



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 09:34 AM UTC

PDB ID : 4GZS / pdb_00004gzs
Title : N2 neuraminidase D151G mutant of a/Tanzania/205/2010 H3N2 in complex with hepes
Authors : Zhu, X.; Wilson, I.A.
Deposited on : 2012-09-06
Resolution : 2.35 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

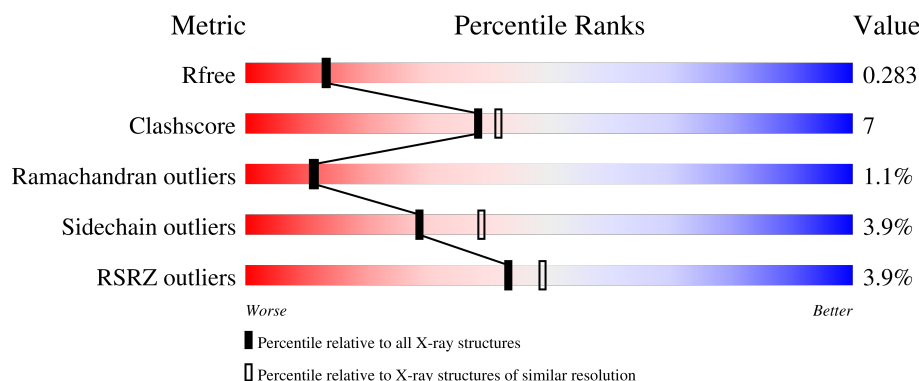
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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.



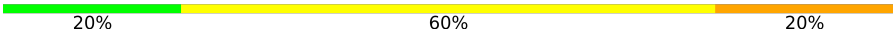
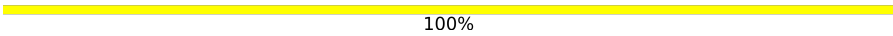
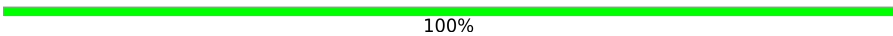
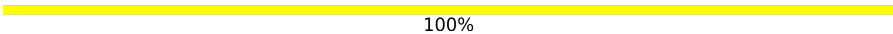
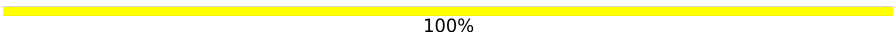
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	393	5% 81% 17% ...
1	B	393	3% 79% 19% ..
1	C	393	5% 79% 17% ..
1	D	393	3% 79% 19% ..
2	E	5	20% 80%

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Mol	Chain	Length	Quality of chain
2	G	5	 20% 60% 20%
2	I	5	 100%
2	K	5	 60% 40%
3	F	2	 50% 50%
3	H	2	 100%
3	J	2	 100%
4	L	2	 100%

2 Entry composition [i](#)

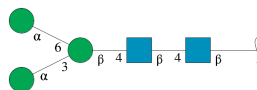
There are 8 unique types of molecules in this entry. The entry contains 12862 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	0	0
			2998	1858	531	587	22			
1	B	388	Total	C	N	O	S	0	0	0
			2998	1858	531	587	22			
1	C	388	Total	C	N	O	S	0	0	0
			2998	1858	531	587	22			
1	D	388	Total	C	N	O	S	0	0	0
			2998	1858	531	587	22			

- Molecule 2 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
2	E	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	G	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	I	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	K	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	2	Total	C	N	O	0	0	0
			24	14	1	9			
3	H	2	Total	C	N	O	0	0	0
			24	14	1	9			
3	J	2	Total	C	N	O	0	0	0
			24	14	1	9			

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

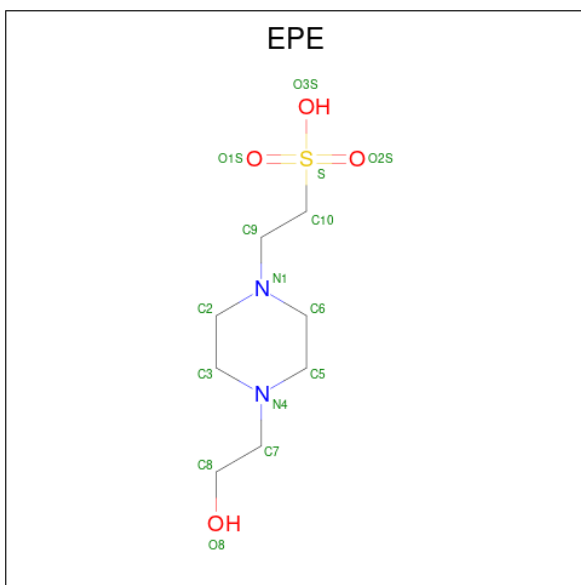


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	L	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

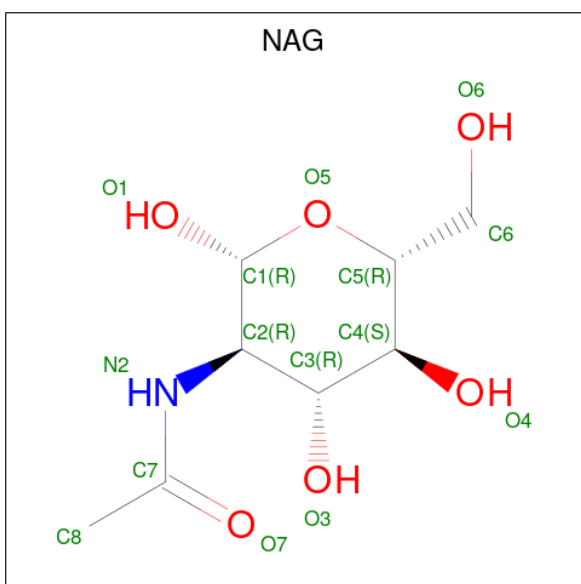
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		
5	B	1	Total	Ca	0	0
			1	1		
5	C	2	Total	Ca	0	0
			2	2		
5	D	1	Total	Ca	0	0
			1	1		

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
6	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
6	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
6	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



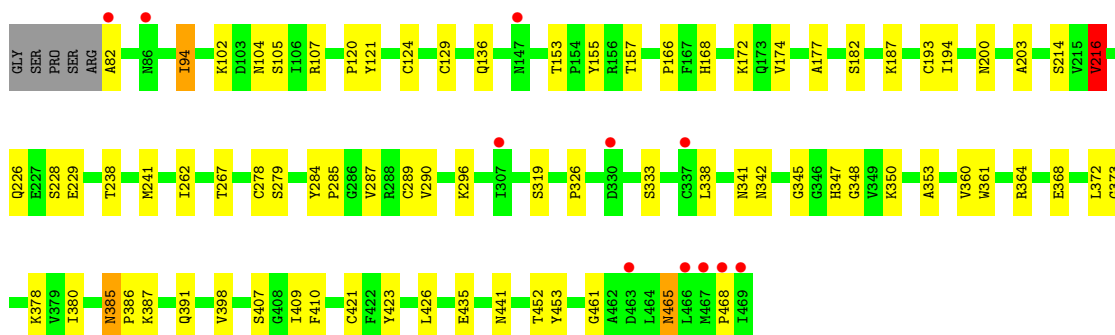
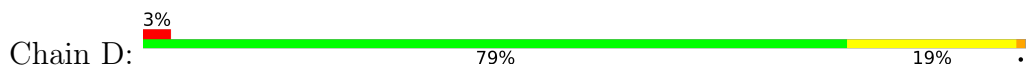
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	91	Total	O	0	0
			91	91		
8	B	89	Total	O	0	0
			89	89		
8	C	93	Total	O	0	0
			93	93		
8	D	90	Total	O	0	0
			90	90		



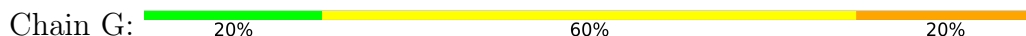
● Molecule 1: Neuraminidase



● Molecule 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



● Molecule 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



● Molecule 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



● Molecule 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





- Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 50% 50%



- Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H: 100%



- Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 100%



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

Chain L: 100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.81Å 110.20Å 110.59Å 90.00° 97.46° 90.00°	Depositor
Resolution (Å)	50.00 – 2.35 50.00 – 2.35	Depositor EDS
% Data completeness (in resolution range)	92.4 (50.00-2.35) 92.3 (50.00-2.35)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.225 , 0.287 0.225 , 0.283	Depositor DCC
R_{free} test set	3724 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	1.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 31.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12862	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% 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: BMA, FUC, NAG, MAN, CA, EPE

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	0.73	0/3065	0.96	2/4156 (0.0%)
1	B	0.70	0/3065	0.92	4/4156 (0.1%)
1	C	0.71	0/3065	0.94	5/4156 (0.1%)
1	D	0.72	0/3065	0.91	3/4156 (0.1%)
All	All	0.71	0/12260	0.93	14/16624 (0.1%)

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	VAL	CB-CA-C	-10.08	97.37	111.28
1	C	216	VAL	CB-CA-C	-9.65	100.98	111.59
1	B	98	ALA	CA-C-N	9.35	129.93	119.93
1	B	98	ALA	C-N-CA	9.35	129.93	119.93
1	C	467	MET	CA-C-N	7.80	129.59	119.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2998	0	2856	39	0
1	B	2998	0	2855	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2998	0	2855	51	0
1	D	2998	0	2855	44	0
2	E	61	0	52	0	0
2	G	61	0	52	1	0
2	I	61	0	52	0	0
2	K	61	0	52	2	0
3	F	24	0	22	1	0
3	H	24	0	22	0	0
3	J	24	0	22	0	0
4	L	28	0	25	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	2	0	0	0	0
5	D	1	0	0	0	0
6	A	15	0	17	2	0
6	B	15	0	17	2	0
6	C	15	0	17	1	0
6	D	15	0	17	2	0
7	A	14	0	13	0	0
7	B	28	0	26	0	0
7	C	28	0	26	0	0
7	D	28	0	26	0	0
8	A	91	0	0	1	0
8	B	89	0	0	2	0
8	C	93	0	0	0	0
8	D	90	0	0	3	0
All	All	12862	0	11879	169	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 7.

The worst 5 of 169 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:452:THR:HB	1:C:216:VAL:CG2	2.02	0.88
1:A:177:ALA:HB2	1:A:193:CYS:HB3	1.60	0.84
1:A:194:ILE:HD11	1:A:241:MET:HE3	1.70	0.74
1:A:216:VAL:HG13	1:D:453:TYR:C	2.13	0.73
1:C:452:THR:HB	1:D:216:VAL:HG22	1.68	0.73

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	386/393 (98%)	361 (94%)	21 (5%)	4 (1%)	12	12
1	B	386/393 (98%)	358 (93%)	24 (6%)	4 (1%)	12	12
1	C	386/393 (98%)	354 (92%)	27 (7%)	5 (1%)	9	8
1	D	386/393 (98%)	357 (92%)	25 (6%)	4 (1%)	12	12
All	All	1544/1572 (98%)	1430 (93%)	97 (6%)	17 (1%)	11	11

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	468	PRO
1	B	333	SER
1	C	234	ASN
1	D	468	PRO
1	A	319	SER

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	337/341 (99%)	320 (95%)	17 (5%)	22	27
1	B	337/341 (99%)	327 (97%)	10 (3%)	36	48
1	C	337/341 (99%)	325 (96%)	12 (4%)	31	41
1	D	337/341 (99%)	324 (96%)	13 (4%)	28	39
All	All	1348/1364 (99%)	1296 (96%)	52 (4%)	28	39

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	136	GLN
1	C	369	THR
1	D	385	ASN
1	C	215	VAL
1	C	276	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	441	ASN
1	D	168	HIS
1	D	136	GLN
1	D	310	HIS
1	B	310	HIS

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 ⓘ

28 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	E	1	1,2	14,14,15	0.64	0	17,19,21	1.17	2 (11%)
2	NAG	E	2	2	14,14,15	0.39	0	17,19,21	1.29	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BMA	E	3	2	11,11,12	0.71	0	15,15,17	0.81	0
2	MAN	E	4	2	11,11,12	0.65	0	15,15,17	1.46	2 (13%)
2	MAN	E	5	2	11,11,12	0.71	0	15,15,17	2.11	3 (20%)
3	NAG	F	1	1,3	14,14,15	0.65	0	17,19,21	1.48	2 (11%)
3	FUC	F	2	3	10,10,11	0.58	0	14,14,16	0.68	0
2	NAG	G	1	1,2	14,14,15	0.44	0	17,19,21	1.34	1 (5%)
2	NAG	G	2	2	14,14,15	0.52	0	17,19,21	0.82	0
2	BMA	G	3	2	11,11,12	0.94	0	15,15,17	1.43	2 (13%)
2	MAN	G	4	2	11,11,12	0.65	0	15,15,17	1.52	3 (20%)
2	MAN	G	5	2	11,11,12	0.58	0	15,15,17	1.98	4 (26%)
3	NAG	H	1	1,3	14,14,15	0.61	0	17,19,21	0.87	0
3	FUC	H	2	3	10,10,11	0.67	0	14,14,16	0.68	0
2	NAG	I	1	1,2	14,14,15	0.77	0	17,19,21	1.19	2 (11%)
2	NAG	I	2	2	14,14,15	0.59	0	17,19,21	1.19	1 (5%)
2	BMA	I	3	2	11,11,12	0.52	0	15,15,17	1.09	1 (6%)
2	MAN	I	4	2	11,11,12	0.56	0	15,15,17	1.87	2 (13%)
2	MAN	I	5	2	11,11,12	0.64	0	15,15,17	1.88	3 (20%)
3	NAG	J	1	1,3	14,14,15	0.54	0	17,19,21	1.09	1 (5%)
3	FUC	J	2	3	10,10,11	0.84	0	14,14,16	1.93	3 (21%)
2	NAG	K	1	1,2	14,14,15	0.70	0	17,19,21	1.29	2 (11%)
2	NAG	K	2	2	14,14,15	0.52	0	17,19,21	1.06	1 (5%)
2	BMA	K	3	2	11,11,12	0.73	0	15,15,17	0.97	1 (6%)
2	MAN	K	4	2	11,11,12	0.57	0	15,15,17	1.32	1 (6%)
2	MAN	K	5	2	11,11,12	0.59	0	15,15,17	1.78	5 (33%)
4	NAG	L	1	1,4	14,14,15	0.46	0	17,19,21	1.56	2 (11%)
4	NAG	L	2	4	14,14,15	0.58	0	17,19,21	1.18	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
2	BMA	E	3	2	-	2/2/19/22	0/1/1/1
2	MAN	E	4	2	-	2/2/19/22	0/1/1/1

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

There are no bond length outliers.

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	5	MAN	C1-C2-C3	6.03	118.42	109.64
2	I	5	MAN	C1-O5-C5	5.39	119.40	112.19
2	I	4	MAN	C1-O5-C5	5.25	119.22	112.19
2	G	5	MAN	C1-O5-C5	4.99	118.87	112.19
4	L	1	NAG	C1-O5-C5	4.78	118.59	112.19

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	K	5	MAN	O5-C5-C6-O6

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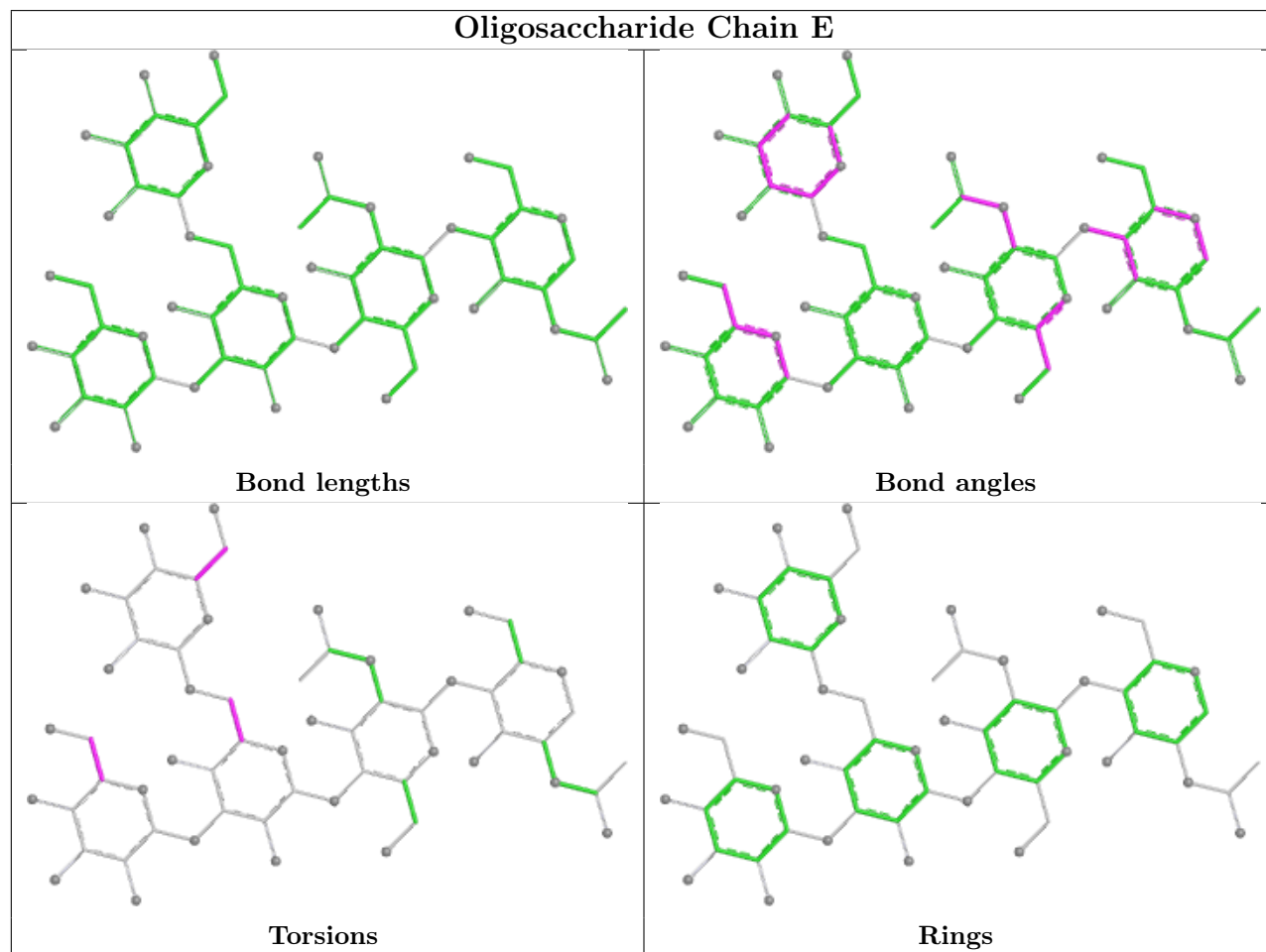
Mol	Chain	Res	Type	Atoms
2	E	4	MAN	O5-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
2	E	5	MAN	O5-C5-C6-O6
2	E	4	MAN	C4-C5-C6-O6

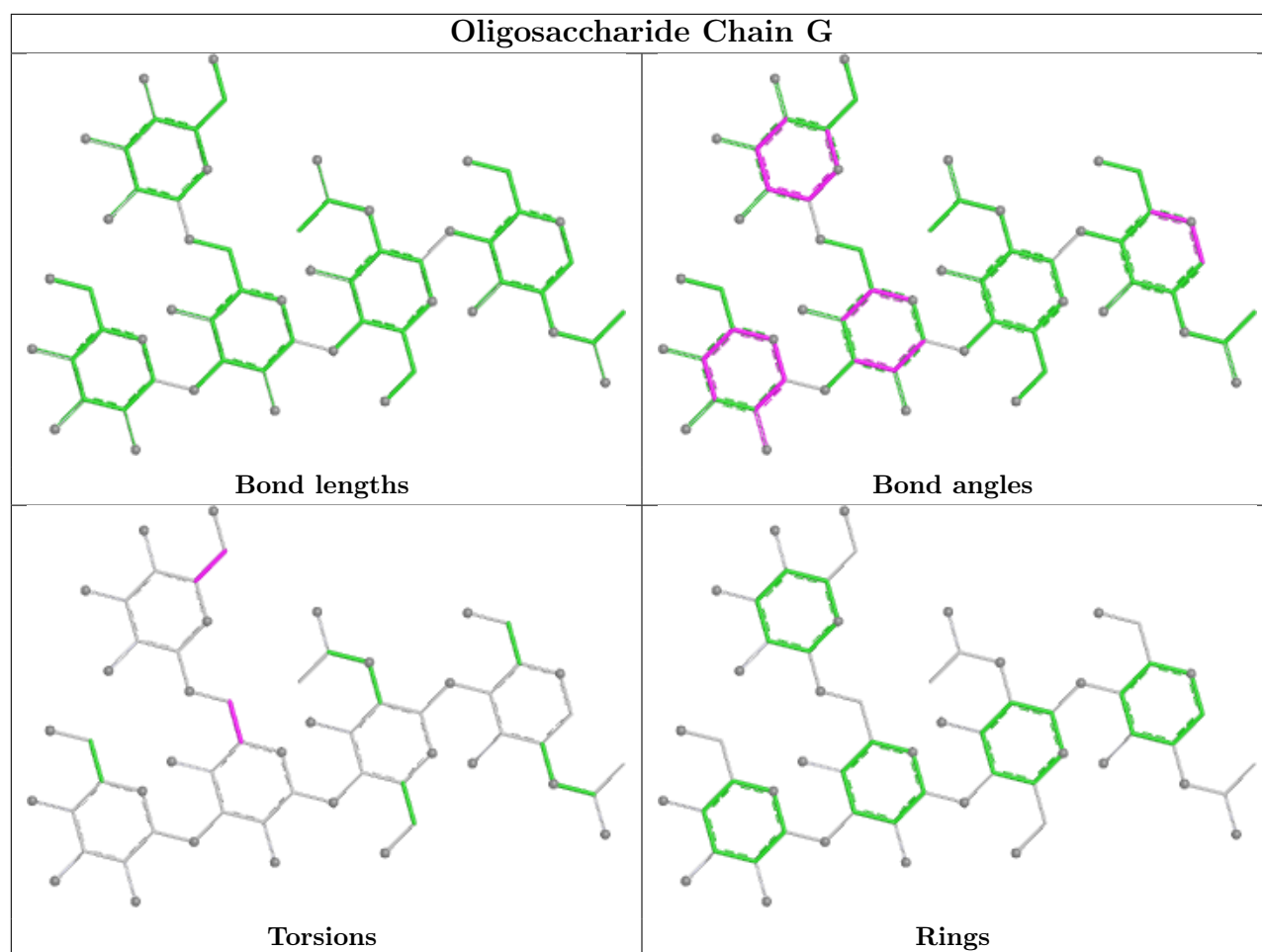
There are no ring outliers.

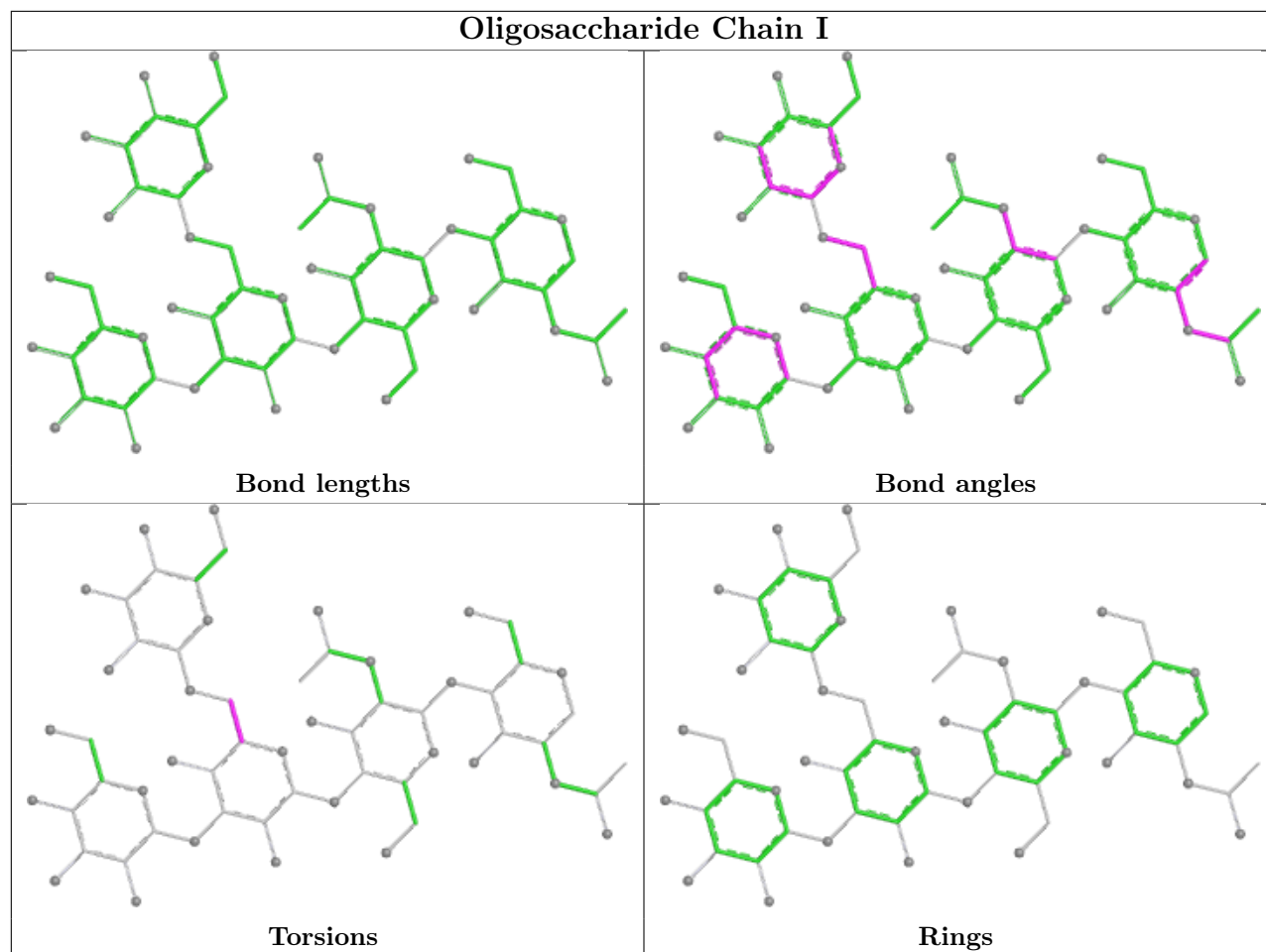
4 monomers are involved in 4 short contacts:

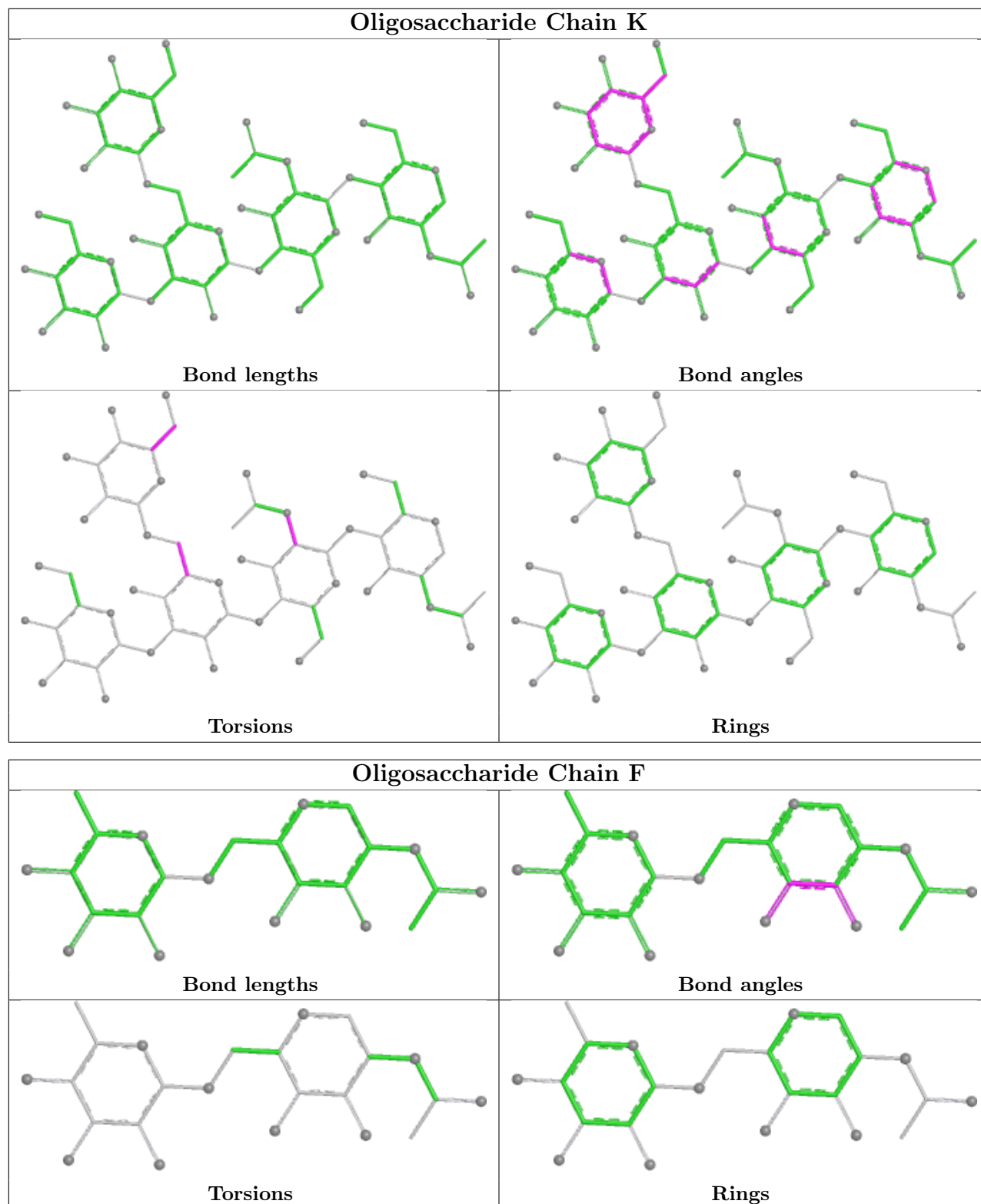
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1	NAG	1	0
2	K	3	BMA	1	0
2	G	1	NAG	1	0
2	K	1	NAG	1	0

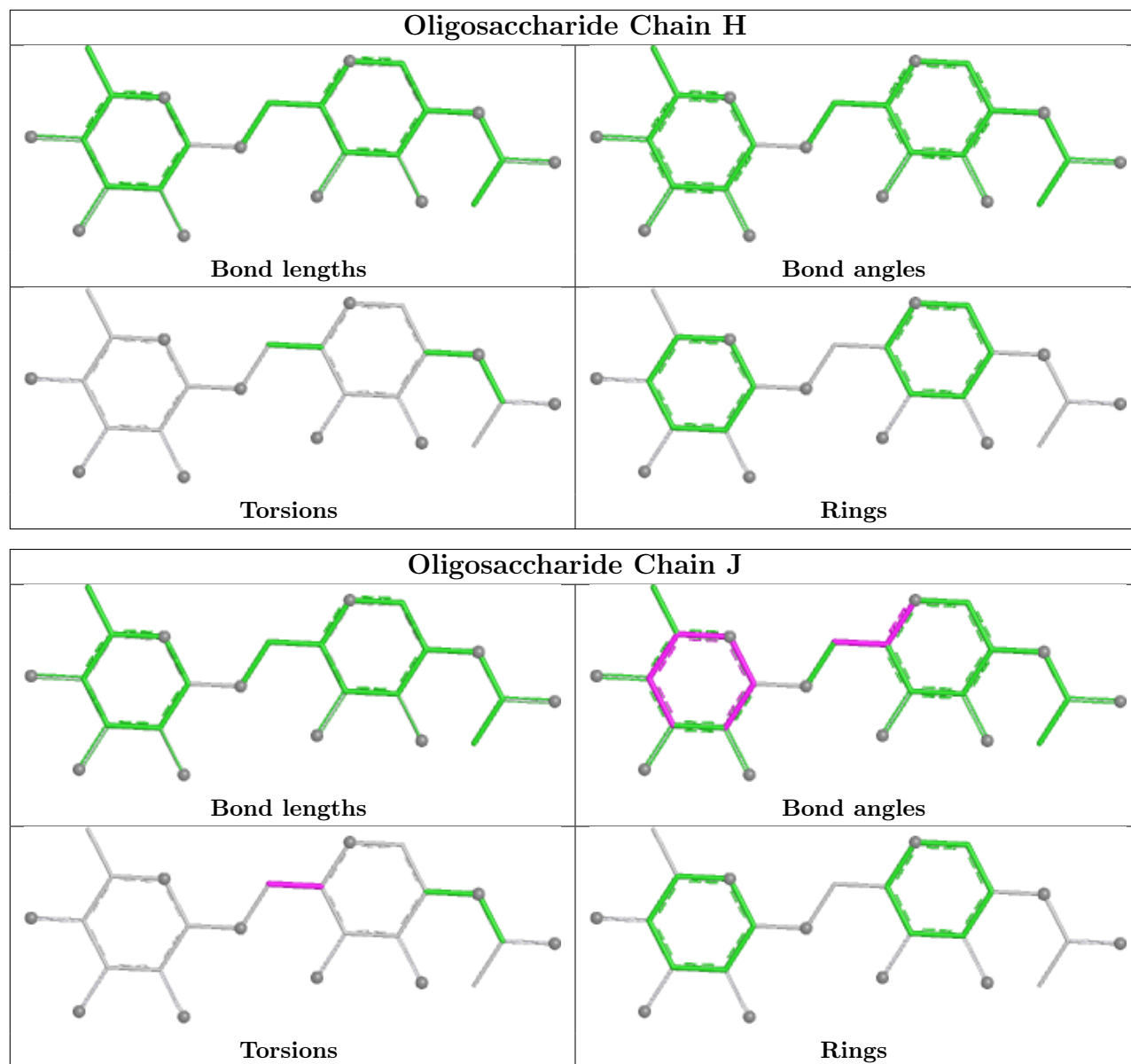
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

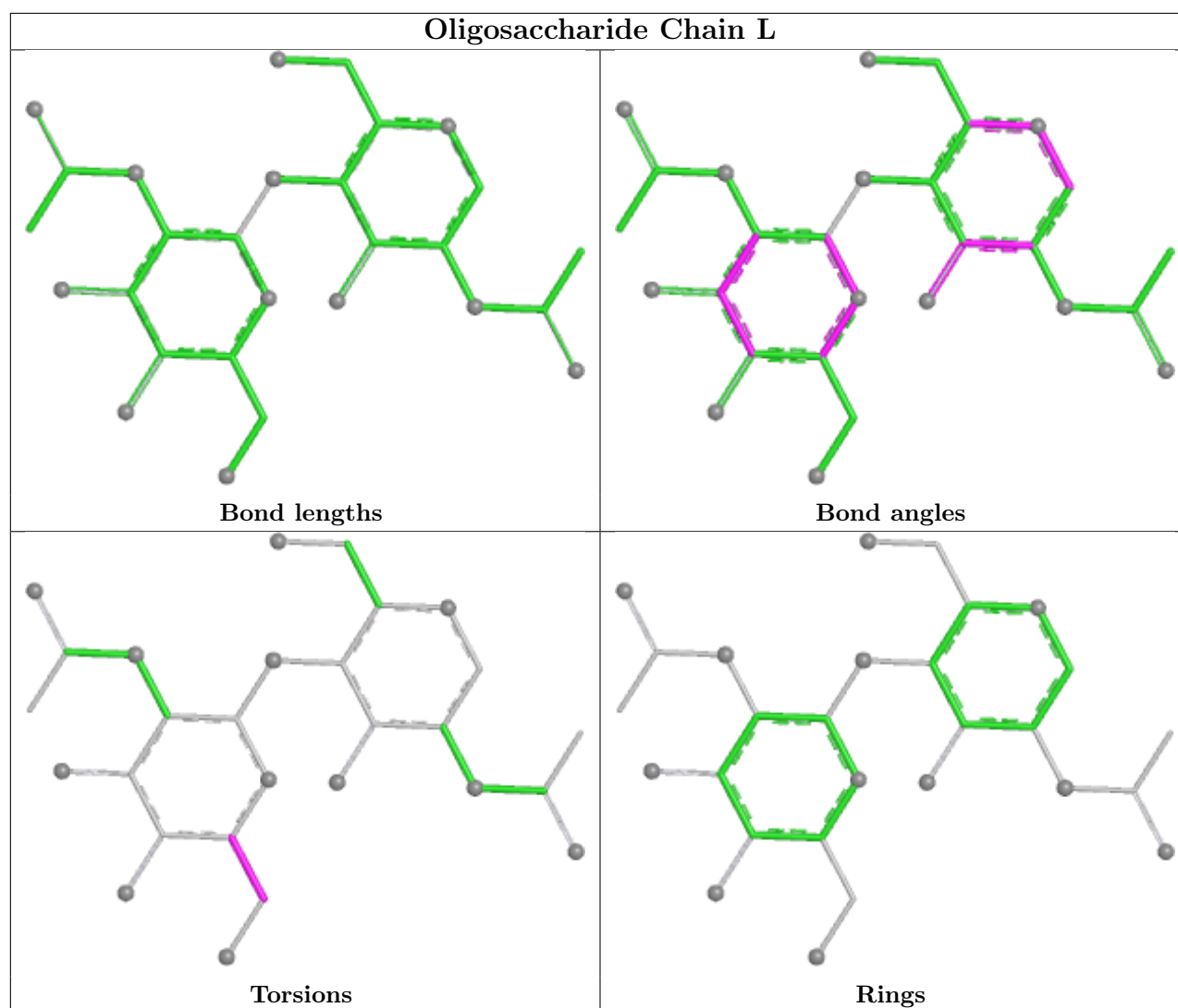












5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 5 are monoatomic - leaving 11 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	EPE	B	502	-	15,15,15	1.05	1 (6%)	19,20,20	2.20	8 (42%)
7	NAG	B	511	1	14,14,15	0.61	0	17,19,21	2.22	2 (11%)
7	NAG	B	508	1	14,14,15	0.46	0	17,19,21	1.77	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	A	510	1	14,14,15	0.71	1 (7%)	17,19,21	1.15	1 (5%)
7	NAG	D	508	1	14,14,15	0.50	0	17,19,21	0.89	1 (5%)
7	NAG	C	512	1	14,14,15	0.71	1 (7%)	17,19,21	1.62	1 (5%)
7	NAG	C	509	1	14,14,15	0.56	0	17,19,21	1.74	4 (23%)
7	NAG	D	511	1	14,14,15	0.47	0	17,19,21	1.87	4 (23%)
6	EPE	A	502	-	15,15,15	1.01	1 (6%)	19,20,20	2.26	5 (26%)
6	EPE	C	503	-	15,15,15	0.91	1 (6%)	19,20,20	2.14	6 (31%)
6	EPE	D	502	-	15,15,15	1.19	1 (6%)	19,20,20	2.32	6 (31%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EPE	B	502	-	-	4/9/19/19	0/1/1/1
7	NAG	B	511	1	-	1/6/23/26	0/1/1/1
7	NAG	B	508	1	-	2/6/23/26	0/1/1/1
7	NAG	A	510	1	-	2/6/23/26	0/1/1/1
7	NAG	D	508	1	-	2/6/23/26	0/1/1/1
7	NAG	C	512	1	-	2/6/23/26	0/1/1/1
7	NAG	C	509	1	-	2/6/23/26	0/1/1/1
7	NAG	D	511	1	-	0/6/23/26	0/1/1/1
6	EPE	A	502	-	-	8/9/19/19	0/1/1/1
6	EPE	C	503	-	-	5/9/19/19	0/1/1/1
6	EPE	D	502	-	-	1/9/19/19	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	502	EPE	C10-S	3.51	1.82	1.77
6	B	502	EPE	C10-S	3.49	1.82	1.77
6	A	502	EPE	C10-S	2.85	1.81	1.77
6	C	503	EPE	C10-S	2.67	1.81	1.77
7	C	512	NAG	C1-C2	2.24	1.55	1.52

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	511	NAG	C1-O5-C5	7.98	122.88	112.19
7	B	508	NAG	C1-O5-C5	6.25	120.56	112.19
6	A	502	EPE	O2S-S-C10	5.81	115.51	106.73
6	D	502	EPE	O2S-S-C10	5.59	115.17	106.73
7	C	512	NAG	C1-O5-C5	5.53	119.59	112.19

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	502	EPE	C10-C9-N1-C6
6	A	502	EPE	C8-C7-N4-C3
6	B	502	EPE	C10-C9-N1-C6
6	B	502	EPE	S-C10-C9-N1
6	C	503	EPE	C9-C10-S-O2S

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	502	EPE	2	0
6	A	502	EPE	2	0
6	C	503	EPE	1	0
6	D	502	EPE	2	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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	388/393 (98%)	0.62	18 (4%) 37 43	14, 28, 42, 58	0
1	B	388/393 (98%)	0.63	12 (3%) 51 58	16, 28, 43, 56	0
1	C	388/393 (98%)	0.71	20 (5%) 33 38	11, 28, 42, 56	0
1	D	388/393 (98%)	0.60	11 (2%) 55 61	12, 27, 42, 58	0
All	All	1552/1572 (98%)	0.64	61 (3%) 43 49	11, 28, 42, 58	0

The worst 5 of 61 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	469	ILE	7.9
1	A	469	ILE	7.5
1	D	469	ILE	6.7
1	D	468	PRO	6.3
1	B	469	ILE	4.9

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	FUC	H	2	10/11	0.55	0.23	70,71,71,72	0
3	NAG	F	1	14/15	0.57	0.20	58,62,65,69	0

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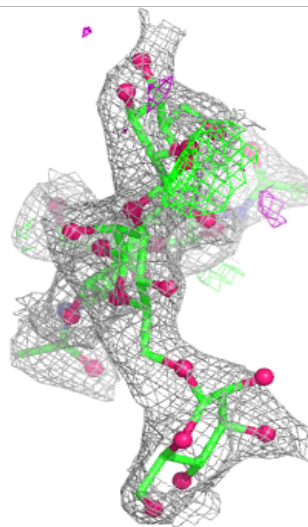
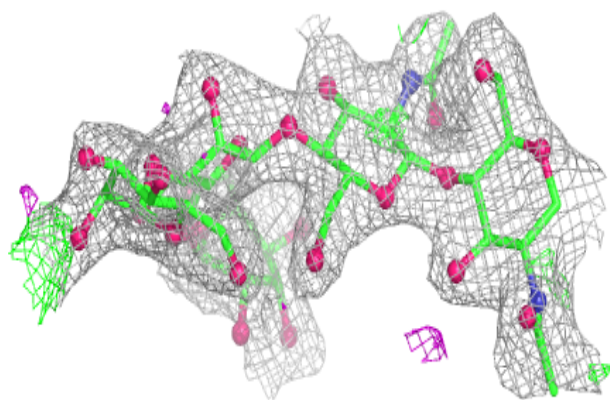
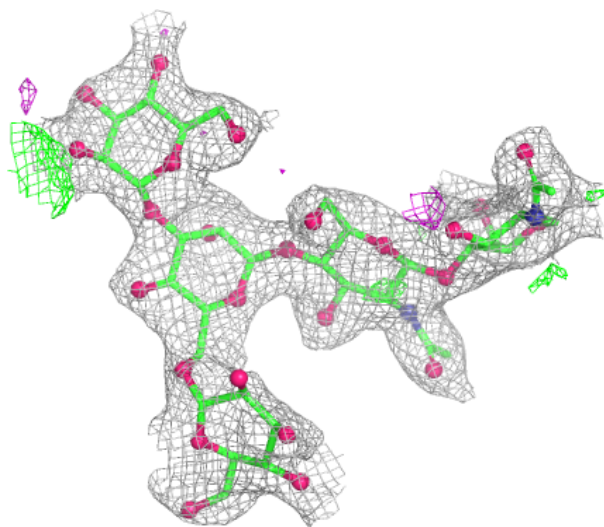
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MAN	K	5	11/12	0.60	0.19	54,54,55,56	0
3	FUC	F	2	10/11	0.64	0.21	66,67,67,68	0
4	NAG	L	2	14/15	0.64	0.18	63,64,66,66	0
3	FUC	J	2	10/11	0.66	0.19	63,64,65,65	0
2	MAN	I	4	11/12	0.66	0.18	48,52,54,56	0
2	MAN	E	5	11/12	0.68	0.17	52,54,54,55	0
2	MAN	G	4	11/12	0.69	0.17	43,46,47,49	0
4	NAG	L	1	14/15	0.73	0.17	54,58,61,62	0
3	NAG	H	1	14/15	0.73	0.17	58,63,68,71	0
2	BMA	I	3	11/12	0.74	0.15	42,46,48,50	0
2	MAN	K	4	11/12	0.74	0.17	49,51,53,55	0
2	MAN	G	5	11/12	0.75	0.14	47,50,51,52	0
2	MAN	E	4	11/12	0.77	0.16	46,48,50,51	0
2	MAN	I	5	11/12	0.77	0.14	50,51,52,53	0
3	NAG	J	1	14/15	0.77	0.14	52,57,62,63	0
2	BMA	E	3	11/12	0.82	0.13	40,44,47,50	0
2	BMA	G	3	11/12	0.83	0.14	42,44,47,50	0
2	BMA	K	3	11/12	0.83	0.11	42,46,48,51	0
2	NAG	K	1	14/15	0.86	0.13	30,36,42,43	0
2	NAG	G	1	14/15	0.86	0.12	22,34,37,38	0
2	NAG	E	1	14/15	0.87	0.11	26,32,38,38	0
2	NAG	K	2	14/15	0.88	0.13	35,36,39,41	0
2	NAG	E	2	14/15	0.88	0.11	31,32,35,36	0
2	NAG	I	1	14/15	0.89	0.11	27,32,38,39	0
2	NAG	I	2	14/15	0.89	0.12	29,31,34,37	0
2	NAG	G	2	14/15	0.89	0.12	35,37,40,40	0

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

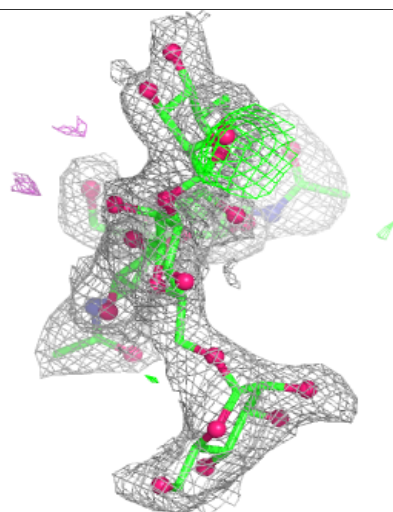
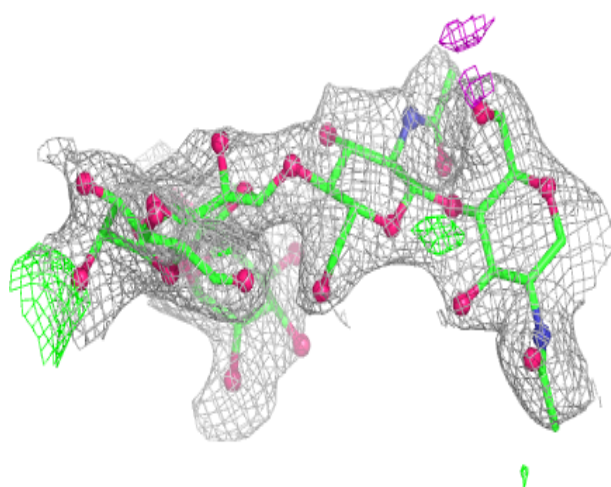
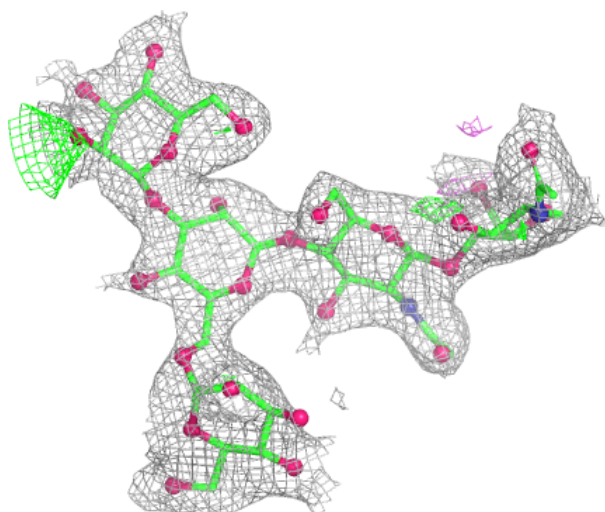
Electron density around Chain E:

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



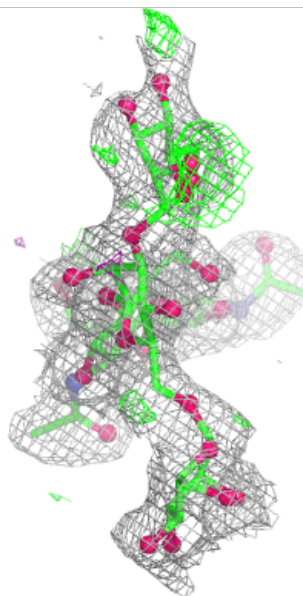
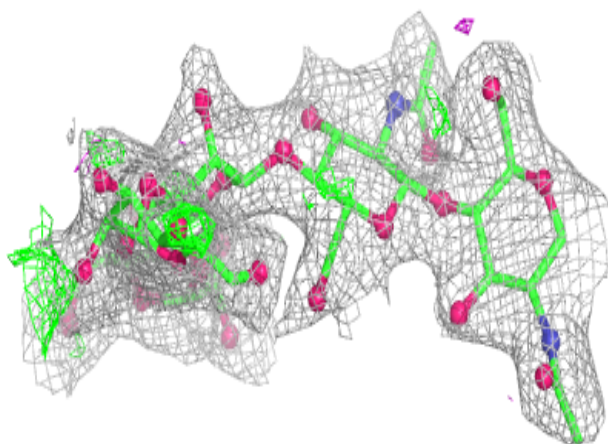
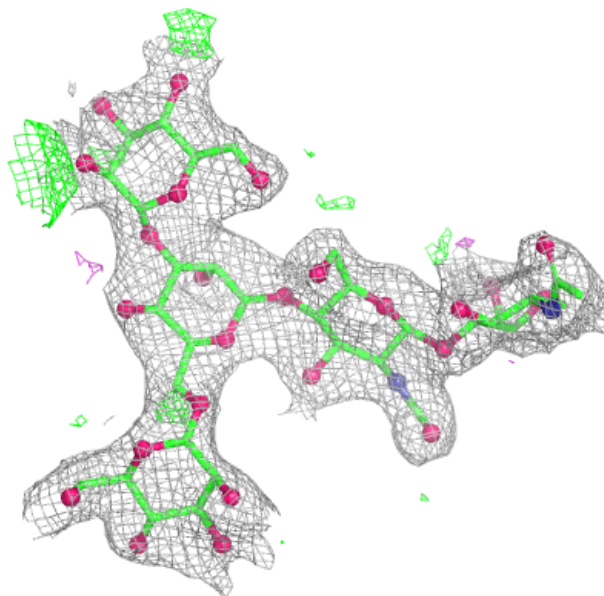
Electron density around Chain G:

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



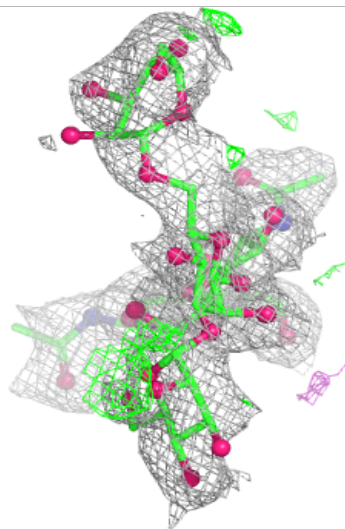
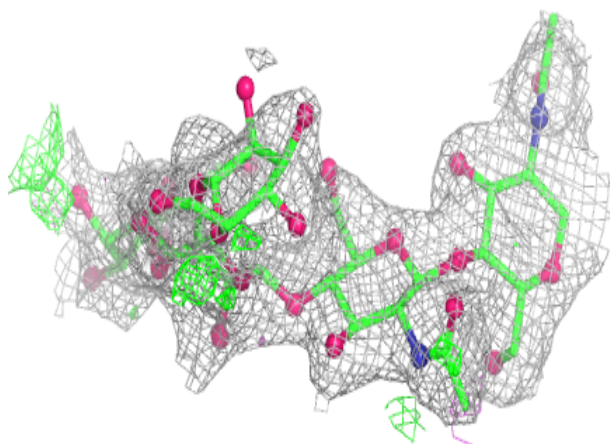
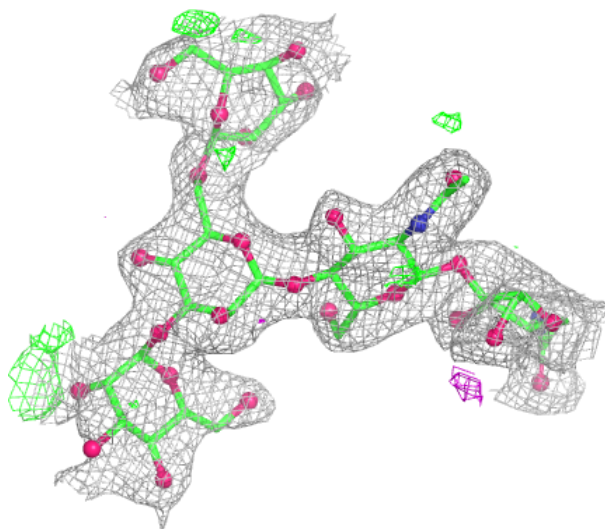
Electron density around Chain I:

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



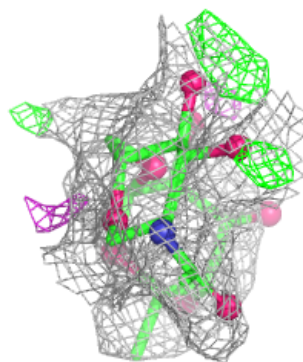
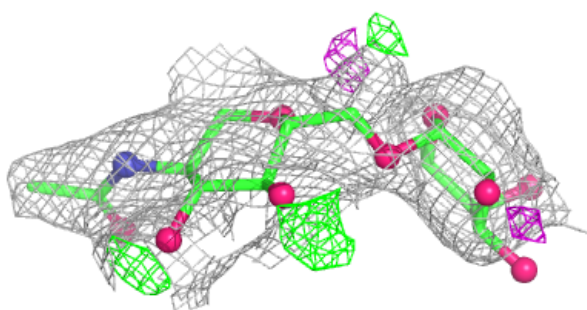
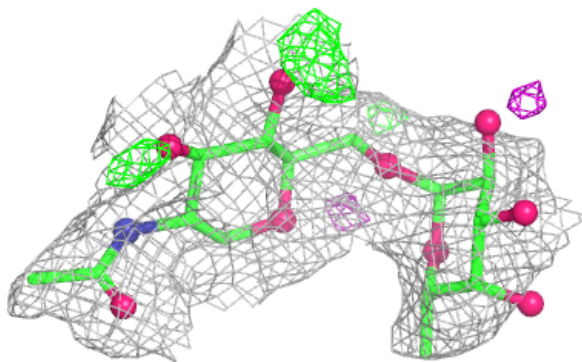
Electron density around Chain K:

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

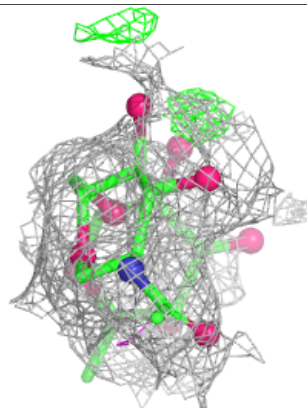
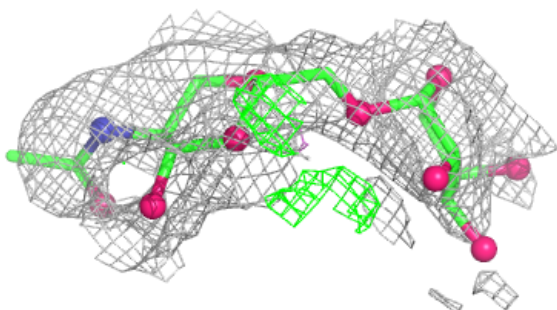
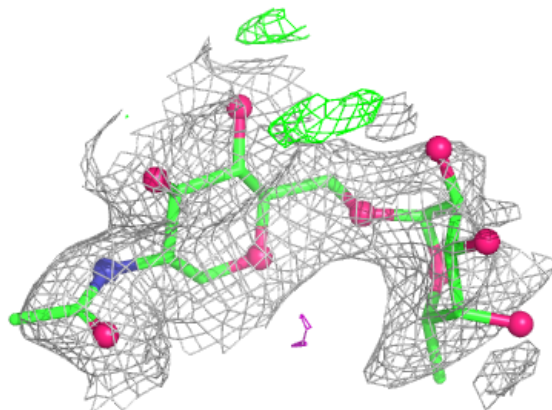


Electron density around Chain F:

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

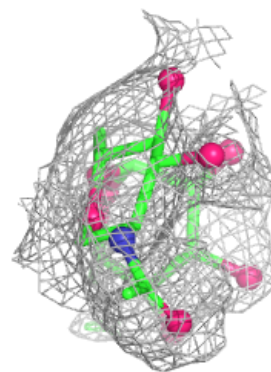
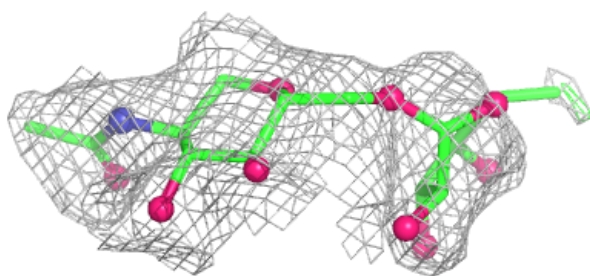
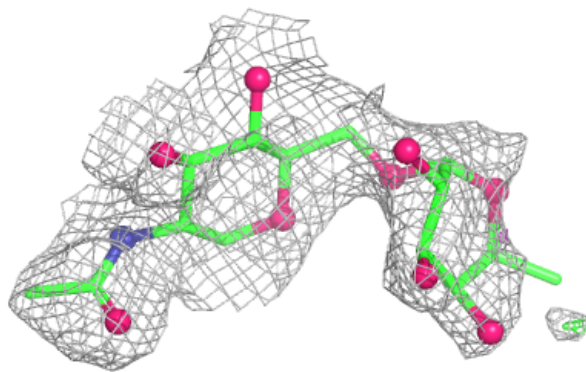
**Electron density around Chain H:**

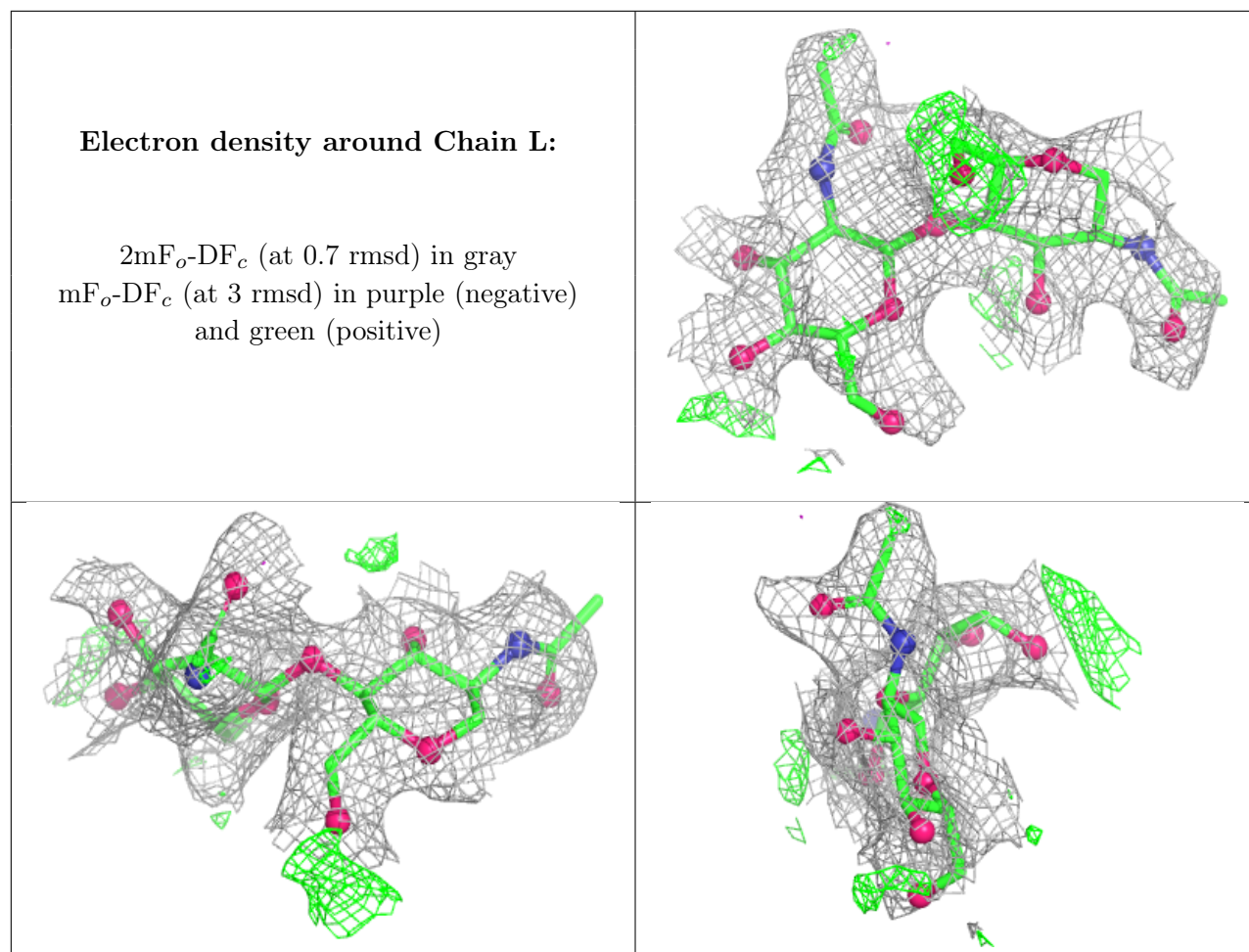
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain J:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	NAG	C	509	14/15	0.51	0.19	60,64,64,64	0
7	NAG	D	508	14/15	0.62	0.17	59,63,65,65	0
7	NAG	C	512	14/15	0.65	0.19	54,56,59,59	0
7	NAG	B	508	14/15	0.65	0.17	50,53,55,55	0
7	NAG	A	510	14/15	0.70	0.17	50,54,55,56	0
7	NAG	B	511	14/15	0.72	0.16	50,53,54,54	0
5	CA	C	501	1/1	0.75	0.16	64,64,64,64	0
7	NAG	D	511	14/15	0.75	0.14	53,56,57,58	0
6	EPE	D	502	15/15	0.83	0.19	38,41,45,45	0
6	EPE	C	503	15/15	0.88	0.18	42,48,51,52	0
6	EPE	B	502	15/15	0.91	0.13	35,38,39,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	EPE	A	502	15/15	0.91	0.14	37,43,45,46	0
5	CA	C	502	1/1	0.92	0.07	34,34,34,34	0
5	CA	A	501	1/1	0.94	0.06	34,34,34,34	0
5	CA	B	501	1/1	0.97	0.04	30,30,30,30	0
5	CA	D	501	1/1	0.99	0.02	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.