



wwPDB X-ray Structure Validation Summary Report ⓘ

May 7, 2025 – 12:28 AM JST

PDB ID : 8X27 / pdb_00008x27
Title : Crystal structure of H5 hemagglutinin from human-infecting H5N8 influenza virus in complex with LSTc
Authors : Jin, X.Y.; Han, P.; Song, H.; Qi, J.X.
Deposited on : 2023-11-09
Resolution : 3.04 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 Phenix2.0rc1
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

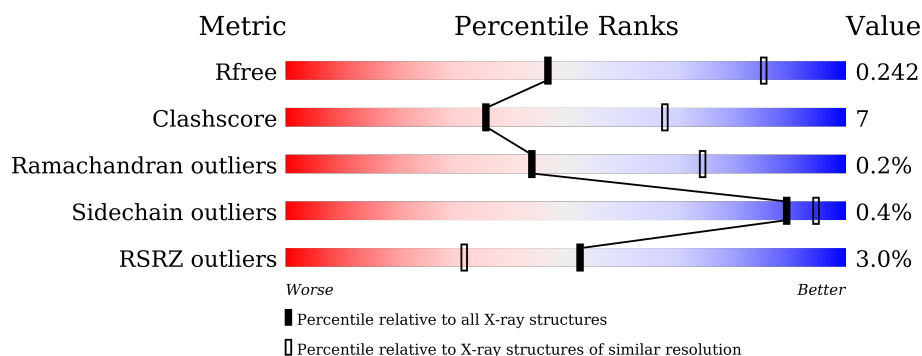
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.04 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.








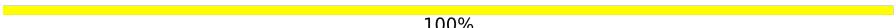
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	3418 (3.08-3.00)
Clashscore	180529	3811 (3.08-3.00)
Ramachandran outliers	177936	3656 (3.08-3.00)
Sidechain outliers	177891	3658 (3.08-3.00)
RSRZ outliers	164620	3430 (3.08-3.00)

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	506	<div> <div>3%</div> <div>81%14%</div> <div>.</div> </div>
1	B	506	<div> <div>4%</div> <div>78%18%</div> <div>.</div> </div>
1	C	506	<div> <div>2%</div> <div>81%14%</div> <div>..</div> </div>
1	D	506	<div> <div>%</div> <div>81%15%</div> <div>.</div> </div>
1	E	506	<div> <div>2%</div> <div>75%21%</div> <div>.</div> </div>
1	F	506	<div> <div>6%</div> <div>75%20%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
2	G	3	 67% 33%
2	J	3	 33% 67%
3	H	4	 50% 25% 25%
3	I	4	 50% 25% 25%
4	K	4	 50% 50%
5	L	2	 100%

2 Entry composition [i](#)

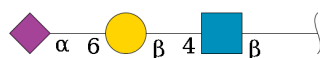
There are 6 unique types of molecules in this entry. The entry contains 23757 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	484	Total	C	N	O	S	0	0	0
			3879	2439	675	743	22			
1	C	484	Total	C	N	O	S	0	0	0
			3878	2438	675	743	22			
1	D	485	Total	C	N	O	S	0	0	0
			3885	2443	676	744	22			
1	B	485	Total	C	N	O	S	0	0	0
			3883	2441	676	744	22			
1	E	485	Total	C	N	O	S	0	0	0
			3882	2440	676	744	22			
1	F	486	Total	C	N	O	S	0	0	0
			3891	2447	677	745	22			

- Molecule 2 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
2	G	3	Total	C	N	O	0	0	0
			46	25	2	19			
2	J	3	Total	C	N	O	0	0	0
			46	25	2	19			

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose.



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

- Molecule 4 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose.



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

- 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
5	L	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

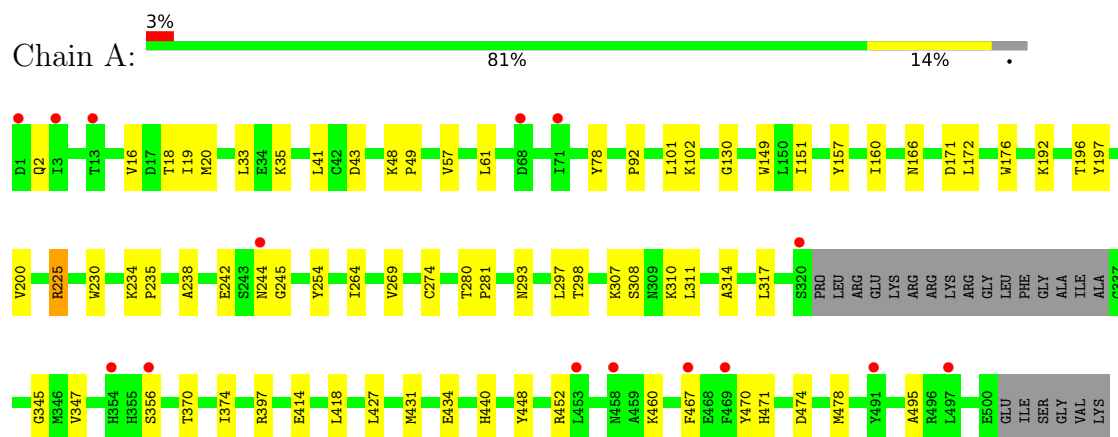


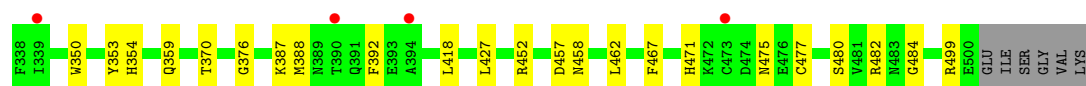
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	E	1	Total	C	N	O	0	0
			14	8	1	5		
6	E	1	Total	C	N	O	0	0
			14	8	1	5		
6	F	1	Total	C	N	O	0	0
			14	8	1	5		

3 Residue-property plots [i](#)

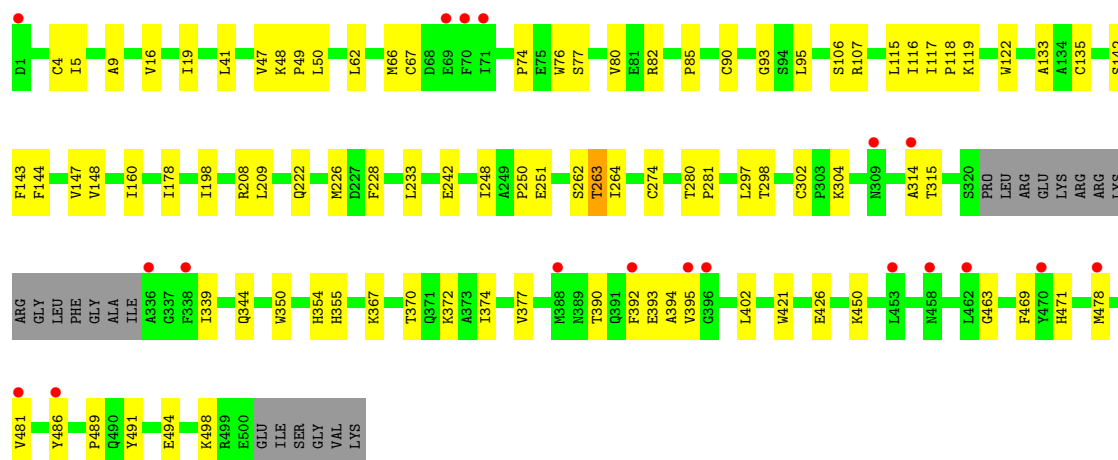
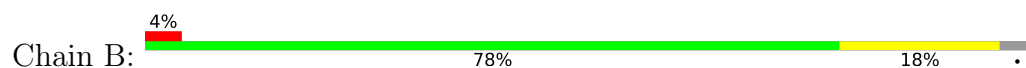
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

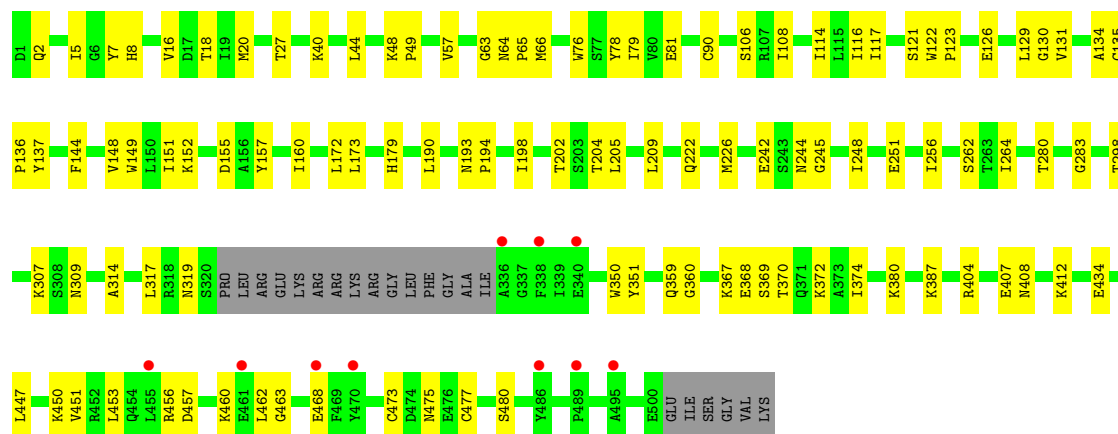
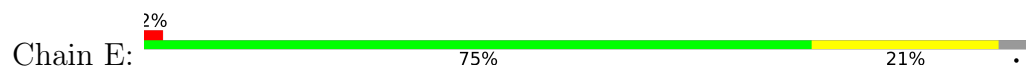




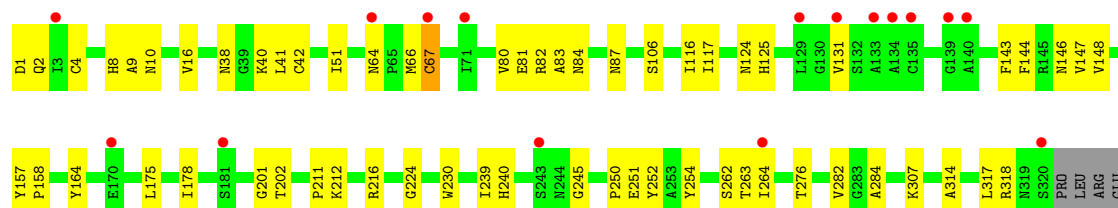
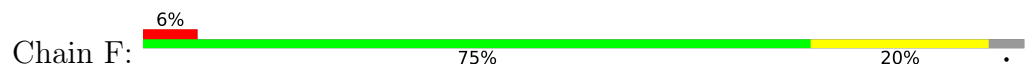
• Molecule 1: Hemagglutinin

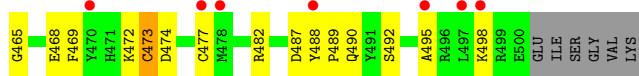


• Molecule 1: Hemagglutinin



• Molecule 1: Hemagglutinin





- NAG1
GAL2
SIA3

- | | |
|------|--|
| NAG1 | |
| GAL2 | |
| SIA3 | |

- GAL1
NAG2
GAL3
SIA4

- | | | | |
|------|------|------|------|
| GAL1 | NAG2 | GAL3 | SIA4 |
|------|------|------|------|

- | | | | |
|------|------|------|------|
| GAL1 | NAG2 | GAL3 | SIA4 |
|------|------|------|------|

- Chain L: 100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.83Å 263.93Å 131.20Å 90.00° 101.08° 90.00°	Depositor
Resolution (Å)	31.72 – 3.04 31.72 – 3.04	Depositor EDS
% Data completeness (in resolution range)	96.0 (31.72-3.04) 90.5 (31.72-3.04)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 3.06Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.211 , 0.242 0.211 , 0.242	Depositor DCC
R_{free} test set	87267 reflections (2.21%)	wwPDB-VP
Wilson B-factor (Å ²)	61.2	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 71.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	23757	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GAL, SIA, NAG

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	0.46	0/3968	0.68	0/5374
1	B	0.39	0/3972	0.55	0/5379
1	C	0.52	0/3967	0.74	3/5372 (0.1%)
1	D	0.47	0/3975	0.65	0/5384
1	E	0.43	0/3971	0.65	1/5377 (0.0%)
1	F	0.35	0/3980	0.52	0/5390
All	All	0.44	0/23833	0.64	4/32276 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	222	GLN	OE1-CD-NE2	8.17	130.77	122.60
1	C	88	ASP	N-CA-C	-5.67	100.69	109.14
1	C	62	LEU	CA-C-N	-5.61	110.41	121.41
1	C	62	LEU	C-N-CA	-5.61	110.41	121.41

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	225	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3879	0	3736	45	0
1	B	3883	0	3740	60	0
1	C	3878	0	3732	46	0
1	D	3885	0	3741	51	0
1	E	3882	0	3735	76	0
1	F	3891	0	3749	67	0
2	G	46	0	40	2	0
2	J	46	0	40	4	0
3	H	57	0	49	1	0
3	I	57	0	49	4	0
4	K	57	0	49	2	0
5	L	28	0	25	0	0
6	A	42	0	39	1	0
6	C	42	0	39	0	0
6	D	42	0	39	0	0
6	E	28	0	26	0	0
6	F	14	0	13	0	0
All	All	23757	0	22841	336	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 336 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:487:ASP:HB2	1:C:490:GLN:HG2	1.57	0.86
1:C:173:LEU:HB2	1:C:256:ILE:HD11	1.58	0.85
1:E:179:HIS:HB2	1:E:226:MET:HE2	1.62	0.80
1:F:81:GLU:HB2	1:F:264:ILE:HD11	1.65	0.79
1:F:124:ASN:HB2	1:F:158:PRO:HG3	1.64	0.79

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	480/506 (95%)	454 (95%)	26 (5%)	0	100	100
1	B	481/506 (95%)	450 (94%)	28 (6%)	3 (1%)	22	54
1	C	480/506 (95%)	465 (97%)	13 (3%)	2 (0%)	30	62
1	D	481/506 (95%)	460 (96%)	20 (4%)	1 (0%)	44	74
1	E	481/506 (95%)	456 (95%)	24 (5%)	1 (0%)	44	74
1	F	482/506 (95%)	453 (94%)	29 (6%)	0	100	100
All	All	2885/3036 (95%)	2738 (95%)	140 (5%)	7 (0%)	44	74

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	89	LEU
1	C	262	SER
1	B	263	THR
1	B	489	PRO
1	D	136	PRO

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	428/445 (96%)	427 (100%)	1 (0%)	92	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	428/445 (96%)	426 (100%)	2 (0%)	86	93
1	C	428/445 (96%)	426 (100%)	2 (0%)	86	93
1	D	429/445 (96%)	429 (100%)	0	100	100
1	E	426/445 (96%)	425 (100%)	1 (0%)	92	96
1	F	429/445 (96%)	426 (99%)	3 (1%)	81	90
All	All	2568/2670 (96%)	2559 (100%)	9 (0%)	89	94

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	282	VAL
1	F	473	CYS
1	B	67	CYS
1	B	274	CYS
1	E	473	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	354	HIS
1	F	45	ASN
1	B	443	ASN
1	E	240	HIS
1	F	218	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

20 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	G	1	2	15,15,15	2.02	6 (40%)	21,21,21	2.59	12 (57%)
2	GAL	G	2	2	11,11,12	1.40	2 (18%)	15,15,17	1.39	2 (13%)
2	SIA	G	3	2	20,20,21	1.88	8 (40%)	24,28,31	2.31	9 (37%)
3	GAL	H	1	3	12,12,12	0.14	0	17,17,17	0.19	0
3	NAG	H	2	3	14,14,15	0.41	0	17,19,21	0.39	0
3	GAL	H	3	3	11,11,12	0.77	0	15,15,17	1.12	1 (6%)
3	SIA	H	4	3	20,20,21	1.93	2 (10%)	24,28,31	1.85	6 (25%)
3	GAL	I	1	3	12,12,12	0.14	0	17,17,17	0.19	0
3	NAG	I	2	3	14,14,15	0.40	0	17,19,21	0.39	0
3	GAL	I	3	3	11,11,12	0.76	0	15,15,17	1.12	1 (6%)
3	SIA	I	4	3	20,20,21	1.94	2 (10%)	24,28,31	1.85	6 (25%)
2	NAG	J	1	2	15,15,15	2.27	7 (46%)	21,21,21	2.31	8 (38%)
2	GAL	J	2	2	11,11,12	1.95	3 (27%)	15,15,17	2.08	4 (26%)
2	SIA	J	3	2	20,20,21	2.45	7 (35%)	24,28,31	2.63	9 (37%)
4	GAL	K	1	4	12,12,12	1.94	4 (33%)	17,17,17	1.51	4 (23%)
4	NAG	K	2	4	14,14,15	2.40	5 (35%)	17,19,21	1.92	5 (29%)
4	GAL	K	3	4	11,11,12	2.41	3 (27%)	15,15,17	2.09	6 (40%)
4	SIA	K	4	4	20,20,21	1.86	3 (15%)	24,28,31	2.76	10 (41%)
5	NAG	L	1	1,5	14,14,15	1.95	2 (14%)	17,19,21	1.59	3 (17%)
5	NAG	L	2	5	14,14,15	2.29	5 (35%)	17,19,21	1.45	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	G	1	2	-	0/6/26/26	0/1/1/1
2	GAL	G	2	2	-	0/2/19/22	0/1/1/1
2	SIA	G	3	2	-	2/18/34/38	0/1/1/1
3	GAL	H	1	3	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	GAL	H	3	3	-	0/2/19/22	0/1/1/1
3	SIA	H	4	3	-	3/18/34/38	0/1/1/1
3	GAL	I	1	3	-	0/2/22/22	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
3	GAL	I	3	3	-	0/2/19/22	0/1/1/1
3	SIA	I	4	3	-	3/18/34/38	0/1/1/1
2	NAG	J	1	2	-	0/6/26/26	0/1/1/1
2	GAL	J	2	2	-	0/2/19/22	0/1/1/1
2	SIA	J	3	2	-	4/18/34/38	0/1/1/1
4	GAL	K	1	4	-	1/2/22/22	0/1/1/1
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1
4	GAL	K	3	4	-	2/2/19/22	0/1/1/1
4	SIA	K	4	4	-	4/18/34/38	0/1/1/1
5	NAG	L	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	L	2	5	-	2/6/23/26	0/1/1/1

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	4	SIA	C2-C1	7.34	1.58	1.52
3	H	4	SIA	C2-C1	7.29	1.58	1.52
2	J	3	SIA	C2-C1	6.77	1.58	1.52
4	K	2	NAG	O5-C1	6.63	1.54	1.43
4	K	4	SIA	O6-C2	6.31	1.52	1.43

The worst 5 of 88 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	3	SIA	C4-C3-C2	6.43	121.34	109.81
2	J	3	SIA	C6-C5-N5	-6.25	100.53	110.91
2	J	2	GAL	C1-O5-C5	-6.06	103.97	112.19
4	K	4	SIA	O9-C9-C8	-6.05	97.89	111.07
4	K	4	SIA	O6-C2-C1	6.01	119.49	107.70

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

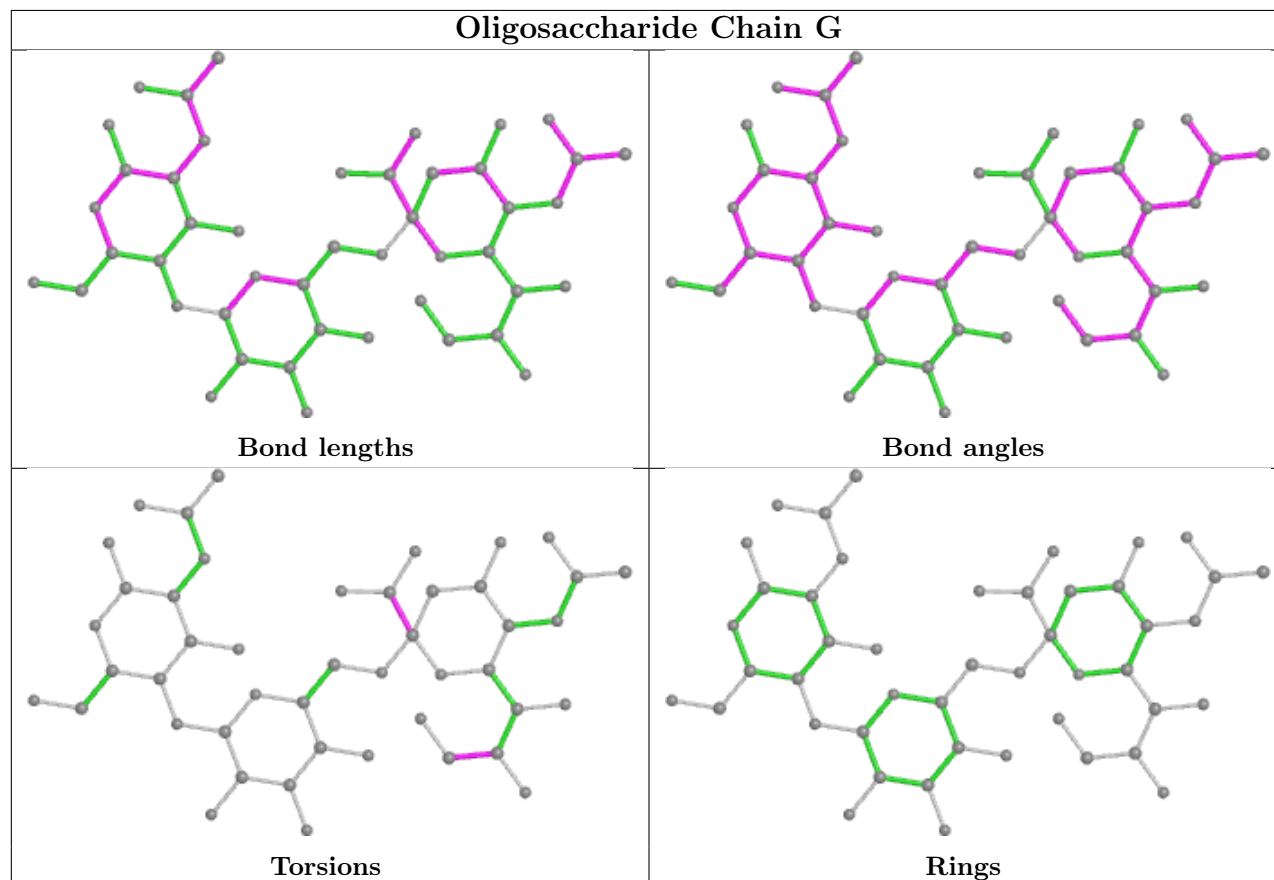
Mol	Chain	Res	Type	Atoms
4	K	4	SIA	C6-C7-C8-C9
4	K	4	SIA	O7-C7-C8-C9
4	K	4	SIA	O7-C7-C8-O8
4	K	3	GAL	O5-C5-C6-O6
4	K	3	GAL	C4-C5-C6-O6

There are no ring outliers.

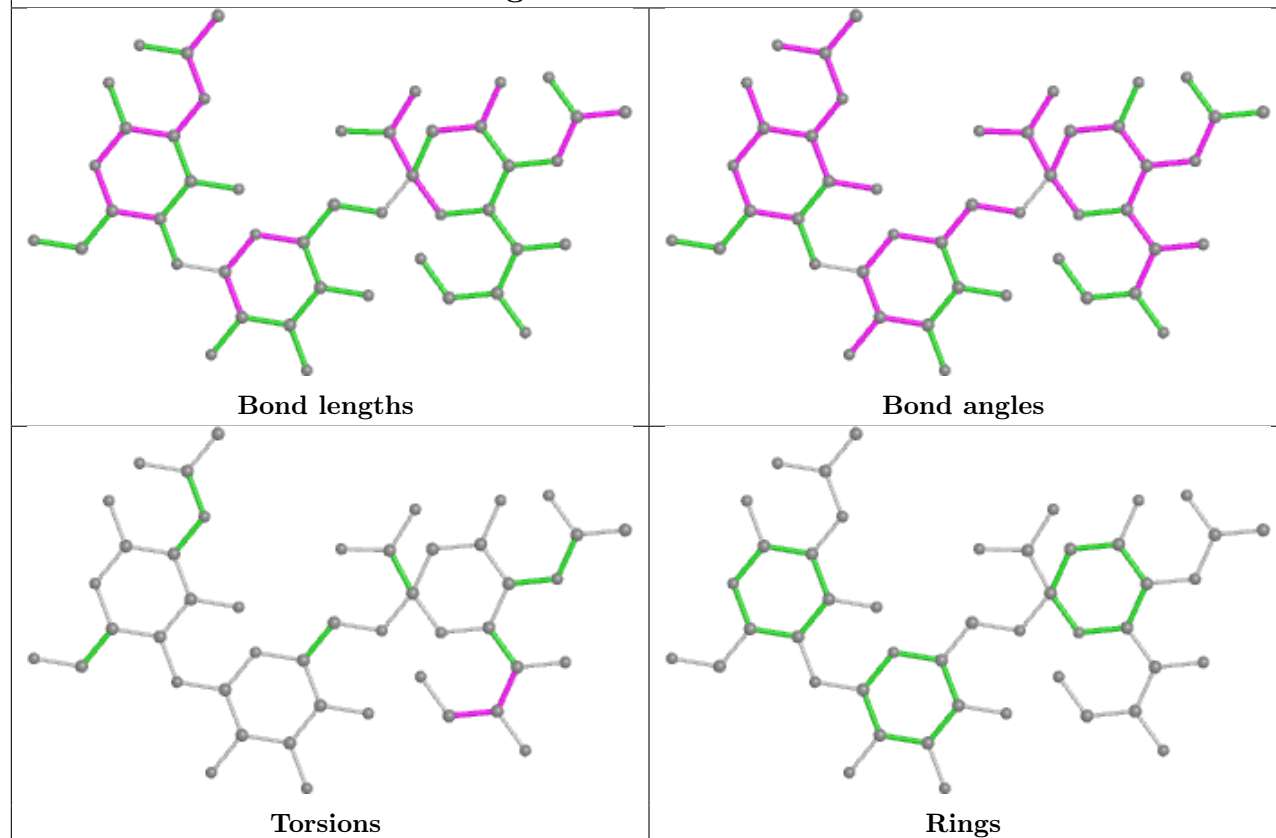
7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	4	SIA	2	0
3	H	4	SIA	1	0
3	I	4	SIA	4	0
4	K	2	NAG	1	0
2	J	2	GAL	2	0
2	J	3	SIA	2	0
2	G	3	SIA	2	0

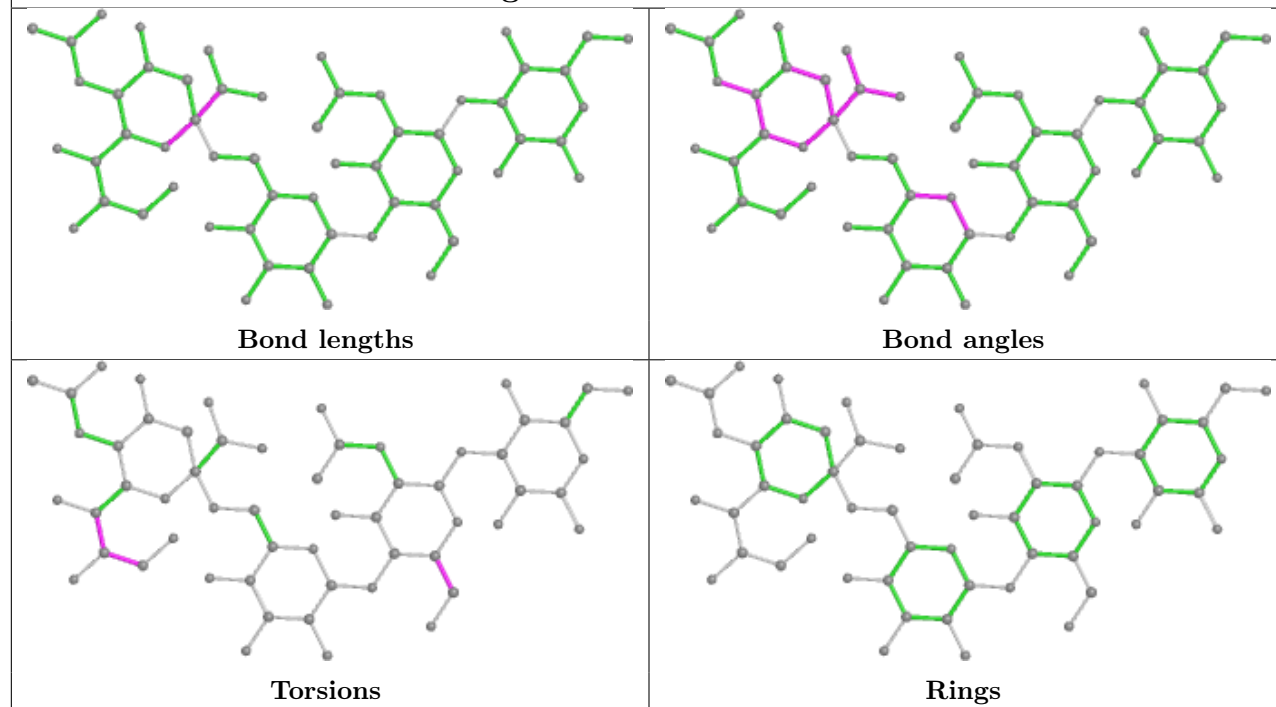
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



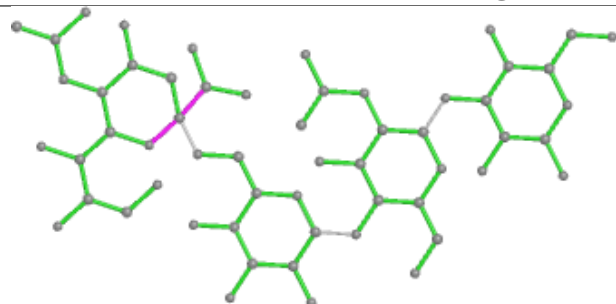
Oligosaccharide Chain J



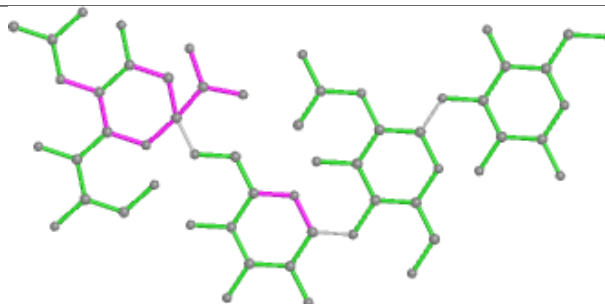
Oligosaccharide Chain H



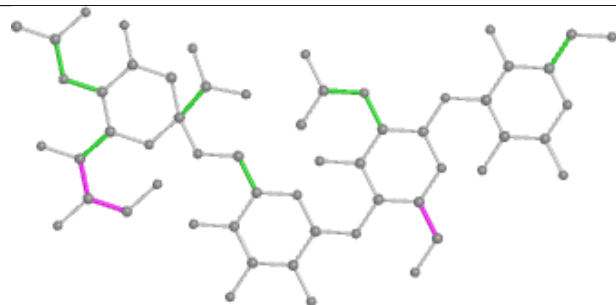
Oligosaccharide Chain I



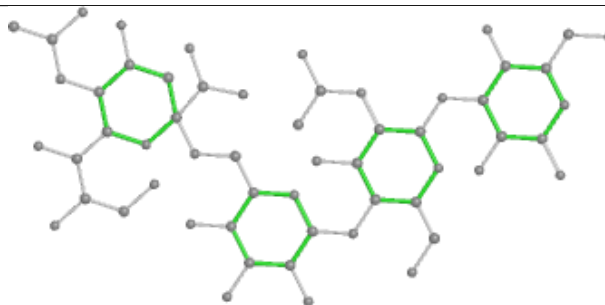
Bond lengths



Bond angles

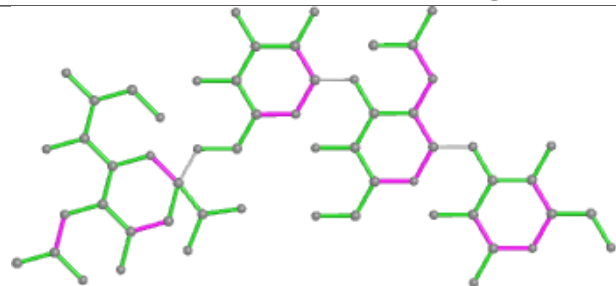


Torsions

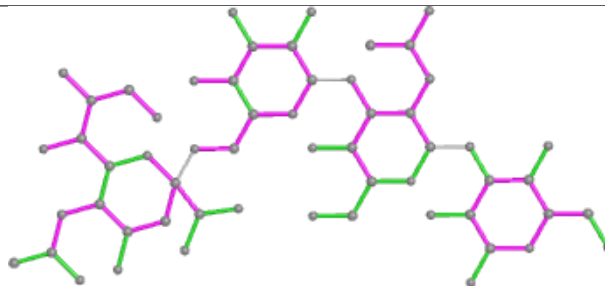


Rings

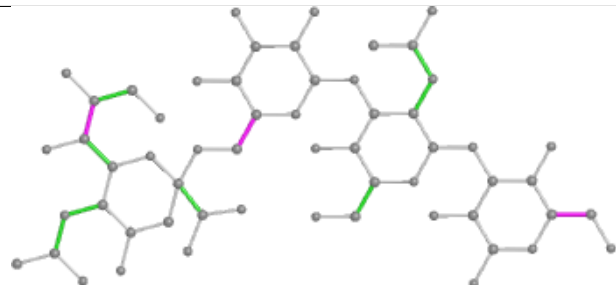
Oligosaccharide Chain K



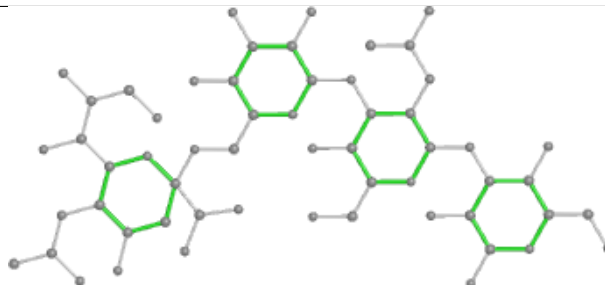
Bond lengths



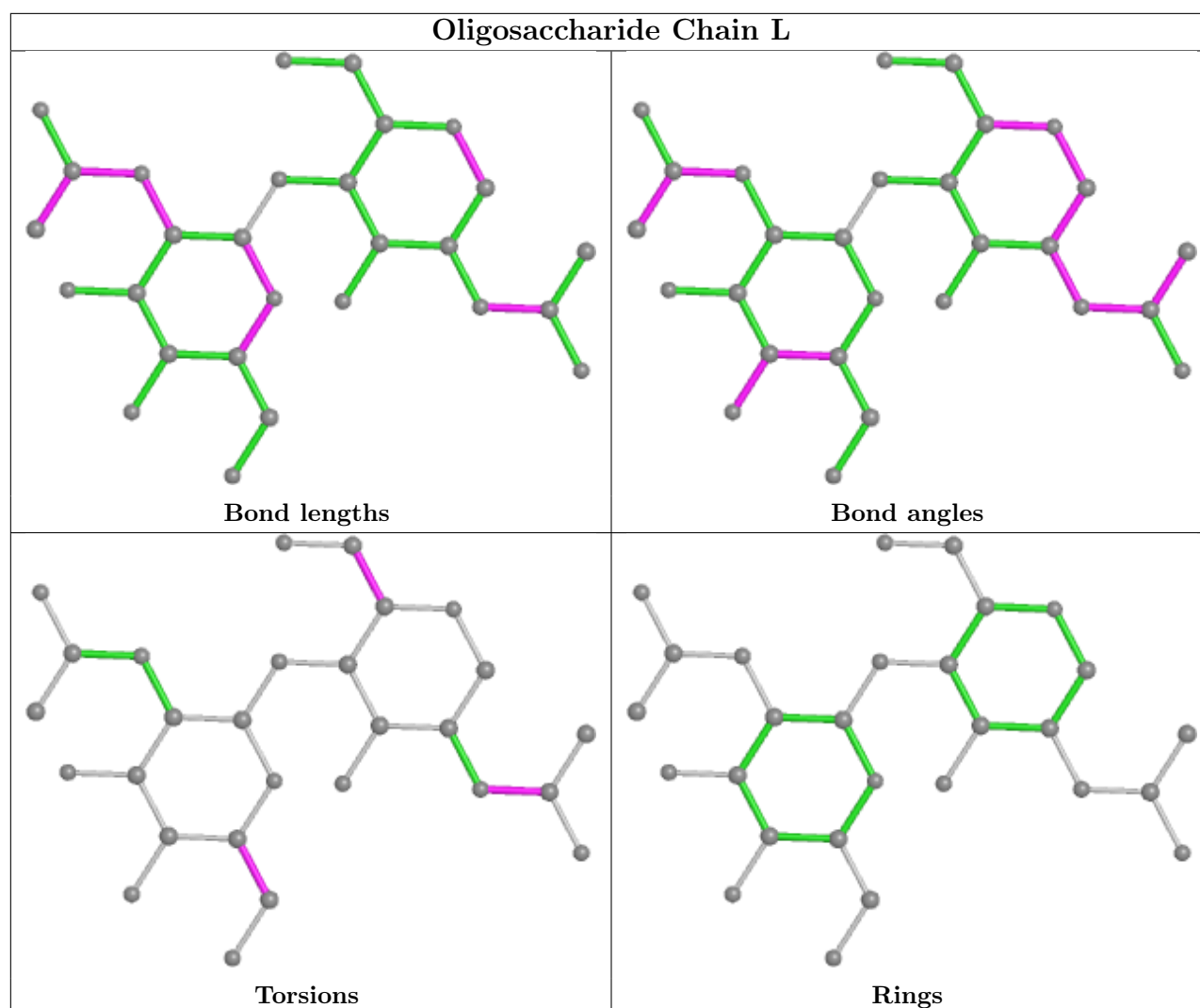
Bond angles



Torsions



Rings



5.6 Ligand geometry [i](#)

12 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	A	602	1	14,14,15	2.40	4 (28%)	17,19,21	1.83	5 (29%)
6	NAG	A	603	1	14,14,15	2.19	4 (28%)	17,19,21	1.33	2 (11%)
6	NAG	F	601	1	14,14,15	2.17	5 (35%)	17,19,21	1.34	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	D	701	1	14,14,15	2.09	5 (35%)	17,19,21	1.70	4 (23%)
6	NAG	C	703	1	14,14,15	2.17	3 (21%)	17,19,21	1.95	3 (17%)
6	NAG	E	602	1	14,14,15	2.24	4 (28%)	17,19,21	1.25	1 (5%)
6	NAG	D	702	1	14,14,15	2.07	4 (28%)	17,19,21	1.08	1 (5%)
6	NAG	E	601	1	14,14,15	2.01	4 (28%)	17,19,21	1.28	3 (17%)
6	NAG	C	702	1	14,14,15	2.10	4 (28%)	17,19,21	1.45	3 (17%)
6	NAG	A	601	1	14,14,15	2.06	4 (28%)	17,19,21	1.16	2 (11%)
6	NAG	D	703	1	14,14,15	2.06	3 (21%)	17,19,21	1.13	1 (5%)
6	NAG	C	701	1	14,14,15	2.09	4 (28%)	17,19,21	1.53	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
6	NAG	A	602	1	-	2/6/23/26	0/1/1/1
6	NAG	A	603	1	-	0/6/23/26	0/1/1/1
6	NAG	F	601	1	-	0/6/23/26	0/1/1/1
6	NAG	D	701	1	-	0/6/23/26	0/1/1/1
6	NAG	C	703	1	-	1/6/23/26	0/1/1/1
6	NAG	E	602	1	-	1/6/23/26	0/1/1/1
6	NAG	D	702	1	-	1/6/23/26	0/1/1/1
6	NAG	E	601	1	-	3/6/23/26	0/1/1/1
6	NAG	C	702	1	-	0/6/23/26	0/1/1/1
6	NAG	A	601	1	-	1/6/23/26	0/1/1/1
6	NAG	D	703	1	-	1/6/23/26	0/1/1/1
6	NAG	C	701	1	-	2/6/23/26	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	602	NAG	O5-C1	5.28	1.52	1.43
6	C	702	NAG	O5-C1	5.21	1.52	1.43
6	F	601	NAG	O5-C1	5.18	1.52	1.43
6	A	603	NAG	O5-C1	5.04	1.51	1.43
6	E	602	NAG	O5-C1	4.97	1.51	1.43

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
6	C	703	NAG	C4-C3-C2	4.61	117.78	111.02
6	D	701	NAG	C1-O5-C5	4.42	118.19	112.19
6	C	703	NAG	C2-N2-C7	4.33	129.07	122.90
6	C	701	NAG	C1-O5-C5	3.97	117.57	112.19
6	A	602	NAG	C8-C7-N2	3.78	122.49	116.10

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	601	NAG	O5-C5-C6-O6
6	E	601	NAG	C4-C5-C6-O6
6	C	703	NAG	C1-C2-N2-C7
6	C	701	NAG	C4-C5-C6-O6
6	D	702	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	602	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	484/506 (95%)	0.01	15 (3%) 51 31	41, 72, 173, 207	0
1	B	485/506 (95%)	0.33	19 (3%) 44 26	48, 101, 184, 201	0
1	C	484/506 (95%)	-0.15	9 (1%) 66 44	33, 58, 168, 180	0
1	D	485/506 (95%)	-0.09	5 (1%) 79 61	39, 68, 153, 185	0
1	E	485/506 (95%)	0.10	10 (2%) 63 42	44, 81, 191, 207	0
1	F	486/506 (96%)	0.55	30 (6%) 28 15	66, 117, 197, 233	0
All	All	2909/3036 (95%)	0.13	88 (3%) 52 32	33, 89, 182, 233	0

The worst 5 of 88 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	170	GLU	6.2
1	F	3	ILE	6.2
1	F	478	MET	5.5
1	A	497	LEU	4.5
1	F	67	CYS	4.2

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](#)

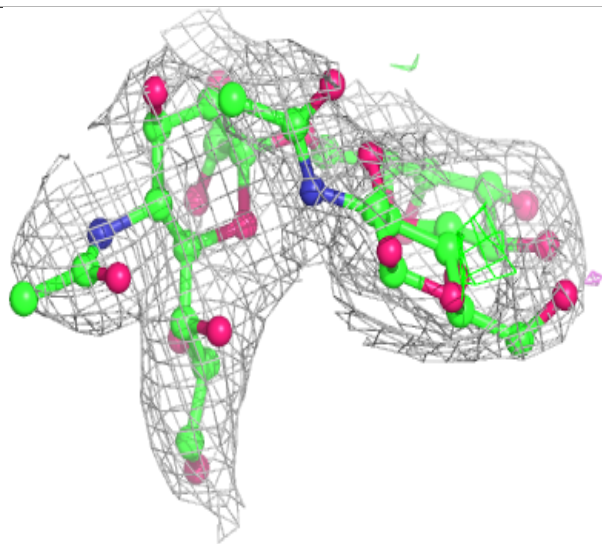
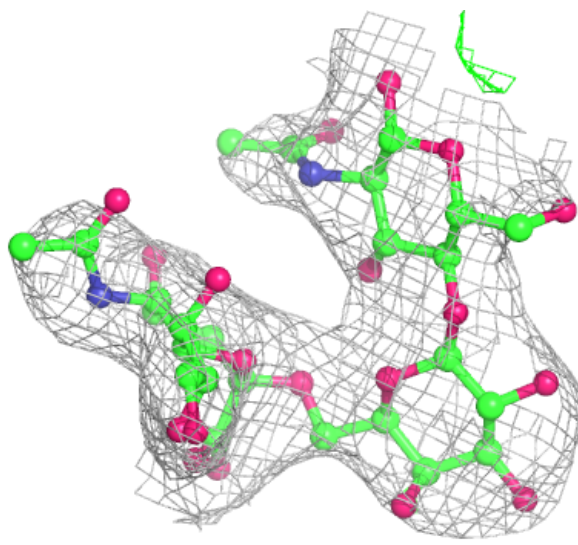
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GAL	K	1	12/12	0.33	0.16	136,143,158,159	0
3	GAL	H	1	12/12	0.43	0.17	63,78,83,87	0
4	NAG	K	2	14/15	0.44	0.17	128,146,165,168	0
3	NAG	I	2	14/15	0.47	0.18	67,72,76,78	0
3	GAL	I	1	12/12	0.56	0.17	63,78,83,87	0
3	NAG	H	2	14/15	0.60	0.19	67,72,76,78	0
2	NAG	J	1	15/15	0.62	0.17	111,121,136,139	0
3	GAL	H	3	11/12	0.62	0.14	57,63,69,69	0
3	GAL	I	3	11/12	0.70	0.13	57,63,69,69	0
2	NAG	G	1	15/15	0.71	0.13	86,115,128,129	0
5	NAG	L	2	14/15	0.75	0.13	82,119,141,144	0
2	GAL	J	2	11/12	0.77	0.12	93,111,126,132	0
2	GAL	G	2	11/12	0.82	0.10	89,102,107,109	0
4	GAL	K	3	11/12	0.83	0.10	97,120,128,133	0
3	SIA	I	4	20/21	0.84	0.14	44,57,65,67	0
5	NAG	L	1	14/15	0.85	0.13	85,99,114,117	0
3	SIA	H	4	20/21	0.88	0.13	44,57,65,67	0
2	SIA	J	3	20/21	0.92	0.12	75,100,121,134	0
4	SIA	K	4	20/21	0.93	0.12	70,87,115,122	0
2	SIA	G	3	20/21	0.96	0.09	54,67,92,101	0

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

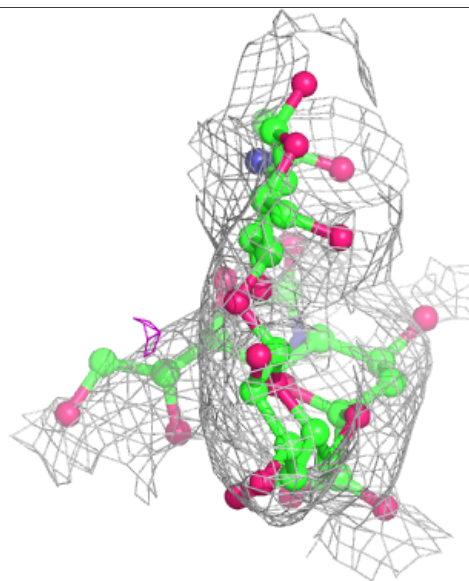
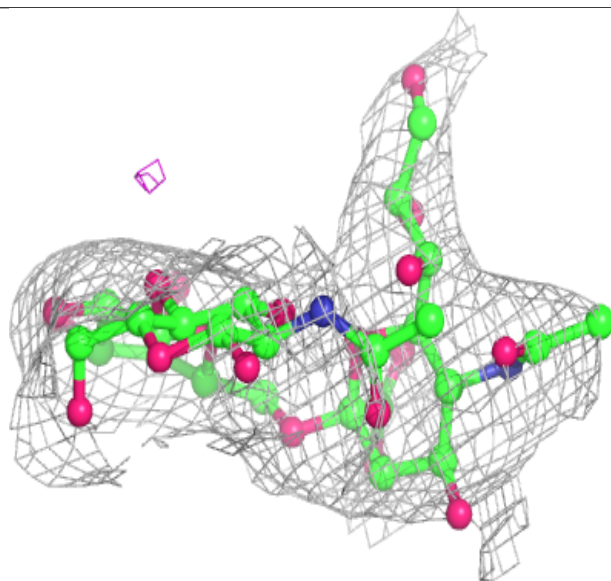
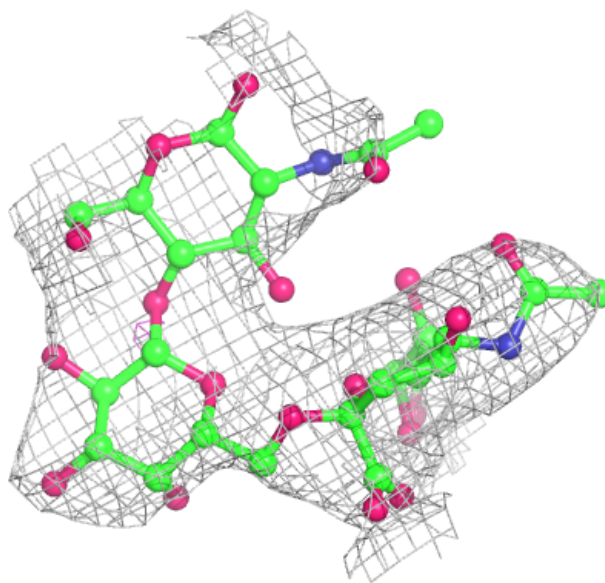
Electron density around Chain G:

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



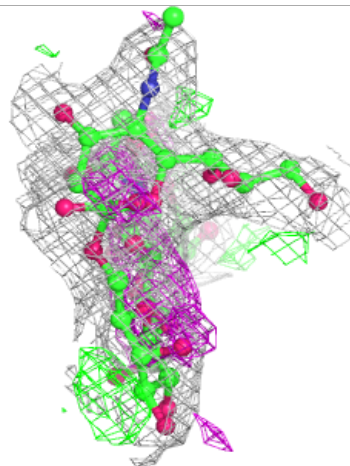
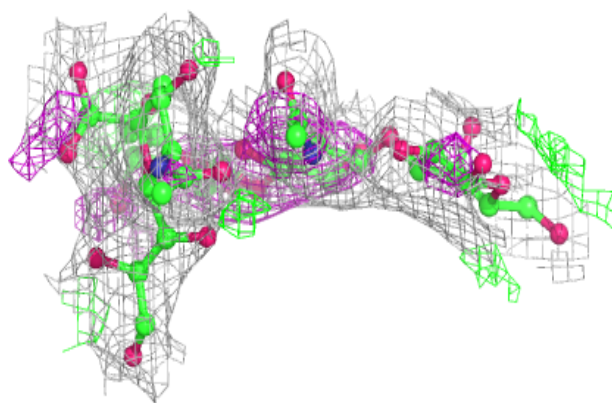
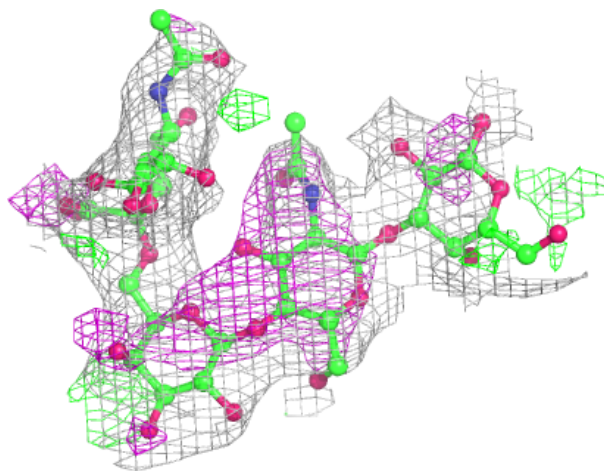
Electron density around Chain J:

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



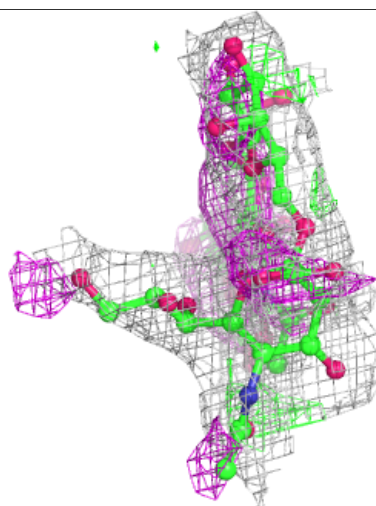
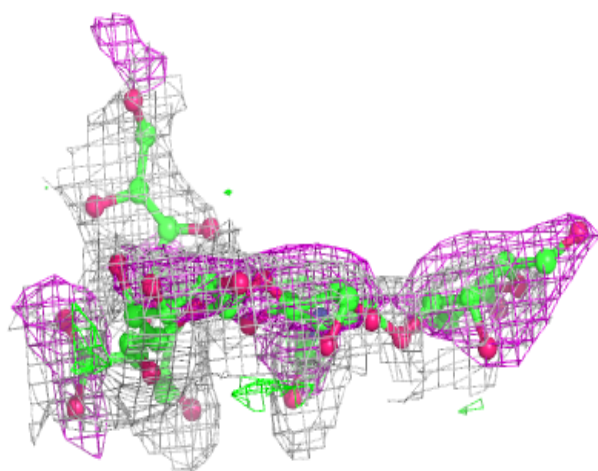
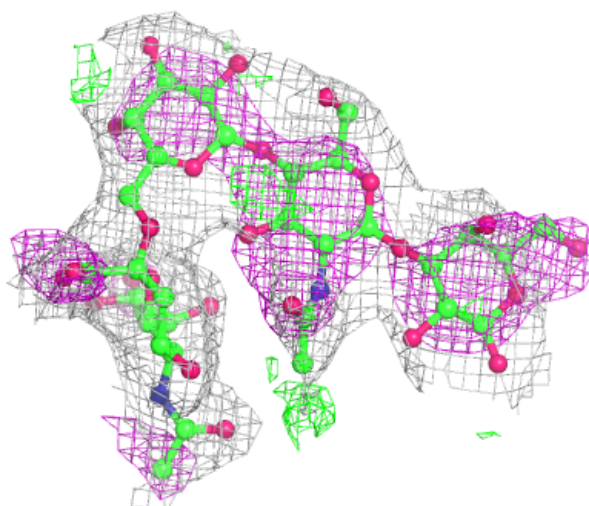
Electron density around Chain H:

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



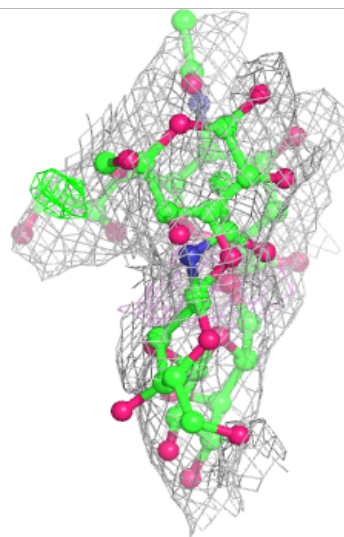
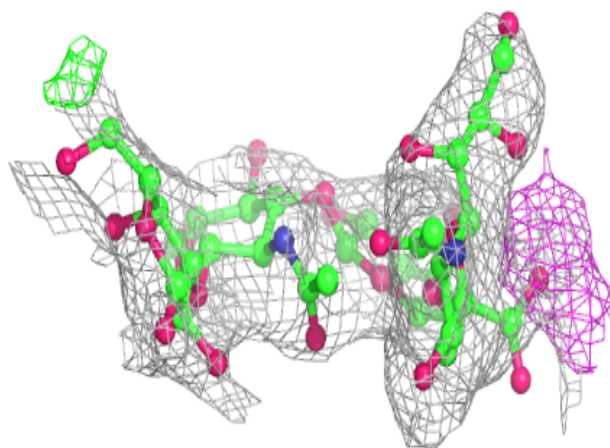
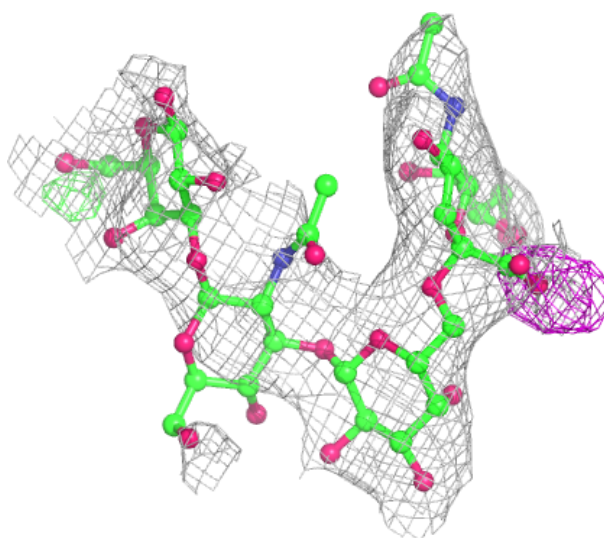
Electron density around Chain I:

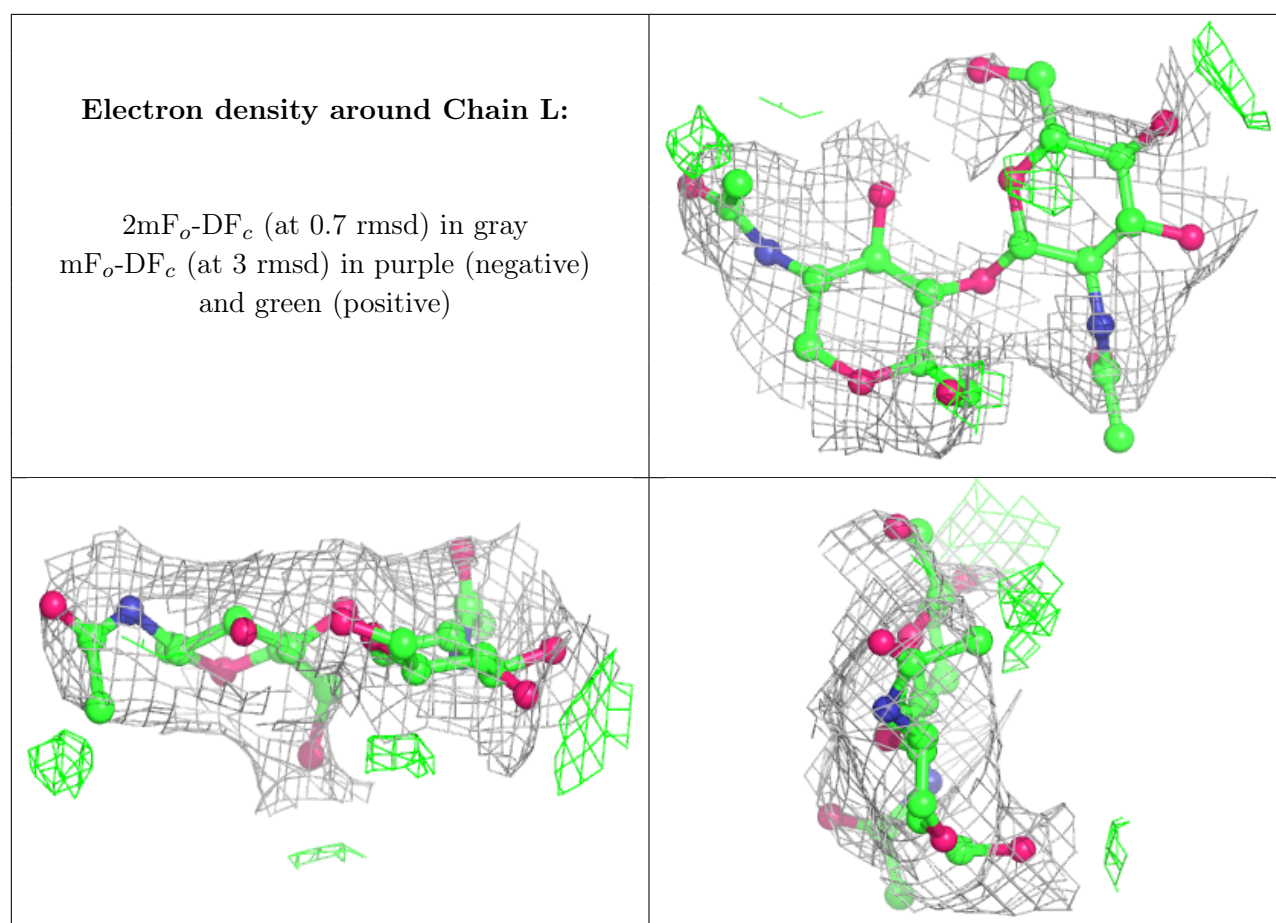
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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, 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
6	NAG	F	601	14/15	0.41	0.16	104,144,159,167	0
6	NAG	D	702	14/15	0.62	0.13	124,141,153,154	0
6	NAG	E	602	14/15	0.65	0.12	78,127,137,141	0
6	NAG	C	702	14/15	0.66	0.11	108,119,134,140	0
6	NAG	A	603	14/15	0.72	0.13	100,122,144,151	0
6	NAG	D	703	14/15	0.72	0.13	100,135,142,148	0
6	NAG	A	601	14/15	0.76	0.10	98,148,168,168	0
6	NAG	C	703	14/15	0.78	0.13	97,117,126,126	0
6	NAG	E	601	14/15	0.83	0.13	81,98,113,121	0
6	NAG	C	701	14/15	0.89	0.11	73,90,104,110	0
6	NAG	A	602	14/15	0.89	0.11	70,82,98,103	0
6	NAG	D	701	14/15	0.91	0.10	50,70,85,86	0

6.5 Other polymers [i](#)

There are no such residues in this entry.