



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 31, 2026 – 11:17 AM UTC

PDB ID : 8OK7 / pdb_00008ok7
Title : Variant Surface Glycoprotein VSG558 NTD
Authors : Zeelen, J.P.; Stebbins, C.E.; van Straaten, M.; Zhong, J.
Deposited on : 2023-03-27
Resolution : 1.74 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
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

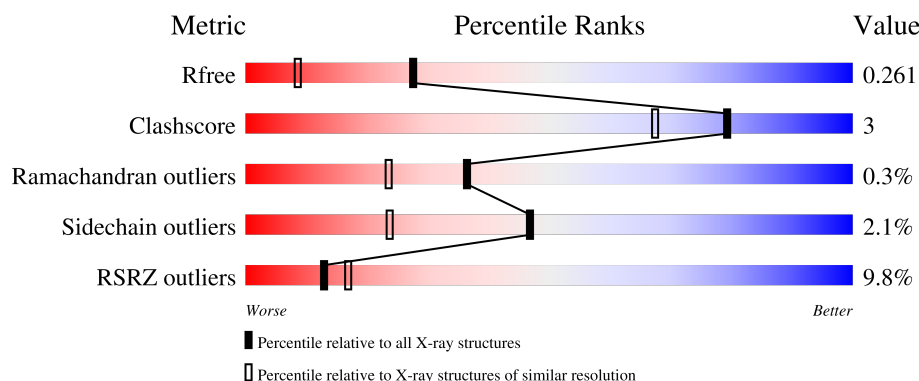
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.74 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	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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	419	3% 83% 14%
1	B	419	7% 79% 6% 14%
1	C	419	18% 73% 12% 14%
1	D	419	5% 80% 6% 14%
2	E	6	100%

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Mol	Chain	Length	Quality of chain
3	F	5	 100%
3	J	5	 60% 40%
3	L	5	 80% 20%
4	G	7	 86% 14%
4	I	7	 71% 29%
5	H	6	 83% 17%
5	K	6	 50% 33% 17%

2 Entry composition [i](#)

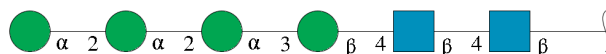
There are 6 unique types of molecules in this entry. The entry contains 12359 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Variant surface glycoprotein 558.

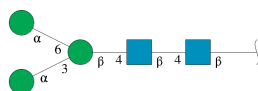
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	361	Total	C	N	O	S	0	5	0
			2769	1692	501	565	11			
1	B	361	Total	C	N	O	S	0	6	0
			2755	1686	496	561	12			
1	C	361	Total	C	N	O	S	0	2	0
			2742	1680	495	556	11			
1	D	361	Total	C	N	O	S	0	4	0
			2767	1692	501	562	12			

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-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
2	E	6	Total	C	N	O	0	0	0
			72	40	2	30			

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



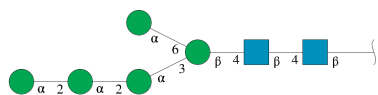
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	5	Total	C	N	O	0	0	0
			61	34	2	25			

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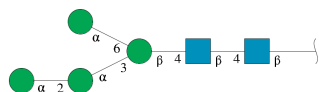
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	J	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	L	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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				ZeroOcc	AltConf	Trace
4	G	7	Total	C	N	O	0	0	0
			83	46	2	35			
4	I	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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				ZeroOcc	AltConf	Trace
5	H	6	Total	C	N	O	0	0	0
			72	40	2	30			
5	K	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	240	Total	O	0	0
			240	240		
6	B	164	Total	O	0	0
			164	164		

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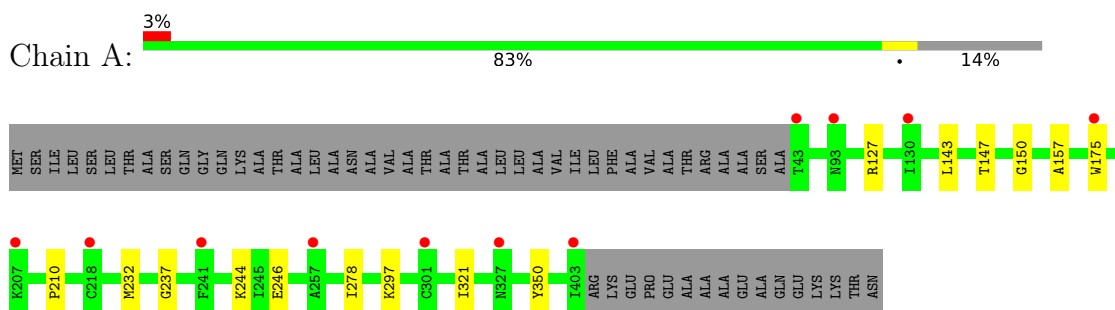
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	181	Total 181	O 181	0	0
6	D	176	Total 176	O 176	0	0

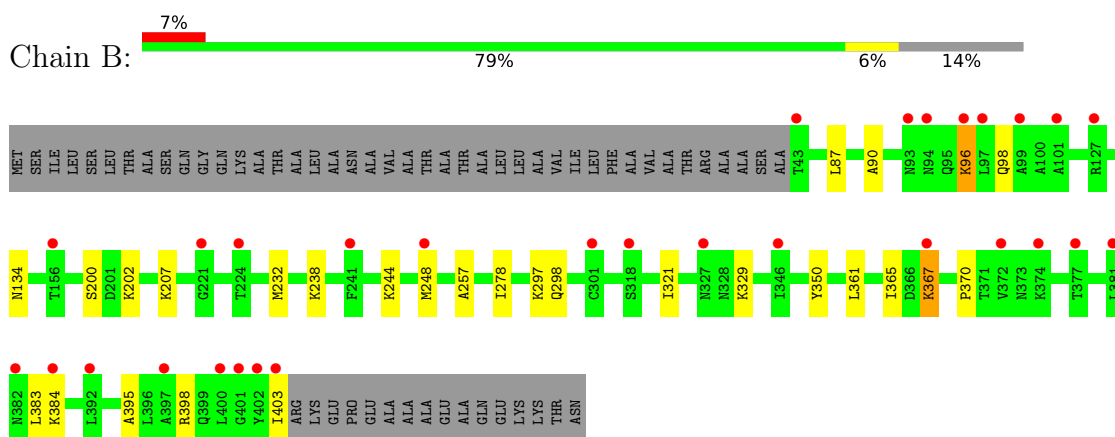
3 Residue-property plots [i](#)

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.

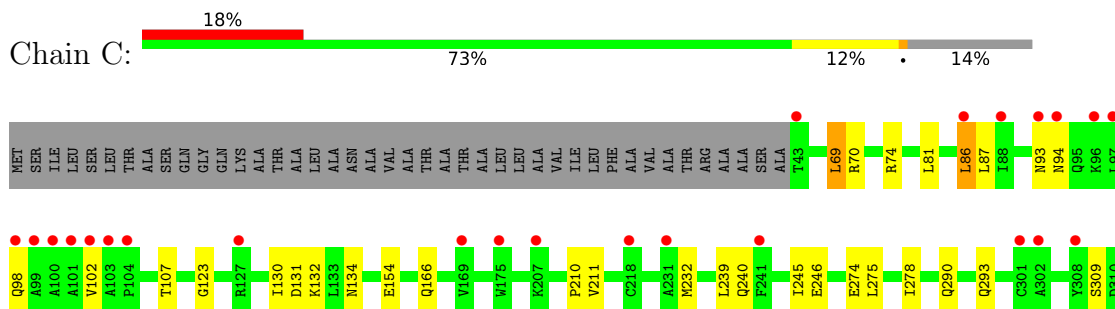
- Molecule 1: Variant surface glycoprotein 558

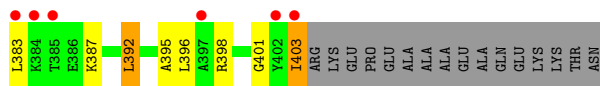
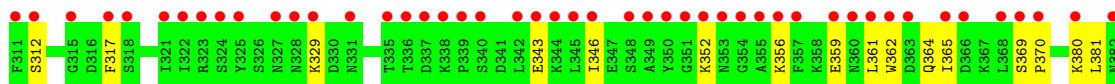


- Molecule 1: Variant surface glycoprotein 558

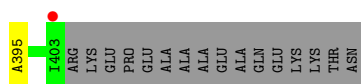
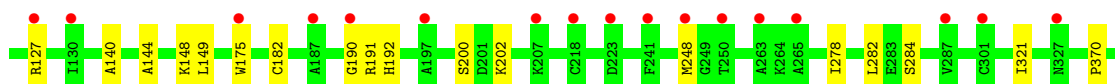
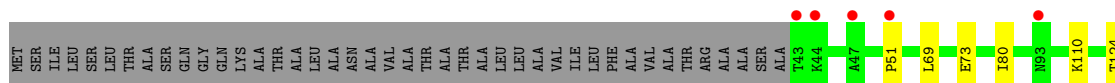
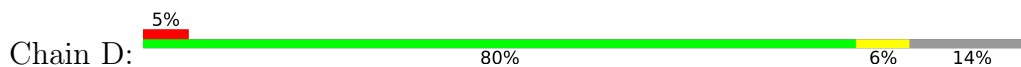


- Molecule 1: Variant surface glycoprotein 558





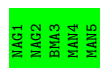
- Molecule 1: Variant surface glycoprotein 558



- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-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



- Molecule 3: alpha-D-mannopyranose-(1-3)-[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



- Molecule 3: alpha-D-mannopyranose-(1-3)-[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



- Molecule 3: alpha-D-mannopyranose-(1-3)-[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 L:  80% 20%



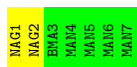
- Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  86% 14%



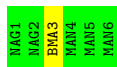
- Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  71% 29%



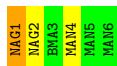
- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  83% 17%



- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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 K:  50% 33% 17%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	103.08Å 64.12Å 155.04Å 90.00° 109.13° 90.00°	Depositor
Resolution (Å)	53.55 – 1.74 53.55 – 1.74	Depositor EDS
% Data completeness (in resolution range)	98.7 (53.55-1.74) 98.7 (53.55-1.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 1.74Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.238 , 0.261 0.238 , 0.261	Depositor DCC
R_{free} test set	9893 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	30.9	Xtriage
Anisotropy	0.467	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.064 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12359	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.84 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.0356e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 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	0.28	0/2802	0.43	0/3777
1	B	0.44	0/2789	0.65	0/3764
1	C	0.55	0/2776	0.80	0/3744
1	D	0.38	0/2800	0.58	0/3773
All	All	0.42	0/11167	0.63	0/15058

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
1	C	0	3
1	D	0	1
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	398	ARG	Sidechain
1	C	398	ARG	Sidechain
1	C	70	ARG	Sidechain
1	C	74	ARG	Sidechain
1	D	191	ARG	Sidechain

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	2769	0	2714	10	0
1	B	2755	0	2674	13	0
1	C	2742	0	2685	27	0
1	D	2767	0	2717	16	0
2	E	72	0	61	0	0
3	F	61	0	52	0	0
3	J	61	0	52	4	0
3	L	61	0	52	0	0
4	G	83	0	70	0	0
4	I	83	0	70	0	0
5	H	72	0	61	0	0
5	K	72	0	61	1	0
6	A	240	0	0	1	0
6	B	164	0	0	0	0
6	C	181	0	0	0	0
6	D	176	0	0	0	0
All	All	12359	0	11269	61	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 3.

All (61) 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:107:THR:HG21	1:C:317:PHE:HB2	1.74	0.67
1:C:81:LEU:HD11	1:C:387:LYS:HA	1.78	0.65
1:C:93:ASN:OD1	1:C:94:ASN:N	2.29	0.62
1:D:182:CYS:HB3	5:K:1:NAG:H82	1.80	0.62
1:B:134:ASN:HD22	1:C:134:ASN:HD22	1.49	0.61
1:D:370:PRO:HB2	1:D:395:ALA:HB1	1.85	0.57
1:B:232:MET:HE3	1:B:238:LYS:C	2.32	0.55
1:A:127:ARG:HH22	1:D:73:GLU:CD	2.14	0.53
1:B:370:PRO:HB2	1:B:395:ALA:HB1	1.90	0.53
1:C:370:PRO:HB2	1:C:395:ALA:HB1	1.91	0.53
1:A:232:MET:HG2	1:A:237:GLY:C	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:THR:CG2	1:C:317:PHE:HB2	2.40	0.52
1:D:124:THR:HA	1:D:127[B]:ARG:NH1	2.25	0.52
1:A:175:TRP:HH2	1:D:175:TRP:HZ3	1.58	0.51
1:B:297:LYS:HG3	1:B:298:GLN:HG3	1.93	0.51
1:C:361:LEU:O	1:C:365:ILE:HG13	2.13	0.49
1:B:87:LEU:HD21	1:C:396:LEU:HD21	1.95	0.48
1:A:157:ALA:HB2	1:A:232:MET:HB3	1.96	0.48
1:B:200:SER:HB2	1:B:202:LYS:HG3	1.96	0.47
1:C:69:LEU:HD11	1:C:123:GLY:HA2	1.97	0.47
1:D:140:ALA:HB2	1:D:282:LEU:HD21	1.97	0.46
1:C:86:LEU:HD11	1:C:362:TRP:CZ3	2.51	0.46
1:C:98:GLN:O	1:C:102:VAL:HG23	2.16	0.46
1:D:148:LYS:O	1:D:148:LYS:HG2	2.15	0.46
1:A:175:TRP:HH2	1:D:175:TRP:CZ3	2.33	0.45
1:A:321:ILE:HD11	1:A:350:TYR:HE2	1.82	0.45
1:C:293:GLN:CB	3:J:1:NAG:H81	2.47	0.44
1:D:149:LEU:HB3	1:D:175:TRP:CD1	2.52	0.44
1:B:207:LYS:O	1:B:248[A]:MET:HG2	2.18	0.44
1:D:248[A]:MET:HE3	1:D:248[A]:MET:HB2	1.86	0.44
1:C:154:GLU:HG3	1:C:240:GLN:HG2	2.01	0.43
1:C:293:GLN:HB3	3:J:1:NAG:H81	2.00	0.43
1:C:392:LEU:HD13	1:C:392:LEU:HA	1.87	0.43
1:D:200:SER:HB2	1:D:202:LYS:HG3	2.00	0.43
1:C:343:GLU:HA	1:C:346:ILE:HD12	2.01	0.43
1:D:80:ILE:HD12	1:D:80:ILE:HA	1.92	0.43
1:C:290:GLN:HA	3:J:1:NAG:C8	2.49	0.42
1:A:143:LEU:O	1:A:147:THR:HG23	2.19	0.42
1:B:321:ILE:HD11	1:B:350:TYR:HE2	1.85	0.42
1:C:232:MET:HE1	1:C:239:LEU:HD22	2.01	0.42
1:D:69:LEU:O	1:D:73:GLU:HG3	2.19	0.42
1:A:150:GLY:HA2	1:A:244:LYS:HE3	2.01	0.42
1:B:367:LYS:HE3	1:B:367:LYS:HB2	1.55	0.42
1:D:190:GLY:HA2	1:D:192:HIS:CE1	2.55	0.42
1:C:69:LEU:HD23	1:C:69:LEU:HA	1.84	0.42
1:B:96:LYS:HE3	1:B:96:LYS:HB3	1.74	0.41
1:B:361:LEU:O	1:B:365:ILE:HG13	2.20	0.41
1:C:211:VAL:HG12	1:C:274:GLU:HA	2.02	0.41
1:C:359:GLU:O	1:C:364:GLN:HG2	2.21	0.41
1:C:381:LEU:HD23	1:C:381:LEU:HA	1.91	0.41
1:A:297:LYS:NZ	6:A:506:HOH:O	2.42	0.41
1:D:321:ILE:HD13	1:D:321:ILE:HA	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:245:ILE:HD12	1:C:275:LEU:HD11	2.02	0.41
1:B:90:ALA:O	1:B:98:GLN:HG2	2.20	0.41
1:C:401:GLY:C	1:C:403:ILE:H	2.29	0.41
3:J:1:NAG:H82	3:J:1:NAG:H2	1.87	0.40
1:A:210:PRO:HA	1:A:246:GLU:O	2.21	0.40
1:C:131:ASP:OD1	1:C:131:ASP:N	2.54	0.40
1:D:51:PRO:HB2	1:D:144:ALA:HB2	2.04	0.40
1:B:257:ALA:HA	1:C:166:GLN:HB2	2.03	0.40
1:C:210:PRO:HA	1:C:246:GLU:O	2.21	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	364/419 (87%)	351 (96%)	12 (3%)	1 (0%)	36	23
1	B	365/419 (87%)	350 (96%)	14 (4%)	1 (0%)	36	23
1	C	361/419 (86%)	343 (95%)	17 (5%)	1 (0%)	36	23
1	D	363/419 (87%)	352 (97%)	10 (3%)	1 (0%)	36	23
All	All	1453/1676 (87%)	1396 (96%)	53 (4%)	4 (0%)	36	23

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	278	ILE
1	B	278	ILE
1	C	278	ILE
1	A	278	ILE

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	291/326 (89%)	291 (100%)	0	100	100
1	B	286/326 (88%)	278 (97%)	8 (3%)	38	15
1	C	286/326 (88%)	271 (95%)	15 (5%)	21	4
1	D	290/326 (89%)	287 (99%)	3 (1%)	68	54
All	All	1153/1304 (88%)	1127 (98%)	26 (2%)	47	20

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	96	LYS
1	B	244[A]	LYS
1	B	244[B]	LYS
1	B	329	LYS
1	B	367	LYS
1	B	383	LEU
1	B	384	LYS
1	B	403	ILE
1	C	69	LEU
1	C	86	LEU
1	C	87	LEU
1	C	130	ILE
1	C	132	LYS
1	C	309	SER
1	C	312	SER
1	C	329	LYS
1	C	352	LYS
1	C	356	LYS
1	C	369	SER
1	C	380	LYS
1	C	383	LEU
1	C	392	LEU
1	C	403	ILE
1	D	110	LYS

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Mol	Chain	Res	Type
1	D	284[A]	SER
1	D	284[B]	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	ASN
1	A	134	ASN
1	A	163	GLN
1	A	230	ASN
1	A	294	ASN
1	A	320	GLN
1	B	82	GLN
1	B	114	ASN
1	B	129	ASN
1	B	230	ASN
1	B	235	ASN
1	B	320	GLN
1	B	373	ASN
1	C	114	ASN
1	C	134	ASN
1	C	183	GLN
1	C	189	GLN
1	C	230	ASN
1	C	235	ASN
1	C	294	ASN
1	C	313	ASN
1	C	320	GLN
1	C	373	ASN
1	C	399	GLN
1	D	93	ASN
1	D	114	ASN
1	D	134	ASN
1	D	230	ASN
1	D	235	ASN
1	D	320	GLN
1	D	399	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

47 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	2,1	14,14,15	0.41	0	17,19,21	0.84	0
2	NAG	E	2	2	14,14,15	0.43	0	17,19,21	0.54	0
2	BMA	E	3	2	11,11,12	0.43	0	15,15,17	0.59	0
2	MAN	E	4	2	11,11,12	0.55	0	15,15,17	0.60	0
2	MAN	E	5	2	11,11,12	0.55	0	15,15,17	0.73	0
2	MAN	E	6	2	11,11,12	0.30	0	15,15,17	0.47	0
3	NAG	F	1	1,3	14,14,15	0.27	0	17,19,21	0.57	0
3	NAG	F	2	3	14,14,15	0.41	0	17,19,21	0.53	0
3	BMA	F	3	3	11,11,12	0.49	0	15,15,17	0.90	0
3	MAN	F	4	3	11,11,12	0.41	0	15,15,17	0.54	0
3	MAN	F	5	3	11,11,12	0.27	0	15,15,17	0.57	0
4	NAG	G	1	4,1	14,14,15	0.42	0	17,19,21	0.87	0
4	NAG	G	2	4	14,14,15	0.40	0	17,19,21	0.79	1 (5%)
4	BMA	G	3	4	11,11,12	0.44	0	15,15,17	0.75	0
4	MAN	G	4	4	11,11,12	0.55	0	15,15,17	0.61	0
4	MAN	G	5	4	11,11,12	0.52	0	15,15,17	0.62	0
4	MAN	G	6	4	11,11,12	0.35	0	15,15,17	0.50	0
4	MAN	G	7	4	11,11,12	0.27	0	15,15,17	0.51	0
5	NAG	H	1	5,1	14,14,15	0.41	0	17,19,21	0.66	0
5	NAG	H	2	5	14,14,15	0.34	0	17,19,21	0.52	0
5	BMA	H	3	5	11,11,12	0.38	0	15,15,17	0.73	1 (6%)
5	MAN	H	4	5	11,11,12	0.27	0	15,15,17	0.51	0
5	MAN	H	5	5	11,11,12	0.21	0	15,15,17	0.56	0
5	MAN	H	6	5	11,11,12	0.36	0	15,15,17	0.54	0
4	NAG	I	1	4,1	14,14,15	0.45	0	17,19,21	0.93	1 (5%)
4	NAG	I	2	4	14,14,15	0.40	0	17,19,21	0.75	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BMA	I	3	4	11,11,12	0.52	0	15,15,17	0.66	0
4	MAN	I	4	4	11,11,12	0.47	0	15,15,17	0.51	0
4	MAN	I	5	4	11,11,12	0.39	0	15,15,17	0.51	0
4	MAN	I	6	4	11,11,12	0.38	0	15,15,17	0.46	0
4	MAN	I	7	4	11,11,12	0.38	0	15,15,17	0.44	0
3	NAG	J	1	1,3	14,14,15	0.40	0	17,19,21	0.61	0
3	NAG	J	2	3	14,14,15	0.34	0	17,19,21	0.48	0
3	BMA	J	3	3	11,11,12	0.23	0	15,15,17	0.79	1 (6%)
3	MAN	J	4	3	11,11,12	0.15	0	15,15,17	0.58	0
3	MAN	J	5	3	11,11,12	0.28	0	15,15,17	0.51	0
5	NAG	K	1	5,1	14,14,15	0.46	0	17,19,21	1.35	3 (17%)
5	NAG	K	2	5	14,14,15	0.41	0	17,19,21	0.79	1 (5%)
5	BMA	K	3	5	11,11,12	0.47	0	15,15,17	0.66	0
5	MAN	K	4	5	11,11,12	0.43	0	15,15,17	1.05	1 (6%)
5	MAN	K	5	5	11,11,12	0.32	0	15,15,17	0.47	0
5	MAN	K	6	5	11,11,12	0.31	0	15,15,17	0.56	0
3	NAG	L	1	1,3	14,14,15	0.42	0	17,19,21	0.79	1 (5%)
3	NAG	L	2	3	14,14,15	0.28	0	17,19,21	0.56	0
3	BMA	L	3	3	11,11,12	0.28	0	15,15,17	0.84	0
3	MAN	L	4	3	11,11,12	0.44	0	15,15,17	0.46	0
3	MAN	L	5	3	11,11,12	0.27	0	15,15,17	0.50	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	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	BMA	E	3	2	-	0/2/19/22	0/1/1/1
2	MAN	E	4	2	-	0/2/19/22	0/1/1/1
2	MAN	E	5	2	-	0/2/19/22	0/1/1/1
2	MAN	E	6	2	-	0/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	BMA	F	3	3	-	2/2/19/22	0/1/1/1
3	MAN	F	4	3	-	2/2/19/22	0/1/1/1
3	MAN	F	5	3	-	2/2/19/22	0/1/1/1
4	NAG	G	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1

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

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	4	MAN	C1-O5-C5	3.67	117.10	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	1	NAG	O5-C1-C2	3.00	115.93	111.29
5	K	1	NAG	C2-N2-C7	2.85	126.71	122.90
4	G	2	NAG	O5-C1-C2	-2.71	107.09	111.29
5	K	1	NAG	C4-C3-C2	2.50	114.68	111.02
5	K	2	NAG	O5-C1-C2	-2.29	107.75	111.29
3	L	1	NAG	C2-N2-C7	-2.23	119.92	122.90
3	J	3	BMA	C1-C2-C3	2.23	112.88	109.64
4	I	2	NAG	O5-C1-C2	-2.10	108.04	111.29
4	I	1	NAG	O5-C1-C2	2.10	114.54	111.29
5	H	3	BMA	C1-C2-C3	2.05	112.63	109.64

There are no chirality outliers.

All (23) torsion outliers are listed below:

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

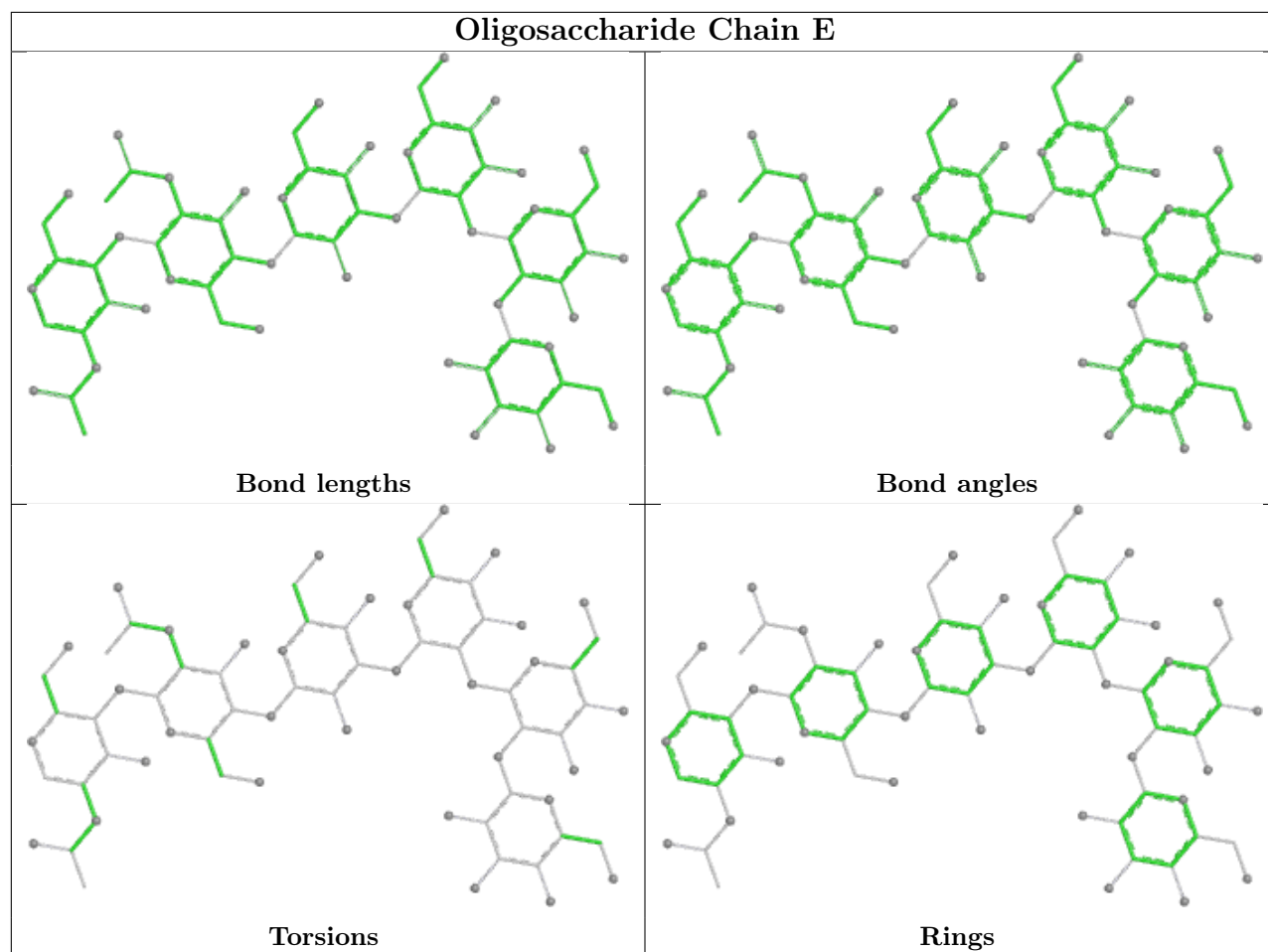
All (1) ring outliers are listed below:

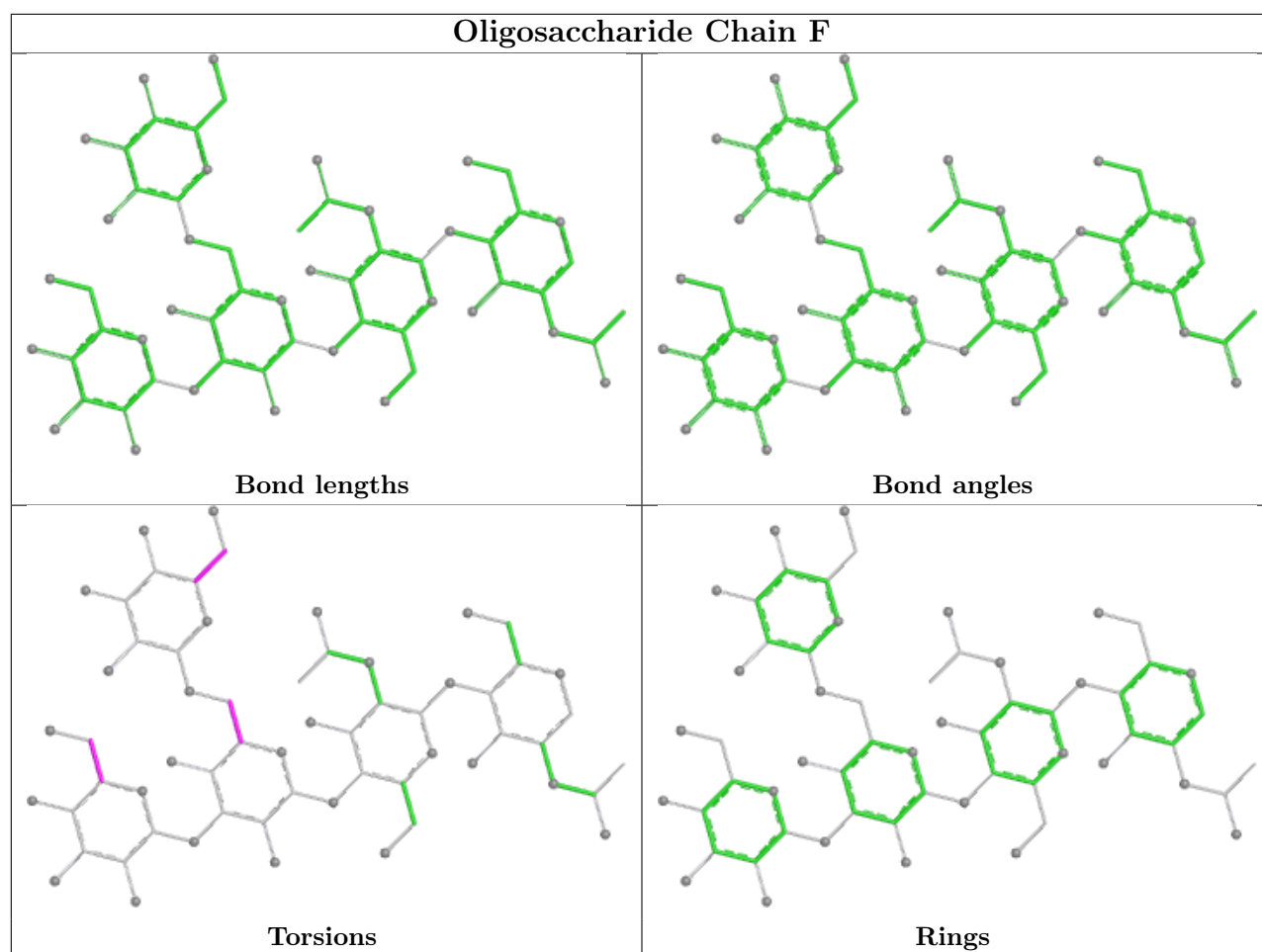
Mol	Chain	Res	Type	Atoms
5	K	4	MAN	C1-C2-C3-C4-C5-O5

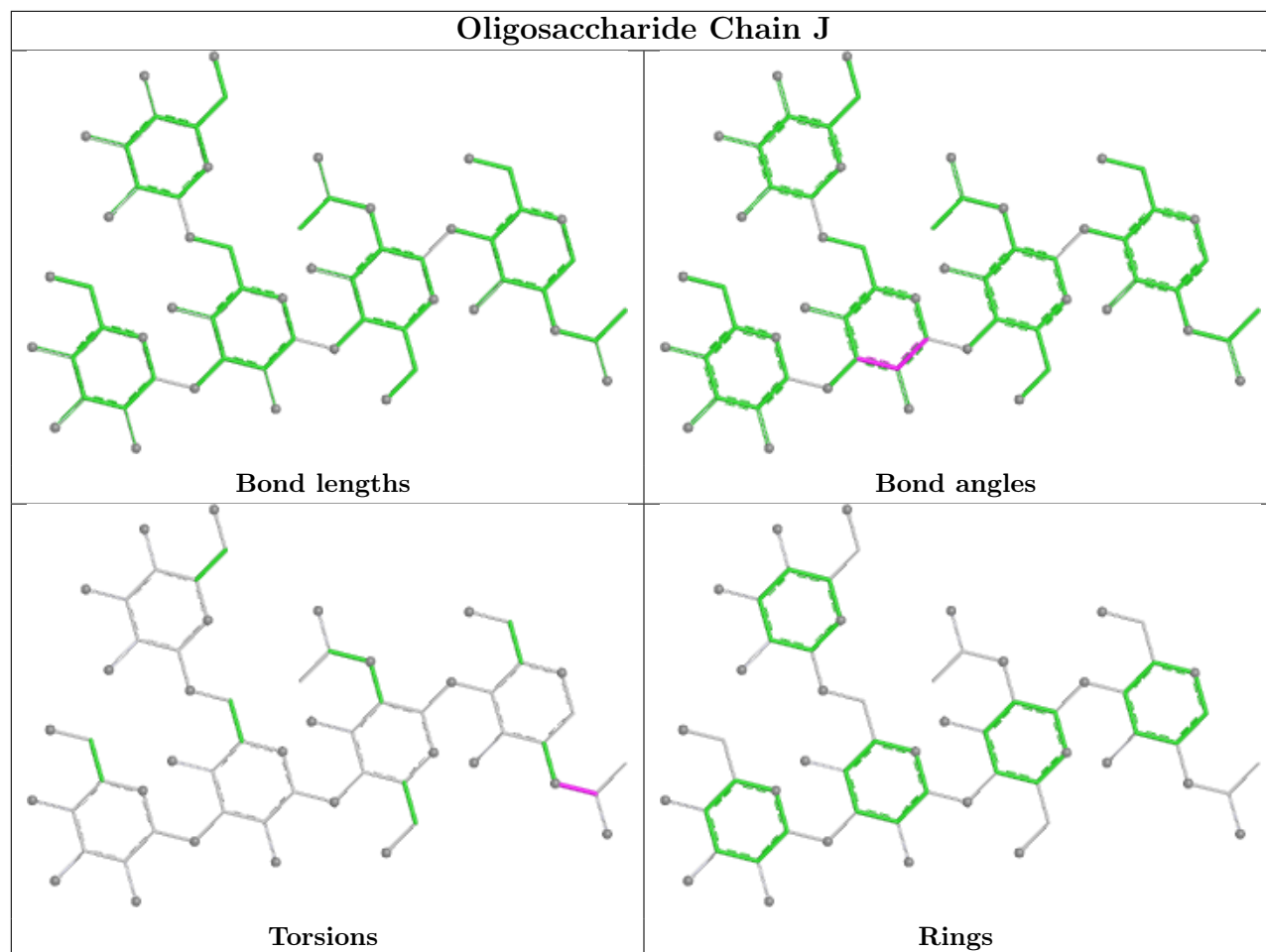
2 monomers are involved in 5 short contacts:

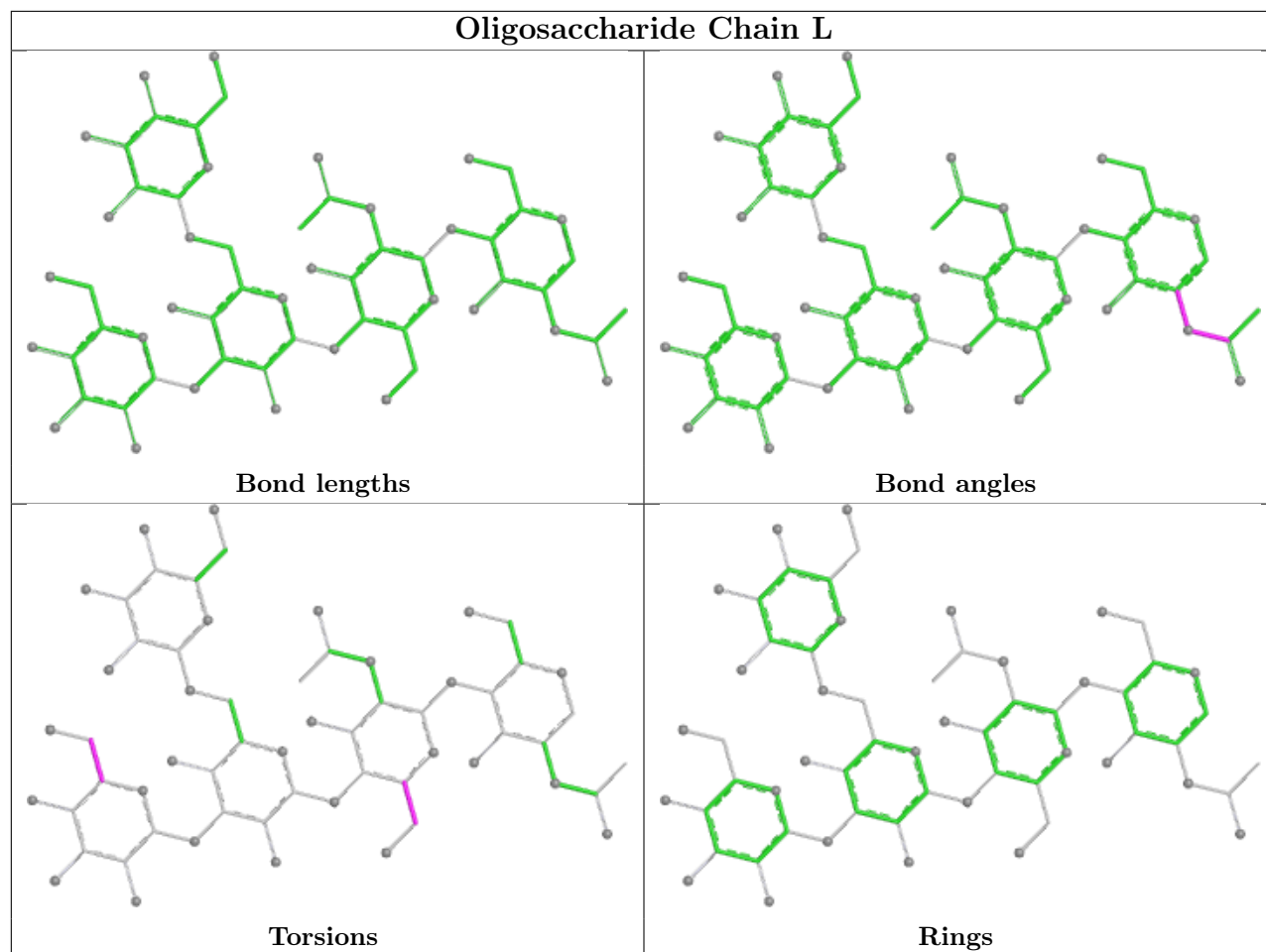
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	1	NAG	1	0
3	J	1	NAG	4	0

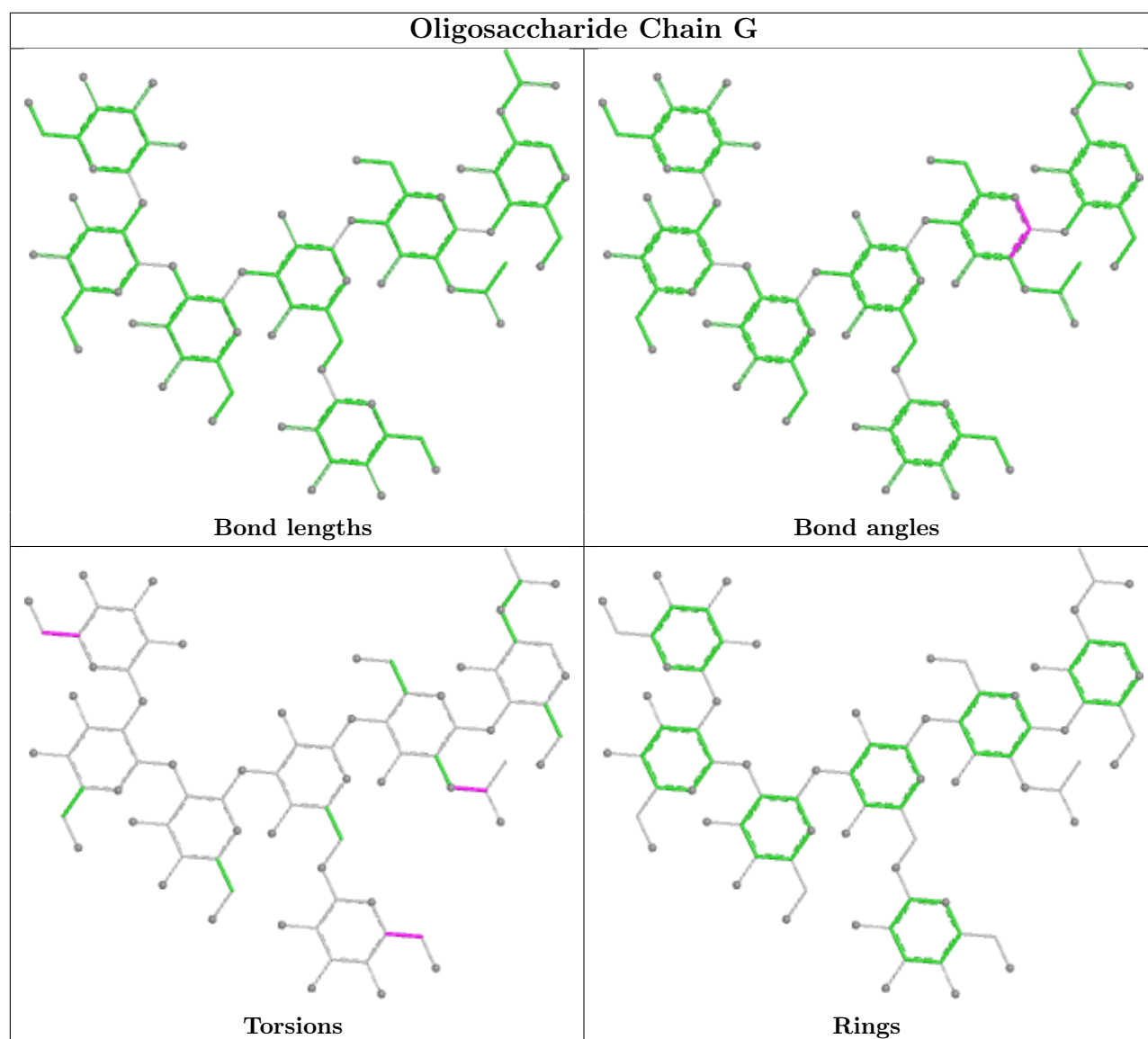
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

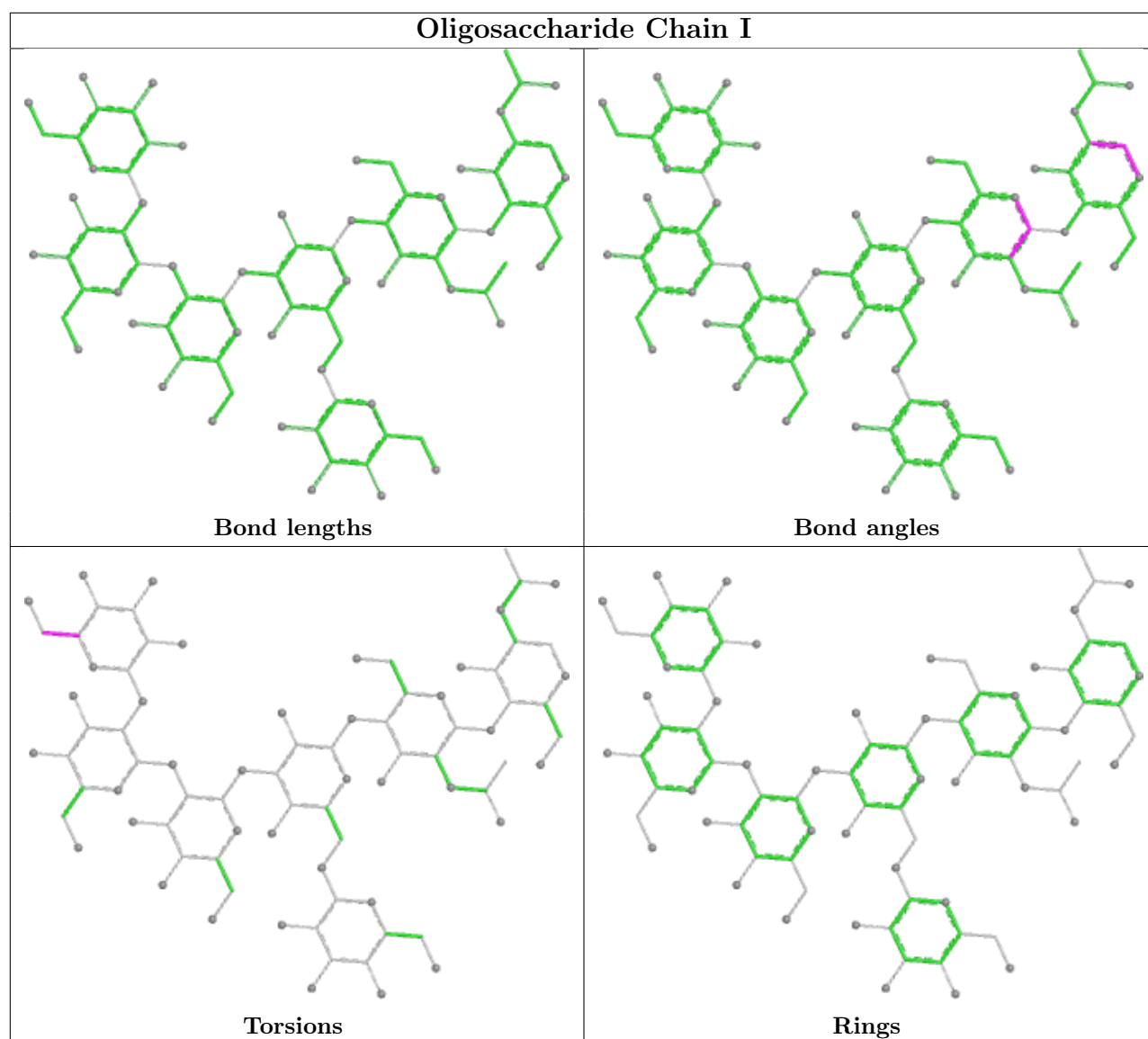




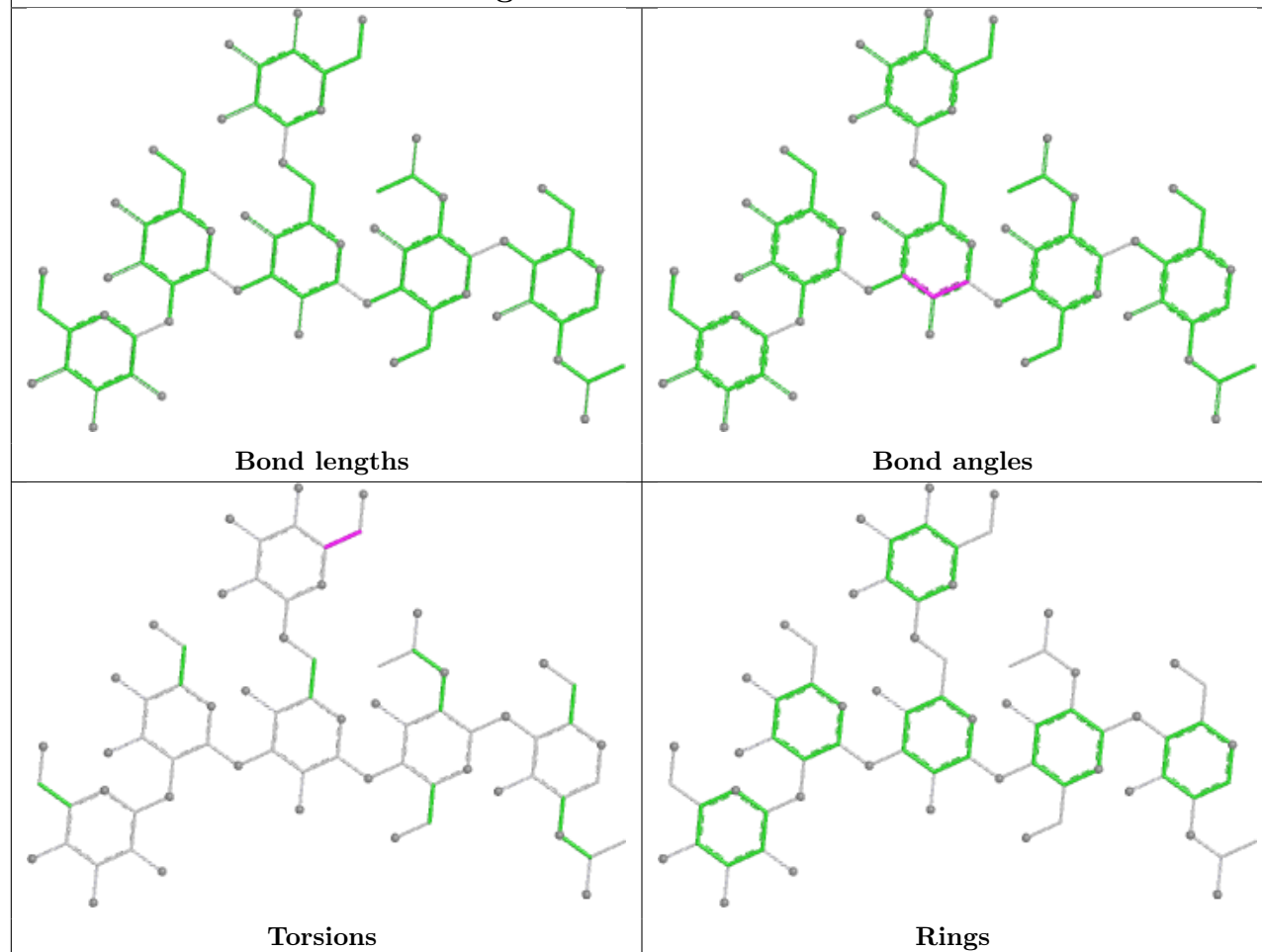


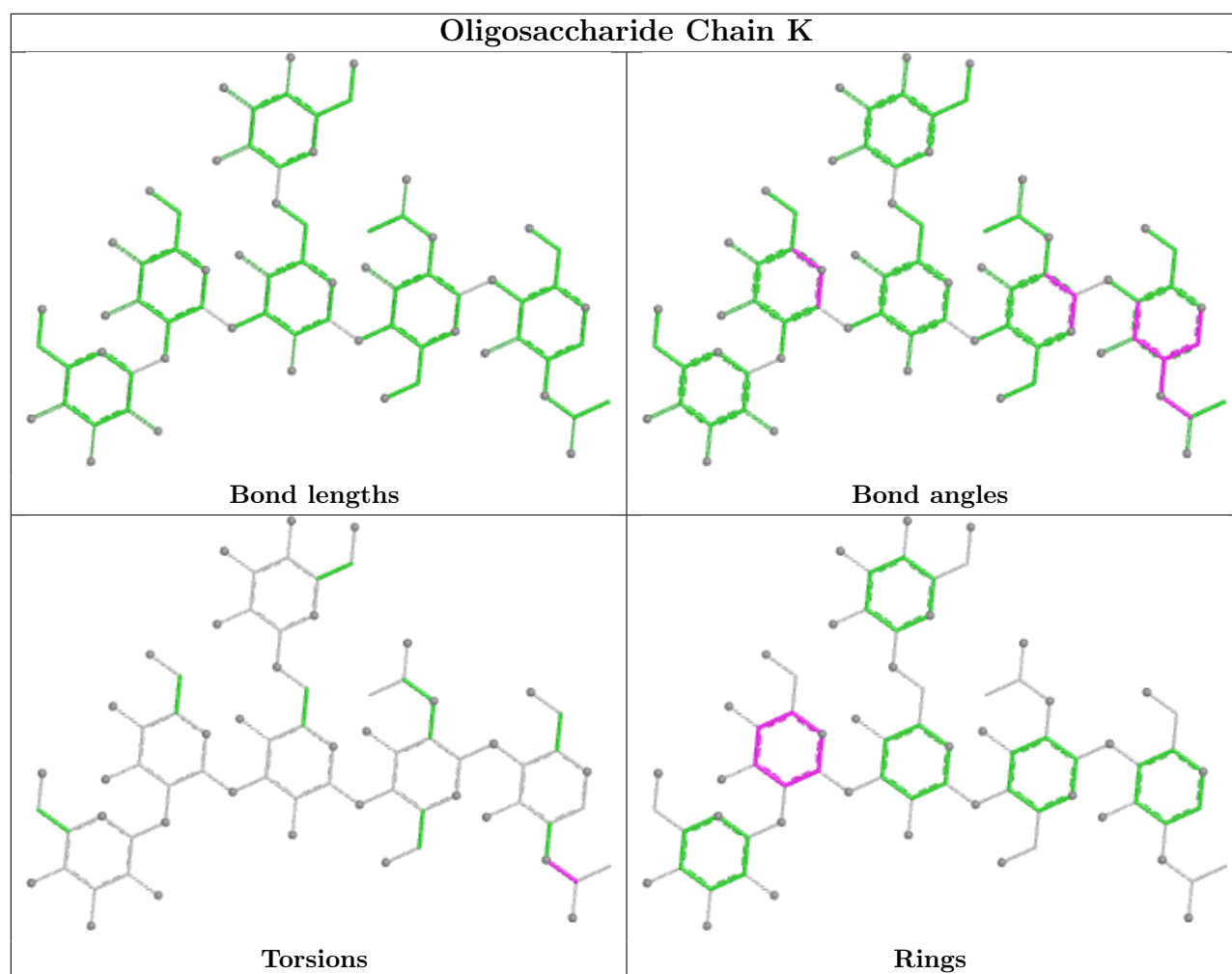






Oligosaccharide Chain H





5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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

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	361/419 (86%)	0.61	11 (3%) 52 61	16, 37, 49, 77	5 (1%)
1	B	361/419 (86%)	0.96	30 (8%) 17 22	16, 42, 63, 80	6 (1%)
1	C	361/419 (86%)	1.30	77 (21%) 2 3	16, 43, 81, 106	2 (0%)
1	D	361/419 (86%)	0.84	23 (6%) 25 31	19, 41, 56, 80	4 (1%)
All	All	1444/1676 (86%)	0.93	141 (9%) 13 17	16, 40, 69, 106	17 (1%)

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	403	ILE	7.9
1	B	403	ILE	5.8
1	C	385	THR	5.3
1	A	403	ILE	5.2
1	A	43	THR	5.2
1	C	348	SER	5.0
1	C	97	LEU	4.8
1	C	301	CYS	4.7
1	C	357	PHE	4.6
1	C	102	VAL	4.6
1	C	339	PRO	4.6
1	C	345	LEU	4.5
1	C	362	TRP	4.5
1	C	350	TYR	4.5
1	D	43	THR	4.4
1	C	354	GLY	4.4
1	C	342	LEU	4.4
1	C	356	LYS	4.3
1	C	338	LYS	4.2
1	B	301	CYS	4.2
1	B	377	THR	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	241	PHE	4.1
1	D	301	CYS	4.1
1	C	361	LEU	3.9
1	A	301	CYS	3.9
1	C	96	LYS	3.8
1	C	99	ALA	3.8
1	C	355	ALA	3.8
1	C	218	CYS	3.8
1	D	93	ASN	3.7
1	C	100	ALA	3.7
1	C	365	ILE	3.5
1	A	218	CYS	3.5
1	B	93	ASN	3.5
1	C	402	TYR	3.5
1	C	351	GLY	3.4
1	C	360	ASN	3.4
1	C	322	ILE	3.3
1	D	403	ILE	3.3
1	D	187	ALA	3.2
1	D	241	PHE	3.2
1	C	329	LYS	3.1
1	B	402	TYR	3.1
1	C	321	ILE	3.1
1	C	325	TYR	3.1
1	D	44	LYS	3.1
1	C	43	THR	3.0
1	C	327	ASN	3.0
1	C	368	LEU	3.0
1	C	103	ALA	2.9
1	D	175	TRP	2.9
1	C	93	ASN	2.9
1	B	401	GLY	2.9
1	C	359	GLU	2.9
1	C	335	THR	2.9
1	C	336	THR	2.9
1	C	349	ALA	2.9
1	C	337	ASP	2.9
1	C	352	LYS	2.8
1	C	311	PHE	2.8
1	C	324	SER	2.8
1	B	43	THR	2.8
1	D	51	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	372	VAL	2.7
1	B	400	LEU	2.7
1	C	346	ILE	2.7
1	C	369	SER	2.7
1	C	94	ASN	2.7
1	C	175	TRP	2.7
1	C	86	LEU	2.7
1	A	175	TRP	2.7
1	C	98	GLN	2.7
1	C	353	ASN	2.7
1	B	127	ARG	2.6
1	C	382	ASN	2.6
1	C	317	PHE	2.6
1	C	344	LYS	2.6
1	C	384	LYS	2.6
1	D	47	ALA	2.6
1	C	318	SER	2.5
1	C	366	ASP	2.5
1	B	392	LEU	2.5
1	C	207	LYS	2.5
1	D	265	ALA	2.5
1	B	346	ILE	2.5
1	C	241[A]	PHE	2.4
1	C	383	LEU	2.4
1	D	127[A]	ARG	2.4
1	C	88	ILE	2.4
1	C	169	VAL	2.4
1	B	94	ASN	2.4
1	C	363	ASP	2.4
1	B	381	LEU	2.4
1	C	104	PRO	2.3
1	B	96	LYS	2.3
1	D	207	LYS	2.3
1	C	308	TYR	2.3
1	A	93	ASN	2.3
1	B	224	THR	2.3
1	A	257	ALA	2.3
1	D	248[A]	MET	2.3
1	C	312	SER	2.3
1	C	323	ARG	2.3
1	D	190	GLY	2.3
1	A	327	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	328	ASN	2.3
1	C	315	GLY	2.3
1	C	101	ALA	2.2
1	C	397	ALA	2.2
1	C	340	SER	2.2
1	C	370	PRO	2.2
1	B	327	ASN	2.2
1	B	374	LYS	2.2
1	B	248[A]	MET	2.2
1	B	221	GLY	2.2
1	C	343	GLU	2.2
1	B	156	THR	2.2
1	B	99	ALA	2.2
1	B	397	ALA	2.2
1	A	207	LYS	2.2
1	B	384	LYS	2.2
1	D	223	ASP	2.1
1	C	231	ALA	2.1
1	C	127	ARG	2.1
1	B	318	SER	2.1
1	A	130	ILE	2.1
1	D	130	ILE	2.1
1	D	287	VAL	2.1
1	C	331	ASN	2.1
1	B	97	LEU	2.1
1	B	367	LYS	2.1
1	B	241[A]	PHE	2.1
1	D	327	ASN	2.0
1	D	218	CYS	2.0
1	D	250	THR	2.0
1	C	380	LYS	2.0
1	B	382	ASN	2.0
1	B	101	ALA	2.0
1	C	302	ALA	2.0
1	D	197	ALA	2.0
1	D	263	ALA	2.0

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

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.

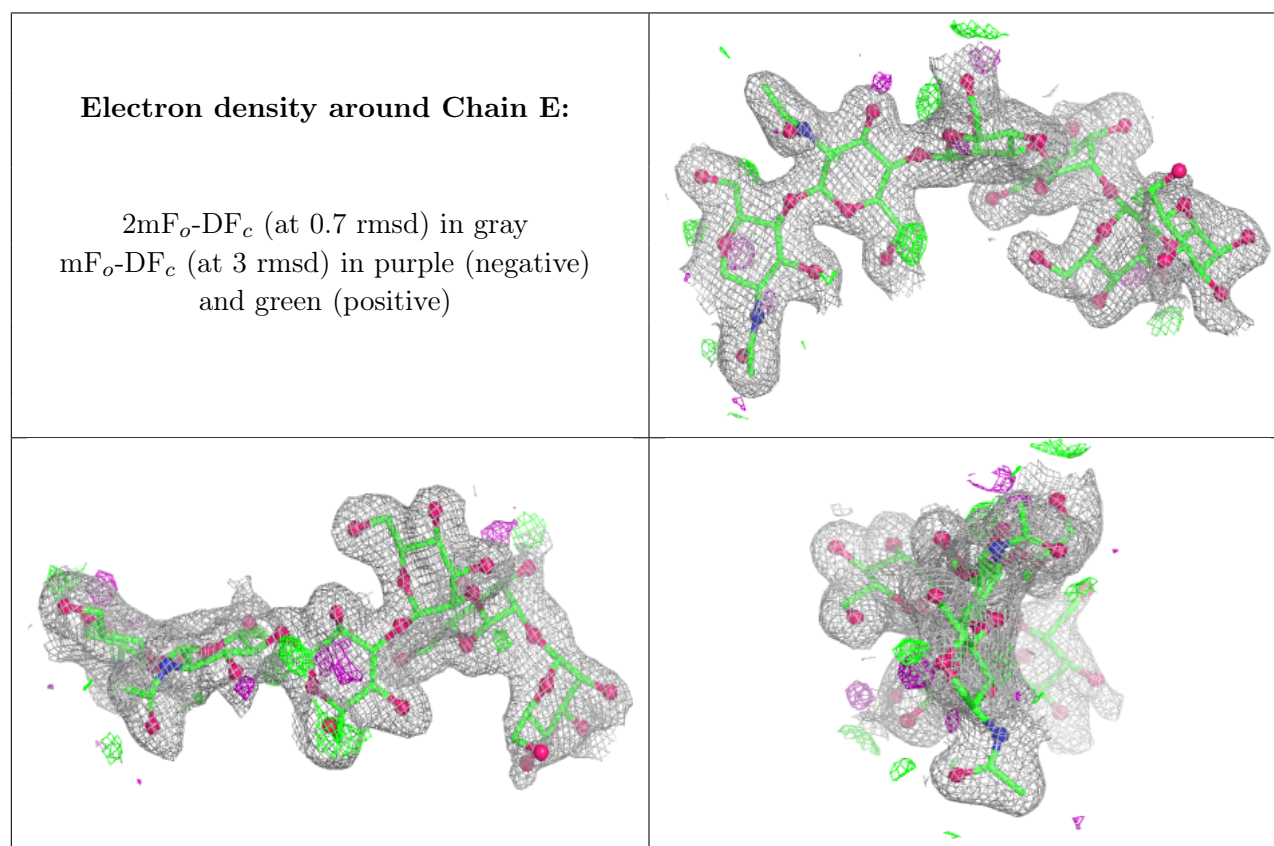
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MAN	F	5	11/12	0.55	0.17	75,79,83,83	0
3	MAN	J	5	11/12	0.55	0.17	76,84,86,87	0
4	MAN	G	7	11/12	0.57	0.18	63,69,72,73	0
4	MAN	I	7	11/12	0.62	0.18	62,67,71,71	0
5	MAN	K	4	11/12	0.67	0.20	36,45,52,54	0
5	MAN	H	6	11/12	0.68	0.16	63,67,70,71	0
5	MAN	K	6	11/12	0.74	0.17	61,65,72,73	0
3	MAN	J	4	11/12	0.75	0.14	49,59,62,62	0
4	MAN	I	6	11/12	0.75	0.14	65,72,84,88	0
2	MAN	E	6	11/12	0.76	0.13	63,69,75,81	0
4	MAN	G	6	11/12	0.76	0.14	54,65,68,79	0
3	MAN	L	5	11/12	0.77	0.14	68,74,75,76	0
3	MAN	F	4	11/12	0.77	0.13	53,68,74,75	0
3	BMA	L	3	11/12	0.78	0.14	55,59,66,71	0
5	MAN	K	5	11/12	0.79	0.14	52,57,64,68	0
5	MAN	H	5	11/12	0.79	0.18	45,57,62,62	0
3	NAG	L	2	14/15	0.81	0.15	38,52,62,65	0
3	NAG	L	1	14/15	0.84	0.15	41,50,56,56	0
3	MAN	L	4	11/12	0.84	0.12	50,59,64,65	0
5	BMA	H	3	11/12	0.87	0.11	44,48,58,60	0
3	BMA	F	3	11/12	0.87	0.12	50,60,68,71	0
4	MAN	G	5	11/12	0.88	0.11	44,50,56,58	0
4	MAN	I	5	11/12	0.88	0.11	36,43,53,54	0
5	MAN	H	4	11/12	0.88	0.11	47,50,54,58	0
2	MAN	E	5	11/12	0.88	0.11	42,49,54,57	0
5	NAG	H	2	14/15	0.89	0.12	31,43,53,53	0
2	BMA	E	3	11/12	0.90	0.10	28,35,43,48	0
5	NAG	H	1	14/15	0.90	0.11	32,38,43,45	0
3	BMA	J	3	11/12	0.91	0.10	43,52,60,67	0
2	NAG	E	2	14/15	0.91	0.10	26,32,37,38	0
4	NAG	I	1	14/15	0.91	0.10	25,30,32,34	0
4	BMA	G	3	11/12	0.91	0.10	29,37,43,48	0
3	NAG	J	1	14/15	0.91	0.10	26,37,41,41	0
3	NAG	J	2	14/15	0.92	0.10	31,38,48,48	0
4	NAG	G	2	14/15	0.92	0.08	27,33,38,43	0
5	NAG	K	1	14/15	0.92	0.10	26,36,41,48	0
4	MAN	G	4	11/12	0.93	0.09	30,33,44,48	0

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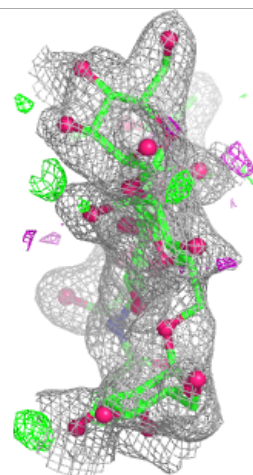
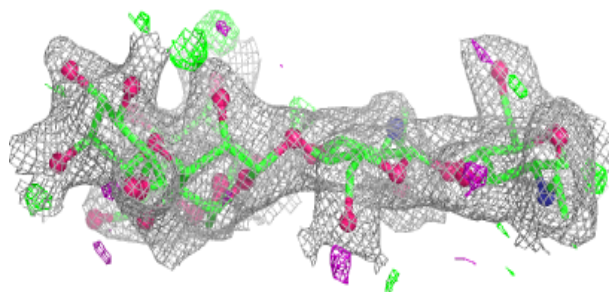
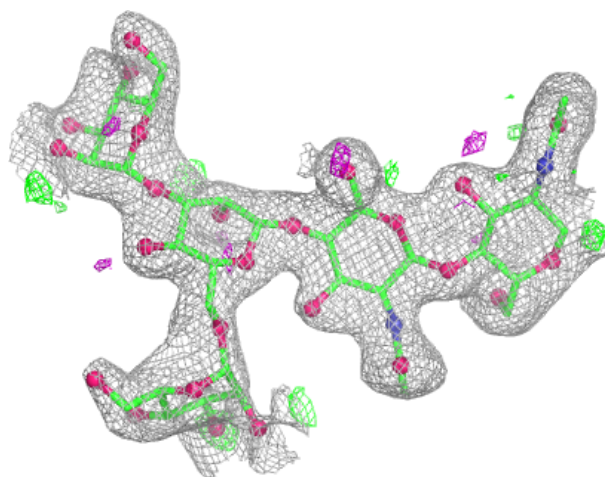
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	I	2	14/15	0.93	0.09	26,32,38,38	0
5	BMA	K	3	11/12	0.93	0.09	37,45,52,59	0
2	NAG	E	1	14/15	0.93	0.09	27,30,34,35	0
2	MAN	E	4	11/12	0.93	0.09	30,36,41,49	0
3	NAG	F	2	14/15	0.93	0.10	33,43,53,54	0
5	NAG	K	2	14/15	0.94	0.08	35,39,42,46	0
4	BMA	I	3	11/12	0.94	0.09	30,35,43,49	0
4	MAN	I	4	11/12	0.94	0.08	31,35,38,39	0
3	NAG	F	1	14/15	0.94	0.08	26,35,40,42	0
4	NAG	G	1	14/15	0.94	0.08	25,30,33,34	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.



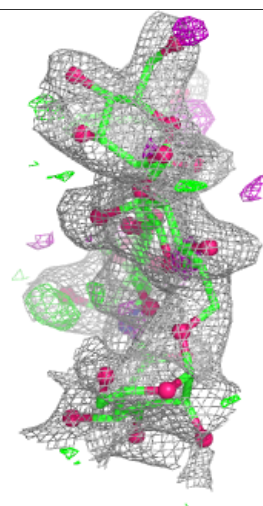
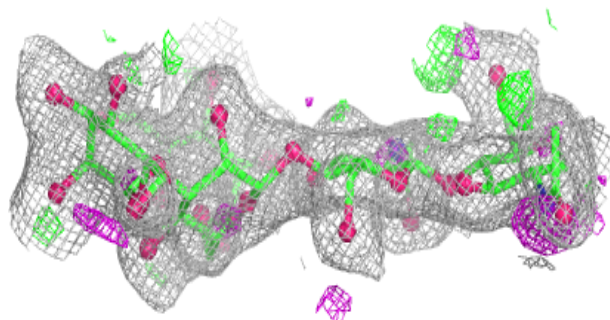
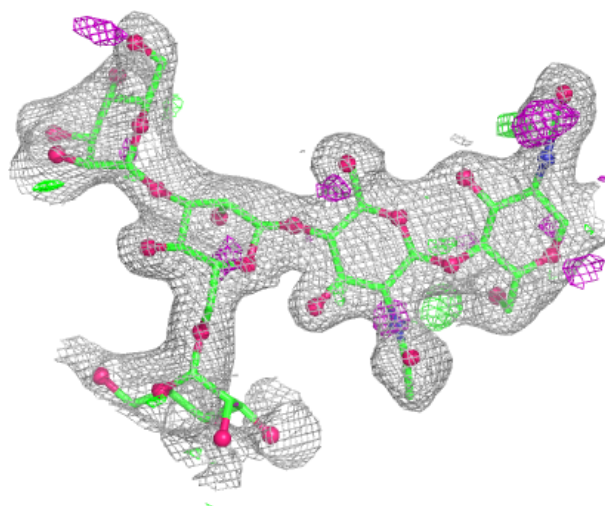
Electron density around Chain F:

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



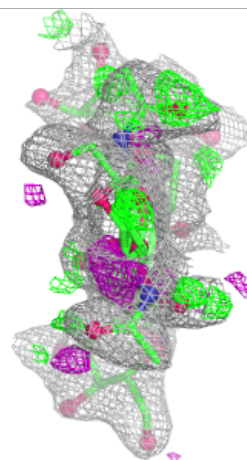
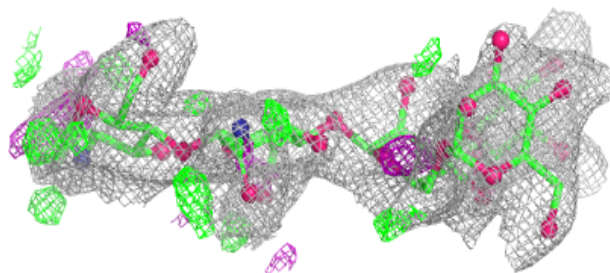
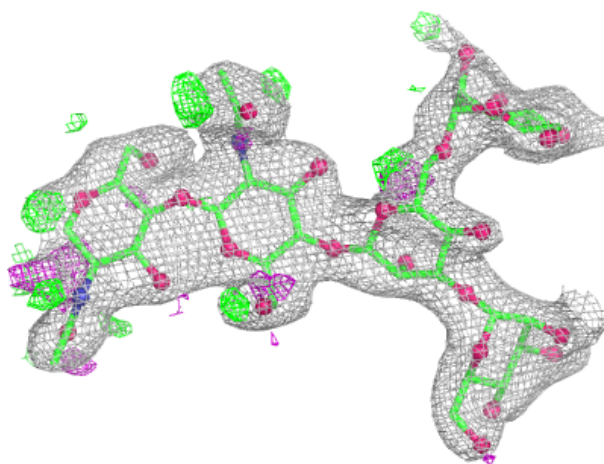
Electron density around Chain J:

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



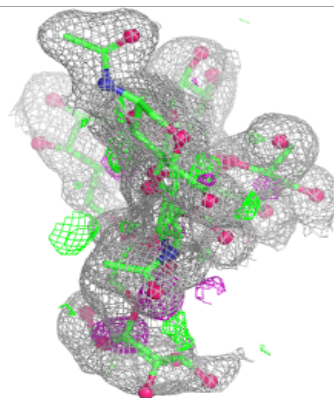
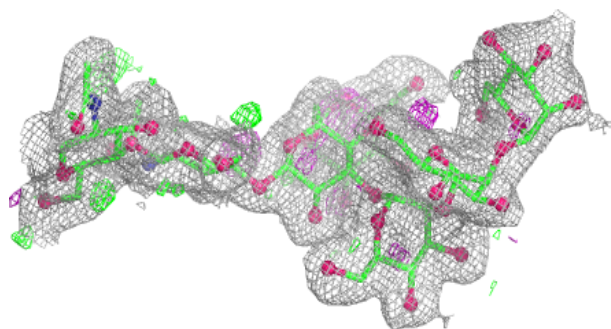
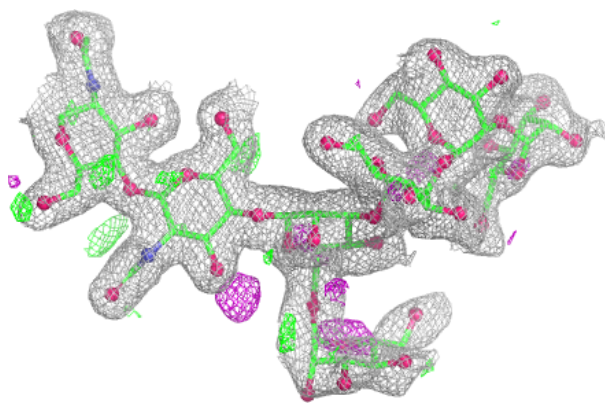
Electron density around Chain L:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



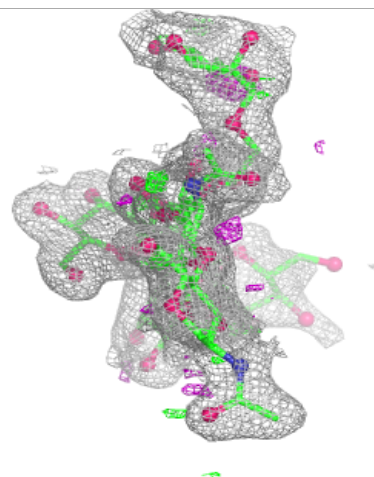
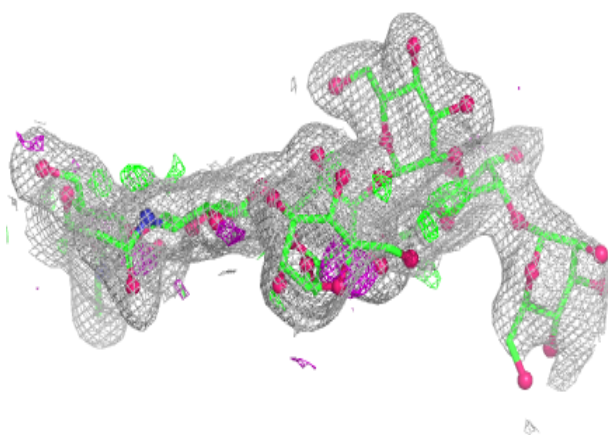
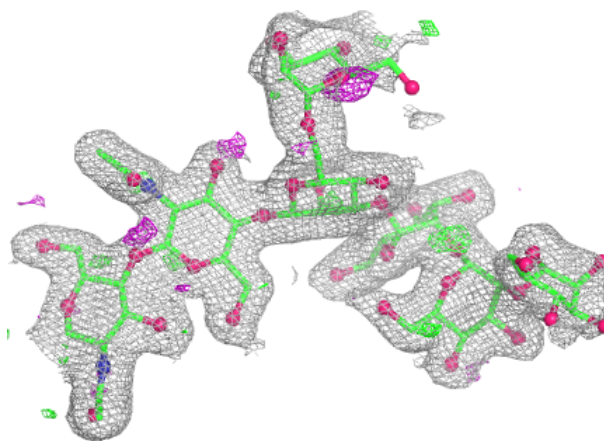
Electron density around Chain G:

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



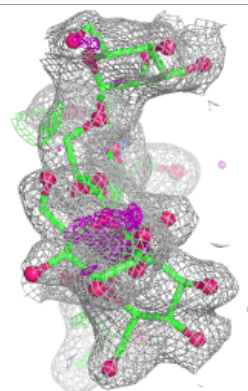
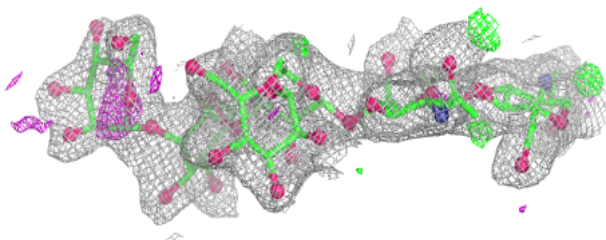
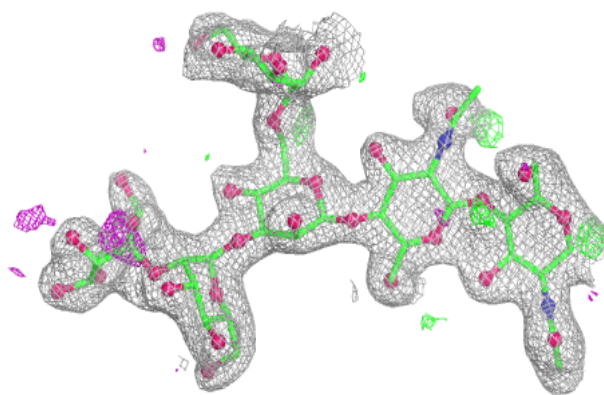
Electron density around Chain I:

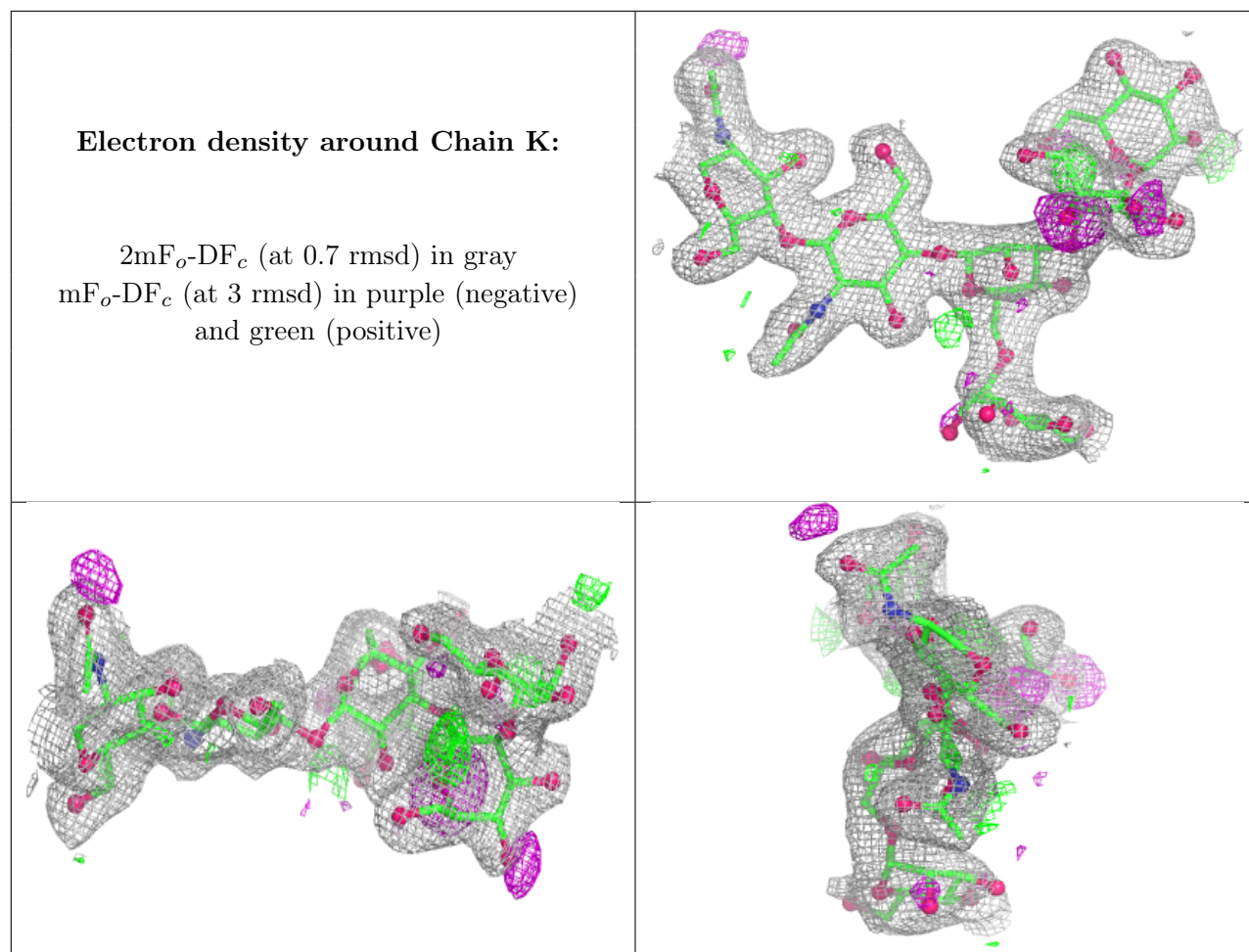
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain H:

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





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.