



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:43 AM UTC

PDB ID : 2B8H / pdb_00002b8h
Title : A/NWS/whale/Maine/1/84 (H1N9) reassortant influenza virus neuraminidase
Authors : Smith, B.J.; Platis, D.; Cox, M.M.J.; Huyton, T.; Joosten, R.P.; McKimm-Breschkin, J.L.; Zhang, J.-G.; Luo, C.S.; Lou, M.-Z.; Garrett, T.P.J.; Labrou, N.E.
Deposited on : 2005-10-07
Resolution : 2.20 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

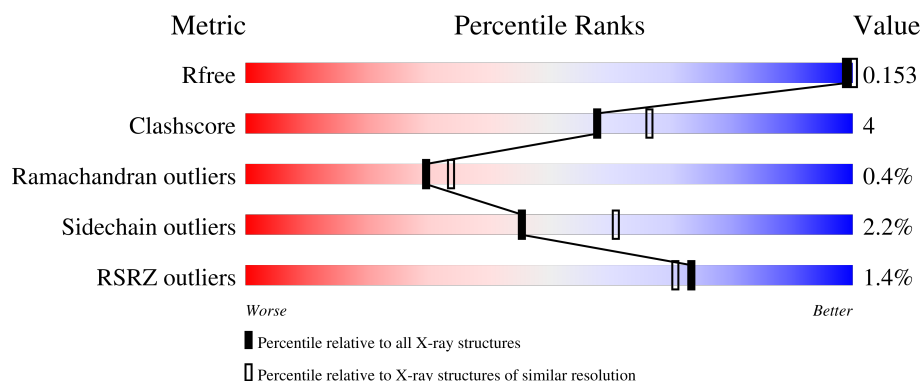
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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.



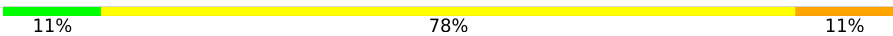
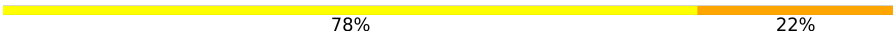
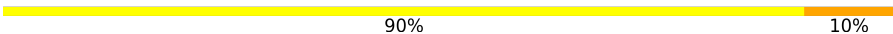
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	388	90% 9% .
1	B	388	% 91% 8% .
1	C	388	% 90% 9% .
1	D	388	3% 85% 12% ..
2	E	2	100%

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Mol	Chain	Length	Quality of chain
2	G	2	 50%50%
2	I	2	 100%
2	K	2	 50%50%
3	F	9	 100%
3	J	9	 11%78%11%
3	L	9	 78%22%
4	H	10	 90%10%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 14424 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 Neuraminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	0	4	0
			3069	1910	539	595	25			
1	B	388	Total	C	N	O	S	0	4	0
			3067	1908	540	594	25			
1	C	388	Total	C	N	O	S	0	4	0
			3067	1909	540	593	25			
1	D	388	Total	C	N	O	S	0	6	0
			3082	1919	544	594	25			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	368	VAL	ILE	conflict	UNP P05803
B	368	VAL	ILE	conflict	UNP P05803
C	368	VAL	ILE	conflict	UNP P05803
D	368	VAL	ILE	conflict	UNP P05803

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



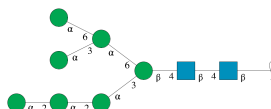
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

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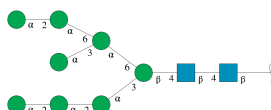
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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	9	Total	C	N	O	0	0	0
			105	58	2	45			
3	J	9	Total	C	N	O	0	0	0
			105	58	2	45			
3	L	9	Total	C	N	O	0	0	0
			105	58	2	45			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[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.



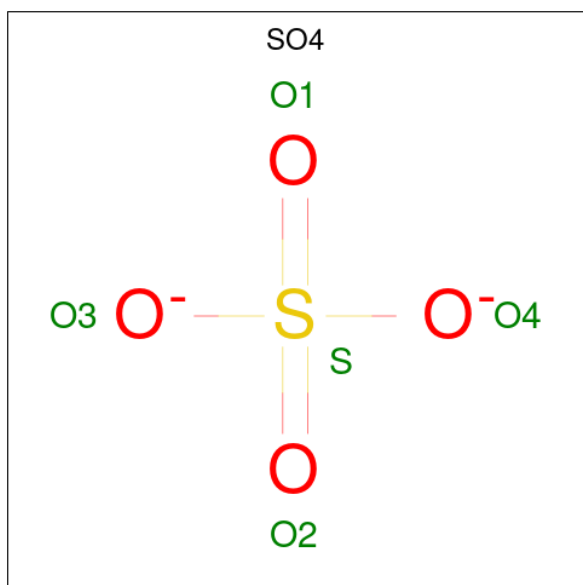
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	10	Total	C	N	O	0	0	0
			116	64	2	50			

- 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	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	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		
7	B	1	Total	Cl	0	0
			1	1		
7	C	1	Total	Cl	0	0
			1	1		
7	D	1	Total	Cl	0	0
			1	1		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



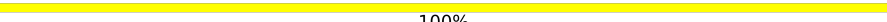
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	369	Total	O	0	0
			369	369		
9	B	315	Total	O	0	0
			315	315		
9	C	324	Total	O	0	0
			324	324		
9	D	365	Total	O	0	0
			365	365		



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

Chain E:  100%

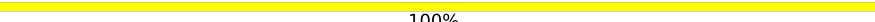
NAG1
NAG2

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

Chain G:  50%

NAG1
NAG2

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

Chain I:  100%

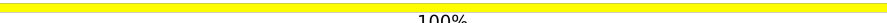
NAG1
NAG2

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

Chain K:  50%

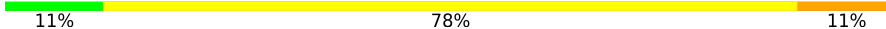
NAG1
NAG2

- Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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 F:  100%

NAG1
NAG2
MAN3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9

- Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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 J:  11% 78% 11%

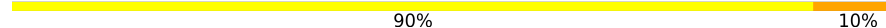
MAN1
MAN2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9

- Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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:  78% 22%

MAN1
MAN2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9

- Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[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:  90% 10%

MAN1
MAN2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9
MAN10

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	107.52Å 107.52Å 338.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.20 20.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-2.20) 99.6 (20.00-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.21 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.139 , 0.189 0.152 , 0.153	Depositor DCC
R_{free} test set	5837 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	21.1	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14424	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, GOL, BMA, NAG, MAN, SO4

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	1.32	3/3169 (0.1%)	1.06	5/4316 (0.1%)
1	B	1.31	4/3167 (0.1%)	1.09	4/4314 (0.1%)
1	C	1.38	8/3169 (0.3%)	1.11	7/4315 (0.2%)
1	D	1.36	7/3195 (0.2%)	1.12	9/4352 (0.2%)
All	All	1.34	22/12700 (0.2%)	1.10	25/17297 (0.1%)

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	C	0	1
1	D	0	1
All	All	0	2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	156	ARG	CD-NE	-7.20	1.36	1.46
1	D	286	ALA	CA-CB	7.18	1.64	1.53
1	B	223	ILE	C-O	-6.71	1.16	1.24
1	B	252	GLU	CA-C	6.46	1.59	1.52
1	D	156	ARG	CD-NE	-6.46	1.37	1.46
1	C	408	SER	N-CA	-6.36	1.38	1.45
1	D	275	HIS	C-O	5.95	1.31	1.23
1	B	274	LYS	CA-C	5.91	1.57	1.52
1	A	240	VAL	C-O	-5.88	1.18	1.24
1	D	270	THR	CA-CB	5.86	1.62	1.53
1	A	333	THR	CA-CB	5.78	1.62	1.53
1	B	201	ASN	C-O	-5.71	1.19	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	293	ARG	NE-CZ	5.69	1.39	1.33
1	C	305	GLN	CA-C	-5.57	1.45	1.52
1	C	105	ALA	CA-CB	-5.56	1.44	1.53
1	C	368	VAL	CA-CB	5.56	1.61	1.54
1	C	421	ALA	C-O	-5.46	1.17	1.23
1	C	404	GLY	C-O	5.46	1.30	1.23
1	D	396	ILE	CA-CB	5.45	1.60	1.55
1	C	289	THR	N-CA	-5.20	1.39	1.46
1	D	389	LYS	CA-C	5.07	1.59	1.52
1	D	276	ILE	C-O	-5.04	1.18	1.23

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	348	GLY	N-CA-C	9.13	134.83	113.18
1	B	277	GLU	N-CA-C	7.85	119.57	108.74
1	C	366	ILE	N-CA-C	-7.19	103.77	110.53
1	C	298	GLY	N-CA-C	7.15	124.39	113.02
1	D	227	GLN	N-CA-C	7.03	119.02	111.36
1	A	227	GLN	N-CA-C	6.75	118.63	111.28
1	D	277	GLU	CB-CG-CD	-6.66	101.29	112.60
1	A	156	ARG	NE-CZ-NH2	-6.60	113.26	119.20
1	D	277	GLU	N-CA-C	6.36	118.44	108.96
1	D	125	ASP	N-CA-C	-6.19	102.88	110.31
1	A	125	ASP	N-CA-C	-5.81	101.52	110.58
1	B	277	GLU	CB-CG-CD	-5.73	102.86	112.60
1	D	295	ASN	N-CA-C	5.72	120.00	113.19
1	C	227	GLN	N-CA-C	5.72	117.60	111.36
1	B	347	ASN	N-CA-C	5.60	122.73	110.80
1	A	181	SER	N-CA-C	5.57	117.54	109.07
1	C	347	ASN	N-CA-C	5.28	117.35	110.43
1	C	277	GLU	N-CA-C	5.25	116.78	108.96
1	B	227	GLN	N-CA-C	5.25	117.00	111.28
1	D	151	ASP	N-CA-C	5.21	117.04	111.36
1	D	156	ARG	NE-CZ-NH2	-5.18	114.54	119.20
1	C	181	SER	N-CA-C	5.17	116.67	108.96
1	A	156	ARG	CB-CG-CD	-5.14	99.49	111.30
1	D	156	ARG	NE-CZ-NH1	5.09	126.59	121.50
1	C	385	ASP	N-CA-C	5.03	116.80	108.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	270	THR	Peptide
1	D	246	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	3069	0	2880	24	0
1	B	3067	0	2878	23	0
1	C	3067	0	2878	20	0
1	D	3082	0	2891	41	0
2	E	28	0	25	0	0
2	G	28	0	25	1	0
2	I	28	0	25	0	0
2	K	28	0	25	1	0
3	F	105	0	87	1	0
3	J	105	0	88	1	0
3	L	105	0	88	2	0
4	H	116	0	97	1	0
5	A	14	0	13	1	0
5	B	14	0	13	1	0
5	C	14	0	13	1	0
5	D	14	0	13	0	0
6	A	40	0	0	1	0
6	B	30	0	0	1	0
6	C	45	0	0	3	0
6	D	30	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	1	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	A	18	0	24	1	0
9	A	369	0	0	4	1
9	B	315	0	0	5	0
9	C	324	0	0	4	0
9	D	365	0	0	11	1
All	All	14424	0	12063	112	1

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 4.

All (112) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:HIS:HB3	1:B:295[A]:ASN:HD21	1.04	1.16
1:B:275:HIS:HB3	1:B:295[A]:ASN:ND2	1.78	0.98
6:A:2516:SO4:O1	9:A:5368:HOH:O	1.84	0.93
1:B:271:GLY:O	1:B:274:LYS:NZ	2.02	0.93
6:B:3516:SO4:O4	9:B:3772:HOH:O	1.86	0.93
1:C:368:VAL:HG22	6:C:3521:SO4:O3	1.71	0.89
1:A:176:CYS:SG	1:A:194[B]:CYS:HB2	2.18	0.84
1:D:176:CYS:SG	1:D:194[B]:CYS:HB2	2.23	0.78
1:D:347:ASN:C	1:D:347:ASN:HD22	1.94	0.76
1:A:82:ARG:HH11	1:A:82:ARG:HB2	1.50	0.75
6:C:3520:SO4:O2	9:C:4826:HOH:O	2.05	0.74
1:B:276:ILE:HD13	1:B:304:ILE:HD11	1.70	0.73
1:C:176:CYS:SG	1:C:194[B]:CYS:HB2	2.28	0.73
1:D:305:GLN:HB3	1:D:314:THR:HG22	1.71	0.72
1:D:270:THR:HG23	9:D:4723:HOH:O	1.89	0.72
1:C:271:GLY:H	1:C:274:LYS:NZ	1.87	0.72
1:A:82:ARG:HH11	1:A:82:ARG:CB	2.03	0.72
1:A:222:ASN:HD21	8:A:5003:GOL:H32	1.55	0.72
7:B:2522:CL:CL	9:B:3822:HOH:O	2.46	0.71
1:D:285:GLN:HG3	9:D:4741:HOH:O	1.88	0.71
1:D:368:VAL:HG23	9:D:4886:HOH:O	1.91	0.70
1:D:295:ASN:O	1:D:346:ASN:HA	1.92	0.69
1:C:402:TRP:CZ3	1:C:433:LYS:HD3	2.28	0.69
1:B:176:CYS:SG	1:B:194[B]:CYS:HB2	2.33	0.68
1:D:269:LEU:O	9:D:4623:HOH:O	2.13	0.67
1:C:271:GLY:H	1:C:274:LYS:HZ3	1.44	0.66
1:D:248:THR:O	1:D:249:GLY:O	2.15	0.63
1:B:275:HIS:CB	1:B:295[A]:ASN:ND2	2.59	0.63
1:D:245:GLY:HA3	1:D:251:ALA:HA	1.80	0.63
1:D:314:THR:HG23	9:D:4679:HOH:O	1.97	0.63
1:D:273:ALA:HA	1:D:317:TYR:CE1	2.36	0.59
1:C:270:THR:HG23	9:C:4801:HOH:O	2.00	0.59
1:D:135:SER:O	1:D:156:ARG:HD2	2.02	0.59
1:B:276:ILE:CD1	1:B:304:ILE:HD11	2.33	0.58
1:D:336:LYS:NZ	9:D:4838:HOH:O	2.36	0.58
1:D:464:LYS:NZ	1:D:464:LYS:HB3	2.21	0.56
6:C:4516:SO4:O3	9:C:4712:HOH:O	2.18	0.55
1:D:269:LEU:HB3	9:D:4623:HOH:O	2.08	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:THR:HG22	9:B:3682:HOH:O	2.08	0.54
1:B:297:GLN:OE1	1:B:342:PRO:HA	2.08	0.53
5:A:500:NAG:H83	9:A:5140:HOH:O	2.07	0.53
1:A:344:ASN:C	1:A:345:ASN:HD22	2.15	0.53
1:D:210[B]:ARG:NE	9:D:4865:HOH:O	2.40	0.53
1:B:344:ASN:ND2	1:B:347:ASN:OD1	2.42	0.53
1:B:415:GLU:HA	1:B:415:GLU:OE1	2.09	0.52
1:B:234:GLN:HG2	1:B:308:PRO:HG2	1.91	0.52
1:A:175:GLU:OE1	9:A:5220:HOH:O	2.19	0.51
1:D:299:SER:OG	1:D:341:TYR:O	2.26	0.51
1:C:402:TRP:CZ3	1:C:433:LYS:CD	2.94	0.51
1:A:234[A]:GLN:HG2	1:A:308:PRO:HG2	1.93	0.51
1:B:171[A]:ASN:HD21	1:C:170:TYR:HB3	1.76	0.50
1:C:402:TRP:CH2	1:C:433:LYS:HD3	2.46	0.50
1:D:464:LYS:HB3	1:D:464:LYS:HZ3	1.77	0.49
5:C:500:NAG:H61	9:C:4718:HOH:O	2.11	0.49
9:B:3715:HOH:O	2:G:2:NAG:O4	2.20	0.49
1:A:378:LYS:O	1:A:390:PRO:HA	2.12	0.49
1:D:210[A]:ARG:HD3	9:D:4865:HOH:O	2.13	0.48
1:D:121:TYR:CG	1:D:229:SER:HA	2.48	0.47
1:C:121:TYR:CG	1:C:229:SER:HA	2.50	0.47
1:D:131:PHE:CE1	1:D:163:LEU:HD12	2.49	0.47
1:D:347:ASN:C	1:D:347:ASN:ND2	2.67	0.47
1:A:262:LYS:NZ	9:A:5332:HOH:O	2.47	0.47
1:C:271:GLY:N	1:C:274:LYS:HZ3	2.11	0.47
1:B:347:ASN:OD1	1:B:347:ASN:N	2.47	0.47
1:D:262:LYS:NZ	9:D:4784:HOH:O	2.47	0.46
1:A:87:LEU:H	1:A:234[B]:GLN:HG2	1.79	0.46
1:A:154:GLN:HG2	1:D:458:ASN:O	2.15	0.46
1:D:193:ILE:HG12	1:D:206:ILE:HG13	1.96	0.46
1:D:275:HIS:O	1:D:276:ILE:CG1	2.64	0.45
1:A:255:ILE:N	1:A:255:ILE:HD12	2.31	0.45
1:B:307:ASP:OD1	1:B:307:ASP:C	2.59	0.45
5:B:500:NAG:H61	9:B:3709:HOH:O	2.15	0.45
1:A:173:ARG:NE	1:A:210:ARG:NH2	2.65	0.45
1:A:135:SER:O	1:A:156:ARG:HD2	2.16	0.45
1:B:222:ASN:HD22	1:B:223:ILE:HG13	1.82	0.45
1:A:121:TYR:CG	1:A:229:SER:HA	2.52	0.44
1:D:263:ILE:HG21	1:D:266[B]:TRP:CE3	2.53	0.44
1:A:135:SER:O	1:A:156:ARG:CD	2.65	0.44
1:A:407:GLY:HA3	1:A:424:TYR:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:234[A]:GLN:HE22	1:D:309:VAL:HG22	1.83	0.43
1:D:297:GLN:NE2	1:D:342:PRO:HA	2.33	0.43
1:A:279:CYS:HB3	1:A:290:CYS:HB3	1.99	0.43
1:B:168:THR:HG1	1:B:171[B]:ASN:CG	2.15	0.43
1:A:393:GLY:HA3	4:H:3:BMA:O2	2.18	0.43
1:D:168:THR:HG1	1:D:171[B]:ASN:CG	2.15	0.43
1:D:135:SER:O	1:D:156:ARG:CD	2.65	0.43
1:C:271:GLY:H	1:C:274:LYS:HZ1	1.64	0.42
1:C:393:GLY:HA3	3:L:3:BMA:O2	2.19	0.42
1:A:82:ARG:HB2	1:A:82:ARG:NH1	2.28	0.42
1:D:393:GLY:HA3	3:F:3:BMA:O2	2.18	0.42
1:C:367:SER:HB3	1:C:372:SER:HB2	2.01	0.42
1:D:263:ILE:HG21	1:D:266[B]:TRP:CZ3	2.54	0.42
1:D:146:ASN:ND2	2:K:1:NAG:O7	2.53	0.42
1:B:182:THR:HG22	1:B:193:ILE:HB	2.00	0.42
1:A:296:TRP:CG	1:A:297:GLN:HG3	2.54	0.42
1:C:276:ILE:HD12	1:C:276:ILE:HA	1.80	0.42
1:D:254:ARG:HD3	1:D:266[A]:TRP:CE3	2.55	0.41
1:C:462:GLY:HA3	1:D:155:TYR:CE1	2.55	0.41
1:A:294:ASP:OD1	1:A:294:ASP:C	2.64	0.41
1:B:458:ASN:O	1:C:154:GLN:HG2	2.21	0.41
1:D:464:LYS:NZ	1:D:464:LYS:CB	2.83	0.41
1:C:330:ASN:HA	3:L:6:MAN:O3	2.19	0.41
1:D:341:TYR:O	1:D:342:PRO:C	2.62	0.41
1:D:140:ILE:HD11	9:D:4619:HOH:O	2.20	0.41
1:B:393:GLY:HA3	3:J:3:BMA:O2	2.21	0.41
1:A:258:PHE:HA	1:A:262:LYS:O	2.21	0.41
1:A:462:GLY:HA3	1:B:155:TYR:CE1	2.56	0.41
1:B:465:ILE:HG23	1:B:465:ILE:HD12	1.79	0.40
1:D:168:THR:OG1	1:D:171[A]:ASN:OD1	2.38	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:5115:HOH:O	9:D:4752:HOH:O[4_565]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	390/388 (100%)	374 (96%)	16 (4%)	0	100	100
1	B	390/388 (100%)	369 (95%)	19 (5%)	2 (0%)	24	27
1	C	390/388 (100%)	366 (94%)	24 (6%)	0	100	100
1	D	392/388 (101%)	365 (93%)	23 (6%)	4 (1%)	12	11
All	All	1562/1552 (101%)	1474 (94%)	82 (5%)	6 (0%)	30	34

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	249	GLY
1	B	348	GLY
1	D	348	GLY
1	D	246	SER
1	B	347	ASN
1	D	248	THR

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	343/340 (101%)	338 (98%)	5 (2%)	57	73
1	B	343/340 (101%)	335 (98%)	8 (2%)	44	59
1	C	343/340 (101%)	333 (97%)	10 (3%)	37	51
1	D	345/340 (102%)	335 (97%)	10 (3%)	37	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1374/1360 (101%)	1341 (98%)	33 (2%)	45 58

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	ARG
1	A	156	ARG
1	A	255	ILE
1	A	284	GLU
1	A	345	ASN
1	B	210	ARG
1	B	221	ARG
1	B	276	ILE
1	B	277	GLU
1	B	295[A]	ASN
1	B	295[B]	ASN
1	B	389	LYS
1	B	466	GLU
1	C	83	GLU
1	C	210	ARG
1	C	234	GLN
1	C	269	LEU
1	C	272	THR
1	C	276	ILE
1	C	284	GLU
1	C	285[A]	GLN
1	C	285[B]	GLN
1	C	299	SER
1	D	83	GLU
1	D	156	ARG
1	D	200	ASN
1	D	234[A]	GLN
1	D	234[B]	GLN
1	D	274	LYS
1	D	276	ILE
1	D	284	GLU
1	D	347	ASN
1	D	464	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	344	ASN
1	A	345	ASN
1	A	458	ASN
1	B	200	ASN
1	B	222	ASN
1	B	235	ASN
1	B	338	ASN
1	B	345	ASN
1	C	95	ASN
1	C	136	GLN
1	C	234	GLN
1	C	458	ASN
1	D	297	GLN
1	D	347	ASN
1	D	458	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 ⓘ

45 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	1.23	2 (14%)	17,19,21	1.82	4 (23%)
2	NAG	E	2	2	14,14,15	0.75	0	17,19,21	1.34	2 (11%)
3	NAG	F	1	1,3	14,14,15	1.16	1 (7%)	17,19,21	1.51	3 (17%)
3	NAG	F	2	3	14,14,15	1.18	1 (7%)	17,19,21	1.83	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	F	3	3	11,11,12	0.89	0	15,15,17	0.88	0
3	MAN	F	4	3	11,11,12	0.72	0	15,15,17	1.73	4 (26%)
3	MAN	F	5	3	11,11,12	1.30	1 (9%)	15,15,17	1.40	2 (13%)
3	MAN	F	6	3	11,11,12	0.88	0	15,15,17	1.44	3 (20%)
3	MAN	F	7	3	11,11,12	1.07	1 (9%)	15,15,17	1.38	1 (6%)
3	MAN	F	8	3	11,11,12	1.13	1 (9%)	15,15,17	1.49	2 (13%)
3	MAN	F	9	3	11,11,12	0.84	0	15,15,17	2.38	7 (46%)
2	NAG	G	1	1,2	14,14,15	1.04	1 (7%)	17,19,21	1.85	4 (23%)
2	NAG	G	2	2	14,14,15	0.72	0	17,19,21	1.75	2 (11%)
4	NAG	H	1	1,4	14,14,15	1.27	2 (14%)	17,19,21	1.84	7 (41%)
4	MAN	H	10	4	11,11,12	0.67	0	15,15,17	1.44	3 (20%)
4	NAG	H	2	4	14,14,15	0.90	0	17,19,21	1.67	3 (17%)
4	BMA	H	3	4	11,11,12	0.98	1 (9%)	15,15,17	1.32	2 (13%)
4	MAN	H	4	4	11,11,12	1.27	1 (9%)	15,15,17	1.96	3 (20%)
4	MAN	H	5	4	11,11,12	0.94	0	15,15,17	1.22	2 (13%)
4	MAN	H	6	4	11,11,12	0.57	0	15,15,17	1.06	1 (6%)
4	MAN	H	7	4	11,11,12	0.96	1 (9%)	15,15,17	1.17	1 (6%)
4	MAN	H	8	4	11,11,12	0.82	0	15,15,17	1.03	1 (6%)
4	MAN	H	9	4	11,11,12	0.75	0	15,15,17	1.35	1 (6%)
2	NAG	I	1	1,2	14,14,15	1.37	2 (14%)	17,19,21	2.27	5 (29%)
2	NAG	I	2	2	14,14,15	1.25	1 (7%)	17,19,21	2.98	3 (17%)
3	NAG	J	1	1,3	14,14,15	0.92	1 (7%)	17,19,21	1.59	5 (29%)
3	NAG	J	2	3	14,14,15	1.14	1 (7%)	17,19,21	1.34	2 (11%)
3	BMA	J	3	3	11,11,12	1.29	1 (9%)	15,15,17	1.38	2 (13%)
3	MAN	J	4	3	11,11,12	1.05	1 (9%)	15,15,17	2.23	6 (40%)
3	MAN	J	5	3	11,11,12	1.07	1 (9%)	15,15,17	1.18	2 (13%)
3	MAN	J	6	3	11,11,12	1.04	0	15,15,17	1.32	1 (6%)
3	MAN	J	7	3	11,11,12	1.17	2 (18%)	15,15,17	0.91	0
3	MAN	J	8	3	11,11,12	0.74	0	15,15,17	1.24	0
3	MAN	J	9	3	11,11,12	1.03	0	15,15,17	2.08	4 (26%)
2	NAG	K	1	1,2	14,14,15	0.98	1 (7%)	17,19,21	2.20	6 (35%)
2	NAG	K	2	2	14,14,15	0.83	0	17,19,21	1.65	4 (23%)
3	NAG	L	1	1,3	14,14,15	1.19	2 (14%)	17,19,21	1.34	3 (17%)
3	NAG	L	2	3	14,14,15	0.95	2 (14%)	17,19,21	1.85	6 (35%)
3	BMA	L	3	3	11,11,12	0.73	0	15,15,17	0.89	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	L	4	3	11,11,12	1.32	1 (9%)	15,15,17	1.78	4 (26%)
3	MAN	L	5	3	11,11,12	0.87	1 (9%)	15,15,17	1.65	2 (13%)
3	MAN	L	6	3	11,11,12	0.88	0	15,15,17	1.18	1 (6%)
3	MAN	L	7	3	11,11,12	0.84	0	15,15,17	1.14	1 (6%)
3	MAN	L	8	3	11,11,12	0.71	0	15,15,17	1.20	1 (6%)
3	MAN	L	9	3	11,11,12	1.00	1 (9%)	15,15,17	1.35	3 (20%)

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	-	0/6/23/26	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	-	0/2/19/22	0/1/1/1
3	MAN	F	4	3	-	0/2/19/22	0/1/1/1
3	MAN	F	5	3	-	0/2/19/22	0/1/1/1
3	MAN	F	6	3	-	0/2/19/22	0/1/1/1
3	MAN	F	7	3	-	0/2/19/22	0/1/1/1
3	MAN	F	8	3	-	2/2/19/22	0/1/1/1
3	MAN	F	9	3	-	1/2/19/22	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
4	NAG	H	1	1,4	-	0/6/23/26	0/1/1/1
4	MAN	H	10	4	-	0/2/19/22	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1
4	BMA	H	3	4	-	0/2/19/22	0/1/1/1
4	MAN	H	4	4	-	0/2/19/22	0/1/1/1
4	MAN	H	5	4	-	0/2/19/22	0/1/1/1
4	MAN	H	6	4	-	0/2/19/22	0/1/1/1
4	MAN	H	7	4	-	0/2/19/22	0/1/1/1
4	MAN	H	8	4	-	0/2/19/22	0/1/1/1
4	MAN	H	9	4	-	0/2/19/22	0/1/1/1
2	NAG	I	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	4/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
3	MAN	J	6	3	-	0/2/19/22	0/1/1/1
3	MAN	J	7	3	-	0/2/19/22	0/1/1/1
3	MAN	J	8	3	-	0/2/19/22	0/1/1/1
3	MAN	J	9	3	-	2/2/19/22	0/1/1/1
2	NAG	K	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
3	NAG	L	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	L	2	3	-	0/6/23/26	0/1/1/1
3	BMA	L	3	3	-	0/2/19/22	0/1/1/1
3	MAN	L	4	3	-	1/2/19/22	0/1/1/1
3	MAN	L	5	3	-	0/2/19/22	0/1/1/1
3	MAN	L	6	3	-	0/2/19/22	0/1/1/1
3	MAN	L	7	3	-	0/2/19/22	0/1/1/1
3	MAN	L	8	3	-	0/2/19/22	0/1/1/1
3	MAN	L	9	3	-	0/2/19/22	0/1/1/1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	2	NAG	C1-C2	3.94	1.57	1.52
3	J	2	NAG	O5-C1	-3.52	1.37	1.43
2	I	1	NAG	O5-C1	-3.34	1.38	1.43
3	F	5	MAN	O3-C3	-3.30	1.34	1.43
2	E	1	NAG	O5-C1	-3.24	1.38	1.43
3	F	2	NAG	O5-C1	-3.17	1.38	1.43
3	L	4	MAN	O5-C1	-3.14	1.38	1.43
3	F	1	NAG	C1-C2	3.06	1.56	1.52
3	L	1	NAG	C1-C2	3.04	1.56	1.52
3	F	8	MAN	O5-C1	-3.02	1.38	1.43
3	J	3	BMA	C2-C3	3.00	1.57	1.52
4	H	4	MAN	C2-C3	2.87	1.56	1.52
4	H	1	NAG	C1-C2	2.83	1.56	1.52
4	H	7	MAN	O2-C2	-2.73	1.37	1.43
2	K	1	NAG	O7-C7	2.70	1.29	1.23
2	G	1	NAG	O7-C7	2.64	1.29	1.23
3	F	7	MAN	O5-C1	-2.54	1.39	1.43
2	I	1	NAG	C3-C2	2.49	1.57	1.52
2	E	1	NAG	O7-C7	2.46	1.28	1.23
4	H	1	NAG	O5-C1	-2.43	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	4	MAN	O5-C1	-2.33	1.39	1.43
3	J	7	MAN	O5-C1	-2.32	1.39	1.43
3	J	7	MAN	O2-C2	-2.25	1.38	1.43
4	H	3	BMA	O3-C3	-2.24	1.37	1.43
3	L	9	MAN	C1-C2	2.23	1.57	1.52
3	J	5	MAN	O5-C1	-2.17	1.40	1.43
3	L	1	NAG	C4-C5	2.16	1.57	1.53
3	J	1	NAG	C1-C2	2.09	1.55	1.52
3	L	2	NAG	O5-C1	-2.08	1.40	1.43
3	L	5	MAN	O5-C1	-2.03	1.40	1.43
3	L	2	NAG	C1-C2	-2.02	1.49	1.52

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	2	NAG	C1-O5-C5	10.79	126.65	112.19
3	J	4	MAN	C1-O5-C5	5.46	119.50	112.19
2	G	2	NAG	C1-O5-C5	4.95	118.82	112.19
3	F	9	MAN	O3-C3-C2	4.93	120.11	110.05
3	J	9	MAN	O2-C2-C1	4.92	120.48	109.22
2	E	1	NAG	O5-C1-C2	-4.87	103.76	111.29
2	I	1	NAG	O3-C3-C4	4.61	121.25	110.38
3	F	4	MAN	O2-C2-C1	-4.48	98.96	109.22
3	L	5	MAN	C1-O5-C5	4.45	118.14	112.19
2	G	1	NAG	C2-N2-C7	-4.44	116.95	122.90
4	H	4	MAN	C1-O5-C5	4.41	118.10	112.19
2	I	1	NAG	C3-C4-C5	-4.34	102.35	110.23
4	H	4	MAN	O2-C2-C1	-4.32	99.33	109.22
2	I	1	NAG	O4-C4-C3	4.31	120.53	110.38
2	E	2	NAG	C2-N2-C7	-4.30	117.14	122.90
3	J	4	MAN	O2-C2-C1	-4.28	99.42	109.22
2	K	1	NAG	C2-N2-C7	-4.27	117.18	122.90
3	F	6	MAN	C1-O5-C5	4.12	117.70	112.19
3	L	2	NAG	C1-C2-N2	4.07	116.85	110.43
2	K	1	NAG	O4-C4-C3	-3.92	101.14	110.38
3	F	9	MAN	O4-C4-C3	-3.76	101.52	110.38
3	L	4	MAN	O2-C2-C1	-3.74	100.67	109.22
4	H	2	NAG	O6-C6-C5	-3.73	98.64	111.33
3	F	2	NAG	C8-C7-N2	3.72	122.29	116.12
3	L	6	MAN	C1-O5-C5	3.59	117.00	112.19
2	K	1	NAG	O5-C1-C2	-3.58	105.75	111.29
3	J	9	MAN	O6-C6-C5	-3.58	99.13	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	5	MAN	C1-C2-C3	-3.57	104.45	109.64
3	F	9	MAN	O2-C2-C3	3.52	117.44	110.15
3	J	1	NAG	O7-C7-N2	3.44	128.07	121.98
2	G	1	NAG	C1-O5-C5	3.43	116.78	112.19
3	F	9	MAN	O2-C2-C1	3.43	117.07	109.22
3	L	7	MAN	O2-C2-C1	3.42	117.05	109.22
3	J	2	NAG	O3-C3-C4	3.37	118.32	110.38
2	K	1	NAG	O7-C7-C8	3.37	128.05	122.05
4	H	2	NAG	O3-C3-C4	3.36	118.31	110.38
3	F	8	MAN	C1-O5-C5	3.36	116.68	112.19
2	K	2	NAG	C2-N2-C7	-3.31	118.47	122.90
4	H	1	NAG	C1-O5-C5	3.30	116.60	112.19
2	K	1	NAG	C8-C7-N2	-3.26	110.71	116.12
3	L	2	NAG	O6-C6-C5	-3.21	100.39	111.33
2	G	1	NAG	O5-C1-C2	-3.19	106.36	111.29
3	L	9	MAN	O2-C2-C1	3.19	116.52	109.22
2	K	2	NAG	C8-C7-N2	3.17	121.37	116.12
4	H	6	MAN	C1-O5-C5	3.09	116.33	112.19
4	H	1	NAG	O4-C4-C3	-3.09	103.09	110.38
2	I	2	NAG	O5-C5-C4	3.08	118.32	110.83
4	H	1	NAG	O5-C1-C2	-3.05	106.57	111.29
3	F	2	NAG	O4-C4-C3	-3.02	103.25	110.38
3	J	6	MAN	C1-O5-C5	2.95	116.14	112.19
3	F	1	NAG	O7-C7-N2	2.94	127.18	121.98
3	L	4	MAN	O6-C6-C5	-2.93	101.35	111.33
3	J	3	BMA	O5-C5-C6	2.92	113.35	107.66
3	F	9	MAN	C1-C2-C3	-2.91	105.41	109.64
3	F	7	MAN	O4-C4-C3	-2.89	103.57	110.38
3	L	8	MAN	O5-C5-C6	2.87	113.25	107.66
2	I	1	NAG	C1-C2-N2	-2.86	105.93	110.43
3	J	5	MAN	O4-C4-C3	-2.85	103.66	110.38
3	J	4	MAN	O2-C2-C3	2.81	115.98	110.15
4	H	9	MAN	O6-C6-C5	-2.74	101.99	111.33
3	F	1	NAG	C2-N2-C7	2.74	126.57	122.90
3	F	6	MAN	C3-C4-C5	-2.70	105.34	110.23
3	L	2	NAG	O5-C1-C2	-2.68	107.15	111.29
3	J	9	MAN	C1-C2-C3	-2.62	105.82	109.64
3	J	2	NAG	O6-C6-C5	-2.62	102.41	111.33
2	E	1	NAG	C2-N2-C7	-2.62	119.39	122.90
2	G	2	NAG	C2-N2-C7	2.61	126.40	122.90
4	H	10	MAN	O3-C3-C4	2.61	116.52	110.38
4	H	10	MAN	O2-C2-C3	2.60	115.54	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2	NAG	C2-N2-C7	-2.59	119.43	122.90
3	J	9	MAN	O4-C4-C3	-2.59	104.27	110.38
3	L	1	NAG	O5-C1-C2	-2.57	107.31	111.29
3	L	2	NAG	O5-C5-C6	2.56	112.64	107.66
3	L	2	NAG	C3-C4-C5	-2.53	105.65	110.23
2	G	1	NAG	O4-C4-C3	-2.52	104.42	110.38
3	L	4	MAN	C1-O5-C5	2.52	115.57	112.19
3	F	2	NAG	O7-C7-C8	-2.49	117.61	122.05
2	E	1	NAG	O4-C4-C3	-2.47	104.55	110.38
4	H	1	NAG	O7-C7-N2	2.47	126.34	121.98
4	H	2	NAG	C3-C4-C5	-2.44	105.81	110.23
3	F	4	MAN	O2-C2-C3	2.42	115.16	110.15
3	F	2	NAG	C6-C5-C4	2.39	118.90	113.02
2	K	2	NAG	O7-C7-C8	-2.38	117.82	122.05
3	J	1	NAG	C1-O5-C5	2.37	115.36	112.19
3	L	1	NAG	O5-C5-C6	2.37	112.28	107.66
3	F	9	MAN	O5-C5-C6	2.36	112.25	107.66
3	J	3	BMA	C6-C5-C4	-2.35	107.26	113.02
3	L	4	MAN	O5-C5-C4	2.33	116.50	110.83
2	I	1	NAG	C4-C3-C2	-2.33	107.60	111.02
3	F	2	NAG	O3-C3-C4	2.32	115.84	110.38
3	J	4	MAN	O4-C4-C3	2.32	115.83	110.38
4	H	7	MAN	C2-C3-C4	2.31	114.93	110.86
3	J	1	NAG	C2-N2-C7	-2.28	119.84	122.90
3	F	9	MAN	O6-C6-C5	-2.27	103.61	111.33
4	H	3	BMA	O3-C3-C2	-2.25	105.47	110.05
3	F	6	MAN	O2-C2-C1	2.24	114.35	109.22
3	J	4	MAN	O6-C6-C5	-2.24	103.71	111.33
2	E	1	NAG	C8-C7-N2	-2.23	112.41	116.12
3	F	1	NAG	C8-C7-N2	-2.23	112.42	116.12
4	H	5	MAN	C1-O5-C5	2.23	115.17	112.19
2	K	1	NAG	C1-O5-C5	2.22	115.16	112.19
4	H	1	NAG	C3-C4-C5	-2.22	106.21	110.23
4	H	3	BMA	C1-C2-C3	-2.21	106.43	109.64
3	L	5	MAN	O6-C6-C5	2.21	118.85	111.33
2	E	2	NAG	O6-C6-C5	-2.20	103.84	111.33
3	J	1	NAG	O7-C7-C8	-2.20	118.14	122.05
4	H	1	NAG	O3-C3-C4	-2.19	105.21	110.38
3	J	5	MAN	O2-C2-C1	-2.19	104.21	109.22
2	I	2	NAG	O3-C3-C2	2.18	113.93	109.40
4	H	10	MAN	C1-C2-C3	-2.17	106.49	109.64
2	K	2	NAG	O5-C5-C6	2.16	111.87	107.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	1	NAG	O7-C7-N2	2.15	125.79	121.98
4	H	4	MAN	O3-C3-C2	2.14	114.43	110.05
3	L	9	MAN	O6-C6-C5	-2.14	104.03	111.33
4	H	5	MAN	O5-C5-C6	2.14	111.83	107.66
3	L	3	BMA	C3-C4-C5	-2.12	106.39	110.23
3	J	4	MAN	C3-C4-C5	-2.12	106.39	110.23
3	F	4	MAN	C1-O5-C5	2.11	115.02	112.19
3	J	1	NAG	O4-C4-C3	-2.11	105.41	110.38
3	L	2	NAG	O3-C3-C4	2.07	115.26	110.38
3	F	5	MAN	O3-C3-C4	-2.06	105.51	110.38
3	F	8	MAN	O3-C3-C2	-2.06	105.85	110.05
4	H	1	NAG	O7-C7-C8	-2.05	118.40	122.05
4	H	8	MAN	C1-O5-C5	2.05	114.93	112.19
3	L	9	MAN	C6-C5-C4	-2.03	108.03	113.02
3	F	4	MAN	O3-C3-C2	2.00	114.14	110.05

There are no chirality outliers.

All (16) torsion outliers are listed below:

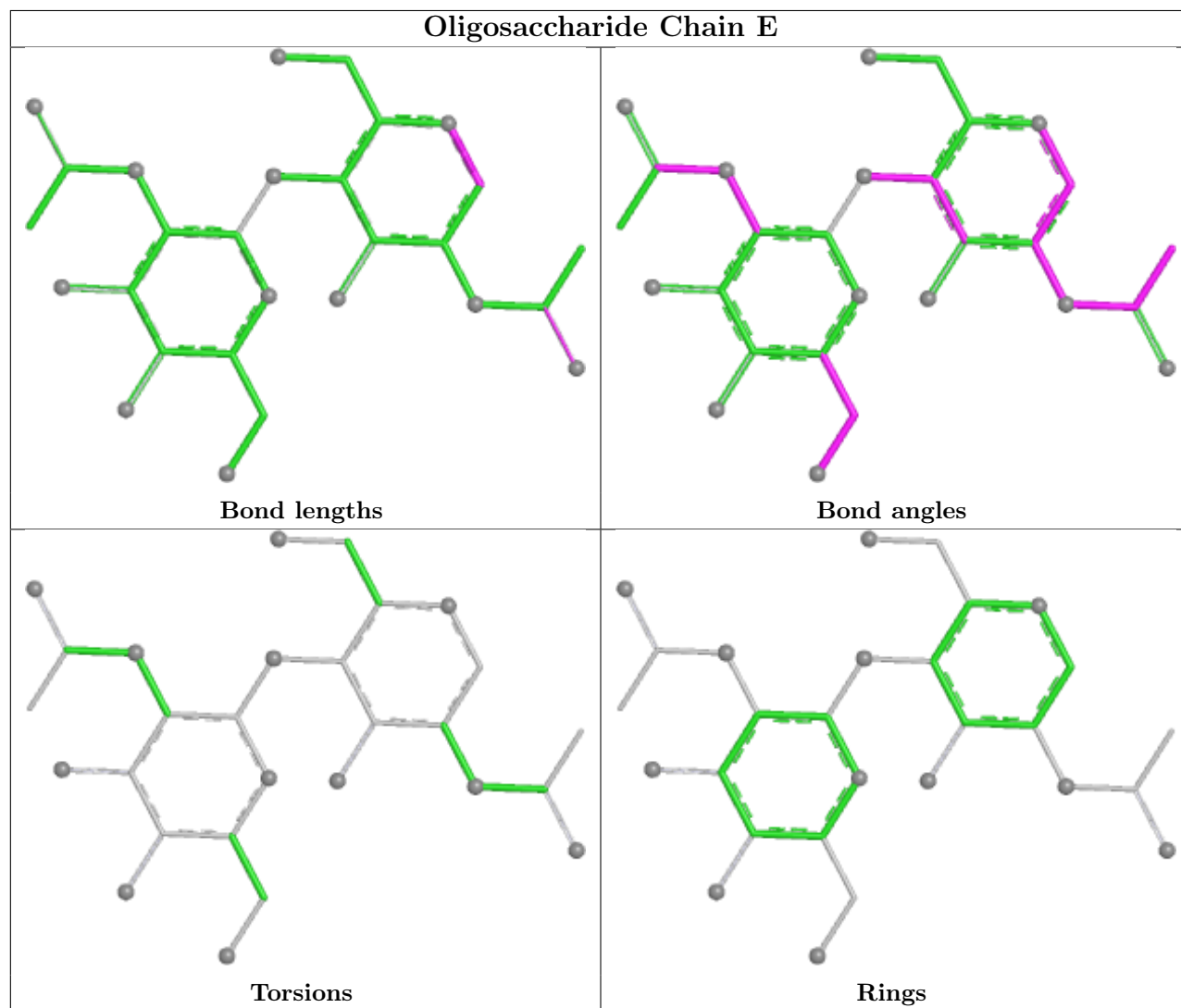
Mol	Chain	Res	Type	Atoms
3	J	9	MAN	O5-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
3	J	9	MAN	C4-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	I	2	NAG	C8-C7-N2-C2
2	I	2	NAG	O7-C7-N2-C2
2	K	2	NAG	O5-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
3	F	8	MAN	C4-C5-C6-O6
3	F	8	MAN	O5-C5-C6-O6
3	F	9	MAN	O5-C5-C6-O6
3	L	4	MAN	C4-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6

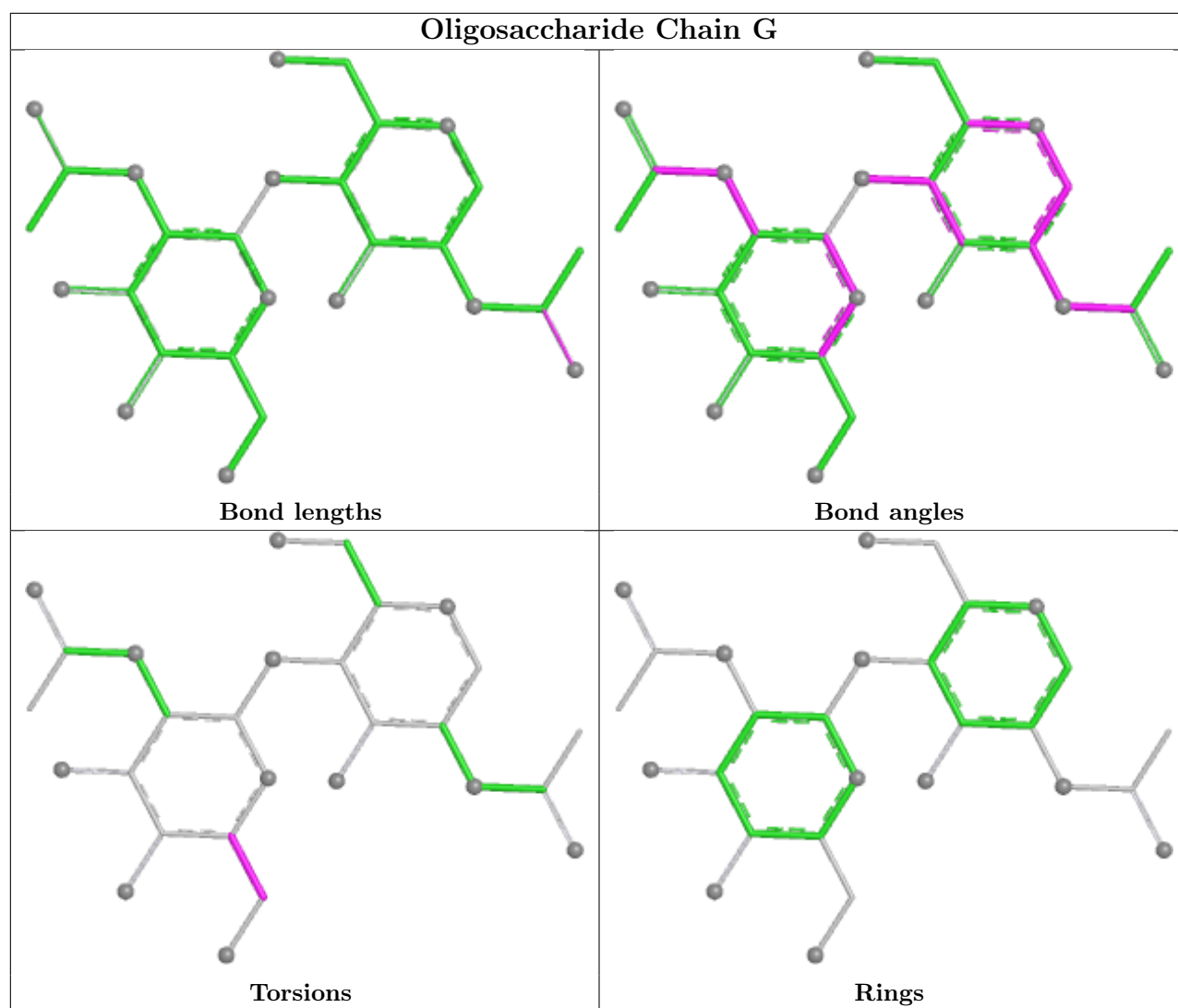
There are no ring outliers.

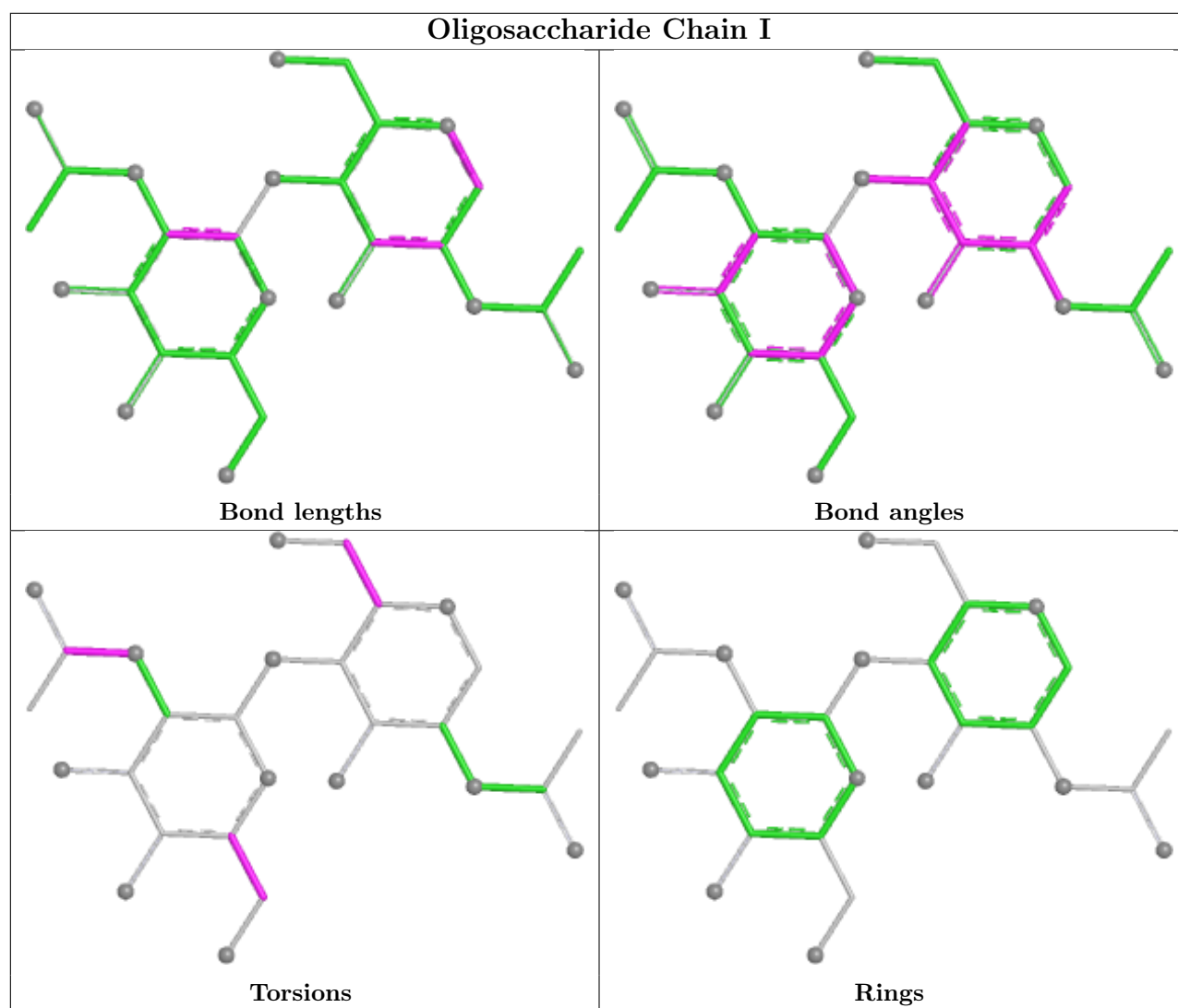
7 monomers are involved in 7 short contacts:

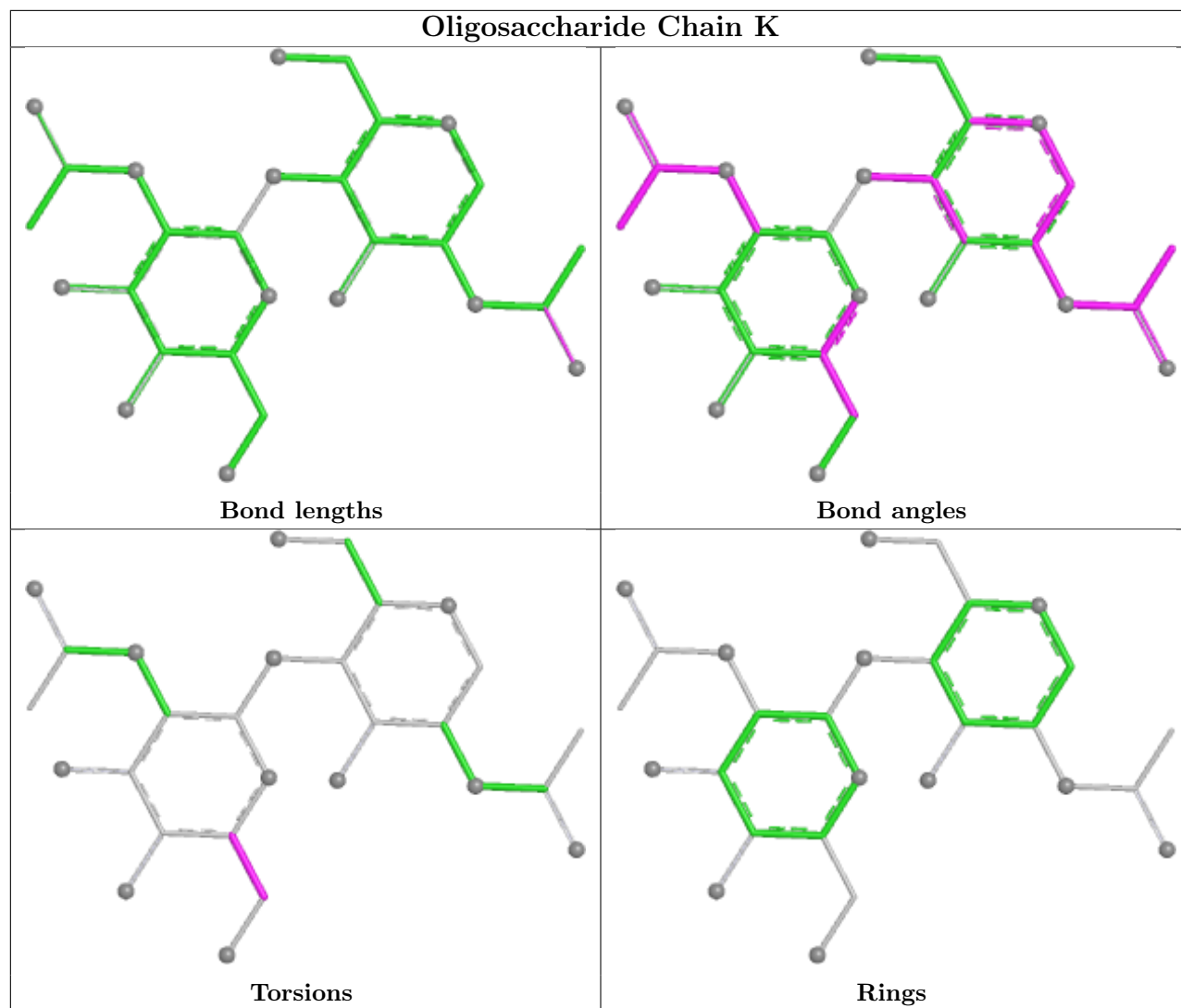
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	3	BMA	1	0
3	J	3	BMA	1	0
2	G	2	NAG	1	0
3	L	3	BMA	1	0
2	K	1	NAG	1	0
3	L	6	MAN	1	0
3	F	3	BMA	1	0

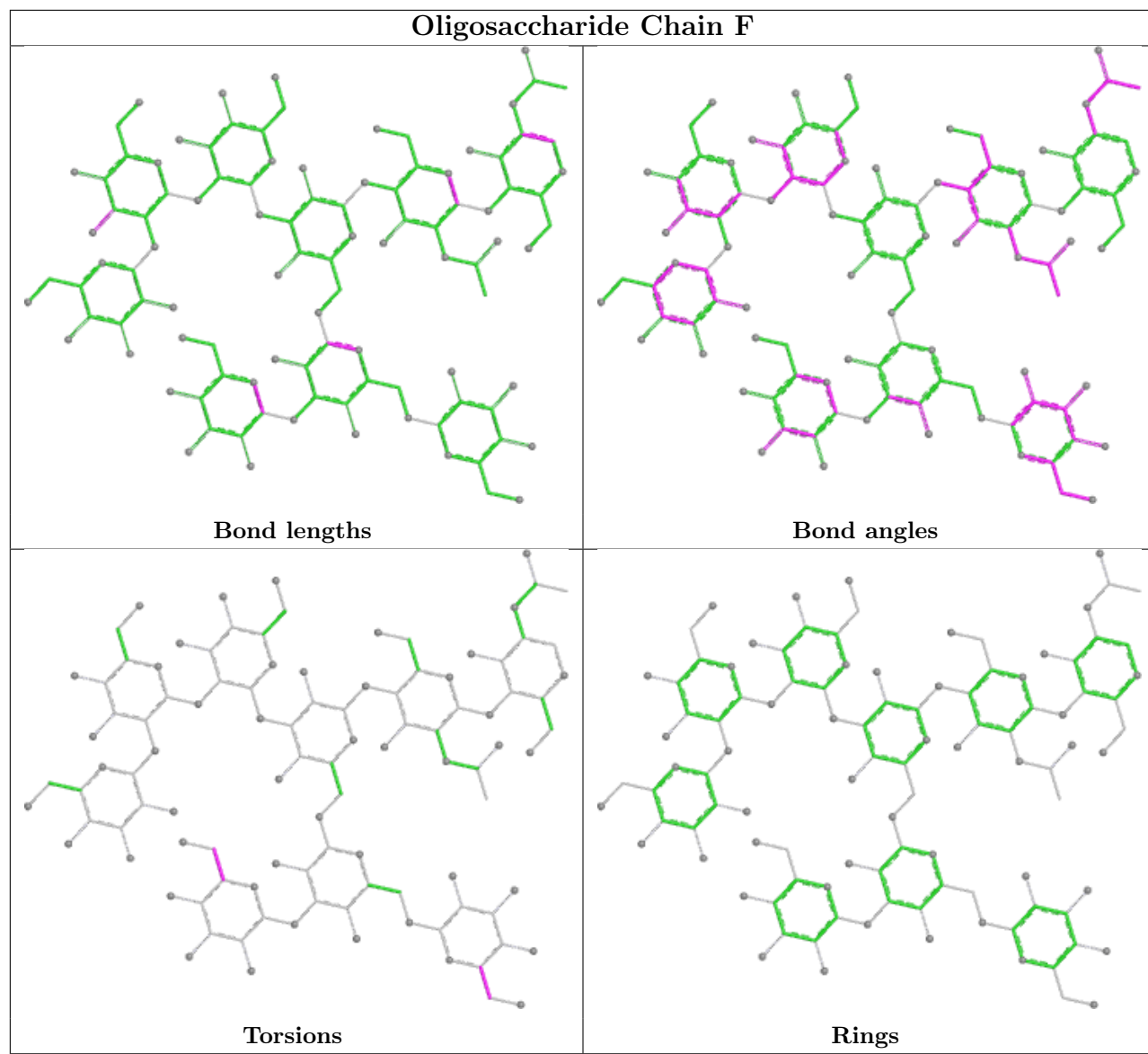
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

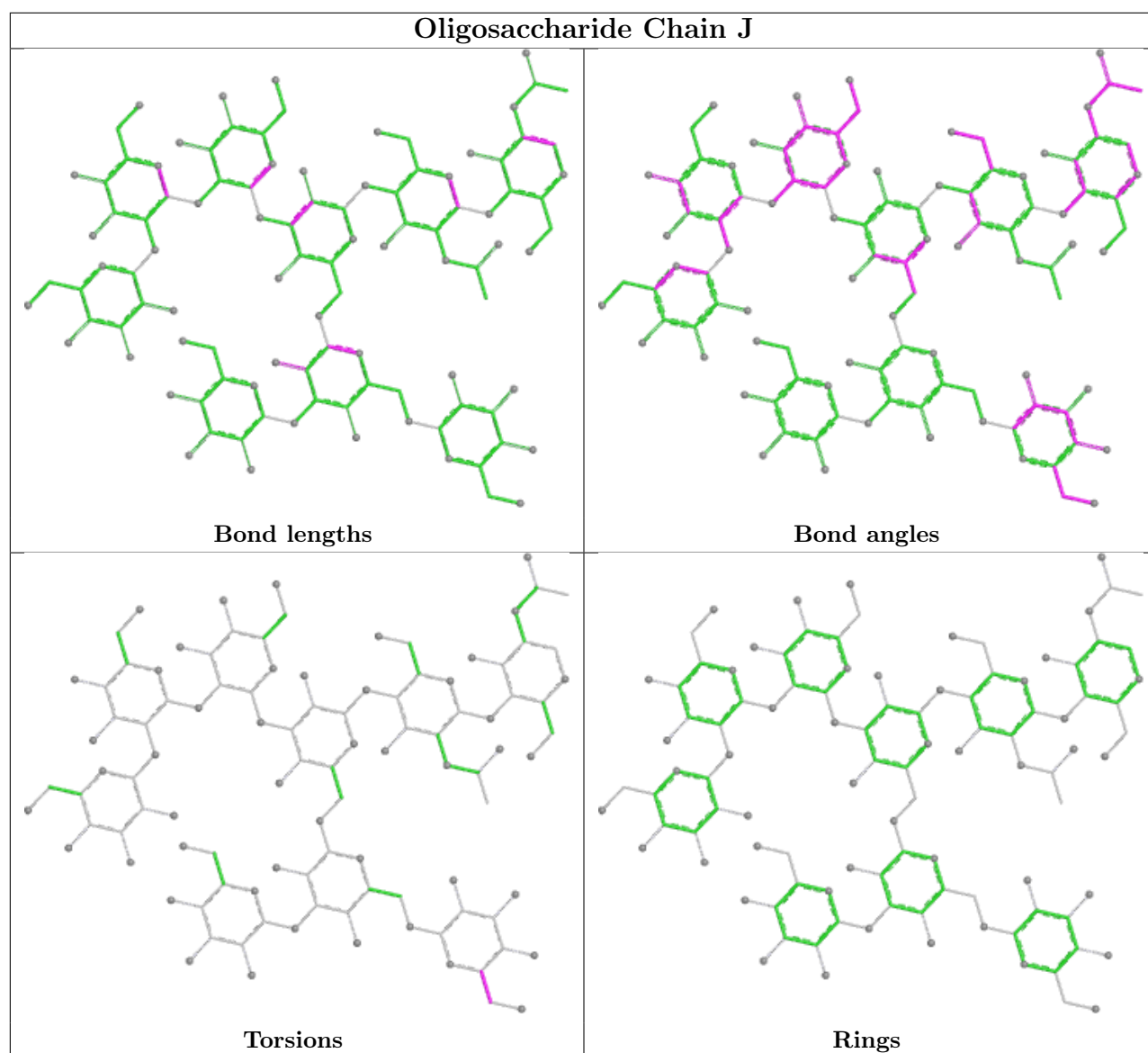


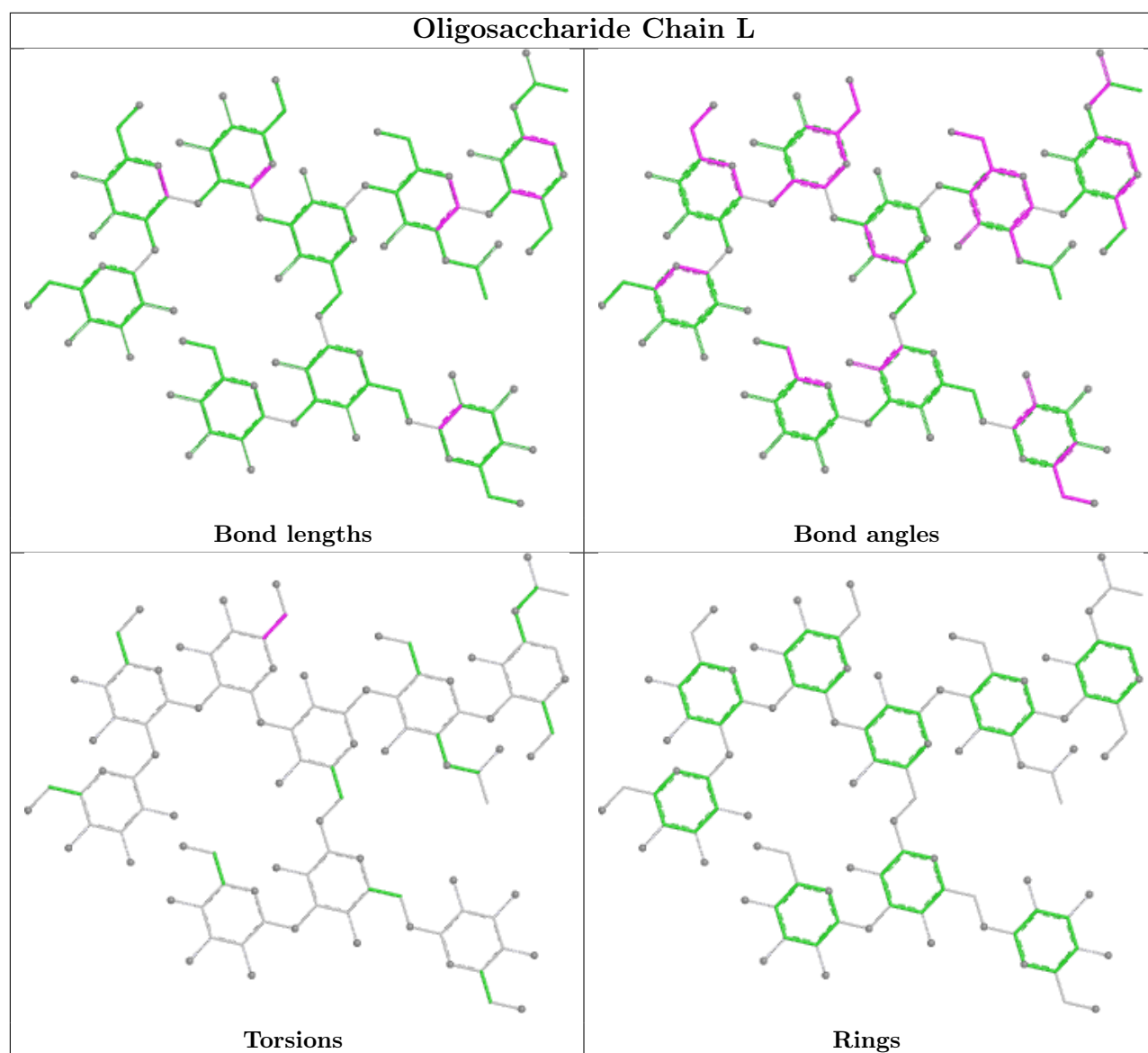


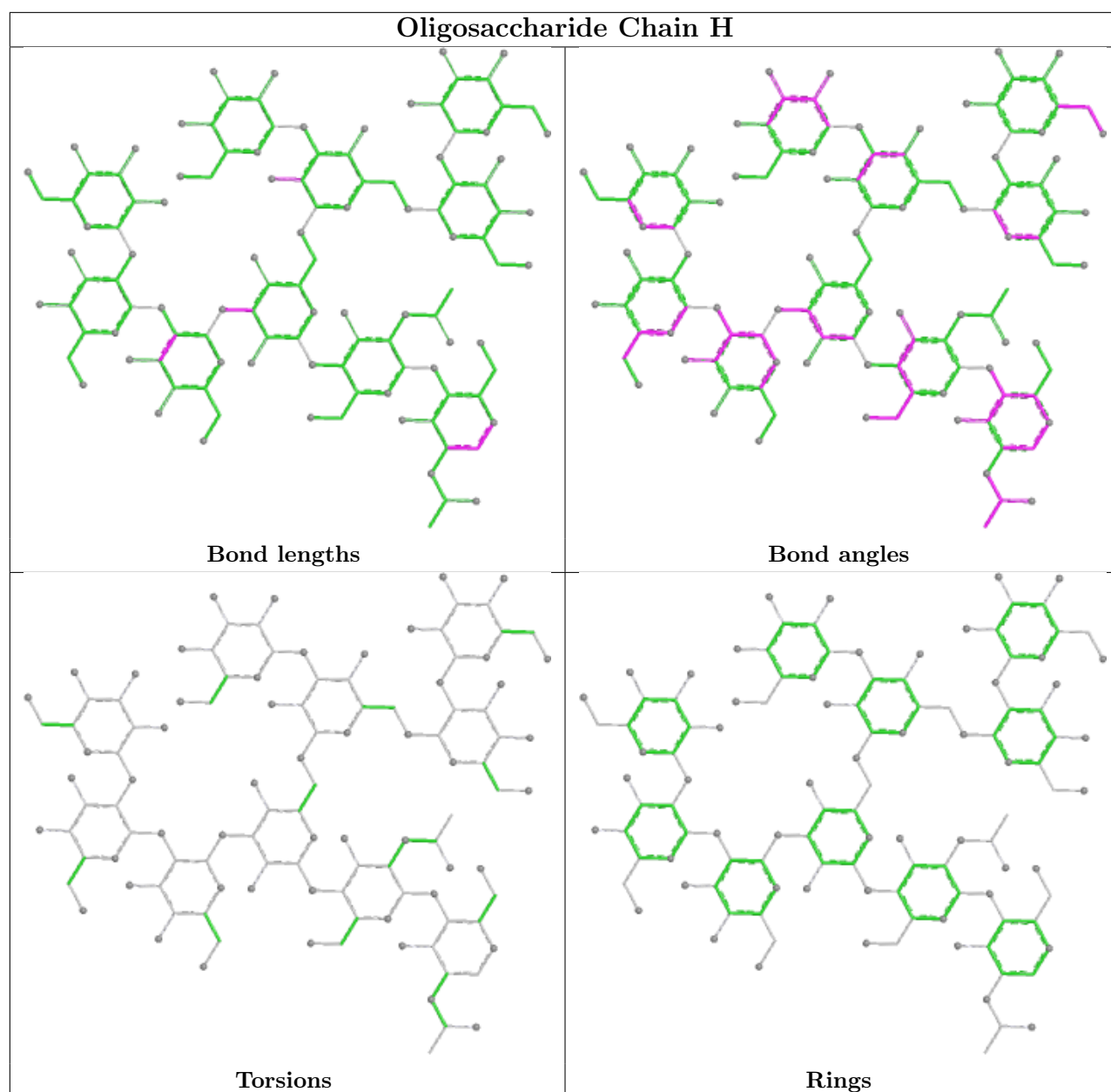












5.6 Ligand geometry [i](#)

Of 40 ligands modelled in this entry, 4 are monoatomic - leaving 36 for Mogul analysis.

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	SO4	A	1517	-	4,4,4	0.33	0	6,6,6	0.50	0
6	SO4	A	2516	-	4,4,4	0.26	0	6,6,6	0.77	0
6	SO4	A	1514	-	4,4,4	0.17	0	6,6,6	0.74	0
6	SO4	B	2520	-	4,4,4	0.11	0	6,6,6	0.72	0
6	SO4	D	4515	-	4,4,4	0.53	0	6,6,6	0.76	0
6	SO4	C	3520	-	4,4,4	0.33	0	6,6,6	0.61	0
6	SO4	C	3519	-	4,4,4	0.45	0	6,6,6	0.52	0
6	SO4	C	4516	-	4,4,4	0.20	0	6,6,6	0.50	0
6	SO4	A	1518	-	4,4,4	0.33	0	6,6,6	0.95	0
6	SO4	A	1513	-	4,4,4	0.45	0	6,6,6	0.80	0
8	GOL	A	5003	-	5,5,5	0.61	0	5,5,5	0.39	0
6	SO4	B	2515	-	4,4,4	0.56	0	6,6,6	0.59	0
6	SO4	B	2514	-	4,4,4	0.25	0	6,6,6	0.65	0
6	SO4	D	4513	-	4,4,4	0.63	0	6,6,6	0.63	0
8	GOL	A	5002	-	5,5,5	0.79	0	5,5,5	1.40	1 (20%)
5	NAG	B	500	1	14,14,15	0.76	0	17,19,21	1.74	2 (11%)
6	SO4	D	4519	-	4,4,4	0.73	0	6,6,6	0.65	0
6	SO4	C	3513	-	4,4,4	0.49	0	6,6,6	0.50	0
6	SO4	A	1519	-	4,4,4	0.49	0	6,6,6	0.37	0
5	NAG	D	500	1	14,14,15	1.03	1 (7%)	17,19,21	2.02	7 (41%)
6	SO4	C	3518	-	4,4,4	0.38	0	6,6,6	1.11	0
8	GOL	A	5001	-	5,5,5	0.76	0	5,5,5	0.93	0
6	SO4	C	3514	-	4,4,4	0.23	0	6,6,6	1.01	0
6	SO4	B	2519	-	4,4,4	0.57	0	6,6,6	0.44	0
6	SO4	B	3516	-	4,4,4	0.31	0	6,6,6	0.77	0
6	SO4	A	1520	-	4,4,4	0.20	0	6,6,6	0.89	0
6	SO4	C	3515	-	4,4,4	0.31	0	6,6,6	1.12	0
6	SO4	D	4514	-	4,4,4	0.60	0	6,6,6	0.65	0
6	SO4	B	2513	-	4,4,4	0.51	0	6,6,6	0.52	0
5	NAG	A	500	1	14,14,15	0.88	0	17,19,21	2.32	9 (52%)
6	SO4	C	3521	-	4,4,4	0.50	0	6,6,6	0.65	0
5	NAG	C	500	1	14,14,15	0.61	0	17,19,21	1.25	1 (5%)
6	SO4	A	1515	-	4,4,4	0.32	0	6,6,6	0.66	0
6	SO4	D	4520	-	4,4,4	0.23	0	6,6,6	0.47	0
6	SO4	D	1516	-	4,4,4	0.35	0	6,6,6	0.64	0
6	SO4	C	3517	-	4,4,4	0.41	0	6,6,6	0.66	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
8	GOL	A	5003	-	-	0/4/4/4	-
5	NAG	C	500	1	-	4/6/23/26	0/1/1/1
8	GOL	A	5001	-	-	4/4/4/4	-
8	GOL	A	5002	-	-	2/4/4/4	-
5	NAG	B	500	1	-	4/6/23/26	0/1/1/1
5	NAG	A	500	1	-	2/6/23/26	0/1/1/1
5	NAG	D	500	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	500	NAG	C4-C5	2.39	1.58	1.53

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	500	NAG	C1-C2-N2	-4.34	103.59	110.43
5	D	500	NAG	C4-C3-C2	-4.22	104.83	111.02
5	A	500	NAG	O3-C3-C4	-3.82	101.36	110.38
5	B	500	NAG	O5-C5-C6	3.73	114.92	107.66
5	A	500	NAG	O5-C5-C6	3.51	114.50	107.66
5	D	500	NAG	O5-C1-C2	3.44	116.61	111.29
5	A	500	NAG	O3-C3-C2	3.00	115.64	109.40
5	A	500	NAG	C1-C2-N2	-2.93	105.81	110.43
5	D	500	NAG	C6-C5-C4	2.91	120.17	113.02
5	A	500	NAG	C2-N2-C7	2.72	126.55	122.90
5	A	500	NAG	O5-C1-C2	2.70	115.47	111.29
5	D	500	NAG	C2-N2-C7	2.63	126.42	122.90
5	A	500	NAG	O4-C4-C5	2.62	115.78	109.32
5	A	500	NAG	O7-C7-N2	2.62	126.61	121.98
5	A	500	NAG	O4-C4-C3	-2.61	104.23	110.38
5	C	500	NAG	O5-C5-C6	2.56	112.65	107.66
5	D	500	NAG	C1-O5-C5	-2.52	108.81	112.19
8	A	5002	GOL	O2-C2-C3	-2.36	99.41	109.18
5	D	500	NAG	O4-C4-C5	2.15	114.62	109.32
5	D	500	NAG	O4-C4-C3	-2.10	105.42	110.38

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	500	NAG	C8-C7-N2-C2
5	A	500	NAG	O7-C7-N2-C2
5	B	500	NAG	C8-C7-N2-C2
5	B	500	NAG	O7-C7-N2-C2
5	C	500	NAG	C8-C7-N2-C2
5	C	500	NAG	O7-C7-N2-C2
5	D	500	NAG	C8-C7-N2-C2
5	D	500	NAG	O7-C7-N2-C2
8	A	5001	GOL	C1-C2-C3-O3
8	A	5002	GOL	O1-C1-C2-O2
8	A	5002	GOL	O1-C1-C2-C3
5	C	500	NAG	O5-C5-C6-O6
5	B	500	NAG	C4-C5-C6-O6
5	B	500	NAG	O5-C5-C6-O6
5	C	500	NAG	C4-C5-C6-O6
8	A	5001	GOL	O1-C1-C2-C3
8	A	5001	GOL	O1-C1-C2-O2
8	A	5001	GOL	O2-C2-C3-O3

There are no ring outliers.

9 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2516	SO4	1	0
6	C	3520	SO4	1	0
6	C	4516	SO4	1	0
8	A	5003	GOL	1	0
5	B	500	NAG	1	0
6	B	3516	SO4	1	0
5	A	500	NAG	1	0
6	C	3521	SO4	1	0
5	C	500	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 ⓘ

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	388/388 (100%)	-0.78	1 (0%)	90	88	10, 18, 30, 44	9 (2%)
1	B	388/388 (100%)	-0.60	4 (1%)	79	77	12, 20, 37, 53	9 (2%)
1	C	388/388 (100%)	-0.61	4 (1%)	79	77	12, 20, 43, 58	4 (1%)
1	D	388/388 (100%)	-0.65	13 (3%)	48	45	11, 17, 38, 58	9 (2%)
All	All	1552/1552 (100%)	-0.66	22 (1%)	73	71	10, 19, 38, 58	31 (1%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	296	TRP	5.0
1	D	247	ALA	5.0
1	D	248	THR	4.7
1	B	347	ASN	4.0
1	B	346	ASN	4.0
1	D	346	ASN	3.5
1	D	298	GLY	3.3
1	D	250	PRO	3.1
1	D	249	GLY	2.9
1	D	271	GLY	2.9
1	D	275	HIS	2.7
1	B	249	GLY	2.7
1	C	347	ASN	2.5
1	B	250	PRO	2.4
1	A	346	ASN	2.4
1	D	251	ALA	2.2
1	D	295	ASN	2.2
1	C	344	ASN	2.2
1	D	274	LYS	2.1
1	C	298	GLY	2.1
1	D	347	ASN	2.1
1	C	299	SER	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.

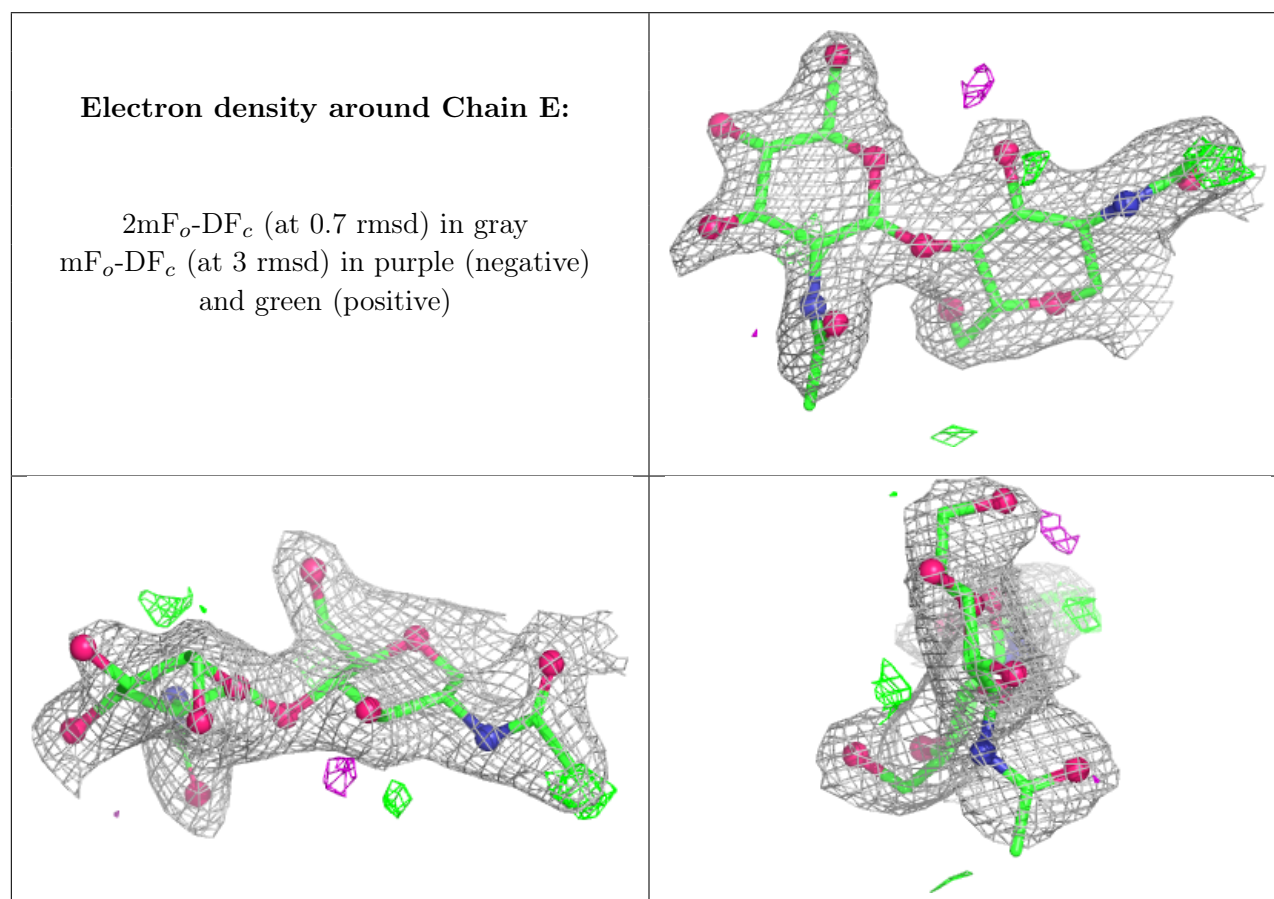
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	I	2	14/15	0.54	0.18	63,67,69,69	0
2	NAG	K	2	14/15	0.71	0.14	46,51,55,56	0
2	NAG	G	2	14/15	0.78	0.13	44,52,57,59	0
4	MAN	H	10	11/12	0.78	0.12	49,52,53,55	0
3	MAN	J	9	11/12	0.79	0.12	46,51,56,57	0
3	MAN	F	9	11/12	0.81	0.11	43,48,50,53	0
4	MAN	H	8	11/12	0.82	0.16	44,50,54,56	0
2	NAG	K	1	14/15	0.83	0.10	25,33,47,47	0
2	NAG	E	2	14/15	0.83	0.11	43,51,56,58	0
2	NAG	G	1	14/15	0.84	0.11	33,39,47,48	0
4	MAN	H	9	11/12	0.85	0.13	52,56,57,57	0
2	NAG	I	1	14/15	0.88	0.10	33,44,48,58	0
3	MAN	J	8	11/12	0.88	0.09	32,39,44,46	0
3	MAN	L	8	11/12	0.90	0.09	32,35,38,39	0
3	MAN	L	9	11/12	0.90	0.09	35,38,41,43	0
4	MAN	H	7	11/12	0.90	0.09	35,39,44,44	0
3	MAN	F	8	11/12	0.91	0.08	32,36,38,43	0
2	NAG	E	1	14/15	0.91	0.08	30,37,41,45	0
4	NAG	H	2	14/15	0.94	0.07	17,22,26,38	0
4	MAN	H	5	11/12	0.94	0.07	22,28,32,33	0
3	MAN	J	7	11/12	0.94	0.07	29,35,38,42	0
3	MAN	L	4	11/12	0.95	0.06	16,21,28,34	0
3	MAN	J	4	11/12	0.95	0.06	18,22,24,31	0
3	NAG	J	1	14/15	0.95	0.06	20,21,25,26	0
3	NAG	L	2	14/15	0.95	0.06	17,21,25,31	0
4	MAN	H	4	11/12	0.95	0.06	16,20,26,33	0
3	NAG	F	2	14/15	0.96	0.06	15,18,24,24	0
3	MAN	J	5	11/12	0.96	0.06	18,21,26,27	0
3	MAN	J	6	11/12	0.96	0.06	16,19,22,22	0
4	MAN	H	6	11/12	0.96	0.05	18,25,26,26	0
3	MAN	L	5	11/12	0.96	0.06	18,20,24,27	0
3	MAN	L	7	11/12	0.96	0.06	24,27,29,31	0

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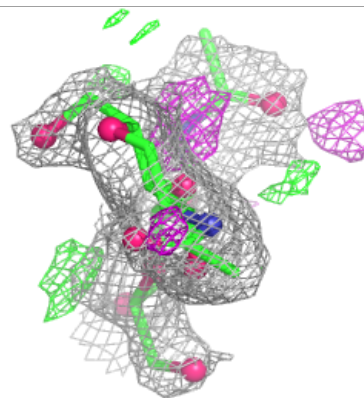
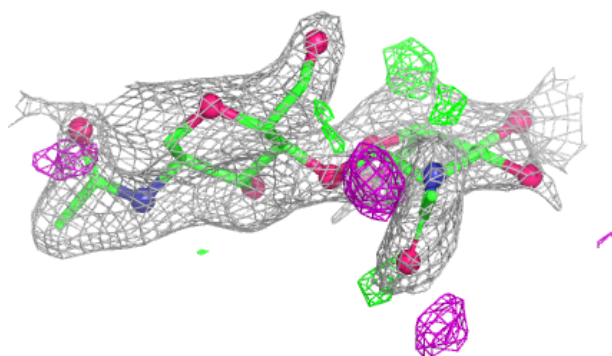
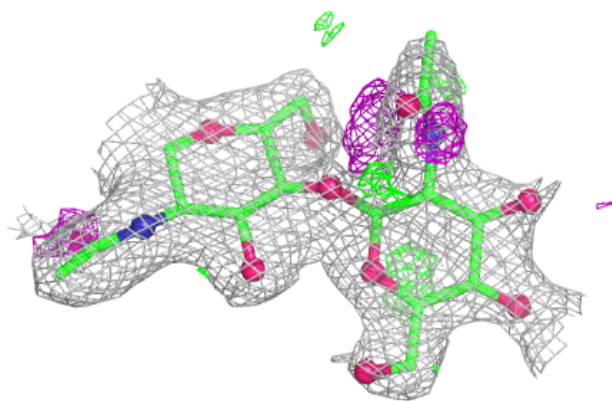
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MAN	F	4	11/12	0.96	0.06	16,19,25,26	0
3	MAN	F	7	11/12	0.96	0.05	21,26,32,37	0
3	BMA	L	3	11/12	0.97	0.05	20,24,26,26	0
4	BMA	H	3	11/12	0.97	0.06	20,22,28,29	0
3	BMA	J	3	11/12	0.97	0.05	18,23,25,29	0
3	NAG	F	1	14/15	0.97	0.06	15,18,27,29	0
3	MAN	L	6	11/12	0.97	0.04	19,21,23,23	0
3	MAN	F	6	11/12	0.97	0.05	15,17,18,21	0
3	NAG	L	1	14/15	0.97	0.05	17,22,28,30	0
3	NAG	J	2	14/15	0.97	0.05	17,21,27,32	0
4	NAG	H	1	14/15	0.97	0.05	18,22,25,26	0
3	BMA	F	3	11/12	0.98	0.04	14,19,22,23	0
3	MAN	F	5	11/12	0.98	0.05	18,20,22,24	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.

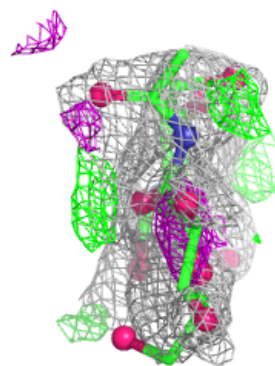
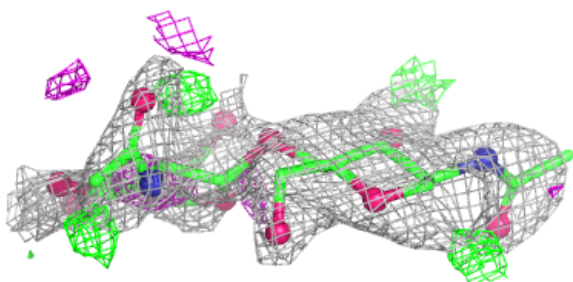
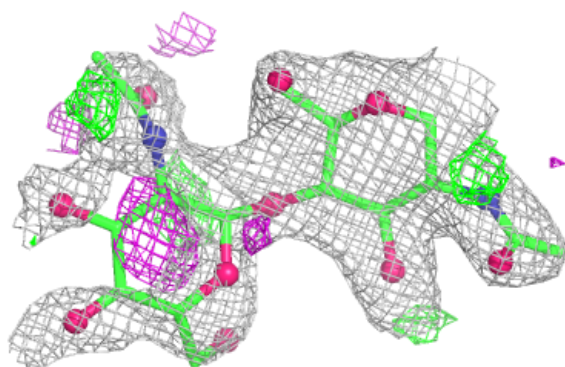


Electron density around Chain G:

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

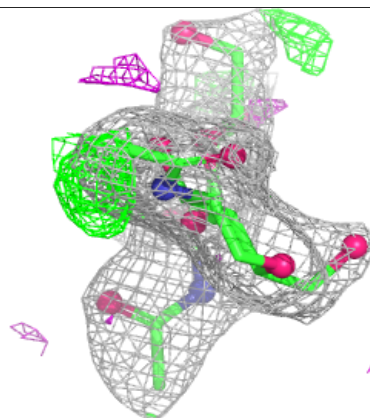
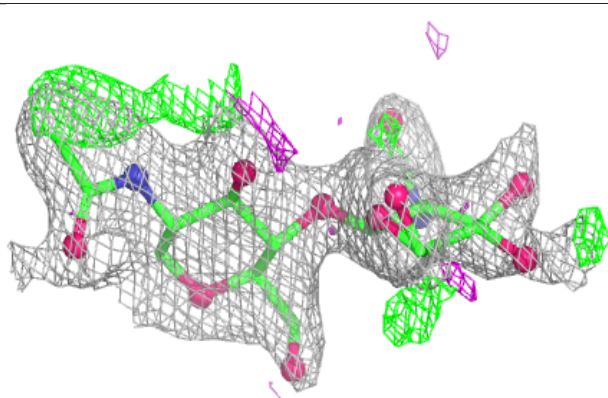
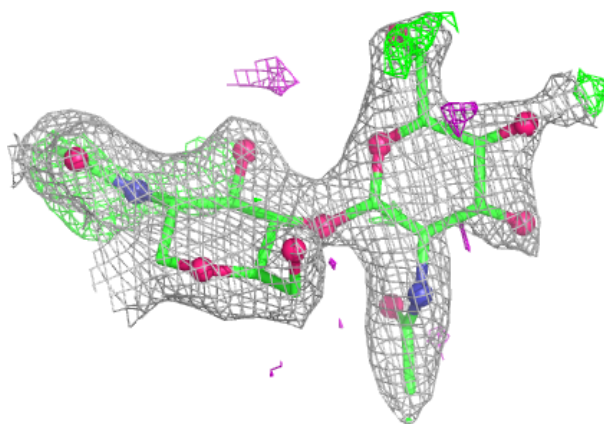
**Electron density around Chain I:**

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



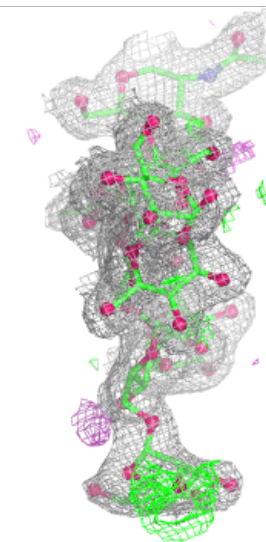
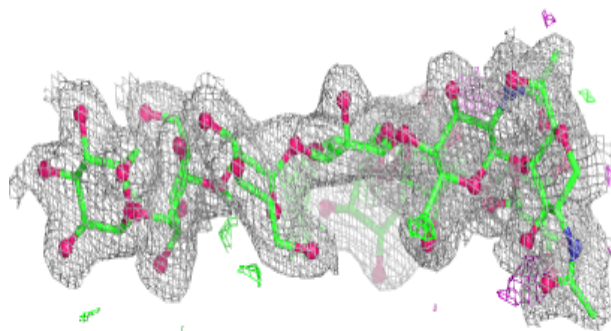
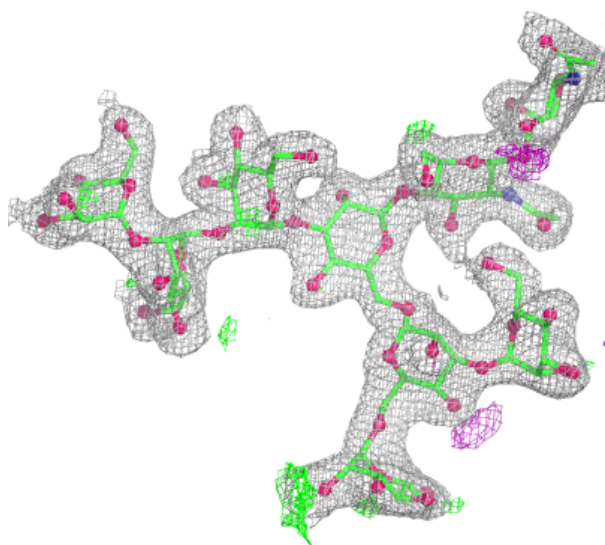
Electron density around Chain K:

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



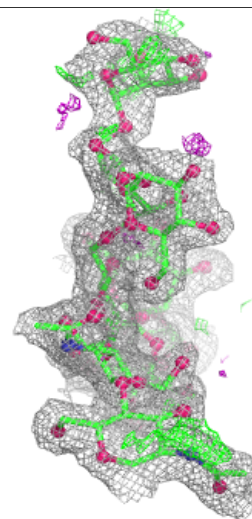
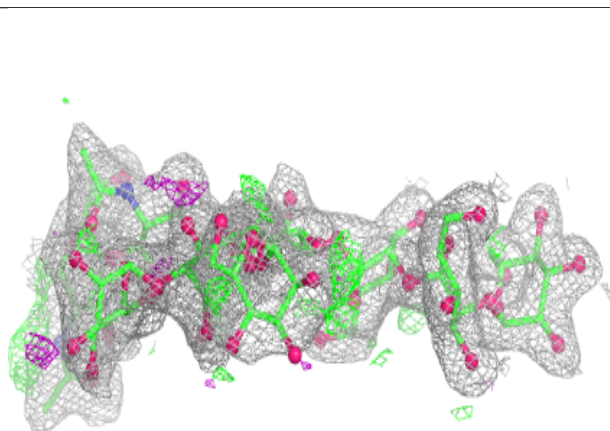
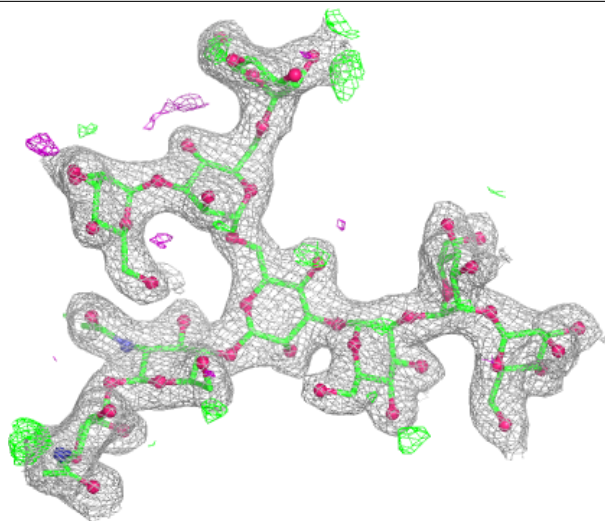
Electron density around Chain F:

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and green (positive)



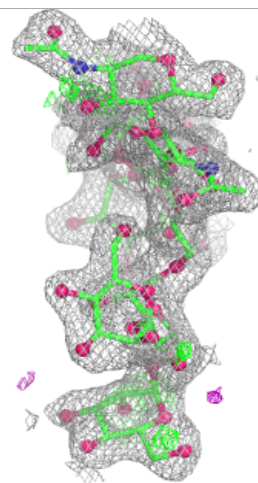
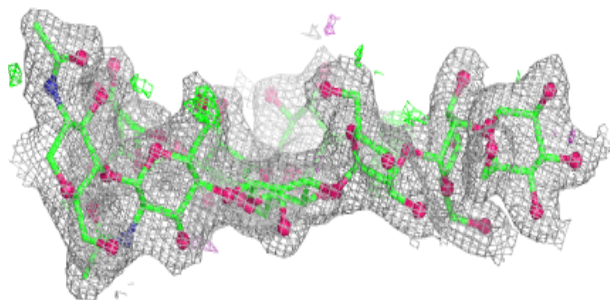
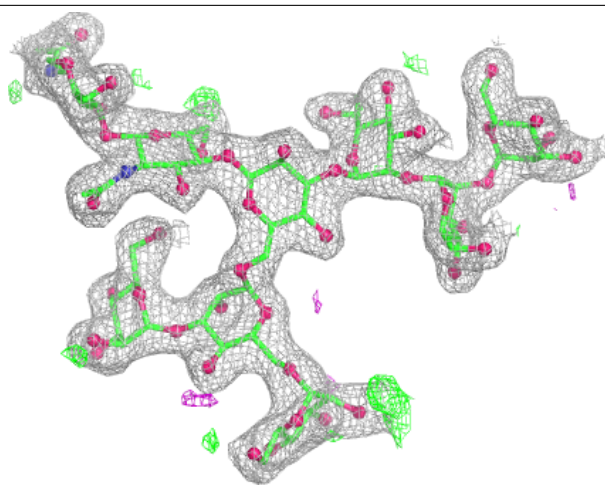
Electron density around Chain J:

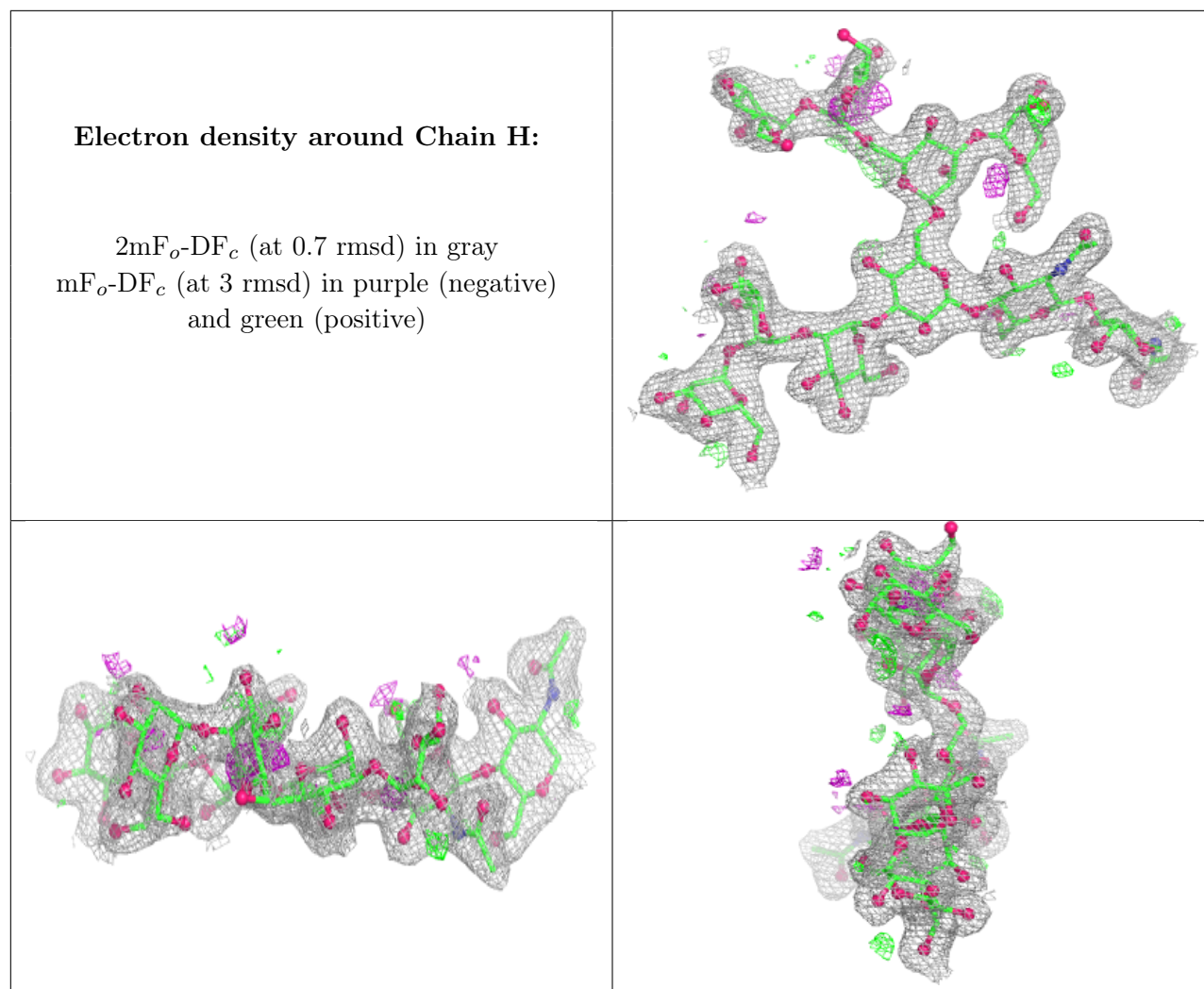
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain L:

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





6.4 Ligands ⓘ

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($\text{\AA}^2$)	Q<0.9
8	GOL	A	5001	6/6	0.70	0.17	55,57,59,59	0
6	SO4	A	1518	5/5	0.75	0.18	76,77,81,81	0
6	SO4	B	2513	5/5	0.77	0.15	70,71,73,75	0
5	NAG	D	500	14/15	0.79	0.13	45,50,57,58	0
6	SO4	C	3513	5/5	0.82	0.15	63,65,66,67	0
8	GOL	A	5003	6/6	0.83	0.16	56,56,58,59	0
5	NAG	A	500	14/15	0.84	0.11	40,48,52,52	0
5	NAG	B	500	14/15	0.84	0.12	45,50,59,61	0
5	NAG	C	500	14/15	0.86	0.11	47,55,58,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	SO4	D	4513	5/5	0.86	0.12	55,59,62,63	0
6	SO4	D	4515	5/5	0.87	0.15	50,54,58,59	0
6	SO4	D	4520	5/5	0.87	0.14	63,64,64,64	0
6	SO4	B	2515	5/5	0.88	0.15	53,55,57,59	0
6	SO4	C	3515	5/5	0.89	0.15	55,56,58,61	0
6	SO4	C	3519	5/5	0.90	0.16	57,61,61,63	0
6	SO4	A	1515	5/5	0.90	0.14	50,54,57,60	0
6	SO4	C	3517	5/5	0.90	0.17	59,61,64,66	0
6	SO4	C	3520	5/5	0.91	0.16	63,64,65,67	0
6	SO4	A	1517	5/5	0.91	0.12	53,56,58,59	0
6	SO4	A	1520	5/5	0.91	0.12	60,63,64,65	0
6	SO4	B	3516	5/5	0.92	0.13	72,73,75,76	0
6	SO4	D	4514	5/5	0.92	0.10	35,48,50,52	0
8	GOL	A	5002	6/6	0.92	0.09	34,40,43,44	0
6	SO4	A	2516	5/5	0.92	0.11	60,61,62,64	0
7	CL	A	1522	1/1	0.93	0.09	46,46,46,46	0
6	SO4	B	2519	5/5	0.94	0.13	46,46,48,52	0
7	CL	D	4522	1/1	0.95	0.15	46,46,46,46	0
6	SO4	D	1516	5/5	0.95	0.13	52,55,57,58	0
7	CL	B	2522	1/1	0.95	0.10	45,45,45,45	0
7	CL	C	3522	1/1	0.95	0.09	50,50,50,50	0
6	SO4	C	3514	5/5	0.96	0.09	32,38,41,43	0
6	SO4	C	4516	5/5	0.96	0.09	56,57,58,60	0
6	SO4	B	2520	5/5	0.96	0.13	47,50,52,52	0
6	SO4	D	4519	5/5	0.96	0.11	40,42,44,45	0
6	SO4	A	1519	5/5	0.97	0.11	40,43,45,45	0
6	SO4	A	1513	5/5	0.97	0.07	40,41,47,47	0
6	SO4	B	2514	5/5	0.97	0.09	40,41,45,45	0
6	SO4	A	1514	5/5	0.99	0.06	29,29,32,32	0
6	SO4	C	3518	5/5	0.99	0.04	21,22,24,25	0
6	SO4	C	3521	5/5	1.00	0.04	17,20,21,23	0

6.5 Other polymers

There are no such residues in this entry.