



Full wwPDB EM Validation Report ⓘ

Jul 8, 2025 – 03:15 PM JST

PDB ID : 8ZJ4 / pdb_00008zj4
EMDB ID : EMD-60137
Title : trypsinogen-EP-N619A
Authors : Song, Q.Y.; Ding, Z.Y.; Huang, H.J.
Deposited on : 2024-05-14
Resolution : 2.67 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 Phenix2.0rc1
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) : 2.44

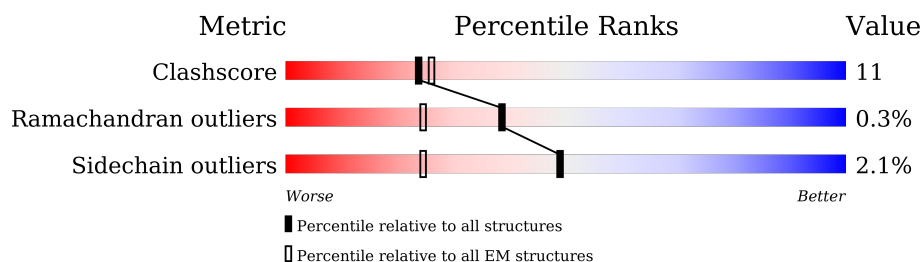
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.67 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.





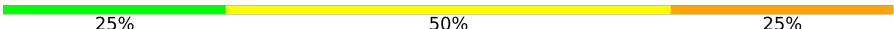

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	D	235	77% 22% .
2	C	232	73% 26% .
3	A	603	78% 21% .
4	B	3	33% 67%
4	J	3	33% 67%
5	E	3	33% 67%
5	G	3	100%
5	M	3	100%
6	F	2	50% 50%

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Mol	Chain	Length	Quality of chain
7	H	4	 75% 25%
8	I	3	 67% 33%
9	K	4	 25% 50% 25%
10	L	4	 25% 25% 50%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 8734 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 Enteropeptidase catalytic light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	235	Total	C	N	O	S	0	0
			1835	1161	319	340	15		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	825	ALA	HIS	engineered mutation	UNP P98073
D	876	ALA	ASP	engineered mutation	UNP P98073
D	971	ALA	SER	engineered mutation	UNP P98073

- Molecule 2 is a protein called Serine protease 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	232	Total	C	N	O	S	0	0
			1755	1095	304	344	12		

- Molecule 3 is a protein called Enteropeptidase non-catalytic heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	603	Total	C	N	O	S	0	0
			4690	2959	774	928	29		

There is a discrepancy between the modelled and reference sequences:

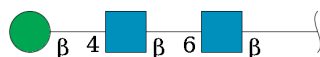
Chain	Residue	Modelled	Actual	Comment	Reference
A	619	ALA	ASN	engineered mutation	UNP P98073

- Molecule 4 is an oligosaccharide called 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
4	B	3	Total	C	N	O	0	0
			39	22	2	15		
4	J	3	Total	C	N	O	0	0
			39	22	2	15		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	3	Total	C	N	O	0	0
			39	22	2	15		
5	G	3	Total	C	N	O	0	0
			39	22	2	15		
5	M	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



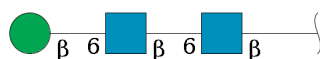
Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
7	H	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 8 is an oligosaccharide called beta-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



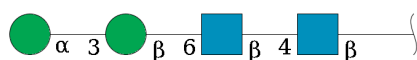
Mol	Chain	Residues	Atoms				AltConf	Trace
8	I	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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
9	K	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
10	L	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

Chain B:  33% 67%

NAG1
NAG2
BMA3

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

Chain J:  33% 67%

NAG1
NAG2
BMA3

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

Chain E:  33% 67%

NAG1
NAG2
BMA3

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

Chain G:  100%

NAG1
NAG2
BMA3

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

Chain M:  100%

NAG1
NAG2
BMA3

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  50% 50%

NAG1
NAG2
BMA3

- Molecule 7: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  75% 25%

NAG1
NAG2
BMA3
MAN4

- Molecule 8: beta-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  67% 33%



- Molecule 9: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  25% 50% 25%



- Molecule 10: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  25% 25% 50%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	410162	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 ($e^-/\text{\AA}^2$)	46	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k 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: MAN, BMA, 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	D	0.11	0/1883	0.33	2/2563 (0.1%)
2	C	0.07	0/1792	0.25	0/2431
3	A	0.15	0/4810	0.28	0/6554
All	All	0.12	0/8485	0.29	2/11548 (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	D	909	ASN	CA-CB-CG	5.64	118.24	112.60
1	D	909	ASN	CB-CA-C	5.21	119.41	110.81

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	D	1835	0	1764	32	0
2	C	1755	0	1695	47	0
3	A	4690	0	4413	105	0
4	B	39	0	34	2	0
4	J	39	0	34	2	0
5	E	39	0	34	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	39	0	34	0	0
5	M	39	0	34	0	0
6	F	28	0	25	1	0
7	H	50	0	43	0	0
8	I	39	0	34	3	0
9	K	50	0	43	2	0
10	L	50	0	43	3	0
11	A	28	0	26	0	0
11	D	14	0	13	0	0
All	All	8734	0	8269	182	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 11.

All (182) 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:27:GLY:HA3	3:A:576:ILE:HD11	1.23	1.10
3:A:578:ASP:HB3	3:A:618:THR:HG22	1.38	1.05
3:A:578:ASP:CB	3:A:618:THR:HG22	1.91	1.00
3:A:574:GLU:OE1	3:A:624:ARG:HD2	1.65	0.96
2:C:27:GLY:HA3	3:A:576:ILE:CD1	2.00	0.91
3:A:573:LEU:O	3:A:624:ARG:HD3	1.71	0.91
2:C:27:GLY:CA	3:A:576:ILE:HD11	1.99	0.91
3:A:579:VAL:HG12	3:A:597:THR:HB	1.55	0.85
3:A:578:ASP:HB3	3:A:618:THR:CG2	2.09	0.83
3:A:578:ASP:HB3	3:A:618:THR:HA	1.62	0.81
5:E:1:NAG:H3	5:E:2:NAG:H82	1.71	0.71
5:E:1:NAG:O3	5:E:1:NAG:O7	2.08	0.70
2:C:47:PHE:HB2	3:A:400:PRO:HG2	1.73	0.70
3:A:579:VAL:CG1	3:A:597:THR:HB	2.21	0.69
2:C:27:GLY:CA	3:A:576:ILE:CD1	2.66	0.68
3:A:578:ASP:CB	3:A:618:THR:HA	2.22	0.68
3:A:578:ASP:HB3	3:A:618:THR:CA	2.24	0.67
10:L:1:NAG:H4	10:L:2:NAG:N2	2.09	0.66
2:C:166:LEU:HD11	2:C:188:PHE:HB3	1.78	0.66
1:D:908:ARG:NH2	1:D:978:GLN:O	2.29	0.65
3:A:574:GLU:OE1	3:A:574:GLU:HA	1.95	0.65
2:C:141:ILE:HD11	2:C:186:VAL:HG11	1.80	0.64
2:C:175:TYR:HB3	2:C:178:LYS:HB2	1.79	0.63
2:C:175:TYR:HB2	2:C:179:ILE:HG12	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:942:GLN:NE2	1:D:949:ASN:O	2.31	0.63
1:D:785:ILE:N	1:D:917:THR:O	2.34	0.61
1:D:997:LEU:HD23	1:D:1000:ARG:HG3	1.80	0.61
2:C:24:ILE:HG22	2:C:26:GLY:H	1.65	0.61
1:D:868:TYR:O	3:A:583:ARG:NH1	2.33	0.61
3:A:480:ASN:ND2	10:L:1:NAG:O7	2.34	0.61
3:A:577:ASN:ND2	3:A:622:LEU:HD12	2.15	0.61
3:A:609:THR:HG23	3:A:611:ARG:H	1.66	0.60
4:B:2:NAG:H3	4:B:2:NAG:H83	1.83	0.60
3:A:554:TRP:HB2	3:A:614:VAL:HB	1.84	0.60
2:C:101:ARG:NH2	3:A:370:GLN:O	2.36	0.59
3:A:709:THR:O	3:A:713:ASN:ND2	2.35	0.59
3:A:577:ASN:HD22	3:A:622:LEU:HD12	1.68	0.59
3:A:529:GLU:OE2	3:A:557:ASN:ND2	2.36	0.59
2:C:189:LEU:HD11	3:A:624:ARG:HG2	1.85	0.58
3:A:586:GLU:HB2	3:A:609:THR:HG21	1.86	0.58
3:A:574:GLU:O	3:A:598:GLY:HA2	2.05	0.57
3:A:578:ASP:OD1	3:A:618:THR:HB	2.05	0.57
5:E:2:NAG:O7	5:E:2:NAG:O3	2.17	0.56
3:A:742:ASN:HB3	3:A:750:ILE:HB	1.85	0.56
3:A:231:LEU:HD12	3:A:257:ILE:HG12	1.86	0.56
3:A:630:ASN:HB2	8:I:1:NAG:H2	1.88	0.56
6:F:2:NAG:H83	6:F:2:NAG:H3	1.88	0.56
9:K:2:NAG:O3	9:K:3:BMA:O2	2.21	0.56
3:A:628:LYS:HG2	8:I:1:NAG:H81	1.88	0.55
2:C:86:GLN:HE22	2:C:118:VAL:HB	1.72	0.55
3:A:647:HIS:HA	3:A:657:PRO:HG3	1.87	0.55
1:D:787:GLY:HA3	1:D:964:ILE:HA	1.87	0.55
2:C:138:LYS:NZ	2:C:162:ASP:OD2	2.40	0.55
1:D:949:ASN:O	1:D:951:THR:N	2.40	0.55
2:C:184:PHE:HB3	2:C:231:LYS:HE2	1.88	0.55
2:C:62:GLY:HA2	2:C:109:MET:HB3	1.88	0.55
3:A:725:ASN:HD22	3:A:768:ASN:HD21	1.55	0.54
3:A:727:SER:OG	3:A:764:ARG:O	2.25	0.54
2:C:31:GLU:OE1	2:C:76:HIS:NE2	2.41	0.54
2:C:109:MET:HE3	2:C:111:ILE:HD11	1.88	0.54
2:C:188:PHE:CZ	3:A:574:GLU:OE2	2.60	0.54
3:A:578:ASP:CB	3:A:618:THR:CG2	2.76	0.54
3:A:583:ARG:HB3	3:A:590:SER:HB2	1.89	0.54
3:A:578:ASP:OD1	3:A:619:ALA:N	2.40	0.53
2:C:77:ASN:ND2	2:C:156:ASP:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:2:NAG:HO3	9:K:3:BMA:HO2	1.53	0.53
3:A:546:TYR:CZ	3:A:623:ALA:HA	2.44	0.53
2:C:141:ILE:HG23	2:C:204:VAL:HG22	1.90	0.52
3:A:369:ILE:HG21	3:A:373:THR:HG22	1.91	0.52
3:A:531:TRP:CD1	3:A:532:GLU:H	2.28	0.52
2:C:193:LYS:O	2:C:197:GLN:NE2	2.42	0.52
1:D:936:LEU:HD22	1:D:1001:PRO:HG3	1.92	0.52
3:A:413:PRO:HG3	3:A:476:LYS:HE2	1.91	0.52
2:C:205:VAL:HG22	2:C:210:LEU:HA	1.91	0.51
2:C:188:PHE:CE1	3:A:574:GLU:OE2	2.63	0.51
2:C:196:CYS:SG	2:C:229:TYR:OH	2.66	0.51
3:A:240:ALA:HB3	3:A:325:VAL:HG12	1.93	0.51
3:A:573:LEU:C	3:A:624:ARG:HD3	2.35	0.51
3:A:578:ASP:OD1	3:A:618:THR:CA	2.59	0.50
3:A:737:PRO:HA	3:A:755:GLN:HB2	1.93	0.50
4:J:1:NAG:H4	4:J:2:NAG:H83	1.93	0.50
3:A:565:GLN:HB3	3:A:632:THR:HG23	1.92	0.50
1:D:982:ARG:NH2	3:A:772:CYS:SG	2.84	0.50
1:D:917:THR:HG22	1:D:924:THR:HA	1.94	0.50
5:E:2:NAG:O4	5:E:2:NAG:O6	2.18	0.50
3:A:415:ASP:OD1	3:A:474:LYS:NZ	2.45	0.50
3:A:578:ASP:OD1	3:A:618:THR:HA	2.11	0.50
3:A:578:ASP:HB3	3:A:618:THR:CB	2.42	0.49
3:A:578:ASP:HB2	3:A:618:THR:HG22	1.86	0.49
1:D:944:GLN:O	1:D:1000:ARG:NH1	2.45	0.49
3:A:548:ASN:HB3	3:A:620:ASP:HA	1.94	0.49
2:C:217:GLY:HA3	2:C:227:GLY:HA2	1.94	0.49
1:D:899:GLU:HG3	1:D:984:PHE:HE2	1.78	0.49
1:D:792:LYS:HB2	1:D:795:ALA:HB2	1.95	0.48
1:D:859:ILE:HG21	1:D:880:MET:HE2	1.95	0.48
3:A:578:ASP:CG	3:A:618:THR:HB	2.39	0.48
1:D:815:VAL:HA	1:D:895:ILE:HG22	1.95	0.48
1:D:954:MET:HA	1:D:1006:ARG:H	1.79	0.48
2:C:31:GLU:HA	2:C:158:LEU:HD13	1.94	0.48
3:A:265:ILE:HD12	3:A:311:VAL:HG23	1.96	0.48
3:A:742:ASN:OD1	3:A:743:THR:N	2.47	0.48
4:B:1:NAG:H3	4:B:2:NAG:H82	1.95	0.48
3:A:643:CYS:H	3:A:649:GLN:NE2	2.12	0.48
3:A:685:THR:HG23	3:A:687:ASN:H	1.79	0.48
10:L:1:NAG:H4	10:L:2:NAG:C7	2.44	0.48
3:A:272:PHE:HE2	3:A:297:TRP:HA	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:435:HIS:HD2	3:A:482:PHE:HB2	1.80	0.47
3:A:575:ASN:OD1	3:A:575:ASN:N	2.39	0.47
2:C:215:SER:HG	2:C:216:TRP:CD1	2.32	0.47
1:D:832:LEU:HD11	3:A:596:TYR:HA	1.95	0.47
1:D:914:GLY:HA3	1:D:971:ALA:HB1	1.96	0.47
1:D:812:ALA:HB2	1:D:822:SER:HB3	1.97	0.47
3:A:258:ARG:NH1	3:A:310:GLN:OE1	2.48	0.47
3:A:458:TYR:CD1	3:A:510:PRO:HB2	2.50	0.47
3:A:678:VAL:HG22	3:A:719:LEU:HD21	1.96	0.47
3:A:578:ASP:HA	3:A:617:ILE:O	2.15	0.46
3:A:700:HIS:HB2	3:A:739:VAL:HG23	1.97	0.46
2:C:216:TRP:O	2:C:228:VAL:N	2.44	0.46
1:D:917:THR:OG1	1:D:919:VAL:O	2.33	0.46
2:C:146:ASN:H	2:C:197:GLN:HG3	1.80	0.45
1:D:856:PRO:O	1:D:857:ARG:NH1	2.45	0.45
3:A:581:GLU:OE1	3:A:583:ARG:NH2	2.43	0.45
2:C:38:GLN:NE2	2:C:39:VAL:O	2.50	0.45
1:D:960:GLU:O	1:D:999:ASN:N	2.50	0.44
1:D:978:GLN:HE21	1:D:983:TRP:HZ3	1.65	0.44
2:C:128:LEU:HD12	2:C:129:PRO:HD2	1.99	0.44
3:A:529:GLU:HG3	3:A:555:ILE:HB	1.99	0.44
3:A:556:LEU:HB3	3:A:631:PHE:CE1	2.53	0.44
3:A:250:SER:OG	3:A:317:ILE:O	2.36	0.44
5:E:1:NAG:O7	5:E:1:NAG:C3	2.63	0.44
2:C:180:THR:HG23	2:C:182:ASN:H	1.83	0.44
3:A:228:ARG:NH2	3:A:237:SER:O	2.51	0.44
1:D:978:GLN:HE22	1:D:981:ASN:HA	1.82	0.44
1:D:975:LEU:HD22	1:D:1004:TYR:HD2	1.82	0.43
3:A:466:GLN:HE21	3:A:502:CYS:HB3	1.83	0.43
1:D:985:LEU:HG	1:D:1007:VAL:HG21	2.00	0.43
3:A:434:VAL:HG13	3:A:490:ILE:HD11	2.01	0.43
3:A:466:GLN:NE2	3:A:502:CYS:HB3	2.33	0.43
2:C:29:ASN:HB3	2:C:160:CYS:HB3	2.01	0.43
3:A:199:LYS:HB3	3:A:202:LEU:HG	2.00	0.43
3:A:426:TRP:HD1	3:A:494:ASP:HB3	1.84	0.43
1:D:888:TYR:CE1	1:D:894:PRO:HG3	2.53	0.42
2:C:191:GLY:HA3	3:A:621:VAL:HG12	2.01	0.42
2:C:193:LYS:HB2	3:A:621:VAL:HG11	2.01	0.42
3:A:584:ASP:HB3	3:A:591:LEU:HB2	2.01	0.42
3:A:648:PHE:HB3	3:A:657:PRO:HA	2.01	0.42
3:A:274:THR:HG21	3:A:326:GLY:HA2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:522:THR:OG1	3:A:523:ASP:N	2.51	0.42
1:D:870:ARG:HH12	3:A:579:VAL:CG2	2.32	0.42
1:D:994:LYS:HD3	1:D:997:LEU:HD22	2.01	0.42
2:C:187:GLY:H	2:C:229:TYR:HE1	1.67	0.42
2:C:194:ASP:OD1	2:C:194:ASP:N	2.52	0.42
3:A:284:GLU:H	3:A:293:ARG:HG2	1.85	0.42
3:A:583:ARG:HB2	3:A:613:THR:HB	2.01	0.42
2:C:77:ASN:OD1	2:C:80:VAL:N	2.52	0.42
3:A:578:ASP:OD1	3:A:618:THR:CB	2.67	0.42
3:A:616:LEU:HD13	3:A:627:PHE:HE1	1.83	0.42
3:A:650:CYS:HB2	3:A:672:SER:OG	2.20	0.42
5:E:2:NAG:HO3	5:E:2:NAG:C7	2.27	0.42
2:C:42:ASN:O	2:C:70:GLN:HB3	2.20	0.42
2:C:205:VAL:HG13	2:C:209:GLN:C	2.45	0.42
2:C:225:LYS:HD3	2:C:225:LYS:H	1.84	0.42
3:A:189:SER:HB2	3:A:203:PHE:CE2	2.55	0.42
3:A:471:GLU:HG3	3:A:473:VAL:H	1.85	0.42
2:C:27:GLY:HA2	3:A:576:ILE:CD1	2.47	0.41
2:C:120:ASN:OD1	2:C:123:VAL:N	2.53	0.41
3:A:223:THR:C	3:A:225:CYS:H	2.28	0.41
3:A:573:LEU:HD13	3:A:573:LEU:HA	1.76	0.41
3:A:630:ASN:HB2	8:I:1:NAG:C2	2.49	0.41
1:D:859:ILE:HG13	1:D:880:MET:HE2	2.02	0.41
1:D:909:ASN:HA	1:D:934:PRO:HA	2.03	0.41
3:A:306:ILE:HG21	3:A:311:VAL:HG22	2.02	0.41
3:A:563:ASN:HD21	3:A:637:LEU:HB2	1.85	0.41
3:A:582:ILE:HG22	3:A:593:LEU:HD12	2.03	0.41
2:C:128:LEU:HD21	2:C:236:VAL:HG13	2.03	0.40
3:A:324:TYR:HD2	3:A:326:GLY:H	1.69	0.40
3:A:307:PHE:HZ	3:A:355:PHE:HB3	1.87	0.40
4:J:1:NAG:H4	4:J:2:NAG:H2	1.82	0.40
3:A:267:LEU:HD12	3:A:282:ILE:HD13	2.02	0.40
1:D:826:CYS:O	1:D:830:ARG:NH1	2.54	0.40
2:C:27:GLY:HA2	3:A:576:ILE:HD13	2.03	0.40
2:C:57:TRP:CZ2	2:C:243:ILE:HA	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	233/235 (99%)	223 (96%)	9 (4%)	1 (0%)	30	52
2	C	230/232 (99%)	222 (96%)	8 (4%)	0	100	100
3	A	601/603 (100%)	551 (92%)	48 (8%)	2 (0%)	37	59
All	All	1064/1070 (99%)	996 (94%)	65 (6%)	3 (0%)	38	59

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	573	LEU
1	D	786	VAL
3	A	224	VAL

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	D	196/196 (100%)	192 (98%)	4 (2%)	50	76
2	C	192/192 (100%)	189 (98%)	3 (2%)	58	80
3	A	528/528 (100%)	516 (98%)	12 (2%)	45	72
All	All	916/916 (100%)	897 (98%)	19 (2%)	49	74

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	800	VAL
1	D	846	LYS
1	D	949	ASN
1	D	981	ASN
2	C	66	LYS
2	C	194	ASP
2	C	225	LYS
3	A	292	LEU
3	A	441	ILE
3	A	470	ASN
3	A	573	LEU
3	A	574	GLU
3	A	575	ASN
3	A	576	ILE
3	A	578	ASP
3	A	579	VAL
3	A	595	VAL
3	A	656	VAL
3	A	678	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	844	HIS
1	D	881	HIS
1	D	929	GLN
2	C	56	GLN
2	C	86	GLN
2	C	105	ASN
2	C	159	GLN
2	C	182	ASN
2	C	222	GLN
2	C	224	ASN
2	C	234	ASN
3	A	435	HIS
3	A	466	GLN
3	A	559	GLN
3	A	577	ASN
3	A	700	HIS
3	A	768	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 ⓘ

32 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	B	1	4,1	14,14,15	0.29	0	17,19,21	0.67	1 (5%)
4	NAG	B	2	4	14,14,15	0.49	0	17,19,21	1.34	2 (11%)
4	BMA	B	3	4	11,11,12	0.60	0	15,15,17	0.72	0
5	NAG	E	1	1,5	14,14,15	1.94	5 (35%)	17,19,21	5.86	7 (41%)
5	NAG	E	2	5	14,14,15	1.56	3 (21%)	17,19,21	2.61	5 (29%)
5	BMA	E	3	5	11,11,12	2.66	7 (63%)	15,15,17	1.82	4 (26%)
6	NAG	F	1	1,6	14,14,15	0.22	0	17,19,21	0.44	0
6	NAG	F	2	6	14,14,15	0.43	0	17,19,21	1.27	1 (5%)
5	NAG	G	1	3,5	14,14,15	0.25	0	17,19,21	0.51	0
5	NAG	G	2	5	14,14,15	0.22	0	17,19,21	0.39	0
5	BMA	G	3	5	11,11,12	0.57	0	15,15,17	0.79	0
7	NAG	H	1	3,7	14,14,15	0.33	0	17,19,21	0.57	0
7	NAG	H	2	7	14,14,15	0.22	0	17,19,21	0.50	0
7	BMA	H	3	7	11,11,12	0.58	0	15,15,17	0.74	0
7	MAN	H	4	7	11,11,12	0.65	0	15,15,17	1.02	2 (13%)
8	NAG	I	1	3,8	14,14,15	0.39	0	17,19,21	0.33	0
8	NAG	I	2	8	14,14,15	0.25	0	17,19,21	0.48	0
8	BMA	I	3	8	11,11,12	0.60	0	15,15,17	0.77	0
4	NAG	J	1	4,3	14,14,15	0.23	0	17,19,21	0.57	0
4	NAG	J	2	4	14,14,15	0.55	0	17,19,21	0.55	0
4	BMA	J	3	4	11,11,12	0.59	0	15,15,17	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	K	1	3,9	14,14,15	0.29	0	17,19,21	0.53	0
9	NAG	K	2	9	14,14,15	0.22	0	17,19,21	0.50	0
9	BMA	K	3	9	11,11,12	0.82	1 (9%)	15,15,17	0.83	0
9	MAN	K	4	9	11,11,12	0.69	0	15,15,17	1.11	2 (13%)
10	NAG	L	1	3,10	14,14,15	0.42	0	17,19,21	0.64	1 (5%)
10	NAG	L	2	10	14,14,15	0.72	1 (7%)	17,19,21	0.68	1 (5%)
10	BMA	L	3	10	11,11,12	0.61	0	15,15,17	0.82	0
10	MAN	L	4	10	11,11,12	0.82	0	15,15,17	1.24	2 (13%)
5	NAG	M	1	3,5	14,14,15	0.21	0	17,19,21	0.44	0
5	NAG	M	2	5	14,14,15	0.22	0	17,19,21	0.41	0
5	BMA	M	3	5	11,11,12	0.58	0	15,15,17	0.76	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	B	2	4	-	3/6/23/26	0/1/1/1
4	BMA	B	3	4	-	0/2/19/22	0/1/1/1
5	NAG	E	1	1,5	-	6/6/23/26	0/1/1/1
5	NAG	E	2	5	-	4/6/23/26	0/1/1/1
5	BMA	E	3	5	-	0/2/19/22	0/1/1/1
6	NAG	F	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	F	2	6	-	5/6/23/26	0/1/1/1
5	NAG	G	1	3,5	-	3/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
5	BMA	G	3	5	-	0/2/19/22	0/1/1/1
7	NAG	H	1	3,7	-	4/6/23/26	0/1/1/1
7	NAG	H	2	7	-	2/6/23/26	0/1/1/1
7	BMA	H	3	7	-	0/2/19/22	0/1/1/1
7	MAN	H	4	7	-	0/2/19/22	0/1/1/1
8	NAG	I	1	3,8	-	2/6/23/26	0/1/1/1
8	NAG	I	2	8	-	2/6/23/26	0/1/1/1
8	BMA	I	3	8	-	0/2/19/22	0/1/1/1
4	NAG	J	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BMA	J	3	4	-	0/2/19/22	0/1/1/1
9	NAG	K	1	3,9	-	4/6/23/26	0/1/1/1
9	NAG	K	2	9	-	2/6/23/26	0/1/1/1
9	BMA	K	3	9	-	1/2/19/22	0/1/1/1
9	MAN	K	4	9	-	1/2/19/22	0/1/1/1
10	NAG	L	1	3,10	-	4/6/23/26	0/1/1/1
10	NAG	L	2	10	-	4/6/23/26	0/1/1/1
10	BMA	L	3	10	-	0/2/19/22	0/1/1/1
10	MAN	L	4	10	-	0/2/19/22	1/1/1/1
5	NAG	M	1	3,5	-	3/6/23/26	0/1/1/1
5	NAG	M	2	5	-	1/6/23/26	0/1/1/1
5	BMA	M	3	5	-	0/2/19/22	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	3	BMA	O5-C1	-5.35	1.35	1.43
5	E	3	BMA	C2-C3	-3.81	1.46	1.52
5	E	3	BMA	O5-C5	-3.60	1.36	1.43
5	E	1	NAG	O5-C5	3.23	1.50	1.43
5	E	1	NAG	C4-C3	-3.12	1.44	1.52
5	E	1	NAG	O7-C7	-3.01	1.16	1.23
5	E	2	NAG	C2-N2	-2.87	1.41	1.46
5	E	2	NAG	C1-C2	-2.84	1.48	1.52
5	E	3	BMA	C1-C2	-2.77	1.45	1.52
5	E	2	NAG	C3-C2	-2.67	1.46	1.52
5	E	1	NAG	C1-C2	-2.44	1.48	1.52
10	L	2	NAG	C1-C2	2.43	1.56	1.52
9	K	3	BMA	C1-C2	2.21	1.57	1.52
5	E	1	NAG	C2-N2	-2.16	1.42	1.46
5	E	3	BMA	C4-C5	-2.09	1.48	1.53
5	E	3	BMA	O3-C3	-2.06	1.38	1.43
5	E	3	BMA	C4-C3	-2.01	1.47	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1	NAG	O5-C5-C6	14.64	130.15	107.20
5	E	1	NAG	C1-C2-N2	-12.95	88.37	110.49
5	E	1	NAG	O5-C1-C2	-8.98	97.11	111.29
5	E	1	NAG	O4-C4-C5	7.98	129.10	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	2	NAG	O5-C1-C2	-6.14	101.59	111.29
5	E	2	NAG	C3-C4-C5	-6.14	99.29	110.24
5	E	1	NAG	C3-C4-C5	-4.75	101.76	110.24
6	F	2	NAG	C2-N2-C7	4.32	129.06	122.90
4	B	2	NAG	C2-N2-C7	4.29	129.01	122.90
5	E	1	NAG	C1-O5-C5	3.93	117.52	112.19
10	L	4	MAN	C1-O5-C5	3.63	117.10	112.19
5	E	1	NAG	C2-N2-C7	3.60	128.03	122.90
5	E	3	BMA	C1-C2-C3	-3.52	105.34	109.67
5	E	2	NAG	C6-C5-C4	-3.28	105.31	113.00
5	E	2	NAG	O4-C4-C3	2.73	116.65	110.35
9	K	4	MAN	C1-O5-C5	2.67	115.82	112.19
5	E	3	BMA	O5-C1-C2	-2.65	106.68	110.77
5	E	3	BMA	O5-C5-C4	-2.65	104.39	110.83
5	E	2	NAG	O5-C5-C6	2.44	111.03	107.20
7	H	4	MAN	C1-O5-C5	2.41	115.45	112.19
5	E	3	BMA	C3-C4-C5	-2.33	106.08	110.24
10	L	2	NAG	C1-O5-C5	2.30	115.31	112.19
4	B	2	NAG	C1-O5-C5	2.25	115.24	112.19
7	H	4	MAN	O2-C2-C3	-2.23	105.67	110.14
10	L	4	MAN	O2-C2-C3	-2.21	105.72	110.14
9	K	4	MAN	O2-C2-C3	-2.21	105.72	110.14
4	B	1	NAG	C1-O5-C5	2.08	115.01	112.19
10	L	1	NAG	C1-O5-C5	2.01	114.92	112.19

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	1	NAG	O7-C7-N2-C2
5	E	2	NAG	C3-C2-N2-C7
5	E	2	NAG	C8-C7-N2-C2
5	E	2	NAG	O7-C7-N2-C2
7	H	1	NAG	C4-C5-C6-O6
8	I	2	NAG	C4-C5-C6-O6
5	E	1	NAG	C8-C7-N2-C2
6	F	2	NAG	O5-C5-C6-O6
7	H	1	NAG	O5-C5-C6-O6
10	L	1	NAG	O5-C5-C6-O6
9	K	1	NAG	C4-C5-C6-O6
6	F	2	NAG	C4-C5-C6-O6
9	K	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
10	L	1	NAG	C4-C5-C6-O6
8	I	2	NAG	O5-C5-C6-O6
10	L	2	NAG	O5-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
5	G	1	NAG	O5-C5-C6-O6
5	G	2	NAG	O5-C5-C6-O6
9	K	1	NAG	O5-C5-C6-O6
9	K	2	NAG	C4-C5-C6-O6
5	E	1	NAG	C1-C2-N2-C7
10	L	2	NAG	C4-C5-C6-O6
4	B	2	NAG	C8-C7-N2-C2
4	B	2	NAG	O7-C7-N2-C2
4	J	2	NAG	C8-C7-N2-C2
4	J	2	NAG	O7-C7-N2-C2
5	M	1	NAG	C8-C7-N2-C2
5	M	1	NAG	O7-C7-N2-C2
6	F	2	NAG	C8-C7-N2-C2
6	F	2	NAG	O7-C7-N2-C2
7	H	1	NAG	C8-C7-N2-C2
7	H	1	NAG	O7-C7-N2-C2
7	H	2	NAG	C8-C7-N2-C2
7	H	2	NAG	O7-C7-N2-C2
9	K	1	NAG	C8-C7-N2-C2
9	K	1	NAG	O7-C7-N2-C2
10	L	1	NAG	C8-C7-N2-C2
10	L	1	NAG	O7-C7-N2-C2
10	L	2	NAG	C8-C7-N2-C2
10	L	2	NAG	O7-C7-N2-C2
5	G	1	NAG	C4-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
4	B	1	NAG	O5-C5-C6-O6
5	E	1	NAG	C4-C5-C6-O6
8	I	1	NAG	O5-C5-C6-O6
9	K	4	MAN	O5-C5-C6-O6
5	E	1	NAG	O5-C5-C6-O6
4	B	1	NAG	C4-C5-C6-O6
5	E	2	NAG	O5-C5-C6-O6
5	M	1	NAG	O5-C5-C6-O6
9	K	3	BMA	O5-C5-C6-O6
5	M	2	NAG	O5-C5-C6-O6
4	B	2	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
5	E	1	NAG	C3-C2-N2-C7
5	G	1	NAG	C3-C2-N2-C7
8	I	1	NAG	C4-C5-C6-O6
6	F	2	NAG	C3-C2-N2-C7

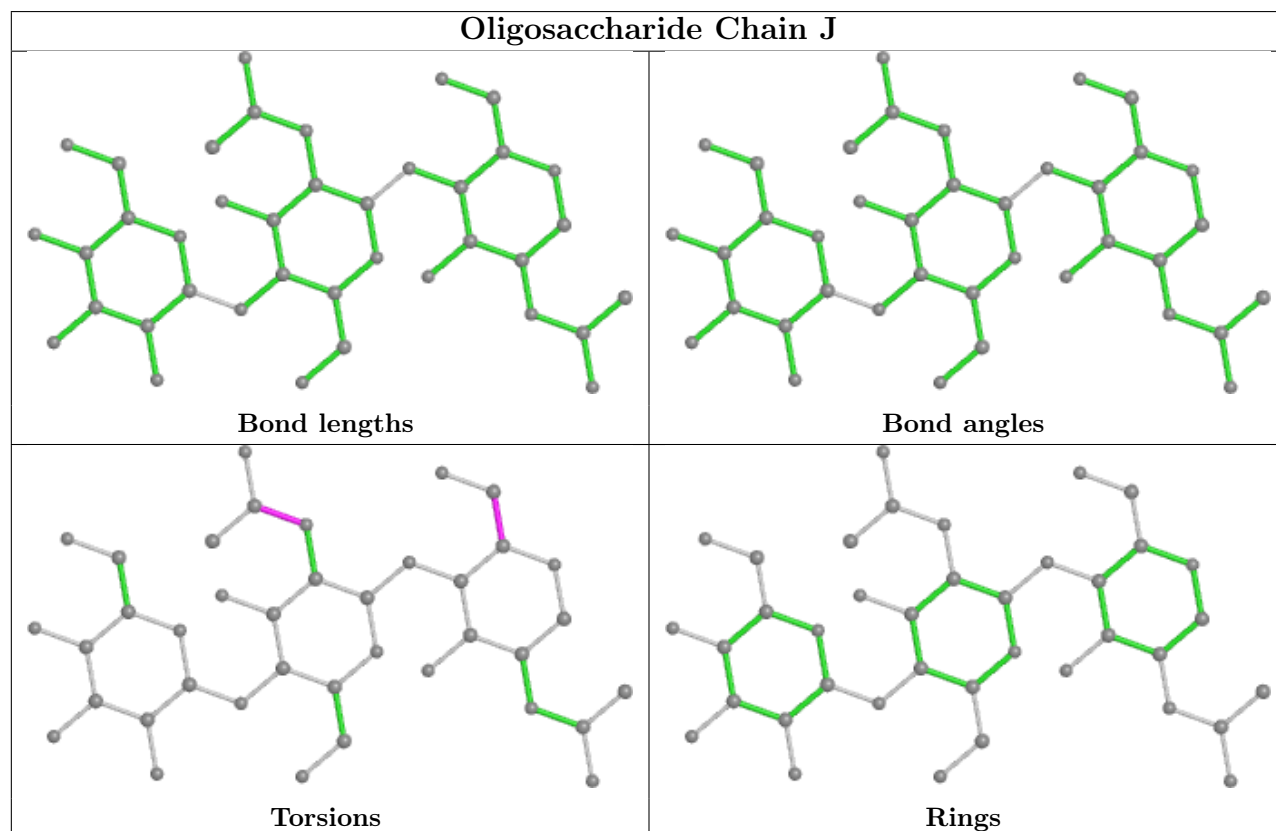
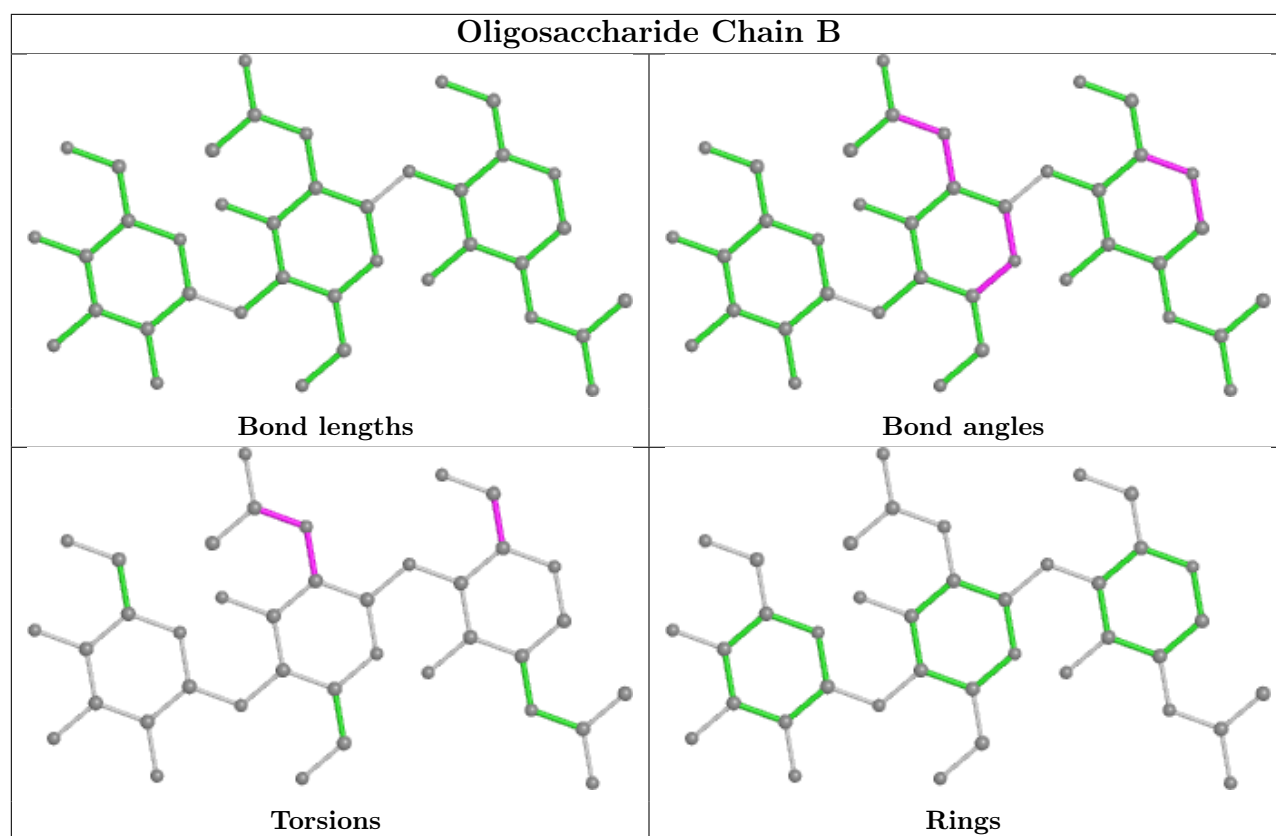
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	L	4	MAN	C1-C2-C3-C4-C5-O5

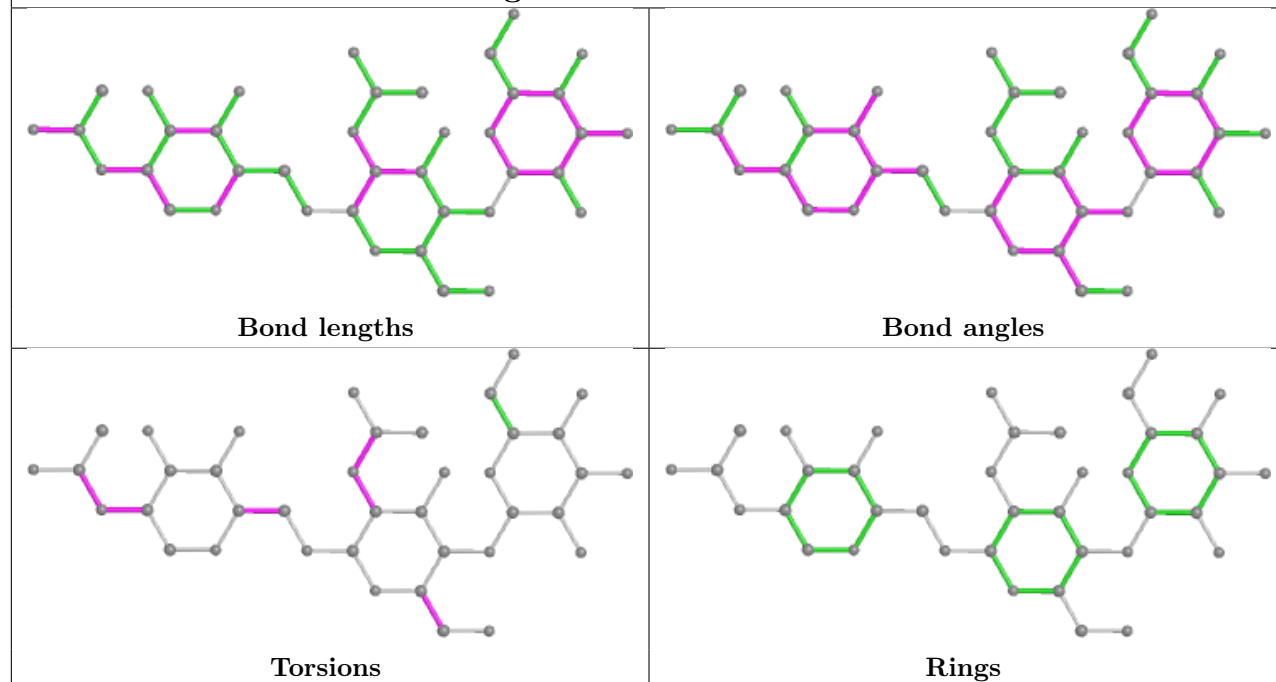
12 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	2	NAG	1	0
5	E	2	NAG	4	0
9	K	2	NAG	2	0
8	I	1	NAG	3	0
10	L	2	NAG	2	0
9	K	3	BMA	2	0
4	B	2	NAG	2	0
4	J	2	NAG	2	0
10	L	1	NAG	3	0
5	E	1	NAG	3	0
4	J	1	NAG	2	0
4	B	1	NAG	1	0

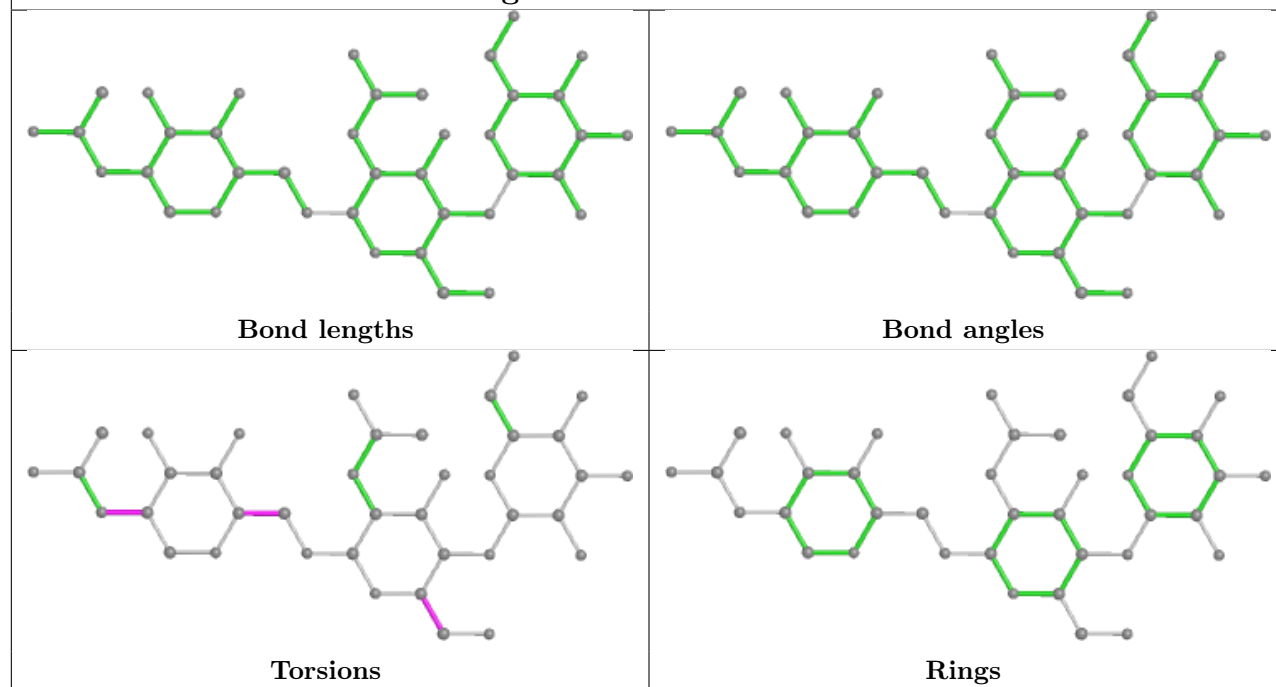
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

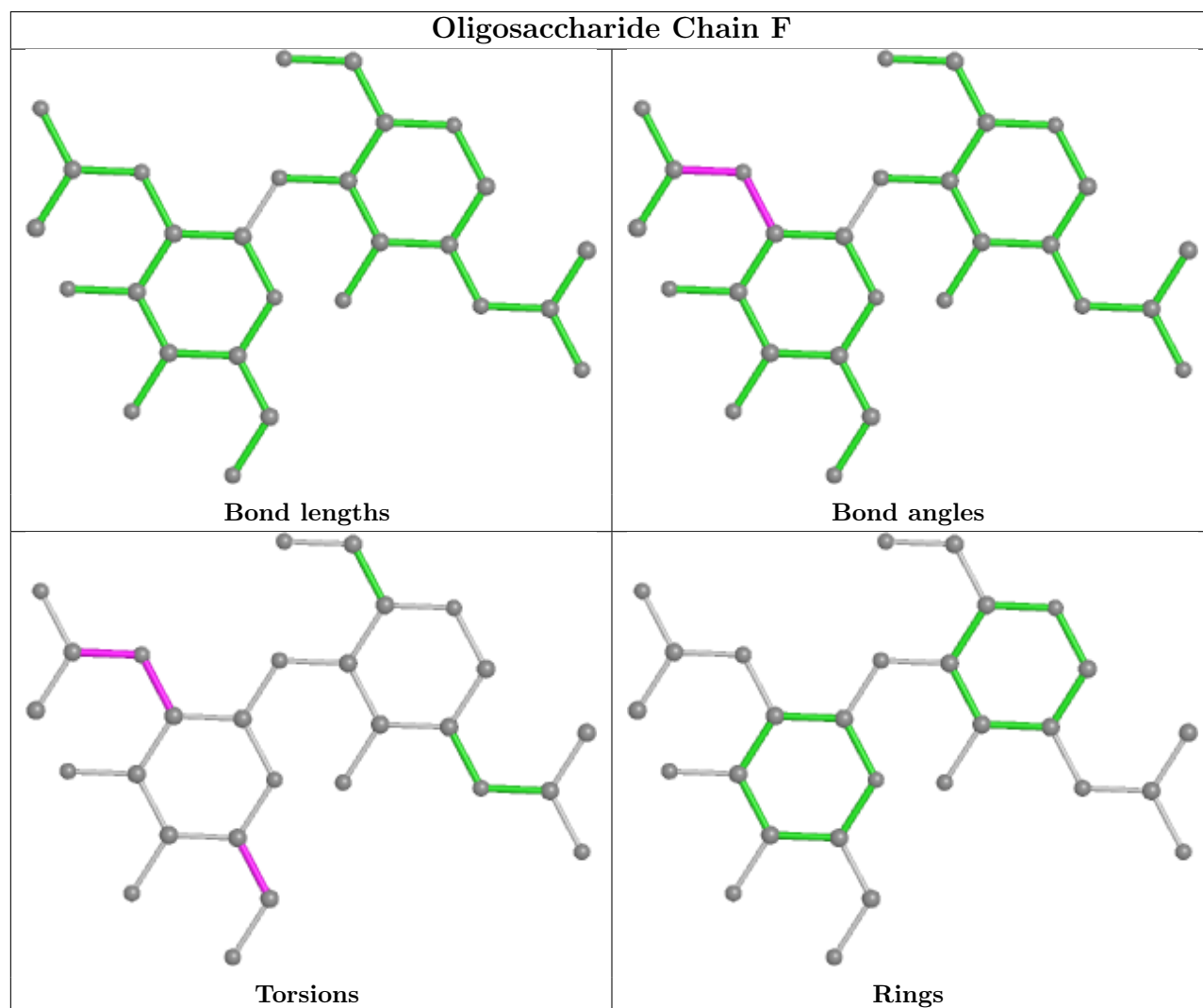
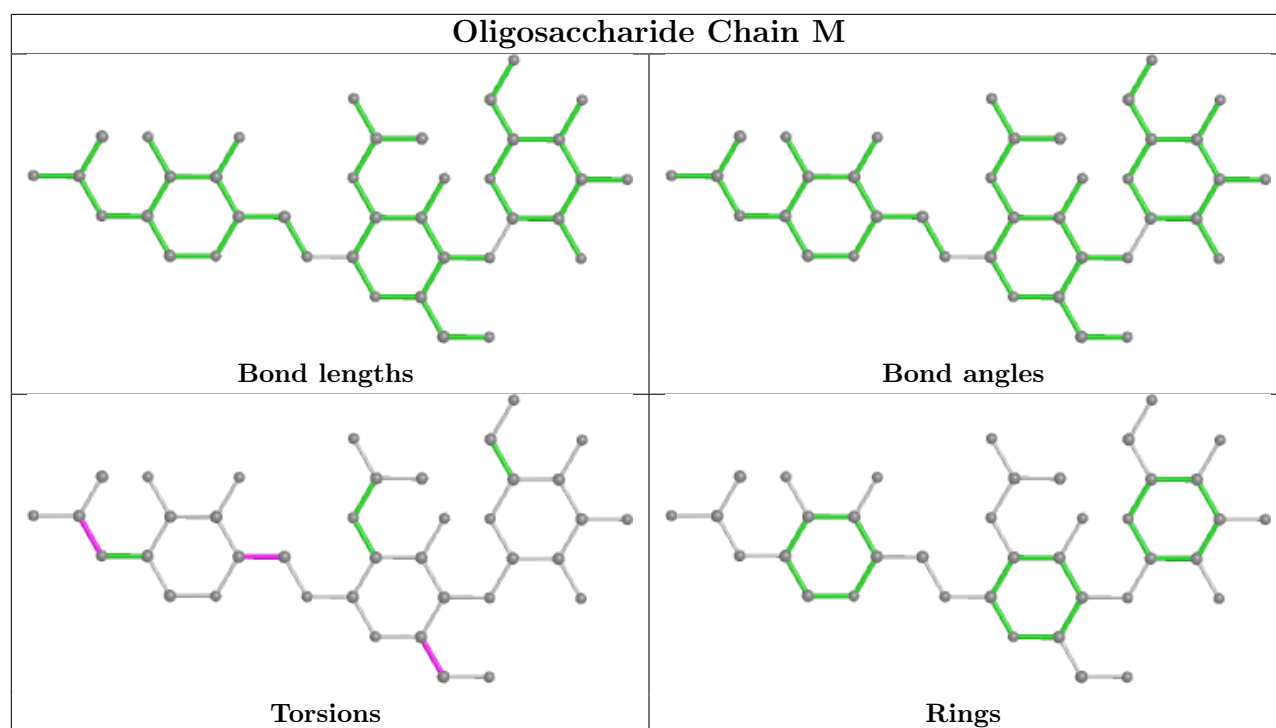


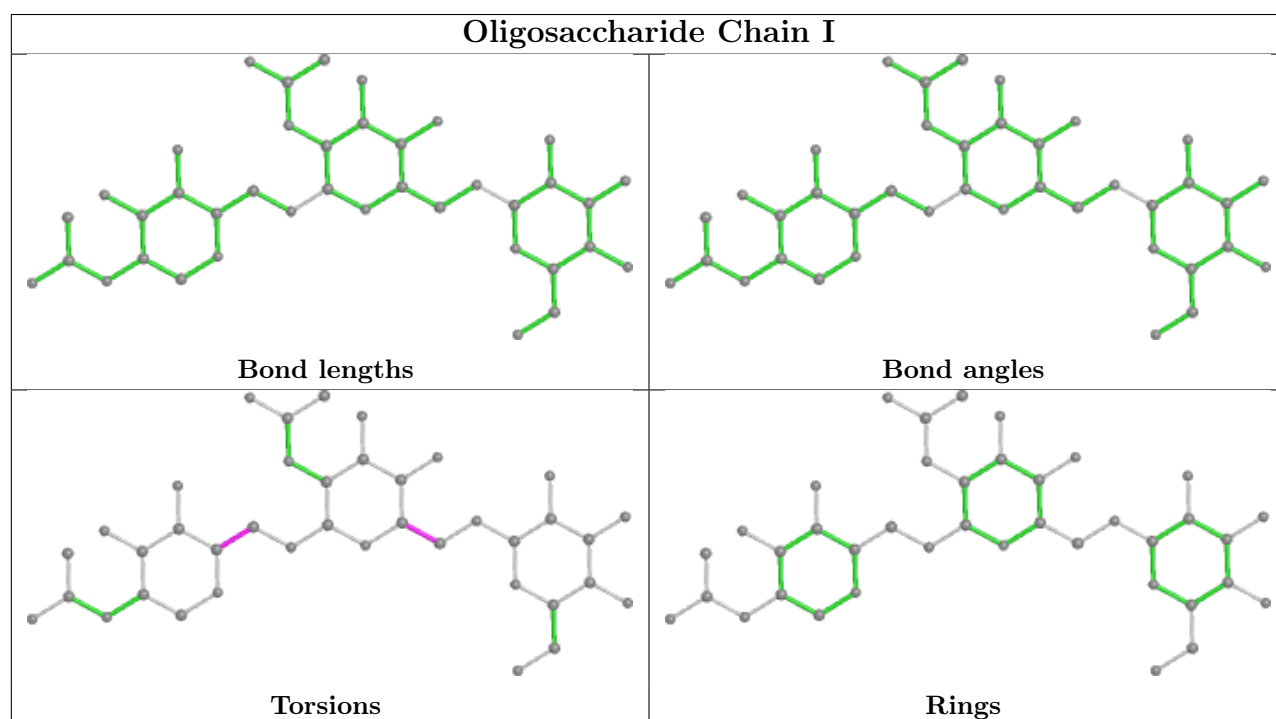
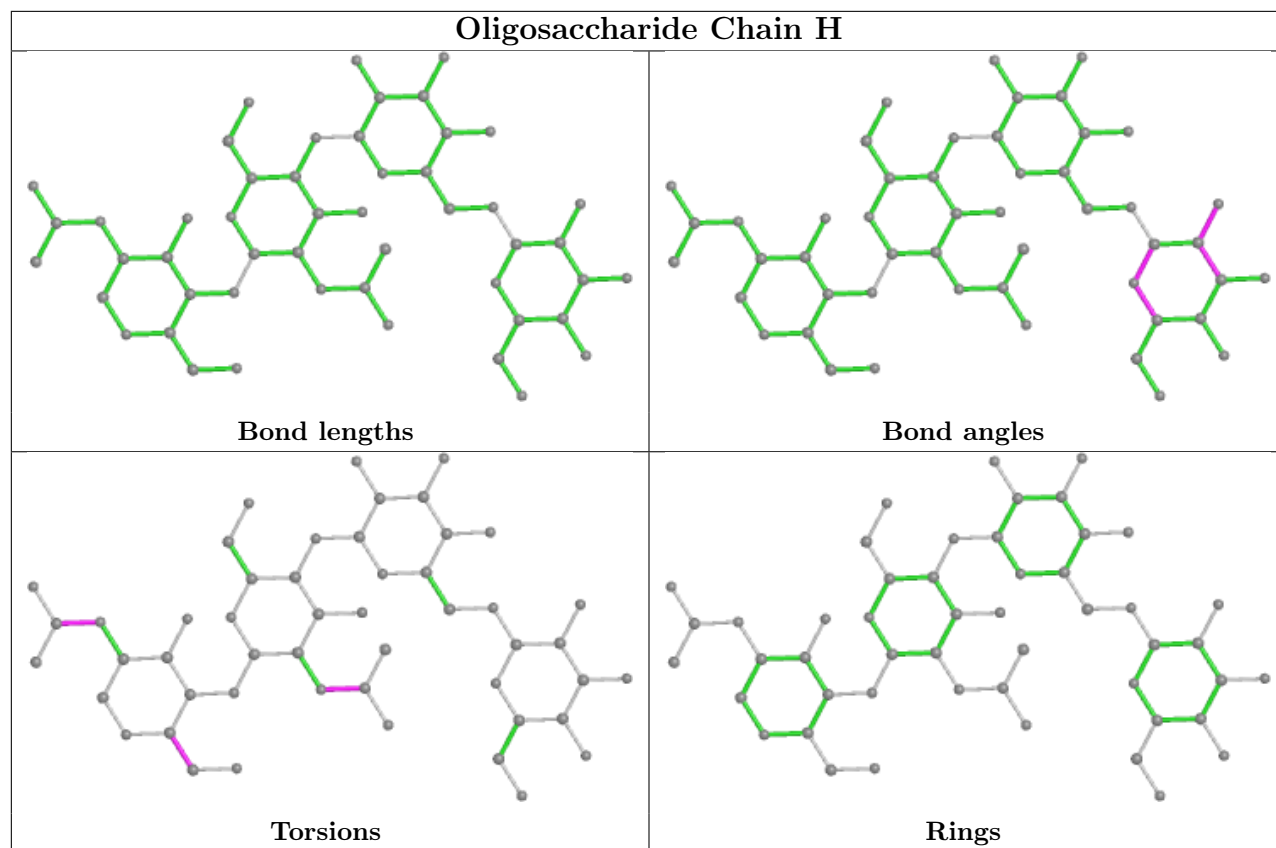
Oligosaccharide Chain E

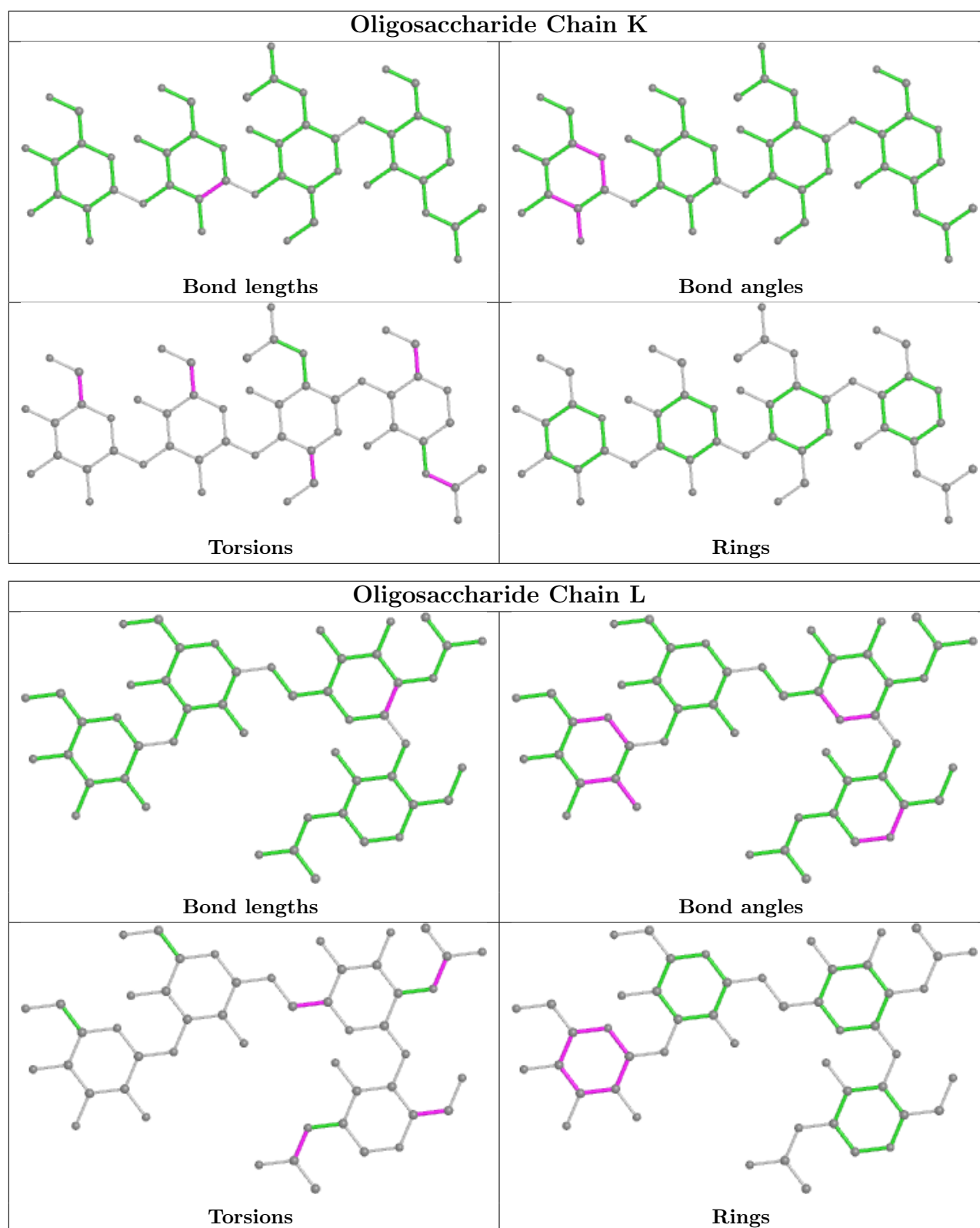


Oligosaccharide Chain G









5.6 Ligand geometry [i](#)

3 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	$\# Z > 2$
11	NAG	D	1101	1	14,14,15	0.25	0	17,19,21	0.51	0
11	NAG	A	802	3	14,14,15	0.26	0	17,19,21	0.53	0
11	NAG	A	801	3	14,14,15	0.22	0	17,19,21	0.42	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
11	NAG	D	1101	1	-	3/6/23/26	0/1/1/1
11	NAG	A	802	3	-	1/6/23/26	0/1/1/1
11	NAG	A	801	3	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	801	NAG	O5-C5-C6-O6
11	D	1101	NAG	O5-C5-C6-O6
11	D	1101	NAG	C4-C5-C6-O6
11	A	801	NAG	C4-C5-C6-O6
11	A	801	NAG	C8-C7-N2-C2
11	A	801	NAG	O7-C7-N2-C2
11	D	1101	NAG	C3-C2-N2-C7
11	A	802	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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.