



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 03:53 AM UTC

PDB ID : 5VMF / pdb\_00005vmf  
Title : Influenza hemagglutinin H1 mutant DH1D in complex with 6'SLN  
Authors : Ni, F.; Kondrashkina, E.; Wang, Q.  
Deposited on : 2017-04-27  
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](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 : 4-5-2 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

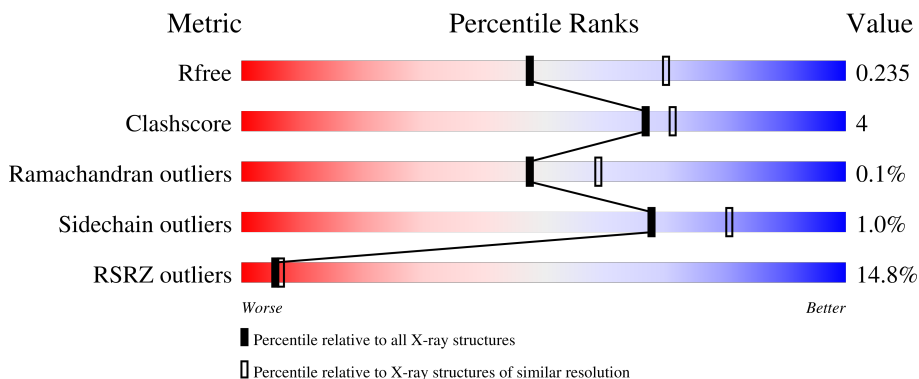
# 1 Overall quality at a glance

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.



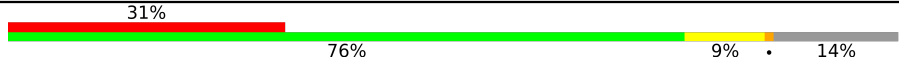
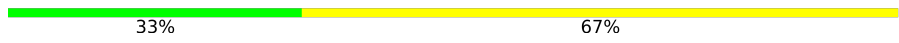



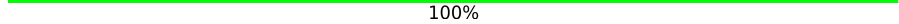
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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  $\geq 3$ , 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	326	5% (poor fit), 92% (0-1 outliers), 7% (2-3 outliers), 0% (4+ outliers)
1	C	326	4% (poor fit), 91% (0-1 outliers), 7% (2-3 outliers), 0% (4+ outliers)
1	E	326	2% (poor fit), 90% (0-1 outliers), 8% (2-3 outliers), 0% (4+ outliers)
2	B	191	28% (poor fit), 79% (0-1 outliers), 6% (2-3 outliers), 14% (4+ outliers)
2	D	191	35% (poor fit), 80% (0-1 outliers), 5% (2-3 outliers), 14% (4+ outliers)

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Mol	Chain	Length	Quality of chain
2	F	191	
3	G	3	
4	H	3	
4	I	3	
4	K	3	
5	J	2	

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 23671 atoms, of which 11123 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Hemagglutinin HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	321	4873	1565	2392	426	479	11	0	0	0
1	C	321	4861	1562	2383	426	479	11	0	0	0
1	E	321	4910	1573	2418	426	482	11	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	222	LEU	GLN	engineered mutation	UNP Q9WFX3
A	224	SER	GLY	engineered mutation	UNP Q9WFX3
C	222	LEU	GLN	engineered mutation	UNP Q9WFX3
C	224	SER	GLY	engineered mutation	UNP Q9WFX3
E	222	LEU	GLN	engineered mutation	UNP Q9WFX3
E	224	SER	GLY	engineered mutation	UNP Q9WFX3

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
2	B	164	2552	825	1235	225	261	6	0	0	0
2	D	164	2552	825	1235	225	261	6	0	0	0
2	F	164	2551	825	1234	225	261	6	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

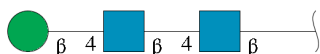
Chain	Residue	Modelled	Actual	Comment	Reference
B	186	GLY	-	expression tag	UNP Q9WFX3
B	187	ALA	-	expression tag	UNP Q9WFX3

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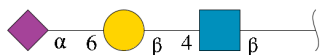
Chain	Residue	Modelled	Actual	Comment	Reference
B	188	LEU	-	expression tag	UNP Q9WFX3
B	189	VAL	-	expression tag	UNP Q9WFX3
B	190	PRO	-	expression tag	UNP Q9WFX3
B	191	ARG	-	expression tag	UNP Q9WFX3
D	186	GLY	-	expression tag	UNP Q9WFX3
D	187	ALA	-	expression tag	UNP Q9WFX3
D	188	LEU	-	expression tag	UNP Q9WFX3
D	189	VAL	-	expression tag	UNP Q9WFX3
D	190	PRO	-	expression tag	UNP Q9WFX3
D	191	ARG	-	expression tag	UNP Q9WFX3
F	186	GLY	-	expression tag	UNP Q9WFX3
F	187	ALA	-	expression tag	UNP Q9WFX3
F	188	LEU	-	expression tag	UNP Q9WFX3
F	189	VAL	-	expression tag	UNP Q9WFX3
F	190	PRO	-	expression tag	UNP Q9WFX3
F	191	ARG	-	expression tag	UNP Q9WFX3

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
3	G	3	75	22	36	2	15	0	0	0

- Molecule 4 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



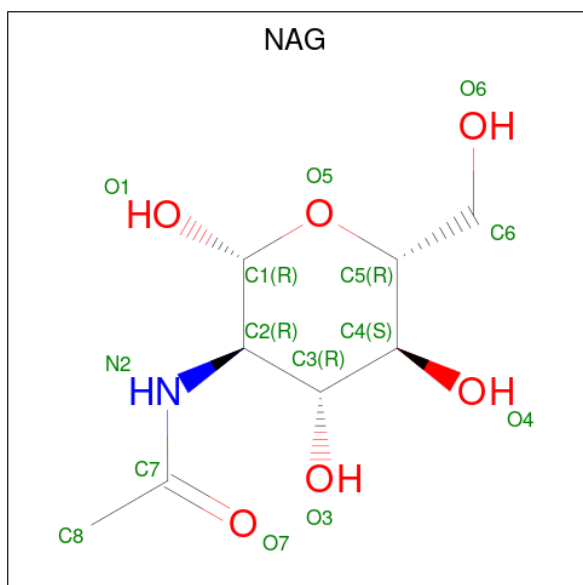
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
4	H	3	87	25	41	2	19	0	0	0
4	I	3	87	25	41	2	19	0	0	0
4	K	3	87	25	41	2	19	0	0	0

- Molecule 5 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	
			Total	C	H	N				O
5	J	2	52	16	25	2	9	0	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	H	N			O
6	A	1	28	8	14	1	5	0	0
6	C	1	28	8	14	1	5	0	0
6	C	1	28	8	14	1	5	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	220	Total	O	0	0
			220	220		
7	B	63	Total	O	0	0
			63	63		

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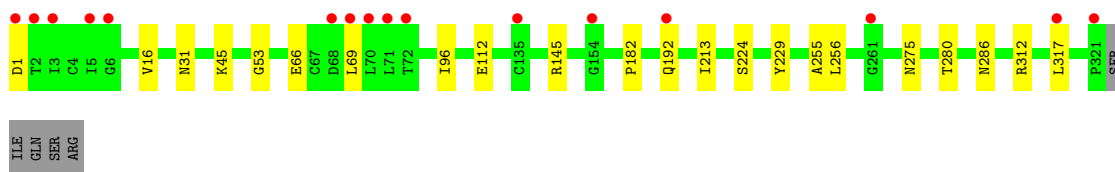
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
7	C	195	Total 195	O 195	0	0
7	D	82	Total 82	O 82	0	0
7	E	257	Total 257	O 257	0	0
7	F	83	Total 83	O 83	0	0

### 3 Residue-property plots [i](#)

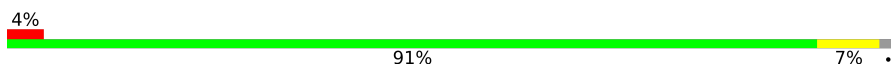
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

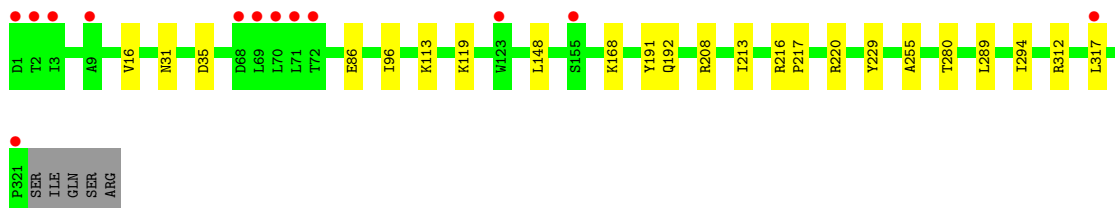
- Molecule 1: Hemagglutinin HA1

Chain A: 




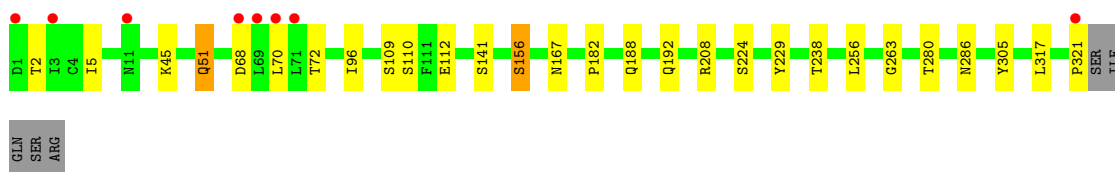
- Molecule 1: Hemagglutinin HA1

Chain C: 




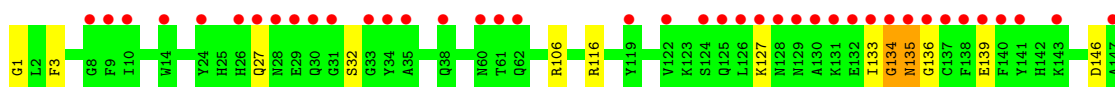
- Molecule 1: Hemagglutinin HA1

Chain E: 



- Molecule 2: Hemagglutinin HA2

Chain B: 





Chain K:  67% 33%

MAG1  
MAG2  
SIA3

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  100%

MAG1  
MAG2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.75Å 80.26Å 121.23Å 90.00° 91.35° 90.00°	Depositor
Resolution (Å)	44.88 – 2.35 44.88 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (44.88-2.35) 99.9 (44.88-2.35)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.45 (at 2.34Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.193 , 0.232 0.199 , 0.235	Depositor DCC
$R_{free}$ test set	3854 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.3	Xtrriage
Anisotropy	0.256	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 48.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.021 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	23671	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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: GAL, NAG, BMA, 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	0.35	0/2545	0.71	0/3469
1	C	0.35	0/2542	0.73	2/3465 (0.1%)
1	E	0.38	0/2556	0.73	1/3484 (0.0%)
2	B	0.35	0/1344	0.73	2/1811 (0.1%)
2	D	0.33	0/1344	0.67	1/1811 (0.1%)
2	F	0.36	0/1344	0.71	1/1811 (0.1%)
All	All	0.36	0/11675	0.71	7/15851 (0.0%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	134	GLY	N-CA-C	-8.76	98.60	110.43
2	F	162	TYR	N-CA-C	5.79	120.04	112.92
1	C	216	ARG	CA-C-N	5.37	125.31	119.78
1	C	216	ARG	C-N-CA	5.37	125.31	119.78
1	E	156	SER	N-CA-C	5.35	117.95	109.50

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	2481	2392	2392	15	0
1	C	2478	2383	2383	15	0
1	E	2492	2418	2418	24	0
2	B	1317	1235	1234	9	0
2	D	1317	1235	1234	8	0
2	F	1317	1234	1234	15	0
3	G	39	36	34	1	0
4	H	46	41	40	0	0
4	I	46	41	40	0	0
4	K	46	41	40	0	0
5	J	27	25	23	0	0
6	A	14	14	13	1	0
6	C	28	28	26	4	0
7	A	220	0	0	10	0
7	B	63	0	0	4	0
7	C	195	0	0	4	0
7	D	82	0	0	5	0
7	E	257	0	0	14	2
7	F	83	0	0	5	1
All	All	12548	11123	11111	83	2

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.

The worst 5 of 83 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:E:286:ASN:ND2	7:E:1101:HOH:O	1.96	0.96
1:A:1:ASP:N	7:A:1101:HOH:O	1.93	0.90
1:A:69:LEU:O	7:A:1102:HOH:O	1.96	0.82
1:E:109:SER:O	7:E:1102:HOH:O	1.98	0.79
2:D:12:GLY:O	7:D:201:HOH:O	2.02	0.77

All (2) 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)
7:E:1333:HOH:O	7:E:1350:HOH:O[2_1059]	1.89	0.31
7:E:1321:HOH:O	7:F:264:HOH:O[2_1049]	1.97	0.23

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	319/326 (98%)	312 (98%)	7 (2%)	0	100	100
1	C	319/326 (98%)	312 (98%)	7 (2%)	0	100	100
1	E	319/326 (98%)	314 (98%)	5 (2%)	0	100	100
2	B	162/191 (85%)	158 (98%)	3 (2%)	1 (1%)	21	24
2	D	162/191 (85%)	159 (98%)	3 (2%)	0	100	100
2	F	162/191 (85%)	159 (98%)	3 (2%)	0	100	100
All	All	1443/1551 (93%)	1414 (98%)	28 (2%)	1 (0%)	48	59

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	135	ASN

### 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	274/283 (97%)	271 (99%)	3 (1%)	65	79
1	C	273/283 (96%)	271 (99%)	2 (1%)	76	86
1	E	278/283 (98%)	275 (99%)	3 (1%)	65	79
2	B	139/162 (86%)	139 (100%)	0	100	100
2	D	139/162 (86%)	137 (99%)	2 (1%)	59	73
2	F	139/162 (86%)	137 (99%)	2 (1%)	59	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1242/1335 (93%)	1230 (99%)	12 (1%)	68 81

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	51	GLN
1	E	280	THR
2	F	164	GLU
1	E	317	LEU
1	C	280	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	246	ASN
2	F	25	HIS
1	C	272	HIS
2	F	62	GLN
2	D	62	GLN

### 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 [i](#)

14 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
3	NAG	G	1	3,1	14,14,15	0.30	0	17,19,21	0.56	0
3	NAG	G	2	3	14,14,15	0.65	1 (7%)	17,19,21	0.40	0
3	BMA	G	3	3	11,11,12	0.74	0	15,15,17	0.79	0
4	NAG	H	1	4	15,15,15	0.40	0	21,21,21	0.51	0
4	GAL	H	2	4	11,11,12	0.87	0	15,15,17	0.98	0
4	SIA	H	3	4	20,20,21	1.24	3 (15%)	21,28,31	1.73	3 (14%)
4	NAG	I	1	4	15,15,15	0.18	0	21,21,21	0.19	0
4	GAL	I	2	4	11,11,12	0.38	0	15,15,17	0.93	0
4	SIA	I	3	4	20,20,21	1.22	3 (15%)	21,28,31	1.76	4 (19%)
5	NAG	J	1	5,1	14,14,15	0.33	0	17,19,21	0.56	0
5	NAG	J	2	5	13,13,15	0.51	0	15,17,21	0.54	0
4	NAG	K	1	4	15,15,15	0.12	0	21,21,21	0.26	0
4	GAL	K	2	4	11,11,12	0.35	0	15,15,17	0.93	0
4	SIA	K	3	4	20,20,21	1.23	3 (15%)	21,28,31	1.75	4 (19%)

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
3	NAG	G	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	BMA	G	3	3	-	2/2/19/22	0/1/1/1
4	NAG	H	1	4	-	0/6/26/26	0/1/1/1
4	GAL	H	2	4	-	0/2/19/22	0/1/1/1
4	SIA	H	3	4	-	0/18/34/38	0/1/1/1
4	NAG	I	1	4	-	0/6/26/26	0/1/1/1
4	GAL	I	2	4	-	0/2/19/22	0/1/1/1
4	SIA	I	3	4	-	2/18/34/38	0/1/1/1
5	NAG	J	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	J	2	5	-	2/6/19/26	0/1/1/1
4	NAG	K	1	4	-	1/6/26/26	0/1/1/1
4	GAL	K	2	4	-	1/2/19/22	0/1/1/1
4	SIA	K	3	4	-	2/18/34/38	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	3	SIA	C4-C5	-2.56	1.50	1.53

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	3	SIA	C10-N5	2.53	1.42	1.34
4	I	3	SIA	C4-C5	-2.52	1.51	1.53
4	K	3	SIA	C10-N5	2.50	1.42	1.34
4	H	3	SIA	C10-N5	2.45	1.42	1.34

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	3	SIA	O6-C2-C3	-4.92	103.94	110.56
4	H	3	SIA	O6-C2-C3	-4.60	104.37	110.56
4	I	3	SIA	O6-C2-C3	-4.33	104.73	110.56
4	I	3	SIA	O6-C2-C1	4.08	115.41	107.72
4	H	3	SIA	O6-C2-C1	3.97	115.21	107.72

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

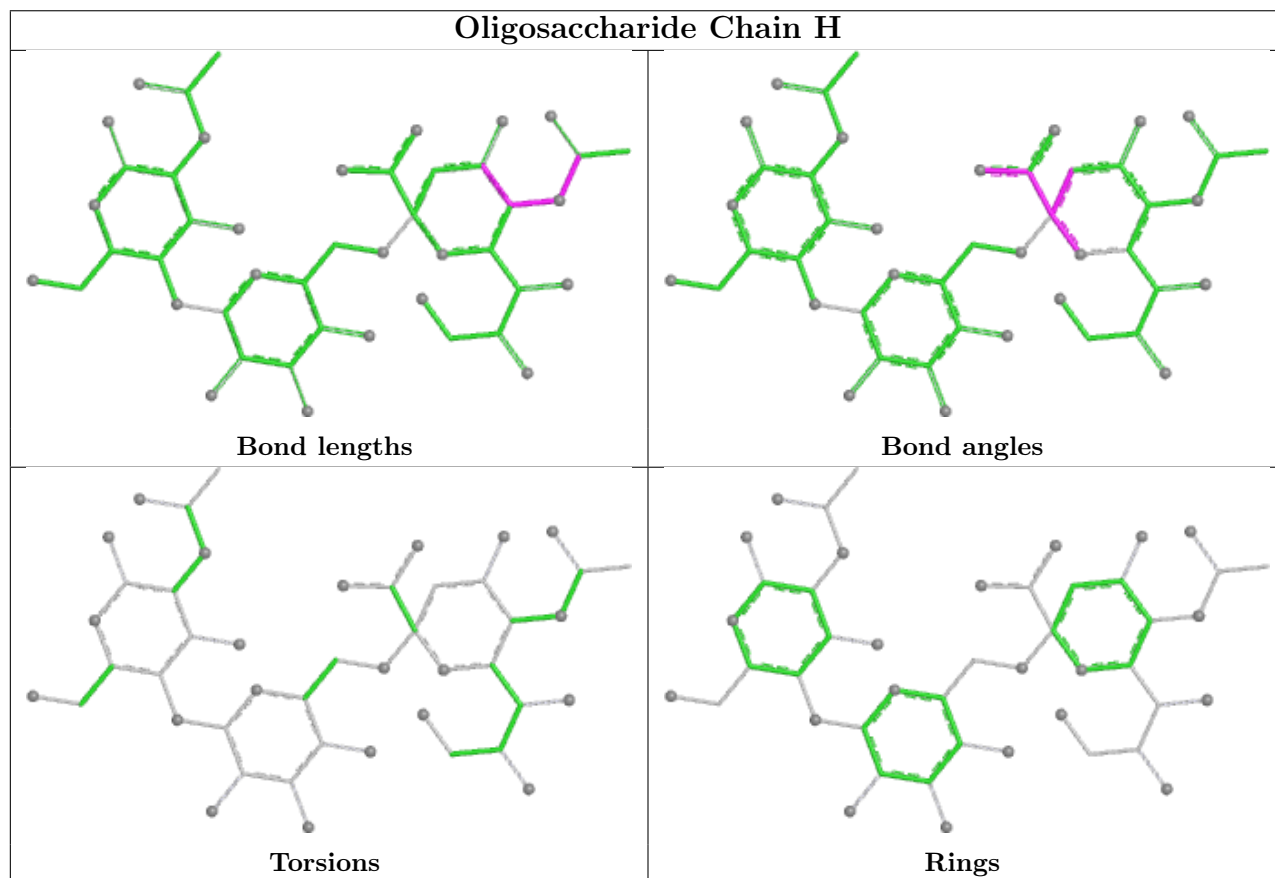
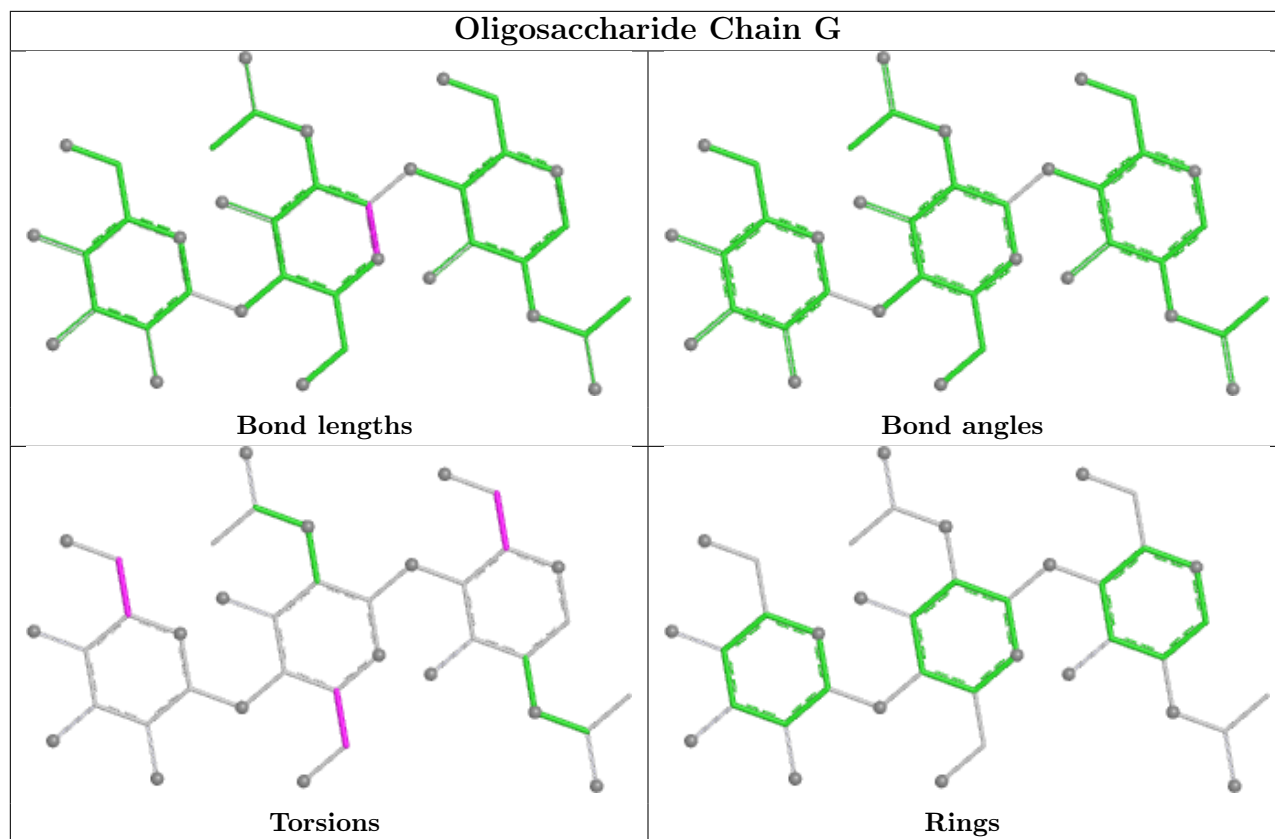
Mol	Chain	Res	Type	Atoms
4	K	3	SIA	C7-C8-C9-O9
4	K	3	SIA	O8-C8-C9-O9
5	J	2	NAG	O5-C5-C6-O6
4	I	3	SIA	O8-C8-C9-O9
5	J	1	NAG	C4-C5-C6-O6

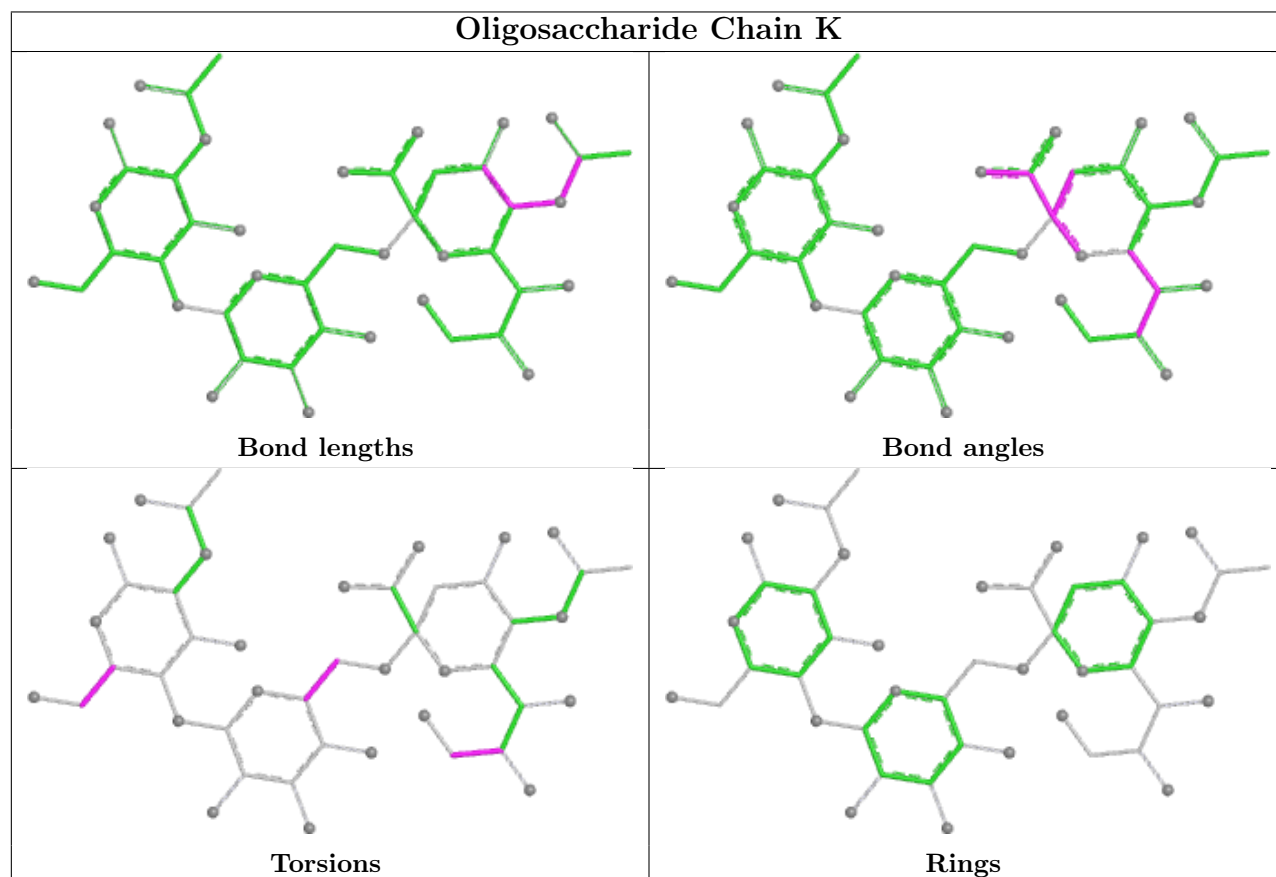
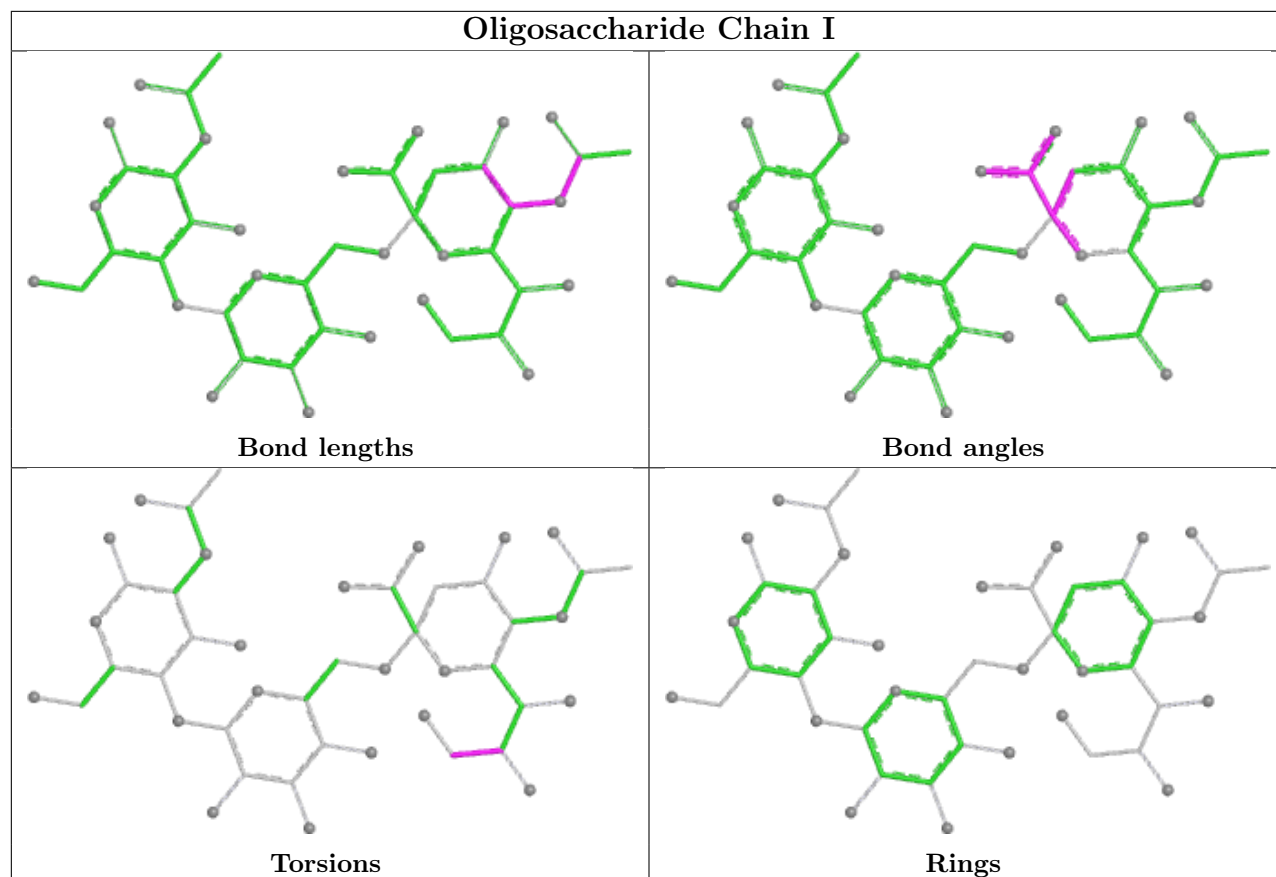
There are no ring outliers.

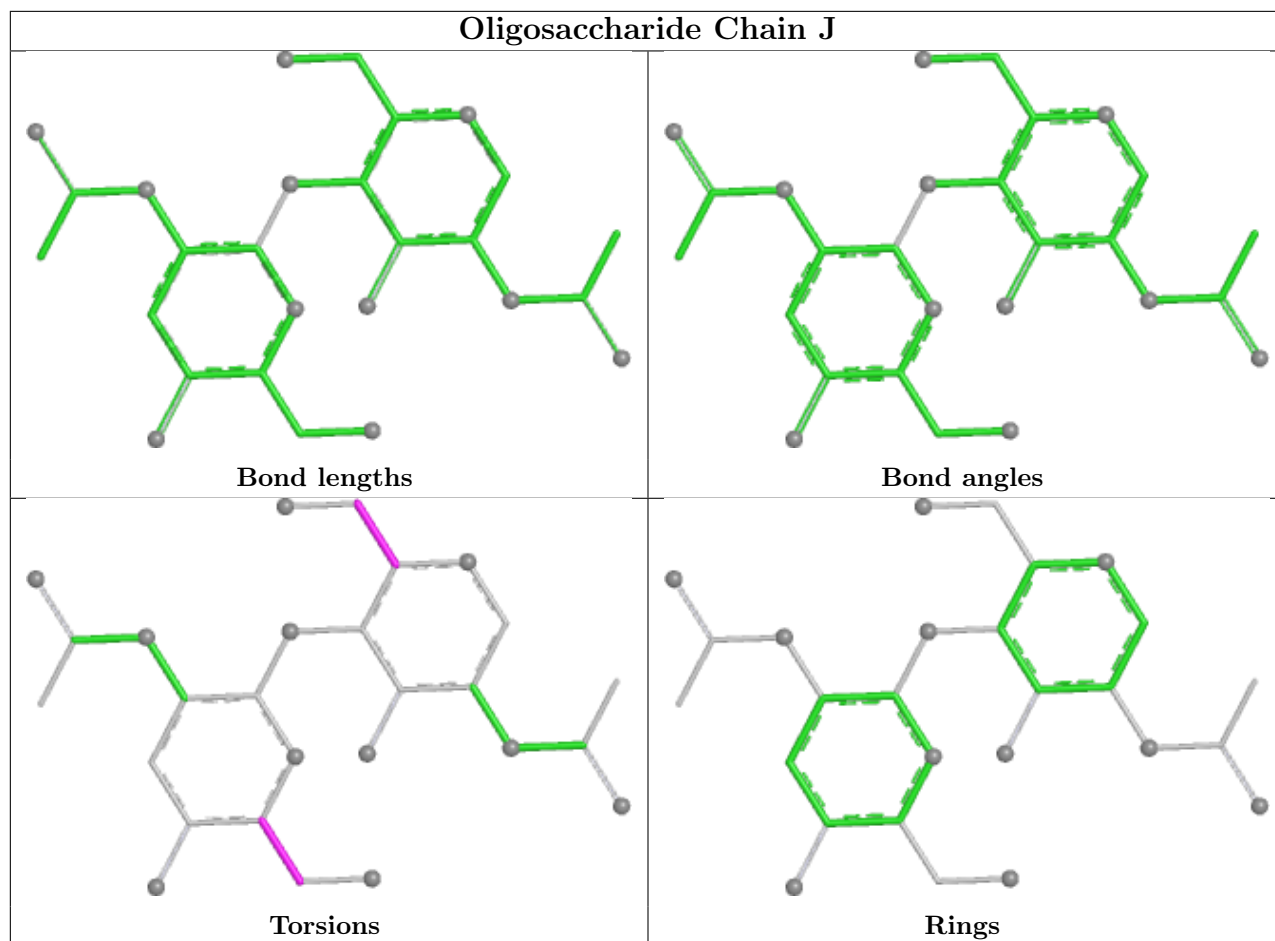
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	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](#)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
6	NAG	C	1002	1	14,14,15	0.61	0	17,19,21	0.83	1 (5%)
6	NAG	C	1001	1	14,14,15	1.00	1 (7%)	17,19,21	0.65	0
6	NAG	A	1004	1	14,14,15	0.72	1 (7%)	17,19,21	0.76	1 (5%)

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	NAG	C	1002	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1001	1	-	3/6/23/26	0/1/1/1
6	NAG	A	1004	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1001	NAG	O5-C1	-3.65	1.37	1.43
6	A	1004	NAG	O5-C1	2.07	1.47	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1002	NAG	C1-O5-C5	3.07	116.31	112.19
6	A	1004	NAG	C1-O5-C5	2.75	115.88	112.19

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	1002	NAG	C4-C5-C6-O6
6	C	1002	NAG	O5-C5-C6-O6
6	C	1001	NAG	O5-C5-C6-O6
6	C	1001	NAG	C1-C2-N2-C7
6	C	1001	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1002	NAG	1	0
6	C	1001	NAG	3	0
6	A	1004	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	321/326 (98%)	0.02	16 (4%) 34 40	14, 28, 56, 104	0
1	C	321/326 (98%)	0.13	13 (4%) 42 48	19, 32, 56, 94	0
1	E	321/326 (98%)	-0.16	8 (2%) 58 64	13, 24, 51, 82	0
2	B	164/191 (85%)	1.21	53 (32%) 1 0	15, 54, 99, 118	0
2	D	164/191 (85%)	1.55	66 (40%) 0 0	16, 59, 106, 118	0
2	F	164/191 (85%)	1.34	59 (35%) 1 0	14, 51, 91, 105	0
All	All	1455/1551 (93%)	0.46	215 (14%) 5 6	13, 33, 91, 118	0

The worst 5 of 215 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	164	GLU	7.2
2	F	164	GLU	7.0
2	F	163	SER	6.7
2	F	134	GLY	6.6
1	A	69	LEU	6.1

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

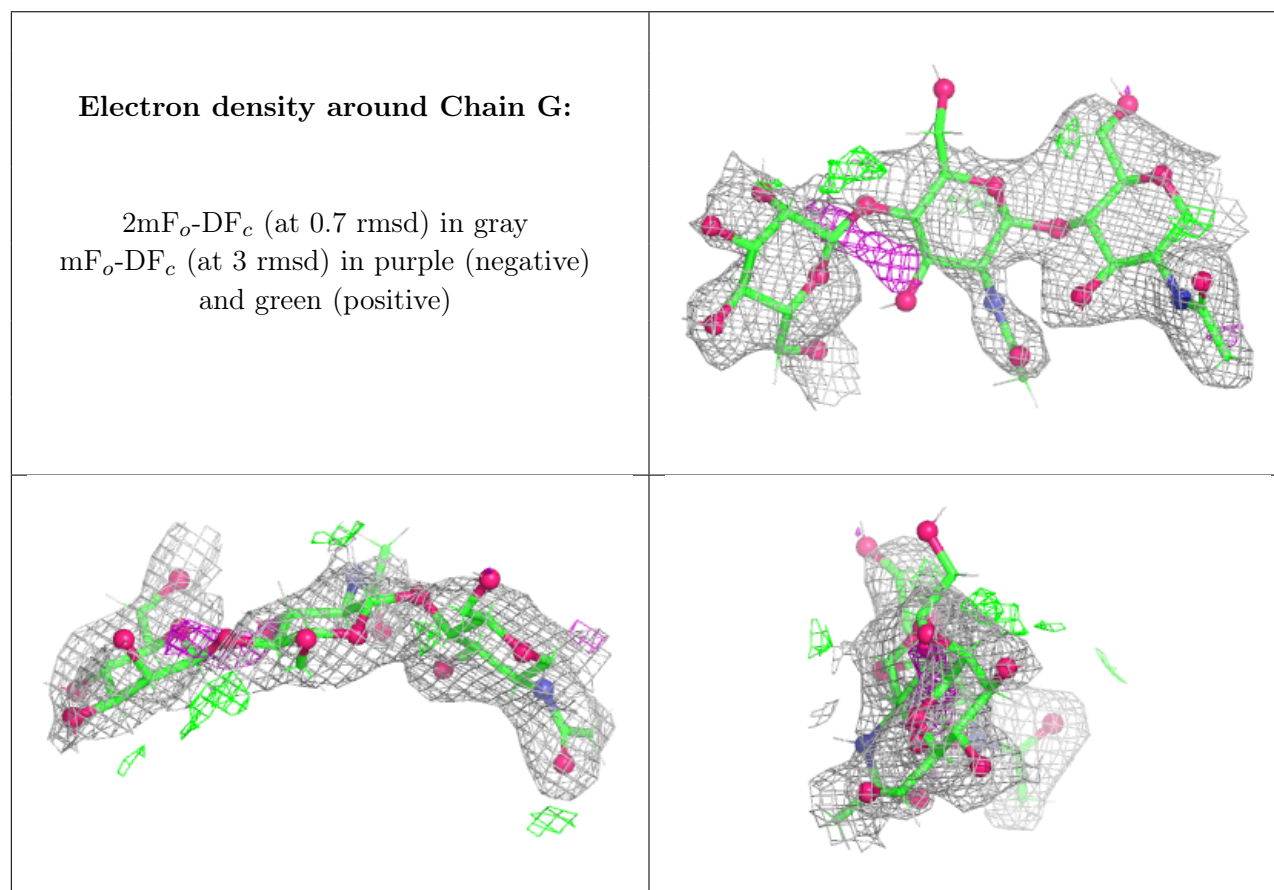
There are no non-standard protein/DNA/RNA residues in this entry.

### 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.

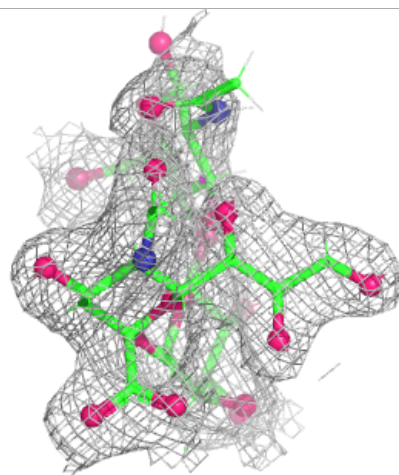
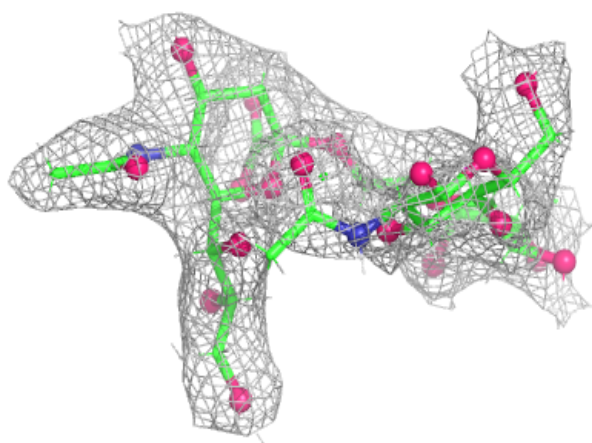
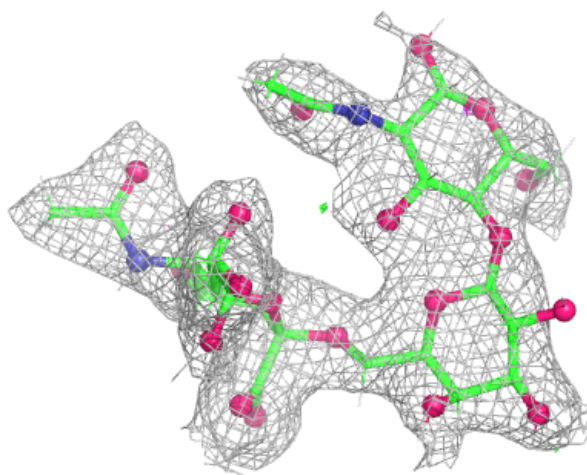
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	BMA	G	3	11/12	0.58	0.16	62,72,82,86	0
3	NAG	G	2	14/15	0.64	0.19	58,71,85,86	0
4	NAG	H	1	15/15	0.70	0.17	53,64,74,77	0
5	NAG	J	2	13/15	0.73	0.21	49,61,73,74	0
4	NAG	I	1	15/15	0.74	0.15	49,59,68,71	0
4	NAG	K	1	15/15	0.83	0.12	38,48,58,70	0
4	GAL	H	2	11/12	0.86	0.12	34,45,60,76	0
4	GAL	K	2	11/12	0.90	0.10	26,37,50,60	0
5	NAG	J	1	14/15	0.90	0.10	24,38,51,51	0
3	NAG	G	1	14/15	0.90	0.11	28,38,57,71	0
4	SIA	I	3	20/21	0.91	0.08	29,35,43,52	0
4	GAL	I	2	11/12	0.94	0.07	32,40,51,61	0
4	SIA	H	3	20/21	0.94	0.07	25,31,43,50	0
4	SIA	K	3	20/21	0.95	0.06	14,21,28,32	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.



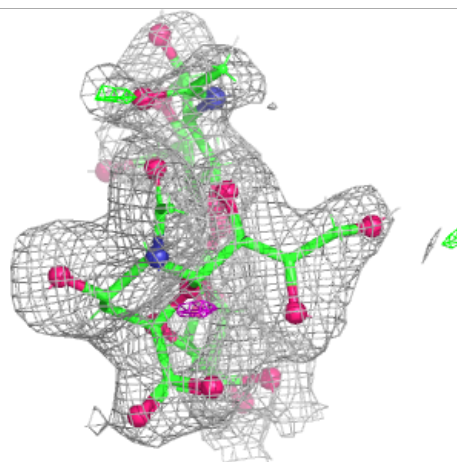
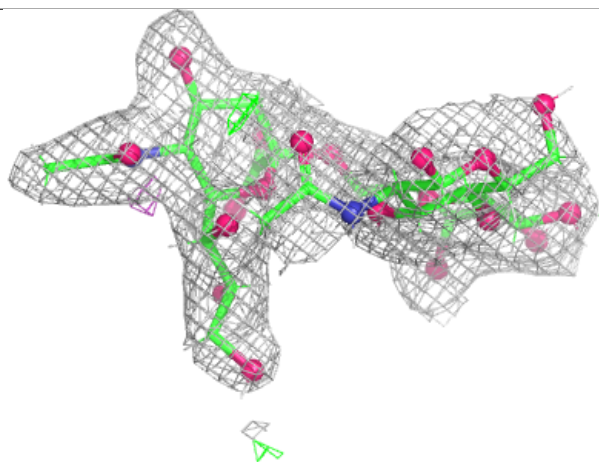
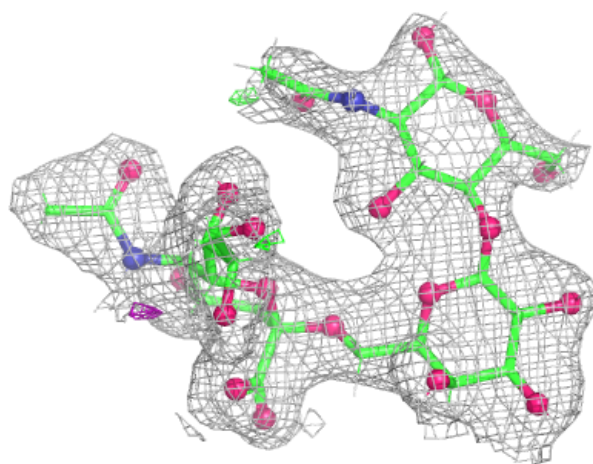
**Electron density around Chain H:**

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



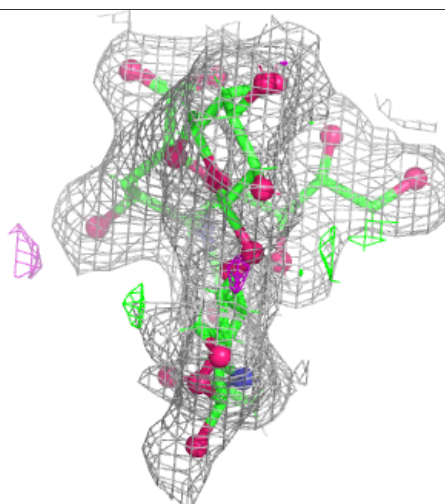
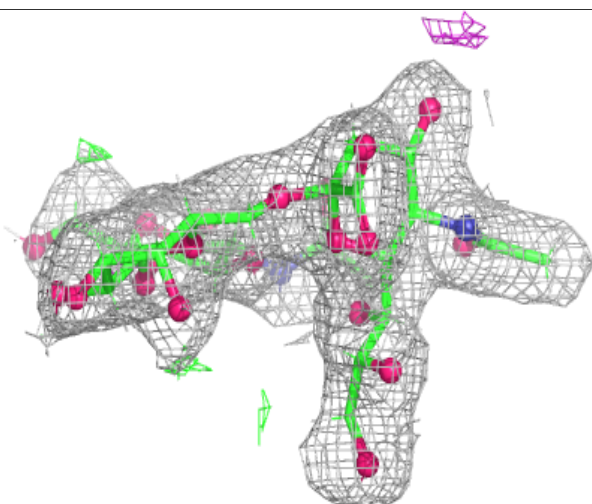
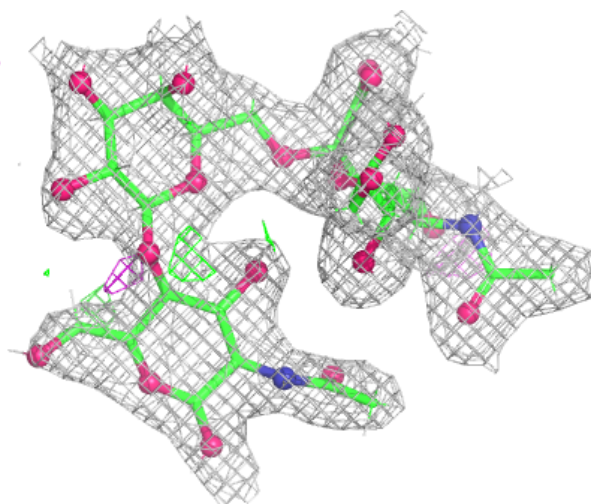
**Electron density around Chain I:**

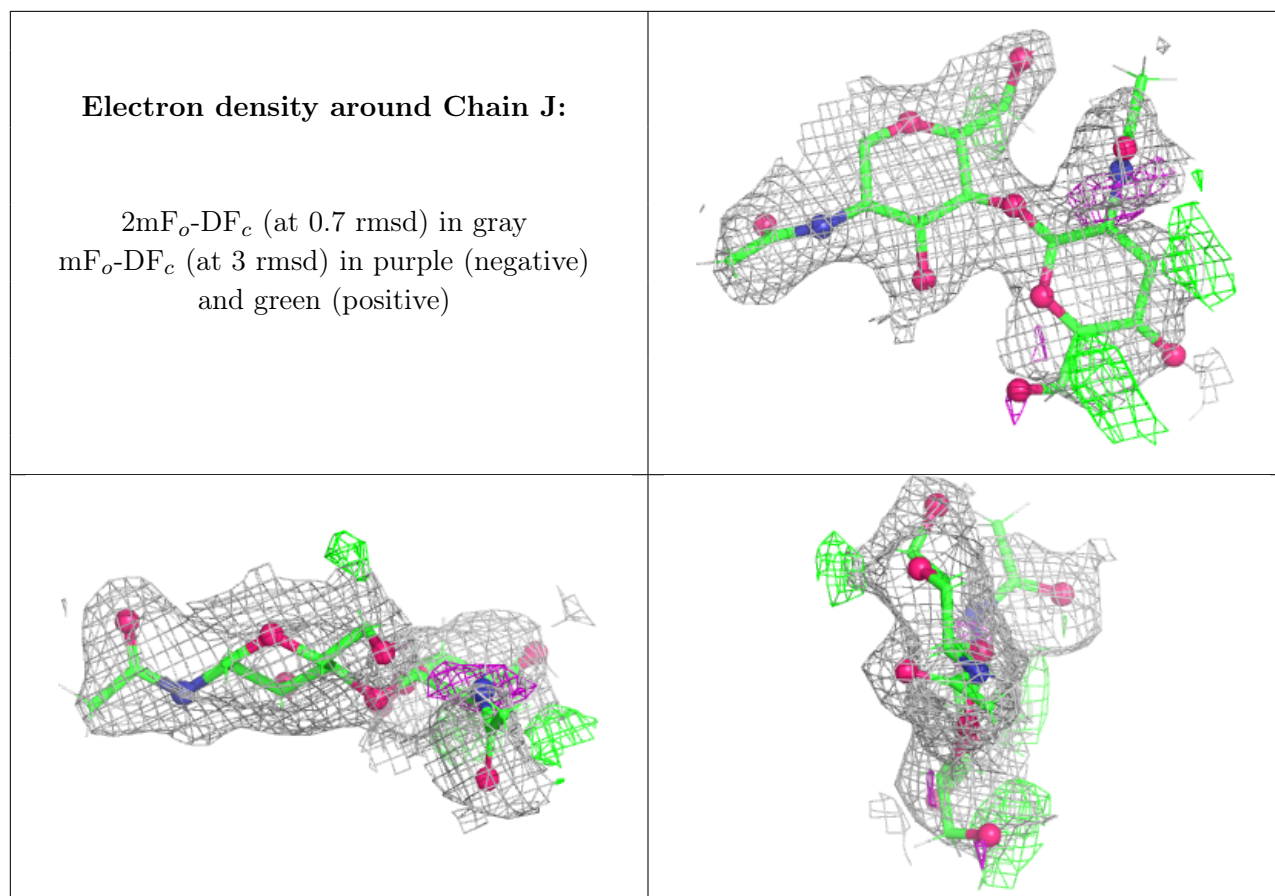
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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)





## 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
6	NAG	A	1004	14/15	0.34	0.20	59,71,85,87	0
6	NAG	C	1002	14/15	0.72	0.17	46,58,70,80	0
6	NAG	C	1001	14/15	0.76	0.18	39,52,65,65	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.