Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 07:16 PM BST

PDB ID	:	3GXP
Title	:	Crystal structure of acid-alpha-galactosidase A complexed with galactose at pH 4.5
Authors	:	Lieberman, R.L.
Deposited on	:	2009-04-02
Resolution	:	2.20 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 ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

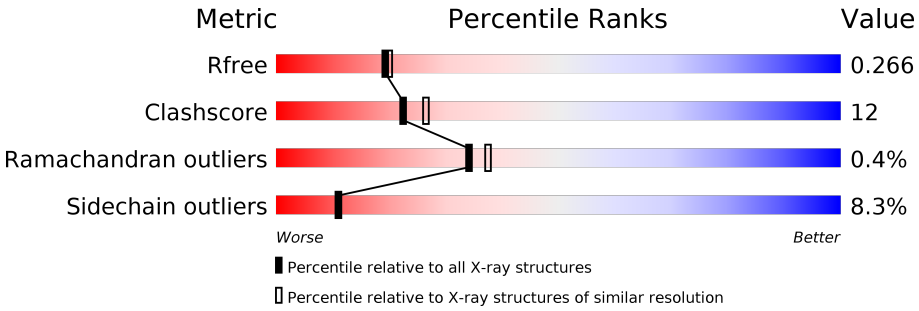
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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 on 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%

Mol	Chain	Length	Quality of chain
1	A	398	72% 22%
1	B	398	70% 25%
2	C	3	67% 33%
3	D	2	50% 50%
3	E	2	50% 50%
3	F	2	100%
3	G	2	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MAN	C	3	X	-	-	-
6	TAM	A	6744	-	-	X	-

2 Entry composition

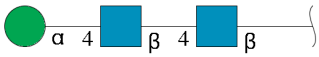
There are 9 unique types of molecules in this entry. The entry contains 6666 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Alpha-galactosidase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	0	0
			3122	1988	534	574	26			
1	B	391	Total	C	N	O	S	0	0	0
			3131	1993	536	576	26			

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

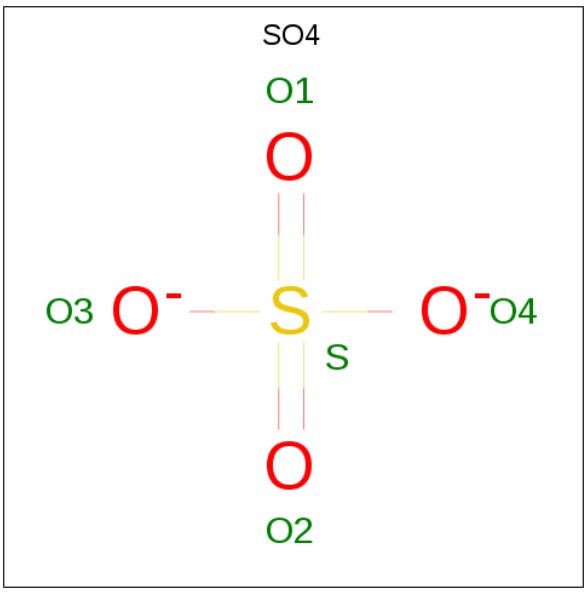


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			39	22	2	15			

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

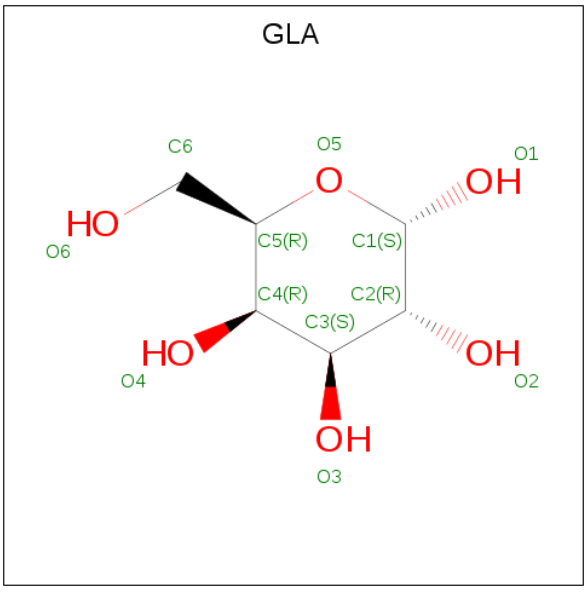
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



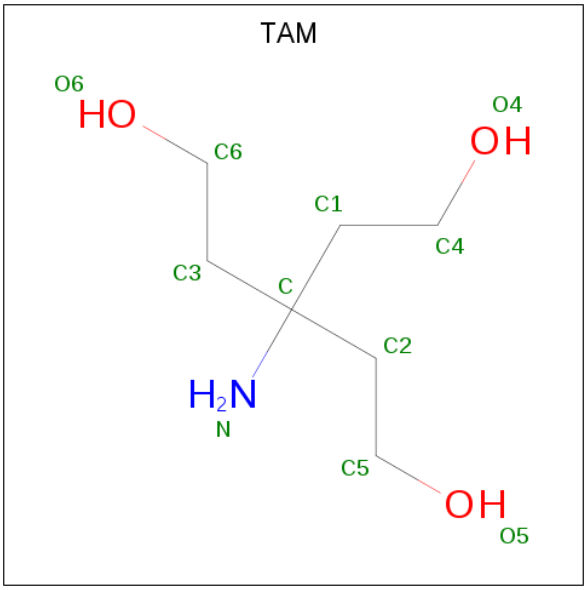
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0

- Molecule 5 is alpha-D-galactopyranose (three-letter code: GLA) (formula: $C_6H_{12}O_6$).



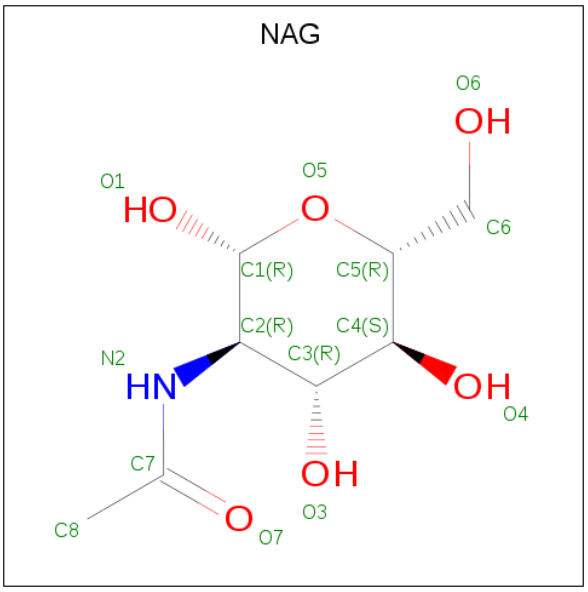
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			12	6	6		
5	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 6 is TRIS(HYDROXYETHYL)AMINOMETHANE (three-letter code: TAM) (formula: $C_7H_{17}NO_3$).



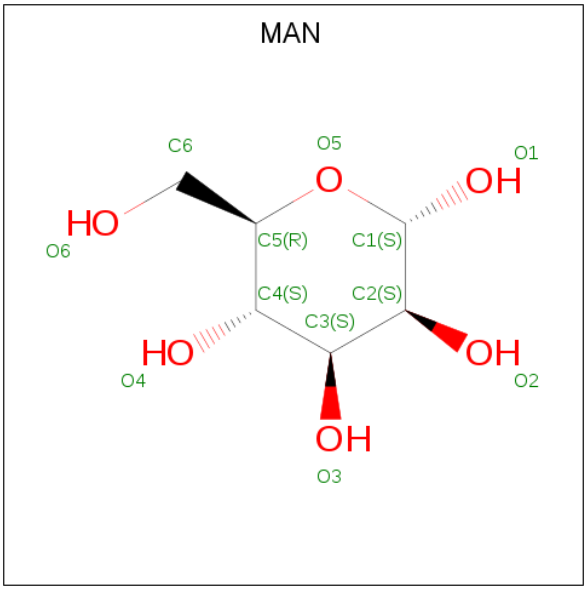
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			11	7	1	3		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 8 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	O		0	0
			11	6	5			
8	B	1	Total	C	O		0	0
			11	6	5			

- Molecule 9 is water.

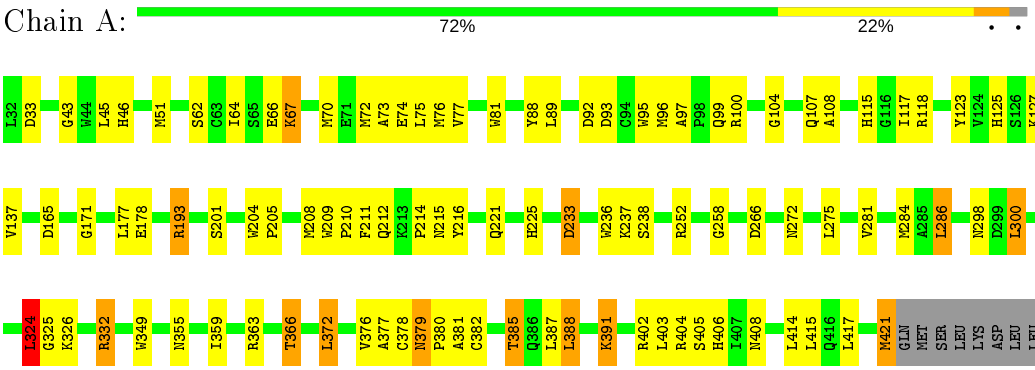
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	86	Total O 86 86	0	0
9	B	71	Total O 71 71	0	0

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. 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. 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.

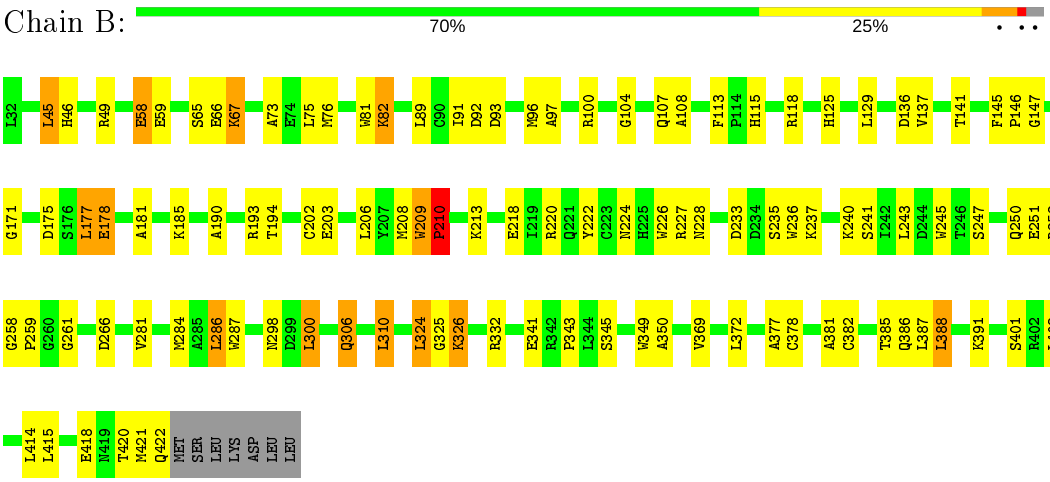
• Molecule 1: Alpha-galactosidase A

Chain A:



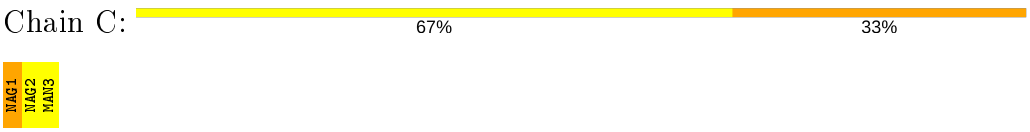
• Molecule 1: Alpha-galactosidase A

Chain B:



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

Chain C:



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

Chain D:

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

Chain E:

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

Chain F:

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

Chain G:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	89.51Å 89.51Å 215.93Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.15 – 2.20 38.15 – 2.20	Depositor EDS
% Data completeness (in resolution range)	81.9 (38.15-2.20) 81.9 (38.15-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.97 (at 2.20Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.201 , 0.265 0.206 , 0.266	Depositor DCC
R_{free} test set	2144 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	46.6	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 56.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6666	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GLA, MAN, NAG, TAM, SO4

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	0.96	2/3209 (0.1%)	0.99	10/4358 (0.2%)
1	B	0.95	1/3218 (0.0%)	0.93	3/4370 (0.1%)
All	All	0.96	3/6427 (0.0%)	0.96	13/8728 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	281	VAL	CB-CG1	-6.01	1.40	1.52
1	A	209	TRP	CB-CG	5.57	1.60	1.50
1	B	254	VAL	CB-CG2	-5.18	1.42	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	286	LEU	CA-CB-CG	-10.05	92.19	115.30
1	B	286	LEU	CA-CB-CG	-7.34	98.41	115.30
1	A	332	ARG	NE-CZ-NH2	-7.03	116.79	120.30
1	A	286	LEU	CB-CG-CD1	6.90	122.73	111.00
1	B	49	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	A	93	ASP	CB-CG-OD1	6.38	124.04	118.30
1	B	49	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	A	193	ARG	NE-CZ-NH1	-5.75	117.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	70	MET	CG-SD-CE	5.70	109.32	100.20
1	A	324	LEU	CA-CB-CG	5.68	128.37	115.30
1	A	275	LEU	CA-CB-CG	5.30	127.48	115.30
1	A	233	ASP	CB-CA-C	-5.12	100.15	110.40
1	A	118	ARG	NE-CZ-NH2	-5.06	117.77	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	209	TRP	Peptide
1	B	210	PRO	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3122	0	2982	66	0
1	B	3131	0	2987	78	0
2	C	39	0	34	1	0
3	D	28	0	25	3	0
3	E	28	0	24	1	0
3	F	28	0	25	1	0
3	G	28	0	22	1	0
4	A	5	0	0	0	0
4	B	15	0	0	0	0
5	A	12	0	12	0	0
5	B	12	0	12	4	0
6	A	11	0	17	11	0
7	A	28	0	25	2	0
8	B	22	0	20	0	0
9	A	86	0	0	6	0
9	B	71	0	0	2	0
All	All	6666	0	6185	147	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 12.

All (147) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ASN:ND2	3:D:1:NAG:C1	2.09	1.15
1:A:215:ASN:HD21	3:D:1:NAG:C1	1.72	0.99
1:A:236:TRP:H	6:A:6744:TAM:H52	1.31	0.94
6:A:6744:TAM:H22	1:B:236:TRP:HB3	1.47	0.94
1:A:66:GLU:OE1	1:A:115:HIS:HD2	1.51	0.93
1:B:170:ASP:OD2	5:B:3681:GLA:H1	1.73	0.86
1:B:65:SER:HB2	1:B:67:LYS:NZ	1.90	0.86
1:A:66:GLU:OE1	1:A:115:HIS:CD2	2.32	0.81
1:B:324:LEU:HD13	1:B:326:LYS:HG3	1.63	0.81
1:B:65:SER:HB2	1:B:67:LYS:HZ3	1.46	0.78
1:B:125:HIS:HE1	1:B:165:ASP:OD2	1.65	0.77
1:A:377:ALA:O	1:A:378:CYS:HB2	1.84	0.76
1:A:379:ASN:HD22	1:A:380:PRO:HA	1.49	0.76
1:A:237:LYS:H	6:A:6744:TAM:HN1	1.32	0.73
1:A:208:MET:CE	1:A:212:GLN:HG3	2.19	0.73
1:B:209:TRP:HE3	1:B:210:PRO:HG3	1.51	0.72
1:B:66:GLU:OE1	1:B:115:HIS:HD2	1.73	0.72
1:A:237:LYS:N	6:A:6744:TAM:N	2.36	0.71
1:A:51:MET:O	1:A:64:ILE:HD11	1.91	0.71
1:A:236:TRP:N	6:A:6744:TAM:H52	2.03	0.70
1:B:306:GLN:HE21	1:B:306:GLN:H	1.37	0.70
1:A:46:HIS:CD2	1:A:92:ASP:H	2.11	0.69
1:B:177:LEU:H	1:B:177:LEU:HD12	1.59	0.68
1:B:46:HIS:CD2	1:B:92:ASP:H	2.12	0.67
1:B:208:MET:O	1:B:210:PRO:HA	1.96	0.66
1:B:236:TRP:CE2	1:B:240:LYS:HD2	2.31	0.66
1:A:97:ALA:HB3	1:A:107:GLN:HG3	1.77	0.66
1:B:306:GLN:HE21	1:B:306:GLN:N	1.94	0.65
1:A:125:HIS:HE1	1:A:165:ASP:OD2	1.80	0.65
1:A:193:ARG:O	1:A:193:ARG:HG3	1.96	0.65
1:A:377:ALA:O	1:A:378:CYS:CB	2.42	0.65
1:B:45:LEU:HD22	1:B:92:ASP:HB2	1.80	0.64
1:A:372:LEU:HD23	1:A:417:LEU:HD21	1.81	0.62
1:B:213:LYS:HD3	1:B:252:ARG:NH1	2.14	0.62
1:B:349:TRP:CD1	1:B:377:ALA:HB2	2.36	0.61
1:B:181:ALA:O	1:B:185:LYS:HG3	2.01	0.61
1:A:349:TRP:CD1	1:A:377:ALA:HB2	2.37	0.60
1:A:237:LYS:H	6:A:6744:TAM:HN2	1.46	0.60
1:A:406:HIS:HE1	1:B:59:GLU:OE2	1.85	0.60
1:A:377:ALA:O	9:A:3476:HOH:O	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:6763:HOH:O	3:G:2:NAG:H2	2.02	0.60
1:B:326:LYS:HB3	1:B:326:LYS:NZ	2.18	0.59
7:A:498:NAG:H4	7:A:430:NAG:C1	2.32	0.59
1:A:403:LEU:HD21	1:A:415:LEU:CD1	2.33	0.59
1:B:388:LEU:HB2	1:B:414:LEU:HB3	1.85	0.58
6:A:6744:TAM:H32	1:B:237:LYS:HB2	1.85	0.58
1:A:72:MET:SD	1:A:300:LEU:HB2	2.43	0.58
1:B:306:GLN:NE2	1:B:306:GLN:H	2.02	0.58
1:A:100:ARG:HD3	1:A:104:GLY:O	2.04	0.57
1:A:379:ASN:HD22	1:A:380:PRO:CA	2.17	0.57
1:A:236:TRP:H	6:A:6744:TAM:C5	2.10	0.57
1:A:385:THR:HG23	9:A:3471:HOH:O	2.05	0.56
1:B:137:VAL:HG12	1:B:171:GLY:HA2	1.86	0.56
1:B:236:TRP:NE1	1:B:240:LYS:HD2	2.20	0.56
1:A:233:ASP:HB2	1:A:238:SER:HB2	1.86	0.56
1:A:212:GLN:HB3	9:A:3474:HOH:O	2.06	0.56
1:B:209:TRP:CE3	1:B:210:PRO:HG3	2.37	0.56
1:A:272:ASN:HD21	1:A:298:ASN:HA	1.71	0.56
1:B:82:LYS:HB2	1:B:129:LEU:HD21	1.87	0.55
1:B:284:MET:HG2	1:B:310:LEU:HD22	1.89	0.55
1:A:403:LEU:HD21	1:A:415:LEU:HD13	1.89	0.55
1:A:324:LEU:HD13	1:A:326:LYS:HG3	1.89	0.54
3:F:1:NAG:H61	3:F:2:NAG:H82	1.89	0.54
1:A:204:TRP:HB3	1:A:205:PRO:HD3	1.89	0.54
1:A:421:MET:HA	9:A:3415:HOH:O	2.07	0.54
1:A:388:LEU:HB2	1:A:414:LEU:HB3	1.90	0.53
1:B:136:ASP:CB	1:B:141:THR:HA	2.39	0.53
1:B:228:ASN:HB3	1:B:245:TRP:CH2	2.42	0.53
1:B:381:ALA:HB3	1:B:422:GLN:HB3	1.90	0.52
1:A:72:MET:O	1:A:76:MET:HG3	2.08	0.52
1:B:243:LEU:O	1:B:247:SER:HB2	2.09	0.51
1:A:214:PRO:HG2	1:A:216:TYR:CE2	2.46	0.51
1:A:74:GLU:OE2	1:A:123:TYR:OH	2.29	0.51
1:B:66:GLU:OE1	1:B:115:HIS:CD2	2.60	0.50
1:B:341:GLU:HA	1:B:350:ALA:O	2.11	0.50
1:A:210:PRO:HD2	1:A:211:PHE:CD2	2.47	0.49
1:B:250:GLN:O	1:B:254:VAL:HG13	2.12	0.49
1:A:117:ILE:HG21	1:A:133:ILE:HD12	1.95	0.49
1:B:224:ASN:O	1:B:261:GLY:HA2	2.13	0.49
1:A:237:LYS:N	6:A:6744:TAM:HN2	2.05	0.49
1:B:404:ARG:HH21	1:B:406:HIS:HE1	1.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:MET:HA	1:B:81:TRP:HB2	1.94	0.49
1:B:108:ALA:HB1	1:B:113:PHE:HB2	1.95	0.48
1:B:378:CYS:HA	1:B:381:ALA:C	2.34	0.48
7:A:498:NAG:C4	7:A:430:NAG:C1	2.92	0.48
1:B:203:GLU:OE2	5:B:3681:GLA:H2	2.14	0.48
1:A:208:MET:HE1	1:A:212:GLN:HG3	1.94	0.48
1:B:136:ASP:HB2	1:B:141:THR:HA	1.96	0.48
9:A:3405:HOH:O	1:B:58:GLU:HG3	2.14	0.48
1:B:203:GLU:HA	1:B:227:ARG:HB2	1.96	0.48
1:B:404:ARG:HH21	1:B:406:HIS:CE1	2.32	0.48
1:A:108:ALA:HB2	1:A:117:ILE:HG12	1.95	0.48
1:A:378:CYS:HA	1:A:382:CYS:HB3	1.96	0.47
1:A:315:ASP:OD2	1:A:391:LYS:HE2	2.13	0.47
1:A:359:ILE:HD12	1:B:233:ASP:HB3	1.96	0.47
1:B:210:PRO:N	9:B:6761:HOH:O	2.46	0.47
1:B:403:LEU:HD21	1:B:415:LEU:HD11	1.97	0.47
1:A:77:VAL:HG21	1:A:127:LYS:HB3	1.95	0.47
1:B:65:SER:HB2	1:B:67:LYS:HZ2	1.75	0.47
1:B:218:GLU:O	1:B:222:TYR:HD2	1.98	0.47
1:A:73:ALA:HB2	1:A:89:LEU:HD22	1.96	0.46
1:A:137:VAL:HG12	1:A:171:GLY:HA2	1.98	0.46
1:A:284:MET:HG2	1:A:310:LEU:HD22	1.98	0.46
6:A:6744:TAM:H21	6:A:6744:TAM:H62	1.70	0.46
1:B:46:HIS:HD2	1:B:92:ASP:H	1.61	0.46
1:A:379:ASN:ND2	1:A:380:PRO:HA	2.26	0.45
1:B:220:ARG:NH2	1:B:259:PRO:O	2.49	0.45
1:A:67:LYS:HE3	1:A:67:LYS:HA	1.98	0.45
1:B:145:PHE:HB3	1:B:146:PRO:CD	2.46	0.45
1:B:178:GLU:H	1:B:178:GLU:HG2	1.49	0.45
1:A:95:TRP:CE2	1:A:96:MET:HG3	2.52	0.45
1:B:298:ASN:OD1	1:B:300:LEU:HD13	2.17	0.45
1:B:45:LEU:CD2	1:B:92:ASP:HB2	2.45	0.45
1:B:213:LYS:HD3	1:B:252:ARG:CZ	2.47	0.44
1:B:175:ASP:N	3:E:1:NAG:O7	2.50	0.44
1:B:202:CYS:O	1:B:226:TRP:HA	2.17	0.44
1:B:170:ASP:OD2	5:B:3681:GLA:C1	2.57	0.44
1:B:190:ALA:O	1:B:194:THR:HG23	2.18	0.44
1:B:258:GLY:HA2	1:B:325:GLY:O	2.17	0.44
1:B:250:GLN:HB2	1:B:254:VAL:CG1	2.48	0.44
1:A:215:ASN:HD22	3:D:1:NAG:C1	2.17	0.44
1:B:100:ARG:NH2	1:B:147:GLY:O	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:GLY:HA3	1:A:88:TYR:O	2.17	0.43
1:B:97:ALA:HB3	1:B:107:GLN:HG3	2.01	0.43
1:A:201:SER:HB2	1:A:225:HIS:CE1	2.54	0.43
1:B:100:ARG:HD2	1:B:104:GLY:O	2.18	0.43
1:B:369:VAL:HB	1:B:401:SER:O	2.17	0.43
1:A:76:MET:HA	1:A:81:TRP:HB2	2.00	0.43
1:B:386:GLN:HA	1:B:415:LEU:HD23	2.01	0.43
1:B:326:LYS:HB2	1:B:343:PRO:HG2	2.01	0.42
1:B:382:CYS:HA	1:B:418:GLU:O	2.19	0.42
1:B:177:LEU:H	1:B:177:LEU:CD1	2.30	0.42
1:B:91:ILE:HG22	1:B:92:ASP:O	2.19	0.42
1:A:355:ASN:HB3	1:A:408:ASN:O	2.20	0.42
1:A:33:ASP:O	2:C:1:NAG:H4	2.19	0.42
1:A:252:ARG:NH2	9:A:6748:HOH:O	2.51	0.41
1:B:73:ALA:HB2	1:B:89:LEU:HD22	2.02	0.41
1:B:125:HIS:CE1	1:B:165:ASP:OD2	2.58	0.41
6:A:6744:TAM:H61	1:B:235:SER:HB2	2.01	0.41
1:A:366:THR:HG22	1:A:404:ARG:HG3	2.01	0.41
1:A:258:GLY:HA2	1:A:325:GLY:O	2.21	0.41
1:A:134:TYR:CD2	1:A:134:TYR:C	2.94	0.41
1:B:93:ASP:HB2	5:B:3681:GLA:C6	2.51	0.41
1:A:177:LEU:HD11	1:A:211:PHE:HB3	2.03	0.41
1:A:378:CYS:HA	1:A:381:ALA:C	2.41	0.40
1:B:145:PHE:HB3	1:B:146:PRO:HD2	2.04	0.40
1:B:203:GLU:O	1:B:206:LEU:HB3	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	388/398 (98%)	370 (95%)	17 (4%)	1 (0%)	41 46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	389/398 (98%)	369 (95%)	18 (5%)	2 (0%)	29 31
All	All	777/796 (98%)	739 (95%)	35 (4%)	3 (0%)	34 37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	266	ASP
1	B	210	PRO
1	B	266	ASP

5.3.2 Protein sidechains

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	331/339 (98%)	306 (92%)	25 (8%)	13 14
1	B	332/339 (98%)	302 (91%)	30 (9%)	9 9
All	All	663/678 (98%)	608 (92%)	55 (8%)	11 11

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	A	62	SER
1	A	67	LYS
1	A	75	LEU
1	A	99	GLN
1	A	178	GLU
1	A	221	GLN
1	A	286	LEU
1	A	300	LEU
1	A	310	LEU
1	A	314	LYS
1	A	324	LEU
1	A	332	ARG

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Mol	Chain	Res	Type
1	A	363	ARG
1	A	366	THR
1	A	372	LEU
1	A	376	VAL
1	A	379	ASN
1	A	385	THR
1	A	387	LEU
1	A	388	LEU
1	A	391	LYS
1	A	402	ARG
1	A	405	SER
1	A	421	MET
1	B	45	LEU
1	B	58	GLU
1	B	67	LYS
1	B	75	LEU
1	B	82	LYS
1	B	96	MET
1	B	118	ARG
1	B	177	LEU
1	B	178	GLU
1	B	193	ARG
1	B	241	SER
1	B	251	GLU
1	B	254	VAL
1	B	281	VAL
1	B	286	LEU
1	B	287	TRP
1	B	300	LEU
1	B	306	GLN
1	B	310	LEU
1	B	324	LEU
1	B	326	LYS
1	B	332	ARG
1	B	345	SER
1	B	372	LEU
1	B	385	THR
1	B	387	LEU
1	B	388	LEU
1	B	391	LYS
1	B	420	THR
1	B	421	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	HIS
1	A	115	HIS
1	A	122	ASN
1	A	125	HIS
1	A	179	ASN
1	A	212	GLN
1	A	272	ASN
1	A	379	ASN
1	A	406	HIS
1	A	416	GLN
1	B	46	HIS
1	B	115	HIS
1	B	125	HIS
1	B	306	GLN
1	B	406	HIS

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

11 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	C	1	1,2	14,14,15	0.51	0	17,19,21	2.07	3 (17%)
2	NAG	C	2	2	14,14,15	0.79	0	17,19,21	1.87	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MAN	C	3	2	11,11,12	0.89	0	15,15,17	1.35	1 (6%)
3	NAG	D	1	3	14,14,15	0.51	0	17,19,21	2.31	4 (23%)
3	NAG	D	2	3	14,14,15	0.81	0	17,19,21	1.33	2 (11%)
3	NAG	E	1	1,3	14,14,15	0.56	0	17,19,21	2.39	3 (17%)
3	NAG	E	2	3	14,14,15	0.92	1 (7%)	17,19,21	1.35	3 (17%)
3	NAG	F	1	1,3	14,14,15	0.66	0	17,19,21	1.40	3 (17%)
3	NAG	F	2	3	14,14,15	0.74	0	17,19,21	1.74	3 (17%)
3	NAG	G	1	1,3	14,14,15	0.41	0	17,19,21	1.72	5 (29%)
3	NAG	G	2	3	14,14,15	0.69	0	17,19,21	1.02	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	C	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	MAN	C	3	2	1/1/4/5	2/2/19/22	0/1/1/1
3	NAG	D	1	3	-	5/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	1/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	3/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2	NAG	C1-C2	2.86	1.56	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	1	NAG	C1-O5-C5	8.07	123.13	112.19
3	D	1	NAG	C2-N2-C7	6.61	132.31	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1	NAG	C1-O5-C5	6.23	120.64	112.19
3	F	2	NAG	C1-O5-C5	5.09	119.08	112.19
2	C	2	NAG	C1-O5-C5	4.52	118.31	112.19
3	D	1	NAG	C1-O5-C5	4.50	118.30	112.19
3	D	2	NAG	C4-C3-C2	3.98	116.85	111.02
2	C	3	MAN	C1-C2-C3	3.53	114.01	109.67
3	G	1	NAG	C2-N2-C7	-3.51	117.91	122.90
2	C	1	NAG	O5-C5-C6	3.17	112.17	107.20
3	F	2	NAG	O5-C5-C6	-3.14	102.29	107.20
3	D	1	NAG	O5-C1-C2	3.07	116.14	111.29
3	E	2	NAG	O5-C1-C2	3.00	116.03	111.29
2	C	2	NAG	C1-C2-N2	2.78	115.23	110.49
2	C	2	NAG	O4-C4-C5	2.77	116.17	109.30
3	F	2	NAG	C2-N2-C7	-2.68	119.08	122.90
3	G	1	NAG	O5-C5-C6	2.63	111.33	107.20
3	D	2	NAG	C3-C4-C5	2.53	114.76	110.24
3	G	1	NAG	O5-C1-C2	-2.53	107.30	111.29
3	G	1	NAG	C3-C4-C5	-2.44	105.88	110.24
2	C	1	NAG	C4-C3-C2	2.43	114.58	111.02
3	F	1	NAG	O5-C1-C2	-2.30	107.66	111.29
3	E	1	NAG	C2-N2-C7	2.26	126.13	122.90
3	E	1	NAG	O5-C5-C4	2.25	116.31	110.83
3	F	1	NAG	C1-O5-C5	2.24	115.23	112.19
3	D	1	NAG	C8-C7-N2	2.20	119.82	116.10
3	E	2	NAG	O4-C4-C5	2.12	114.57	109.30
3	E	2	NAG	O5-C5-C4	-2.09	105.75	110.83
2	C	2	NAG	O7-C7-C8	-2.06	118.23	122.06
2	C	2	NAG	O7-C7-N2	2.05	125.72	121.95
3	F	1	NAG	O4-C4-C3	-2.02	105.68	110.35
3	G	1	NAG	C1-O5-C5	2.01	114.92	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	3	MAN	C1

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1	NAG	C1-C2-N2-C7
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	C	1	NAG	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	F	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O5-C5-C6-O6
2	C	3	MAN	O5-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
3	F	2	NAG	O7-C7-N2-C2
3	F	1	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
2	C	3	MAN	C4-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	D	2	NAG	C8-C7-N2-C2
3	D	2	NAG	O7-C7-N2-C2
3	E	2	NAG	C4-C5-C6-O6

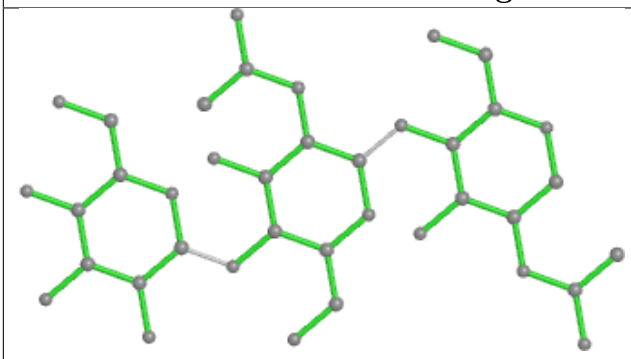
There are no ring outliers.

6 monomers are involved in 7 short contacts:

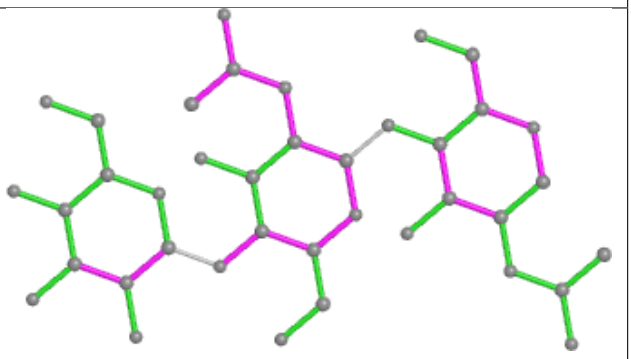
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1	NAG	1	0
3	D	1	NAG	3	0
3	F	2	NAG	1	0
2	C	1	NAG	1	0
3	G	2	NAG	1	0
3	E	1	NAG	1	0

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

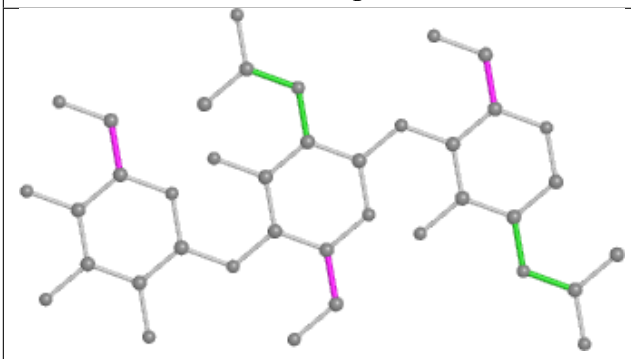
Oligosaccharide Chain C



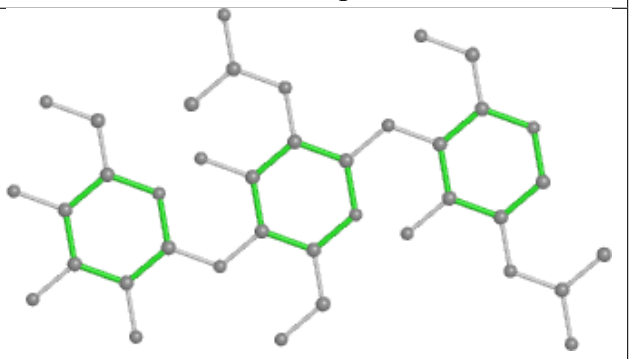
Bond lengths



Bond angles

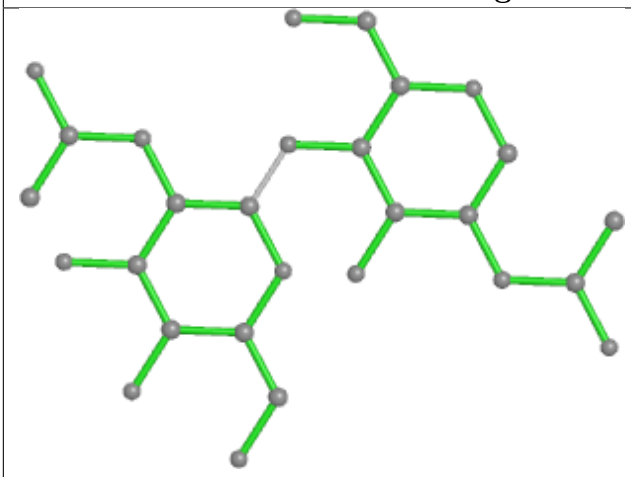


Torsions

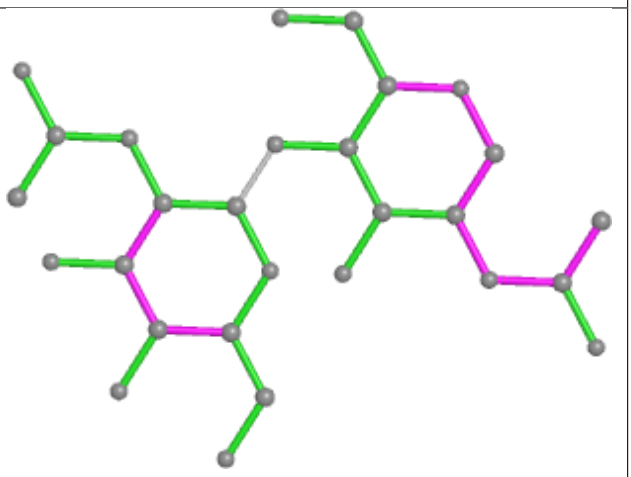


Rings

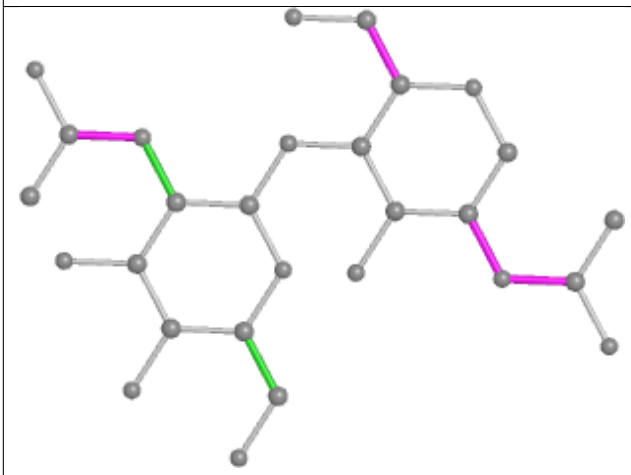
Oligosaccharide Chain D



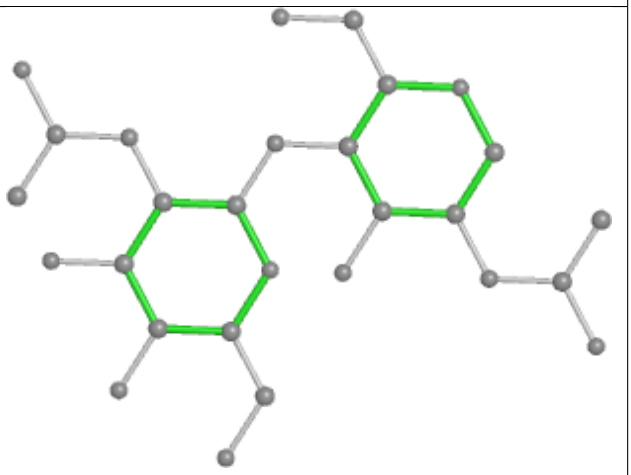
Bond lengths



Bond angles

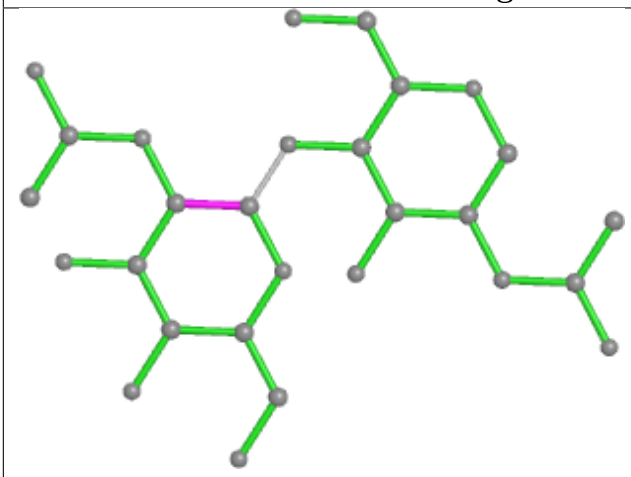


Torsions

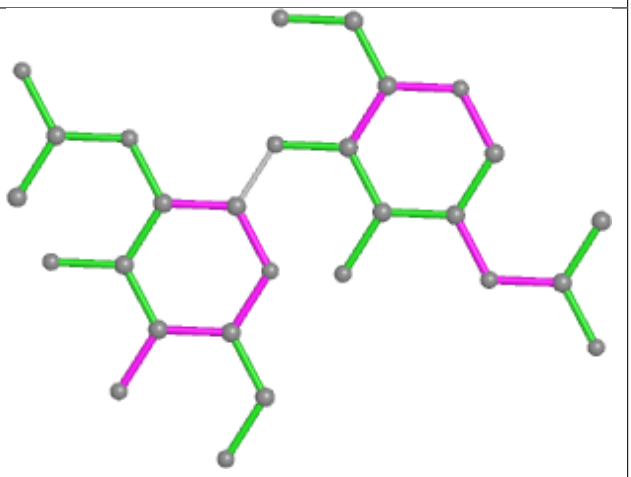


Rings

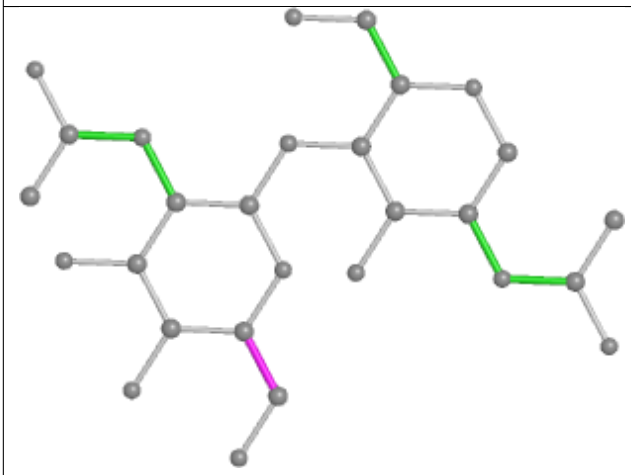
Oligosaccharide Chain E



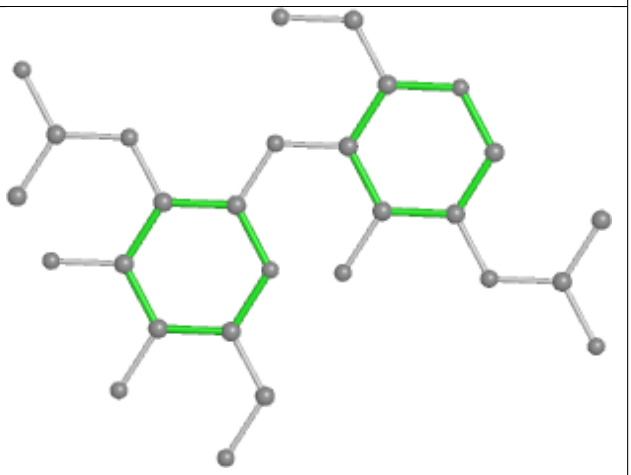
Bond lengths



Bond angles

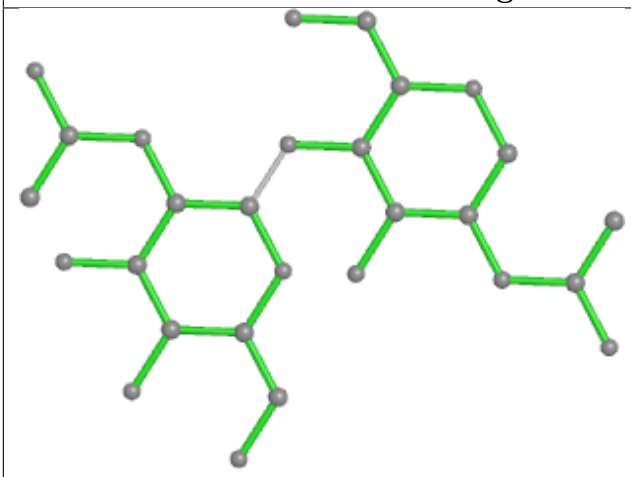


Torsions

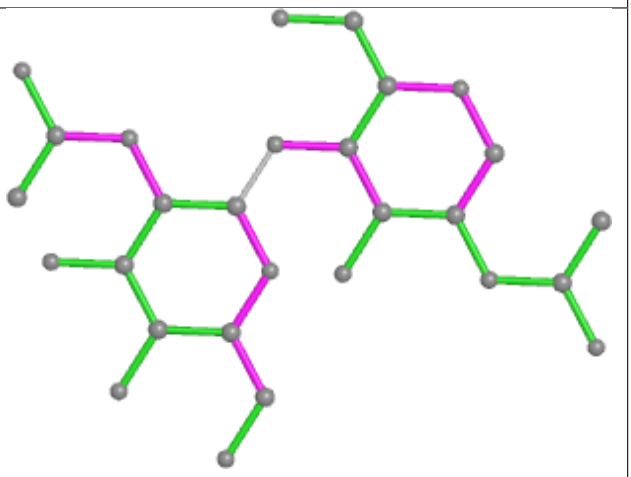


Rings

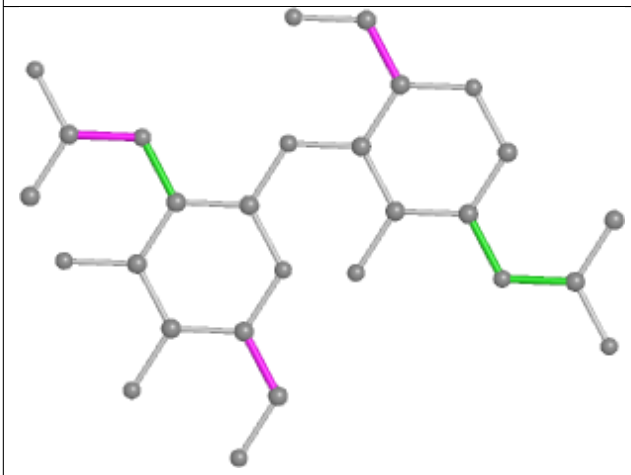
Oligosaccharide Chain F



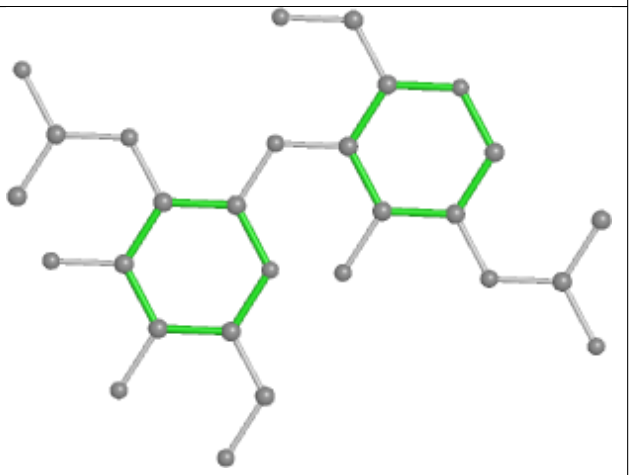
Bond lengths



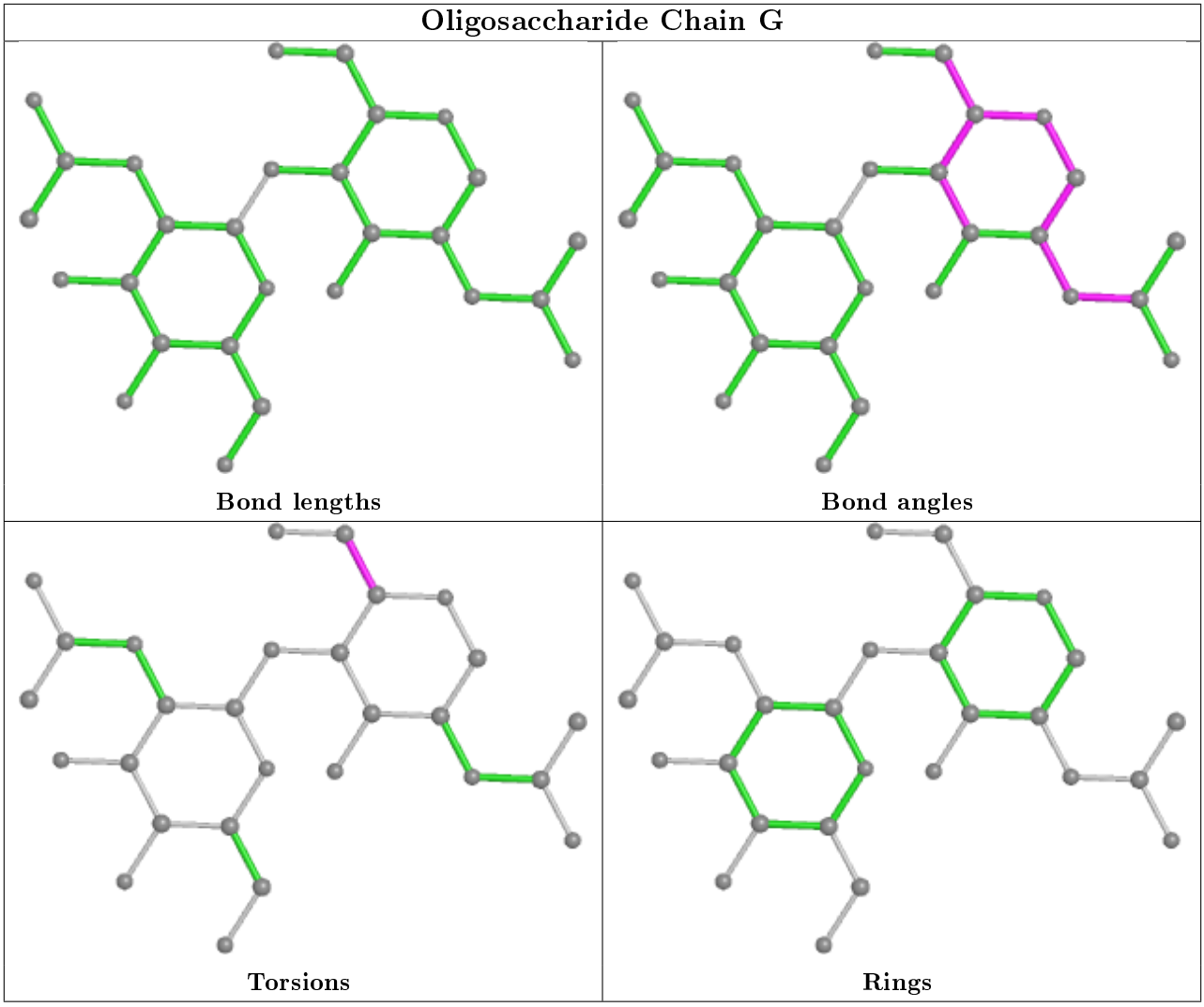
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

11 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SO4	B	4	-	4,4,4	0.16	0	6,6,6	0.36	0
8	MAN	B	695	-	11,11,12	0.79	1 (9%)	15,15,17	1.75	6 (40%)
7	NAG	A	430	-	14,14,15	0.59	0	17,19,21	1.67	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	GLA	B	3681	-	12,12,12	0.78	0	17,17,17	1.86	4 (23%)
5	GLA	A	3681	-	12,12,12	1.39	1 (8%)	17,17,17	1.98	7 (41%)
4	SO4	B	3	-	4,4,4	0.27	0	6,6,6	0.56	0
4	SO4	B	2	-	4,4,4	0.08	0	6,6,6	0.70	0
7	NAG	A	498	1	14,14,15	1.02	1 (7%)	17,19,21	1.76	5 (29%)
4	SO4	A	1	-	4,4,4	0.21	0	6,6,6	1.08	0
6	TAM	A	6744	-	7,10,10	1.97	2 (28%)	9,12,12	3.41	3 (33%)
8	MAN	B	694	-	11,11,12	0.67	0	15,15,17	1.88	3 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	430	-	-	4/6/23/26	0/1/1/1
8	MAN	B	695	-	-	2/2/19/22	0/1/1/1
5	GLA	B	3681	-	-	0/2/22/22	0/1/1/1
5	GLA	A	3681	-	-	0/2/22/22	0/1/1/1
7	NAG	A	498	1	-	1/6/23/26	0/1/1/1
6	TAM	A	6744	-	-	6/12/12/12	-
8	MAN	B	694	-	-	1/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	6744	TAM	C-N	-3.86	1.36	1.49
5	A	3681	GLA	O5-C5	-3.83	1.35	1.44
6	A	6744	TAM	C1-C4	2.71	1.57	1.52
8	B	695	MAN	C2-C3	2.17	1.55	1.52
7	A	498	NAG	C1-C2	2.03	1.55	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	6744	TAM	C2-C-C1	7.07	122.97	110.50
6	A	6744	TAM	C2-C-N	-5.58	92.19	108.09
8	B	694	MAN	C1-C2-C3	5.49	116.41	109.67
5	B	3681	GLA	O5-C1-C2	4.42	118.18	110.28
7	A	498	NAG	C3-C4-C5	4.20	117.73	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	6744	TAM	O6-C6-C3	-4.19	100.19	111.39
5	B	3681	GLA	C1-O5-C5	3.93	121.08	113.66
5	A	3681	GLA	O2-C2-C3	3.52	118.49	110.35
5	A	3681	GLA	O1-C1-C2	3.36	118.49	109.03
8	B	694	MAN	O5-C5-C6	2.97	111.86	107.20
7	A	498	NAG	O4-C4-C3	-2.91	103.61	110.35
5	B	3681	GLA	O1-C1-O5	-2.88	101.72	110.38
5	A	3681	GLA	C4-C3-C2	-2.86	105.83	110.82
7	A	430	NAG	O5-C1-C2	2.83	115.75	111.29
7	A	430	NAG	O5-C5-C6	2.79	111.58	107.20
8	B	695	MAN	C1-C2-C3	2.79	113.10	109.67
8	B	694	MAN	C2-C3-C4	2.73	115.62	110.89
7	A	498	NAG	O5-C5-C6	2.72	111.46	107.20
5	A	3681	GLA	C1-O5-C5	2.72	118.79	113.66
7	A	430	NAG	C1-C2-N2	-2.71	105.87	110.49
8	B	695	MAN	O5-C5-C6	2.60	111.27	107.20
7	A	430	NAG	C1-O5-C5	2.52	115.60	112.19
8	B	695	MAN	O3-C3-C2	2.49	114.76	109.99
8	B	695	MAN	O5-C5-C4	-2.46	104.84	110.83
5	A	3681	GLA	O1-C1-O5	-2.46	103.00	110.38
7	A	498	NAG	C1-C2-N2	2.42	114.63	110.49
5	A	3681	GLA	O3-C3-C2	2.41	115.92	110.35
5	A	3681	GLA	O5-C5-C6	-2.30	100.72	106.44
7	A	430	NAG	O5-C5-C4	-2.26	105.34	110.83
8	B	695	MAN	O5-C1-C2	2.16	114.11	110.77
5	B	3681	GLA	C4-C3-C2	-2.08	107.20	110.82
8	B	695	MAN	C3-C4-C5	-2.07	106.54	110.24
7	A	498	NAG	C2-N2-C7	-2.01	120.04	122.90

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	6744	TAM	C2-C-C1-C4
6	A	6744	TAM	C3-C-C1-C4
6	A	6744	TAM	N-C-C1-C4
6	A	6744	TAM	C2-C-C3-C6
6	A	6744	TAM	N-C-C3-C6
7	A	430	NAG	O5-C5-C6-O6
8	B	695	MAN	O5-C5-C6-O6
7	A	430	NAG	C4-C5-C6-O6
7	A	430	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
7	A	430	NAG	O7-C7-N2-C2
8	B	695	MAN	C4-C5-C6-O6
8	B	694	MAN	O5-C5-C6-O6
7	A	498	NAG	C4-C5-C6-O6
6	A	6744	TAM	C1-C-C3-C6

There are no ring outliers.

4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	430	NAG	2	0
5	B	3681	GLA	4	0
7	A	498	NAG	2	0
6	A	6744	TAM	11	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

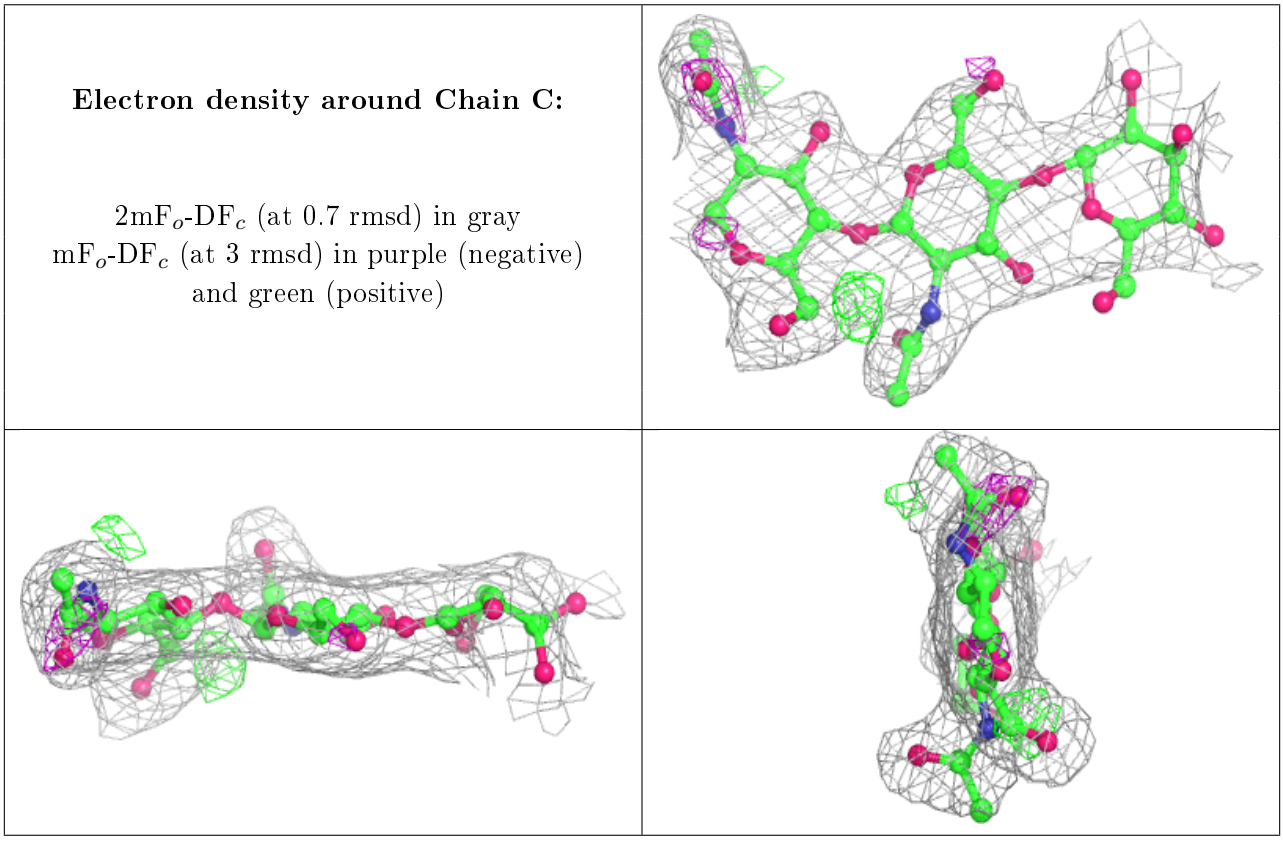
6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

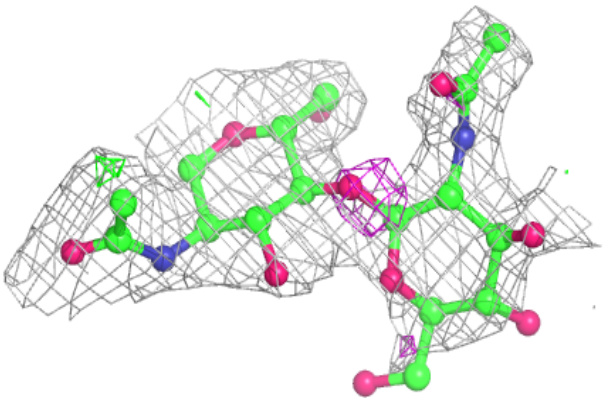
Unable to reproduce the depositors R factor - this section is therefore empty.

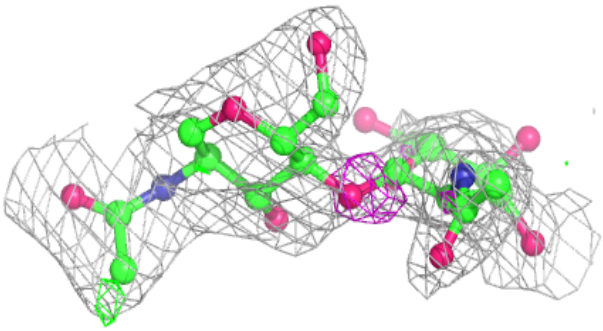
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

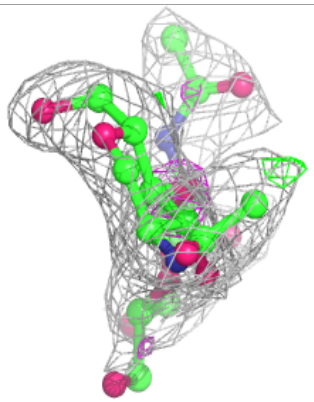


Electron density around Chain D:

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

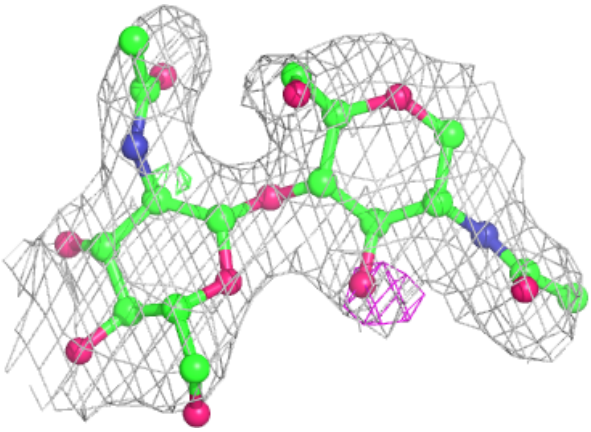


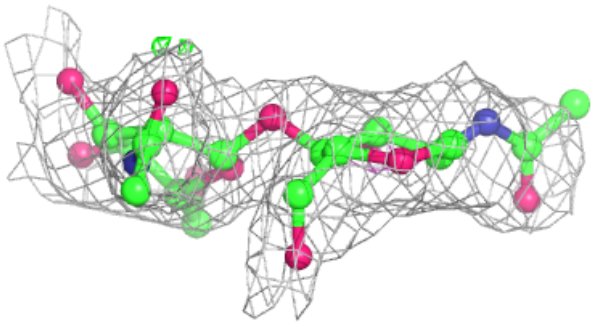


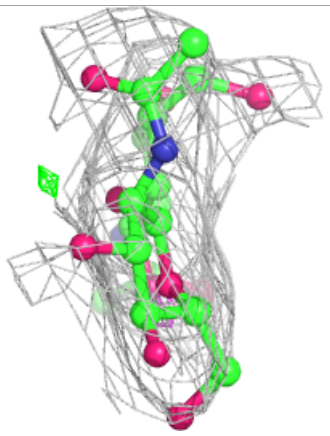


Electron density around Chain E:

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

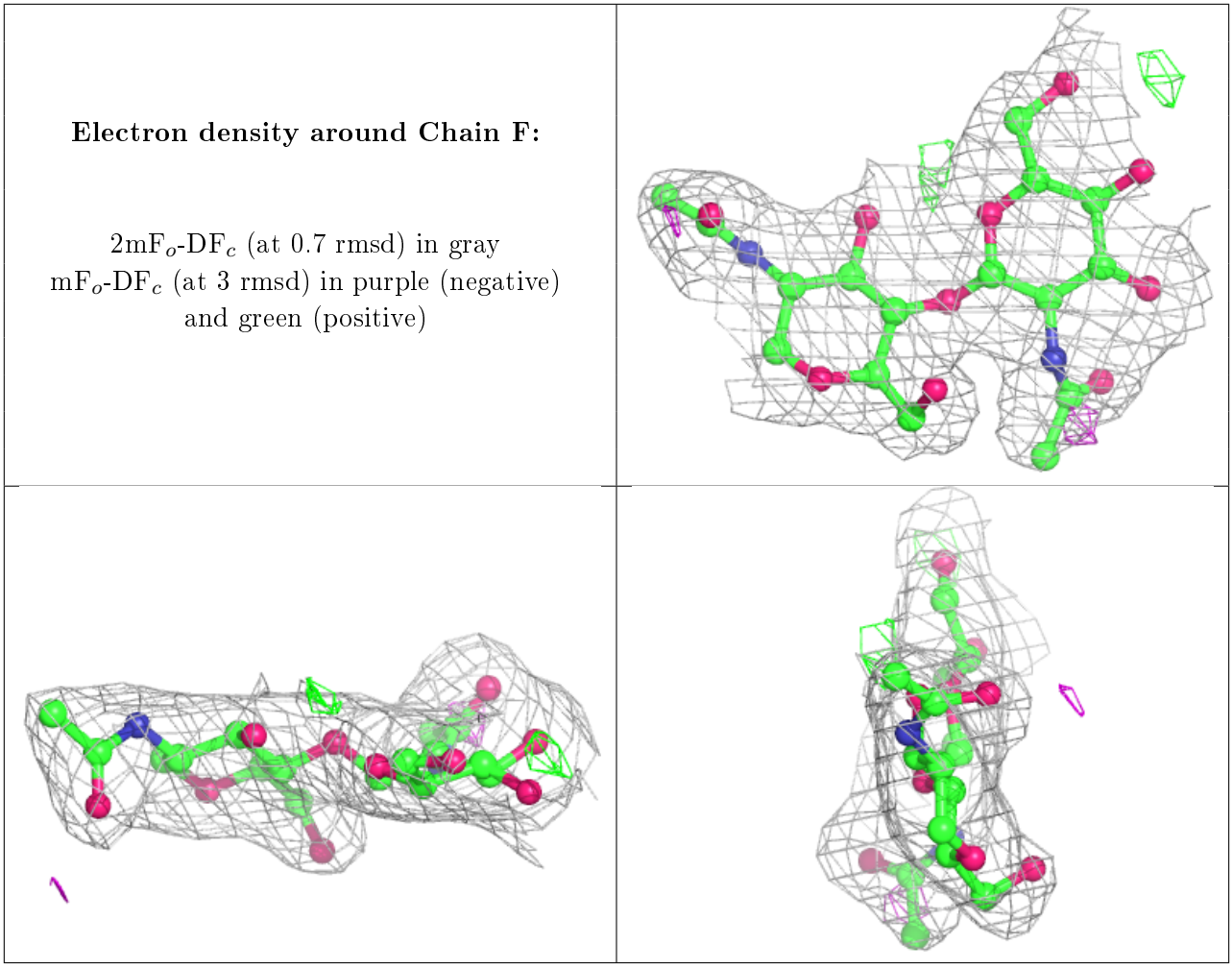






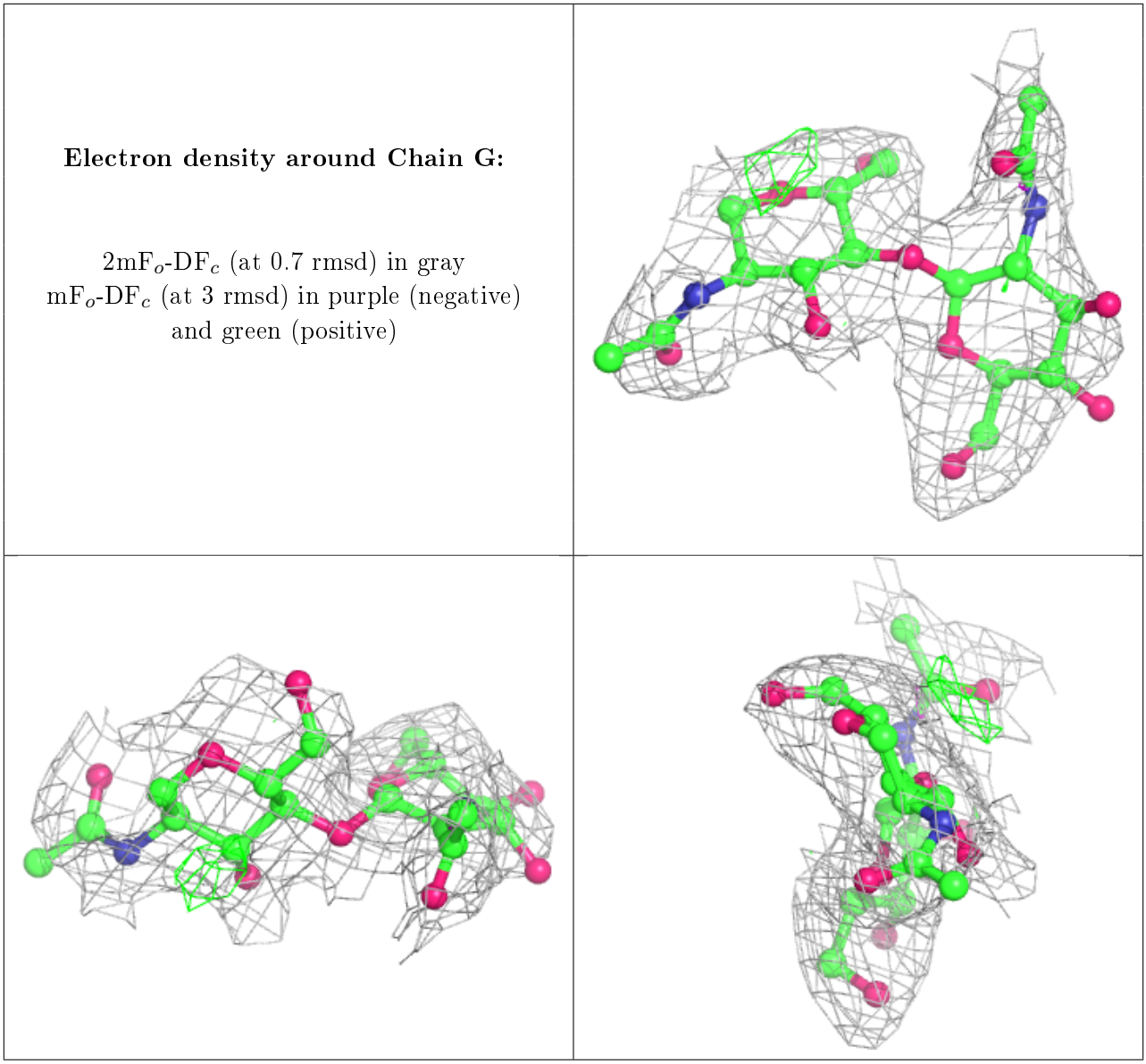
Electron density around Chain F:

$2mF_o$-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 G:

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



6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.