wwPDB X-ray Structure Validation Summary Report (i)

Aug 6, 2020 – 05:57 PM BST

PDB ID	:	3D12
Title	:	Crystal Structures of Nipah Virus G Attachment Glycoprotein in Complex with its Receptor Ephrin-B3
Authors	:	Xu, K.; Rajashankar, K.R.; Chan, Y.P.; Himanen, P.; Broder, C.C.; Nikolov, D.B.
Deposited on	:	2008-05-02
Resolution	:	3.00 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

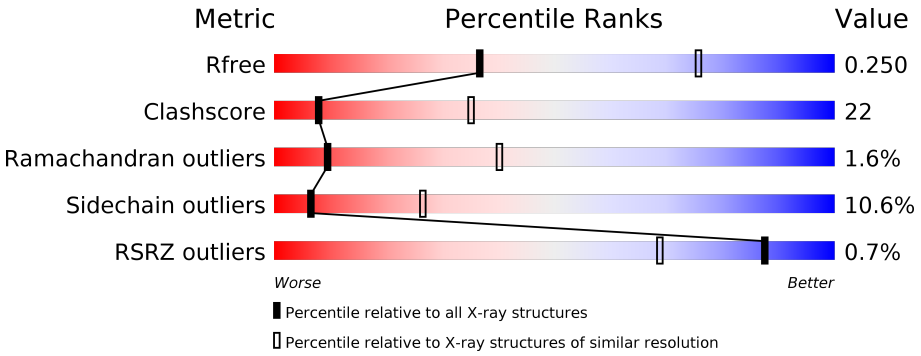
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 on 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 <=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	428	% 57% 36% 6%
1	D	428	58% 35% 7%
2	B	141	% 57% 37% 6%
2	E	141	53% 40% 6%
3	C	5	60% 40%
4	F	7	57% 14% 29%

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Mol	Chain	Length	Quality of chain
5	G	2	
5	J	2	
6	H	5	
7	I	7	

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
4	NGA	F	2	X	-	-	-
4	GL0	F	3	X	-	-	-
4	GLC	F	5	X	-	-	-
4	BGC	F	6	X	-	-	-
4	GLC	F	7	X	-	-	-
5	NAG	G	1	X	-	-	-
5	NAG	G	2	X	-	-	-
5	NAG	J	1	X	-	-	-
5	NAG	J	2	X	-	-	-
6	BMA	H	3	-	-	-	X
6	BGC	H	4	-	-	-	X
6	MAN	H	5	-	-	-	X
7	NGZ	I	2	X	-	-	-
7	GL0	I	3	X	-	-	-
7	BGC	I	4	-	-	-	X
7	GLC	I	5	X	-	-	-
7	BGC	I	6	X	-	-	-
7	GXL	I	7	X	-	-	-
8	NAG	D	1310	X	-	-	-
9	SO4	A	1368	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 9598 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-neuraminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	0	0
			3370	2146	568	635	21			
1	D	428	Total	C	N	O	S	0	0	0
			3370	2146	568	635	21			

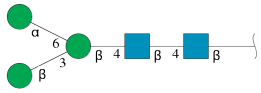
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	603	ALA	-	expression tag	UNP Q9IH62
D	603	ALA	-	expression tag	UNP Q9IH62

- Molecule 2 is a protein called Ephrin-B3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	141	Total	C	N	O	S	0	0	0
			1132	720	201	206	5			
2	E	141	Total	C	N	O	S	0	0	0
			1132	720	201	206	5			

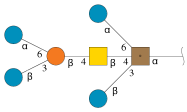
- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 4 is an oligosaccharide called beta-D-glucopyranose-(1-3)-[alpha-D-glucopyranose-

(1-6)]beta-D-gulopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[beta-D-glucopyranose-(1-3)][alpha-D-glucopyranose-(1-6)]2-acetamido-2-deoxy-alpha-D-idopyranose.

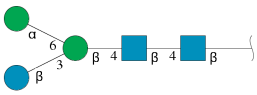


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

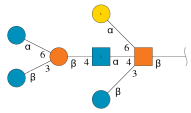
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is an oligosaccharide called beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



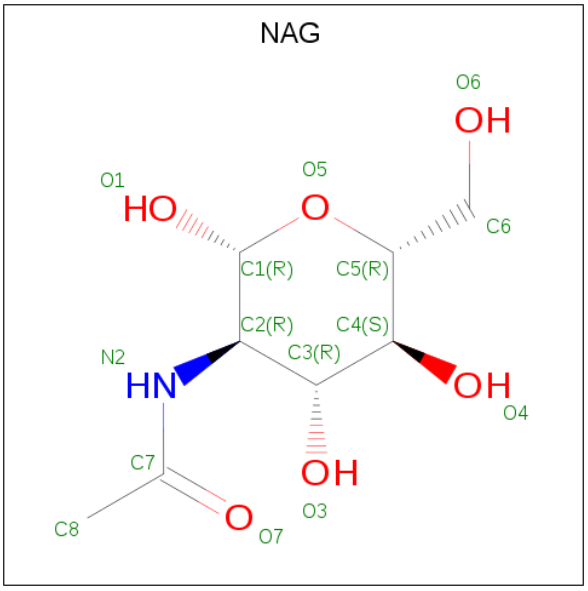
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	H	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 7 is an oligosaccharide called beta-D-glucopyranose-(1-3)-[alpha-D-glucopyranose-(1-6)]beta-D-gulopyranose-(1-4)-2-acetamido-2-deoxy-alpha-L-glucopyranose-(1-4)-[beta-D-glucopyranose-(1-3)][alpha-L-galactopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-gulopyranose.



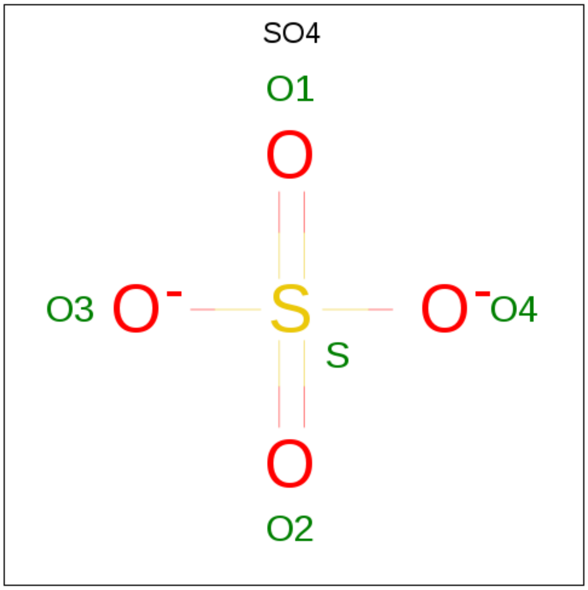
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	I	7	Total C N O 83 46 2 35	0	0	0

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	D	1	Total O S 5 4 1	0	0
9	D	1	Total O S 5 4 1	0	0
9	D	1	Total O S 5 4 1	0	0
9	D	1	Total O S 5 4 1	0	0
9	D	1	Total O S 5 4 1	0	0
9	D	1	Total O S 5 4 1	0	0
9	D	1	Total O S 5 4 1	0	0
9	E	1	Total O S 5 4 1	0	0

- Molecule 10 is water.

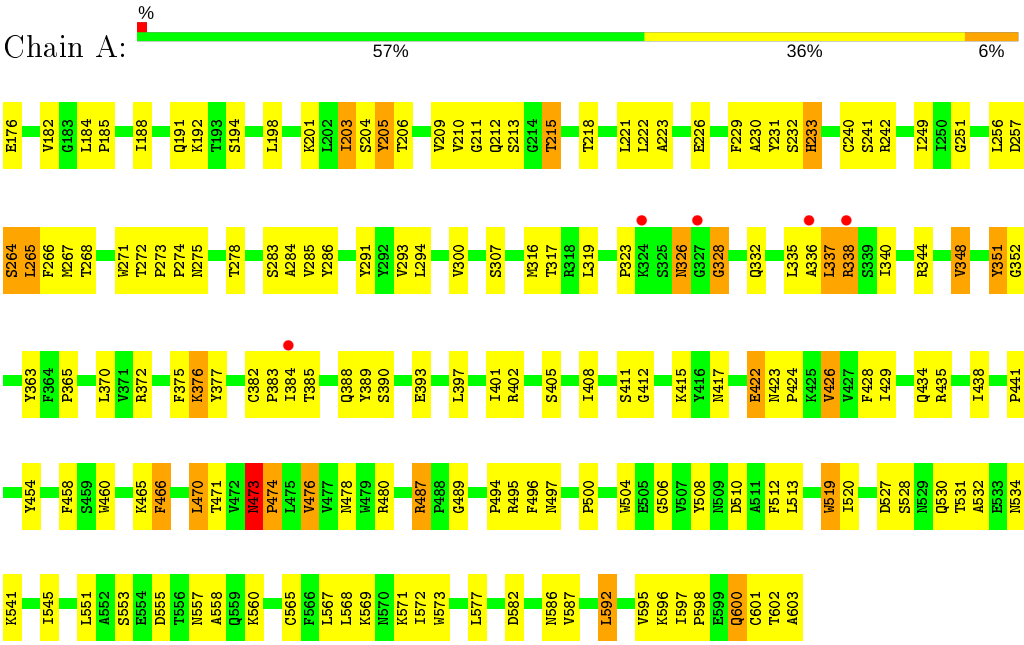
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	46	Total O 46 46	0	0
10	B	9	Total O 9 9	0	0
10	D	44	Total O 44 44	0	0
10	E	13	Total O 13 13	0	0

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.

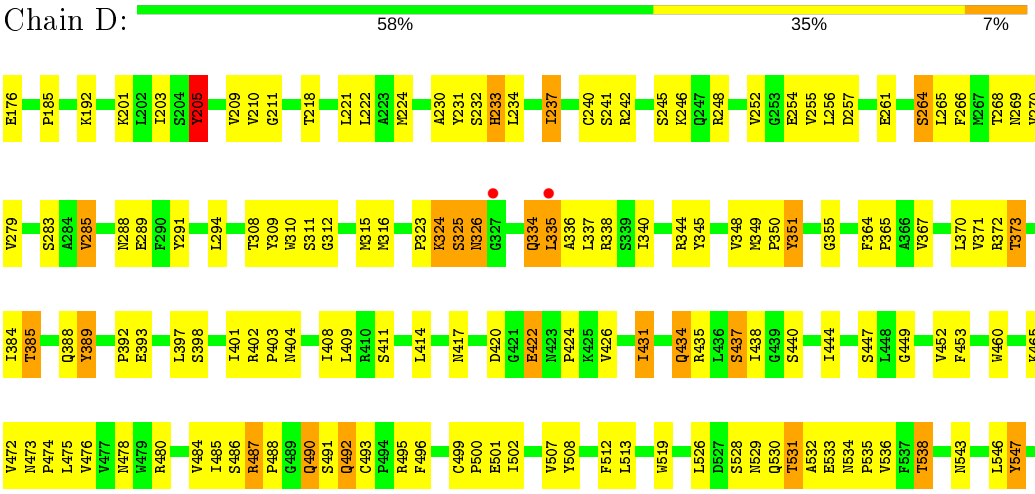
- Molecule 1: Hemagglutinin-neuraminidase

Chain A:



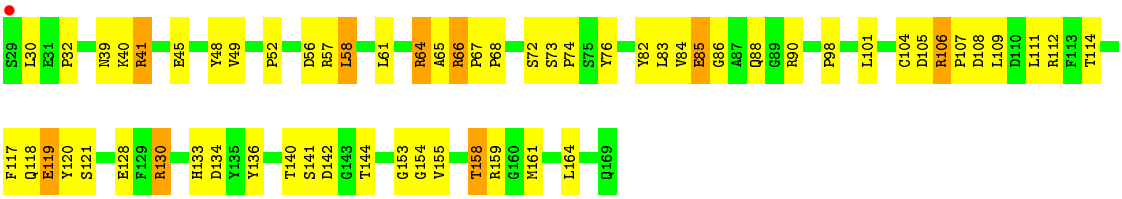
- Molecule 1: Hemagglutinin-neuraminidase

Chain D:



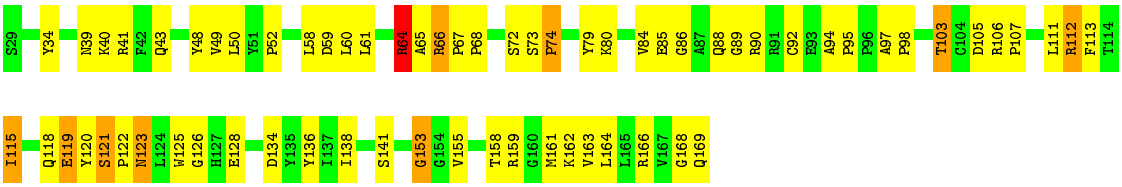
• Molecule 2: Ephrin-B3

Chain B:



• Molecule 2: Ephrin-B3

Chain E:



• Molecule 3: beta-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

• Molecule 4: beta-D-glucopyranose-(1-3)-[alpha-D-glucopyranose-(1-6)]beta-D-gulopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[beta-D-glucopyranose-(1-3)][alpha-D-glucopyranose-(1-6)]2-acetamido-2-deoxy-alpha-D-idopyranose

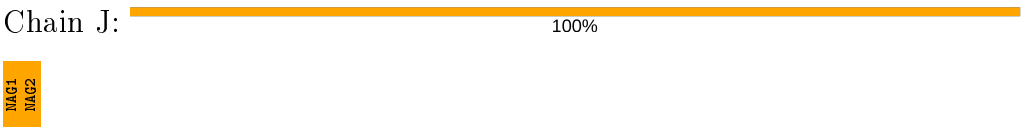
Chain F:

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

Chain G:

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

Chain J:



• Molecule 6: beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

• Molecule 7: beta-D-glucopyranose-(1-3)-[alpha-D-glucopyranose-(1-6)]beta-D-gulopyranose-(1-4)-2-acetamido-2-deoxy-alpha-L-glucopyranose-(1-4)-[beta-D-glucopyranose-(1-3)][alpha-L-galactopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-gulopyranose

Chain I:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	189.49Å 189.49Å 277.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.34 – 3.00 39.34 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.3 (39.34-3.00) 91.4 (39.34-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.57 (at 3.01Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.221 , 0.265 0.212 , 0.250	Depositor DCC
R_{free} test set	2911 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	62.2	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 48.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9598	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: BGC, NAG, GXL, GLC, LXZ, NGA, BMA, SO4, GL0, MAN, NGZ, LXB

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	1/3451 (0.0%)	0.54	0/4694
1	D	0.45	1/3451 (0.0%)	0.54	0/4694
2	B	0.37	0/1165	0.54	0/1582
2	E	0.39	0/1165	0.54	0/1582
All	All	0.44	2/9232 (0.0%)	0.54	0/12552

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
1	D	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	176	GLU	CD-OE2	7.35	1.33	1.25
1	D	176	GLU	CD-OE2	7.19	1.33	1.25

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	473	ASN	Peptide
1	D	473	ASN	Peptide

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	3370	0	3313	145	0
1	D	3370	0	3313	143	0
2	B	1132	0	1094	53	0
2	E	1132	0	1094	66	0
3	C	61	0	52	1	0
4	F	83	0	70	1	0
5	G	28	0	25	2	0
5	J	28	0	25	1	0
6	H	61	0	52	3	0
7	I	83	0	70	5	0
8	A	14	0	13	0	0
8	D	14	0	13	0	0
9	A	45	0	0	4	0
9	B	10	0	0	1	0
9	D	50	0	0	0	0
9	E	5	0	0	1	0
10	A	46	0	0	2	0
10	B	9	0	0	0	0
10	D	44	0	0	2	0
10	E	13	0	0	1	0
All	All	9598	0	9134	401	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 22.

The worst 5 of 401 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:LYS:H	1:A:376:LYS:HD3	1.26	0.97
1:D:403:PRO:HG3	1:D:502:ILE:HD11	1.44	0.97
1:A:376:LYS:N	1:A:376:LYS:HD3	1.81	0.94
1:D:531:THR:HG21	1:D:533:GLU:OE2	1.71	0.90
2:B:86:GLY:HA2	2:B:136:TYR:HD1	1.37	0.90

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	426/428 (100%)	382 (90%)	40 (9%)	4 (1%)	17 55
1	D	426/428 (100%)	372 (87%)	50 (12%)	4 (1%)	17 55
2	B	139/141 (99%)	120 (86%)	13 (9%)	6 (4%)	2 15
2	E	139/141 (99%)	118 (85%)	17 (12%)	4 (3%)	4 24
All	All	1130/1138 (99%)	992 (88%)	120 (11%)	18 (2%)	9 40

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	64	ARG
2	E	64	ARG
1	A	338	ARG
2	B	45	GLU
2	B	153	GLY

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	382/382 (100%)	344 (90%)	38 (10%)	8 30
1	D	382/382 (100%)	335 (88%)	47 (12%)	4 21
2	B	121/121 (100%)	111 (92%)	10 (8%)	11 39
2	E	121/121 (100%)	109 (90%)	12 (10%)	8 30
All	All	1006/1006 (100%)	899 (89%)	107 (11%)	6 26

5 of 107 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	201	LYS
1	D	308	THR
2	E	64	ARG
1	D	205	TYR
1	D	264	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	326	ASN
1	D	334	GLN
2	E	123	ASN
1	D	332	GLN
1	D	423	ASN

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)

28 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	C	1	1,3	14,14,15	1.91	4 (28%)	17,19,21	2.00	5 (29%)
3	NAG	C	2	3	14,14,15	2.52	6 (42%)	17,19,21	1.42	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	BMA	C	3	3	11,11,12	2.02	5 (45%)	15,15,17	1.61	3 (20%)
3	BMA	C	4	3	11,11,12	1.63	3 (27%)	15,15,17	1.83	4 (26%)
3	MAN	C	5	3	11,11,12	1.65	3 (27%)	15,15,17	1.67	3 (20%)
4	LXZ	F	1	1,4	14,14,15	2.38	4 (28%)	17,19,21	1.81	5 (29%)
4	NGA	F	2	4	14,14,15	2.30	6 (42%)	17,19,21	2.37	6 (35%)
4	GL0	F	3	4	11,11,12	2.43	4 (36%)	15,15,17	2.31	5 (33%)
4	BGC	F	4	4	11,11,12	1.67	3 (27%)	15,15,17	1.44	2 (13%)
4	GLC	F	5	4	11,11,12	1.64	4 (36%)	15,15,17	1.32	2 (13%)
4	BGC	F	6	4	11,11,12	1.32	2 (18%)	15,15,17	2.43	4 (26%)
4	GLC	F	7	4	11,11,12	1.55	3 (27%)	15,15,17	1.63	3 (20%)
5	NAG	G	1	1,5	14,14,15	1.95	4 (28%)	17,19,21	2.09	5 (29%)
5	NAG	G	2	5	14,14,15	2.21	4 (28%)	17,19,21	1.70	4 (23%)
6	NAG	H	1	1,6	14,14,15	2.02	6 (42%)	17,19,21	1.36	2 (11%)
6	NAG	H	2	6	14,14,15	2.46	8 (57%)	17,19,21	1.68	6 (35%)
6	BMA	H	3	6	11,11,12	2.17	5 (45%)	15,15,17	1.55	4 (26%)
6	BGC	H	4	6	11,11,12	1.86	4 (36%)	15,15,17	2.58	7 (46%)
6	MAN	H	5	6	11,11,12	1.80	3 (27%)	15,15,17	1.23	2 (13%)
7	LXB	I	1	1,7	14,14,15	2.37	4 (28%)	17,19,21	1.67	4 (23%)
7	NGZ	I	2	7	14,14,15	2.41	7 (50%)	17,19,21	1.85	5 (29%)
7	GL0	I	3	7	11,11,12	2.43	4 (36%)	15,15,17	2.65	6 (40%)
7	BGC	I	4	7	11,11,12	1.59	3 (27%)	15,15,17	1.25	2 (13%)
7	GLC	I	5	7	11,11,12	1.58	3 (27%)	15,15,17	1.60	3 (20%)
7	BGC	I	6	7	11,11,12	1.30	1 (9%)	15,15,17	2.56	4 (26%)
7	GXL	I	7	7	11,11,12	1.54	4 (36%)	15,15,17	1.17	0
5	NAG	J	1	1,5	14,14,15	1.96	4 (28%)	17,19,21	1.83	5 (29%)
5	NAG	J	2	5	14,14,15	2.29	4 (28%)	17,19,21	1.64	3 (17%)

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	C	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	C	4	3	-	2/2/19/22	0/1/1/1
3	MAN	C	5	3	-	2/2/19/22	0/1/1/1
4	LXZ	F	1	1,4	-	2/6/23/26	0/1/1/1
4	NGA	F	2	4	5/5/5/7	2/6/23/26	0/1/1/1
4	GL0	F	3	4	1/1/4/5	2/2/19/22	0/1/1/1
4	BGC	F	4	4	-	2/2/19/22	0/1/1/1
4	GLC	F	5	4	5/5/4/5	2/2/19/22	0/1/1/1
4	BGC	F	6	4	1/1/4/5	0/2/19/22	0/1/1/1
4	GLC	F	7	4	5/5/4/5	2/2/19/22	0/1/1/1
5	NAG	G	1	1,5	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	G	2	5	1/1/5/7	2/6/23/26	0/1/1/1
6	NAG	H	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	H	2	6	-	1/6/23/26	0/1/1/1
6	BMA	H	3	6	-	2/2/19/22	0/1/1/1
6	BGC	H	4	6	-	0/2/19/22	0/1/1/1
6	MAN	H	5	6	-	1/2/19/22	1/1/1/1
7	LXB	I	1	1,7	-	2/6/23/26	0/1/1/1
7	NGZ	I	2	7	1/1/5/7	0/6/23/26	0/1/1/1
7	GL0	I	3	7	1/1/4/5	0/2/19/22	0/1/1/1
7	BGC	I	4	7	-	0/2/19/22	0/1/1/1
7	GLC	I	5	7	5/5/4/5	2/2/19/22	0/1/1/1
7	BGC	I	6	7	1/1/4/5	2/2/19/22	0/1/1/1
7	GXL	I	7	7	1/1/4/5	2/2/19/22	0/1/1/1
5	NAG	J	1	1,5	2/2/5/7	5/6/23/26	0/1/1/1
5	NAG	J	2	5	1/1/5/7	2/6/23/26	0/1/1/1

The worst 5 of 115 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	NAG	C1-C2	5.23	1.60	1.52
7	I	2	NGZ	C1-C2	5.17	1.60	1.52
5	J	2	NAG	C1-C2	4.90	1.59	1.52
7	I	1	LXB	C4-C5	4.74	1.63	1.53
4	F	1	LXZ	C4-C5	4.67	1.62	1.53

The worst 5 of 107 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	I	6	BGC	O5-C1-C2	6.95	121.50	110.77
7	I	3	GL0	C1-C2-C3	6.57	117.74	109.67
6	H	4	BGC	C1-C2-C3	5.88	116.90	109.67
5	G	1	NAG	C1-O5-C5	5.76	120.00	112.19
4	F	6	BGC	C1-C2-C3	5.71	116.69	109.67

5 of 31 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	I	6	BGC	C5
5	J	1	NAG	C2
5	J	1	NAG	C1
5	G	2	NAG	C1
7	I	3	GL0	C1

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	J	1	NAG	C1-C2-N2-C7
5	J	1	NAG	O7-C7-N2-C2
4	F	2	NGA	C1-C2-N2-C7
3	C	3	BMA	O5-C5-C6-O6
7	I	7	GXL	O5-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	H	5	MAN	C1-C2-C3-C4-C5-O5

13 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	4	BGC	2	0
7	I	4	BGC	1	0
3	C	4	BMA	1	0
7	I	1	LXB	4	0
5	G	2	NAG	1	0
7	I	3	GL0	1	0
6	H	1	NAG	1	0
5	G	1	NAG	1	0
3	C	3	BMA	1	0
4	F	7	GLC	1	0
5	J	2	NAG	1	0

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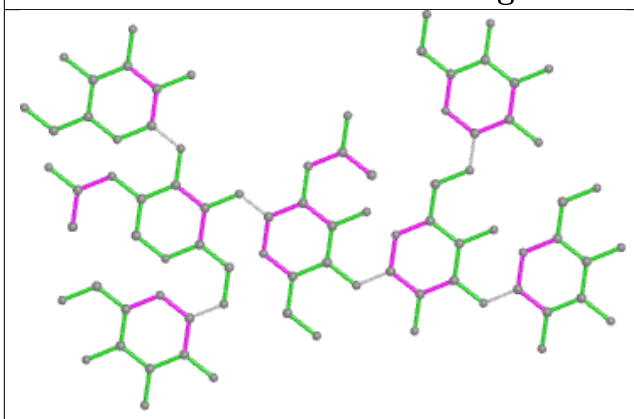
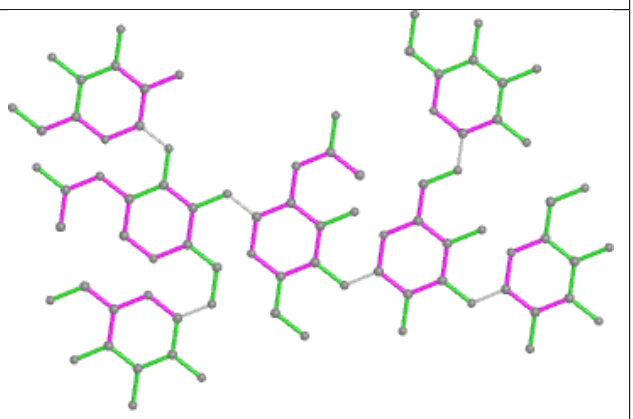
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	3	BMA	2	0
4	F	2	NGA	1	0

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

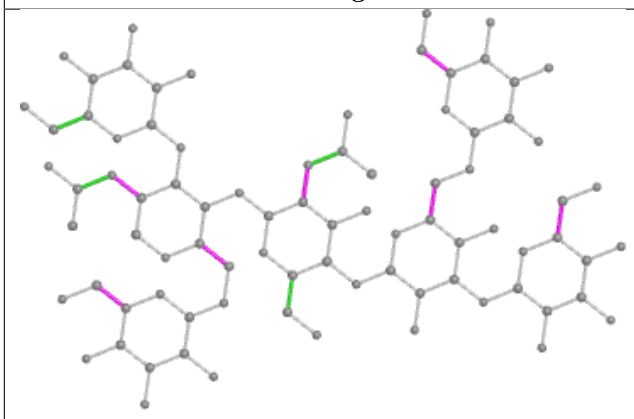
Oligosaccharide Chain F



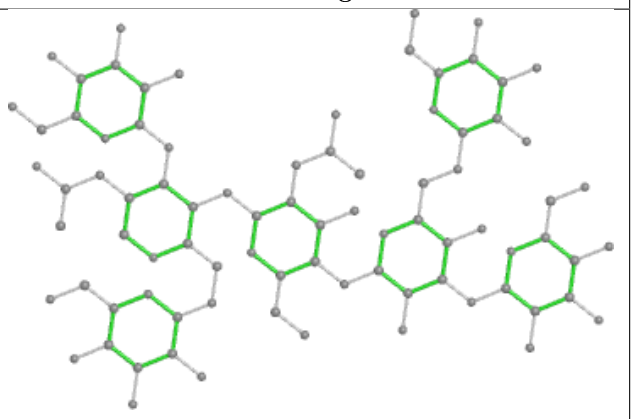
Bond lengths



Bond angles

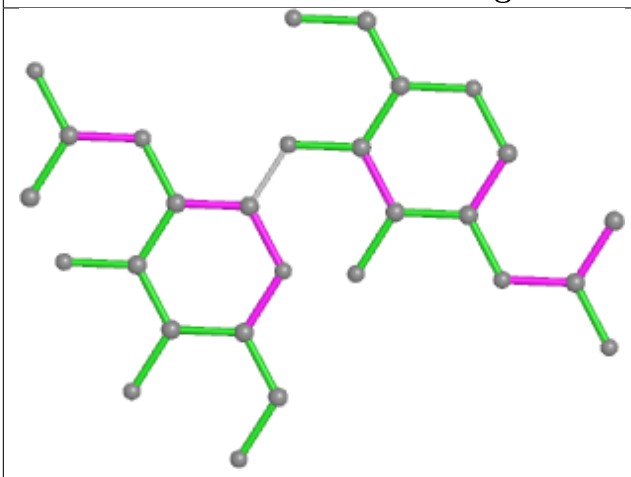


Torsions

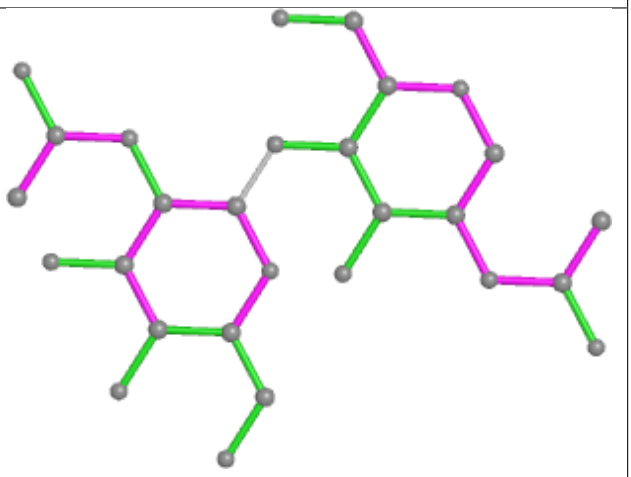


Rings

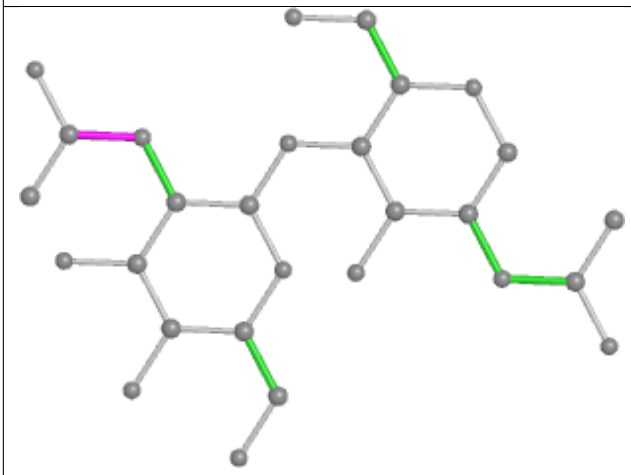
Oligosaccharide Chain G



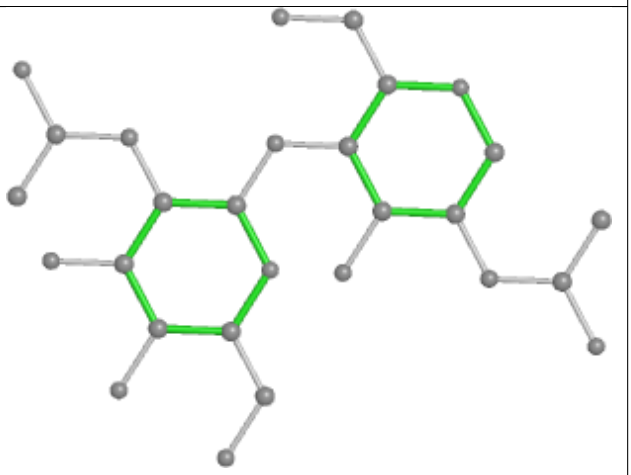
Bond lengths



Bond angles

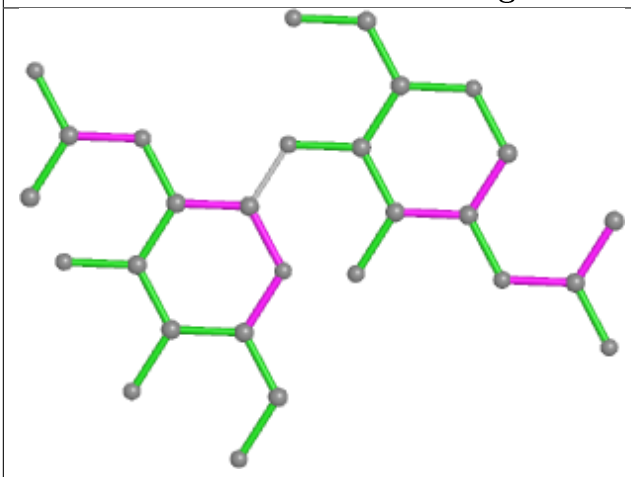


Torsions

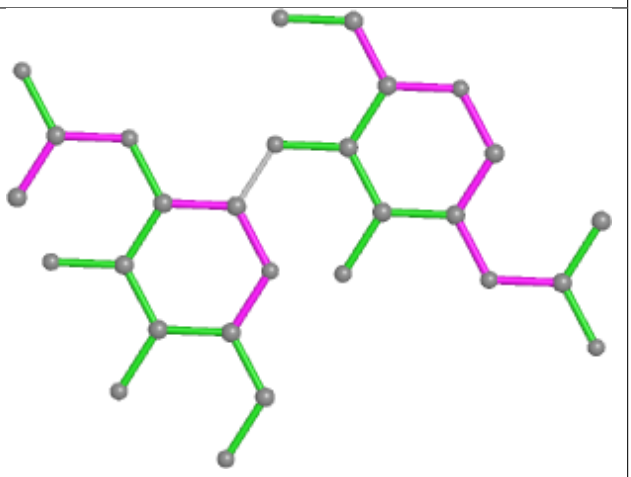


Rings

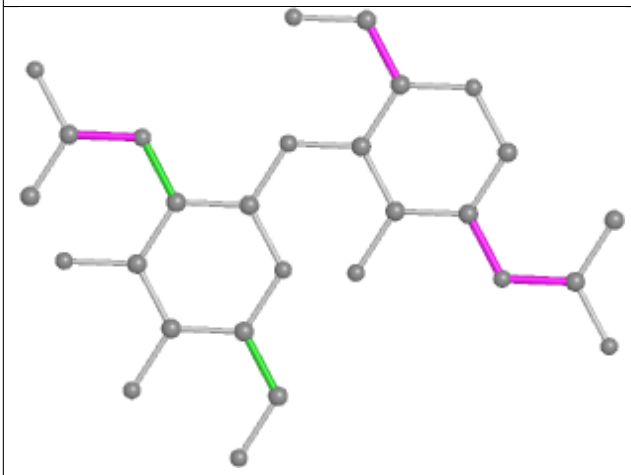
Oligosaccharide Chain J



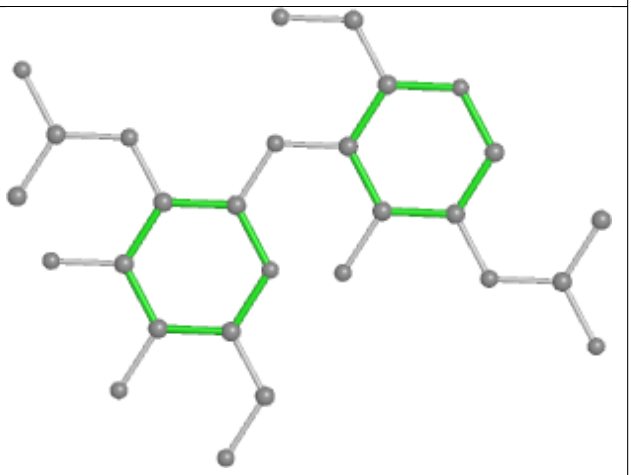
Bond lengths



Bond angles

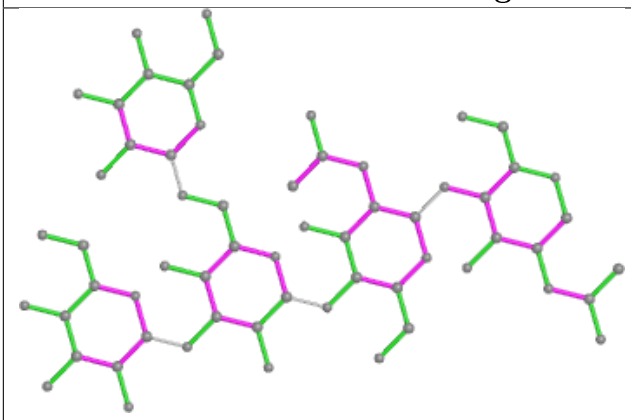


Torsions

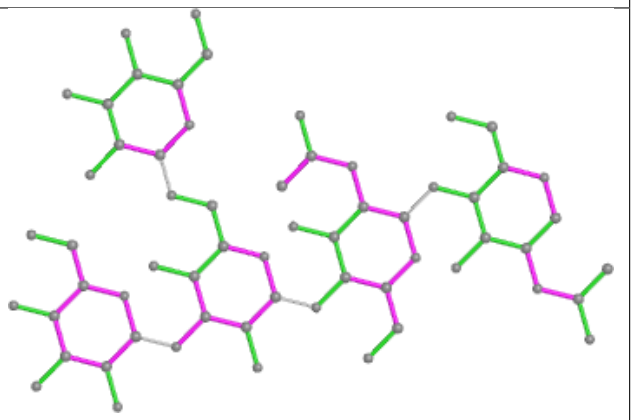


Rings

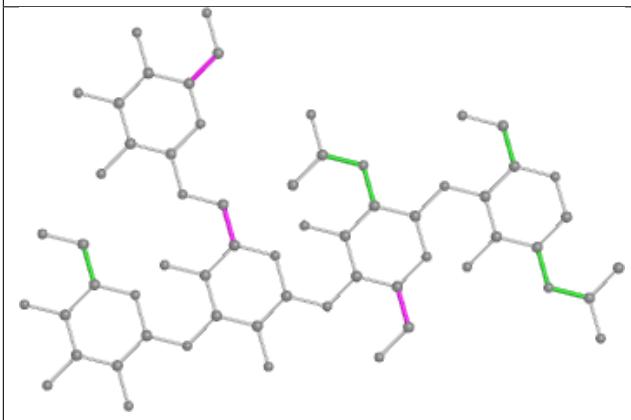
Oligosaccharide Chain H



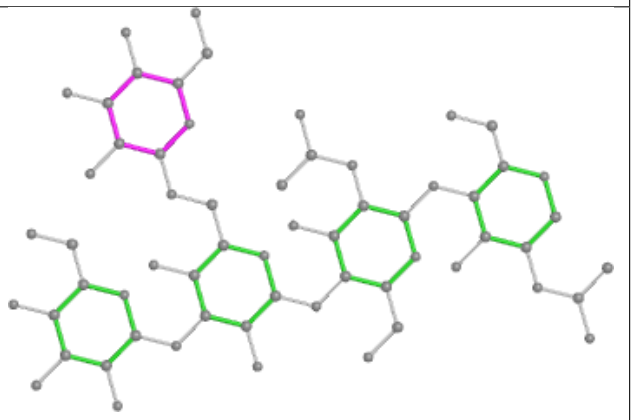
Bond lengths



Bond angles

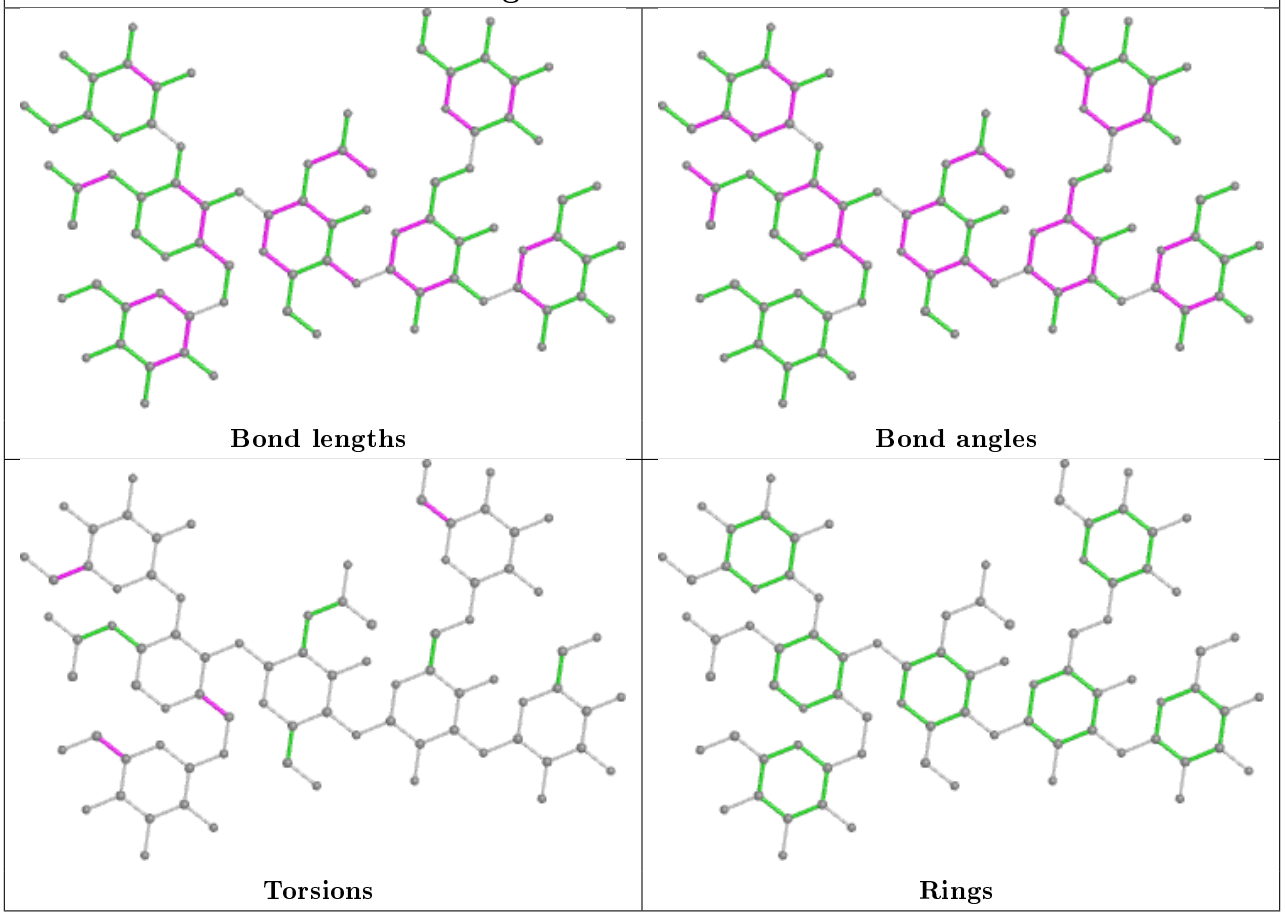


Torsions



Rings

Oligosaccharide Chain I



5.6 Ligand geometry (i)

24 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	$\#\|Z\| > 2$
9	SO4	D	1471	-	4,4,4	0.22	0	6,6,6	0.16	0
8	NAG	A	1210	1	14,14,15	1.69	3 (21%)	17,19,21	1.58	3 (17%)
9	SO4	D	1476	-	4,4,4	0.16	0	6,6,6	0.18	0
9	SO4	B	202	-	4,4,4	0.19	0	6,6,6	0.12	0
9	SO4	E	190	-	4,4,4	0.14	0	6,6,6	0.20	0
9	SO4	D	1477	-	4,4,4	0.15	0	6,6,6	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	SO4	D	1473	-	4,4,4	0.18	0	6,6,6	0.12	0
9	SO4	D	1474	-	4,4,4	0.28	0	6,6,6	0.27	0
9	SO4	A	1370	-	4,4,4	0.18	0	6,6,6	0.09	0
9	SO4	D	1472	-	4,4,4	0.16	0	6,6,6	0.18	0
8	NAG	D	1310	1	14,14,15	1.72	3 (21%)	17,19,21	1.24	2 (11%)
9	SO4	A	1368	-	4,4,4	0.24	0	6,6,6	0.28	0
9	SO4	A	1372	-	4,4,4	0.24	0	6,6,6	0.11	0
9	SO4	D	1469	-	4,4,4	0.16	0	6,6,6	0.10	0
9	SO4	A	1371	-	4,4,4	0.17	0	6,6,6	0.14	0
9	SO4	A	1369	-	4,4,4	0.27	0	6,6,6	0.29	0
9	SO4	B	203	-	4,4,4	0.16	0	6,6,6	0.11	0
9	SO4	D	1468	-	4,4,4	0.23	0	6,6,6	0.14	0
9	SO4	D	1470	-	4,4,4	0.18	0	6,6,6	0.14	0
9	SO4	A	1374	-	4,4,4	0.21	0	6,6,6	0.21	0
9	SO4	A	1373	-	4,4,4	0.19	0	6,6,6	0.17	0
9	SO4	D	1475	-	4,4,4	0.21	0	6,6,6	0.08	0
9	SO4	A	1375	-	4,4,4	0.30	0	6,6,6	0.37	0
9	SO4	A	1376	-	4,4,4	0.19	0	6,6,6	0.14	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
8	NAG	A	1210	1	-	5/6/23/26	0/1/1/1
8	NAG	D	1310	1	1/1/5/7	2/6/23/26	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1210	NAG	C7-N2	3.88	1.47	1.34
8	D	1310	NAG	C7-N2	3.72	1.47	1.34
8	D	1310	NAG	C1-C2	3.13	1.57	1.52
8	A	1210	NAG	C1-C2	3.01	1.56	1.52
8	A	1210	NAG	C8-C7	2.08	1.54	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	1210	NAG	C8-C7-N2	3.41	121.87	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	1210	NAG	C1-O5-C5	3.40	116.80	112.19
8	A	1210	NAG	C6-C5-C4	-2.24	107.76	113.00
8	D	1310	NAG	O5-C1-C2	2.19	114.74	111.29
8	D	1310	NAG	C1-O5-C5	2.14	115.09	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	D	1310	NAG	C1

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1210	NAG	C8-C7-N2-C2
8	A	1210	NAG	O5-C5-C6-O6
8	A	1210	NAG	O7-C7-N2-C2
8	A	1210	NAG	C4-C5-C6-O6
8	D	1310	NAG	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	E	190	SO4	1	0
9	A	1368	SO4	3	0
9	A	1371	SO4	1	0
9	B	203	SO4	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

6.1 Protein, DNA and RNA chains

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^{th} 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	428/428 (100%)	-0.25	5 (1%)	79	54	43, 59, 85, 110	0
1	D	428/428 (100%)	-0.29	2 (0%)	91	75	45, 61, 86, 104	0
2	B	141/141 (100%)	-0.21	1 (0%)	87	69	45, 72, 94, 106	0
2	E	141/141 (100%)	-0.30	0	100	100	48, 70, 97, 99	0
All	All	1138/1138 (100%)	-0.27	8 (0%)	87	69	43, 63, 90, 110	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	336	ALA	3.2
1	A	324	LYS	2.5
1	A	338	ARG	2.2
1	A	327	GLY	2.1
1	A	384	ILE	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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, 95^{th} 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	MAN	H	5	11/12	0.56	0.76	108,118,121,122	0
6	BGC	H	4	11/12	0.69	0.60	75,98,105,106	0

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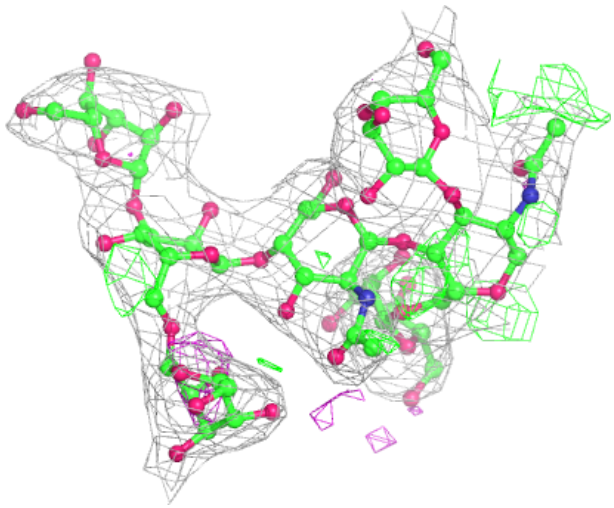
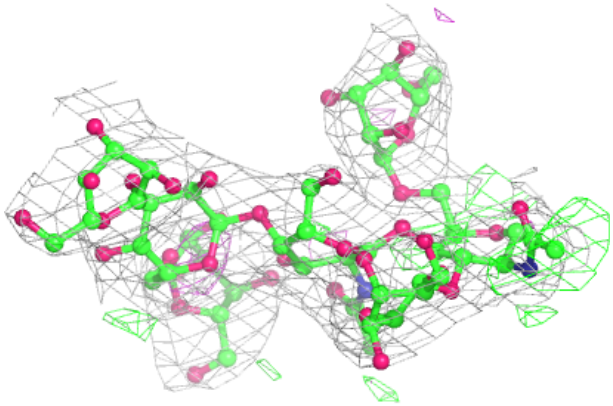
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	BMA	H	3	11/12	0.78	0.48	101,110,116,117	0
7	BGC	I	4	11/12	0.79	0.40	113,120,124,125	0
6	NAG	H	2	14/15	0.80	0.31	90,103,113,116	0
7	GL0	I	3	11/12	0.83	0.34	110,116,119,121	0
3	MAN	C	5	11/12	0.84	0.33	87,91,96,96	0
5	NAG	J	2	14/15	0.85	0.37	89,102,109,110	0
4	GLC	F	5	11/12	0.87	0.43	87,97,101,101	0
4	BGC	F	4	11/12	0.87	0.39	93,103,106,106	0
7	GLC	I	5	11/12	0.88	0.41	98,107,112,113	0
5	NAG	G	2	14/15	0.88	0.36	85,95,100,100	0
6	NAG	H	1	14/15	0.89	0.26	85,90,100,104	0
4	LXZ	F	1	14/15	0.91	0.16	65,70,80,81	0
3	BMA	C	4	11/12	0.91	0.29	86,90,93,93	0
4	BGC	F	6	11/12	0.91	0.21	75,81,87,90	0
5	NAG	J	1	14/15	0.91	0.18	72,83,92,104	0
5	NAG	G	1	14/15	0.92	0.21	62,79,89,97	0
7	GXL	I	7	11/12	0.92	0.20	69,79,90,91	0
4	GL0	F	3	11/12	0.93	0.26	93,97,99,101	0
7	BGC	I	6	11/12	0.93	0.19	79,82,87,89	0
4	NGA	F	2	14/15	0.93	0.18	71,80,84,91	0
7	NGZ	I	2	14/15	0.94	0.25	70,92,99,106	0
7	LXB	I	1	14/15	0.94	0.15	73,76,80,85	0
3	NAG	C	1	14/15	0.94	0.15	55,59,65,67	0
4	GLC	F	7	11/12	0.94	0.21	69,75,82,90	0
3	BMA	C	3	11/12	0.95	0.16	75,81,86,89	0
3	NAG	C	2	14/15	0.96	0.14	60,67,72,73	0

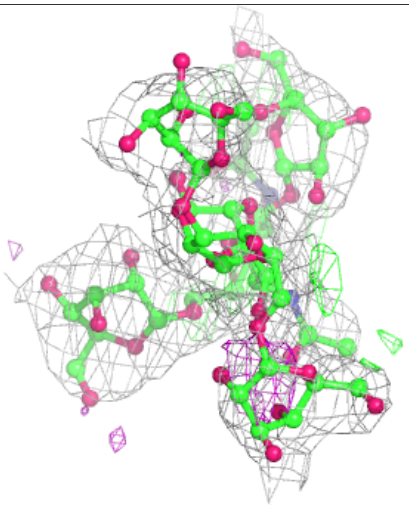
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain F:

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

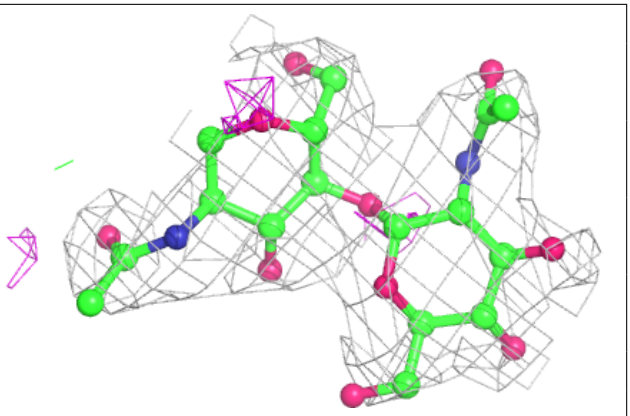


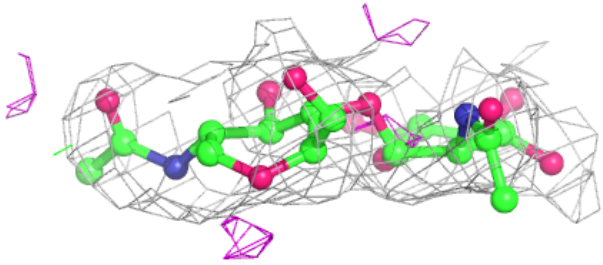


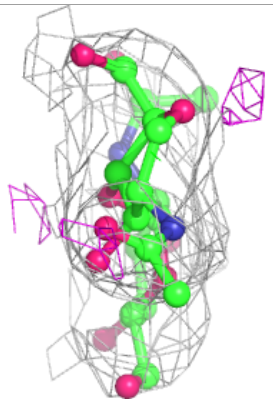


Electron density around Chain G:

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

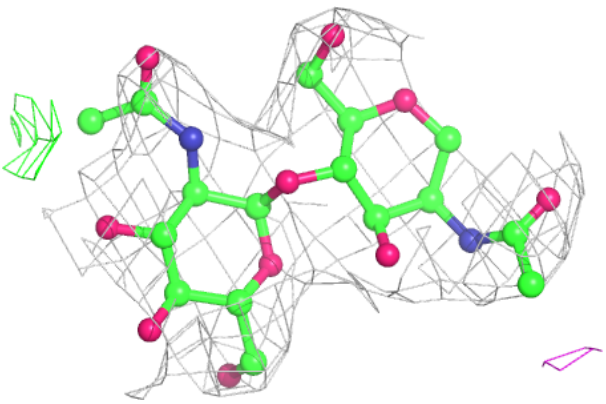


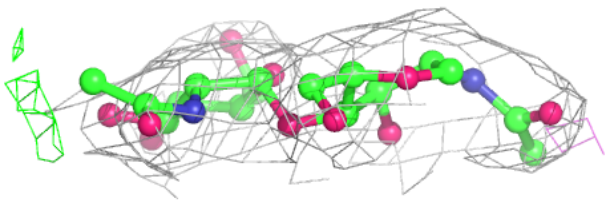


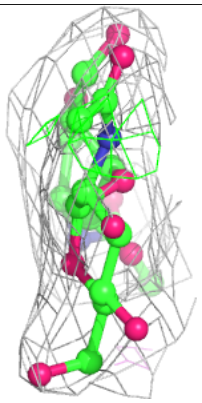


Electron density around Chain J:

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

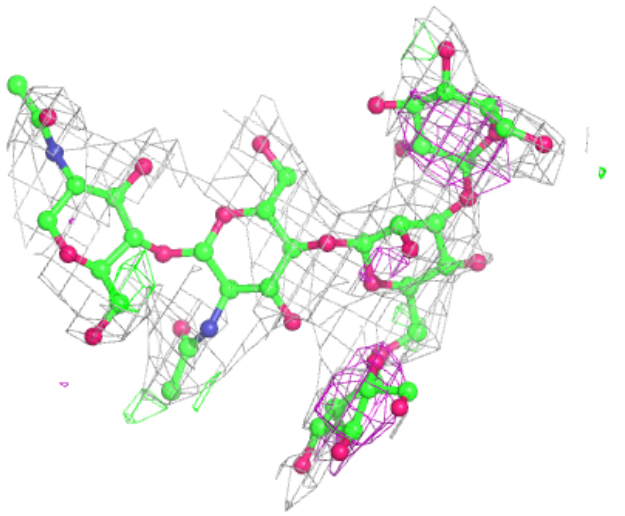


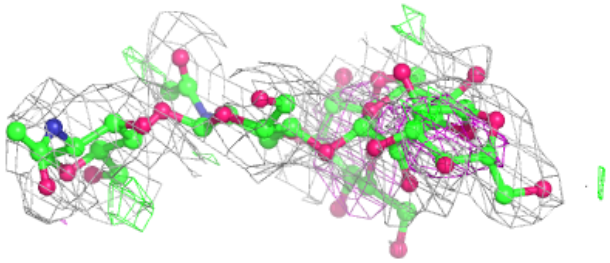


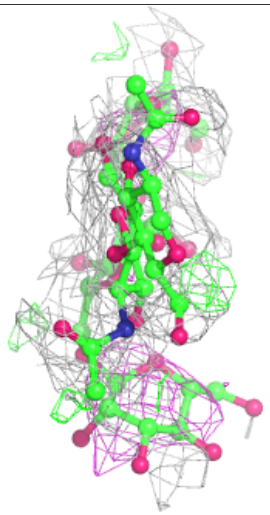


Electron density around Chain H:

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

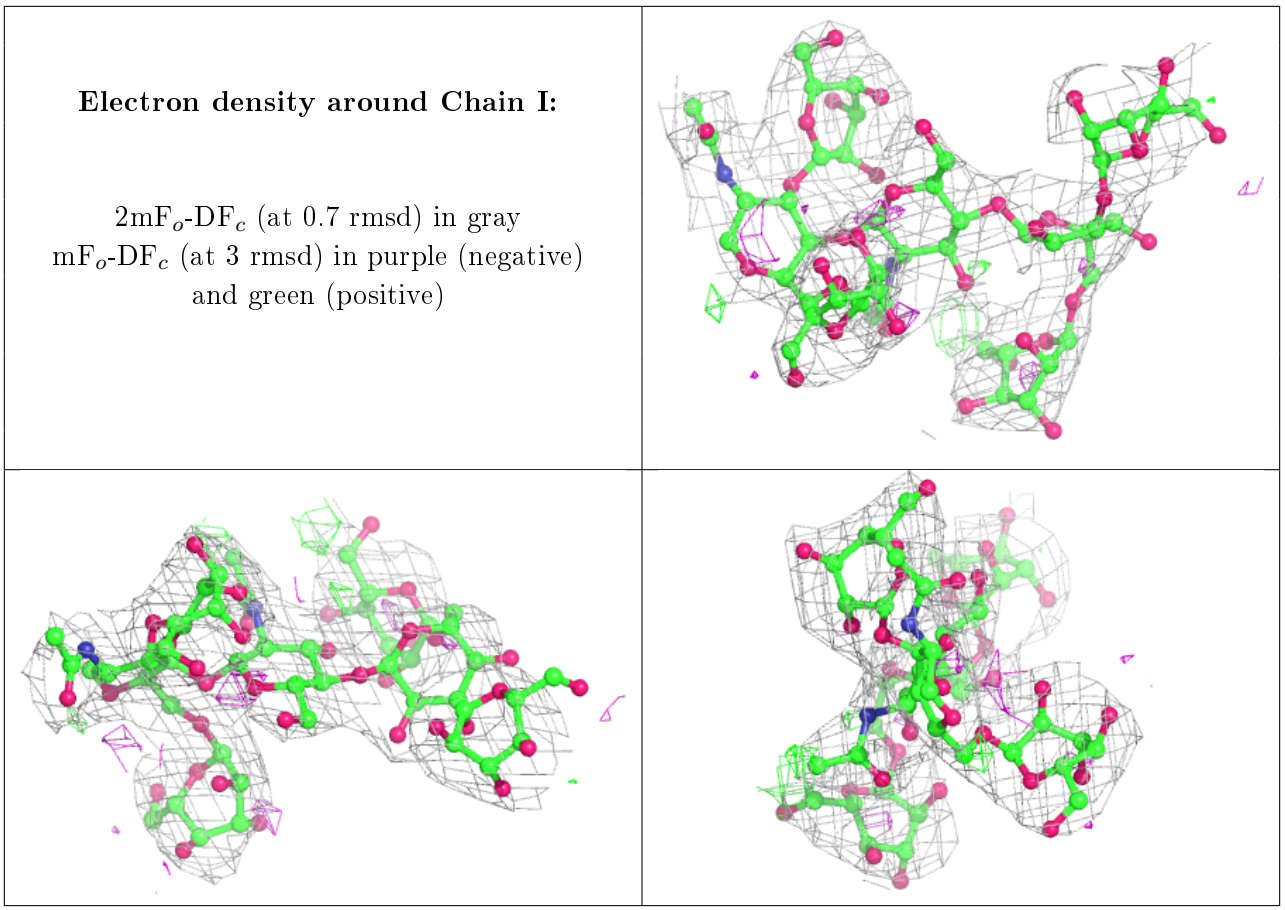






Electron density around Chain I:

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



6.4 Ligands

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^{th} 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
9	SO4	D	1477	5/5	0.74	0.32	105,107,117,130	0
9	SO4	D	1470	5/5	0.75	0.30	109,117,128,134	0
9	SO4	D	1469	5/5	0.81	0.34	124,128,134,144	0
9	SO4	D	1471	5/5	0.82	0.59	84,97,109,120	0
8	NAG	D	1310	14/15	0.82	0.35	95,105,108,108	0
9	SO4	D	1473	5/5	0.83	0.45	105,111,123,131	0
9	SO4	A	1372	5/5	0.83	0.38	81,92,102,116	0
9	SO4	A	1373	5/5	0.83	0.31	93,99,118,124	0
9	SO4	A	1375	5/5	0.84	0.38	82,83,103,104	0
9	SO4	D	1472	5/5	0.85	0.37	98,103,119,121	0
9	SO4	D	1474	5/5	0.85	0.41	90,95,109,114	0
9	SO4	A	1371	5/5	0.85	0.32	108,110,117,129	0
8	NAG	A	1210	14/15	0.87	0.30	88,92,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	SO4	A	1374	5/5	0.87	0.31	92,99,110,121	0
9	SO4	B	203	5/5	0.88	0.33	108,108,125,130	0
9	SO4	E	190	5/5	0.89	0.37	105,109,123,130	0
9	SO4	A	1370	5/5	0.89	0.28	116,121,126,139	0
9	SO4	B	202	5/5	0.94	0.36	102,106,112,126	0
9	SO4	D	1475	5/5	0.94	0.23	88,88,100,108	0
9	SO4	D	1468	5/5	0.94	0.12	81,86,90,97	0
9	SO4	A	1368	5/5	0.95	0.21	58,60,64,67	0
9	SO4	A	1369	5/5	0.96	0.16	57,66,73,79	0
9	SO4	D	1476	5/5	0.96	0.14	86,89,99,105	0
9	SO4	A	1376	5/5	0.96	0.22	86,88,100,108	0

6.5 Other polymers (i)

There are no such residues in this entry.