



Full wwPDB EM Validation Report ⓘ

May 31, 2026 – 12:15 AM JST

PDB ID : 9J93 / pdb_00009j93
EMDB ID : EMD-61251
Title : Native GluA1/GluA4 ATD dimer binding with 1D8 and 11B8
Authors : Li, X.; Li, R.; Wei, Y.; Zhao, Y.
Deposited on : 2024-08-22
Resolution : 3.54 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

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 : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

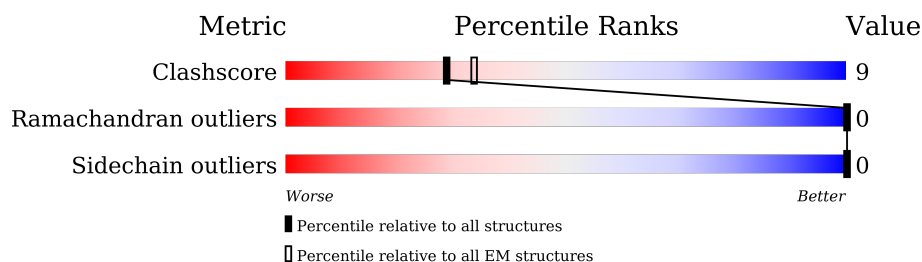
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.54 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.



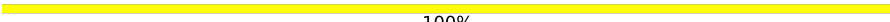
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	B	884	37% 6% 57%
2	A	906	34% 7% 59%
3	H	218	93% 6%
3	L	218	94% 6%
4	C	275	55% 28% 17%
5	D	2	50% 50%
5	E	2	100%
5	F	2	50% 50%
5	G	2	50% 50%

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Mol	Chain	Length	Quality of chain
5	I	2	 100%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10138 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 Glutamate receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	377	Total	C	N	O	S	0	0
			3028	1931	527	557	13		

- Molecule 2 is a protein called Glutamate receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	373	Total	C	N	O	S	1	0
			3026	1930	528	556	12		

- Molecule 3 is a protein called 1D8 Fab.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	H	217	Total	C	N	O	0	0
			1085	651	217	217		
3	L	216	Total	C	N	O	0	0
			1080	648	216	216		

- Molecule 4 is a protein called 11B8 scFV.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	229	Total	C	N	O	S	0	0
			1765	1117	295	347	6		

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



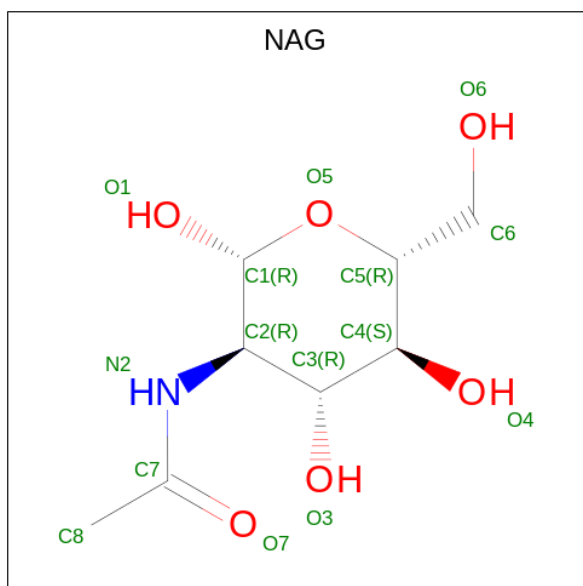
Mol	Chain	Residues	Atoms				AltConf	Trace
5	D	2	Total	C	N	O	0	0
			28	16	2	10		

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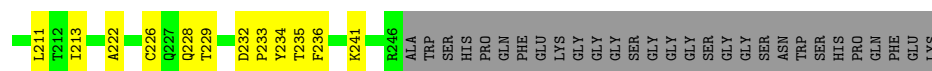
Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	2	Total	C	N	O	0	0
			28	16	2	10		
5	F	2	Total	C	N	O	0	0
			28	16	2	10		
5	G	2	Total	C	N	O	0	0
			28	16	2	10		
5	I	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

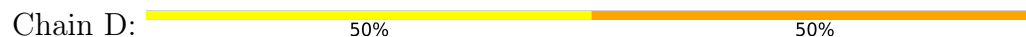


Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	1	5	





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



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



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



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	138139	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (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: NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	B	0.15	0/3099	0.33	0/4198
2	A	0.18	0/3100	0.39	0/4193
4	C	0.30	0/1805	0.53	3/2448 (0.1%)
All	All	0.20	0/8004	0.41	3/10839 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	29	PHE	N-CA-CB	-5.55	103.88	111.65
4	C	229	THR	N-CA-C	-5.32	105.89	112.38
4	C	234	TYR	N-CA-C	-5.01	107.32	112.93

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3028	0	2969	38	0
2	A	3026	0	2979	52	0
3	H	1085	0	242	7	0
3	L	1080	0	232	6	0
4	C	1765	0	1727	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	28	0	25	2	0
5	E	28	0	25	0	0
5	F	28	0	25	1	0
5	G	28	0	25	1	0
5	I	28	0	25	1	0
6	A	14	0	13	4	0
All	All	10138	0	8287	173	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 9.

All (173) 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:A:231:ASN:OD1	2:A:354:LYS:HG3	1.38	1.21
2:A:231:ASN:HD22	6:A:901:NAG:C1	1.56	1.18
4:C:173:TRP:CZ3	4:C:226:CYS:SG	2.43	1.12
2:A:231:ASN:ND2	6:A:901:NAG:C1	2.17	1.07
4:C:98:ARG:HH22	4:C:106:MET:HB2	1.34	0.93
2:A:231:ASN:ND2	6:A:901:NAG:O5	2.05	0.89
2:A:242:ASP:OD1	2:A:243:THR:N	2.06	0.88
4:C:105:VAL:HG13	4:C:106:MET:HG3	1.61	0.81
4:C:173:TRP:CH2	4:C:226:CYS:SG	2.81	0.73
1:B:262:LEU:HD12	1:B:267:TYR:HD2	1.52	0.73
2:A:195:LEU:O	2:A:199:ILE:HD12	1.89	0.70
4:C:232:ASP:HB2	4:C:233:PRO:HD3	1.74	0.69
1:B:95:ILE:HD11	1:B:304:ARG:HH21	1.58	0.69
2:A:199:ILE:HD13	2:A:224:LYS:HG2	1.75	0.69
2:A:199:ILE:HG23	2:A:202:GLU:OE2	1.93	0.68
2:A:250:GLN:NE2	4:C:54:ASP:O	2.27	0.67
4:C:98:ARG:NH1	4:C:106:MET:O	2.26	0.67
2:A:352:GLU:OE2	2:A:354:LYS:NZ	2.28	0.67
4:C:192:LEU:HD21	4:C:201:SER:HA	1.76	0.67
4:C:136:ILE:HD13	4:C:235:THR:HB	1.76	0.66
1:B:191:ILE:HB	1:B:219:ILE:HG22	1.77	0.66
1:B:180:GLU:OE2	1:B:184:ARG:NH2	2.29	0.66
4:C:169:SER:OG	4:C:206:ARG:NH1	2.29	0.64
2:A:135:ARG:NH1	2:A:187:GLU:OE1	2.31	0.64
4:C:138:LEU:HD11	4:C:228:GLN:HG3	1.81	0.63
4:C:199:ARG:HG3	4:C:213:ILE:HG23	1.81	0.62
1:B:109:GLN:O	1:B:330:LYS:NZ	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:136:ILE:HG13	4:C:228:GLN:HB2	1.80	0.62
1:B:225:LYS:HE3	1:B:357:PHE:HE2	1.65	0.61
4:C:98:ARG:HB3	4:C:99:PRO:HD2	1.84	0.60
2:A:262:ARG:NH1	4:C:101:GLY:O	2.35	0.60
2:A:218:MET:HA	2:A:218:MET:HE3	1.84	0.59
4:C:175:GLN:HG3	4:C:185:LEU:HD11	1.83	0.59
1:B:290:GLU:OE1	1:B:293:ARG:NH1	2.35	0.59
4:C:29:PHE:HD2	4:C:32:TYR:HB2	1.68	0.59
1:B:20:GLU:OE2	1:B:277:THR:OG1	2.21	0.59
2:A:178:LYS:HA	2:A:205:GLY:HA2	1.85	0.58
2:A:3:PHE:HD1	2:A:4:PRO:HD2	1.69	0.58
1:B:238:ASN:ND2	5:D:1:NAG:O5	2.36	0.57
2:A:108:ARG:NH2	2:A:270:TYR:OH	2.37	0.57
1:B:123:LEU:HD12	1:B:153:LYS:HD3	1.87	0.57
2:A:231:ASN:OD1	2:A:354:LYS:CG	2.32	0.57
3:H:159:UNK:N	3:H:199:UNK:O	2.39	0.56
4:C:163:VAL:HG11	4:C:206:ARG:HB2	1.87	0.56
4:C:109:TRP:HH2	4:C:236:PHE:CE2	2.23	0.55
4:C:34:MET:CE	4:C:98:ARG:HD2	2.36	0.55
4:C:33:TRP:HE3	4:C:53:PRO:HD2	1.72	0.55
4:C:140:GLN:NE2	4:C:226:CYS:SG	2.78	0.55
4:C:144:SER:HA	4:C:241:LYS:HD2	1.88	0.54
4:C:52:ASN:O	4:C:56:SER:HB2	2.07	0.54
4:C:58:ILE:HD12	4:C:71:SER:HA	1.90	0.54
6:A:901:NAG:H83	6:A:901:NAG:H3	1.89	0.54
4:C:169:SER:HB2	4:C:206:ARG:HD2	1.89	0.54
2:A:72:GLU:HG2	2:A:73:ARG:H	1.73	0.53
3:H:140:UNK:N	3:H:188:UNK:O	2.41	0.53
4:C:67:LYS:HG2	4:C:85:LYS:HE2	1.91	0.53
1:B:75:PHE:HE2	1:B:284:GLY:HA3	1.74	0.53
2:A:47:SER:O	5:F:1:NAG:O6	2.27	0.53
4:C:51:ILE:HG23	4:C:58:ILE:HG12	1.90	0.53
4:C:20:LEU:HD21	4:C:113:THR:HG21	1.91	0.53
3:L:138:UNK:O	3:L:177:UNK:N	2.42	0.52
3:H:157:UNK:O	3:H:201:UNK:N	2.42	0.52
4:C:45:LEU:HD22	4:C:109:TRP:HZ3	1.75	0.52
3:L:9:UNK:O	3:L:103:UNK:N	2.42	0.52
2:A:164:GLU:O	2:A:168:ARG:HG2	2.10	0.51
2:A:262:ARG:HG2	4:C:191:LYS:NZ	2.25	0.51
4:C:111:GLN:O	4:C:111:GLN:NE2	2.42	0.51
1:B:256:MET:HA	1:B:256:MET:HE3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:173:TRP:CE3	4:C:226:CYS:SG	3.00	0.51
5:D:1:NAG:H62	5:D:2:NAG:H62	1.93	0.51
4:C:66:ASP:OD1	4:C:66:ASP:N	2.44	0.51
3:L:151:UNK:O	3:L:195:UNK:N	2.44	0.50
1:B:106:GLY:O	1:B:348:ARG:NH2	2.44	0.50
1:B:255:LEU:HD22	1:B:337:LEU:HD21	1.94	0.50
1:B:374:ASP:OD1	1:B:374:ASP:N	2.42	0.50
2:A:17:GLN:O	2:A:17:GLN:HG2	2.12	0.49
4:C:58:ILE:HG21	4:C:70:ILE:HB	1.92	0.49
2:A:159:ILE:HA	2:A:162:THR:HG22	1.93	0.49
4:C:44:GLY:HA3	4:C:236:PHE:O	2.12	0.49
4:C:148:SER:H	4:C:151:GLN:NE2	2.09	0.49
4:C:155:ILE:HD12	4:C:211:LEU:HD23	1.93	0.49
4:C:136:ILE:CG1	4:C:228:GLN:HB2	2.43	0.48
1:B:19:GLN:HE21	1:B:259:TRP:HZ2	1.59	0.48
4:C:241:LYS:C	4:C:241:LYS:HD3	2.39	0.48
1:B:136:PHE:CE2	1:B:138:TYR:HB3	2.49	0.47
2:A:179:GLU:OE2	2:A:179:GLU:N	2.47	0.47
4:C:173:TRP:HB2	4:C:186:ILE:HG22	1.96	0.47
2:A:258:ARG:HH12	2:A:262:ARG:NH1	2.13	0.47
4:C:29:PHE:CD2	4:C:29:PHE:O	2.68	0.47
1:B:104:THR:H	1:B:113:GLN:NE2	2.12	0.47
2:A:289:LEU:HD21	2:A:322:ALA:HB2	1.97	0.47
4:C:176:GLN:O	4:C:222:ALA:HB1	2.15	0.46
1:B:300:ILE:HG13	1:B:300:ILE:O	2.16	0.46
4:C:20:LEU:HD11	4:C:94:TYR:HD2	1.79	0.46
2:A:180:ARG:O	2:A:208:TYR:HA	2.14	0.46
4:C:51:ILE:HG22	4:C:53:PRO:HD3	1.96	0.46
2:A:96:PRO:HA	2:A:106:GLN:OE1	2.14	0.46
3:H:150:UNK:HA	3:H:151:UNK:HA	1.66	0.46
4:C:35:SER:HB2	4:C:47:TRP:HE1	1.80	0.46
3:H:168:UNK:N	3:H:185:UNK:O	2.49	0.45
4:C:188:LEU:C	4:C:206:ARG:HH12	2.24	0.45
2:A:126:LYS:HE3	2:A:175:GLU:OE2	2.17	0.45
2:A:366:GLU:O	2:A:369:LYS:NZ	2.49	0.45
1:B:340:ASN:O	1:B:349:ARG:NH2	2.49	0.45
2:A:9:ILE:HG21	2:A:282:MET:CE	2.47	0.45
2:A:258:ARG:HA	2:A:258:ARG:HD2	1.69	0.45
4:C:39:GLN:HA	4:C:45:LEU:HA	1.97	0.45
4:C:177:LYS:HB2	4:C:180:GLN:HB2	1.97	0.45
2:A:354:LYS:HB2	2:A:354:LYS:HE2	1.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:174:TYR:CE1	4:C:182:PRO:HB2	2.52	0.45
2:A:44:VAL:HG12	2:A:55:ARG:HG3	1.99	0.45
2:A:301:ASN:OD1	2:A:302:ALA:N	2.50	0.45
2:A:159:ILE:HD12	2:A:194:ILE:HD11	1.99	0.45
4:C:34:MET:HE3	4:C:98:ARG:HD2	1.98	0.45
2:A:233:THR:HG22	2:A:234:GLY:H	1.82	0.45
4:C:53:PRO:HG3	4:C:74:ASN:HD22	1.82	0.44
1:B:38:SER:O	1:B:296:ARG:NH2	2.51	0.44
4:C:45:LEU:HD12	4:C:45:LEU:H	1.82	0.44
4:C:115:VAL:HG13	4:C:117:VAL:HG23	2.00	0.44
1:B:225:LYS:HE3	1:B:357:PHE:CE2	2.49	0.44
2:A:253:LYS:HD3	4:C:33:TRP:HZ2	1.83	0.44
1:B:314:ASN:HB2	2:A:54:TYR:CE2	2.53	0.44
2:A:20:GLU:N	2:A:20:GLU:OE1	2.50	0.44
1:B:256:MET:HE3	1:B:259:TRP:HB3	1.98	0.44
1:B:345:HIS:C	1:B:345:HIS:HD1	2.25	0.44
1:B:371:ASN:OD1	1:B:372:ASP:N	2.45	0.44
2:A:260:HIS:HB3	2:A:261:THR:H	1.59	0.44
1:B:138:TYR:HE1	1:B:163:ALA:HB1	1.83	0.43
4:C:100:ARG:HG3	4:C:107:ASP:CG	2.43	0.43
2:A:262:ARG:HA	2:A:262:ARG:HE	1.82	0.43
4:C:29:PHE:HE2	4:C:34:MET:HG2	1.83	0.43
4:C:135:ASN:OD1	4:C:233:PRO:HG3	2.19	0.43
5:I:1:NAG:O3	5:I:2:NAG:H83	2.19	0.43
1:B:206:VAL:HG13	1:B:211:HIS:CE1	2.53	0.43
2:A:315:GLN:N	2:A:315:GLN:OE1	2.51	0.43
1:B:345:HIS:C	1:B:345:HIS:ND1	2.76	0.43
4:C:169:SER:O	4:C:206:ARG:NH1	2.52	0.43
2:A:178:LYS:HD2	2:A:205:GLY:HA2	2.00	0.43
4:C:98:ARG:CZ	4:C:106:MET:O	2.66	0.43
3:H:18:UNK:O	3:H:83:UNK:HA	2.19	0.43
2:A:46:ILE:HG22	2:A:52:MET:HE3	2.02	0.42
3:L:139:UNK:HA	3:L:176:UNK:HA	2.00	0.42
4:C:98:ARG:O	4:C:100:ARG:NE	2.22	0.42
3:L:136:UNK:N	3:L:179:UNK:O	2.52	0.42
4:C:34:MET:SD	4:C:98:ARG:HA	2.59	0.42
4:C:187:PHE:C	4:C:189:ALA:H	2.27	0.42
1:B:8:GLN:N	1:B:8:GLN:OE1	2.51	0.42
4:C:181:PRO:HA	4:C:182:PRO:HD3	1.84	0.42
2:A:105:LEU:HD11	2:A:323:LEU:HB3	2.00	0.42
4:C:173:TRP:HB2	4:C:186:ILE:CG2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:51:ILE:HG12	4:C:58:ILE:HG23	2.02	0.42
4:C:186:ILE:HD11	4:C:201:SER:O	2.19	0.42
1:B:138:TYR:CE1	1:B:163:ALA:HB1	2.55	0.42
1:B:345:HIS:ND1	1:B:345:HIS:O	2.52	0.41
4:C:176:GLN:HA	4:C:182:PRO:HB3	2.01	0.41
1:B:123:LEU:HD13	1:B:123:LEU:HA	1.93	0.41
2:A:147:ALA:HB1	2:A:152:TRP:HB2	2.02	0.41
3:L:149:UNK:N	3:L:197:UNK:O	2.54	0.41
4:C:33:TRP:O	4:C:99:PRO:HD3	2.21	0.41
5:G:1:NAG:H4	5:G:2:NAG:H2	1.65	0.41
1:B:144:TYR:O	1:B:148:GLN:HG3	2.21	0.41
2:A:9:ILE:HG21	2:A:282:MET:HE1	2.02	0.41
3:H:100:UNK:HA	3:H:103:UNK:O	2.21	0.41
4:C:2:VAL:HB	4:C:26:GLY:HA3	2.01	0.41
1:B:90:CYS:SG	1:B:91:SER:N	2.94	0.41
2:A:199:ILE:O	2:A:202:GLU:HG2	2.21	0.41
2:A:254:THR:O	2:A:254:THR:OG1	2.38	0.40
2:A:336:GLN:HE22	2:A:345:ASN:HD22	1.67	0.40
4:C:177:LYS:HD3	4:C:222:ALA:HB2	2.03	0.40
1:B:175:ARG:O	1:B:179:GLU:HG3	2.21	0.40
1:B:349:ARG:HE	1:B:349:ARG:HB3	1.55	0.40
2:A:253:LYS:HD3	4:C:33:TRP:CZ2	2.57	0.40
1:B:262:LEU:HD12	1:B:267:TYR:CD2	2.42	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	375/884 (42%)	352 (94%)	23 (6%)	0	100	100
2	A	372/906 (41%)	346 (93%)	26 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	C	225/275 (82%)	196 (87%)	29 (13%)	0	100	100
All	All	972/2065 (47%)	894 (92%)	78 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	329/757 (44%)	329 (100%)	0	100	100
2	A	327/769 (42%)	327 (100%)	0	100	100
4	C	193/220 (88%)	193 (100%)	0	100	100
All	All	849/1746 (49%)	849 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	84	HIS
1	B	314	ASN
2	A	2	ASN
2	A	101	ASN
2	A	251	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 ⓘ

10 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	D	1	5	14,14,15	0.20	0	17,19,21	0.47	0
5	NAG	D	2	5	14,14,15	0.88	1 (7%)	17,19,21	1.04	1 (5%)
5	NAG	E	1	1,5	14,14,15	0.19	0	17,19,21	0.44	0
5	NAG	E	2	5	14,14,15	0.26	0	17,19,21	0.51	0
5	NAG	F	1	5,2	14,14,15	0.26	0	17,19,21	0.50	0
5	NAG	F	2	5	14,14,15	0.38	0	17,19,21	0.36	0
5	NAG	G	1	5,2	14,14,15	0.33	0	17,19,21	0.60	0
5	NAG	G	2	5	14,14,15	0.62	1 (7%)	17,19,21	0.58	0
5	NAG	I	1	5,2	14,14,15	0.28	0	17,19,21	0.41	0
5	NAG	I	2	5	14,14,15	0.41	0	17,19,21	0.39	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	D	1	5	-	0/6/23/26	0/1/1/1
5	NAG	D	2	5	-	2/6/23/26	0/1/1/1
5	NAG	E	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	2	5	-	3/6/23/26	0/1/1/1
5	NAG	F	1	5,2	-	2/6/23/26	0/1/1/1
5	NAG	F	2	5	-	4/6/23/26	0/1/1/1
5	NAG	G	1	5,2	-	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
5	NAG	I	1	5,2	-	1/6/23/26	0/1/1/1
5	NAG	I	2	5	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	2	NAG	O5-C1	2.88	1.48	1.43
5	G	2	NAG	C1-C2	2.14	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	2	NAG	C1-O5-C5	4.00	117.61	112.19

There are no chirality outliers.

All (18) torsion outliers are listed below:

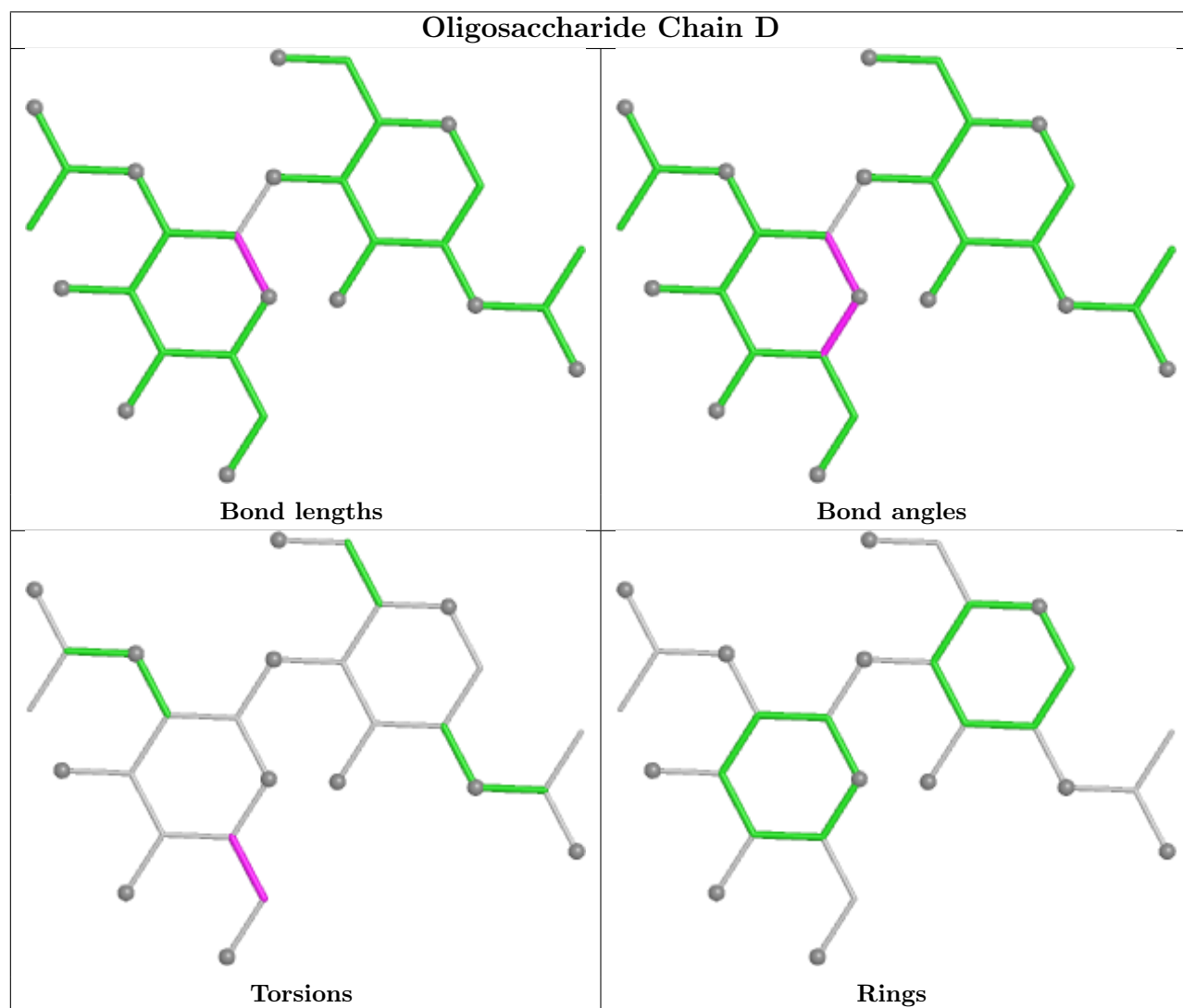
Mol	Chain	Res	Type	Atoms
5	G	1	NAG	O5-C5-C6-O6
5	F	2	NAG	C4-C5-C6-O6
5	D	2	NAG	O5-C5-C6-O6
5	F	2	NAG	O5-C5-C6-O6
5	G	1	NAG	C4-C5-C6-O6
5	F	2	NAG	C8-C7-N2-C2
5	F	2	NAG	O7-C7-N2-C2
5	I	2	NAG	C8-C7-N2-C2
5	I	2	NAG	O7-C7-N2-C2
5	E	2	NAG	O5-C5-C6-O6
5	I	1	NAG	O5-C5-C6-O6
5	F	1	NAG	C4-C5-C6-O6
5	D	2	NAG	C4-C5-C6-O6
5	G	2	NAG	O5-C5-C6-O6
5	E	2	NAG	C3-C2-N2-C7
5	G	2	NAG	C3-C2-N2-C7
5	E	2	NAG	C4-C5-C6-O6
5	F	1	NAG	O5-C5-C6-O6

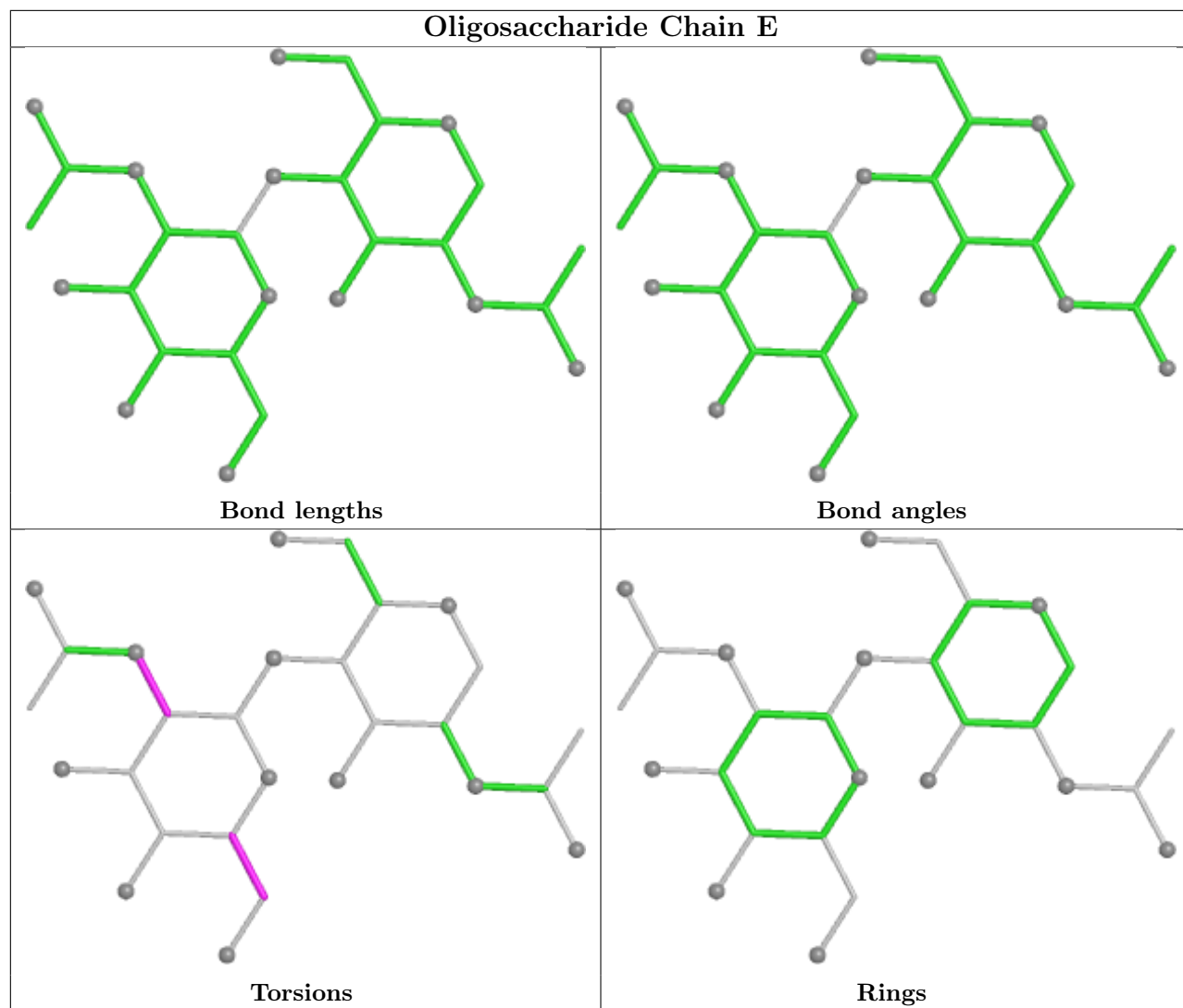
There are no ring outliers.

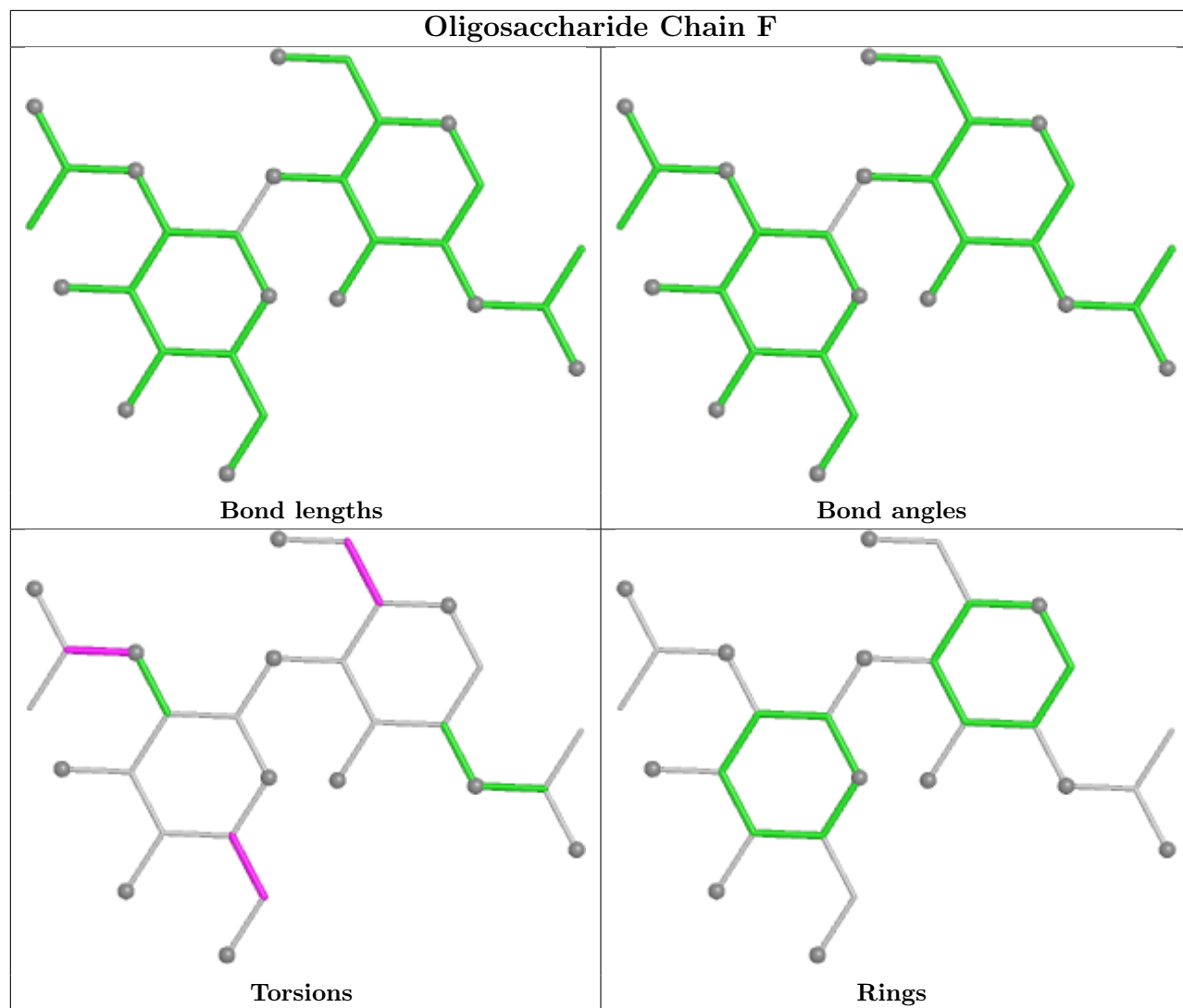
7 monomers are involved in 5 short contacts:

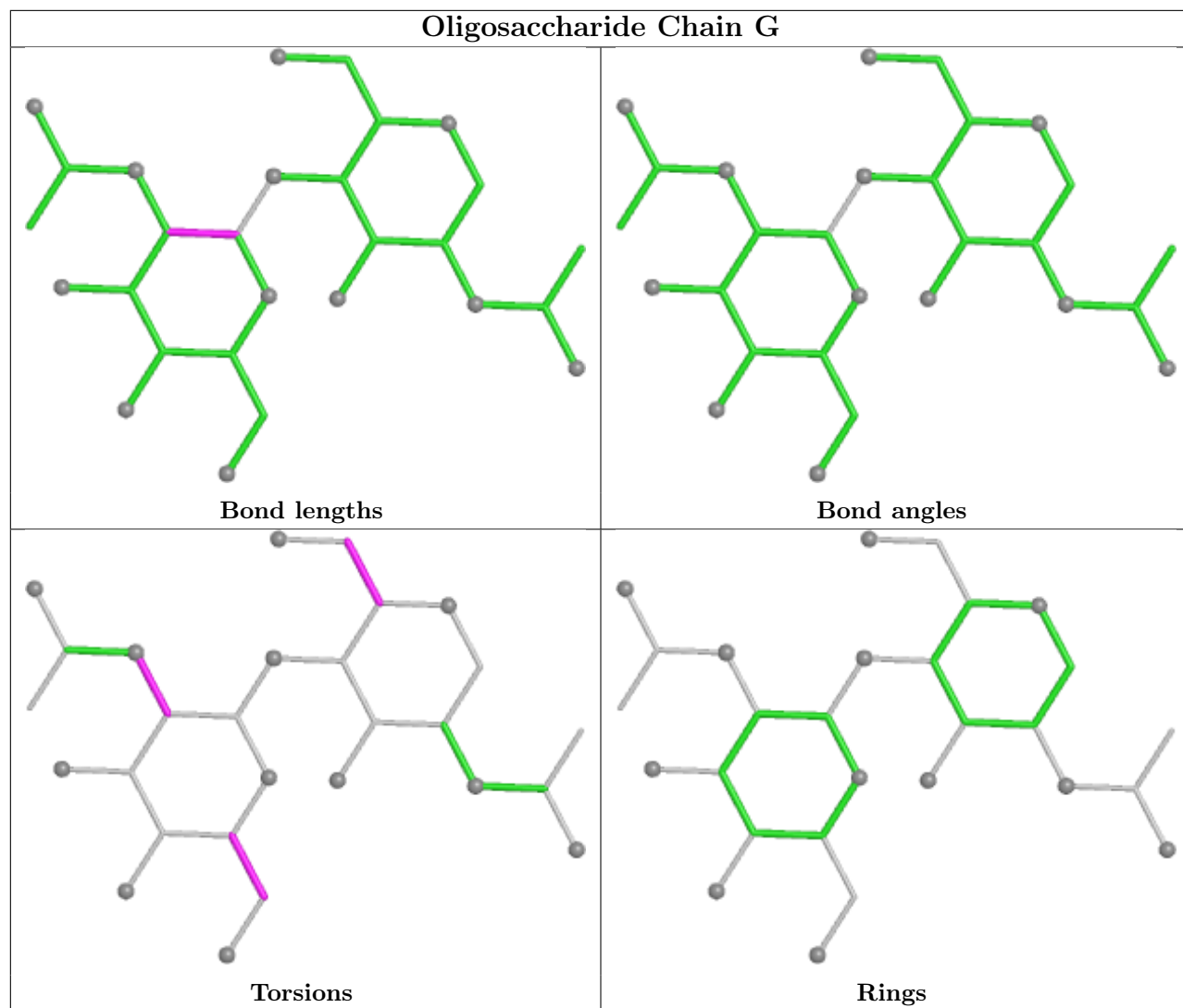
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	2	NAG	1	0
5	G	1	NAG	1	0
5	D	1	NAG	2	0
5	I	1	NAG	1	0
5	F	1	NAG	1	0
5	G	2	NAG	1	0
5	I	2	NAG	1	0

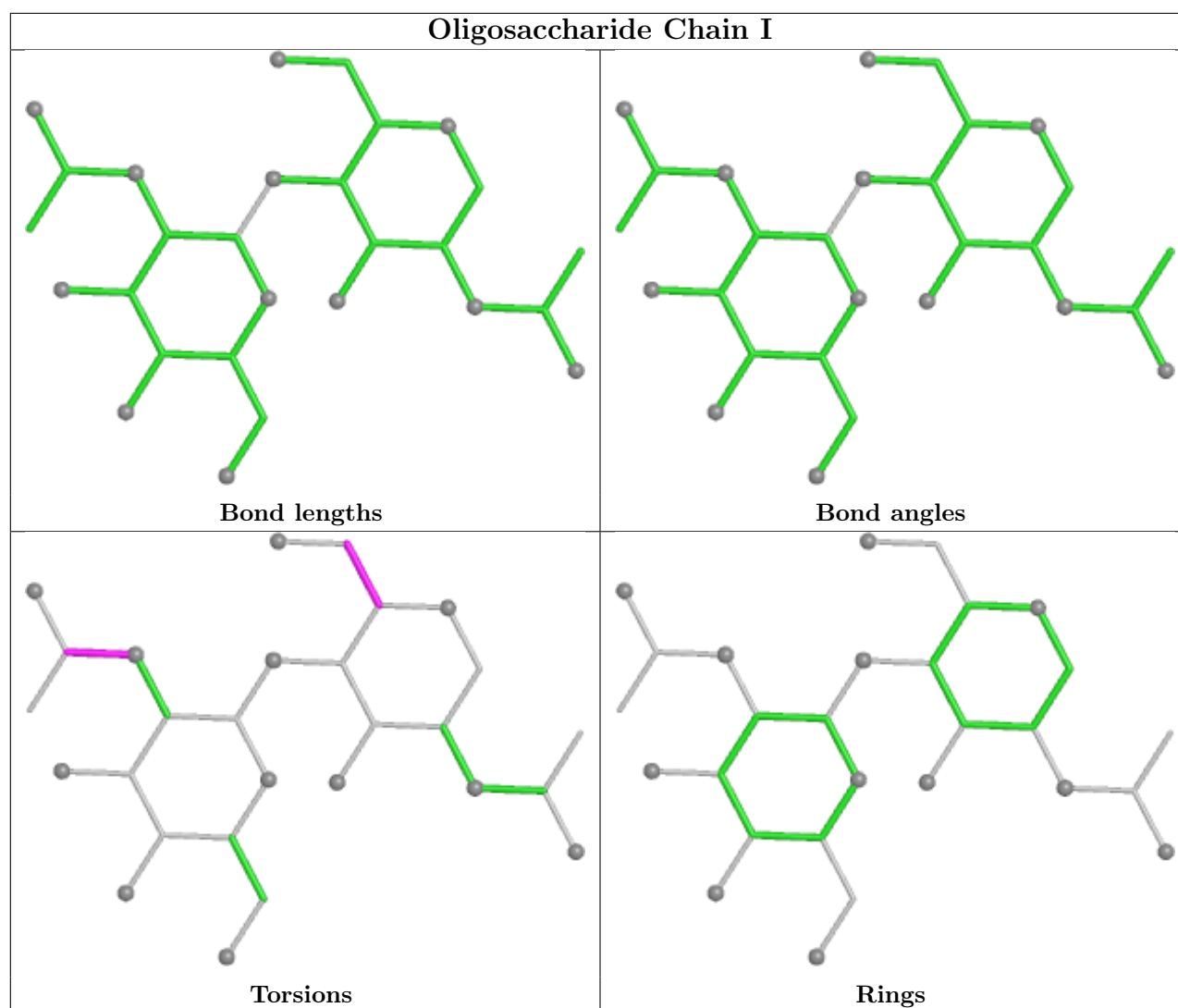
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
6	NAG	A	901	-	14,14,15	0.39	0	17,19,21	1.24	1 (5%)

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
6	NAG	A	901	-	-	5/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	901	NAG	C2-N2-C7	4.31	129.04	122.90

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	901	NAG	C8-C7-N2-C2
6	A	901	NAG	O7-C7-N2-C2
6	A	901	NAG	C4-C5-C6-O6
6	A	901	NAG	O5-C5-C6-O6
6	A	901	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	901	NAG	4	0

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.