Full wwPDB X-ray Structure Validation Report (i)

Sep 6, 2023 – 10:41 am BST

PDB ID	:	8OK7
Title	:	Variant Surface Glycoprotein VSG558 NTD
Authors	:	Zeelen, J.P.; Stebbins, C.E.; van Straaten, M.; Zhong, J.
Deposited on	:	2023-03-27
Resolution	:	1.74 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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:

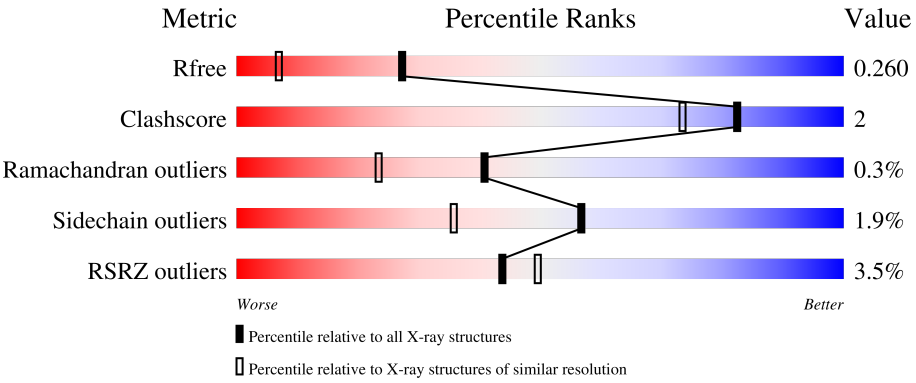
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.74 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	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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	419	83% · 14%
1	B	419	80% 5% 14%
1	C	419	7% 74% 12% · 14%
1	D	419	80% 6% 14%
2	E	6	100%

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Mol	Chain	Length	Quality of chain
3	F	5	80% 20%
3	J	5	60% 40%
3	L	5	60% 40%
4	G	7	86% 14%
4	I	7	71% 29%
5	H	6	83% 17%
5	K	6	50% 33% 17%

2 Entry composition

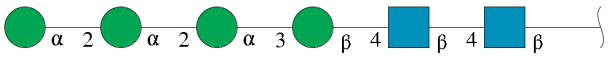
There are 6 unique types of molecules in this entry. The entry contains 12359 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Variant surface glycoprotein 558.

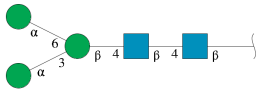
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	361	Total	C	N	O	S	0	5	0
			2769	1692	501	565	11			
1	B	361	Total	C	N	O	S	0	6	0
			2755	1686	496	561	12			
1	C	361	Total	C	N	O	S	0	2	0
			2742	1680	495	556	11			
1	D	361	Total	C	N	O	S	0	4	0
			2767	1692	501	562	12			

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-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
2	E	6	Total	C	N	O	0	0	0
			72	40	2	30			

- 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	F	5	Total	C	N	O	0	0	0
			61	34	2	25			

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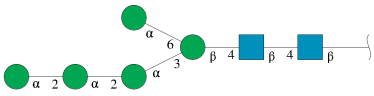
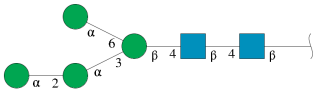
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	J	5	Total C N O 61 34 2 25	0	0	0
3	L	5	Total C N O 61 34 2 25	0	0	0

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-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
4	G	7	Total C N O 83 46 2 35	0	0	0
4	I	7	Total C N O 83 46 2 35	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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
5	H	6	Total C N O 72 40 2 30	0	0	0
5	K	6	Total C N O 72 40 2 30	0	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	240	Total O 240 240	0	0
6	B	164	Total O 164 164	0	0

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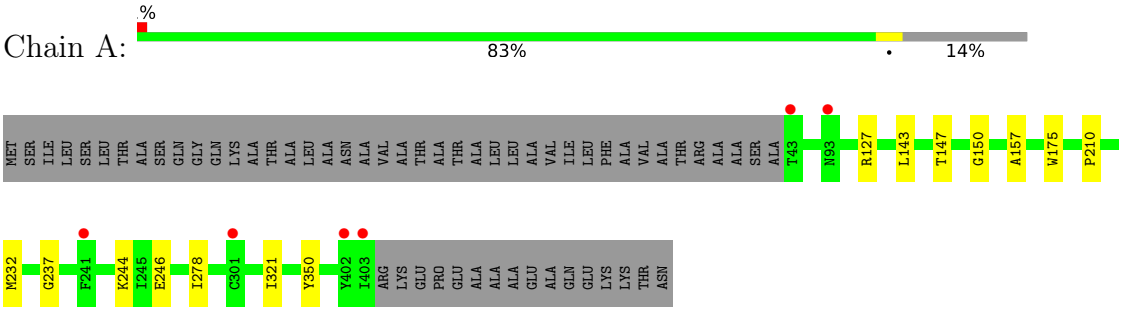
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	181	Total O 181 181	0	0
6	D	176	Total O 176 176	0	0

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.

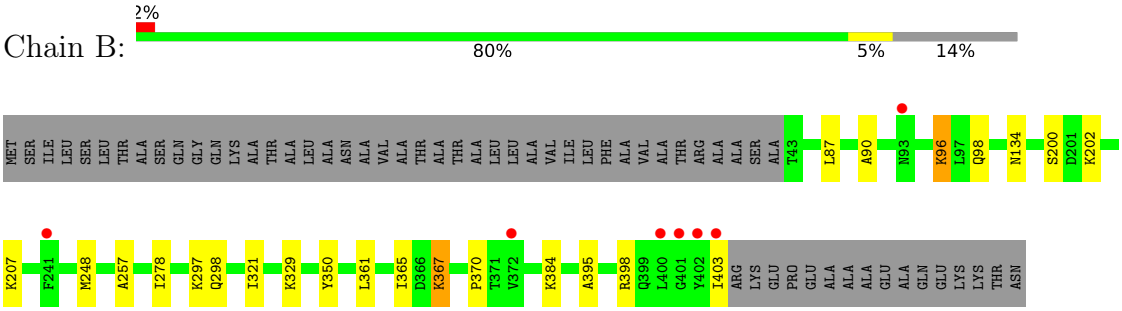
• Molecule 1: Variant surface glycoprotein 558

Chain A:



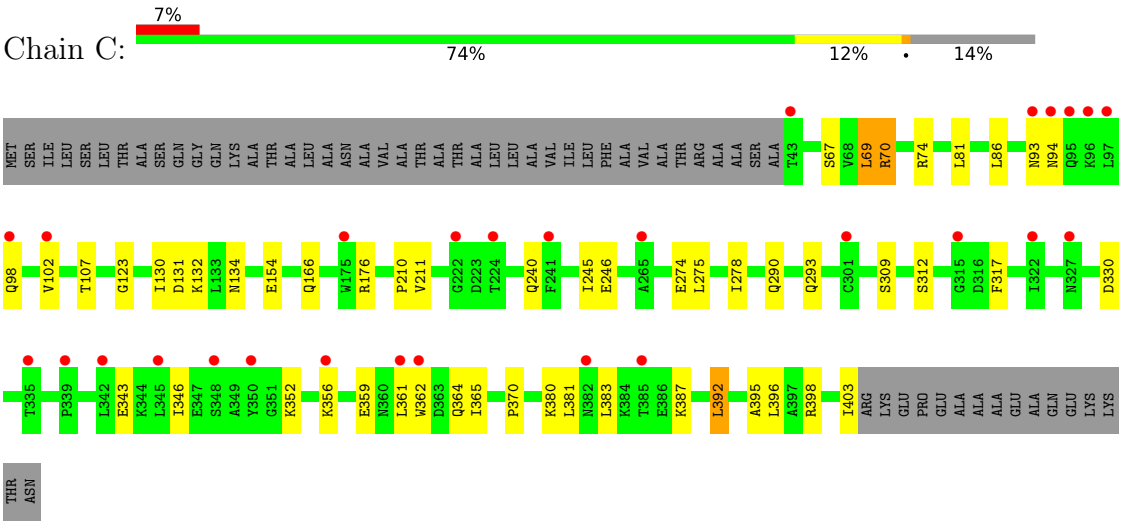
• Molecule 1: Variant surface glycoprotein 558

Chain B:



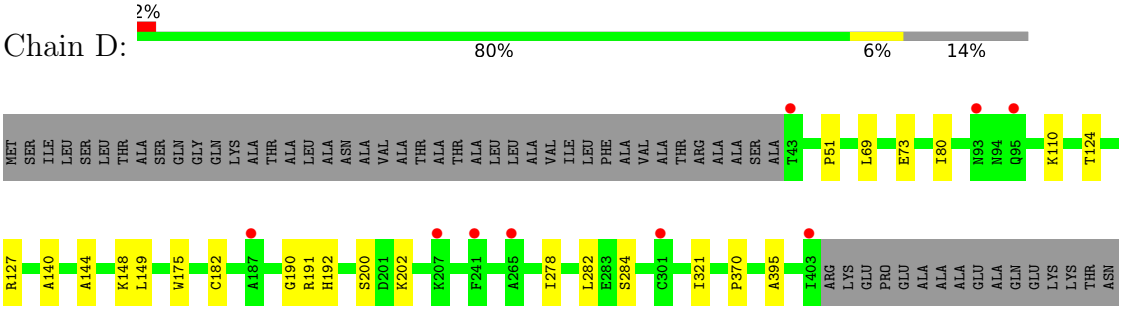
• Molecule 1: Variant surface glycoprotein 558

Chain C:



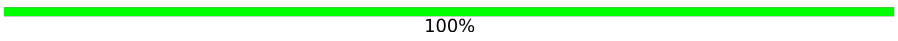
• Molecule 1: Variant surface glycoprotein 558

Chain D:



• Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-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 E:



• 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 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 J:

• 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 L:

• Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-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

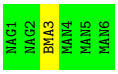
Chain G:

• Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-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 5: alpha-D-mannopyranose-(1-2)-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 H:



• Molecule 5: alpha-D-mannopyranose-(1-2)-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:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	103.08Å 64.12Å 155.04Å 90.00° 109.13° 90.00°	Depositor
Resolution (Å)	53.55 – 1.74 53.55 – 1.74	Depositor EDS
% Data completeness (in resolution range)	98.7 (53.55-1.74) 98.7 (53.55-1.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.03 (at 1.74Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.238 , 0.261 0.237 , 0.260	Depositor DCC
R_{free} test set	9780 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	30.9	Xtriage
Anisotropy	0.467	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 39.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.064 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12359	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.84 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.0356e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: MAN, BMA, NAG

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	0.31	0/2802	0.49	0/3777
1	B	0.36	0/2789	0.53	0/3764
1	C	0.41	0/2776	0.56	0/3744
1	D	0.33	0/2800	0.52	0/3773
All	All	0.35	0/11167	0.52	0/15058

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	B	0	1
1	C	0	3
1	D	0	1
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	398	ARG	Sidechain
1	C	398	ARG	Sidechain
1	C	70	ARG	Sidechain
1	C	74	ARG	Sidechain
1	D	191	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2769	0	2714	9	0
1	B	2755	0	2674	12	0
1	C	2742	0	2685	25	0
1	D	2767	0	2717	15	0
2	E	72	0	61	0	0
3	F	61	0	52	0	0
3	J	61	0	52	4	0
3	L	61	0	52	0	0
4	G	83	0	70	0	0
4	I	83	0	70	0	0
5	H	72	0	61	0	0
5	K	72	0	61	1	0
6	A	240	0	0	0	0
6	B	164	0	0	0	0
6	C	181	0	0	0	0
6	D	176	0	0	0	0
All	All	12359	0	11269	56	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (56) 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:C:107:THR:HG21	1:C:317:PHE:HB2	1.74	0.67
1:C:81:LEU:HD11	1:C:387:LYS:HA	1.78	0.65
1:C:93:ASN:OD1	1:C:94:ASN:N	2.29	0.62
1:D:182:CYS:HB3	5:K:1:NAG:H82	1.80	0.62
1:B:134:ASN:HD22	1:C:134:ASN:HD22	1.49	0.61
1:D:370:PRO:HB2	1:D:395:ALA:HB1	1.85	0.57
1:B:370:PRO:HB2	1:B:395:ALA:HB1	1.90	0.53
1:C:370:PRO:HB2	1:C:395:ALA:HB1	1.91	0.53
1:C:107:THR:CG2	1:C:317:PHE:HB2	2.40	0.52
1:D:124:THR:HA	1:D:127[B]:ARG:NH1	2.25	0.52
1:A:175:TRP:HH2	1:D:175:TRP:HZ3	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:LYS:HG3	1:B:298:GLN:HG3	1.93	0.51
1:C:361:LEU:O	1:C:365:ILE:HG13	2.13	0.49
1:A:127:ARG:HH22	1:D:73:GLU:CD	2.14	0.49
1:B:87:LEU:HD21	1:C:396:LEU:HD21	1.95	0.48
1:A:157:ALA:HB2	1:A:232:MET:HB3	1.96	0.48
1:B:200:SER:HB2	1:B:202:LYS:HG3	1.96	0.47
1:A:232:MET:HG2	1:A:237:GLY:C	2.34	0.47
1:C:69:LEU:HD11	1:C:123:GLY:HA2	1.97	0.47
1:D:140:ALA:HB2	1:D:282:LEU:HD21	1.97	0.46
1:C:86:LEU:HD11	1:C:362:TRP:CZ3	2.51	0.46
1:C:98:GLN:O	1:C:102:VAL:HG23	2.16	0.46
1:D:148:LYS:O	1:D:148:LYS:HG2	2.15	0.46
1:A:175:TRP:HH2	1:D:175:TRP:CZ3	2.33	0.45
1:A:321:ILE:HD11	1:A:350:TYR:HE2	1.82	0.45
1:C:293:GLN:CB	3:J:1:NAG:H81	2.47	0.44
1:D:149:LEU:HB3	1:D:175:TRP:CD1	2.52	0.44
1:B:207:LYS:O	1:B:248[A]:MET:HG2	2.18	0.44
1:C:154:GLU:HG3	1:C:240:GLN:HG2	2.01	0.43
1:C:293:GLN:HB3	3:J:1:NAG:H81	2.00	0.43
1:C:392:LEU:HD13	1:C:392:LEU:HA	1.87	0.43
1:D:200:SER:HB2	1:D:202:LYS:HG3	2.00	0.43
1:C:343:GLU:HA	1:C:346:ILE:HD12	2.01	0.43
1:D:80:ILE:HD12	1:D:80:ILE:HA	1.92	0.43
1:C:290:GLN:HA	3:J:1:NAG:C8	2.49	0.42
1:A:143:LEU:O	1:A:147:THR:HG23	2.19	0.42
1:B:321:ILE:HD11	1:B:350:TYR:HE2	1.85	0.42
1:D:69:LEU:O	1:D:73:GLU:HG3	2.19	0.42
1:A:150:GLY:HA2	1:A:244:LYS:HE3	2.01	0.42
1:B:367:LYS:HE3	1:B:367:LYS:HB2	1.55	0.42
1:D:190:GLY:HA2	1:D:192:HIS:CE1	2.55	0.42
1:C:69:LEU:HD23	1:C:69:LEU:HA	1.84	0.42
1:B:96:LYS:HE3	1:B:96:LYS:HB3	1.74	0.41
1:B:361:LEU:O	1:B:365:ILE:HG13	2.20	0.41
1:C:211:VAL:HG12	1:C:274:GLU:HA	2.02	0.41
1:C:359:GLU:O	1:C:364:GLN:HG2	2.21	0.41
1:C:381:LEU:HD23	1:C:381:LEU:HA	1.91	0.41
1:D:321:ILE:HD13	1:D:321:ILE:HA	1.87	0.41
1:C:245:ILE:HD12	1:C:275:LEU:HD11	2.02	0.41
1:B:90:ALA:O	1:B:98:GLN:HG2	2.20	0.41
3:J:1:NAG:H82	3:J:1:NAG:H2	1.87	0.40
1:A:210:PRO:HA	1:A:246:GLU:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:ASP:OD1	1:C:131:ASP:N	2.54	0.40
1:D:51:PRO:HB2	1:D:144:ALA:HB2	2.04	0.40
1:B:257:ALA:HA	1:C:166:GLN:HB2	2.03	0.40
1:C:210:PRO:HA	1:C:246:GLU:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	364/419 (87%)	351 (96%)	12 (3%)	1 (0%)	41	23
1	B	365/419 (87%)	350 (96%)	14 (4%)	1 (0%)	41	23
1	C	361/419 (86%)	343 (95%)	17 (5%)	1 (0%)	41	23
1	D	363/419 (87%)	352 (97%)	10 (3%)	1 (0%)	41	23
All	All	1453/1676 (87%)	1396 (96%)	53 (4%)	4 (0%)	41	23

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	278	ILE
1	B	278	ILE
1	C	278	ILE
1	A	278	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	291/326 (89%)	291 (100%)	0	100 100
1	B	286/326 (88%)	281 (98%)	5 (2%)	60 41
1	C	286/326 (88%)	271 (95%)	15 (5%)	23 5
1	D	290/326 (89%)	287 (99%)	3 (1%)	76 63
All	All	1153/1304 (88%)	1130 (98%)	23 (2%)	57 33

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	96	LYS
1	B	329	LYS
1	B	367	LYS
1	B	384	LYS
1	B	403	ILE
1	C	67	SER
1	C	69	LEU
1	C	70	ARG
1	C	130	ILE
1	C	132	LYS
1	C	176	ARG
1	C	309	SER
1	C	312	SER
1	C	330	ASP
1	C	352	LYS
1	C	356	LYS
1	C	380	LYS
1	C	383	LEU
1	C	392	LEU
1	C	403	ILE
1	D	110	LYS
1	D	284[A]	SER
1	D	284[B]	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	373	ASN
1	C	134	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

47 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	E	1	2,1	14,14,15	0.43	0	17,19,21	0.83	0
2	NAG	E	2	2	14,14,15	0.44	0	17,19,21	0.52	0
2	BMA	E	3	2	11,11,12	0.46	0	15,15,17	0.61	0
2	MAN	E	4	2	11,11,12	0.58	0	15,15,17	0.64	0
2	MAN	E	5	2	11,11,12	0.58	0	15,15,17	0.78	0
2	MAN	E	6	2	11,11,12	0.30	0	15,15,17	0.53	0
3	NAG	F	1	1,3	14,14,15	0.27	0	17,19,21	0.60	0
3	NAG	F	2	3	14,14,15	0.39	0	17,19,21	0.62	0
3	BMA	F	3	3	11,11,12	0.50	0	15,15,17	0.98	1 (6%)
3	MAN	F	4	3	11,11,12	0.43	0	15,15,17	0.54	0
3	MAN	F	5	3	11,11,12	0.28	0	15,15,17	0.64	0
4	NAG	G	1	1,4	14,14,15	0.44	0	17,19,21	0.86	0
4	NAG	G	2	4	14,14,15	0.42	0	17,19,21	0.77	1 (5%)
4	BMA	G	3	4	11,11,12	0.47	0	15,15,17	0.76	0
4	MAN	G	4	4	11,11,12	0.58	0	15,15,17	0.65	0
4	MAN	G	5	4	11,11,12	0.54	0	15,15,17	0.69	0
4	MAN	G	6	4	11,11,12	0.36	0	15,15,17	0.59	0
4	MAN	G	7	4	11,11,12	0.27	0	15,15,17	0.55	0
5	NAG	H	1	1,5	14,14,15	0.42	0	17,19,21	0.63	0
5	NAG	H	2	5	14,14,15	0.33	0	17,19,21	0.59	0
5	BMA	H	3	5	11,11,12	0.39	0	15,15,17	0.83	1 (6%)
5	MAN	H	4	5	11,11,12	0.28	0	15,15,17	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	MAN	H	5	5	11,11,12	0.22	0	15,15,17	0.61	0
5	MAN	H	6	5	11,11,12	0.37	0	15,15,17	0.65	0
4	NAG	I	1	1,4	14,14,15	0.46	0	17,19,21	0.91	1 (5%)
4	NAG	I	2	4	14,14,15	0.41	0	17,19,21	0.73	1 (5%)
4	BMA	I	3	4	11,11,12	0.55	0	15,15,17	0.67	0
4	MAN	I	4	4	11,11,12	0.49	0	15,15,17	0.54	0
4	MAN	I	5	4	11,11,12	0.40	0	15,15,17	0.58	0
4	MAN	I	6	4	11,11,12	0.40	0	15,15,17	0.55	0
4	MAN	I	7	4	11,11,12	0.39	0	15,15,17	0.52	0
3	NAG	J	1	1,3	14,14,15	0.42	0	17,19,21	0.60	0
3	NAG	J	2	3	14,14,15	0.33	0	17,19,21	0.56	0
3	BMA	J	3	3	11,11,12	0.24	0	15,15,17	0.87	1 (6%)
3	MAN	J	4	3	11,11,12	0.16	0	15,15,17	0.61	0
3	MAN	J	5	3	11,11,12	0.28	0	15,15,17	0.63	0
5	NAG	K	1	1,5	14,14,15	0.47	0	17,19,21	1.31	3 (17%)
5	NAG	K	2	5	14,14,15	0.42	0	17,19,21	0.77	1 (5%)
5	BMA	K	3	5	11,11,12	0.50	0	15,15,17	0.67	0
5	MAN	K	4	5	11,11,12	0.44	0	15,15,17	1.04	1 (6%)
5	MAN	K	5	5	11,11,12	0.34	0	15,15,17	0.55	0
5	MAN	K	6	5	11,11,12	0.32	0	15,15,17	0.68	0
3	NAG	L	1	1,3	14,14,15	0.43	0	17,19,21	0.76	1 (5%)
3	NAG	L	2	3	14,14,15	0.27	0	17,19,21	0.61	0
3	BMA	L	3	3	11,11,12	0.30	0	15,15,17	0.92	1 (6%)
3	MAN	L	4	3	11,11,12	0.46	0	15,15,17	0.47	0
3	MAN	L	5	3	11,11,12	0.27	0	15,15,17	0.53	0

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	F	4	3	-	2/2/19/22	0/1/1/1
3	MAN	F	5	3	-	2/2/19/22	0/1/1/1
4	NAG	G	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
4	MAN	G	4	4	-	0/2/19/22	0/1/1/1
4	MAN	G	5	4	-	0/2/19/22	0/1/1/1
4	MAN	G	6	4	-	1/2/19/22	0/1/1/1
4	MAN	G	7	4	-	2/2/19/22	0/1/1/1
5	NAG	H	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	H	2	5	-	0/6/23/26	0/1/1/1
5	BMA	H	3	5	-	0/2/19/22	0/1/1/1
5	MAN	H	4	5	-	0/2/19/22	0/1/1/1
5	MAN	H	5	5	-	0/2/19/22	0/1/1/1
5	MAN	H	6	5	-	2/2/19/22	0/1/1/1
4	NAG	I	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1
4	BMA	I	3	4	-	0/2/19/22	0/1/1/1
4	MAN	I	4	4	-	0/2/19/22	0/1/1/1
4	MAN	I	5	4	-	0/2/19/22	0/1/1/1
4	MAN	I	6	4	-	2/2/19/22	0/1/1/1
4	MAN	I	7	4	-	0/2/19/22	0/1/1/1
3	NAG	J	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1
3	BMA	J	3	3	-	0/2/19/22	0/1/1/1
3	MAN	J	4	3	-	0/2/19/22	0/1/1/1
3	MAN	J	5	3	-	0/2/19/22	0/1/1/1
5	NAG	K	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	K	2	5	-	0/6/23/26	0/1/1/1
5	BMA	K	3	5	-	0/2/19/22	0/1/1/1
5	MAN	K	4	5	-	0/2/19/22	1/1/1/1
5	MAN	K	5	5	-	0/2/19/22	0/1/1/1
5	MAN	K	6	5	-	0/2/19/22	0/1/1/1
3	NAG	L	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	L	2	3	-	2/6/23/26	0/1/1/1
3	BMA	L	3	3	-	0/2/19/22	0/1/1/1
3	MAN	L	4	3	-	2/2/19/22	0/1/1/1
3	MAN	L	5	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	K	4	MAN	C1-O5-C5	3.62	117.10	112.19
5	K	1	NAG	O5-C1-C2	2.94	115.93	111.29
5	K	1	NAG	C2-N2-C7	2.68	126.71	122.90
4	G	2	NAG	O5-C1-C2	-2.66	107.09	111.29
3	J	3	BMA	C1-C2-C3	2.62	112.88	109.67
5	K	1	NAG	C4-C3-C2	2.50	114.68	111.02
5	H	3	BMA	C1-C2-C3	2.41	112.63	109.67
5	K	2	NAG	O5-C1-C2	-2.24	107.75	111.29
3	F	3	BMA	C1-C2-C3	2.21	112.39	109.67
3	L	3	BMA	C1-C2-C3	2.19	112.36	109.67
3	L	1	NAG	C2-N2-C7	-2.10	119.92	122.90
4	I	2	NAG	O5-C1-C2	-2.06	108.04	111.29
4	I	1	NAG	O5-C1-C2	2.06	114.54	111.29

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	K	1	NAG	C8-C7-N2-C2
3	F	5	MAN	O5-C5-C6-O6
5	H	6	MAN	O5-C5-C6-O6
4	I	6	MAN	C4-C5-C6-O6
3	L	4	MAN	C4-C5-C6-O6
4	I	6	MAN	O5-C5-C6-O6
3	F	5	MAN	C4-C5-C6-O6
5	H	6	MAN	C4-C5-C6-O6
3	F	4	MAN	C4-C5-C6-O6
5	K	1	NAG	O7-C7-N2-C2
4	G	7	MAN	C4-C5-C6-O6
3	J	1	NAG	C8-C7-N2-C2
3	J	1	NAG	O7-C7-N2-C2
4	G	2	NAG	C8-C7-N2-C2
4	G	2	NAG	O7-C7-N2-C2
4	G	7	MAN	O5-C5-C6-O6
3	F	3	BMA	O5-C5-C6-O6
3	L	4	MAN	O5-C5-C6-O6
3	F	4	MAN	O5-C5-C6-O6
3	F	3	BMA	C4-C5-C6-O6
3	L	2	NAG	C4-C5-C6-O6
4	G	6	MAN	O5-C5-C6-O6
3	L	2	NAG	O5-C5-C6-O6

All (1) ring outliers are listed below:

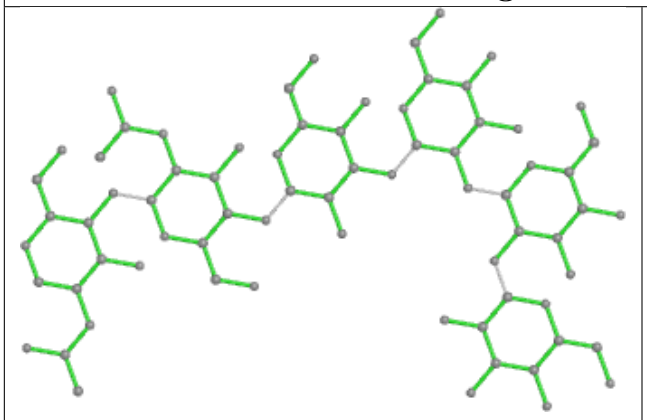
Mol	Chain	Res	Type	Atoms
5	K	4	MAN	C1-C2-C3-C4-C5-O5

2 monomers are involved in 5 short contacts:

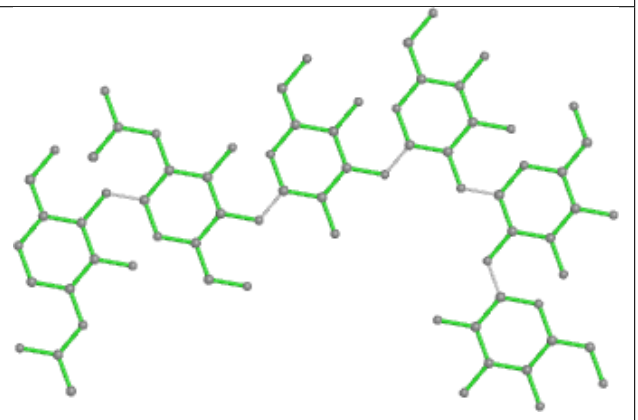
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	1	NAG	1	0
3	J	1	NAG	4	0

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

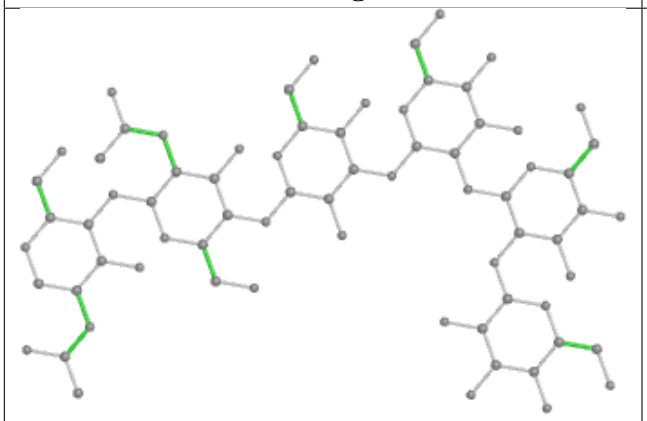
Oligosaccharide Chain E



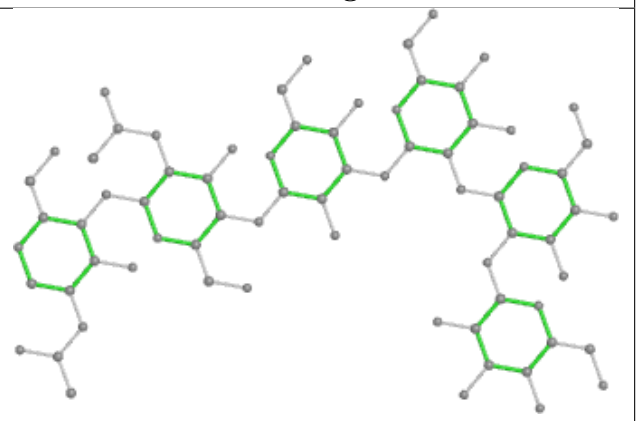
Bond lengths



Bond angles

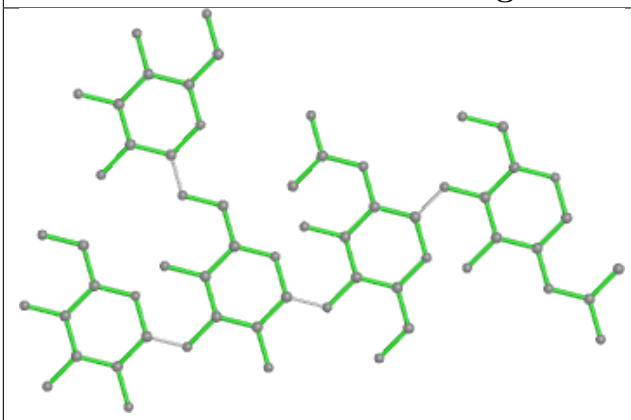


Torsions

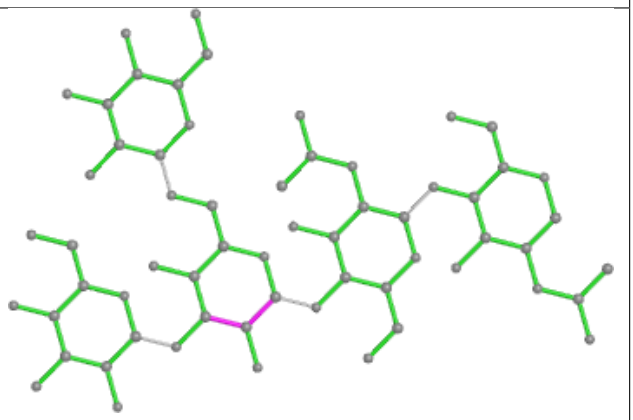


Rings

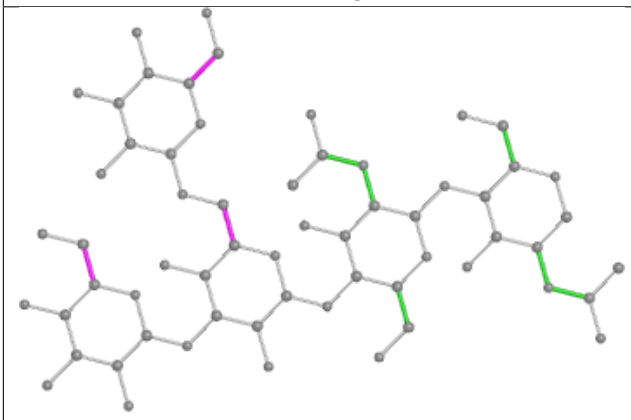
Oligosaccharide Chain F



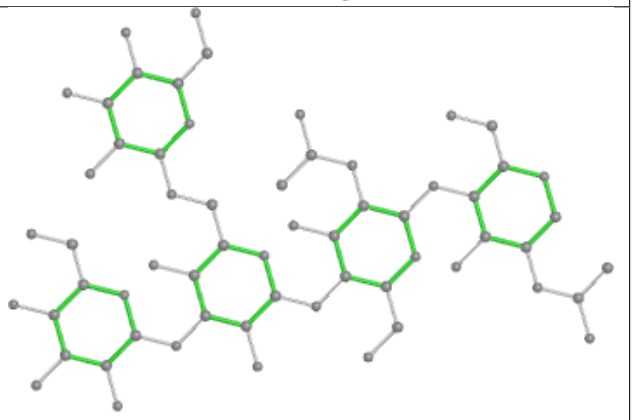
Bond lengths



Bond angles

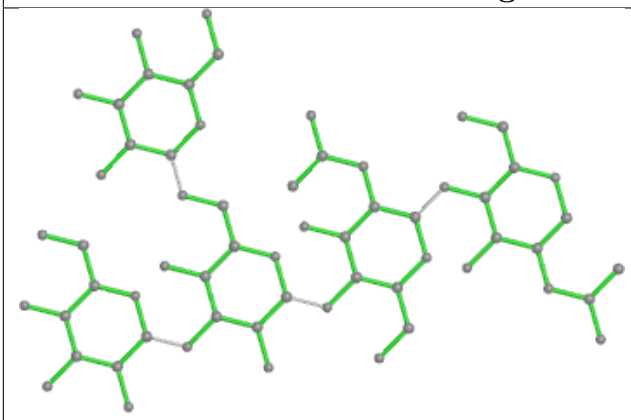


Torsions

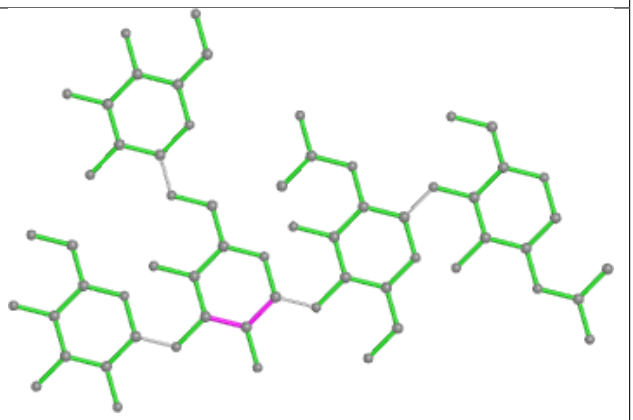


Rings

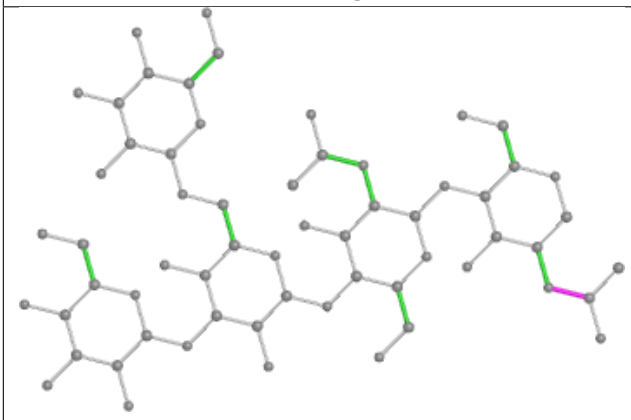
Oligosaccharide Chain J



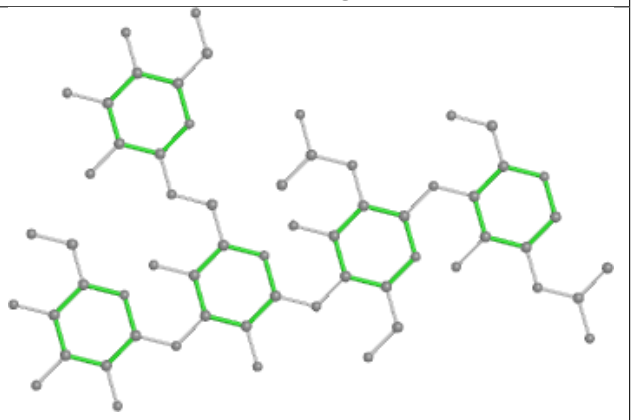
Bond lengths



Bond angles

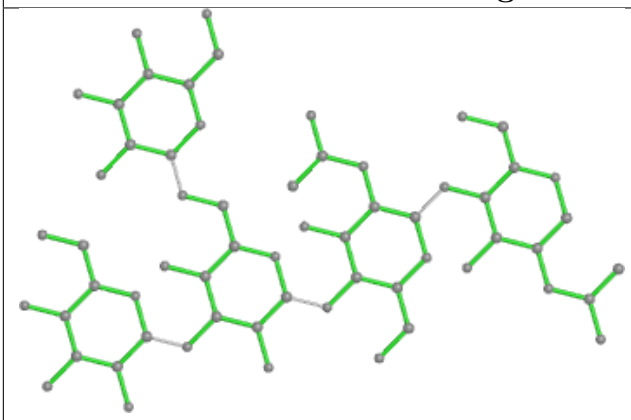


Torsions

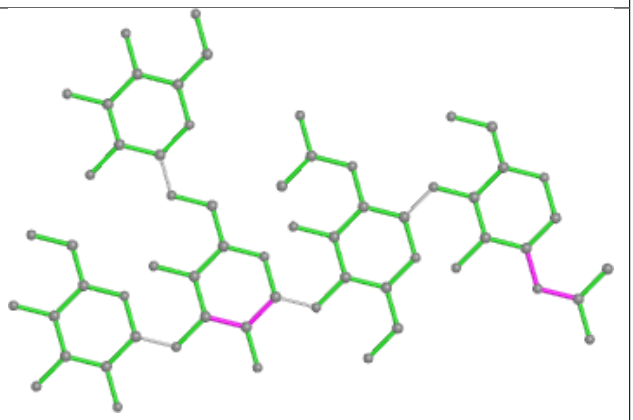


Rings

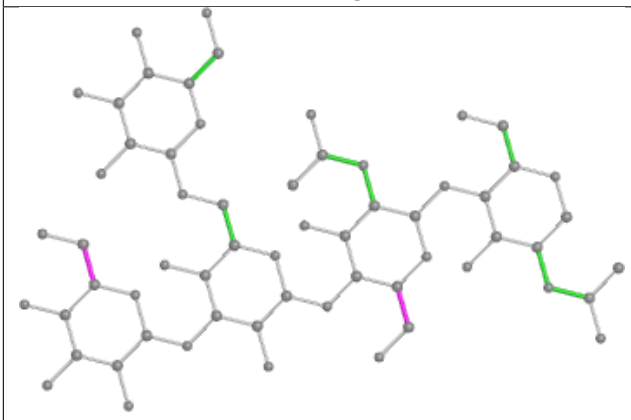
Oligosaccharide Chain L



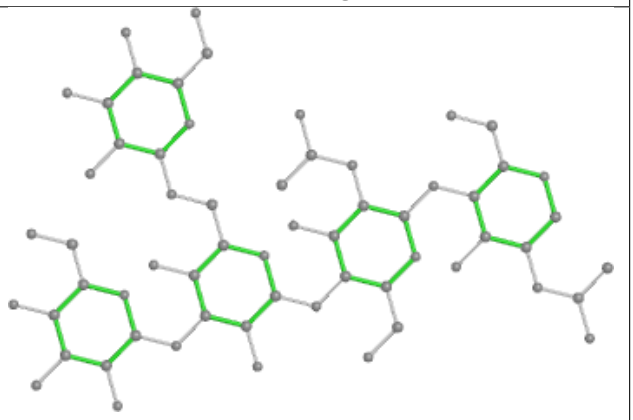
Bond lengths



Bond angles

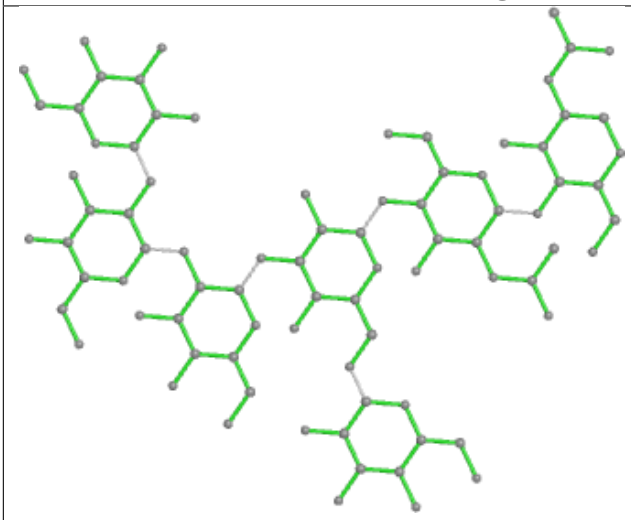


Torsions

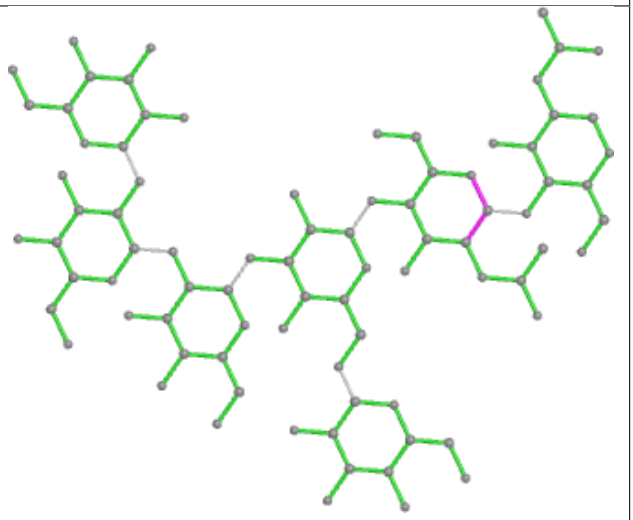


Rings

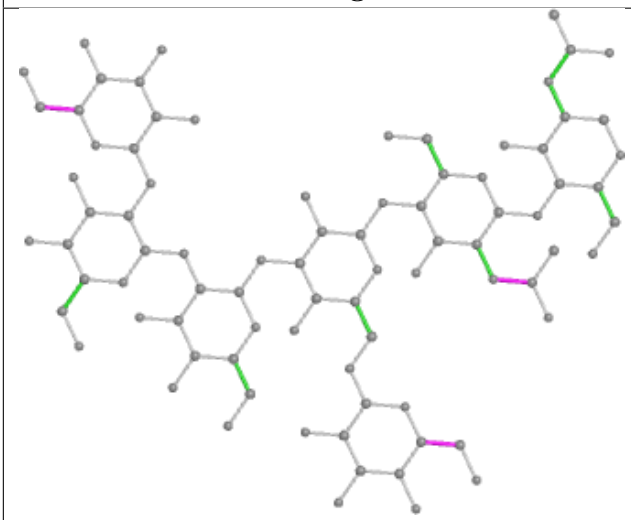
Oligosaccharide Chain G



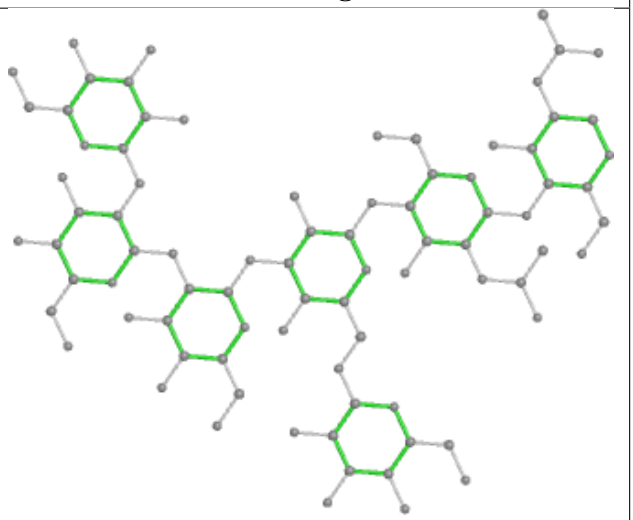
Bond lengths



Bond angles

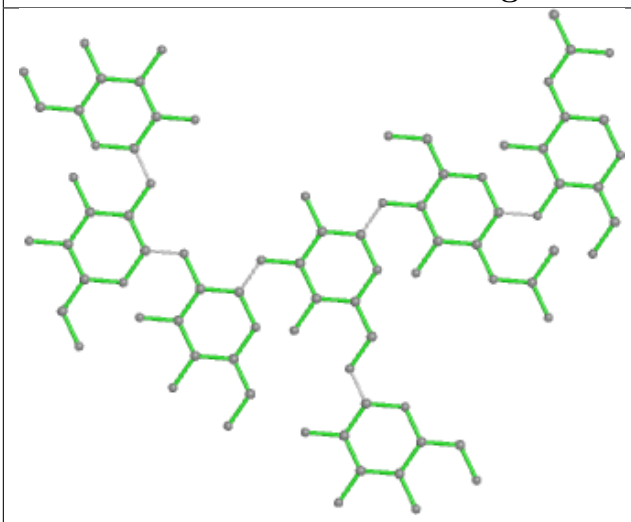


Torsions

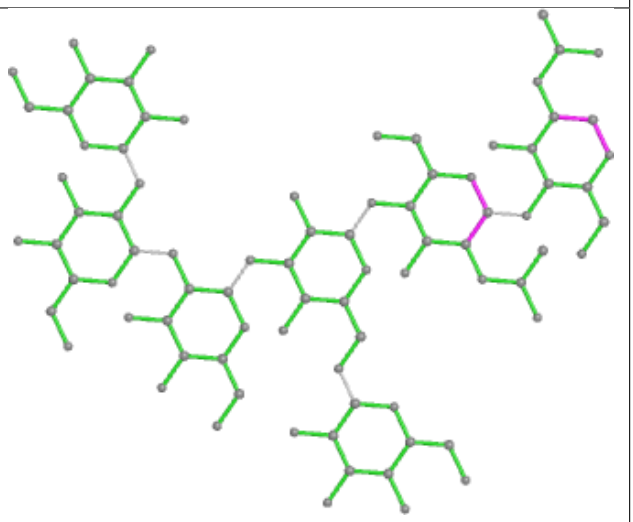


Rings

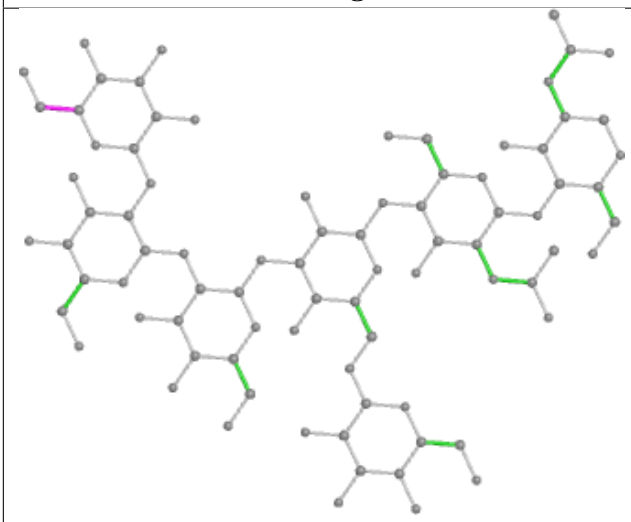
Oligosaccharide Chain I



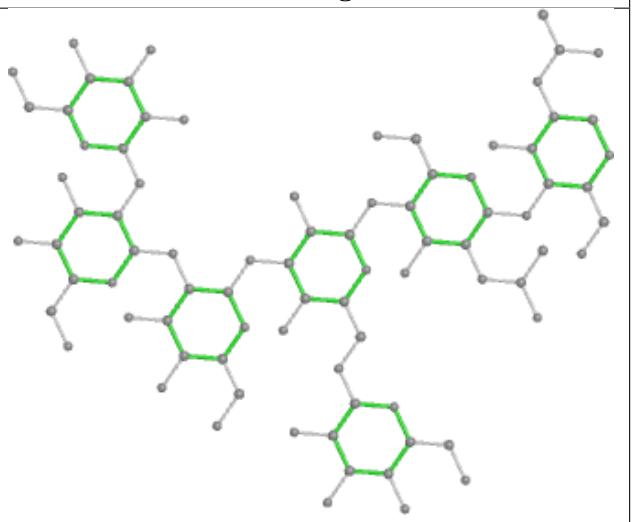
Bond lengths



Bond angles

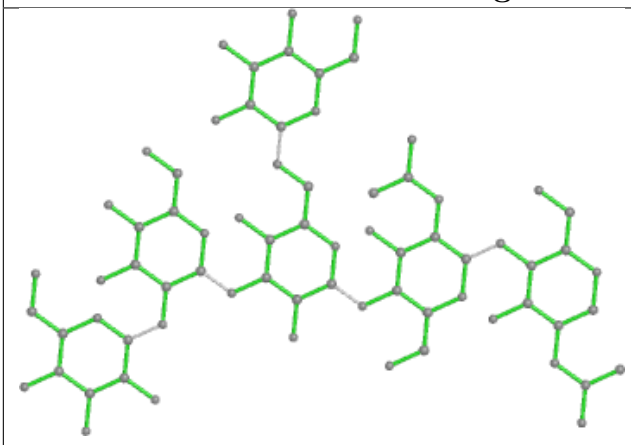


Torsions

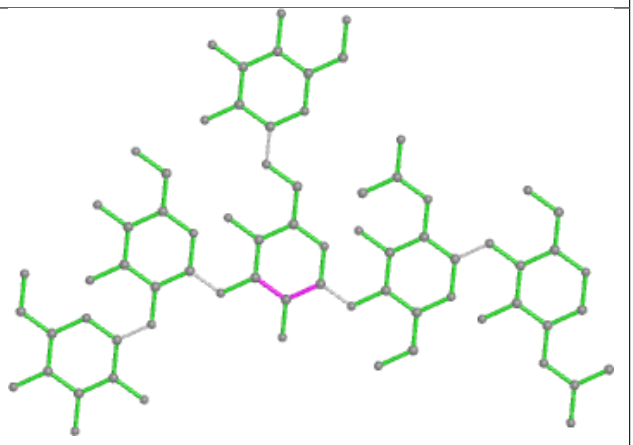


Rings

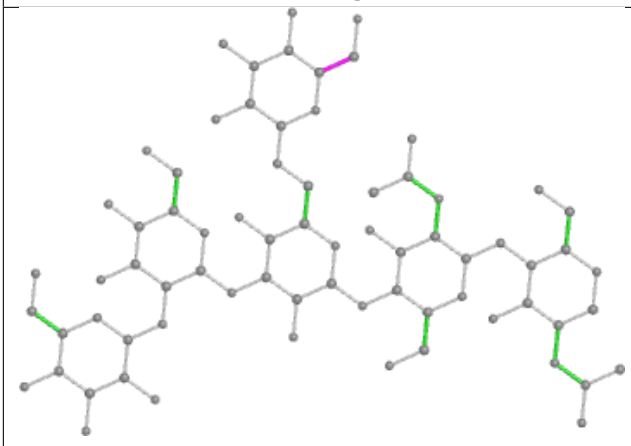
Oligosaccharide Chain H



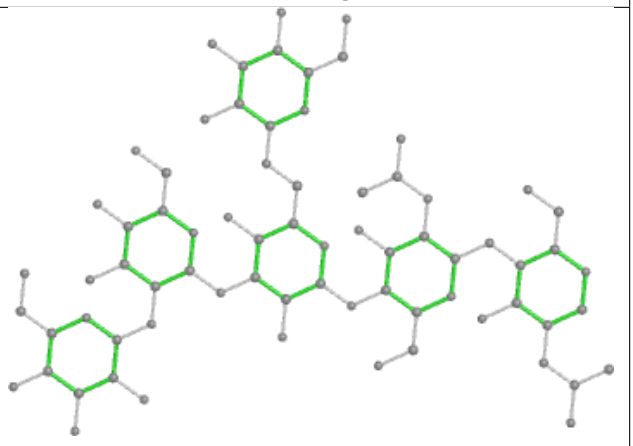
Bond lengths



Bond angles

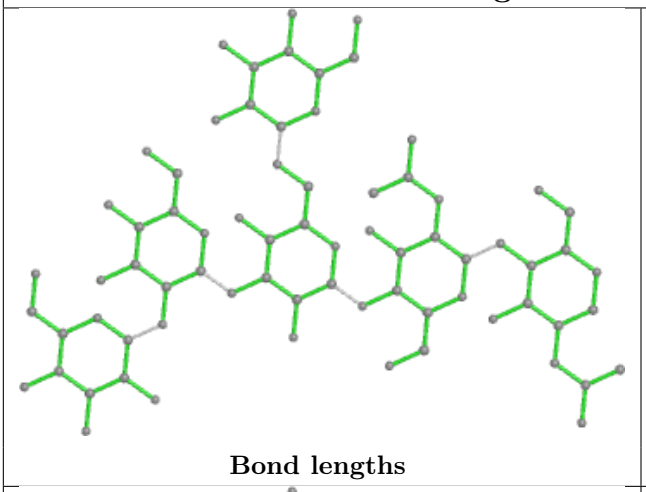


Torsions

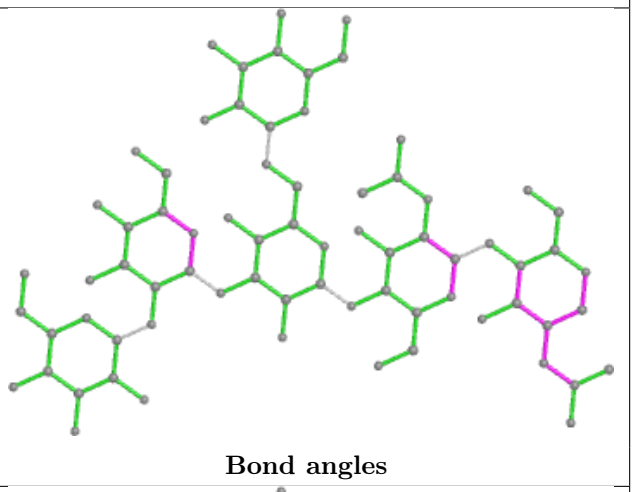


Rings

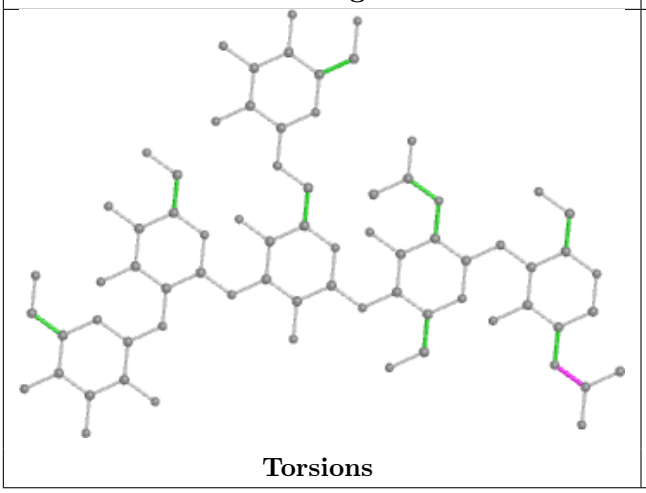
Oligosaccharide Chain K



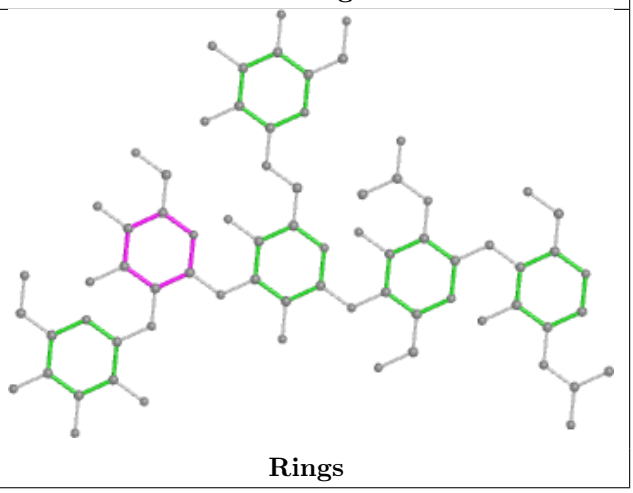
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	361/419 (86%)	0.16	6 (1%)	70	76	27, 37, 49, 77	0
1	B	361/419 (86%)	0.36	7 (1%)	66	73	29, 42, 63, 80	0
1	C	361/419 (86%)	0.53	28 (7%)	13	17	27, 43, 81, 106	0
1	D	361/419 (86%)	0.28	9 (2%)	57	63	26, 42, 57, 80	0
All	All	1444/1676 (86%)	0.33	50 (3%)	44	49	26, 41, 69, 106	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	348	SER	5.1
1	C	96	LYS	4.5
1	B	93	ASN	4.4
1	A	43	THR	4.4
1	A	403	ILE	4.3
1	D	403	ILE	4.1
1	B	241[A]	PHE	3.9
1	D	93	ASN	3.8
1	C	241[A]	PHE	3.6
1	D	207	LYS	3.6
1	C	361	LEU	3.5
1	D	187	ALA	3.3
1	B	372	VAL	3.2
1	A	93	ASN	3.2
1	A	301	CYS	3.2
1	C	43	THR	3.0
1	D	241	PHE	3.0
1	C	322	ILE	3.0
1	B	403	ILE	3.0
1	D	43	THR	2.9
1	D	301	CYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	342	LEU	2.9
1	C	265	ALA	2.9
1	B	401	GLY	2.8
1	C	385	THR	2.8
1	C	362	TRP	2.7
1	C	339	PRO	2.7
1	C	335	THR	2.7
1	C	350	TYR	2.7
1	C	102	VAL	2.7
1	C	345	LEU	2.7
1	C	222	GLY	2.6
1	C	93	ASN	2.6
1	C	97	LEU	2.6
1	C	356	LYS	2.6
1	A	241	PHE	2.5
1	C	94	ASN	2.5
1	C	301	CYS	2.4
1	C	327	ASN	2.4
1	B	402	TYR	2.3
1	C	382	ASN	2.3
1	C	175	TRP	2.2
1	A	402	TYR	2.2
1	C	315	GLY	2.1
1	C	224	THR	2.1
1	B	400	LEU	2.1
1	C	95	GLN	2.1
1	C	98	GLN	2.0
1	D	265	ALA	2.0
1	D	95	GLN	2.0

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, 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	J	5	11/12	0.25	0.34	76,84,86,87	0
3	MAN	F	5	11/12	0.45	0.25	75,79,83,83	0
5	MAN	K	4	11/12	0.52	0.26	36,45,52,54	0
4	MAN	G	7	11/12	0.56	0.34	63,69,72,73	0
4	MAN	I	7	11/12	0.67	0.25	62,67,71,71	0
5	MAN	K	6	11/12	0.67	0.36	61,65,72,73	0
5	MAN	H	5	11/12	0.69	0.26	45,57,62,62	0
3	MAN	F	4	11/12	0.69	0.19	53,68,74,75	0
3	MAN	L	5	11/12	0.69	0.31	68,74,75,76	0
3	MAN	J	4	11/12	0.71	0.23	49,59,62,62	0
3	BMA	L	3	11/12	0.74	0.20	55,59,66,71	0
4	MAN	G	6	11/12	0.75	0.22	54,65,68,79	0
2	MAN	E	6	11/12	0.76	0.30	63,69,75,81	0
3	BMA	J	3	11/12	0.77	0.13	43,52,60,67	0
3	NAG	L	2	14/15	0.79	0.13	38,52,62,65	0
3	NAG	L	1	14/15	0.80	0.13	41,50,56,56	0
5	MAN	H	6	11/12	0.82	0.17	63,67,70,71	0
4	BMA	G	3	11/12	0.83	0.10	29,37,43,48	0
5	MAN	K	5	11/12	0.83	0.17	52,57,64,68	0
3	BMA	F	3	11/12	0.83	0.17	50,60,68,71	0
4	MAN	G	5	11/12	0.85	0.10	44,50,56,58	0
4	MAN	G	4	11/12	0.86	0.11	30,33,44,48	0
3	NAG	J	1	14/15	0.86	0.10	26,37,41,41	0
3	MAN	L	4	11/12	0.86	0.21	50,59,64,65	0
2	BMA	E	3	11/12	0.86	0.10	28,35,43,48	0
2	MAN	E	5	11/12	0.86	0.10	42,49,54,57	0
5	NAG	K	1	14/15	0.87	0.10	26,36,41,48	0
5	NAG	K	2	14/15	0.88	0.08	35,39,42,46	0
4	BMA	I	3	11/12	0.88	0.09	30,35,43,49	0
4	MAN	I	5	11/12	0.88	0.12	36,43,53,54	0
4	NAG	I	1	14/15	0.88	0.11	25,30,32,34	0
2	NAG	E	2	14/15	0.89	0.09	26,32,37,38	0
5	NAG	H	1	14/15	0.89	0.11	32,38,43,45	0
5	NAG	H	2	14/15	0.89	0.12	31,43,53,53	0
2	NAG	E	1	14/15	0.89	0.11	27,30,34,35	0
4	MAN	I	6	11/12	0.89	0.41	65,72,84,88	0
5	BMA	H	3	11/12	0.90	0.09	44,48,58,60	0
2	MAN	E	4	11/12	0.90	0.09	30,36,41,49	0
3	NAG	J	2	14/15	0.90	0.11	31,38,48,48	0
4	NAG	I	2	14/15	0.90	0.11	26,32,38,38	0
5	MAN	H	4	11/12	0.91	0.12	47,50,54,58	0
5	BMA	K	3	11/12	0.91	0.10	37,45,52,59	0
3	NAG	F	2	14/15	0.91	0.10	33,43,53,54	0

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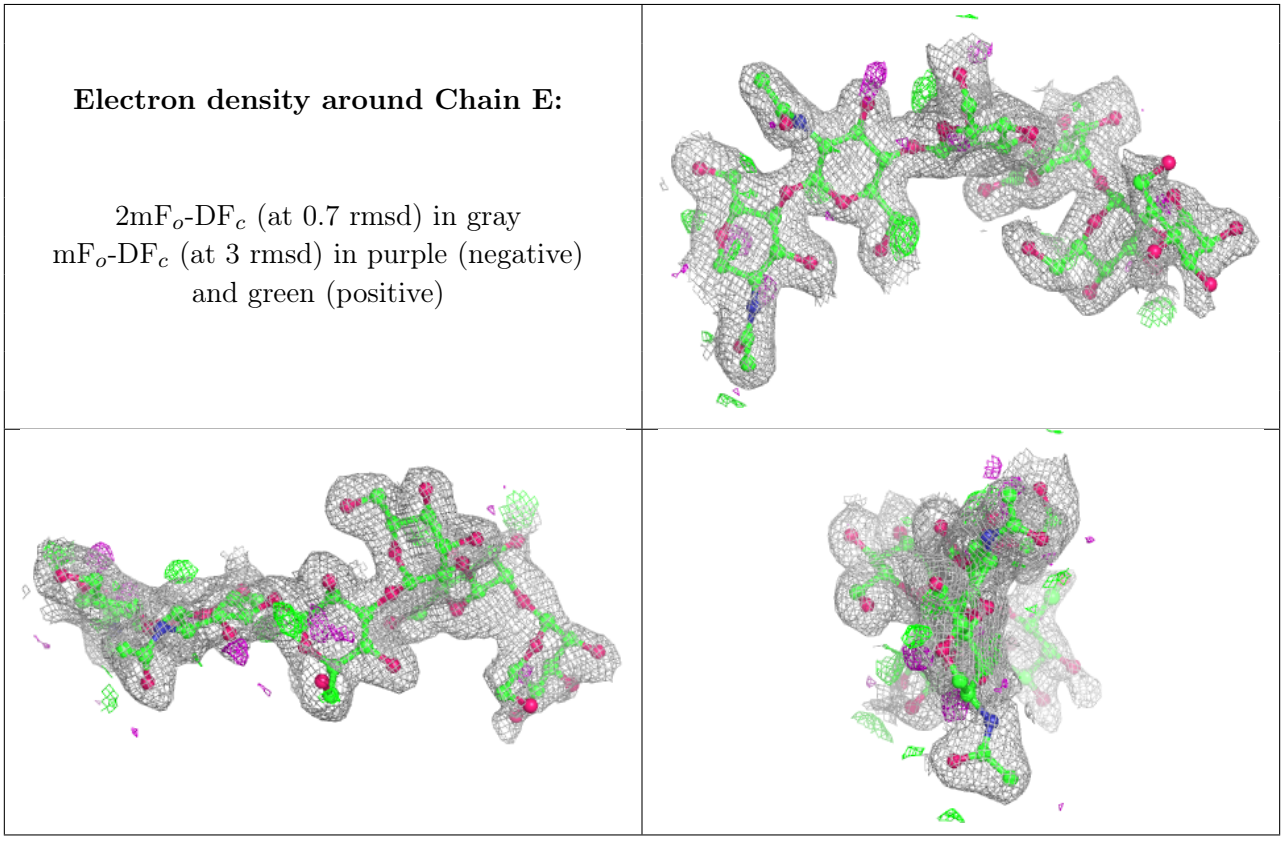
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	G	1	14/15	0.91	0.10	25,30,33,34	0
4	MAN	I	4	11/12	0.91	0.08	31,35,38,39	0
4	NAG	G	2	14/15	0.92	0.08	27,33,38,43	0
3	NAG	F	1	14/15	0.94	0.07	26,35,40,42	0

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.

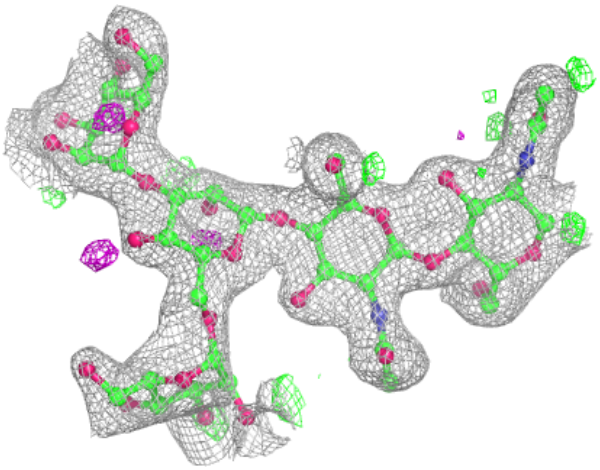
Electron density around Chain E:

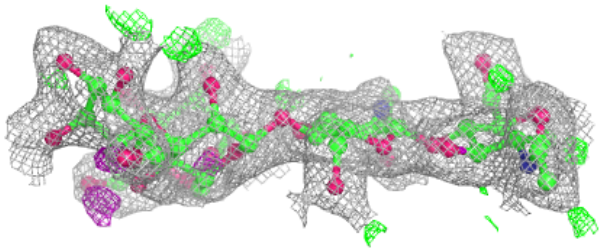
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

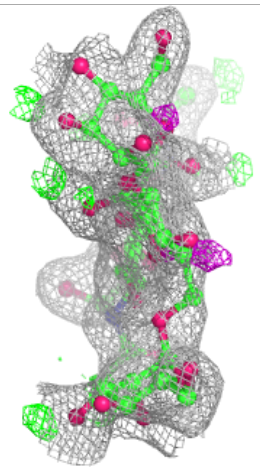


Electron density around Chain F:

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

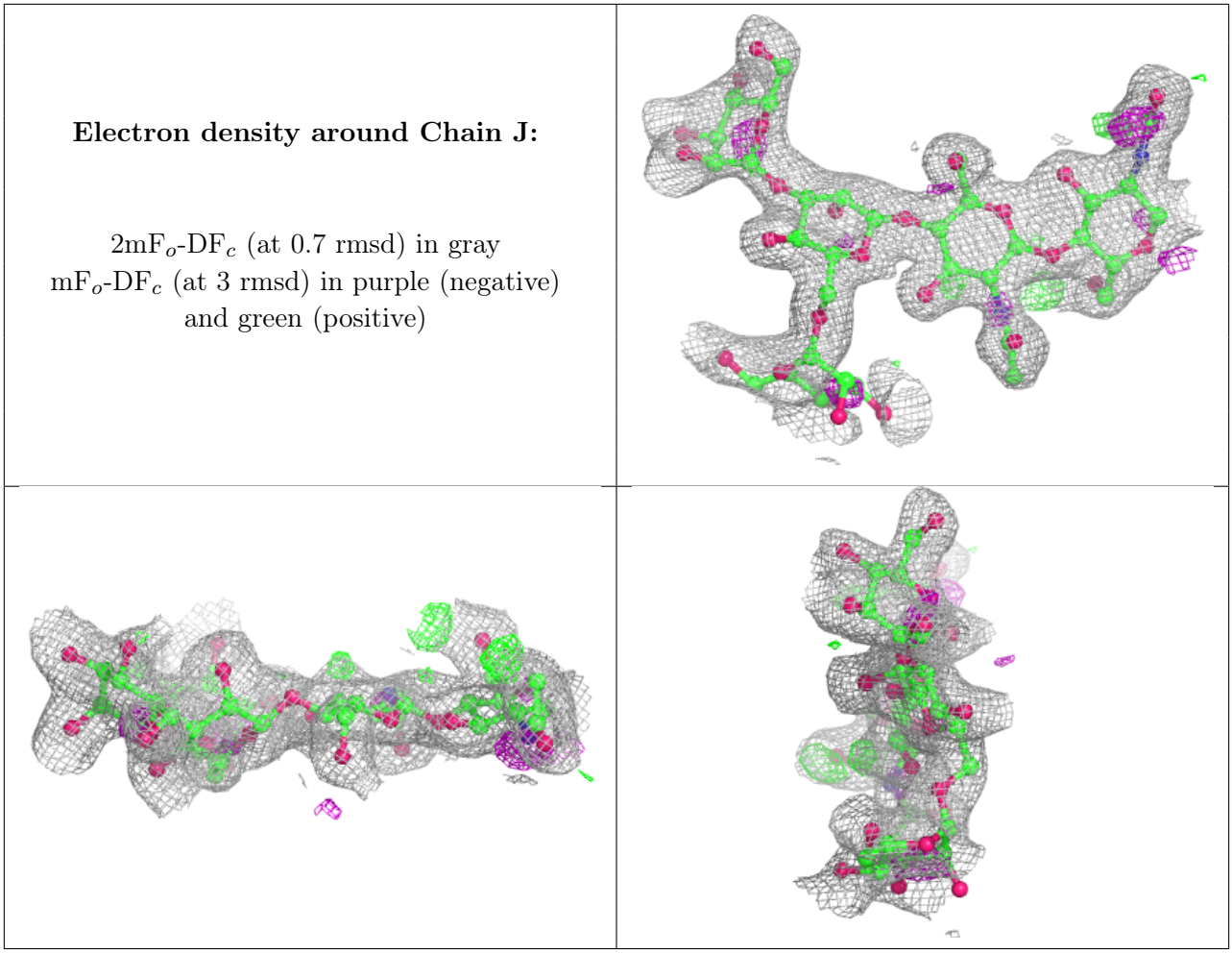






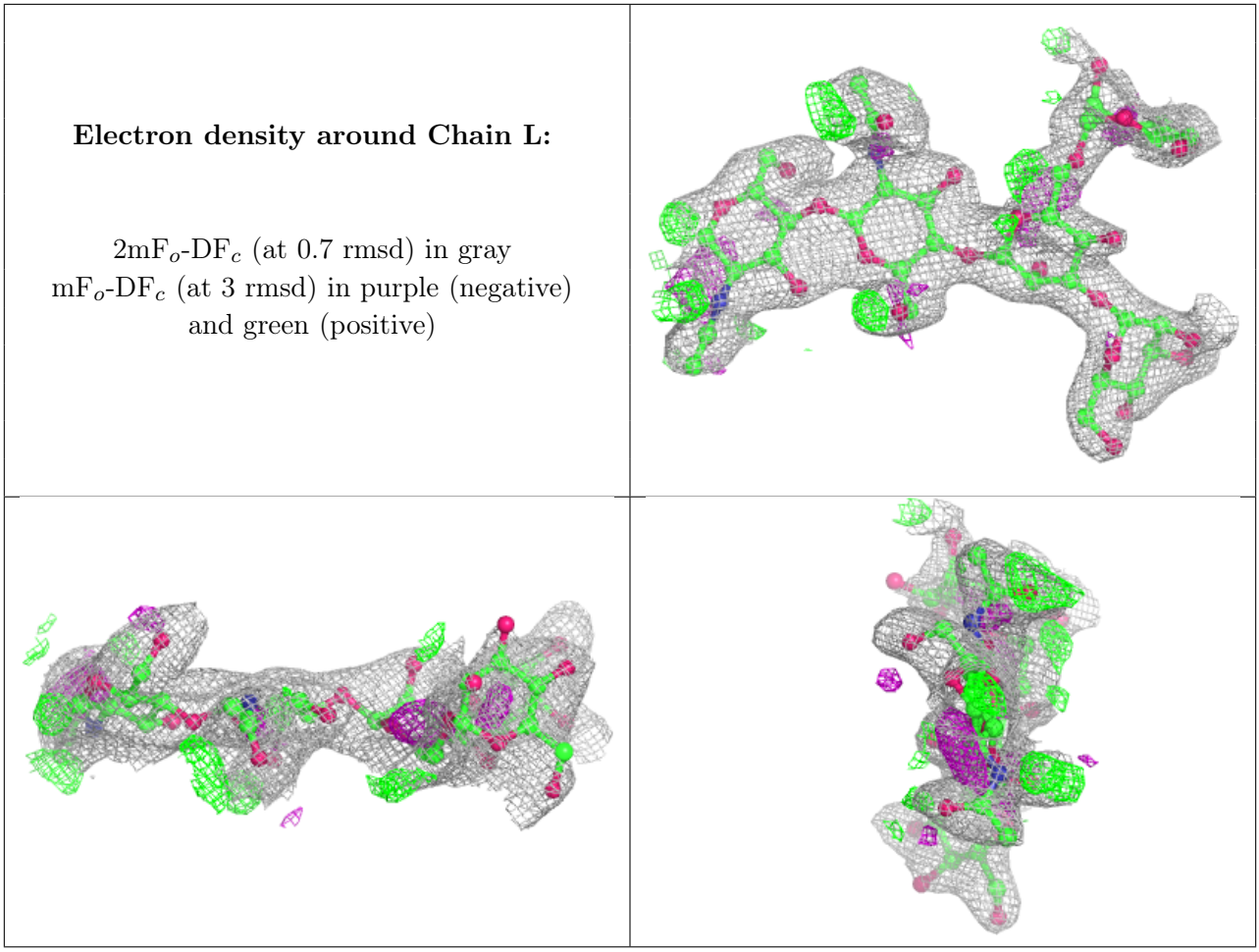
Electron density around Chain J:

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



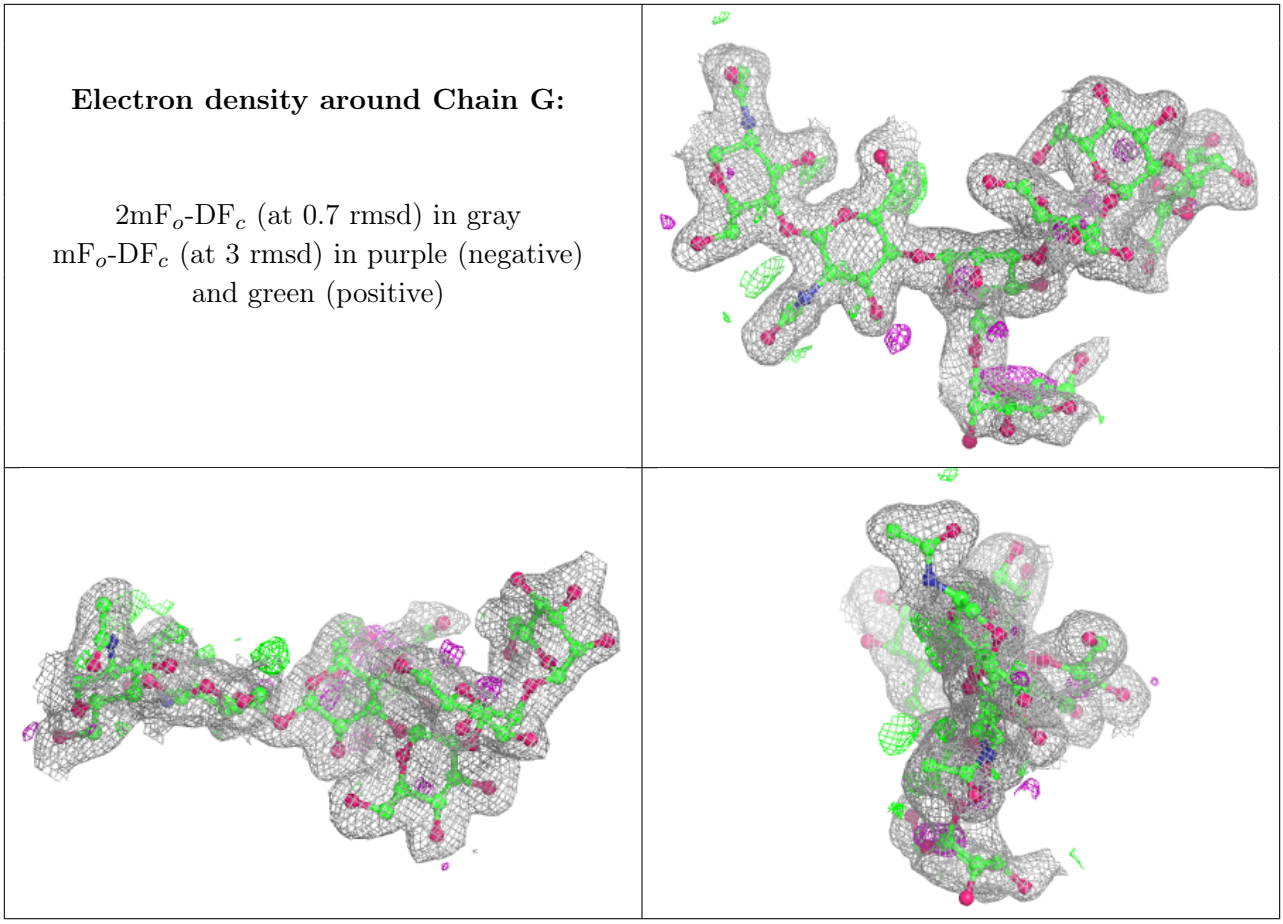
Electron density around Chain L:

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



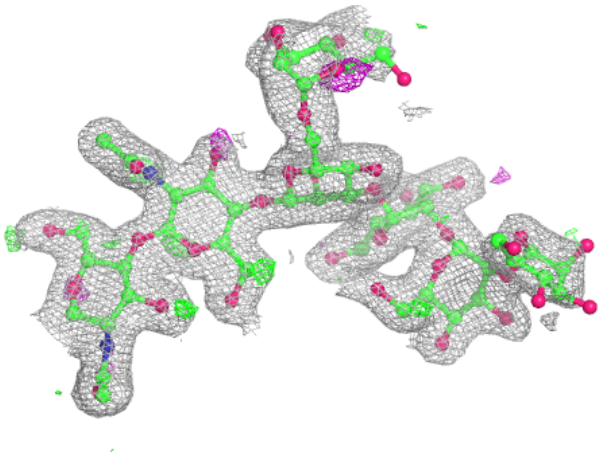
Electron density around Chain G:

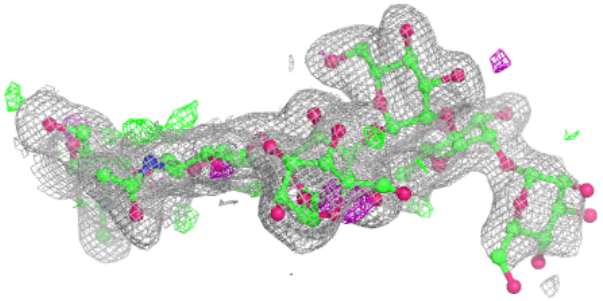
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

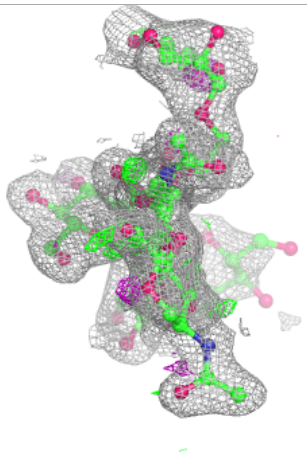


Electron density around Chain I:

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

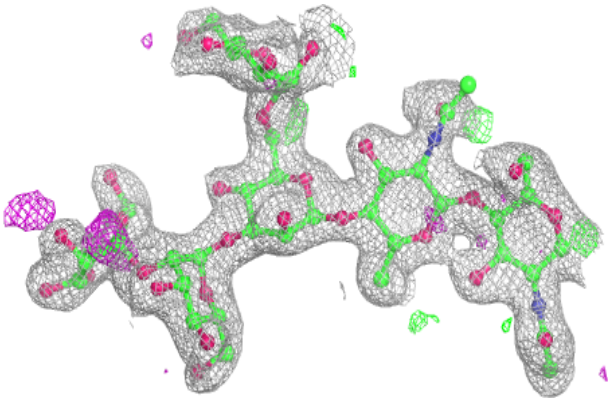


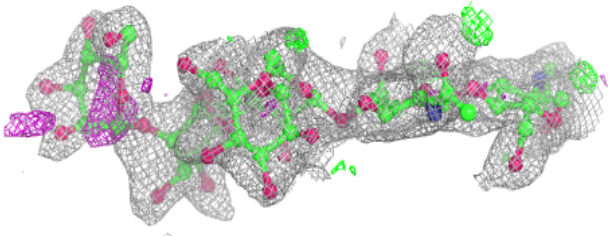


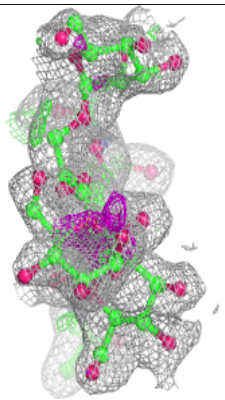


Electron density around Chain H:

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

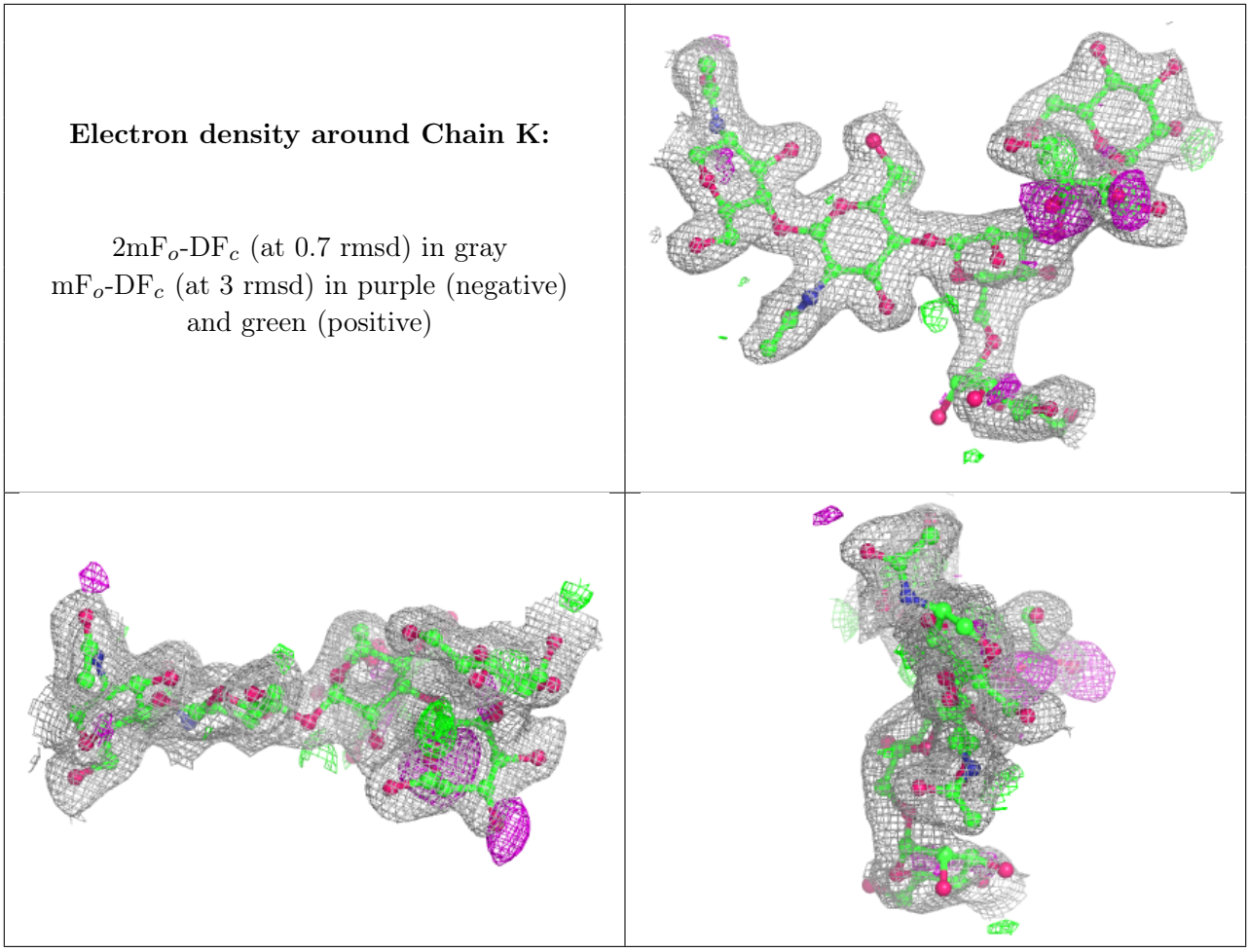






Electron density around Chain K:

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



6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.