



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 11:57 PM UTC

PDB ID : 3SEJ / pdb_00003sej
Title : Structural characterization of a GII.4 2004 norovirus variant (TCH05) bound to Secretor Lewis HBGA (LeB)
Authors : Shanker, S.; Choi, J.-M.; Sankaran, B.; Atmar, R.L.; Estes, M.K.; Prasad, B.V.V.
Deposited on : 2011-06-10
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 Phenix2.0
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

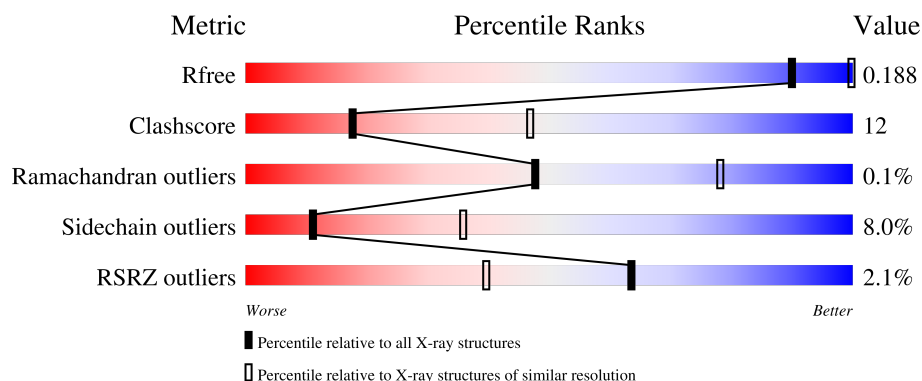
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



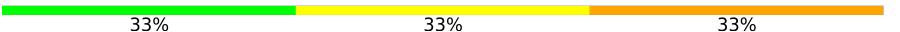
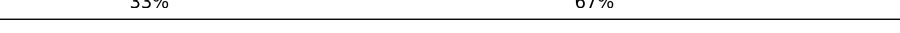
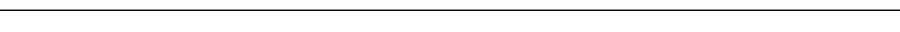
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3685 (3.08-3.00)
Clashscore	190562	4007 (3.08-3.00)
Ramachandran outliers	187476	3834 (3.08-3.00)
Sidechain outliers	187428	3836 (3.08-3.00)
RSRZ outliers	180081	3684 (3.08-3.00)

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	311	% 76% 21% ..
1	B	311	76% 21% ..
1	C	311	79% 19% .
1	D	311	% 75% 20% ..
1	E	311	74% 22% ..

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Mol	Chain	Length	Quality of chain
1	F	311	
1	G	311	
1	H	311	
1	I	311	
1	J	311	
2	K	6	
2	L	6	
2	M	6	
2	N	6	
2	O	6	
2	P	6	
2	Q	6	
2	R	6	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FUC	M	5	-	-	X	-
2	FUC	M	6	-	-	X	-
2	FUC	N	5	-	-	X	-
2	FUC	N	6	-	-	X	-
2	FUC	Q	5	-	-	X	-
2	BGC	R	1	-	-	X	-
2	GAL	R	2	-	-	X	-
2	FUC	R	6	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24569 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 Capsid.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2403	1517	415	461	10			
1	B	307	Total	C	N	O	S	0	0	0
			2382	1505	407	460	10			
1	C	311	Total	C	N	O	S	0	0	0
			2416	1524	417	465	10			
1	D	307	Total	C	N	O	S	0	0	0
			2386	1507	410	459	10			
1	E	309	Total	C	N	O	S	0	0	0
			2406	1518	415	463	10			
1	F	308	Total	C	N	O	S	0	0	0
			2393	1511	411	461	10			
1	G	308	Total	C	N	O	S	0	0	0
			2380	1505	407	458	10			
1	H	300	Total	C	N	O	S	0	0	0
			2291	1456	393	432	10			
1	I	284	Total	C	N	O	S	0	0	0
			2128	1347	371	402	8			
1	J	307	Total	C	N	O	S	0	0	0
			2383	1506	410	457	10			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
A	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
A	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
B	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
B	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
B	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
C	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
C	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
C	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
D	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
D	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
E	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
E	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
E	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
F	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
F	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
F	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
G	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
G	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
G	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
H	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
H	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
H	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
I	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
I	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
I	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
J	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
J	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
J	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8

-

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	K	6	Total 68	C 38	N 1	O 29	0	0	0
2	L	6	Total 68	C 38	N 1	O 29	0	0	0
2	M	6	Total 68	C 38	N 1	O 29	0	0	0
2	N	6	Total 68	C 38	N 1	O 29	0	0	0
2	O	6	Total 68	C 38	N 1	O 29	0	0	0



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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	6	Total	C	N	O	0	0	0
			68	38	1	29			
2	Q	6	Total	C	N	O	0	0	0
			68	38	1	29			
2	R	6	Total	C	N	O	0	0	0
			68	38	1	29			

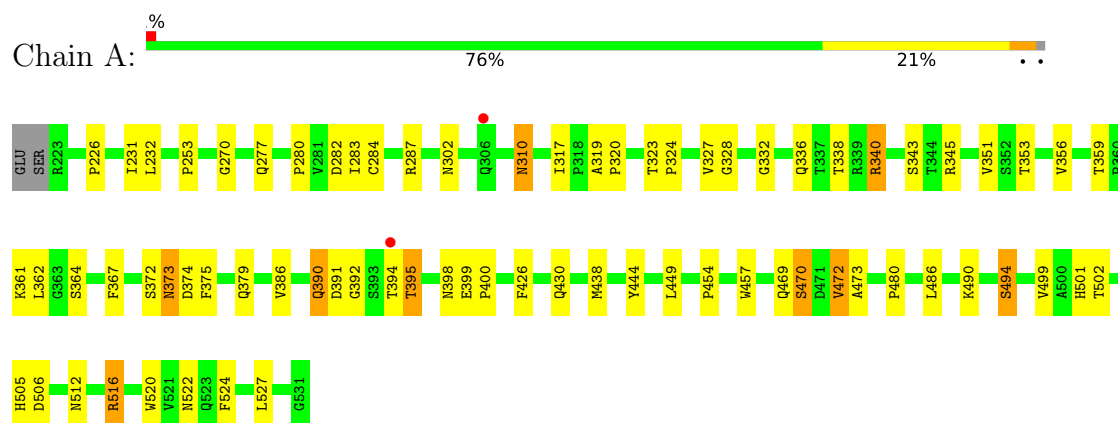
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	68	Total	O	0	0
			68	68		
3	B	54	Total	O	0	0
			54	54		
3	C	53	Total	O	0	0
			53	53		
3	D	57	Total	O	0	0
			57	57		
3	E	46	Total	O	0	0
			46	46		
3	F	45	Total	O	0	0
			45	45		
3	G	41	Total	O	0	0
			41	41		
3	H	36	Total	O	0	0
			36	36		
3	I	18	Total	O	0	0
			18	18		
3	J	39	Total	O	0	0
			39	39		

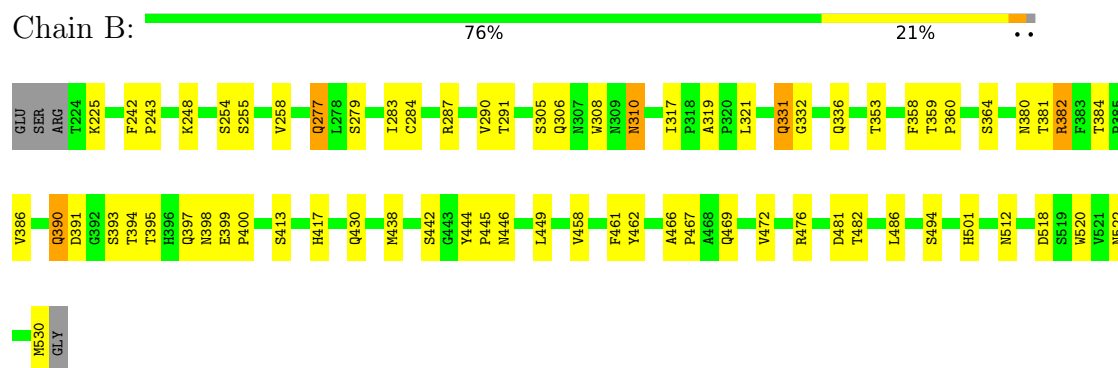
3 Residue-property plots

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.

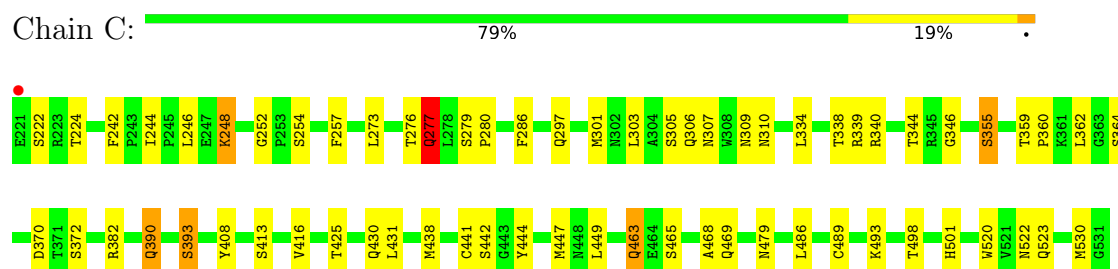
• Molecule 1: Capsid



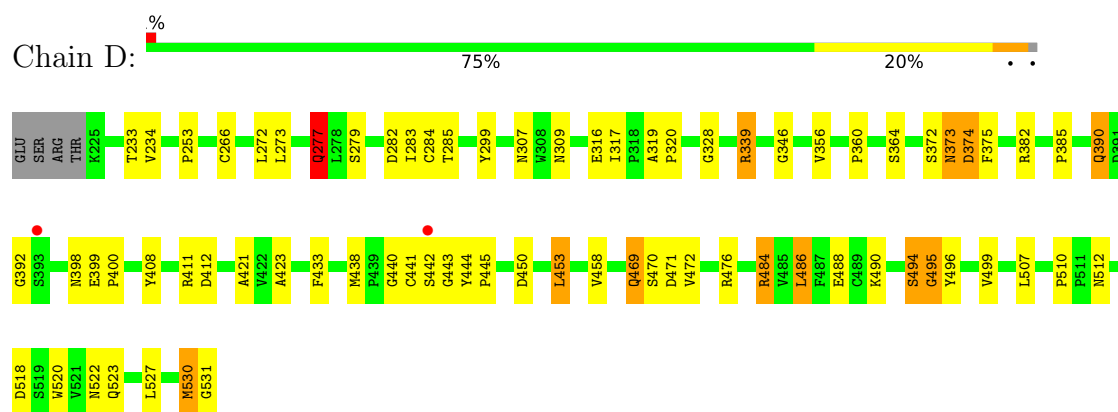
• Molecule 1: Capsid



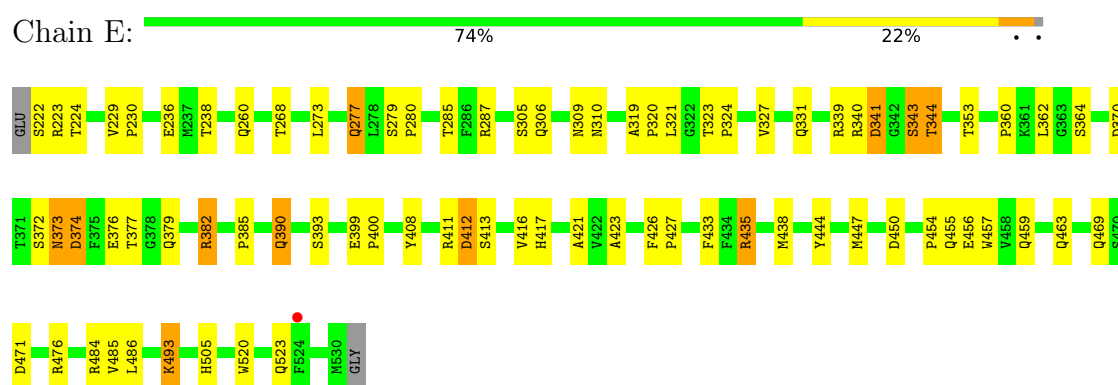
• Molecule 1: Capsid



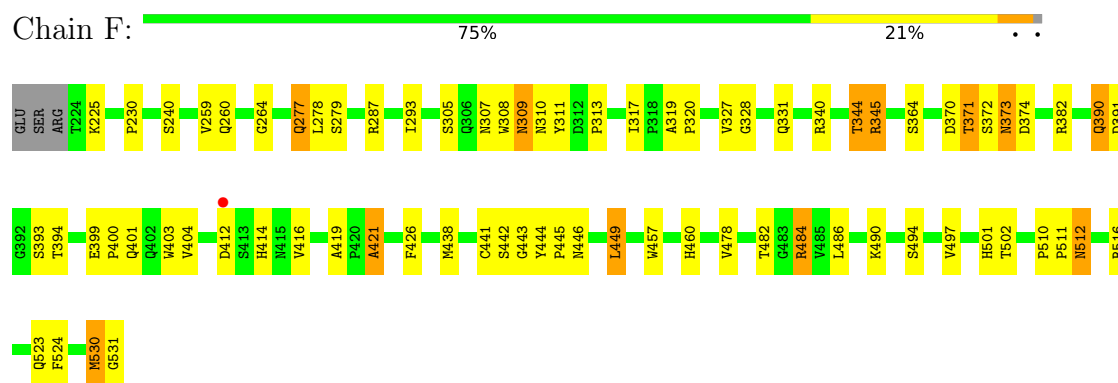
• Molecule 1: Capsid



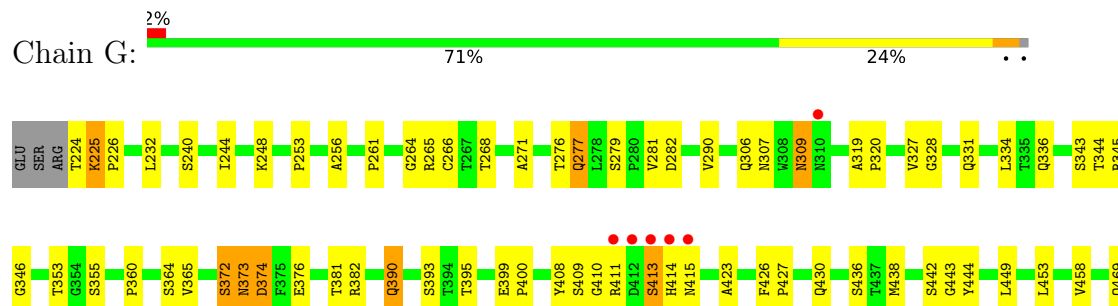
• Molecule 1: Capsid



• Molecule 1: Capsid

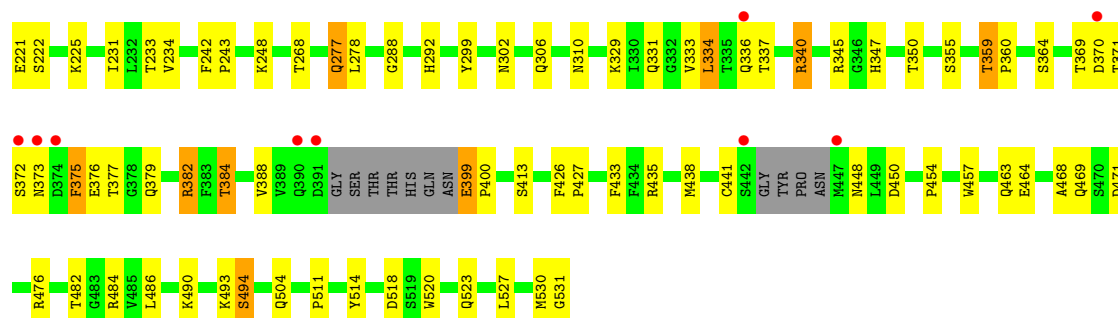


• Molecule 1: Capsid

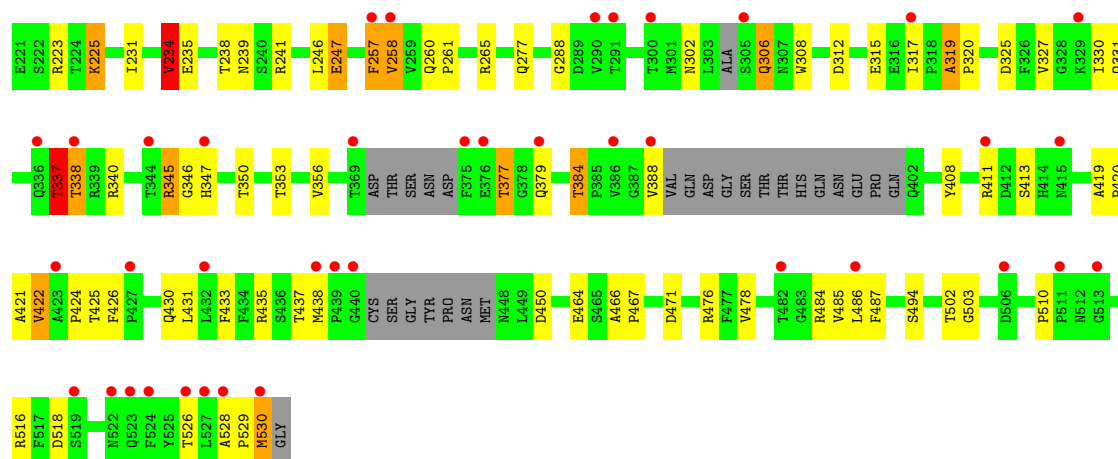




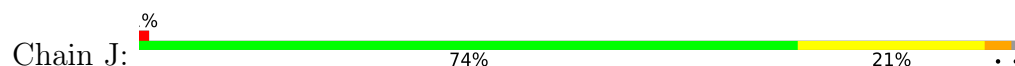
• Molecule 1: Capsid



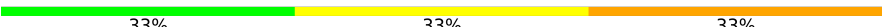
• Molecule 1: Capsid

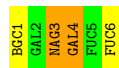


• Molecule 1: Capsid



- Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-3)-[alpha-L-fucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain K:  33% 33% 33%



- Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-3)-[alpha-L-fucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain L:  17% 83%



- Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-3)-[alpha-L-fucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain M:  33% 67%



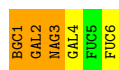
- Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-3)-[alpha-L-fucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain N:  33% 67%



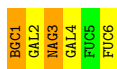
- Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-3)-[alpha-L-fucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain O:  17% 33% 50%

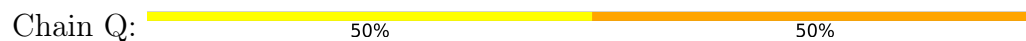


- Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-3)-[alpha-L-fucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain P:  17% 50% 33%



- Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-3)-[alpha-L-fucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose



- Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-3)-[alpha-L-fucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	242.74Å 339.78Å 125.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.38 – 3.04 49.38 – 3.04	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.38-3.04) 99.7 (49.38-3.04)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 3.07Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.166 , 0.223 (Not available) , 0.188	Depositor DCC
R_{free} test set	4924 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	40.5	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 32.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	24569	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.95% 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: FUC, BGC, NAG, GAL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.12	2/2473 (0.1%)	1.18	4/3384 (0.1%)
1	B	1.05	0/2452	1.13	4/3357 (0.1%)
1	C	1.04	2/2486 (0.1%)	1.12	2/3401 (0.1%)
1	D	1.04	4/2456 (0.2%)	1.15	7/3361 (0.2%)
1	E	1.03	1/2476 (0.0%)	1.17	5/3388 (0.1%)
1	F	0.97	2/2463 (0.1%)	1.16	8/3371 (0.2%)
1	G	0.99	0/2450	1.14	12/3355 (0.4%)
1	H	1.02	0/2356	1.14	8/3225 (0.2%)
1	I	1.15	4/2188 (0.2%)	1.12	15/2993 (0.5%)
1	J	1.05	1/2453 (0.0%)	1.12	6/3357 (0.2%)
All	All	1.05	16/24253 (0.1%)	1.14	71/33192 (0.2%)

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	E	0	1
1	J	0	1
All	All	0	2

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	317	ILE	C-O	-8.61	1.18	1.24
1	D	423	ALA	CA-CB	-7.28	1.44	1.54
1	F	317	ILE	C-O	-6.44	1.19	1.24
1	C	277	GLN	CA-C	5.99	1.59	1.52
1	I	510	PRO	CA-C	5.89	1.56	1.52

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	374	ASP	N-CA-C	13.66	126.25	111.36
1	E	374	ASP	N-CA-C	12.53	124.67	111.14
1	F	374	ASP	N-CA-C	11.75	124.17	111.36
1	A	374	ASP	N-CA-C	11.38	123.76	111.36
1	G	495	GLY	N-CA-C	11.06	130.54	114.95

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	344	THR	Peptide
1	J	345	ARG	Sidechain

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	2403	0	2292	60	0
1	B	2382	0	2264	39	0
1	C	2416	0	2304	46	0
1	D	2386	0	2275	49	0
1	E	2406	0	2297	49	0
1	F	2393	0	2282	58	0
1	G	2380	0	2263	67	0
1	H	2291	0	2167	55	0
1	I	2128	0	1939	50	0
1	J	2383	0	2273	58	0
2	K	68	0	60	2	0
2	L	68	0	60	8	0
2	M	68	0	60	15	0
2	N	68	0	60	18	0
2	O	68	0	60	6	0
2	P	68	0	60	6	0
2	Q	68	0	60	21	0
2	R	68	0	60	21	0
3	A	68	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	54	0	0	12	0
3	C	53	0	0	13	0
3	D	57	0	0	10	0
3	E	46	0	0	13	0
3	F	45	0	0	15	0
3	G	41	0	0	8	0
3	H	36	0	0	16	0
3	I	18	0	0	10	0
3	J	39	0	0	6	0
All	All	24569	0	22836	583	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 12.

The worst 5 of 583 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:J:345:ARG:HD3	2:Q:5:FUC:O3	1.40	1.20
1:J:345:ARG:HG2	1:J:345:ARG:HH21	1.07	1.18
1:H:231:ILE:HB	3:H:545:HOH:O	1.40	1.18
1:B:481:ASP:HB2	3:B:181:HOH:O	1.43	1.16
1:F:512:ASN:HB3	3:F:544:HOH:O	1.50	1.12

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	307/311 (99%)	293 (95%)	14 (5%)	0	100	100
1	B	305/311 (98%)	294 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	309/311 (99%)	294 (95%)	15 (5%)	0	100	100
1	D	305/311 (98%)	297 (97%)	8 (3%)	0	100	100
1	E	307/311 (99%)	290 (94%)	17 (6%)	0	100	100
1	F	306/311 (98%)	290 (95%)	16 (5%)	0	100	100
1	G	306/311 (98%)	295 (96%)	11 (4%)	0	100	100
1	H	294/311 (94%)	278 (95%)	16 (5%)	0	100	100
1	I	274/311 (88%)	252 (92%)	20 (7%)	2 (1%)	18	49
1	J	305/311 (98%)	295 (97%)	10 (3%)	0	100	100
All	All	3018/3110 (97%)	2878 (95%)	138 (5%)	2 (0%)	48	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	425	THR
1	I	231	ILE

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	269/272 (99%)	253 (94%)	16 (6%)	18	47
1	B	268/272 (98%)	248 (92%)	20 (8%)	12	38
1	C	271/272 (100%)	248 (92%)	23 (8%)	10	34
1	D	268/272 (98%)	250 (93%)	18 (7%)	15	43
1	E	271/272 (100%)	248 (92%)	23 (8%)	10	34
1	F	269/272 (99%)	250 (93%)	19 (7%)	13	40
1	G	266/272 (98%)	246 (92%)	20 (8%)	12	38
1	H	249/272 (92%)	226 (91%)	23 (9%)	8	30
1	I	219/272 (80%)	196 (90%)	23 (10%)	6	25
1	J	267/272 (98%)	243 (91%)	24 (9%)	9	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2617/2720 (96%)	2408 (92%)	209 (8%)	11	36

5 of 209 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	484	ARG
1	H	329	LYS
1	J	382	ARG
1	G	224	THR
1	G	376	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	469	GLN
1	J	306	GLN
1	D	505	HIS
1	D	417	HIS
1	J	390	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 ⓘ

48 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	BGC	K	1	2	12,12,12	0.50	0	17,17,17	0.75	1 (5%)
2	GAL	K	2	2	11,11,12	0.37	0	15,15,17	0.81	0
2	NAG	K	3	2	14,14,15	0.56	0	17,19,21	0.89	1 (5%)
2	GAL	K	4	2	11,11,12	0.32	0	15,15,17	0.75	1 (6%)
2	FUC	K	5	2	10,10,11	0.42	0	14,14,16	0.81	0
2	FUC	K	6	2	10,10,11	0.42	0	14,14,16	0.81	0
2	BGC	L	1	2	12,12,12	0.53	0	17,17,17	1.52	4 (23%)
2	GAL	L	2	2	11,11,12	0.54	0	15,15,17	1.23	2 (13%)
2	NAG	L	3	2	14,14,15	0.98	1 (7%)	17,19,21	2.08	5 (29%)
2	GAL	L	4	2	11,11,12	1.97	3 (27%)	15,15,17	2.41	5 (33%)
2	FUC	L	5	2	10,10,11	1.89	3 (30%)	14,14,16	3.64	5 (35%)
2	FUC	L	6	2	10,10,11	1.66	3 (30%)	14,14,16	2.60	6 (42%)
2	BGC	M	1	2	12,12,12	0.48	0	17,17,17	0.94	1 (5%)
2	GAL	M	2	2	11,11,12	0.33	0	15,15,17	0.79	0
2	NAG	M	3	2	14,14,15	0.97	1 (7%)	17,19,21	2.28	3 (17%)
2	GAL	M	4	2	11,11,12	1.58	2 (18%)	15,15,17	2.41	3 (20%)
2	FUC	M	5	2	10,10,11	1.40	1 (10%)	14,14,16	2.78	4 (28%)
2	FUC	M	6	2	10,10,11	0.41	0	14,14,16	0.82	0
2	BGC	N	1	2	12,12,12	0.84	0	17,17,17	2.15	6 (35%)
2	GAL	N	2	2	11,11,12	0.68	0	15,15,17	1.75	3 (20%)
2	NAG	N	3	2	14,14,15	0.90	1 (7%)	17,19,21	2.40	2 (11%)
2	GAL	N	4	2	11,11,12	1.74	3 (27%)	15,15,17	2.76	6 (40%)
2	FUC	N	5	2	10,10,11	0.44	0	14,14,16	0.75	0
2	FUC	N	6	2	10,10,11	0.45	0	14,14,16	0.91	0
2	BGC	O	1	2	12,12,12	1.15	1 (8%)	17,17,17	2.12	5 (29%)
2	GAL	O	2	2	11,11,12	1.04	1 (9%)	15,15,17	2.15	7 (46%)
2	NAG	O	3	2	14,14,15	0.99	1 (7%)	17,19,21	1.73	4 (23%)
2	GAL	O	4	2	11,11,12	2.02	2 (18%)	15,15,17	2.30	6 (40%)
2	FUC	O	5	2	10,10,11	0.63	0	14,14,16	0.95	0
2	FUC	O	6	2	10,10,11	0.40	0	14,14,16	0.81	0
2	BGC	P	1	2	12,12,12	0.50	0	17,17,17	0.75	1 (5%)
2	GAL	P	2	2	11,11,12	0.36	0	15,15,17	0.81	1 (6%)
2	NAG	P	3	2	14,14,15	0.55	0	17,19,21	0.89	1 (5%)
2	GAL	P	4	2	11,11,12	0.33	0	15,15,17	0.75	0
2	FUC	P	5	2	10,10,11	0.42	0	14,14,16	0.81	0
2	FUC	P	6	2	10,10,11	0.43	0	14,14,16	0.81	0
2	BGC	Q	1	2	12,12,12	0.50	0	17,17,17	0.75	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GAL	Q	2	2	11,11,12	0.37	0	15,15,17	0.82	1 (6%)
2	NAG	Q	3	2	14,14,15	0.56	0	17,19,21	0.88	1 (5%)
2	GAL	Q	4	2	11,11,12	0.33	0	15,15,17	0.75	0
2	FUC	Q	5	2	10,10,11	0.41	0	14,14,16	0.81	0
2	FUC	Q	6	2	10,10,11	0.41	0	14,14,16	0.81	0
2	BGC	R	1	2	12,12,12	0.50	0	17,17,17	0.75	1 (5%)
2	GAL	R	2	2	11,11,12	0.36	0	15,15,17	0.81	1 (6%)
2	NAG	R	3	2	14,14,15	0.55	0	17,19,21	0.88	0
2	GAL	R	4	2	11,11,12	0.32	0	15,15,17	0.75	0
2	FUC	R	5	2	10,10,11	0.42	0	14,14,16	0.81	0
2	FUC	R	6	2	10,10,11	0.42	0	14,14,16	0.81	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
2	BGC	K	1	2	-	2/2/22/22	0/1/1/1
2	GAL	K	2	2	-	0/2/19/22	0/1/1/1
2	NAG	K	3	2	-	2/6/23/26	0/1/1/1
2	GAL	K	4	2	-	2/2/19/22	0/1/1/1
2	FUC	K	5	2	-	-	0/1/1/1
2	FUC	K	6	2	-	-	0/1/1/1
2	BGC	L	1	2	-	2/2/22/22	0/1/1/1
2	GAL	L	2	2	-	2/2/19/22	0/1/1/1
2	NAG	L	3	2	-	2/6/23/26	0/1/1/1
2	GAL	L	4	2	-	1/2/19/22	0/1/1/1
2	FUC	L	5	2	-	-	0/1/1/1
2	FUC	L	6	2	-	-	0/1/1/1
2	BGC	M	1	2	-	2/2/22/22	0/1/1/1
2	GAL	M	2	2	-	0/2/19/22	0/1/1/1
2	NAG	M	3	2	-	0/6/23/26	0/1/1/1
2	GAL	M	4	2	-	2/2/19/22	0/1/1/1
2	FUC	M	5	2	-	-	0/1/1/1
2	FUC	M	6	2	-	-	0/1/1/1
2	BGC	N	1	2	-	2/2/22/22	0/1/1/1
2	GAL	N	2	2	-	1/2/19/22	0/1/1/1
2	NAG	N	3	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GAL	N	4	2	-	2/2/19/22	0/1/1/1
2	FUC	N	5	2	-	-	0/1/1/1
2	FUC	N	6	2	-	-	0/1/1/1
2	BGC	O	1	2	-	2/2/22/22	0/1/1/1
2	GAL	O	2	2	-	0/2/19/22	0/1/1/1
2	NAG	O	3	2	-	2/6/23/26	0/1/1/1
2	GAL	O	4	2	-	2/2/19/22	0/1/1/1
2	FUC	O	5	2	-	-	0/1/1/1
2	FUC	O	6	2	-	-	0/1/1/1
2	BGC	P	1	2	-	2/2/22/22	0/1/1/1
2	GAL	P	2	2	-	2/2/19/22	0/1/1/1
2	NAG	P	3	2	-	2/6/23/26	0/1/1/1
2	GAL	P	4	2	-	0/2/19/22	0/1/1/1
2	FUC	P	5	2	-	-	0/1/1/1
2	FUC	P	6	2	-	-	0/1/1/1
2	BGC	Q	1	2	-	2/2/22/22	0/1/1/1
2	GAL	Q	2	2	-	2/2/19/22	0/1/1/1
2	NAG	Q	3	2	-	0/6/23/26	0/1/1/1
2	GAL	Q	4	2	-	1/2/19/22	0/1/1/1
2	FUC	Q	5	2	-	-	0/1/1/1
2	FUC	Q	6	2	-	-	0/1/1/1
2	BGC	R	1	2	-	0/2/22/22	0/1/1/1
2	GAL	R	2	2	-	2/2/19/22	0/1/1/1
2	NAG	R	3	2	-	0/6/23/26	0/1/1/1
2	GAL	R	4	2	-	1/2/19/22	0/1/1/1
2	FUC	R	5	2	-	-	0/1/1/1
2	FUC	R	6	2	-	-	0/1/1/1

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	4	GAL	O5-C1	-4.58	1.36	1.43
2	O	4	GAL	O5-C5	-4.20	1.35	1.43
2	L	5	FUC	O5-C5	-4.03	1.35	1.43
2	M	4	GAL	O5-C1	-3.97	1.37	1.43
2	M	5	FUC	O5-C1	-3.93	1.37	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	5	FUC	C6-C5-C4	-9.93	94.92	113.08
2	N	3	NAG	C6-C5-C4	-8.70	91.65	113.02
2	M	3	NAG	C6-C5-C4	-7.56	94.45	113.02
2	L	5	FUC	O5-C5-C4	-7.06	96.85	109.55
2	N	4	GAL	C1-O5-C5	-6.91	102.93	112.19

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	1	BGC	C4-C5-C6-O6
2	O	3	NAG	O5-C5-C6-O6
2	O	4	GAL	O5-C5-C6-O6
2	L	2	GAL	O5-C5-C6-O6
2	O	1	BGC	O5-C5-C6-O6

There are no ring outliers.

40 monomers are involved in 97 short contacts:

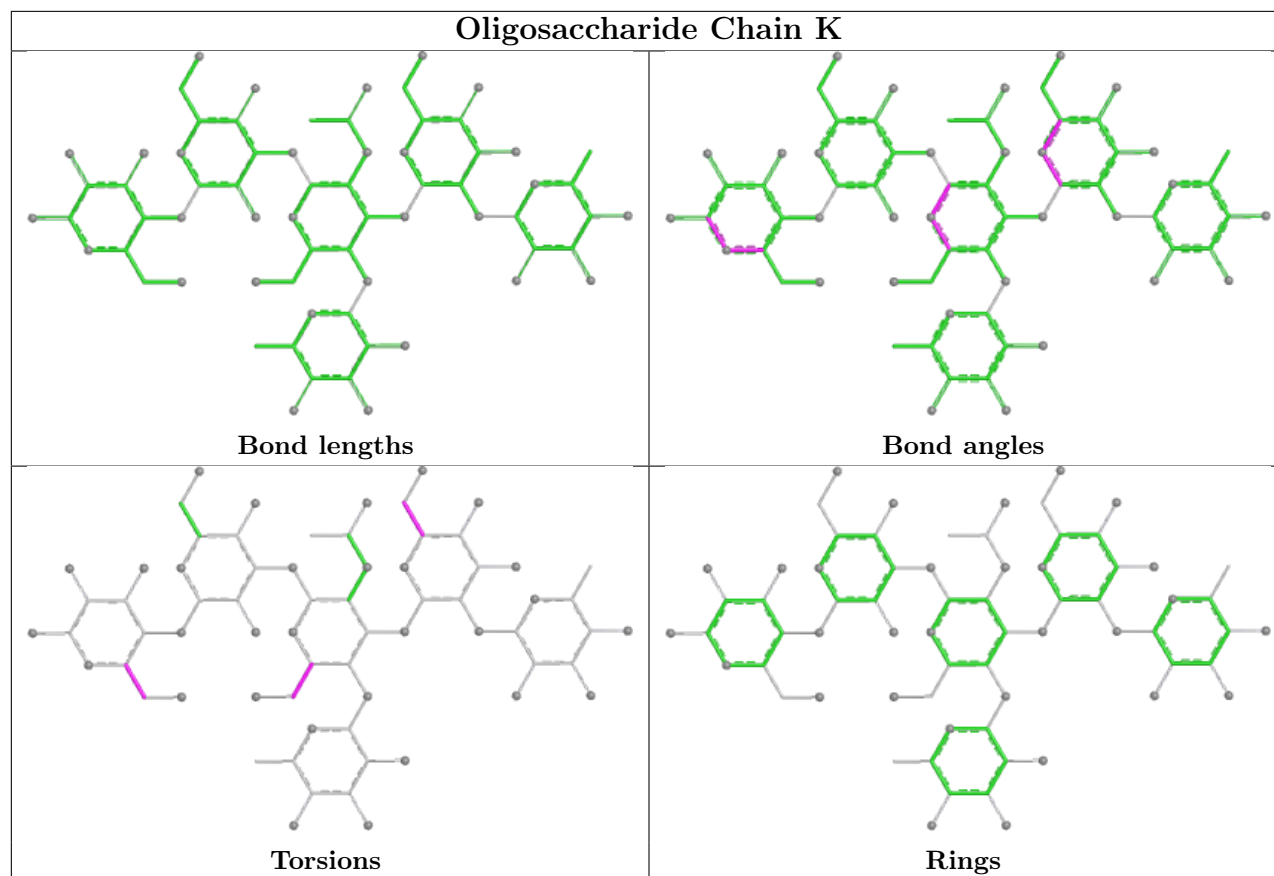
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	1	BGC	2	0
2	O	3	NAG	2	0
2	P	3	NAG	2	0
2	K	3	NAG	1	0
2	N	2	GAL	1	0
2	R	6	FUC	14	0
2	N	6	FUC	14	0
2	K	6	FUC	2	0
2	M	4	GAL	5	0
2	Q	5	FUC	13	0
2	N	1	BGC	1	0
2	P	4	GAL	3	0
2	K	4	GAL	1	0
2	M	3	NAG	3	0
2	N	3	NAG	4	0
2	R	5	FUC	5	0
2	N	4	GAL	4	0
2	P	6	FUC	4	0
2	L	6	FUC	4	0
2	O	1	BGC	4	0
2	Q	1	BGC	2	0
2	Q	2	GAL	4	0

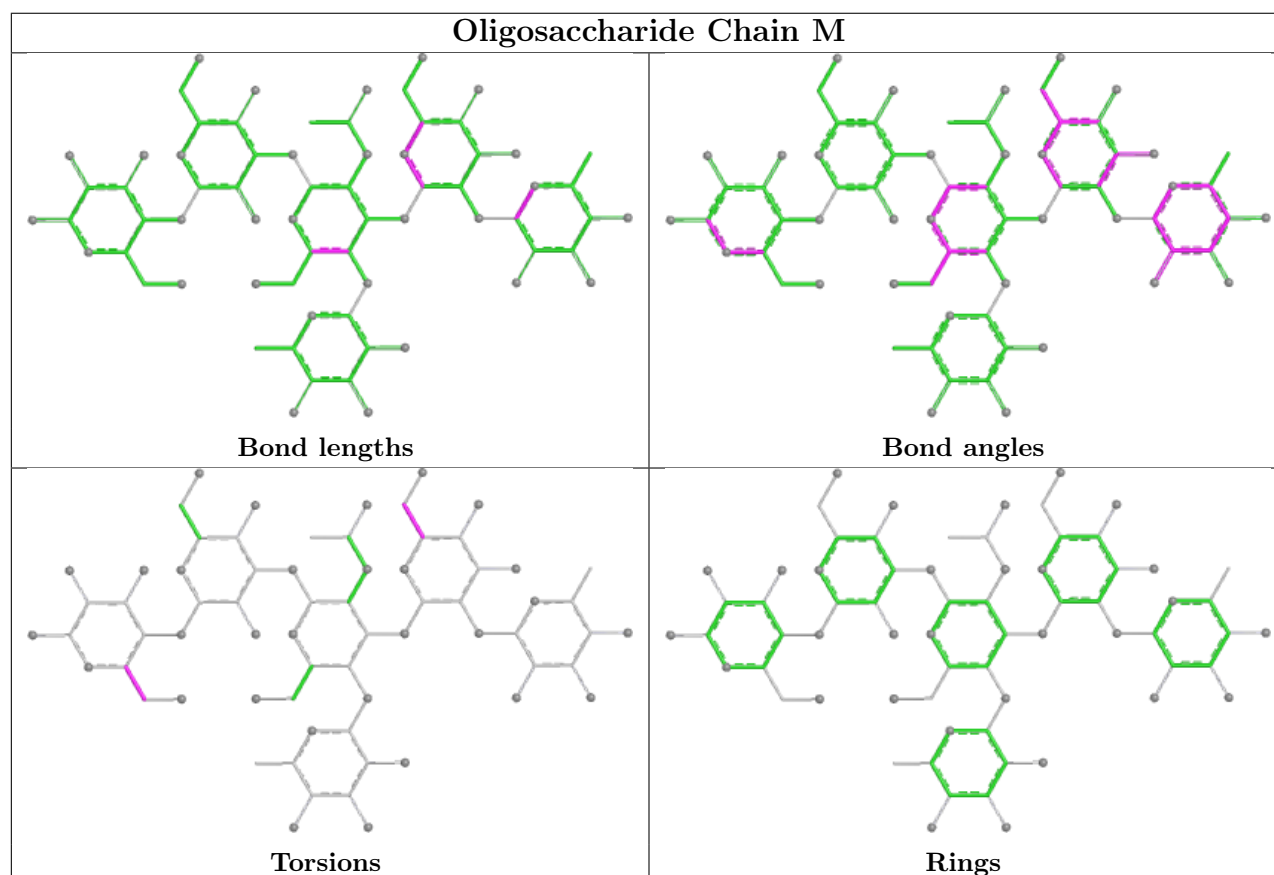
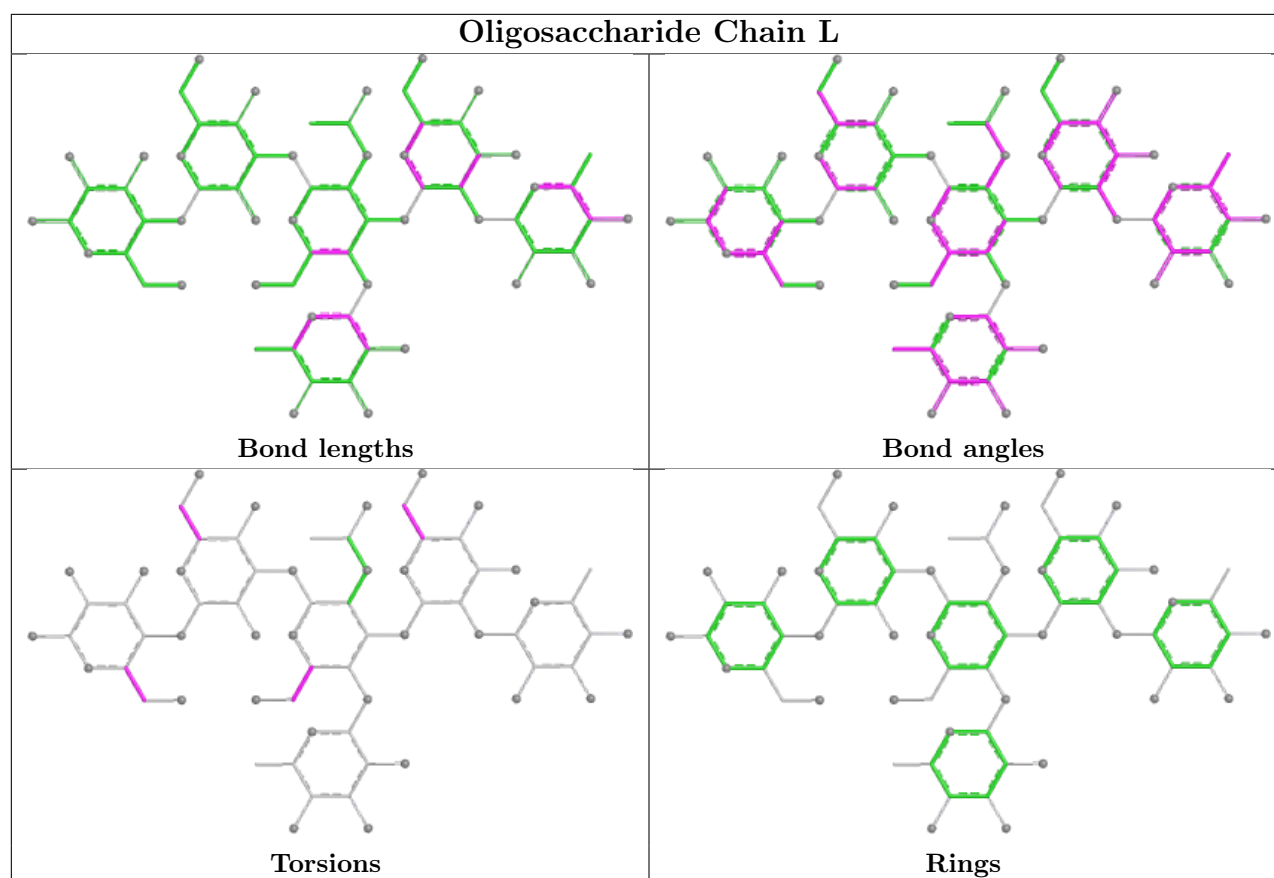
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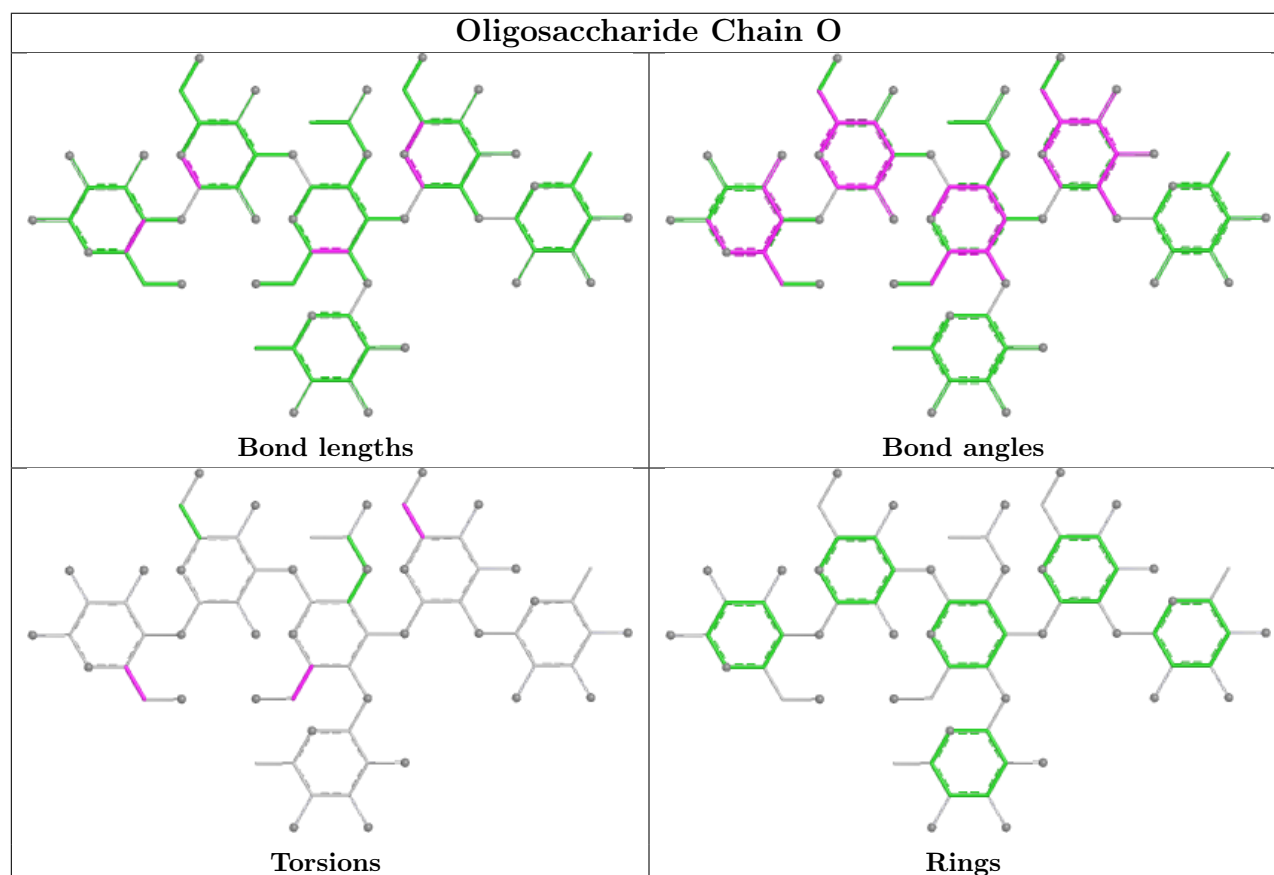
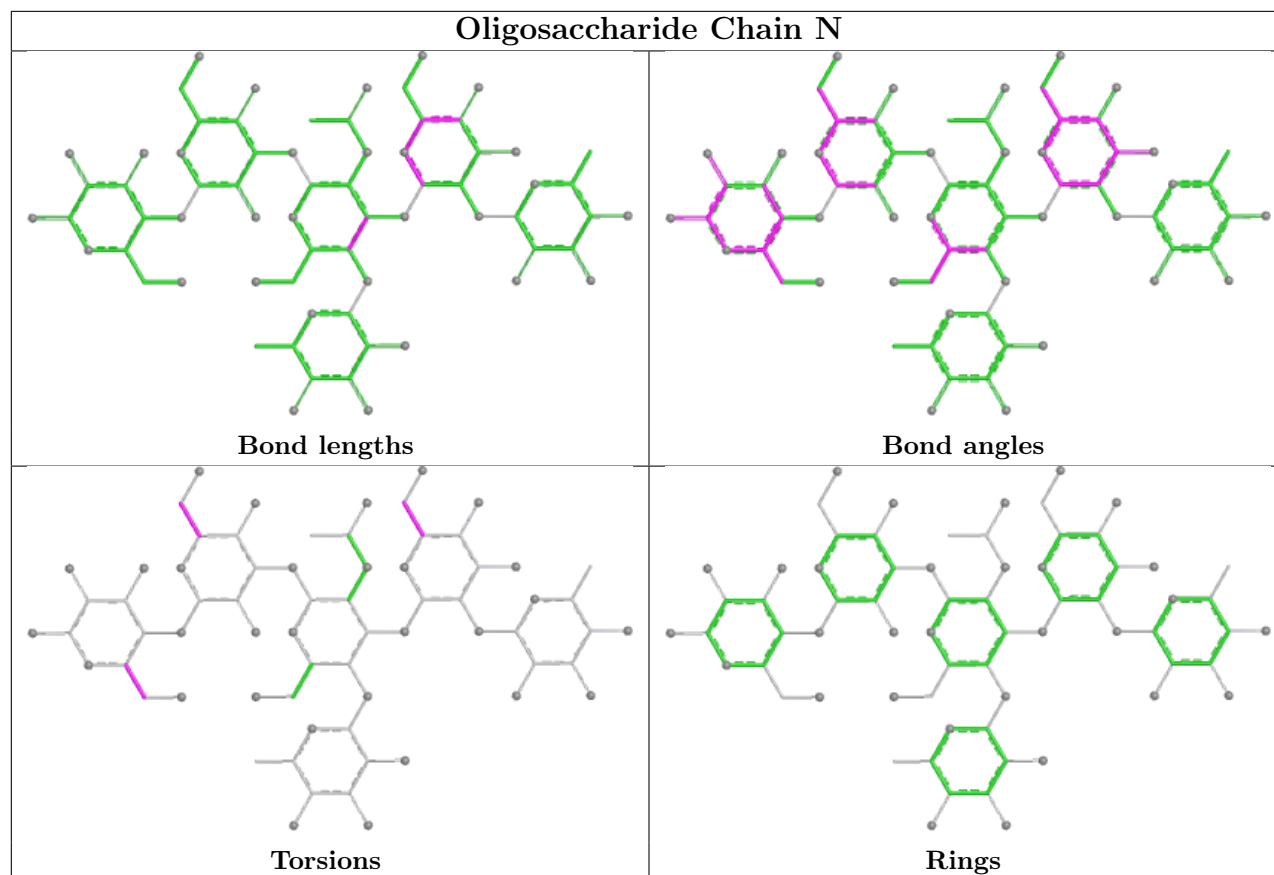
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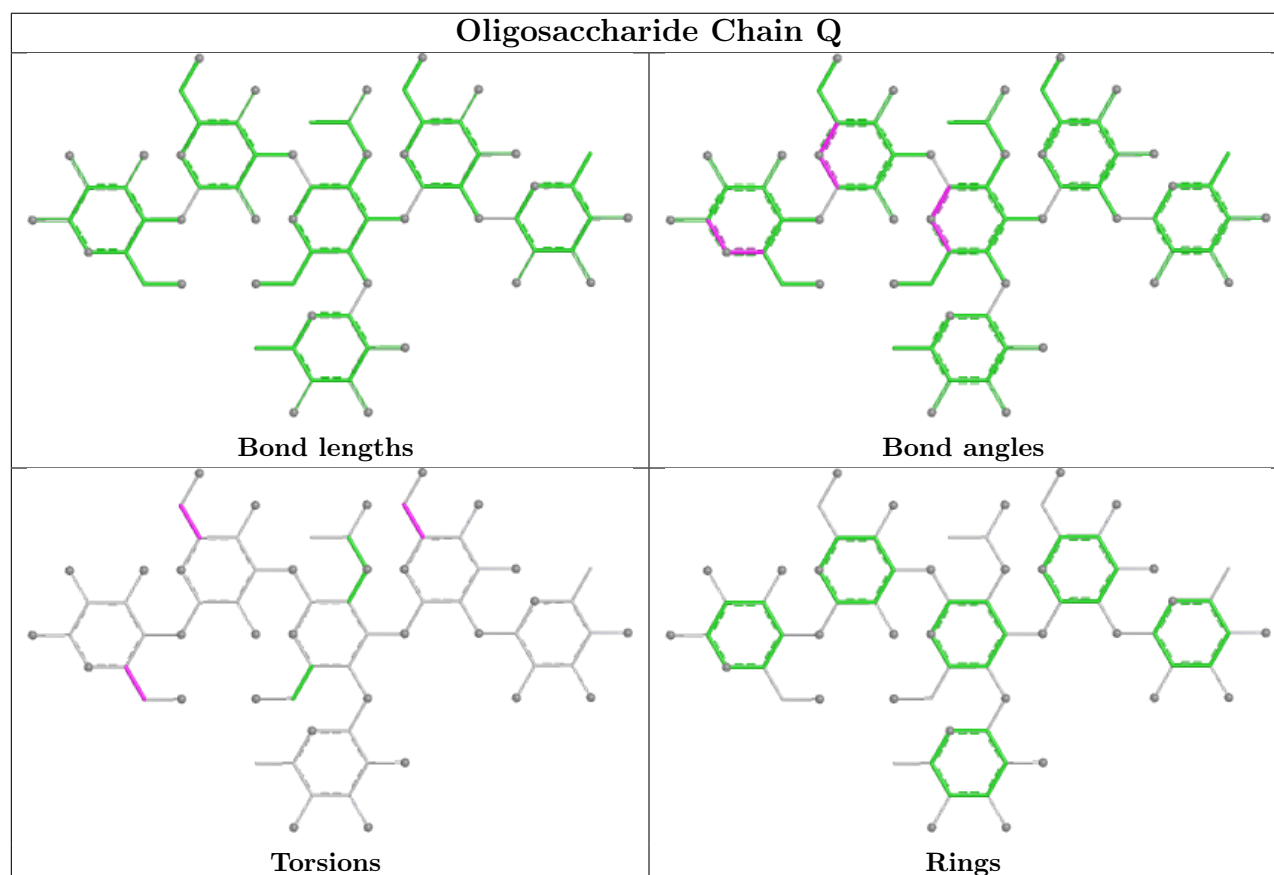
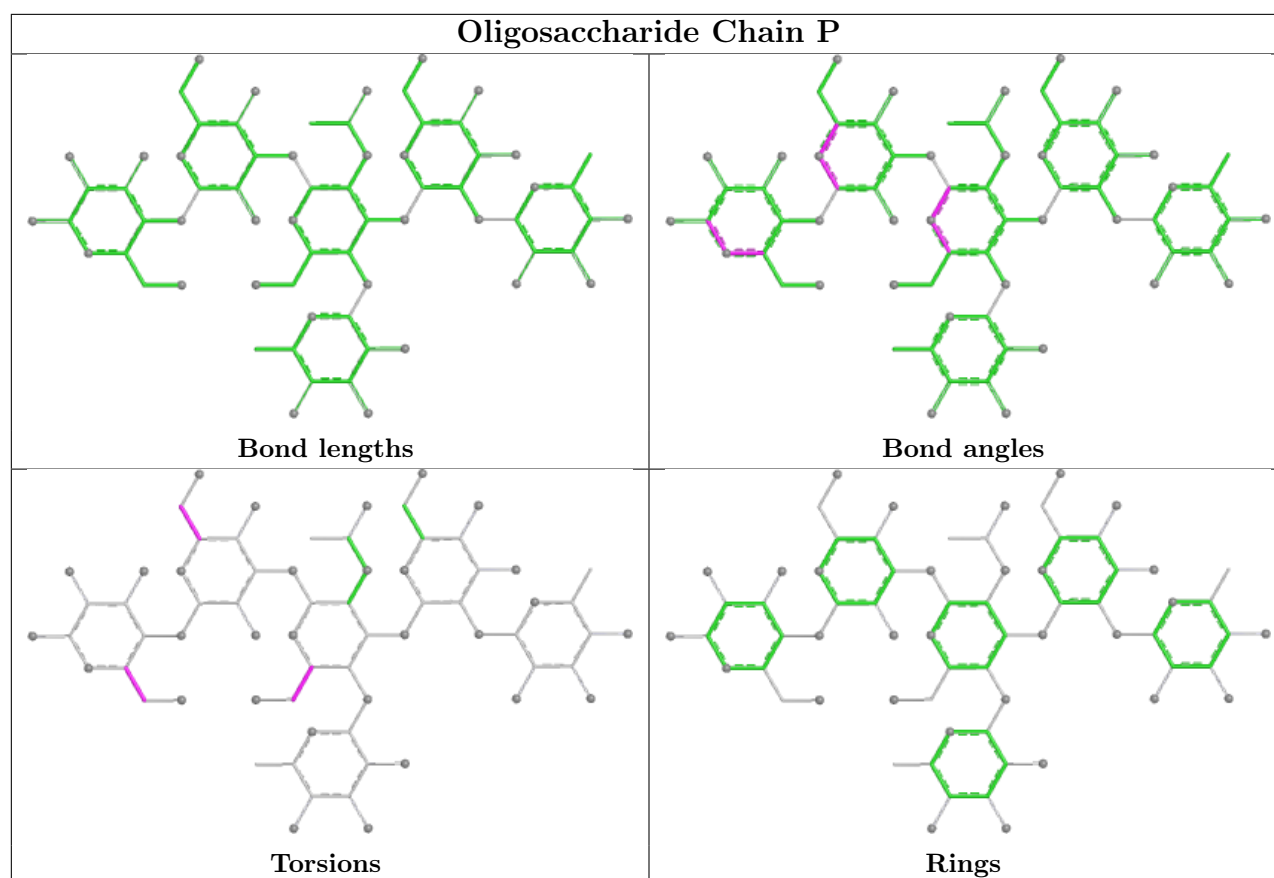
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	N	5	FUC	8	0
2	P	1	BGC	1	0
2	Q	3	NAG	2	0
2	L	1	BGC	2	0
2	L	5	FUC	2	0
2	Q	4	GAL	3	0
2	L	3	NAG	4	0
2	M	2	GAL	2	0
2	R	2	GAL	6	0
2	M	5	FUC	8	0
2	O	2	GAL	1	0
2	M	6	FUC	8	0
2	Q	6	FUC	5	0
2	R	1	BGC	6	0
2	O	6	FUC	2	0
2	R	4	GAL	3	0
2	R	3	NAG	2	0
2	L	2	GAL	1	0

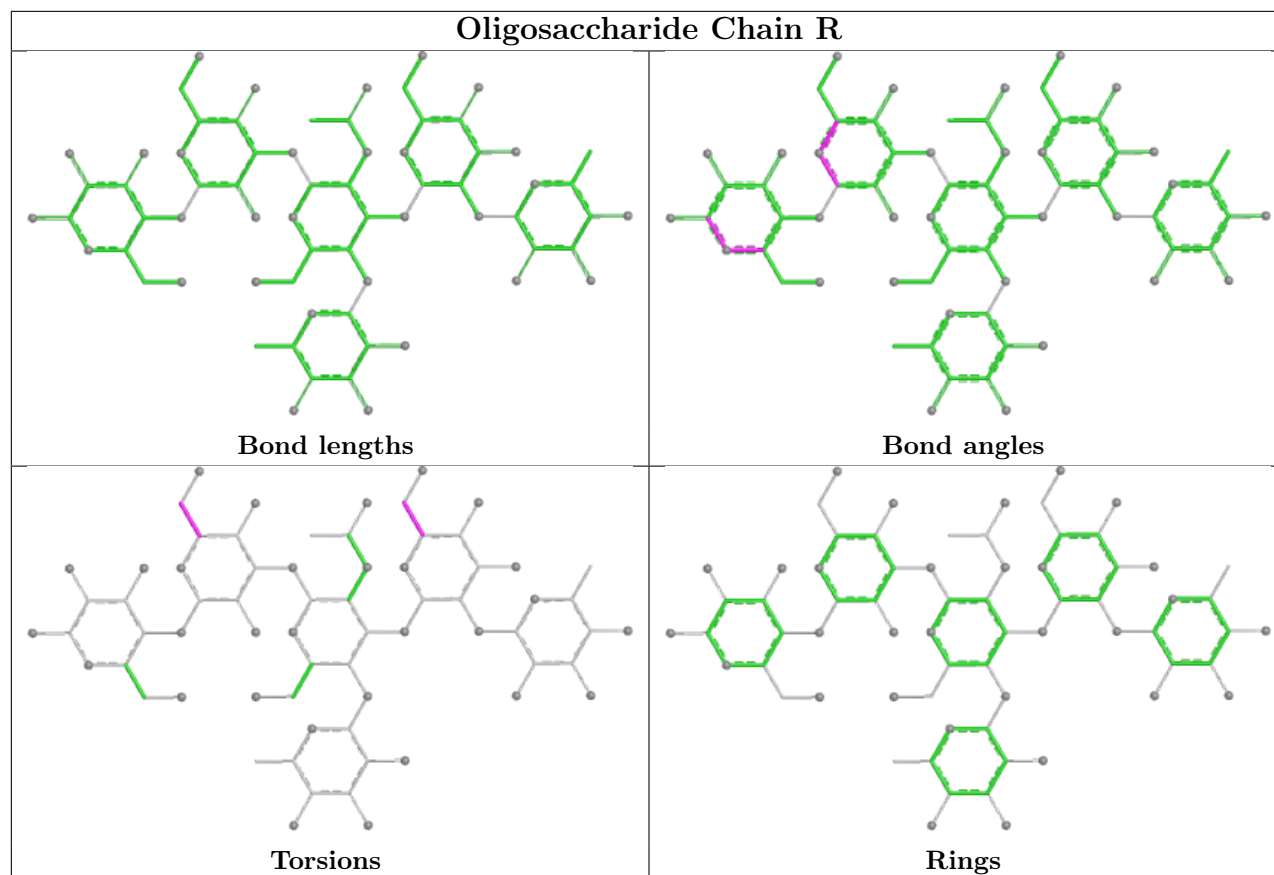
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	309/311 (99%)	-0.82	2 (0%) 85 69	10, 22, 54, 90	0
1	B	307/311 (98%)	-0.80	0 100 100	15, 26, 51, 65	0
1	C	311/311 (100%)	-0.82	1 (0%) 90 79	13, 27, 49, 64	0
1	D	307/311 (98%)	-0.75	2 (0%) 84 66	11, 27, 59, 82	0
1	E	309/311 (99%)	-0.77	1 (0%) 90 79	15, 28, 60, 74	0
1	F	308/311 (99%)	-0.57	1 (0%) 90 79	20, 39, 68, 83	0
1	G	308/311 (99%)	-0.55	7 (2%) 61 37	22, 38, 63, 104	0
1	H	300/311 (96%)	-0.33	9 (3%) 52 29	17, 41, 79, 109	0
1	I	284/311 (91%)	0.93	39 (13%) 6 4	51, 81, 110, 140	0
1	J	307/311 (98%)	-0.63	2 (0%) 84 66	17, 33, 62, 79	0
All	All	3050/3110 (98%)	-0.52	64 (2%) 63 39	10, 33, 83, 140	0

The worst 5 of 64 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	413	SER	5.6
1	H	391	ASP	4.6
1	I	388	VAL	4.5
1	G	412	ASP	4.4
1	H	442	SER	4.3

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

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

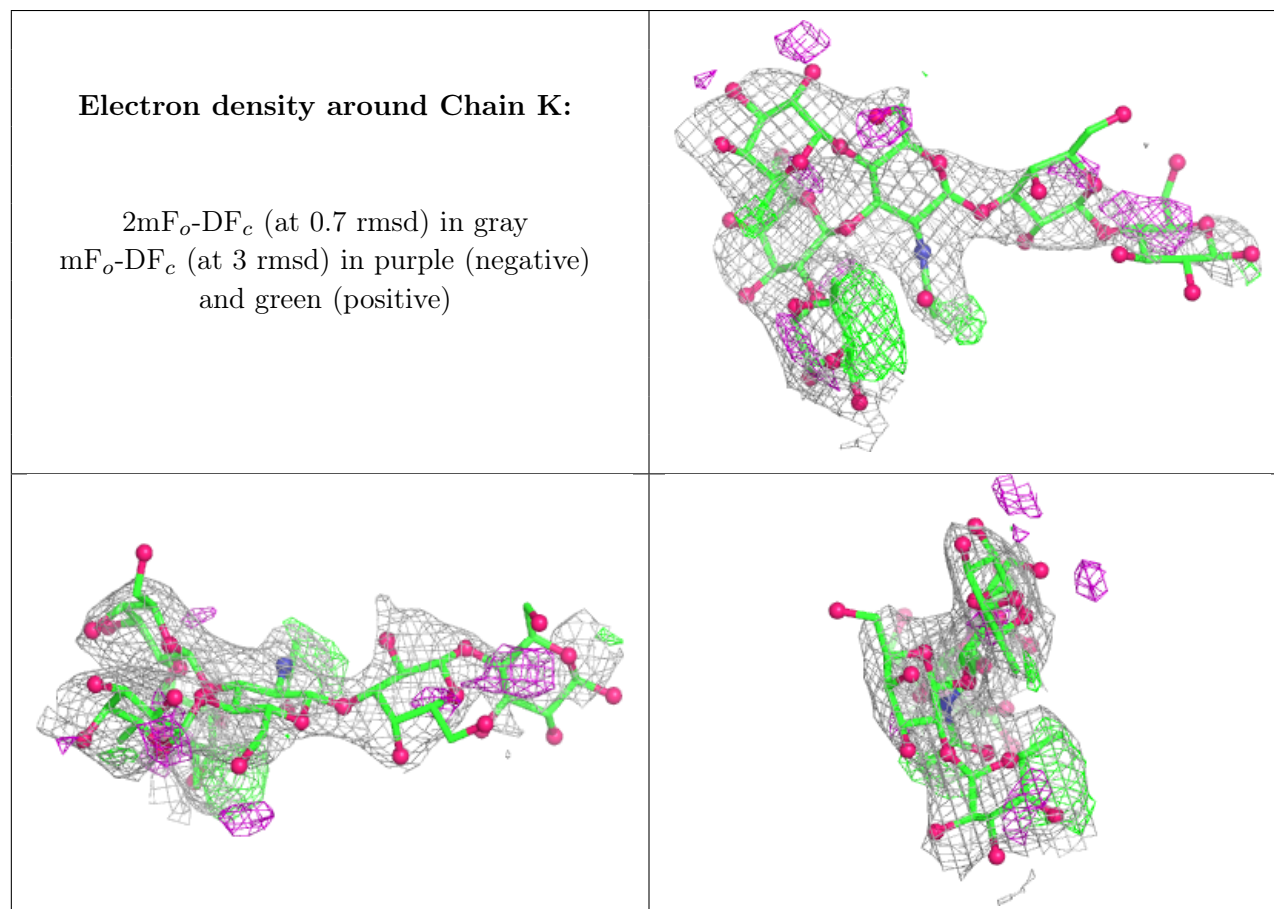
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BGC	K	1	12/12	0.13	0.18	126,130,130,131	0
2	BGC	M	1	12/12	0.19	0.17	122,125,126,126	0
2	GAL	M	2	11/12	0.30	0.20	108,115,118,118	0
2	BGC	L	1	12/12	0.34	0.19	124,130,130,130	0
2	BGC	N	1	12/12	0.39	0.16	123,126,126,127	0
2	BGC	R	1	12/12	0.41	0.16	129,133,133,133	0
2	GAL	N	2	11/12	0.45	0.18	111,115,119,120	0
2	GAL	K	2	11/12	0.47	0.17	113,119,122,123	0
2	GAL	P	2	11/12	0.51	0.16	126,130,131,132	0
2	GAL	R	2	11/12	0.53	0.16	119,122,125,126	0
2	BGC	O	1	12/12	0.61	0.21	105,109,109,109	0
2	BGC	P	1	12/12	0.62	0.16	134,136,136,136	0
2	GAL	O	2	11/12	0.63	0.19	93,97,101,101	0
2	NAG	Q	3	14/15	0.64	0.22	97,103,106,106	0
2	FUC	L	6	10/11	0.65	0.22	92,96,97,98	0
2	NAG	K	3	14/15	0.65	0.20	98,104,107,108	0
2	GAL	L	2	11/12	0.66	0.16	111,116,119,120	0
2	FUC	M	6	10/11	0.69	0.20	91,93,94,95	0
2	GAL	L	4	11/12	0.69	0.15	85,91,93,93	0
2	GAL	M	4	11/12	0.70	0.15	83,88,89,90	0
2	GAL	Q	4	11/12	0.70	0.15	85,96,97,97	0
2	FUC	K	6	10/11	0.70	0.19	99,100,101,101	0
2	GAL	Q	2	11/12	0.70	0.18	110,113,114,114	0
2	FUC	Q	5	10/11	0.71	0.19	70,74,76,79	0
2	FUC	N	6	10/11	0.72	0.18	97,99,99,99	0
2	NAG	O	3	14/15	0.73	0.18	79,83,86,88	0
2	NAG	L	3	14/15	0.73	0.20	98,102,104,106	0
2	FUC	K	5	10/11	0.73	0.20	74,77,78,80	0
2	FUC	R	6	10/11	0.73	0.17	107,108,109,109	0
2	GAL	N	4	11/12	0.74	0.14	92,94,96,96	0
2	GAL	R	4	11/12	0.74	0.13	92,96,99,99	0
2	NAG	M	3	14/15	0.74	0.17	93,97,101,103	0
2	NAG	R	3	14/15	0.75	0.16	104,111,112,114	0
2	GAL	P	4	11/12	0.75	0.16	108,112,113,114	0
2	BGC	Q	1	12/12	0.75	0.23	113,116,117,117	0
2	FUC	R	5	10/11	0.77	0.17	83,84,86,88	0
2	NAG	P	3	14/15	0.77	0.17	117,121,123,124	0

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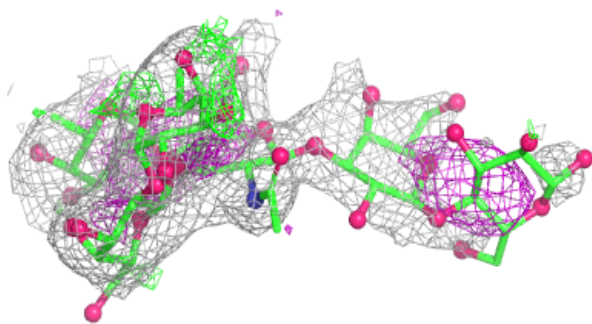
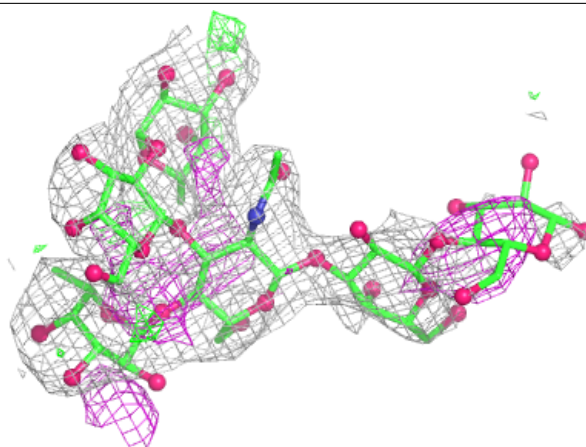
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FUC	N	5	10/11	0.78	0.20	84,87,88,89	0
2	FUC	Q	6	10/11	0.78	0.16	100,101,102,102	0
2	FUC	O	6	10/11	0.79	0.16	73,75,76,77	0
2	FUC	P	6	10/11	0.80	0.17	119,120,121,121	0
2	FUC	M	5	10/11	0.81	0.18	73,74,77,79	0
2	FUC	L	5	10/11	0.81	0.18	71,72,75,78	0
2	NAG	N	3	14/15	0.81	0.16	97,102,105,106	0
2	FUC	O	5	10/11	0.82	0.17	57,61,62,63	0
2	GAL	O	4	11/12	0.83	0.12	68,72,74,75	0
2	GAL	K	4	11/12	0.86	0.10	84,91,92,92	0
2	FUC	P	5	10/11	0.89	0.15	100,101,102,104	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.



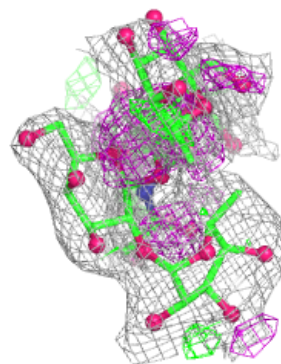
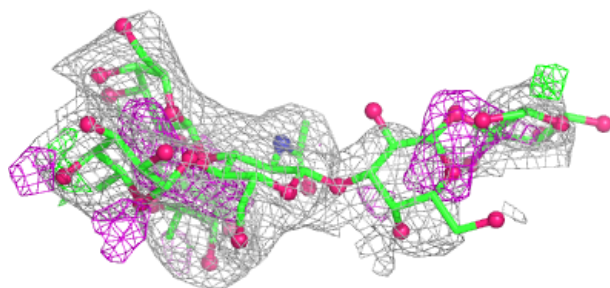
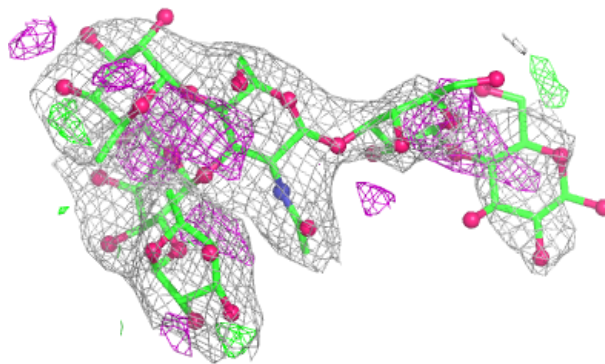
Electron density around Chain L:

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



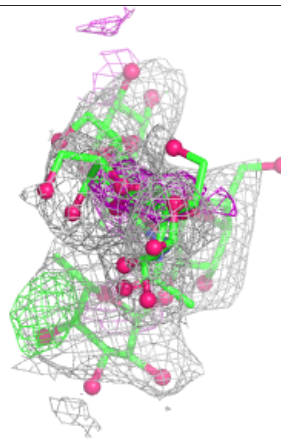
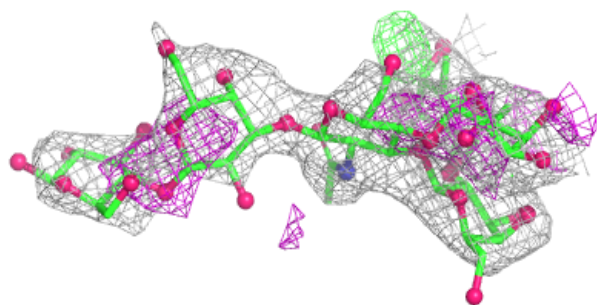
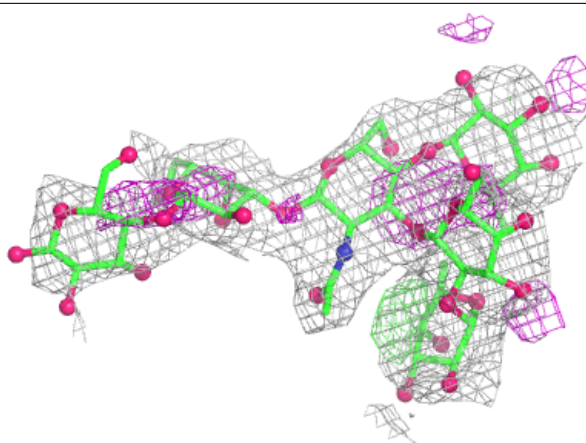
Electron density around Chain M:

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



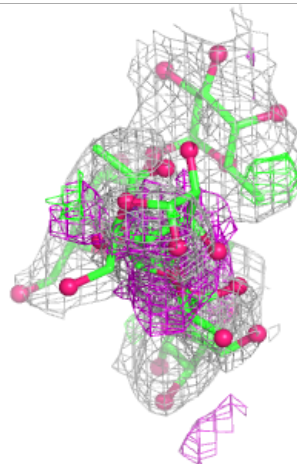
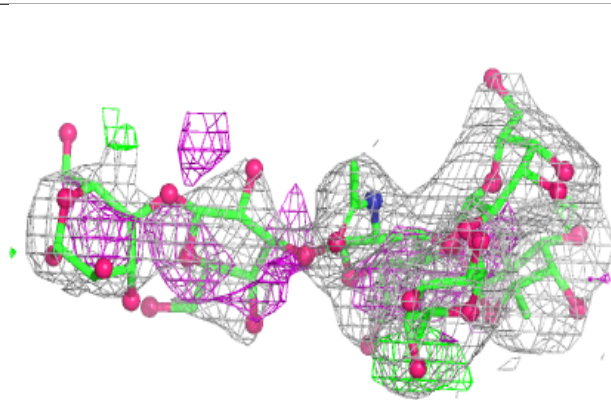
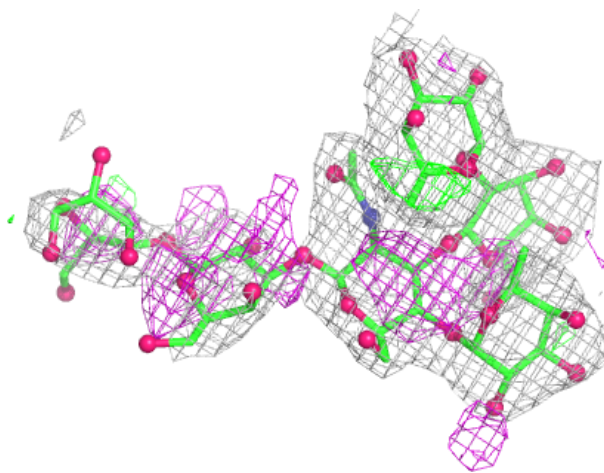
Electron density around Chain N:

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



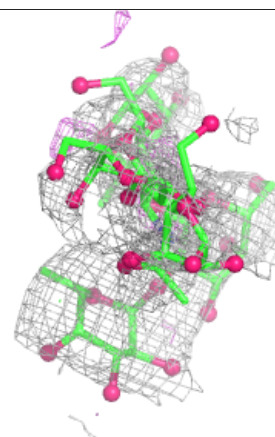
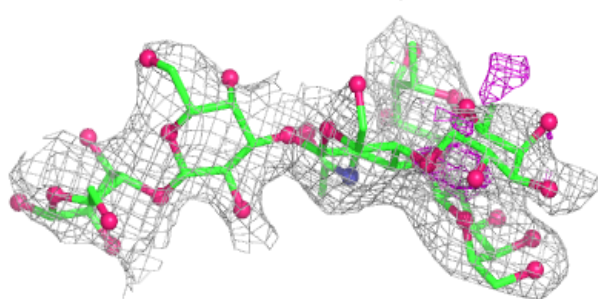
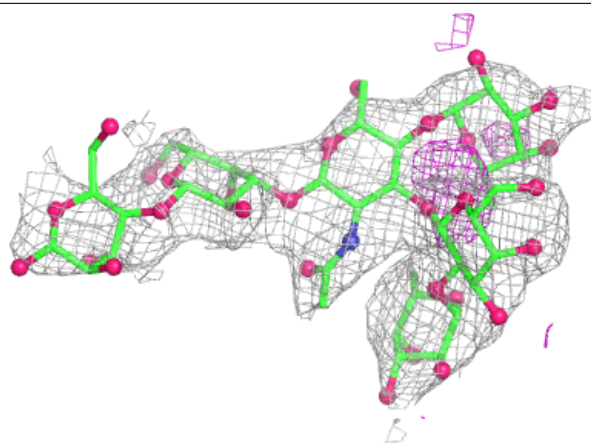
Electron density around Chain O:

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



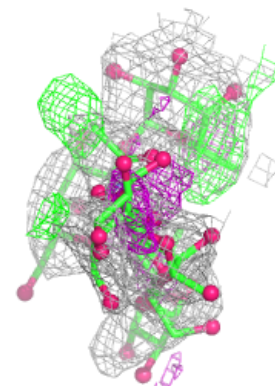
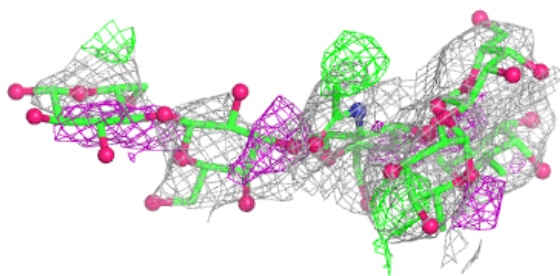
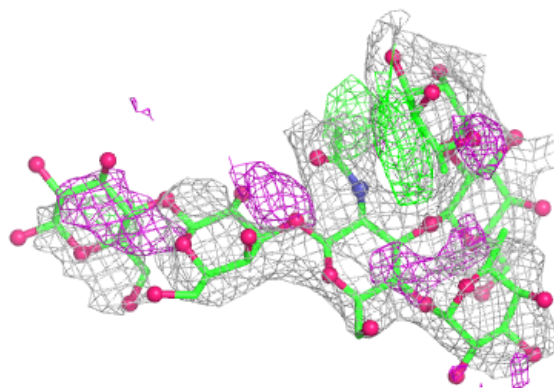
Electron density around Chain P:

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

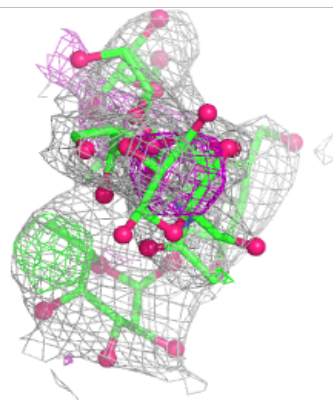
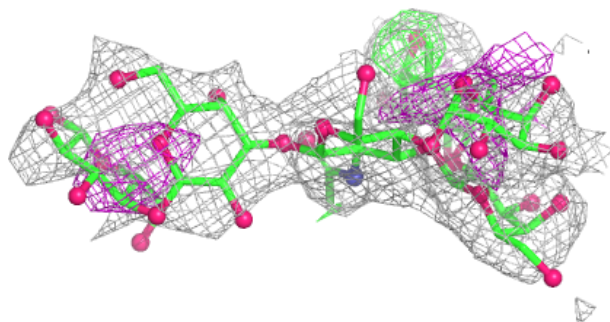
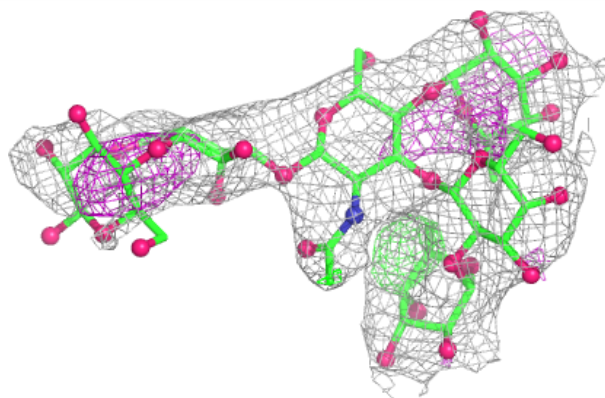


Electron density around Chain Q:

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

**Electron density around Chain R:**

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



6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.