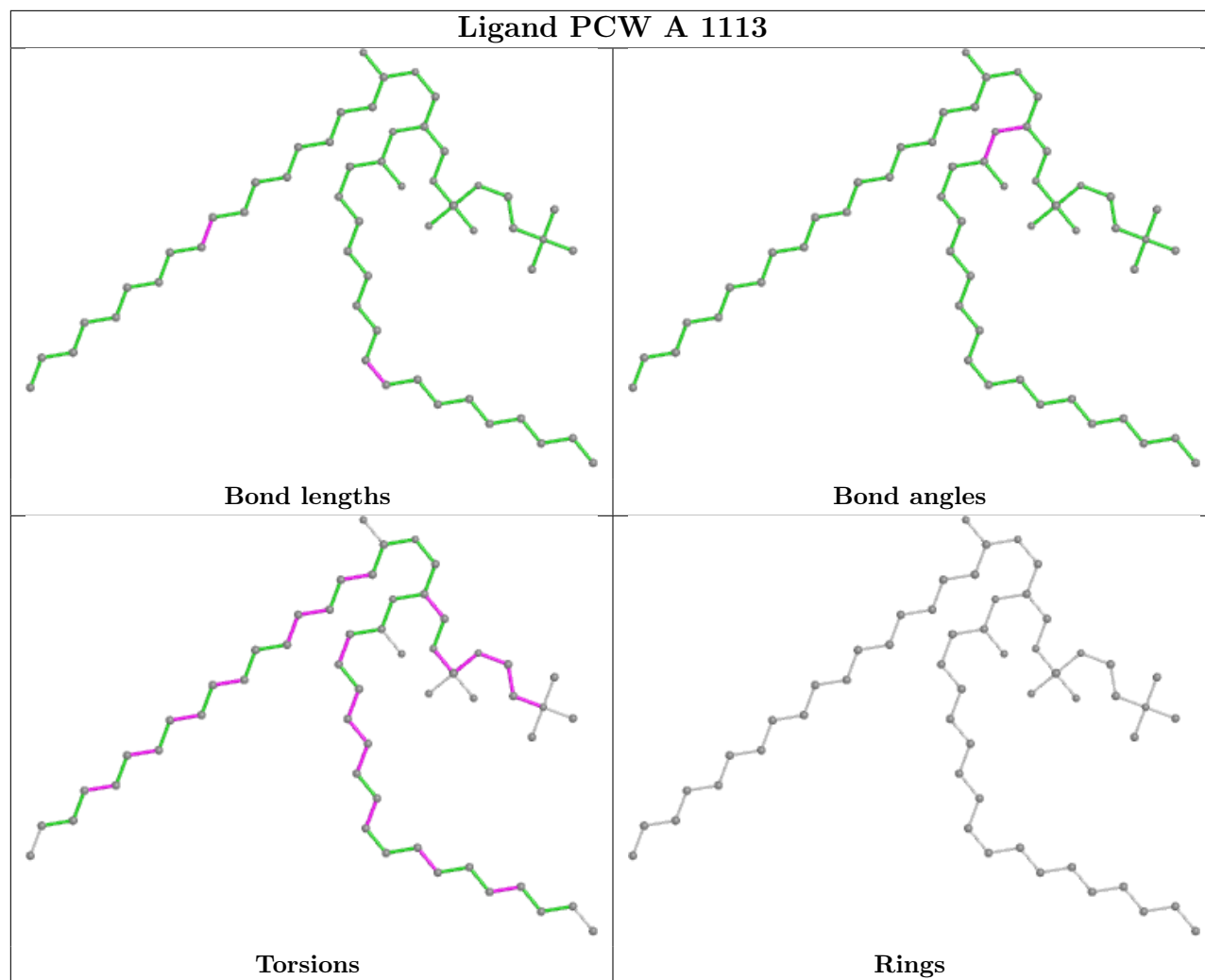
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



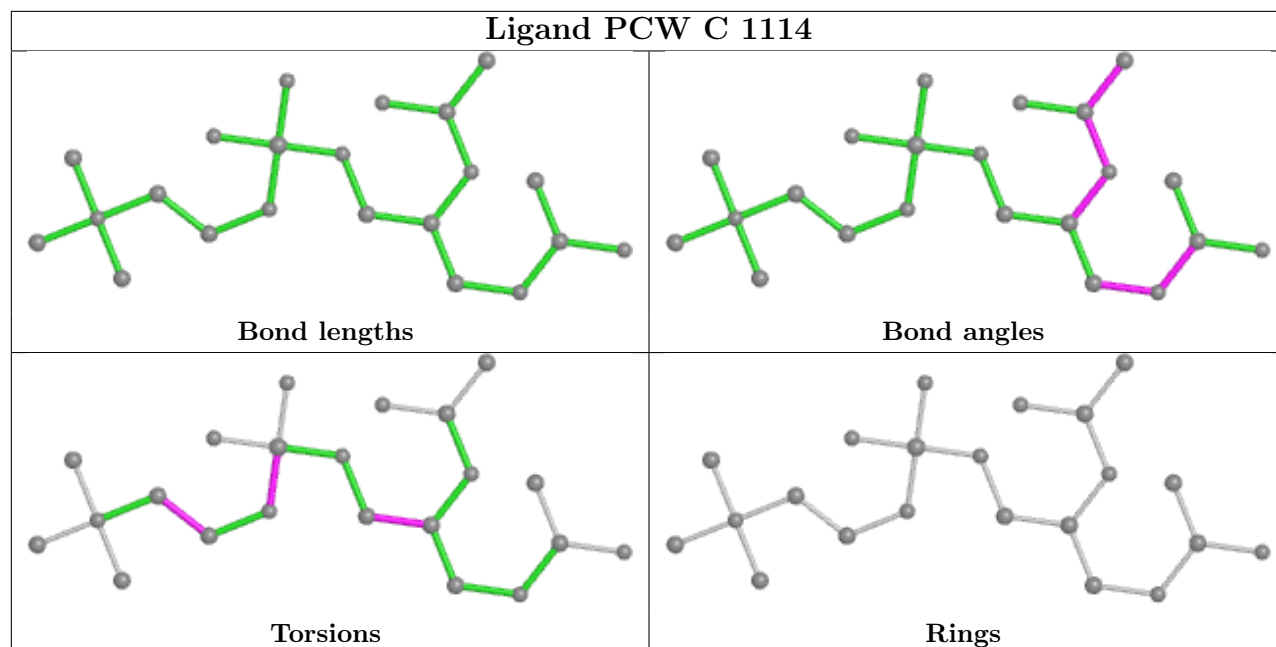




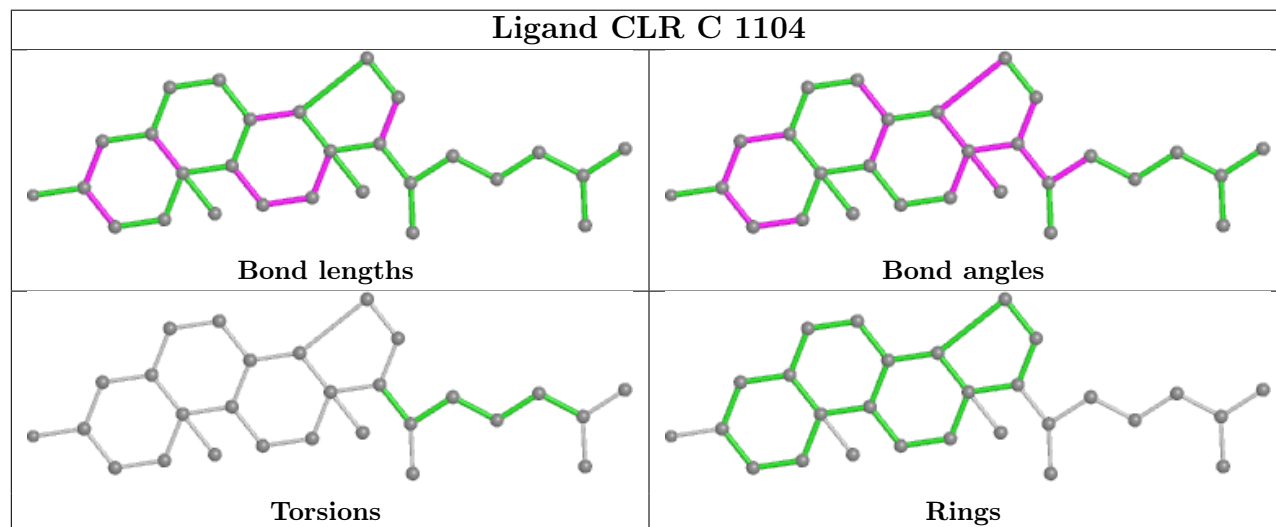


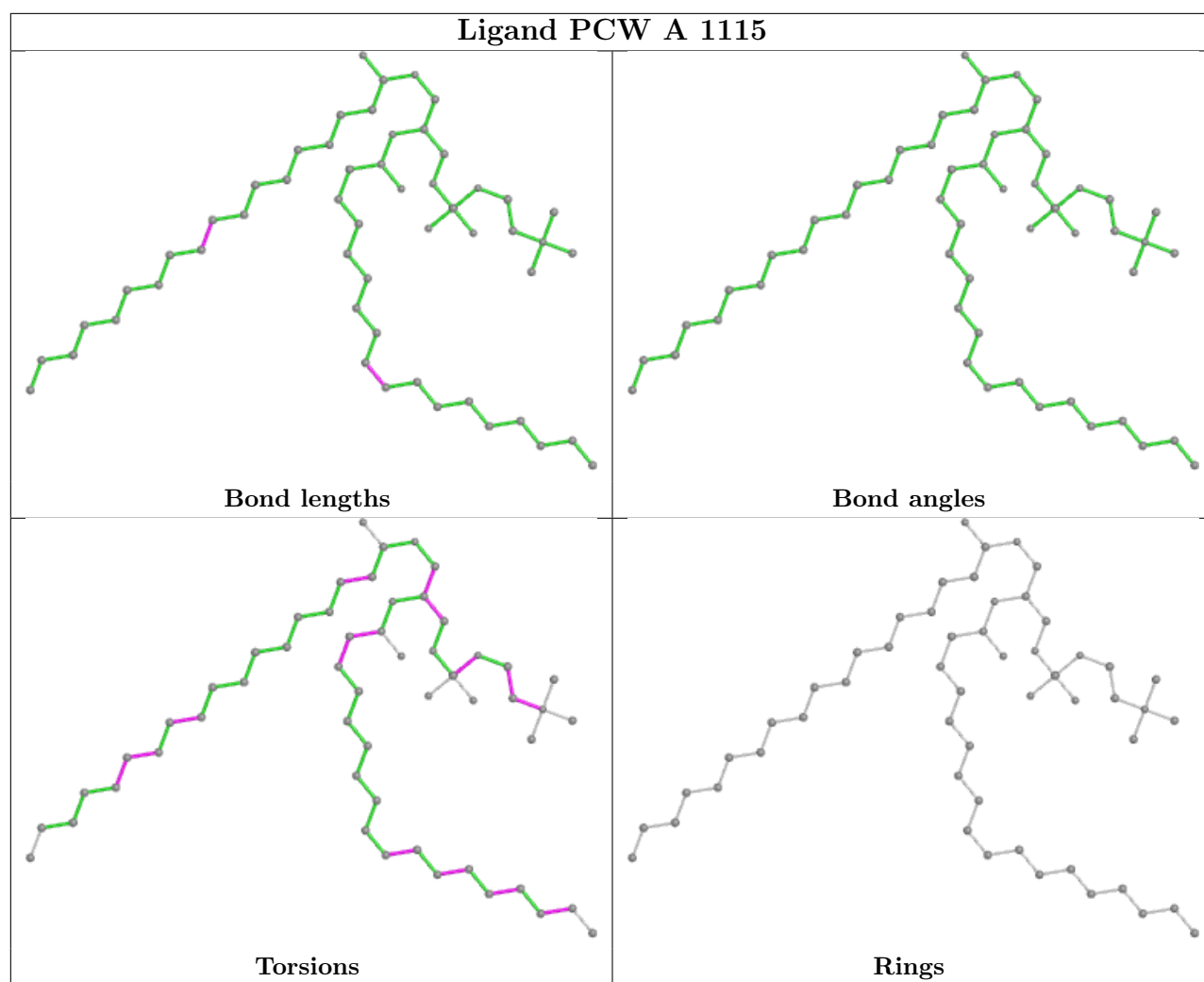


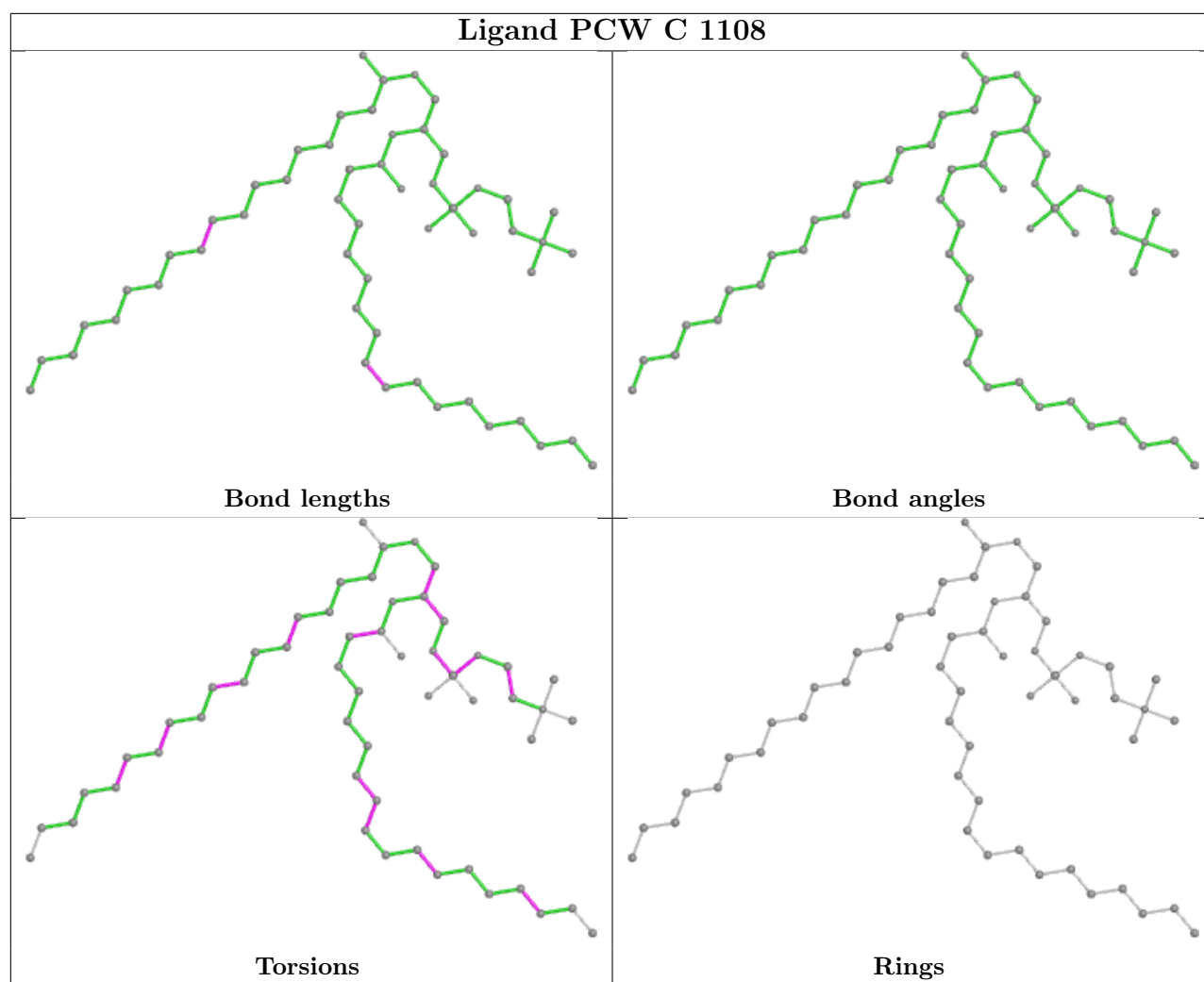
Ligand PCW C 1114

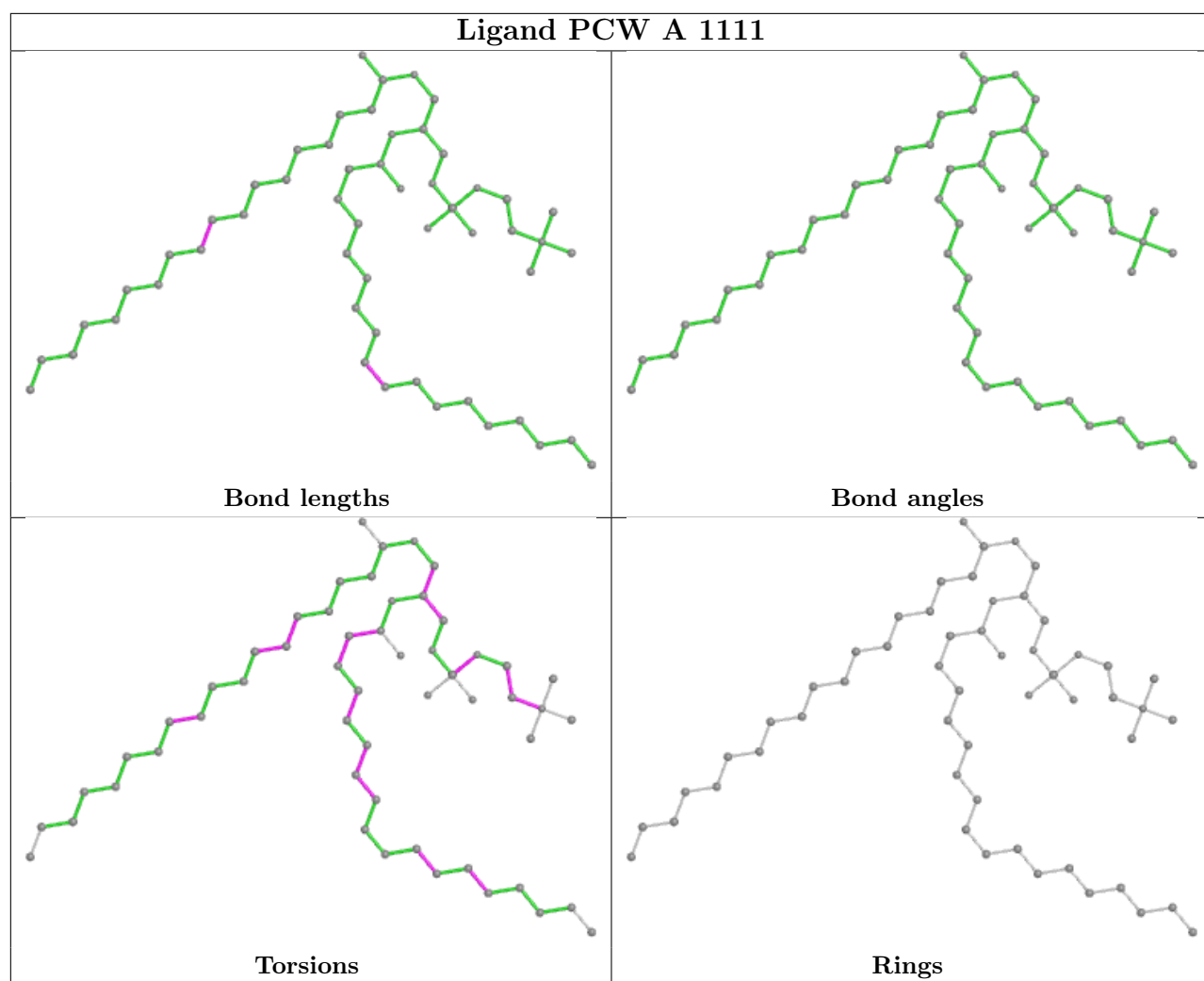


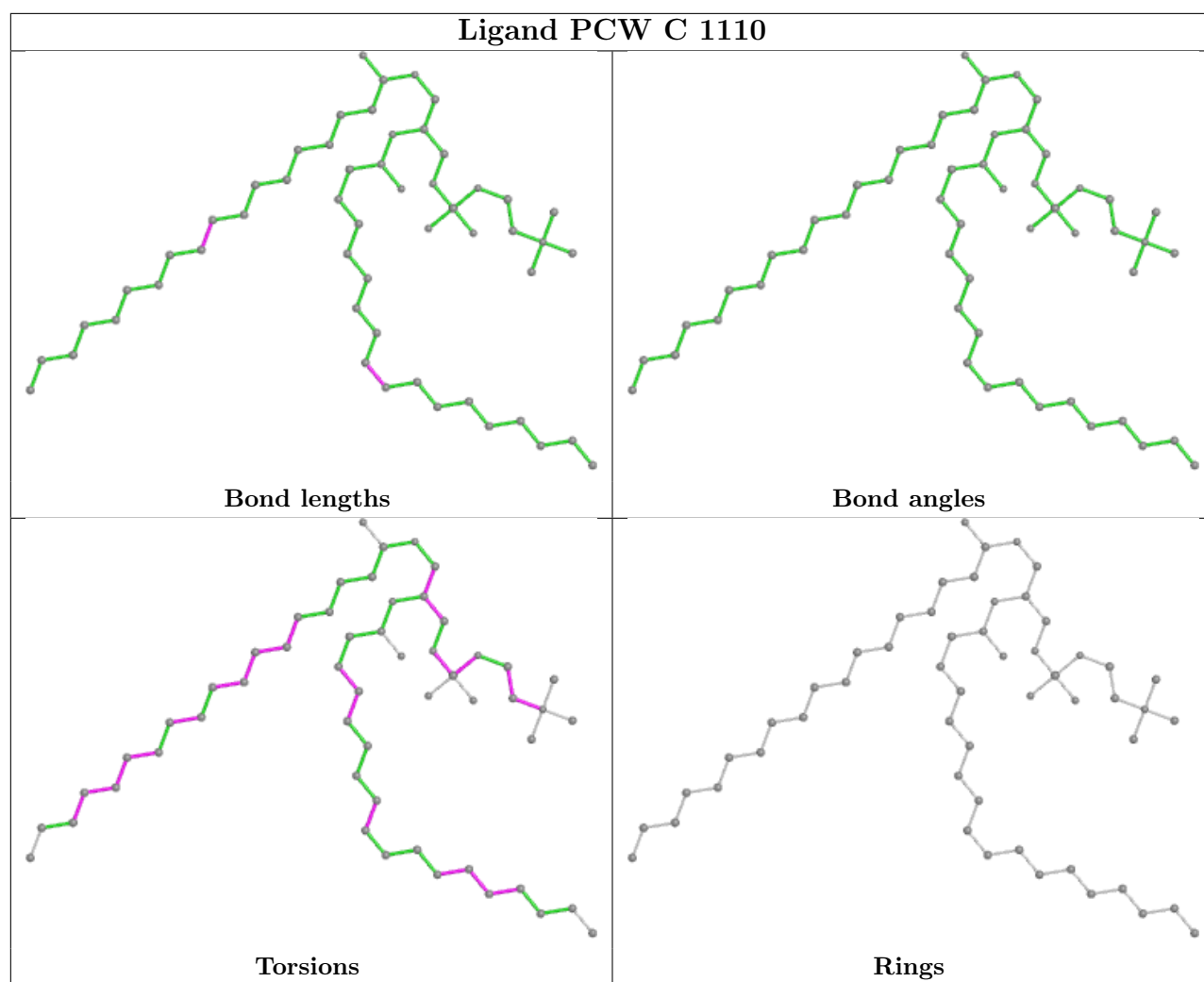
Ligand CLR C 1104

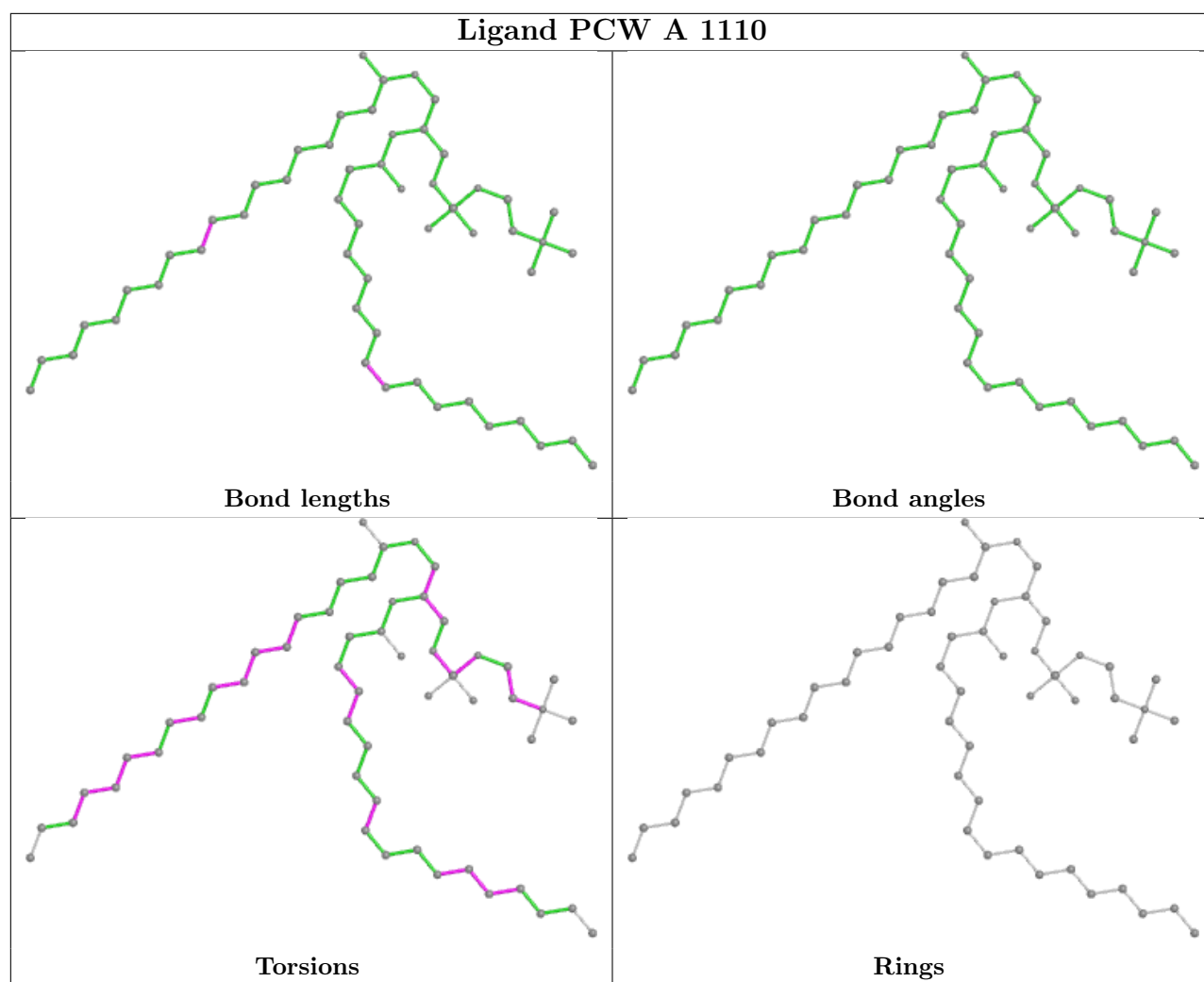


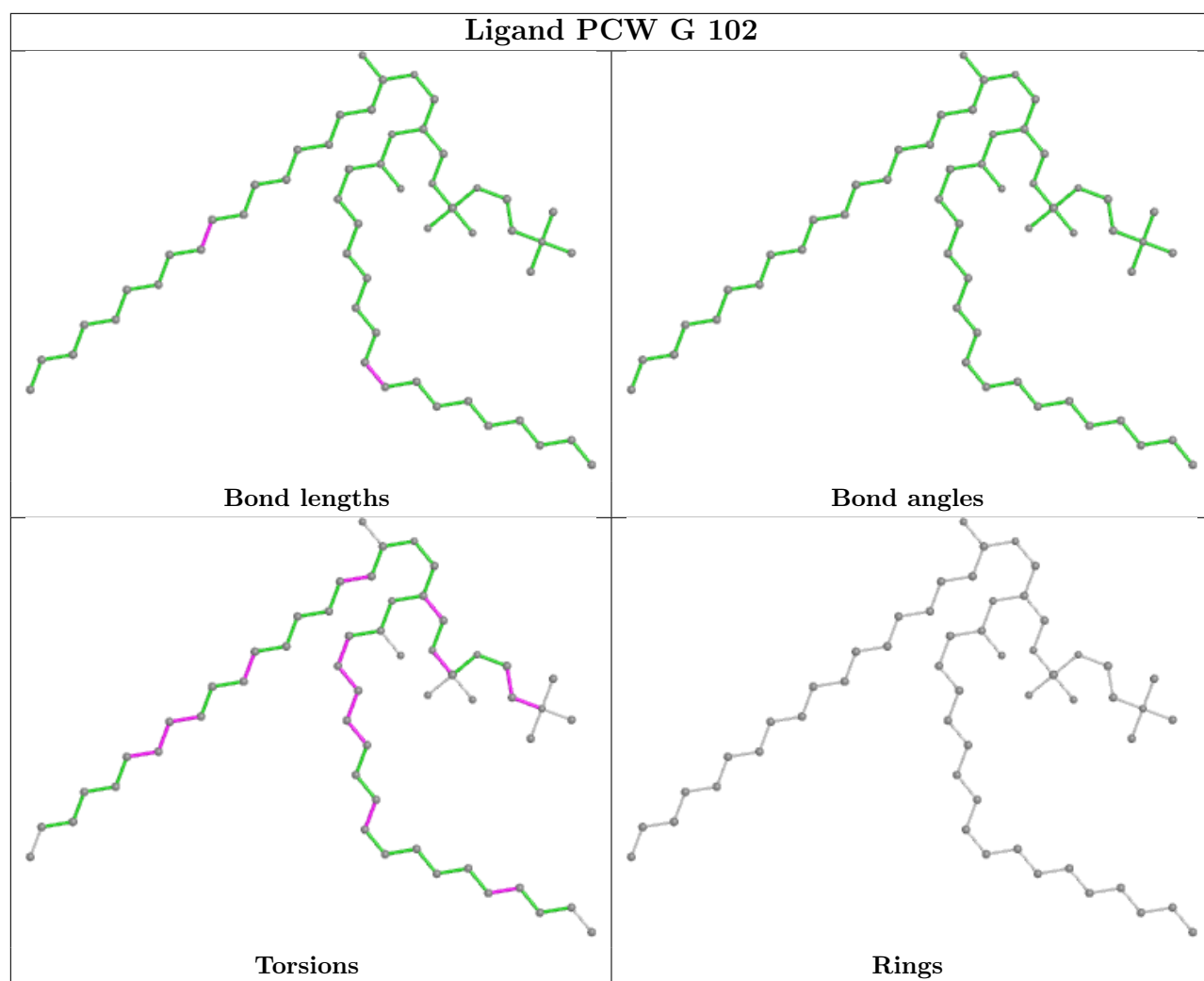


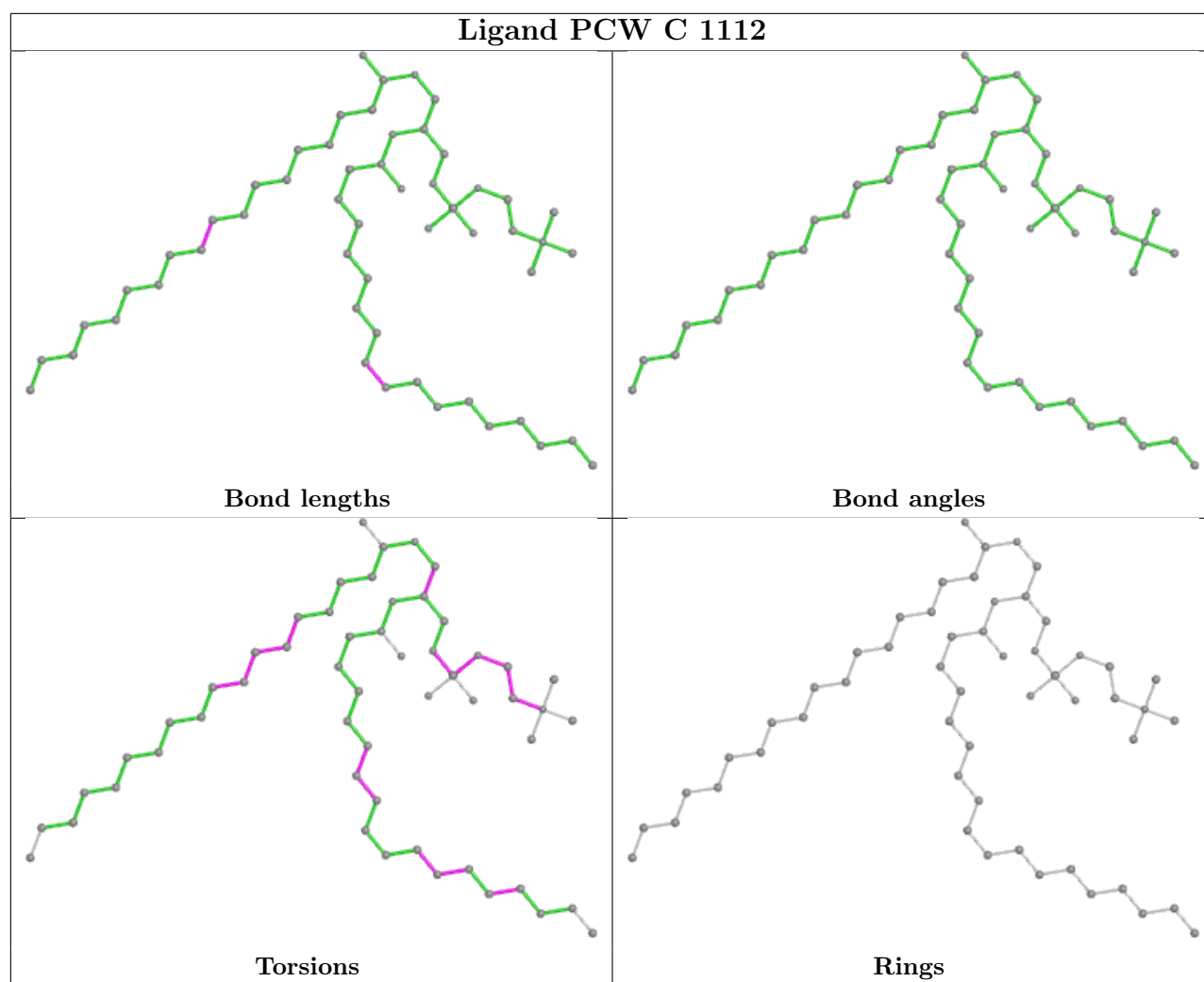




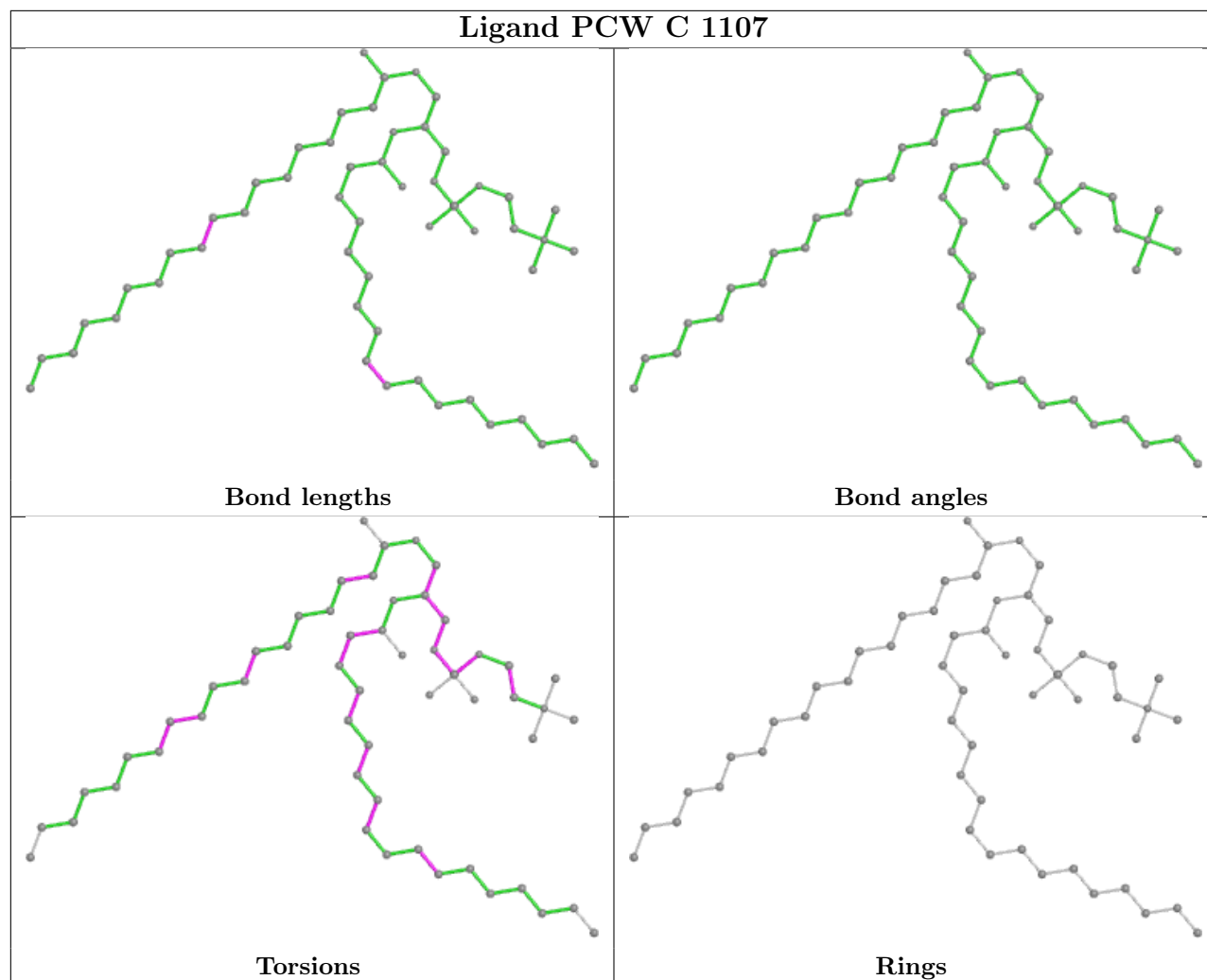




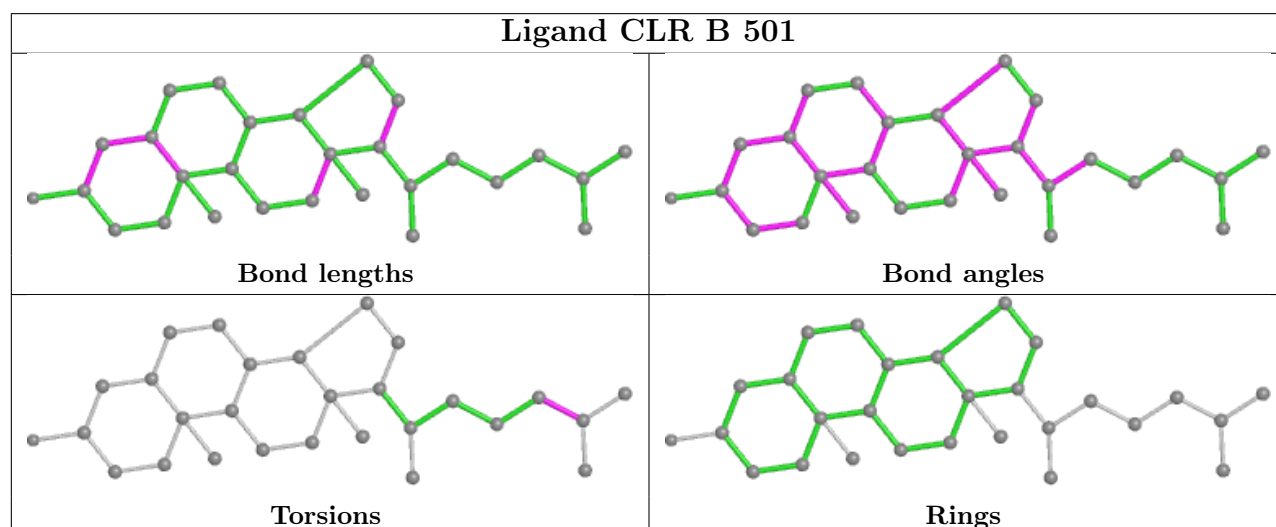


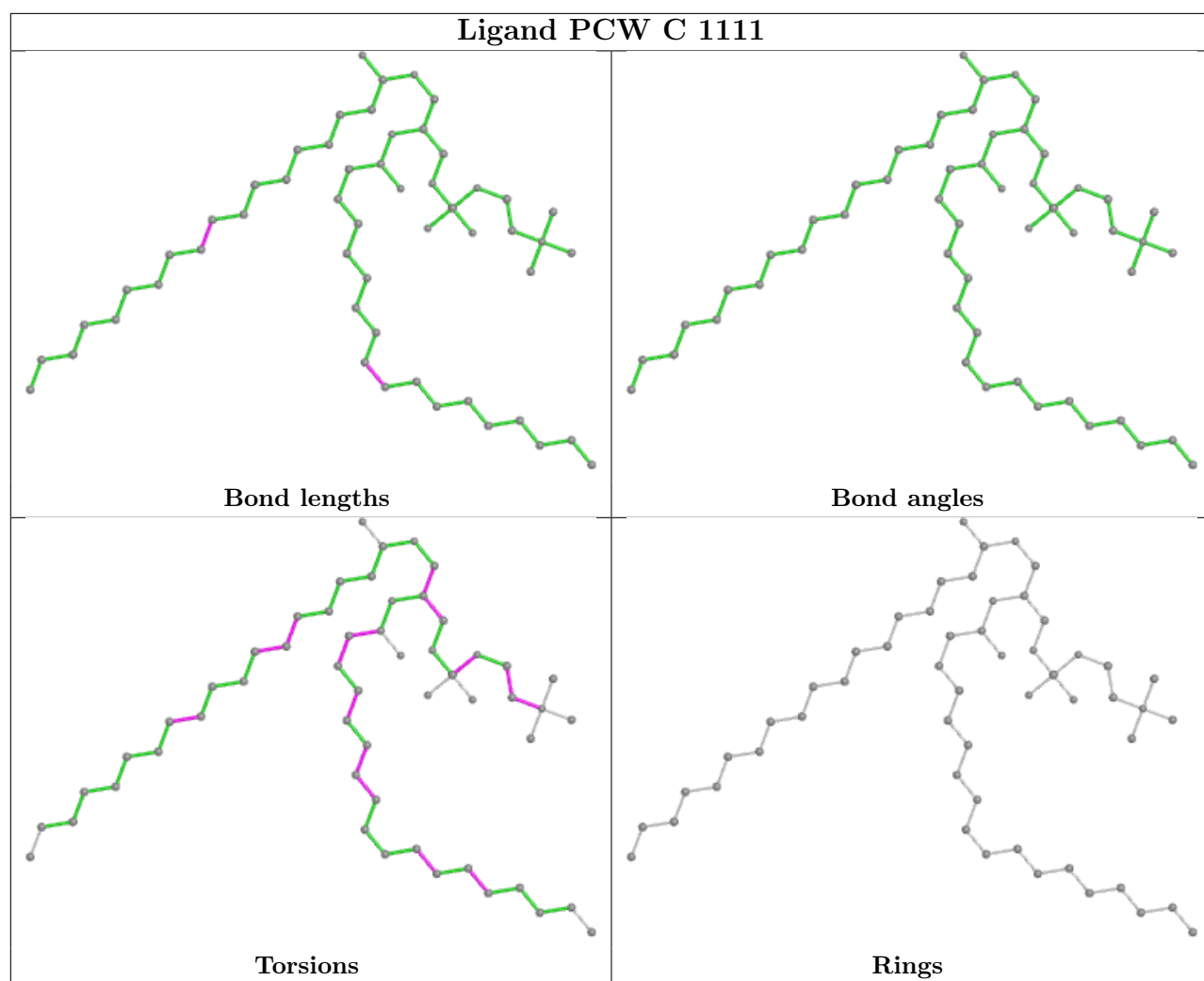


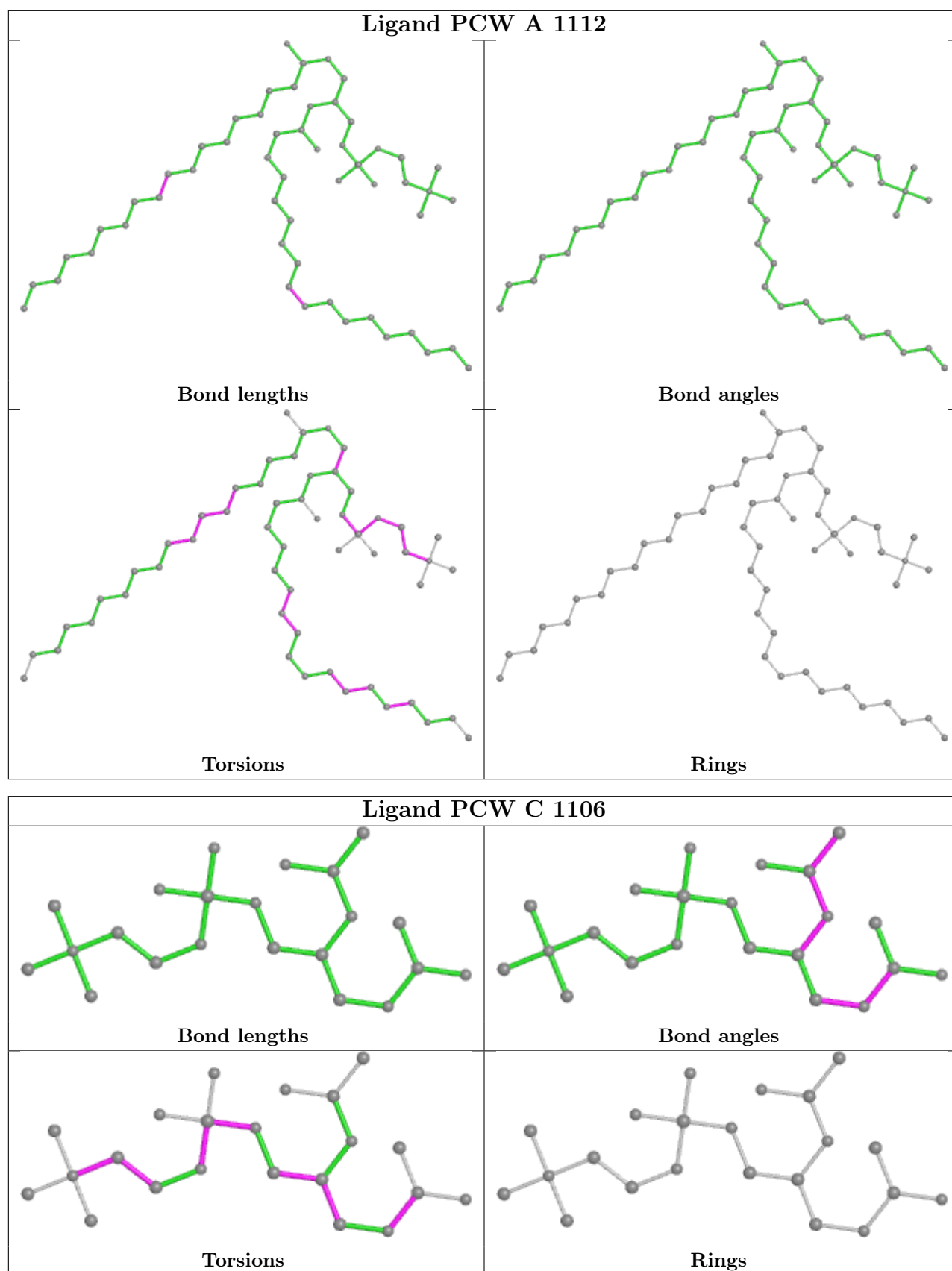
Ligand PCW C 1107

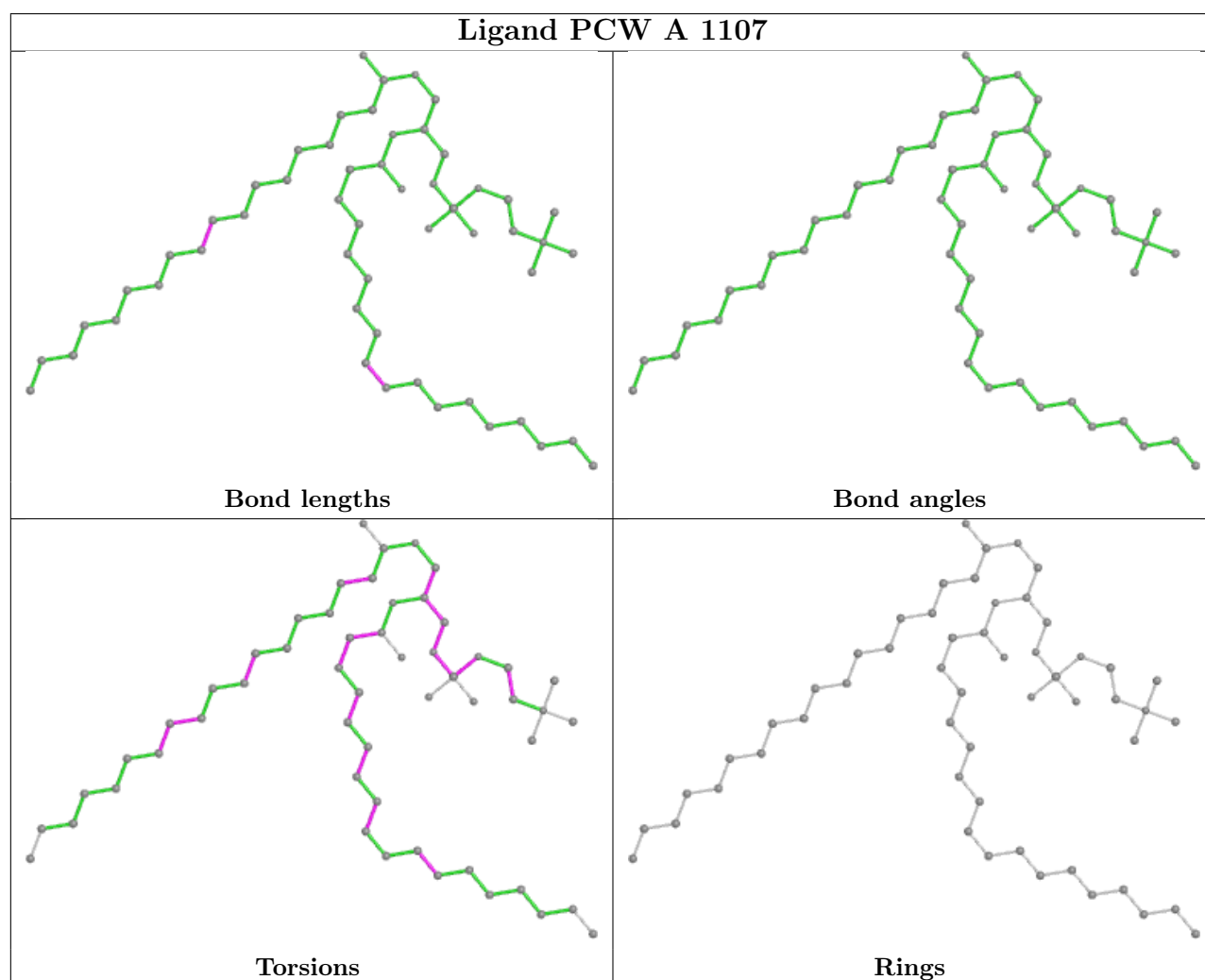
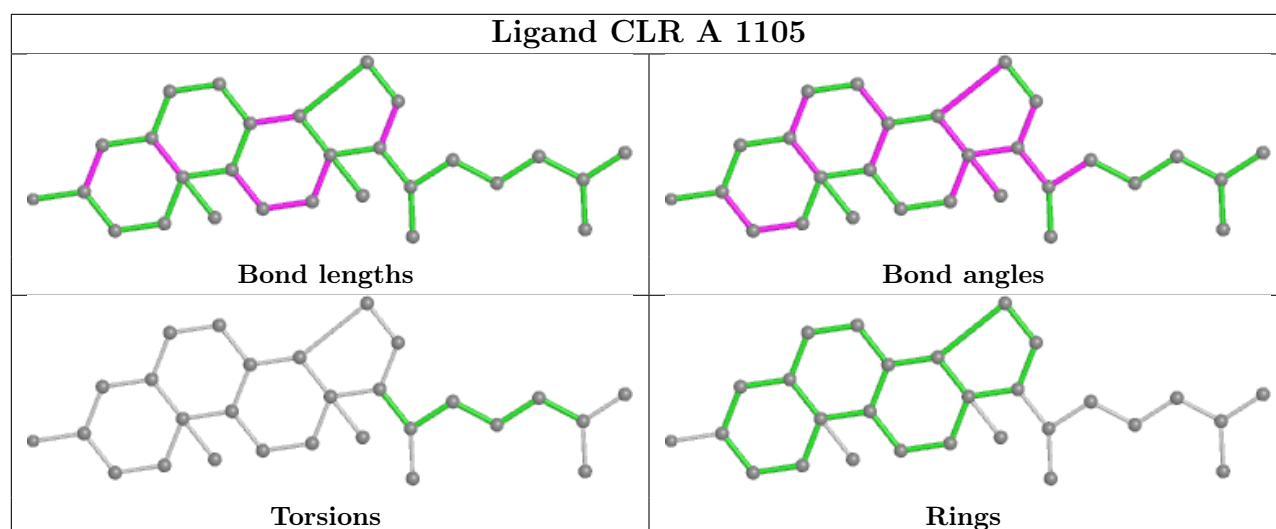


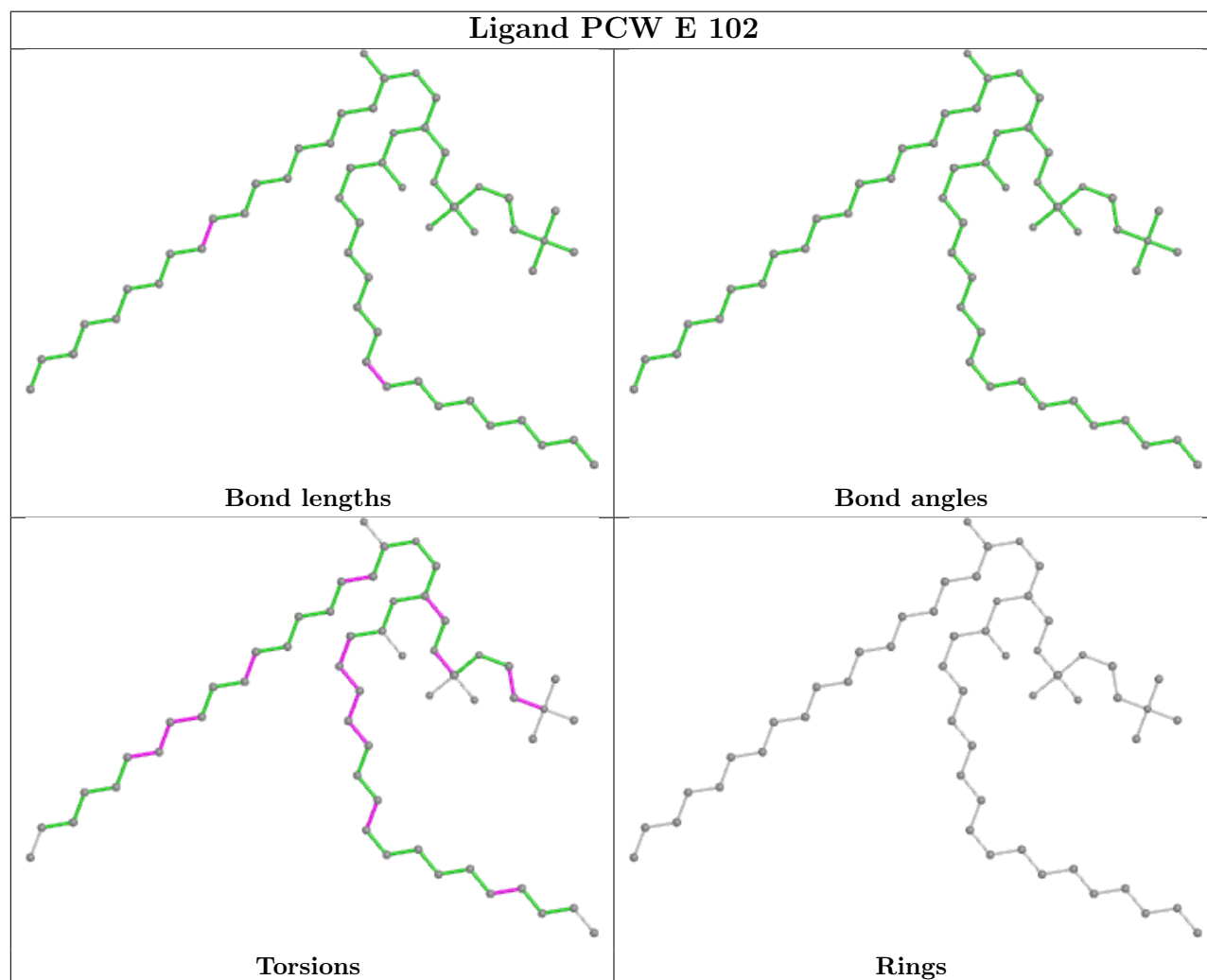
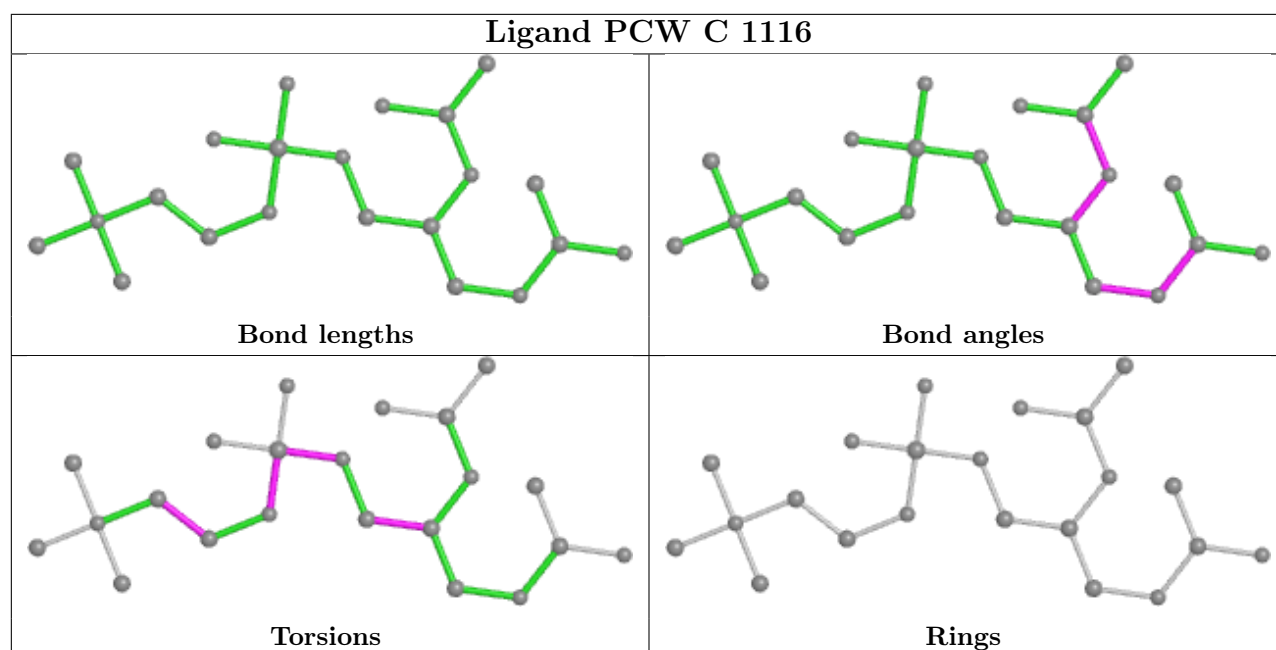
Ligand CLR B 501

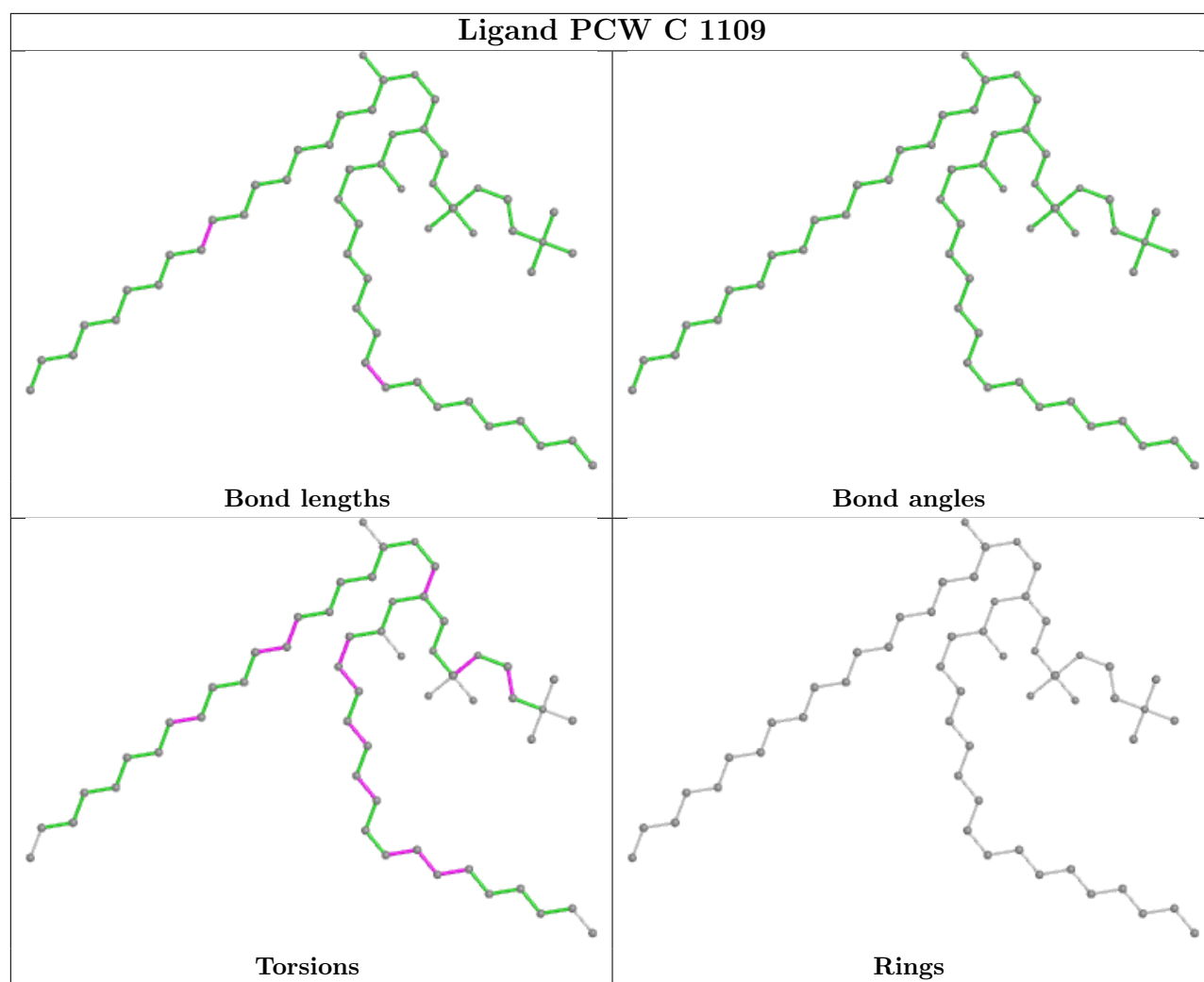




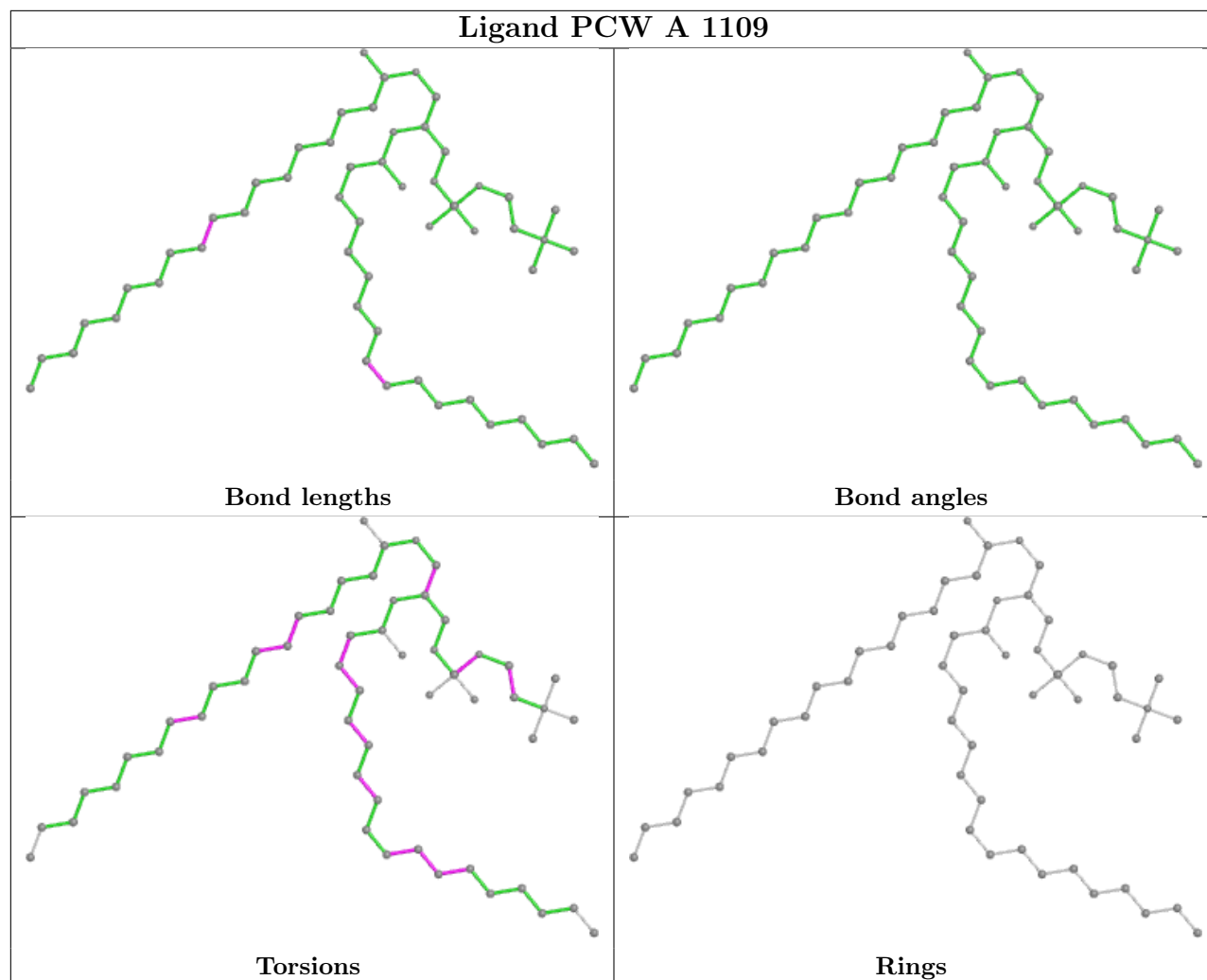




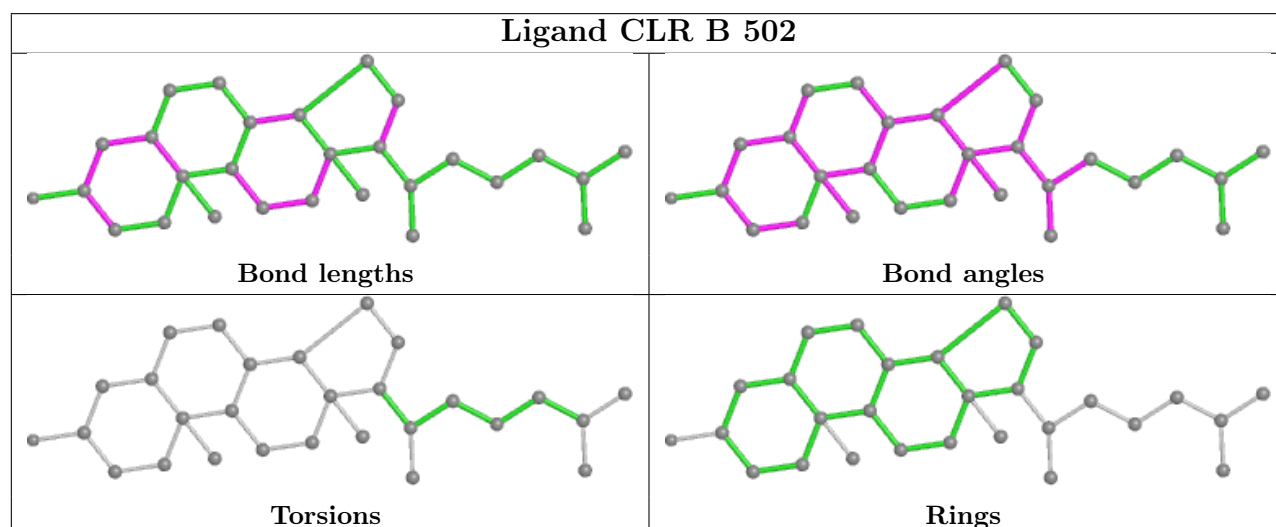


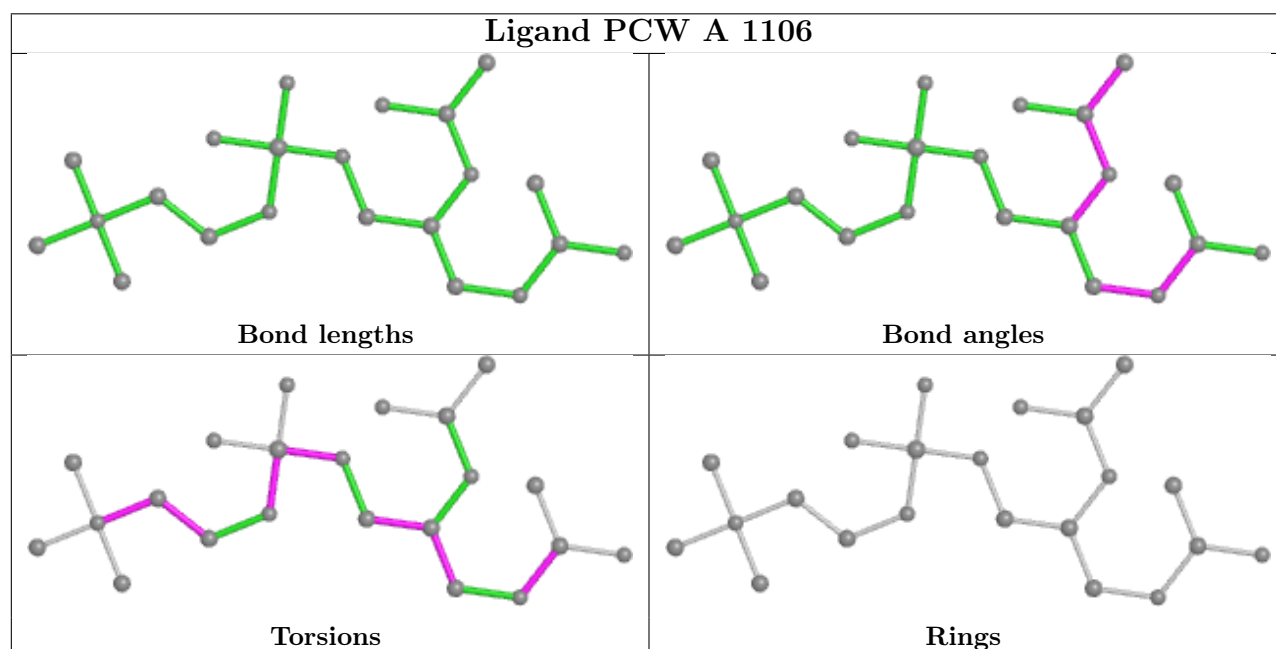
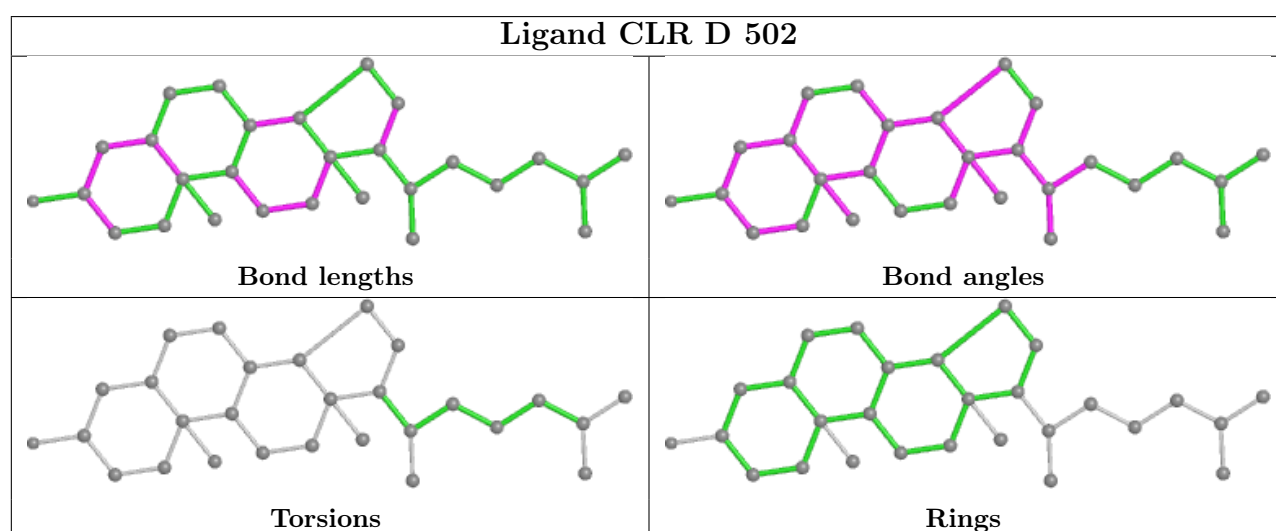
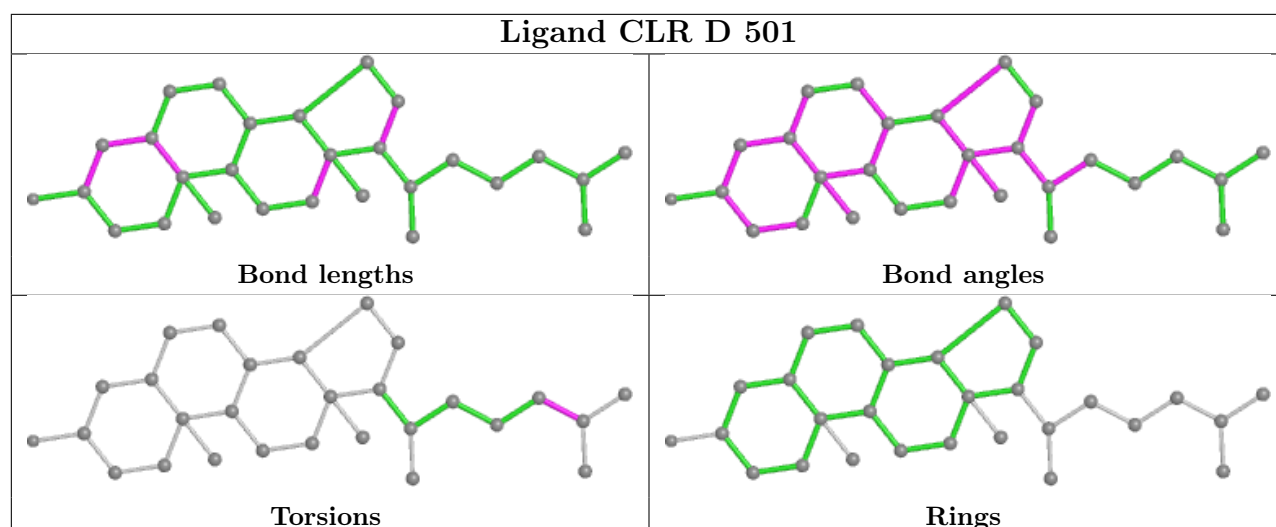


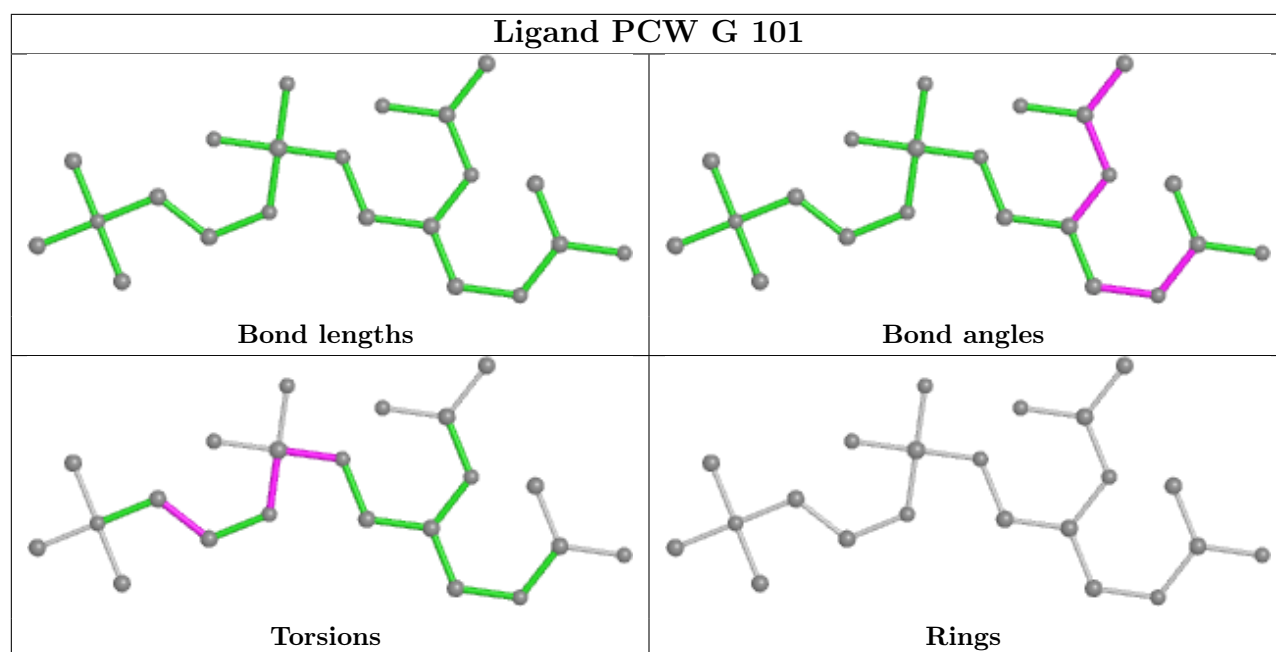
Ligand PCW A 1109



Ligand CLR B 502







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.

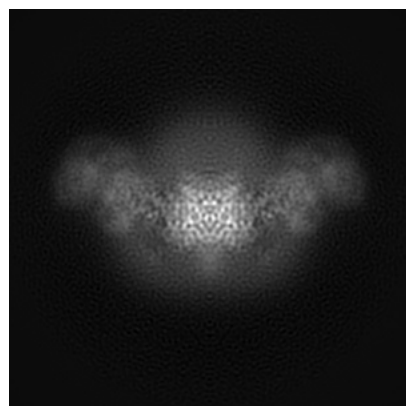
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33601. These allow visual inspection of the internal detail of the map and identification of artifacts.

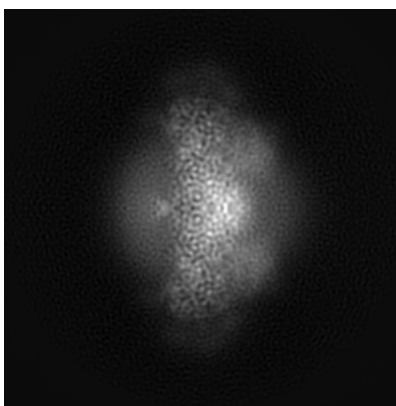
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

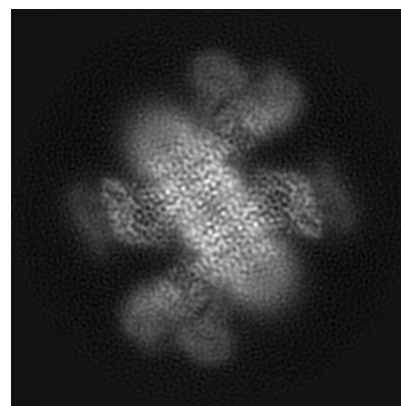
6.1.1 Primary map



X

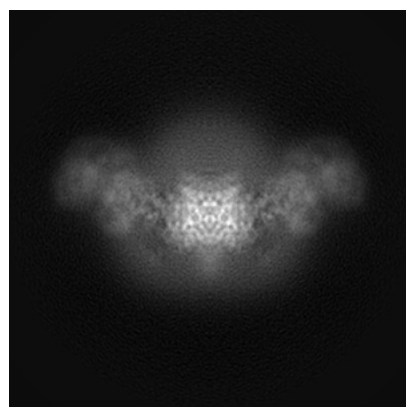


Y

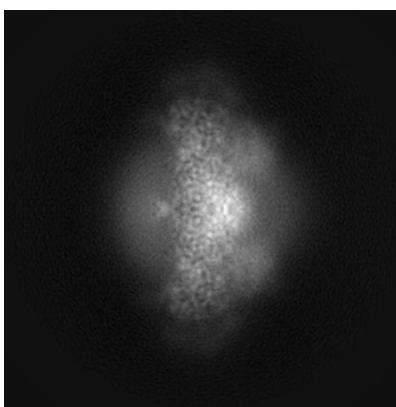


Z

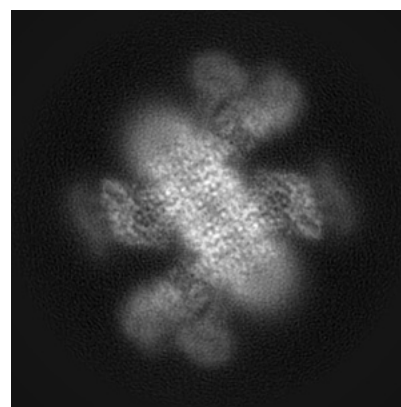
6.1.2 Raw map



X



Y

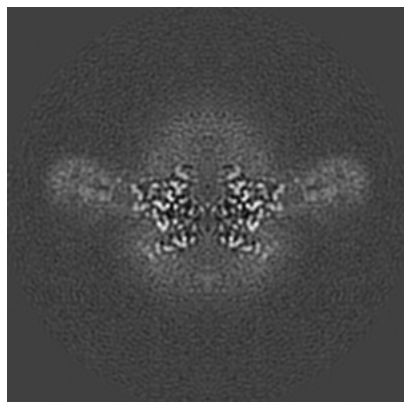


Z

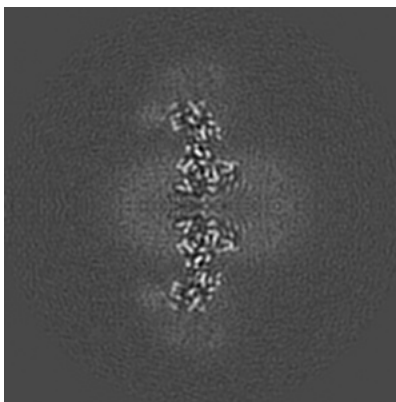
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

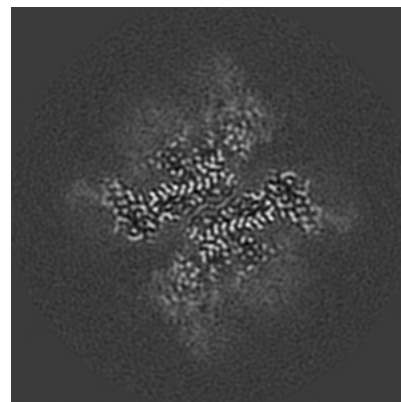
6.2.1 Primary map



X Index: 120

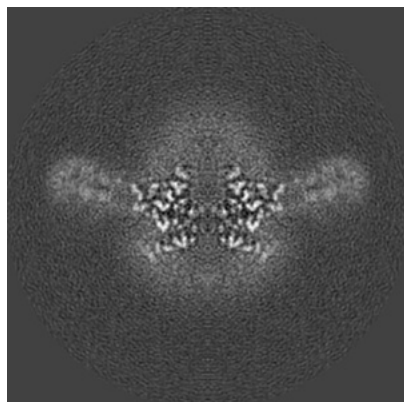


Y Index: 120

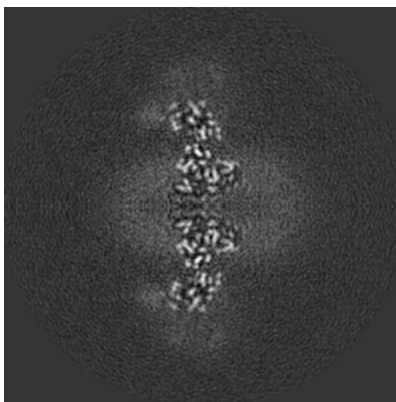


Z Index: 120

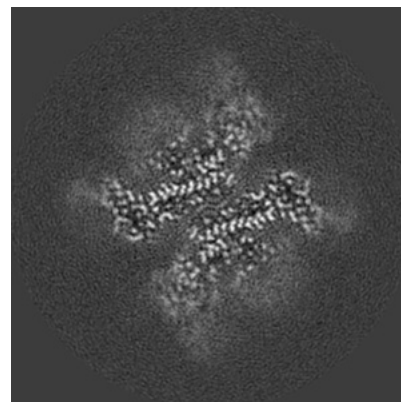
6.2.2 Raw map



X Index: 120



Y Index: 120

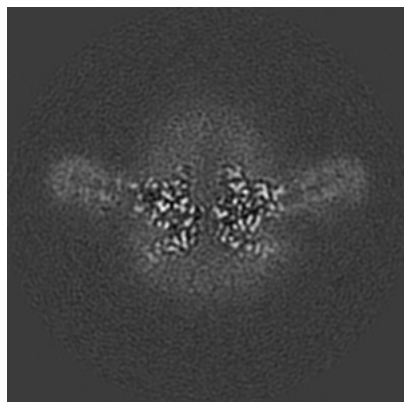


Z Index: 120

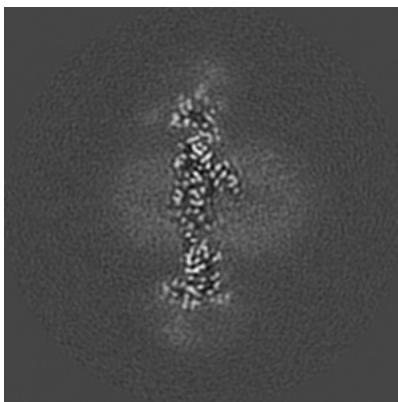
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

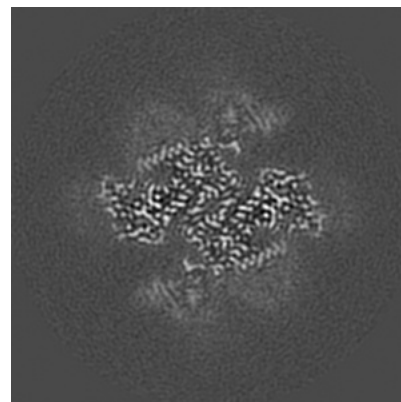
6.3.1 Primary map



X Index: 119

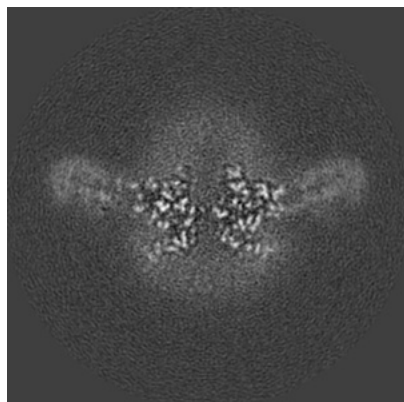


Y Index: 114

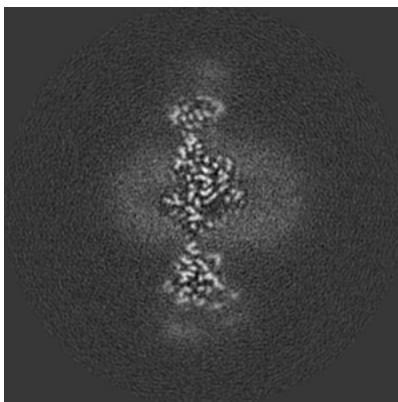


Z Index: 116

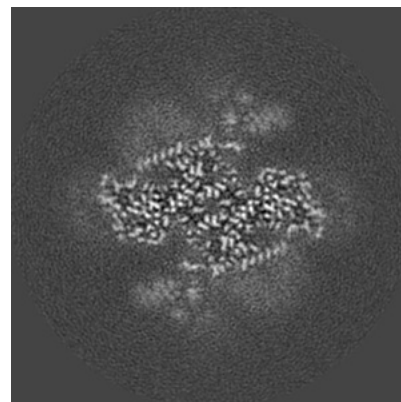
6.3.2 Raw map



X Index: 119



Y Index: 109

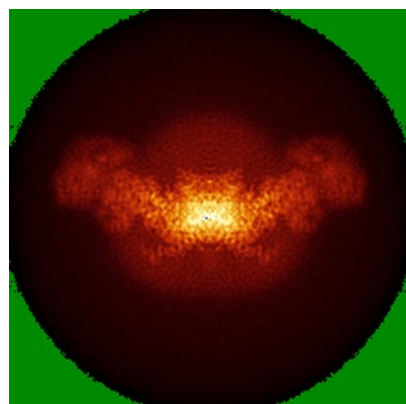


Z Index: 115

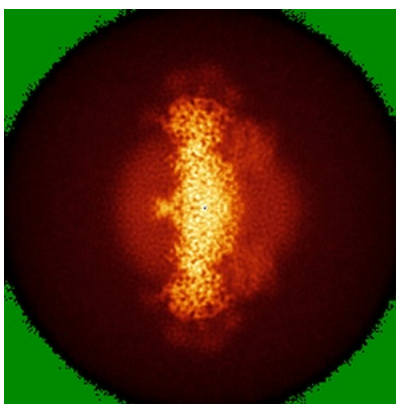
The images above show the largest variance slices of the map in three orthogonal directions.

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

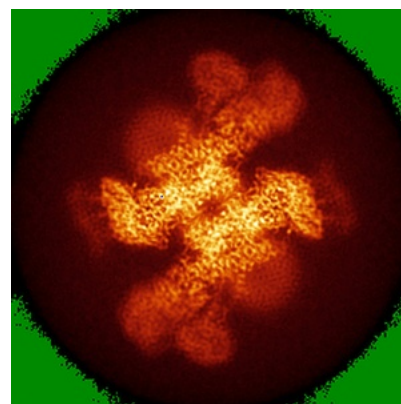
6.4.1 Primary map



X

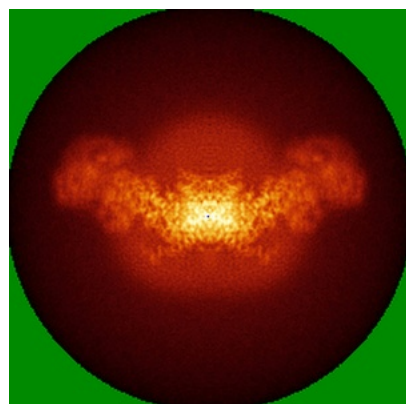


Y

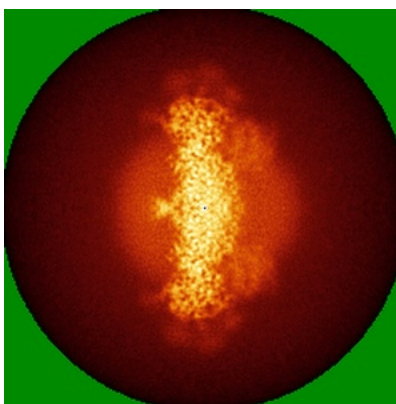


Z

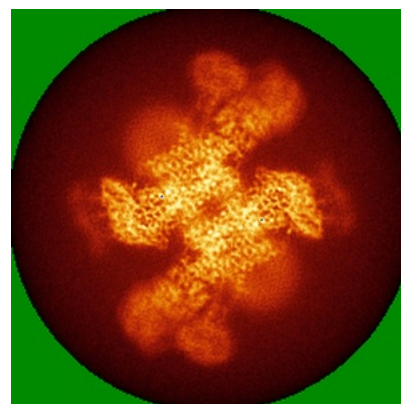
6.4.2 Raw map



X



Y

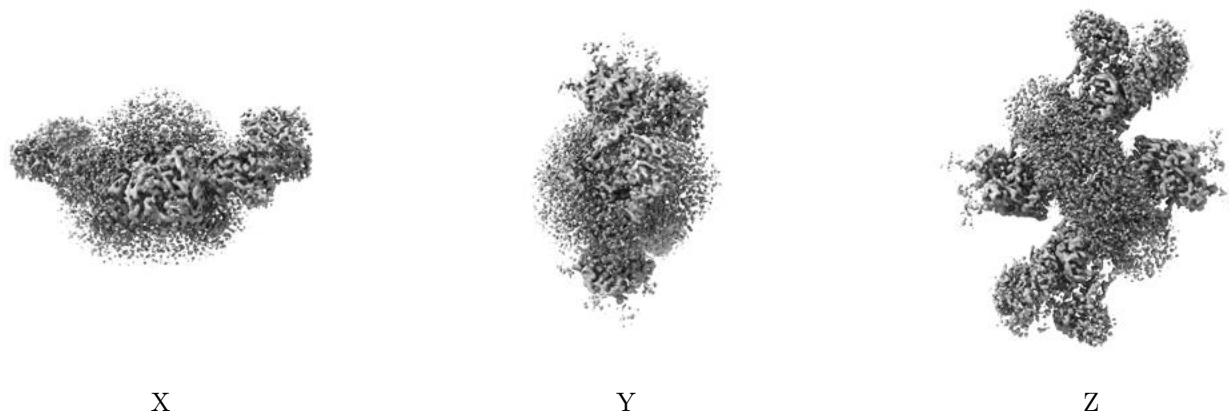


Z

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

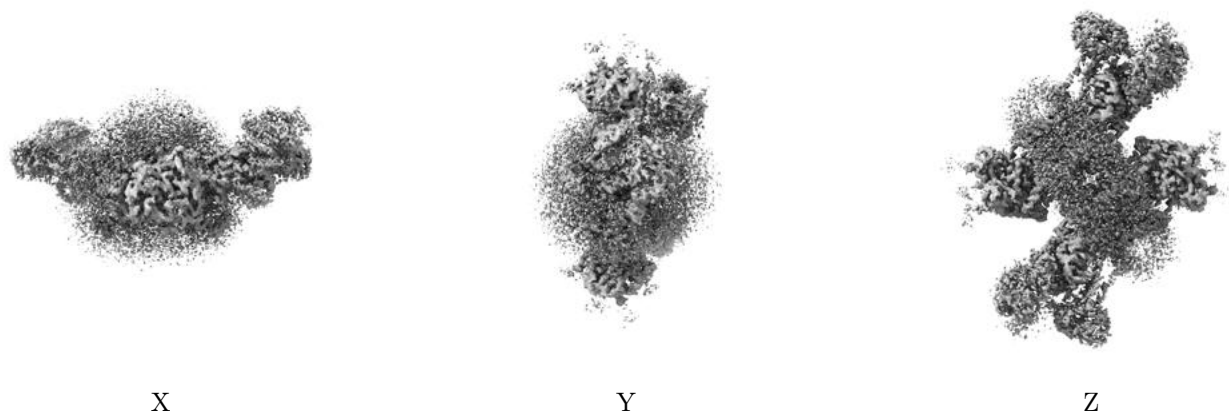
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0199. 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.

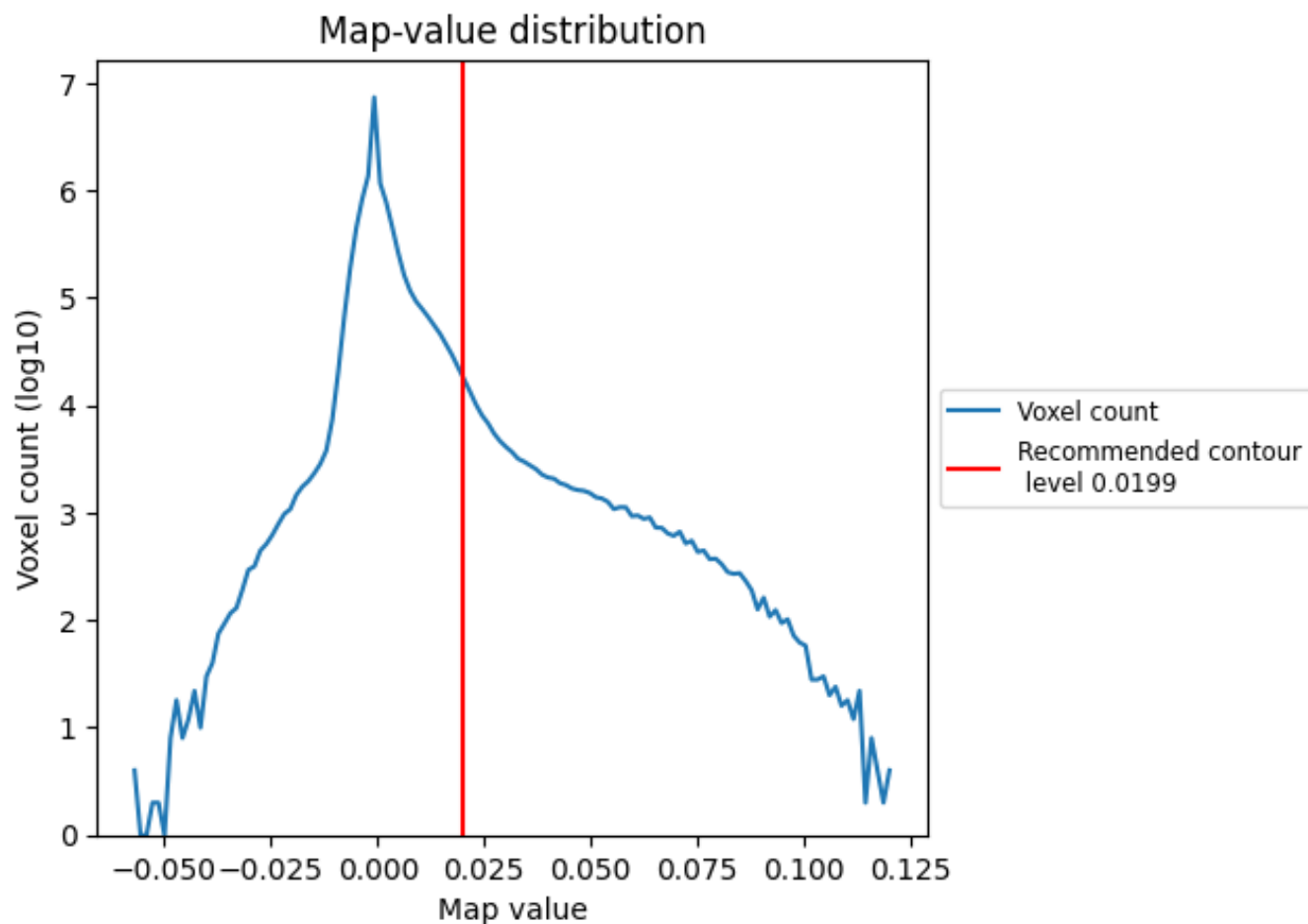
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

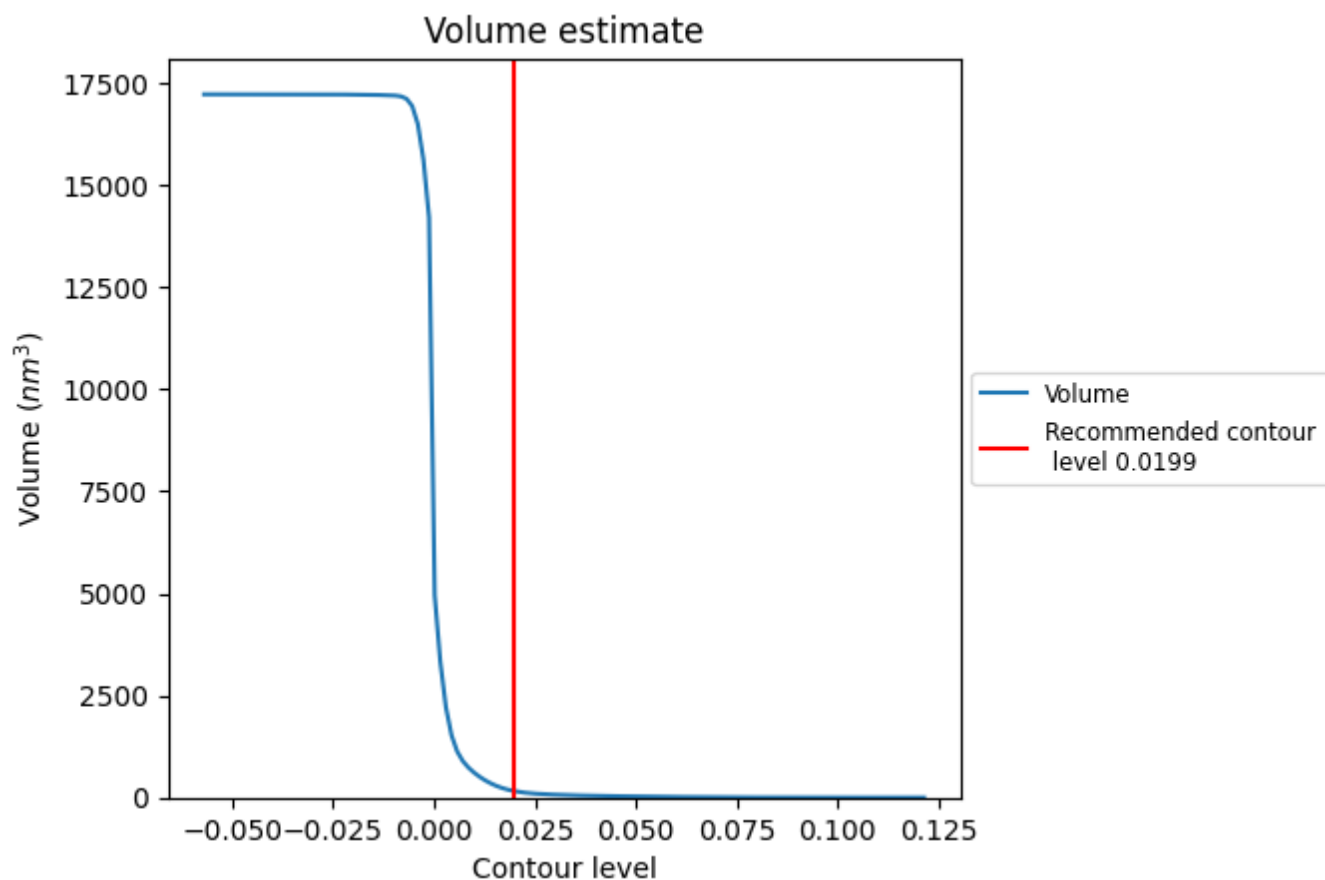
This section contains the results of statistical analysis of the map.

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.

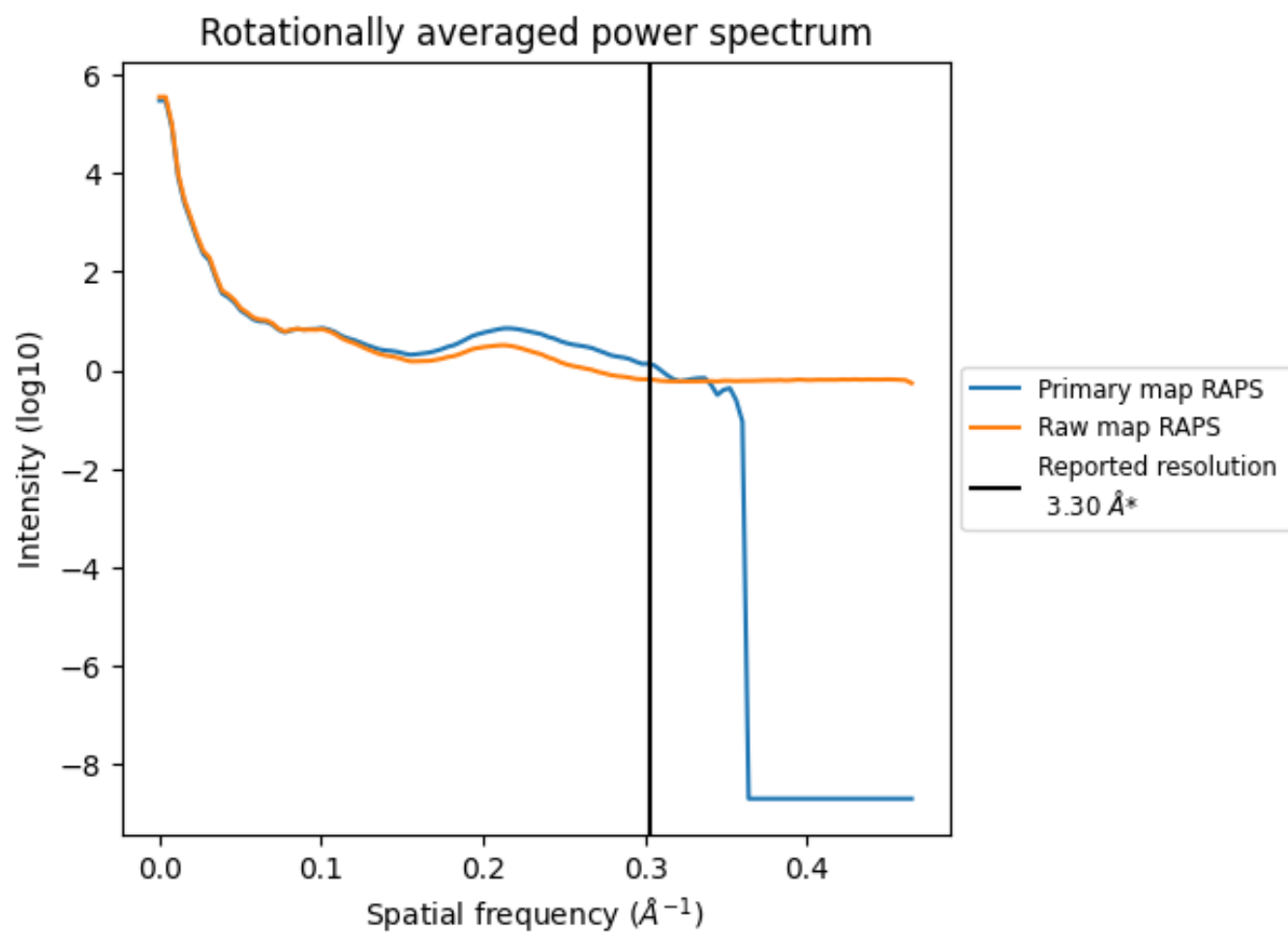
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 159 nm³; this corresponds to an approximate mass of 144 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 ⓘ

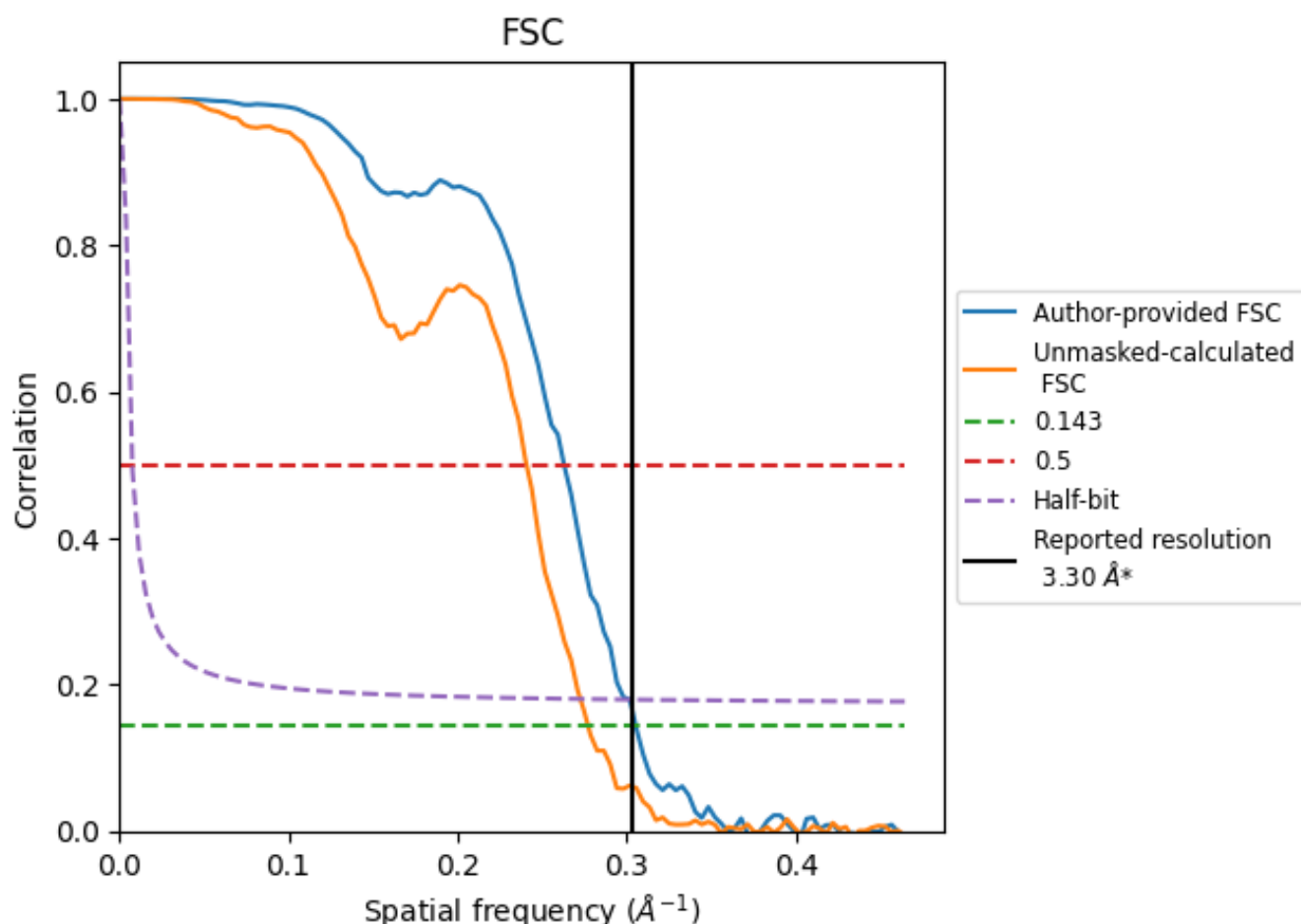


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 Å⁻¹

8.2 Resolution estimates [i](#)

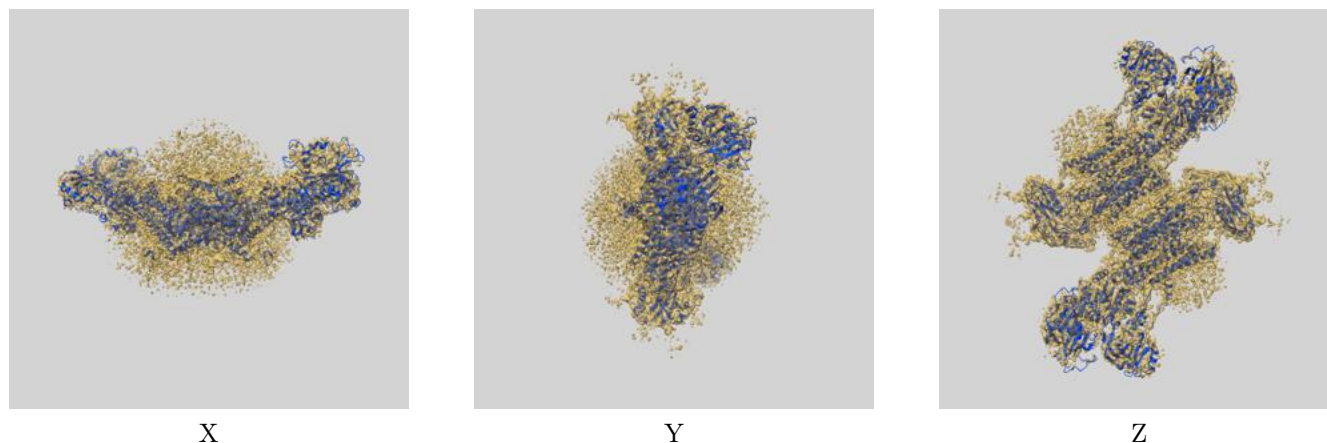
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.27	3.80	3.31
Unmasked-calculated*	3.61	4.15	3.67

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

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-33601 and PDB model 7Y45. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

9.1 Map-model overlay [i](#)



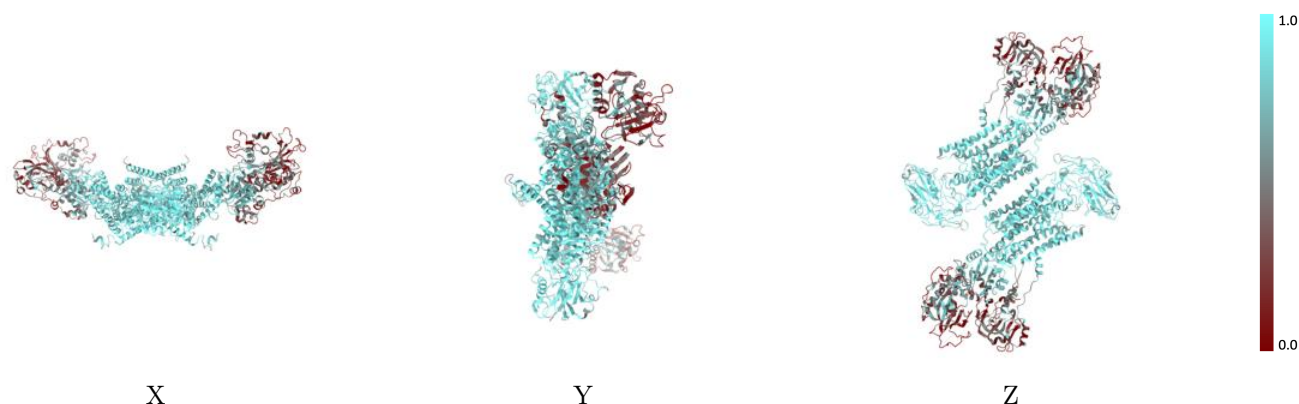
The images above show the 3D surface view of the map at the recommended contour level 0.0199 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



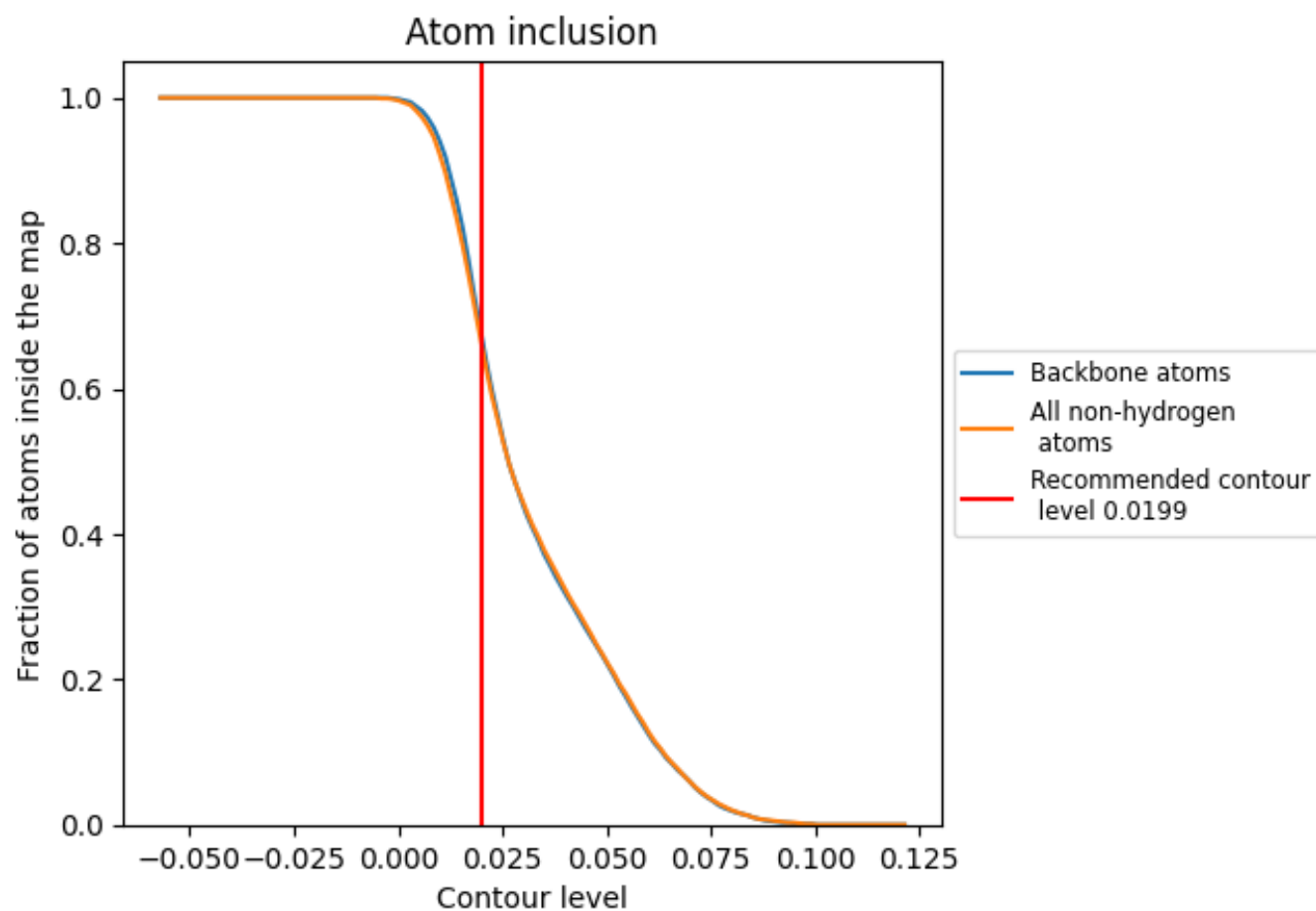
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0199).































9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 66% 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 (0.0199) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6640	 0.4040
A	 0.6200	 0.3790
B	 0.8670	 0.5090
C	 0.6190	 0.3770
D	 0.8560	 0.5000
E	 0.7350	 0.4620
F	 0.4510	 0.2770
G	 0.7460	 0.4800
H	 0.1330	 -0.0060
I	 0.2830	 0.1640
J	 0.1430	 -0.0160
K	 0.4790	 0.2940
L	 0.1470	 -0.0190
M	 0.2830	 0.1770
N	 0.1790	 0.0590

