



## Full wwPDB EM Validation Report ⓘ

Apr 20, 2025 – 12:08 AM JST

PDB ID : 8KCT / pdb\_00008ket  
EMDB ID : EMD-37109  
Title : Cryo-EM structure of human gamma-secretase in complex with Nirogacestat  
Authors : Guo, X.; Li, H.; Kai, U.; Yan, C.; Lei, J.; Zhou, R.; Shi, Y.  
Deposited on : 2023-08-08  
Resolution : 2.60 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

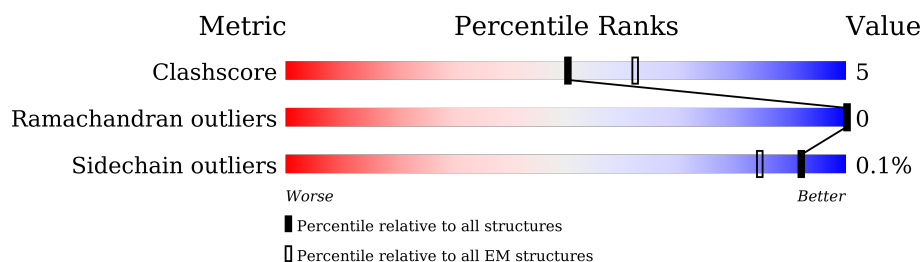
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.60 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.



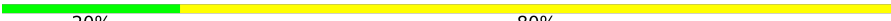
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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% 10% 5%
2	C	265	83% 8% 8%
3	D	101	83% 12% 5%
4	B	467	55% 10% 34%
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	 A horizontal bar chart showing the quality of chain F. The bar is divided into two segments: a green segment on the left representing 20% and a yellow segment on the right representing 80%. The labels '20%' and '80%' are placed below their respective segments.

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 10839 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 Gamma-secretase subunit APH-1A.

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

- Molecule 3 is a protein called Gamma-secretase subunit PEN-2.

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

- Molecule 4 is a protein called Presenilin-1.

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

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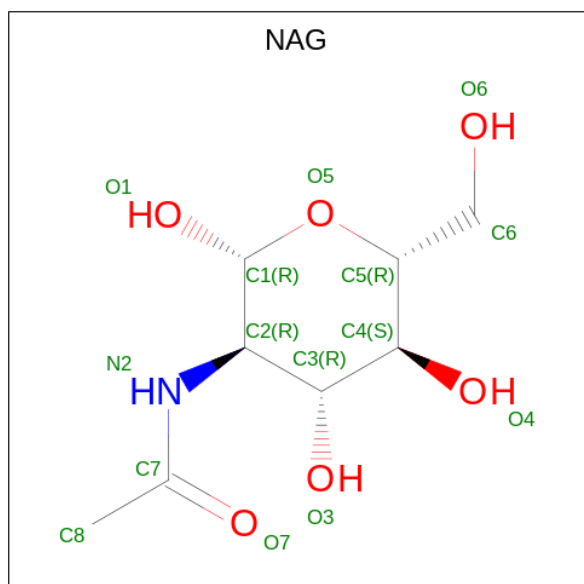
Mol	Chain	Residues	Atoms				AltConf	Trace
5	H	2	Total	C	N	O	0	0
			28	16	2	10		
5	I	2	Total	C	N	O	0	0
			28	16	2	10		
5	J	2	Total	C	N	O	0	0
			28	16	2	10		

- 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>).



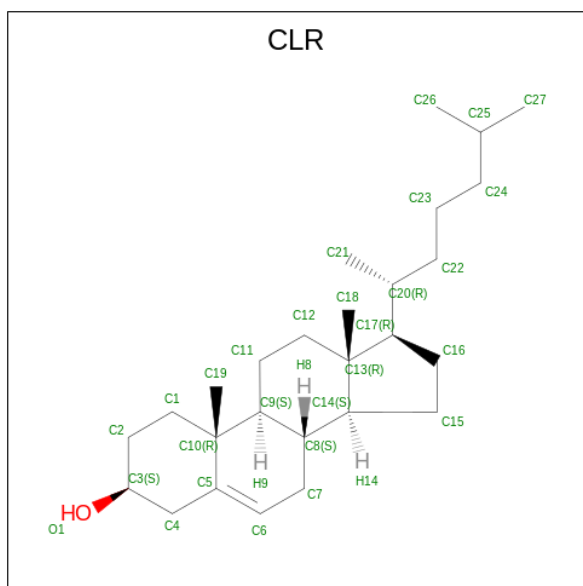
Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			14	8	1	5	

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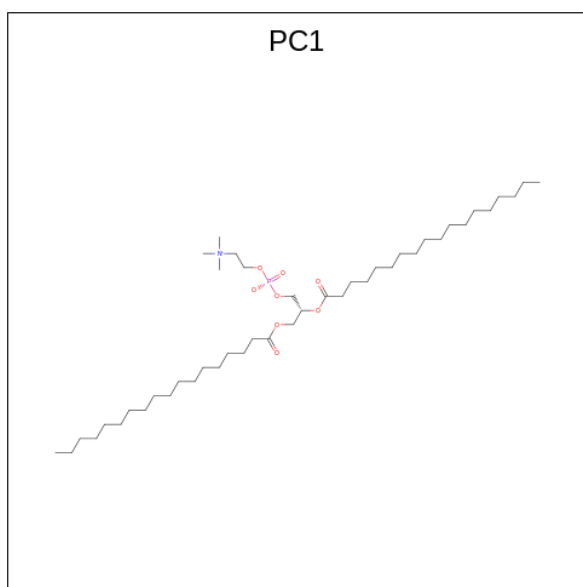
Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	

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



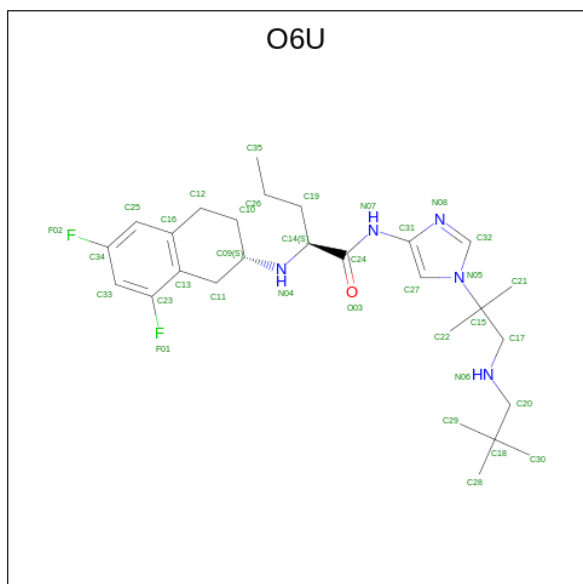
Mol	Chain	Residues	Atoms				AltConf
8	C	1	Total	C	O		0
			28	27	1		
8	C	1	Total	C	O		0
			28	27	1		
8	C	1	Total	C	O		0
			28	27	1		

- Molecule 9 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula:  $C_{44}H_{88}NO_8P$ ).



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

- Molecule 10 is Nirogacestat (CCD ID: O6U) (formula:  $C_{27}H_{41}F_2N_5O$ ) (labeled as "Ligand of Interest" by depositor).




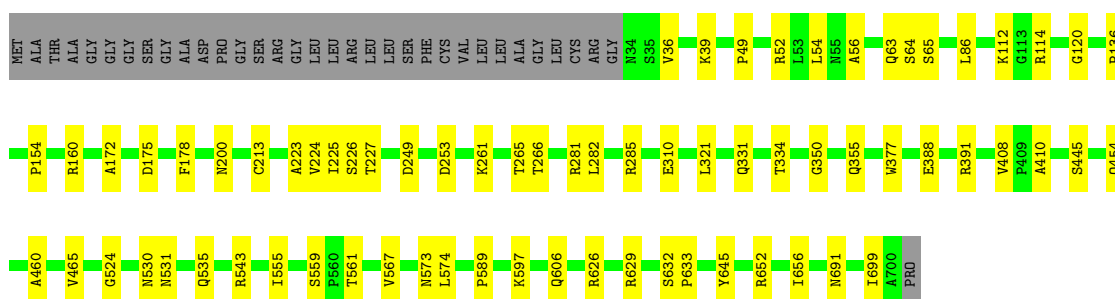
Mol	Chain	Residues	Atoms					AltConf
10	B	1	Total	C	F	N	O	0
			35	27	2	5	1	

### 3 Residue-property plots


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

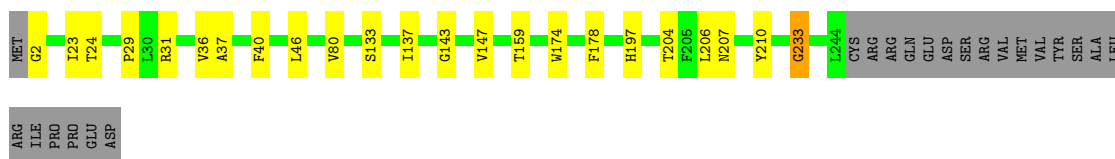
#### • Molecule 1: Nicastrin

Chain A: 




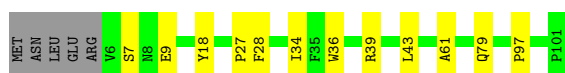
#### • Molecule 2: Gamma-secretase subunit APh-1A

Chain C: 



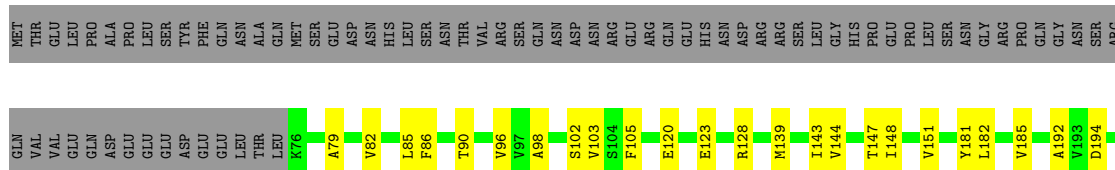
#### • Molecule 3: Gamma-secretase subunit PEN-2

Chain D: 

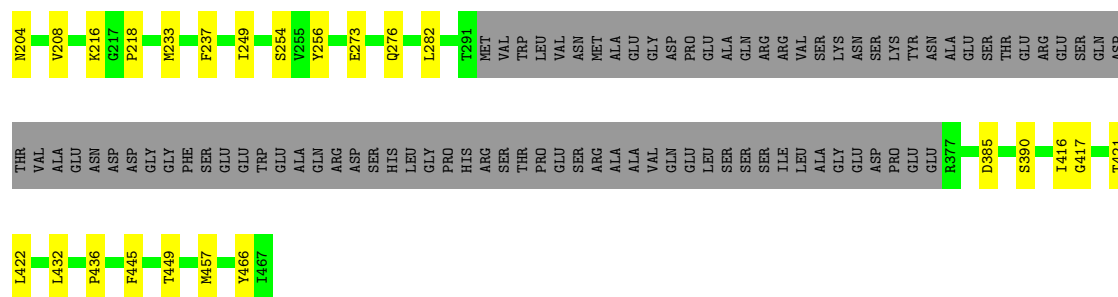


#### • Molecule 4: Presenilin-1

Chain B: 







- 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

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## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1047939	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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: O6U, NAG, BMA, CLR, PC1

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	C	0.39	0/1924	0.61	1/2624 (0.0%)
3	D	0.35	0/847	0.48	0/1157
4	B	0.27	0/2499	0.40	0/3410
All	All	0.35	0/10628	0.51	2/14493 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	233	GLY	N-CA-C	12.38	144.04	113.10
1	A	226	SER	N-CA-CB	5.98	119.47	110.50

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5235	0	5126	41	0
2	C	1872	0	1911	24	0
3	D	814	0	804	13	0
4	B	2436	0	2558	58	0
5	E	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	C	84	0	135	7	0
9	B	37	0	48	0	0
9	C	41	0	56	1	0
10	B	35	0	0	1	0
All	All	10839	0	10893	118	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 (118) 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)
2:C:206:LEU:HD21	8:C:301:CLR:C21	1.70	1.20
4:B:233:MET:CE	4:B:237:PHE:CZ	2.25	1.19
4:B:233:MET:HE3	4:B:237:PHE:CE2	1.76	1.19
4:B:233:MET:CE	4:B:237:PHE:CE2	2.29	1.14
4:B:233:MET:O	4:B:237:PHE:CD2	2.02	1.13
4:B:233:MET:HE3	4:B:237:PHE:CZ	1.86	1.08
2:C:206:LEU:CD2	8:C:301:CLR:H212	1.89	1.02
4:B:233:MET:O	4:B:237:PHE:HD2	1.35	1.01
2:C:206:LEU:HD21	8:C:301:CLR:H212	1.39	1.00
1:A:224:VAL:HG12	1:A:225:ILE:HG13	1.49	0.94
2:C:206:LEU:CD2	8:C:301:CLR:C21	2.48	0.91
2:C:206:LEU:HD21	8:C:301:CLR:H211	1.51	0.91
4:B:233:MET:HE2	4:B:237:PHE:CE2	2.06	0.90
4:B:254:SER:OG	4:B:436:PRO:HA	1.72	0.89
2:C:29:PRO:HB2	4:B:79:ALA:O	1.78	0.84
4:B:233:MET:CE	4:B:237:PHE:HZ	1.90	0.83
4:B:139:MET:SD	4:B:249:ILE:HD13	2.21	0.81
4:B:233:MET:HE2	4:B:237:PHE:CZ	2.19	0.77
4:B:233:MET:HB3	4:B:237:PHE:HE2	1.53	0.73
4:B:233:MET:HE2	4:B:237:PHE:HE2	1.54	0.71
4:B:233:MET:CE	4:B:237:PHE:HE2	1.98	0.69
3:D:27:PRO:HD2	4:B:204:ASN:HD21	1.58	0.67
1:A:39:LYS:HB3	2:C:147:VAL:HG13	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:97:PRO:HD3	4:B:192:ALA:HB2	1.79	0.65
1:A:350:GLY:HA2	1:A:355:GLN:HE22	1.62	0.64
3:D:79:GLN:NE2	4:B:192:ALA:O	2.29	0.62
4:B:98:ALA:O	4:B:102:SER:OG	2.18	0.60
3:D:28:PHE:HD2	4:B:208:VAL:HG21	1.67	0.60
1:A:632:SER:OG	1:A:645:TYR:O	2.21	0.59
3:D:18:TYR:OH	4:B:216:LYS:O	2.19	0.58
4:B:82:VAL:HG22	4:B:422:LEU:HD22	1.85	0.58
1:A:86:LEU:HD22	1:A:114:ARG:HD2	1.86	0.58
1:A:530:ASN:OD1	1:A:535:GLN:NE2	2.36	0.58
1:A:261:LYS:NZ	1:A:321:LEU:O	2.37	0.57
1:A:36:VAL:HG21	2:C:137:ILE:HG22	1.85	0.56
1:A:691:ASN:HD22	2:C:23:ILE:HG22	1.71	0.56
2:C:133:SER:HG	4:B:466:TYR:HE2	1.55	0.55
1:A:699:ILE:HG13	2:C:233:GLY:O	2.07	0.54
1:A:559:SER:HB3	1:A:629:ARG:HH12	1.72	0.54
9:C:304:PC1:H362	9:C:304:PC1:H2A1	1.89	0.54
4:B:233:MET:HE1	4:B:237:PHE:CZ	2.37	0.54
2:C:206:LEU:HD23	8:C:301:CLR:H212	1.82	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	1.73	0.53
2:C:204:THR:HB	2:C:207:ASN:HD21	1.76	0.51
3:D:27:PRO:CD	4:B:204:ASN:HD21	2.21	0.51
4:B:120:GLU:HG2	4:B:128:ARG:HE	1.74	0.51
1:A:136:PRO:HB2	1:A:172:ALA:HB2	1.93	0.51
1:A:249:ASP:OD2	1:A:652:ARG:NH1	2.40	0.50
1:A:54:LEU:HD11	1:A:223:ALA:HB1	1.93	0.50
4:B:96:VAL:HG21	4:B:390:SER:HB3	1.93	0.50
2:C:80:VAL:HG13	2:C:197:HIS:CD2	2.45	0.50
1:A:265:THR:OG1	1:A:626:ARG:NH1	2.44	0.50
1:A:253:ASP:OD1	1:A:561:THR:OG1	2.26	0.49
1:A:524:GLY:HA2	1:A:531:ASN:HD21	1.77	0.49
1:A:120:GLY:H	1:A:178:PHE:HB2	1.77	0.49
1:A:281:ARG:NH2	1:A:334:THR:OG1	2.45	0.49
1:A:460:ALA:HB1	1:A:465:VAL:HB	1.95	0.48
1:A:266:THR:HB	7:A:804:NAG:HN2	1.78	0.48
2:C:204:THR:HB	2:C:207:ASN:ND2	2.28	0.48
2:C:36:VAL:HG12	4:B:416:ILE:HG12	1.96	0.48
1:A:285:ARG:HG2	1:A:454:GLN:HE21	1.79	0.48
4:B:86:PHE:O	4:B:90:THR:HG22	2.14	0.48
4:B:254:SER:HG	4:B:436:PRO:HA	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:GLU:OE1	1:A:391:ARG:NH2	2.47	0.47
4:B:85:LEU:HD12	4:B:422:LEU:HD12	1.97	0.47
4:B:120:GLU:HG2	4:B:128:ARG:HH11	1.80	0.47
2:C:2:GLY:N	2:C:143:GLY:O	2.48	0.47
3:D:36:TRP:CG	4:B:218:PRO:HG3	2.49	0.47
1:A:112:LYS:NZ	1:A:175:ASP:O	2.40	0.46
1:A:310:GLU:HB2	1:A:574:LEU:HD23	1.98	0.46
8:C:303:CLR:H162	8:C:303:CLR:H221	1.62	0.46
1:A:224:VAL:HG12	1:A:225:ILE:CG1	2.35	0.46
4:B:254:SER:OG	4:B:436:PRO:CA	2.55	0.46
4:B:148:ILE:HA	4:B:151:VAL:HG12	1.97	0.46
4:B:233:MET:C	4:B:237:PHE:HD2	2.13	0.46
1:A:154:PRO:O	1:A:160:ARG:NH1	2.49	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:49:PRO:HG3	1:A:656:ILE:HD13	1.98	0.45
3:D:27:PRO:HD2	4:B:204:ASN:ND2	2.29	0.45
2:C:37:ALA:HA	4:B:416:ILE:HD11	1.97	0.45
1:A:331:GLN:HE21	1:A:555:ILE:HB	1.81	0.45
2:C:46:LEU:HD11	4:B:457:MET:HE3	1.97	0.45
4:B:233:MET:HE1	4:B:237:PHE:HZ	1.73	0.45
3:D:34:ILE:HD11	3:D:61:ALA:HA	1.99	0.44
4:B:139:MET:O	4:B:143:ILE:HG13	2.18	0.44
4:B:417:GLY:O	4:B:421:THR:HG22	2.17	0.44
3:D:39:ARG:HG3	3:D:43:LEU:HD22	2.00	0.43
1:A:253:ASP:HB3	1:A:331:GLN:HG2	2.00	0.43
2:C:159:THR:HG21	2:C:210:TYR:CD1	2.53	0.43
4:B:194:ASP:OD1	4:B:194:ASP:N	2.37	0.43
4:B:432:LEU:O	10:B:502:O6U:N04	2.51	0.43
2:C:133:SER:OG	4:B:466:TYR:HE2	2.02	0.43
3:D:39:ARG:HA	3:D:43:LEU:HD13	2.01	0.42
4:B:103:VAL:HG12	4:B:105:PHE:H	1.83	0.42
1:A:56:ALA:HA	1:A:227:THR:HG22	2.01	0.42
1:A:589:PRO:HD2	1:A:597:LYS:HD2	2.01	0.42
4:B:144:VAL:O	4:B:147:THR:HG22	2.19	0.42
2:C:24:THR:O	2:C:31:ARG:NH1	2.50	0.42
3:D:7:SER:OG	3:D:9:GLU:OE1	2.38	0.42
4:B:181:TYR:O	4:B:185:VAL:HG12	2.20	0.41
1:A:64:SER:OG	1:A:65:SER:N	2.53	0.41
4:B:445:PHE:O	4:B:449:THR:OG1	2.30	0.41
3:D:36:TRP:CD1	4:B:218:PRO:HG3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:385:ASP:N	4:B:385:ASP:OD1	2.53	0.41
1:A:377:TRP:CE2	1:A:445:SER:HB3	2.55	0.41
1:A:589:PRO:HG2	1:A:597:LYS:HB2	2.02	0.41
4:B:182:LEU:HD12	4:B:182:LEU:HA	1.95	0.41
1:A:200:ASN:HD21	1:A:213:CYS:HB3	1.86	0.41
4:B:273:GLU:HA	4:B:276:GLN:HG3	2.03	0.41
2:C:40:PHE:HB2	4:B:416:ILE:HG13	2.02	0.41
1:A:632:SER:HA	1:A:633:PRO:HD3	1.97	0.40
2:C:174:TRP:O	2:C:178:PHE:HB2	2.21	0.40
4:B:147:THR:HG21	4:B:256:TYR:OH	2.21	0.40
4:B:233:MET:C	4:B:237:PHE:CD2	2.86	0.40
4:B:123:GLU:H	4:B:123:GLU:CD	2.23	0.40
4:B:282:LEU:HD23	4:B:282:LEU:HA	1.81	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	C	241/265 (91%)	234 (97%)	7 (3%)	0	100	100
3	D	94/101 (93%)	90 (96%)	4 (4%)	0	100	100
4	B	303/467 (65%)	295 (97%)	8 (3%)	0	100	100
All	All	1303/1534 (85%)	1245 (96%)	58 (4%)	0	100	100

There are no Ramachandran outliers to report.



### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	584/606 (96%)	583 (100%)	1 (0%)	92	98
2	C	193/214 (90%)	193 (100%)	0	100	100
3	D	84/89 (94%)	84 (100%)	0	100	100
4	B	265/408 (65%)	265 (100%)	0	100	100
All	All	1126/1317 (86%)	1125 (100%)	1 (0%)	92	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	573	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) 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	C	207	ASN
4	B	204	ASN
4	B	279	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	5,1	14,14,15	0.28	0	17,19,21	0.41	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	0.26	0	17,19,21	0.54	0
6	NAG	F	2	6	14,14,15	0.20	0	17,19,21	0.66	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	0.92	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	5,1	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	0.49	0
5	NAG	H	1	5,1	14,14,15	0.22	0	17,19,21	0.48	0
5	NAG	H	2	5	14,14,15	0.20	0	17,19,21	0.55	0
5	NAG	I	1	5,1	14,14,15	0.23	0	17,19,21	0.51	0
5	NAG	I	2	5	14,14,15	0.74	1 (7%)	17,19,21	2.24	3 (17%)
5	NAG	J	1	5,1	14,14,15	0.32	0	17,19,21	0.54	0
5	NAG	J	2	5	14,14,15	0.26	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	5,1	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
5	NAG	G	1	5,1	-	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	5,1	-	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	5,1	-	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	5,1	-	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	3.08	1.57	1.52
6	F	5	BMA	C1-C2	3.01	1.59	1.52
5	I	2	NAG	C1-C2	2.09	1.55	1.52
6	F	5	BMA	O5-C1	2.08	1.47	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	2	NAG	C2-N2-C7	7.80	134.01	122.90
6	F	5	BMA	C1-O5-C5	4.99	118.96	112.19
5	I	2	NAG	C1-C2-N2	3.65	116.73	110.49
5	G	1	NAG	C2-N2-C7	3.13	127.36	122.90
6	F	5	BMA	C1-C2-C3	3.01	113.37	109.67
6	F	5	BMA	O5-C1-C2	2.74	115.00	110.77
6	F	2	NAG	C1-O5-C5	2.24	115.23	112.19
6	F	5	BMA	C2-C3-C4	2.19	114.69	110.89
5	I	2	NAG	C8-C7-N2	2.14	119.72	116.10
6	F	4	BMA	C1-O5-C5	2.06	114.98	112.19
6	F	3	BMA	O2-C2-C3	-2.05	106.03	110.14

There are no chirality outliers.

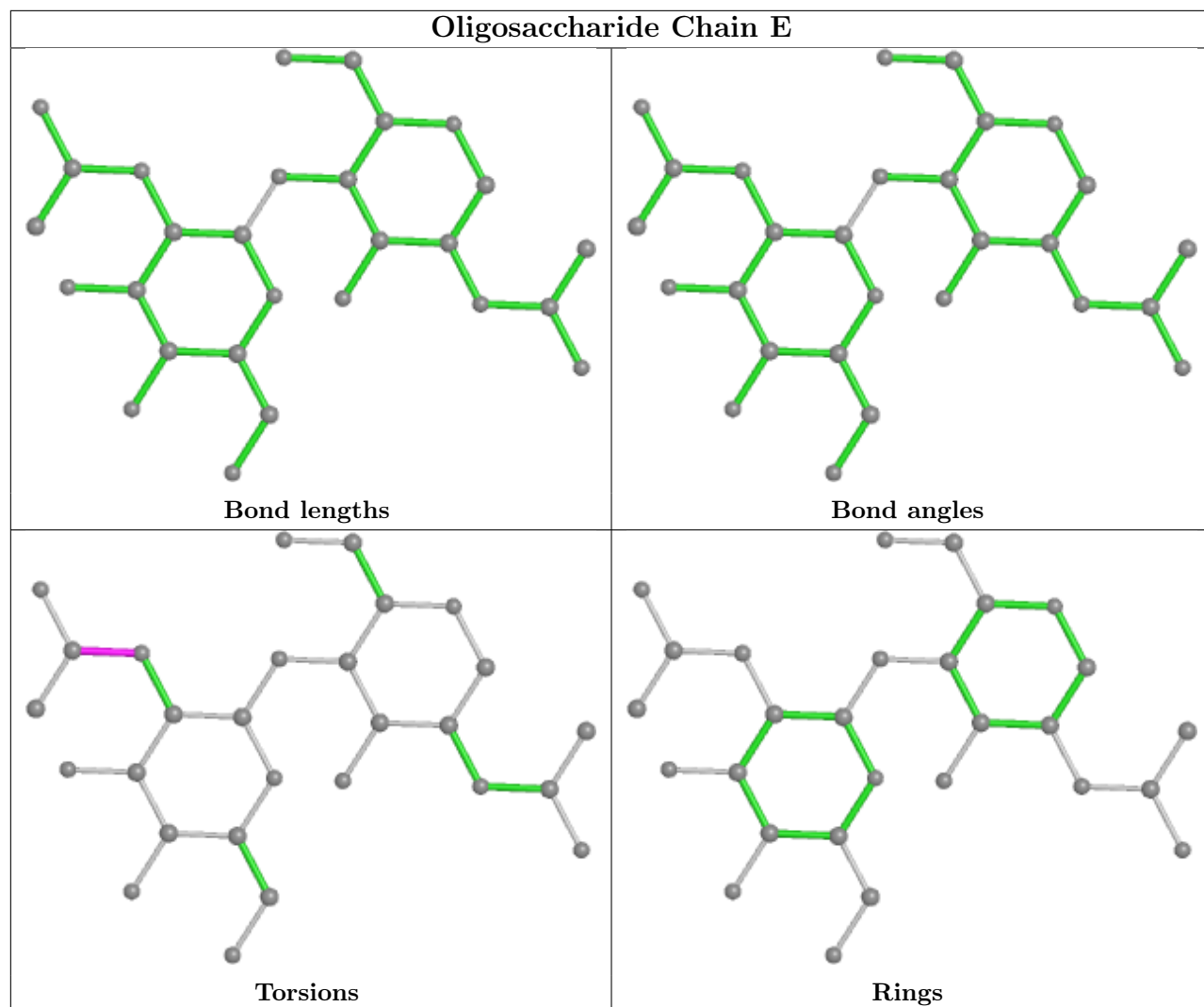
All (28) torsion outliers are listed below:

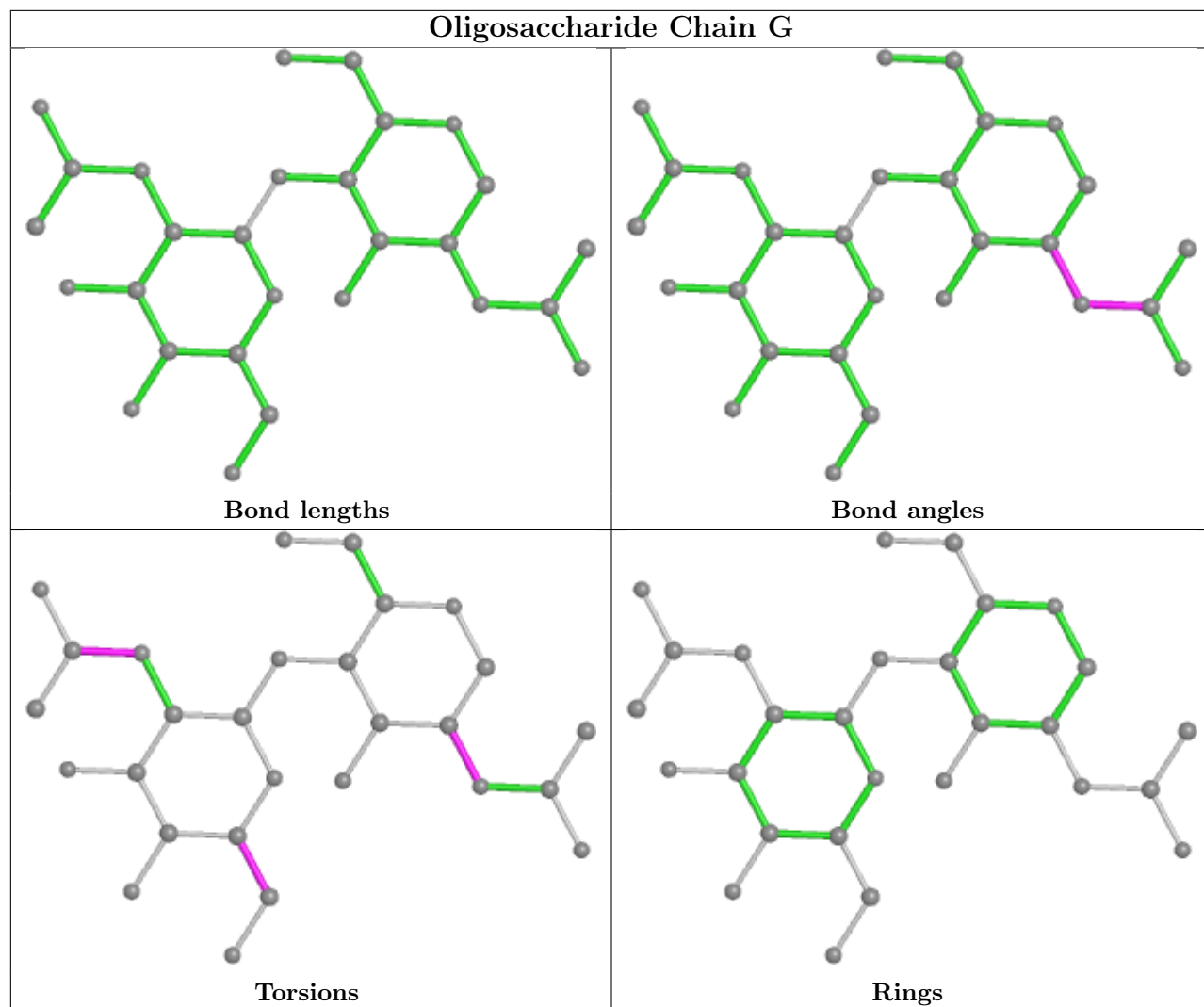
Mol	Chain	Res	Type	Atoms
5	I	1	NAG	O5-C5-C6-O6
6	F	3	BMA	C4-C5-C6-O6
5	J	1	NAG	O5-C5-C6-O6
5	I	1	NAG	C4-C5-C6-O6
6	F	3	BMA	O5-C5-C6-O6
5	J	1	NAG	C4-C5-C6-O6
5	E	2	NAG	C8-C7-N2-C2
5	E	2	NAG	O7-C7-N2-C2
5	G	2	NAG	C8-C7-N2-C2
5	G	2	NAG	O7-C7-N2-C2
5	H	2	NAG	C8-C7-N2-C2
5	H	2	NAG	O7-C7-N2-C2
5	I	2	NAG	C8-C7-N2-C2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

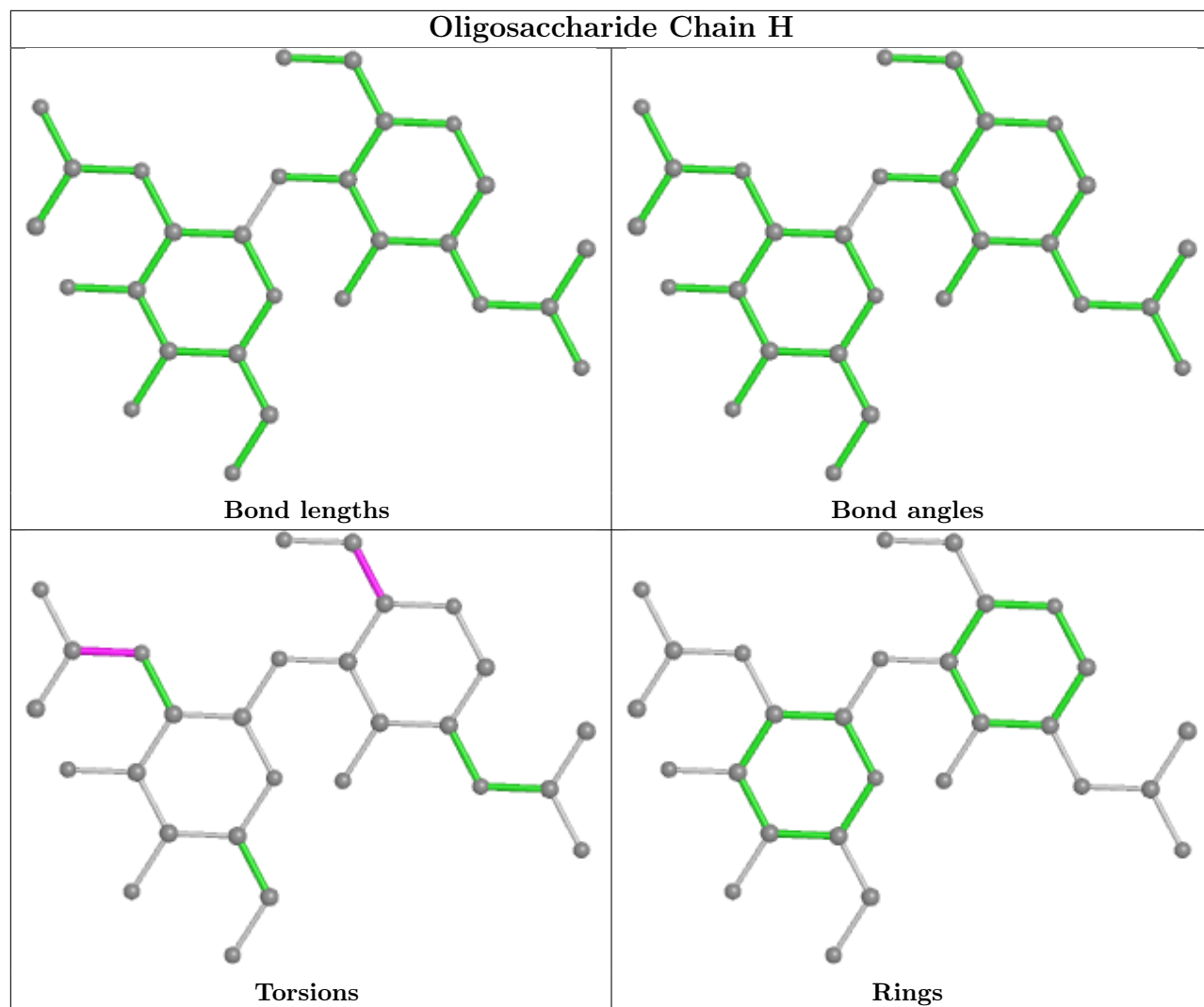
There are no ring outliers.

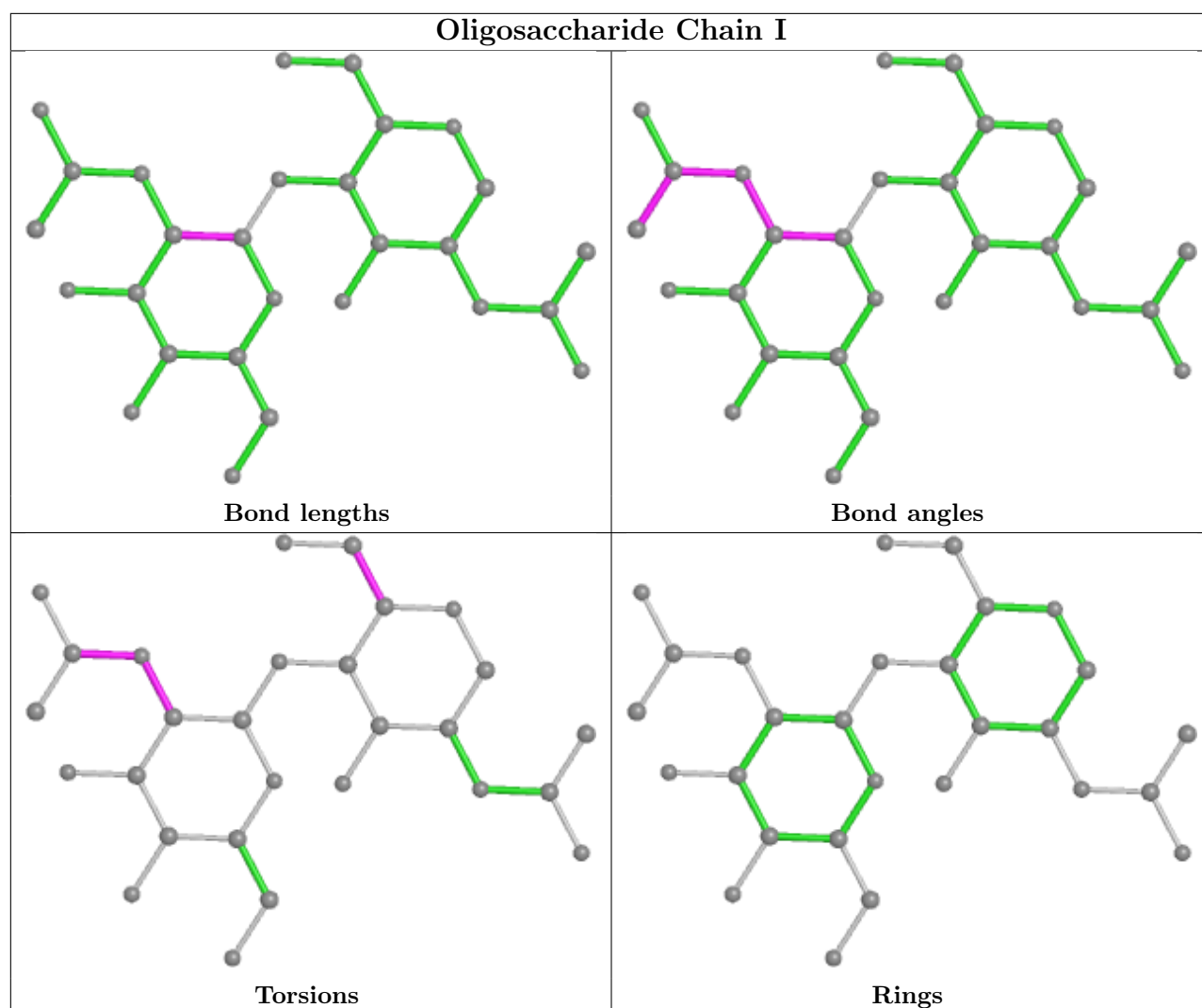
No monomer is involved in short contacts.

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

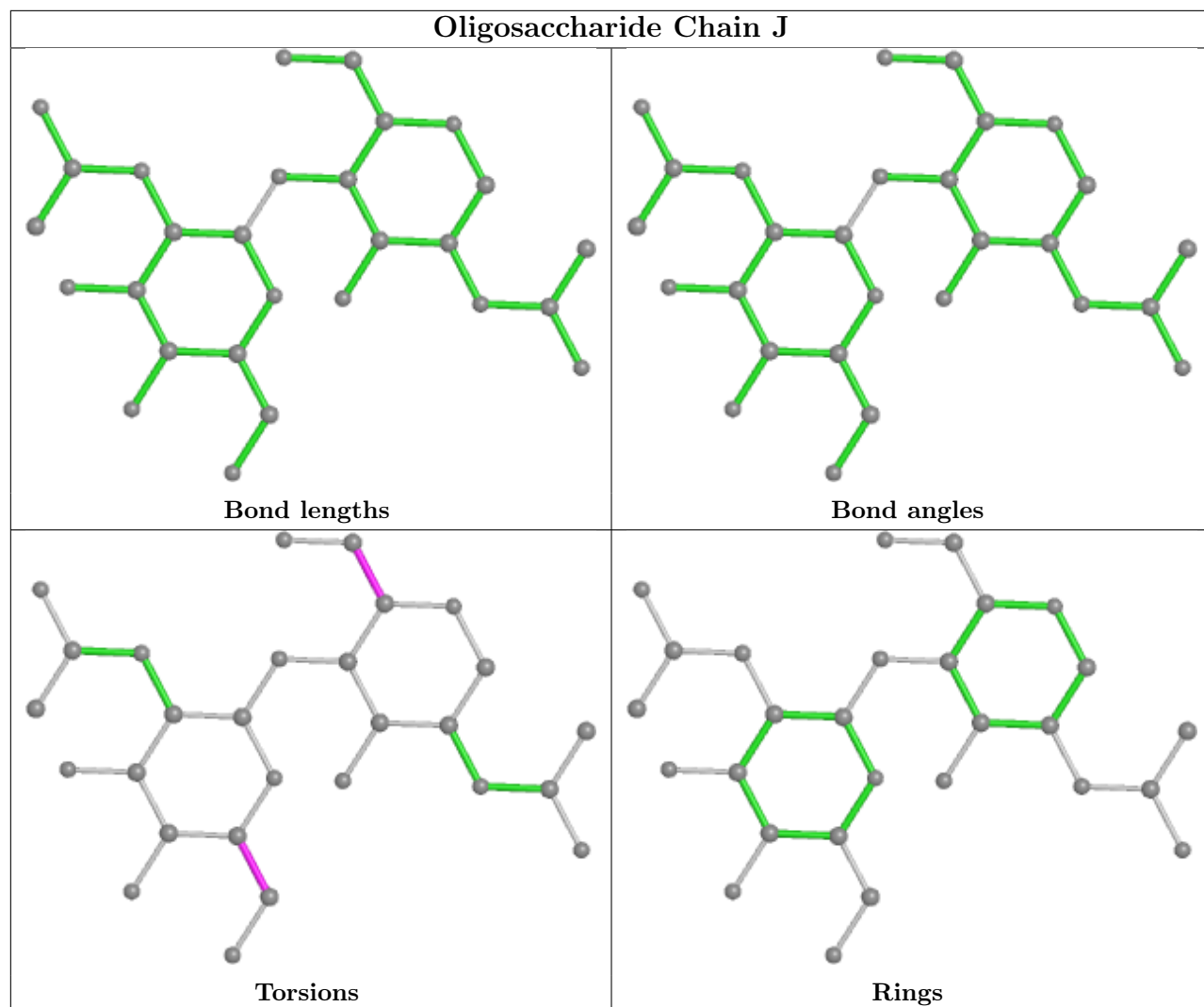


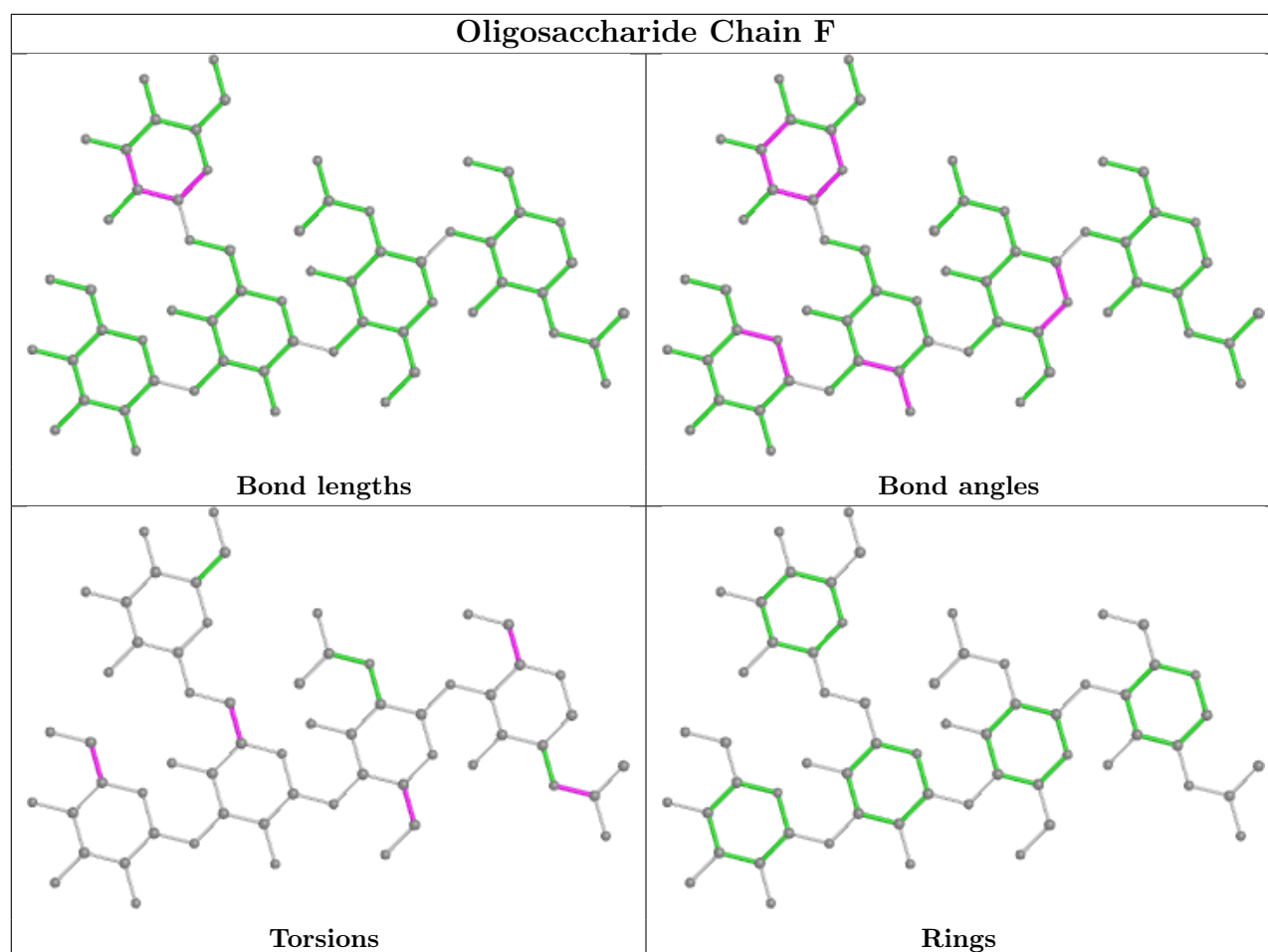












## 5.6 Ligand geometry [i](#)

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	$\# Z  > 2$
9	PC1	B	501	-	36,36,53	0.31	0	42,44,61	0.37	0
8	CLR	C	301	-	31,31,31	0.34	0	48,48,48	0.51	0
7	NAG	A	804	1	14,14,15	0.92	1 (7%)	17,19,21	2.27	3 (17%)
8	CLR	C	303	-	31,31,31	0.29	0	48,48,48	0.54	0
7	NAG	A	806	1	14,14,15	0.22	0	17,19,21	0.60	1 (5%)
10	O6U	B	502	-	32,37,37	4.61	13 (40%)	38,54,54	2.44	9 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	NAG	A	803	1	14,14,15	0.44	0	17,19,21	0.46	0
7	NAG	A	802	1	14,14,15	0.53	0	17,19,21	1.00	1 (5%)
7	NAG	A	805	1	14,14,15	0.25	0	17,19,21	0.48	0
9	PC1	C	304	-	40,40,53	0.30	0	46,48,61	0.41	0
7	NAG	A	801	1	14,14,15	0.36	0	17,19,21	0.57	0
8	CLR	C	302	-	31,31,31	0.29	0	48,48,48	0.59	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	PC1	B	501	-	-	5/40/40/57	-
8	CLR	C	301	-	-	1/10/68/68	0/4/4/4
7	NAG	A	804	1	-	5/6/23/26	0/1/1/1
8	CLR	C	303	-	-	6/10/68/68	0/4/4/4
7	NAG	A	806	1	-	0/6/23/26	0/1/1/1
10	O6U	B	502	-	-	12/25/38/38	0/3/3/3
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
9	PC1	C	304	-	-	8/44/44/57	-
7	NAG	A	801	1	-	0/6/23/26	0/1/1/1
8	CLR	C	302	-	-	5/10/68/68	0/4/4/4

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	502	O6U	C33-C34	10.92	1.55	1.37
10	B	502	O6U	C16-C13	10.23	1.54	1.40
10	B	502	O6U	C25-C34	10.11	1.54	1.37
10	B	502	O6U	C13-C23	9.87	1.53	1.38
10	B	502	O6U	C33-C23	9.72	1.54	1.37
10	B	502	O6U	C25-C16	8.08	1.53	1.39
10	B	502	O6U	C24-N07	4.47	1.45	1.35
10	B	502	O6U	C15-N05	-4.21	1.45	1.51
10	B	502	O6U	C12-C16	4.08	1.58	1.51
10	B	502	O6U	C11-C13	3.99	1.57	1.51
7	A	804	NAG	C1-C2	2.93	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	502	O6U	C11-C09	-2.65	1.50	1.52
10	B	502	O6U	C31-N07	2.45	1.45	1.40
10	B	502	O6U	O03-C24	-2.36	1.18	1.23

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	804	NAG	C2-N2-C7	7.90	134.15	122.90
10	B	502	O6U	C33-C23-C13	-7.28	119.48	124.59
10	B	502	O6U	C12-C16-C13	-6.51	111.22	121.38
10	B	502	O6U	C10-C09-C11	5.73	114.35	110.12
10	B	502	O6U	C11-C13-C16	-4.48	112.91	121.55
10	B	502	O6U	C12-C16-C25	3.99	127.91	119.91
7	A	804	NAG	C1-C2-N2	3.67	116.76	110.49
10	B	502	O6U	C23-C33-C34	3.41	120.20	116.62
10	B	502	O6U	C31-N07-C24	-3.37	122.78	127.55
7	A	802	NAG	C2-N2-C7	3.08	127.29	122.90
10	B	502	O6U	C33-C34-C25	-2.79	120.00	123.52
7	A	804	NAG	C8-C7-N2	2.16	119.76	116.10
10	B	502	O6U	C22-C15-N05	2.11	110.32	108.04
7	A	806	NAG	C1-O5-C5	2.11	115.05	112.19

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	303	CLR	C16-C17-C20-C22
9	C	304	PC1	C11-O13-P-O14
9	C	304	PC1	O22-C21-O21-C2
9	B	501	PC1	C11-O13-P-O14
9	B	501	PC1	O32-C31-O31-C3
9	B	501	PC1	C32-C31-O31-C3
10	B	502	O6U	C21-C15-C17-N06
10	B	502	O6U	C22-C15-C17-N06
10	B	502	O6U	N05-C15-C17-N06
10	B	502	O6U	C28-C18-C20-N06
10	B	502	O6U	C29-C18-C20-N06
8	C	303	CLR	C13-C17-C20-C21
7	A	802	NAG	O5-C5-C6-O6
7	A	804	NAG	O5-C5-C6-O6
9	C	304	PC1	C22-C21-O21-C2
8	C	303	CLR	C16-C17-C20-C21

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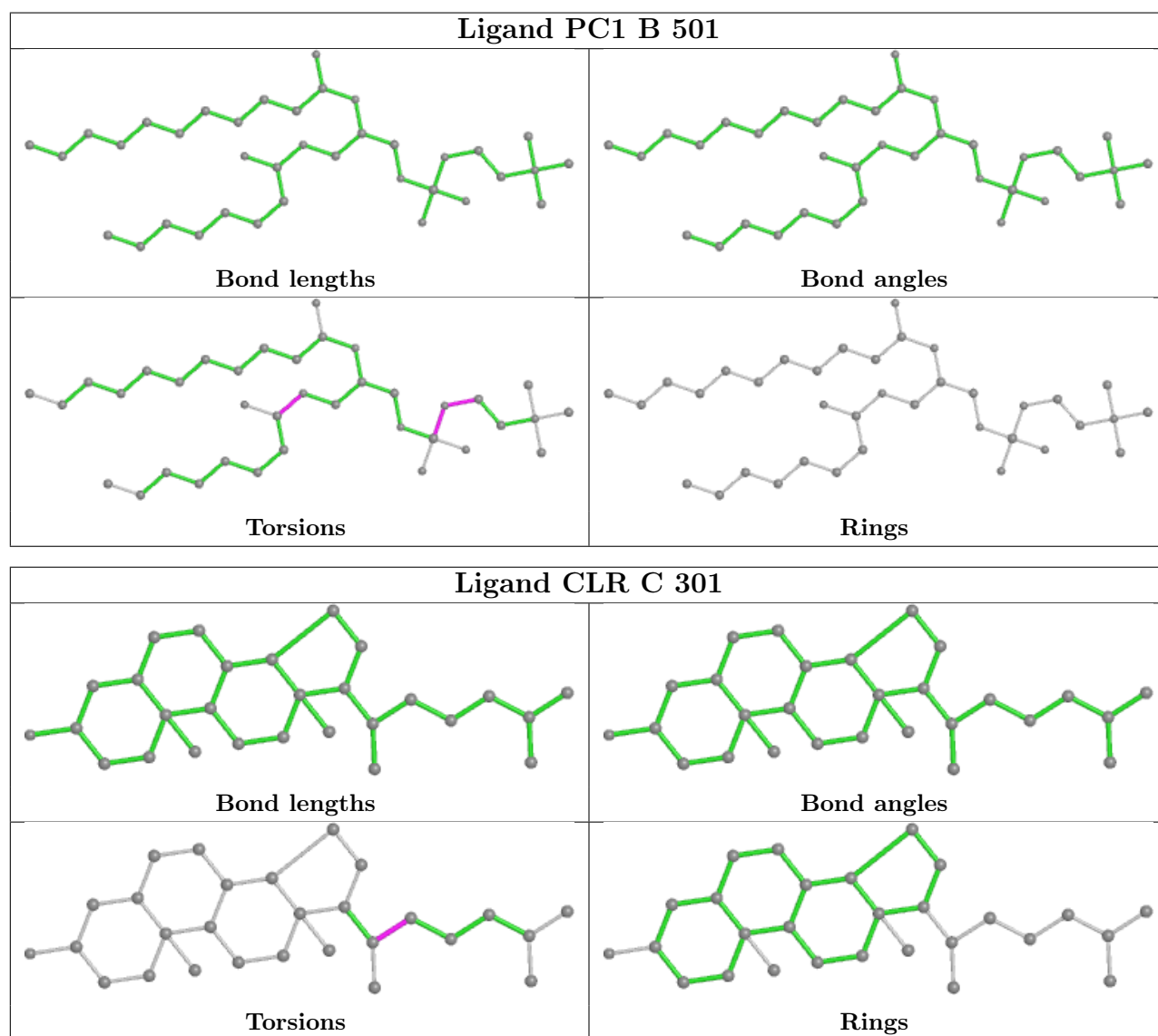
Mol	Chain	Res	Type	Atoms
8	C	303	CLR	C13-C17-C20-C22
7	A	802	NAG	C4-C5-C6-O6
7	A	804	NAG	C4-C5-C6-O6
8	C	303	CLR	C17-C20-C22-C23
7	A	804	NAG	C8-C7-N2-C2
7	A	804	NAG	O7-C7-N2-C2
8	C	303	CLR	C21-C20-C22-C23
10	B	502	O6U	C30-C18-C20-N06
8	C	302	CLR	C20-C22-C23-C24
7	A	803	NAG	O5-C5-C6-O6
8	C	301	CLR	C17-C20-C22-C23
10	B	502	O6U	C15-C17-N06-C20
9	C	304	PC1	C11-O13-P-O11
8	C	302	CLR	C16-C17-C20-C22
7	A	803	NAG	C4-C5-C6-O6
9	C	304	PC1	C12-C11-O13-P
9	B	501	PC1	C12-C11-O13-P
9	C	304	PC1	C21-C22-C23-C24
9	C	304	PC1	O13-C11-C12-N
8	C	302	CLR	C13-C17-C20-C22
8	C	302	CLR	C16-C17-C20-C21
9	B	501	PC1	C11-O13-P-O11
8	C	302	CLR	C13-C17-C20-C21
10	B	502	O6U	C18-C20-N06-C17
10	B	502	O6U	C21-C15-N05-C27
10	B	502	O6U	C21-C15-N05-C32
10	B	502	O6U	C22-C15-N05-C27
10	B	502	O6U	C22-C15-N05-C32
9	C	304	PC1	C1-C2-O21-C21
7	A	802	NAG	C3-C2-N2-C7
7	A	804	NAG	C3-C2-N2-C7

There are no ring outliers.

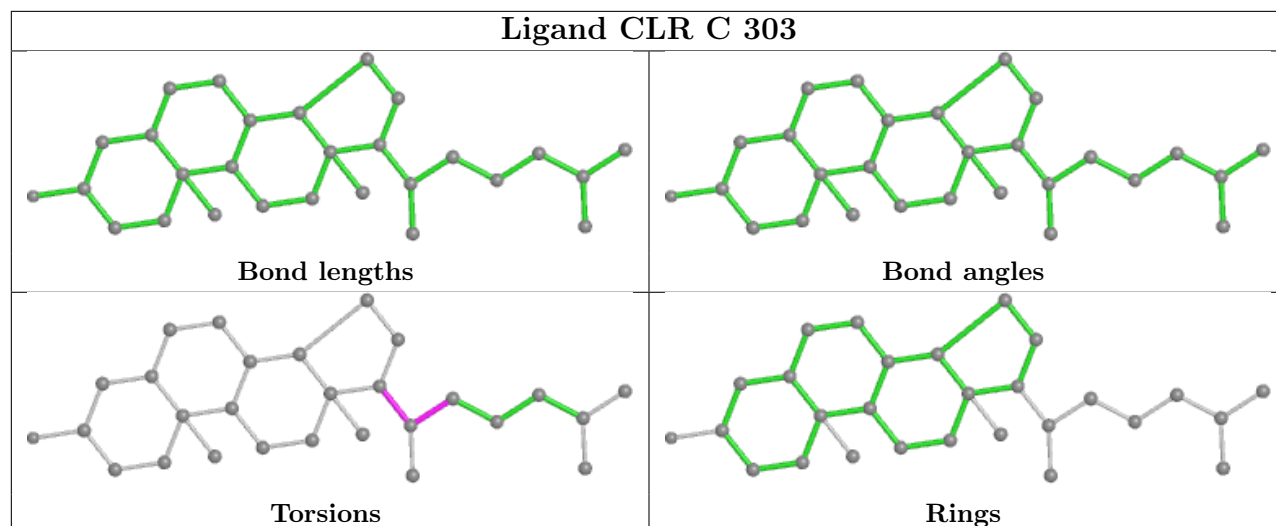
5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	301	CLR	6	0
7	A	804	NAG	1	0
8	C	303	CLR	1	0
10	B	502	O6U	1	0
9	C	304	PC1	1	0

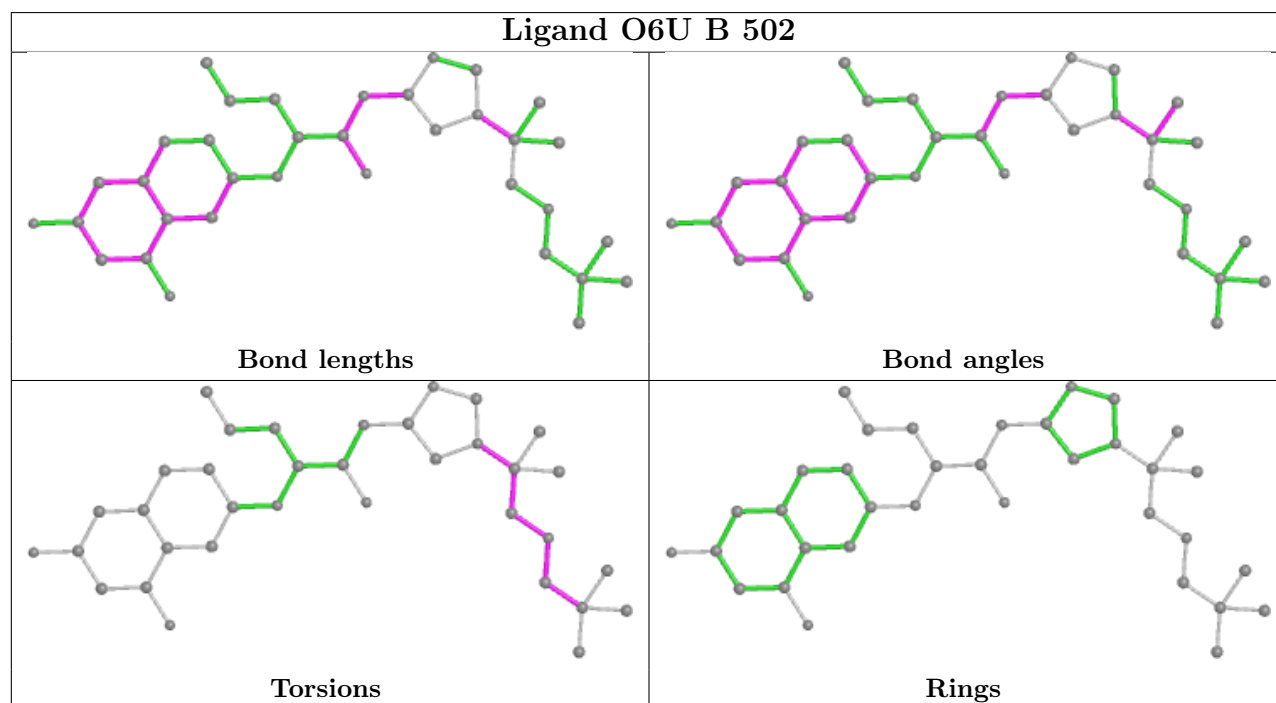
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



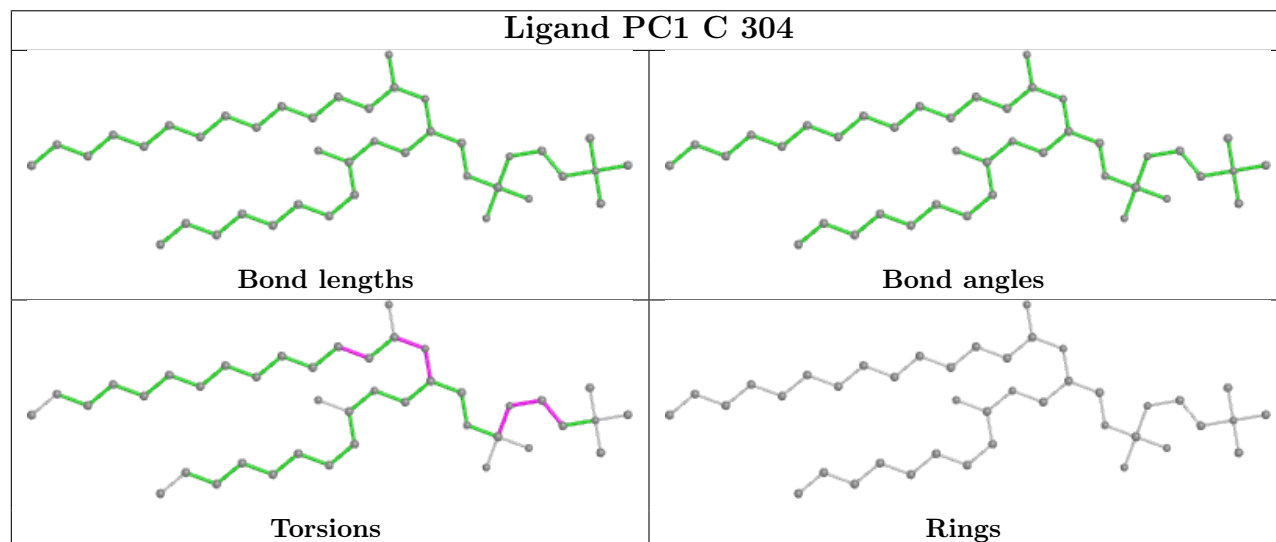
## Ligand CLR C 303

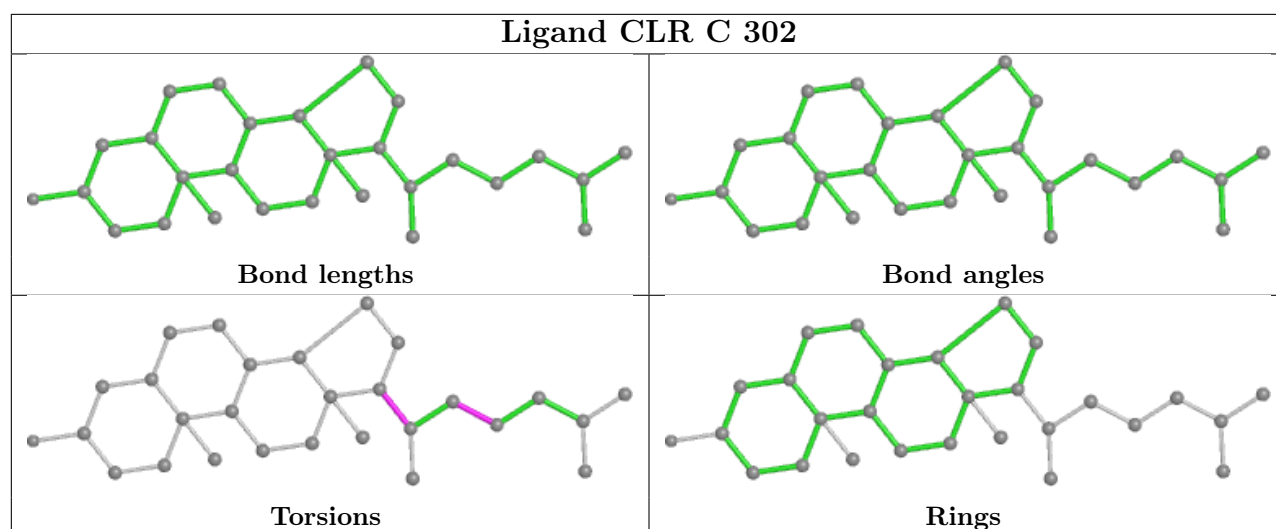


## Ligand O6U B 502



## Ligand PC1 C 304





## 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.