Full wwPDB X-ray Structure Validation Report (i)

Nov 16, 2023 – 03:48 AM JST

PDB ID	:	6KRU
Title	:	Crystal structure of mouse IgG2b Fc
Authors	:	Taniguchi, Y.; Satoh, T.; Yagi, H.; Kato, K.
Deposited on	:	2019-08-22
Resolution	:	2.30 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 (i)) were used in the production of this report:

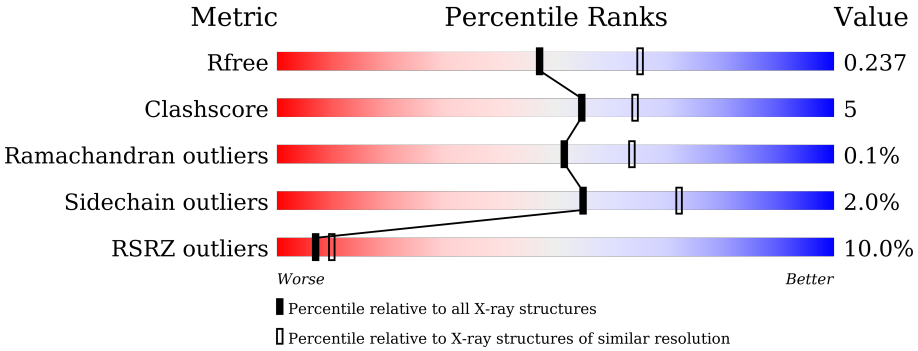
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 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	218	8%, 85%, 9%, • 5%
1	B	218	9%, 83%, 11%, • 5%
1	C	218	9%, 86%, 7%, 7%
1	D	218	10%, 83%, 9%, 8%
1	E	218	9%, 73%, 14%, 12%
1	F	218	11%, 81%, 10%, • 6%

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Mol	Chain	Length	Quality of chain
2	G	9	11% 78% 11%
2	H	9	33% 67%
2	I	9	22% 67% 11%
2	J	9	22% 67% 11%
2	L	9	33% 44% 22%
3	K	8	25% 50% 25%

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
2	NAG	G	8	-	-	-	X

2 Entry composition (i)

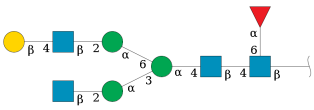
There are 4 unique types of molecules in this entry. The entry contains 10678 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ig gamma-2B chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	208	1658	1052	279	320	7	0	0	0
1	B	208	1658	1052	279	320	7	0	0	0
1	C	203	1620	1028	273	312	7	0	0	0
1	D	201	1602	1020	271	304	7	0	0	0
1	E	191	1522	973	257	285	7	0	0	0
1	F	204	1627	1033	274	313	7	0	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	G	9	110	62	4	44	0	0	0
2	H	9	110	62	4	44	0	0	0
2	I	9	110	62	4	44	0	0	0
2	J	9	110	62	4	44	0	0	0

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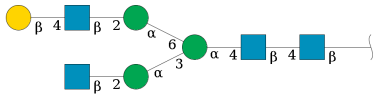
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	L	9	110	62	4	44	0	0	0

- Molecule 3 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]alpha-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			
3	K	8	100	56	4	40	0	0	0

- Molecule 4 is water.

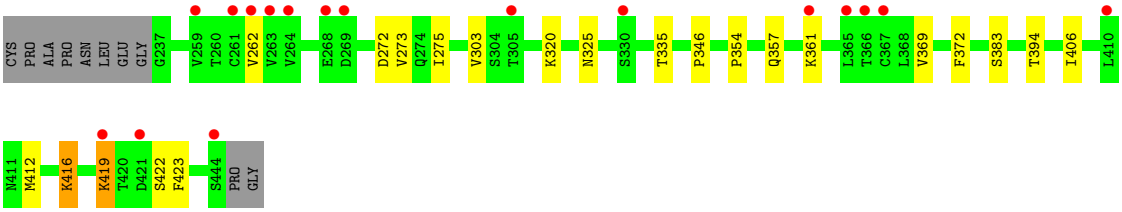
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	62	62	62	0	0
4	B	67	67	67	0	0
4	C	44	44	44	0	0
4	D	53	53	53	0	0
4	E	49	49	49	0	0
4	F	66	66	66	0	0

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.

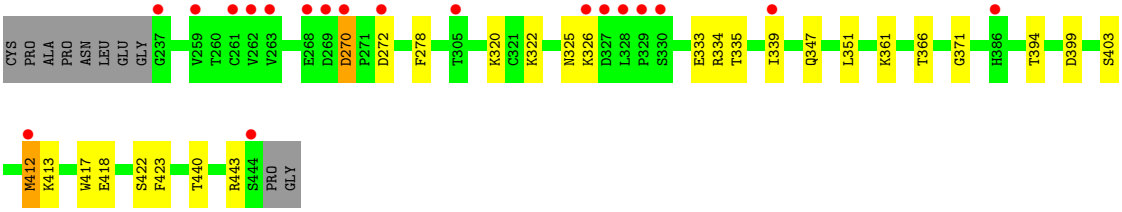
• Molecule 1: Ig gamma-2B chain C region

Chain A:



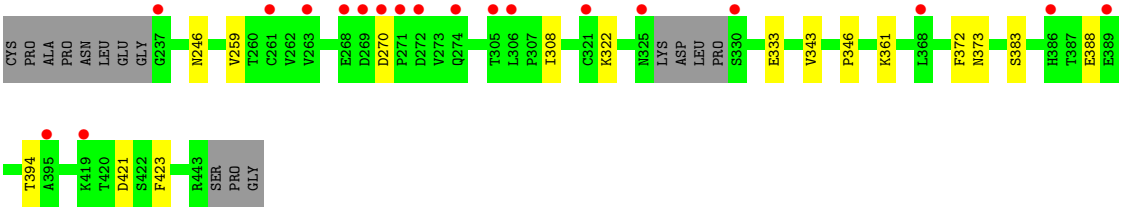
• Molecule 1: Ig gamma-2B chain C region

Chain B:



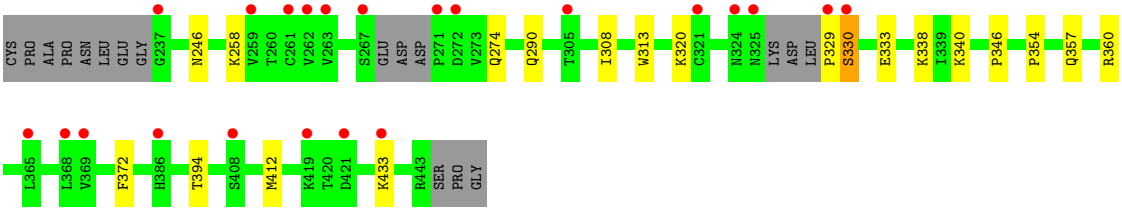
• Molecule 1: Ig gamma-2B chain C region

Chain C:



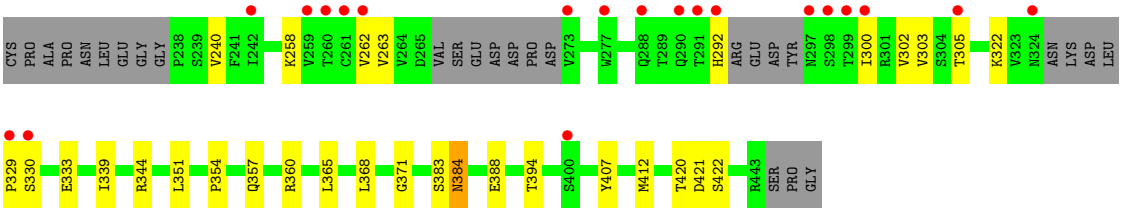
• Molecule 1: Ig gamma-2B chain C region

Chain D:



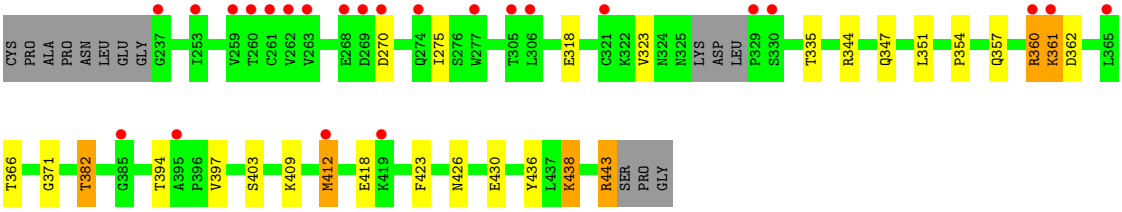
• Molecule 1: Ig gamma-2B chain C region

Chain E:



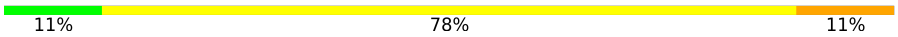
• Molecule 1: Ig gamma-2B chain C region

Chain F:



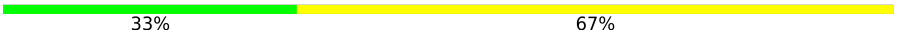
• Molecule 2: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



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

Chain H:



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

Chain I:

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

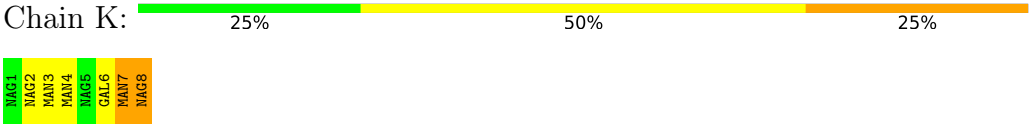
Chain J:

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

Chain L:

• Molecule 3: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]alpha-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 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	112.55Å 130.16Å 134.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.30 19.98 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.98-2.30) 99.9 (19.98-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 2.30Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.198 , 0.237 0.198 , 0.237	Depositor DCC
R_{free} test set	4487 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	49.8	Xtriage
Anisotropy	0.561	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 43.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.005 for -h,l,k	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10678	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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: FUC, NAG, MAN, GAL

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	0.52	0/1698	0.65	1/2311 (0.0%)
1	B	0.49	0/1698	0.61	0/2311
1	C	0.46	0/1658	0.58	0/2255
1	D	0.44	0/1640	0.57	0/2228
1	E	0.48	0/1557	0.60	0/2113
1	F	0.45	0/1666	0.61	0/2266
All	All	0.48	0/9917	0.60	1/13484 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	416	LYS	CD-CE-NZ	-5.52	99.00	111.70

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	1658	0	1640	16	0
1	B	1658	0	1640	27	0
1	C	1620	0	1599	9	0
1	D	1602	0	1593	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1522	0	1526	23	0
1	F	1627	0	1607	29	0
2	G	110	0	94	1	0
2	H	110	0	94	0	0
2	I	110	0	94	1	0
2	J	110	0	94	1	0
2	L	110	0	94	1	0
3	K	100	0	85	1	0
4	A	62	0	0	1	0
4	B	67	0	0	4	0
4	C	44	0	0	3	0
4	D	53	0	0	1	0
4	E	49	0	0	1	0
4	F	66	0	0	1	0
All	All	10678	0	10160	107	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 5.

All (107) 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:F:412:MET:HE1	1:F:423:PHE:CE2	1.88	1.08
1:B:412:MET:HE1	1:B:417:TRP:HB2	1.33	1.07
1:F:412:MET:CE	1:F:423:PHE:CE2	2.46	0.97
1:B:272:ASP:O	4:B:701:HOH:O	1.87	0.93
1:B:326:LYS:NZ	4:B:701:HOH:O	2.01	0.91
1:F:426:ASN:OD1	1:F:438:LYS:NZ	2.07	0.88
1:B:412:MET:CE	1:B:417:TRP:HB2	2.07	0.84
1:B:325:ASN:ND2	4:B:701:HOH:O	2.11	0.84
1:F:418:GLU:HG2	1:F:443:ARG:HE	1.46	0.79
1:C:361:LYS:HB3	4:C:742:HOH:O	1.81	0.79
1:F:436:TYR:OH	1:F:438:LYS:NZ	2.16	0.79
1:B:270:ASP:HB3	1:B:326:LYS:HE2	1.67	0.74
1:F:412:MET:HE2	1:F:423:PHE:CE2	2.26	0.70
1:A:361:LYS:NZ	1:F:362:ASP:CG	2.46	0.69
1:E:240:VAL:HG13	1:E:263:VAL:HG12	1.75	0.68
1:F:412:MET:CE	1:F:423:PHE:CZ	2.78	0.65
1:B:339:ILE:H	1:B:339:ILE:HD12	1.62	0.65
1:E:365:LEU:HG	1:E:412:MET:HE2	1.78	0.65
1:F:430:GLU:OE2	4:F:701:HOH:O	2.14	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:383:SER:OG	1:E:388:GLU:OE2	2.13	0.64
1:F:412:MET:HE1	1:F:423:PHE:CD2	2.33	0.64
1:B:347:GLN:NE2	4:B:705:HOH:O	2.29	0.63
1:B:412:MET:HE1	1:B:417:TRP:CB	2.22	0.63
1:E:344:ARG:HG2	1:E:371:GLY:O	1.98	0.63
1:A:320:LYS:HB2	1:A:335:THR:HG22	1.81	0.62
1:A:361:LYS:NZ	1:F:362:ASP:OD1	2.33	0.62
1:E:263:VAL:HG22	1:E:302:VAL:HB	1.82	0.62
1:E:322:LYS:HG2	1:E:333:GLU:HG2	1.80	0.62
1:E:339:ILE:HD12	4:E:746:HOH:O	1.99	0.62
4:C:701:HOH:O	2:I:6:GAL:O3	2.16	0.61
1:A:361:LYS:HZ1	1:F:362:ASP:CG	2.04	0.61
1:B:322:LYS:HG2	1:B:333:GLU:HG2	1.86	0.57
1:B:417:TRP:CD1	1:B:443:ARG:HD2	2.39	0.57
1:A:262:VAL:HG22	1:A:303:VAL:HG13	1.87	0.57
1:B:361:LYS:HE2	1:B:413:LYS:NZ	2.20	0.56
1:C:346:PRO:HB3	1:C:372:PHE:HB3	1.88	0.56
1:F:412:MET:HE2	1:F:423:PHE:CZ	2.40	0.55
1:A:346:PRO:HB3	1:A:372:PHE:HB3	1.90	0.54
1:C:394:THR:HG21	1:D:394:THR:HG21	1.92	0.52
1:E:394:THR:HG22	1:F:397:VAL:HG21	1.92	0.52
1:B:412:MET:HE3	1:B:417:TRP:N	2.25	0.51
1:E:394:THR:HG21	1:F:394:THR:HG21	1.92	0.50
1:E:360:ARG:NH1	1:F:347:GLN:OE1	2.44	0.50
1:C:322:LYS:HE3	1:C:333:GLU:OE2	2.12	0.50
1:F:360:ARG:HH11	1:F:360:ARG:HG2	1.77	0.49
4:A:701:HOH:O	2:G:6:GAL:O3	2.20	0.48
1:A:273:VAL:HG12	1:A:275:ILE:HG13	1.95	0.48
1:E:258:LYS:HB3	1:E:305:THR:HG23	1.95	0.48
1:F:361:LYS:H	1:F:361:LYS:CD	2.26	0.48
1:E:365:LEU:HD11	1:E:412:MET:HE1	1.96	0.48
1:B:422:SER:HB2	1:B:440:THR:CG2	2.44	0.48
1:F:351:LEU:HB2	1:F:366:THR:HB	1.95	0.48
1:E:354:PRO:HG2	1:E:357:GLN:HB2	1.95	0.47
1:D:346:PRO:HB3	1:D:372:PHE:HB3	1.96	0.47
1:A:394:THR:HG21	1:B:394:THR:HG21	1.96	0.47
1:D:320:LYS:HD2	1:D:333:GLU:OE2	2.15	0.46
1:A:361:LYS:NZ	1:F:362:ASP:OD2	2.48	0.46
1:A:416:LYS:HA	1:A:419:LYS:HG3	1.97	0.46
1:B:270:ASP:HB3	1:B:326:LYS:CE	2.43	0.46
1:B:270:ASP:OD2	1:B:326:LYS:HE2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:360:ARG:HG2	1:F:360:ARG:NH1	2.29	0.46
1:A:383:SER:HB3	1:A:423:PHE:CE1	2.51	0.46
1:E:420:THR:HG22	1:E:422:SER:H	1.80	0.46
1:F:382:THR:HB	1:F:426:ASN:HD21	1.80	0.46
1:B:270:ASP:CB	1:B:326:LYS:HE2	2.41	0.46
1:E:329:PRO:HB2	1:E:330:SER:H	1.56	0.45
1:D:354:PRO:HG2	1:D:357:GLN:HB2	1.98	0.45
1:E:368:LEU:HD13	1:E:407:TYR:CZ	2.52	0.45
1:A:272:ASP:O	1:A:325:ASN:ND2	2.46	0.45
1:B:278:PHE:CE1	1:B:322:LYS:HD2	2.52	0.45
1:B:320:LYS:HB2	1:B:335:THR:HG22	1.98	0.45
2:L:2:NAG:H83	2:L:4:MAN:O3	2.16	0.45
1:B:339:ILE:HG22	1:D:340:LYS:HE2	1.99	0.45
1:B:418:GLU:HA	1:B:443:ARG:HD3	1.99	0.45
1:B:412:MET:SD	1:B:423:PHE:CE2	3.10	0.45
1:A:354:PRO:HG2	1:A:357:GLN:HB2	1.99	0.45
1:E:351:LEU:HD23	1:F:351:LEU:HD23	2.00	0.43
1:C:246:ASN:HB2	4:C:720:HOH:O	2.19	0.43
1:E:292:HIS:O	1:E:300:ILE:HD12	2.19	0.43
1:B:351:LEU:HB2	1:B:366:THR:HB	2.00	0.43
1:B:412:MET:SD	1:B:423:PHE:CZ	3.11	0.43
1:F:354:PRO:HG2	1:F:357:GLN:HB2	2.00	0.43
1:A:412:MET:HB3	1:A:412:MET:HE3	1.65	0.43
1:E:263:VAL:CG2	1:E:302:VAL:HB	2.46	0.43
1:D:340:LYS:HE3	1:D:340:LYS:HB3	1.88	0.43
1:E:368:LEU:HD13	1:E:407:TYR:CE1	2.54	0.42
1:E:384:ASN:OD1	1:E:421:ASP:HB2	2.19	0.42
1:C:259:VAL:HG23	1:C:308:ILE:HD13	2.01	0.42
1:C:383:SER:OG	1:C:388:GLU:OE2	2.26	0.42
1:A:416:LYS:HG2	1:A:419:LYS:HE3	2.01	0.42
1:D:329:PRO:HB2	1:D:330:SER:H	1.67	0.42
1:F:418:GLU:HG2	1:F:443:ARG:NE	2.25	0.42
1:F:275:ILE:HG12	1:F:323:VAL:HG22	2.00	0.42
1:D:308:ILE:HD12	1:D:313:TRP:HB2	2.01	0.42
1:B:320:LYS:HA	1:B:334:ARG:O	2.20	0.41
1:E:262:VAL:HG22	1:E:303:VAL:HG12	2.01	0.41
1:D:246:ASN:HB2	2:J:6:GAL:O4	2.20	0.41
1:D:338:LYS:HE3	4:D:708:HOH:O	2.20	0.41
1:F:412:MET:HB3	1:F:412:MET:HE3	1.64	0.41
1:B:371:GLY:HA2	1:B:403:SER:OG	2.20	0.41
1:C:383:SER:HB3	1:C:423:PHE:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:258:LYS:NZ	1:E:305:THR:HG21	2.35	0.41
3:K:7:MAN:O3	3:K:8:NAG:O5	2.29	0.41
1:F:371:GLY:HA2	1:F:403:SER:OG	2.19	0.41
1:F:318:GLU:HG3	1:F:335:THR:OG1	2.20	0.41
1:A:369:VAL:HB	1:A:406:ILE:HG22	2.03	0.40
1:C:343:VAL:HA	1:C:373:ASN:O	2.22	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	206/218 (94%)	204 (99%)	2 (1%)	0	100	100
1	B	206/218 (94%)	203 (98%)	3 (2%)	0	100	100
1	C	199/218 (91%)	197 (99%)	2 (1%)	0	100	100
1	D	195/218 (89%)	191 (98%)	4 (2%)	0	100	100
1	E	183/218 (84%)	182 (100%)	0	1 (0%)	29	35
1	F	200/218 (92%)	196 (98%)	4 (2%)	0	100	100
All	All	1189/1308 (91%)	1173 (99%)	15 (1%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	384	ASN

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	196/203 (97%)	194 (99%)	2 (1%)	76	87
1	B	196/203 (97%)	193 (98%)	3 (2%)	65	79
1	C	191/203 (94%)	189 (99%)	2 (1%)	76	87
1	D	189/203 (93%)	182 (96%)	7 (4%)	34	48
1	E	180/203 (89%)	180 (100%)	0	100	100
1	F	192/203 (95%)	183 (95%)	9 (5%)	26	37
All	All	1144/1218 (94%)	1121 (98%)	23 (2%)	55	72

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

Mol	Chain	Res	Type
1	A	419	LYS
1	A	422	SER
1	B	270	ASP
1	B	399	ASP
1	B	412	MET
1	C	270	ASP
1	C	421	ASP
1	D	258	LYS
1	D	274	GLN
1	D	290	GLN
1	D	330	SER
1	D	360	ARG
1	D	412	MET
1	D	433	LYS
1	F	270	ASP
1	F	344	ARG
1	F	360	ARG
1	F	361	LYS
1	F	382	THR
1	F	409	LYS
1	F	412	MET
1	F	438	LYS
1	F	443	ARG

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

Mol	Chain	Res	Type
1	A	290	GLN
1	E	290	GLN

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)

53 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	G	1	1,2	14,14,15	0.66	1 (7%)	17,19,21	0.86	1 (5%)
2	NAG	G	2	2	14,14,15	0.39	0	17,19,21	0.89	1 (5%)
2	MAN	G	3	2	11,11,12	1.25	1 (9%)	15,15,17	1.37	3 (20%)
2	MAN	G	4	2	11,11,12	0.77	0	15,15,17	1.57	2 (13%)
2	NAG	G	5	2	14,14,15	1.39	2 (14%)	17,19,21	0.86	1 (5%)
2	GAL	G	6	2	11,11,12	1.43	2 (18%)	15,15,17	1.00	1 (6%)
2	MAN	G	7	2	11,11,12	1.56	4 (36%)	15,15,17	2.41	4 (26%)
2	NAG	G	8	2	14,14,15	0.93	1 (7%)	17,19,21	1.00	1 (5%)
2	FUC	G	9	2	10,10,11	0.90	0	14,14,16	0.95	0
2	NAG	H	1	1,2	14,14,15	0.44	0	17,19,21	0.72	0
2	NAG	H	2	2	14,14,15	0.85	1 (7%)	17,19,21	1.09	1 (5%)
2	MAN	H	3	2	11,11,12	1.35	1 (9%)	15,15,17	1.55	4 (26%)
2	MAN	H	4	2	11,11,12	1.19	2 (18%)	15,15,17	1.38	2 (13%)
2	NAG	H	5	2	14,14,15	0.24	0	17,19,21	0.56	0
2	GAL	H	6	2	11,11,12	1.87	2 (18%)	15,15,17	1.31	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	MAN	H	7	2	11,11,12	0.80	0	15,15,17	1.32	1 (6%)
2	NAG	H	8	2	14,14,15	0.41	0	17,19,21	0.45	0
2	FUC	H	9	2	10,10,11	0.76	0	14,14,16	1.10	1 (7%)
2	NAG	I	1	1,2	14,14,15	0.66	0	17,19,21	0.52	0
2	NAG	I	2	2	14,14,15	0.30	0	17,19,21	0.99	1 (5%)
2	MAN	I	3	2	11,11,12	1.32	1 (9%)	15,15,17	1.75	2 (13%)
2	MAN	I	4	2	11,11,12	0.81	0	15,15,17	1.27	2 (13%)
2	NAG	I	5	2	14,14,15	0.61	1 (7%)	17,19,21	0.48	0
2	GAL	I	6	2	11,11,12	1.50	2 (18%)	15,15,17	1.07	2 (13%)
2	MAN	I	7	2	11,11,12	1.07	1 (9%)	15,15,17	1.81	1 (6%)
2	NAG	I	8	2	14,14,15	0.53	0	17,19,21	0.69	0
2	FUC	I	9	2	10,10,11	1.10	1 (10%)	14,14,16	0.87	0
2	NAG	J	1	1,2	14,14,15	0.22	0	17,19,21	0.89	1 (5%)
2	NAG	J	2	2	14,14,15	0.35	0	17,19,21	0.95	1 (5%)
2	MAN	J	3	2	11,11,12	1.72	1 (9%)	15,15,17	1.63	2 (13%)
2	MAN	J	4	2	11,11,12	0.79	0	15,15,17	1.70	2 (13%)
2	NAG	J	5	2	14,14,15	0.27	0	17,19,21	0.54	0
2	GAL	J	6	2	11,11,12	1.52	3 (27%)	15,15,17	1.72	3 (20%)
2	MAN	J	7	2	11,11,12	1.37	2 (18%)	15,15,17	1.34	2 (13%)
2	NAG	J	8	2	14,14,15	0.67	0	17,19,21	0.56	0
2	FUC	J	9	2	10,10,11	1.11	1 (10%)	14,14,16	0.89	0
3	NAG	K	1	1,3	14,14,15	0.50	0	17,19,21	0.79	0
3	NAG	K	2	3	14,14,15	0.48	0	17,19,21	0.77	1 (5%)
3	MAN	K	3	3	11,11,12	1.37	2 (18%)	15,15,17	1.32	3 (20%)
3	MAN	K	4	3	11,11,12	0.83	0	15,15,17	1.38	2 (13%)
3	NAG	K	5	3	14,14,15	0.24	0	17,19,21	0.60	0
3	GAL	K	6	3	11,11,12	1.07	1 (9%)	15,15,17	1.00	1 (6%)
3	MAN	K	7	3	11,11,12	1.28	3 (27%)	15,15,17	1.16	3 (20%)
3	NAG	K	8	3	14,14,15	0.56	0	17,19,21	0.71	1 (5%)
2	NAG	L	1	1,2	14,14,15	0.42	0	17,19,21	0.62	0
2	NAG	L	2	2	14,14,15	0.48	0	17,19,21	1.08	1 (5%)
2	MAN	L	3	2	11,11,12	1.39	1 (9%)	15,15,17	1.87	2 (13%)
2	MAN	L	4	2	11,11,12	1.47	3 (27%)	15,15,17	1.04	1 (6%)
2	NAG	L	5	2	14,14,15	0.49	0	17,19,21	0.47	0
2	GAL	L	6	2	11,11,12	1.34	1 (9%)	15,15,17	1.37	2 (13%)
2	MAN	L	7	2	11,11,12	1.03	1 (9%)	15,15,17	1.43	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	L	8	2	14,14,15	0.79	1 (7%)	17,19,21	0.86	2 (11%)
2	FUC	L	9	2	10,10,11	0.84	0	14,14,16	0.77	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	G	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	MAN	G	3	2	-	0/2/19/22	1/1/1/1
2	MAN	G	4	2	-	0/2/19/22	0/1/1/1
2	NAG	G	5	2	-	0/6/23/26	0/1/1/1
2	GAL	G	6	2	-	0/2/19/22	0/1/1/1
2	MAN	G	7	2	-	2/2/19/22	0/1/1/1
2	NAG	G	8	2	-	0/6/23/26	0/1/1/1
2	FUC	G	9	2	-	-	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	MAN	H	3	2	-	0/2/19/22	1/1/1/1
2	MAN	H	4	2	-	1/2/19/22	0/1/1/1
2	NAG	H	5	2	-	0/6/23/26	0/1/1/1
2	GAL	H	6	2	-	0/2/19/22	0/1/1/1
2	MAN	H	7	2	-	1/2/19/22	0/1/1/1
2	NAG	H	8	2	-	2/6/23/26	0/1/1/1
2	FUC	H	9	2	-	-	0/1/1/1
2	NAG	I	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
2	MAN	I	3	2	-	0/2/19/22	1/1/1/1
2	MAN	I	4	2	-	2/2/19/22	0/1/1/1
2	NAG	I	5	2	-	0/6/23/26	0/1/1/1
2	GAL	I	6	2	-	1/2/19/22	0/1/1/1
2	MAN	I	7	2	-	0/2/19/22	0/1/1/1
2	NAG	I	8	2	-	3/6/23/26	0/1/1/1
2	FUC	I	9	2	-	-	0/1/1/1
2	NAG	J	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	MAN	J	3	2	-	0/2/19/22	0/1/1/1
2	MAN	J	4	2	-	0/2/19/22	0/1/1/1
2	NAG	J	5	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GAL	J	6	2	-	0/2/19/22	0/1/1/1
2	MAN	J	7	2	-	0/2/19/22	0/1/1/1
2	NAG	J	8	2	-	2/6/23/26	0/1/1/1
2	FUC	J	9	2	-	-	0/1/1/1
3	NAG	K	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	1/6/23/26	0/1/1/1
3	MAN	K	3	3	-	1/2/19/22	1/1/1/1
3	MAN	K	4	3	-	0/2/19/22	0/1/1/1
3	NAG	K	5	3	-	0/6/23/26	0/1/1/1
3	GAL	K	6	3	-	2/2/19/22	0/1/1/1
3	MAN	K	7	3	-	2/2/19/22	0/1/1/1
3	NAG	K	8	3	-	3/6/23/26	0/1/1/1
2	NAG	L	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	L	2	2	-	2/6/23/26	0/1/1/1
2	MAN	L	3	2	-	0/2/19/22	1/1/1/1
2	MAN	L	4	2	-	0/2/19/22	0/1/1/1
2	NAG	L	5	2	-	0/6/23/26	0/1/1/1
2	GAL	L	6	2	-	1/2/19/22	0/1/1/1
2	MAN	L	7	2	-	1/2/19/22	0/1/1/1
2	NAG	L	8	2	-	2/6/23/26	0/1/1/1
2	FUC	L	9	2	-	-	0/1/1/1

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	3	MAN	O5-C1	-5.43	1.35	1.43
2	H	6	GAL	O2-C2	4.11	1.52	1.43
2	G	5	NAG	O5-C1	-4.02	1.37	1.43
2	L	3	MAN	O5-C1	-3.76	1.37	1.43
2	H	6	GAL	C1-C2	3.71	1.60	1.52
2	G	6	GAL	O2-C2	3.66	1.51	1.43
2	I	3	MAN	O5-C1	-3.61	1.37	1.43
2	L	6	GAL	C1-C2	3.53	1.60	1.52
3	K	3	MAN	C1-C2	3.49	1.60	1.52
2	G	8	NAG	O5-C1	3.31	1.49	1.43
2	I	6	GAL	O2-C2	3.10	1.49	1.43
2	G	5	NAG	C1-C2	3.04	1.56	1.52
2	H	2	NAG	O5-C1	-3.04	1.38	1.43
2	J	7	MAN	C4-C5	2.97	1.59	1.53
2	G	3	MAN	O5-C5	2.92	1.49	1.43
2	L	4	MAN	C2-C3	2.84	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	6	GAL	C1-C2	2.78	1.58	1.52
2	G	7	MAN	C4-C5	2.56	1.58	1.53
2	J	6	GAL	C1-C2	2.54	1.58	1.52
3	K	3	MAN	O5-C5	2.51	1.48	1.43
2	H	4	MAN	C2-C3	2.43	1.56	1.52
2	H	3	MAN	C1-C2	2.43	1.57	1.52
2	L	4	MAN	O5-C1	-2.43	1.39	1.43
2	G	7	MAN	O5-C5	2.39	1.48	1.43
2	L	8	NAG	O5-C1	-2.39	1.39	1.43
2	H	4	MAN	O5-C1	-2.38	1.39	1.43
2	J	6	GAL	O2-C2	2.33	1.48	1.43
3	K	7	MAN	C2-C3	2.32	1.55	1.52
3	K	7	MAN	O5-C5	2.32	1.48	1.43
2	J	7	MAN	O5-C5	2.26	1.48	1.43
2	G	1	NAG	O5-C1	-2.26	1.40	1.43
2	L	7	MAN	C4-C5	2.25	1.57	1.53
2	L	4	MAN	O5-C5	2.25	1.48	1.43
2	G	7	MAN	C1-C2	2.23	1.57	1.52
2	I	5	NAG	O5-C1	-2.23	1.40	1.43
2	J	6	GAL	O5-C5	2.23	1.48	1.43
2	J	9	FUC	C2-C3	2.20	1.55	1.52
2	I	7	MAN	O5-C5	2.16	1.47	1.43
2	I	9	FUC	C2-C3	2.13	1.55	1.52
2	G	7	MAN	O2-C2	2.12	1.47	1.43
3	K	6	GAL	C4-C3	2.10	1.57	1.52
2	G	6	GAL	C1-C2	2.08	1.56	1.52
3	K	7	MAN	O2-C2	2.05	1.47	1.43

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	7	MAN	C1-O5-C5	6.97	121.63	112.19
2	I	7	MAN	C1-O5-C5	5.53	119.69	112.19
2	L	3	MAN	C1-O5-C5	5.51	119.65	112.19
2	J	4	MAN	C1-O5-C5	5.15	119.17	112.19
2	I	3	MAN	C1-O5-C5	5.11	119.11	112.19
2	J	6	GAL	C1-O5-C5	4.61	118.43	112.19
2	J	3	MAN	C1-O5-C5	4.57	118.38	112.19
2	G	4	MAN	C1-O5-C5	4.38	118.12	112.19
2	J	7	MAN	C1-O5-C5	4.17	117.84	112.19
3	K	4	MAN	C1-O5-C5	4.15	117.82	112.19
2	L	7	MAN	C1-O5-C5	3.83	117.38	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	7	MAN	C1-O5-C5	3.73	117.25	112.19
2	L	6	GAL	O2-C2-C1	3.33	115.97	109.15
2	G	8	NAG	C1-O5-C5	3.31	116.68	112.19
2	H	4	MAN	C1-O5-C5	3.28	116.64	112.19
2	L	3	MAN	C1-C2-C3	3.26	113.68	109.67
2	H	3	MAN	C1-C2-C3	3.26	113.67	109.67
2	J	3	MAN	C1-C2-C3	3.23	113.64	109.67
2	H	6	GAL	O2-C2-C1	3.22	115.75	109.15
2	I	3	MAN	C1-C2-C3	3.19	113.58	109.67
2	J	4	MAN	O2-C2-C3	-3.17	103.78	110.14
2	G	7	MAN	C3-C4-C5	3.15	115.85	110.24
2	H	3	MAN	C1-O5-C5	3.13	116.43	112.19
2	G	3	MAN	C1-O5-C5	3.07	116.35	112.19
3	K	4	MAN	O2-C2-C3	-2.92	104.28	110.14
2	G	7	MAN	O2-C2-C1	2.92	115.12	109.15
2	I	4	MAN	C1-O5-C5	2.91	116.14	112.19
2	I	2	NAG	O4-C4-C3	2.91	117.08	110.35
3	K	3	MAN	O2-C2-C3	-2.88	104.37	110.14
2	L	2	NAG	O4-C4-C3	2.88	117.00	110.35
2	J	2	NAG	O4-C4-C5	-2.87	102.17	109.30
2	H	2	NAG	O4-C4-C5	-2.77	102.42	109.30
2	J	6	GAL	O2-C2-C1	2.76	114.81	109.15
2	G	2	NAG	O4-C4-C5	-2.72	102.55	109.30
2	G	3	MAN	C1-C2-C3	2.71	112.99	109.67
3	K	3	MAN	C1-C2-C3	2.65	112.93	109.67
2	I	4	MAN	O2-C2-C3	-2.65	104.83	110.14
2	G	4	MAN	O2-C2-C3	-2.63	104.87	110.14
3	K	2	NAG	O4-C4-C5	-2.63	102.77	109.30
2	L	7	MAN	O2-C2-C3	-2.62	104.89	110.14
3	K	6	GAL	O2-C2-C1	2.54	114.36	109.15
2	G	6	GAL	O2-C2-C1	2.52	114.31	109.15
2	G	7	MAN	O5-C5-C4	2.49	116.89	110.83
2	I	6	GAL	O2-C2-C1	2.47	114.20	109.15
2	G	1	NAG	C1-O5-C5	2.45	115.51	112.19
3	K	3	MAN	C1-O5-C5	2.37	115.40	112.19
2	J	1	NAG	C1-O5-C5	2.34	115.36	112.19
2	I	6	GAL	C1-C2-C3	2.29	112.49	109.67
2	L	8	NAG	C4-C3-C2	2.28	114.36	111.02
2	H	4	MAN	O2-C2-C3	-2.24	105.65	110.14
2	H	3	MAN	O6-C6-C5	-2.23	103.64	111.29
3	K	7	MAN	C1-O5-C5	2.22	115.21	112.19
2	J	6	GAL	O5-C1-C2	2.19	114.15	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	5	NAG	C4-C3-C2	2.19	114.23	111.02
2	L	4	MAN	O3-C3-C2	2.19	114.18	109.99
3	K	7	MAN	C1-C2-C3	-2.14	107.04	109.67
2	H	6	GAL	C1-O5-C5	2.09	115.03	112.19
2	L	8	NAG	C3-C4-C5	2.09	113.97	110.24
2	G	3	MAN	O6-C6-C5	-2.09	104.14	111.29
2	J	7	MAN	O2-C2-C3	-2.07	106.00	110.14
3	K	7	MAN	O3-C3-C2	2.06	113.94	109.99
2	H	9	FUC	C3-C4-C5	-2.06	106.56	109.77
2	H	3	MAN	O2-C2-C3	-2.04	106.05	110.14
3	K	8	NAG	C1-O5-C5	2.04	114.96	112.19
2	L	6	GAL	O2-C2-C3	-2.04	106.06	110.14

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	K	8	NAG	C3-C2-N2-C7
3	K	7	MAN	O5-C5-C6-O6
2	H	8	NAG	O5-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
3	K	6	GAL	C4-C5-C6-O6
3	K	7	MAN	C4-C5-C6-O6
3	K	6	GAL	O5-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	H	8	NAG	C4-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
2	L	2	NAG	O5-C5-C6-O6
2	I	8	NAG	C4-C5-C6-O6
3	K	8	NAG	C4-C5-C6-O6
2	G	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
2	I	8	NAG	O5-C5-C6-O6
2	L	8	NAG	C4-C5-C6-O6
2	L	2	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	J	8	NAG	O5-C5-C6-O6
3	K	8	NAG	O5-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
2	L	8	NAG	O5-C5-C6-O6
2	G	7	MAN	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	H	2	NAG	O5-C5-C6-O6
2	I	4	MAN	C4-C5-C6-O6
2	I	6	GAL	O5-C5-C6-O6
2	J	8	NAG	C4-C5-C6-O6
2	L	7	MAN	C4-C5-C6-O6
3	K	3	MAN	O5-C5-C6-O6
2	H	4	MAN	C4-C5-C6-O6
2	H	7	MAN	C4-C5-C6-O6
2	I	8	NAG	C3-C2-N2-C7
2	G	7	MAN	O5-C5-C6-O6
2	I	4	MAN	O5-C5-C6-O6
2	L	6	GAL	C4-C5-C6-O6

All (5) ring outliers are listed below:

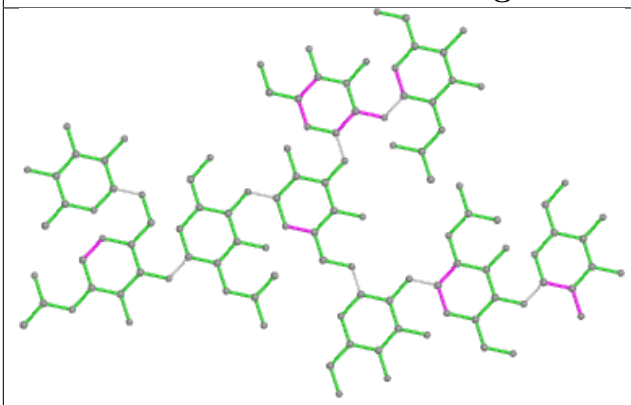
Mol	Chain	Res	Type	Atoms
2	I	3	MAN	C1-C2-C3-C4-C5-O5
3	K	3	MAN	C1-C2-C3-C4-C5-O5
2	G	3	MAN	C1-C2-C3-C4-C5-O5
2	L	3	MAN	C1-C2-C3-C4-C5-O5
2	H	3	MAN	C1-C2-C3-C4-C5-O5

7 monomers are involved in 5 short contacts:

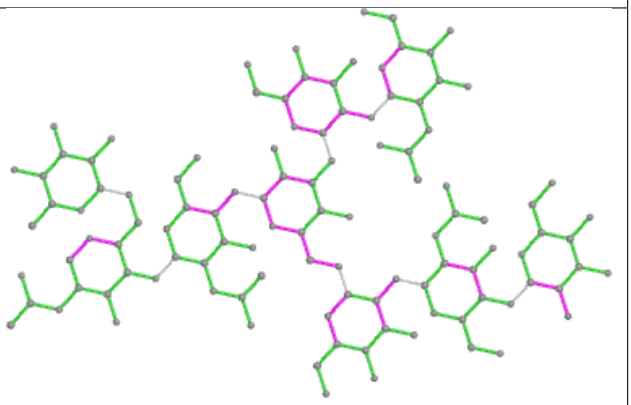
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	6	GAL	1	0
3	K	8	NAG	1	0
2	J	6	GAL	1	0
2	L	4	MAN	1	0
3	K	7	MAN	1	0
2	I	6	GAL	1	0
2	L	2	NAG	1	0

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

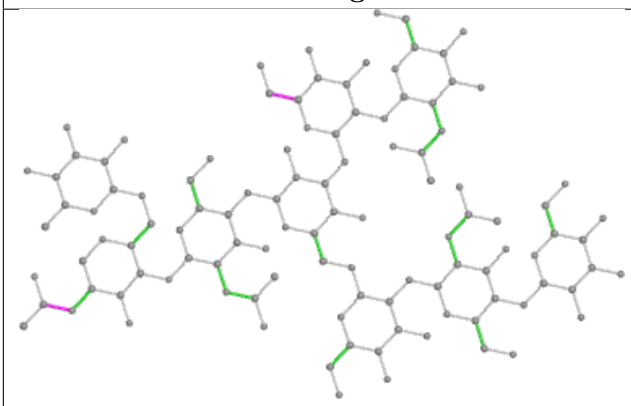
Oligosaccharide Chain G



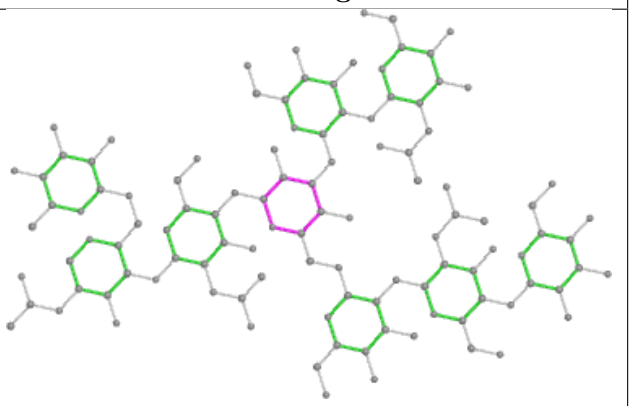
Bond lengths



Bond angles

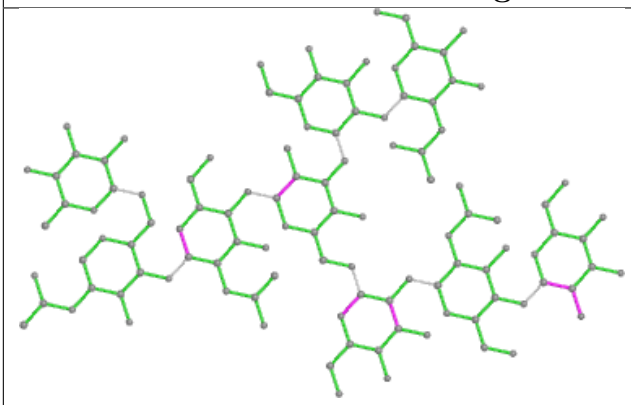


Torsions

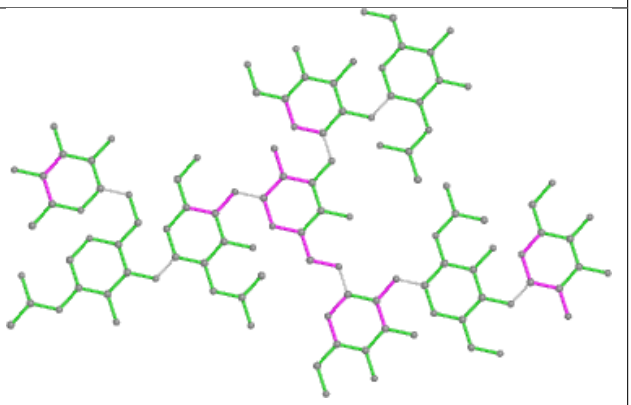


Rings

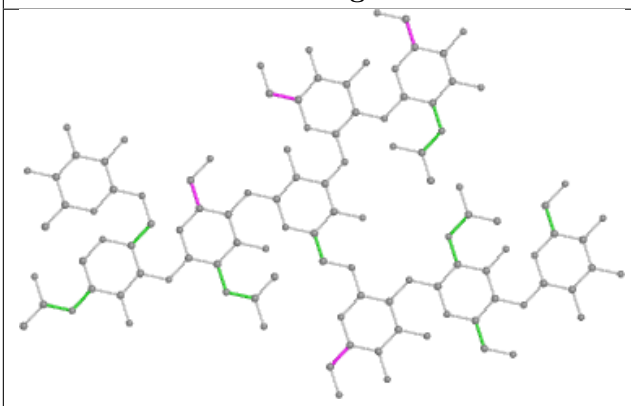
Oligosaccharide Chain H



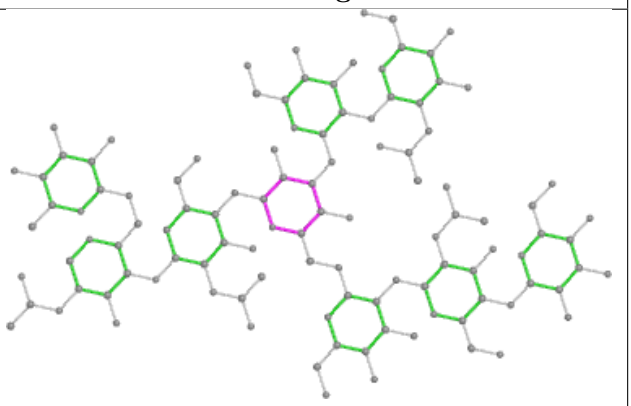
Bond lengths



Bond angles

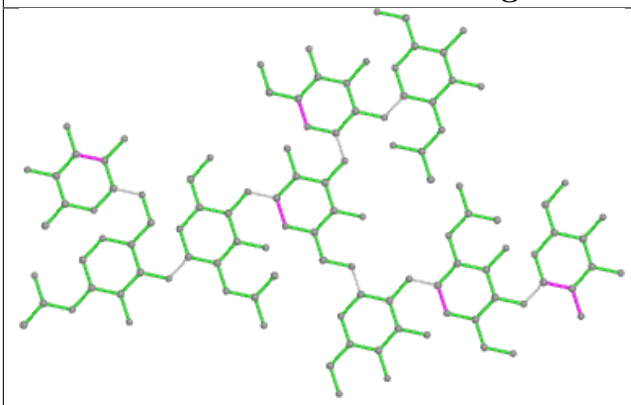


Torsions

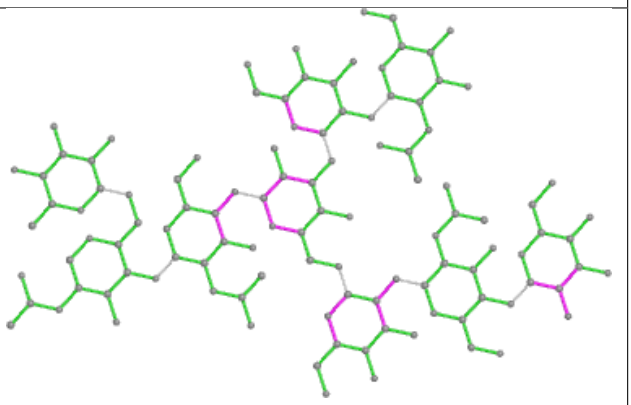


Rings

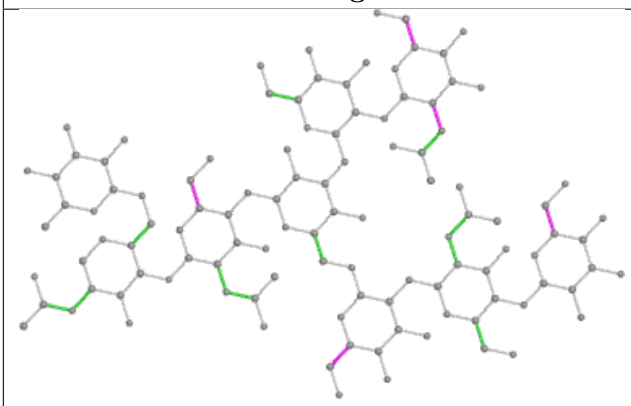
Oligosaccharide Chain I



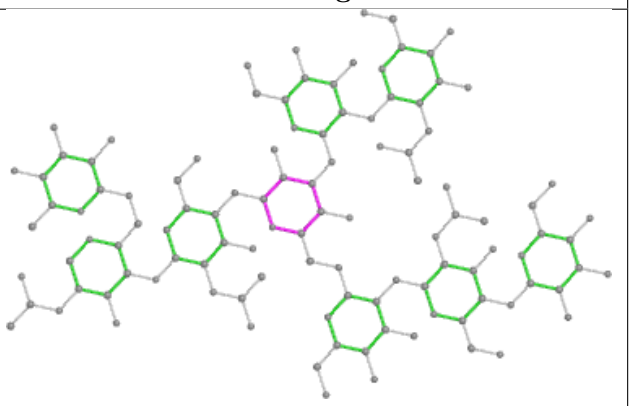
Bond lengths



Bond angles

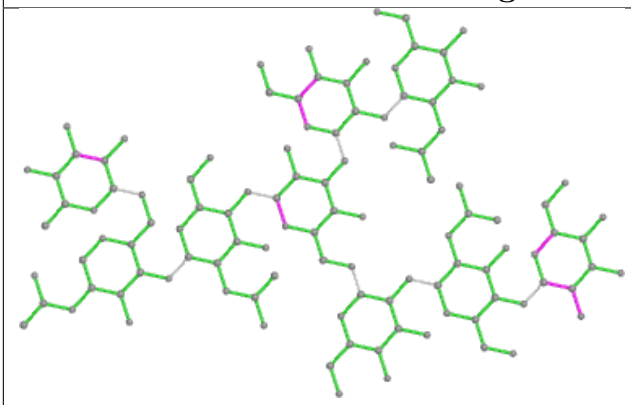


Torsions

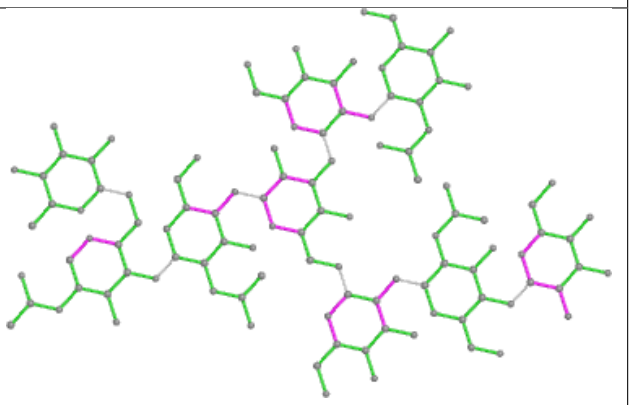


Rings

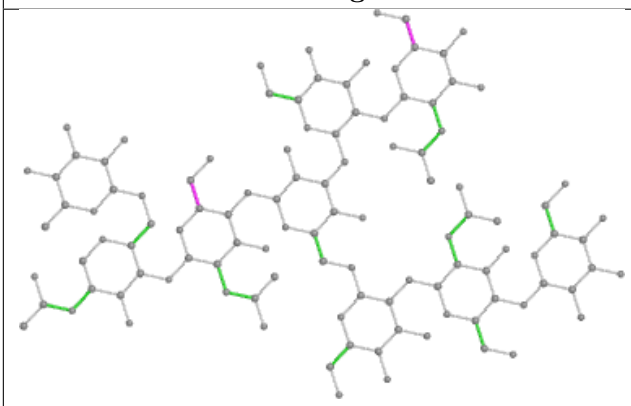
Oligosaccharide Chain J



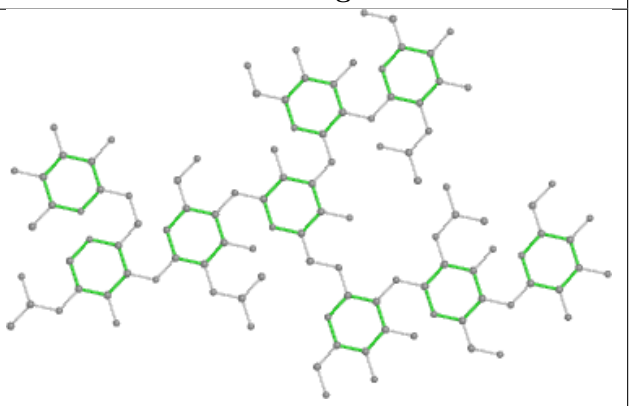
Bond lengths



Bond angles

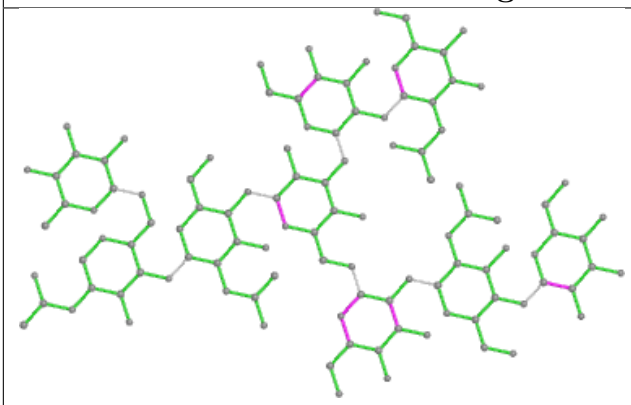


Torsions

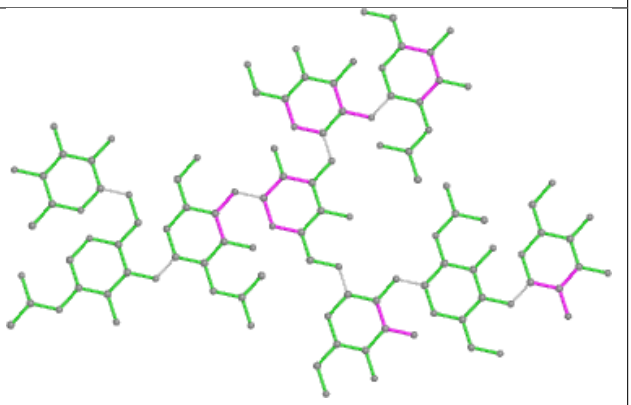


Rings

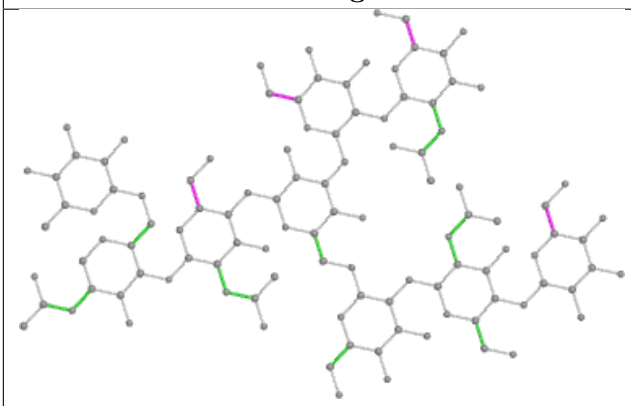
Oligosaccharide Chain L



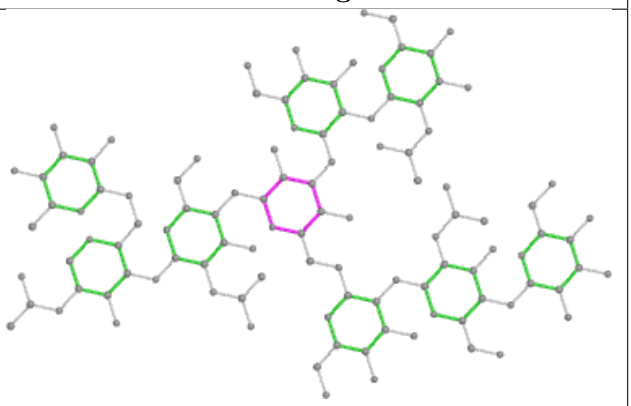
Bond lengths



Bond angles

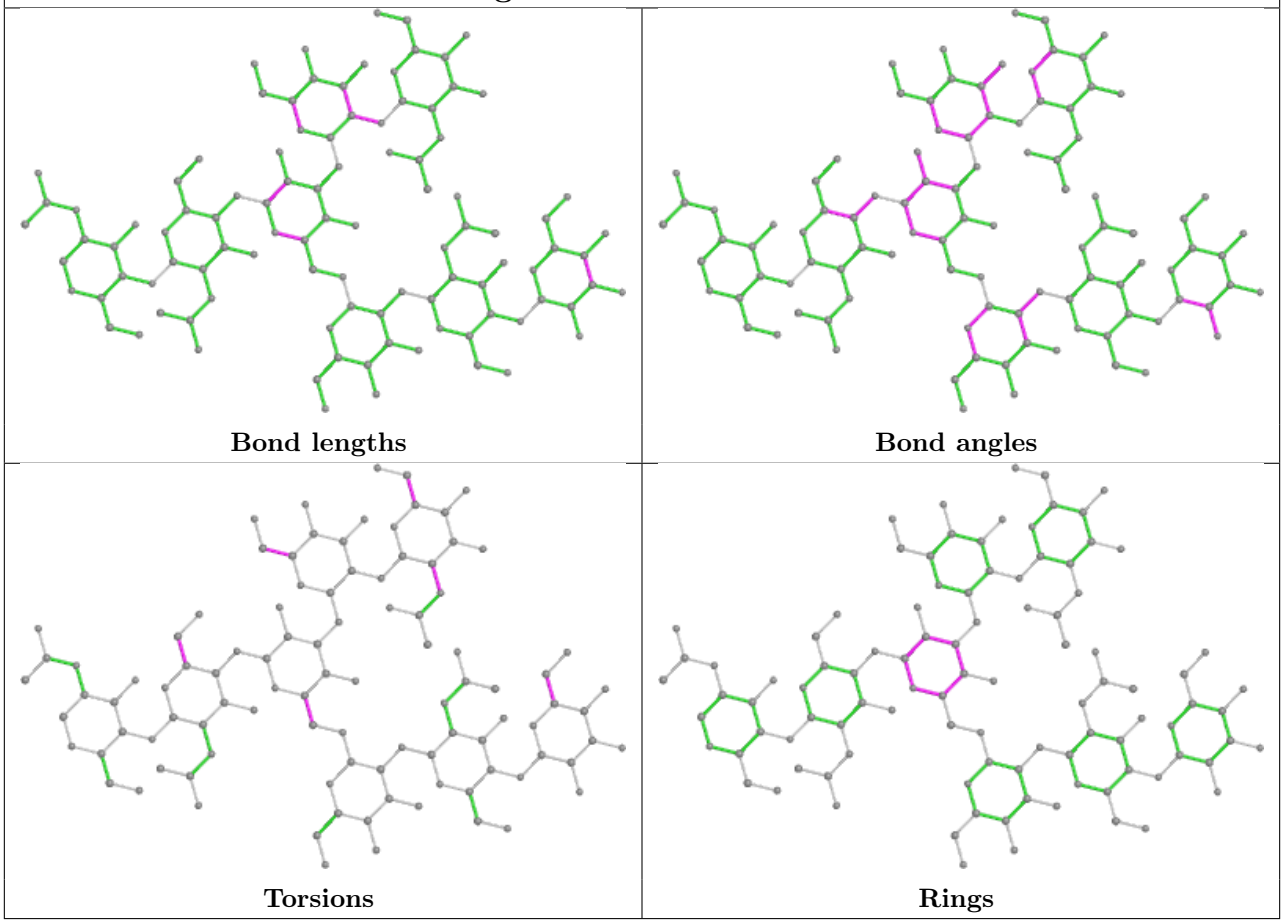


Torsions



Rings

Oligosaccharide Chain K



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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	208/218 (95%)	0.43	17 (8%)	11	15	38, 54, 75, 92	0
1	B	208/218 (95%)	0.48	19 (9%)	9	12	38, 51, 89, 126	0
1	C	203/218 (93%)	0.36	19 (9%)	8	11	42, 55, 91, 112	0
1	D	201/218 (92%)	0.51	22 (10%)	5	8	42, 56, 88, 123	0
1	E	191/218 (87%)	0.60	20 (10%)	6	8	39, 56, 105, 147	0
1	F	204/218 (93%)	0.55	24 (11%)	4	6	40, 55, 91, 116	0
All	All	1215/1308 (92%)	0.49	121 (9%)	7	10	38, 55, 91, 147	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	298	SER	7.3
1	A	421	ASP	5.4
1	C	330	SER	5.2
1	E	299	THR	5.0
1	B	326	LYS	5.0
1	B	329	PRO	4.9
1	C	269	ASP	4.7
1	E	261	CYS	4.7
1	D	272	ASP	4.6
1	E	260	THR	4.6
1	E	292	HIS	4.5
1	D	329	PRO	4.4
1	A	263	VAL	4.3
1	E	330	SER	4.2
1	B	330	SER	4.0
1	B	328	LEU	4.0
1	D	330	SER	4.0
1	F	237	GLY	4.0
1	B	268	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	300	ILE	3.8
1	B	386	HIS	3.8
1	C	419	LYS	3.7
1	B	269	ASP	3.7
1	D	368	LEU	3.6
1	B	327	ASP	3.6
1	A	419	LYS	3.6
1	C	263	VAL	3.6
1	E	262	VAL	3.6
1	E	259	VAL	3.5
1	B	270	ASP	3.5
1	F	269	ASP	3.4
1	D	271	PRO	3.3
1	E	297	ASN	3.3
1	F	259	VAL	3.3
1	B	272	ASP	3.2
1	F	274	GLN	3.1
1	C	271	PRO	3.1
1	F	261	CYS	3.1
1	B	444	SER	3.1
1	D	421	ASP	3.1
1	F	277	TRP	3.1
1	B	259	VAL	3.1
1	A	262	VAL	3.0
1	D	263	VAL	3.0
1	F	365	LEU	3.0
1	E	329	PRO	3.0
1	B	263	VAL	3.0
1	A	365	LEU	3.0
1	D	386	HIS	3.0
1	A	269	ASP	2.9
1	C	268	GLU	2.9
1	B	339	ILE	2.9
1	E	291	THR	2.9
1	F	268	GLU	2.9
1	F	270	ASP	2.8
1	A	264	VAL	2.8
1	B	261	CYS	2.8
1	C	261	CYS	2.7
1	A	305	THR	2.7
1	C	305	THR	2.7
1	F	253	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	261	CYS	2.7
1	D	259	VAL	2.7
1	F	260	THR	2.7
1	D	419	LYS	2.7
1	A	444	SER	2.7
1	C	270	ASP	2.7
1	C	274	GLN	2.6
1	D	325	ASN	2.6
1	A	367	CYS	2.6
1	F	305	THR	2.6
1	C	325	ASN	2.6
1	D	267	SER	2.6
1	C	386	HIS	2.6
1	C	395	ALA	2.6
1	D	365	LEU	2.6
1	C	272	ASP	2.6
1	C	321	CYS	2.5
1	D	237	GLY	2.5
1	F	321	CYS	2.5
1	A	366	THR	2.5
1	C	237	GLY	2.5
1	E	288	GLN	2.5
1	A	259	VAL	2.5
1	F	263	VAL	2.4
1	E	290	GLN	2.4
1	D	261	CYS	2.4
1	F	395	ALA	2.4
1	F	330	SER	2.4
1	B	305	THR	2.3
1	E	277	TRP	2.3
1	E	273	VAL	2.3
1	C	389	GLU	2.3
1	B	412	MET	2.3
1	F	262	VAL	2.3
1	D	305	THR	2.3
1	E	324	ASN	2.3
1	F	419	LYS	2.3
1	F	306	LEU	2.2
1	F	361	LYS	2.2
1	F	385	GLY	2.2
1	E	400	SER	2.2
1	E	305	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	360	ARG	2.2
1	A	330	SER	2.2
1	B	262	VAL	2.2
1	D	369	VAL	2.2
1	A	361	LYS	2.2
1	D	262	VAL	2.1
1	F	329	PRO	2.1
1	D	408	SER	2.1
1	A	268	GLU	2.1
1	D	324	ASN	2.1
1	F	412	MET	2.1
1	D	433	LYS	2.1
1	A	410	LEU	2.0
1	C	306	LEU	2.0
1	E	242	ILE	2.0
1	B	237	GLY	2.0
1	D	321	CYS	2.0
1	C	368	LEU	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	K	1	14/15	0.68	0.29	108,118,132,132	0
3	NAG	K	5	14/15	0.71	0.26	87,100,109,109	0
3	GAL	K	6	11/12	0.74	0.33	77,91,107,109	0
2	NAG	G	8	14/15	0.77	0.44	109,119,120,127	0
3	NAG	K	8	14/15	0.78	0.38	115,129,134,134	0
2	GAL	I	6	11/12	0.81	0.39	63,82,95,96	0
2	NAG	H	8	14/15	0.82	0.37	75,97,101,103	0
2	NAG	J	8	14/15	0.82	0.39	89,102,113,113	0
3	MAN	K	4	11/12	0.83	0.35	102,106,111,112	0
2	GAL	G	6	11/12	0.84	0.41	57,72,87,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	L	8	14/15	0.86	0.42	79,100,109,112	0
2	NAG	G	5	14/15	0.87	0.23	61,71,78,83	0
2	MAN	I	7	11/12	0.88	0.29	82,90,93,97	0
2	NAG	I	8	14/15	0.89	0.32	92,102,109,116	0
2	GAL	H	6	11/12	0.89	0.36	49,61,68,68	0
2	NAG	J	5	14/15	0.90	0.17	53,58,65,65	0
2	GAL	J	6	11/12	0.90	0.30	52,65,70,70	0
2	NAG	H	5	14/15	0.90	0.17	49,56,60,60	0
2	GAL	L	6	11/12	0.90	0.31	54,62,71,72	0
2	MAN	G	7	11/12	0.90	0.35	90,98,104,105	0
2	NAG	L	5	14/15	0.91	0.20	56,59,64,65	0
2	NAG	G	1	14/15	0.91	0.12	59,65,67,71	0
2	MAN	J	7	11/12	0.91	0.31	78,82,88,95	0
2	NAG	I	5	14/15	0.91	0.19	60,66,72,73	0
2	MAN	G	4	11/12	0.92	0.17	67,68,72,75	0
2	MAN	G	3	11/12	0.93	0.10	60,66,71,81	0
2	MAN	L	7	11/12	0.93	0.23	79,82,86,91	0
2	MAN	L	4	11/12	0.93	0.15	48,53,56,56	0
2	MAN	H	7	11/12	0.93	0.27	77,83,91,92	0
3	NAG	K	2	14/15	0.94	0.14	100,102,107,108	0
2	NAG	I	2	14/15	0.94	0.12	50,60,65,66	0
2	NAG	L	1	14/15	0.94	0.12	51,54,60,61	0
2	MAN	I	4	11/12	0.94	0.17	62,64,68,73	0
3	MAN	K	7	11/12	0.94	0.36	115,121,125,126	0
2	NAG	G	2	14/15	0.94	0.15	59,62,66,66	0
2	NAG	H	1	14/15	0.95	0.10	44,51,54,54	0
2	NAG	J	1	14/15	0.95	0.09	50,55,60,62	0
2	NAG	J	2	14/15	0.95	0.10	47,54,62,65	0
3	MAN	K	3	11/12	0.95	0.14	97,98,103,107	0
2	MAN	L	3	11/12	0.95	0.11	55,59,66,74	0
2	MAN	J	3	11/12	0.95	0.16	51,58,68,75	0
2	MAN	J	4	11/12	0.95	0.16	54,56,61,64	0
2	MAN	I	3	11/12	0.95	0.11	60,63,72,79	0
2	MAN	H	3	11/12	0.95	0.12	54,60,70,71	0
2	FUC	I	9	10/11	0.96	0.16	53,57,60,62	0
2	MAN	H	4	11/12	0.96	0.16	51,53,60,69	0
2	NAG	H	2	14/15	0.96	0.11	45,50,55,58	0
2	FUC	G	9	10/11	0.96	0.12	60,63,67,72	0
2	FUC	J	9	10/11	0.97	0.10	52,54,56,59	0
2	FUC	L	9	10/11	0.97	0.09	51,54,58,61	0
2	FUC	H	9	10/11	0.97	0.09	47,50,58,59	0
2	NAG	L	2	14/15	0.97	0.09	48,53,59,62	0

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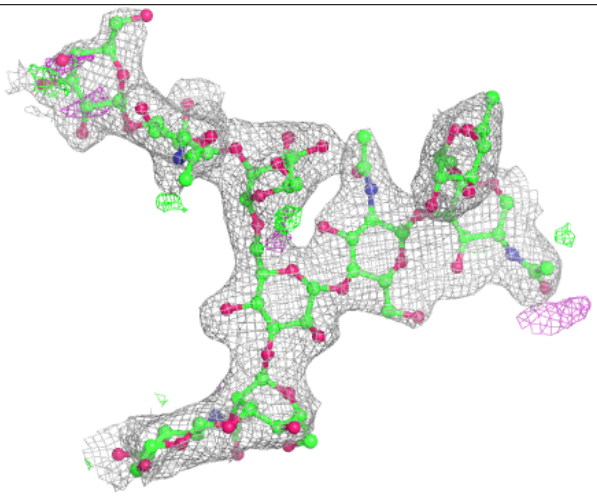
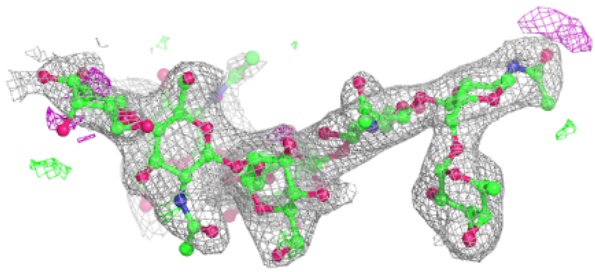
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	I	1	14/15	0.97	0.09	49,58,60,62	0

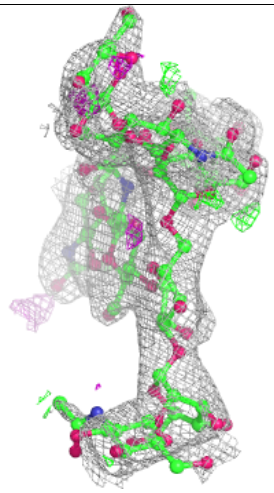
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

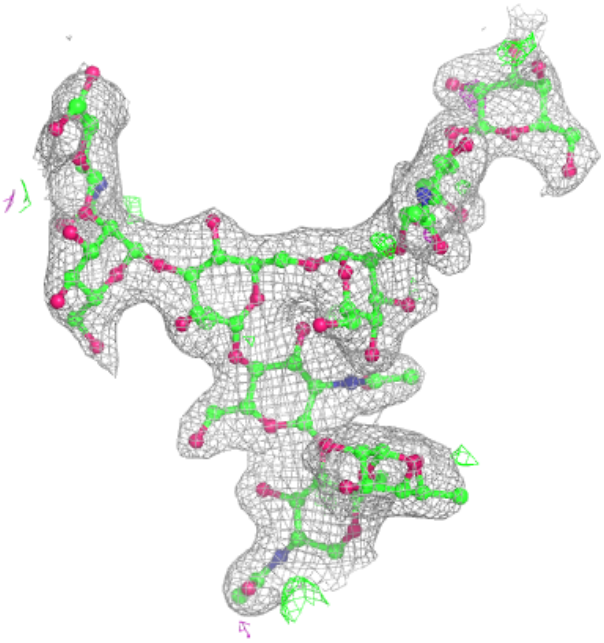


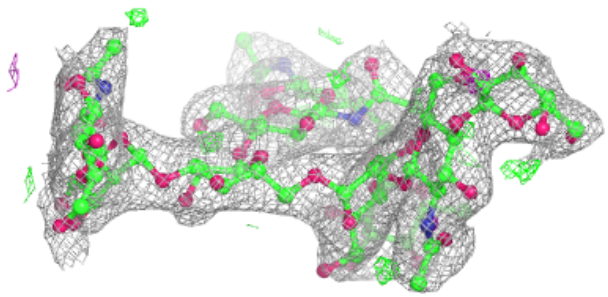


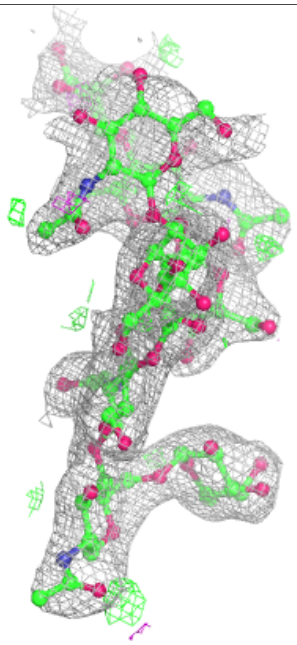


Electron density around Chain H:

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

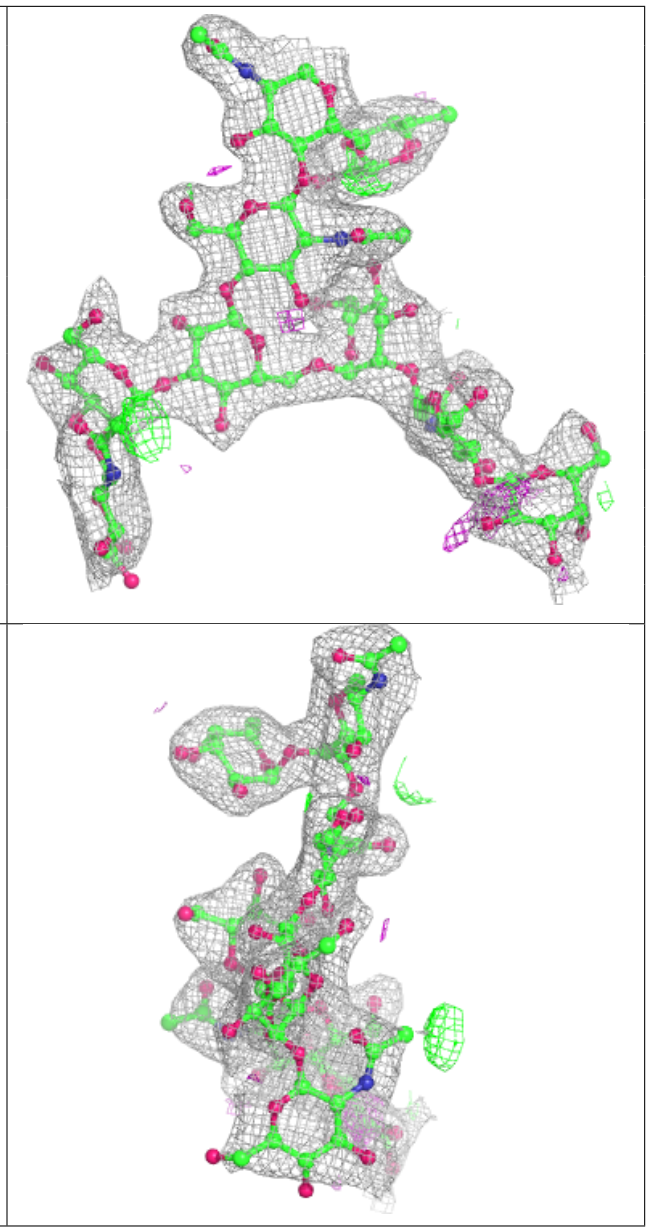






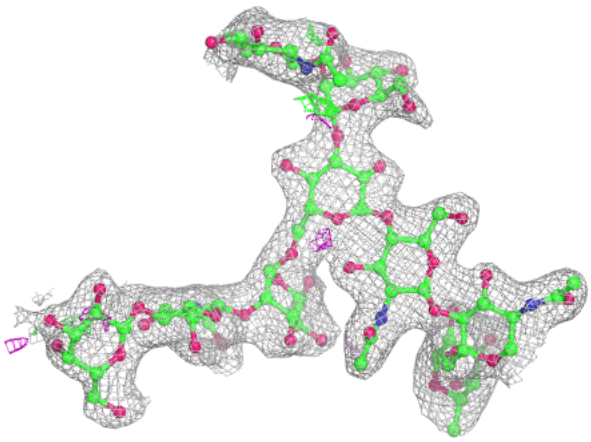
Electron density around Chain I:

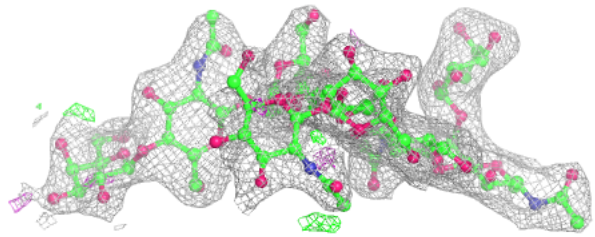
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

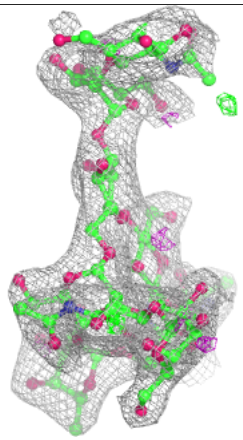


Electron density around Chain J:

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

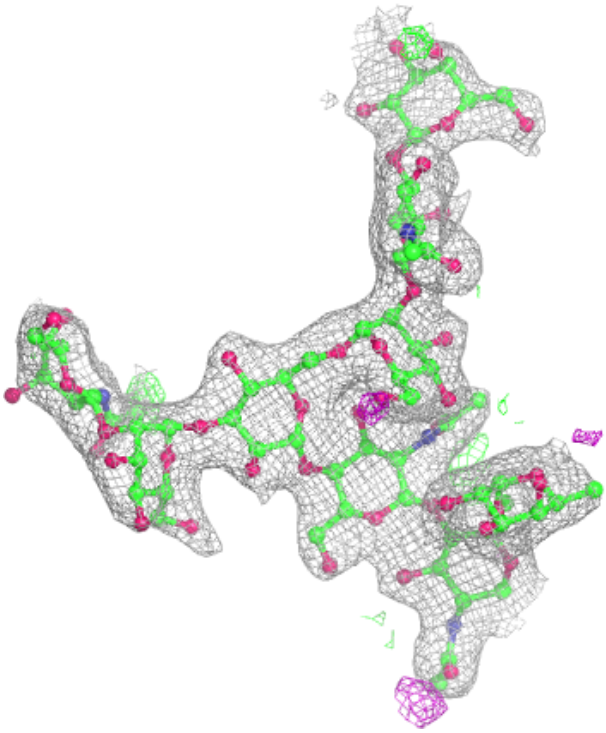


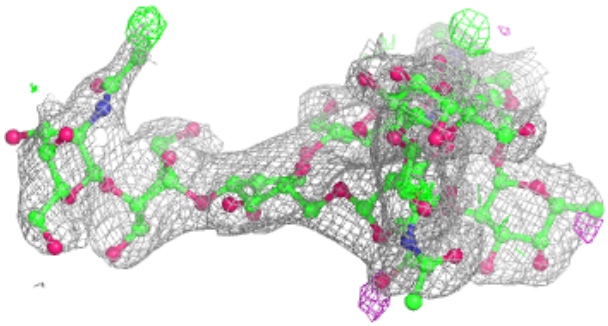


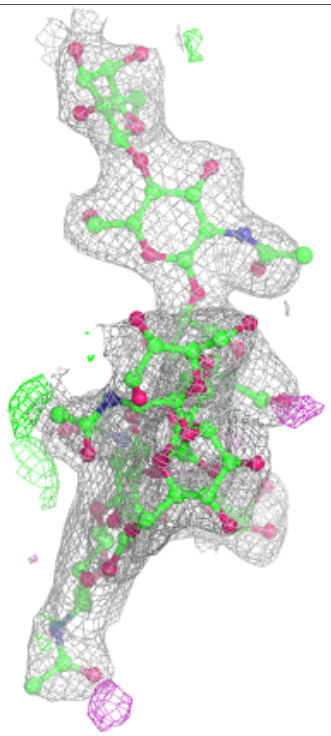


Electron density around Chain L:

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

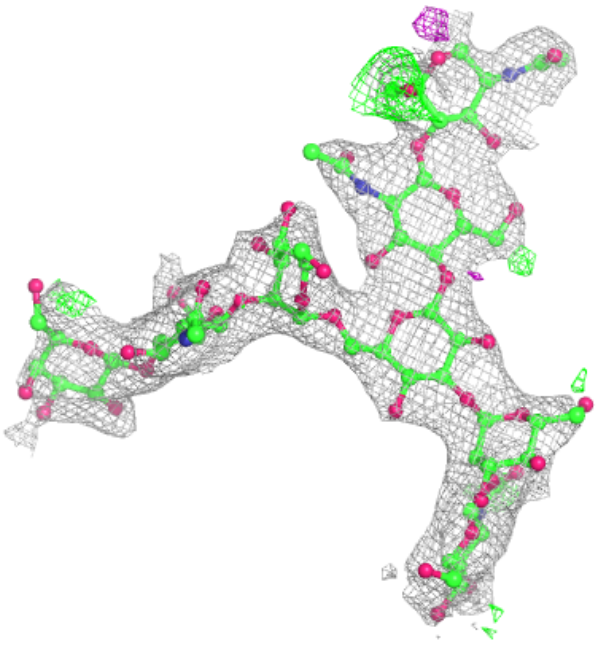


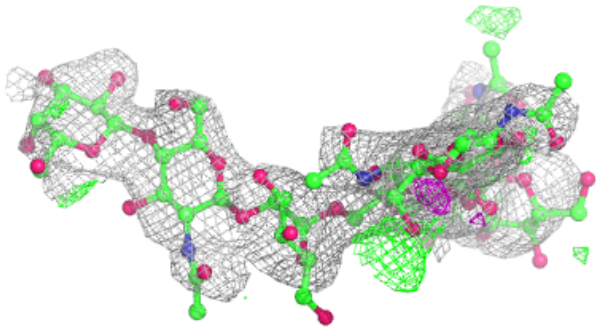


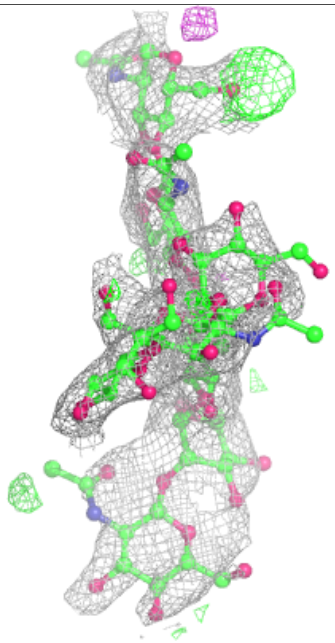


Electron density around Chain K:

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







6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.