Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2023 – 11:53 PM JST

PDB ID	:	6IK5
Title	:	Crystal structure of tomato beta-galactosidase (TBG) 4 in complex with galactose
Authors	:	Matsuyama, K.; Nakae, S.; Igarashi, K.; Tada, T.; Ishimaru, M.
Deposited on	:	2018-10-15
Resolution	:	1.82 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

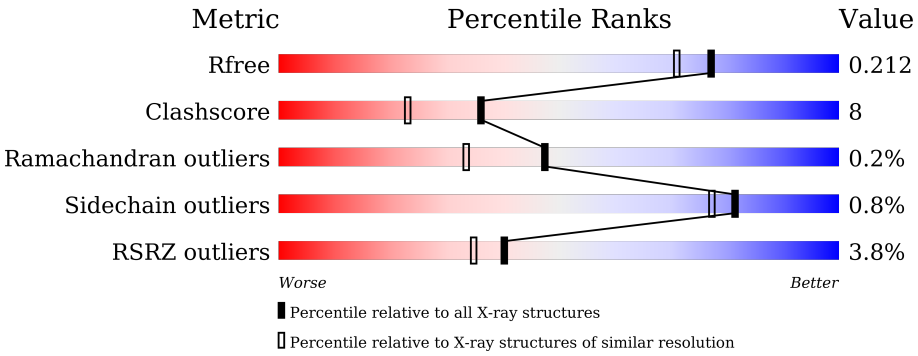
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.82 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	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	718	4% 84% 13%
1	B	718	4% 88% 10%
2	C	2	50% 50%
2	D	2	50% 50%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	C	2	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12055 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-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	705	Total	C	N	O	S	0	0	0
			5531	3535	944	1025	27			
1	B	705	Total	C	N	O	S	0	0	0
			5531	3535	944	1025	27			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	GLU	-	expression tag	UNP O81100
A	19	ALA	-	expression tag	UNP O81100
A	20	GLU	-	expression tag	UNP O81100
A	21	ALA	-	expression tag	UNP O81100
A	22	GLU	-	expression tag	UNP O81100
A	23	PHE	-	expression tag	UNP O81100
A	725	SER	-	expression tag	UNP O81100
A	726	ALA	-	expression tag	UNP O81100
A	727	ALA	-	expression tag	UNP O81100
A	728	ALA	-	expression tag	UNP O81100
A	729	ALA	-	expression tag	UNP O81100
A	730	SER	-	expression tag	UNP O81100
A	731	PHE	-	expression tag	UNP O81100
A	732	LEU	-	expression tag	UNP O81100
A	733	GLU	-	expression tag	UNP O81100
A	734	GLN	-	expression tag	UNP O81100
A	735	LYS	-	expression tag	UNP O81100
B	18	GLU	-	expression tag	UNP O81100
B	19	ALA	-	expression tag	UNP O81100
B	20	GLU	-	expression tag	UNP O81100
B	21	ALA	-	expression tag	UNP O81100
B	22	GLU	-	expression tag	UNP O81100
B	23	PHE	-	expression tag	UNP O81100
B	725	SER	-	expression tag	UNP O81100
B	726	ALA	-	expression tag	UNP O81100

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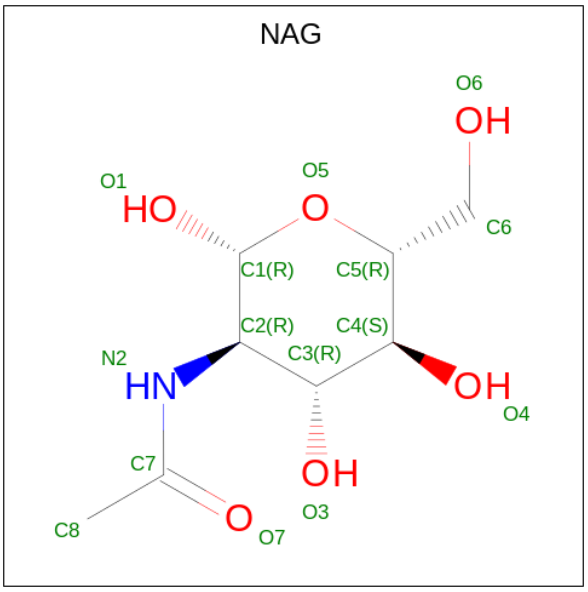
Chain	Residue	Modelled	Actual	Comment	Reference
B	727	ALA	-	expression tag	UNP O81100
B	728	ALA	-	expression tag	UNP O81100
B	729	ALA	-	expression tag	UNP O81100
B	730	SER	-	expression tag	UNP O81100
B	731	PHE	-	expression tag	UNP O81100
B	732	LEU	-	expression tag	UNP O81100
B	733	GLU	-	expression tag	UNP O81100
B	734	GLN	-	expression tag	UNP O81100
B	735	LYS	-	expression tag	UNP O81100

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

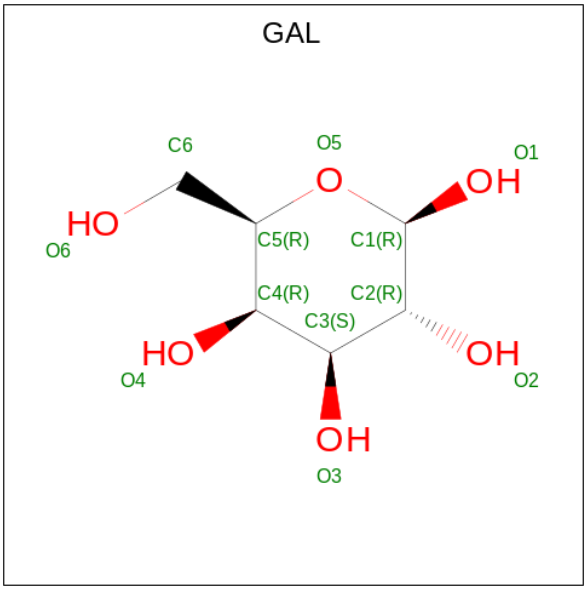
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	C	2	Total C N O 28 16 2 10	0	0	0
2	D	2	Total C N O 28 16 2 10	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 4 is beta-D-galactopyranose (three-letter code: GAL) (formula: $C_6H_{12}O_6$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is water.

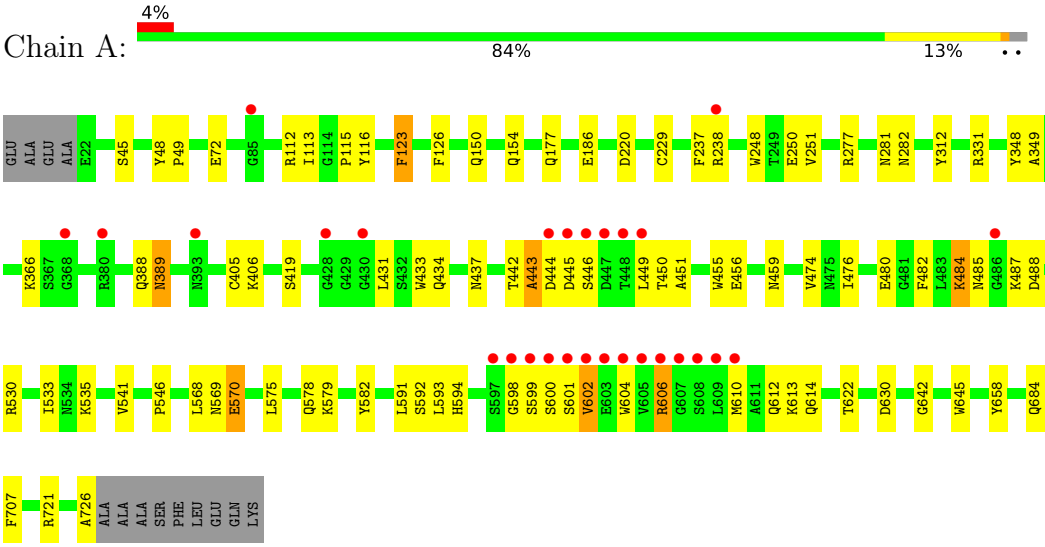
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	453	Total O 453 453	0	0
5	B	432	Total O 432 432	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

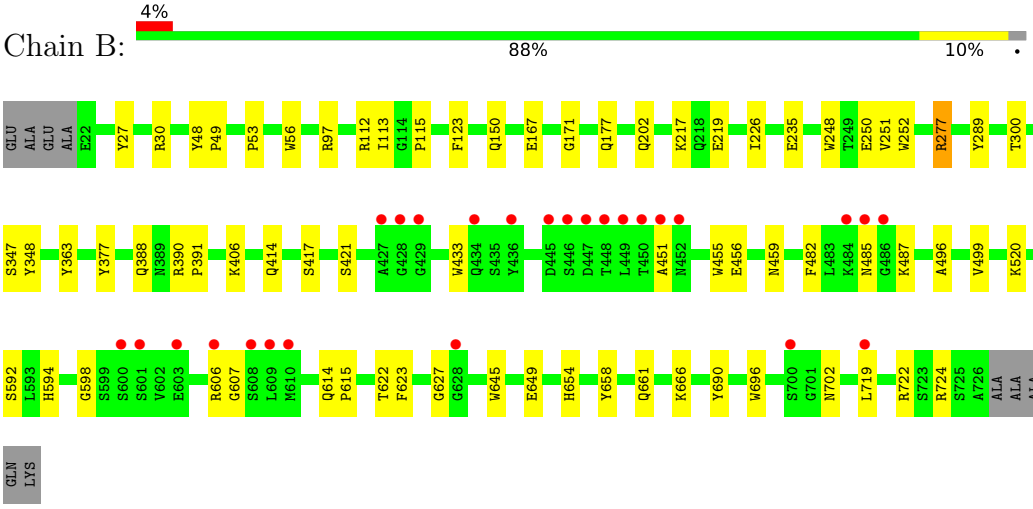
• Molecule 1: Beta-galactosidase

Chain A:



• Molecule 1: Beta-galactosidase

Chain B:



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

Chain C:

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

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	92.14Å 95.33Å 158.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.28 – 1.82 41.28 – 1.82	Depositor EDS
% Data completeness (in resolution range)	98.0 (41.28-1.82) 98.1 (41.28-1.82)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.27 (at 1.82Å)	Xtriage
Refinement program	PHENIX, REFMAC 5.8.0232	Depositor
R, R_{free}	0.172 , 0.209 0.173 , 0.212	Depositor DCC
R_{free} test set	6178 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	23.1	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 58.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12055	wwPDB-VP
Average B, all atoms (Å^2)	27.0	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: NAG, GAL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.48	0/5694	0.82	2/7739 (0.0%)
1	B	0.49	0/5694	0.81	6/7739 (0.1%)
All	All	0.49	0/11388	0.82	8/15478 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	570	GLU	C-N-CA	-7.95	105.61	122.30
1	B	30	ARG	CG-CD-NE	-7.20	96.67	111.80
1	B	277	ARG	NE-CZ-NH1	-7.13	116.74	120.30
1	B	277	ARG	NE-CZ-NH2	6.91	123.75	120.30
1	B	97	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	B	331	ARG	CG-CD-NE	-5.47	100.32	111.80
1	A	331	ARG	CG-CD-NE	-5.22	100.83	111.80
1	B	722	ARG	CG-CD-NE	5.06	122.42	111.80

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	5531	0	5349	113	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5531	0	5350	63	0
2	C	28	0	25	2	0
2	D	28	0	25	1	0
3	A	14	0	13	5	0
3	B	14	0	13	6	0
4	A	12	0	12	1	0
4	B	12	0	12	1	0
5	A	453	0	0	13	0
5	B	432	0	0	10	0
All	All	12055	0	10799	176	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 8.

All (176) 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:593:LEU:CD2	1:A:599:SER:O	1.73	1.35
1:A:600:SER:HB2	5:A:907:HOH:O	1.24	1.29
1:A:593:LEU:HD23	1:A:599:SER:O	1.15	1.26
1:A:600:SER:CB	5:A:907:HOH:O	1.72	1.24
1:A:601:SER:HA	1:A:604:TRP:HH2	1.01	1.10
1:A:433:TRP:O	1:A:610:MET:HE1	1.52	1.08
1:A:591:LEU:O	1:A:599:SER:C	1.91	1.08
1:A:601:SER:O	1:A:602:VAL:HG22	1.54	1.08
1:A:601:SER:HA	1:A:604:TRP:CH2	1.89	1.06
1:A:591:LEU:HB3	1:A:600:SER:HB3	1.10	1.06
1:A:456:GLU:H	3:A:803:NAG:H81	1.18	1.04
1:B:235:GLU:CD	1:B:277:ARG:HE	1.61	1.02
1:B:235:GLU:CG	1:B:277:ARG:HE	1.74	1.00
1:B:300:THR:HG22	5:B:943:HOH:O	1.63	0.98
1:A:591:LEU:CB	1:A:600:SER:HB3	1.93	0.98
1:A:600:SER:CA	5:A:907:HOH:O	2.03	0.98
1:B:456:GLU:H	3:B:803:NAG:H81	1.29	0.96
1:A:591:LEU:HD22	1:A:600:SER:OG	1.65	0.95
1:A:575:LEU:O	1:A:578:GLN:HG2	1.66	0.94
1:B:456:GLU:H	3:B:803:NAG:C8	1.81	0.93
1:A:591:LEU:O	1:A:599:SER:CA	2.18	0.91
1:B:606:ARG:HD2	1:B:607:GLY:H	1.34	0.91
1:B:235:GLU:HG3	1:B:277:ARG:HE	1.36	0.90
1:B:485:ASN:ND2	1:B:487:LYS:HD2	1.86	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:601:SER:CA	1:A:604:TRP:HH2	1.84	0.89
1:A:593:LEU:HD21	1:A:599:SER:O	1.72	0.88
1:B:451:ALA:HB2	1:B:455:TRP:CZ2	2.09	0.88
1:A:600:SER:HA	5:A:907:HOH:O	1.69	0.88
1:B:235:GLU:HG3	1:B:277:ARG:NE	1.89	0.87
1:A:480:GLU:O	1:A:484:LYS:HE2	1.74	0.87
1:A:591:LEU:HB3	1:A:600:SER:CB	2.02	0.87
1:A:433:TRP:O	1:A:610:MET:CE	2.24	0.85
1:A:450:THR:HG21	1:A:579:LYS:HE2	1.58	0.85
1:A:601:SER:CA	1:A:604:TRP:CH2	2.58	0.84
1:A:593:LEU:HD23	1:A:599:SER:C	1.87	0.83
1:A:434:GLN:HA	1:A:610:MET:HE2	1.61	0.83
1:A:591:LEU:HD22	1:A:600:SER:CB	2.08	0.82
1:A:601:SER:CB	5:A:901:HOH:O	2.22	0.81
1:A:601:SER:O	1:A:602:VAL:CG2	2.28	0.81
1:A:150:GLN:HE21	1:A:154:GLN:NE2	1.78	0.81
1:A:591:LEU:O	1:A:600:SER:N	2.14	0.80
1:A:150:GLN:HE21	1:A:154:GLN:HE21	1.29	0.78
1:B:150:GLN:HG2	5:B:1281:HOH:O	1.82	0.78
1:A:601:SER:C	1:A:604:TRP:CH2	2.57	0.77
1:A:456:GLU:H	3:A:803:NAG:C8	1.96	0.77
1:A:459:ASN:HD22	3:A:803:NAG:H83	1.48	0.77
1:B:235:GLU:CD	1:B:277:ARG:NE	2.38	0.76
1:A:591:LEU:O	1:A:599:SER:HA	1.85	0.74
1:B:496:ALA:HA	1:B:520:LYS:HD3	1.68	0.73
1:A:238:ARG:NH2	1:A:282:ASN:HD22	1.86	0.73
1:B:459:ASN:HD22	3:B:803:NAG:H83	1.54	0.73
1:B:485:ASN:OD1	1:B:487:LYS:HB2	1.89	0.72
1:A:602:VAL:O	1:A:604:TRP:CE3	2.43	0.71
1:B:235:GLU:CG	1:B:277:ARG:NE	2.49	0.71
1:A:443:ALA:O	5:A:902:HOH:O	2.10	0.69
1:B:606:ARG:HD2	1:B:607:GLY:N	2.06	0.69
1:A:449:LEU:HB3	1:A:582:TYR:HB2	1.75	0.68
1:A:601:SER:OG	1:A:602:VAL:N	2.24	0.67
1:B:390:ARG:NH1	1:B:406:LYS:HD2	2.10	0.66
1:A:434:GLN:CA	1:A:610:MET:HE2	2.25	0.65
1:A:238:ARG:HH22	1:A:282:ASN:HD22	1.44	0.64
1:A:601:SER:O	1:A:602:VAL:HG13	1.97	0.64
1:A:610:MET:CE	5:A:1103:HOH:O	2.45	0.63
1:A:450:THR:CG2	1:A:579:LYS:HE2	2.29	0.62
1:B:414:GLN:HB2	5:B:1273:HOH:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:GLN:NE2	1:B:406:LYS:HE2	2.15	0.62
1:B:433:TRP:O	1:B:606:ARG:HD3	1.99	0.62
1:B:202:GLN:HG3	5:B:1241:HOH:O	1.99	0.61
1:A:592:SER:O	1:A:599:SER:CA	2.37	0.61
1:A:433:TRP:C	1:A:610:MET:HE1	2.19	0.61
1:B:277:ARG:NH1	1:B:377:TYR:CE1	2.69	0.61
1:B:456:GLU:N	3:B:803:NAG:H81	2.10	0.61
1:B:482:PHE:O	1:B:485:ASN:O	2.18	0.61
1:A:575:LEU:HD22	1:A:578:GLN:OE1	2.00	0.61
1:A:456:GLU:N	3:A:803:NAG:H81	2.03	0.59
1:A:482:PHE:HA	1:A:485:ASN:OD1	2.03	0.58
1:A:610:MET:HE1	5:A:1103:HOH:O	2.02	0.58
1:A:601:SER:O	1:A:602:VAL:CB	2.52	0.57
1:A:592:SER:O	1:A:599:SER:HA	2.04	0.57
1:B:485:ASN:HD21	1:B:487:LYS:HD2	1.66	0.57
1:A:575:LEU:O	1:A:578:GLN:CG	2.48	0.57
1:A:366:LYS:HG2	5:A:949:HOH:O	2.04	0.56
1:A:444:ASP:C	1:A:446:SER:H	2.06	0.56
1:A:444:ASP:C	1:A:446:SER:N	2.58	0.56
1:A:123:PHE:HA	1:A:546:PRO:O	2.07	0.55
1:A:598:GLY:O	5:A:903:HOH:O	2.17	0.54
1:A:431:LEU:H	1:A:431:LEU:HD12	1.73	0.54
1:A:446:SER:OG	1:A:446:SER:O	2.23	0.54
1:A:568:LEU:O	1:A:570:GLU:O	2.25	0.53
1:A:598:GLY:O	5:A:904:HOH:O	2.19	0.52
1:A:601:SER:O	1:A:602:VAL:CG1	2.57	0.52
1:A:684:GLN:HB3	1:A:685:PRO:HD2	1.92	0.52
1:B:300:THR:HG23	5:B:1232:HOH:O	2.09	0.52
1:A:444:ASP:OD1	5:A:905:HOH:O	2.19	0.52
1:A:444:ASP:O	1:A:446:SER:N	2.42	0.52
1:A:602:VAL:O	1:A:604:TRP:CZ3	2.63	0.51
1:B:235:GLU:CB	1:B:277:ARG:HG2	2.40	0.51
1:A:405:CYS:O	1:A:406:LYS:HD3	2.11	0.51
1:A:433:TRP:C	1:A:610:MET:CE	2.77	0.51
1:B:250:GLU:OE1	4:B:804:GAL:H1	2.11	0.51
1:A:591:LEU:CD2	1:A:600:SER:CB	2.84	0.51
1:A:250:GLU:OE1	4:A:804:GAL:H1	2.12	0.50
1:A:388:GLN:O	1:A:389:ASN:HB2	2.11	0.50
1:B:455:TRP:HA	3:B:803:NAG:H82	1.93	0.50
1:A:437:ASN:HD21	1:A:614:GLN:HG2	1.76	0.50
1:A:116:TYR:HB2	1:A:126:PHE:CZ	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:TYR:CD2	2:C:1:NAG:H62	2.48	0.49
1:A:451:ALA:HB2	1:A:455:TRP:CZ2	2.48	0.49
1:A:455:TRP:HA	3:A:803:NAG:H82	1.95	0.49
1:B:654:HIS:HA	1:B:690:TYR:CE2	2.48	0.48
1:B:594:HIS:HB2	1:B:645:TRP:CG	2.49	0.48
1:A:476:ILE:HG23	1:A:480:GLU:HG3	1.95	0.48
1:A:529:LEU:O	1:A:530:ARG:HD2	2.14	0.48
1:A:591:LEU:CB	1:A:600:SER:CB	2.76	0.47
1:A:622:THR:HA	1:A:702:ASN:O	2.14	0.47
1:B:27:TYR:CD2	1:B:226:ILE:HD11	2.49	0.47
1:B:499:VAL:HB	1:B:541:VAL:HB	1.97	0.47
1:A:150:GLN:O	1:A:154:GLN:HG3	2.15	0.47
1:B:649:GLU:HG3	1:B:696:TRP:CH2	2.50	0.46
1:B:217:LYS:HG2	5:B:1165:HOH:O	2.15	0.46
1:B:248:TRP:CD2	1:B:251:VAL:HG22	2.51	0.46
1:A:113:ILE:O	1:A:115:PRO:HA	2.16	0.46
1:B:328:GLY:HA3	1:B:417:SER:OG	2.16	0.46
1:B:406:LYS:HA	1:B:406:LYS:HD3	1.71	0.46
1:A:238:ARG:HH22	1:A:282:ASN:ND2	2.11	0.45
1:B:388:GLN:HE21	1:B:406:LYS:HE2	1.82	0.45
1:A:186:GLU:OE2	1:A:220:ASP:OD2	2.34	0.45
1:A:601:SER:OG	5:A:901:HOH:O	1.77	0.44
1:A:450:THR:HG21	1:A:579:LYS:CE	2.38	0.44
1:A:388:GLN:HE21	1:A:406:LYS:HE2	1.82	0.44
1:B:348:TYR:CD1	2:D:1:NAG:H62	2.52	0.44
1:B:456:GLU:N	3:B:803:NAG:C8	2.65	0.44
1:A:630:ASP:OD2	1:A:721:ARG:HB3	2.17	0.44
1:B:485:ASN:OD1	1:B:487:LYS:CB	2.62	0.44
1:A:112:ARG:HA	1:A:177:GLN:HB3	2.00	0.43
1:B:666:LYS:HD2	5:B:1293:HOH:O	2.18	0.43
1:A:594:HIS:HB2	1:A:645:TRP:CG	2.53	0.43
1:B:623:PHE:CE2	1:B:719:LEU:HD11	2.53	0.43
1:A:569:ASN:C	1:A:570:GLU:O	2.57	0.43
1:B:622:THR:HA	1:B:702:ASN:O	2.18	0.43
1:A:474:VAL:HG23	1:A:474:VAL:O	2.18	0.43
1:B:112:ARG:HA	1:B:177:GLN:HB3	2.00	0.43
1:A:281:ASN:O	1:A:282:ASN:HB2	2.19	0.43
1:A:487:LYS:HG2	1:A:488:ASP:N	2.34	0.43
1:A:499:VAL:HB	1:A:541:VAL:HB	2.01	0.43
1:B:113:ILE:O	1:B:115:PRO:HA	2.19	0.42
1:A:351:VAL:HG23	2:C:1:NAG:H83	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:642:GLY:HA3	1:A:707:PHE:O	2.19	0.42
1:B:167:GLU:HA	1:B:171:GLY:O	2.20	0.42
1:B:451:ALA:HB2	1:B:455:TRP:CE2	2.51	0.42
1:B:614:GLN:HG2	1:B:615:PRO:HD2	2.01	0.42
1:A:45:SER:HA	1:A:72:GLU:O	2.20	0.42
1:A:248:TRP:CD2	1:A:251:VAL:HG22	2.54	0.42
1:B:252:TRP:HA	1:B:289:TYR:O	2.20	0.42
1:B:347:SER:OG	1:B:363:TYR:HB3	2.19	0.42
1:A:419:SER:O	1:A:726:ALA:HA	2.19	0.41
1:B:390:ARG:HA	1:B:391:PRO:HD3	1.93	0.41
1:A:238:ARG:HD3	1:A:238:ARG:HA	1.84	0.41
1:A:388:GLN:NE2	1:A:406:LYS:HE2	2.36	0.41
1:B:53:PRO:HA	1:B:56:TRP:CD2	2.54	0.41
1:B:627:GLY:HA3	5:B:974:HOH:O	2.19	0.41
1:A:48:TYR:CG	1:A:49:PRO:HD3	2.55	0.41
1:A:229:CYS:HB2	1:A:237:PHE:CG	2.54	0.41
1:B:661:GLN:NE2	5:B:925:HOH:O	2.54	0.41
1:A:442:THR:HG21	1:A:535:LYS:HD2	2.02	0.41
1:A:533:ILE:HD13	1:A:533:ILE:HA	1.98	0.41
1:B:724:ARG:HH11	1:B:724:ARG:HD2	1.73	0.41
1:B:248:TRP:CE2	1:B:251:VAL:HG22	2.56	0.41
1:A:349:ALA:HB2	1:A:363:TYR:CZ	2.56	0.40
1:A:150:GLN:NE2	1:A:154:GLN:HE21	2.06	0.40
1:A:612:GLN:O	1:A:613:LYS:C	2.60	0.40
1:B:219:GLU:HG2	5:B:1306:HOH:O	2.20	0.40
1:B:592:SER:O	1:B:598:GLY:HA3	2.21	0.40
1:B:421:SER:O	1:B:724:ARG:HA	2.21	0.40
1:A:434:GLN:HG2	1:A:606:ARG:HB2	2.04	0.40
1:B:48:TYR:CG	1:B:49:PRO:HD3	2.57	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	703/718 (98%)	674 (96%)	26 (4%)	3 (0%)	34 21
1	B	703/718 (98%)	679 (97%)	24 (3%)	0	100 100
All	All	1406/1436 (98%)	1353 (96%)	50 (4%)	3 (0%)	47 33

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	602	VAL
1	A	445	ASP
1	A	443	ALA

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	591/599 (99%)	584 (99%)	7 (1%)	71 64
1	B	591/599 (99%)	588 (100%)	3 (0%)	88 87
All	All	1182/1198 (99%)	1172 (99%)	10 (1%)	81 77

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	PHE
1	A	277	ARG
1	A	312	TYR
1	A	389	ASN
1	A	484	LYS
1	A	606	ARG
1	A	658	TYR
1	B	123	PHE
1	B	587	LYS
1	B	658	TYR

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

Mol	Chain	Res	Type
1	A	154	GLN
1	A	437	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

4 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	0.79	0	17,19,21	1.69	2 (11%)
2	NAG	C	2	2	14,14,15	0.70	0	17,19,21	1.22	1 (5%)
2	NAG	D	1	1,2	14,14,15	0.70	0	17,19,21	1.87	8 (47%)
2	NAG	D	2	2	14,14,15	0.65	0	17,19,21	1.35	3 (17%)

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	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1	NAG	C1-O5-C5	5.62	119.81	112.19
2	D	1	NAG	C1-C2-N2	-3.20	105.02	110.49
2	C	1	NAG	C1-C2-N2	-3.10	105.19	110.49
2	D	1	NAG	C2-N2-C7	-2.87	118.82	122.90
2	D	1	NAG	O3-C3-C2	-2.74	103.79	109.47
2	C	2	NAG	C2-N2-C7	2.66	126.70	122.90
2	D	2	NAG	O5-C5-C6	2.53	111.16	107.20
2	D	1	NAG	O3-C3-C4	2.32	115.72	110.35
2	D	1	NAG	O7-C7-N2	-2.20	117.91	121.95
2	D	1	NAG	O7-C7-C8	2.19	126.13	122.06
2	D	2	NAG	O5-C1-C2	2.13	114.65	111.29
2	D	2	NAG	C3-C4-C5	-2.12	106.46	110.24
2	D	1	NAG	O4-C4-C3	2.07	115.14	110.35
2	D	1	NAG	O5-C1-C2	-2.05	108.06	111.29

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6

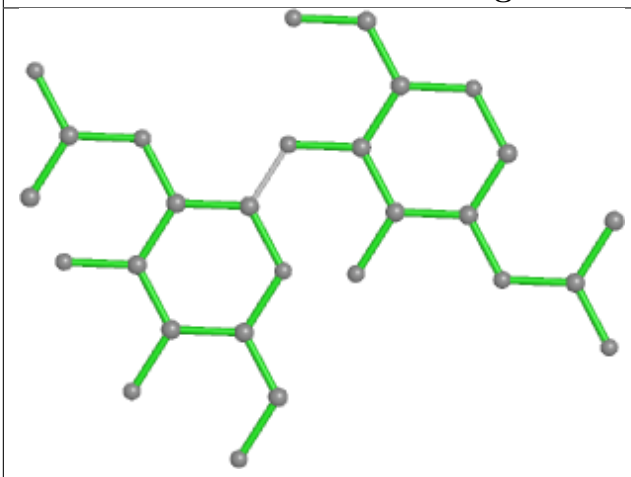
There are no ring outliers.

2 monomers are involved in 3 short contacts:

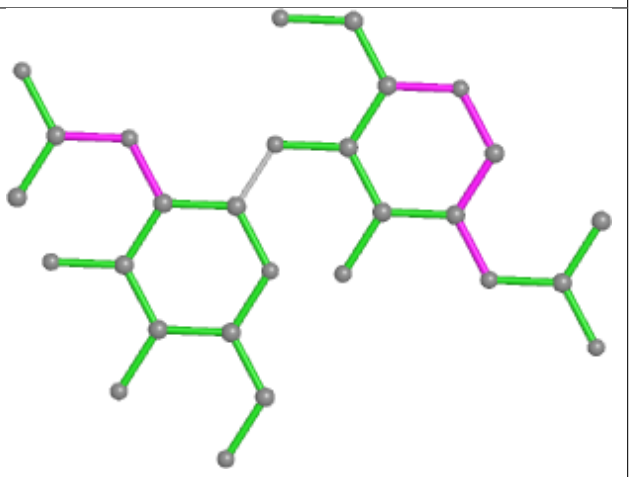
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	2	0
2	D	1	NAG	1	0

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

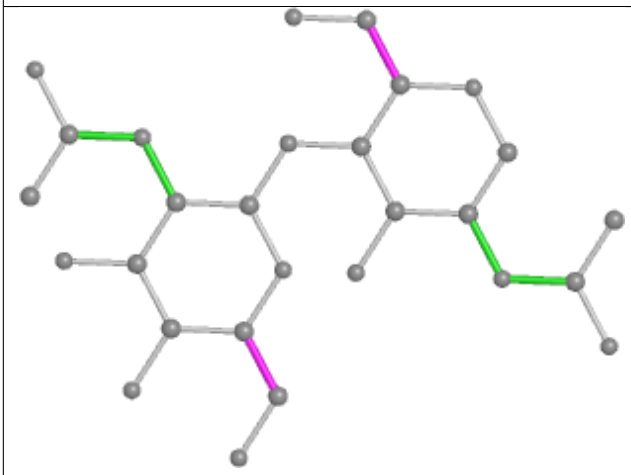
Oligosaccharide Chain C



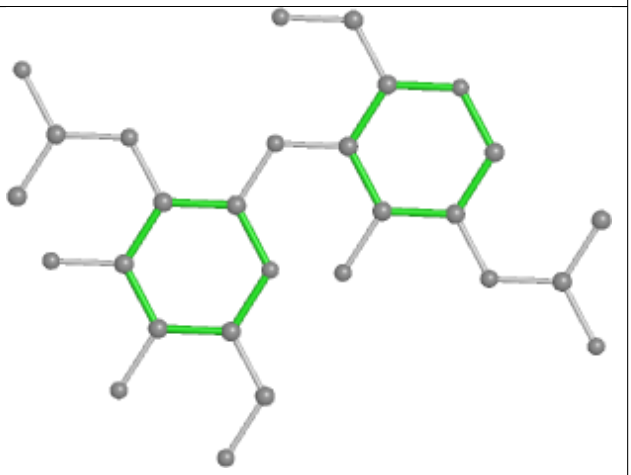
Bond lengths



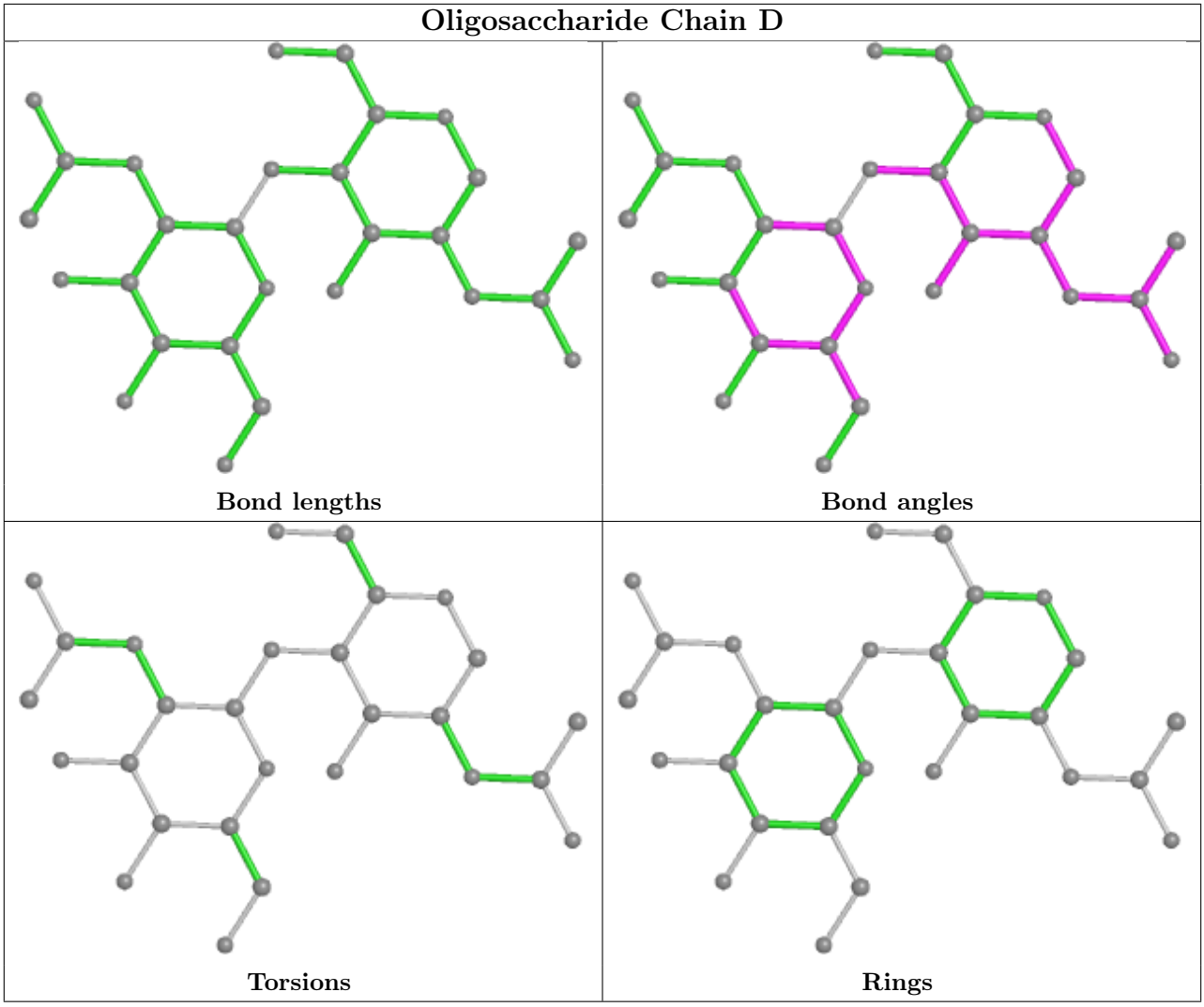
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

4 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	$\#\|Z\| > 2$
3	NAG	A	803	1	14,14,15	0.96	1 (7%)	17,19,21	1.69	5 (29%)
4	GAL	A	804	-	12,12,12	0.95	1 (8%)	17,17,17	1.44	3 (17%)
3	NAG	B	803	1	14,14,15	0.95	0	17,19,21	1.82	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	GAL	B	804	-	12,12,12	0.69	0	17,17,17	1.12	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	803	1	-	2/6/23/26	0/1/1/1
4	GAL	A	804	-	-	1/2/22/22	0/1/1/1
3	NAG	B	803	1	-	2/6/23/26	0/1/1/1
4	GAL	B	804	-	-	1/2/22/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	803	NAG	C1-C2	2.20	1.55	1.52
4	A	804	GAL	O4-C4	2.11	1.47	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	804	GAL	O1-C1-O5	-3.70	99.27	110.38
4	A	804	GAL	C1-O5-C5	-3.65	106.78	113.66
3	B	803	NAG	C2-N2-C7	3.54	127.94	122.90
3	B	803	NAG	O7-C7-C8	-3.52	115.53	122.06
3	A	803	NAG	C1-O5-C5	3.29	116.64	112.19
3	A	803	NAG	C1-C2-N2	3.00	115.61	110.49
4	A	804	GAL	O1-C1-O5	-2.97	101.48	110.38
3	B	803	NAG	C8-C7-N2	2.68	120.64	116.10
3	A	803	NAG	C6-C5-C4	-2.52	107.09	113.00
3	A	803	NAG	O5-C5-C6	2.41	110.99	107.20
3	B	803	NAG	O6-C6-C5	-2.28	103.47	111.29
3	B	803	NAG	O5-C1-C2	-2.18	107.84	111.29
4	A	804	GAL	O5-C5-C4	-2.15	105.78	109.69
3	A	803	NAG	C2-N2-C7	2.15	125.97	122.90

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	803	NAG	C8-C7-N2-C2
3	A	803	NAG	O7-C7-N2-C2
3	B	803	NAG	C8-C7-N2-C2
3	B	803	NAG	O7-C7-N2-C2
4	B	804	GAL	O5-C5-C6-O6
4	A	804	GAL	O5-C5-C6-O6

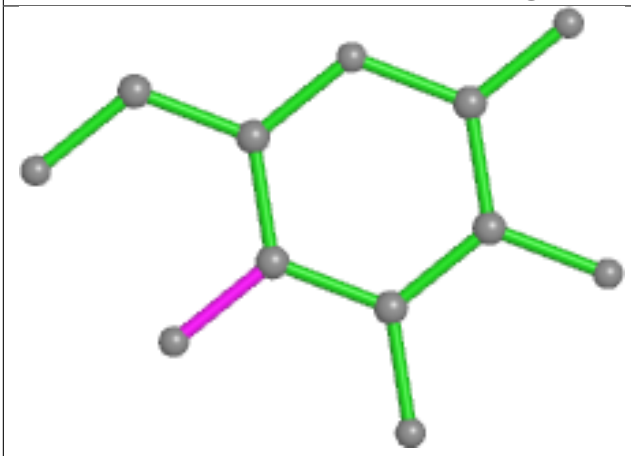
There are no ring outliers.

4 monomers are involved in 13 short contacts:

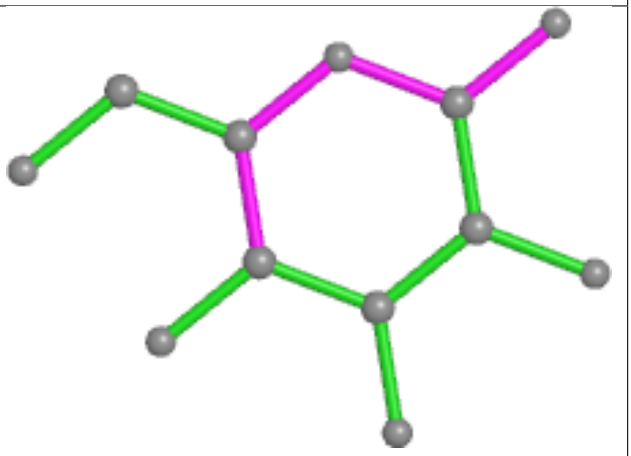
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	803	NAG	5	0
4	A	804	GAL	1	0
3	B	803	NAG	6	0
4	B	804	GAL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

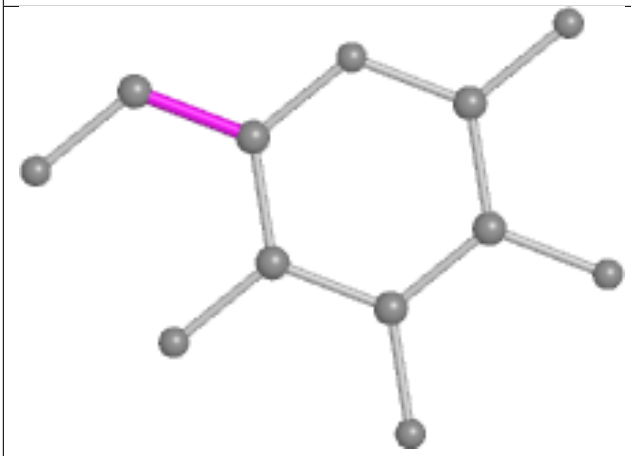
Ligand GAL A 804



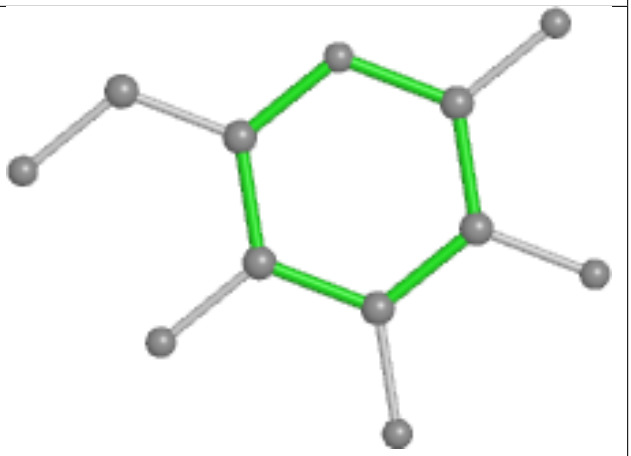
Bond lengths



Bond angles

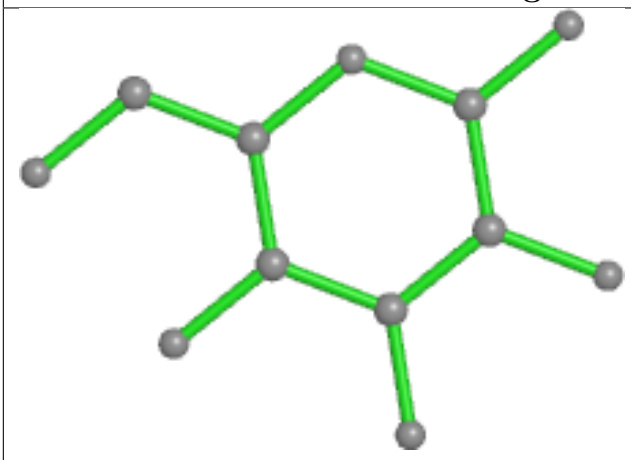


Torsions

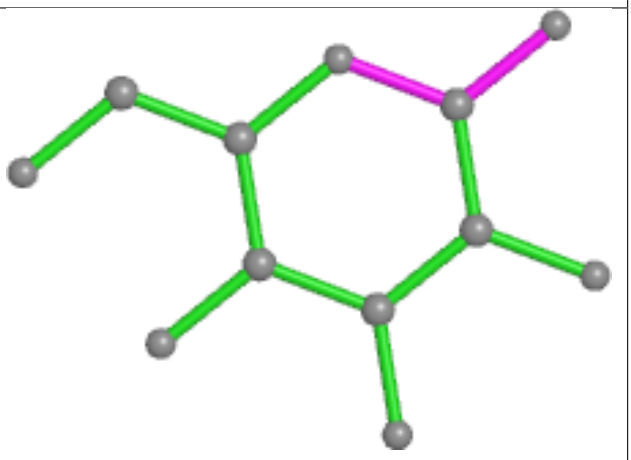


Rings

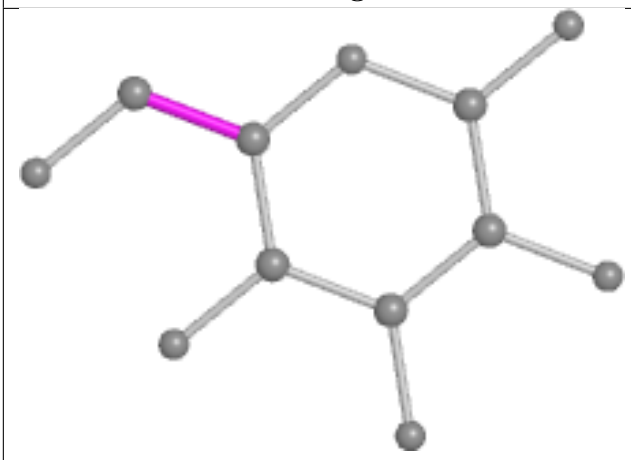
Ligand GAL B 804



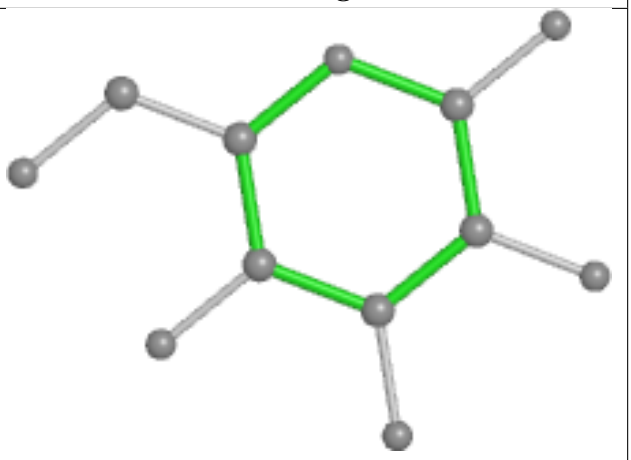
Bond lengths



Bond angles



Torsions



Rings

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

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	705/718 (98%)	-0.06	28 (3%)	38	32	13, 24, 46, 149	0
1	B	705/718 (98%)	-0.09	26 (3%)	41	36	14, 23, 52, 96	0
All	All	1410/1436 (98%)	-0.07	54 (3%)	40	35	13, 24, 49, 149	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	445	ASP	21.4
1	A	448	THR	17.1
1	A	599	SER	15.5
1	A	446	SER	13.0
1	A	600	SER	9.3
1	B	428	GLY	9.1
1	A	486	GLY	6.9
1	A	601	SER	6.4
1	B	448	THR	6.3
1	B	449	LEU	5.7
1	B	450	THR	4.8
1	B	606	ARG	4.7
1	A	449	LEU	4.7
1	B	429	GLY	4.6
1	A	604	TRP	4.4
1	A	608	SER	4.3
1	B	609	LEU	3.9
1	B	603	GLU	3.8
1	B	446	SER	3.8
1	A	597	SER	3.6
1	A	609	LEU	3.6
1	A	447	ASP	3.5
1	B	486	GLY	3.4
1	B	485	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	368	GLY	3.1
1	B	447	ASP	3.1
1	A	428	GLY	3.0
1	B	601	SER	3.0
1	A	380	ARG	2.9
1	B	452	ASN	2.9
1	A	603	GLU	2.8
1	B	600	SER	2.8
1	A	607	GLY	2.8
1	B	451	ALA	2.7
1	A	610	MET	2.6
1	A	85	GLY	2.6
1	A	444	ASP	2.6
1	A	598	GLY	2.6
1	A	605	VAL	2.6
1	A	430	GLY	2.5
1	A	602	VAL	2.5
1	B	608	SER	2.5
1	B	628	GLY	2.4
1	B	700	SER	2.4
1	B	427	ALA	2.4
1	B	445	ASP	2.3
1	B	434	GLN	2.3
1	B	484	LYS	2.2
1	B	719	LEU	2.1
1	B	436	TYR	2.1
1	A	238	ARG	2.1
1	A	393	ASN	2.1
1	B	610	MET	2.1
1	A	606	ARG	2.1

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

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

6.3 Carbohydrates (i)

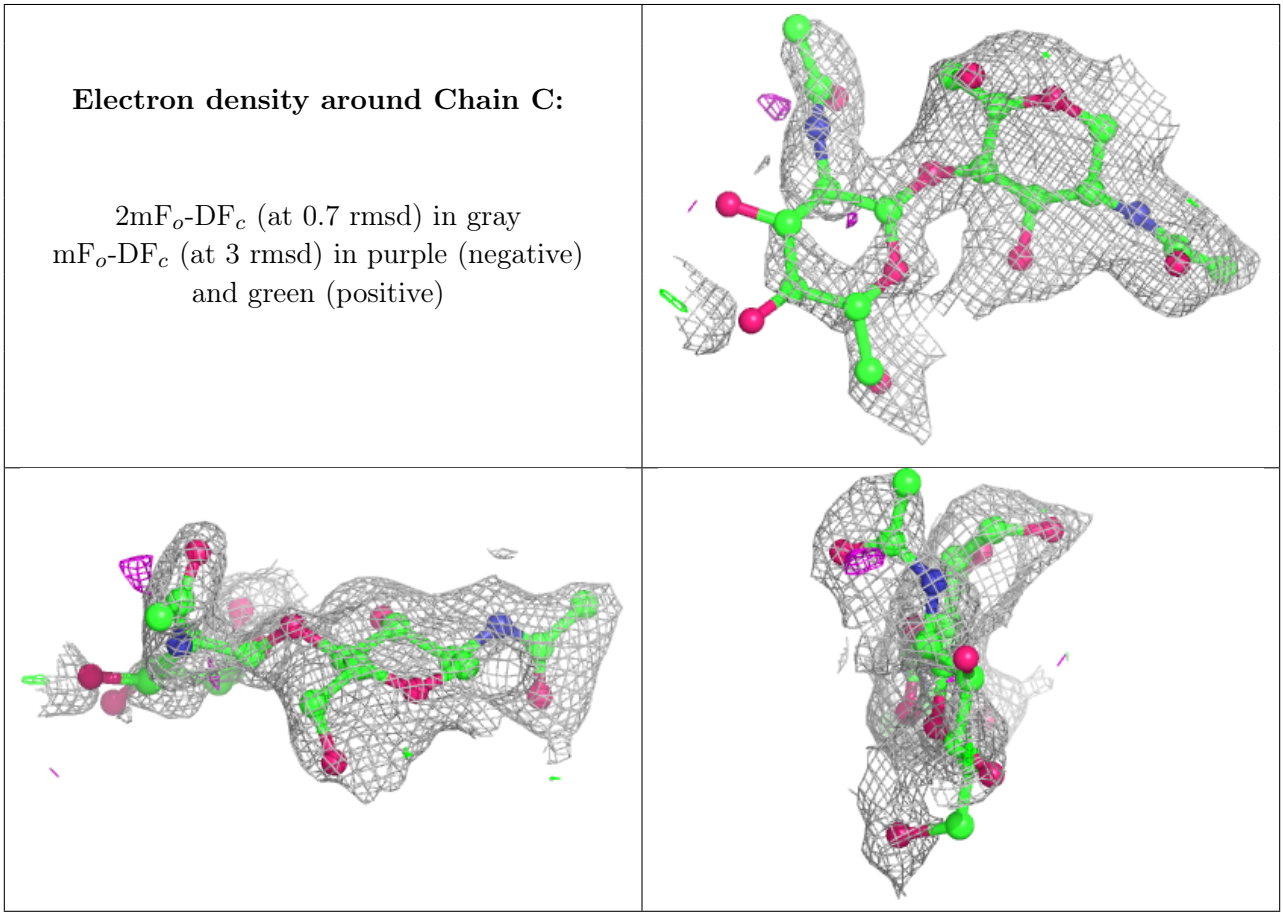
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	C	2	14/15	0.56	0.41	52,73,83,88	0
2	NAG	D	2	14/15	0.76	0.23	65,75,92,96	0
2	NAG	C	1	14/15	0.89	0.12	37,42,63,65	0
2	NAG	D	1	14/15	0.94	0.08	28,35,44,52	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.

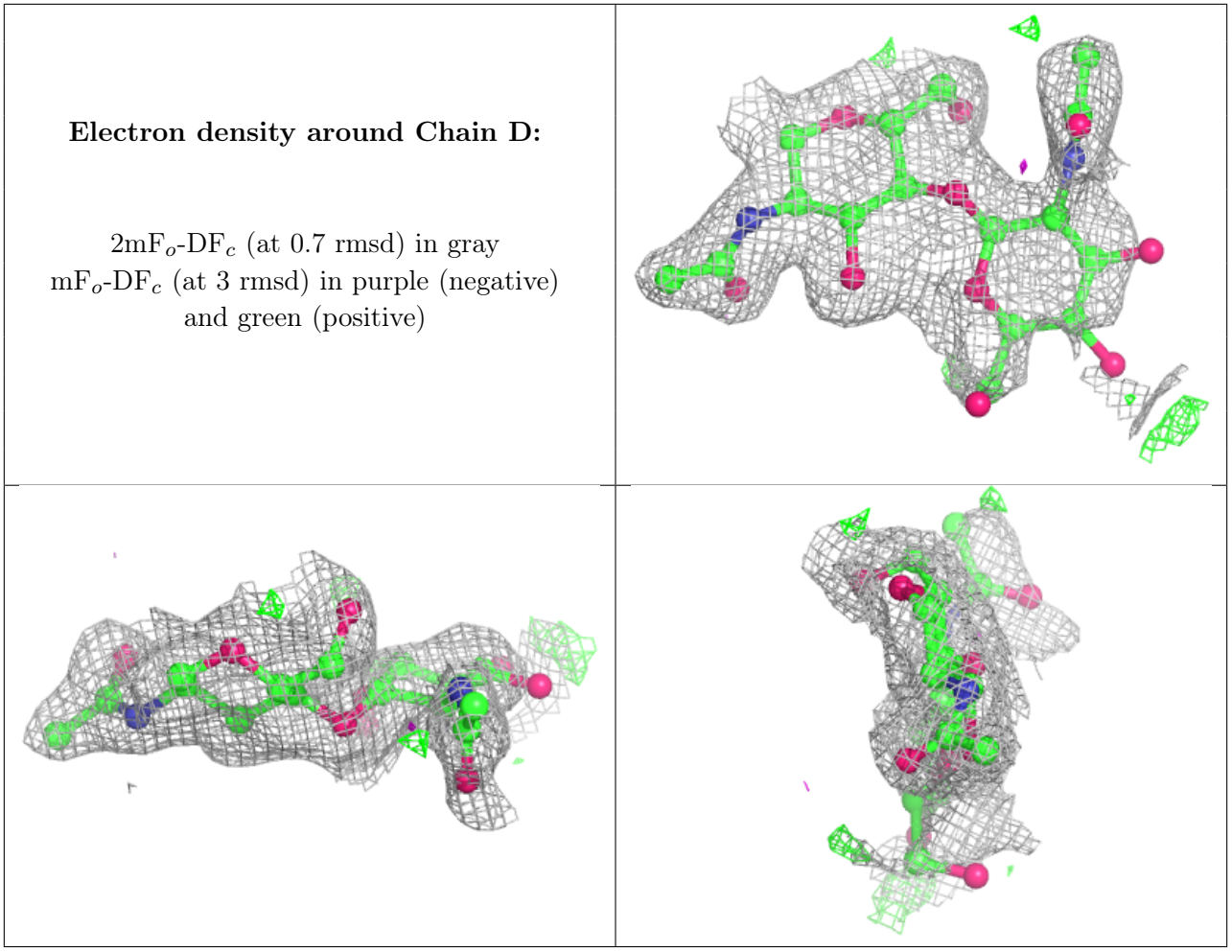
Electron density around Chain C:

$2mF_o$-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)



6.4 Ligands

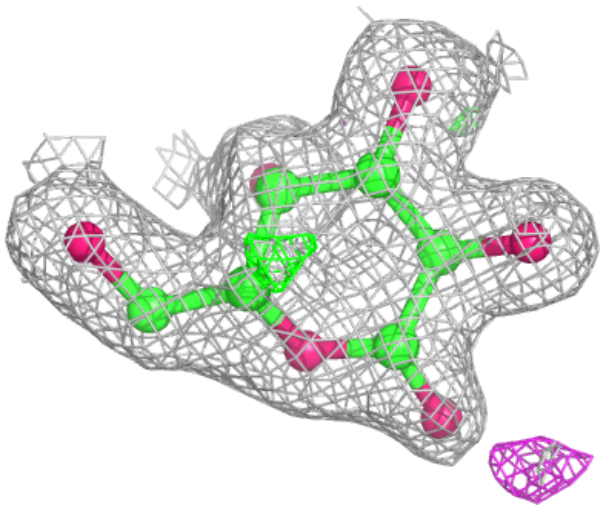
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

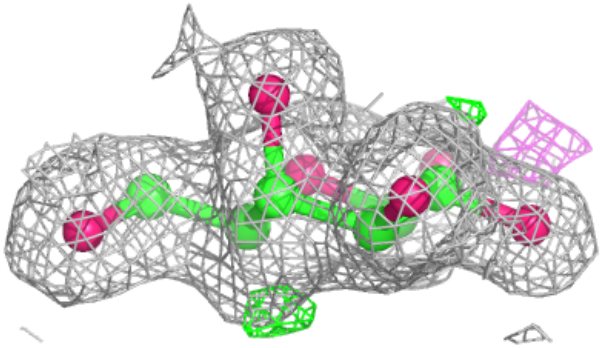
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	A	803	14/15	0.81	0.26	32,45,54,59	0
3	NAG	B	803	14/15	0.82	0.20	24,40,48,48	0
4	GAL	A	804	12/12	0.93	0.10	19,21,26,32	0
4	GAL	B	804	12/12	0.96	0.13	17,18,20,26	0

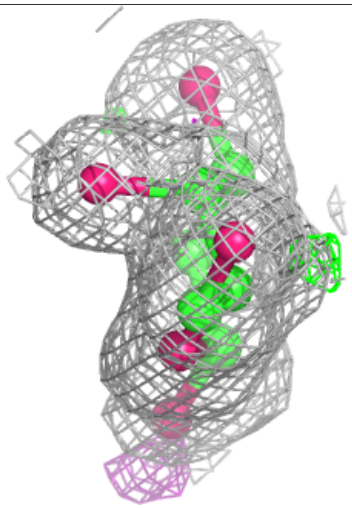
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around GAL A 804:

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

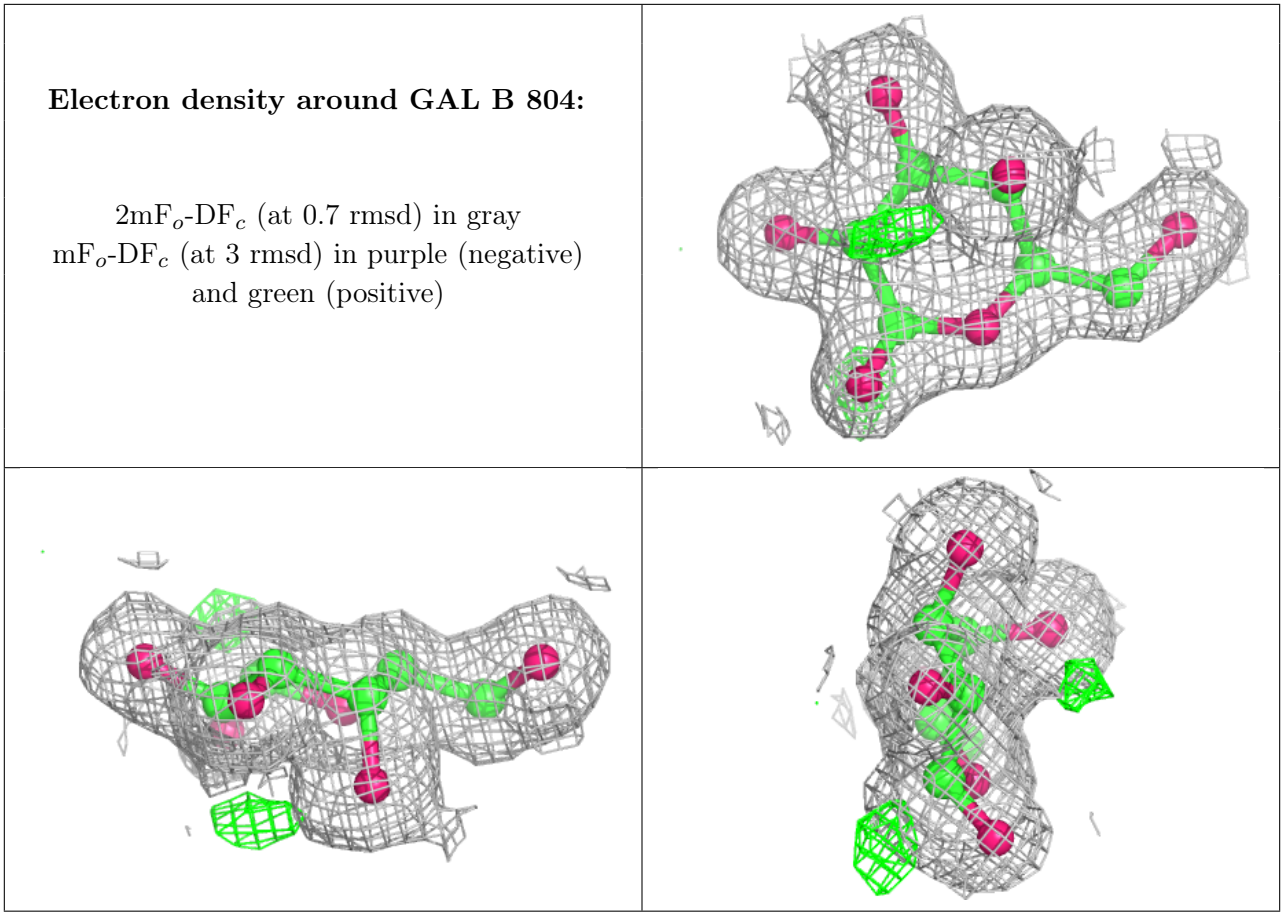






Electron density around GAL B 804:

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



6.5 Other polymers

There are no such residues in this entry.