



Full wwPDB EM Validation Report ⓘ

Mar 2, 2025 – 02:30 PM JST

PDB ID : 9JMZ
EMDB ID : EMD-61616
Title : Cryo-EM structure of a human-infecting bovine influenza H5N1 hemagglutinin complexed with avian receptor analog LSTa
Authors : Wang, H.C.; Han, P.; Song, H.; Gao, G.F.
Deposited on : 2024-09-22
Resolution : 2.91 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 : 4.02b-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) : 2.41.2

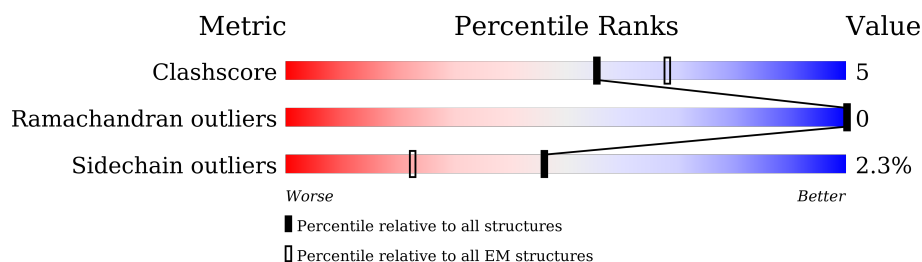
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.91 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	506	85% 11% .
1	B	506	82% 13% . .
1	C	506	84% 11% .
2	D	2	100%
2	E	2	50% 50%
3	F	2	50% 50%
4	G	3	100%
4	H	3	67% 33%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12001 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	487	Total	C	N	O	S	0	0
			3897	2449	679	746	23		
1	B	486	Total	C	N	O	S	0	0
			3892	2446	678	745	23		
1	C	486	Total	C	N	O	S	0	0
			3892	2446	678	745	23		

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



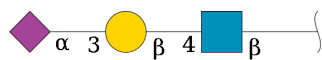
Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



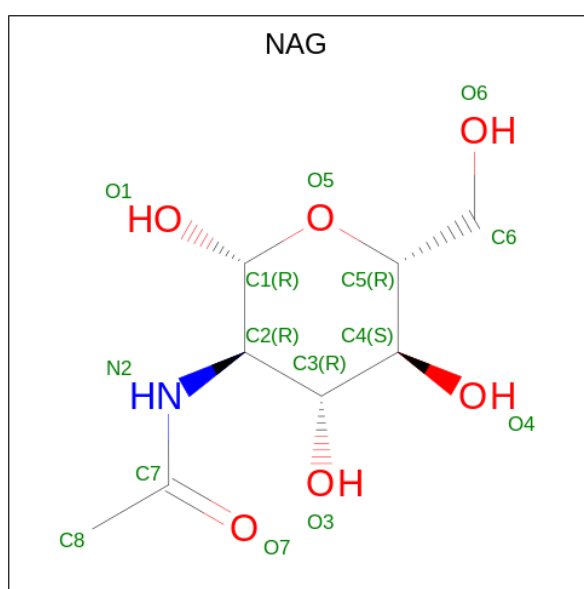
Mol	Chain	Residues	Atoms				AltConf	Trace
3	F	2	Total	C	N	O	0	0
			26	14	1	11		

- Molecule 4 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
4	G	3	Total	C	N	O	0	0
			46	25	2	19		
4	H	3	Total	C	N	O	0	0
			46	25	2	19		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



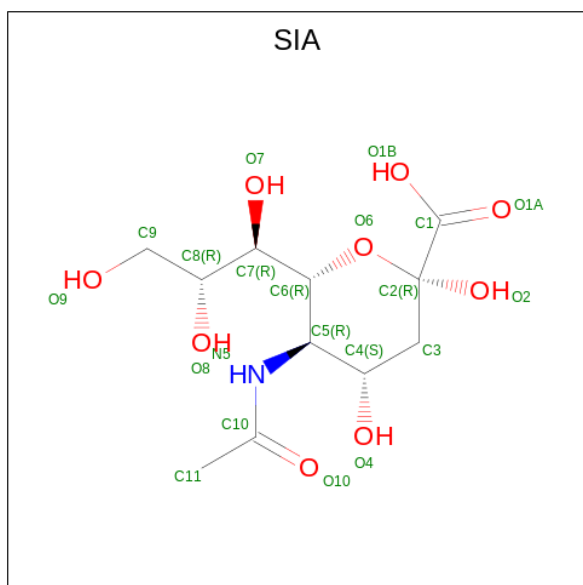
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	

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

- Molecule 6 is N-acetyl-alpha-neuraminic acid (three-letter code: SIA) (formula: $C_{11}H_{19}NO_9$).



Mol	Chain	Residues	Atoms				AltConf
6	F	1	Total	C	N	O	0
			20	11	1	8	

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

Chain D:  100%


MAG1
MAG2

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

Chain E:  50% 50%


MAG1
MAG2

- Molecule 3: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  50% 50%


MAG1
GAL2

- Molecule 4: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  100%


MAG1
GAL2
SIA3

- Molecule 4: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  67% 33%


MAG1
GAL2
SIA3

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	352780	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)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (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: SIA, GAL, 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	A	0.25	0/3986	0.52	2/5397 (0.0%)
1	B	0.25	0/3981	0.50	0/5390
1	C	0.25	0/3981	0.50	0/5390
All	All	0.25	0/11948	0.51	2/16177 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	453	LEU	CA-CB-CG	7.64	132.88	115.30
1	A	438	ASP	CB-CG-OD1	6.39	124.06	118.30

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	3897	0	3751	35	0
1	B	3892	0	3746	40	0
1	C	3892	0	3747	35	0
2	D	28	0	25	0	0
2	E	28	0	25	1	0
3	F	26	0	23	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	46	0	40	1	0
4	H	46	0	40	0	0
5	A	56	0	52	1	0
5	B	28	0	26	1	0
5	C	42	0	39	0	0
6	F	20	0	17	3	0
All	All	12001	0	11531	112	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 (112) 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:F:2:GAL:O3	6:F:3:SIA:C2	1.65	1.41
4:G:1:NAG:H62	4:G:2:GAL:C1	2.14	0.77
1:B:286:ASN:OD1	5:B:602:NAG:N2	2.18	0.77
1:B:450:LYS:HZ1	1:B:454:GLN:HB2	1.47	0.76
1:B:462:LEU:HD23	1:B:466:CYS:HB2	1.70	0.73
1:A:445:LYS:O	1:A:445:LYS:NZ	2.21	0.72
3:F:2:GAL:O3	6:F:3:SIA:O6	2.08	0.71
1:C:14:GLU:N	1:C:14:GLU:OE2	2.24	0.71
1:B:48:LYS:HD3	1:B:49:PRO:HD2	1.73	0.70
1:C:450:LYS:O	1:C:450:LYS:NZ	2.22	0.70
1:C:452:ARG:HH22	1:C:456:ARG:H	1.43	0.66
1:A:463:GLY:HA3	1:B:453:LEU:HD11	1.79	0.65
1:C:401:ASN:OD1	1:C:404:ARG:NH2	2.32	0.63
1:A:66:MET:HB3	1:A:87:ASN:HD22	1.65	0.62
1:C:21:GLU:N	1:C:21:GLU:OE2	2.33	0.62
1:B:450:LYS:O	1:B:450:LYS:NZ	2.30	0.62
1:C:61:LEU:O	1:C:146:ASN:ND2	2.34	0.61
1:B:270:GLU:OE2	1:B:270:GLU:N	2.23	0.61
1:B:280:THR:HG22	1:B:298:THR:HG22	1.82	0.61
1:B:15:GLN:HB3	1:B:23:ASN:HB2	1.82	0.61
1:B:64:ASN:HB3	1:B:67:CYS:HB3	1.82	0.61
1:A:280:THR:HG22	1:A:282:VAL:H	1.66	0.60
1:B:258:LYS:NZ	1:B:260:GLY:O	2.35	0.59
1:A:307:LYS:HG3	1:A:418:LEU:HD11	1.84	0.59
1:B:48:LYS:HE2	1:B:271:TYR:CZ	2.36	0.59
1:B:450:LYS:NZ	1:B:454:GLN:HB2	2.18	0.58
1:B:42:CYS:HA	1:B:274:CYS:HB3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:TRP:HB2	1:B:370:THR:HG22	1.86	0.57
1:B:61:LEU:O	1:B:146:ASN:ND2	2.37	0.57
1:A:18:THR:OG1	1:A:21:GLU:OE1	2.23	0.57
1:B:455:LEU:HD11	1:B:459:ALA:HB3	1.87	0.56
1:C:368:GLU:N	1:C:368:GLU:OE1	2.33	0.56
1:C:270:GLU:N	1:C:270:GLU:OE1	2.38	0.56
1:C:41:LEU:HG	1:C:269:VAL:HG23	1.87	0.56
1:C:234:LYS:HB2	1:C:237:ASP:HB2	1.87	0.56
1:B:493:GLU:O	1:B:497:LEU:HG	2.06	0.55
1:C:68:ASP:OD2	1:C:145:ARG:NH1	2.40	0.54
1:B:234:LYS:HB2	1:B:237:ASP:HB2	1.88	0.54
1:C:280:THR:HG22	1:C:298:THR:HG22	1.90	0.54
1:B:311:LEU:HG	1:B:429:VAL:HG21	1.91	0.51
1:B:9:ALA:HB2	1:B:342:GLY:HA3	1.93	0.51
1:B:473:CYS:SG	1:B:478:MET:HG2	2.50	0.51
1:C:452:ARG:HH22	1:C:456:ARG:N	2.09	0.51
1:C:452:ARG:CZ	1:C:453:LEU:H	2.24	0.51
1:A:398:GLU:OE1	1:A:398:GLU:N	2.44	0.51
1:A:452:ARG:O	1:A:453:LEU:HD23	2.12	0.50
1:B:447:LEU:O	1:B:451:VAL:HG12	2.12	0.50
1:A:311:LEU:HD22	1:A:429:VAL:HG21	1.94	0.49
1:A:1:ASP:N	1:A:356:SER:O	2.45	0.49
1:C:3:ILE:HD11	1:C:353:TYR:HB3	1.93	0.49
1:B:410:ASN:O	1:B:413:MET:HB3	2.13	0.49
1:A:457:ASP:OD1	1:A:457:ASP:N	2.45	0.48
1:B:346:MET:HB2	1:B:363:TYR:CD2	2.47	0.48
3:F:2:GAL:C3	6:F:3:SIA:C2	2.82	0.48
1:A:61:LEU:O	1:A:146:ASN:ND2	2.47	0.48
1:B:338:PHE:HE2	1:B:445:LYS:HD2	1.78	0.48
1:C:452:ARG:NH1	1:C:453:LEU:H	2.12	0.48
1:A:496:ARG:O	1:A:496:ARG:NE	2.47	0.48
1:B:22:LYS:HB2	2:E:1:NAG:H82	1.96	0.48
1:A:446:ASN:HA	1:A:449:ASP:OD1	2.15	0.47
1:A:42:CYS:HB3	1:A:274:CYS:HB2	1.38	0.47
1:A:452:ARG:HG2	1:A:453:LEU:H	1.79	0.47
1:A:471:HIS:CE1	1:A:473:CYS:HB2	2.50	0.47
1:C:20:MET:HB2	1:C:21:GLU:OE2	2.15	0.46
1:C:126:GLU:OE2	1:C:128:SER:OG	2.27	0.46
1:C:304:LYS:HD2	1:C:421:TRP:CE2	2.50	0.46
1:C:216:ARG:O	1:C:223:ARG:NH1	2.49	0.46
1:C:39:GLY:HA2	1:C:282:VAL:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:SER:O	1:A:108:ILE:HG12	2.15	0.45
1:C:34:GLU:OE2	1:C:36:THR:N	2.41	0.45
1:A:339:ILE:HD12	1:A:340:GLU:N	2.31	0.45
1:B:397:ARG:HA	1:B:397:ARG:HD3	1.81	0.45
1:C:455:LEU:HD21	1:C:459:ALA:HB3	1.99	0.45
1:C:459:ALA:HB2	1:C:469:PHE:HA	1.99	0.45
1:A:165:ASN:OD1	5:A:601:NAG:N2	2.50	0.44
1:B:16:VAL:HG21	1:B:314:ALA:HB2	1.99	0.44
1:B:449:ASP:OD2	1:B:449:ASP:N	2.50	0.44
1:C:262:SER:OG	1:C:263:THR:N	2.50	0.44
1:C:493:GLU:O	1:C:497:LEU:HD22	2.17	0.44
1:C:175:LEU:O	1:C:250:PRO:HB3	2.18	0.44
1:A:450:LYS:HE2	1:A:450:LYS:HA	1.99	0.43
1:B:7:TYR:HB2	1:B:317:LEU:HD13	1.99	0.43
1:B:401:ASN:OD1	1:B:404:ARG:NH2	2.51	0.43
1:A:336:ALA:O	1:A:465:GLY:HA3	2.18	0.43
1:A:175:LEU:O	1:A:250:PRO:HB3	2.18	0.43
1:B:462:LEU:HD22	1:B:462:LEU:H	1.83	0.43
1:B:42:CYS:HB2	1:B:276:THR:HG22	2.00	0.43
1:A:224:GLY:O	1:A:225:ARG:NH1	2.39	0.43
1:A:478:MET:O	1:A:481:VAL:HG12	2.19	0.43
1:B:70:PHE:CG	1:B:71:ILE:N	2.87	0.43
1:B:357:ASN:ND2	1:B:475:ASN:OD1	2.45	0.43
1:B:70:PHE:CD1	1:B:72:ARG:HG3	2.54	0.42
1:A:335:ILE:HG12	1:A:464:ASN:HD21	1.84	0.42
1:C:53:LYS:HG3	1:C:70:PHE:CZ	2.55	0.42
1:A:419:ASP:OD1	1:B:389:ASN:ND2	2.53	0.42
1:A:462:LEU:HD22	1:A:462:LEU:H	1.84	0.42
1:C:42:CYS:HB3	1:C:274:CYS:HB2	1.61	0.42
1:A:166:ASN:ND2	1:A:234:LYS:O	2.46	0.42
1:A:340:GLU:H	1:A:340:GLU:HG3	1.68	0.41
1:C:129:LEU:HD12	1:C:151:ILE:HD11	2.02	0.41
1:C:234:LYS:HA	1:C:234:LYS:HD3	1.82	0.41
1:C:435:ARG:HA	1:C:438:ASP:OD1	2.20	0.41
1:A:181:SER:O	1:A:216:ARG:NH2	2.49	0.41
1:C:452:ARG:O	1:C:453:LEU:HG	2.20	0.41
1:C:498:LYS:O	1:C:498:LYS:NZ	2.35	0.41
1:A:335:ILE:HG12	1:A:464:ASN:ND2	2.36	0.41
1:B:355:HIS:HB2	1:B:478:MET:CE	2.51	0.41
1:A:108:ILE:HD13	1:A:108:ILE:HA	1.91	0.41
1:A:437:LEU:HD23	1:A:437:LEU:HA	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:449:ASP:OD1	1:C:449:ASP:N	2.54	0.41
1:A:338:PHE:HZ	1:A:448:TYR:CZ	2.39	0.40
1:B:172:LEU:HD12	1:B:172:LEU:HA	1.93	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	483/506 (96%)	463 (96%)	20 (4%)	0	100	100
1	B	482/506 (95%)	461 (96%)	21 (4%)	0	100	100
1	C	482/506 (95%)	470 (98%)	12 (2%)	0	100	100
All	All	1447/1518 (95%)	1394 (96%)	53 (4%)	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	428/444 (96%)	420 (98%)	8 (2%)	52	79
1	B	428/444 (96%)	415 (97%)	13 (3%)	36	69
1	C	428/444 (96%)	419 (98%)	9 (2%)	48	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1284/1332 (96%)	1254 (98%)	30 (2%)	46 75

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	286	ASN
1	A	338	PHE
1	A	353	TYR
1	A	441	ASP
1	A	453	LEU
1	A	469	PHE
1	A	474	ASP
1	A	477	CYS
1	B	48	LYS
1	B	66	MET
1	B	70	PHE
1	B	165	ASN
1	B	236	ASP
1	B	286	ASN
1	B	346	MET
1	B	441	ASP
1	B	443	ASN
1	B	447	LEU
1	B	469	PHE
1	B	477	CYS
1	B	491	TYR
1	C	72	ARG
1	C	171	ASP
1	C	274	CYS
1	C	308	SER
1	C	338	PHE
1	C	355	HIS
1	C	445	LYS
1	C	469	PHE
1	C	491	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	218	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 ⓘ

12 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$
2	NAG	D	1	2,1	14,14,15	0.48	0	17,19,21	0.47	0
2	NAG	D	2	2	14,14,15	0.33	0	17,19,21	0.36	0
2	NAG	E	1	2,1	14,14,15	0.54	0	17,19,21	0.88	1 (5%)
2	NAG	E	2	2	14,14,15	0.28	0	17,19,21	0.45	0
3	NAG	F	1	3	15,15,15	0.09	0	21,21,21	0.13	0
3	GAL	F	2	3	11,11,12	0.69	0	15,15,17	0.93	0
4	NAG	G	1	4	15,15,15	0.10	0	21,21,21	0.14	0
4	GAL	G	2	4	11,11,12	0.67	0	15,15,17	0.93	0
4	SIA	G	3	4	20,20,21	1.94	2 (10%)	24,28,31	1.62	4 (16%)
4	NAG	H	1	4	15,15,15	0.09	0	21,21,21	0.14	0
4	GAL	H	2	4	11,11,12	0.68	0	15,15,17	0.93	0
4	SIA	H	3	4	20,20,21	1.94	2 (10%)	24,28,31	1.64	4 (16%)

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
2	NAG	D	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
3	NAG	F	1	3	-	2/6/26/26	0/1/1/1
3	GAL	F	2	3	-	1/2/19/22	0/1/1/1
4	NAG	G	1	4	-	2/6/26/26	0/1/1/1
4	GAL	G	2	4	-	1/2/19/22	0/1/1/1
4	SIA	G	3	4	-	0/18/34/38	0/1/1/1
4	NAG	H	1	4	-	2/6/26/26	0/1/1/1
4	GAL	H	2	4	-	1/2/19/22	0/1/1/1
4	SIA	H	3	4	-	0/18/34/38	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	3	SIA	C2-C1	7.39	1.59	1.52
4	H	3	SIA	C2-C1	7.34	1.58	1.52
4	H	3	SIA	O6-C2	2.79	1.47	1.43
4	G	3	SIA	O6-C2	2.75	1.47	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	3	SIA	O1A-C1-C2	-4.31	112.39	122.57
4	G	3	SIA	O1A-C1-C2	-4.27	112.48	122.57
4	H	3	SIA	C6-O6-C2	3.62	119.08	111.34
4	G	3	SIA	C6-O6-C2	3.45	118.73	111.34
4	G	3	SIA	O1B-C1-O1A	2.44	129.63	124.09
4	H	3	SIA	O1B-C1-O1A	2.44	129.62	124.09
4	G	3	SIA	O6-C2-C3	-2.39	107.17	110.46
4	H	3	SIA	O6-C2-C3	-2.33	107.25	110.46
2	E	1	NAG	C3-C4-C5	2.06	113.91	110.24

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	2	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6

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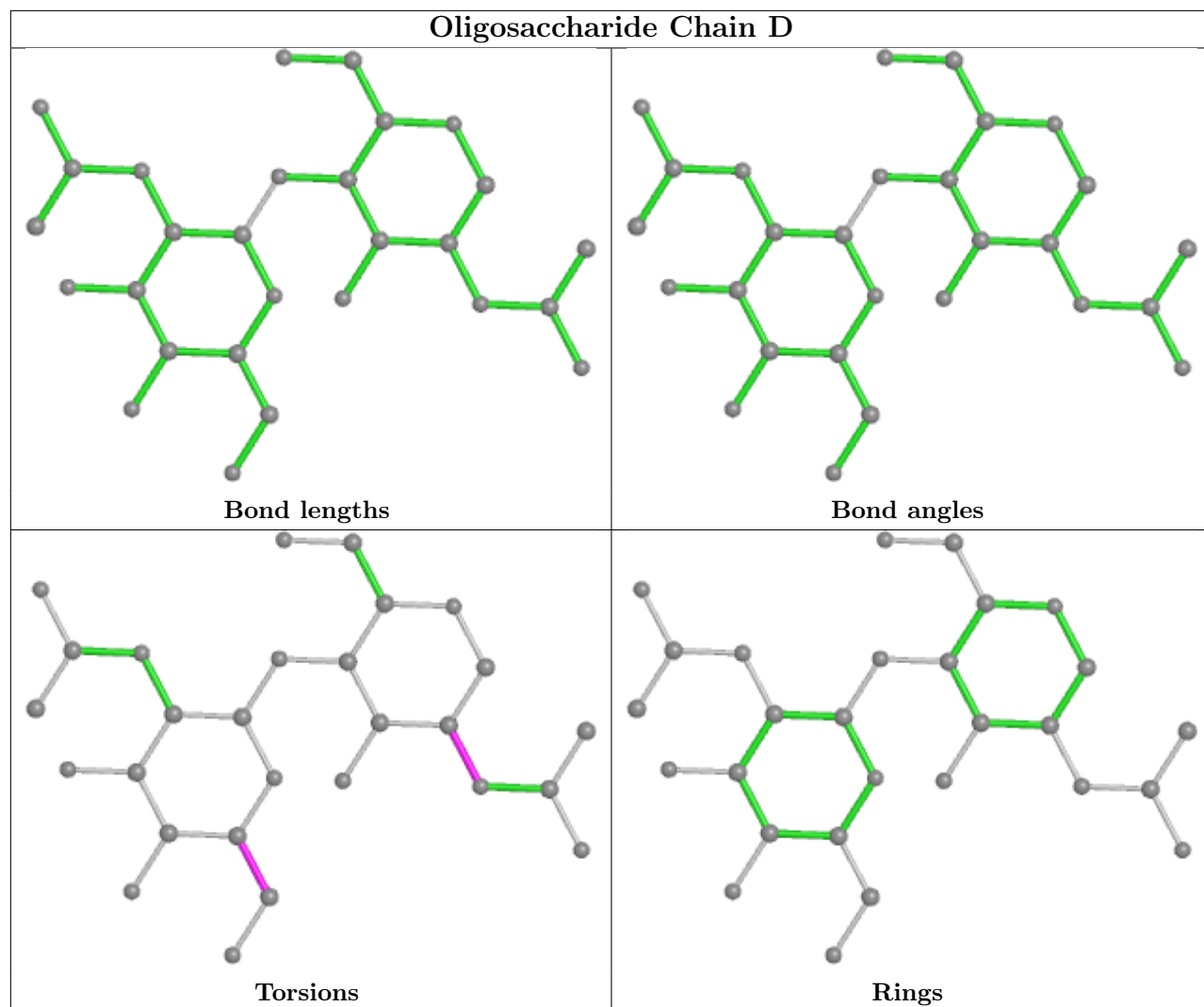
Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C4-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
4	H	1	NAG	C4-C5-C6-O6
2	D	1	NAG	C1-C2-N2-C7
3	F	1	NAG	O5-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6
3	F	2	GAL	C4-C5-C6-O6
4	H	2	GAL	C4-C5-C6-O6
4	G	2	GAL	C4-C5-C6-O6
2	D	1	NAG	C3-C2-N2-C7
2	E	1	NAG	C1-C2-N2-C7

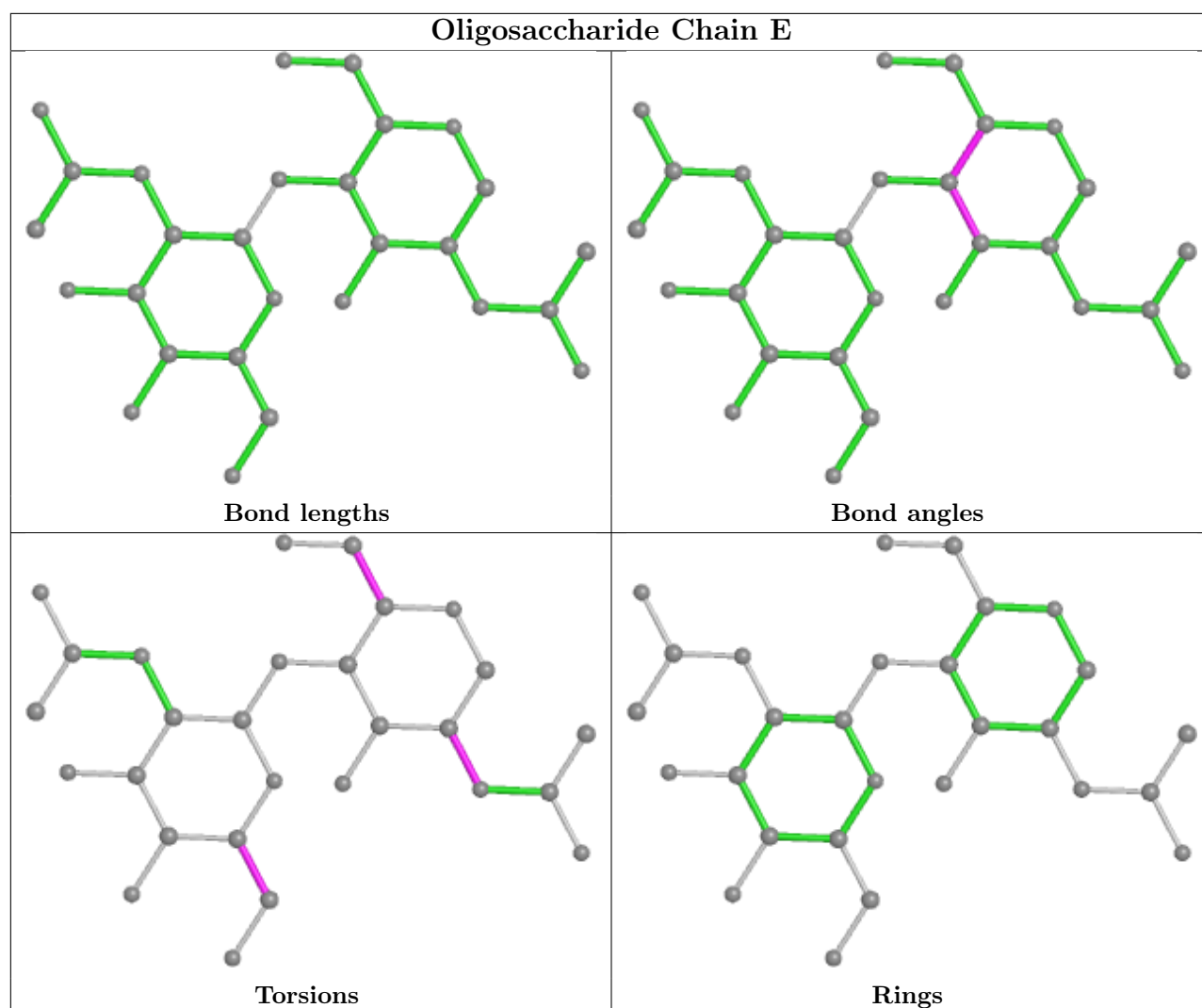
There are no ring outliers.

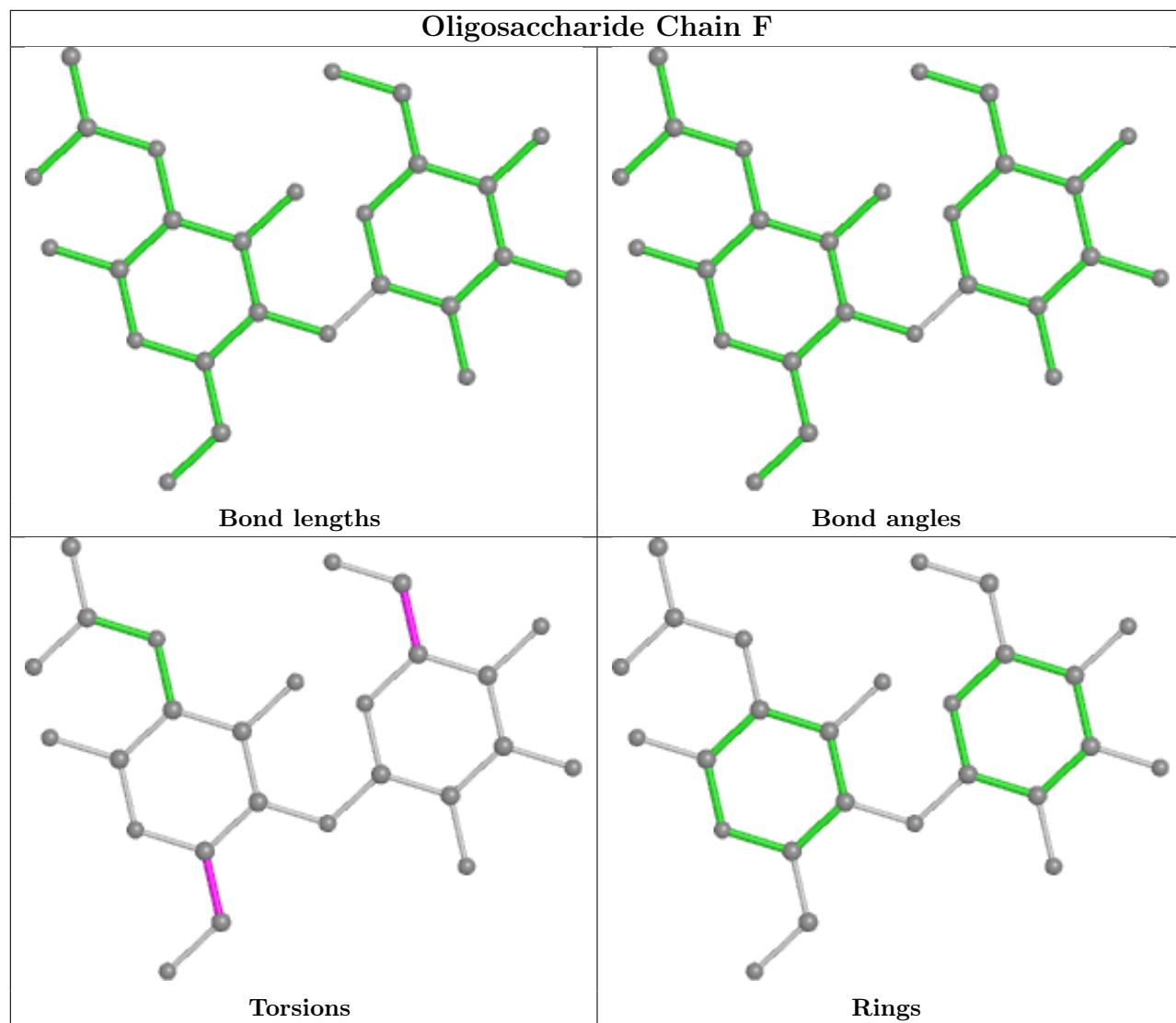
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	2	GAL	1	0
2	E	1	NAG	1	0
4	G	1	NAG	1	0
3	F	2	GAL	3	0

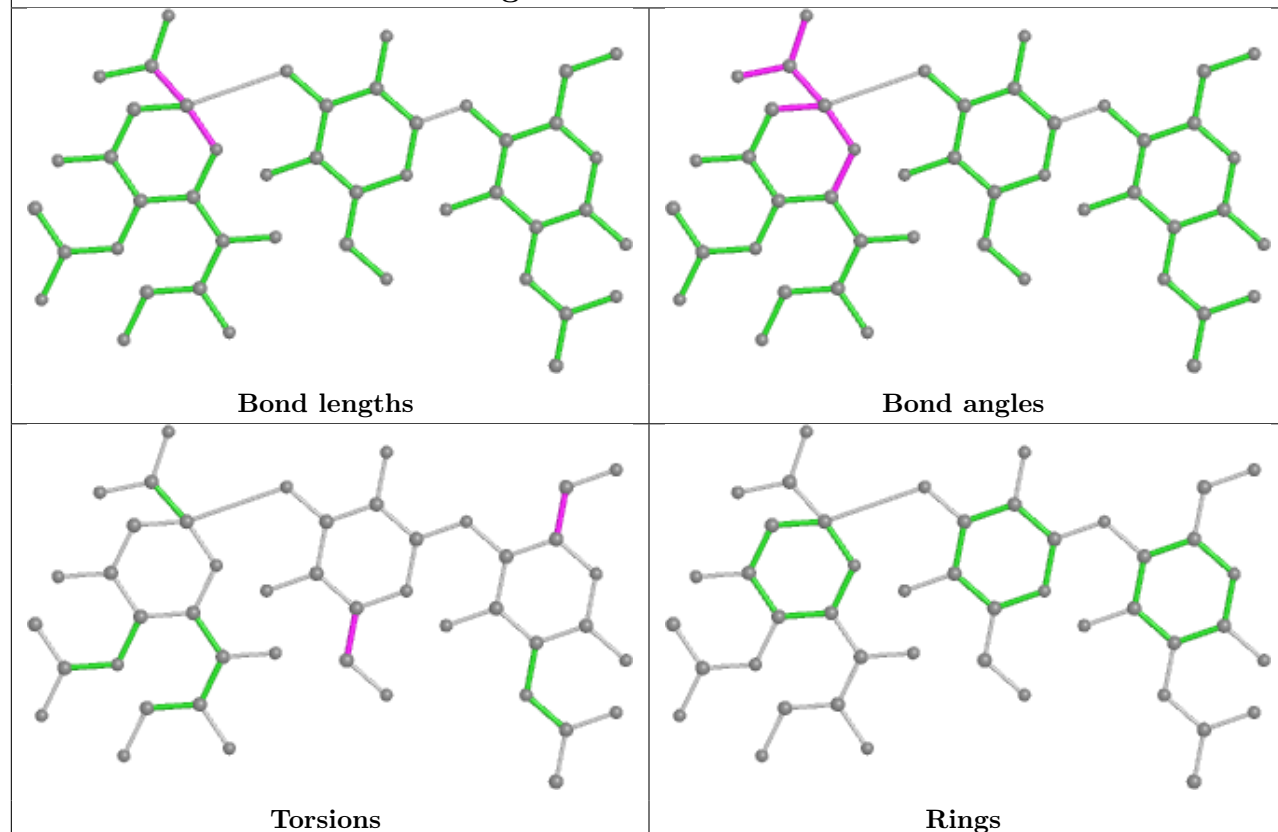
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



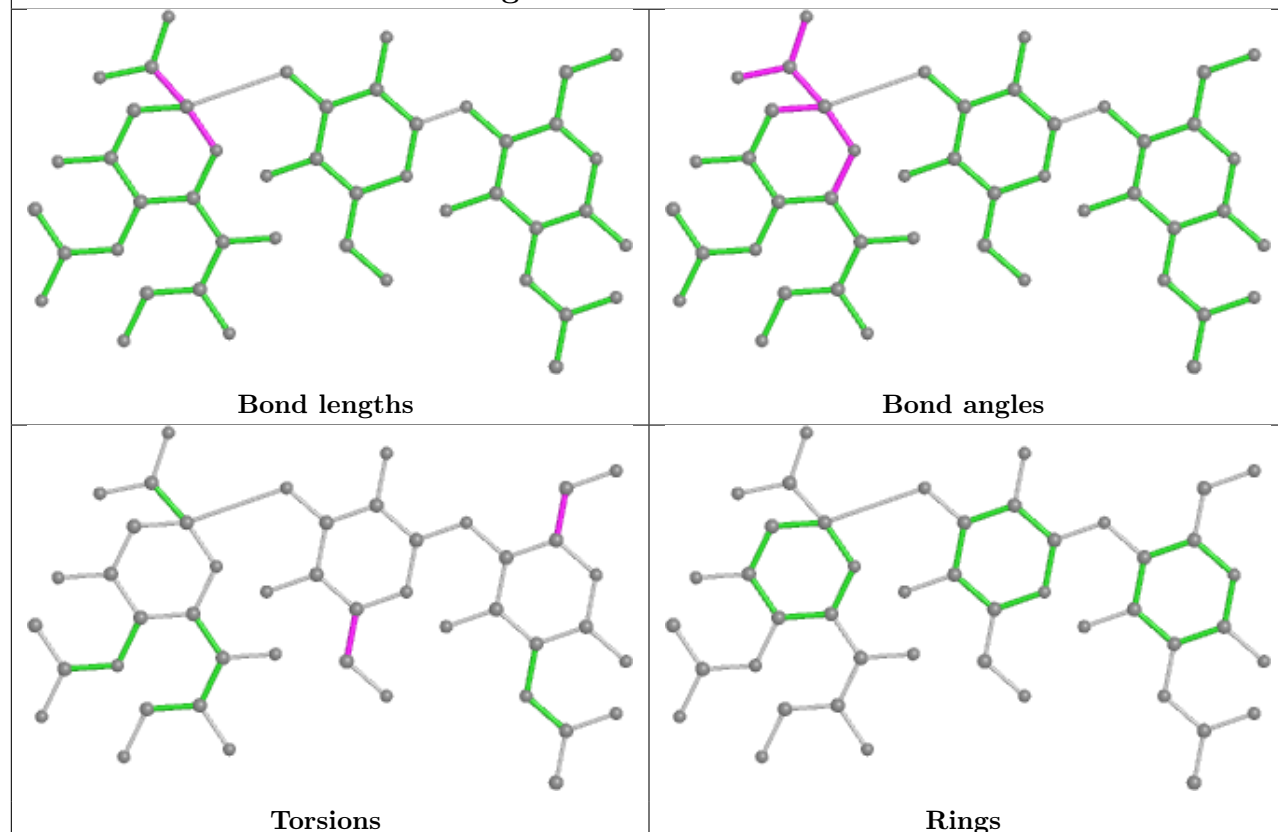




Oligosaccharide Chain G



Oligosaccharide Chain H



5.6 Ligand geometry

10 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
5	NAG	B	601	1	14,14,15	0.30	0	17,19,21	0.46	0
6	SIA	F	3	-	20,20,21	1.94	2 (10%)	24,28,31	1.63	4 (16%)
5	NAG	B	602	1	14,14,15	0.47	0	17,19,21	0.75	1 (5%)
5	NAG	A	604	1	14,14,15	0.27	0	17,19,21	0.51	0
5	NAG	A	603	1	14,14,15	0.57	0	17,19,21	0.86	1 (5%)
5	NAG	A	601	1	14,14,15	0.72	1 (7%)	17,19,21	0.72	1 (5%)
5	NAG	C	603	1	14,14,15	0.31	0	17,19,21	0.52	0
5	NAG	C	601	1	14,14,15	0.27	0	17,19,21	0.55	0
5	NAG	A	602	1	14,14,15	0.28	0	17,19,21	0.56	0
5	NAG	C	602	1	14,14,15	0.28	0	17,19,21	0.58	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	B	601	1	-	2/6/23/26	0/1/1/1
6	SIA	F	3	-	-	1/18/34/38	0/1/1/1
5	NAG	B	602	1	-	2/6/23/26	0/1/1/1
5	NAG	A	604	1	-	0/6/23/26	0/1/1/1
5	NAG	A	603	1	-	0/6/23/26	0/1/1/1
5	NAG	A	601	1	-	2/6/23/26	0/1/1/1
5	NAG	C	603	1	-	2/6/23/26	0/1/1/1
5	NAG	C	601	1	-	2/6/23/26	0/1/1/1
5	NAG	A	602	1	-	2/6/23/26	0/1/1/1
5	NAG	C	602	1	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	3	SIA	C2-C1	7.38	1.59	1.52
6	F	3	SIA	O6-C2	2.72	1.47	1.43
5	A	601	NAG	O5-C1	2.25	1.47	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	3	SIA	O1A-C1-C2	-4.27	112.50	122.57
6	F	3	SIA	C6-O6-C2	3.52	118.87	111.34
5	A	603	NAG	C1-O5-C5	2.73	115.90	112.19
5	B	602	NAG	C1-O5-C5	2.51	115.59	112.19
5	A	601	NAG	C1-O5-C5	2.45	115.51	112.19
6	F	3	SIA	O1B-C1-O1A	2.41	129.57	124.09
6	F	3	SIA	O6-C2-C3	-2.37	107.20	110.46

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	601	NAG	C4-C5-C6-O6
5	B	601	NAG	C4-C5-C6-O6
5	A	601	NAG	O5-C5-C6-O6
5	B	601	NAG	O5-C5-C6-O6
5	C	601	NAG	C4-C5-C6-O6
5	A	602	NAG	C4-C5-C6-O6
5	B	602	NAG	C4-C5-C6-O6
5	C	601	NAG	O5-C5-C6-O6
5	B	602	NAG	O5-C5-C6-O6
5	A	602	NAG	O5-C5-C6-O6
6	F	3	SIA	C6-C7-C8-O8
5	C	603	NAG	C3-C2-N2-C7
5	C	603	NAG	C1-C2-N2-C7

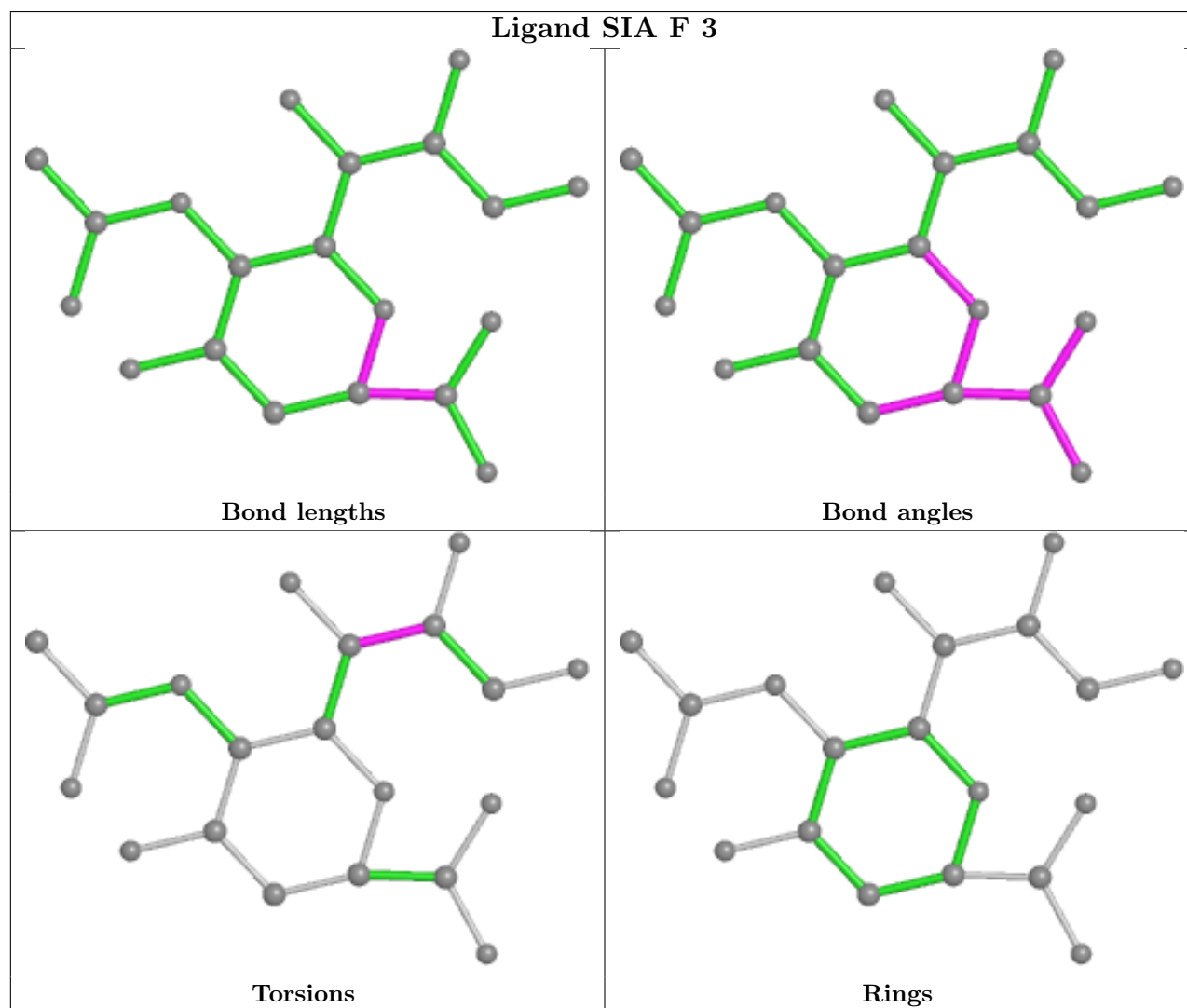
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	3	SIA	3	0
5	B	602	NAG	1	0
5	A	601	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 ⓘ

There are no chain breaks in this entry.