wwPDB X-ray Structure Validation Summary Report (i)

Sep 28, 2024 – 09:26 AM EDT

PDB ID	:	4QBZ
Title	:	Crystal structure of human TLR8 in complex with DS-802
Authors	:	Tanji, H.; Ohto, U.; Shimizu, T.
Deposited on	:	2014-05-09
Resolution	:	2.00 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

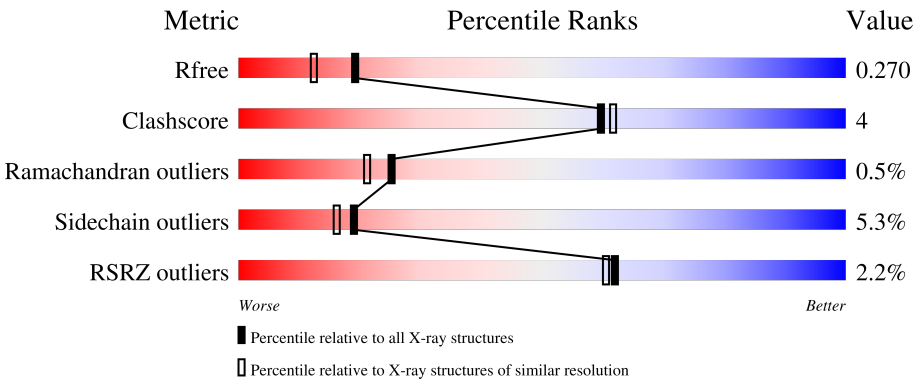
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.00 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}	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

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 <=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	811	2%, 81%, 10%, •, 7%
1	B	811	2%, 80%, 11%, •, 7%
2	C	5	80%, 20%
3	D	2	100%
3	G	2	100%

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Mol	Chain	Length	Quality of chain
4	E	3	67% 33%
4	H	3	100%
5	F	4	100%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 13074 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 Toll-like receptor 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	754	6071	3882	1029	1141	19	0	0	0
1	B	751	6062	3878	1031	1134	19	0	1	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	ARG	-	expression tag	UNP Q9NR97
A	24	SER	-	expression tag	UNP Q9NR97
A	25	PRO	-	expression tag	UNP Q9NR97
A	26	TRP	-	expression tag	UNP Q9NR97
A	828	GLU	-	expression tag	UNP Q9NR97
A	829	PHE	-	expression tag	UNP Q9NR97
A	830	LEU	-	expression tag	UNP Q9NR97
A	831	VAL	-	expression tag	UNP Q9NR97
A	832	PRO	-	expression tag	UNP Q9NR97
A	833	ARG	-	expression tag	UNP Q9NR97
B	23	ARG	-	expression tag	UNP Q9NR97
B	24	SER	-	expression tag	UNP Q9NR97
B	25	PRO	-	expression tag	UNP Q9NR97
B	26	TRP	-	expression tag	UNP Q9NR97
B	828	GLU	-	expression tag	UNP Q9NR97
B	829	PHE	-	expression tag	UNP Q9NR97
B	830	LEU	-	expression tag	UNP Q9NR97
B	831	VAL	-	expression tag	UNP Q9NR97
B	832	PRO	-	expression tag	UNP Q9NR97
B	833	ARG	-	expression tag	UNP Q9NR97

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(2-3)-[beta-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
			Total	C	N	O			
2	C	5	61	34	2	25	0	0	0

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

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

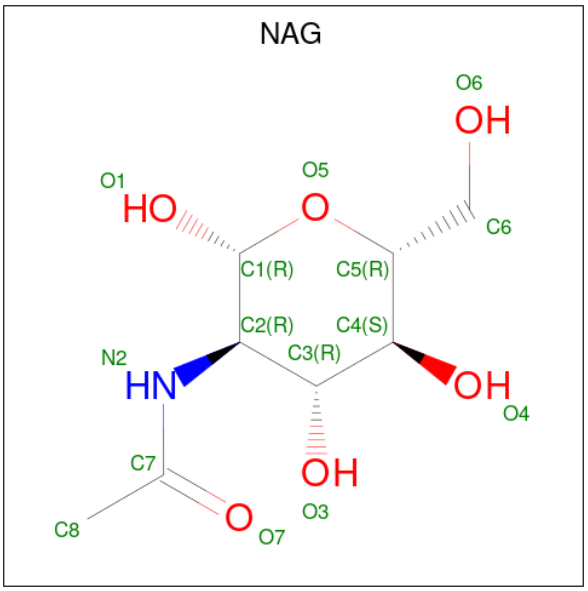
- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	E	3	39	22	2	15	0	0	0
4	H	3	39	22	2	15	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

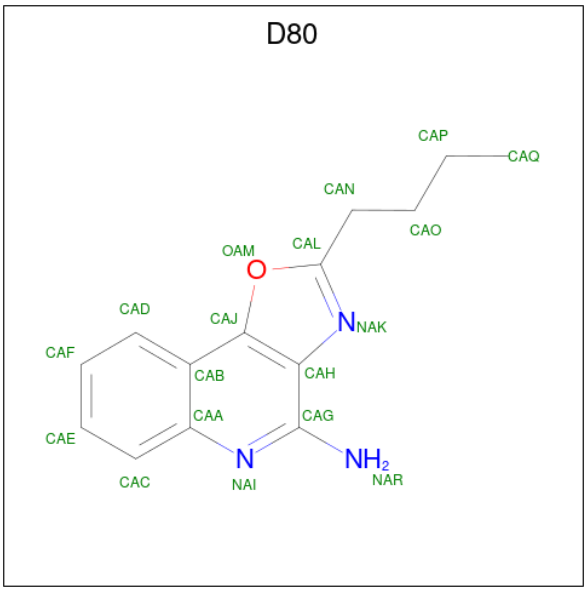
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	F	4	50	28	2	20	0	0	0

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



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

- Molecule 7 is 2-butyl[1,3]oxazolo[4,5-c]quinolin-4-amine (three-letter code: D80) (formula: $C_{14}H_{15}N_3O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	A	1	18	14	3	1	0	0
			Total	C	N	O		
7	B	1	18	14	3	1	0	0

- Molecule 8 is water.

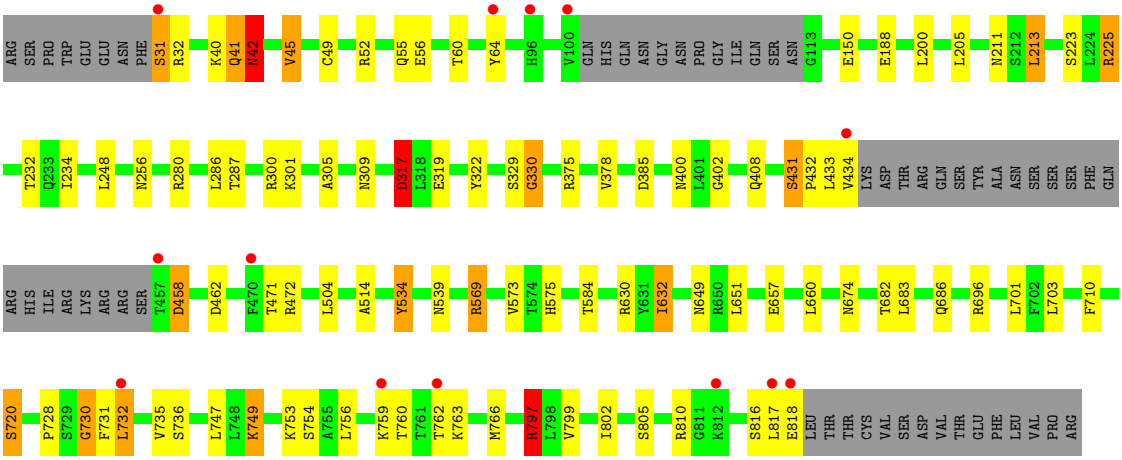
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	277	277	277	0	0
			Total	O		
8	B	229	229	229	0	0

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.

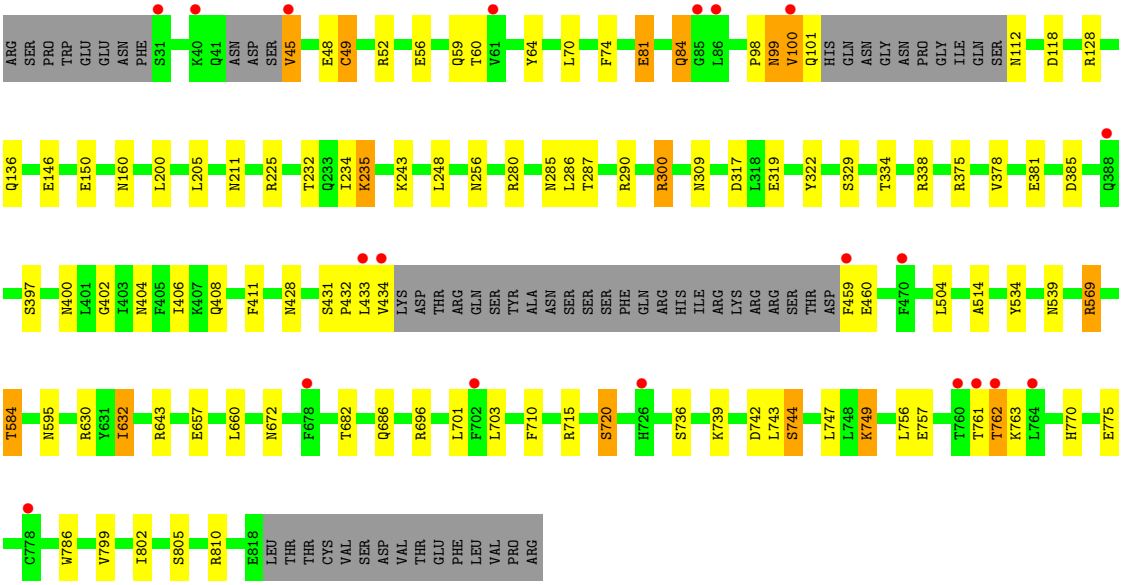
- Molecule 1: Toll-like receptor 8

Chain A:



- Molecule 1: Toll-like receptor 8

Chain B:



• Molecule 2: alpha-D-mannopyranose-(2-3)-[beta-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: 80% 20%

NAG1 NAG2 BMA3 MAN4 BMA5

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 100%

NAG1 NAG2

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G: 100%

NAG1 NAG2

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

Chain E: 67% 33%

NAG1 NAG2 BMA3

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

Chain H: 100%

NAG1 NAG2 BMA3

• Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 100%

NAG1 NAG2 BMA3 MAN4

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	72.15Å 156.72Å 86.16Å 90.00° 77.10° 90.00°	Depositor
Resolution (Å)	26.38 – 2.00 26.38 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.1 (26.38-2.00) 99.5 (26.38-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.209 , 0.264 0.218 , 0.270	Depositor DCC
R_{free} test set	6265 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	31.3	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 34.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13074	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 3.34% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, NAG, D80, BMA

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	0.51	0/6196	0.92	9/8404 (0.1%)
1	B	0.47	0/6186	0.90	6/8387 (0.1%)
All	All	0.49	0/12382	0.91	15/16791 (0.1%)

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	2
1	B	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	290	ARG	NE-CZ-NH1	8.44	124.52	120.30
1	A	569	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	B	643	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	A	630	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	B	290	ARG	NE-CZ-NH2	-5.82	117.39	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	42	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	A	458	ASP	Peptide
1	B	99	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	6071	0	6055	48	1
1	B	6062	0	6055	58	0
2	C	61	0	52	1	0
3	D	28	0	25	0	0
3	G	28	0	25	0	0
4	E	39	0	34	2	0
4	H	39	0	34	0	0
5	F	50	0	43	0	0
6	A	84	0	78	1	0
6	B	70	0	65	1	0
7	A	18	0	15	0	0
7	B	18	0	15	0	0
8	A	277	0	0	1	1
8	B	229	0	0	2	0
All	All	13074	0	12496	104	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 104 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:818:GLU:N	1:A:818:GLU:OE1	1.88	1.05
1:A:433:LEU:HD23	1:A:434:VAL:N	1.95	0.82
1:B:99:ASN:HB3	1:B:100:VAL:HG23	1.64	0.80
1:B:317:ASP:OD2	1:B:319:GLU:OE1	2.03	0.76
1:A:31:SER:OG	1:A:32:ARG:N	2.18	0.75

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:759:LYS:NZ	8:A:1277:HOH:O[1_556]	2.02	0.18

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	748/811 (92%)	698 (93%)	46 (6%)	4 (0%)	25	21
1	B	744/811 (92%)	693 (93%)	48 (6%)	3 (0%)	30	27
All	All	1492/1622 (92%)	1391 (93%)	94 (6%)	7 (0%)	25	21

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	B	762	THR
1	B	100	VAL
1	A	330	GLY
1	B	378	VAL

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	701/755 (93%)	663 (95%)	38 (5%)	18	16
1	B	699/755 (93%)	663 (95%)	36 (5%)	19	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1400/1510 (93%)	1326 (95%)	74 (5%)	19 16

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	334	THR
1	B	747	LEU
1	B	397	SER
1	B	632	ILE
1	A	584	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	135	ASN
1	B	136	GLN
1	B	531	HIS
1	B	428	ASN
1	B	469	HIS

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)

19 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	C	1	2,1	14,14,15	0.82	0	17,19,21	1.37	4 (23%)
2	NAG	C	2	2	14,14,15	0.62	0	17,19,21	1.57	4 (23%)
2	BMA	C	3	2	11,11,12	0.44	0	15,15,17	1.70	3 (20%)
2	MAN	C	4	2	11,11,12	0.70	0	13,15,17	3.37	7 (53%)
2	BMA	C	5	2	11,11,12	0.29	0	15,15,17	2.37	9 (60%)
3	NAG	D	1	3,1	14,14,15	1.03	1 (7%)	17,19,21	1.88	5 (29%)
3	NAG	D	2	3	14,14,15	0.52	0	17,19,21	1.83	4 (23%)
4	NAG	E	1	4,1	14,14,15	0.60	0	17,19,21	1.56	2 (11%)
4	NAG	E	2	4	14,14,15	0.96	1 (7%)	17,19,21	2.29	6 (35%)
4	BMA	E	3	4	11,11,12	0.43	0	15,15,17	1.93	6 (40%)
5	NAG	F	1	1,5	14,14,15	0.62	0	17,19,21	1.84	7 (41%)
5	NAG	F	2	5	14,14,15	0.92	1 (7%)	17,19,21	1.66	3 (17%)
5	BMA	F	3	5	11,11,12	0.47	0	15,15,17	1.81	4 (26%)
5	MAN	F	4	5	11,11,12	0.53	0	15,15,17	2.51	8 (53%)
3	NAG	G	1	3,1	14,14,15	0.79	1 (7%)	17,19,21	2.01	5 (29%)
3	NAG	G	2	3	14,14,15	0.60	0	17,19,21	2.94	7 (41%)
4	NAG	H	1	4,1	14,14,15	0.79	0	17,19,21	1.53	2 (11%)
4	NAG	H	2	4	14,14,15	0.75	0	17,19,21	1.64	4 (23%)
4	BMA	H	3	4	11,11,12	0.53	0	15,15,17	1.84	4 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	2/2/19/22	0/1/1/1
2	MAN	C	4	2	-	1/2/18/22	0/1/1/1
2	BMA	C	5	2	-	1/2/19/22	0/1/1/1
3	NAG	D	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
4	NAG	E	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	3/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
5	NAG	F	1	1,5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	F	2	5	-	2/6/23/26	0/1/1/1
5	BMA	F	3	5	-	0/2/19/22	0/1/1/1
5	MAN	F	4	5	-	1/2/19/22	0/1/1/1
3	NAG	G	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
4	NAG	H	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	1/6/23/26	0/1/1/1
4	BMA	H	3	4	-	2/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1	NAG	O5-C1	-2.59	1.39	1.43
4	E	2	NAG	C8-C7	-2.33	1.45	1.50
3	G	1	NAG	O5-C1	-2.14	1.40	1.43
5	F	2	NAG	O5-C1	-2.07	1.40	1.43

The worst 5 of 94 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	2	NAG	C1-O5-C5	8.77	123.94	112.19
2	C	4	MAN	C2-C3-C4	-8.17	98.89	110.67
2	C	4	MAN	C3-C4-C5	-5.59	104.38	109.99
5	F	4	MAN	O3-C3-C2	-5.42	99.00	110.05
4	E	2	NAG	O7-C7-C8	-5.10	112.97	122.05

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	2	NAG	C4-C5-C6-O6
5	F	2	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
4	E	2	NAG	C8-C7-N2-C2

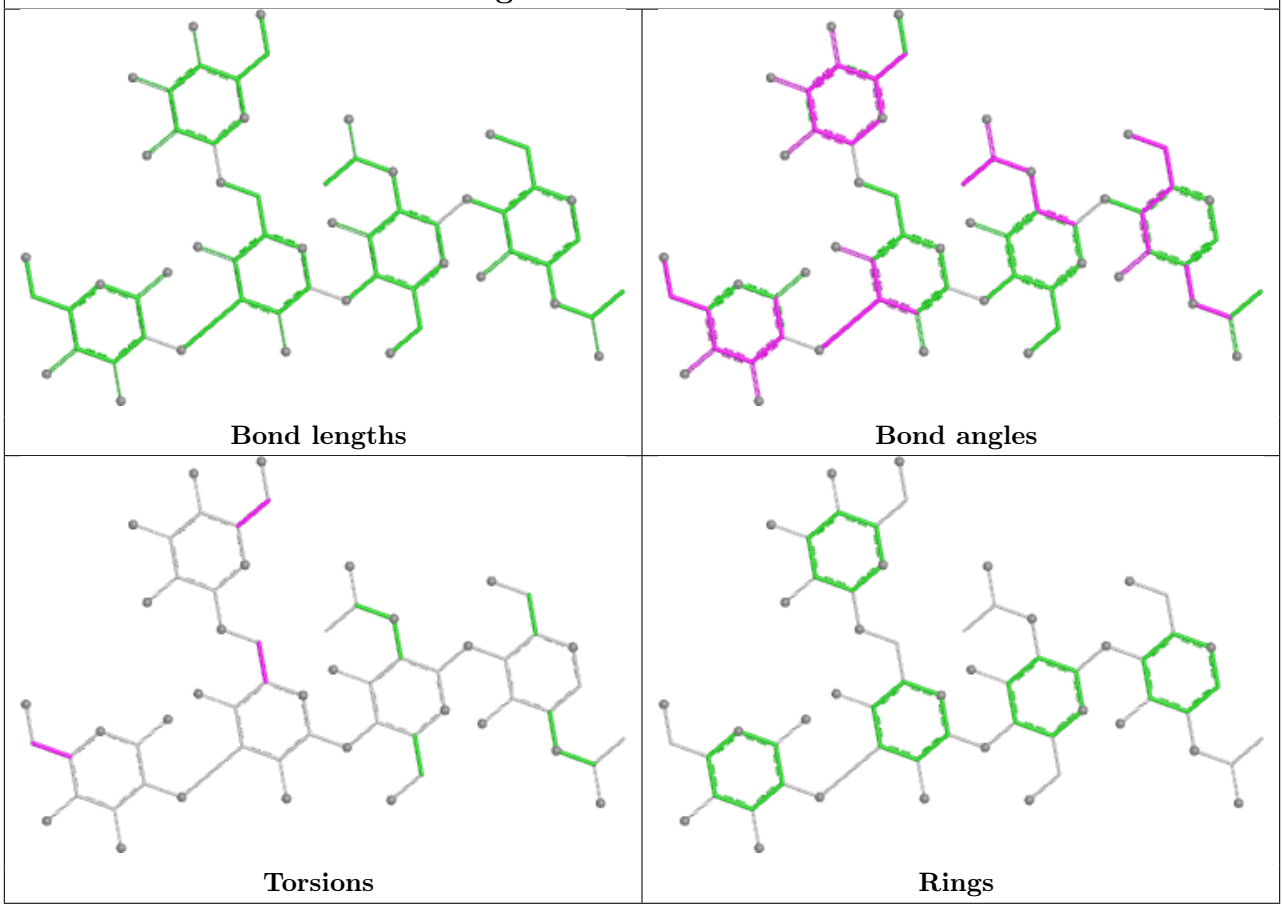
There are no ring outliers.

2 monomers are involved in 3 short contacts:

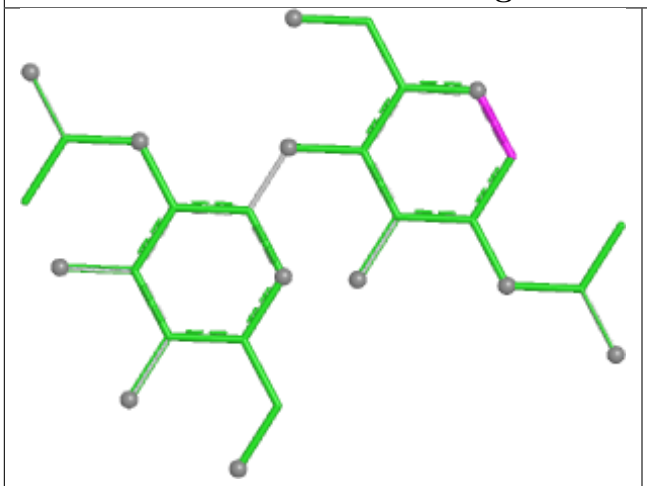
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	2	NAG	2	0
2	C	4	MAN	1	0

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

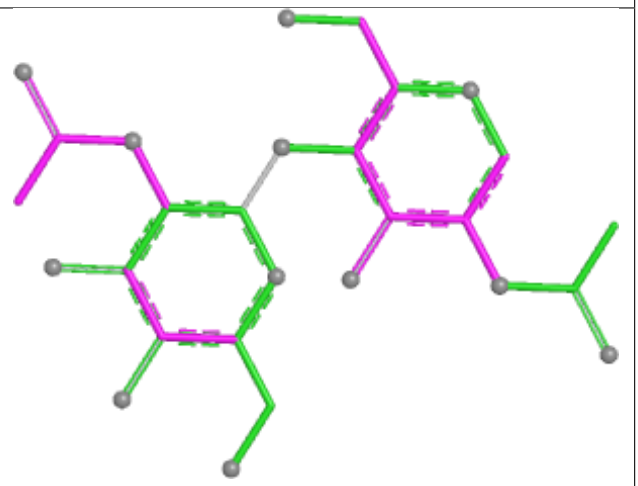
Oligosaccharide Chain C



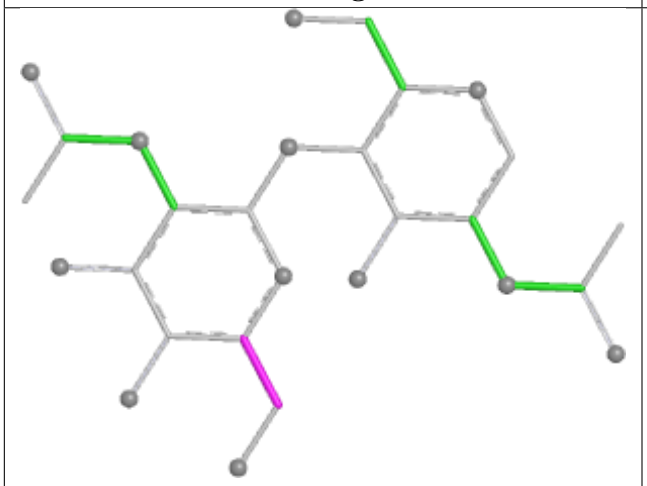
Oligosaccharide Chain D



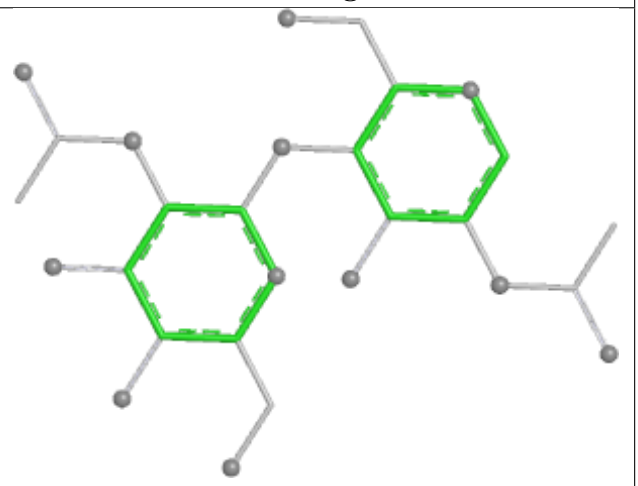
Bond lengths



Bond angles

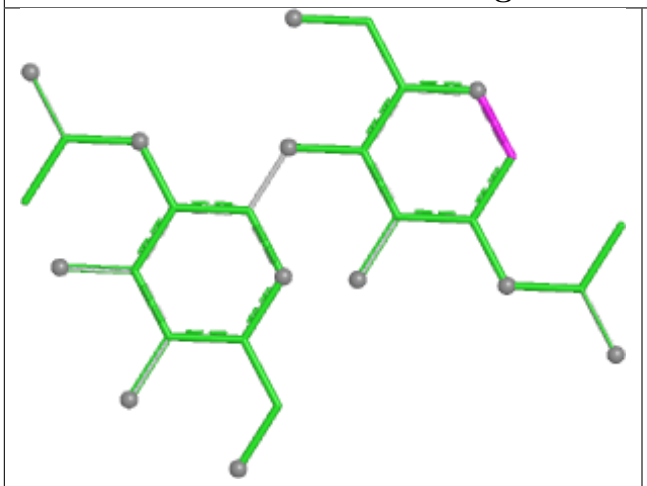


Torsions

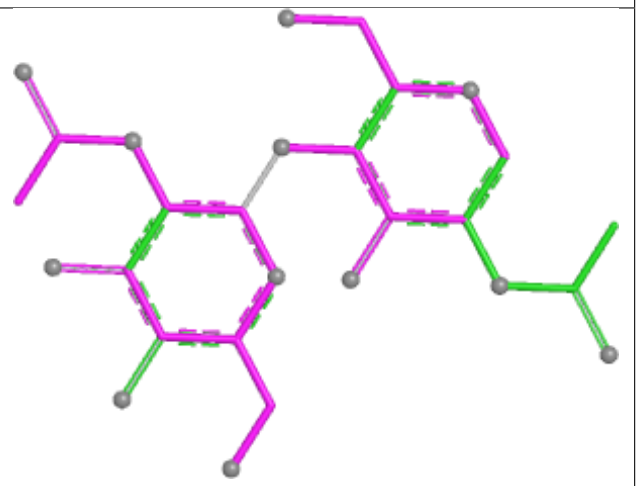


Rings

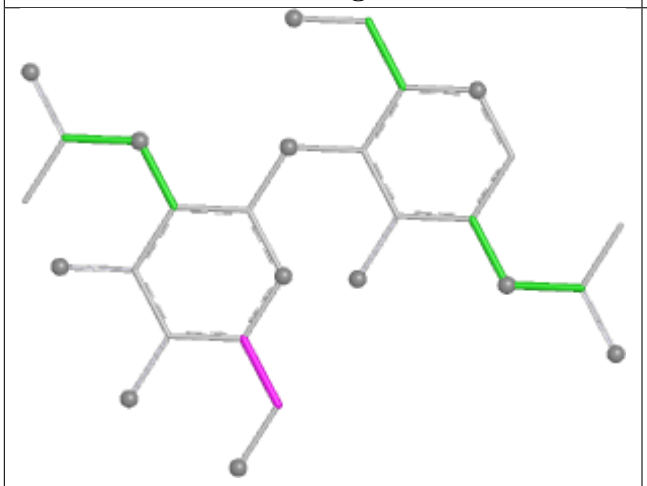
Oligosaccharide Chain G



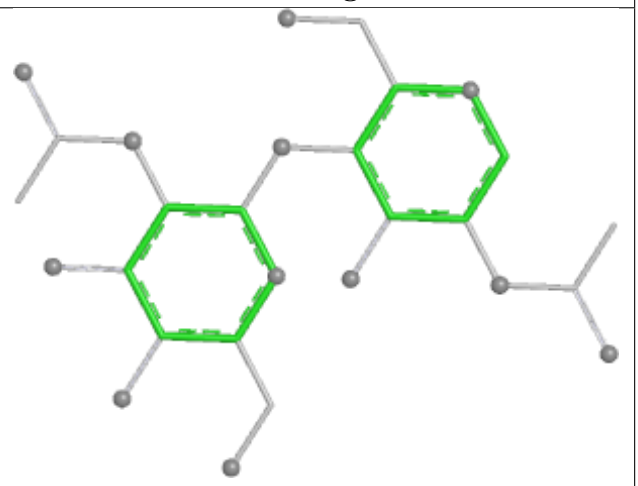
Bond lengths



Bond angles

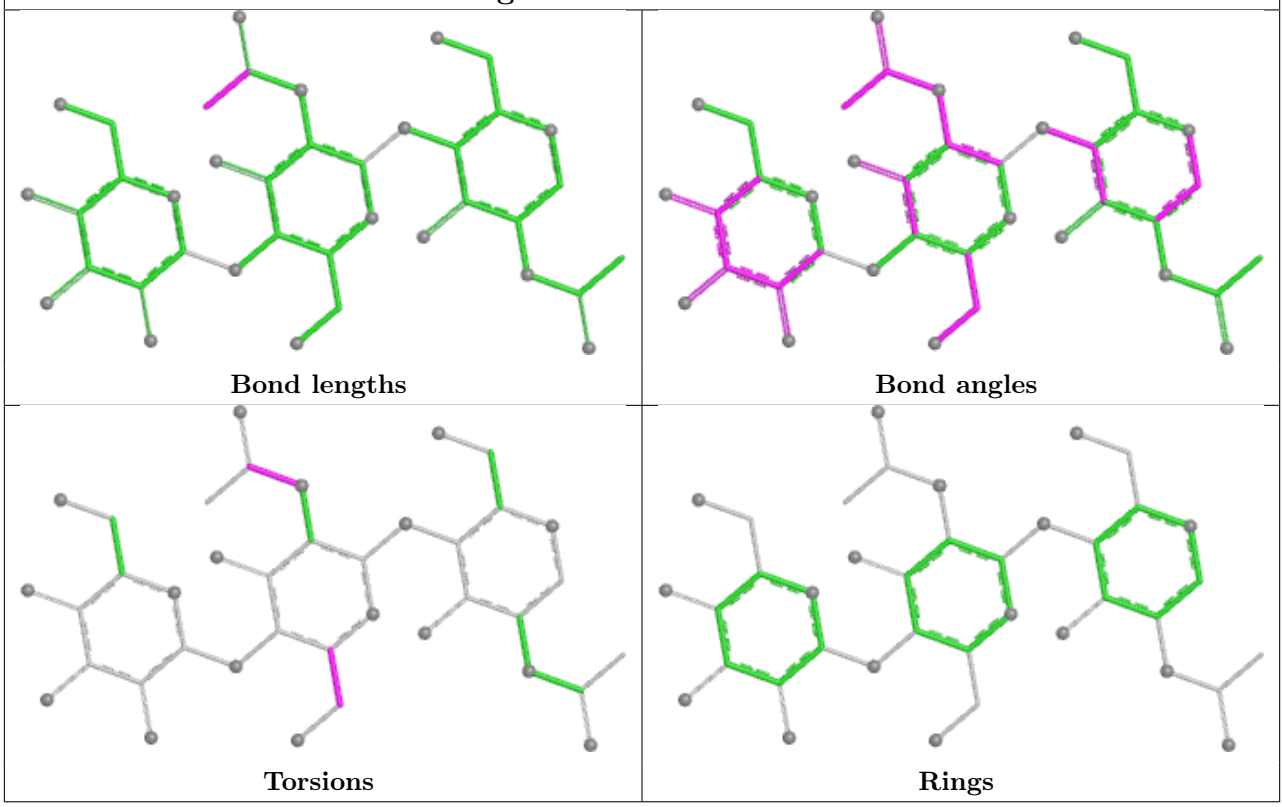


Torsions

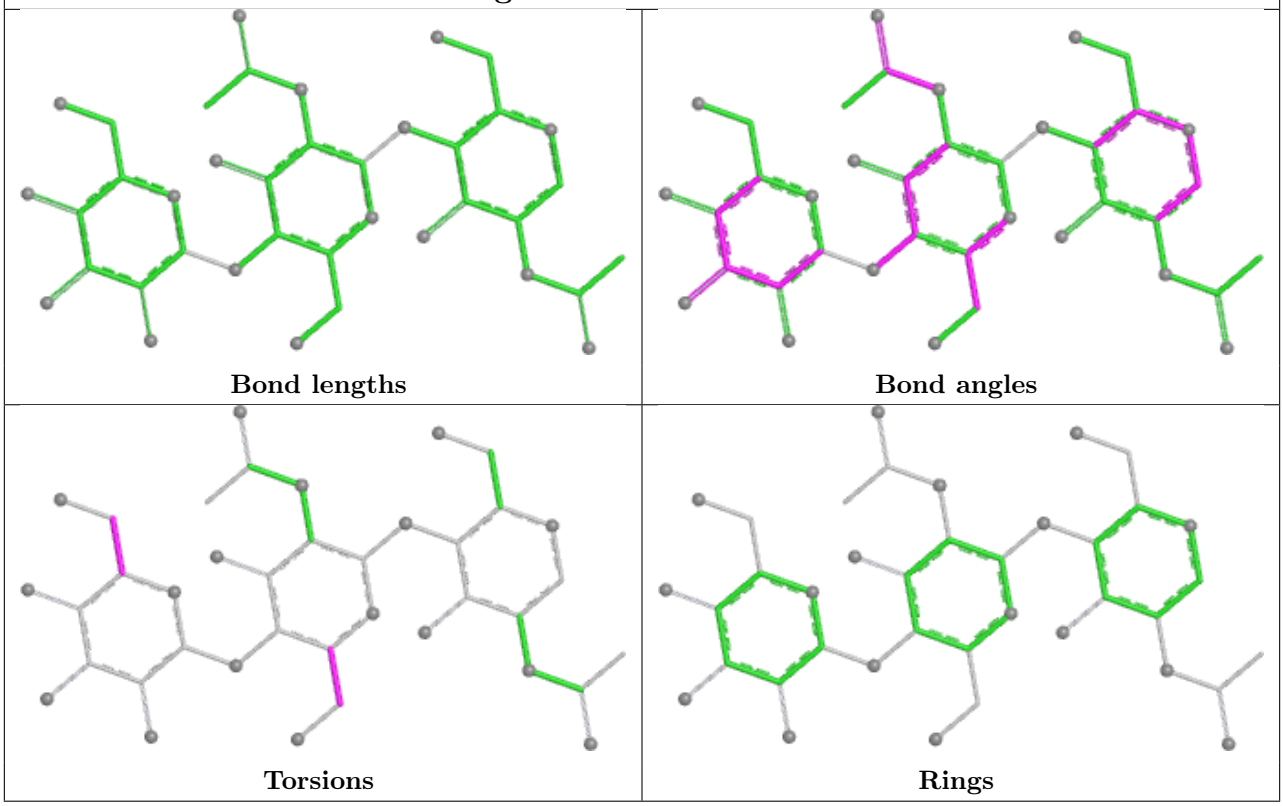


Rings

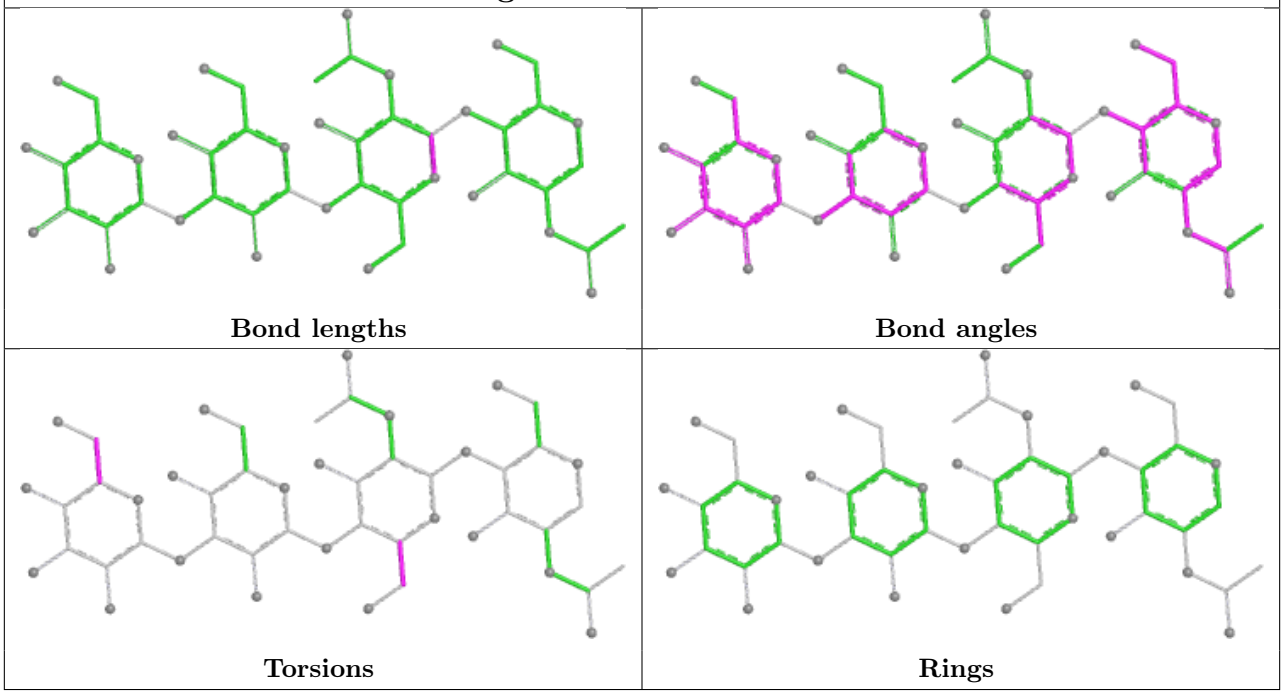
Oligosaccharide Chain E



Oligosaccharide Chain H



Oligosaccharide Chain F



5.6 Ligand geometry (i)

13 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	907	1	14,14,15	0.47	0	17,19,21	1.13	2 (11%)
6	NAG	B	906	1	14,14,15	0.43	0	17,19,21	2.31	9 (52%)
7	D80	B	901	-	16,20,20	1.17	1 (6%)	17,28,28	1.02	0
6	NAG	B	915	1	14,14,15	0.50	0	17,19,21	3.43	8 (47%)
6	NAG	B	910	1	14,14,15	0.37	0	17,19,21	2.12	3 (17%)
6	NAG	B	909	1	14,14,15	0.55	0	17,19,21	2.07	6 (35%)
6	NAG	A	901	1	14,14,15	0.65	0	17,19,21	1.58	4 (23%)
6	NAG	B	914	1	14,14,15	0.73	0	17,19,21	2.28	8 (47%)
6	NAG	A	915	1	14,14,15	0.89	1 (7%)	17,19,21	2.80	6 (35%)
7	D80	A	917	-	16,20,20	1.08	1 (6%)	17,28,28	1.56	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	A	916	1	14,14,15	0.62	0	17,19,21	2.97	7 (41%)
6	NAG	A	910	1	14,14,15	0.76	0	17,19,21	1.69	3 (17%)
6	NAG	A	911	1	14,14,15	0.41	0	17,19,21	2.70	4 (23%)

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	907	1	-	0/6/23/26	0/1/1/1
6	NAG	B	906	1	-	2/6/23/26	0/1/1/1
7	D80	B	901	-	-	2/3/4/4	0/3/3/3
6	NAG	B	915	1	-	0/6/23/26	0/1/1/1
6	NAG	B	910	1	-	3/6/23/26	0/1/1/1
6	NAG	B	909	1	-	0/6/23/26	0/1/1/1
6	NAG	A	901	1	-	2/6/23/26	0/1/1/1
6	NAG	B	914	1	-	0/6/23/26	0/1/1/1
6	NAG	A	915	1	-	2/6/23/26	0/1/1/1
7	D80	A	917	-	-	1/3/4/4	0/3/3/3
6	NAG	A	916	1	-	2/6/23/26	0/1/1/1
6	NAG	A	910	1	-	2/6/23/26	0/1/1/1
6	NAG	A	911	1	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	917	D80	CAB-CAJ	-2.70	1.38	1.41
7	B	901	D80	CAC-CAA	-2.16	1.38	1.41
6	A	915	NAG	O5-C1	-2.04	1.40	1.43

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	915	NAG	C1-O5-C5	11.06	127.00	112.19
6	A	911	NAG	C1-O5-C5	9.56	125.00	112.19
6	A	916	NAG	C1-O5-C5	-6.91	102.93	112.19
6	A	916	NAG	C1-C2-N2	6.27	120.32	110.43
6	B	910	NAG	C1-C2-N2	5.64	119.33	110.43

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	917	D80	NAK-CAL-CAN-CAO
7	B	901	D80	NAK-CAL-CAN-CAO
6	A	911	NAG	O5-C5-C6-O6
6	A	915	NAG	C4-C5-C6-O6
6	A	915	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	909	NAG	1	0
6	A	916	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	754/811 (92%)	-0.05	13 (1%)	69	67	20, 34, 59, 90	0
1	B	751/811 (92%)	0.18	20 (2%)	56	54	16, 38, 68, 96	1 (0%)
All	All	1505/1622 (92%)	0.07	33 (2%)	62	60	16, 36, 63, 96	1 (0%)

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	817	LEU	5.3
1	B	434	VAL	4.5
1	B	762	THR	4.3
1	B	459	PHE	4.2
1	B	760	THR	4.0

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(Å^2)	Q<0.9
5	MAN	F	4	11/12	0.68	0.19	58,67,77,79	0
2	MAN	C	4	11/12	0.76	0.19	44,63,72,94	0
2	BMA	C	5	11/12	0.77	0.14	59,65,68,70	0
4	BMA	H	3	11/12	0.81	0.11	44,51,61,63	0
4	BMA	E	3	11/12	0.84	0.09	42,47,50,61	0

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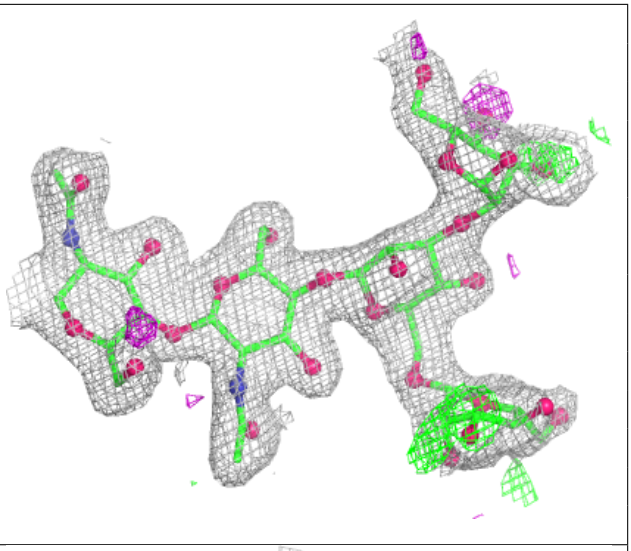
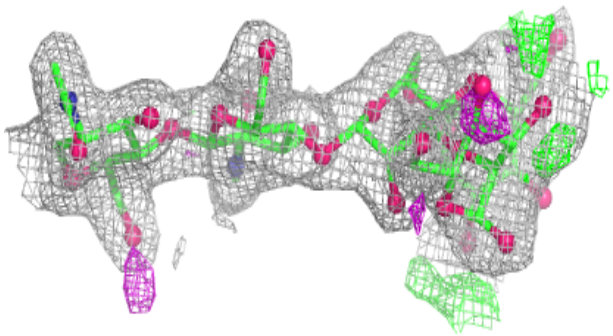
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	G	2	14/15	0.85	0.12	40,51,56,56	0
5	BMA	F	3	11/12	0.88	0.09	41,46,48,52	0
3	NAG	D	2	14/15	0.91	0.08	36,44,54,55	0
5	NAG	F	2	14/15	0.91	0.08	29,35,42,44	0
2	NAG	C	2	14/15	0.93	0.07	27,33,39,48	0
2	BMA	C	3	11/12	0.93	0.08	42,46,51,55	0
5	NAG	F	1	14/15	0.93	0.09	28,31,37,47	0
4	NAG	H	2	14/15	0.94	0.08	31,33,39,45	0
4	NAG	E	2	14/15	0.94	0.07	25,30,38,38	0
3	NAG	G	1	14/15	0.95	0.06	24,26,30,32	0
2	NAG	C	1	14/15	0.95	0.07	23,26,30,38	0
4	NAG	E	1	14/15	0.97	0.05	20,23,27,27	0
4	NAG	H	1	14/15	0.97	0.05	24,28,29,30	0
3	NAG	D	1	14/15	0.98	0.05	22,25,30,32	0

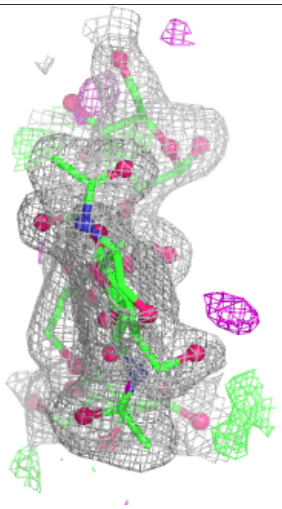
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

$2mF_o$-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 D:

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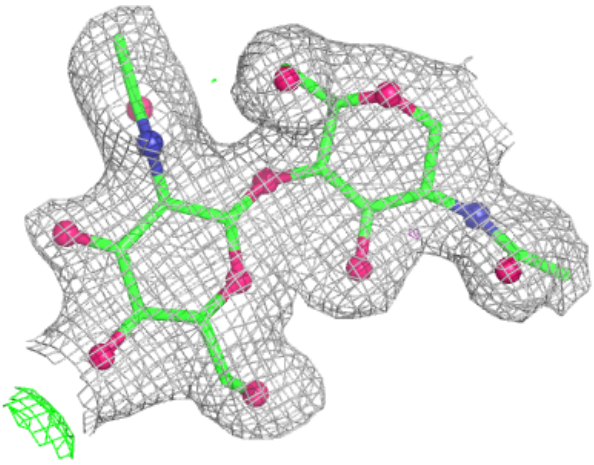
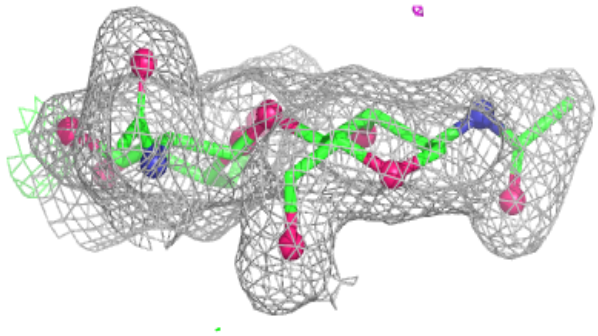
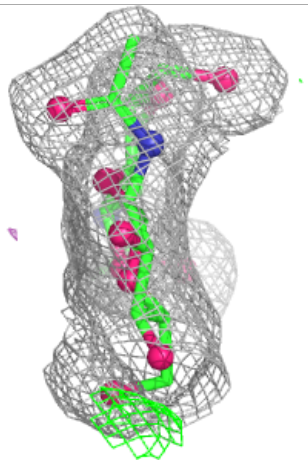
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

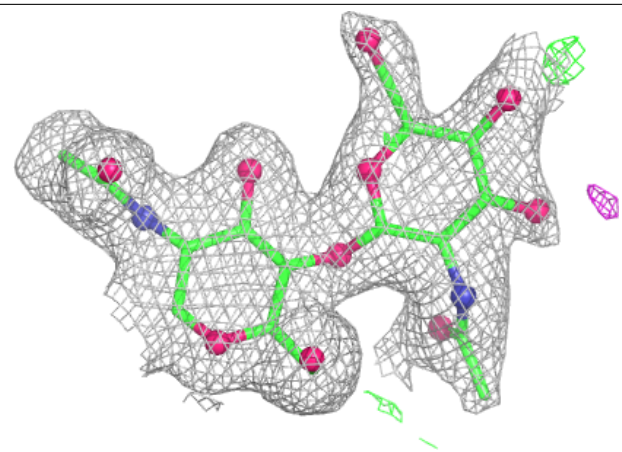


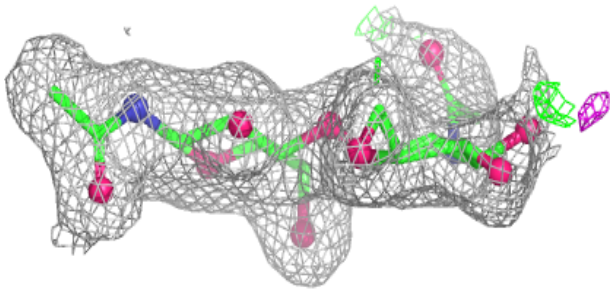


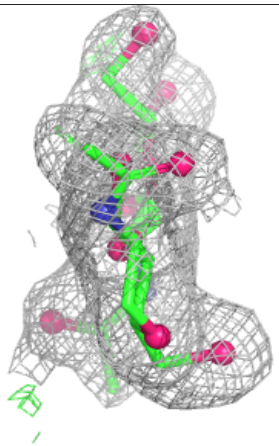


Electron density around Chain G:

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

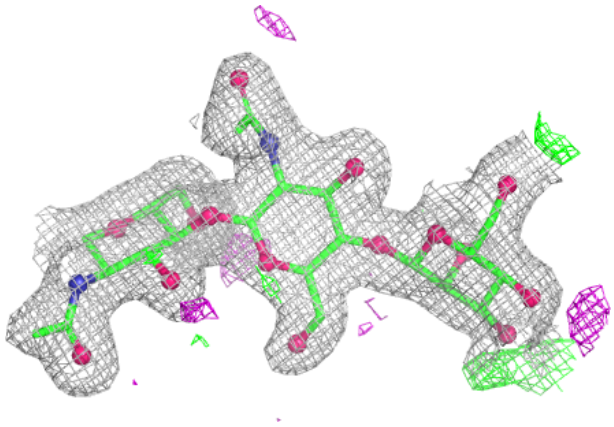


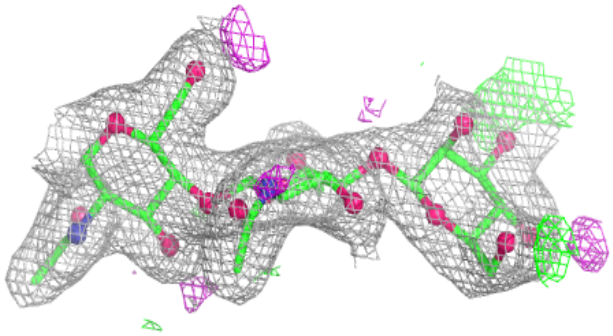


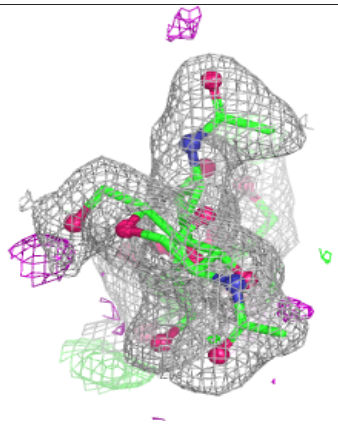


Electron density around Chain E:

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

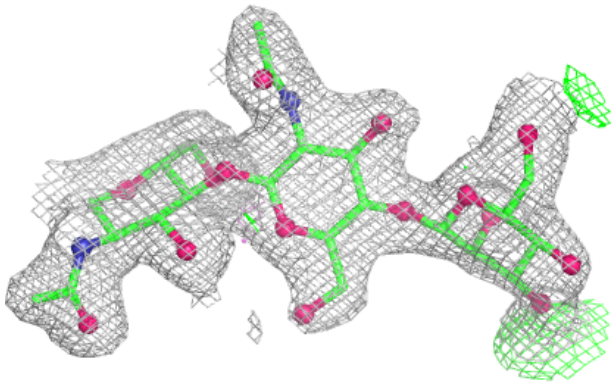


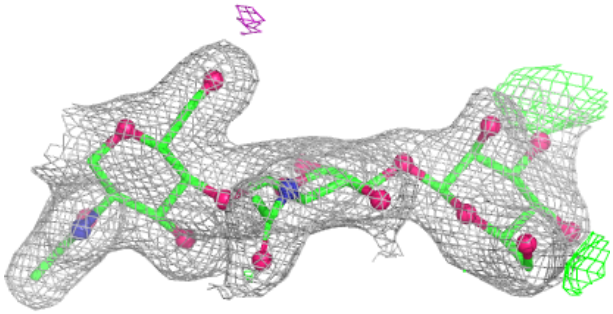


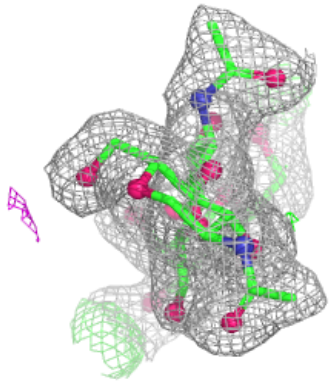


Electron density around Chain H:

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

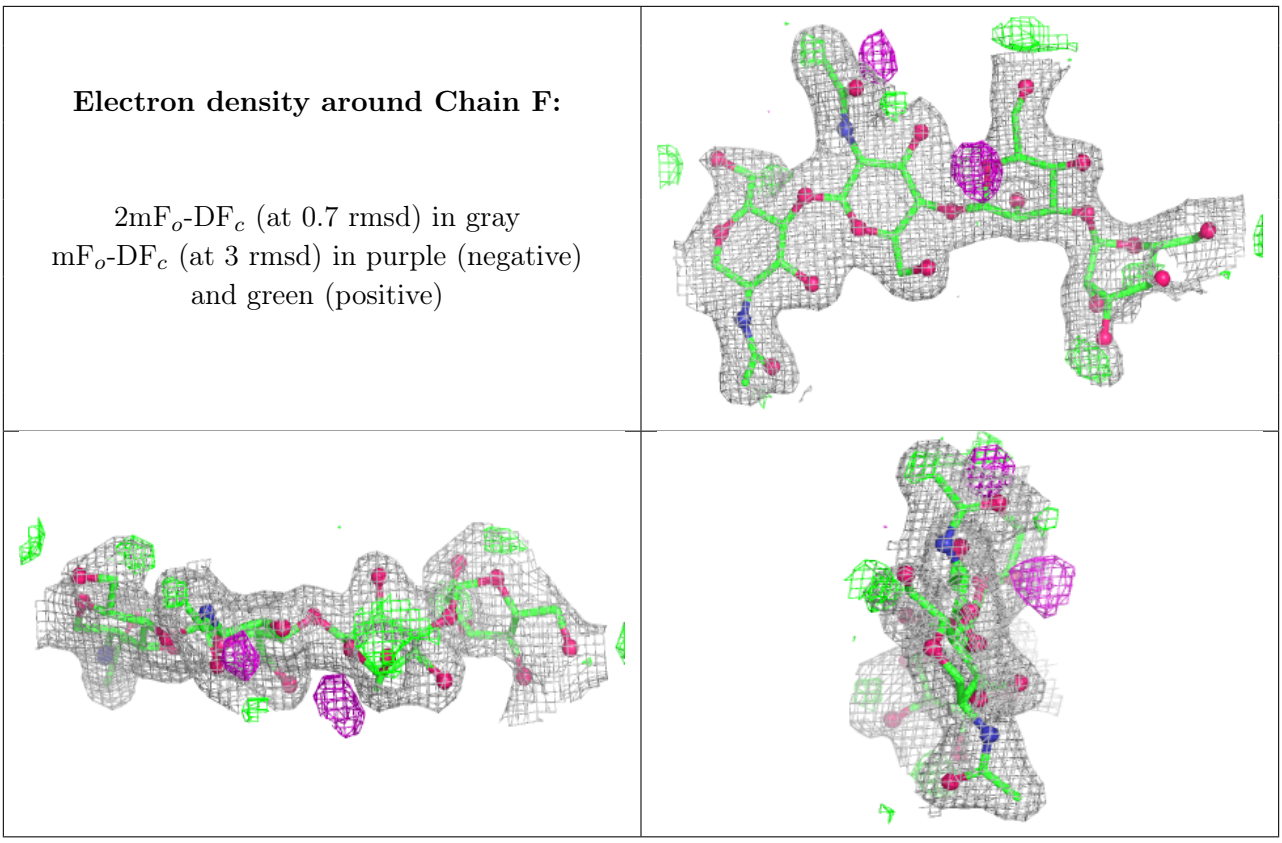






Electron density around Chain F:

$2mF_o$-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	A	901	14/15	0.72	0.12	48,57,63,66	0
6	NAG	A	911	14/15	0.78	0.13	57,62,68,71	0
6	NAG	B	910	14/15	0.81	0.12	55,62,65,66	0
6	NAG	B	906	14/15	0.85	0.11	33,43,46,57	0
6	NAG	B	915	14/15	0.86	0.12	48,54,64,65	0
6	NAG	A	910	14/15	0.88	0.09	45,56,60,67	0
6	NAG	B	909	14/15	0.88	0.12	41,54,64,67	0
6	NAG	A	915	14/15	0.88	0.10	33,43,48,50	0
6	NAG	A	916	14/15	0.88	0.11	45,51,63,67	0
6	NAG	B	914	14/15	0.91	0.09	27,40,53,55	0
6	NAG	A	907	14/15	0.92	0.09	33,39,44,47	0
7	D80	A	917	18/18	0.96	0.05	21,25,28,28	0
7	D80	B	901	18/18	0.96	0.06	21,24,28,30	0

6.5 Other polymers (i)

There are no such residues in this entry.