



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:24 AM UTC

PDB ID : 2ID5 / pdb_00002id5
Title : Crystal Structure of the Lingo-1 Ectodomain
Authors : Mosyak, L.; Wood, A.; Dwyer, B.; Johnson, M.; Stahl, M.L.; Somers, W.S.
Deposited on : 2006-09-14
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

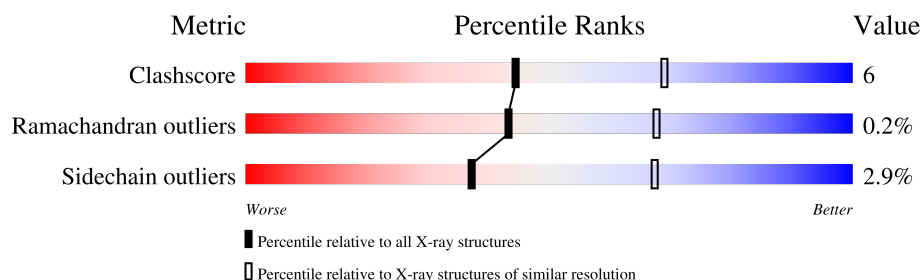
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

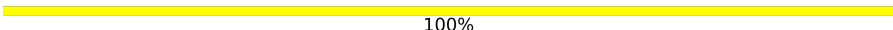
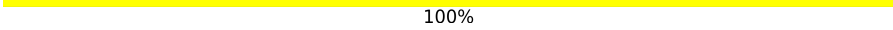
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	477	
1	B	477	
1	C	477	
1	D	477	
2	E	3	
2	F	3	
2	H	3	
2	J	3	

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Mol	Chain	Length	Quality of chain
2	K	3	 100%
2	L	3	 33% 67%
2	M	3	 67% 33%
2	N	3	 33% 67%
2	Q	3	 33% 67%
3	G	2	 100%
3	P	2	 50% 50%
4	I	4	 75% 25%
4	O	4	 25% 25% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MAN	E	3	X	-	-	-
2	MAN	F	3	X	-	-	-
2	MAN	H	3	X	-	-	-
2	MAN	J	3	X	-	-	-
2	MAN	K	3	X	-	-	-
2	MAN	L	3	X	-	-	-
2	MAN	M	3	X	-	-	-
2	MAN	N	3	X	-	-	-
3	NAG	G	1	X	-	-	-
3	NAG	G	2	X	-	-	-
4	MAN	I	3	X	-	-	-
4	MAN	O	3	X	-	-	-
5	NAG	B	501	X	-	-	-
5	NAG	C	502	X	-	-	-

2 Entry composition [i](#)

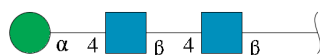
There are 6 unique types of molecules in this entry. The entry contains 16119 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Leucine rich repeat neuronal 6A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	470	Total	C	N	O	S	0	0	0
			3769	2402	671	679	17			
1	B	473	Total	C	N	O	S	0	0	0
			3790	2414	676	683	17			
1	C	472	Total	C	N	O	S	0	0	0
			3785	2410	677	681	17			
1	D	471	Total	C	N	O	S	0	0	0
			3778	2407	677	677	17			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	3	Total	C	N	O		0	0	0
			39	22	2	15				
2	F	3	Total	C	N	O		0	0	0
			39	22	2	15				
2	H	3	Total	C	N	O		0	0	0
			39	22	2	15				
2	J	3	Total	C	N	O		0	0	0
			39	22	2	15				
2	K	3	Total	C	N	O		0	0	0
			39	22	2	15				
2	L	3	Total	C	N	O		0	0	0
			39	22	2	15				
2	M	3	Total	C	N	O		0	0	0
			39	22	2	15				
2	N	3	Total	C	N	O		0	0	0
			39	22	2	15				

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

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	P	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	78	Total 78	O 78	0	0
6	B	100	Total 100	O 100	0	0
6	C	68	Total 68	O 68	0	0
6	D	62	Total 62	O 62	0	0

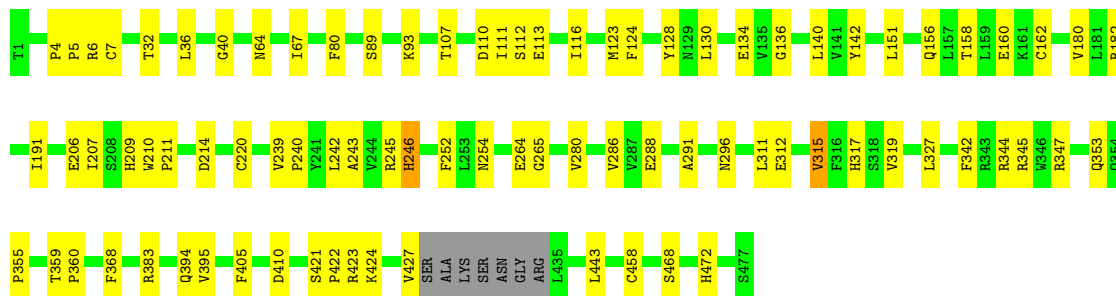
3 Residue-property plots

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.

Note EDS was not executed.

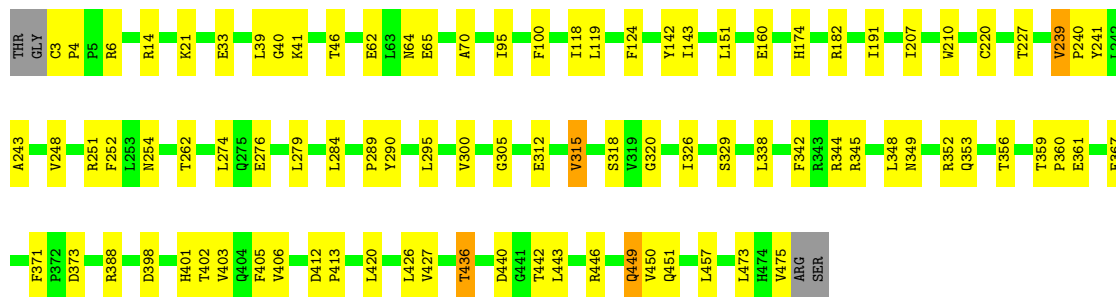
• Molecule 1: Leucine rich repeat neuronal 6A

Chain A: 



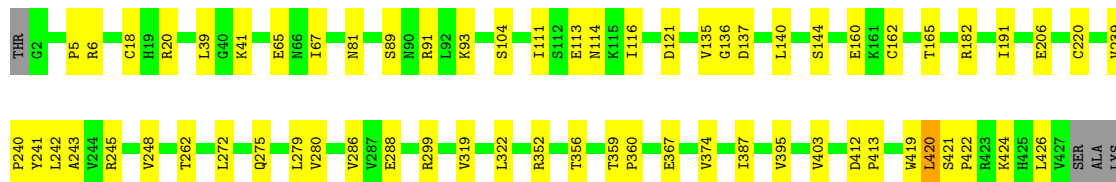
• Molecule 1: Leucine rich repeat neuronal 6A

Chain B: 



• Molecule 1: Leucine rich repeat neuronal 6A

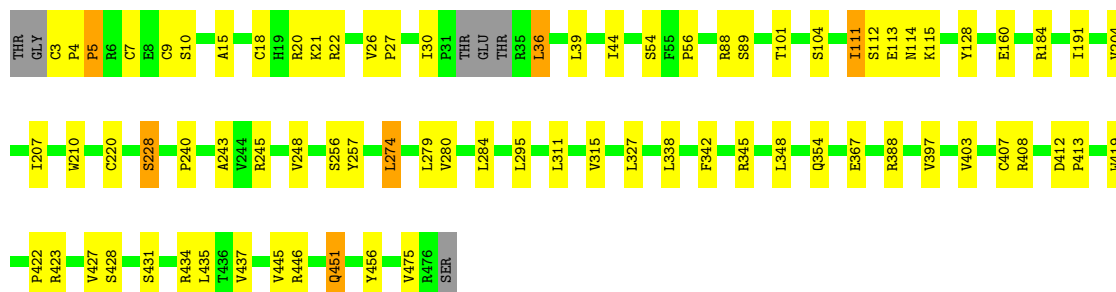
Chain C: 





- Molecule 1: Leucine rich repeat neuronal 6A

Chain D: 82% 15% ..



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

Chain E: 100%



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

Chain F: 33% 33% 33%



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

Chain H: 33% 67%

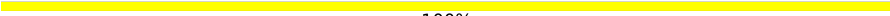


- Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 67% 33%



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

Chain K:  100%

NAG1
NAG2
MAN3

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

Chain L:  33% 67%

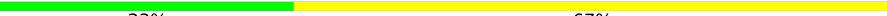
NAG1
NAG2
MAN3

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

Chain M:  67% 33%

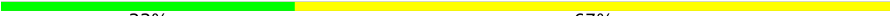
NAG1
NAG2
MAN3

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

Chain N:  33% 67%

NAG1
NAG2
MAN3

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

Chain Q:  33% 67%

NAG1
NAG2
MAN3

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

Chain G:  100%

NAG1
NAG2

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

Chain P:  50% 50%

NAG1
NAG2

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

Chain I:  75% 25%

MAG1
MAG2
MAN3
MAN4

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

Chain O:  25% 25% 50%

MAG1
MAG2
MAN3
MAN4

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	201.52Å 149.72Å 157.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	158.11 – 2.70	Depositor
% Data completeness (in resolution range)	98.7 (158.11-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.214 , 0.255	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16119	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, 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	0.57	1/3850 (0.0%)	0.83	3/5233 (0.1%)
1	B	0.56	1/3872 (0.0%)	0.83	1/5263 (0.0%)
1	C	0.52	0/3866	0.78	0/5253
1	D	0.51	1/3859 (0.0%)	0.79	2/5242 (0.0%)
All	All	0.54	3/15447 (0.0%)	0.81	6/20991 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	449	GLN	CD-OE1	5.27	1.33	1.23
1	D	451	GLN	CD-OE1	5.23	1.33	1.23
1	A	246	HIS	ND1-CE1	5.18	1.37	1.32

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	246	HIS	CB-CG-CD2	-6.43	122.84	131.20
1	B	239	VAL	O-C-N	5.68	127.27	121.14
1	A	214	ASP	CB-CA-C	-5.67	101.94	110.90
1	A	246	HIS	CB-CG-ND1	5.59	131.09	122.70
1	D	3	CYS	CA-C-N	5.56	126.11	120.38
1	D	3	CYS	C-N-CA	5.56	126.11	120.38

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	344	ARG	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3769	0	3787	48	0
1	B	3790	0	3807	59	0
1	C	3785	0	3797	42	0
1	D	3778	0	3801	42	0
2	E	39	0	34	0	0
2	F	39	0	34	1	0
2	H	39	0	34	0	0
2	J	39	0	34	2	0
2	K	39	0	34	0	0
2	L	39	0	34	0	0
2	M	39	0	34	2	0
2	N	39	0	34	0	0
2	Q	39	0	34	0	0
3	G	28	0	25	0	0
3	P	28	0	25	0	0
4	I	50	0	43	1	0
4	O	50	0	43	1	0
5	A	42	0	39	1	0
5	B	56	0	52	0	0
5	C	56	0	52	2	0
5	D	28	0	26	0	0
6	A	78	0	0	0	0
6	B	100	0	0	5	0
6	C	68	0	0	0	0
6	D	62	0	0	0	0
All	All	16119	0	15803	189	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 6.

All (189) 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)
1:C:352:ARG:HH12	2:M:3:MAN:H3	1.24	0.97
1:C:41:LYS:HE3	1:C:65:GLU:OE1	1.74	0.86
1:B:276:GLU:HG2	1:B:300:VAL:HB	1.58	0.85
1:B:356:THR:HG22	1:B:367:GLU:HG2	1.60	0.82
1:B:46:THR:HG22	1:B:70:ALA:HB3	1.60	0.81
1:C:395:VAL:HG11	1:C:403:VAL:CG2	2.11	0.81
1:B:62:GLU:HG3	1:B:64:ASN:ND2	1.96	0.81
1:A:245:ARG:HH21	1:A:246:HIS:CD2	1.99	0.81
1:A:245:ARG:NH2	1:A:246:HIS:NE2	2.29	0.80
1:B:3:CYS:HB2	1:B:4:PRO:HD2	1.65	0.78
1:C:420:LEU:HD13	1:C:459:ILE:HD11	1.67	0.76
1:C:395:VAL:HG11	1:C:403:VAL:HG21	1.66	0.76
1:A:245:ARG:NH2	1:A:246:HIS:CD2	2.53	0.76
1:B:352:ARG:NH1	2:J:3:MAN:H5	2.03	0.74
1:C:412:ASP:OD1	1:C:413:PRO:HA	1.88	0.73
1:A:242:LEU:O	1:A:245:ARG:HG2	1.90	0.72
1:B:352:ARG:HH12	2:J:3:MAN:H5	1.54	0.71
1:B:174:HIS:HE1	6:B:612:HOH:O	1.73	0.71
1:B:227:THR:HG21	1:B:251:ARG:HH21	1.54	0.70
1:B:342:PHE:O	1:B:345:ARG:HB3	1.92	0.70
1:A:383:ARG:HH12	1:A:410:ASP:HB3	1.55	0.69
1:B:191:ILE:HG22	1:B:220:CYS:HB2	1.75	0.69
1:C:395:VAL:CG1	1:C:403:VAL:HG21	2.24	0.68
1:B:356:THR:CG2	1:B:367:GLU:HG2	2.25	0.67
1:A:191:ILE:HG22	1:A:220:CYS:HB2	1.78	0.65
1:B:356:THR:HG22	1:B:367:GLU:CG	2.25	0.65
1:C:20:ARG:HE	1:C:41:LYS:HD3	1.61	0.65
1:C:191:ILE:HG22	1:C:220:CYS:HB2	1.80	0.65
6:B:682:HOH:O	4:I:2:NAG:H3	1.96	0.64
1:B:62:GLU:HG3	1:B:64:ASN:HD21	1.64	0.62
1:A:296:ASN:OD1	1:A:317:HIS:CD2	2.53	0.62
1:B:239:VAL:HG13	1:B:240:PRO:HD2	1.82	0.60
1:D:423:ARG:NH1	1:D:451:GLN:OE1	2.35	0.59
1:A:182:ARG:HG2	1:A:206:GLU:HB3	1.83	0.59
1:B:3:CYS:CB	1:B:4:PRO:HD2	2.33	0.59
1:A:142:TYR:HE2	1:B:426:LEU:HD22	1.67	0.59
1:A:142:TYR:CE2	1:B:426:LEU:HD22	2.38	0.58
1:C:239:VAL:HG13	1:C:240:PRO:HD2	1.85	0.58
1:B:14:ARG:HE	1:B:33:GLU:HB2	1.68	0.58
1:C:121:ASP:OD1	1:C:144:SER:HB3	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:352:ARG:NH1	2:M:3:MAN:H3	2.08	0.58
1:D:240:PRO:HB2	1:D:243:ALA:HB3	1.85	0.58
1:B:207:ILE:HG23	1:B:210:TRP:CE2	2.39	0.58
1:B:46:THR:CG2	1:B:70:ALA:HB3	2.31	0.57
1:C:41:LYS:CE	1:C:65:GLU:OE1	2.48	0.57
1:D:397:VAL:HB	1:D:403:VAL:HG21	1.86	0.57
1:D:397:VAL:CG2	1:D:403:VAL:HG21	2.36	0.56
1:D:54:SER:C	1:D:56:PRO:HD3	2.30	0.56
1:B:124:PHE:HB3	1:B:151:LEU:HD21	1.88	0.56
1:C:421:SER:HB2	1:C:422:PRO:HD2	1.87	0.55
1:A:134:GLU:HG2	1:A:158:THR:HB	1.87	0.55
1:B:240:PRO:HB2	1:B:243:ALA:HB3	1.89	0.54
1:B:345:ARG:NH1	1:B:373:ASP:OD1	2.41	0.54
1:D:10:SER:HB3	1:D:15:ALA:HB3	1.89	0.54
1:D:397:VAL:CG2	1:D:403:VAL:CG2	2.86	0.53
1:C:240:PRO:HB2	1:C:243:ALA:HB3	1.90	0.53
1:C:140:LEU:HD23	1:C:162:CYS:SG	2.49	0.53
1:A:355:PRO:HG2	1:A:368:PHE:CG	2.44	0.53
1:D:354:GLN:HG2	1:D:367:GLU:HB3	1.90	0.53
1:D:15:ALA:HA	1:D:36:LEU:HB3	1.92	0.52
1:D:428:SER:H	1:D:431:SER:HB2	1.74	0.52
1:A:458:CYS:O	1:A:468:SER:HA	2.10	0.52
1:B:406:VAL:HA	1:B:442:THR:HG22	1.91	0.52
1:D:427:VAL:HG12	1:D:437:VAL:HG23	1.92	0.51
1:A:136:GLY:HA3	1:A:160:GLU:O	2.11	0.51
1:C:67:ILE:HG12	1:C:91:ARG:HG3	1.93	0.51
1:D:279:LEU:HD13	1:D:284:LEU:HD11	1.93	0.51
1:C:356:THR:HG22	1:C:367:GLU:HG2	1.92	0.51
1:D:434:ARG:HB2	1:D:446:ARG:HB3	1.92	0.51
1:B:262:THR:HG22	6:B:632:HOH:O	2.11	0.51
1:A:5:PRO:O	1:A:6:ARG:HB2	2.10	0.51
1:A:89:SER:HA	1:A:113:GLU:O	2.11	0.50
1:C:420:LEU:HD23	1:C:424:LYS:HA	1.93	0.50
1:B:252:PHE:CE2	1:B:254:ASN:HB2	2.46	0.50
1:B:359:THR:HB	1:B:360:PRO:HA	1.93	0.50
1:C:104:SER:HB2	5:C:501:NAG:H83	1.94	0.50
1:A:359:THR:HB	1:A:360:PRO:HA	1.94	0.50
1:D:20:ARG:HH22	1:D:22:ARG:HH11	1.60	0.50
1:B:40:GLY:HA2	1:B:64:ASN:O	2.12	0.49
1:B:450:VAL:HA	1:B:475:VAL:HG11	1.94	0.49
1:D:388:ARG:NH1	1:D:408:ARG:HD3	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:402:THR:HG23	1:B:446:ARG:HA	1.95	0.49
1:A:239:VAL:HG13	1:A:240:PRO:HD2	1.95	0.49
1:A:264:GLU:HA	1:A:288:GLU:HG3	1.95	0.49
1:C:182:ARG:HG2	1:C:206:GLU:HB3	1.95	0.49
1:C:114:ASN:N	1:C:137:ASP:OD1	2.44	0.48
1:A:405:PHE:HD2	1:A:443:LEU:HD23	1.78	0.48
1:C:136:GLY:HA3	1:C:160:GLU:O	2.13	0.48
1:B:95:ILE:HG21	1:B:100:PHE:CE2	2.48	0.48
1:A:124:PHE:HB3	1:A:151:LEU:HD21	1.95	0.48
1:B:312:GLU:O	1:B:315:VAL:HG13	2.13	0.48
1:B:305:GLY:HA2	1:B:329:SER:HB2	1.94	0.48
1:C:89:SER:HA	1:C:113:GLU:O	2.13	0.48
1:D:7:CYS:HA	1:D:21:LYS:HE3	1.96	0.48
1:B:449:GLN:HG3	1:B:451:GLN:HB2	1.96	0.48
1:A:107:THR:HA	1:A:130:LEU:HA	1.96	0.47
1:D:89:SER:HA	1:D:113:GLU:O	2.15	0.47
1:B:326:ILE:HG23	1:B:353:GLN:HB3	1.96	0.47
1:A:421:SER:HB2	1:A:422:PRO:HD2	1.97	0.47
1:A:123:MET:HE2	1:A:124:PHE:CE1	2.50	0.47
1:D:435:LEU:HD23	1:D:445:VAL:HG22	1.96	0.47
1:C:5:PRO:O	1:C:6:ARG:HB2	2.15	0.47
1:A:311:LEU:HD22	1:A:327:LEU:HD21	1.97	0.47
1:C:359:THR:HB	1:C:360:PRO:HA	1.96	0.47
1:A:240:PRO:HB2	1:A:243:ALA:HB3	1.97	0.46
1:D:422:PRO:HD3	1:D:456:TYR:CE1	2.50	0.46
1:A:342:PHE:O	1:A:345:ARG:HG3	2.16	0.46
1:D:412:ASP:HA	1:D:413:PRO:C	2.41	0.46
1:A:156:GLN:HG3	1:A:180:VAL:HB	1.98	0.46
1:A:252:PHE:HE2	1:A:254:ASN:HB2	1.81	0.46
1:A:265:GLY:HA2	1:A:291:ALA:HA	1.97	0.46
1:A:4:PRO:HB2	1:A:7:CYS:SG	2.56	0.46
1:B:412:ASP:HA	1:B:413:PRO:C	2.41	0.46
1:C:137:ASP:O	1:C:162:CYS:HA	2.16	0.46
1:A:209:HIS:O	1:A:211:PRO:HD3	2.17	0.45
1:C:412:ASP:HA	1:C:413:PRO:C	2.40	0.45
1:B:182:ARG:NE	6:B:601:HOH:O	2.19	0.45
1:B:252:PHE:HB2	6:B:669:HOH:O	2.15	0.45
1:D:204:VAL:HG22	1:D:228:SER:HB2	1.97	0.45
1:C:419:TRP:CZ2	1:C:458:CYS:HB3	2.51	0.45
1:D:207:ILE:HG23	1:D:210:TRP:CE2	2.51	0.45
1:C:81:ASN:OD1	5:C:501:NAG:H61	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:PHE:CE2	1:A:254:ASN:HB2	2.52	0.45
1:A:395:VAL:HG22	1:A:405:PHE:CE1	2.51	0.45
1:B:119:LEU:HD12	1:B:143:ILE:HG12	1.99	0.45
1:A:344:ARG:HG2	1:A:347:ARG:HH21	1.83	0.44
1:C:67:ILE:HD11	1:C:91:ARG:NH1	2.33	0.44
1:D:39:LEU:HD23	1:D:44:ILE:HD11	1.98	0.44
1:B:398:ASP:HB2	1:B:401:HIS:ND1	2.32	0.44
1:B:41:LYS:HE2	1:B:65:GLU:OE1	2.18	0.44
1:B:440:ASP:OD1	1:B:442:THR:HG23	2.17	0.44
1:C:239:VAL:HB	1:C:241:TYR:CZ	2.52	0.44
1:A:207:ILE:HG23	1:A:210:TRP:CE2	2.52	0.44
1:D:191:ILE:HG22	1:D:220:CYS:HB2	2.00	0.43
1:D:397:VAL:HG21	1:D:403:VAL:CG2	2.48	0.43
1:A:312:GLU:O	1:A:315:VAL:HG13	2.18	0.43
1:C:18:CYS:HB2	1:C:39:LEU:HD23	2.00	0.43
1:C:412:ASP:OD1	1:C:413:PRO:CA	2.63	0.43
1:D:27:PRO:HG2	1:D:30:ILE:HG13	1.99	0.43
1:C:419:TRP:CH2	1:C:458:CYS:HB3	2.53	0.43
4:O:1:NAG:H61	4:O:2:NAG:HN2	1.83	0.43
1:A:93:LYS:O	1:A:116:ILE:HA	2.19	0.43
1:B:436:THR:O	1:B:443:LEU:HA	2.19	0.43
1:C:93:LYS:O	1:C:116:ILE:HA	2.19	0.43
1:D:311:LEU:HD22	1:D:327:LEU:HD21	2.01	0.43
1:B:239:VAL:HB	1:B:241:TYR:CE1	2.53	0.43
1:B:420:LEU:HB3	1:B:457:LEU:HB3	2.00	0.43
1:D:114:ASN:HB3	1:D:115:LYS:H	1.70	0.43
1:B:289:PRO:O	1:B:290:TYR:HB2	2.18	0.43
1:D:89:SER:HB2	1:D:113:GLU:HG3	2.00	0.43
1:B:353:GLN:N	1:B:353:GLN:OE1	2.52	0.43
1:A:353:GLN:NE2	2:F:2:NAG:H2	2.33	0.43
1:D:4:PRO:HA	1:D:5:PRO:HD3	1.83	0.43
1:A:394:GLN:HG2	1:A:472:HIS:HB2	2.00	0.42
1:D:20:ARG:HA	1:D:20:ARG:HD2	1.90	0.42
1:D:160:GLU:HA	1:D:184:ARG:O	2.19	0.42
1:D:274:LEU:HD23	1:D:295:LEU:HD21	2.01	0.42
1:D:342:PHE:O	1:D:345:ARG:HG3	2.20	0.42
1:B:405:PHE:HZ	1:B:473:LEU:HB2	1.85	0.42
1:C:322:LEU:HD12	1:C:322:LEU:HA	1.91	0.42
1:B:342:PHE:CE1	1:B:371:PHE:HB2	2.54	0.42
1:B:239:VAL:CG1	1:B:240:PRO:HD2	2.49	0.42
1:D:256:SER:HB3	1:D:257:TYR:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:397:VAL:CB	1:D:403:VAL:HG21	2.48	0.42
1:B:342:PHE:HE1	1:B:371:PHE:HB2	1.84	0.42
1:C:275:GLN:OE1	1:C:299:ARG:NH2	2.53	0.42
1:A:110:ASP:OD1	1:A:112:SER:OG	2.35	0.42
1:B:279:LEU:HD13	1:B:284:LEU:HD11	2.00	0.42
1:C:242:LEU:O	1:C:245:ARG:HG2	2.20	0.41
1:D:397:VAL:HG21	1:D:403:VAL:HG23	2.02	0.41
1:C:356:THR:HG22	1:C:367:GLU:CG	2.51	0.41
1:A:423:ARG:O	1:A:424:LYS:HB2	2.20	0.41
1:A:40:GLY:HA2	1:A:64:ASN:O	2.19	0.41
1:A:128:TYR:CE2	1:B:320:GLY:HA3	2.56	0.41
1:D:104:SER:HB2	1:D:128:TYR:CZ	2.56	0.41
1:A:140:LEU:HD23	1:A:162:CYS:SG	2.61	0.41
1:A:111:ILE:HD13	1:A:111:ILE:HA	1.93	0.41
1:B:142:TYR:HB2	1:C:420:LEU:HD21	2.03	0.41
1:C:420:LEU:CD1	1:C:459:ILE:HD11	2.44	0.41
1:B:6:ARG:HB3	1:B:21:LYS:HD2	2.03	0.41
1:B:274:LEU:HD23	1:B:295:LEU:HD21	2.03	0.40
1:B:348:LEU:O	1:B:349:ASN:C	2.64	0.40
1:B:227:THR:HG21	1:B:251:ARG:NH2	2.29	0.40
1:A:296:ASN:OD1	1:A:317:HIS:NE2	2.54	0.40
1:D:407:CYS:HB2	1:D:419:TRP:CZ2	2.56	0.40
1:D:7:CYS:HB3	1:D:18:CYS:HB2	1.94	0.40
1:D:112:SER:C	1:D:113:GLU:HG2	2.47	0.40
1:A:80:PHE:O	5:A:501:NAG:H2	2.21	0.40
1:D:111:ILE:O	1:D:111:ILE:CG2	2.69	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 X-ray entries followed by that with respect to entries of similar resolution.

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	466/477 (98%)	439 (94%)	27 (6%)	0	100	100
1	B	471/477 (99%)	445 (94%)	24 (5%)	2 (0%)	30	54
1	C	468/477 (98%)	443 (95%)	25 (5%)	0	100	100
1	D	467/477 (98%)	422 (90%)	44 (9%)	1 (0%)	43	68
All	All	1872/1908 (98%)	1749 (93%)	120 (6%)	3 (0%)	43	68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	361	GLU
1	D	5	PRO
1	B	388	ARG

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 X-ray entries followed by that with respect to entries of similar resolution.

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	422/427 (99%)	414 (98%)	8 (2%)	50	77
1	B	424/427 (99%)	414 (98%)	10 (2%)	43	72
1	C	423/427 (99%)	407 (96%)	16 (4%)	29	58
1	D	422/427 (99%)	407 (96%)	15 (4%)	31	60
All	All	1691/1708 (99%)	1642 (97%)	49 (3%)	37	67

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	THR
1	A	36	LEU
1	A	67	ILE
1	A	280	VAL
1	A	286	VAL
1	A	315	VAL
1	A	319	VAL
1	A	427	VAL

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Mol	Chain	Res	Type
1	B	39	LEU
1	B	118	ILE
1	B	160	GLU
1	B	248	VAL
1	B	315	VAL
1	B	318	SER
1	B	338	LEU
1	B	403	VAL
1	B	427	VAL
1	B	436	THR
1	C	111	ILE
1	C	135	VAL
1	C	165	THR
1	C	248	VAL
1	C	262	THR
1	C	272	LEU
1	C	279	LEU
1	C	280	VAL
1	C	286	VAL
1	C	288	GLU
1	C	319	VAL
1	C	374	VAL
1	C	387	ILE
1	C	420	LEU
1	C	426	LEU
1	C	437	VAL
1	D	9	CYS
1	D	26	VAL
1	D	36	LEU
1	D	88	ARG
1	D	101	THR
1	D	111	ILE
1	D	228	SER
1	D	245	ARG
1	D	248	VAL
1	D	274	LEU
1	D	280	VAL
1	D	315	VAL
1	D	338	LEU
1	D	348	LEU
1	D	475	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	152	ASN
1	A	174	HIS
1	A	187	ASN
1	A	209	HIS
1	A	233	HIS
1	A	349	ASN
1	B	174	HIS
1	B	176	HIS
1	B	349	ASN
1	C	57	HIS
1	C	64	ASN
1	C	145	HIS
1	C	187	ASN
1	C	233	HIS
1	C	317	HIS
1	C	401	HIS
1	C	462	ASN
1	D	81	ASN
1	D	185	HIS
1	D	209	HIS
1	D	296	ASN
1	D	472	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

39 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	E	1	1,2	14,14,15	0.52	0	17,19,21	1.23	2 (11%)
2	NAG	E	2	2	14,14,15	0.61	0	17,19,21	1.37	3 (17%)
2	MAN	E	3	2	11,11,12	0.65	0	15,15,17	0.86	1 (6%)
2	NAG	F	1	1,2	14,14,15	0.50	0	17,19,21	0.85	0
2	NAG	F	2	2	14,14,15	0.54	0	17,19,21	1.07	1 (5%)
2	MAN	F	3	2	11,11,12	0.58	0	15,15,17	0.87	1 (6%)
3	NAG	G	1	1,3	14,14,15	0.43	0	17,19,21	1.57	2 (11%)
3	NAG	G	2	3	14,14,15	0.49	0	17,19,21	1.18	2 (11%)
2	NAG	H	1	1,2	14,14,15	0.52	0	17,19,21	1.08	0
2	NAG	H	2	2	14,14,15	0.61	0	17,19,21	1.46	2 (11%)
2	MAN	H	3	2	11,11,12	0.75	0	15,15,17	1.10	1 (6%)
4	NAG	I	1	1,4	14,14,15	0.50	0	17,19,21	1.74	3 (17%)
4	NAG	I	2	4	14,14,15	0.59	0	17,19,21	1.42	2 (11%)
4	MAN	I	3	4	11,11,12	0.63	0	15,15,17	1.23	1 (6%)
4	MAN	I	4	4	11,11,12	0.64	0	15,15,17	1.02	1 (6%)
2	NAG	J	1	1,2	14,14,15	0.60	0	17,19,21	0.98	1 (5%)
2	NAG	J	2	2	14,14,15	0.55	0	17,19,21	0.91	1 (5%)
2	MAN	J	3	2	11,11,12	0.73	0	15,15,17	1.03	1 (6%)
2	NAG	K	1	1,2	14,14,15	0.59	0	17,19,21	1.14	2 (11%)
2	NAG	K	2	2	14,14,15	0.69	0	17,19,21	1.46	3 (17%)
2	MAN	K	3	2	11,11,12	0.72	0	15,15,17	1.25	2 (13%)
2	NAG	L	1	1,2	14,14,15	0.51	0	17,19,21	1.30	2 (11%)
2	NAG	L	2	2	14,14,15	0.54	0	17,19,21	0.82	0
2	MAN	L	3	2	11,11,12	0.63	0	15,15,17	0.79	1 (6%)
2	NAG	M	1	1,2	14,14,15	0.53	0	17,19,21	1.14	1 (5%)
2	NAG	M	2	2	14,14,15	0.42	0	17,19,21	1.85	2 (11%)
2	MAN	M	3	2	11,11,12	0.56	0	15,15,17	1.06	1 (6%)
2	NAG	N	1	1,2	14,14,15	0.50	0	17,19,21	1.12	0
2	NAG	N	2	2	14,14,15	0.67	0	17,19,21	1.68	4 (23%)
2	MAN	N	3	2	11,11,12	0.61	0	15,15,17	1.83	2 (13%)
4	NAG	O	1	1,4	14,14,15	0.50	0	17,19,21	1.21	1 (5%)
4	NAG	O	2	4	14,14,15	0.52	0	17,19,21	1.19	2 (11%)
4	MAN	O	3	4	11,11,12	0.72	0	15,15,17	0.89	0
4	MAN	O	4	4	11,11,12	0.56	0	15,15,17	1.35	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	P	1	1,3	14,14,15	0.51	0	17,19,21	0.87	0
3	NAG	P	2	3	14,14,15	0.46	0	17,19,21	1.07	1 (5%)
2	NAG	Q	1	1,2	14,14,15	0.51	0	17,19,21	0.89	0
2	NAG	Q	2	2	14,14,15	0.56	0	17,19,21	1.11	1 (5%)
2	MAN	Q	3	2	11,11,12	0.59	0	15,15,17	1.51	2 (13%)

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	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	3/6/23/26	0/1/1/1
2	MAN	E	3	2	1/1/4/5	0/2/19/22	0/1/1/1
2	NAG	F	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	MAN	F	3	2	1/1/4/5	2/2/19/22	0/1/1/1
3	NAG	G	1	1,3	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	G	2	3	1/1/5/7	4/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	H	2	2	-	4/6/23/26	0/1/1/1
2	MAN	H	3	2	1/1/4/5	2/2/19/22	0/1/1/1
4	NAG	I	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	4/6/23/26	0/1/1/1
4	MAN	I	3	4	1/1/4/5	2/2/19/22	0/1/1/1
4	MAN	I	4	4	-	0/2/19/22	0/1/1/1
2	NAG	J	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	MAN	J	3	2	1/1/4/5	2/2/19/22	0/1/1/1
2	NAG	K	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	K	2	2	-	4/6/23/26	0/1/1/1
2	MAN	K	3	2	1/1/4/5	1/2/19/22	0/1/1/1
2	NAG	L	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	L	2	2	-	4/6/23/26	0/1/1/1
2	MAN	L	3	2	1/1/4/5	2/2/19/22	0/1/1/1
2	NAG	M	1	1,2	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	M	2	2	-	2/6/23/26	0/1/1/1
2	MAN	M	3	2	1/1/4/5	2/2/19/22	0/1/1/1
2	NAG	N	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	N	2	2	-	3/6/23/26	0/1/1/1
2	MAN	N	3	2	1/1/4/5	1/2/19/22	1/1/1/1
4	NAG	O	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	O	2	4	-	4/6/23/26	0/1/1/1
4	MAN	O	3	4	1/1/4/5	2/2/19/22	0/1/1/1
4	MAN	O	4	4	-	1/2/19/22	0/1/1/1
3	NAG	P	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	P	2	3	-	2/6/23/26	0/1/1/1
2	NAG	Q	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	4/6/23/26	0/1/1/1
2	MAN	Q	3	2	-	2/2/19/22	1/1/1/1

There are no bond length outliers.

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	2	NAG	C1-O5-C5	6.27	120.58	112.19
2	N	3	MAN	C1-O5-C5	5.78	119.93	112.19
4	I	1	NAG	C1-O5-C5	4.98	118.86	112.19
2	Q	3	MAN	C1-O5-C5	4.80	118.62	112.19
3	G	1	NAG	C1-O5-C5	4.60	118.35	112.19
2	H	2	NAG	C4-C3-C2	4.58	117.74	111.02
4	O	4	MAN	C1-O5-C5	4.26	117.89	112.19
2	N	2	NAG	O4-C4-C3	3.95	119.68	110.38
2	K	2	NAG	C4-C3-C2	3.88	116.71	111.02
2	M	3	MAN	C1-O5-C5	3.52	116.90	112.19
2	L	1	NAG	C1-O5-C5	3.45	116.81	112.19
4	I	2	NAG	C4-C3-C2	3.36	115.94	111.02
2	N	3	MAN	C1-C2-C3	3.28	114.41	109.64
2	F	2	NAG	C1-O5-C5	3.22	116.50	112.19
2	M	1	NAG	O5-C1-C2	-3.20	106.34	111.29
3	P	2	NAG	C1-O5-C5	3.17	116.43	112.19
2	N	2	NAG	O4-C4-C5	3.10	116.97	109.32
4	I	1	NAG	C8-C7-N2	3.10	121.26	116.12
4	O	1	NAG	C1-O5-C5	3.07	116.30	112.19
2	E	1	NAG	C1-O5-C5	3.07	116.30	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	2	NAG	C1-O5-C5	3.05	116.28	112.19
2	J	3	MAN	C1-C2-C3	3.03	114.06	109.64
2	Q	2	NAG	C4-C3-C2	2.90	115.26	111.02
3	G	2	NAG	C1-O5-C5	2.88	116.04	112.19
4	I	3	MAN	C1-C2-C3	2.87	113.82	109.64
2	K	1	NAG	C1-O5-C5	2.85	116.00	112.19
2	N	2	NAG	C3-C4-C5	-2.68	105.37	110.23
4	I	4	MAN	C1-O5-C5	2.63	115.71	112.19
2	E	2	NAG	C4-C3-C2	2.63	114.87	111.02
2	L	3	MAN	C1-O5-C5	2.59	115.66	112.19
2	J	1	NAG	C1-C2-N2	-2.47	106.53	110.43
2	K	3	MAN	C1-C2-C3	2.47	113.24	109.64
4	I	2	NAG	O5-C5-C6	2.39	112.32	107.66
2	E	3	MAN	O5-C5-C6	2.39	112.31	107.66
3	G	1	NAG	O5-C5-C6	2.36	112.25	107.66
2	H	2	NAG	O4-C4-C3	-2.35	104.84	110.38
2	E	2	NAG	O5-C1-C2	-2.34	107.67	111.29
4	I	1	NAG	C2-N2-C7	2.33	126.02	122.90
2	N	2	NAG	C4-C3-C2	-2.31	107.64	111.02
2	E	2	NAG	C3-C4-C5	2.30	114.41	110.23
2	K	2	NAG	C1-O5-C5	2.28	115.24	112.19
2	M	2	NAG	O5-C1-C2	2.23	114.75	111.29
3	G	2	NAG	C4-C3-C2	-2.21	107.77	111.02
4	O	2	NAG	C2-N2-C7	2.19	125.83	122.90
2	K	2	NAG	O4-C4-C3	-2.18	105.25	110.38
2	E	1	NAG	C3-C4-C5	-2.16	106.32	110.23
2	K	1	NAG	O5-C1-C2	-2.14	107.98	111.29
2	H	3	MAN	C1-C2-C3	2.13	112.75	109.64
2	Q	3	MAN	C1-C2-C3	2.10	112.70	109.64
2	K	3	MAN	C1-O5-C5	2.05	114.94	112.19
4	O	2	NAG	C8-C7-N2	2.05	119.51	116.12
2	F	3	MAN	C1-O5-C5	2.03	114.91	112.19
4	O	4	MAN	C1-C2-C3	2.03	112.60	109.64
2	L	1	NAG	C8-C7-N2	2.02	119.47	116.12

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	E	3	MAN	C1
2	F	3	MAN	C1
2	H	3	MAN	C1
2	J	3	MAN	C1

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Mol	Chain	Res	Type	Atom
2	K	3	MAN	C1
2	L	3	MAN	C1
2	M	3	MAN	C1
2	N	3	MAN	C1
3	G	1	NAG	C1
3	G	2	NAG	C1
4	I	3	MAN	C5
4	O	3	MAN	C1

All (85) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	2	NAG	C8-C7-N2-C2
2	H	2	NAG	O7-C7-N2-C2
2	K	1	NAG	C8-C7-N2-C2
2	K	1	NAG	O7-C7-N2-C2
2	L	1	NAG	C8-C7-N2-C2
2	L	1	NAG	O7-C7-N2-C2
2	L	2	NAG	C8-C7-N2-C2
2	N	2	NAG	C8-C7-N2-C2
2	N	2	NAG	O7-C7-N2-C2
3	G	2	NAG	C8-C7-N2-C2
3	G	2	NAG	O7-C7-N2-C2
3	P	2	NAG	C8-C7-N2-C2
3	P	2	NAG	O7-C7-N2-C2
3	G	1	NAG	C8-C7-N2-C2
3	P	1	NAG	C8-C7-N2-C2
3	P	1	NAG	O7-C7-N2-C2
4	O	3	MAN	O5-C5-C6-O6
2	M	2	NAG	O5-C5-C6-O6
2	L	2	NAG	O7-C7-N2-C2
3	G	1	NAG	O7-C7-N2-C2
4	O	2	NAG	C8-C7-N2-C2
2	K	2	NAG	O5-C5-C6-O6
2	Q	3	MAN	O5-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
4	I	3	MAN	O5-C5-C6-O6
4	O	3	MAN	C4-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
4	I	3	MAN	C4-C5-C6-O6
2	J	3	MAN	O5-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	M	2	NAG	C4-C5-C6-O6
2	F	1	NAG	C8-C7-N2-C2
2	M	1	NAG	C8-C7-N2-C2
2	N	1	NAG	C8-C7-N2-C2
2	N	1	NAG	O7-C7-N2-C2
2	J	2	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
2	M	3	MAN	O5-C5-C6-O6
2	L	3	MAN	O5-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
2	M	3	MAN	C4-C5-C6-O6
2	E	2	NAG	C8-C7-N2-C2
4	O	2	NAG	O7-C7-N2-C2
2	J	3	MAN	C4-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6
4	O	2	NAG	O5-C5-C6-O6
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	M	1	NAG	O7-C7-N2-C2
2	Q	1	NAG	C8-C7-N2-C2
4	I	1	NAG	C8-C7-N2-C2
4	I	1	NAG	O7-C7-N2-C2
4	I	2	NAG	C8-C7-N2-C2
4	I	2	NAG	O7-C7-N2-C2
2	H	3	MAN	O5-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	F	3	MAN	O5-C5-C6-O6
2	Q	3	MAN	C4-C5-C6-O6
2	J	1	NAG	C8-C7-N2-C2
2	Q	1	NAG	O7-C7-N2-C2
2	H	2	NAG	C4-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	J	1	NAG	O7-C7-N2-C2
2	Q	2	NAG	C8-C7-N2-C2
4	O	4	MAN	O5-C5-C6-O6
2	L	3	MAN	C4-C5-C6-O6
2	K	3	MAN	O5-C5-C6-O6
2	Q	2	NAG	C4-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
4	O	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	N	3	MAN	O5-C5-C6-O6
2	L	2	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	Q	2	NAG	O7-C7-N2-C2
2	H	3	MAN	C4-C5-C6-O6
2	Q	2	NAG	O5-C5-C6-O6
2	M	1	NAG	C4-C5-C6-O6
2	F	3	MAN	C4-C5-C6-O6
2	L	2	NAG	O5-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
2	N	2	NAG	C4-C5-C6-O6
2	K	2	NAG	C8-C7-N2-C2
2	K	2	NAG	O7-C7-N2-C2

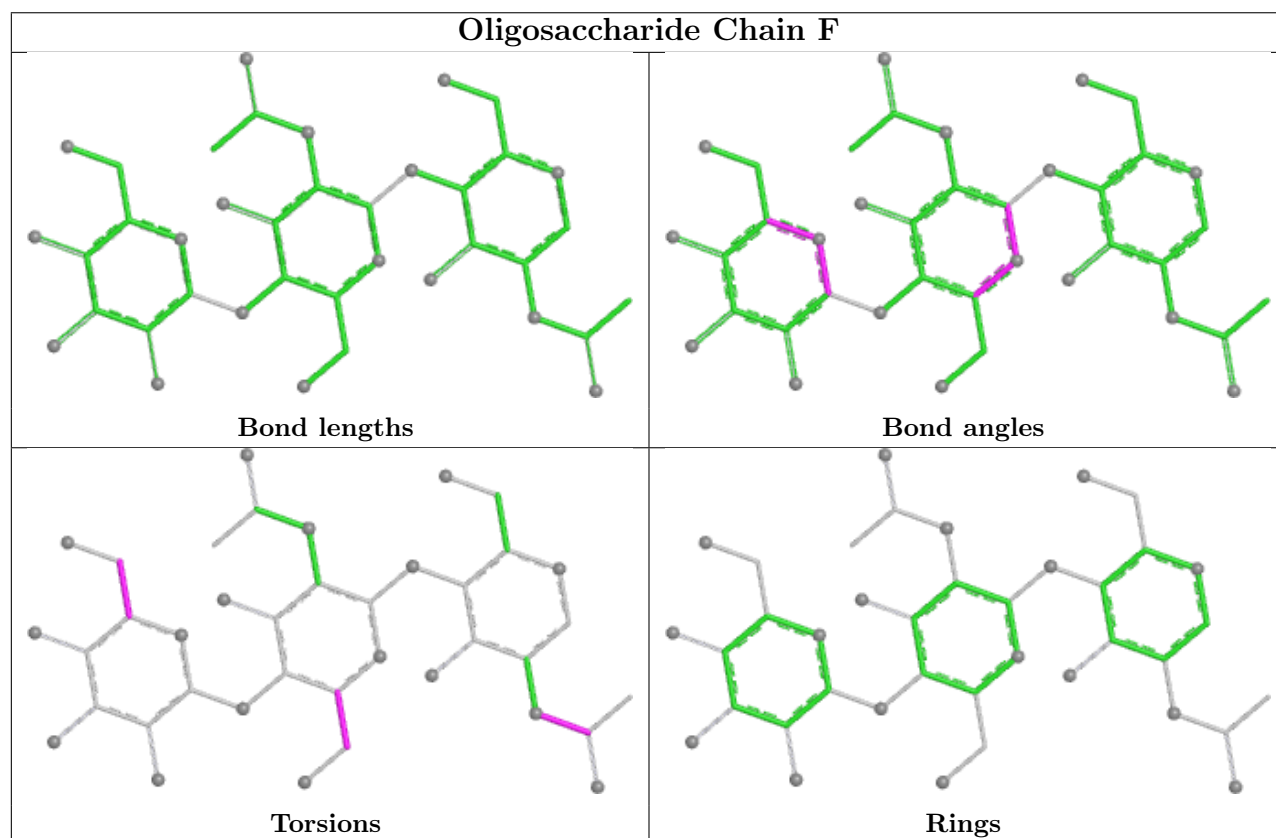
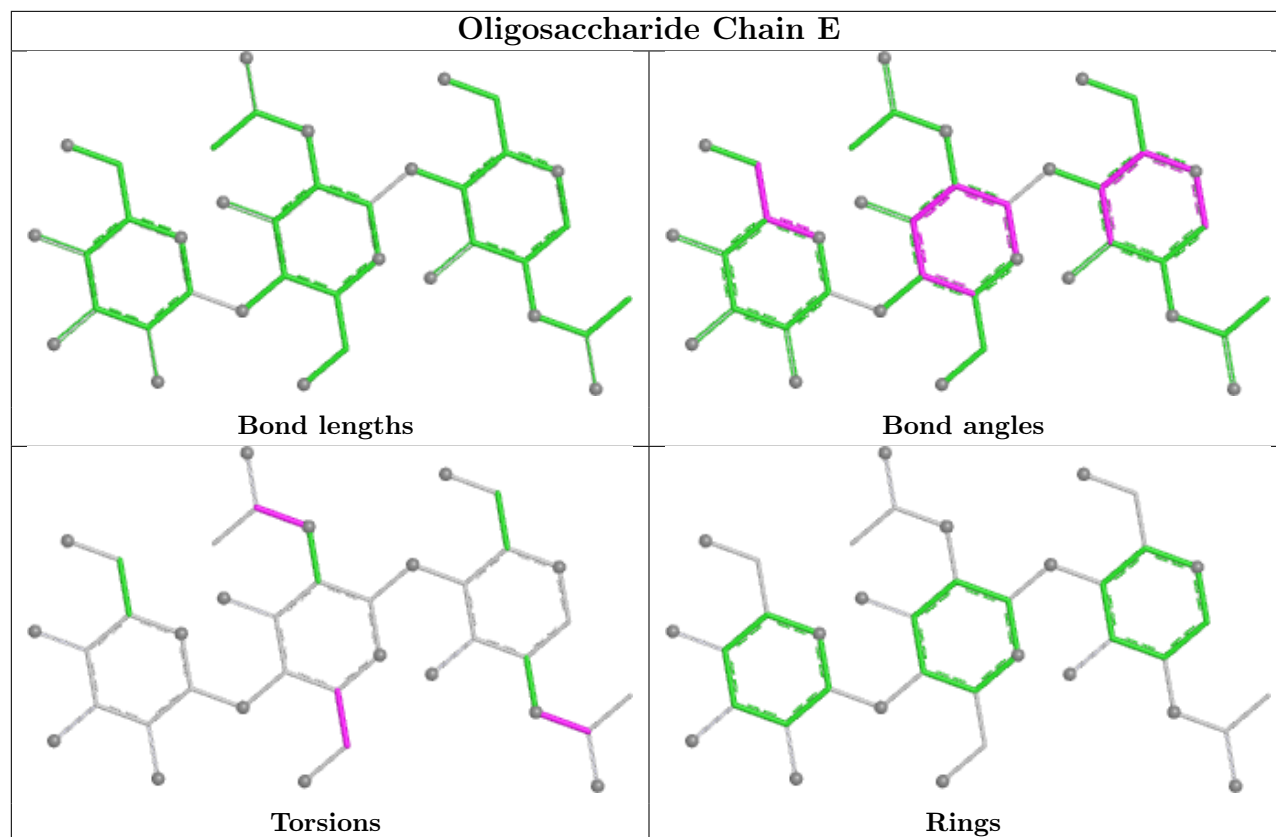
All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	N	3	MAN	C1-C2-C3-C4-C5-O5
2	Q	3	MAN	C1-C2-C3-C4-C5-O5

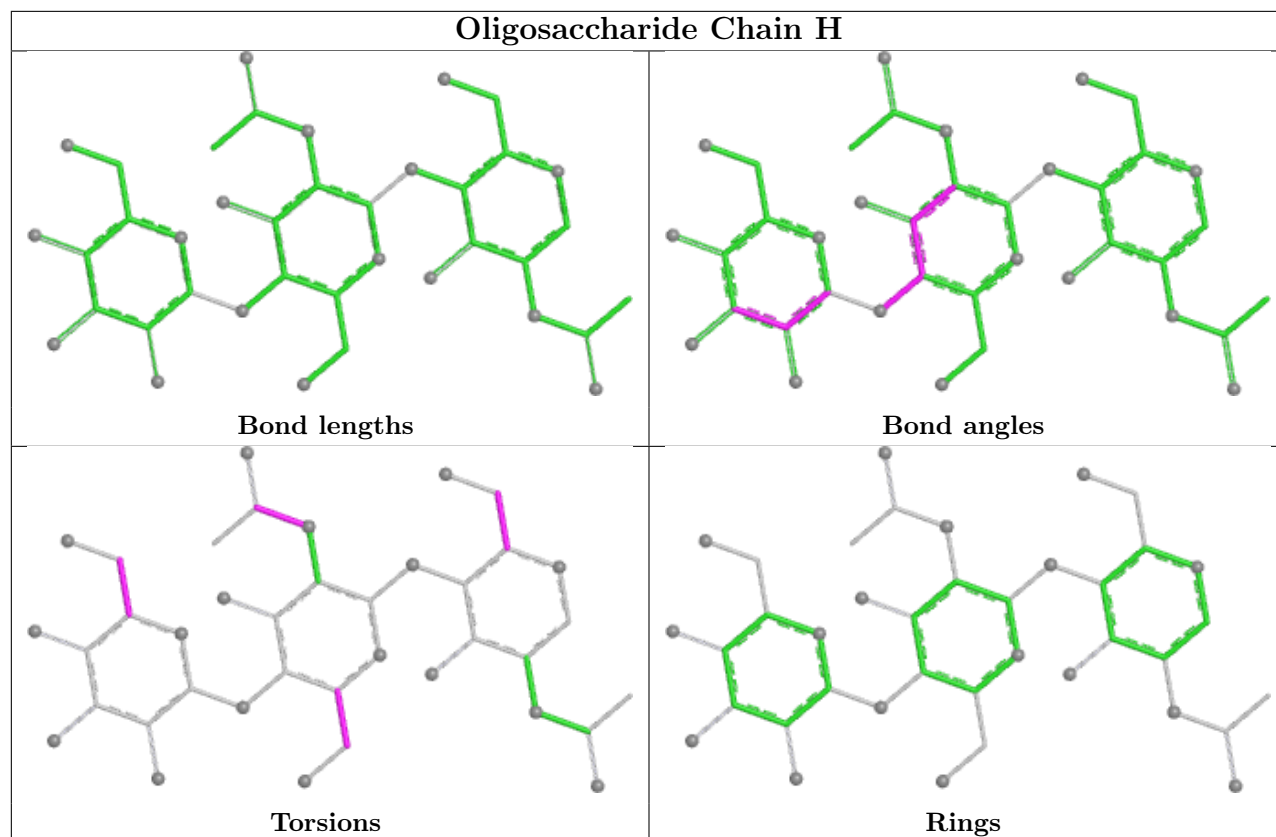
6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	2	NAG	1	0
4	O	2	NAG	1	0
4	O	1	NAG	1	0
2	M	3	MAN	2	0
2	F	2	NAG	1	0
2	J	3	MAN	2	0

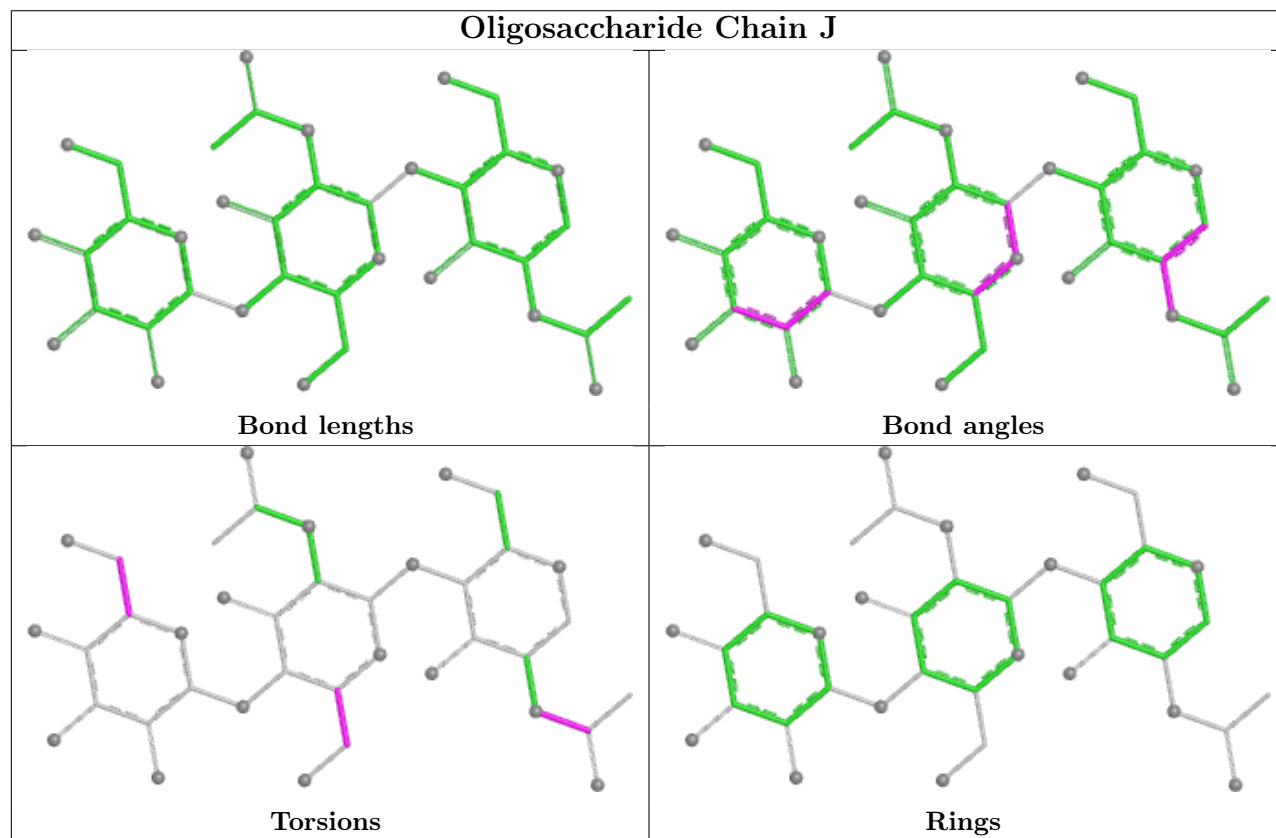
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

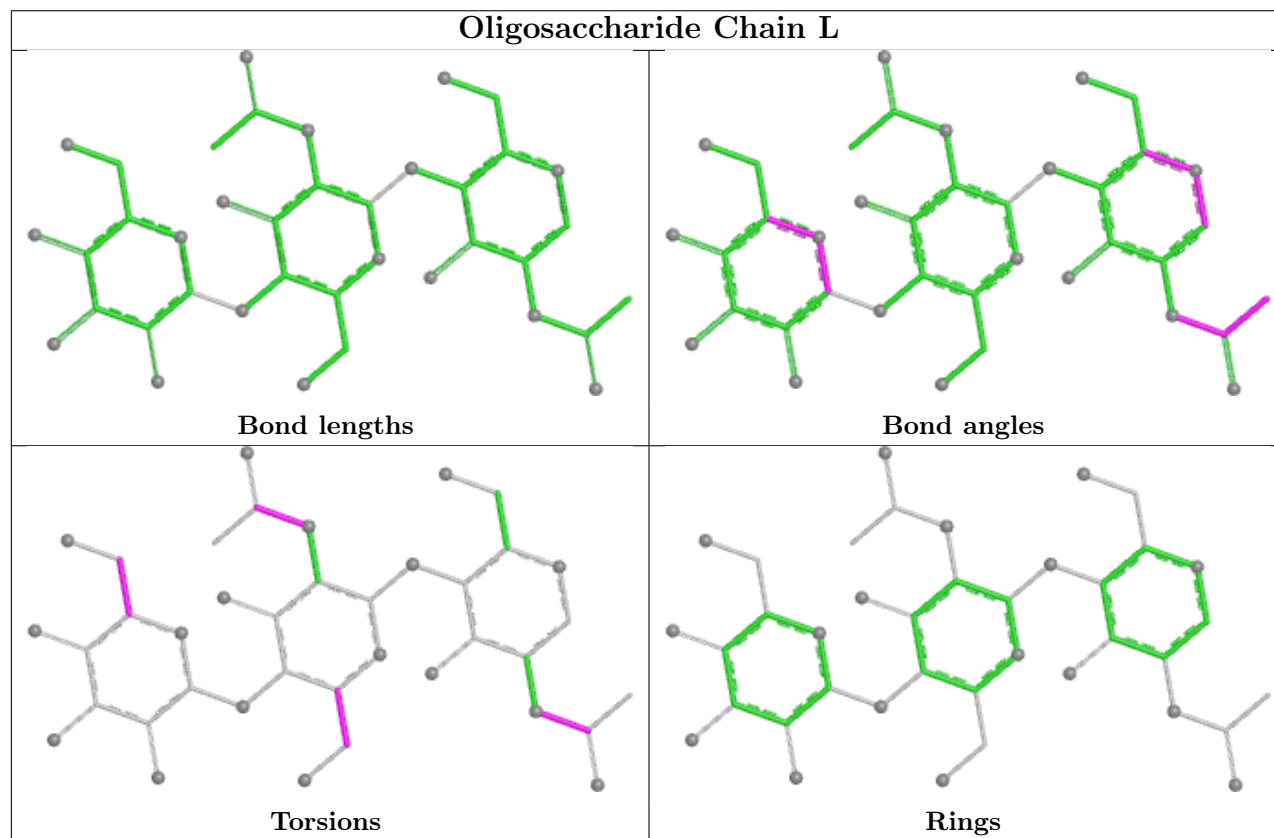
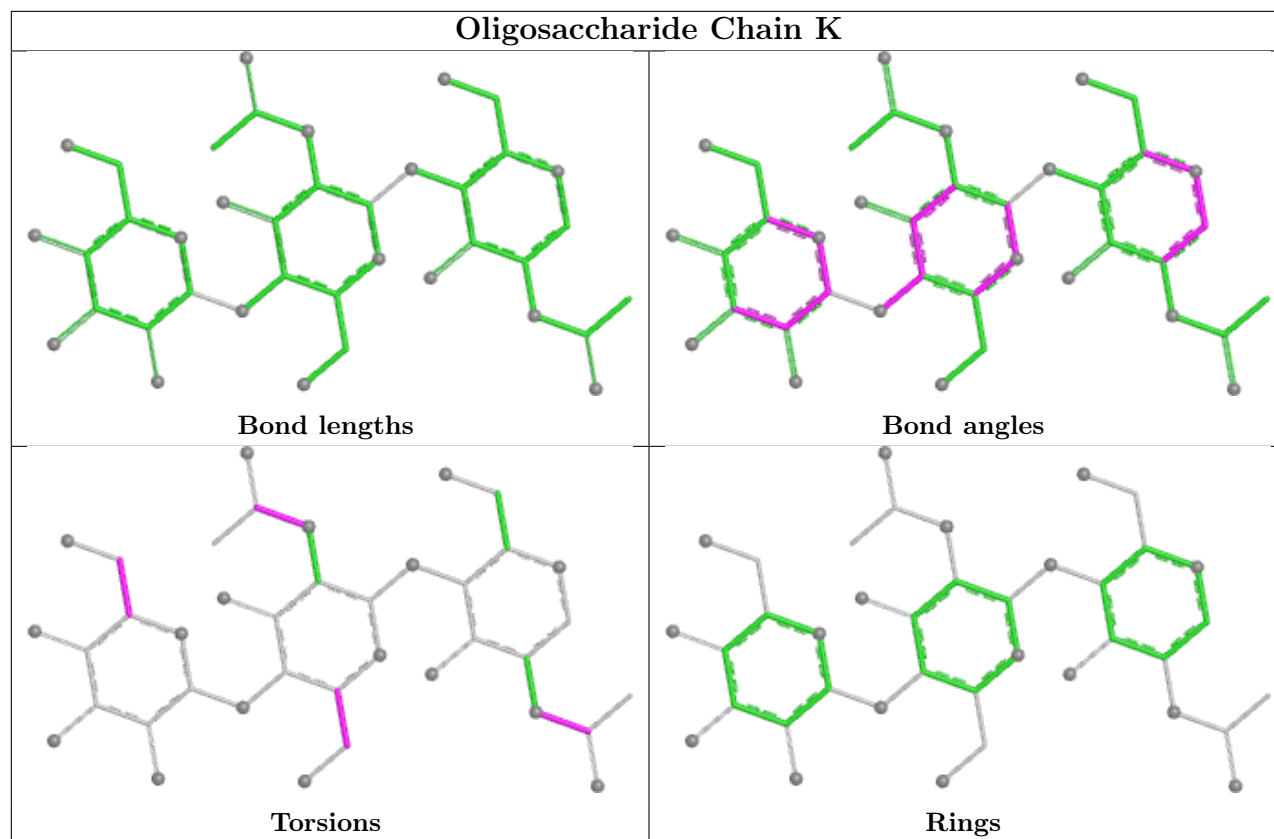


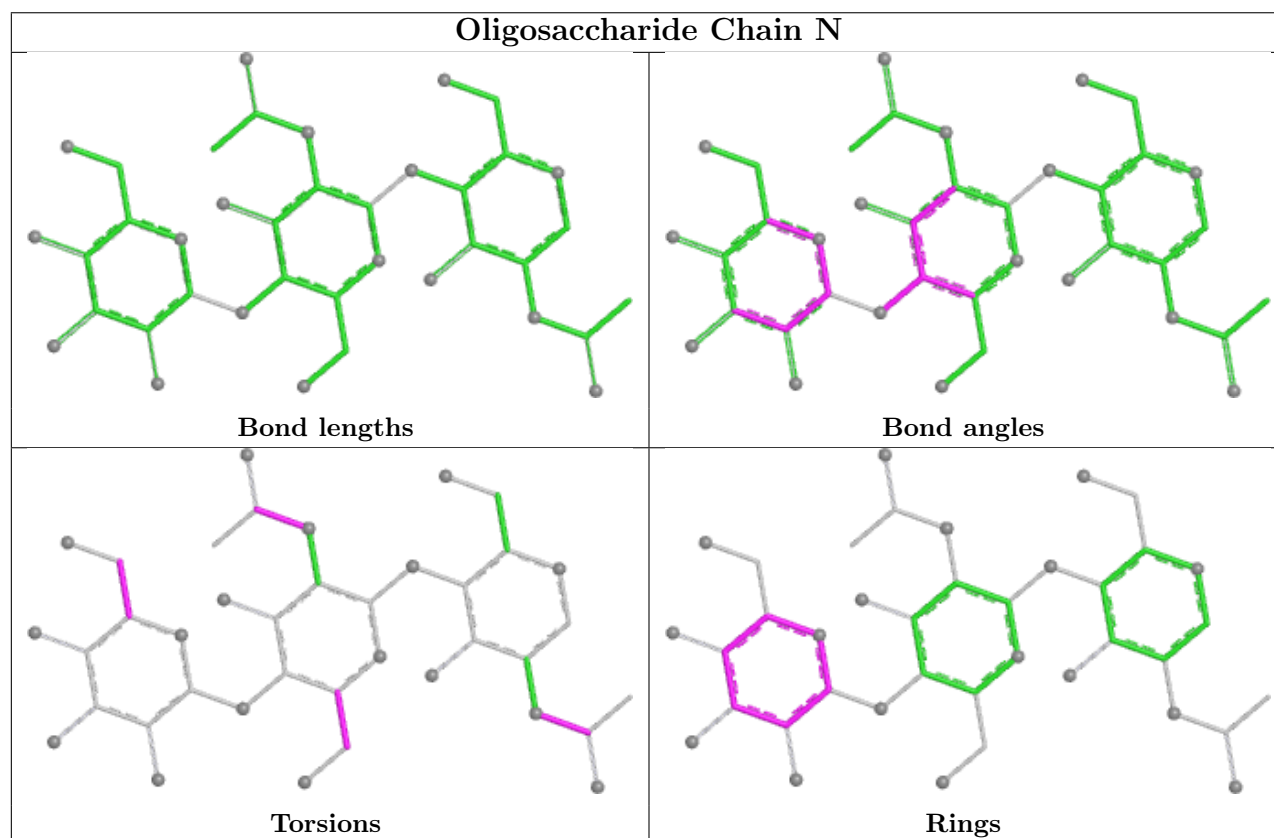
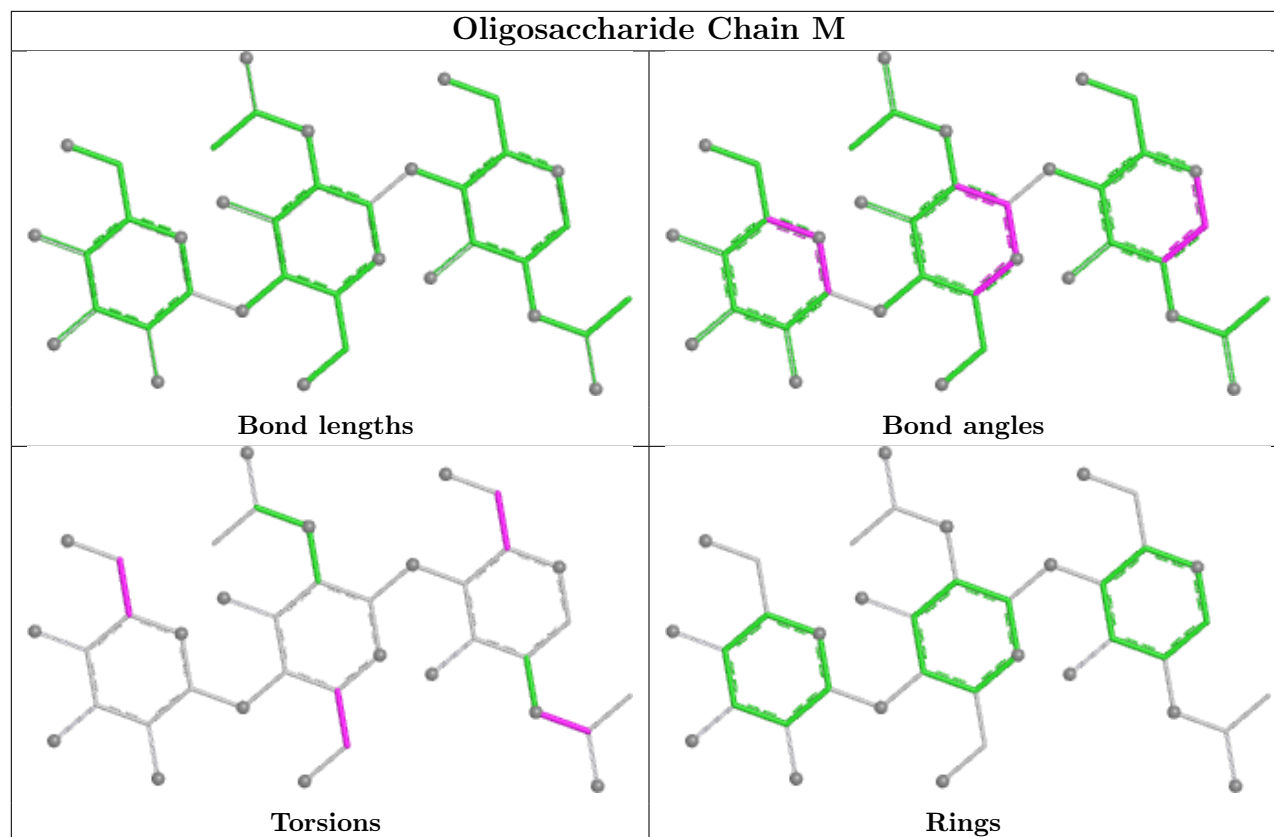
Oligosaccharide Chain H

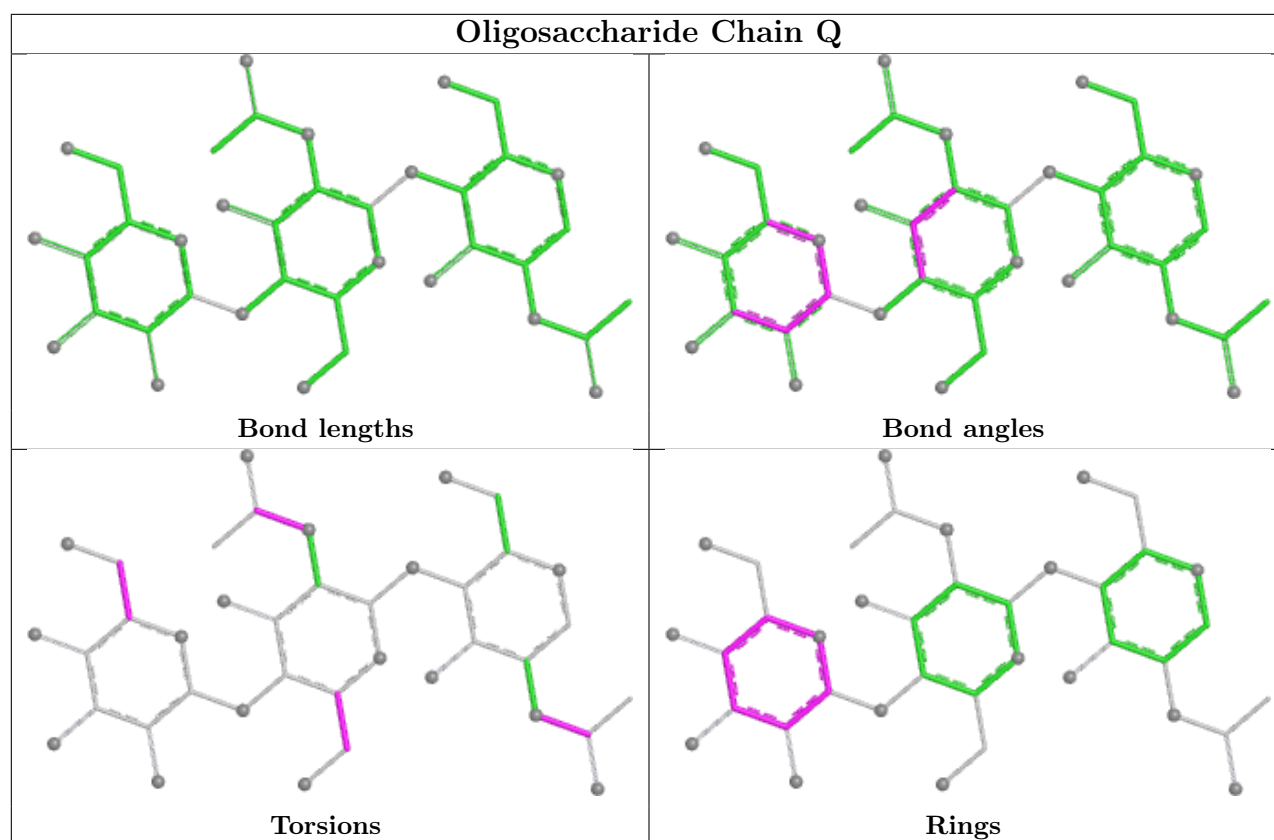


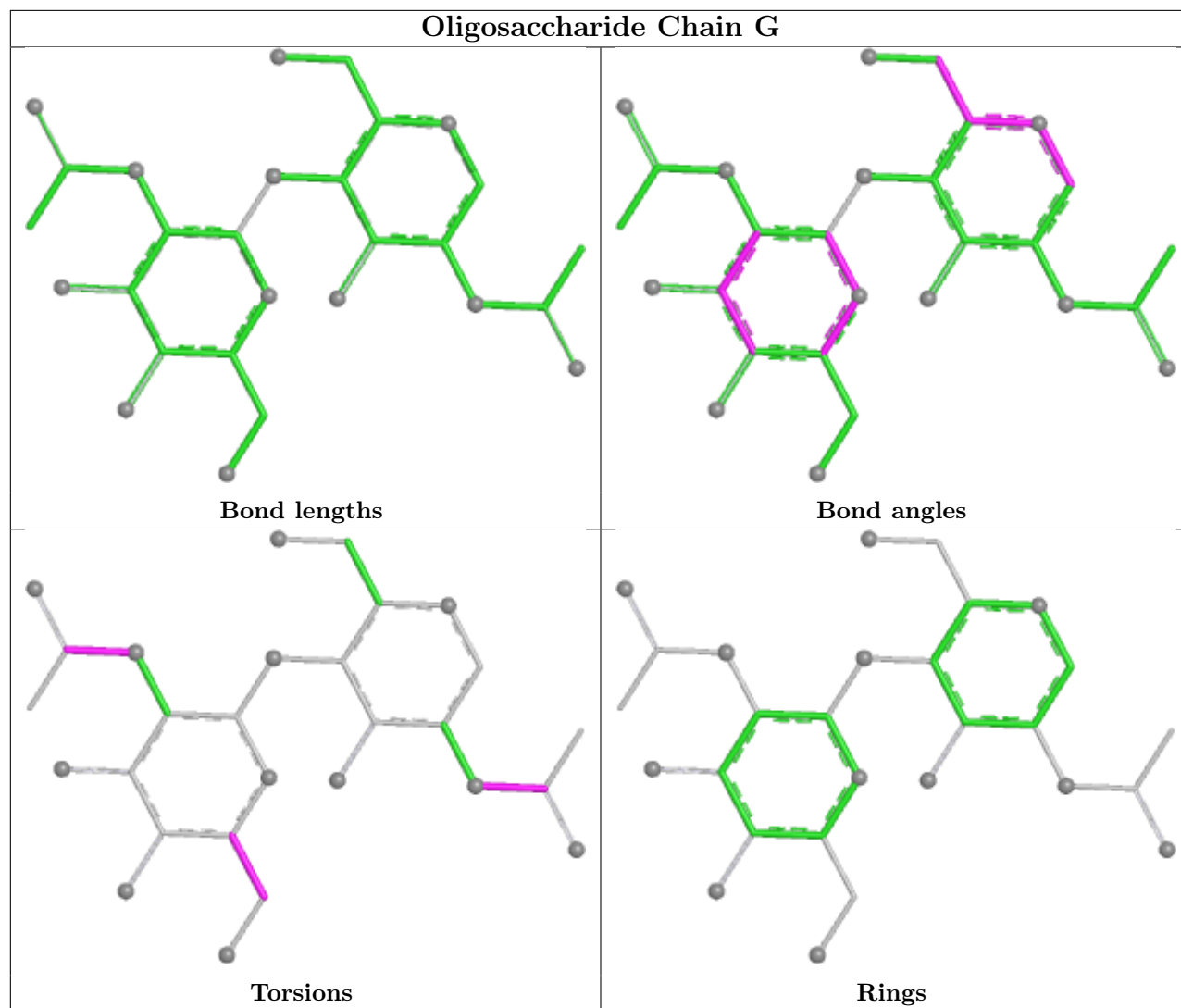
Oligosaccharide Chain J

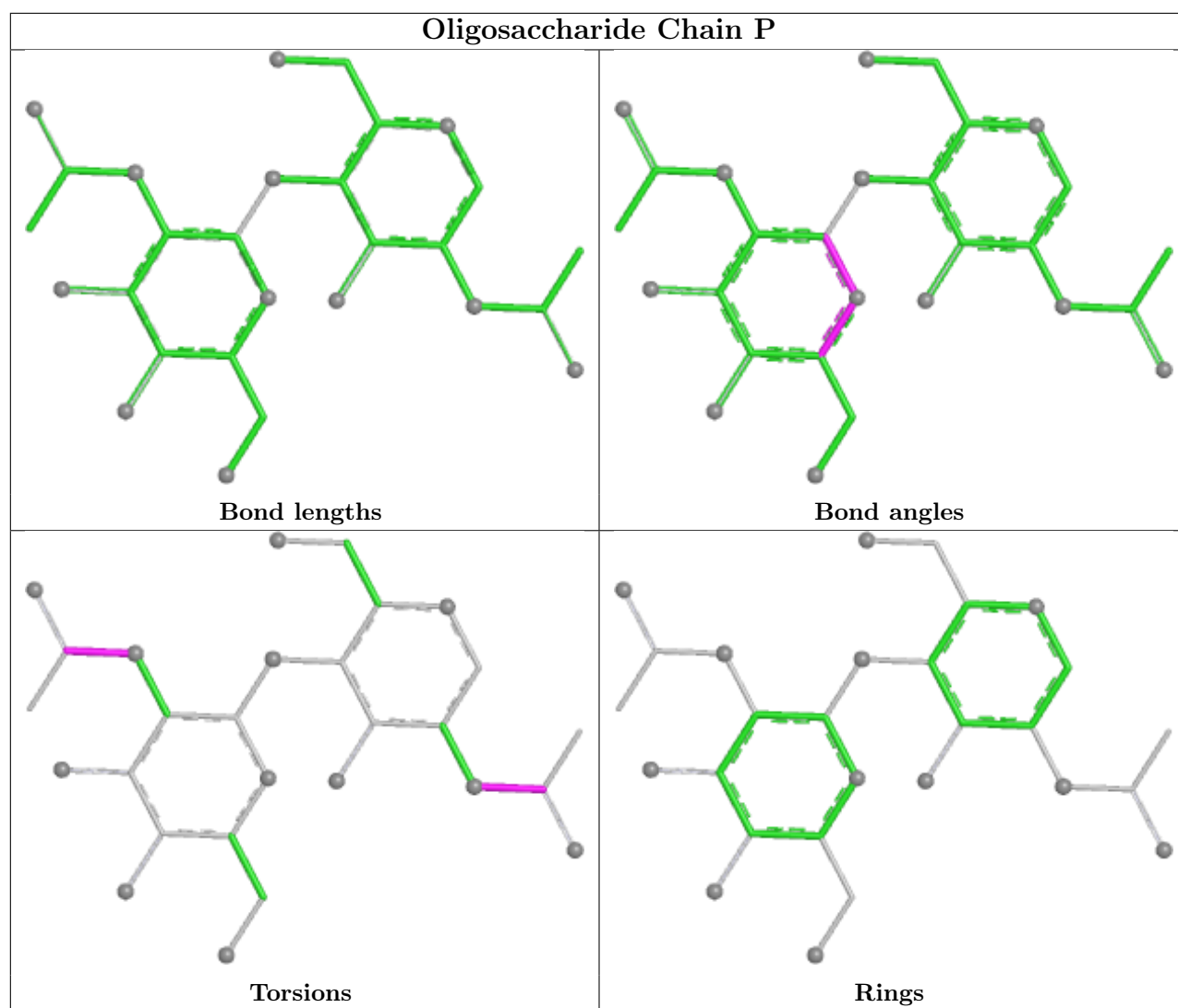


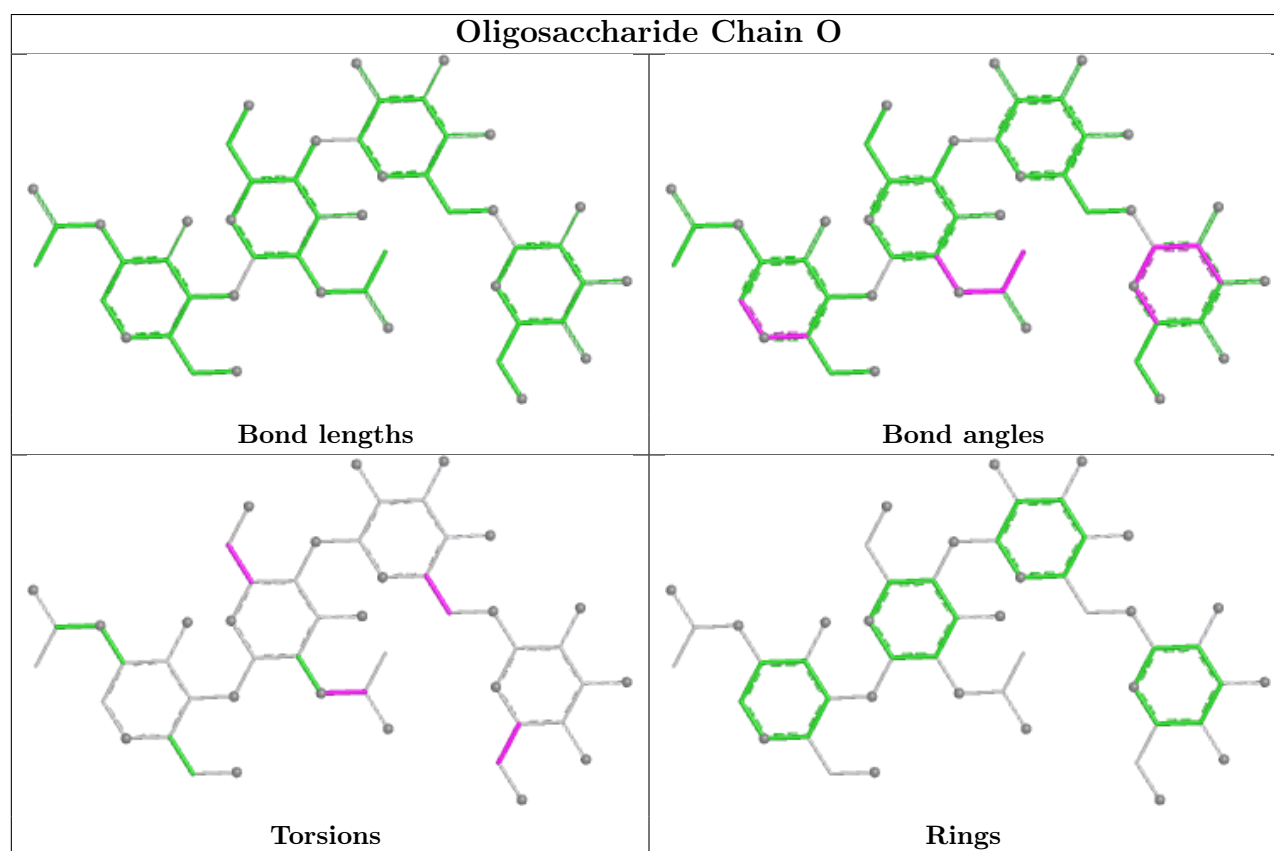
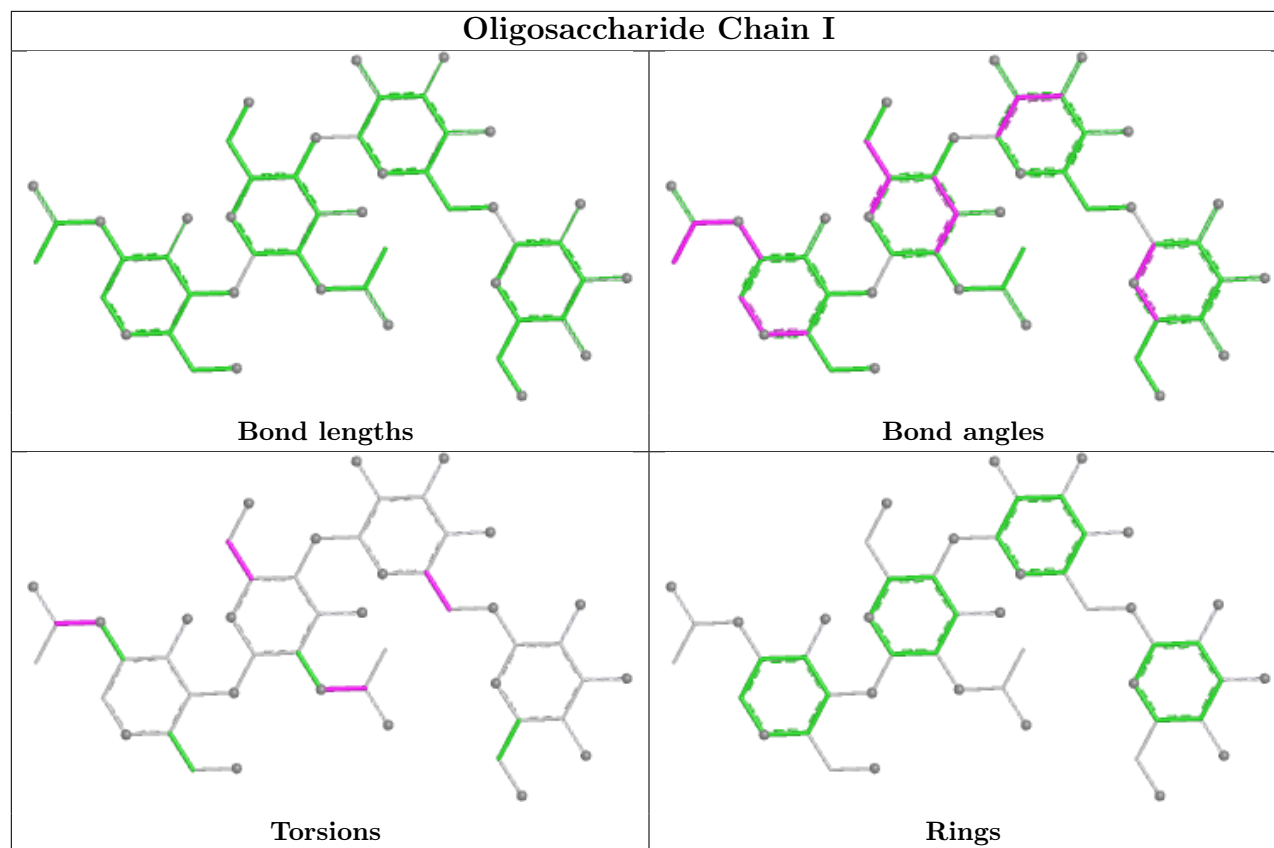












5.6 Ligand geometry

13 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	D	501	1	14,14,15	0.62	0	17,19,21	0.84	0
5	NAG	C	501	1	14,14,15	0.74	0	17,19,21	1.52	2 (11%)
5	NAG	A	502	1	14,14,15	0.46	0	17,19,21	0.97	2 (11%)
5	NAG	C	503	1	14,14,15	1.15	1 (7%)	17,19,21	1.57	4 (23%)
5	NAG	D	502	1	14,14,15	0.49	0	17,19,21	1.15	2 (11%)
5	NAG	A	503	1	14,14,15	0.58	0	17,19,21	0.81	0
5	NAG	C	502	1	14,14,15	0.67	0	17,19,21	0.98	0
5	NAG	B	501	1	14,14,15	0.71	0	17,19,21	1.66	5 (29%)
5	NAG	C	504	1	14,14,15	0.48	0	17,19,21	1.54	4 (23%)
5	NAG	B	503	1	14,14,15	0.55	0	17,19,21	1.38	1 (5%)
5	NAG	B	504	1	14,14,15	0.55	0	17,19,21	0.89	0
5	NAG	B	502	1	14,14,15	0.56	0	17,19,21	0.62	0
5	NAG	A	501	1	14,14,15	0.90	1 (7%)	17,19,21	1.38	2 (11%)

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	501	1	-	0/6/23/26	0/1/1/1
5	NAG	C	501	1	-	3/6/23/26	0/1/1/1
5	NAG	A	502	1	-	3/6/23/26	0/1/1/1
5	NAG	C	503	1	-	6/6/23/26	0/1/1/1
5	NAG	D	502	1	-	3/6/23/26	0/1/1/1
5	NAG	A	503	1	-	4/6/23/26	0/1/1/1
5	NAG	C	502	1	1/1/5/7	4/6/23/26	0/1/1/1
5	NAG	B	501	1	1/1/5/7	4/6/23/26	1/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	504	1	-	3/6/23/26	0/1/1/1
5	NAG	B	503	1	-	2/6/23/26	0/1/1/1
5	NAG	B	504	1	-	2/6/23/26	0/1/1/1
5	NAG	B	502	1	-	5/6/23/26	0/1/1/1
5	NAG	A	501	1	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	503	NAG	O5-C1	-4.03	1.36	1.43
5	A	501	NAG	C1-C2	2.80	1.56	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	503	NAG	C1-O5-C5	4.14	117.73	112.19
5	C	501	NAG	C2-N2-C7	3.62	127.75	122.90
5	C	503	NAG	C1-O5-C5	3.57	116.98	112.19
5	C	504	NAG	O5-C1-C2	-3.24	106.28	111.29
5	D	502	NAG	C1-O5-C5	3.06	116.28	112.19
5	C	504	NAG	C4-C3-C2	-3.06	106.54	111.02
5	A	501	NAG	C1-O5-C5	3.04	116.26	112.19
5	C	503	NAG	O5-C1-C2	-3.03	106.60	111.29
5	B	501	NAG	C1-C2-N2	3.03	115.21	110.43
5	A	501	NAG	C2-N2-C7	2.73	126.56	122.90
5	C	503	NAG	C4-C3-C2	-2.71	107.05	111.02
5	B	501	NAG	C4-C3-C2	-2.61	107.19	111.02
5	B	501	NAG	O5-C5-C6	2.60	112.72	107.66
5	B	501	NAG	C8-C7-N2	2.46	120.19	116.12
5	C	503	NAG	C1-C2-N2	2.36	114.15	110.43
5	B	501	NAG	O7-C7-C8	-2.28	117.99	122.05
5	C	501	NAG	O5-C5-C4	-2.20	105.46	110.83
5	D	502	NAG	O5-C1-C2	-2.17	107.93	111.29
5	C	504	NAG	C1-O5-C5	2.17	115.09	112.19
5	C	504	NAG	C1-C2-N2	2.17	113.85	110.43
5	A	502	NAG	C2-N2-C7	2.08	125.69	122.90
5	A	502	NAG	C1-O5-C5	2.03	114.91	112.19

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	501	NAG	C5
5	C	502	NAG	C1

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	502	NAG	C3-C2-N2-C7
5	A	502	NAG	C8-C7-N2-C2
5	A	502	NAG	O7-C7-N2-C2
5	B	502	NAG	C8-C7-N2-C2
5	B	502	NAG	O7-C7-N2-C2
5	B	504	NAG	C8-C7-N2-C2
5	B	504	NAG	O7-C7-N2-C2
5	C	501	NAG	C1-C2-N2-C7
5	C	501	NAG	C8-C7-N2-C2
5	C	501	NAG	O7-C7-N2-C2
5	C	502	NAG	C8-C7-N2-C2
5	C	502	NAG	O7-C7-N2-C2
5	C	504	NAG	C8-C7-N2-C2
5	C	504	NAG	O7-C7-N2-C2
5	D	502	NAG	C8-C7-N2-C2
5	D	502	NAG	O7-C7-N2-C2
5	A	503	NAG	C8-C7-N2-C2
5	A	503	NAG	O7-C7-N2-C2
5	C	503	NAG	C8-C7-N2-C2
5	C	503	NAG	O7-C7-N2-C2
5	B	501	NAG	O5-C5-C6-O6
5	B	501	NAG	C4-C5-C6-O6
5	B	503	NAG	C8-C7-N2-C2
5	C	503	NAG	C4-C5-C6-O6
5	B	501	NAG	C8-C7-N2-C2
5	B	501	NAG	O7-C7-N2-C2
5	B	503	NAG	O7-C7-N2-C2
5	C	503	NAG	O5-C5-C6-O6
5	B	502	NAG	O5-C5-C6-O6
5	C	504	NAG	O5-C5-C6-O6
5	B	502	NAG	C3-C2-N2-C7
5	C	502	NAG	C4-C5-C6-O6
5	A	503	NAG	C4-C5-C6-O6
5	D	502	NAG	C4-C5-C6-O6
5	B	502	NAG	C4-C5-C6-O6
5	A	503	NAG	O5-C5-C6-O6
5	A	501	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
5	C	503	NAG	C3-C2-N2-C7
5	C	502	NAG	O5-C5-C6-O6
5	C	503	NAG	C1-C2-N2-C7

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	501	NAG	C1-C2-C3-C4-C5-O5

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	501	NAG	2	0
5	A	501	NAG	1	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.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.