



## Full wwPDB EM Validation Report ⓘ

Apr 20, 2025 – 12:07 AM JST

PDB ID : 8KCP / pdb\_00008kcp  
EMDB ID : EMD-37107  
Title : Cryo-EM structure of human gamma-secretase in complex with Crenigacestat  
Authors : Guo, X.; Li, H.; Kai, U.; Yan, C.; Lei, J.; Zhou, R.; Shi, Y.  
Deposited on : 2023-08-08  
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : **FAILED**  
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 : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

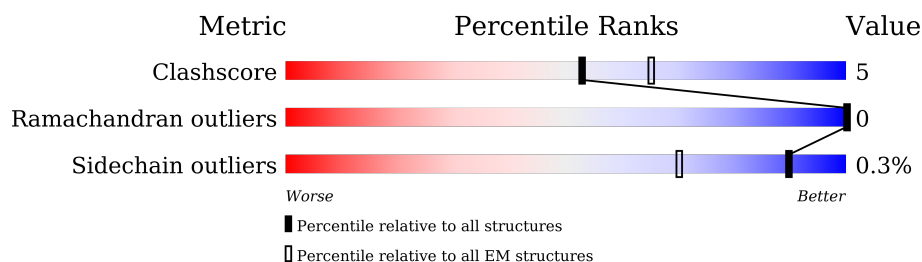
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	701	85% 11% 5%
2	B	467	57% 8% 34%
3	C	265	85% 7% 8%
4	D	101	85% 10% 5%
5	E	2	100%
5	G	2	50% 50%
5	H	2	100%
5	I	2	50% 50%
5	J	2	100%

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Mol	Chain	Length	Quality of chain
6	F	5	<div><div></div><div>20%</div><div>80%</div></div>

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 10837 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 Nicastrin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	667	Total	C	N	O	S	0	0
			5235	3321	890	1003	21		

- Molecule 2 is a protein called Presenilin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	307	Total	C	N	O	S	0	0
			2436	1649	370	403	14		

- Molecule 3 is a protein called Gamma-secretase subunit APH-1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	243	Total	C	N	O	S	0	0
			1872	1254	299	315	4		

- Molecule 4 is a protein called Gamma-secretase subunit PEN-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	96	Total	C	N	O	S	0	0
			814	559	126	128	1		

- Molecule 5 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
5	E	2	Total	C	N	O		0	0
			28	16	2	10			
5	G	2	Total	C	N	O		0	0
			28	16	2	10			

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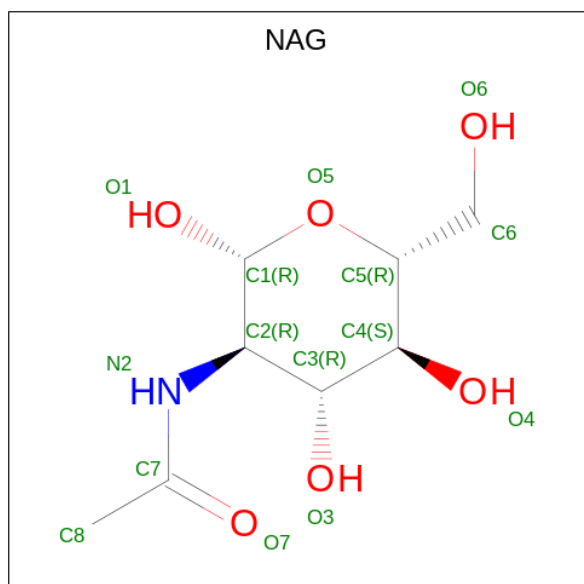
Mol	Chain	Residues	Atoms				AltConf	Trace
5	H	2	Total	C	N	O	0	0
			28	16	2	10		
5	I	2	Total	C	N	O	0	0
			28	16	2	10		
5	J	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[beta-D-mannopyranos e-(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
6	F	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



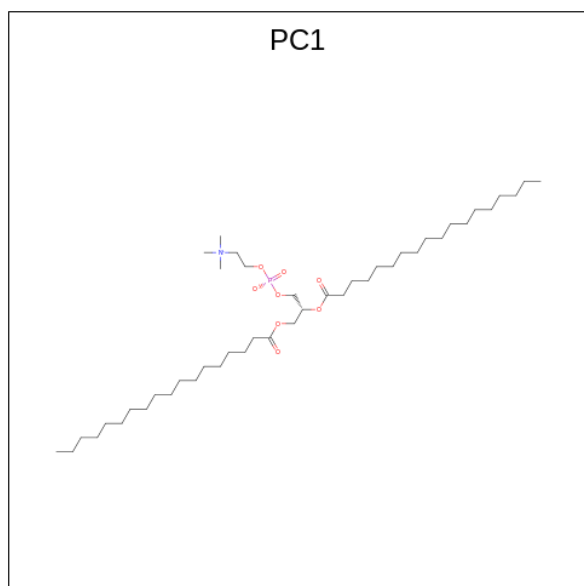
Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			14	8	1	5	

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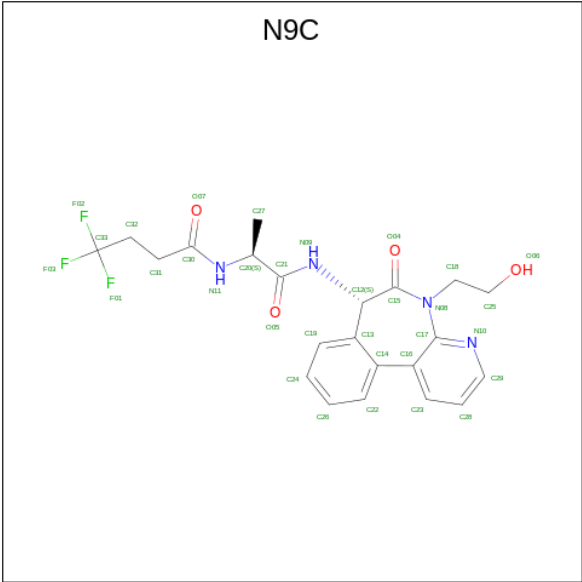
Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 8 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula:  $C_{44}H_{88}NO_8P$ ).



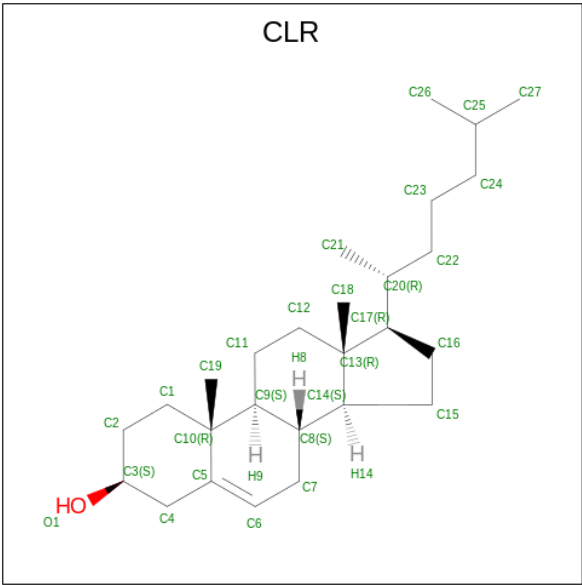
Mol	Chain	Residues	Atoms					AltConf
8	B	1	Total	C	N	O	P	0
			37	27	1	8	1	
8	C	1	Total	C	N	O	P	0
			41	31	1	8	1	

- Molecule 9 is 4,4,4-tris(fluoranyl)-N-[(2S)-1-[[[(7S)-5-(2-hydroxyethyl)-6-oxidanylidene-7H-pyrido[2,3-d][3]benzazepin-7-yl]amino]-1-oxidanylidene-propan-2-yl]butanamide (CCD ID: N9C) (formula:  $C_{22}H_{23}F_3N_4O_4$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
9	B	1	Total	C	F	N	O	0
			33	22	3	4	4	

- Molecule 10 is CHOLESTEROL (CCD ID: CLR) (formula: C<sub>27</sub>H<sub>46</sub>O).



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







- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  50%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  50%



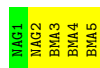
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  100%



- Molecule 6: beta-D-mannopyranose-(1-3)-[beta-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 F:  20%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	2022327	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, PC1, N9C, NAG, CLR

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.36	0/5358	0.53	1/7302 (0.0%)
2	B	0.38	0/2499	0.55	1/3410 (0.0%)
3	C	0.39	0/1924	0.61	1/2624 (0.0%)
4	D	0.34	0/847	0.48	0/1157
All	All	0.37	0/10628	0.54	3/14493 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	233	GLY	N-CA-C	12.38	144.05	113.10
2	B	286	LEU	CA-CB-CG	6.89	131.14	115.30
1	A	226	SER	N-CA-CB	5.99	119.49	110.50

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5235	0	5126	42	0
2	B	2436	0	2558	49	0
3	C	1872	0	1911	26	0
4	D	814	0	804	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	28	0	25	0	0
5	G	28	0	25	0	0
5	H	28	0	25	0	0
5	I	28	0	25	0	0
5	J	28	0	25	0	0
6	F	61	0	52	0	0
7	A	84	0	78	1	0
8	B	37	0	48	0	0
8	C	41	0	56	1	0
9	B	33	0	0	0	0
10	C	84	0	135	7	0
All	All	10837	0	10893	110	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (110) 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)
3:C:206:LEU:HD21	10:C:301:CLR:C21	1.70	1.20
2:B:433:PRO:HB2	2:B:436:PRO:CG	1.77	1.14
2:B:433:PRO:HB2	2:B:436:PRO:HG2	1.26	1.10
2:B:83:ILE:HD11	3:C:29:PRO:HA	1.35	1.06
2:B:83:ILE:HD12	3:C:29:PRO:HB3	1.39	1.02
3:C:206:LEU:CD2	10:C:301:CLR:H212	1.90	1.02
3:C:206:LEU:HD21	10:C:301:CLR:H212	1.39	1.00
2:B:435:LEU:HD22	2:B:439:ILE:HG13	1.42	0.98
2:B:83:ILE:HD12	3:C:29:PRO:CB	1.95	0.96
1:A:224:VAL:HG12	1:A:225:ILE:HG13	1.49	0.94
2:B:433:PRO:CB	2:B:436:PRO:HG2	1.98	0.93
3:C:206:LEU:CD2	10:C:301:CLR:C21	2.48	0.91
2:B:83:ILE:CD1	3:C:29:PRO:HA	2.01	0.91
3:C:206:LEU:HD21	10:C:301:CLR:H211	1.51	0.90
2:B:83:ILE:HD11	3:C:29:PRO:CA	2.05	0.85
2:B:435:LEU:CD2	2:B:439:ILE:HG13	2.07	0.83
2:B:435:LEU:CD2	2:B:439:ILE:CG1	2.56	0.83
2:B:405:ASN:HD22	2:B:454:GLN:HE22	1.32	0.76
2:B:83:ILE:CD1	3:C:29:PRO:CA	2.63	0.75
2:B:83:ILE:CD1	3:C:29:PRO:CB	2.64	0.74
2:B:433:PRO:HB2	2:B:436:PRO:CD	2.19	0.73
2:B:435:LEU:HD23	2:B:439:ILE:CG1	2.19	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:80:LYS:HG3	2:B:84:MET:HE3	1.75	0.69
2:B:435:LEU:N	2:B:436:PRO:CD	2.57	0.68
2:B:435:LEU:HD23	2:B:439:ILE:HG12	1.76	0.66
1:A:39:LYS:HB3	3:C:147:VAL:HG13	1.78	0.65
2:B:433:PRO:CG	2:B:436:PRO:HG2	2.25	0.65
1:A:350:GLY:HA2	1:A:355:GLN:HE22	1.62	0.64
2:B:83:ILE:CD1	3:C:29:PRO:HB3	2.24	0.62
2:B:106:TYR:HA	2:B:239:LYS:HD3	1.84	0.60
2:B:287:ILE:O	2:B:287:ILE:HG22	2.01	0.59
1:A:530:ASN:OD1	1:A:535:GLN:NE2	2.36	0.58
1:A:632:SER:OG	1:A:645:TYR:O	2.21	0.58
1:A:86:LEU:HD22	1:A:114:ARG:HD2	1.86	0.58
1:A:261:LYS:NZ	1:A:321:LEU:O	2.38	0.57
1:A:36:VAL:HG21	3:C:137:ILE:HG22	1.85	0.56
1:A:691:ASN:HD22	3:C:23:ILE:HG22	1.71	0.56
2:B:437:ILE:O	2:B:440:THR:N	2.38	0.55
1:A:699:ILE:HG13	3:C:233:GLY:O	2.07	0.54
3:C:206:LEU:HD23	10:C:301:CLR:H212	1.82	0.54
1:A:559:SER:HB3	1:A:629:ARG:HH12	1.72	0.54
2:B:392:LEU:HD22	2:B:414:ILE:HD11	1.90	0.54
8:C:304:PC1:H362	8:C:304:PC1:H2A1	1.89	0.53
1:A:52:ARG:NH2	1:A:63:GLN:OE1	2.41	0.53
1:A:543:ARG:HD3	1:A:606:GLN:HE22	1.72	0.53
2:B:435:LEU:N	2:B:436:PRO:HD2	2.25	0.52
3:C:204:THR:HB	3:C:207:ASN:HD21	1.76	0.51
1:A:249:ASP:OD2	1:A:652:ARG:NH1	2.40	0.51
1:A:136:PRO:HB2	1:A:172:ALA:HB2	1.93	0.51
1:A:54:LEU:HD11	1:A:223:ALA:HB1	1.93	0.51
3:C:80:VAL:HG13	3:C:197:HIS:CD2	2.45	0.50
2:B:192:ALA:HB2	4:D:97:PRO:HD3	1.93	0.50
1:A:120:GLY:H	1:A:178:PHE:HB2	1.76	0.50
1:A:524:GLY:HA2	1:A:531:ASN:HD21	1.77	0.50
1:A:265:THR:OG1	1:A:626:ARG:NH1	2.44	0.50
1:A:281:ARG:NH2	1:A:334:THR:OG1	2.45	0.49
2:B:166:LEU:HD21	2:B:285:ALA:HB3	1.95	0.49
2:B:96:VAL:HG21	2:B:390:SER:HB3	1.94	0.49
1:A:460:ALA:HB1	1:A:465:VAL:HB	1.95	0.48
2:B:288:TYR:C	2:B:288:TYR:CD1	2.86	0.48
1:A:266:THR:HB	7:A:804:NAG:HN2	1.78	0.48
2:B:192:ALA:O	4:D:79:GLN:NE2	2.36	0.48
3:C:204:THR:HB	3:C:207:ASN:ND2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ASP:OD1	1:A:561:THR:OG1	2.26	0.48
1:A:285:ARG:HG2	1:A:454:GLN:HE21	1.79	0.48
2:B:258:LEU:HD12	2:B:436:PRO:HB3	1.95	0.48
2:B:150:LEU:HD12	2:B:165:TRP:HZ3	1.79	0.47
1:A:224:VAL:HG12	1:A:225:ILE:CG1	2.35	0.47
3:C:2:GLY:N	3:C:143:GLY:O	2.48	0.47
1:A:112:LYS:NZ	1:A:175:ASP:O	2.40	0.47
1:A:388:GLU:OE1	1:A:391:ARG:NH2	2.47	0.47
2:B:421:THR:HG21	2:B:434:ALA:HA	1.96	0.47
2:B:435:LEU:CD2	2:B:439:ILE:HD11	2.44	0.47
1:A:310:GLU:HB2	1:A:574:LEU:HD23	1.98	0.46
2:B:194:ASP:OD2	4:D:74:TRP:NE1	2.40	0.46
2:B:435:LEU:H	2:B:436:PRO:CD	2.27	0.46
1:A:282:LEU:HD11	1:A:567:VAL:HG21	1.97	0.46
1:A:408:VAL:HG22	1:A:410:ALA:H	1.80	0.46
1:A:154:PRO:O	1:A:160:ARG:NH1	2.49	0.46
1:A:49:PRO:HG3	1:A:656:ILE:HD13	1.98	0.45
1:A:331:GLN:HE21	1:A:555:ILE:HB	1.81	0.45
10:C:303:CLR:H162	10:C:303:CLR:H221	1.62	0.45
2:B:433:PRO:HG2	2:B:436:PRO:HG2	1.97	0.45
2:B:81:HIS:HD2	2:B:84:MET:CE	2.29	0.45
4:D:34:ILE:HD11	4:D:61:ALA:HA	1.99	0.44
2:B:433:PRO:C	2:B:436:PRO:HD2	2.36	0.44
2:B:435:LEU:CD2	2:B:439:ILE:CD1	2.95	0.44
1:A:130:PRO:O	1:A:452:TYR:OH	2.30	0.44
1:A:253:ASP:HB3	1:A:331:GLN:HG2	2.00	0.43
2:B:145:VAL:HA	2:B:148:ILE:HG22	1.99	0.43
4:D:39:ARG:HG3	4:D:43:LEU:HD22	2.00	0.43
3:C:159:THR:HG21	3:C:210:TYR:CD1	2.54	0.43
2:B:291:THR:HG22	2:B:378:GLY:HA3	2.01	0.43
1:A:56:ALA:HA	1:A:227:THR:HG22	2.01	0.43
2:B:437:ILE:O	2:B:440:THR:HB	2.19	0.42
4:D:39:ARG:HA	4:D:43:LEU:HD13	2.01	0.42
2:B:208:VAL:HG21	4:D:28:PHE:HD2	1.85	0.42
1:A:589:PRO:HD2	1:A:597:LYS:HD2	2.01	0.42
2:B:256:TYR:HA	2:B:259:VAL:HG12	2.01	0.42
1:A:64:SER:OG	1:A:65:SER:N	2.53	0.42
2:B:435:LEU:H	2:B:436:PRO:HD3	1.85	0.42
3:C:24:THR:O	3:C:31:ARG:NH1	2.50	0.42
4:D:7:SER:OG	4:D:9:GLU:OE1	2.38	0.42
1:A:377:TRP:CE2	1:A:445:SER:HB3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:589:PRO:HG2	1:A:597:LYS:HB2	2.02	0.41
2:B:194:ASP:N	2:B:194:ASP:OD1	2.52	0.41
2:B:464:GLN:NE2	3:C:160:SER:OG	2.54	0.41
3:C:174:TRP:O	3:C:178:PHE:HB2	2.21	0.41
1:A:200:ASN:HD21	1:A:213:CYS:HB3	1.86	0.40
1:A:632:SER:HA	1:A:633:PRO:HD3	1.97	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	665/701 (95%)	626 (94%)	39 (6%)	0	100	100
2	B	303/467 (65%)	291 (96%)	12 (4%)	0	100	100
3	C	241/265 (91%)	234 (97%)	7 (3%)	0	100	100
4	D	94/101 (93%)	90 (96%)	4 (4%)	0	100	100
All	All	1303/1534 (85%)	1241 (95%)	62 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	584/606 (96%)	583 (100%)	1 (0%)	92	97
2	B	265/408 (65%)	263 (99%)	2 (1%)	79	90
3	C	193/214 (90%)	193 (100%)	0	100	100
4	D	84/89 (94%)	84 (100%)	0	100	100
All	All	1126/1317 (86%)	1123 (100%)	3 (0%)	90	96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	573	ASN
2	B	287	ILE
2	B	380	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	163	GLN
1	A	331	GLN
1	A	355	GLN
1	A	358	ASN
1	A	454	GLN
1	A	531	ASN
1	A	606	GLN
1	A	691	ASN
2	B	81	HIS
2	B	454	GLN
2	B	464	GLN
3	C	207	ASN

### 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 ⓘ

15 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$
5	NAG	E	1	1,5	14,14,15	0.26	0	17,19,21	0.42	0
5	NAG	E	2	5	14,14,15	0.24	0	17,19,21	0.59	0
6	NAG	F	1	6,1	14,14,15	0.25	0	17,19,21	0.54	0
6	NAG	F	2	6	14,14,15	0.20	0	17,19,21	0.65	1 (5%)
6	BMA	F	3	6	11,11,12	0.66	0	15,15,17	0.90	1 (6%)
6	BMA	F	4	6	11,11,12	0.66	0	15,15,17	0.93	1 (6%)
6	BMA	F	5	6	11,11,12	1.60	3 (27%)	15,15,17	1.89	4 (26%)
5	NAG	G	1	1,5	14,14,15	0.32	0	17,19,21	1.05	1 (5%)
5	NAG	G	2	5	14,14,15	0.38	0	17,19,21	0.50	0
5	NAG	H	1	1,5	14,14,15	0.22	0	17,19,21	0.47	0
5	NAG	H	2	5	14,14,15	0.20	0	17,19,21	0.56	0
5	NAG	I	1	1,5	14,14,15	0.23	0	17,19,21	0.50	0
5	NAG	I	2	5	14,14,15	0.73	1 (7%)	17,19,21	2.24	3 (17%)
5	NAG	J	1	1,5	14,14,15	0.32	0	17,19,21	0.54	0
5	NAG	J	2	5	14,14,15	0.25	0	17,19,21	0.48	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
5	NAG	E	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1
6	NAG	F	1	6,1	-	4/6/23/26	0/1/1/1
6	NAG	F	2	6	-	1/6/23/26	0/1/1/1
6	BMA	F	3	6	-	2/2/19/22	0/1/1/1
6	BMA	F	4	6	-	1/2/19/22	0/1/1/1
6	BMA	F	5	6	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	G	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	G	2	5	-	4/6/23/26	0/1/1/1
5	NAG	H	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	H	2	5	-	2/6/23/26	0/1/1/1
5	NAG	I	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	I	2	5	-	3/6/23/26	0/1/1/1
5	NAG	J	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	J	2	5	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	5	BMA	C2-C3	3.09	1.57	1.52
6	F	5	BMA	C1-C2	2.98	1.59	1.52
6	F	5	BMA	O5-C1	2.11	1.47	1.43
5	I	2	NAG	C1-C2	2.05	1.55	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	2	NAG	C2-N2-C7	7.81	134.02	122.90
6	F	5	BMA	C1-O5-C5	4.99	118.95	112.19
5	I	2	NAG	C1-C2-N2	3.68	116.77	110.49
5	G	1	NAG	C2-N2-C7	3.11	127.34	122.90
6	F	5	BMA	C1-C2-C3	3.02	113.37	109.67
6	F	5	BMA	O5-C1-C2	2.74	115.00	110.77
6	F	2	NAG	C1-O5-C5	2.23	115.22	112.19
6	F	5	BMA	C2-C3-C4	2.19	114.69	110.89
5	I	2	NAG	C8-C7-N2	2.12	119.69	116.10
6	F	4	BMA	C1-O5-C5	2.07	115.00	112.19
6	F	3	BMA	O2-C2-C3	-2.05	106.03	110.14

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	1	NAG	O5-C5-C6-O6
6	F	3	BMA	C4-C5-C6-O6
5	J	1	NAG	O5-C5-C6-O6
5	I	1	NAG	C4-C5-C6-O6

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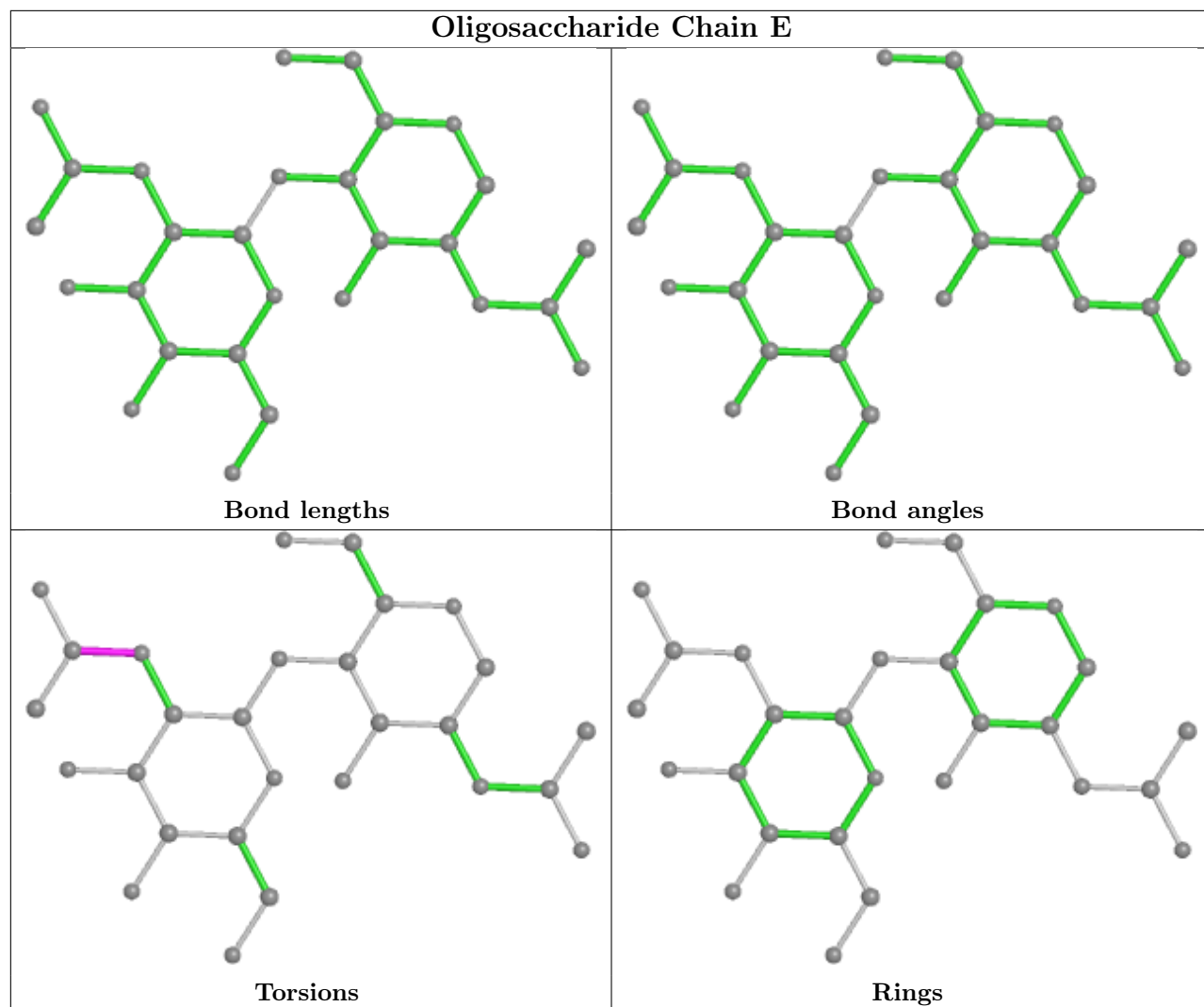
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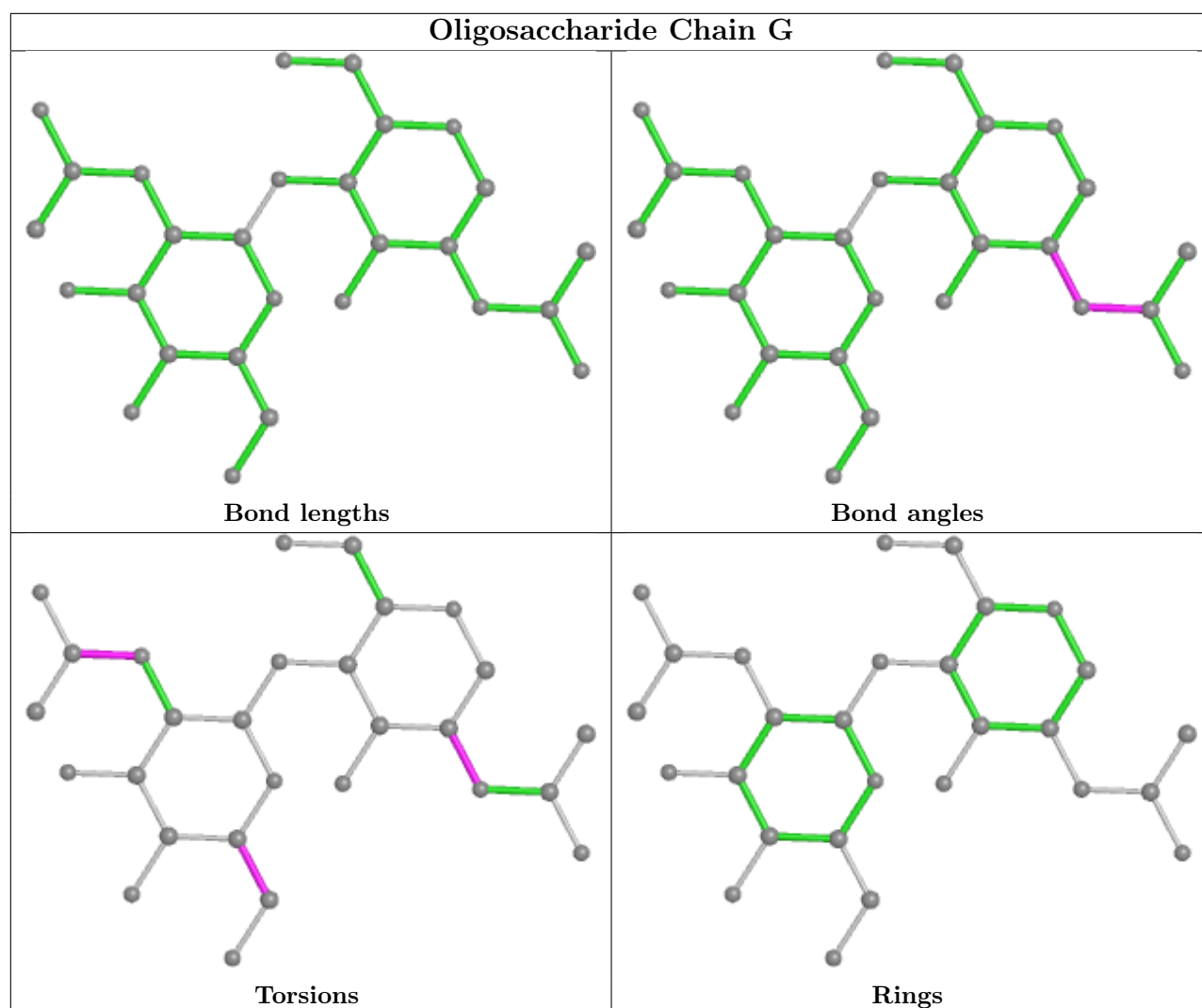
Mol	Chain	Res	Type	Atoms
6	F	3	BMA	O5-C5-C6-O6
5	J	1	NAG	C4-C5-C6-O6
5	E	2	NAG	C8-C7-N2-C2
5	E	2	NAG	O7-C7-N2-C2
5	G	2	NAG	C8-C7-N2-C2
5	G	2	NAG	O7-C7-N2-C2
5	H	2	NAG	C8-C7-N2-C2
5	H	2	NAG	O7-C7-N2-C2
5	I	2	NAG	C8-C7-N2-C2
5	I	2	NAG	O7-C7-N2-C2
6	F	1	NAG	C8-C7-N2-C2
6	F	1	NAG	O7-C7-N2-C2
5	G	2	NAG	O5-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
6	F	4	BMA	O5-C5-C6-O6
6	F	1	NAG	C4-C5-C6-O6
5	J	2	NAG	C4-C5-C6-O6
6	F	2	NAG	O5-C5-C6-O6
5	H	1	NAG	C4-C5-C6-O6
6	F	1	NAG	O5-C5-C6-O6
5	J	2	NAG	O5-C5-C6-O6
5	H	1	NAG	O5-C5-C6-O6
5	G	1	NAG	C3-C2-N2-C7
5	I	2	NAG	C3-C2-N2-C7

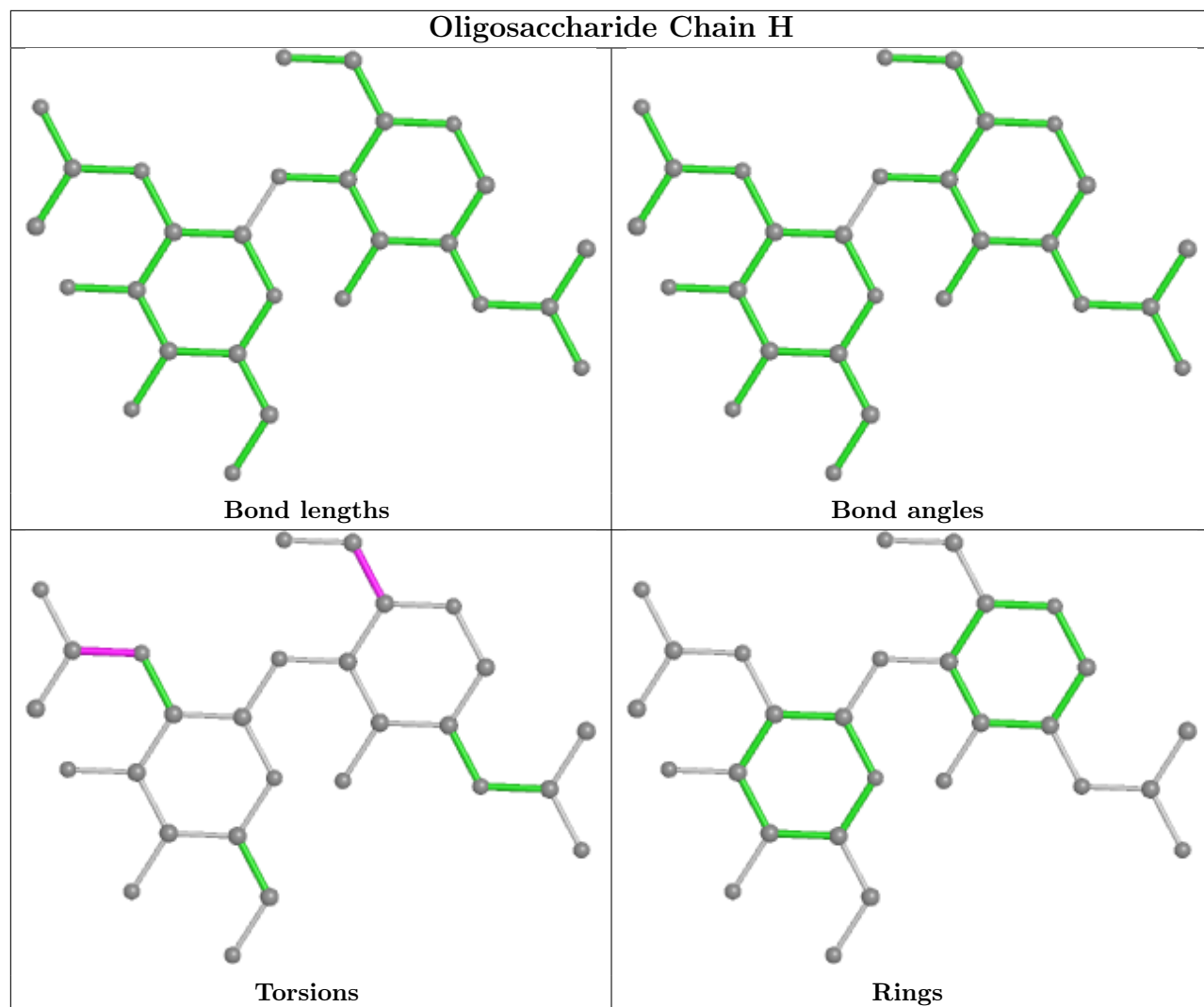
There are no ring outliers.

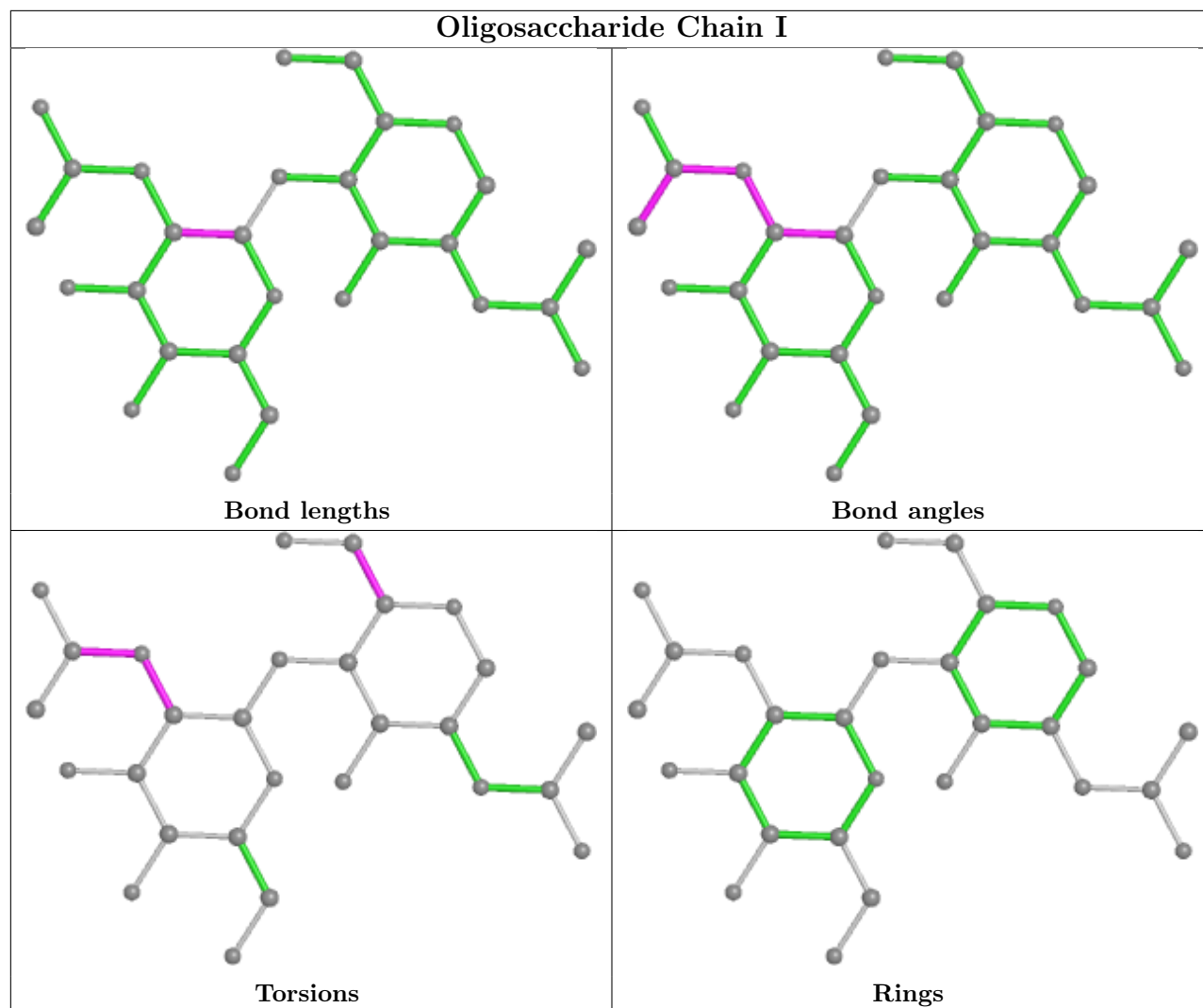
No monomer is involved in short contacts.

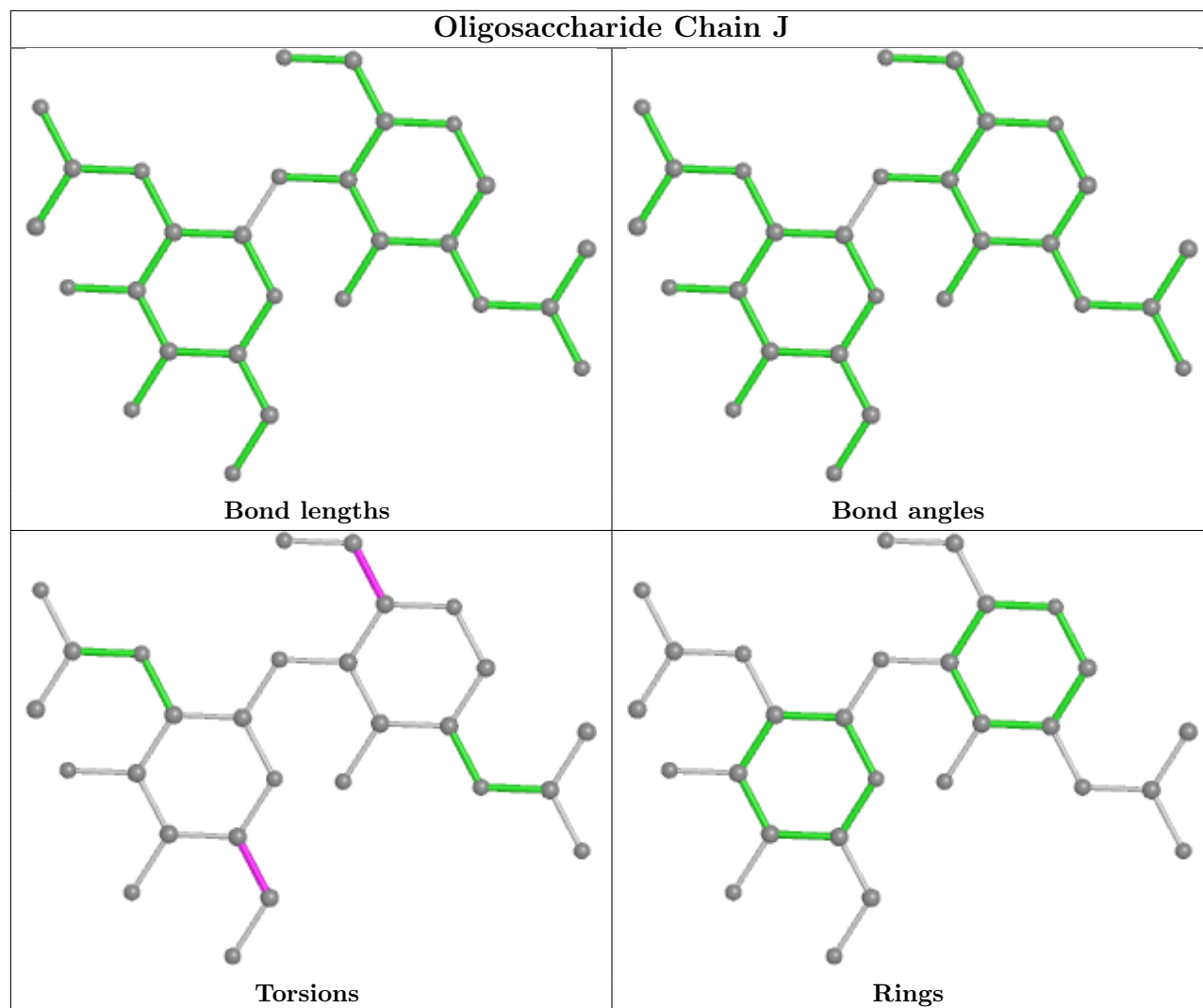
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



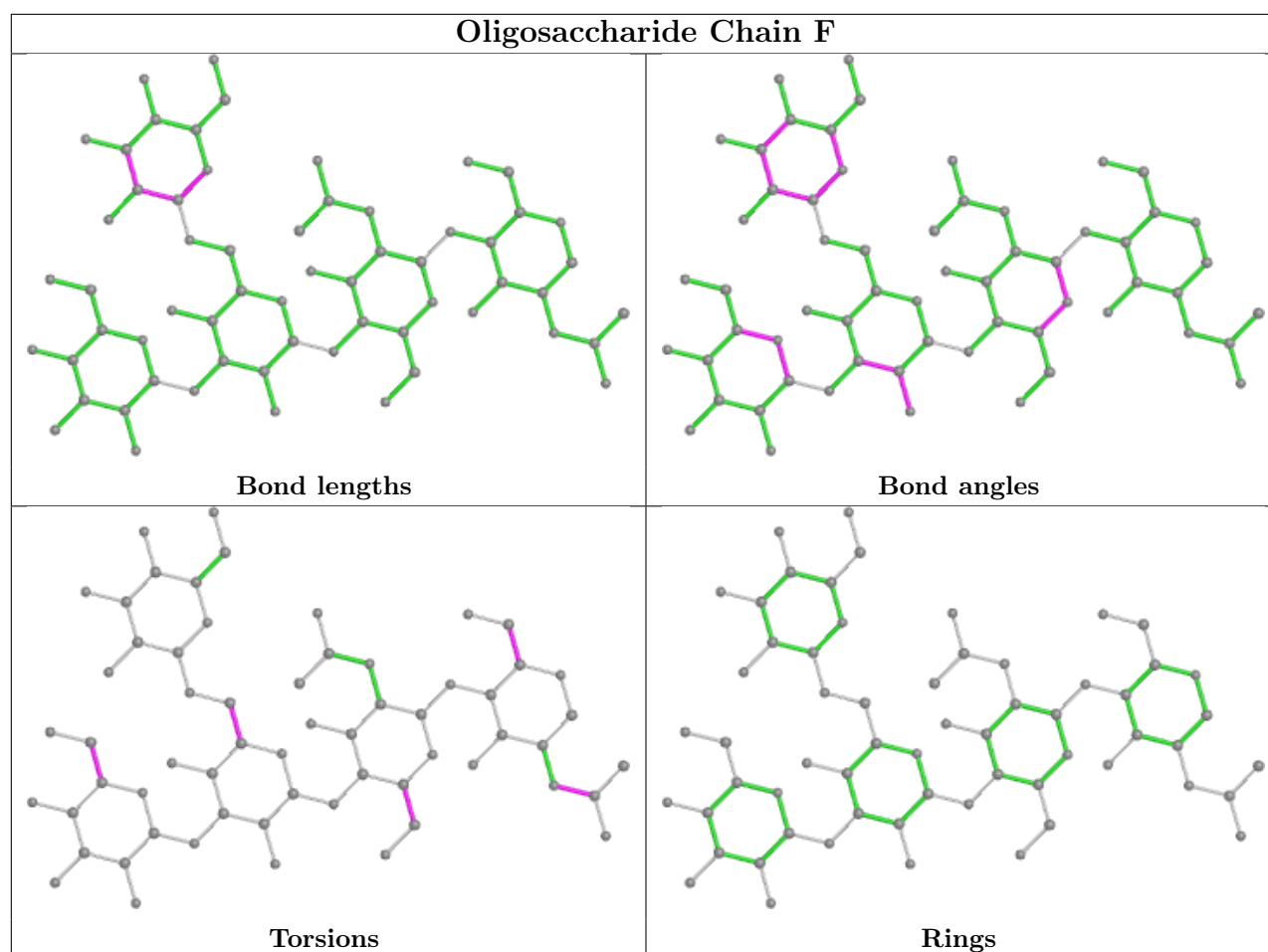












## 5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
10	CLR	C	303	-	31,31,31	0.29	0	48,48,48	0.54	0
10	CLR	C	302	-	31,31,31	0.29	0	48,48,48	0.59	0
9	N9C	B	502	-	33,35,35	4.84	19 (57%)	45,50,50	1.33	8 (17%)
8	PC1	B	501	-	36,36,53	0.33	0	42,44,61	0.47	0
7	NAG	A	806	1	14,14,15	0.22	0	17,19,21	0.60	1 (5%)
7	NAG	A	801	1	14,14,15	0.36	0	17,19,21	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	PC1	C	304	-	40,40,53	0.30	0	46,48,61	0.41	0
10	CLR	C	301	-	31,31,31	0.34	0	48,48,48	0.52	0
7	NAG	A	804	1	14,14,15	0.92	1 (7%)	17,19,21	2.26	3 (17%)
7	NAG	A	803	1	14,14,15	0.45	0	17,19,21	0.46	0
7	NAG	A	802	1	14,14,15	0.52	0	17,19,21	1.00	1 (5%)
7	NAG	A	805	1	14,14,15	0.26	0	17,19,21	0.47	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLR	C	303	-	-	6/10/68/68	0/4/4/4
10	CLR	C	302	-	-	5/10/68/68	0/4/4/4
9	N9C	B	502	-	-	3/21/41/41	0/3/3/3
8	PC1	B	501	-	-	5/40/40/57	-
7	NAG	A	806	1	-	0/6/23/26	0/1/1/1
7	NAG	A	801	1	-	0/6/23/26	0/1/1/1
8	PC1	C	304	-	-	8/44/44/57	-
10	CLR	C	301	-	-	1/10/68/68	0/4/4/4
7	NAG	A	804	1	-	5/6/23/26	0/1/1/1
7	NAG	A	803	1	-	2/6/23/26	0/1/1/1
7	NAG	A	802	1	-	3/6/23/26	0/1/1/1
7	NAG	A	805	1	-	0/6/23/26	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	502	N9C	C19-C13	11.19	1.54	1.39
9	B	502	N9C	C22-C14	9.18	1.54	1.40
9	B	502	N9C	C17-N10	8.30	1.50	1.34
9	B	502	N9C	C14-C13	7.57	1.50	1.40
9	B	502	N9C	C23-C16	7.26	1.51	1.40
9	B	502	N9C	C26-C22	7.05	1.53	1.38
9	B	502	N9C	C24-C19	6.96	1.53	1.38
9	B	502	N9C	C29-N10	6.91	1.49	1.34
9	B	502	N9C	C26-C24	6.26	1.54	1.38
9	B	502	N9C	C16-C17	5.90	1.51	1.43
9	B	502	N9C	C28-C29	5.81	1.54	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	502	N9C	C28-C23	5.58	1.50	1.38
9	B	502	N9C	C30-N11	5.03	1.44	1.34
9	B	502	N9C	C21-N09	5.01	1.45	1.34
9	B	502	N9C	C16-C14	3.63	1.55	1.49
9	B	502	N9C	C15-N08	3.35	1.43	1.37
7	A	804	NAG	C1-C2	2.92	1.56	1.52
9	B	502	N9C	O05-C21	-2.53	1.18	1.23
9	B	502	N9C	O07-C30	-2.39	1.18	1.23
9	B	502	N9C	O04-C15	-2.33	1.18	1.22

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	804	NAG	C2-N2-C7	7.89	134.14	122.90
7	A	804	NAG	C1-C2-N2	3.67	116.77	110.49
7	A	802	NAG	C2-N2-C7	3.08	127.28	122.90
9	B	502	N9C	C31-C32-C33	-2.90	108.43	113.00
9	B	502	N9C	C17-N08-C15	2.66	127.37	123.04
9	B	502	N9C	C31-C30-N11	2.58	120.31	115.83
9	B	502	N9C	N10-C17-N08	2.51	118.00	114.86
9	B	502	N9C	C23-C16-C17	2.41	119.72	117.33
9	B	502	N9C	C28-C29-N10	-2.37	119.56	123.43
9	B	502	N9C	C29-N10-C17	2.27	120.39	115.14
7	A	804	NAG	C8-C7-N2	2.16	119.75	116.10
7	A	806	NAG	C1-O5-C5	2.13	115.08	112.19
9	B	502	N9C	C18-N08-C17	-2.09	116.09	118.37

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	501	PC1	O32-C31-O31-C3
8	B	501	PC1	C32-C31-O31-C3
8	C	304	PC1	C11-O13-P-O14
8	C	304	PC1	O22-C21-O21-C2
10	C	303	CLR	C16-C17-C20-C22
10	C	303	CLR	C13-C17-C20-C21
7	A	802	NAG	O5-C5-C6-O6
7	A	804	NAG	O5-C5-C6-O6
8	C	304	PC1	C22-C21-O21-C2
10	C	303	CLR	C16-C17-C20-C21
10	C	303	CLR	C13-C17-C20-C22

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Mol	Chain	Res	Type	Atoms
7	A	802	NAG	C4-C5-C6-O6
7	A	804	NAG	C4-C5-C6-O6
10	C	303	CLR	C17-C20-C22-C23
7	A	804	NAG	C8-C7-N2-C2
7	A	804	NAG	O7-C7-N2-C2
10	C	303	CLR	C21-C20-C22-C23
10	C	302	CLR	C20-C22-C23-C24
7	A	803	NAG	O5-C5-C6-O6
9	B	502	N9C	N08-C18-C25-O06
10	C	301	CLR	C17-C20-C22-C23
8	C	304	PC1	C11-O13-P-O11
10	C	302	CLR	C16-C17-C20-C22
7	A	803	NAG	C4-C5-C6-O6
8	B	501	PC1	C12-C11-O13-P
8	C	304	PC1	C12-C11-O13-P
8	C	304	PC1	C21-C22-C23-C24
8	C	304	PC1	O13-C11-C12-N
9	B	502	N9C	C30-C31-C32-C33
10	C	302	CLR	C13-C17-C20-C22
10	C	302	CLR	C16-C17-C20-C21
10	C	302	CLR	C13-C17-C20-C21
8	C	304	PC1	C1-C2-O21-C21
8	B	501	PC1	O21-C21-C22-C23
7	A	802	NAG	C3-C2-N2-C7
7	A	804	NAG	C3-C2-N2-C7
8	B	501	PC1	O22-C21-C22-C23
9	B	502	N9C	C31-C32-C33-F01

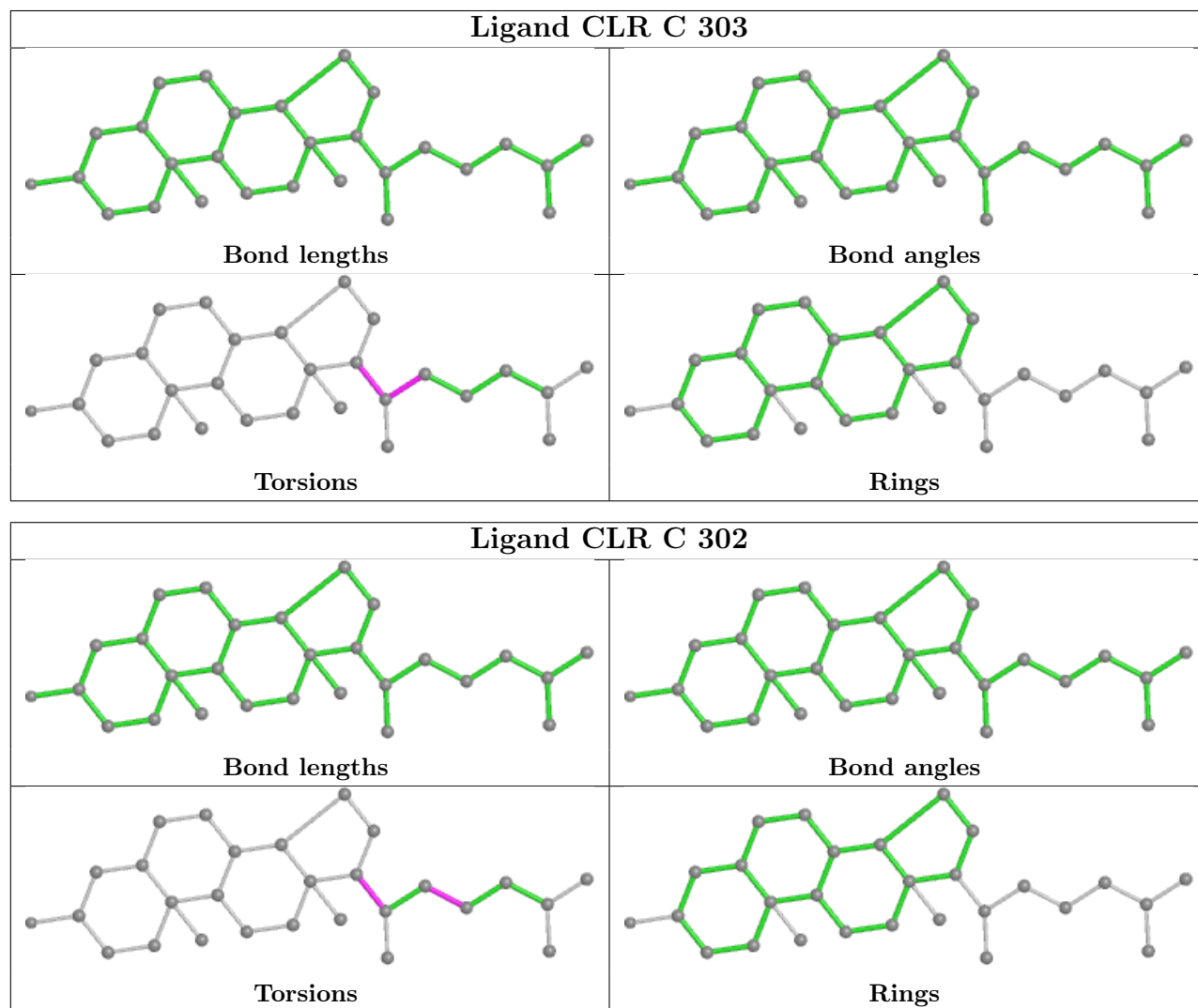
There are no ring outliers.

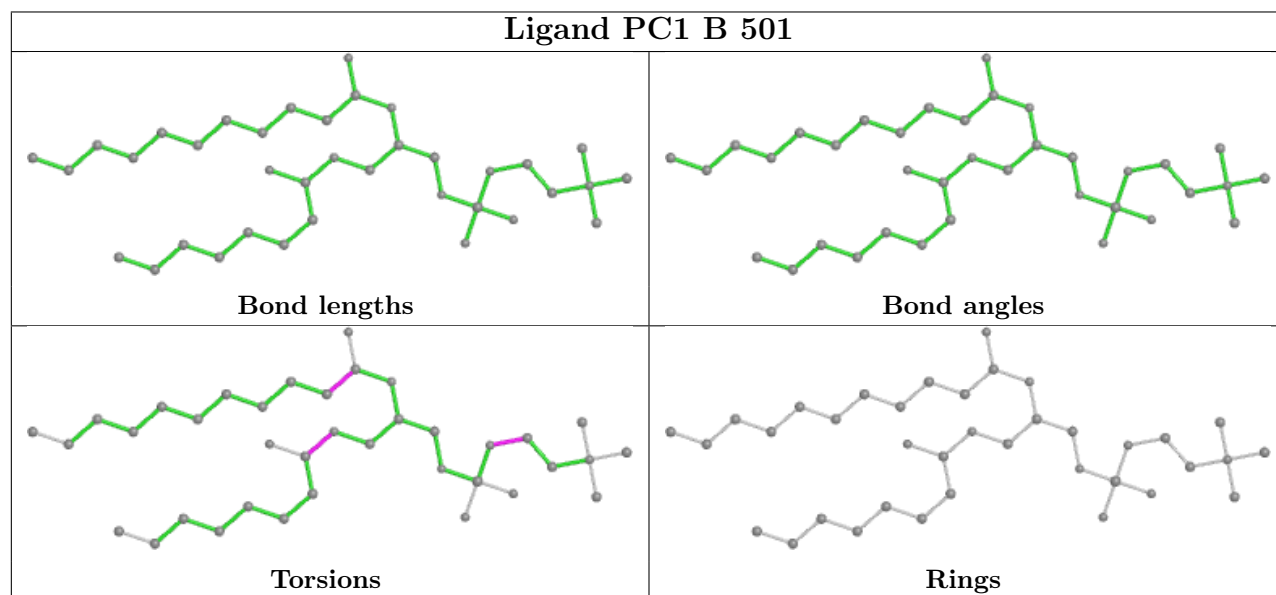
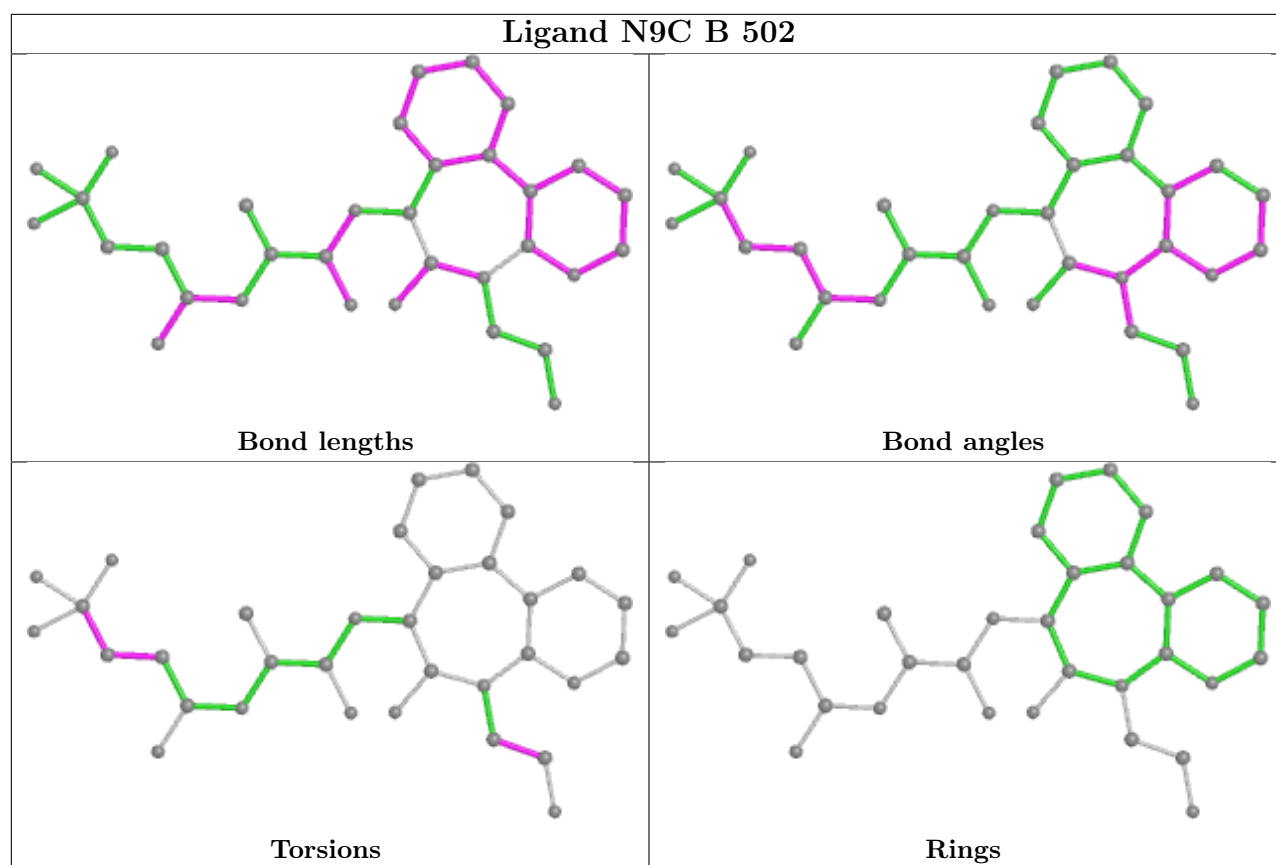
4 monomers are involved in 9 short contacts:

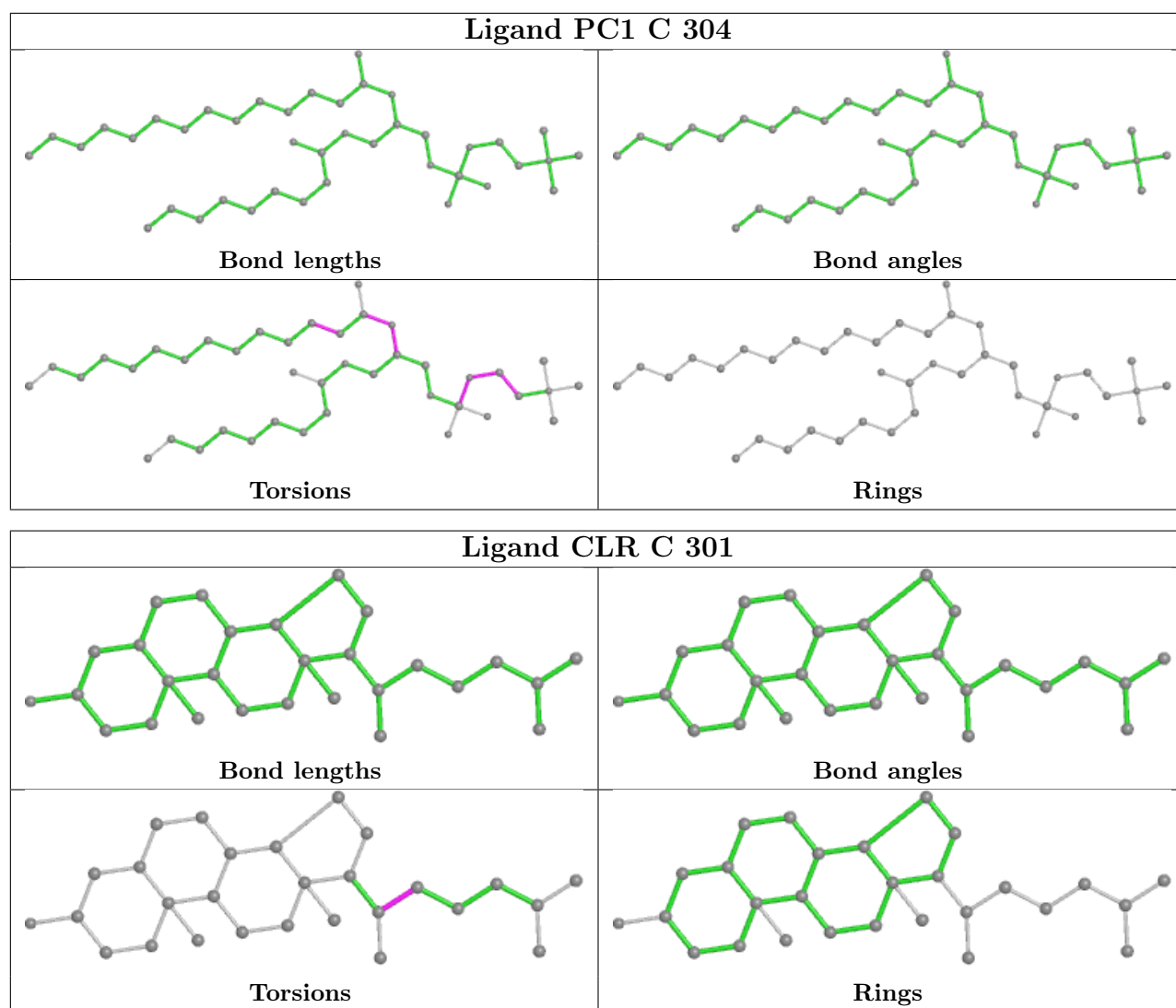
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	303	CLR	1	0
8	C	304	PC1	1	0
10	C	301	CLR	6	0
7	A	804	NAG	1	0

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







## 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.