wwPDB X-ray Structure Validation Summary Report (i)

Dec 16, 2023 – 11:24 AM EST

PDB ID	:	4P5M
Title	:	Structural Basis of Chronic Beryllium Disease: Bridging the Gap Between Allergic Hypersensitivity and Autoimmunity
Authors	:	Wang, Y.; Dai, S.; Kappler, J.
Deposited on	:	2014-03-18
Resolution	:	1.70 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 (1)) were used in the production of this report:

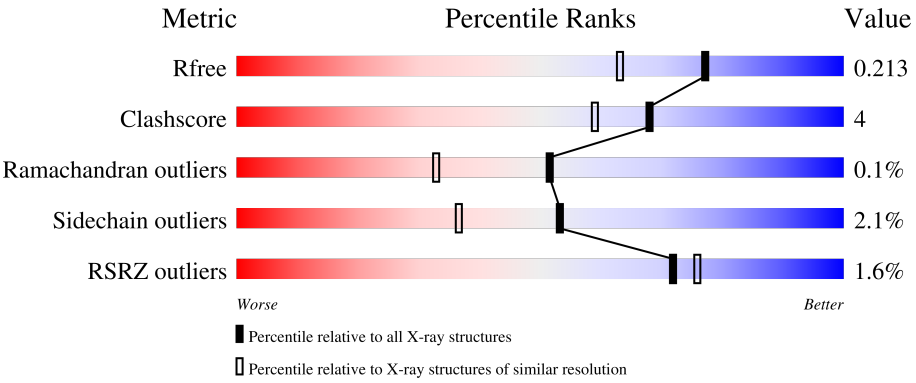
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	183	89% 8%
1	C	183	92% 6%
1	E	183	87% 9%
1	G	183	91% 7%
2	B	212	3% 85% 7% 6%

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Mol	Chain	Length	Quality of chain
2	D	212	2% 79% 11% • 6%
2	F	212	2% 79% 9% • 10%
2	H	212	2% 78% 10% • 10%
3	I	2	100%
3	K	2	100%
3	N	2	100%
4	J	4	50% 50%
5	L	3	33% 67%
6	M	4	50% 50%
7	O	3	100%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 14385 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 HLA class II histocompatibility antigen, DP alpha 1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	S	0	2	0
			1487	962	240	279	6			
1	C	180	Total	C	N	O	S	0	3	0
			1495	968	240	281	6			
1	E	180	Total	C	N	O	S	0	3	0
			1494	967	240	282	5			
1	G	180	Total	C	N	O	S	0	3	0
			1494	965	240	284	5			

- Molecule 2 is a protein called peptide,HLA class II histocompatibility antigen, DP beta 1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	199	Total	C	N	O	S	0	1	0
			1638	1031	288	311	8			
2	D	199	Total	C	N	O	S	0	2	0
			1646	1035	289	313	9			
2	F	190	Total	C	N	O	S	0	5	0
			1598	1002	278	309	9			
2	H	191	Total	C	N	O	S	0	3	0
			1583	997	273	305	8			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	GLY	-	linker	PDB ?
B	-12	GLY	-	linker	PDB ?
B	-11	SER	-	linker	PDB ?
B	-10	LEU	-	linker	PDB ?
B	-9	VAL	-	linker	PDB ?
B	-8	PRO	-	linker	PDB ?
B	-7	ARG	-	linker	PDB ?
B	-6	GLY	-	linker	PDB ?

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	SER	-	linker	PDB ?
B	-4	GLY	-	linker	PDB ?
B	-3	GLY	-	linker	PDB ?
B	-2	GLY	-	linker	PDB ?
B	-1	GLY	-	linker	PDB ?
B	3	SER	THR	variant	UNP Q5EP54
D	-13	GLY	-	linker	PDB ?
D	-12	GLY	-	linker	PDB ?
D	-11	SER	-	linker	PDB ?
D	-10	LEU	-	linker	PDB ?
D	-9	VAL	-	linker	PDB ?
D	-8	PRO	-	linker	PDB ?
D	-7	ARG	-	linker	PDB ?
D	-6	GLY	-	linker	PDB ?
D	-5	SER	-	linker	PDB ?
D	-4	GLY	-	linker	PDB ?
D	-3	GLY	-	linker	PDB ?
D	-2	GLY	-	linker	PDB ?
D	-1	GLY	-	linker	PDB ?
D	3	SER	THR	variant	UNP Q5EP54
F	-13	GLY	-	linker	PDB ?
F	-12	GLY	-	linker	PDB ?
F	-11	SER	-	linker	PDB ?
F	-10	LEU	-	linker	PDB ?
F	-9	VAL	-	linker	PDB ?
F	-8	PRO	-	linker	PDB ?
F	-7	ARG	-	linker	PDB ?
F	-6	GLY	-	linker	PDB ?
F	-5	SER	-	linker	PDB ?
F	-4	GLY	-	linker	PDB ?
F	-3	GLY	-	linker	PDB ?
F	-2	GLY	-	linker	PDB ?
F	-1	GLY	-	linker	PDB ?
F	3	SER	THR	variant	UNP Q5EP54
H	-13	GLY	-	linker	PDB ?
H	-12	GLY	-	linker	PDB ?
H	-11	SER	-	linker	PDB ?
H	-10	LEU	-	linker	PDB ?
H	-9	VAL	-	linker	PDB ?
H	-8	PRO	-	linker	PDB ?
H	-7	ARG	-	linker	PDB ?
H	-6	GLY	-	linker	PDB ?

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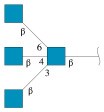
Chain	Residue	Modelled	Actual	Comment	Reference
H	-5	SER	-	linker	PDB ?
H	-4	GLY	-	linker	PDB ?
H	-3	GLY	-	linker	PDB ?
H	-2	GLY	-	linker	PDB ?
H	-1	GLY	-	linker	PDB ?
H	3	SER	THR	variant	UNP Q5EP54

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

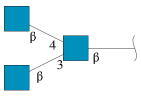
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	N	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



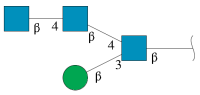
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	J	4	Total	C	N	O	0	0	0
			56	32	4	20			

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



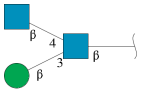
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	L	3	Total	C	N	O	0	0	0
			42	24	3	15			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	M	4	Total	C	N	O	0	0	0
			53	30	3	20			

- Molecule 7 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose.

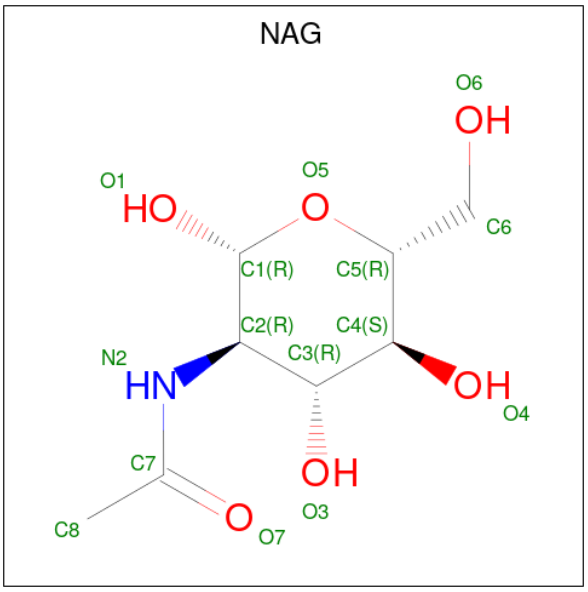


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	O	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Na	0	0
			1	1		
8	C	1	Total	Na	0	0
			1	1		

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	E	1	Total C N O 14 8 1 5	0	0

- Molecule 10 is water.

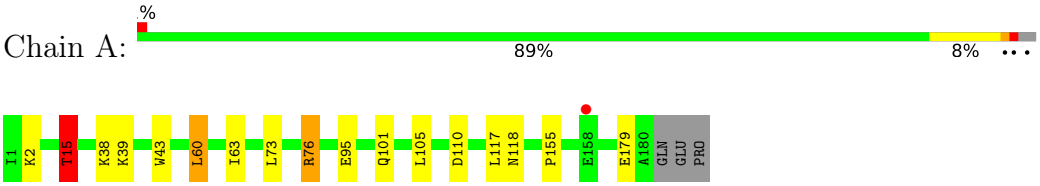
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	205	Total O 205 205	0	0
10	B	192	Total O 192 192	0	0
10	C	225	Total O 225 225	0	0
10	D	195	Total O 195 195	0	0
10	E	222	Total O 222 222	0	0
10	F	207	Total O 207 207	0	0
10	G	200	Total O 200 200	0	0
10	H	214	Total O 214 214	0	0

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.

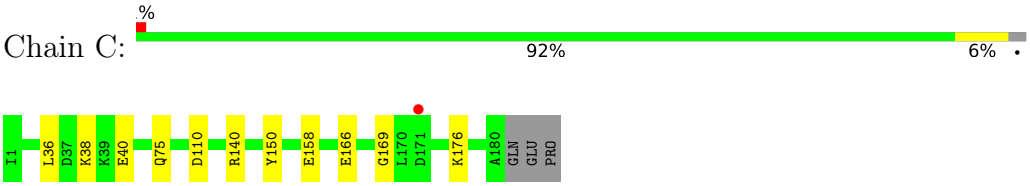
• Molecule 1: HLA class II histocompatibility antigen, DP alpha 1 chain

Chain A:



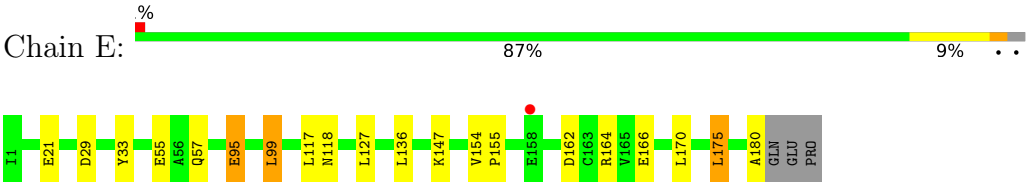
• Molecule 1: HLA class II histocompatibility antigen, DP alpha 1 chain

Chain C:



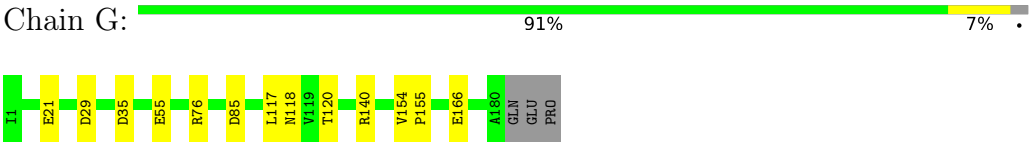
• Molecule 1: HLA class II histocompatibility antigen, DP alpha 1 chain

Chain E:



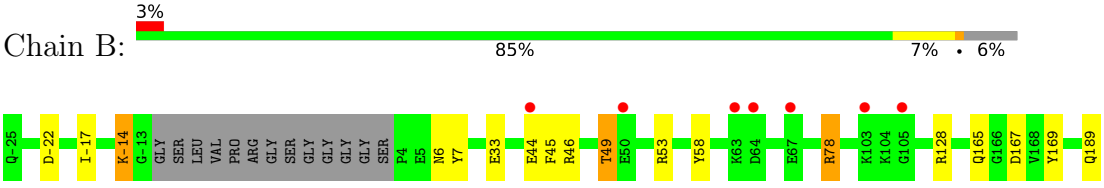
• Molecule 1: HLA class II histocompatibility antigen, DP alpha 1 chain

Chain G:



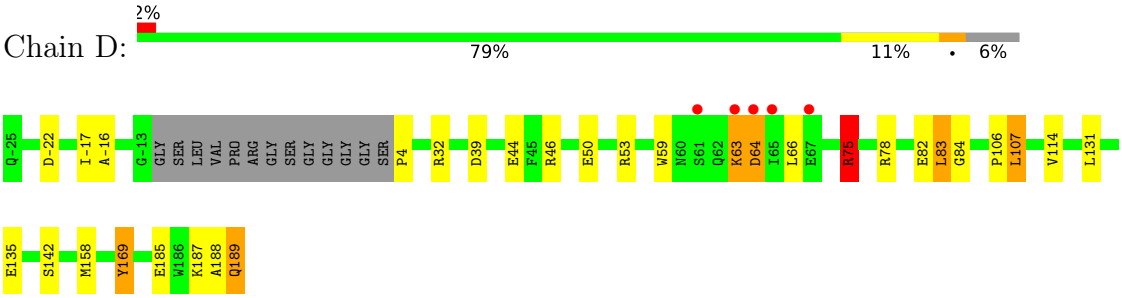
• Molecule 2: peptide,HLA class II histocompatibility antigen, DP beta 1 chain

Chain B:



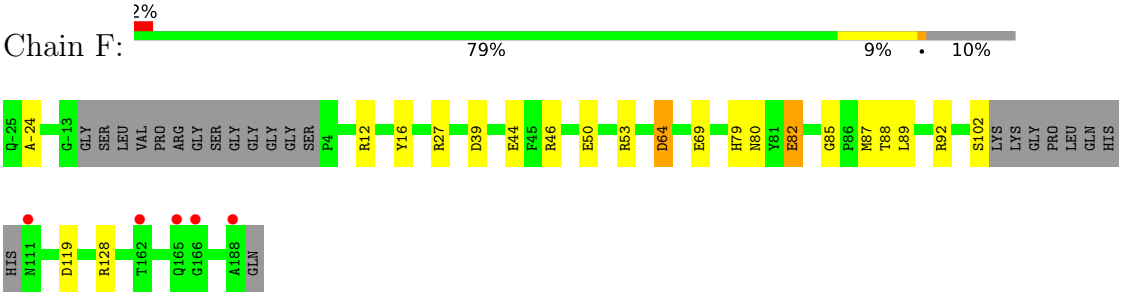
• Molecule 2: peptide,HLA class II histocompatibility antigen, DP beta 1 chain

Chain D:



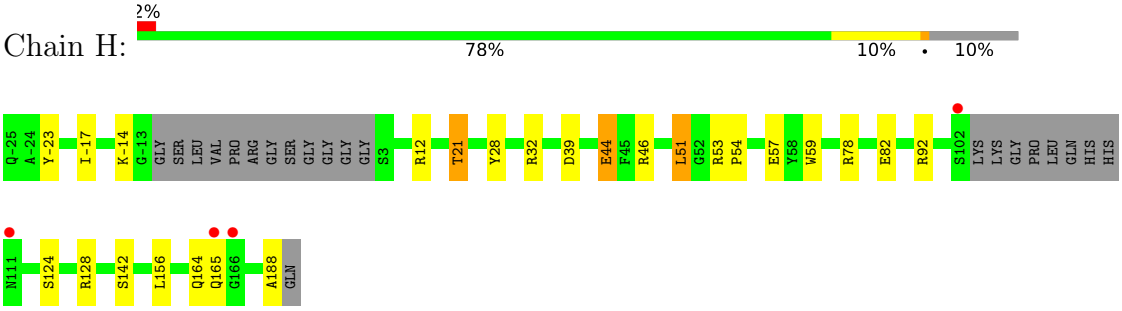
• Molecule 2: peptide,HLA class II histocompatibility antigen, DP beta 1 chain

Chain F:



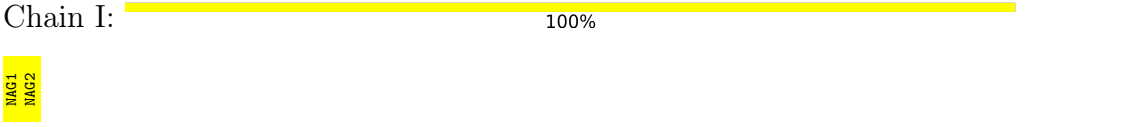
• Molecule 2: peptide,HLA class II histocompatibility antigen, DP beta 1 chain

Chain H:



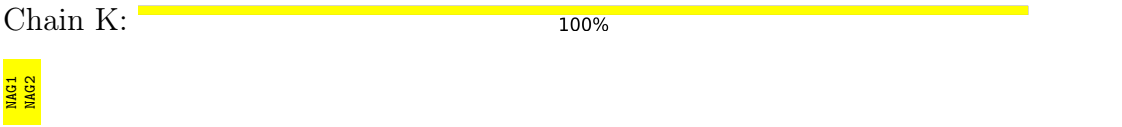
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



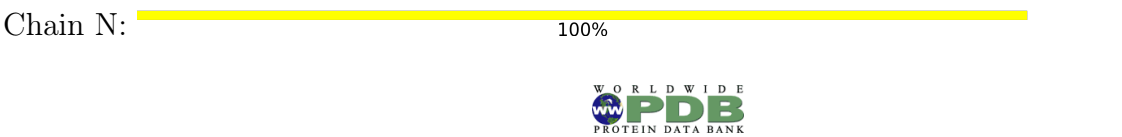
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



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

Chain N:



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

Chain J:

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

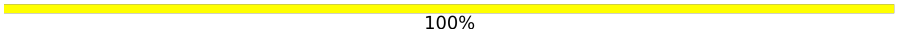
Chain L:

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

Chain M:

• Molecule 7: beta-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	81.63Å 130.47Å 107.99Å 90.00° 107.16° 90.00°	Depositor
Resolution (Å)	47.98 – 1.70 47.98 – 1.70	Depositor EDS
% Data completeness (in resolution range)	87.5 (47.98-1.70) 87.5 (47.98-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.02 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.168 , 0.204 0.178 , 0.213	Depositor DCC
R_{free} test set	10564 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	18.9	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 50.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14385	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.39% 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: NA, NAG, 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	1.11	2/1538 (0.1%)	1.09	8/2098 (0.4%)
1	C	1.20	6/1546 (0.4%)	1.06	3/2109 (0.1%)
1	E	1.16	4/1545 (0.3%)	1.08	6/2109 (0.3%)
1	G	1.10	1/1545 (0.1%)	1.03	5/2111 (0.2%)
2	B	1.11	0/1681	1.09	4/2279 (0.2%)
2	D	1.13	2/1689 (0.1%)	1.06	4/2288 (0.2%)
2	F	1.21	3/1635 (0.2%)	1.15	6/2215 (0.3%)
2	H	1.19	5/1625 (0.3%)	1.16	5/2203 (0.2%)
All	All	1.15	23/12804 (0.2%)	1.09	41/17412 (0.2%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	55	GLU	CD-OE2	8.10	1.34	1.25
2	F	82	GLU	CD-OE2	7.80	1.34	1.25
1	E	95	GLU	CD-OE2	7.69	1.34	1.25
1	E	55	GLU	CD-OE1	6.96	1.33	1.25
1	C	40	GLU	CD-OE1	6.87	1.33	1.25

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	12	ARG	NE-CZ-NH2	-12.07	114.27	120.30
2	H	12	ARG	NE-CZ-NH1	11.71	126.15	120.30
2	B	78	ARG	NE-CZ-NH2	9.76	125.18	120.30
1	A	76	ARG	NE-CZ-NH2	9.63	125.11	120.30
1	A	76	ARG	NE-CZ-NH1	-9.47	115.56	120.30

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	1487	0	1392	9	1
1	C	1495	0	1401	3	0
1	E	1494	0	1398	11	0
1	G	1494	0	1393	8	0
2	B	1638	0	1553	12	0
2	D	1646	0	1555	20	0
2	F	1598	0	1489	16	1
2	H	1583	0	1495	17	0
3	I	28	0	25	0	0
3	K	28	0	25	0	0
3	N	28	0	25	0	0
4	J	56	0	49	1	0
5	L	42	0	37	1	0
6	M	53	0	45	1	0
7	O	39	0	34	0	0
8	A	1	0	0	0	0
8	C	1	0	0	0	0
9	E	14	0	13	0	0
10	A	205	0	0	2	1
10	B	192	0	0	3	0
10	C	225	0	0	2	0
10	D	195	0	0	8	0
10	E	222	0	0	7	0
10	F	207	0	0	2	0
10	G	200	0	0	5	1
10	H	214	0	0	6	0
All	All	14385	0	11929	93	2

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 93 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:82:GLU:HG3	10:F:377:HOH:O	1.58	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:44:GLU:CD	2:F:46:ARG:HH12	1.69	0.95
2:F:44:GLU:OE2	2:F:46:ARG:NH1	2.04	0.90
2:D:78:ARG:HD2	10:D:473:HOH:O	1.76	0.85
1:G:85[B]:ASP:OD1	10:G:368:HOH:O	1.94	0.85

All (2) 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)
10:A:301:HOH:O	10:G:313:HOH:O[2_645]	2.01	0.19
1:A:39:LYS:NZ	2:F:64[A]:ASP:OD2[2_545]	2.19	0.01

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	180/183 (98%)	179 (99%)	1 (1%)	0	100	100
1	C	181/183 (99%)	180 (99%)	1 (1%)	0	100	100
1	E	181/183 (99%)	180 (99%)	1 (1%)	0	100	100
1	G	181/183 (99%)	180 (99%)	1 (1%)	0	100	100
2	B	196/212 (92%)	193 (98%)	3 (2%)	0	100	100
2	D	197/212 (93%)	195 (99%)	2 (1%)	0	100	100
2	F	189/212 (89%)	185 (98%)	3 (2%)	1 (0%)	29	13
2	H	188/212 (89%)	182 (97%)	6 (3%)	0	100	100
All	All	1493/1580 (94%)	1474 (99%)	18 (1%)	1 (0%)	51	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	85	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	163/164 (99%)	158 (97%)	5 (3%)	40	21
1	C	164/164 (100%)	162 (99%)	2 (1%)	71	59
1	E	164/164 (100%)	162 (99%)	2 (1%)	71	59
1	G	164/164 (100%)	164 (100%)	0	100	100
2	B	178/185 (96%)	174 (98%)	4 (2%)	52	34
2	D	179/185 (97%)	171 (96%)	8 (4%)	27	10
2	F	174/185 (94%)	172 (99%)	2 (1%)	73	63
2	H	173/185 (94%)	167 (96%)	6 (4%)	36	17
All	All	1359/1396 (97%)	1330 (98%)	29 (2%)	53	36

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	75	ARG
2	H	164	GLN
2	D	187	LYS
2	H	21[A]	THR
2	D	107	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	62	GLN
2	D	189	GLN
2	H	31	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

20 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	I	1	3,1	14,14,15	0.70	0	17,19,21	1.42	2 (11%)
3	NAG	I	2	3	14,14,15	0.59	0	17,19,21	2.47	6 (35%)
4	NAG	J	1	2,4	14,14,15	1.06	1 (7%)	17,19,21	3.55	8 (47%)
4	NAG	J	2	4	14,14,15	0.98	1 (7%)	17,19,21	2.74	7 (41%)
4	NAG	J	3	4	14,14,15	0.72	0	17,19,21	1.81	3 (17%)
4	NAG	J	4	4	14,14,15	0.64	0	17,19,21	2.22	4 (23%)
3	NAG	K	1	3,1	14,14,15	1.21	1 (7%)	17,19,21	1.95	4 (23%)
3	NAG	K	2	3	14,14,15	0.61	0	17,19,21	2.06	4 (23%)
5	NAG	L	1	2,5	14,14,15	1.14	2 (14%)	17,19,21	2.24	6 (35%)
5	NAG	L	2	5	14,14,15	0.77	0	17,19,21	3.10	12 (70%)
5	NAG	L	3	5	14,14,15	0.69	0	17,19,21	1.73	2 (11%)
6	NAG	M	1	6,2	14,14,15	1.59	2 (14%)	17,19,21	1.66	3 (17%)
6	NAG	M	2	6	14,14,15	0.86	0	17,19,21	1.81	5 (29%)
6	NAG	M	3	6	14,14,15	0.79	0	17,19,21	2.16	7 (41%)
6	BMA	M	4	6	11,11,12	0.73	0	15,15,17	5.51	10 (66%)
3	NAG	N	1	3,1	14,14,15	0.98	0	17,19,21	2.07	6 (35%)
3	NAG	N	2	3	14,14,15	0.58	0	17,19,21	1.97	2 (11%)
7	NAG	O	1	2,7	14,14,15	1.23	2 (14%)	17,19,21	1.25	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	BMA	O	2	7	11,11,12	2.28	4 (36%)	15,15,17	4.05	9 (60%)
7	NAG	O	3	7	14,14,15	1.19	1 (7%)	17,19,21	2.37	5 (29%)

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	I	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
4	NAG	J	1	2,4	-	1/6/23/26	0/1/1/1
4	NAG	J	2	4	-	1/6/23/26	0/1/1/1
4	NAG	J	3	4	-	0/6/23/26	0/1/1/1
4	NAG	J	4	4	-	3/6/23/26	0/1/1/1
3	NAG	K	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
5	NAG	L	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	L	2	5	-	0/6/23/26	0/1/1/1
5	NAG	L	3	5	-	0/6/23/26	0/1/1/1
6	NAG	M	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	M	2	6	-	0/6/23/26	0/1/1/1
6	NAG	M	3	6	-	0/6/23/26	0/1/1/1
6	BMA	M	4	6	-	1/2/19/22	0/1/1/1
3	NAG	N	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	2/6/23/26	0/1/1/1
7	NAG	O	1	2,7	-	0/6/23/26	0/1/1/1
7	BMA	O	2	7	-	2/2/19/22	0/1/1/1
7	NAG	O	3	7	-	1/6/23/26	0/1/1/1

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	O	2	BMA	O5-C1	-5.55	1.34	1.43
6	M	1	NAG	O5-C1	-4.24	1.36	1.43
7	O	1	NAG	O5-C1	-3.58	1.38	1.43
7	O	3	NAG	C1-C2	2.99	1.56	1.52
7	O	2	BMA	C6-C5	-2.99	1.41	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	M	4	BMA	O4-C4-C3	-10.78	85.44	110.35
6	M	4	BMA	O5-C5-C6	9.94	122.79	107.20
6	M	4	BMA	C1-O5-C5	9.20	124.66	112.19
7	O	2	BMA	O4-C4-C3	-8.86	89.86	110.35
6	M	4	BMA	O4-C4-C5	-8.52	88.13	109.30

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	N	2	NAG	O5-C5-C6-O6
4	J	4	NAG	O5-C5-C6-O6
7	O	2	BMA	O5-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6

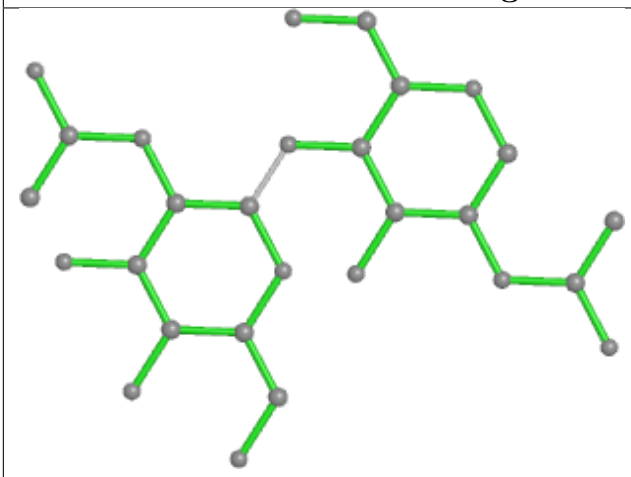
There are no ring outliers.

6 monomers are involved in 3 short contacts:

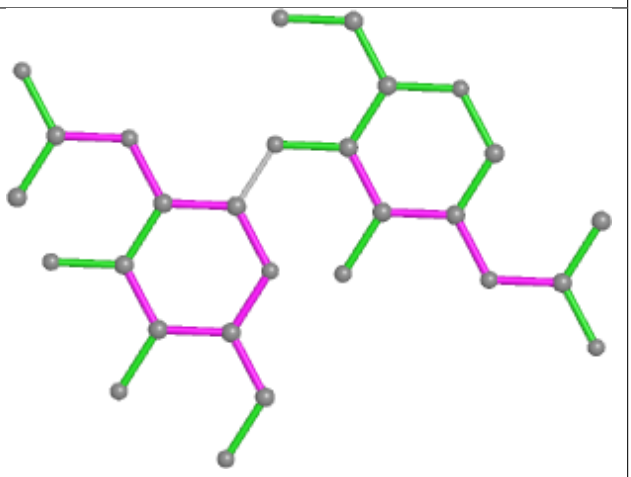
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	2	NAG	1	0
4	J	3	NAG	1	0
6	M	2	NAG	1	0
5	L	3	NAG	1	0
5	L	2	NAG	1	0
6	M	4	BMA	1	0

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

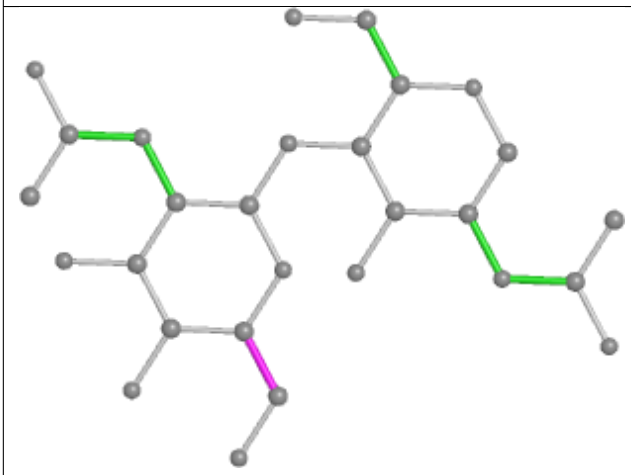
Oligosaccharide Chain I



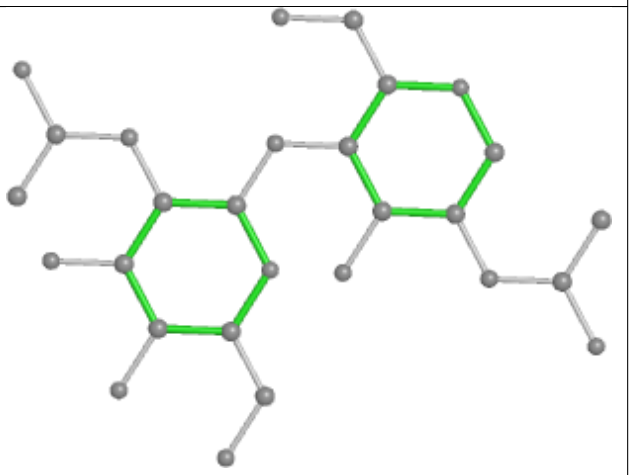
Bond lengths



Bond angles

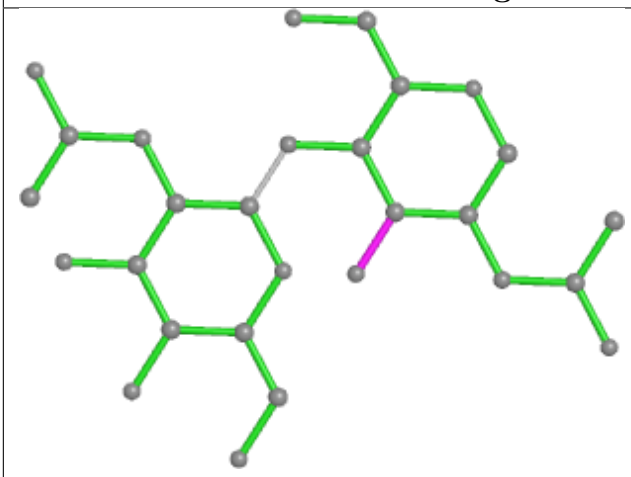


Torsions

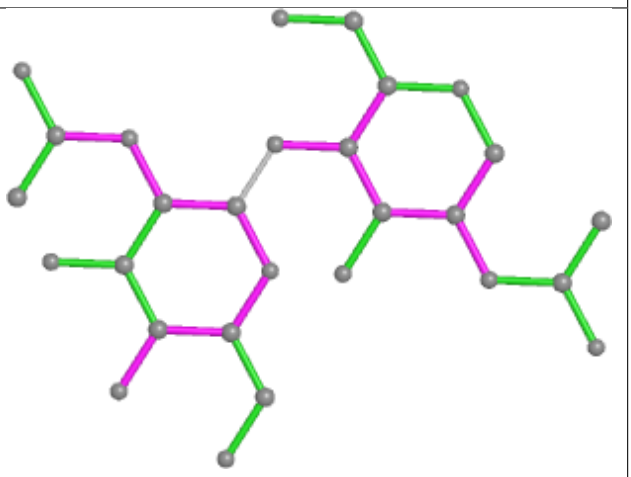


Rings

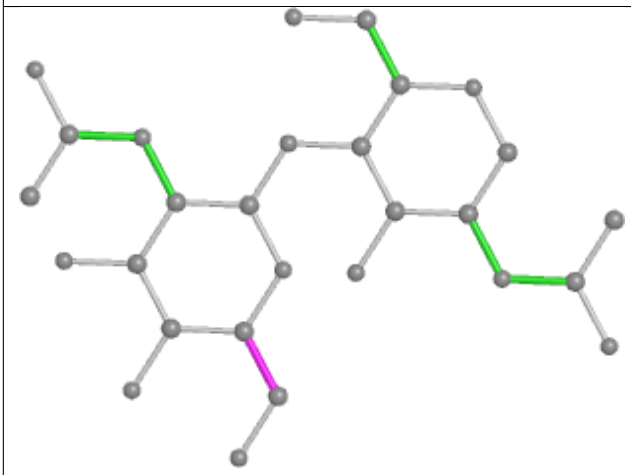
Oligosaccharide Chain K



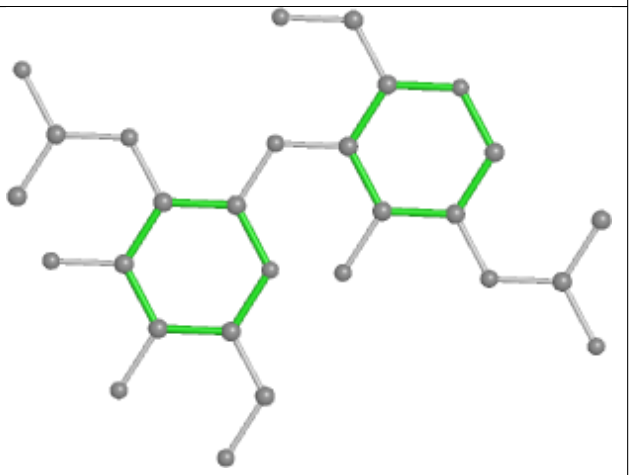
Bond lengths



Bond angles

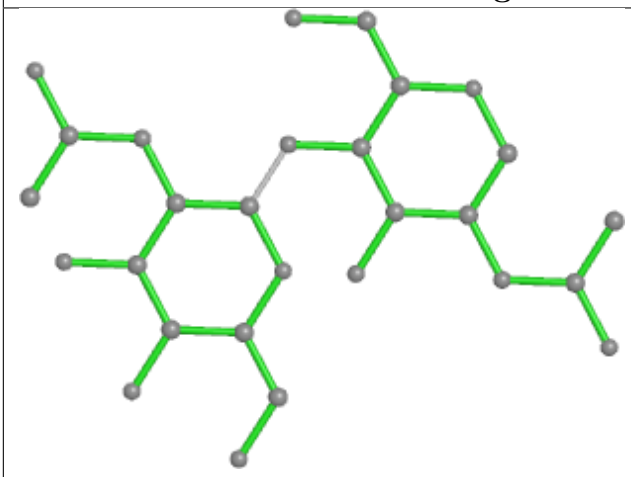


Torsions

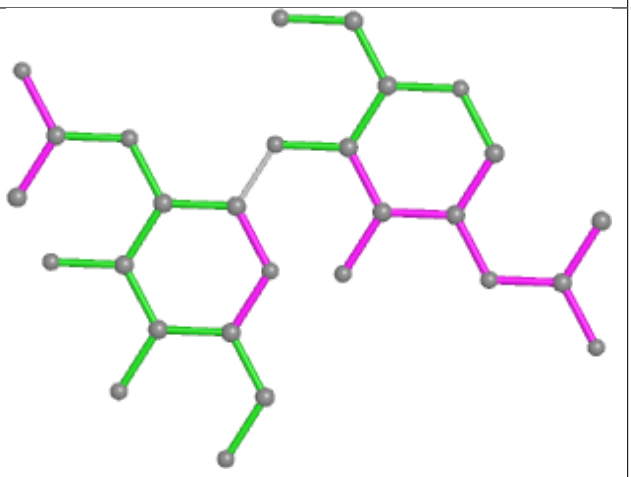


Rings

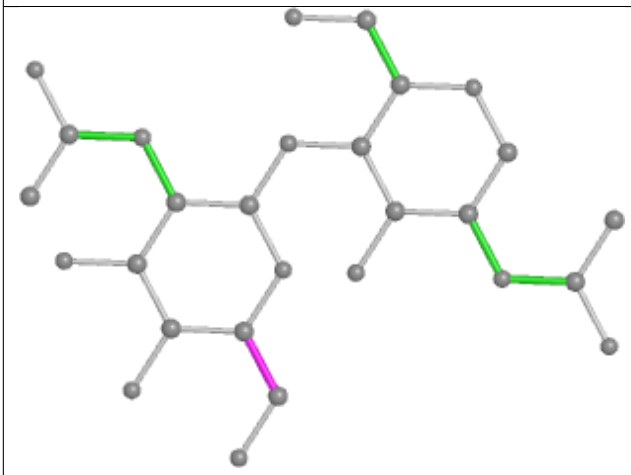
Oligosaccharide Chain N



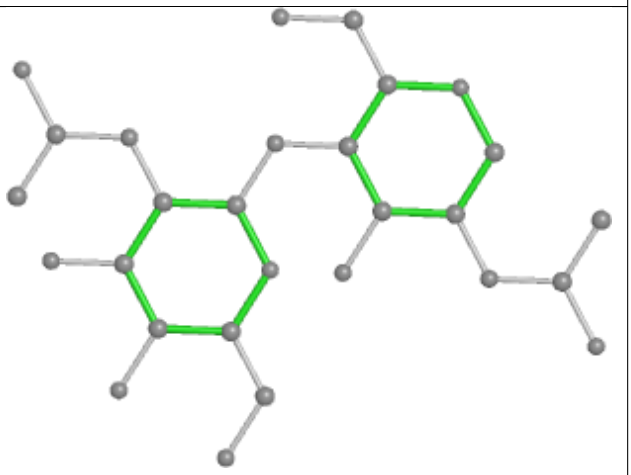
Bond lengths



Bond angles

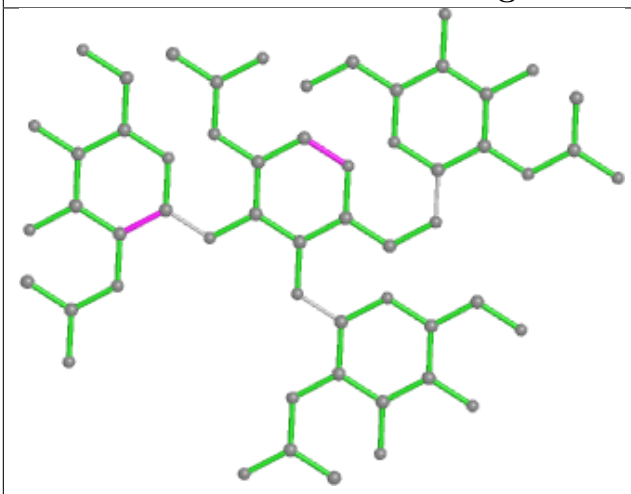


Torsions

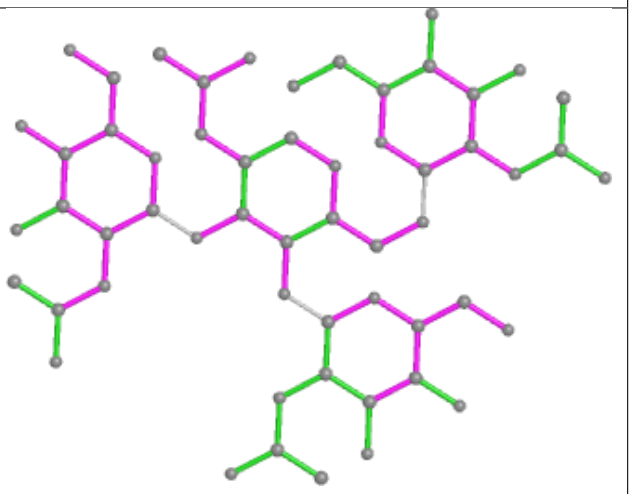


Rings

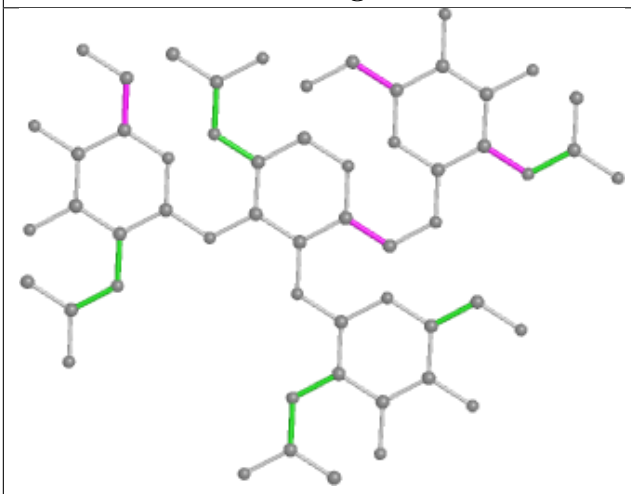
Oligosaccharide Chain J



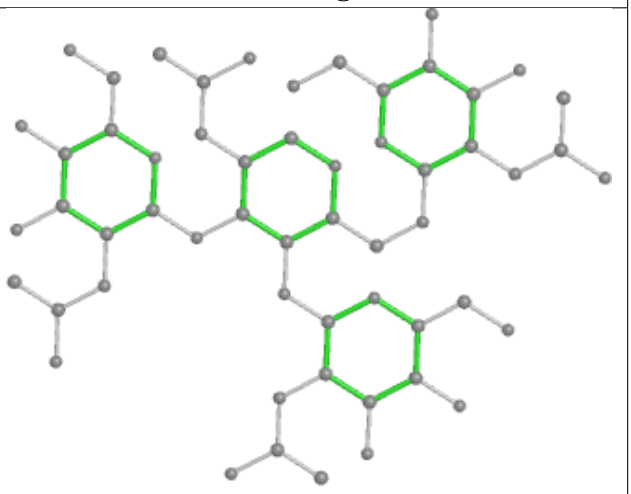
Bond lengths



Bond angles

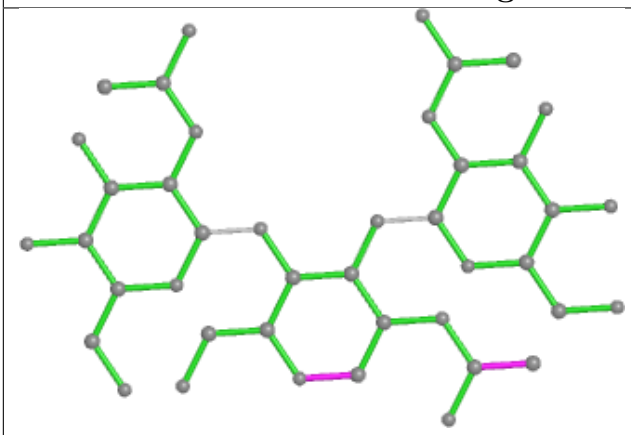


Torsions

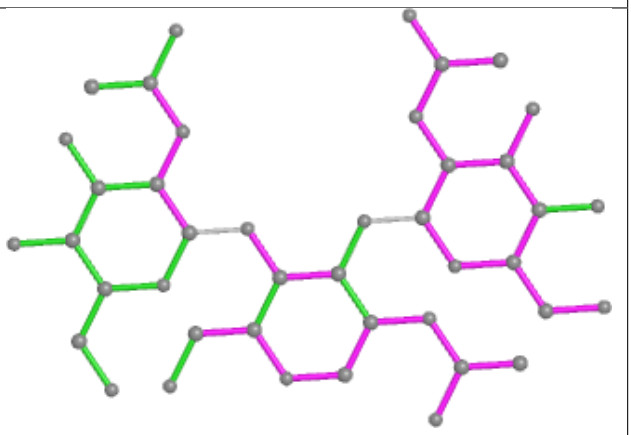


Rings

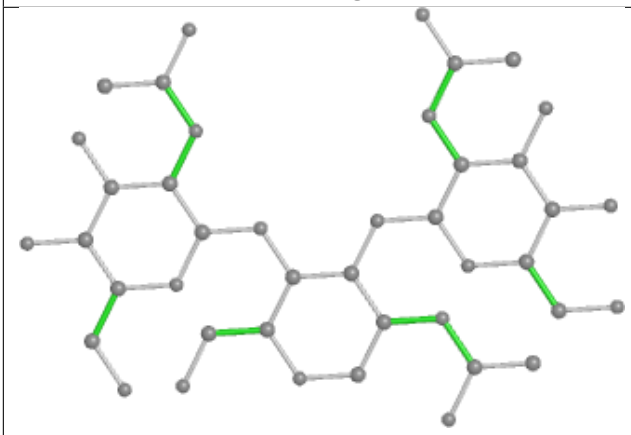
Oligosaccharide Chain L



Bond lengths



Bond angles



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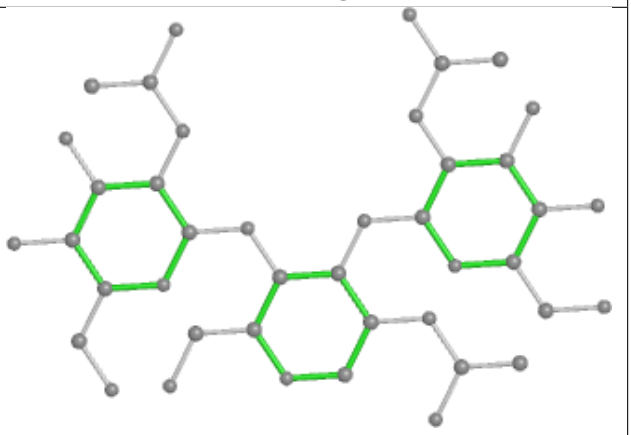
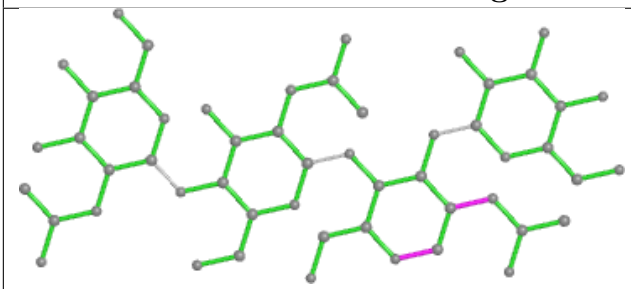
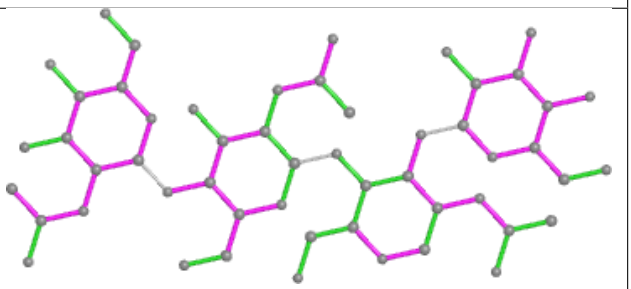


Rings

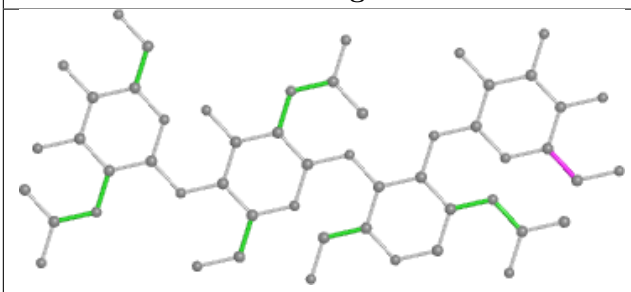
Oligosaccharide Chain M



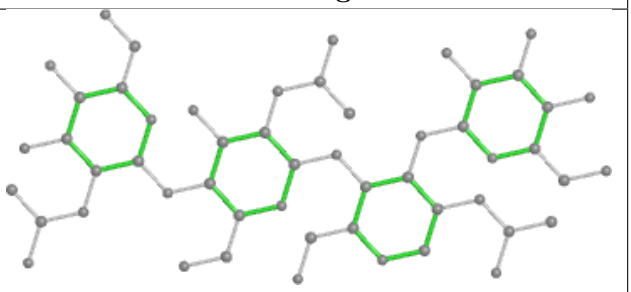
Bond lengths



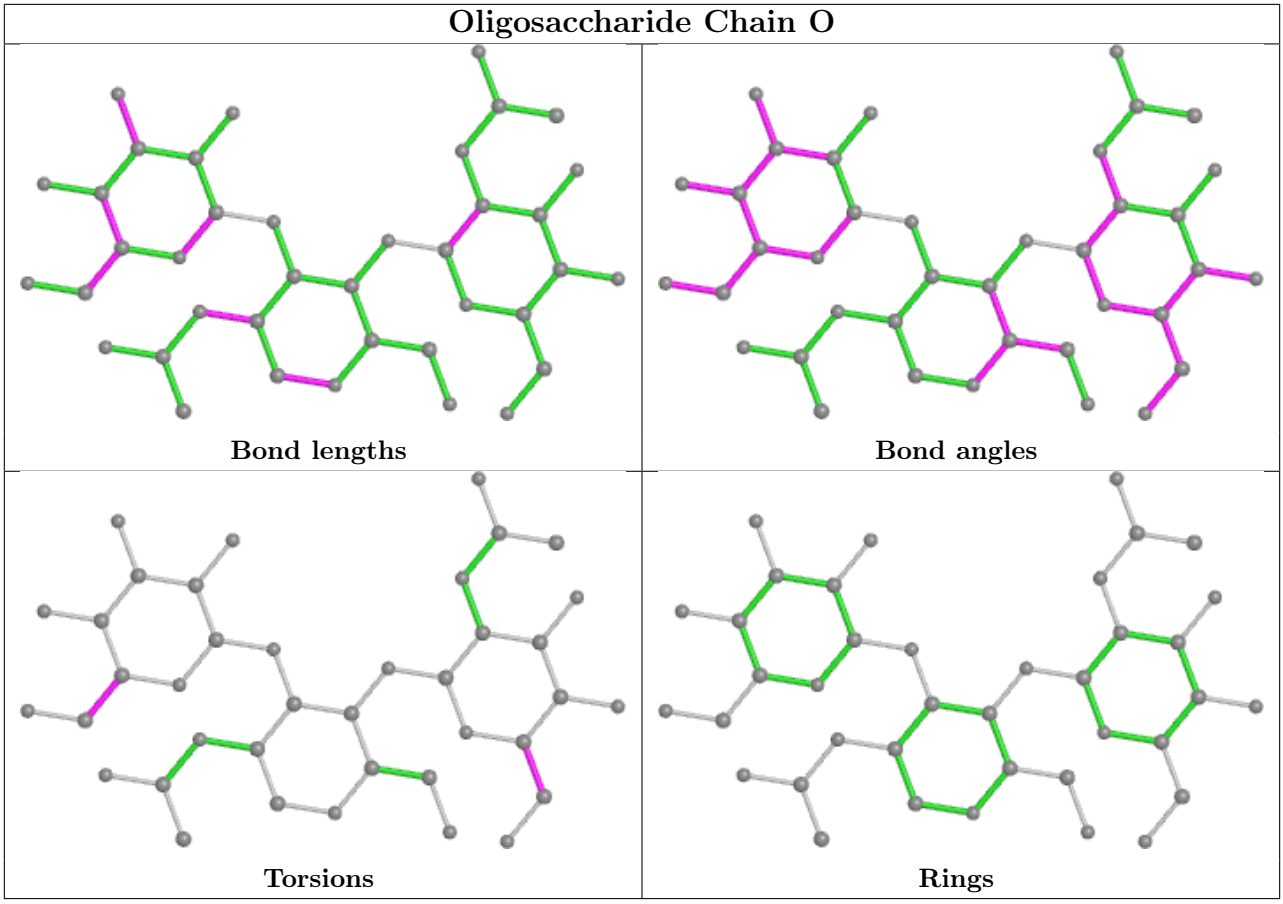
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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	NAG	E	201	1	14,14,15	1.02	0	17,19,21	1.74	5 (29%)

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
9	NAG	E	201	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	E	201	NAG	O7-C7-C8	-3.47	115.62	122.06
9	E	201	NAG	O4-C4-C5	3.04	116.85	109.30
9	E	201	NAG	C8-C7-N2	3.00	121.18	116.10
9	E	201	NAG	C3-C4-C5	-2.85	105.16	110.24
9	E	201	NAG	O5-C1-C2	-2.75	106.94	111.29

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	E	201	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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	180/183 (98%)	-0.26	1 (0%)	89	91	13, 21, 38, 56	0
1	C	180/183 (98%)	-0.37	1 (0%)	89	91	12, 20, 34, 52	0
1	E	180/183 (98%)	-0.31	1 (0%)	89	91	11, 20, 39, 56	0
1	G	180/183 (98%)	-0.28	0	100	100	10, 20, 37, 50	0
2	B	199/212 (93%)	-0.09	7 (3%)	44	49	11, 23, 50, 68	0
2	D	199/212 (93%)	-0.08	5 (2%)	57	61	10, 23, 48, 68	0
2	F	190/212 (89%)	-0.18	5 (2%)	56	60	11, 20, 42, 64	0
2	H	191/212 (90%)	-0.25	4 (2%)	63	67	11, 20, 42, 56	0
All	All	1499/1580 (94%)	-0.22	24 (1%)	72	76	10, 21, 42, 68	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	165	GLN	4.9
2	H	165	GLN	4.7
2	H	166	GLY	4.2
2	F	166	GLY	4.0
2	F	188	ALA	3.5

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,

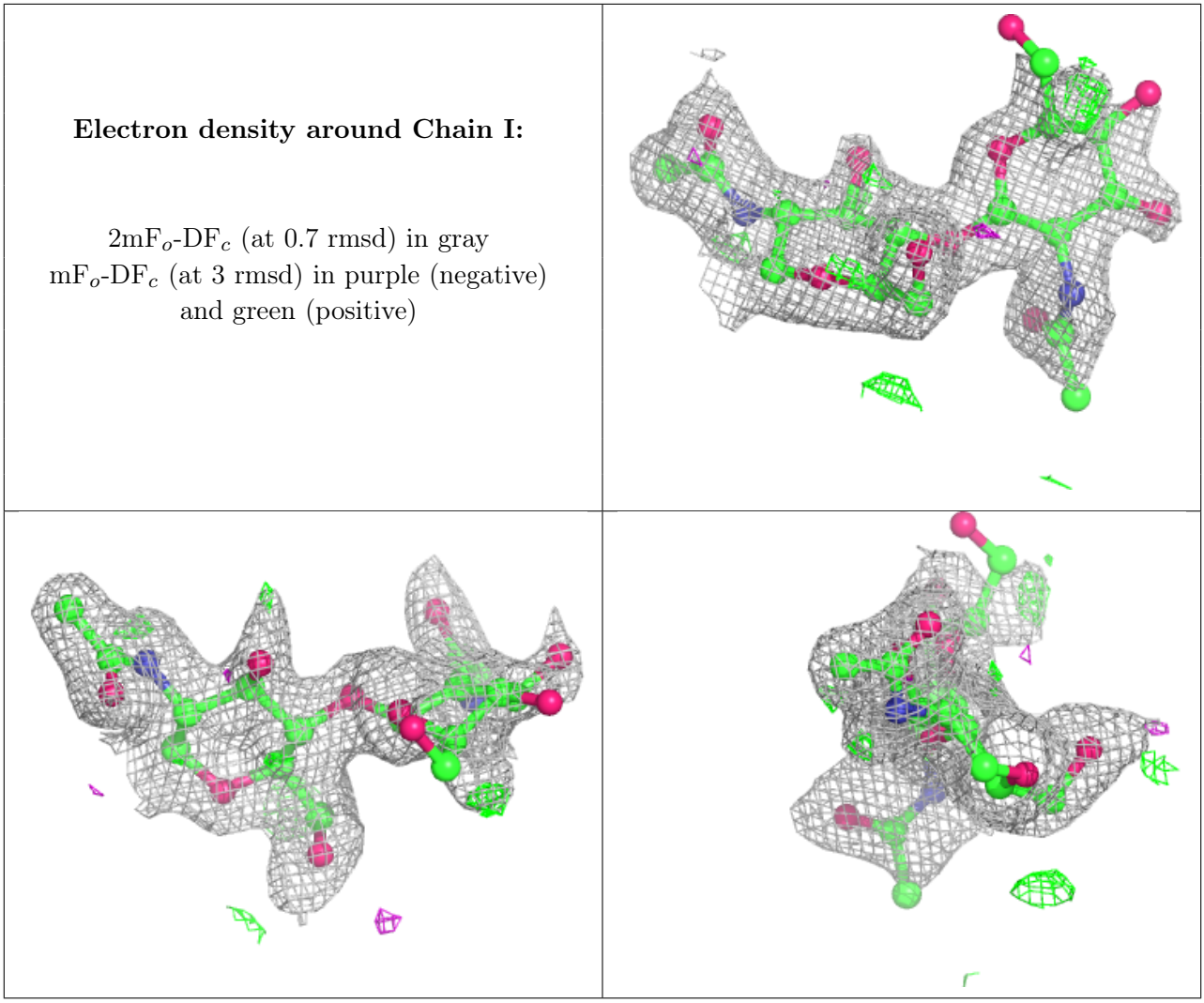
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	J	4	14/15	0.72	0.33	60,72,83,84	0
3	NAG	K	2	14/15	0.78	0.21	46,53,64,65	0
6	NAG	M	3	14/15	0.79	0.26	45,55,77,86	0
5	NAG	L	3	14/15	0.83	0.18	41,45,55,65	0
3	NAG	I	2	14/15	0.84	0.21	47,57,74,80	0
4	NAG	J	3	14/15	0.85	0.18	36,42,52,62	0
3	NAG	I	1	14/15	0.87	0.11	25,35,46,48	0
3	NAG	N	2	14/15	0.87	0.23	50,60,73,74	0
4	NAG	J	2	14/15	0.88	0.18	33,48,72,87	0
5	NAG	L	2	14/15	0.89	0.18	37,54,72,85	0
3	NAG	K	1	14/15	0.90	0.09	28,32,45,47	0
7	NAG	O	3	14/15	0.91	0.10	24,28,33,41	0
7	BMA	O	2	11/12	0.92	0.09	21,29,32,37	0
3	NAG	N	1	14/15	0.92	0.10	26,31,43,47	0
4	NAG	J	1	14/15	0.94	0.07	22,28,41,54	0
6	BMA	M	4	11/12	0.94	0.09	21,27,35,53	0
5	NAG	L	1	14/15	0.95	0.07	24,30,37,47	0
6	NAG	M	2	14/15	0.95	0.11	21,28,34,40	0
6	NAG	M	1	14/15	0.97	0.06	14,17,24,24	0
7	NAG	O	1	14/15	0.98	0.06	15,17,22,25	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.

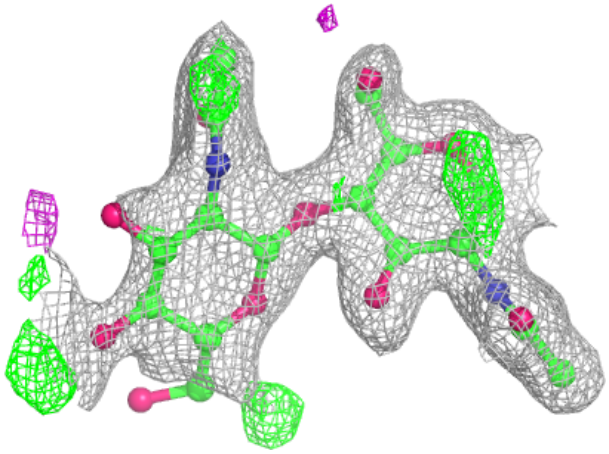
Electron density around Chain I:

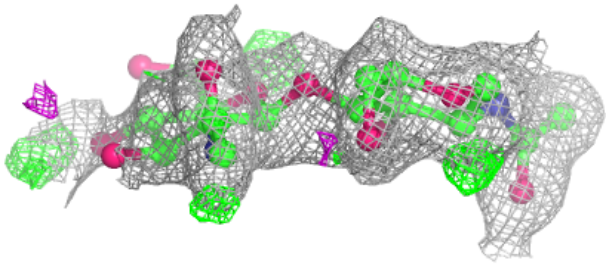
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

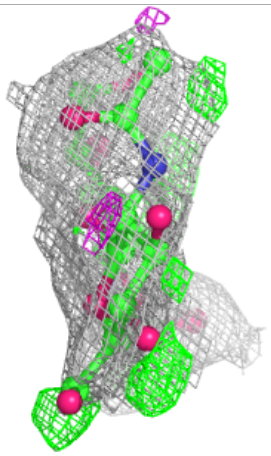


Electron density around Chain K:

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

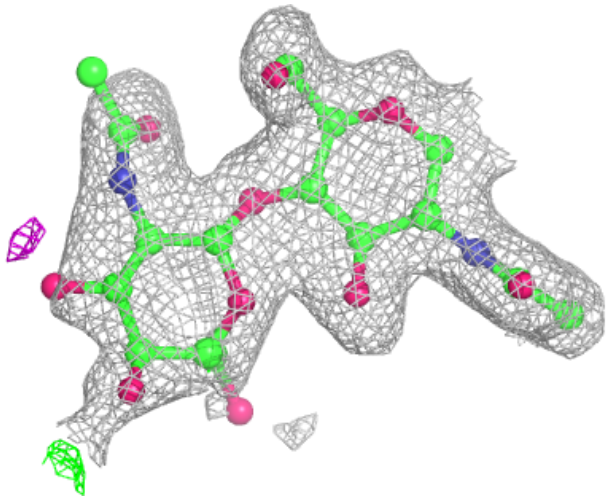


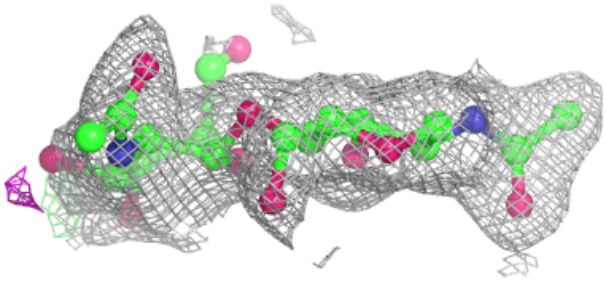


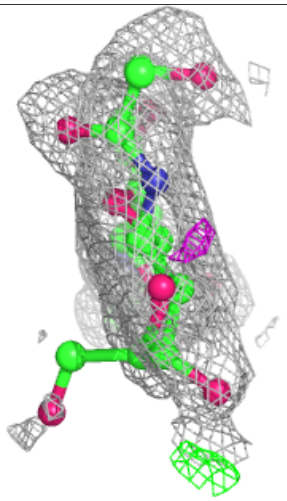


Electron density around Chain N:

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

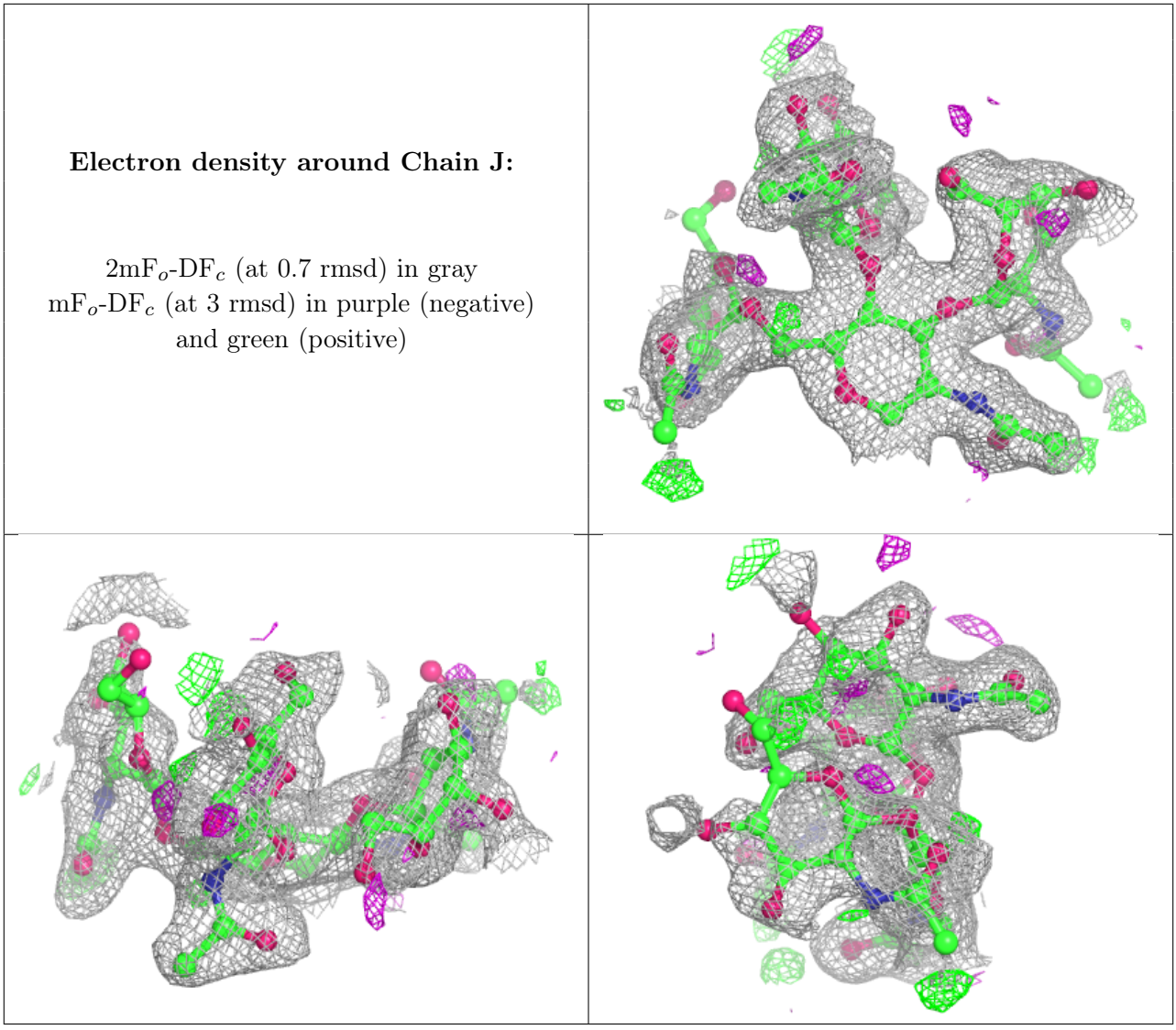






Electron density around Chain J:

$2mF_o$-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 L:

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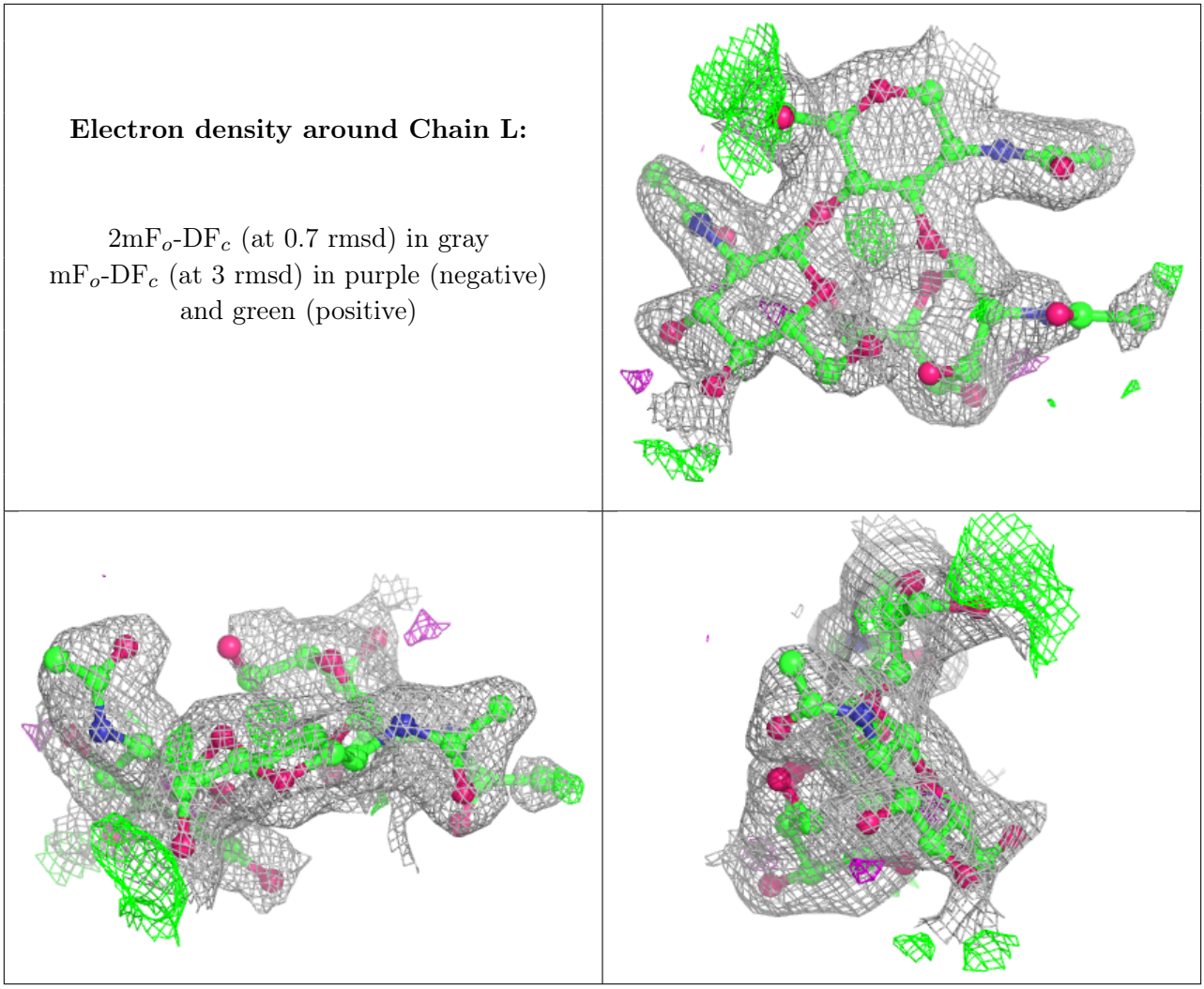
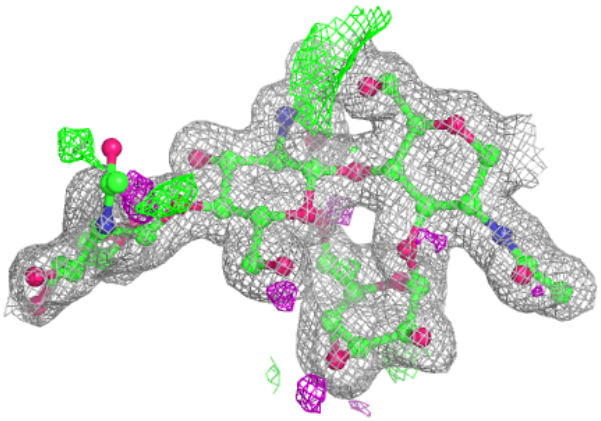
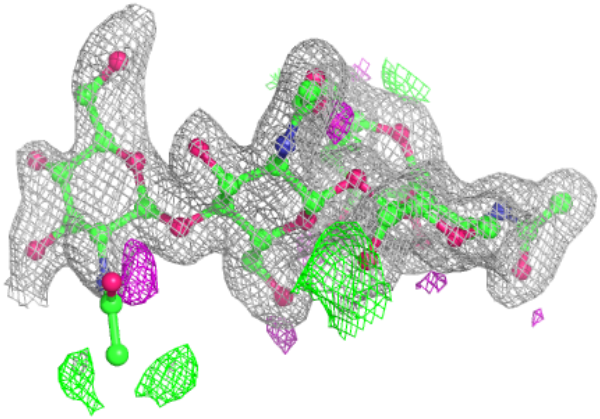
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

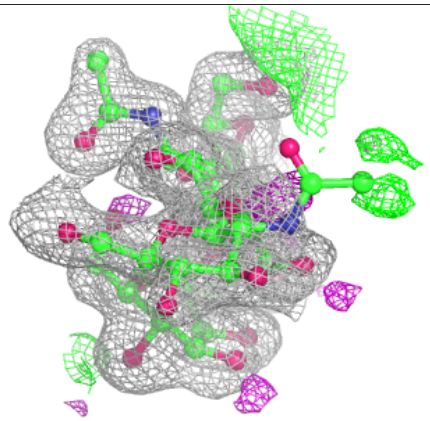


Electron density around Chain M:

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

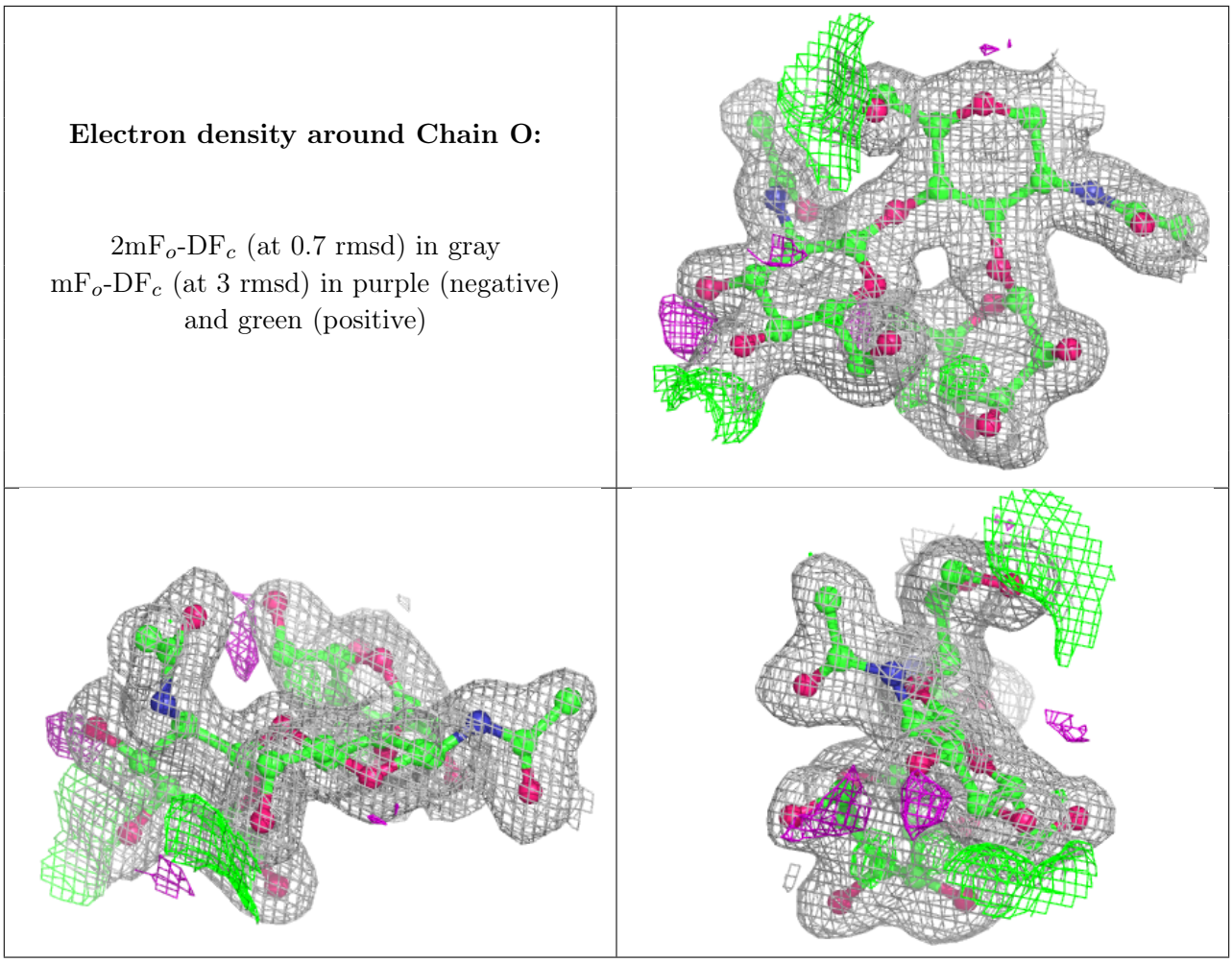






Electron density around Chain O:

$2mF_o$-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	NAG	E	201	14/15	0.91	0.12	27,37,51,52	0
8	NA	A	201	1/1	0.98	0.06	31,31,31,31	0
8	NA	C	201	1/1	0.99	0.05	32,32,32,32	0

6.5 Other polymers

There are no such residues in this entry.