



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 28, 2024 – 09:14 AM JST

PDB ID : 6JJM  
Title : Crystal structure of Mumps virus hemagglutinin-neuraminidase bound to the oligosaccharide portion of the GM2 ganglioside  
Authors : Kubota, M.; Matsuoka, R.; Suzuki, T.; Yonekura, K.; Yanagi, Y.; Hashiguchi, T.  
Deposited on : 2019-02-26  
Resolution : 2.05 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

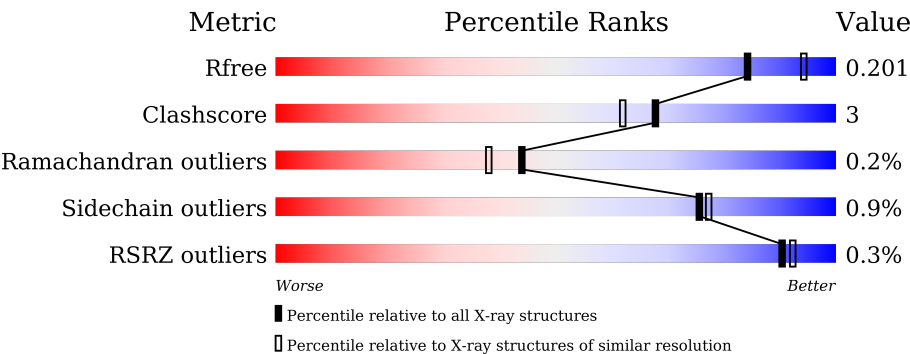
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.05 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.



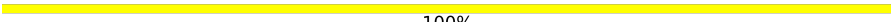
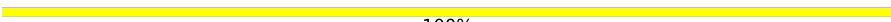
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	2096 (2.04-2.04)
Clashscore	180529	2229 (2.04-2.04)
Ramachandran outliers	177936	2217 (2.04-2.04)
Sidechain outliers	177891	2217 (2.04-2.04)
RSRZ outliers	164620	2096 (2.04-2.04)

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  $\geq 3$ , 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	489	<div><div>85%</div><div>7% • 8%</div></div>
1	B	489	<div><div>83%</div><div>9% 8%</div></div>
2	C	2	<div><div>100%</div></div>
2	D	2	<div><div>100%</div></div>
2	F	2	<div><div>100%</div></div>
2	G	2	<div><div>100%</div></div>

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Mol	Chain	Length	Quality of chain
3	E	4	 100%
3	H	4	 100%

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7819 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 HN protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	452	Total	C	N	O	S	0	0	0
			3530	2256	584	669	21			
1	B	452	Total	C	N	O	S	0	0	0
			3530	2256	584	669	21			

There are 24 discrepancies between the modelled and reference sequences:

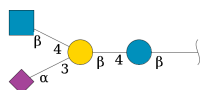
Chain	Residue	Modelled	Actual	Comment	Reference
A	103	GLU	-	expression tag	UNP Q9WAF5
A	104	THR	-	expression tag	UNP Q9WAF5
A	105	GLY	-	expression tag	UNP Q9WAF5
A	583	GLY	-	expression tag	UNP Q9WAF5
A	584	THR	-	expression tag	UNP Q9WAF5
A	585	LYS	-	expression tag	UNP Q9WAF5
A	586	HIS	-	expression tag	UNP Q9WAF5
A	587	HIS	-	expression tag	UNP Q9WAF5
A	588	HIS	-	expression tag	UNP Q9WAF5
A	589	HIS	-	expression tag	UNP Q9WAF5
A	590	HIS	-	expression tag	UNP Q9WAF5
A	591	HIS	-	expression tag	UNP Q9WAF5
B	103	GLU	-	expression tag	UNP Q9WAF5
B	104	THR	-	expression tag	UNP Q9WAF5
B	105	GLY	-	expression tag	UNP Q9WAF5
B	583	GLY	-	expression tag	UNP Q9WAF5
B	584	THR	-	expression tag	UNP Q9WAF5
B	585	LYS	-	expression tag	UNP Q9WAF5
B	586	HIS	-	expression tag	UNP Q9WAF5
B	587	HIS	-	expression tag	UNP Q9WAF5
B	588	HIS	-	expression tag	UNP Q9WAF5
B	589	HIS	-	expression tag	UNP Q9WAF5
B	590	HIS	-	expression tag	UNP Q9WAF5
B	591	HIS	-	expression tag	UNP Q9WAF5

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



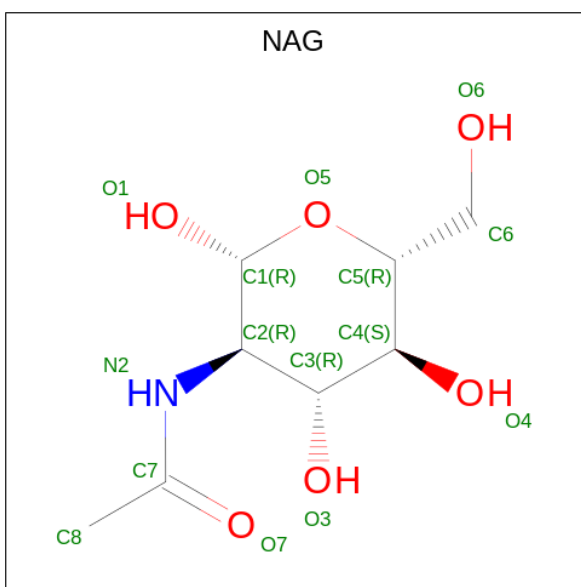
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]beta-D-galactopyranose-(1-4)-beta-D-glucopyranose.



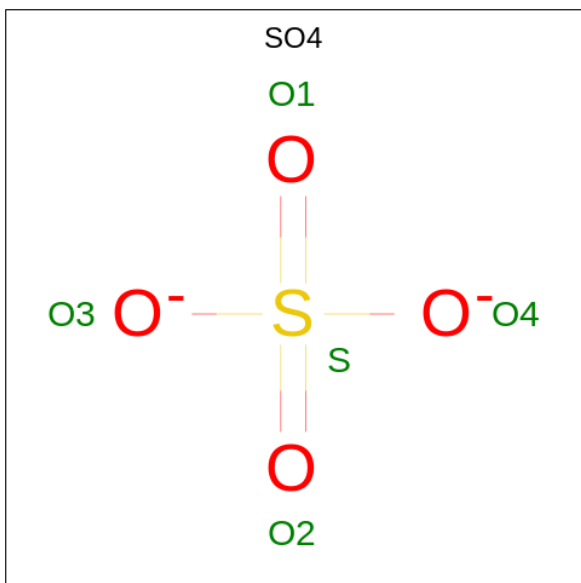
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	4	Total	C	N	O	0	0	0
			57	31	2	24			
3	H	4	Total	C	N	O	0	0	0
			57	31	2	24			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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


- Molecule 6 is water.

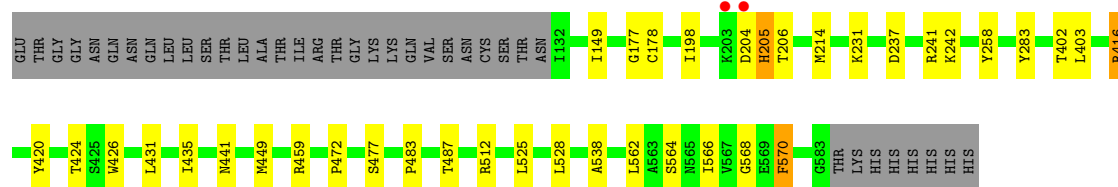
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	248	Total	O	0	0
			248	248		
6	B	219	Total	O	0	0
			219	219		

### 3 Residue-property plots


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

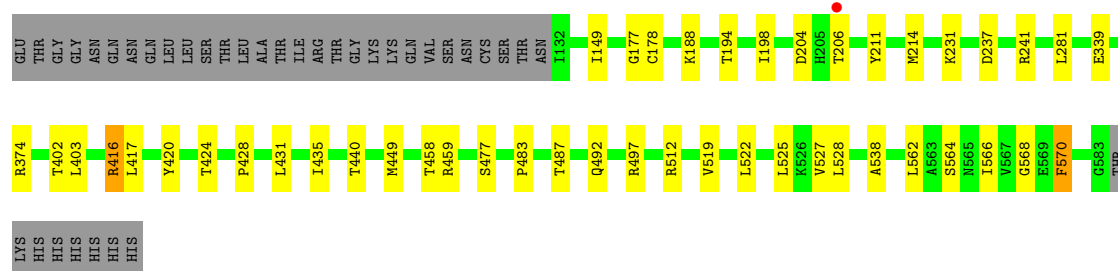
- Molecule 1: HN protein

Chain A: 

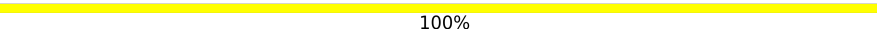


- Molecule 1: HN protein

Chain B: 



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

Chain C: 



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

Chain D: 





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

Chain F:  100%

NAG1  
NAG2

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

Chain G:  100%


NAG1  
NAG2

- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain E:  100%

BGC1  
GAL2  
STA3  
NAG4

- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain H:  100%

BGC1  
GAL2  
STA3  
NAG4

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	137.26Å 137.26Å 178.01Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.93 – 2.05 44.93 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.93-2.05) 99.8 (44.93-2.05)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.77 (at 2.05Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, $R_{free}$	0.183 , 0.201 0.183 , 0.201	Depositor DCC
$R_{free}$ test set	5877 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.3	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 44.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.165 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	7819	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: SO4, GAL, BGC, NAG, SIA

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	0.27	0/3628	0.50	0/4962
1	B	0.27	0/3628	0.50	0/4962
All	All	0.27	0/7256	0.50	0/9924

There are no bond length outliers.

There are no bond angle outliers.

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	3530	0	3409	26	0
1	B	3530	0	3409	26	0
2	C	28	0	25	0	0
2	D	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
3	E	57	0	48	0	0
3	H	57	0	48	0	0
4	A	28	0	26	0	0
4	B	28	0	26	0	0
5	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	5	0	0	0	0
6	A	248	0	0	2	0
6	B	219	0	0	1	0
All	All	7819	0	7066	50	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 (50) 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:A:416:ARG:NH1	1:A:435:ILE:O	2.12	0.83
1:B:525:LEU:HD13	1:B:528:LEU:HD21	1.67	0.75
1:B:562:LEU:O	1:B:570:PHE:HA	1.90	0.72
1:B:416:ARG:NH2	1:B:417:LEU:O	2.23	0.71
1:A:525:LEU:HD13	1:A:528:LEU:HD21	1.76	0.68
1:A:562:LEU:O	1:A:570:PHE:HA	2.00	0.61
1:B:339:GLU:O	1:B:374:ARG:NH2	2.35	0.58
1:B:188:LYS:NZ	6:B:705:HOH:O	2.37	0.57
1:A:178:CYS:HB3	1:A:198:ILE:HB	1.87	0.56
1:A:205:HIS:NE2	1:A:242:LYS:HD2	2.21	0.56
1:B:214:MET:HG2	1:B:231:LYS:HB2	1.88	0.56
1:B:204:ASP:OD1	1:B:206:THR:HG22	2.06	0.55
1:A:204:ASP:OD1	1:A:206:THR:HG22	2.08	0.54
1:B:402:THR:HB	1:B:449:MET:HE1	1.89	0.54
1:A:402:THR:HB	1:A:449:MET:CE	2.38	0.53
1:B:428:PRO:HB2	1:B:458:THR:OG1	2.08	0.53
1:A:416:ARG:NH1	6:A:708:HOH:O	2.42	0.52
1:B:149:ILE:HB	1:B:487:THR:HG22	1.92	0.51
1:B:403:LEU:HD12	1:B:431:LEU:HD11	1.92	0.51
1:B:402:THR:HB	1:B:449:MET:CE	2.42	0.49
1:A:403:LEU:HD12	1:A:431:LEU:HD11	1.94	0.49
1:A:214:MET:HG2	1:A:231:LYS:HB2	1.94	0.49
1:A:204:ASP:OD1	1:A:205:HIS:N	2.48	0.47
1:B:435:ILE:HG22	1:B:449:MET:HG2	1.96	0.47
1:B:420:TYR:CD1	1:B:483:PRO:HD3	2.50	0.47
1:A:149:ILE:HB	1:A:487:THR:HG22	1.98	0.45
1:A:402:THR:HB	1:A:449:MET:HE1	1.98	0.45
1:A:420:TYR:CD1	1:A:483:PRO:HD3	2.52	0.45
1:B:497:ARG:HD3	1:B:522:LEU:HD12	1.99	0.45
1:B:440:THR:HG22	1:B:440:THR:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:519:VAL:HB	1:B:527:VAL:HG12	1.99	0.44
1:B:237:ASP:CG	1:B:241:ARG:HH22	2.20	0.44
1:A:564:SER:HB2	1:B:566:ILE:HD11	2.00	0.44
1:A:283:TYR:OH	6:A:701:HOH:O	2.21	0.44
1:A:426:TRP:CG	1:A:472:PRO:HA	2.53	0.43
1:A:426:TRP:CD2	1:A:472:PRO:HA	2.54	0.43
1:A:402:THR:HB	1:A:449:MET:HE3	2.00	0.43
1:A:512:ARG:HB3	1:A:538:ALA:O	2.18	0.42
1:A:435:ILE:HG22	1:A:449:MET:HG2	2.01	0.42
1:B:178:CYS:HB3	1:B:198:ILE:HB	2.00	0.42
1:A:424:THR:HA	1:A:477:SER:O	2.20	0.42
1:B:177:GLY:O	1:B:568:GLY:HA3	2.20	0.42
1:A:566:ILE:HD11	1:B:564:SER:HB2	2.02	0.42
1:A:177:GLY:O	1:A:568:GLY:HA3	2.20	0.41
1:B:424:THR:HA	1:B:477:SER:O	2.20	0.41
1:B:492:GLN:CD	1:B:492:GLN:H	2.24	0.41
1:B:512:ARG:HB3	1:B:538:ALA:O	2.20	0.41
1:A:237:ASP:CG	1:A:241:ARG:HH22	2.24	0.41
1:A:242:LYS:HD3	1:A:258:TYR:OH	2.21	0.40
1:B:194:THR:HA	1:B:211:TYR:O	2.21	0.40

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	450/489 (92%)	428 (95%)	21 (5%)	1 (0%)	44	38
1	B	450/489 (92%)	430 (96%)	19 (4%)	1 (0%)	44	38
All	All	900/978 (92%)	858 (95%)	40 (4%)	2 (0%)	44	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	570	PHE
1	A	570	PHE

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	399/432 (92%)	395 (99%)	4 (1%)	73	74
1	B	399/432 (92%)	396 (99%)	3 (1%)	79	80
All	All	798/864 (92%)	791 (99%)	7 (1%)	75	77

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	205	HIS
1	A	416	ARG
1	A	441	ASN
1	A	459	ARG
1	B	281	LEU
1	B	416	ARG
1	B	459	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

16 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	C	1	2,1	14,14,15	0.43	0	17,19,21	1.56	3 (17%)
2	NAG	C	2	2	14,14,15	0.69	0	17,19,21	1.25	2 (11%)
2	NAG	D	1	2,1	14,14,15	0.28	0	17,19,21	0.68	0
2	NAG	D	2	2	14,14,15	0.35	0	17,19,21	0.76	0
3	BGC	E	1	3	12,12,12	1.29	1 (8%)	17,17,17	0.74	0
3	GAL	E	2	3	11,11,12	1.01	0	15,15,17	1.12	1 (6%)
3	SIA	E	3	3	20,20,21	2.00	3 (15%)	24,28,31	1.94	4 (16%)
3	NAG	E	4	3	14,14,15	0.23	0	17,19,21	1.34	2 (11%)
2	NAG	F	1	2,1	14,14,15	0.30	0	17,19,21	0.84	1 (5%)
2	NAG	F	2	2	14,14,15	0.45	0	17,19,21	2.46	5 (29%)
2	NAG	G	1	2,1	14,14,15	0.30	0	17,19,21	0.63	0
2	NAG	G	2	2	14,14,15	0.33	0	17,19,21	0.60	0
3	BGC	H	1	3	12,12,12	1.28	1 (8%)	17,17,17	0.88	1 (5%)
3	GAL	H	2	3	11,11,12	1.01	1 (9%)	15,15,17	1.35	3 (20%)
3	SIA	H	3	3	20,20,21	1.91	3 (15%)	24,28,31	2.22	5 (20%)
3	NAG	H	4	3	14,14,15	0.21	0	17,19,21	1.33	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	C	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
3	BGC	E	1	3	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GAL	E	2	3	-	0/2/19/22	0/1/1/1
3	SIA	E	3	3	-	0/18/34/38	0/1/1/1
3	NAG	E	4	3	-	0/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
3	BGC	H	1	3	-	0/2/22/22	0/1/1/1
3	GAL	H	2	3	-	0/2/19/22	0/1/1/1
3	SIA	H	3	3	-	0/18/34/38	0/1/1/1
3	NAG	H	4	3	-	0/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	3	SIA	C2-C1	7.40	1.59	1.52
3	H	3	SIA	C2-C1	6.90	1.58	1.52
3	E	1	BGC	O5-C1	3.34	1.51	1.42
3	H	1	BGC	O5-C1	3.30	1.51	1.42
3	E	3	SIA	O6-C2	3.11	1.47	1.43
3	H	3	SIA	O6-C2	2.92	1.47	1.43
3	H	3	SIA	C7-C6	2.03	1.55	1.53
3	E	3	SIA	C7-C6	2.01	1.55	1.53
3	H	2	GAL	O4-C4	-2.00	1.38	1.43

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	3	SIA	C4-C3-C2	5.70	120.04	109.81
2	F	2	NAG	O5-C5-C6	-5.61	98.41	107.20
3	H	3	SIA	C4-C3-C2	5.16	119.05	109.81
3	H	3	SIA	C6-O6-C2	4.96	121.94	111.34
3	E	3	SIA	C6-O6-C2	4.90	121.83	111.34
3	H	3	SIA	O1A-C1-C2	-4.88	111.05	122.57
2	F	2	NAG	C1-O5-C5	4.56	118.38	112.19
2	F	2	NAG	C2-N2-C7	-4.37	116.68	122.90
3	H	3	SIA	O6-C2-C3	4.24	116.30	110.46
2	C	1	NAG	O4-C4-C5	-3.99	99.39	109.30
2	F	2	NAG	C6-C5-C4	-3.67	104.41	113.00
2	F	2	NAG	C4-C3-C2	-3.55	105.81	111.02
3	E	3	SIA	O6-C2-C3	3.55	115.34	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	4	NAG	C3-C4-C5	-3.11	104.69	110.24
3	H	4	NAG	C3-C4-C5	-3.09	104.72	110.24
2	C	1	NAG	O5-C5-C6	3.02	111.94	107.20
2	C	2	NAG	C4-C3-C2	-2.92	106.74	111.02
3	H	2	GAL	O4-C4-C5	2.84	116.34	109.30
2	C	2	NAG	C1-O5-C5	2.79	115.97	112.19
3	E	4	NAG	C4-C3-C2	-2.79	106.93	111.02
3	H	3	SIA	O1B-C1-O1A	2.76	130.36	124.09
3	H	4	NAG	C4-C3-C2	-2.72	107.03	111.02
2	C	1	NAG	O4-C4-C3	2.69	116.58	110.35
3	E	3	SIA	O1B-C1-O1A	2.49	129.75	124.09
3	H	2	GAL	O4-C4-C3	-2.26	105.13	110.35
3	H	2	GAL	C2-C3-C4	-2.23	107.03	110.89
3	E	2	GAL	C2-C3-C4	-2.07	107.31	110.89
3	H	1	BGC	O4-C4-C3	-2.05	105.61	110.35
2	F	1	NAG	O4-C4-C5	-2.03	104.25	109.30

There are no chirality outliers.

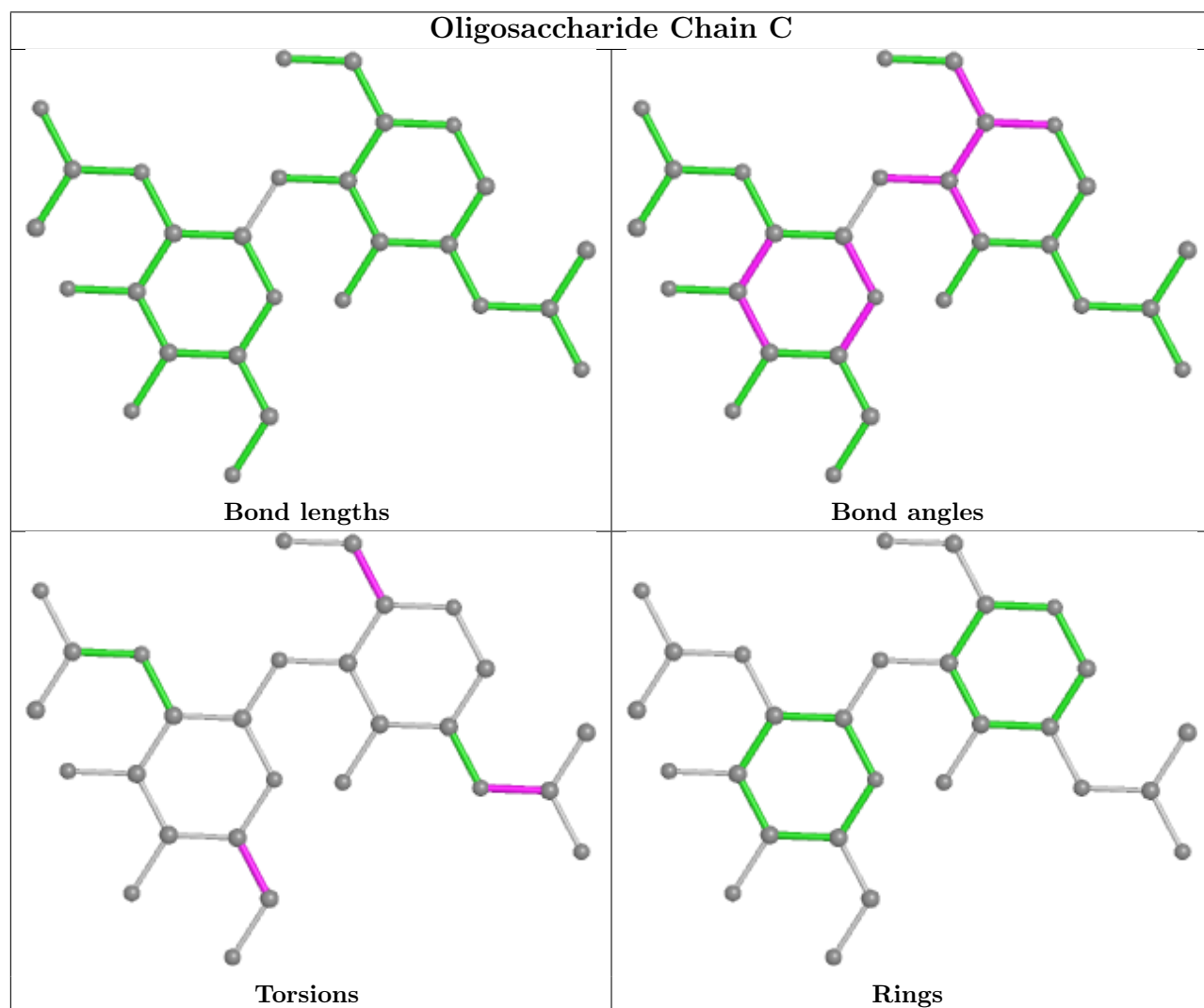
All (18) torsion outliers are listed below:

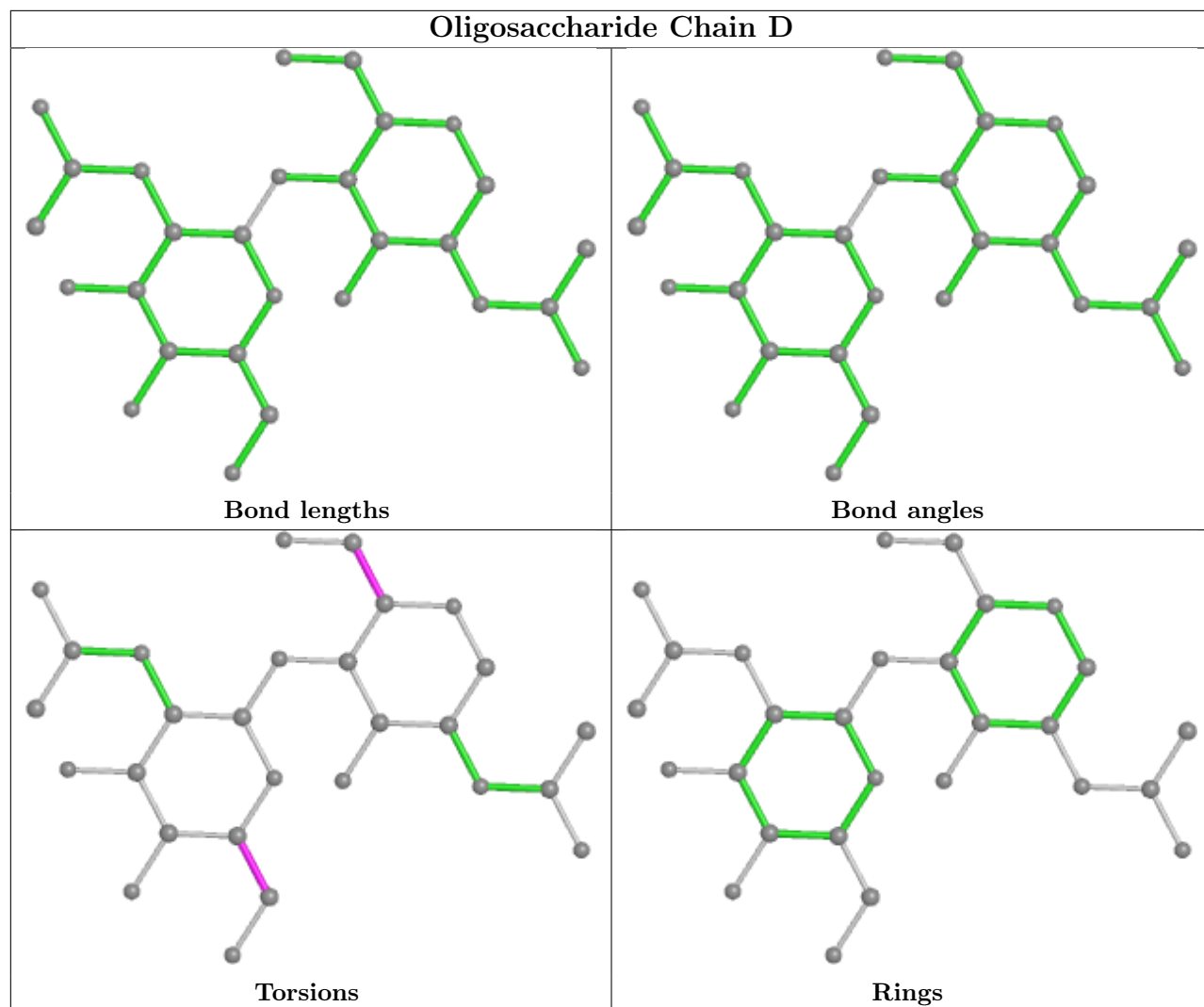
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	O5-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	G	2	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6

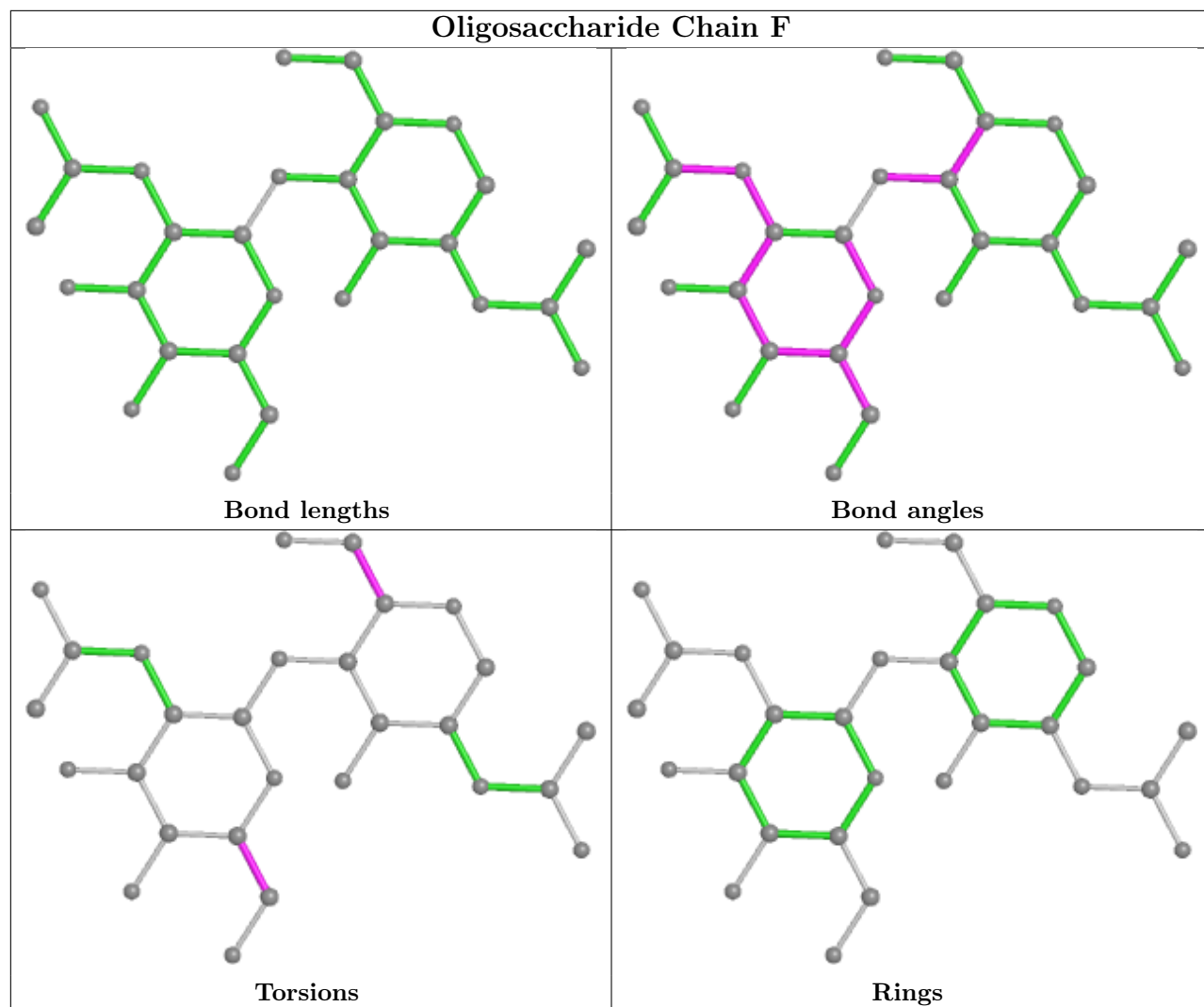
There are no ring outliers.

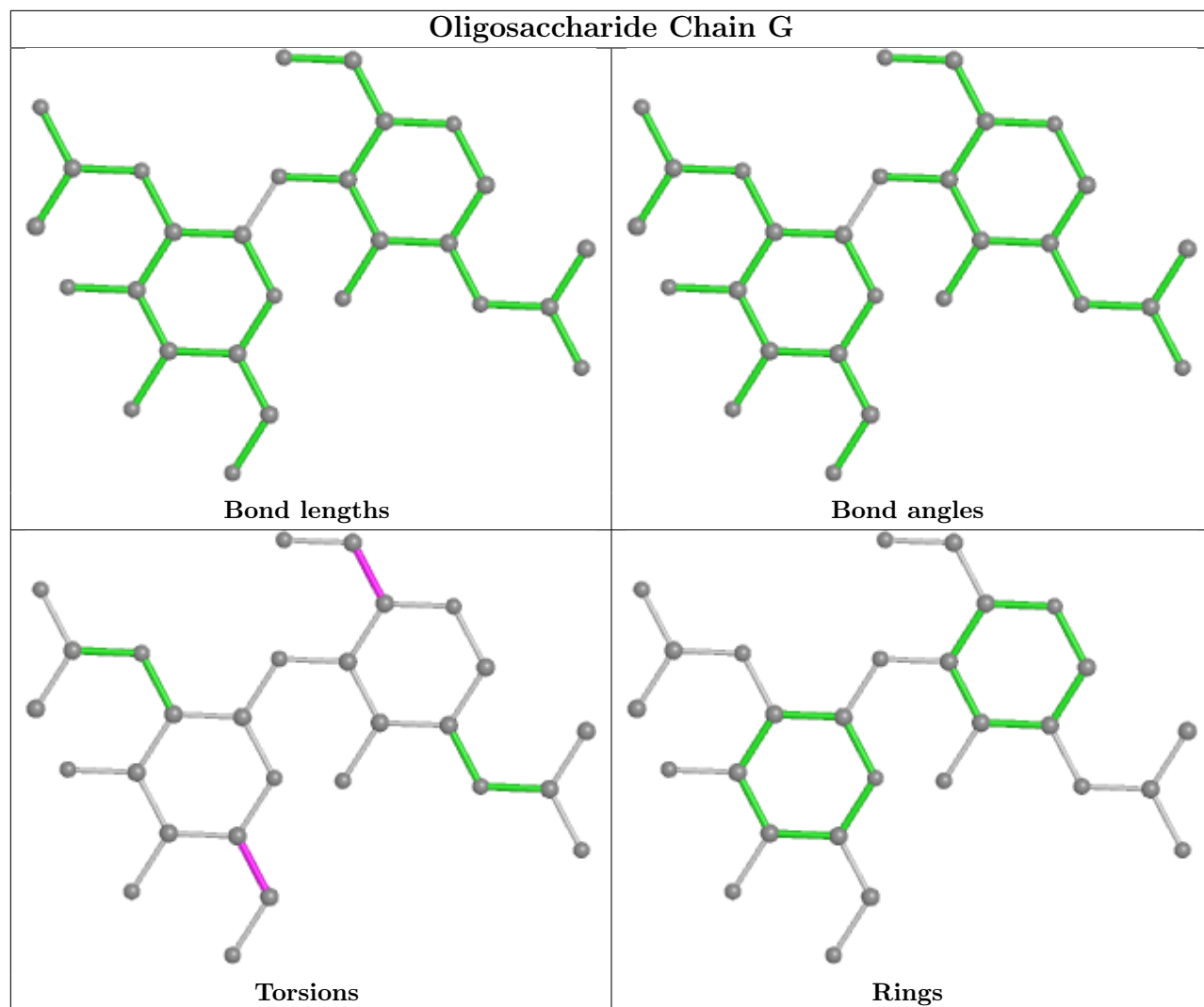
No monomer is involved in short contacts.

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

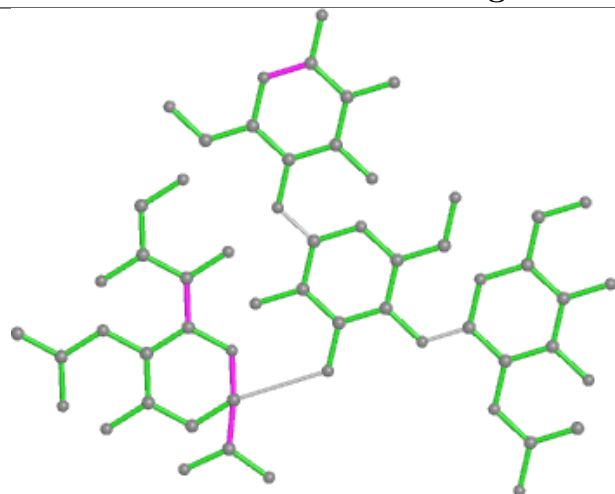




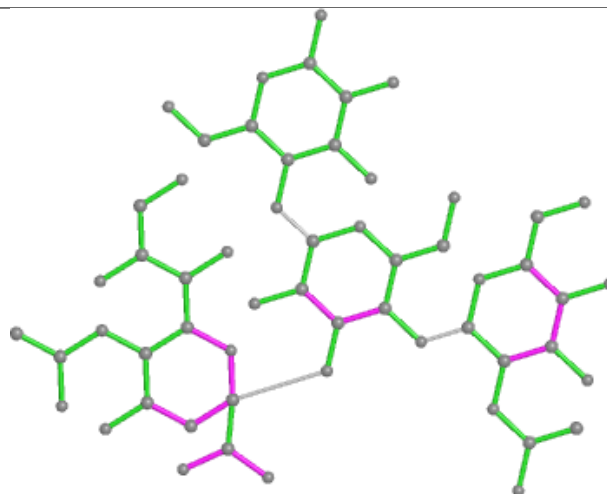




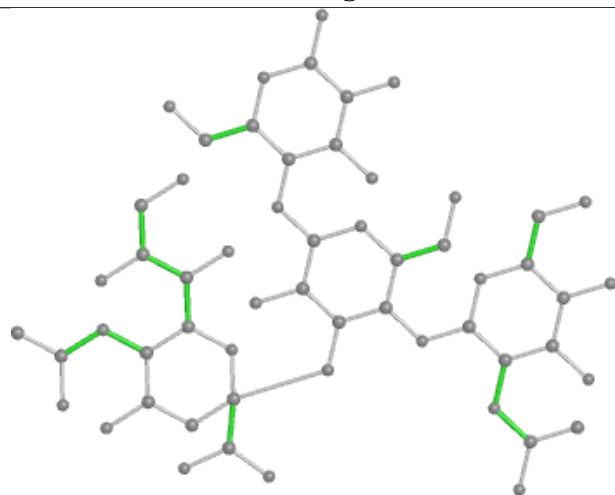
## Oligosaccharide Chain E



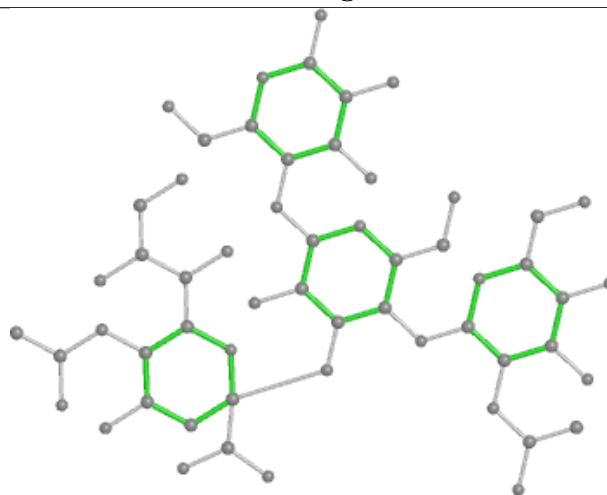
Bond lengths



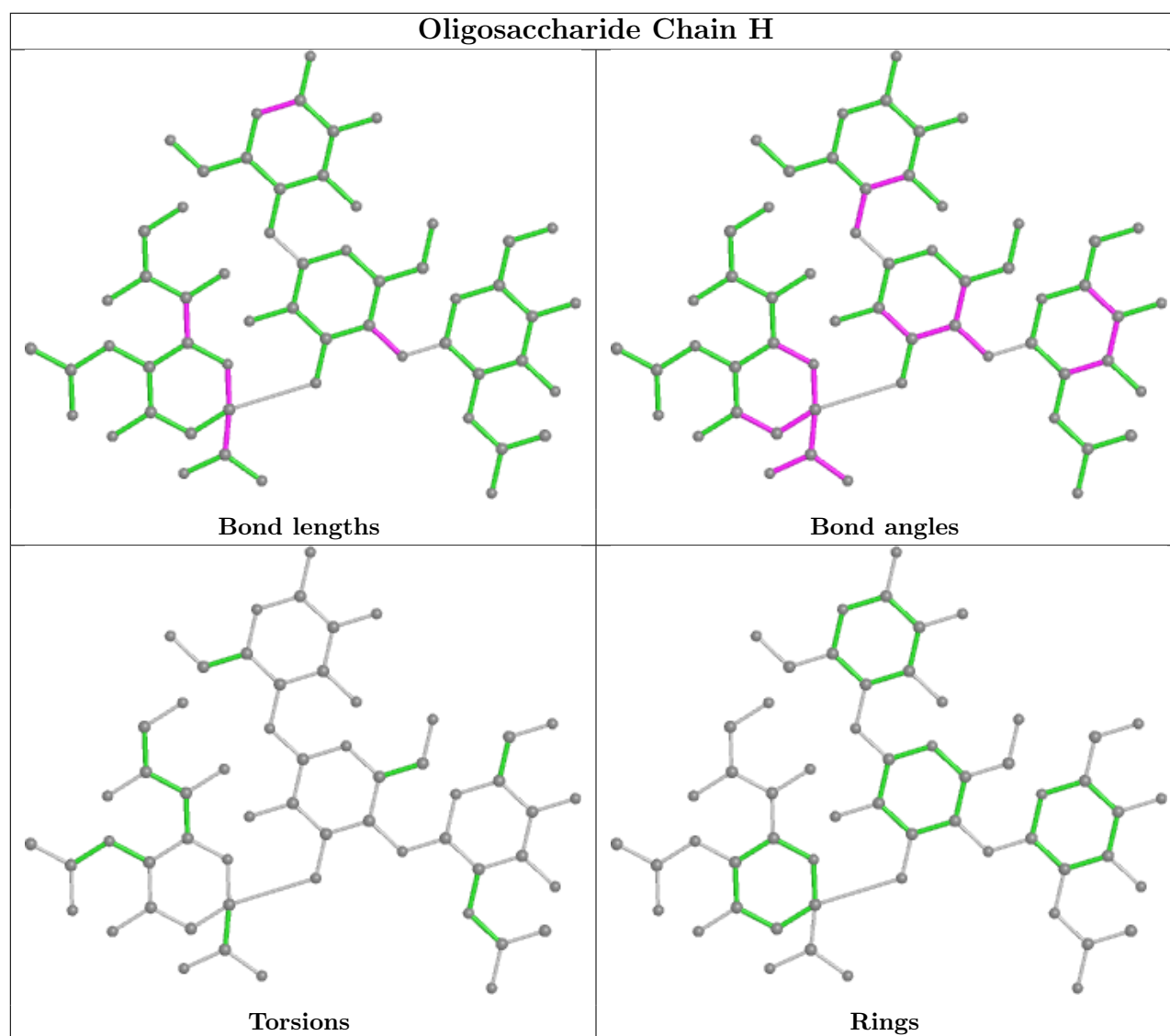
Bond angles



Torsions



Rings



## 5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	SO4	B	611	-	4,4,4	0.14	0	6,6,6	0.09	0
4	NAG	B	606	1	14,14,15	0.34	0	17,19,21	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	SO4	A	611	-	4,4,4	0.15	0	6,6,6	0.06	0
4	NAG	B	603	1	14,14,15	0.30	0	17,19,21	0.63	0
4	NAG	A	606	1	14,14,15	0.32	0	17,19,21	0.68	0
4	NAG	A	603	1	14,14,15	0.27	0	17,19,21	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
4	NAG	B	603	1	-	0/6/23/26	0/1/1/1
4	NAG	A	606	1	-	2/6/23/26	0/1/1/1
4	NAG	B	606	1	-	2/6/23/26	0/1/1/1
4	NAG	A	603	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	606	NAG	C4-C5-C6-O6
4	B	606	NAG	C4-C5-C6-O6
4	A	606	NAG	O5-C5-C6-O6
4	B	606	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	452/489 (92%)	-1.28	2 (0%) 89 90	29, 44, 75, 123	0
1	B	452/489 (92%)	-1.26	1 (0%) 92 93	29, 45, 75, 124	0
All	All	904/978 (92%)	-1.27	3 (0%) 90 92	29, 45, 75, 124	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	204	ASP	2.8
1	B	206	THR	2.5
1	A	203	LYS	2.3

### 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, 95<sup>th</sup> 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.

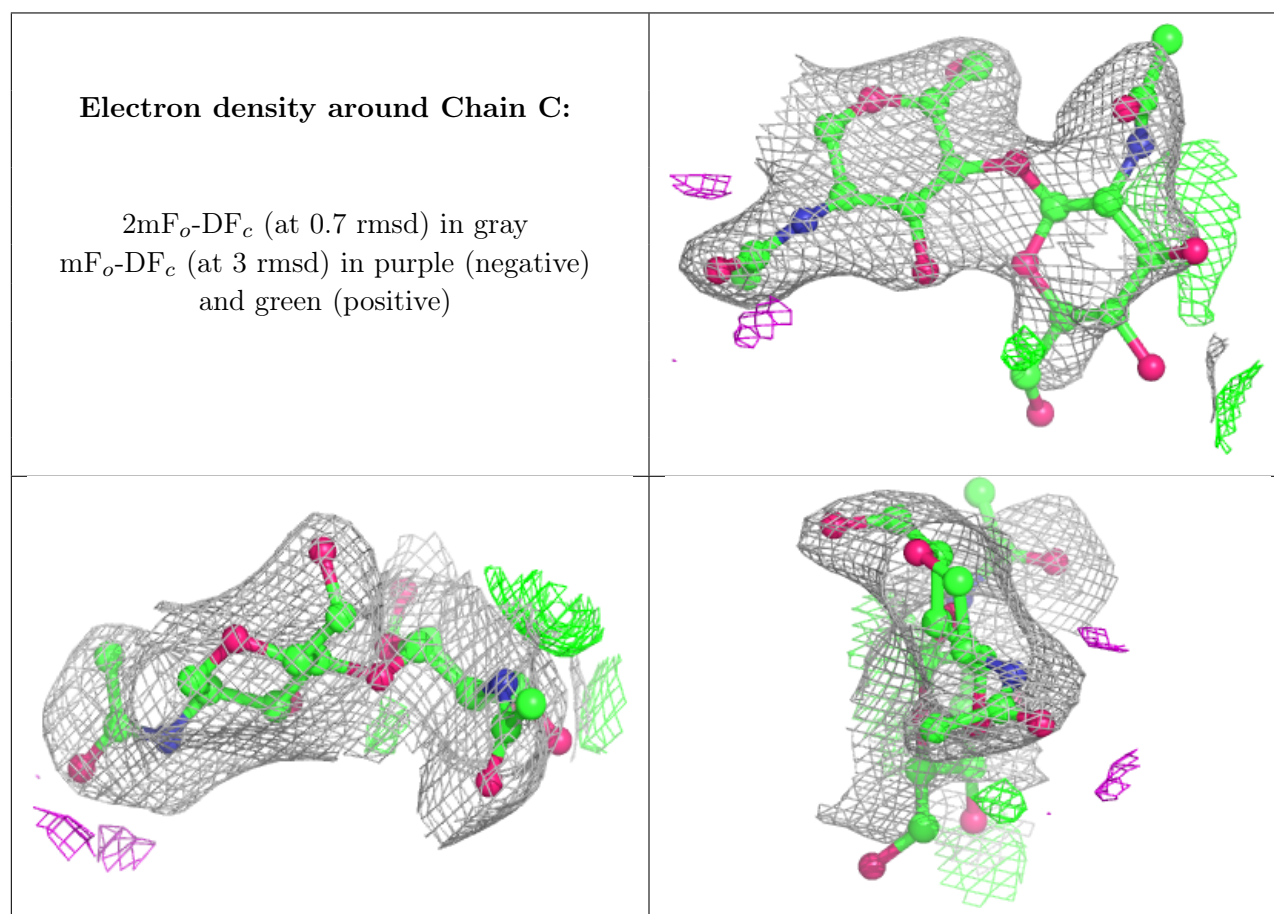
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	G	2	14/15	0.95	0.07	96,98,100,100	0
2	NAG	D	1	14/15	0.96	0.07	68,82,93,94	0
2	NAG	D	2	14/15	0.96	0.07	94,99,101,102	0
2	NAG	C	2	14/15	0.96	0.09	94,102,105,106	0
2	NAG	F	2	14/15	0.97	0.08	83,89,91,93	0
2	NAG	G	1	14/15	0.98	0.05	64,80,84,89	0

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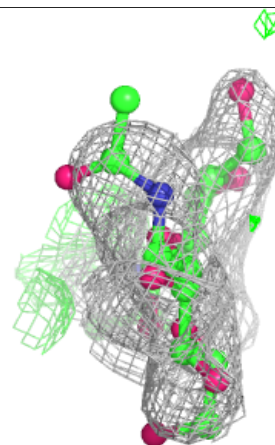
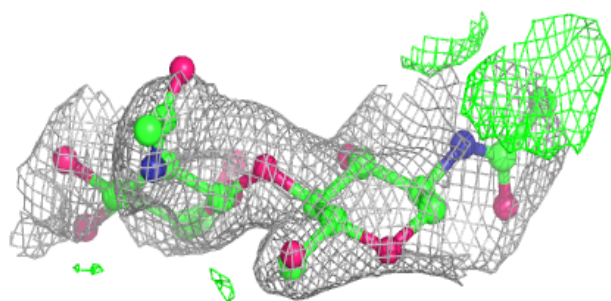
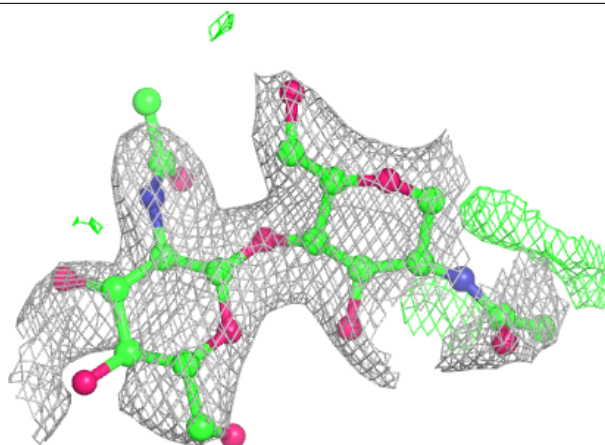
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	C	1	14/15	0.98	0.05	56,76,84,94	0
2	NAG	F	1	14/15	0.99	0.04	50,67,73,76	0
3	BGC	E	1	12/12	0.99	0.04	52,65,75,78	0
3	GAL	E	2	11/12	0.99	0.03	37,44,48,53	0
3	NAG	E	4	14/15	0.99	0.04	42,47,52,69	0
3	BGC	H	1	12/12	0.99	0.04	62,75,83,86	0
3	GAL	H	2	11/12	0.99	0.03	40,46,51,53	0
3	SIA	H	3	20/21	0.99	0.03	30,39,42,44	0
3	NAG	H	4	14/15	0.99	0.04	46,52,55,71	0
3	SIA	E	3	20/21	1.00	0.02	30,36,40,43	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.

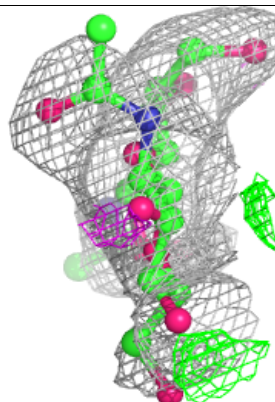
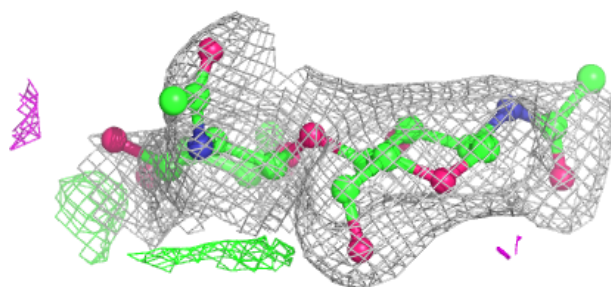
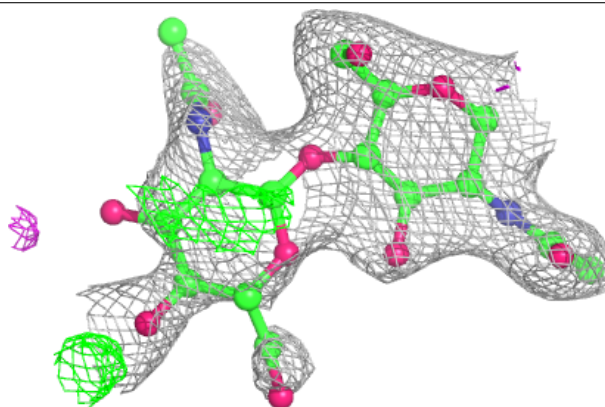


**Electron density around Chain D:**

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

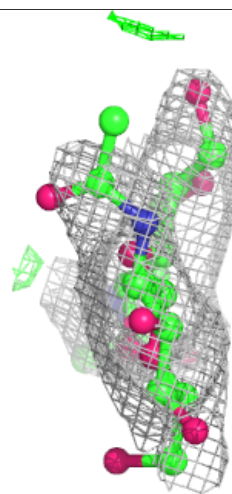
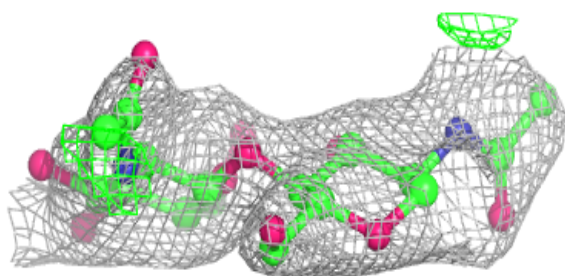
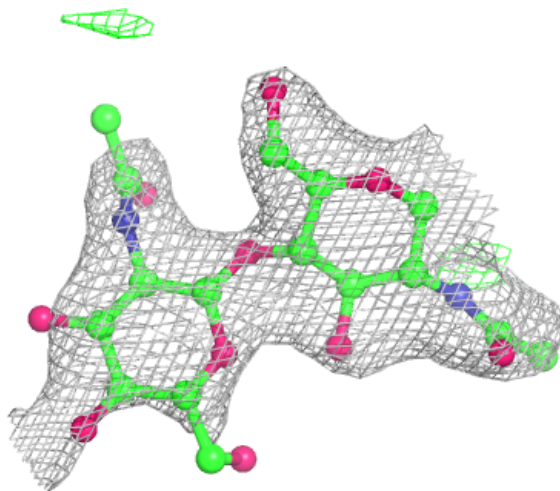
**Electron density around Chain F:**

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



**Electron density around Chain G:**

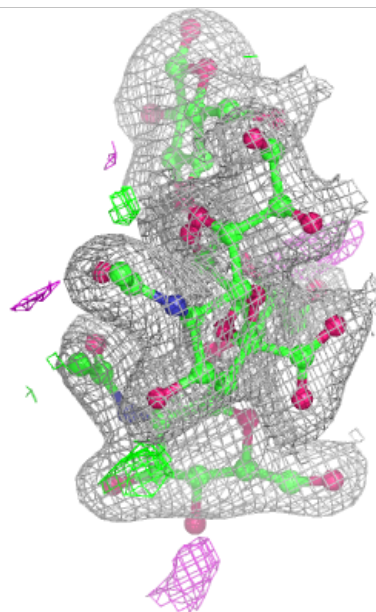
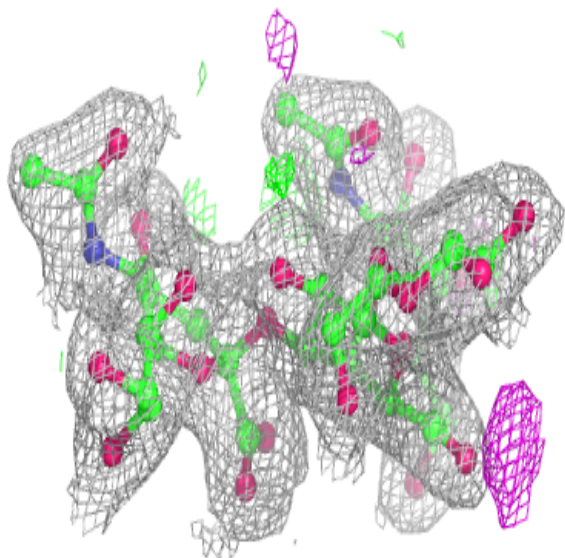
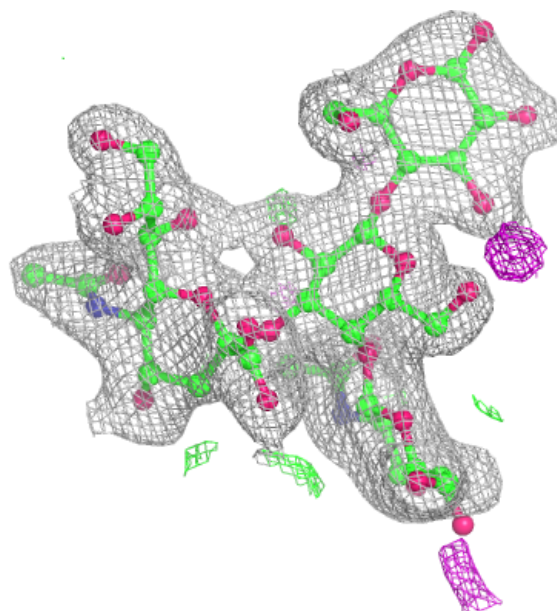
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

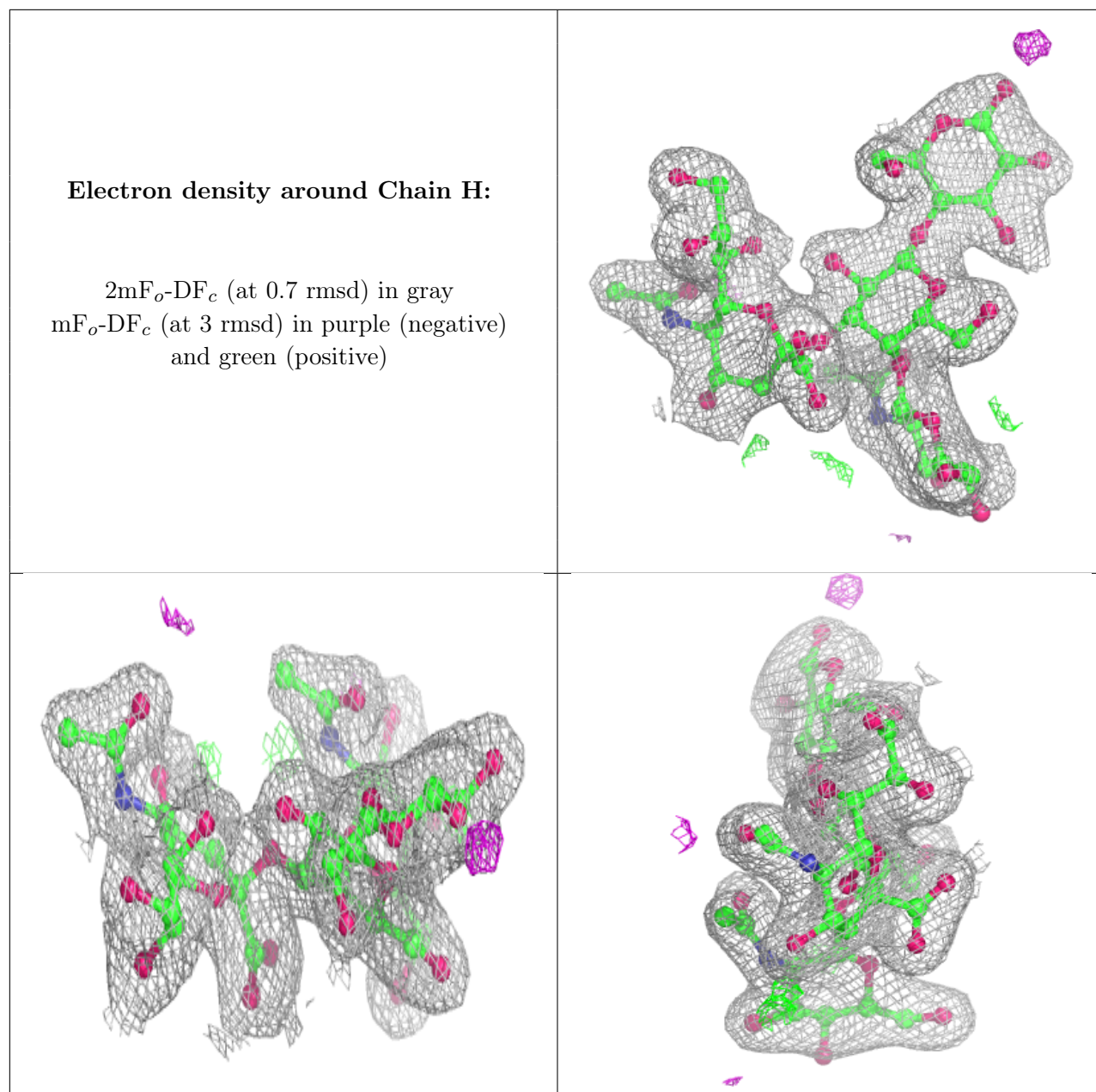




**Electron density around Chain E:**

$2mF_o-DF_c$  (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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	NAG	A	603	14/15	0.97	0.05	64,77,81,82	0
4	NAG	A	606	14/15	0.98	0.06	48,59,67,72	0
4	NAG	B	603	14/15	0.98	0.05	59,72,76,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	B	606	14/15	0.98	0.06	50,62,73,78	0
5	SO4	A	611	5/5	0.99	0.06	89,90,91,92	0
5	SO4	B	611	5/5	1.00	0.03	66,67,69,74	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.