wwPDB X-ray Structure Validation Summary Report (i)

Jun 19, 2024 – 02:06 PM EDT

PDB ID	:	4CYV
Title	:	Structure of the A_mallard_Sweden_51_2002 H10 Avian Haemmaglutinin
Authors	:	Vachieri, S.G.; Xiong, X.; Collins, P.J.; Walker, P.A.; Martin, S.R.; Haire, L.F.; McCauley, J.W.; Gamblin, S.J.; Skehel, J.J.
Deposited on	:	2014-04-15
Resolution	:	2.30 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:

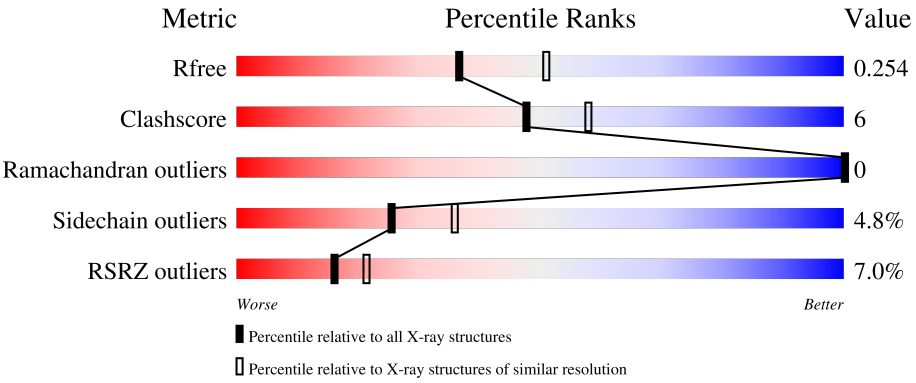
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	324	3% 81% 15%
1	C	324	% 89% 8%
1	E	324	8% 82% 15%
2	B	172	6% 86% 13%
2	D	172	15% 95%

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Mol	Chain	Length	Quality of chain
2	F	172	16% 88% 12%
3	G	5	80% 20%
3	I	5	20% 60% 20%
3	K	5	60% 40%
4	H	3	67% 33%
5	J	2	100%

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
3	MAN	K	4	-	-	-	X
3	MAN	K	5	X	-	-	-
4	BMA	H	3	-	-	-	X
5	NAG	J	2	X	-	-	-
6	NAG	A	401	X	-	-	-
6	NAG	A	420	X	-	-	-
6	NAG	C	420	X	-	-	-
6	NAG	E	420	X	-	-	-
7	EDO	E	1327	-	-	-	X
7	EDO	E	1328	-	-	X	-
7	EDO	F	1175	-	-	-	X
7	EDO	F	1176	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 12135 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

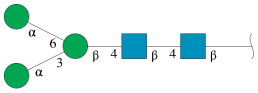
- Molecule 1 is a protein called HEMAGGLUTININ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	1	0
			2427	1501	436	474	16			
1	C	319	Total	C	N	O	S	0	0	0
			2430	1504	437	473	16			
1	E	319	Total	C	N	O	S	0	0	0
			2426	1501	436	473	16			

- Molecule 2 is a protein called HEMAGGLUTININ.

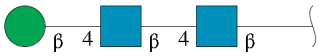
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	0	0
			1384	855	239	282	8			
2	D	172	Total	C	N	O	S	0	0	0
			1377	851	240	278	8			
2	F	172	Total	C	N	O	S	0	0	0
			1380	851	239	282	8			

- Molecule 3 is an oligosaccharide called alpha-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	G	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	I	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	K	5	Total	C	N	O	0	0	0
			61	34	2	25			

- 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.

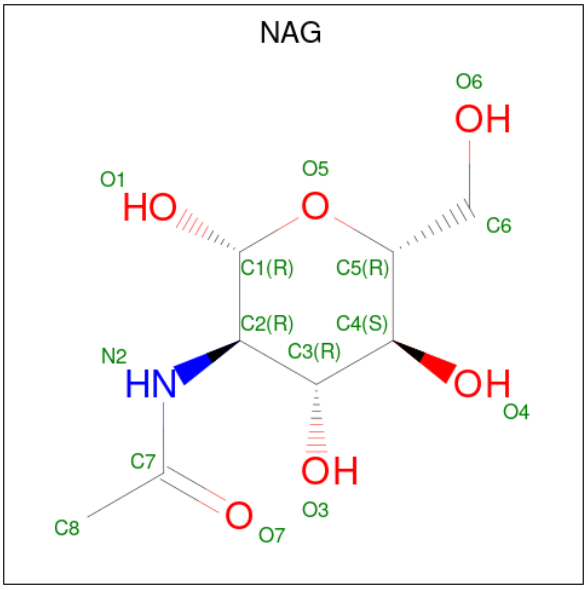


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	H	3	39	22	2	15	0	0	0

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

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

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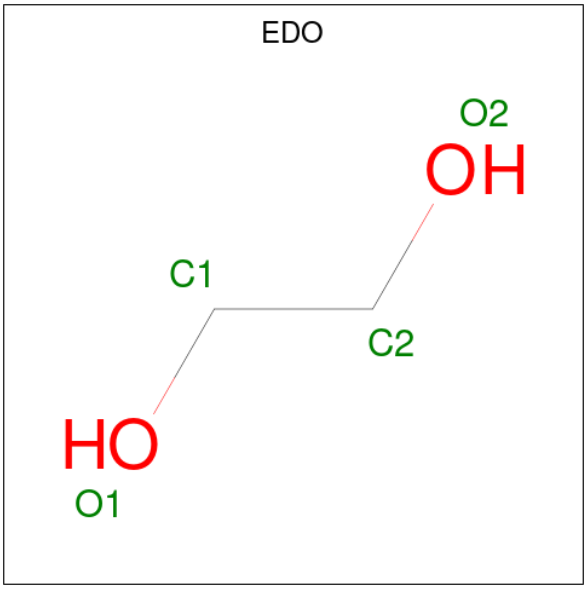
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O 14 8 1 5	0	0
6	B	1	Total C N O 14 8 1 5	0	0
6	C	1	Total C N O 14 8 1 5	0	0
6	D	1	Total C N O 14 8 1 5	0	0
6	E	1	Total C N O 14 8 1 5	0	0

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C O 4 2 2	0	0
7	C	1	Total C O 4 2 2	0	0
7	C	1	Total C O 4 2 2	0	0
7	C	1	Total C O 4 2 2	0	0
7	D	1	Total C O 4 2 2	0	0
7	E	1	Total C O 4 2 2	0	0
7	E	1	Total C O 4 2 2	0	0
7	E	1	Total C O 4 2 2	0	0
7	F	1	Total C O 4 2 2	0	0
7	F	1	Total C O 4 2 2	0	0
7	F	1	Total C O 4 2 2	0	0
7	F	1	Total C O 4 2 2	0	0

- Molecule 8 is water.

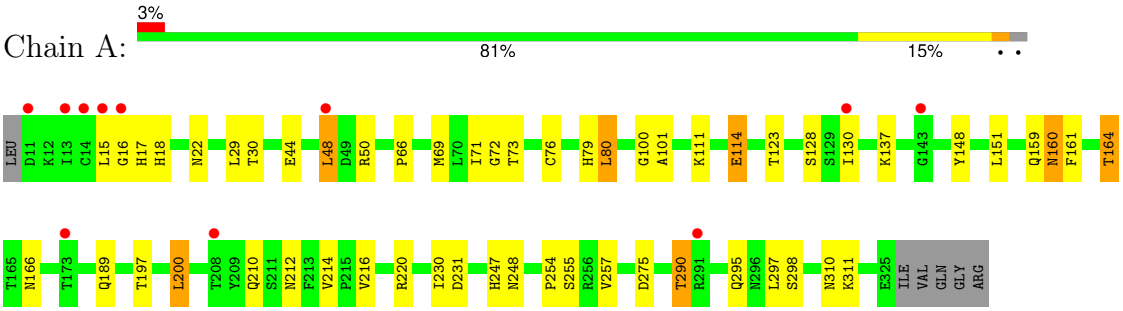
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	69	Total O 69 69	0	0
8	B	43	Total O 43 43	0	0
8	C	98	Total O 98 98	0	0
8	D	27	Total O 27 27	0	0
8	E	52	Total O 52 52	0	0
8	F	16	Total O 16 16	0	0

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.

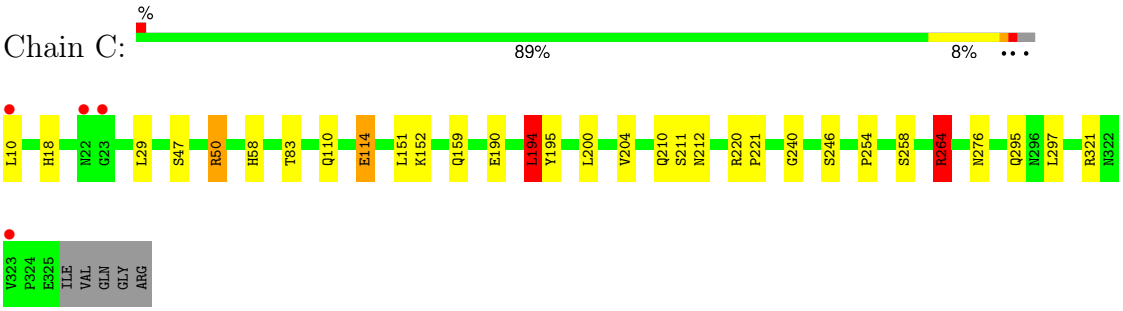
• Molecule 1: HEMAGGLUTININ

Chain A:



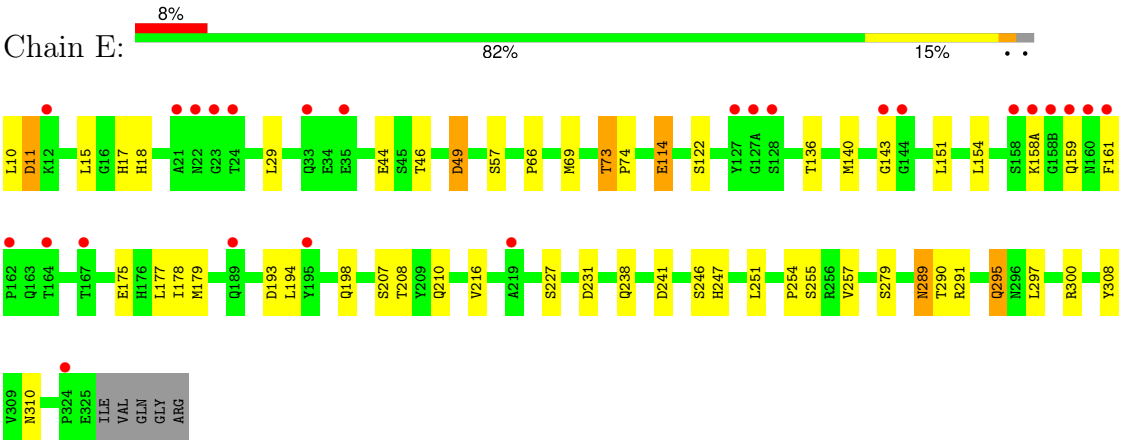
• Molecule 1: HEMAGGLUTININ

Chain C:



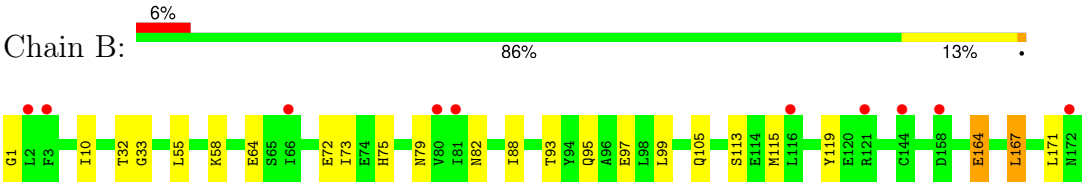
• Molecule 1: HEMAGGLUTININ

Chain E:



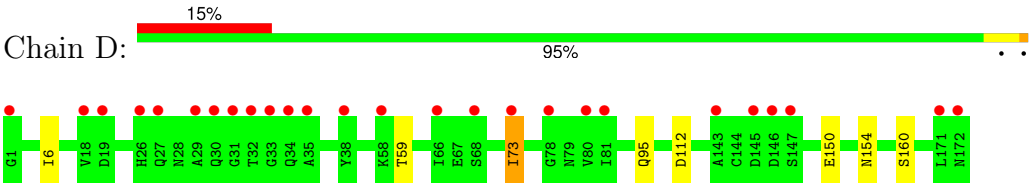
• Molecule 2: HEMAGGLUTININ

Chain B:



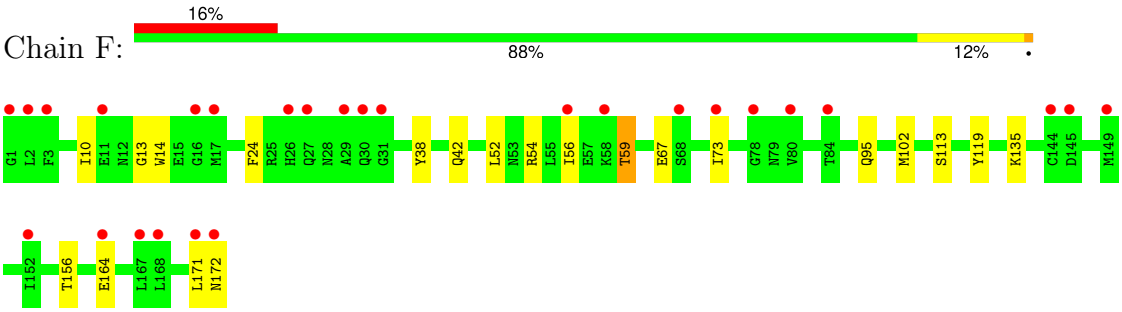
• Molecule 2: HEMAGGLUTININ

Chain D:



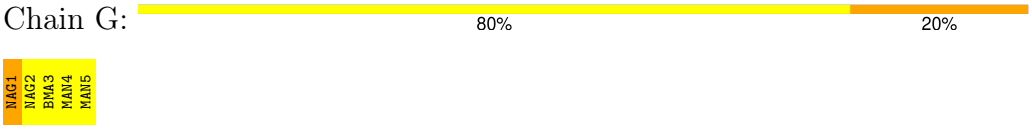
• Molecule 2: HEMAGGLUTININ

Chain F:



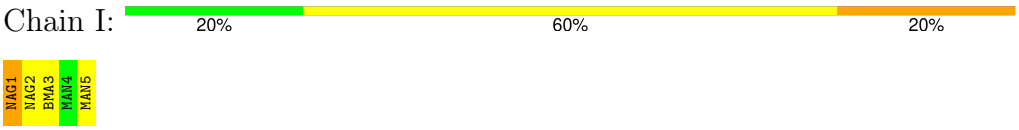
• Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



• Molecule 3: alpha-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 I:



• Molecule 3: alpha-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

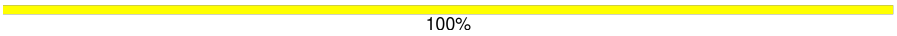
Chain K:

• 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:

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

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	67.61Å 227.99Å 68.72Å 90.00° 110.32° 90.00°	Depositor
Resolution (Å)	113.99 – 2.30 49.15 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.4 (113.99-2.30) 98.4 (49.15-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.51 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.214 , 0.252 0.217 , 0.254	Depositor DCC
R_{free} test set	4237 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	41.6	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 43.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.022 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12135	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% 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: NAG, MAN, BMA, EDO

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	0.65	2/2479 (0.1%)	0.76	3/3361 (0.1%)
1	C	0.76	3/2479 (0.1%)	0.85	6/3361 (0.2%)
1	E	0.65	2/2475 (0.1%)	0.76	4/3357 (0.1%)
2	B	0.52	0/1409	0.65	0/1902
2	D	0.56	0/1402	0.66	0/1892
2	F	0.56	0/1405	0.66	0/1897
All	All	0.64	7/11649 (0.1%)	0.75	13/15770 (0.1%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	114	GLU	CD-OE2	16.48	1.43	1.25
1	A	114	GLU	CD-OE2	14.82	1.42	1.25
1	E	114	GLU	CD-OE2	11.45	1.38	1.25
1	E	114	GLU	CB-CG	9.31	1.69	1.52
1	C	114	GLU	CB-CG	8.72	1.68	1.52

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	114	GLU	CA-CB-CG	8.99	133.19	113.40
1	C	114	GLU	CA-CB-CG	8.40	131.87	113.40
1	C	114	GLU	CG-CD-OE1	-7.93	102.43	118.30
1	C	264	ARG	NE-CZ-NH1	6.99	123.80	120.30
1	E	114	GLU	CG-CD-OE1	-6.94	104.42	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2427	0	2360	45	0
1	C	2430	0	2367	17	1
1	E	2426	0	2356	36	1
2	B	1384	0	1276	29	0
2	D	1377	0	1270	7	0
2	F	1380	0	1266	27	0
3	G	61	0	50	3	0
3	I	61	0	52	1	0
3	K	61	0	52	2	0
4	H	39	0	34	4	0
5	J	28	0	25	0	0
6	A	28	0	26	0	0
6	B	14	0	13	0	0
6	C	14	0	13	0	0
6	D	14	0	13	1	0
6	E	14	0	13	0	0
7	A	12	0	18	2	0
7	B	12	0	18	1	0
7	C	16	0	24	2	0
7	D	4	0	6	0	0
7	E	12	0	18	7	0
7	F	16	0	24	8	0
8	A	69	0	0	1	0
8	B	43	0	0	4	0
8	C	98	0	0	1	0
8	D	27	0	0	0	0
8	E	52	0	0	3	0
8	F	16	0	0	0	0
All	All	12135	0	11294	141	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 6.

The worst 5 of 141 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)
2:F:10:ILE:HG21	7:F:1176:EDO:O1	1.72	0.88
2:F:56:ILE:HG22	2:F:56:ILE:O	1.82	0.78
1:E:158(A):LYS:O	1:E:193:ASP:O	2.06	0.74
2:F:14:TRP:CE2	7:F:1176:EDO:H21	2.23	0.73
1:E:291:ARG:HB3	2:F:56:ILE:HG21	1.69	0.72

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:THR:OG1	1:E:49:ASP:OD2[1_655]	2.16	0.04

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	317/324 (98%)	304 (96%)	13 (4%)	0	100	100
1	C	317/324 (98%)	306 (96%)	11 (4%)	0	100	100
1	E	317/324 (98%)	299 (94%)	18 (6%)	0	100	100
2	B	170/172 (99%)	159 (94%)	11 (6%)	0	100	100
2	D	170/172 (99%)	166 (98%)	4 (2%)	0	100	100
2	F	170/172 (99%)	161 (95%)	9 (5%)	0	100	100
All	All	1461/1488 (98%)	1395 (96%)	66 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	270/275 (98%)	256 (95%)	14 (5%)	23	32
1	C	270/275 (98%)	258 (96%)	12 (4%)	28	39
1	E	269/275 (98%)	250 (93%)	19 (7%)	14	19
2	B	145/146 (99%)	140 (97%)	5 (3%)	37	51
2	D	143/146 (98%)	140 (98%)	3 (2%)	53	70
2	F	144/146 (99%)	138 (96%)	6 (4%)	30	42
All	All	1241/1263 (98%)	1182 (95%)	59 (5%)	25	36

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	264	ARG
2	F	113	SER
1	E	11	ASP
2	F	59	THR
1	E	255	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	58	HIS
2	D	95	GLN
1	C	276	ASN
1	E	22	ASN
1	A	224	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)

20 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	G	1	3,2	14,14,15	1.95	3 (21%)	17,19,21	5.12	8 (47%)
3	NAG	G	2	3	14,14,15	0.92	1 (7%)	17,19,21	1.52	4 (23%)
3	BMA	G	3	3	11,11,12	0.80	0	15,15,17	1.97	3 (20%)
3	MAN	G	4	3	11,11,12	0.58	0	15,15,17	1.09	1 (6%)
3	MAN	G	5	3	11,11,12	0.66	0	15,15,17	1.39	2 (13%)
4	NAG	H	1	4,1	14,14,15	0.53	0	17,19,21	1.40	4 (23%)
4	NAG	H	2	4	14,14,15	0.76	0	17,19,21	1.41	3 (17%)
4	BMA	H	3	4	11,11,12	0.56	0	15,15,17	2.28	3 (20%)
3	NAG	I	1	3,2	14,14,15	0.73	0	17,19,21	1.75	6 (35%)
3	NAG	I	2	3	14,14,15	0.54	0	17,19,21	1.16	1 (5%)
3	BMA	I	3	3	11,11,12	0.65	0	15,15,17	2.19	2 (13%)
3	MAN	I	4	3	11,11,12	0.44	0	15,15,17	0.97	0
3	MAN	I	5	3	11,11,12	0.62	0	15,15,17	1.52	3 (20%)
5	NAG	J	1	5,1	14,14,15	0.52	0	17,19,21	1.60	3 (17%)
5	NAG	J	2	5	14,14,15	0.55	0	17,19,21	1.68	4 (23%)
3	NAG	K	1	3,2	14,14,15	0.65	0	17,19,21	1.75	5 (29%)
3	NAG	K	2	3	14,14,15	0.76	0	17,19,21	1.54	3 (17%)
3	BMA	K	3	3	11,11,12	0.65	0	15,15,17	1.56	2 (13%)
3	MAN	K	4	3	11,11,12	0.54	0	15,15,17	1.35	2 (13%)
3	MAN	K	5	3	11,11,12	0.72	0	15,15,17	2.05	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
3	NAG	G	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	BMA	G	3	3	-	2/2/19/22	0/1/1/1
3	MAN	G	4	3	-	2/2/19/22	0/1/1/1
3	MAN	G	5	3	-	0/2/19/22	1/1/1/1
4	NAG	H	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
4	BMA	H	3	4	-	1/2/19/22	0/1/1/1
3	NAG	I	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	BMA	I	3	3	-	1/2/19/22	0/1/1/1
3	MAN	I	4	3	-	0/2/19/22	0/1/1/1
3	MAN	I	5	3	-	0/2/19/22	1/1/1/1
5	NAG	J	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	J	2	5	1/1/5/7	4/6/23/26	0/1/1/1
3	NAG	K	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
3	BMA	K	3	3	-	1/2/19/22	0/1/1/1
3	MAN	K	4	3	-	0/2/19/22	1/1/1/1
3	MAN	K	5	3	1/1/4/5	1/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	1	NAG	C1-C2	5.89	1.60	1.52
3	G	1	NAG	C8-C7	3.13	1.57	1.50
3	G	1	NAG	C3-C2	2.47	1.57	1.52
3	G	2	NAG	O5-C1	-2.26	1.39	1.43

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	1	NAG	O5-C1-C2	-12.09	92.59	111.29
3	G	1	NAG	C1-C2-N2	8.69	124.13	110.43
3	G	1	NAG	C8-C7-N2	7.85	129.14	116.12
4	H	3	BMA	C1-O5-C5	7.57	122.33	112.19
3	G	1	NAG	O7-C7-N2	-7.38	108.94	121.98

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	K	5	MAN	C1
5	J	2	NAG	C1

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	2	NAG	O5-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
3	G	4	MAN	O5-C5-C6-O6
5	J	2	NAG	O5-C5-C6-O6

All (3) ring outliers are listed below:

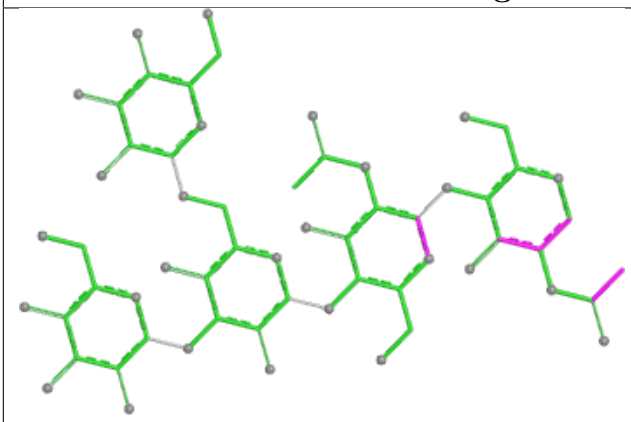
Mol	Chain	Res	Type	Atoms
3	K	4	MAN	C1-C2-C3-C4-C5-O5
3	I	5	MAN	C1-C2-C3-C4-C5-O5
3	G	5	MAN	C1-C2-C3-C4-C5-O5

5 monomers are involved in 10 short contacts:

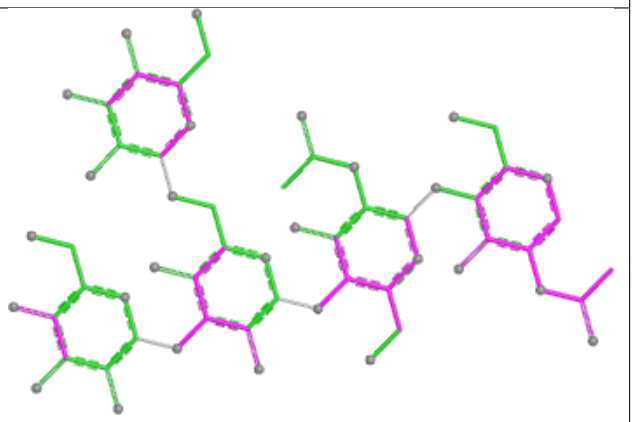
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	1	NAG	1	0
4	H	1	NAG	4	0
3	K	1	NAG	2	0
3	K	2	NAG	1	0
3	G	1	NAG	3	0

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

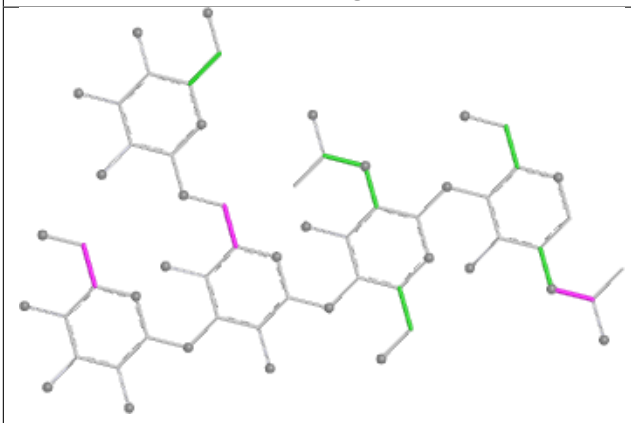
Oligosaccharide Chain G



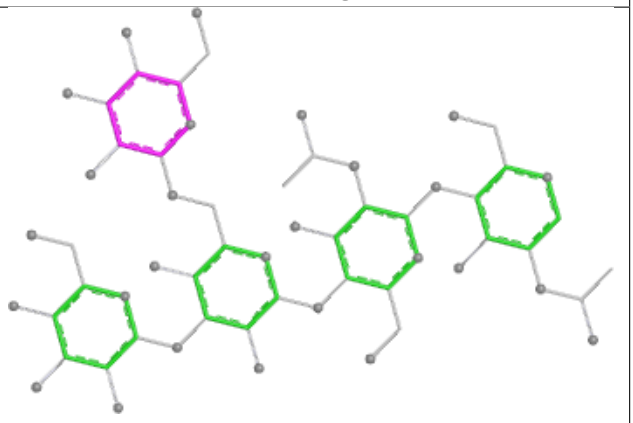
Bond lengths



Bond angles

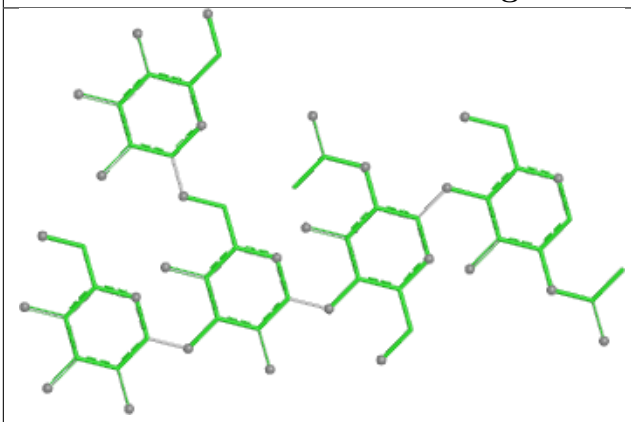


Torsions

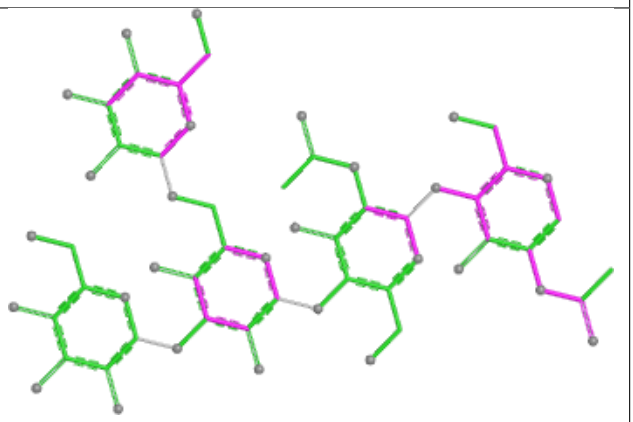


Rings

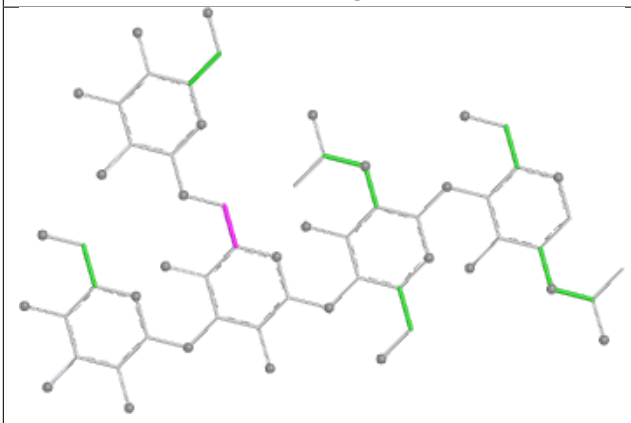
Oligosaccharide Chain I



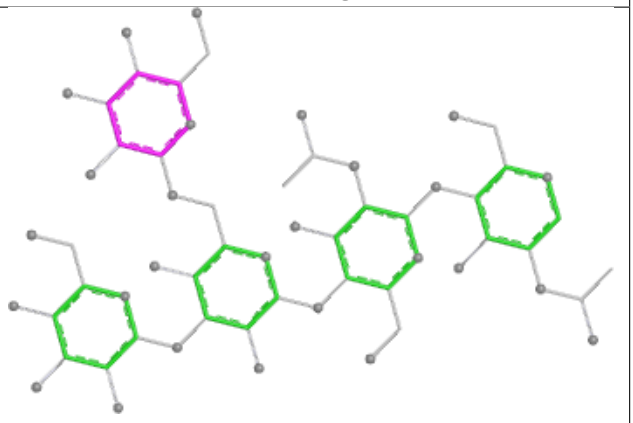
Bond lengths



Bond angles

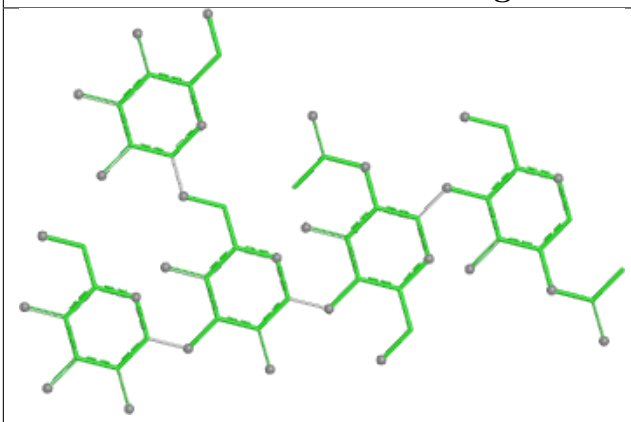


Torsions

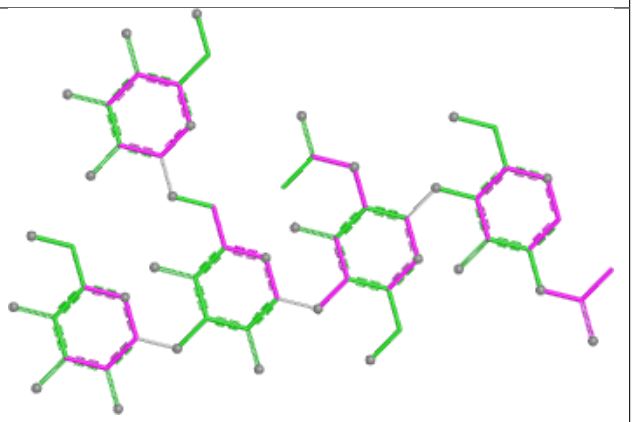


Rings

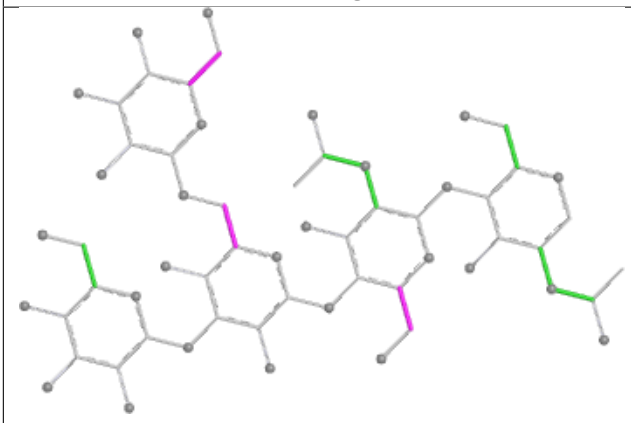
Oligosaccharide Chain K



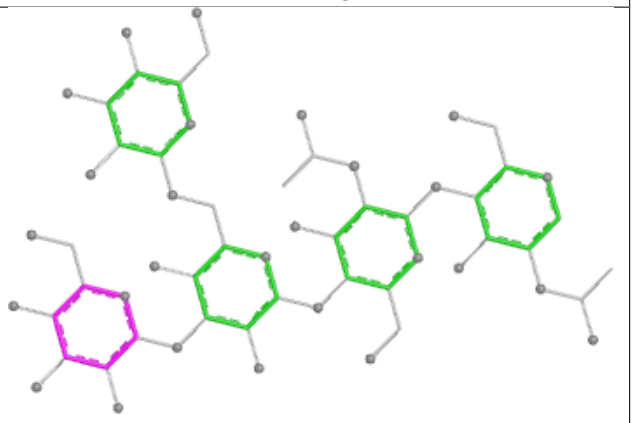
Bond lengths



Bond angles

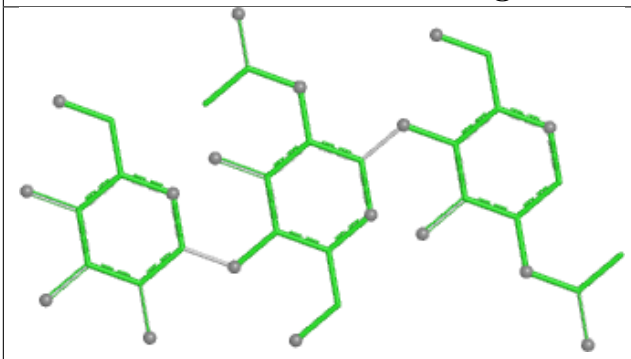


Torsions

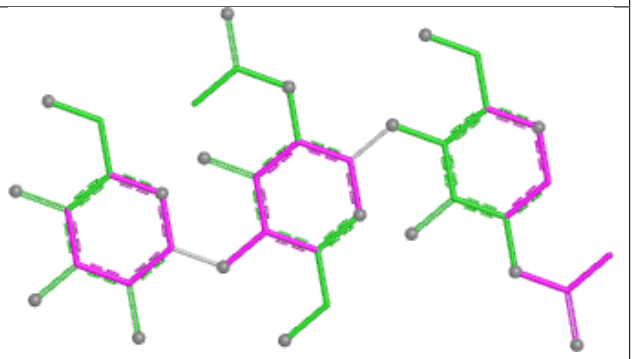


Rings

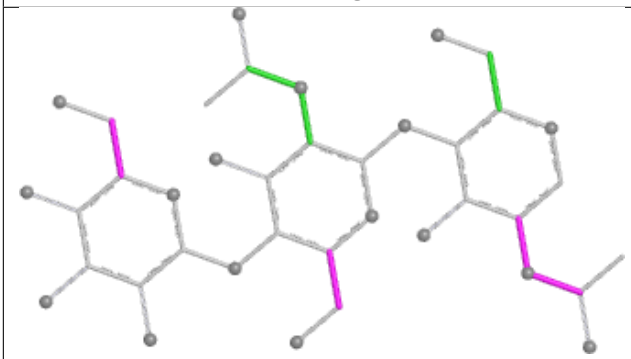
Oligosaccharide Chain H



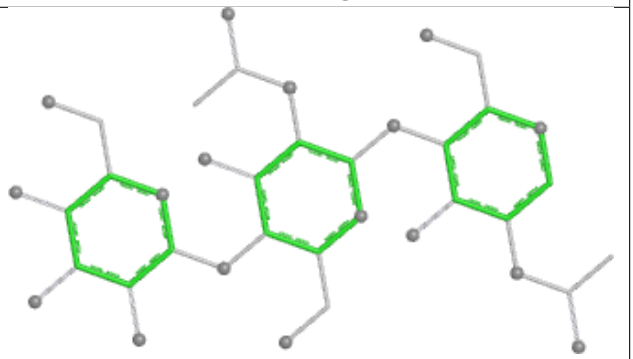
Bond lengths



Bond angles

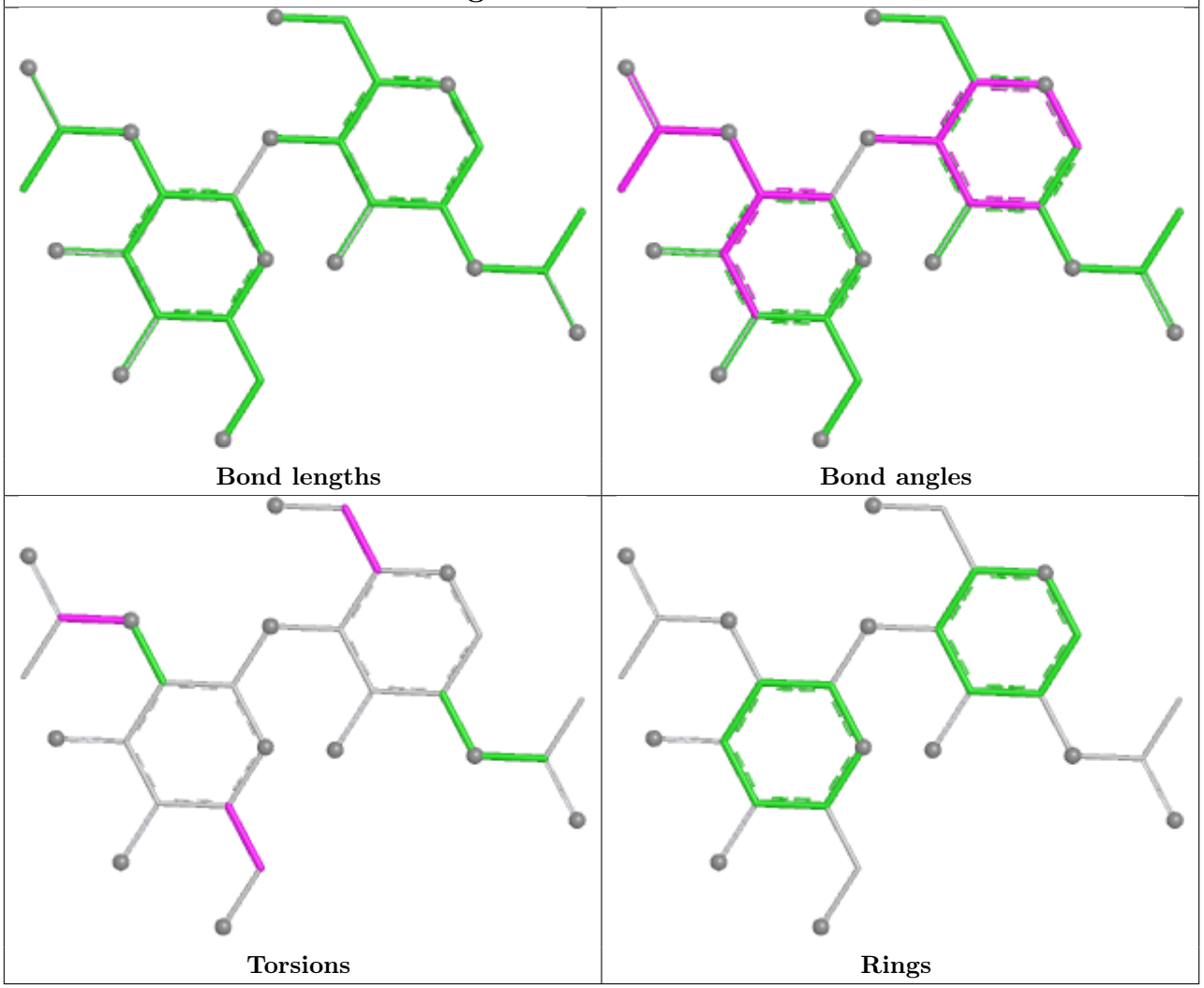


Torsions



Rings

Oligosaccharide Chain J



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	$\#\|Z\| > 2$
7	EDO	D	1173	-	3,3,3	0.53	0	2,2,2	0.35	0
7	EDO	C	1327	-	3,3,3	0.40	0	2,2,2	0.37	0
7	EDO	F	1174	-	3,3,3	0.35	0	2,2,2	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	EDO	B	1174	-	3,3,3	0.50	0	2,2,2	0.33	0
7	EDO	C	1329	-	3,3,3	0.51	0	2,2,2	0.54	0
7	EDO	A	1327	-	3,3,3	0.59	0	2,2,2	0.32	0
6	NAG	A	401	1	14,14,15	0.53	0	17,19,21	1.67	3 (17%)
6	NAG	D	211	2	14,14,15	0.78	1 (7%)	17,19,21	1.36	2 (11%)
7	EDO	B	1173	-	3,3,3	0.58	0	2,2,2	0.20	0
7	EDO	A	1326	-	3,3,3	0.59	0	2,2,2	0.32	0
6	NAG	E	420	1	14,14,15	0.54	0	17,19,21	1.81	3 (17%)
7	EDO	C	1328	-	3,3,3	0.61	0	2,2,2	0.20	0
7	EDO	F	1173	-	3,3,3	0.45	0	2,2,2	0.08	0
6	NAG	A	420	1	14,14,15	0.56	0	17,19,21	1.87	3 (17%)
7	EDO	F	1176	-	3,3,3	0.48	0	2,2,2	0.52	0
7	EDO	F	1175	-	3,3,3	0.60	0	2,2,2	0.19	0
7	EDO	E	1327	-	3,3,3	0.58	0	2,2,2	0.09	0
7	EDO	B	1175	-	3,3,3	0.37	0	2,2,2	0.55	0
7	EDO	E	1326	-	3,3,3	0.39	0	2,2,2	0.69	0
7	EDO	C	1326	-	3,3,3	0.57	0	2,2,2	0.50	0
7	EDO	E	1328	-	3,3,3	0.55	0	2,2,2	0.24	0
7	EDO	A	1328	-	3,3,3	0.67	0	2,2,2	0.29	0
6	NAG	B	211	2	14,14,15	0.68	0	17,19,21	1.32	3 (17%)
6	NAG	C	420	1	14,14,15	0.59	0	17,19,21	2.63	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
7	EDO	D	1173	-	-	1/1/1/1	-
7	EDO	C	1327	-	-	1/1/1/1	-
7	EDO	F	1174	-	-	1/1/1/1	-
7	EDO	B	1174	-	-	1/1/1/1	-
7	EDO	C	1329	-	-	0/1/1/1	-
7	EDO	A	1327	-	-	1/1/1/1	-
6	NAG	A	401	1	1/1/5/7	2/6/23/26	0/1/1/1
6	NAG	D	211	2	-	1/6/23/26	0/1/1/1
7	EDO	B	1173	-	-	1/1/1/1	-
7	EDO	A	1326	-	-	1/1/1/1	-
6	NAG	E	420	1	1/1/5/7	4/6/23/26	0/1/1/1
7	EDO	C	1328	-	-	1/1/1/1	-
7	EDO	F	1173	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	420	1	1/1/5/7	2/6/23/26	0/1/1/1
7	EDO	F	1176	-	-	1/1/1/1	-
7	EDO	F	1175	-	-	1/1/1/1	-
7	EDO	E	1327	-	-	1/1/1/1	-
7	EDO	B	1175	-	-	1/1/1/1	-
7	EDO	E	1326	-	-	0/1/1/1	-
7	EDO	C	1326	-	-	0/1/1/1	-
7	EDO	E	1328	-	-	1/1/1/1	-
7	EDO	A	1328	-	-	1/1/1/1	-
6	NAG	B	211	2	-	0/6/23/26	0/1/1/1
6	NAG	C	420	1	1/1/5/7	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	211	NAG	C1-C2	2.63	1.55	1.52

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	420	NAG	O5-C1-C2	-8.38	98.32	111.29
6	A	420	NAG	O5-C1-C2	-5.84	102.25	111.29
6	E	420	NAG	O5-C1-C2	-5.29	103.11	111.29
6	A	401	NAG	C1-O5-C5	5.15	119.09	112.19
6	C	420	NAG	C2-N2-C7	-4.05	117.47	122.90

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	401	NAG	C1
6	A	420	NAG	C1
6	C	420	NAG	C1
6	E	420	NAG	C1

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	401	NAG	O5-C5-C6-O6
6	C	420	NAG	O5-C5-C6-O6
6	E	420	NAG	O5-C5-C6-O6
6	A	401	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	C	420	NAG	C4-C5-C6-O6

There are no ring outliers.

9 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	1329	EDO	1	0
6	D	211	NAG	1	0
7	C	1328	EDO	1	0
7	F	1176	EDO	5	0
7	F	1175	EDO	3	0
7	B	1175	EDO	1	0
7	E	1326	EDO	1	0
7	E	1328	EDO	6	0
7	A	1328	EDO	2	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	318/324 (98%)	0.11	11 (3%) 44 51	31, 51, 77, 149	0
1	C	319/324 (98%)	-0.03	4 (1%) 77 81	24, 42, 76, 140	0
1	E	319/324 (98%)	0.33	25 (7%) 13 17	33, 56, 88, 141	0
2	B	172/172 (100%)	0.67	10 (5%) 23 29	30, 66, 87, 91	0
2	D	172/172 (100%)	0.86	26 (15%) 2 3	30, 65, 94, 99	0
2	F	172/172 (100%)	0.95	27 (15%) 2 2	34, 71, 101, 108	0
All	All	1472/1488 (98%)	0.38	103 (6%) 16 21	24, 56, 91, 149	0

The worst 5 of 103 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	16	GLY	5.8
2	D	27	GLN	4.7
2	F	168	LEU	4.6
2	D	33	GLY	4.5
1	E	127	TYR	4.5

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

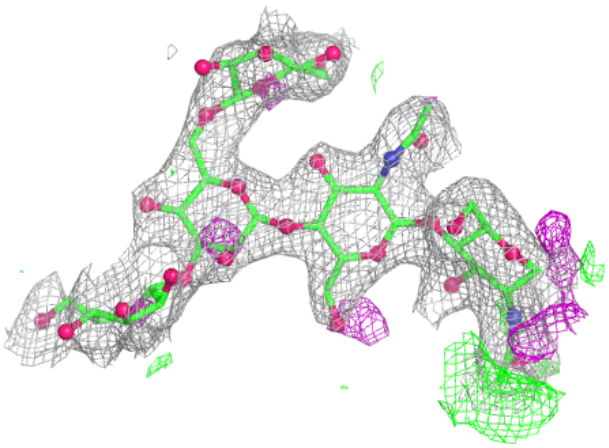
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

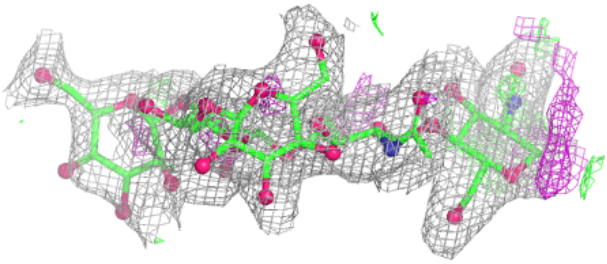
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MAN	K	5	11/12	0.46	0.39	107,119,126,129	0
3	BMA	K	3	11/12	0.68	0.37	98,107,117,118	0
5	NAG	J	2	14/15	0.72	0.40	89,93,98,99	0
4	BMA	H	3	11/12	0.73	0.41	97,100,106,107	0
3	MAN	I	5	11/12	0.73	0.21	75,79,85,88	0
3	MAN	G	4	11/12	0.76	0.32	81,85,94,95	0
3	BMA	I	3	11/12	0.77	0.21	76,85,90,93	0
3	MAN	K	4	11/12	0.78	0.43	116,122,132,134	0
3	MAN	I	4	11/12	0.78	0.17	92,96,106,108	0
3	MAN	G	5	11/12	0.81	0.31	71,74,80,83	0
4	NAG	H	2	14/15	0.83	0.45	83,89,92,95	0
3	BMA	G	3	11/12	0.84	0.27	68,75,80,82	0
3	NAG	K	2	14/15	0.85	0.19	69,73,83,89	0
5	NAG	J	1	14/15	0.86	0.26	73,77,85,87	0
4	NAG	H	1	14/15	0.87	0.27	63,67,74,78	0
3	NAG	G	2	14/15	0.89	0.17	51,54,61,64	0
3	NAG	I	2	14/15	0.89	0.12	53,56,64,70	0
3	NAG	K	1	14/15	0.92	0.24	47,51,57,62	0
3	NAG	G	1	14/15	0.92	0.19	37,40,45,47	0
3	NAG	I	1	14/15	0.95	0.19	39,42,46,49	0

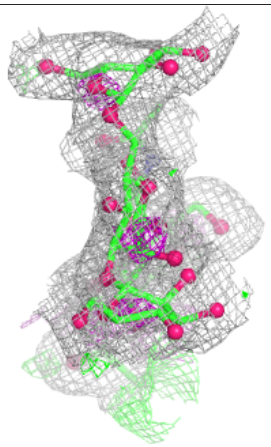
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain G:

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

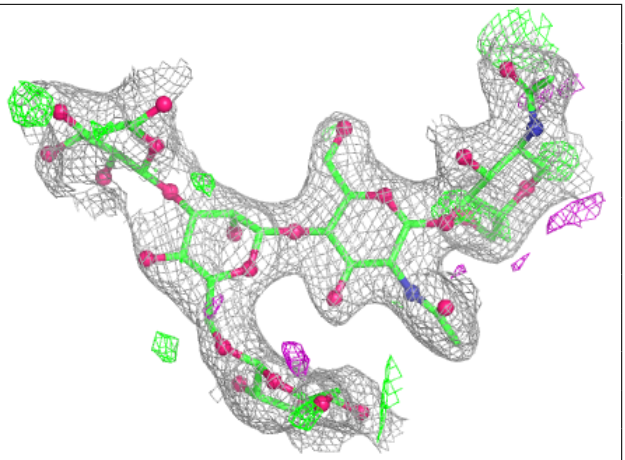


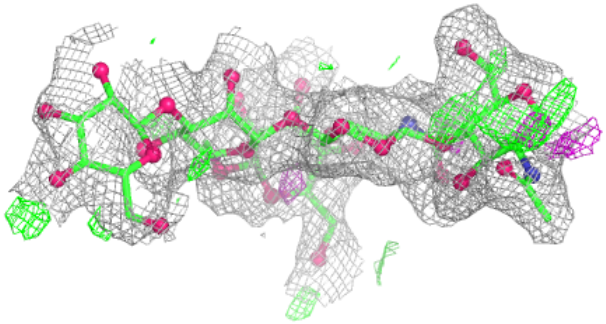


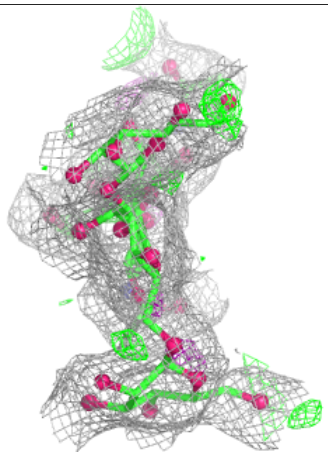


Electron density around Chain I:

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

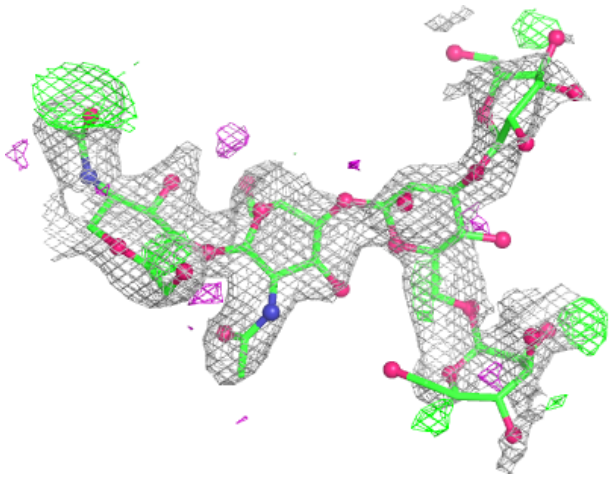


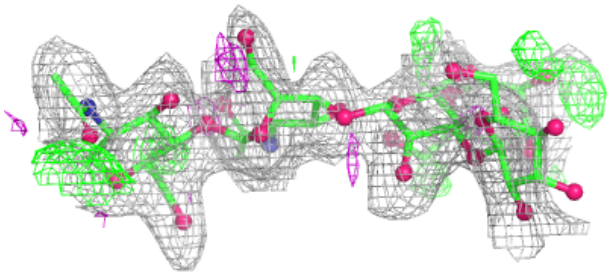


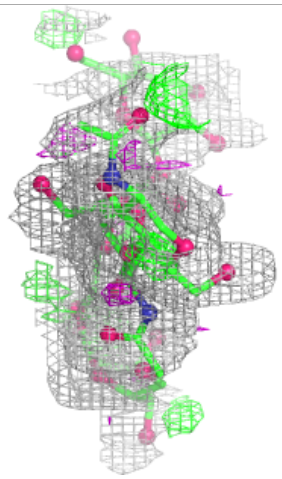


Electron density around Chain K:

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

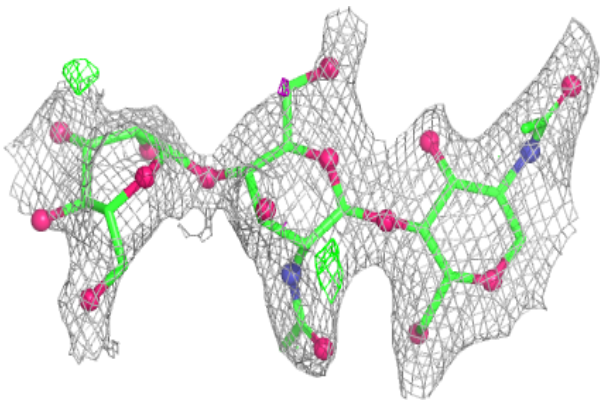


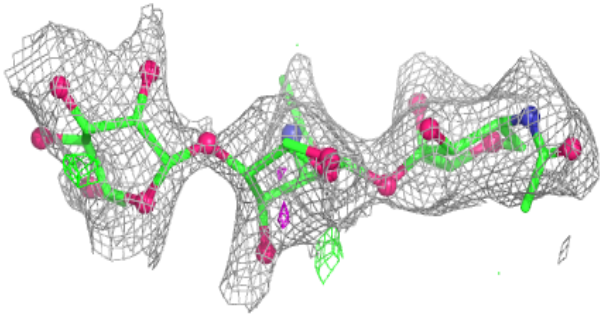


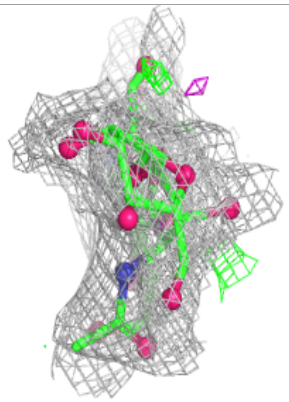


Electron density around Chain H:

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

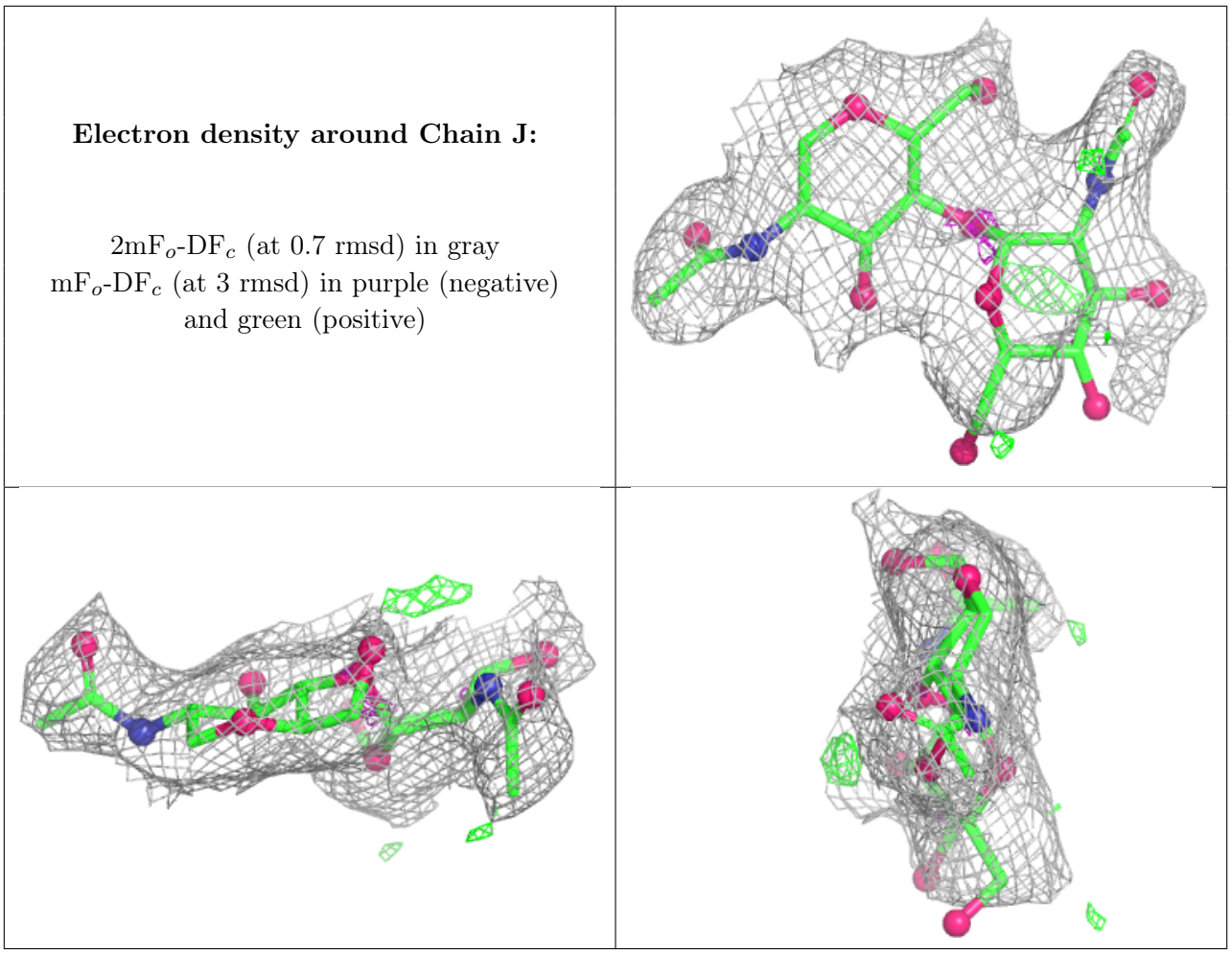






Electron density around Chain J:

$2mF_o$-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
6	NAG	D	211	14/15	0.64	0.35	94,100,105,106	0
6	NAG	C	420	14/15	0.73	0.28	61,67,72,73	0
6	NAG	B	211	14/15	0.74	0.29	93,100,103,105	0
7	EDO	E	1327	4/4	0.79	0.61	53,55,55,56	0
6	NAG	A	420	14/15	0.80	0.33	72,78,84,84	0
7	EDO	F	1175	4/4	0.80	0.46	67,68,71,71	0
7	EDO	E	1328	4/4	0.82	0.54	58,58,60,62	0
7	EDO	D	1173	4/4	0.82	0.18	50,52,56,58	0
7	EDO	F	1176	4/4	0.83	0.59	63,64,64,68	0
7	EDO	C	1329	4/4	0.86	0.28	48,49,50,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	A	401	14/15	0.86	0.30	81,85,93,93	0
6	NAG	E	420	14/15	0.88	0.30	68,74,79,79	0
7	EDO	A	1327	4/4	0.90	0.26	49,52,54,57	0
7	EDO	C	1328	4/4	0.91	0.24	39,48,50,51	0
7	EDO	F	1174	4/4	0.91	0.20	39,40,40,50	0
7	EDO	B	1175	4/4	0.92	0.44	40,44,45,45	0
7	EDO	C	1327	4/4	0.92	0.32	47,47,50,50	0
7	EDO	E	1326	4/4	0.93	0.32	46,46,49,52	0
7	EDO	F	1173	4/4	0.94	0.15	41,42,43,48	0
7	EDO	A	1328	4/4	0.95	0.21	44,44,45,47	0
7	EDO	B	1174	4/4	0.95	0.18	43,45,45,46	0
7	EDO	B	1173	4/4	0.96	0.26	34,34,38,39	0
7	EDO	A	1326	4/4	0.96	0.13	30,32,35,35	0
7	EDO	C	1326	4/4	0.97	0.15	30,30,33,34	0

6.5 Other polymers (i)

There are no such residues in this entry.