Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 11:25 PM BST

PDB ID	:	5A7M
Title	:	The structure of Hypocrea jecorina beta-xylosidase Xyl3A (Bxl1)
Authors	:	Mikkelsen, N.E.; Gudmundsson, M.; Karkehabadi, S.; Hansson, H.; Sandgren, M.; Larenas, E.; Mitchinson, C.; Keleman, B.; Kaper, T.
Deposited on	:	2015-07-08
Resolution	:	1.80 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:

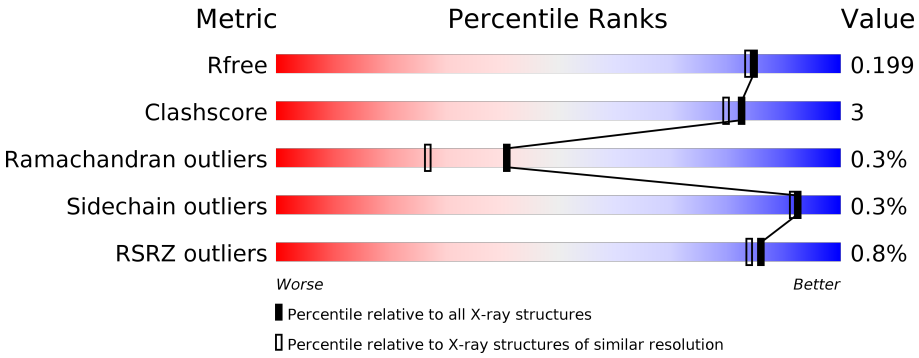
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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% 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	766	% 94% 5%
1	B	766	% 96%
2	C	7	29% 71%
3	D	2	100%
3	F	2	100%
3	J	2	50% 50%

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Mol	Chain	Length	Quality of chain
3	K	2	100%
4	E	5	40% 60%
4	I	5	40% 60%
5	G	3	100%
6	H	4	75% 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
8	ZN	B	1906[A]	-	-	X	-

2 Entry composition

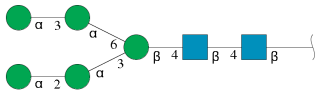
There are 12 unique types of molecules in this entry. The entry contains 14532 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BETA-XYLOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	761	Total	C	N	O	S	0	18	0
			5988	3821	999	1155	13			
1	B	766	Total	C	N	O	S	0	21	0
			6055	3859	1017	1167	12			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	7	Total	C	N	O	0	0	0
			83	46	2	35			

- 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	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

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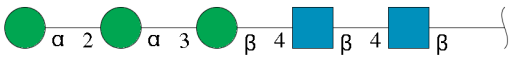
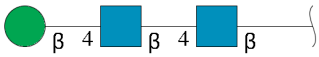
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	5	Total	C	N	O	0	0	0
			61	34	2	25			
4	I	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



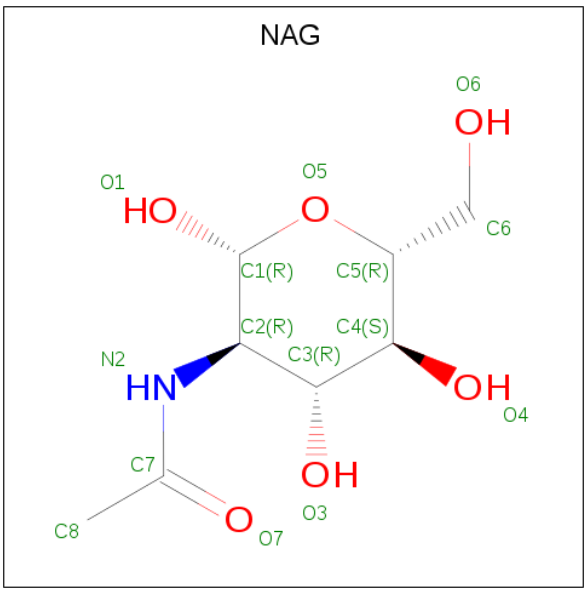
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	3	Total	C	N	O	0	0	0
			39	22	2	15			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	H	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:

$C_8H_{15}NO_6$).



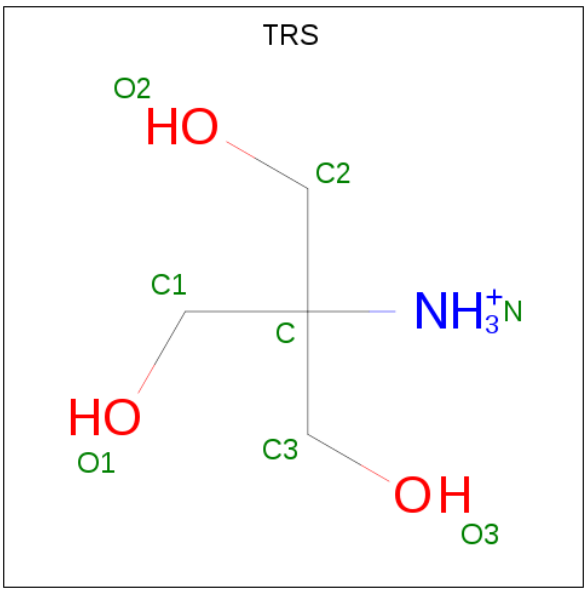
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C N O 14 8 1 5	0	0
7	A	1	Total C N O 14 8 1 5	0	0
7	A	1	Total C N O 14 8 1 5	0	0
7	A	1	Total C N O 14 8 1 5	0	0
7	A	1	Total C N O 14 8 1 5	0	0
7	B	1	Total C N O 14 8 1 5	0	0
7	B	1	Total C N O 14 8 1 5	0	0
7	B	1	Total C N O 14 8 1 5	0	0

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	11	Total Zn 11 11	0	2
8	A	10	Total Zn 11 11	0	2

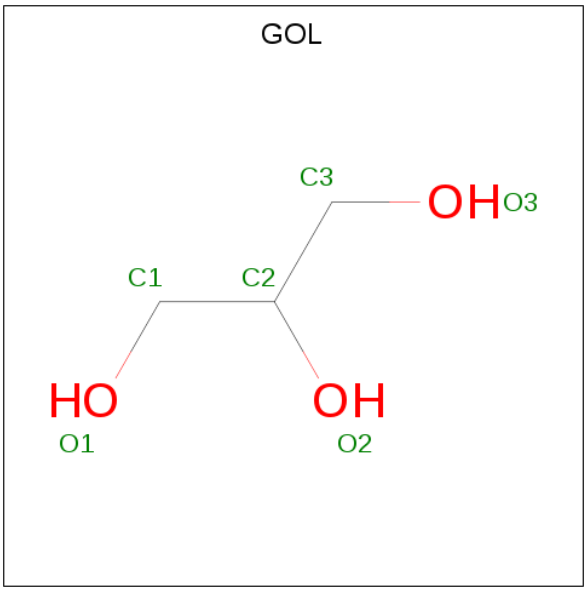
- Molecule 9 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code:

TRS) (formula: $C_4H_{12}NO_3$).



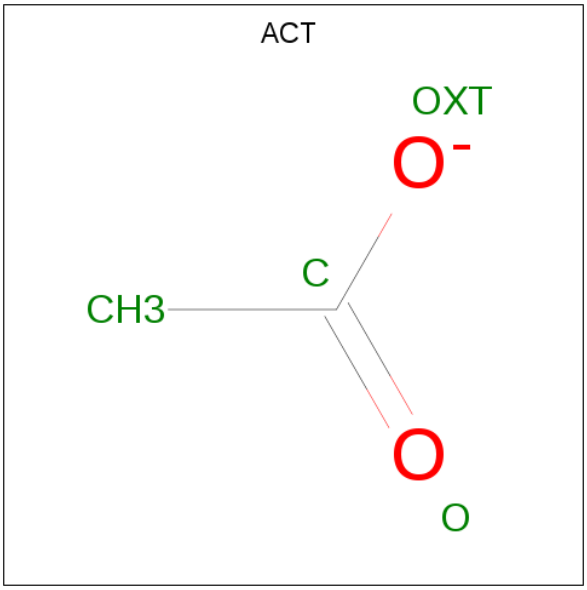
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C N O 8 4 1 3	0	0
9	A	1	Total C N O 8 4 1 3	0	0
9	B	1	Total C N O 8 4 1 3	0	0

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C O 6 3 3	0	0
10	B	1	Total C O 6 3 3	0	0
10	B	1	Total C O 6 3 3	0	0

- Molecule 11 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 12 is water.

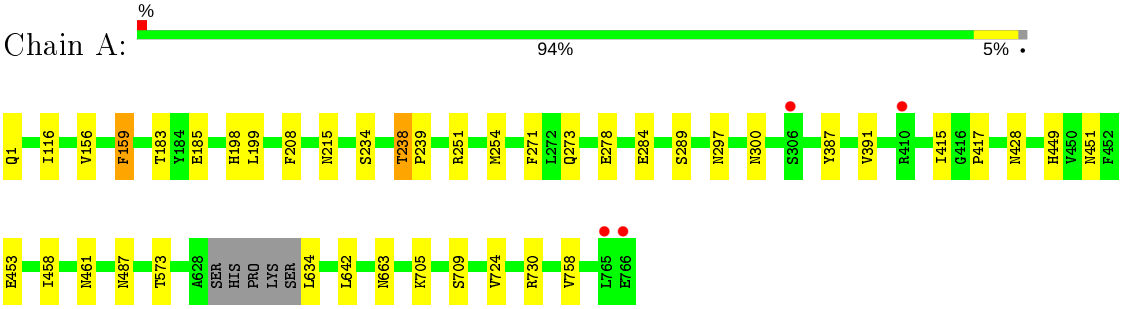
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	956	Total O 958 958	0	11
12	B	941	Total O 941 941	0	5

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.

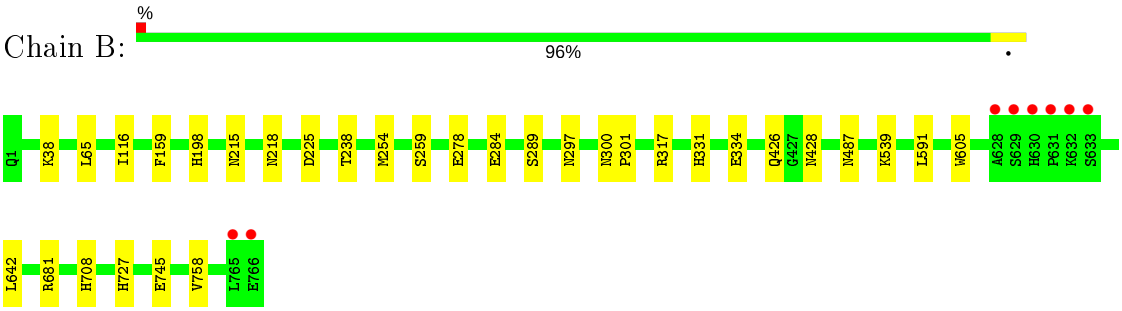
• Molecule 1: BETA-XYLOSIDASE

Chain A:



• Molecule 1: BETA-XYLOSIDASE

Chain B:

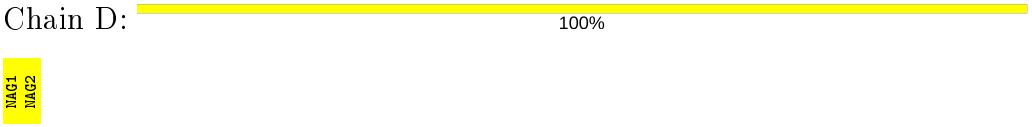


• Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

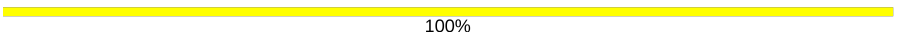
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



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

Chain F:

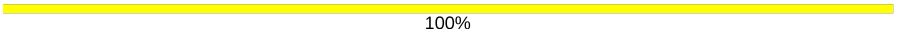


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

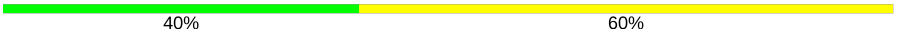
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



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

Chain E:



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

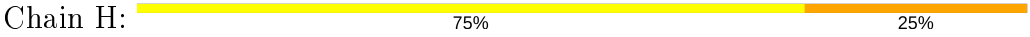
Chain I:

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

Chain G:

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

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	99.91Å 203.72Å 82.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	204.12 – 1.80 26.57 – 1.80	Depositor EDS
% Data completeness (in resolution range)	94.5 (204.12-1.80) 94.5 (26.57-1.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.02 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.161 , 0.199 0.161 , 0.199	Depositor DCC
R_{free} test set	7364 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	14.1	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 50.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14532	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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: GOL, ZN, BMA, NAG, ACT, TRS, PCA, MAN

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	0.53	0/6192	0.65	0/8437
1	B	0.55	0/6260	0.66	0/8529
All	All	0.54	0/12452	0.65	0/16966

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	5988	0	5809	27	0
1	B	6055	0	5865	33	0
2	C	83	0	70	0	0
3	D	28	0	25	0	0
3	F	28	0	25	0	0
3	J	28	0	25	1	0
3	K	28	0	25	0	0
4	E	61	0	52	0	0
4	I	61	0	52	0	0
5	G	39	0	34	0	0
6	H	50	0	43	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	70	0	65	0	0
7	B	42	0	39	1	0
8	A	11	0	0	0	0
8	B	11	0	0	2	0
9	A	16	0	24	1	0
9	B	8	0	12	0	0
10	A	6	0	8	0	0
10	B	12	0	16	1	0
11	A	4	0	3	0	0
11	B	4	0	3	0	0
12	A	958	0	0	11	0
12	B	941	0	0	23	0
All	All	14532	0	12195	63	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 3.

All (63) 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:B:331[B]:HIS:CE1	12:B:2496[B]:HOH:O	1.89	1.23
8:B:1906[A]:ZN:ZN	12:B:2362:HOH:O	1.24	0.85
1:A:449:HIS:NE2	12:A:2626:HOH:O	2.13	0.81
1:B:198[B]:HIS:HE1	12:B:2368:HOH:O	1.64	0.79
1:A:705:LYS:NZ	12:A:2837:HOH:O	2.26	0.67
1:B:198[A]:HIS:CE1	12:B:2370:HOH:O	2.49	0.65
1:B:198[B]:HIS:HE1	12:B:2369:HOH:O	1.78	0.65
1:B:331[B]:HIS:NE2	12:B:2496[B]:HOH:O	2.12	0.64
1:A:273[B]:GLN:NE2	12:A:2460:HOH:O	1.71	0.64
8:B:1906[A]:ZN:ZN	12:B:2368:HOH:O	1.45	0.63
1:B:681:ARG:HH22	1:B:745:GLU:CD	2.05	0.60
1:B:334:GLU:OE2	12:B:2512:HOH:O	2.16	0.60
1:A:185:GLU:OE1	12:A:2241:HOH:O	2.17	0.60
1:B:331[B]:HIS:HE1	12:B:2496[B]:HOH:O	1.48	0.59
1:B:198[A]:HIS:HE1	12:B:2370:HOH:O	1.83	0.59
1:B:198[B]:HIS:CE1	12:B:2368:HOH:O	2.44	0.58
1:B:198[B]:HIS:CE1	12:B:2362:HOH:O	2.56	0.57
1:B:317:ARG:NH2	12:B:2504:HOH:O	2.30	0.57
7:B:1001:NAG:H83	12:B:2024:HOH:O	2.04	0.57
1:A:724:VAL:HG22	1:A:730[B]:ARG:HG2	1.89	0.55
1:A:284:GLU:CD	1:B:284:GLU:HB2	2.27	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1921:TRS:H12	12:A:2955:HOH:O	2.08	0.52
1:A:634:LEU:N	12:A:2790:HOH:O	2.43	0.50
1:A:451:ASN:ND2	12:A:2626:HOH:O	2.15	0.50
1:A:284:GLU:HB2	1:B:284:GLU:CD	2.32	0.50
1:B:38:LYS:HE3	12:B:2115:HOH:O	2.11	0.50
1:B:539:LYS:HE2	12:B:2678:HOH:O	2.12	0.50
1:A:387:TYR:CZ	1:A:391:VAL:HG21	2.48	0.49
1:A:663[A]:ASN:HD21	1:A:709:SER:HB3	1.78	0.48
1:A:461:ASN:HB3	12:A:2642:HOH:O	2.13	0.48
1:B:218:ASN:ND2	12:B:2396:HOH:O	2.46	0.48
1:A:428:ASN:HB3	1:A:487:ASN:ND2	2.28	0.48
1:A:297:ASN:HA	1:A:300:ASN:O	2.14	0.48
1:A:234:SER:O	1:A:730[B]:ARG:NH1	2.48	0.47
1:B:426:GLN:HA	12:B:2193:HOH:O	2.13	0.47
1:B:708:HIS:ND1	12:B:2864:HOH:O	2.27	0.47
1:B:591:LEU:HB3	1:B:605:TRP:CD1	2.49	0.47
1:A:208:PHE:CE2	1:A:271:PHE:HB3	2.49	0.46
1:A:417:PRO:HB2	1:A:458:ILE:HG12	1.96	0.46
1:A:642:LEU:HD12	1:A:758:VAL:HG11	1.97	0.45
1:B:254:MET:HA	1:B:289:SER:O	2.16	0.45
1:A:449:HIS:ND1	12:A:2625:HOH:O	2.13	0.44
1:A:198:HIS:NE2	12:A:2339:HOH:O	2.17	0.44
1:A:415:ILE:HA	1:A:453:GLU:O	2.17	0.44
1:B:727:HIS:CG	10:B:1923:GOL:H11	2.53	0.43
1:B:300:ASN:HA	1:B:301:PRO:HA	1.82	0.43
1:A:199:LEU:HD13	1:A:251:ARG:HG3	2.01	0.43
1:A:254:MET:HA	1:A:289:SER:O	2.19	0.43
1:B:642:LEU:HD12	1:B:758:VAL:HG11	1.99	0.43
1:B:681:ARG:NE	12:B:2829:HOH:O	2.51	0.42
1:B:428:ASN:HB3	1:B:487:ASN:ND2	2.34	0.42
12:A:2804:HOH:O	1:B:65:LEU:HD11	2.19	0.42
1:B:225:ASP:HA	1:B:259[B]:SER:OG	2.20	0.42
1:B:334:GLU:HG2	6:H:1:NAG:H82	2.01	0.42
1:B:297:ASN:HA	1:B:300:ASN:O	2.19	0.41
1:A:278[A]:GLU:OE2	1:B:278[A]:GLU:OE2	2.38	0.41
1:B:539:LYS:CE	12:B:2678:HOH:O	2.68	0.41
1:B:198[B]:HIS:CE1	12:B:2369:HOH:O	2.61	0.41
6:H:3:BMA:H3	6:H:4:MAN:C5	2.51	0.41
1:A:156:VAL:HG11	1:A:183:THR:OG1	2.21	0.41
1:A:238:THR:N	1:A:239:PRO:CD	2.84	0.41
1:A:159:PHE:CD2	1:A:573:THR:HG21	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:2925:HOH:O	3:J:1:NAG:H62	2.20	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	775/766 (101%)	750 (97%)	23 (3%)	2 (0%)	41	27
1	B	785/766 (102%)	759 (97%)	24 (3%)	2 (0%)	41	27
All	All	1560/1532 (102%)	1509 (97%)	47 (3%)	4 (0%)	41	27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	215	ASN
1	B	215	ASN
1	B	238	THR
1	A	238	THR

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	643/630 (102%)	641 (100%)	2 (0%)	92	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	650/630 (103%)	648 (100%)	2 (0%)	92 91
All	All	1293/1260 (103%)	1289 (100%)	4 (0%)	92 91

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	ILE
1	A	159	PHE
1	B	116	ILE
1	B	159	PHE

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

Mol	Chain	Res	Type
1	A	487	ASN
1	B	487	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	PCA	A	1	1	7,8,9	0.48	0	9,10,12	1.29	1 (11%)
1	PCA	B	1	1	7,8,9	0.69	0	9,10,12	1.15	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
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1
1	PCA	B	1	1	-	0/0/11/13	0/1/1/1

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	1	PCA	CB-CA-C	-2.28	109.57	112.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

32 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	0.47	0	17,19,21	1.28	1 (5%)
2	NAG	C	2	2	14,14,15	0.76	0	17,19,21	1.15	2 (11%)
2	BMA	C	3	2	11,11,12	0.32	0	15,15,17	0.83	0
2	MAN	C	4	2	11,11,12	0.60	0	15,15,17	1.08	1 (6%)
2	MAN	C	5	2	11,11,12	0.26	0	15,15,17	0.64	0
2	MAN	C	6	2	11,11,12	0.65	0	15,15,17	0.79	1 (6%)
2	MAN	C	7	2	11,11,12	0.73	0	15,15,17	0.86	1 (6%)
3	NAG	D	1	1,3	14,14,15	0.46	0	17,19,21	0.96	1 (5%)
3	NAG	D	2	3	14,14,15	0.58	0	17,19,21	1.47	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	E	1	1,4	14,14,15	0.80	0	17,19,21	0.81	0
4	NAG	E	2	4	14,14,15	0.58	0	17,19,21	1.04	0
4	BMA	E	3	4	11,11,12	0.33	0	15,15,17	0.93	1 (6%)
4	MAN	E	4	4	11,11,12	0.58	0	15,15,17	1.32	2 (13%)
4	MAN	E	5	4	11,11,12	0.68	0	15,15,17	1.23	1 (6%)
3	NAG	F	1	1,3	14,14,15	0.53	0	17,19,21	1.11	2 (11%)
3	NAG	F	2	3	14,14,15	0.45	0	17,19,21	1.22	2 (11%)
5	NAG	G	1	1,5	14,14,15	0.47	0	17,19,21	1.27	1 (5%)
5	NAG	G	2	5	14,14,15	0.68	0	17,19,21	1.11	1 (5%)
5	BMA	G	3	5	11,11,12	0.43	0	15,15,17	1.67	2 (13%)
6	NAG	H	1	1,6	14,14,15	0.55	0	17,19,21	1.02	0
6	NAG	H	2	6	14,14,15	0.51	0	17,19,21	1.01	1 (5%)
6	BMA	H	3	6	11,11,12	0.41	0	15,15,17	1.70	3 (20%)
6	MAN	H	4	6	11,11,12	0.27	0	15,15,17	0.63	0
4	NAG	I	1	1,4	14,14,15	0.74	0	17,19,21	0.98	0
4	NAG	I	2	4	14,14,15	0.69	0	17,19,21	0.98	1 (5%)
4	BMA	I	3	4	11,11,12	0.45	0	15,15,17	0.78	0
4	MAN	I	4	4	11,11,12	0.77	0	15,15,17	1.12	1 (6%)
4	MAN	I	5	4	11,11,12	0.82	0	15,15,17	1.31	1 (6%)
3	NAG	J	1	1,3	14,14,15	0.52	0	17,19,21	1.23	2 (11%)
3	NAG	J	2	3	14,14,15	0.45	0	17,19,21	1.30	2 (11%)
3	NAG	K	1	1,3	14,14,15	0.44	0	17,19,21	1.36	2 (11%)
3	NAG	K	2	3	14,14,15	0.53	0	17,19,21	1.27	2 (11%)

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	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	2/2/19/22	0/1/1/1
2	MAN	C	5	2	-	2/2/19/22	0/1/1/1
2	MAN	C	6	2	-	0/2/19/22	0/1/1/1
2	MAN	C	7	2	-	0/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1

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

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	3	BMA	C1-O5-C5	5.20	119.23	112.19
6	H	3	BMA	C1-C2-C3	4.75	115.51	109.67
2	C	1	NAG	O5-C5-C6	3.68	112.97	107.20
5	G	1	NAG	O5-C5-C6	3.66	112.95	107.20
3	K	2	NAG	C1-O5-C5	3.63	117.11	112.19
3	F	2	NAG	C1-O5-C5	3.51	116.95	112.19
4	E	4	MAN	C1-O5-C5	3.47	116.90	112.19
3	D	2	NAG	C2-N2-C7	-3.29	118.22	122.90
3	F	1	NAG	C1-O5-C5	3.27	116.62	112.19
2	C	4	MAN	C1-O5-C5	3.18	116.50	112.19
6	H	2	NAG	O5-C5-C6	3.02	111.94	107.20
3	K	1	NAG	O5-C1-C2	-2.91	106.70	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	H	3	BMA	O3-C3-C2	-2.84	104.56	109.99
4	I	5	MAN	O3-C3-C2	-2.69	104.84	109.99
3	K	1	NAG	C2-N2-C7	-2.65	119.13	122.90
4	I	4	MAN	O5-C5-C6	2.64	111.35	107.20
3	J	2	NAG	O5-C5-C6	2.51	111.14	107.20
3	D	2	NAG	O5-C5-C6	2.47	111.07	107.20
4	E	3	BMA	C1-C2-C3	2.45	112.67	109.67
3	J	1	NAG	O5-C5-C6	2.43	111.02	107.20
2	C	7	MAN	C1-O5-C5	2.38	115.41	112.19
2	C	2	NAG	O4-C4-C5	-2.38	103.40	109.30
3	J	2	NAG	C3-C4-C5	-2.32	106.10	110.24
2	C	6	MAN	O5-C5-C6	2.28	110.78	107.20
4	I	2	NAG	O5-C1-C2	-2.27	107.70	111.29
5	G	2	NAG	C4-C3-C2	2.27	114.35	111.02
3	D	2	NAG	O5-C5-C4	-2.27	105.31	110.83
5	G	3	BMA	C1-C2-C3	2.19	112.35	109.67
2	C	2	NAG	O5-C5-C6	2.18	110.63	107.20
3	F	1	NAG	C4-C3-C2	2.18	114.21	111.02
3	J	1	NAG	O5-C1-C2	-2.17	107.86	111.29
3	D	2	NAG	C3-C4-C5	-2.16	106.38	110.24
4	E	4	MAN	O5-C5-C6	2.14	110.56	107.20
3	K	2	NAG	C1-C2-N2	2.14	114.14	110.49
3	F	2	NAG	C1-C2-N2	2.08	114.03	110.49
4	E	5	MAN	O2-C2-C1	2.07	113.38	109.15
6	H	3	BMA	O5-C5-C6	2.04	110.41	107.20
3	D	1	NAG	C1-O5-C5	2.02	114.93	112.19

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	5	MAN	O5-C5-C6-O6
4	E	5	MAN	O5-C5-C6-O6
6	H	2	NAG	O5-C5-C6-O6
2	C	5	MAN	C4-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
3	J	1	NAG	C8-C7-N2-C2
3	J	1	NAG	O7-C7-N2-C2
4	E	5	MAN	C4-C5-C6-O6
4	I	5	MAN	O5-C5-C6-O6
6	H	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	H	4	MAN	O5-C5-C6-O6
2	C	4	MAN	C4-C5-C6-O6
4	I	5	MAN	C4-C5-C6-O6
2	C	4	MAN	O5-C5-C6-O6
4	I	4	MAN	O5-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6
4	E	3	BMA	C4-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6

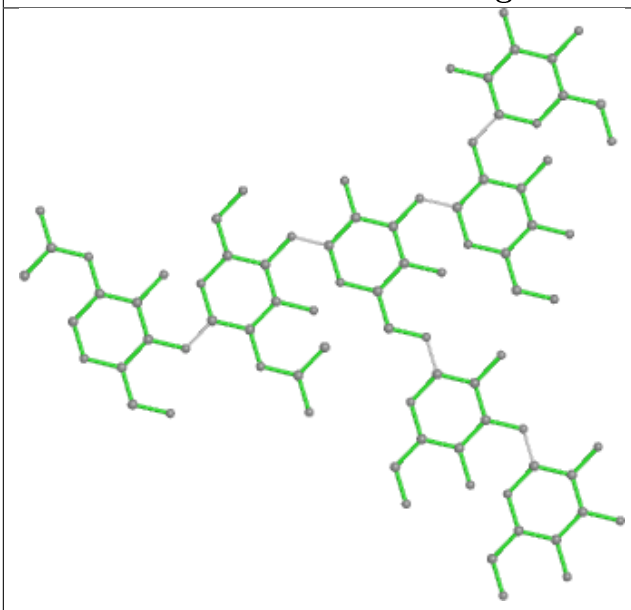
There are no ring outliers.

4 monomers are involved in 3 short contacts:

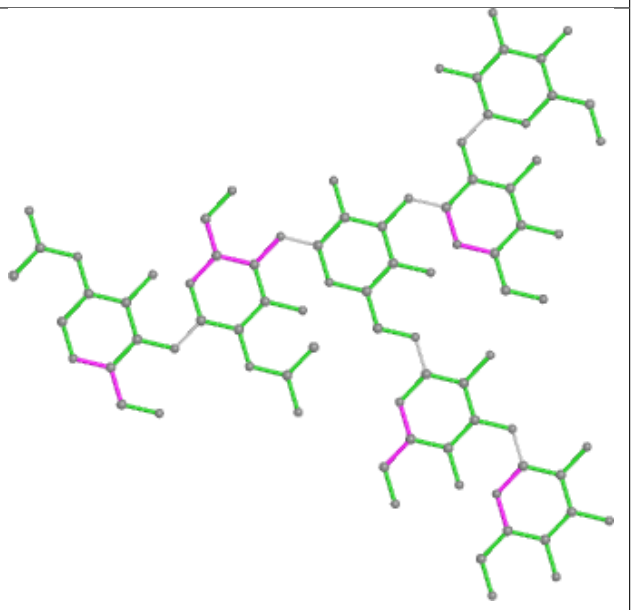
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	1	NAG	1	0
6	H	4	MAN	1	0
6	H	3	BMA	1	0
6	H	1	NAG	1	0

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

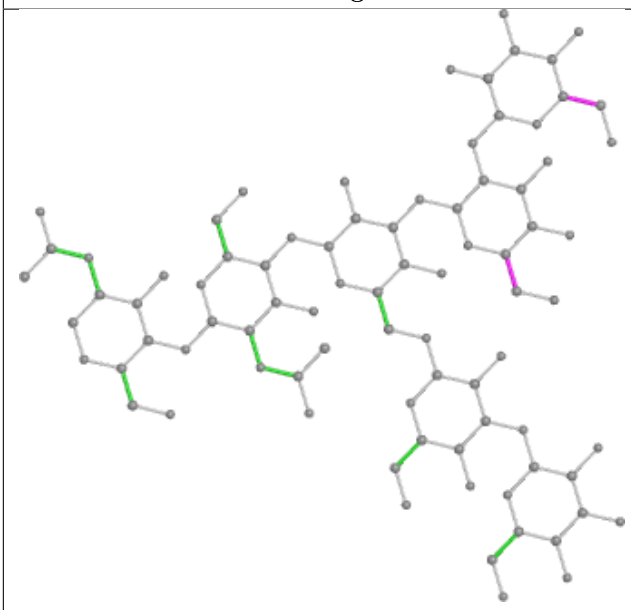
Oligosaccharide Chain C



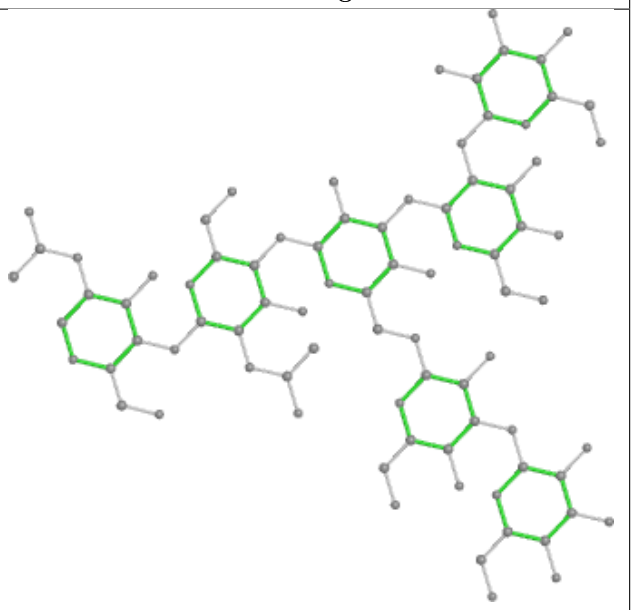
Bond lengths



Bond angles

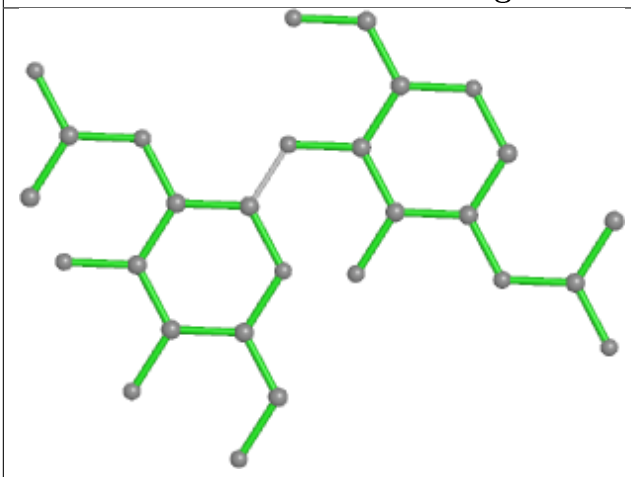


Torsions

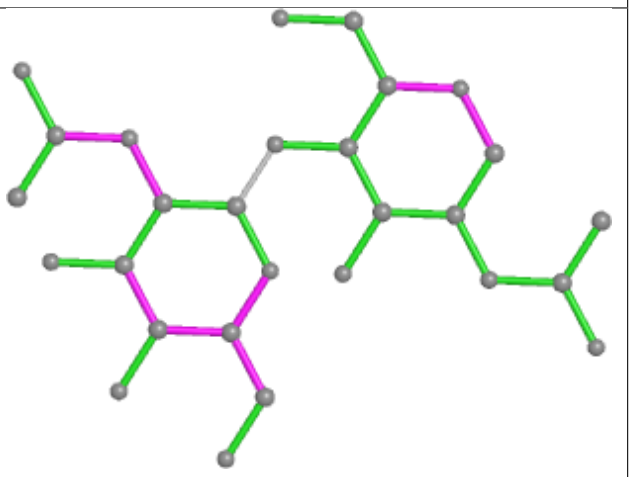


Rings

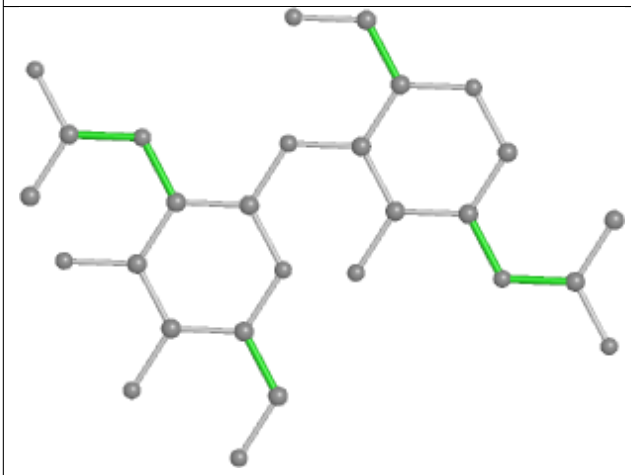
Oligosaccharide Chain D



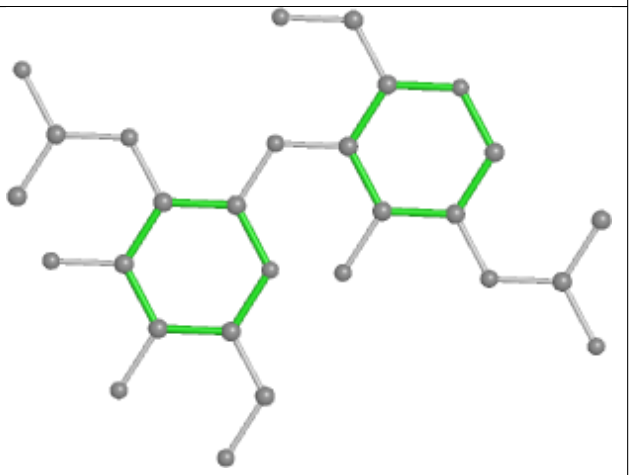
Bond lengths



Bond angles

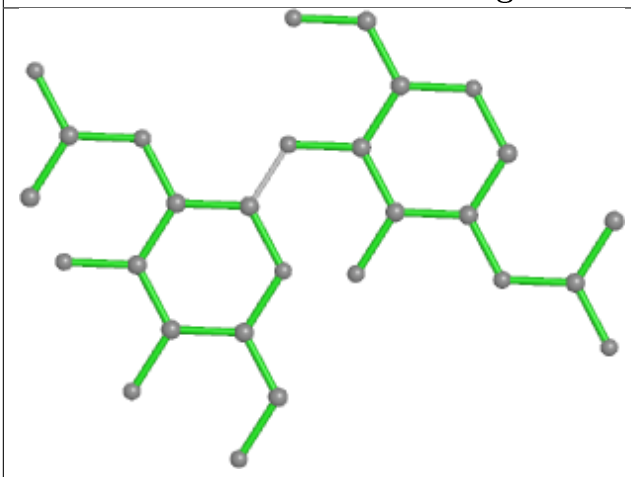


Torsions

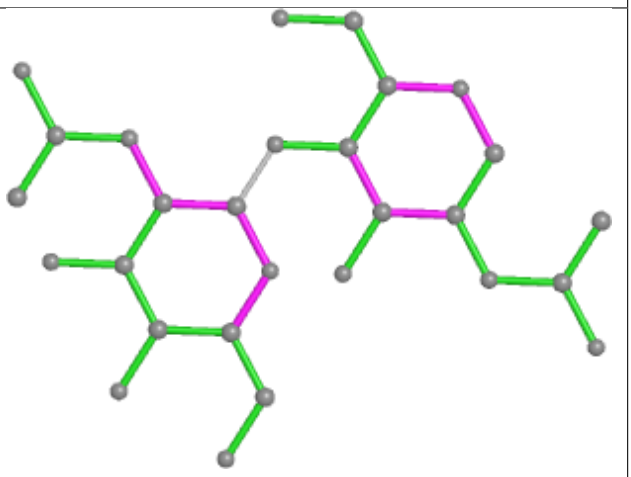


Rings

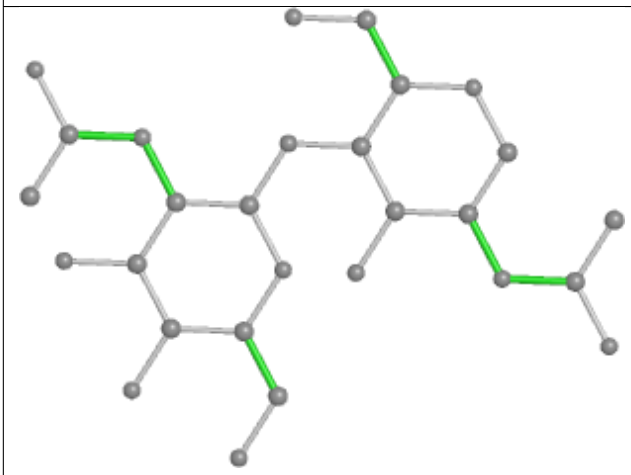
Oligosaccharide Chain F



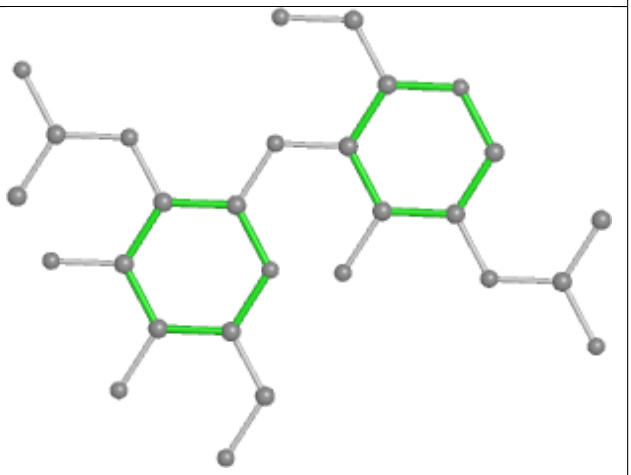
Bond lengths



Bond angles

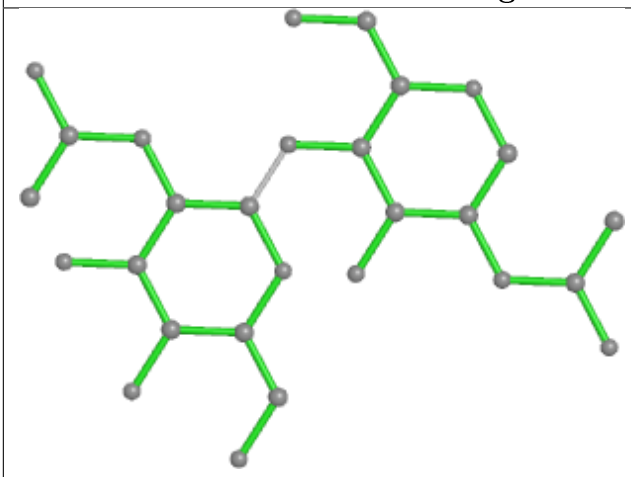


Torsions

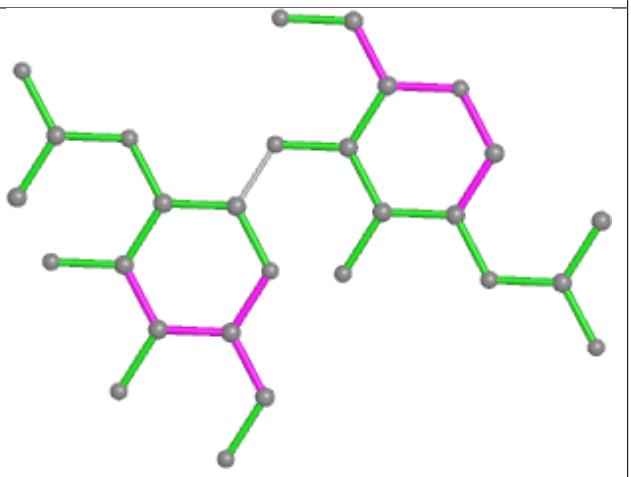


Rings

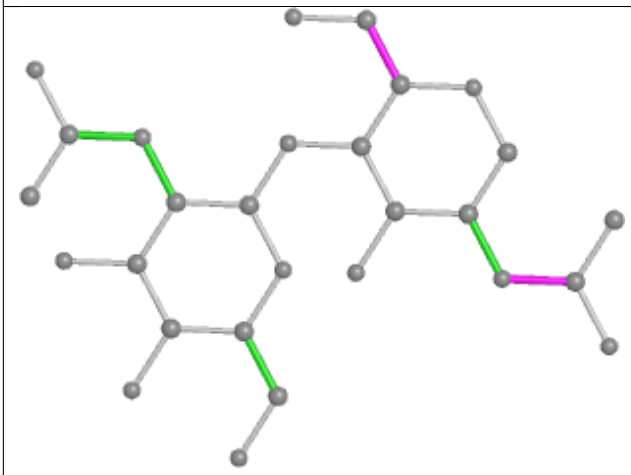
Oligosaccharide Chain J



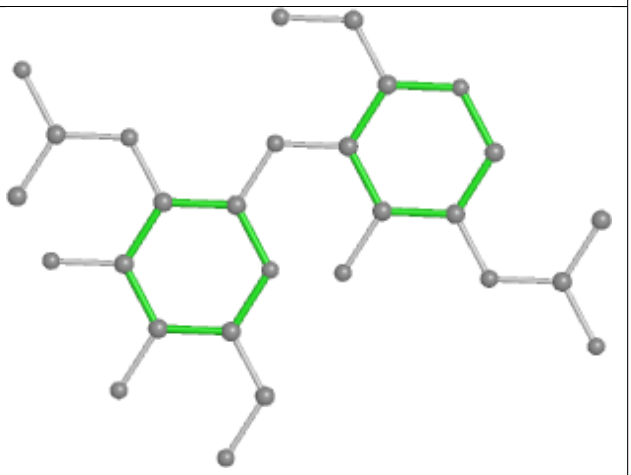
Bond lengths



Bond angles

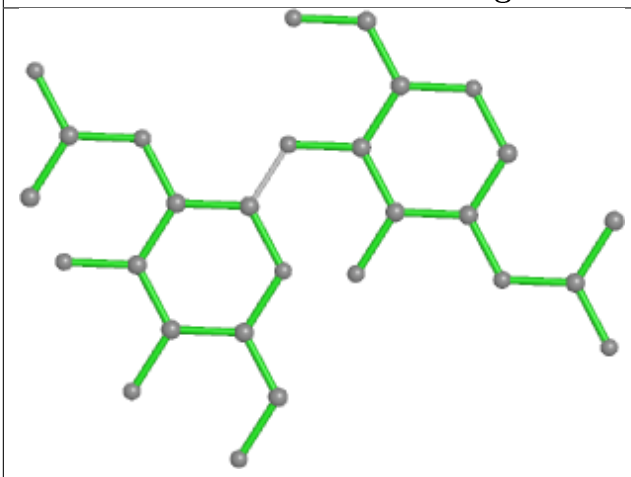


Torsions

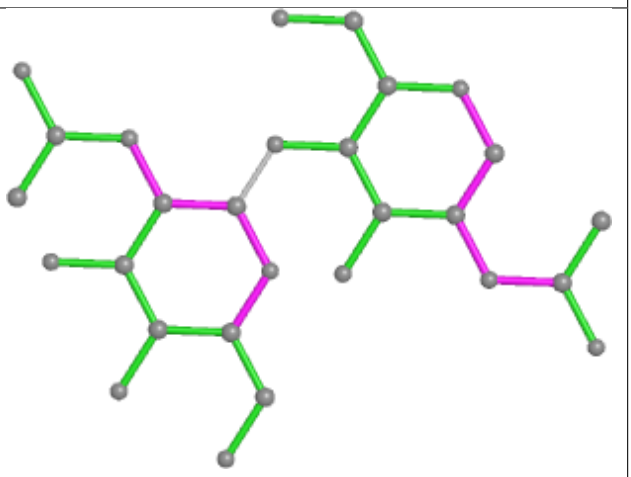


Rings

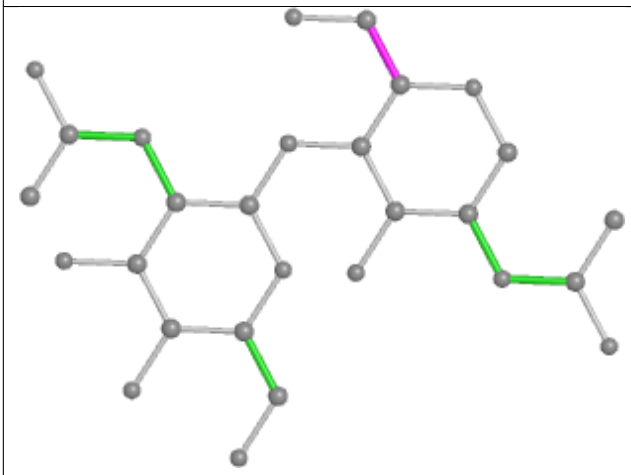
Oligosaccharide Chain K



Bond lengths



Bond angles



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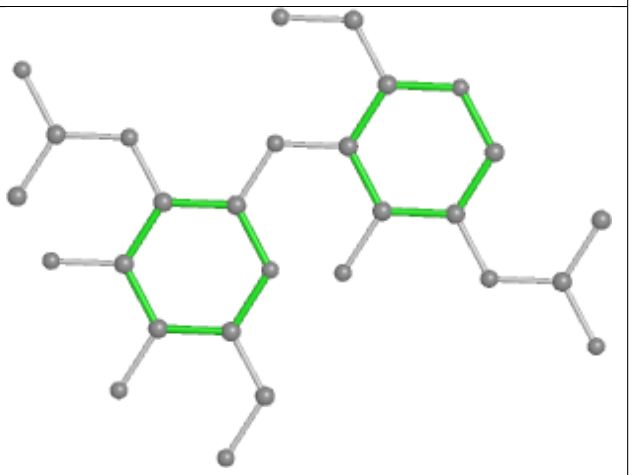
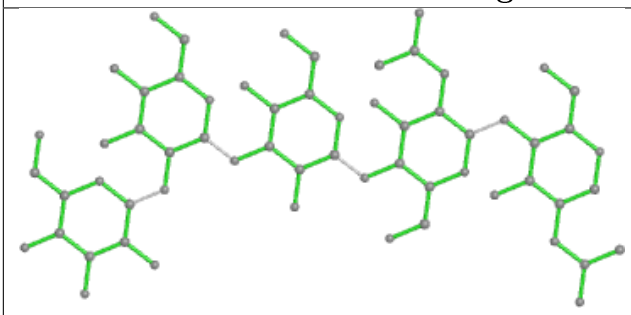
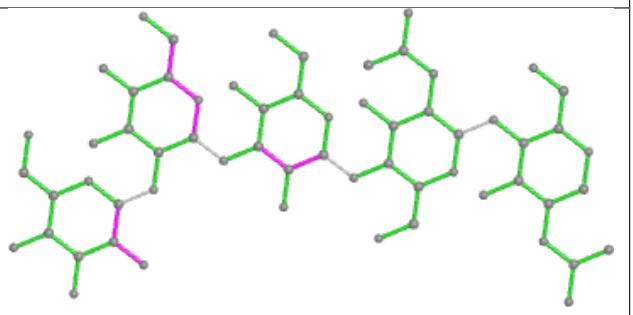


Rings

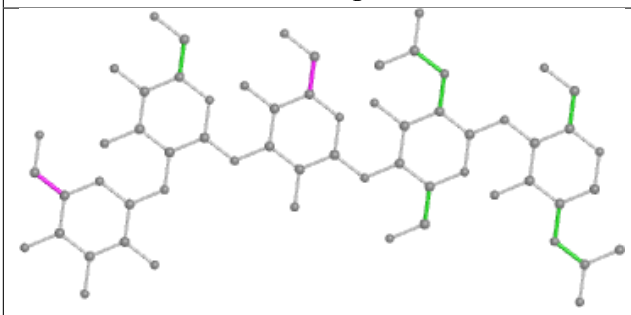
Oligosaccharide Chain E



Bond lengths



Bond angles



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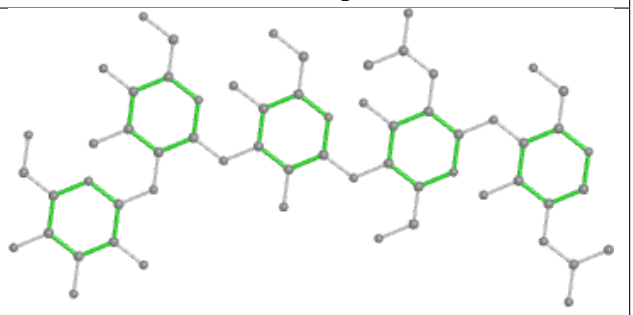
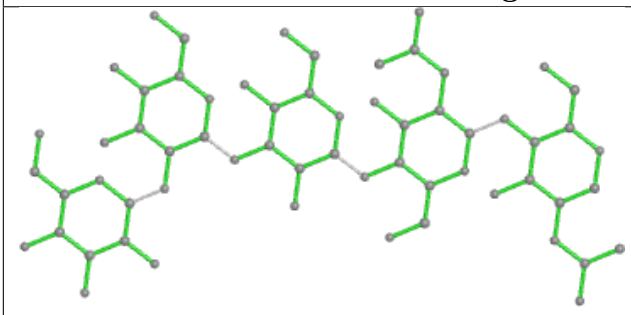
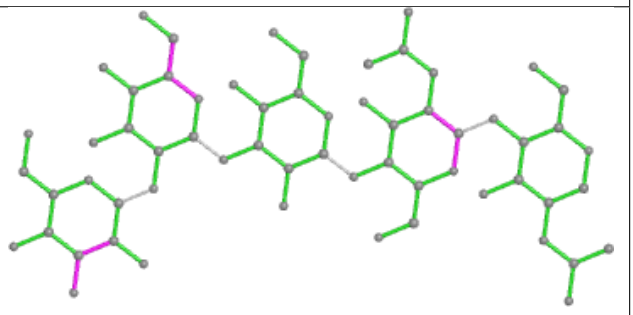


Rings

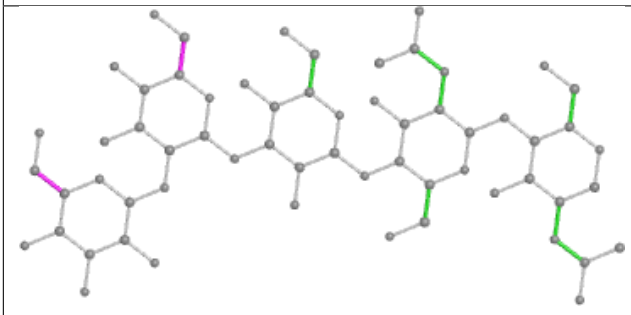
Oligosaccharide Chain I



Bond lengths



Bond angles



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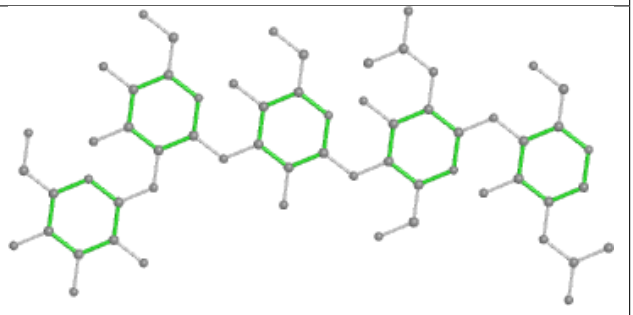
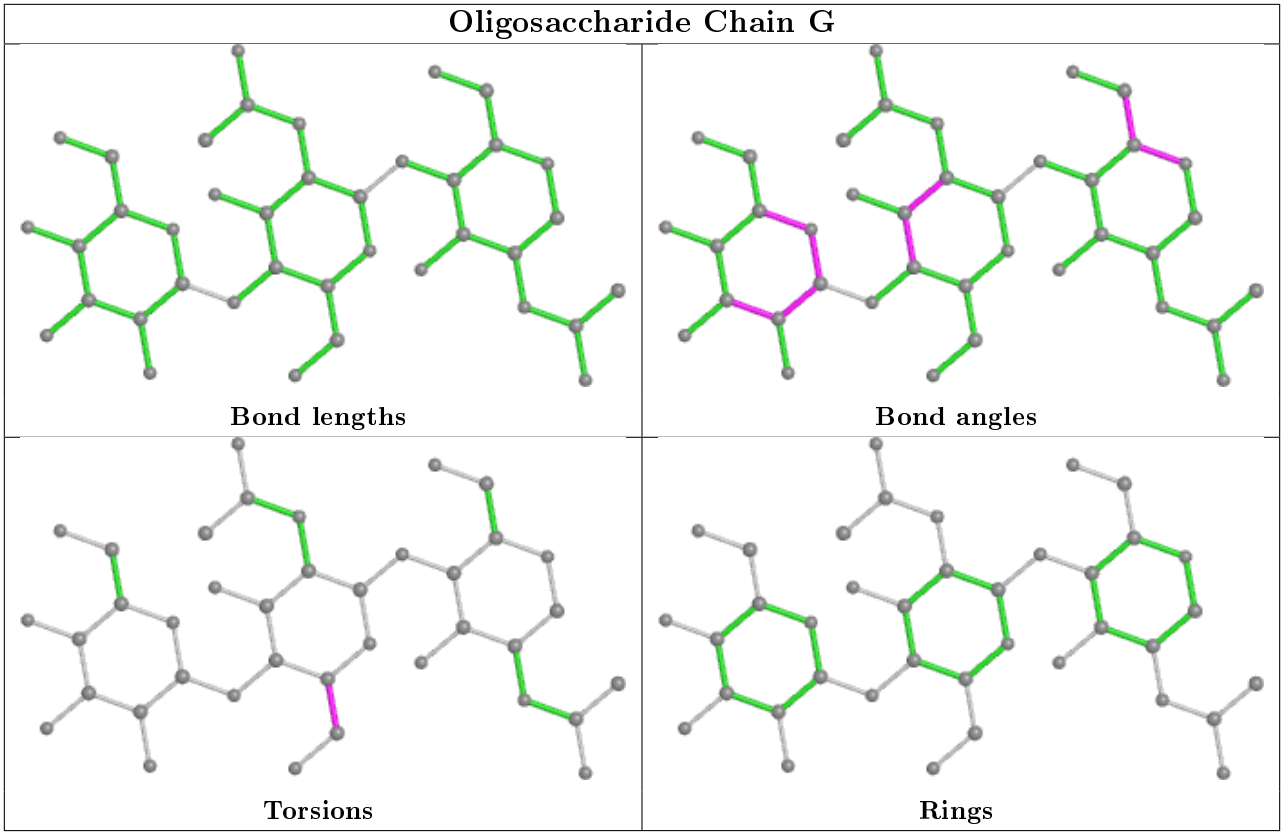
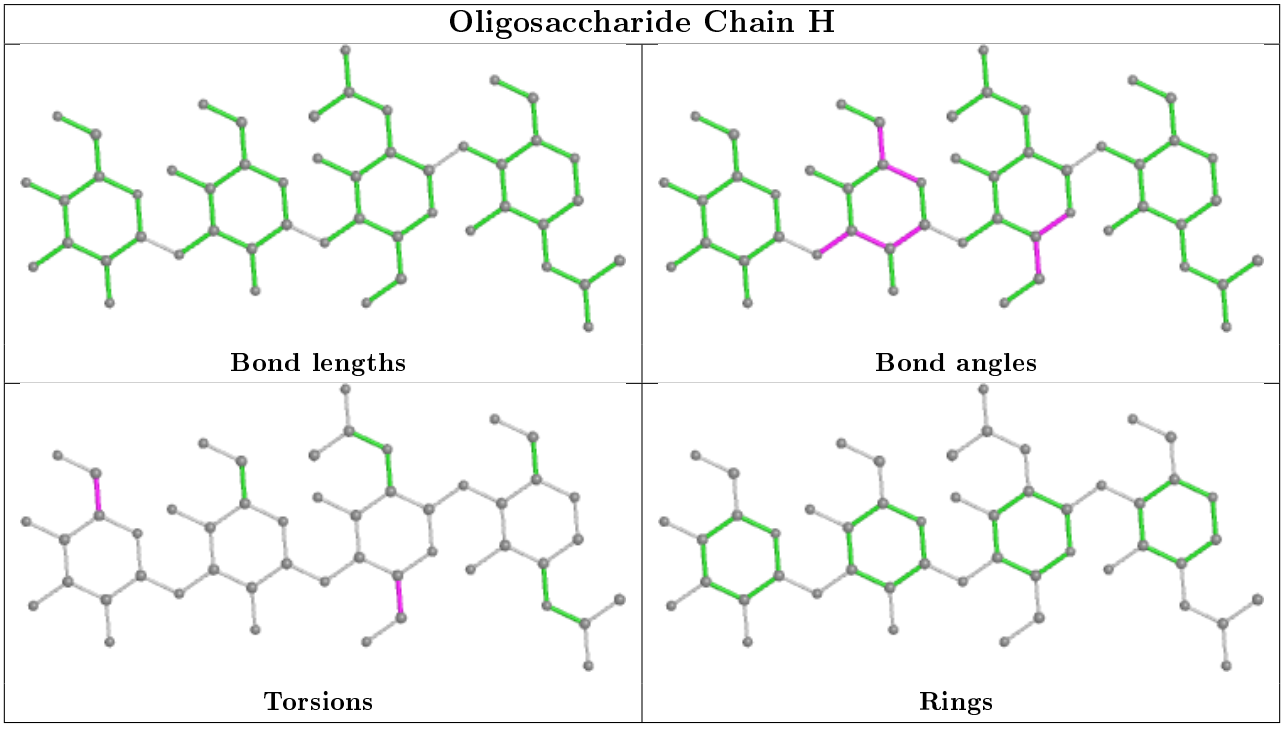


Rings





5.6 Ligand geometry

Of 38 ligands modelled in this entry, 22 are monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	ACT	B	1924	8	1,3,3	1.56	0	0,3,3	0.00	-
7	NAG	A	1801	1	14,14,15	0.52	0	17,19,21	0.90	1 (5%)
7	NAG	A	1201	1	14,14,15	0.60	0	17,19,21	0.84	0
11	ACT	A	1923	8	1,3,3	1.26	0	0,3,3	0.00	-
10	GOL	B	1923	-	5,5,5	0.34	0	5,5,5	0.51	0
7	NAG	A	1301	1	14,14,15	0.55	0	17,19,21	1.76	2 (11%)
7	NAG	A	1001	1	14,14,15	0.64	0	17,19,21	1.11	2 (11%)
9	TRS	A	1920	-	7,7,7	0.57	0	9,9,9	0.40	0
7	NAG	B	901	1	14,14,15	0.64	0	17,19,21	1.23	1 (5%)
10	GOL	B	1922	-	5,5,5	0.40	0	5,5,5	0.56	0
9	TRS	B	1920	-	7,7,7	0.27	0	9,9,9	0.82	0
7	NAG	A	901	1	14,14,15	0.58	0	17,19,21	1.08	0
7	NAG	B	1701	1	14,14,15	0.69	0	17,19,21	1.20	1 (5%)
9	TRS	A	1921	-	7,7,7	0.36	0	9,9,9	0.60	0
7	NAG	B	1001	1	14,14,15	0.73	1 (7%)	17,19,21	1.16	2 (11%)
10	GOL	A	1922	-	5,5,5	0.38	0	5,5,5	0.27	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
7	NAG	A	1801	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1201	1	-	0/6/23/26	0/1/1/1
9	TRS	A	1920	-	-	0/9/9/9	-
10	GOL	B	1923	-	-	2/4/4/4	-
7	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1001	1	-	0/6/23/26	0/1/1/1
7	NAG	B	901	1	-	0/6/23/26	0/1/1/1
10	GOL	B	1922	-	-	0/4/4/4	-
9	TRS	B	1920	-	-	0/9/9/9	-
7	NAG	A	901	1	-	0/6/23/26	0/1/1/1
7	NAG	B	1701	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	TRS	A	1921	-	-	9/9/9/9	-
7	NAG	B	1001	1	-	2/6/23/26	0/1/1/1
10	GOL	A	1922	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1001	NAG	O5-C1	-2.11	1.40	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	1301	NAG	C1-O5-C5	6.05	120.39	112.19
7	B	901	NAG	C1-O5-C5	3.31	116.67	112.19
7	A	1001	NAG	C1-O5-C5	2.81	116.00	112.19
7	B	1001	NAG	O5-C1-C2	-2.59	107.20	111.29
7	A	1001	NAG	O5-C5-C6	2.26	110.74	107.20
7	B	1001	NAG	C6-C5-C4	-2.26	107.72	113.00
7	A	1801	NAG	C1-O5-C5	2.19	115.16	112.19
7	A	1301	NAG	C1-C2-N2	-2.09	106.92	110.49
7	B	1701	NAG	O5-C5-C6	2.07	110.45	107.20

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	B	1923	GOL	O1-C1-C2-O2
10	B	1923	GOL	O1-C1-C2-C3
9	A	1921	TRS	C1-C-C2-O2
9	A	1921	TRS	C3-C-C2-O2
9	A	1921	TRS	C2-C-C3-O3
9	A	1921	TRS	N-C-C3-O3
7	B	1001	NAG	C8-C7-N2-C2
7	B	1001	NAG	O7-C7-N2-C2
7	A	1801	NAG	O5-C5-C6-O6
7	A	1801	NAG	C4-C5-C6-O6
9	A	1921	TRS	C2-C-C1-O1
9	A	1921	TRS	N-C-C1-O1
9	A	1921	TRS	N-C-C2-O2
9	A	1921	TRS	C1-C-C3-O3
9	A	1921	TRS	C3-C-C1-O1

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	1923	GOL	1	0
9	A	1921	TRS	1	0
7	B	1001	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	760/766 (99%)	-0.44	4 (0%)	91	89	7, 12, 25, 52	1 (0%)
1	B	765/766 (99%)	-0.49	8 (1%)	82	80	6, 11, 23, 52	0
All	All	1525/1532 (99%)	-0.47	12 (0%)	86	84	6, 12, 24, 52	1 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	631	PRO	4.0
1	B	632	LYS	3.7
1	B	629	SER	3.7
1	A	766	GLU	3.4
1	B	630	HIS	3.2
1	B	633	SER	2.7
1	A	306	SER	2.2
1	A	765	LEU	2.2
1	B	628	ALA	2.1
1	B	766	GLU	2.1
1	A	410	ARG	2.1
1	B	765	LEU	2.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	PCA	A	1	8/9	0.92	0.12	17,17,19,19	0
1	PCA	B	1	8/9	0.96	0.08	13,14,15,16	0

6.3 Carbohydrates (i)

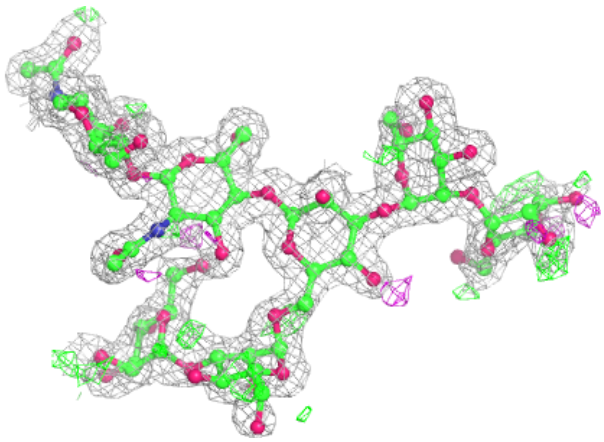
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

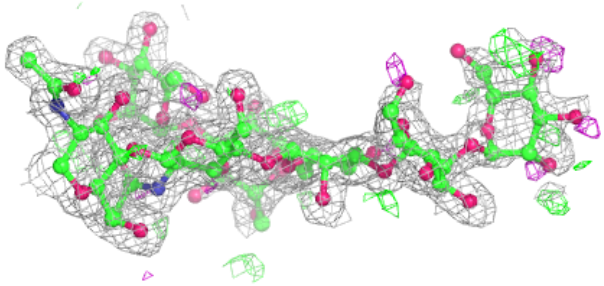
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MAN	H	4	11/12	0.59	0.23	22,25,26,27	11
2	MAN	C	5	11/12	0.67	0.34	29,32,35,37	11
4	MAN	E	4	11/12	0.73	0.24	27,34,36,38	11
6	BMA	H	3	11/12	0.73	0.24	29,31,34,37	11
6	NAG	H	2	14/15	0.78	0.29	27,30,32,36	0
5	BMA	G	3	11/12	0.79	0.28	33,34,34,35	11
3	NAG	K	2	14/15	0.79	0.29	34,37,40,40	0
3	NAG	D	2	14/15	0.79	0.28	29,34,39,40	0
4	MAN	I	5	11/12	0.80	0.14	18,19,19,20	11
4	MAN	E	5	11/12	0.80	0.25	37,39,40,41	11
2	MAN	C	6	11/12	0.81	0.21	30,32,37,38	11
3	NAG	F	2	14/15	0.83	0.37	47,52,54,55	0
4	MAN	I	4	11/12	0.83	0.17	14,17,17,18	11
3	NAG	J	2	14/15	0.83	0.33	35,39,44,44	0
2	MAN	C	4	11/12	0.85	0.14	22,23,26,27	11
4	BMA	E	3	11/12	0.85	0.27	28,31,33,34	11
4	BMA	I	3	11/12	0.87	0.18	19,22,23,27	11
3	NAG	D	1	14/15	0.87	0.16	23,26,30,30	0
3	NAG	F	1	14/15	0.88	0.17	29,32,35,41	0
2	MAN	C	7	11/12	0.88	0.21	25,27,29,29	11
5	NAG	G	2	14/15	0.90	0.20	22,28,32,33	0
5	NAG	G	1	14/15	0.91	0.13	11,12,15,16	0
2	NAG	C	2	14/15	0.92	0.12	16,18,19,23	0
2	BMA	C	3	11/12	0.92	0.16	19,21,25,27	0
6	NAG	H	1	14/15	0.92	0.16	21,24,33,34	0
3	NAG	K	1	14/15	0.93	0.11	20,23,26,29	0
4	NAG	E	2	14/15	0.93	0.20	20,24,29,29	0
3	NAG	J	1	14/15	0.93	0.14	22,26,30,32	0
4	NAG	I	2	14/15	0.94	0.16	18,22,25,27	0
4	NAG	E	1	14/15	0.94	0.12	15,17,19,19	0
2	NAG	C	1	14/15	0.96	0.07	11,12,15,16	0
4	NAG	I	1	14/15	0.97	0.10	15,17,19,19	0

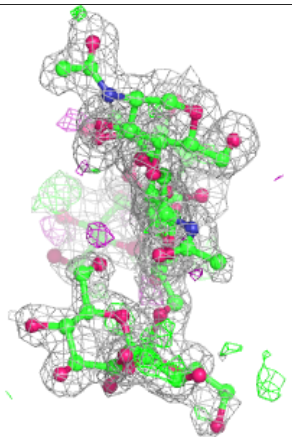
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

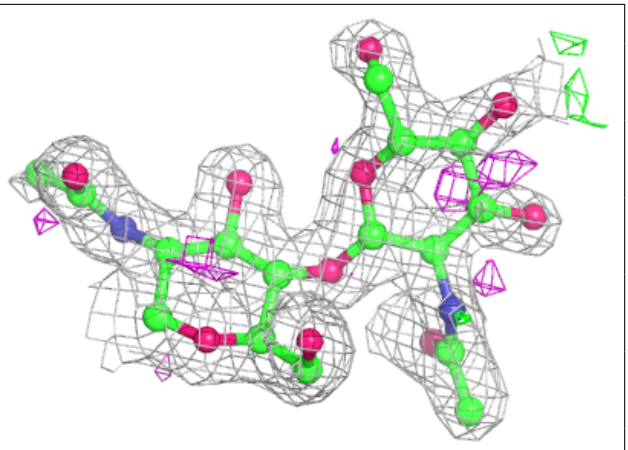


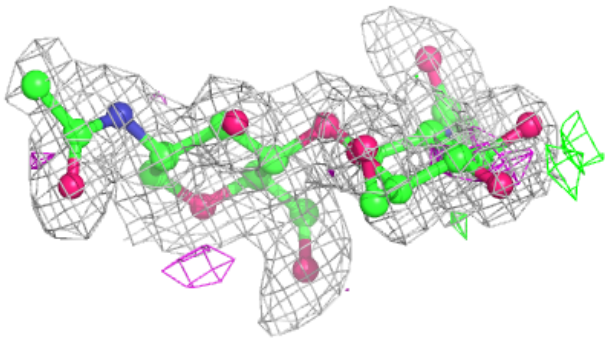




Electron density around Chain D:

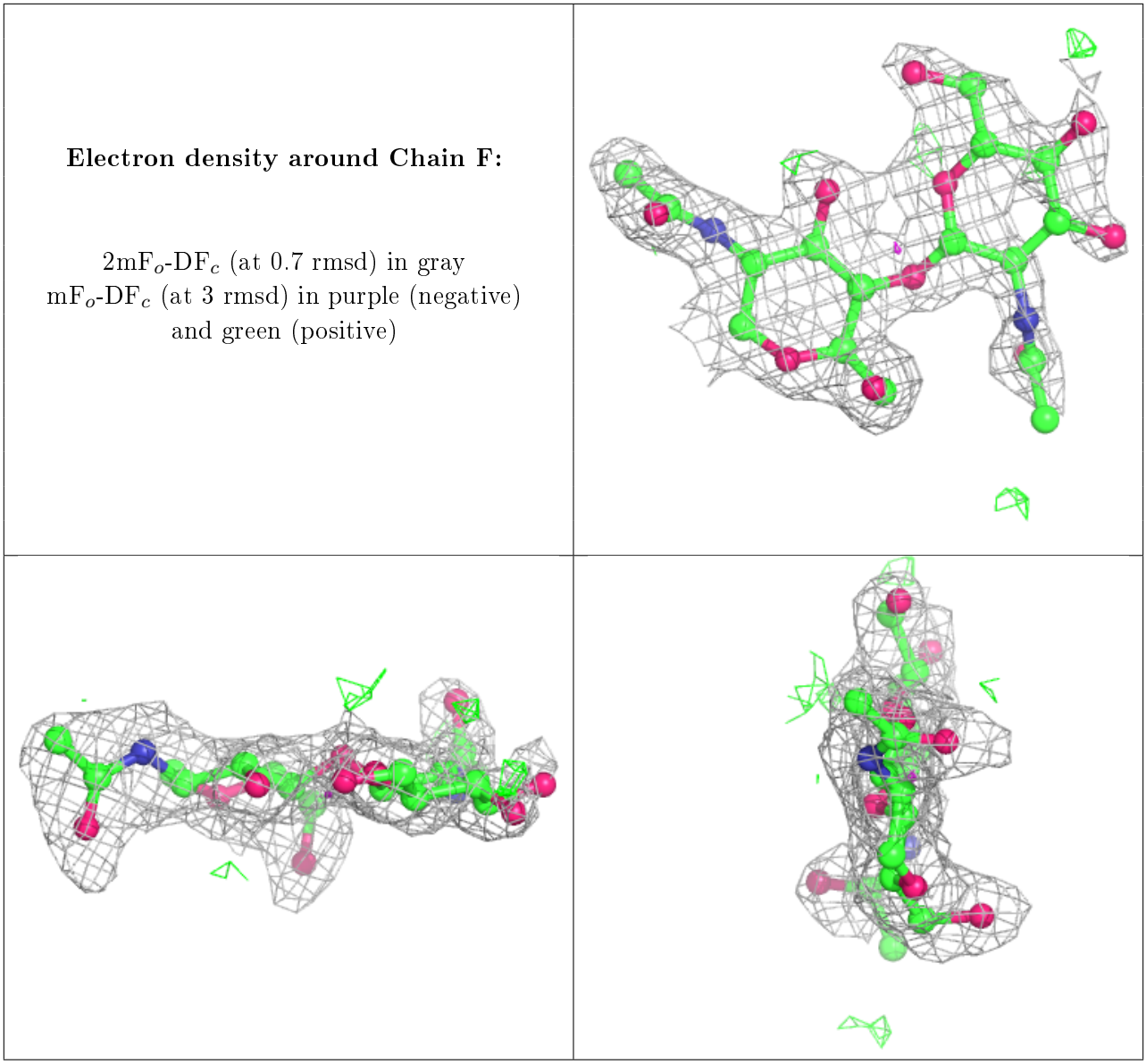
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





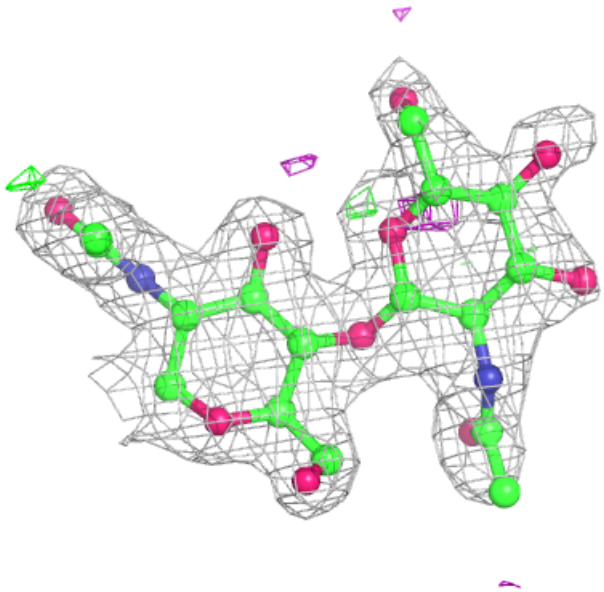
Electron density around Chain F:

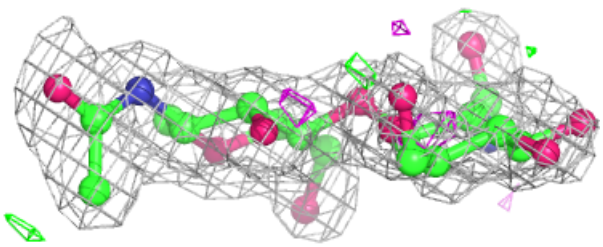
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

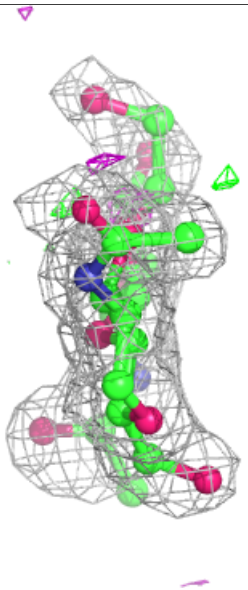


Electron density around Chain J:

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

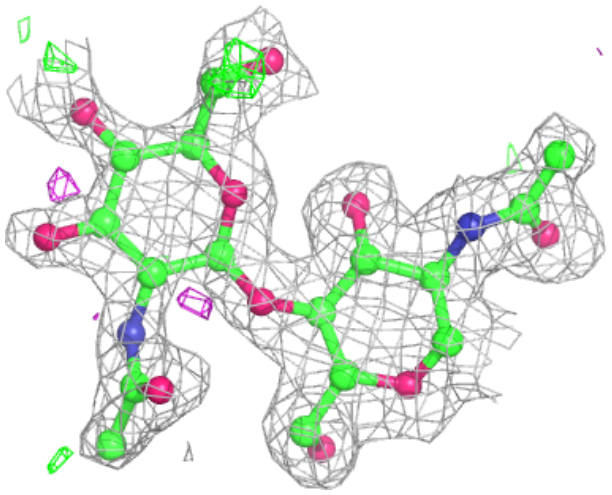


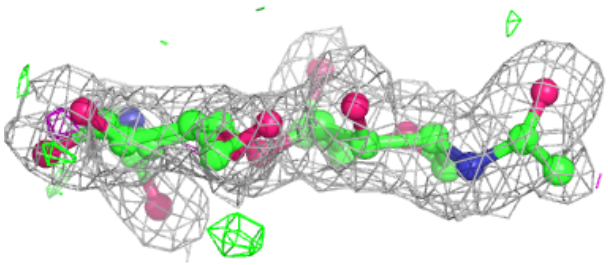


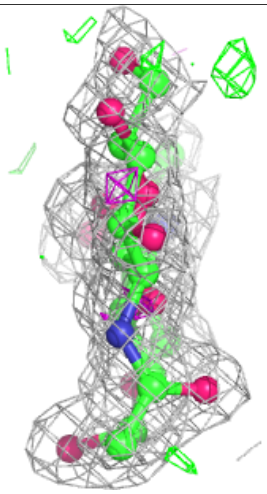


Electron density around Chain K:

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

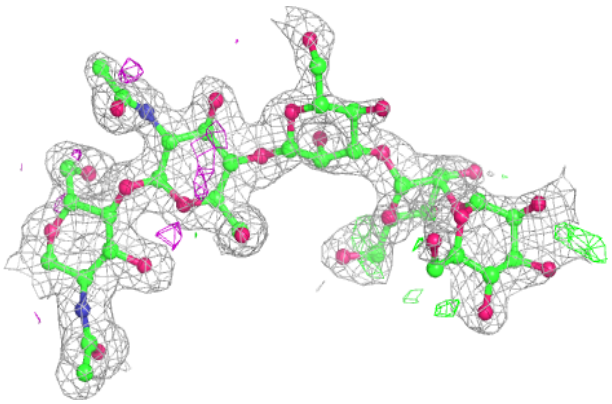


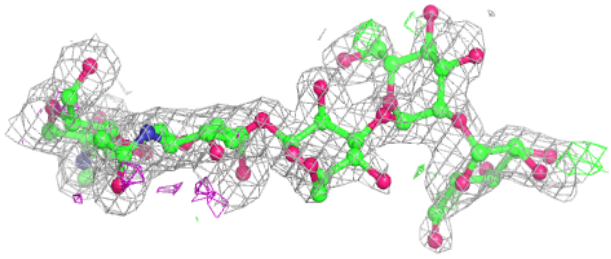


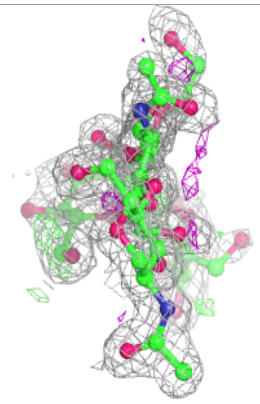


Electron density around Chain E:

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

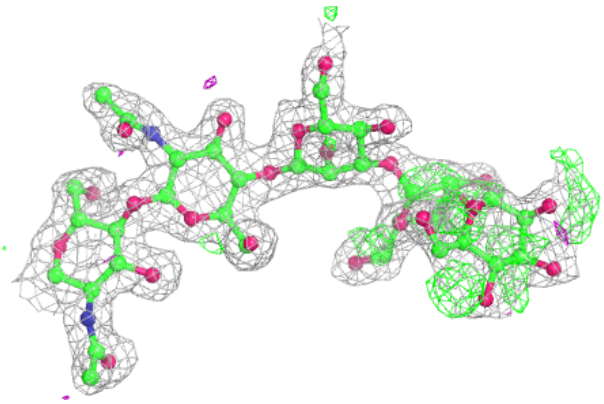


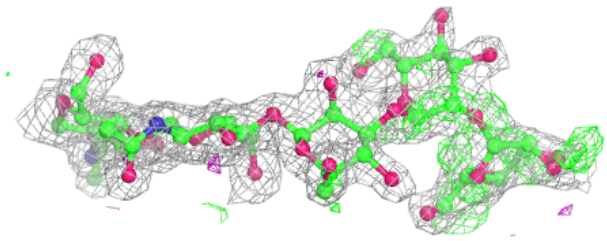


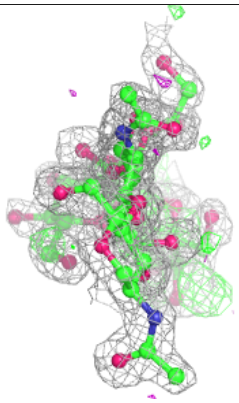


Electron density around Chain I:

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

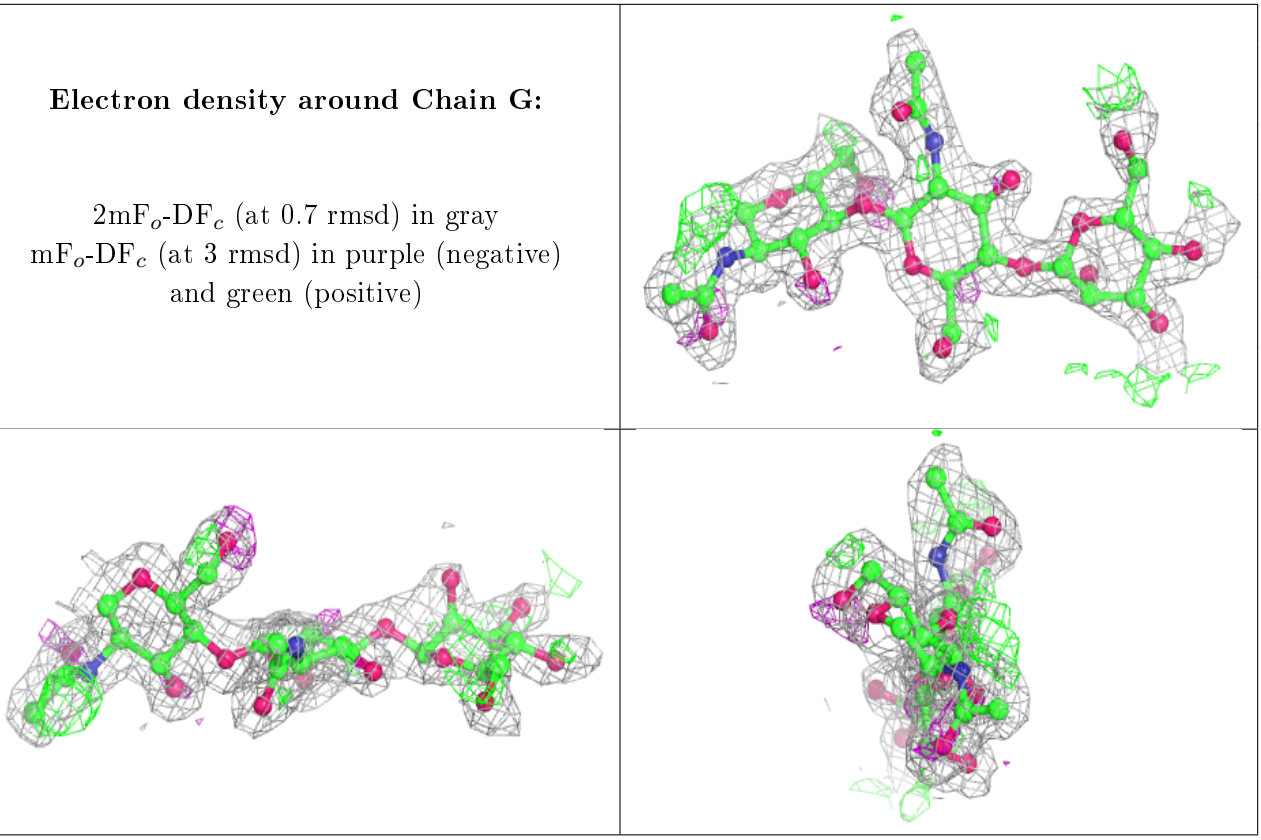






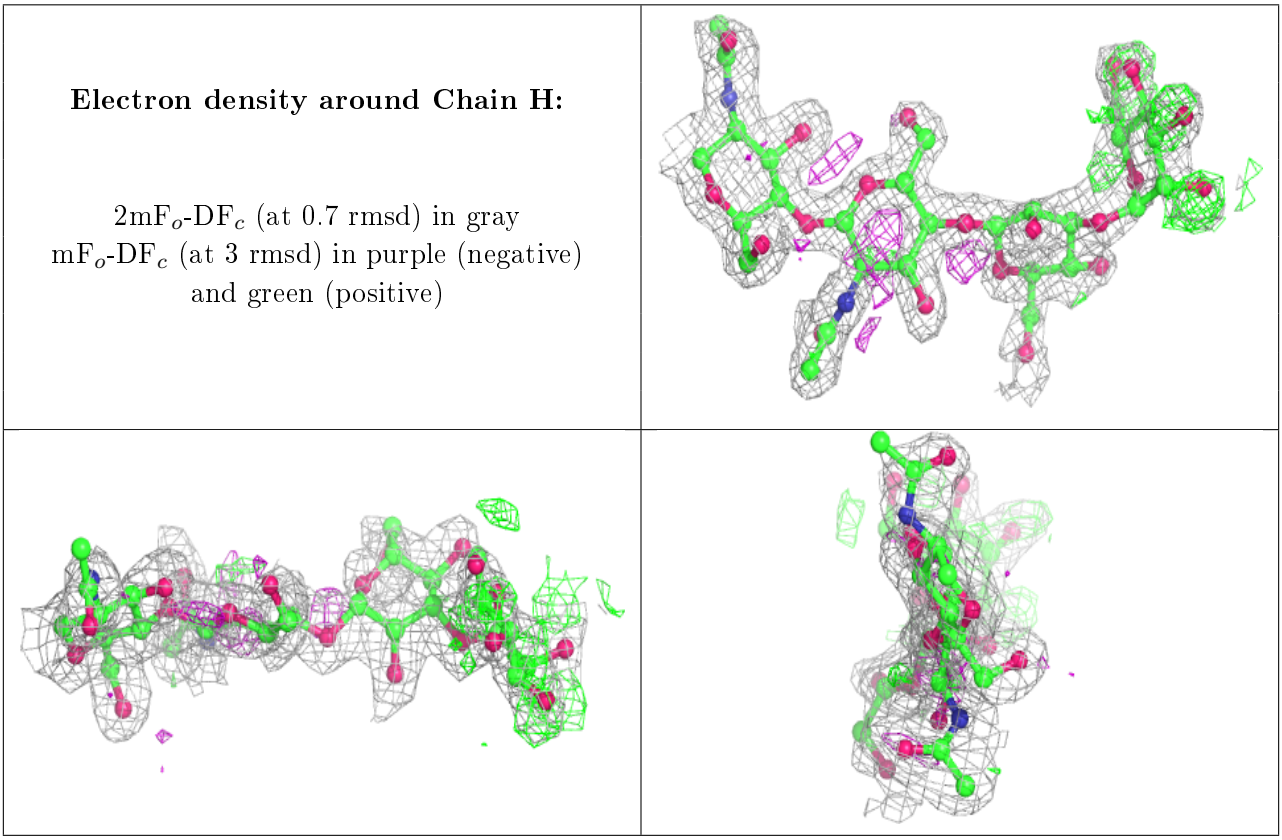
Electron density around Chain G:

$2mF_o$-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)



6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	NAG	A	1201	14/15	0.82	0.32	32,38,45,49	0
9	TRS	A	1921	8/8	0.83	0.24	32,38,42,42	0
8	ZN	B	1916	1/1	0.85	0.16	73,73,73,73	0
7	NAG	A	1801	14/15	0.86	0.22	35,40,45,46	0
7	NAG	B	1701	14/15	0.90	0.16	16,20,25,26	0
7	NAG	B	901	14/15	0.90	0.15	19,24,28,29	0
7	NAG	A	1001	14/15	0.92	0.19	20,24,31,32	0
7	NAG	A	901	14/15	0.92	0.14	20,26,29,30	0
7	NAG	B	1001	14/15	0.93	0.10	18,20,26,27	0
10	GOL	B	1923	6/6	0.93	0.09	22,24,26,28	0
7	NAG	A	1301	14/15	0.93	0.20	21,24,26,26	0
8	ZN	A	1902	1/1	0.94	0.06	47,47,47,47	0
11	ACT	A	1923	4/4	0.94	0.14	15,15,16,16	0
9	TRS	B	1920	8/8	0.95	0.09	10,11,12,12	0
11	ACT	B	1924	4/4	0.96	0.08	14,15,15,15	0
8	ZN	B	1905	1/1	0.96	0.17	50,50,50,50	1
9	TRS	A	1920	8/8	0.96	0.08	13,14,15,16	0
8	ZN	A	1909[A]	1/1	0.98	0.05	29,29,29,29	1
8	ZN	B	1906[A]	1/1	0.98	0.06	19,19,19,19	1
10	GOL	B	1922	6/6	0.98	0.07	8,8,8,9	0
8	ZN	B	1912	1/1	0.98	0.07	31,31,31,31	1
8	ZN	A	1909[B]	1/1	0.98	0.05	22,22,22,22	1
8	ZN	B	1913	1/1	0.98	0.10	42,42,42,42	0
8	ZN	B	1911[A]	1/1	0.99	0.05	24,24,24,24	1
8	ZN	A	1904	1/1	0.99	0.06	21,21,21,21	0
8	ZN	B	1904	1/1	0.99	0.06	22,22,22,22	0
8	ZN	A	1911[B]	1/1	0.99	0.05	17,17,17,17	1
10	GOL	A	1922	6/6	0.99	0.06	10,11,11,11	0
8	ZN	B	1914	1/1	0.99	0.03	20,20,20,20	0
8	ZN	A	1908	1/1	0.99	0.09	35,35,35,35	0
8	ZN	A	1916	1/1	0.99	0.03	21,21,21,21	0
8	ZN	B	1901	1/1	1.00	0.02	14,14,14,14	0
8	ZN	A	1903	1/1	1.00	0.04	20,20,20,20	0
8	ZN	A	1901	1/1	1.00	0.02	14,14,14,14	0
8	ZN	A	1915	1/1	1.00	0.07	7,7,7,7	1
8	ZN	B	1903	1/1	1.00	0.03	17,17,17,17	0
8	ZN	B	1907	1/1	1.00	0.03	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	ZN	A	1907	1/1	1.00	0.02	16,16,16,16	0

6.5 Other polymers (i)

There are no such residues in this entry.