



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:23 AM UTC

PDB ID : 3I27 / pdb_00003i27
Title : Structure of bovine torovirus Hemagglutinin-Esterase in complex with receptor
Authors : Zeng, Q.H.; Huizinga, E.G.
Deposited on : 2009-06-29
Resolution : 2.00 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:

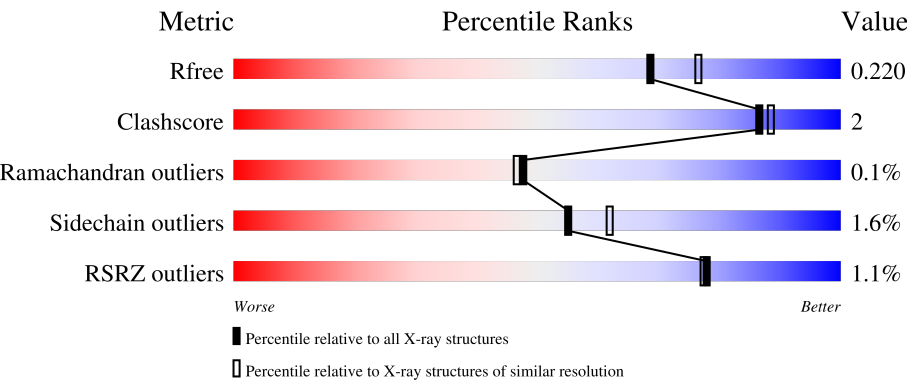
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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.



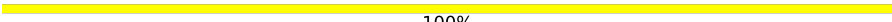
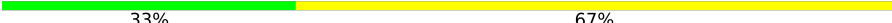
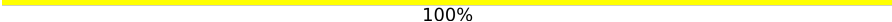
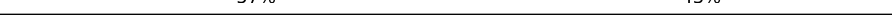
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	384	90%5%5%
1	B	384	90%•5%
1	C	384	2% 84%8%•7%
1	D	384	2% 92%•••
2	E	3	100%

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Mol	Chain	Length	Quality of chain
2	H	3	 100%
2	J	3	 33% 67%
3	F	2	 100%
3	G	2	 50% 50%
3	I	2	 50% 50%
3	K	2	 50% 50%
3	L	2	 50% 50%
4	M	7	 57% 43%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12866 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 Hemagglutinin-esterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total	C	N	O	S	0	0	0
			2862	1821	455	559	27			
1	B	364	Total	C	N	O	S	0	0	0
			2855	1819	454	555	27			
1	C	358	Total	C	N	O	S	0	0	0
			2813	1795	447	544	27			
1	D	369	Total	C	N	O	S	0	0	0
			2889	1837	460	565	27			

There are 24 discrepancies between the modelled and reference sequences:

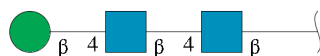
Chain	Residue	Modelled	Actual	Comment	Reference
A	393	ASP	-	expression tag	UNP P0C0V9
A	394	PRO	-	expression tag	UNP P0C0V9
A	395	LEU	-	expression tag	UNP P0C0V9
A	396	VAL	-	expression tag	UNP P0C0V9
A	397	PRO	-	expression tag	UNP P0C0V9
A	398	ARG	-	expression tag	UNP P0C0V9
B	393	ASP	-	expression tag	UNP P0C0V9
B	394	PRO	-	expression tag	UNP P0C0V9
B	395	LEU	-	expression tag	UNP P0C0V9
B	396	VAL	-	expression tag	UNP P0C0V9
B	397	PRO	-	expression tag	UNP P0C0V9
B	398	ARG	-	expression tag	UNP P0C0V9
C	393	ASP	-	expression tag	UNP P0C0V9
C	394	PRO	-	expression tag	UNP P0C0V9
C	395	LEU	-	expression tag	UNP P0C0V9
C	396	VAL	-	expression tag	UNP P0C0V9
C	397	PRO	-	expression tag	UNP P0C0V9
C	398	ARG	-	expression tag	UNP P0C0V9
D	393	ASP	-	expression tag	UNP P0C0V9
D	394	PRO	-	expression tag	UNP P0C0V9
D	395	LEU	-	expression tag	UNP P0C0V9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	396	VAL	-	expression tag	UNP P0C0V9
D	397	PRO	-	expression tag	UNP P0C0V9
D	398	ARG	-	expression tag	UNP P0C0V9

- Molecule 2 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.



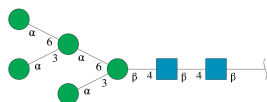
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	H	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	J	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



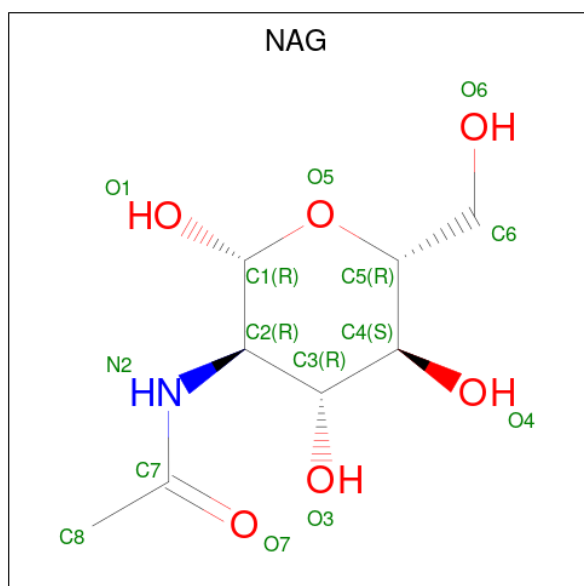
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	L	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[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.



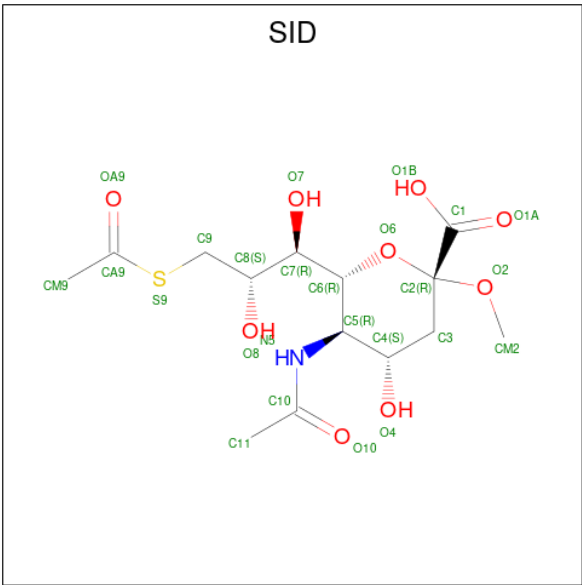
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	M	7	Total	C	N	O	0	0	0
			83	46	2	35			

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



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	B	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 methyl 9-S-acetyl-5-acetamido-3,5-dideoxy-9-thio-D-glycero-alpha-D-galacto-n-on-2-ulopyranosidonic acid (CCD ID: SID) (formula: $C_{14}H_{23}NO_9S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	D	1	Total	C	N	O	S	0	0
			25	14	1	9	1		

- Molecule 7 is water.

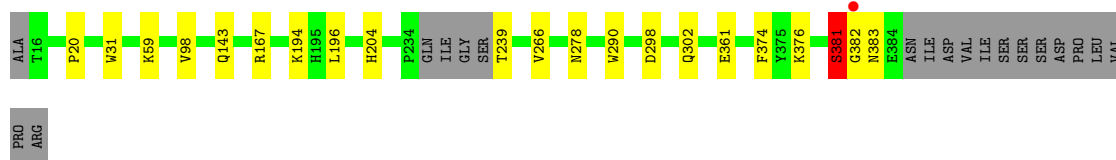
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	347	Total	O	0	0
			347	347		
7	B	338	Total	O	0	0
			338	338		
7	C	65	Total	O	0	0
			65	65		
7	D	262	Total	O	0	0
			262	262		

3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Hemagglutinin-esterase

Chain A: 



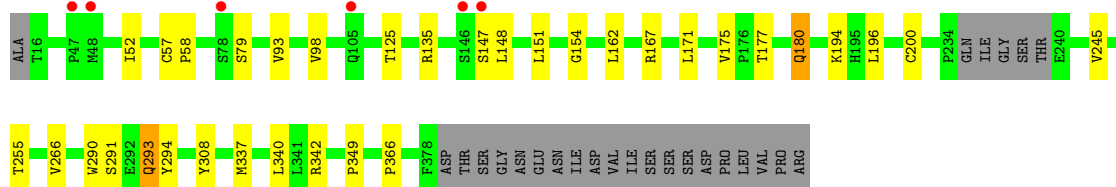
- Molecule 1: Hemagglutinin-esterase

Chain B: 

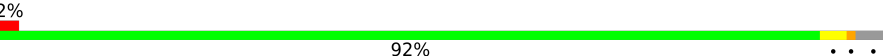


- Molecule 1: Hemagglutinin-esterase

Chain C: 



- Molecule 1: Hemagglutinin-esterase

Chain D: 



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

Chain E:  100%

MAG1
MAG2
BMA3

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

Chain H:  100%

MAG1
MAG2
BMA3

- Molecule 2: 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%

MAG1
MAG2
BMA3

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

Chain F:  100%

MAG1
MAG2

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

Chain G:  50% 50%

MAG1
MAG2

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

Chain I:  50% 50%

MAG1
MAG2

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

Chain K:  50% 50%

MAG1
MAG2

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

Chain L:  50% 50%

MAG1
MAG2

- Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[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 M:  57% 43%

MAG1
MAG2
MAN3
MAN4
MAN5
MAN6
MAN7

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.63Å 112.89Å 273.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.92 – 2.00 48.92 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.92-2.00) 99.6 (48.92-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.179 , 0.210 0.190 , 0.220	Depositor DCC
R_{free} test set	7106 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	22.8	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12866	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SID, MAN, NAG, BMA

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	0.81	0/2949	0.84	1/4021 (0.0%)
1	B	0.80	0/2943	0.81	0/4014
1	C	0.58	0/2900	0.73	0/3954
1	D	0.75	0/2977	0.83	2/4060 (0.0%)
All	All	0.74	0/11769	0.80	3/16049 (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	A	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	D	211	GLY	CA-C-N	5.42	131.46	121.70
1	D	211	GLY	C-N-CA	5.42	131.46	121.70
1	A	381	SER	N-CA-C	5.20	117.03	111.36

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	381	SER	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	2862	0	2669	12	0
1	B	2855	0	2672	10	0
1	C	2813	0	2635	15	0
1	D	2889	0	2697	10	0
2	E	39	0	34	0	0
2	H	39	0	34	0	0
2	J	39	0	34	0	0
3	F	28	0	25	0	0
3	G	28	0	25	0	0
3	I	28	0	25	0	0
3	K	28	0	25	0	0
3	L	28	0	25	0	0
4	M	83	0	70	0	0
5	A	28	0	26	0	0
5	B	14	0	13	1	0
5	D	28	0	26	0	0
6	D	25	0	22	2	0
7	A	347	0	0	3	0
7	B	338	0	0	0	0
7	C	65	0	0	0	0
7	D	262	0	0	0	0
All	All	12866	0	11057	47	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 2.

All (47) 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:D:211:GLY:HA3	1:D:212:SER:CB	2.15	0.76
1:D:211:GLY:HA3	1:D:212:SER:HB2	1.78	0.64
1:C:98:VAL:HG22	1:C:290:TRP:CE2	2.33	0.64
1:A:381:SER:HB2	1:A:383:ASN:H	1.64	0.62
1:B:63:LYS:HD3	1:B:64:SER:N	2.20	0.56
1:D:211:GLY:HA3	1:D:212:SER:HB3	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:PHE:HB3	5:B:5154:NAG:H5	1.87	0.55
1:D:167:ARG:O	1:D:266:VAL:HA	2.07	0.55
1:A:204:HIS:ND1	7:A:671:HOH:O	2.32	0.54
1:D:78:SER:O	1:D:79:SER:CB	2.56	0.53
1:B:378:PHE:O	1:B:379:ASP:HB2	2.10	0.52
1:B:63:LYS:HD3	1:B:63:LYS:C	2.36	0.51
1:B:70:LEU:C	1:B:70:LEU:HD23	2.37	0.50
1:D:207:PHE:CE2	6:D:1001:SID:HM9B	2.48	0.48
1:D:207:PHE:CZ	6:D:1001:SID:HM9B	2.49	0.48
1:C:154:GLY:O	1:C:162:LEU:HD22	2.13	0.48
1:C:196:LEU:C	1:C:196:LEU:HD23	2.38	0.48
1:D:78:SER:O	1:D:79:SER:HB3	2.14	0.48
1:A:98:VAL:HG22	1:A:290:TRP:CE2	2.48	0.47
1:C:93:VAL:HG21	1:C:340:LEU:HD21	1.95	0.47
1:D:98:VAL:HG22	1:D:290:TRP:CE2	2.49	0.47
1:C:349:PRO:HD3	1:C:366:PRO:O	2.16	0.46
1:D:169:ALA:C	1:D:170:LEU:HD12	2.41	0.46
1:B:196:LEU:C	1:B:196:LEU:HD23	2.40	0.46
1:B:108:CYS:O	1:B:156:CYS:HB3	2.17	0.45
1:A:381:SER:CB	1:A:383:ASN:H	2.29	0.45
1:C:167:ARG:O	1:C:266:VAL:HA	2.16	0.45
1:A:167:ARG:O	1:A:266:VAL:HA	2.18	0.44
1:B:167:ARG:O	1:B:266:VAL:HA	2.19	0.43
1:C:180:GLN:HG2	1:C:255:THR:CG2	2.48	0.43
1:A:278:ASN:ND2	7:A:1019:HOH:O	2.52	0.43
1:A:382:GLY:HA2	7:A:959:HOH:O	2.18	0.43
1:C:154:GLY:C	1:C:162:LEU:HD22	2.43	0.43
1:A:196:LEU:C	1:A:196:LEU:HD23	2.44	0.42
1:B:98:VAL:HG22	1:B:290:TRP:CE2	2.54	0.42
1:C:52:ILE:HG22	1:C:337:MET:HG3	2.01	0.42
1:B:111:GLU:H	1:B:111:GLU:CD	2.28	0.42
1:C:291:SER:OG	1:C:293:GLN:NE2	2.47	0.42
1:C:125:THR:HG23	1:C:308:TYR:OH	2.19	0.42
1:C:293:GLN:HG2	1:C:294:TYR:CD1	2.55	0.41
1:A:298:ASP:O	1:A:302:GLN:HG2	2.19	0.41
1:A:374:PHE:CZ	1:A:376:LYS:HD2	2.54	0.41
1:C:57:CYS:N	1:C:58:PRO:CD	2.84	0.41
1:A:20:PRO:HD2	1:A:361:GLU:HG2	2.04	0.40
1:C:151:LEU:HD23	1:C:171:LEU:HD23	2.02	0.40
1:A:31:TRP:CZ2	1:A:59:LYS:HG3	2.56	0.40
1:C:200:CYS:HA	1:C:245:VAL:O	2.22	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	361/384 (94%)	345 (96%)	16 (4%)	0	100	100
1	B	362/384 (94%)	347 (96%)	15 (4%)	0	100	100
1	C	354/384 (92%)	341 (96%)	13 (4%)	0	100	100
1	D	367/384 (96%)	349 (95%)	17 (5%)	1 (0%)	36	35
All	All	1444/1536 (94%)	1382 (96%)	61 (4%)	1 (0%)	48	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	212	SER

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 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	327/344 (95%)	324 (99%)	3 (1%)	70	78
1	B	326/344 (95%)	321 (98%)	5 (2%)	57	64
1	C	321/344 (93%)	311 (97%)	10 (3%)	35	37
1	D	330/344 (96%)	327 (99%)	3 (1%)	70	78
All	All	1304/1376 (95%)	1283 (98%)	21 (2%)	55	62

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	GLN
1	A	194	LYS
1	A	239	THR
1	B	16	THR
1	B	63	LYS
1	B	178	SER
1	B	194	LYS
1	B	342	ARG
1	C	79	SER
1	C	135	ARG
1	C	147	SER
1	C	148	LEU
1	C	175	VAL
1	C	177	THR
1	C	180	GLN
1	C	194	LYS
1	C	293	GLN
1	C	342	ARG
1	D	143	GLN
1	D	236	ILE
1	D	238	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	278	ASN
1	A	373	GLN
1	B	161	GLN
1	B	293	GLN
1	B	302	GLN
1	C	141	GLN
1	C	180	GLN
1	D	43	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 ⓘ

26 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	0.80	1 (7%)	17,19,21	1.25	1 (5%)
2	NAG	E	2	2	14,14,15	0.76	1 (7%)	17,19,21	1.04	2 (11%)
2	BMA	E	3	2	11,11,12	0.52	0	15,15,17	1.11	1 (6%)
3	NAG	F	1	3,1	14,14,15	0.55	0	17,19,21	1.02	1 (5%)
3	NAG	F	2	3	14,14,15	0.61	0	17,19,21	1.33	2 (11%)
3	NAG	G	1	3,1	14,14,15	0.69	0	17,19,21	0.79	0
3	NAG	G	2	3	14,14,15	0.57	0	17,19,21	1.05	2 (11%)
2	NAG	H	1	1,2	14,14,15	0.63	0	17,19,21	1.45	2 (11%)
2	NAG	H	2	2	14,14,15	0.59	0	17,19,21	1.37	3 (17%)
2	BMA	H	3	2	11,11,12	0.50	0	15,15,17	1.35	3 (20%)
3	NAG	I	1	3,1	14,14,15	0.53	0	17,19,21	1.46	3 (17%)
3	NAG	I	2	3	14,14,15	0.67	0	17,19,21	0.70	0
2	NAG	J	1	1,2	14,14,15	0.55	0	17,19,21	1.09	1 (5%)
2	NAG	J	2	2	14,14,15	0.54	0	17,19,21	1.03	1 (5%)
2	BMA	J	3	2	11,11,12	0.44	0	15,15,17	0.70	0
3	NAG	K	1	3,1	14,14,15	0.98	0	17,19,21	1.58	3 (17%)
3	NAG	K	2	3	14,14,15	0.55	0	17,19,21	0.95	0
3	NAG	L	1	3,1	14,14,15	0.85	0	17,19,21	1.24	1 (5%)
3	NAG	L	2	3	14,14,15	0.49	0	17,19,21	0.85	0
4	NAG	M	1	1,4	14,14,15	0.81	0	17,19,21	1.21	1 (5%)
4	NAG	M	2	4	14,14,15	0.78	0	17,19,21	0.96	0
4	BMA	M	3	4	11,11,12	0.27	0	15,15,17	0.90	0
4	MAN	M	4	4	11,11,12	0.68	0	15,15,17	1.27	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	M	5	4	11,11,12	0.61	0	15,15,17	0.73	0
4	MAN	M	6	4	11,11,12	0.53	0	15,15,17	1.00	1 (6%)
4	MAN	M	7	4	11,11,12	0.54	0	15,15,17	0.84	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
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	BMA	E	3	2	-	2/2/19/22	0/1/1/1
3	NAG	F	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	NAG	G	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	1/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	BMA	H	3	2	-	0/2/19/22	0/1/1/1
3	NAG	I	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	1/6/23/26	0/1/1/1
2	BMA	J	3	2	-	0/2/19/22	0/1/1/1
3	NAG	K	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	0/6/23/26	0/1/1/1
3	NAG	L	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	L	2	3	-	2/6/23/26	0/1/1/1
4	NAG	M	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	M	2	4	-	0/6/23/26	0/1/1/1
4	BMA	M	3	4	-	0/2/19/22	0/1/1/1
4	MAN	M	4	4	-	0/2/19/22	0/1/1/1
4	MAN	M	5	4	-	2/2/19/22	0/1/1/1
4	MAN	M	6	4	-	0/2/19/22	0/1/1/1
4	MAN	M	7	4	-	1/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	NAG	O5-C1	-2.35	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2	NAG	O5-C1	-2.11	1.40	1.43

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	1	NAG	O5-C1-C2	-4.11	104.93	111.29
3	I	1	NAG	C1-C2-N2	3.80	116.42	110.43
2	H	2	NAG	C1-O5-C5	3.66	117.09	112.19
2	E	1	NAG	C1-O5-C5	3.58	116.98	112.19
2	H	1	NAG	C1-O5-C5	3.37	116.71	112.19
3	K	1	NAG	C1-O5-C5	3.36	116.69	112.19
2	H	1	NAG	C1-C2-N2	-3.21	105.37	110.43
4	M	4	MAN	C1-O5-C5	3.14	116.39	112.19
3	F	2	NAG	C4-C3-C2	-2.93	106.72	111.02
2	J	1	NAG	C1-O5-C5	2.89	116.06	112.19
3	F	2	NAG	C1-C2-N2	2.87	114.96	110.43
3	F	1	NAG	O5-C1-C2	-2.62	107.24	111.29
2	H	3	BMA	C1-C2-C3	2.56	113.38	109.64
3	G	2	NAG	O6-C6-C5	-2.46	102.95	111.33
2	E	2	NAG	O5-C5-C6	2.39	112.32	107.66
2	E	2	NAG	O5-C1-C2	-2.34	107.67	111.29
4	M	1	NAG	C3-C4-C5	-2.33	106.00	110.23
3	K	1	NAG	O4-C4-C5	-2.26	103.75	109.32
2	H	3	BMA	O5-C5-C6	2.25	112.05	107.66
3	L	1	NAG	O3-C3-C2	-2.25	104.72	109.40
2	H	2	NAG	C2-N2-C7	2.25	125.91	122.90
2	H	2	NAG	O7-C7-N2	2.23	125.92	121.98
3	I	1	NAG	C1-O5-C5	2.16	115.08	112.19
2	E	3	BMA	C2-C3-C4	-2.13	107.12	110.86
3	I	1	NAG	O3-C3-C2	-2.13	104.99	109.40
3	G	2	NAG	C3-C4-C5	-2.03	106.55	110.23
2	J	2	NAG	O5-C5-C6	2.03	111.61	107.66
4	M	6	MAN	C1-O5-C5	2.01	114.88	112.19
2	H	3	BMA	C3-C4-C5	-2.01	106.58	110.23

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	5	MAN	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
4	M	5	MAN	C4-C5-C6-O6

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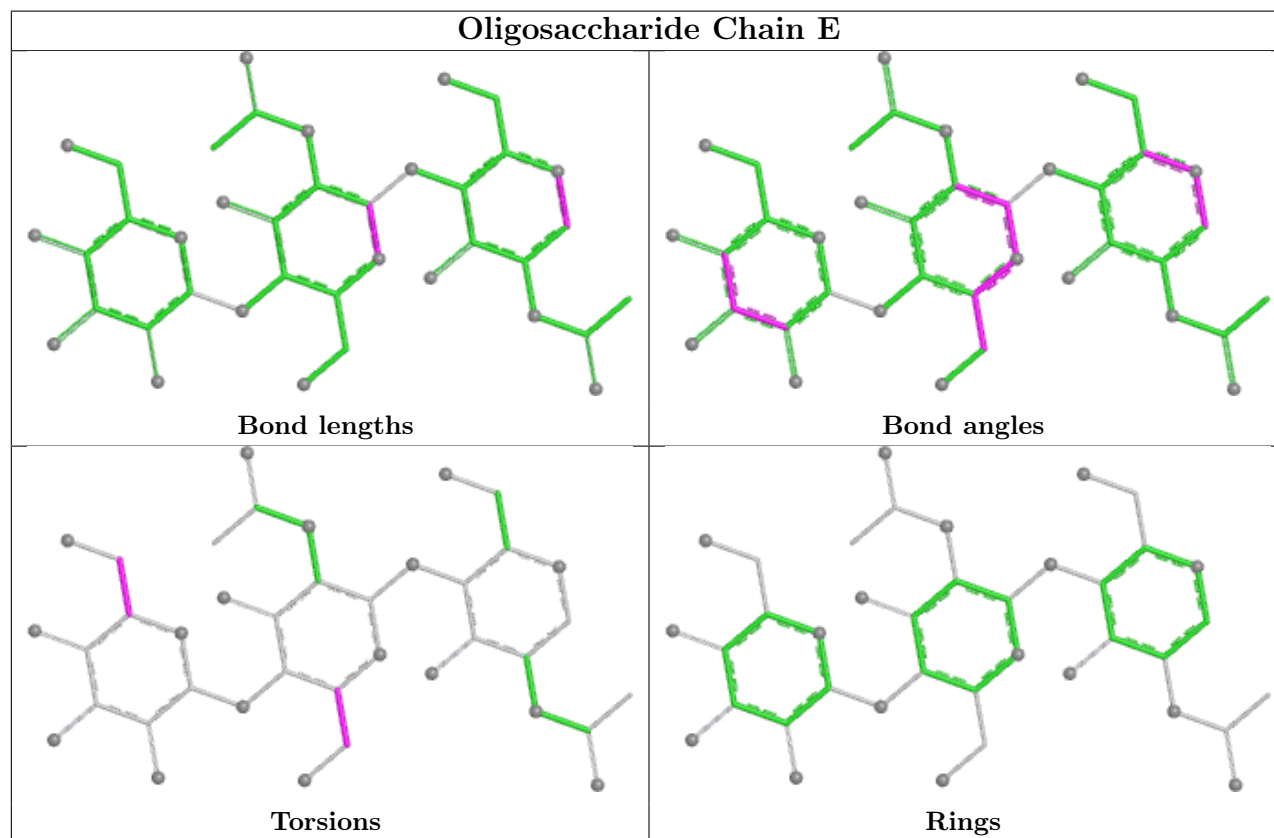
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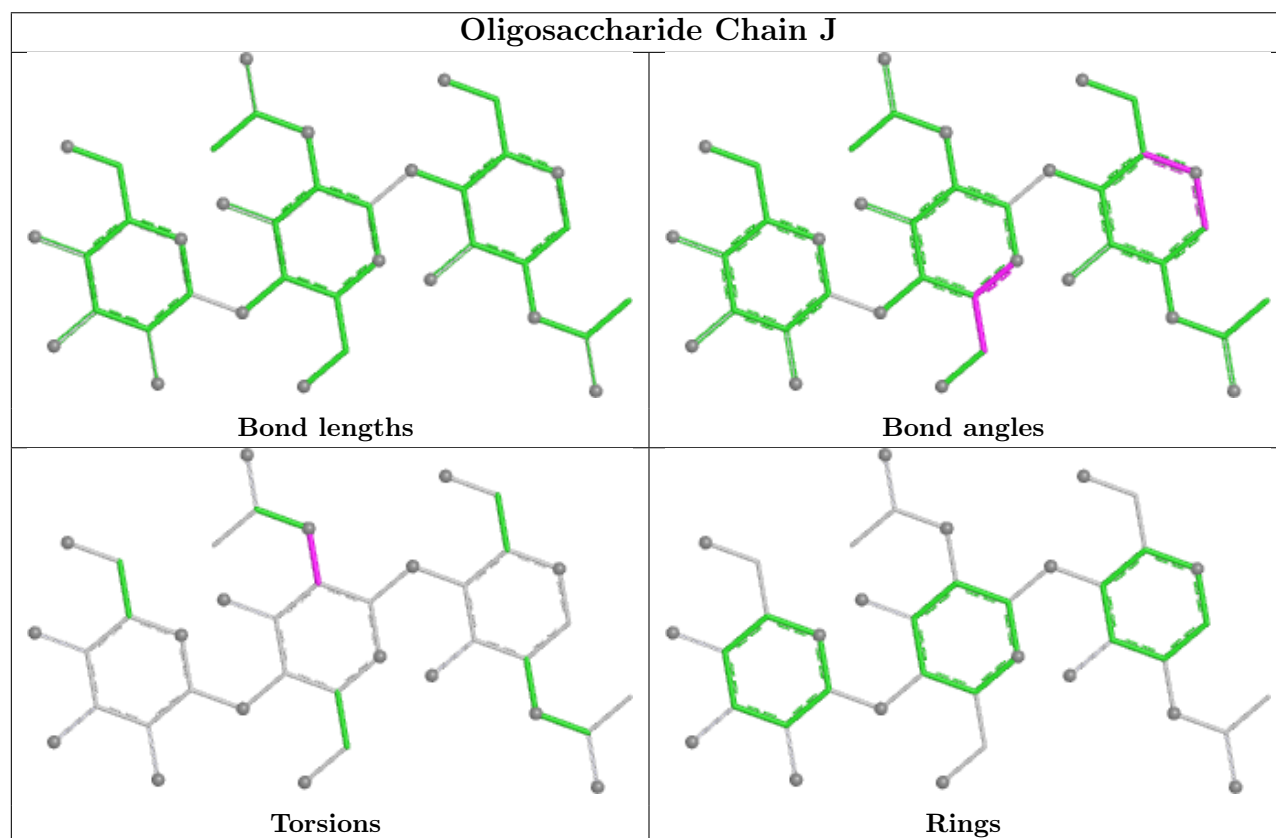
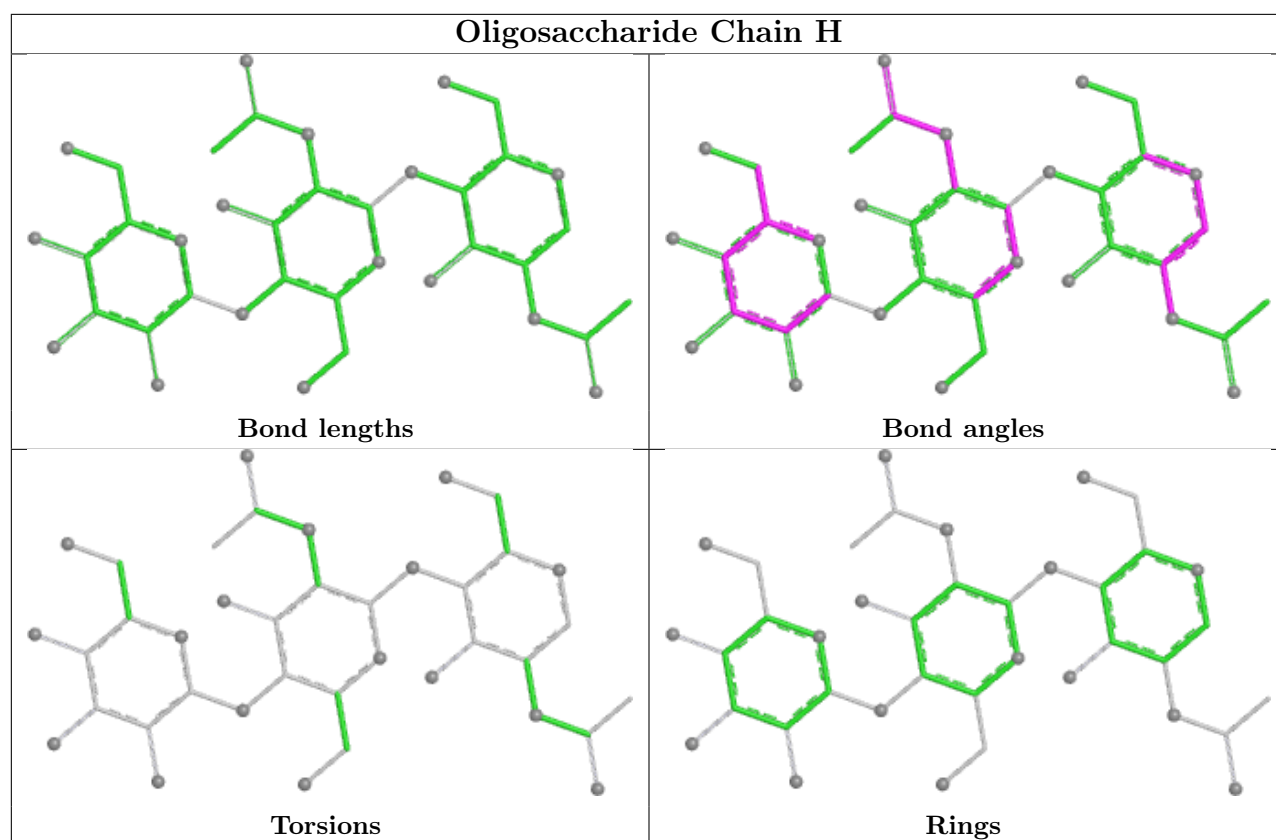
Mol	Chain	Res	Type	Atoms
2	E	2	NAG	O5-C5-C6-O6
3	L	2	NAG	O5-C5-C6-O6
4	M	7	MAN	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
2	E	3	BMA	C4-C5-C6-O6
3	L	2	NAG	C4-C5-C6-O6
2	E	3	BMA	O5-C5-C6-O6
2	J	2	NAG	C1-C2-N2-C7

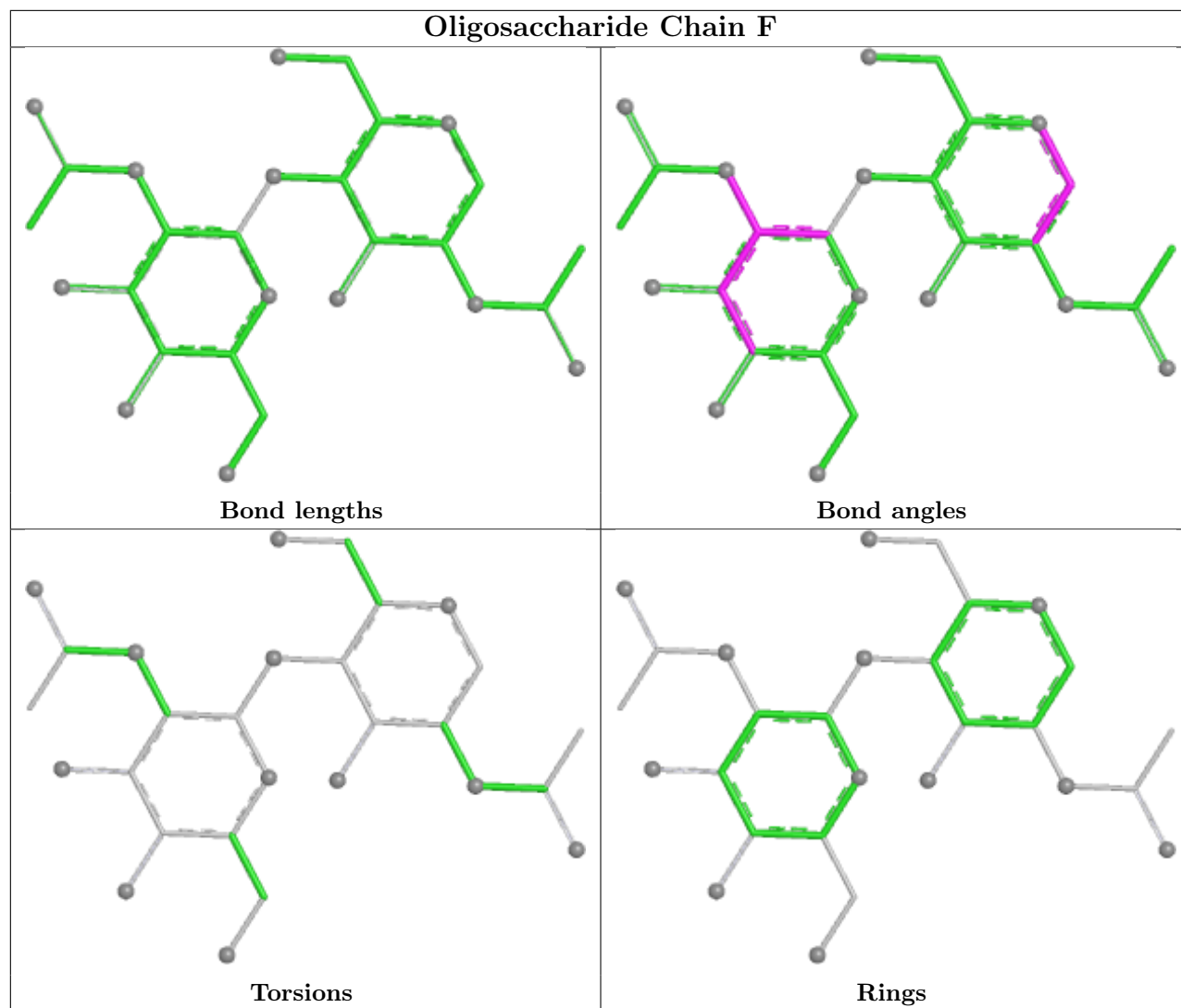
There are no ring outliers.

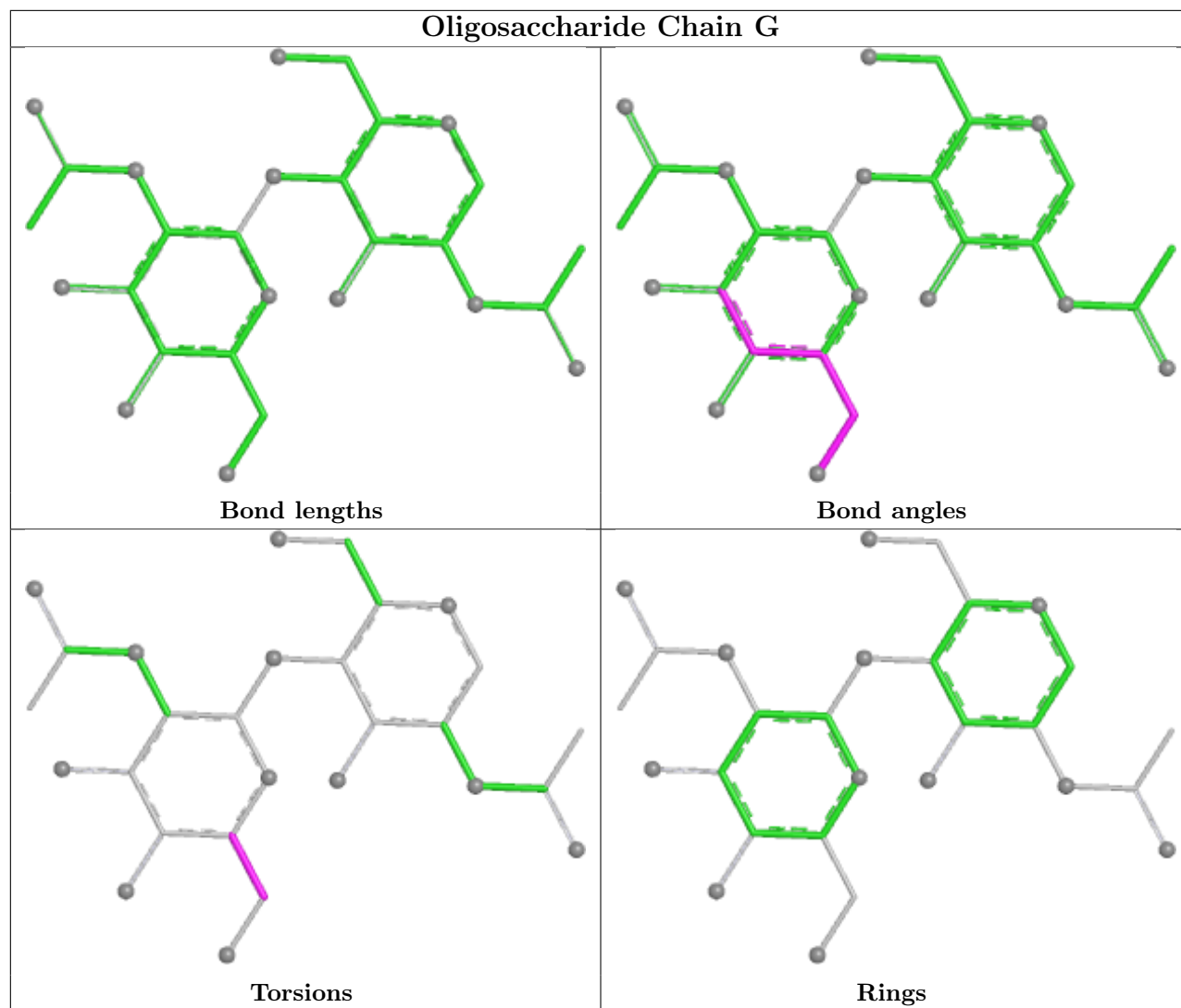
No monomer is involved in short contacts.

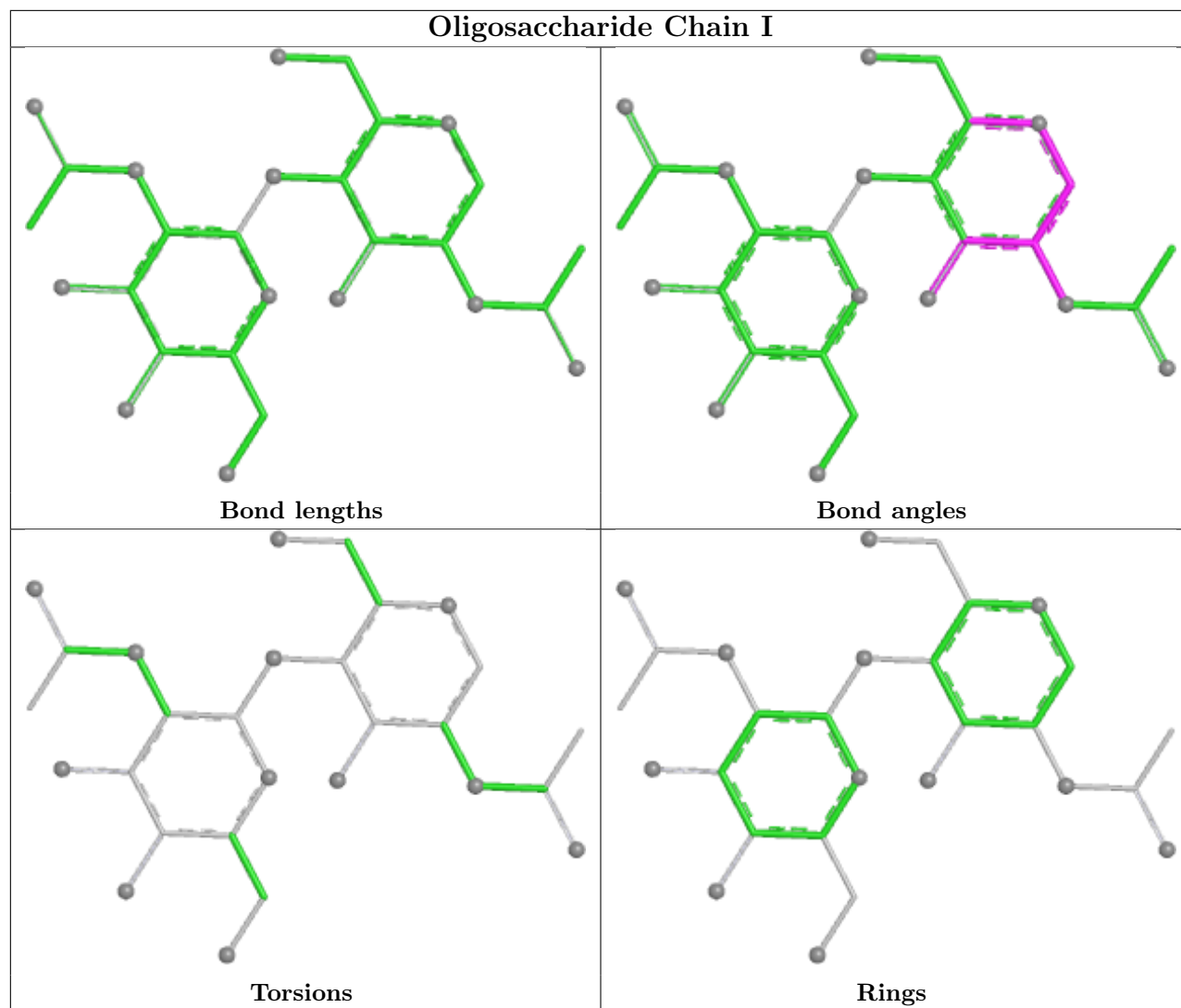
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

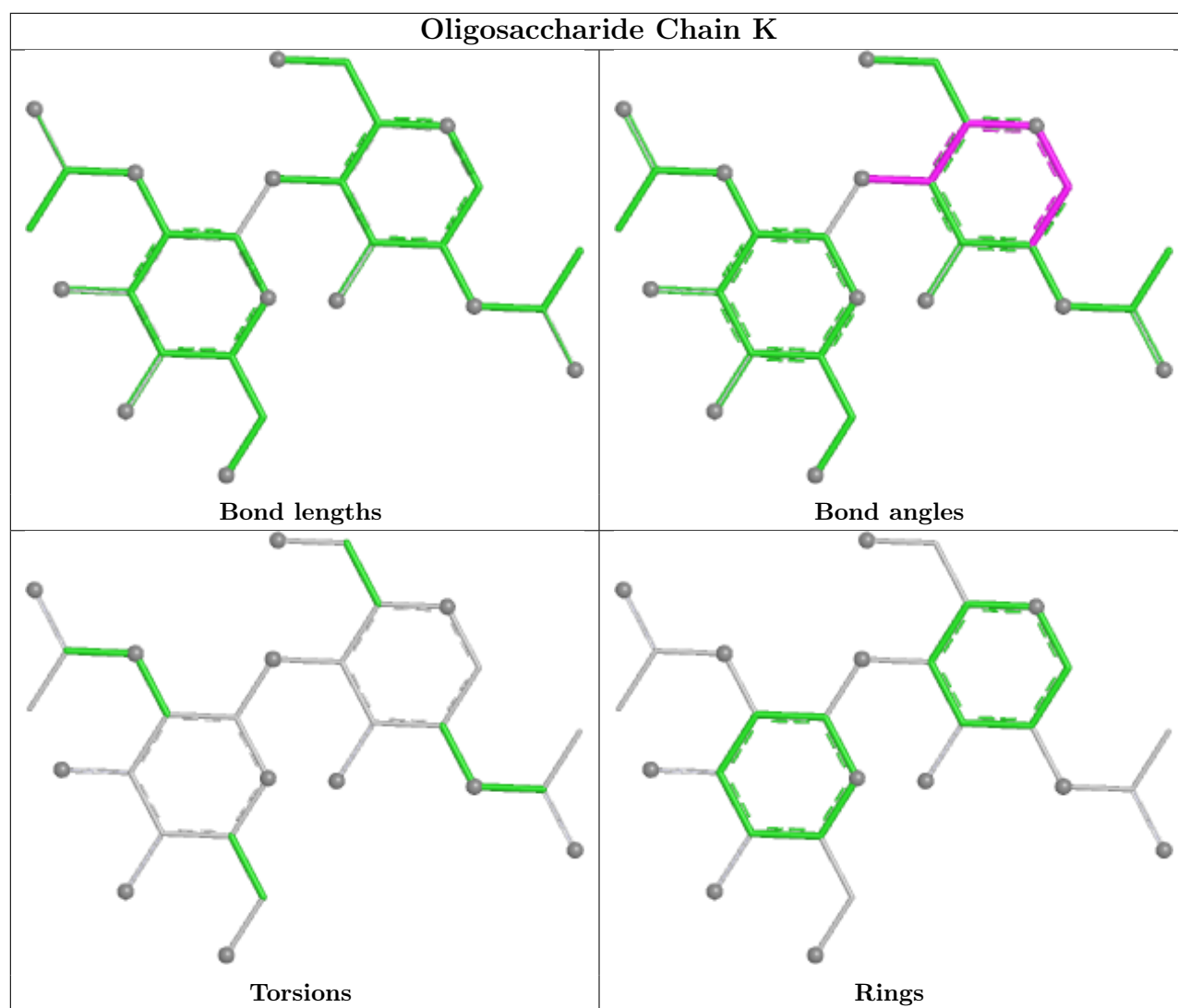


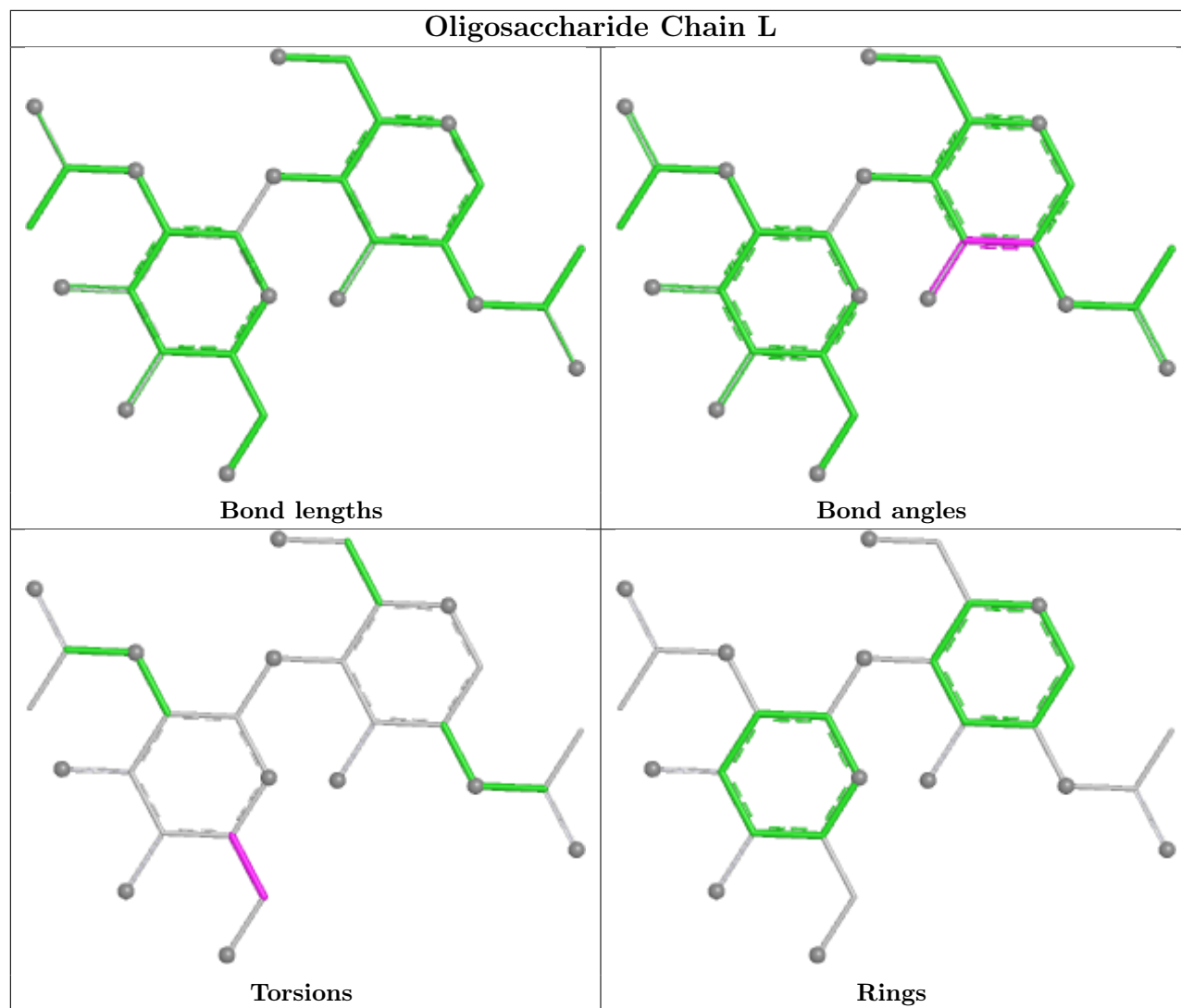


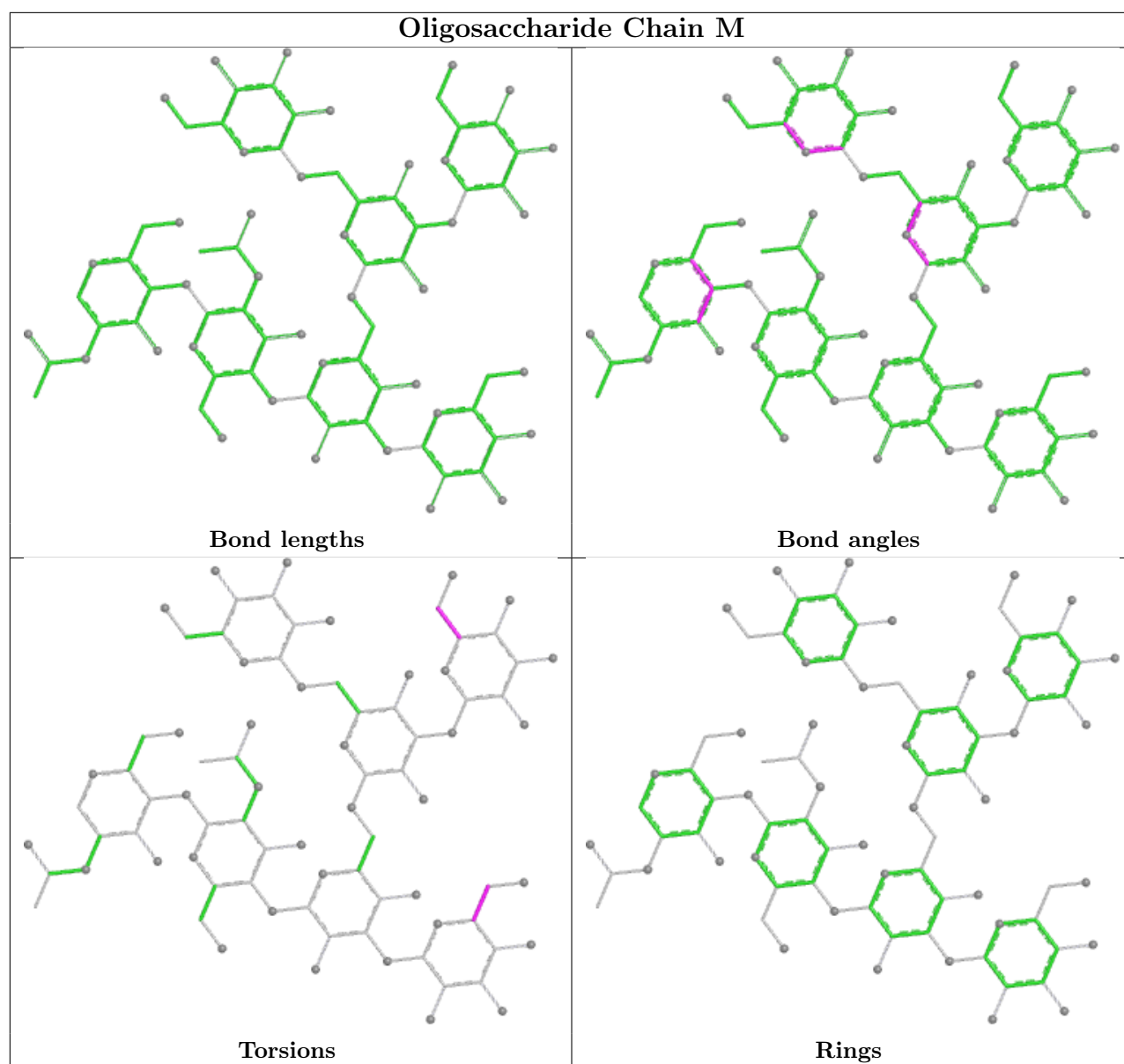












5.6 Ligand geometry [i](#)

6 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
6	SID	D	1001	-	24,25,25	1.26	3 (12%)	27,36,36	1.17	3 (11%)
5	NAG	D	5157	1	14,14,15	0.54	0	17,19,21	0.76	0
5	NAG	A	5156	1	14,14,15	0.83	1 (7%)	17,19,21	1.57	4 (23%)
5	NAG	B	5154	1	14,14,15	0.68	0	17,19,21	1.19	1 (5%)
5	NAG	A	5157	1	14,14,15	0.49	0	17,19,21	0.93	1 (5%)
5	NAG	D	5156	1	14,14,15	0.43	0	17,19,21	1.62	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
6	SID	D	1001	-	-	5/26/44/44	0/1/1/1
5	NAG	D	5157	1	-	2/6/23/26	0/1/1/1
5	NAG	A	5156	1	-	2/6/23/26	0/1/1/1
5	NAG	B	5154	1	-	0/6/23/26	0/1/1/1
5	NAG	A	5157	1	-	2/6/23/26	0/1/1/1
5	NAG	D	5156	1	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1001	SID	O6-C2	3.04	1.46	1.42
6	D	1001	SID	C3-C2	2.69	1.56	1.52
5	A	5156	NAG	C1-C2	2.57	1.55	1.52
6	D	1001	SID	C3-C4	2.21	1.56	1.53

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	5156	NAG	C1-O5-C5	4.54	118.27	112.19
6	D	1001	SID	C8-C7-C6	-3.32	106.83	113.05
5	A	5156	NAG	C1-O5-C5	2.85	116.01	112.19
5	B	5154	NAG	C1-C2-N2	-2.79	106.03	110.43
5	A	5156	NAG	C3-C4-C5	-2.60	105.52	110.23
5	A	5156	NAG	O7-C7-C8	-2.42	117.75	122.05
5	A	5157	NAG	O5-C5-C6	2.32	112.17	107.66
5	D	5156	NAG	C3-C4-C5	2.14	114.12	110.23
5	A	5156	NAG	C1-C2-N2	2.13	113.79	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	1001	SID	C3-C4-C5	2.02	112.85	109.72
6	D	1001	SID	O1A-C1-C2	-2.01	117.73	123.79

There are no chirality outliers.

All (13) torsion outliers are listed below:

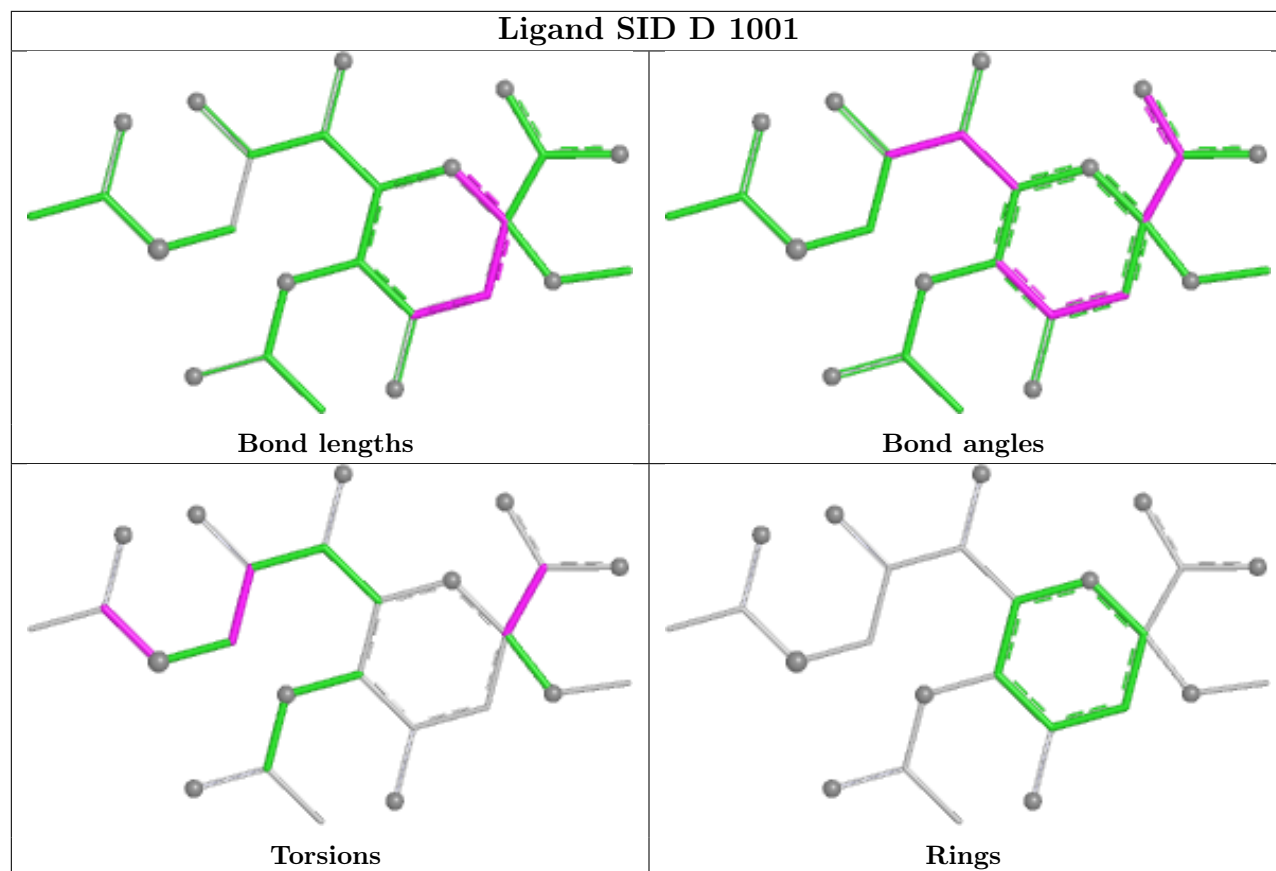
Mol	Chain	Res	Type	Atoms
6	D	1001	SID	O1B-C1-C2-O2
6	D	1001	SID	C7-C8-C9-S9
6	D	1001	SID	O8-C8-C9-S9
6	D	1001	SID	OA9-CA9-S9-C9
6	D	1001	SID	CM9-CA9-S9-C9
5	D	5157	NAG	C4-C5-C6-O6
5	D	5157	NAG	O5-C5-C6-O6
5	A	5157	NAG	O5-C5-C6-O6
5	D	5156	NAG	C4-C5-C6-O6
5	A	5157	NAG	C4-C5-C6-O6
5	A	5156	NAG	O5-C5-C6-O6
5	A	5156	NAG	C4-C5-C6-O6
5	D	5156	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	1001	SID	2	0
5	B	5154	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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	365/384 (95%)	-0.60	1 (0%) 90 89	9, 13, 21, 35	0
1	B	364/384 (94%)	-0.55	1 (0%) 90 89	8, 13, 21, 30	0
1	C	358/384 (93%)	0.46	6 (1%) 69 68	15, 25, 32, 37	0
1	D	369/384 (96%)	-0.37	8 (2%) 62 61	10, 17, 28, 45	0
All	All	1456/1536 (94%)	-0.27	16 (1%) 78 77	8, 17, 29, 45	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	237	GLY	4.9
1	D	236	ILE	3.6
1	D	239	THR	3.5
1	D	238	SER	3.4
1	B	223	ASP	3.3
1	C	78	SER	3.1
1	C	147	SER	3.1
1	C	146	SER	3.1
1	D	210	GLY	2.6
1	C	48	MET	2.6
1	C	105	GLN	2.5
1	D	211	GLY	2.5
1	D	308	TYR	2.2
1	D	224	SER	2.2
1	C	47	PRO	2.1
1	A	382	GLY	2.0

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

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

6.3 Carbohydrates

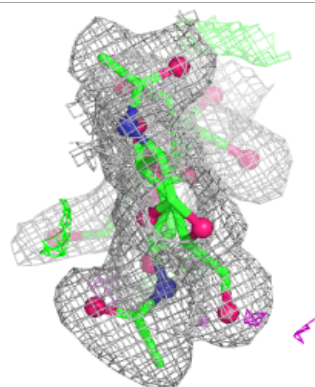
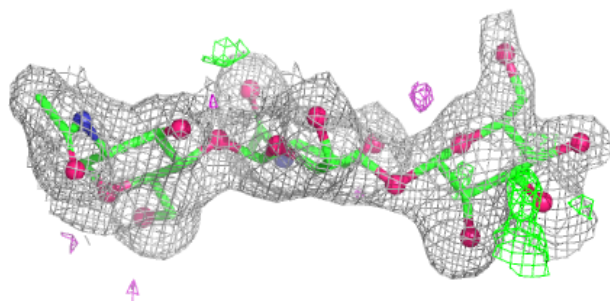
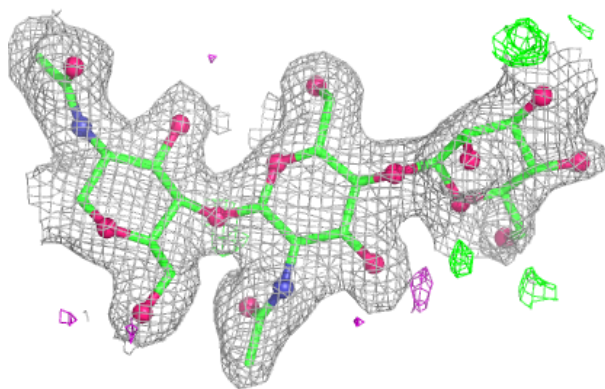
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BMA	J	3	11/12	0.54	0.17	64,66,67,67	0
4	MAN	M	7	11/12	0.60	0.15	63,66,66,67	0
2	NAG	J	2	14/15	0.68	0.16	55,57,60,63	0
2	BMA	H	3	11/12	0.77	0.14	44,48,49,52	0
3	NAG	F	2	14/15	0.79	0.14	38,45,49,49	0
2	BMA	E	3	11/12	0.80	0.12	41,47,50,50	0
4	MAN	M	6	11/12	0.82	0.12	53,55,56,57	0
4	BMA	M	3	11/12	0.84	0.12	49,51,54,59	0
4	MAN	M	4	11/12	0.86	0.11	46,47,51,53	0
3	NAG	G	2	14/15	0.86	0.11	30,35,39,41	0
2	NAG	J	1	14/15	0.86	0.11	38,42,46,50	0
4	MAN	M	5	11/12	0.87	0.12	36,43,45,48	0
3	NAG	I	2	14/15	0.87	0.10	34,36,42,42	0
3	NAG	L	2	14/15	0.87	0.10	40,42,47,49	0
4	NAG	M	2	14/15	0.90	0.10	31,36,40,46	0
3	NAG	L	1	14/15	0.91	0.09	33,36,37,37	0
2	NAG	H	2	14/15	0.92	0.09	31,34,41,42	0
3	NAG	K	2	14/15	0.92	0.08	29,31,34,35	0
2	NAG	E	2	14/15	0.93	0.09	27,32,35,40	0
4	NAG	M	1	14/15	0.93	0.07	22,25,29,32	0
2	NAG	H	1	14/15	0.94	0.08	22,24,26,29	0
3	NAG	I	1	14/15	0.95	0.07	19,22,27,30	0
2	NAG	E	1	14/15	0.95	0.06	17,20,26,28	0
3	NAG	F	1	14/15	0.95	0.06	20,24,27,31	0
3	NAG	G	1	14/15	0.97	0.06	19,22,25,27	0
3	NAG	K	1	14/15	0.97	0.05	15,18,25,27	0

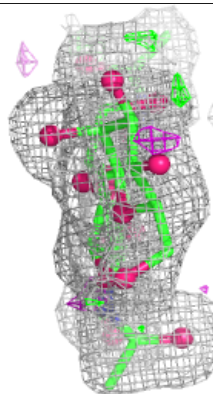
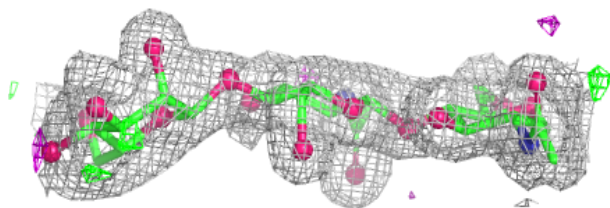
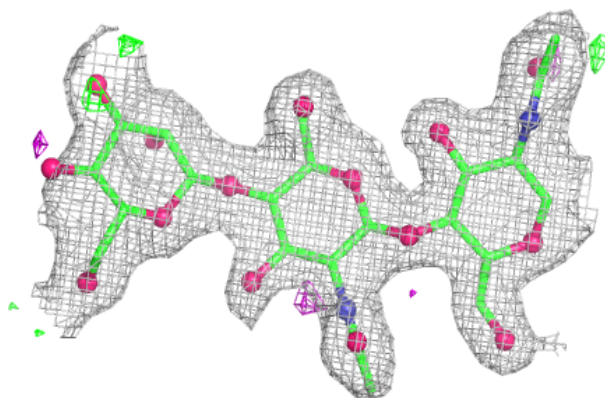
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

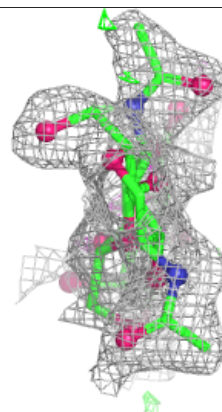
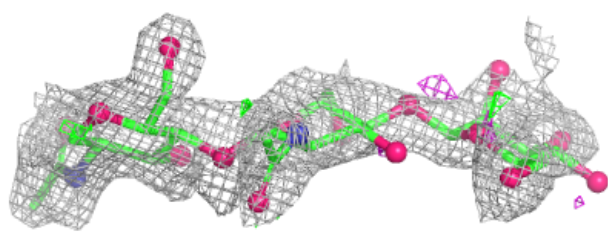
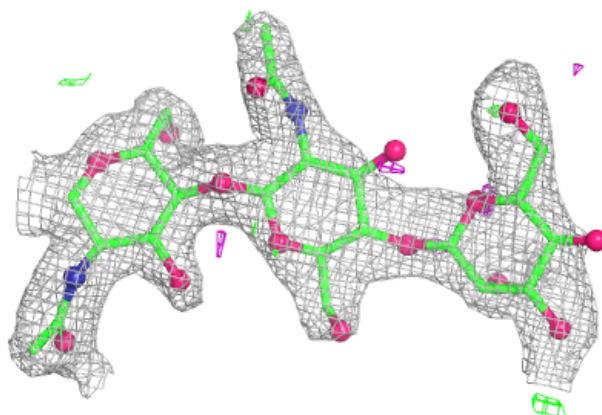
**Electron density around Chain H:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

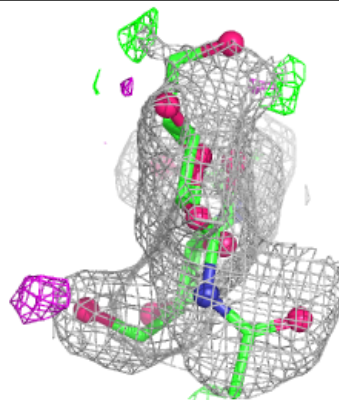
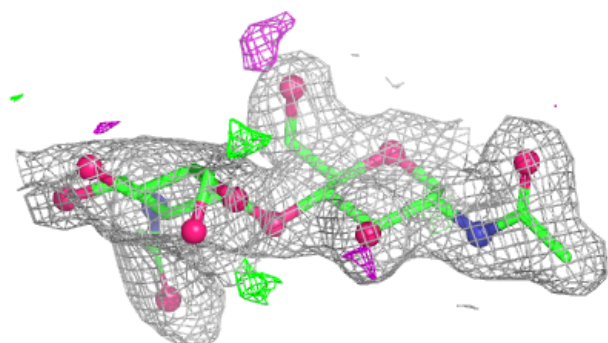
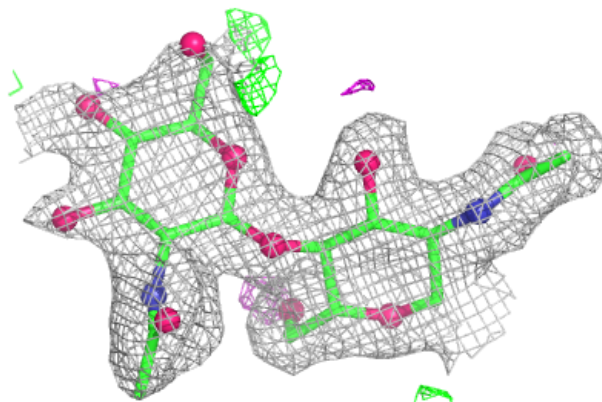


Electron density around Chain J:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

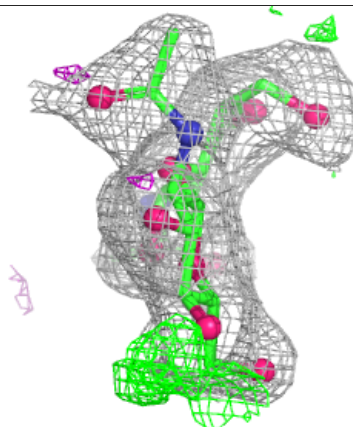
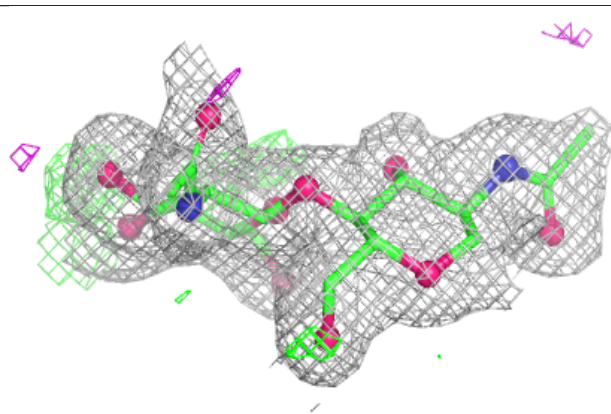
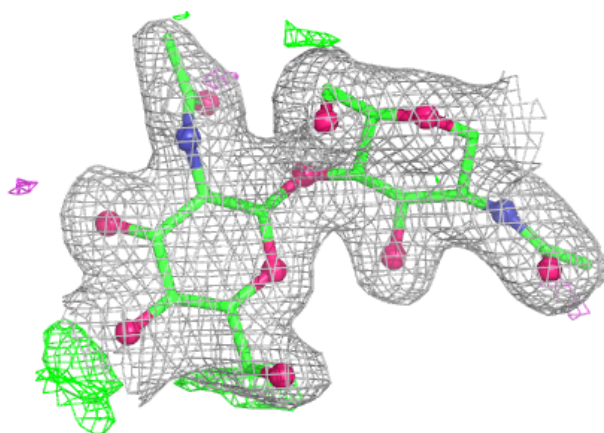
**Electron density around Chain F:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



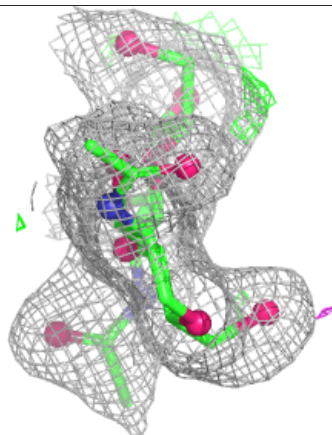
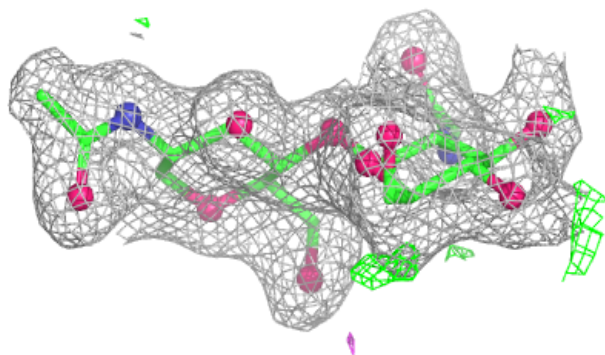
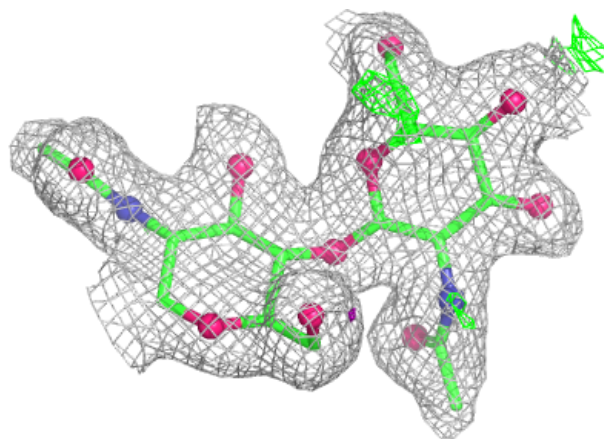
Electron density around Chain G:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



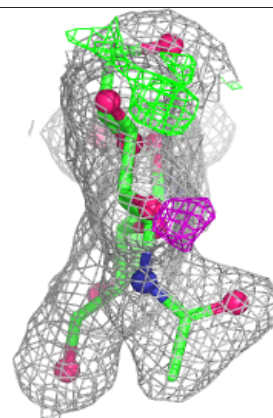
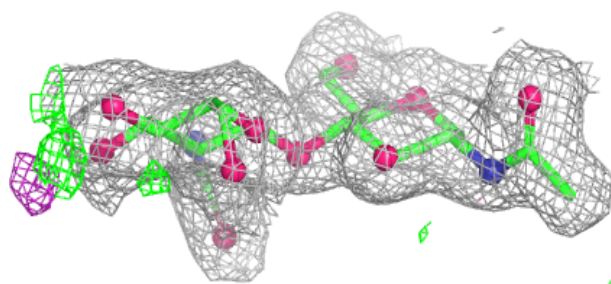
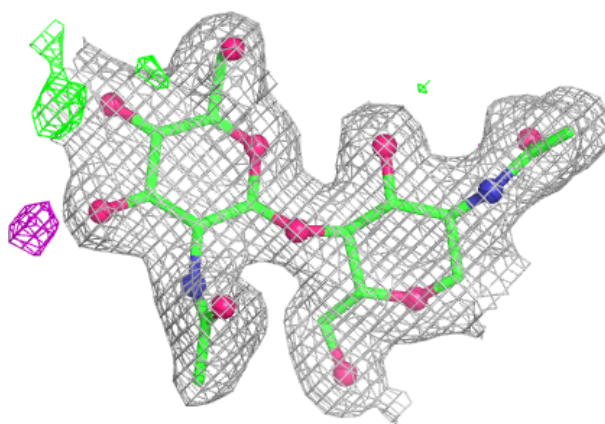
Electron density around Chain I:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

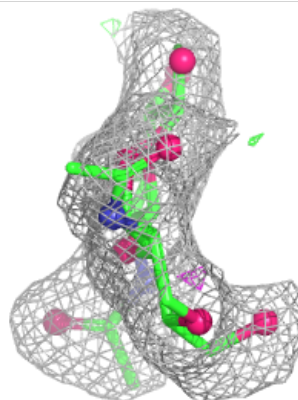
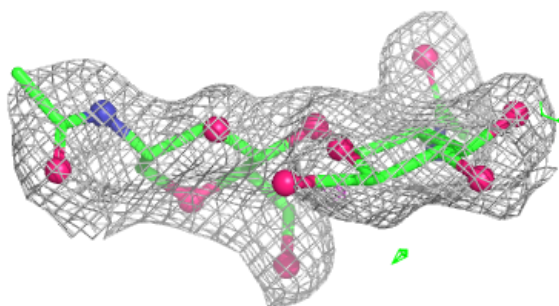
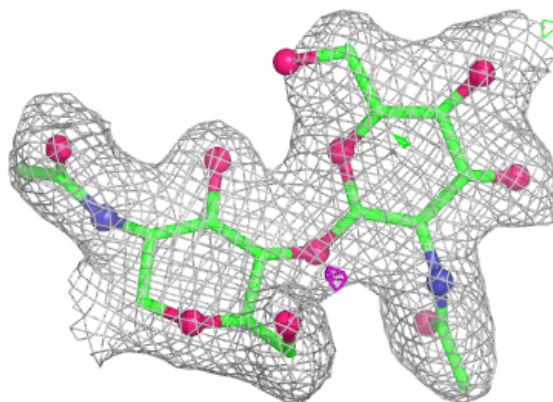


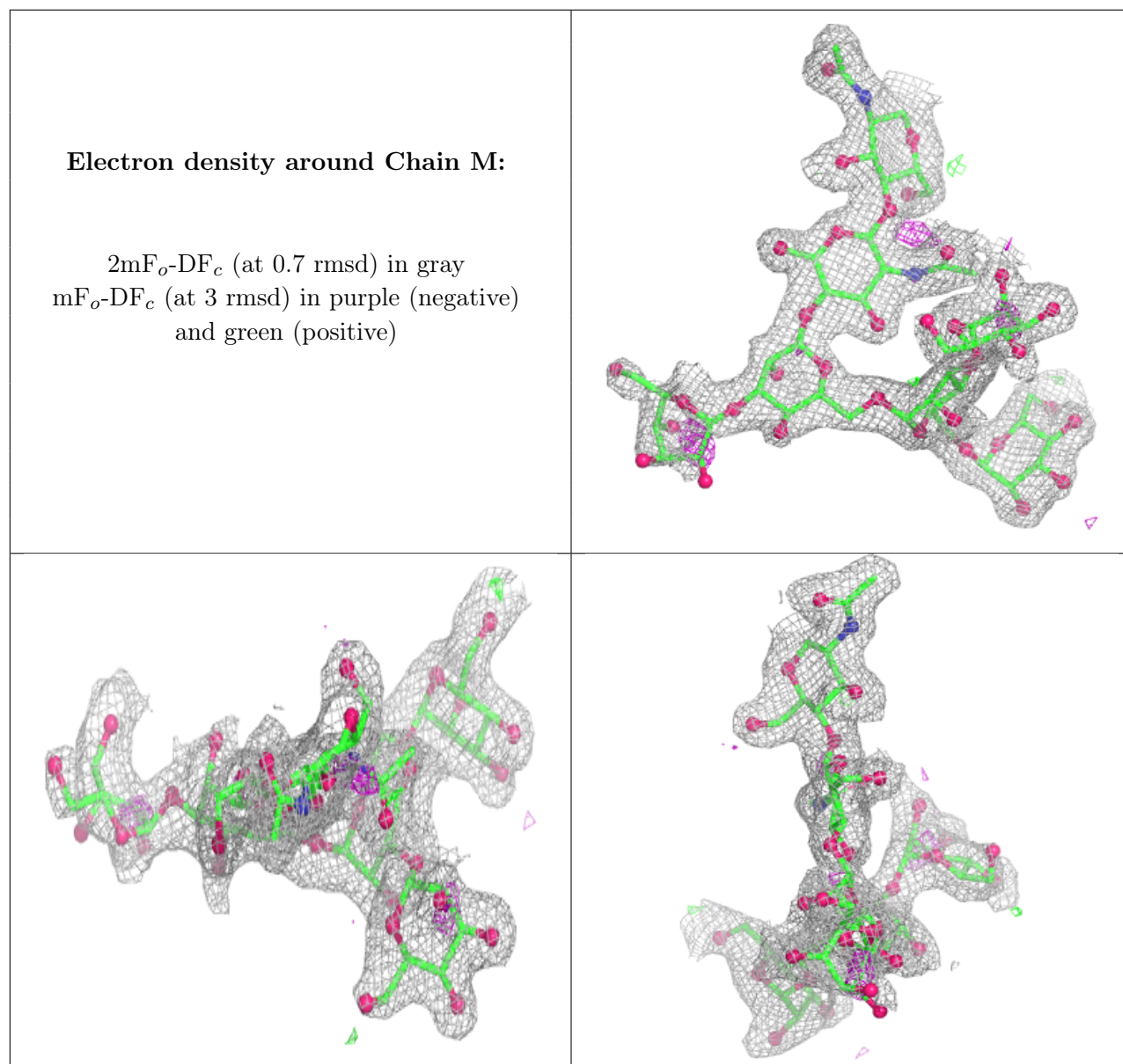
Electron density around Chain K:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around Chain L:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

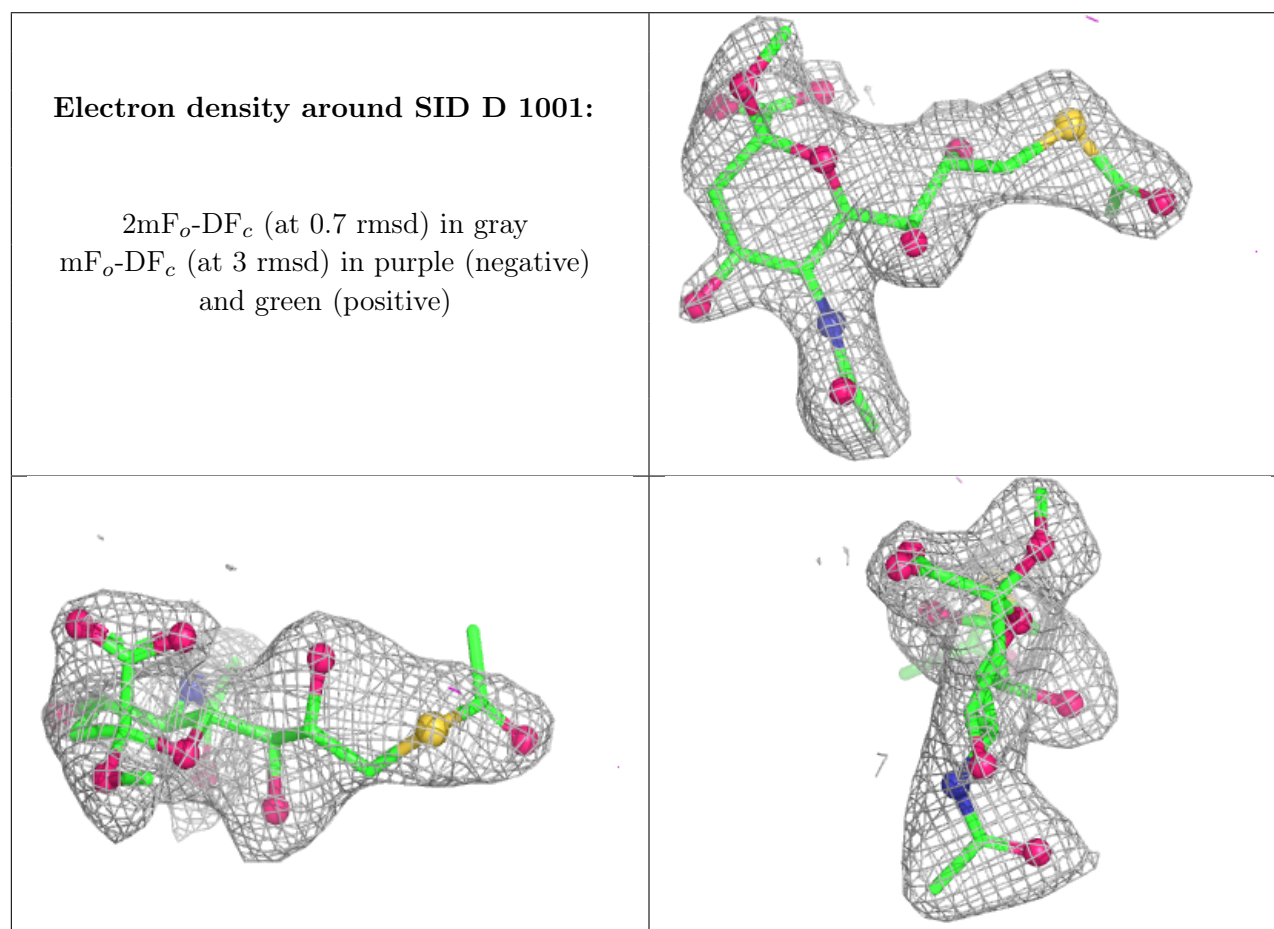
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	B	5154	14/15	0.64	0.16	50,55,57,57	0
5	NAG	A	5157	14/15	0.72	0.16	47,54,56,57	0
5	NAG	A	5156	14/15	0.81	0.13	32,36,40,40	0
5	NAG	D	5156	14/15	0.84	0.13	36,42,45,46	0
5	NAG	D	5157	14/15	0.85	0.11	41,47,50,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	SID	D	1001	25/25	0.88	0.14	49,55,62,62	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers ⓘ

There are no such residues in this entry.