



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 07:48 AM BST

PDB ID : 3HG2
Title : Human alpha-galactosidase catalytic mechanism 1. Empty active site
Authors : Guce, A.I.; Clark, N.E.; Garman, S.C.
Deposited on : 2009-05-13
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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 : 2.13.1
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

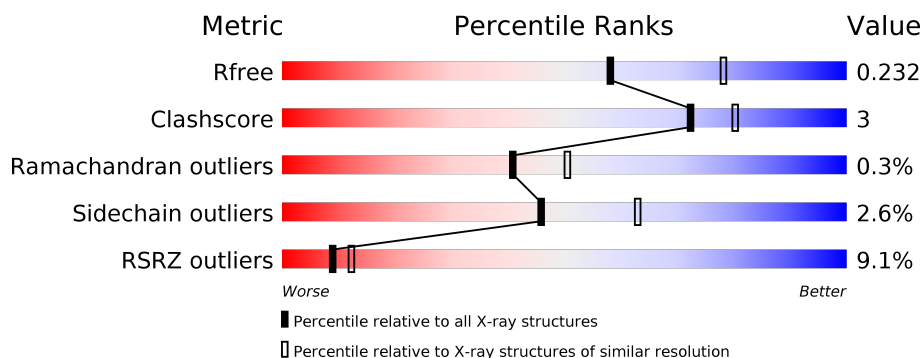
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. 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	398	<div> <div>8%</div> <div> <div></div> <div>91%</div> <div>6% ..</div> </div> </div>
1	B	398	<div> <div>10%</div> <div> <div></div> <div>88%</div> <div>10% ..</div> </div> </div>
2	C	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>
3	D	3	<div> <div></div> <div> <div>67%</div> <div>33%</div> </div> </div>
3	E	3	<div> <div></div> <div>100%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FUC	C	2	-	-	-	X
4	NAG	B	715	-	-	-	X

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6765 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Alpha-galactosidase A.

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

- Molecule 2 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 3 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
3	D	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	E	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 5 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



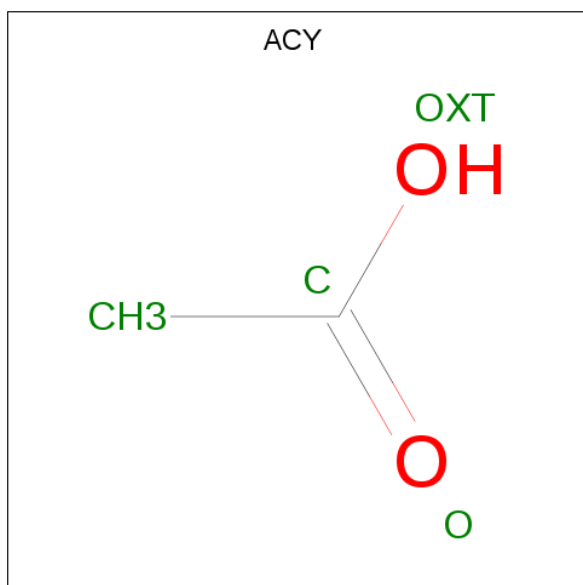
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		

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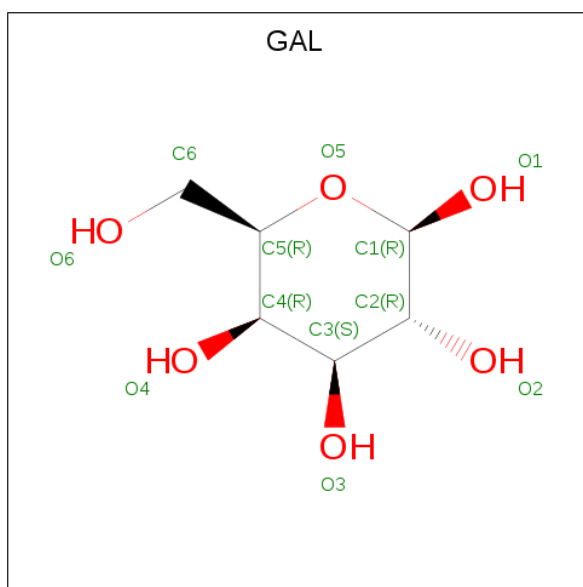
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is ACETIC ACID (three-letter code: ACY) (formula: C₂H₄O₂).



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

- Molecule 7 is beta-D-galactopyranose (three-letter code: GAL) (formula: C₆H₁₂O₆).



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

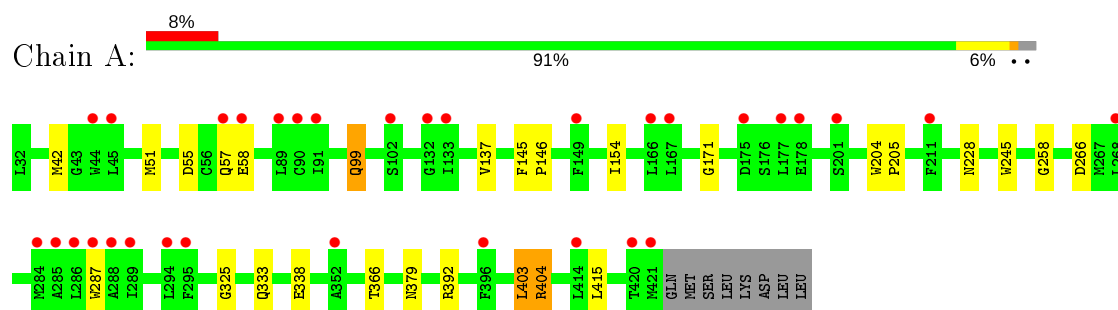
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	194	Total	O	0	0
			194	194		
8	B	135	Total	O	0	0
			135	135		

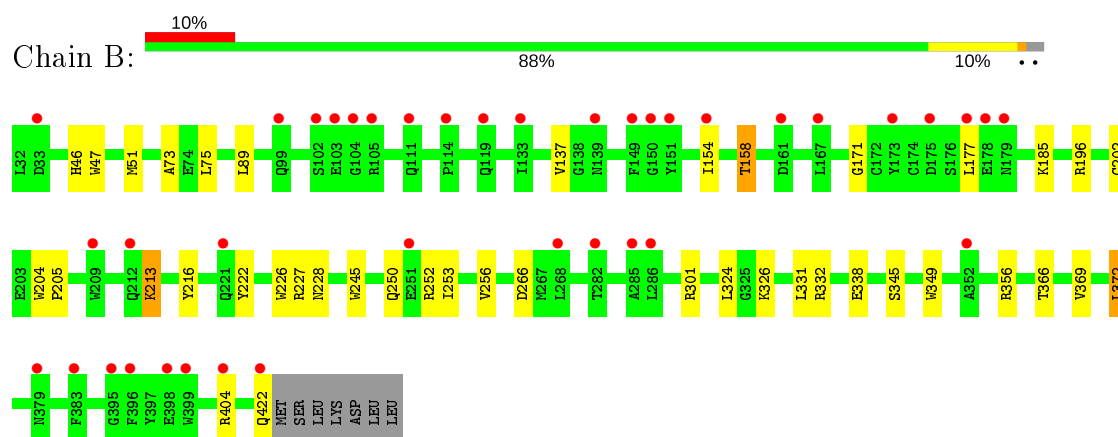
3 Residue-property plots [i](#)

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: Alpha-galactosidase A



- Molecule 1: Alpha-galactosidase A



- Molecule 2: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



MAG1
MAG2
B/M3

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

Chain E:

100%

MAG1
MAG2
B/M3

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	90.81Å 90.81Å 217.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.31 – 2.30 28.30 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.3 (28.31-2.30) 97.3 (28.30-2.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.38 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.176 , 0.202 0.215 , 0.232	Depositor DCC
R_{free} test set	2339 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	33.9	Xtriage
Anisotropy	0.002	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6765	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: BMA, NAG, GAL, SO4, ACY, FUC

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	0.41	0/3209	0.55	0/4358
1	B	0.41	0/3218	0.53	0/4370
All	All	0.41	0/6427	0.54	0/8728

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	3122	0	2981	18	0
1	B	3131	0	2989	24	0
2	C	24	0	22	0	0
3	D	39	0	34	0	0
3	E	39	0	34	0	0
4	A	14	0	13	0	0
4	B	28	0	26	0	0
5	A	10	0	0	0	0
5	B	5	0	0	0	0
6	A	4	0	3	0	0
6	B	8	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	12	0	12	2	0
8	A	194	0	0	5	0
8	B	135	0	0	1	0
All	All	6765	0	6120	42	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 (42) 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:366:THR:HG22	1:A:404:ARG:HD3	1.75	0.68
1:A:403:LEU:HD11	1:A:415:LEU:HD13	1.78	0.64
1:B:250:GLN:NE2	7:B:803:GAL:H1	2.16	0.61
1:B:137:VAL:HG12	1:B:171:GLY:HA2	1.88	0.56
1:B:250:GLN:HE21	7:B:803:GAL:H1	1.71	0.55
1:B:75:LEU:CD1	1:B:301:ARG:HG2	2.37	0.55
1:B:154:ILE:O	1:B:158:THR:HG22	2.07	0.54
1:A:403:LEU:HD11	1:A:415:LEU:CD1	2.37	0.54
1:B:369:VAL:HA	1:B:372:LEU:HD22	1.89	0.54
1:B:213:LYS:HD2	8:B:1294:HOH:O	2.08	0.54
1:A:154:ILE:HG12	8:A:1306:HOH:O	2.07	0.54
1:A:99:GLN:HB3	8:A:1328:HOH:O	2.08	0.53
1:A:55:ASP:OD2	1:A:58:GLU:HB2	2.08	0.52
1:B:75:LEU:HD11	1:B:301:ARG:HG2	1.91	0.52
1:B:366:THR:HG22	1:B:404:ARG:HG2	1.92	0.51
1:A:42:MET:HE1	8:A:1258:HOH:O	2.10	0.51
1:A:228:ASN:HB3	1:A:245:TRP:CH2	2.46	0.50
1:B:228:ASN:HB3	1:B:245:TRP:CH2	2.47	0.49
1:A:204:TRP:HB3	1:A:205:PRO:HD3	1.95	0.49
1:B:366:THR:CG2	1:B:404:ARG:HG2	2.45	0.46
1:A:42:MET:CE	8:A:1169:HOH:O	2.63	0.46
1:A:137:VAL:HG12	1:A:171:GLY:HA2	1.99	0.45
1:A:333:GLN:HG3	1:A:338:GLU:HG2	2.00	0.44
1:B:216:TYR:HE1	1:B:228:ASN:HD21	1.65	0.44
1:B:253:ILE:O	1:B:256:VAL:HG22	2.17	0.44
1:A:204:TRP:HB3	1:A:205:PRO:CD	2.48	0.44
1:A:392:ARG:NH2	8:A:1040:HOH:O	2.47	0.43
1:B:202:CYS:O	1:B:226:TRP:HA	2.19	0.42
1:A:145:PHE:HB3	1:A:146:PRO:CD	2.49	0.42
1:B:204:TRP:HB3	1:B:205:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:GLN:HE21	1:B:422:GLN:HB2	1.68	0.41
1:A:145:PHE:HB3	1:A:146:PRO:HD2	2.02	0.41
1:B:213:LYS:NZ	1:B:252:ARG:HH22	2.19	0.41
1:B:331:LEU:HG	1:B:332:ARG:HG3	2.01	0.41
1:B:73:ALA:HB2	1:B:89:LEU:HD22	2.03	0.41
1:A:366:THR:CG2	1:A:404:ARG:HD3	2.48	0.40
1:A:258:GLY:HA2	1:A:325:GLY:O	2.22	0.40
1:B:213:LYS:HG3	1:B:252:ARG:HH12	1.86	0.40
1:B:185:LYS:HG2	1:B:222:TYR:CZ	2.56	0.40
1:B:47:TRP:O	1:B:51:MET:HG2	2.21	0.40
1:B:338:GLU:OE2	1:B:356:ARG:NH1	2.55	0.40
1:B:205:PRO:HG2	1:B:227:ARG:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	388/398 (98%)	375 (97%)	12 (3%)	1 (0%)	41	50
1	B	389/398 (98%)	378 (97%)	10 (3%)	1 (0%)	41	50
All	All	777/796 (98%)	753 (97%)	22 (3%)	2 (0%)	41	50

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	331/339 (98%)	324 (98%)	7 (2%)	53	70
1	B	332/339 (98%)	322 (97%)	10 (3%)	41	57
All	All	663/678 (98%)	646 (97%)	17 (3%)	46	63

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	MET
1	A	57	GLN
1	A	99	GLN
1	A	287	TRP
1	A	379	ASN
1	A	403	LEU
1	A	404	ARG
1	B	46	HIS
1	B	158	THR
1	B	177	LEU
1	B	196	ARG
1	B	213	LYS
1	B	324	LEU
1	B	326	LYS
1	B	345	SER
1	B	349	TRP
1	B	372	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	111	GLN
1	A	228	ASN
1	A	249	ASN
1	A	379	ASN

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Mol	Chain	Res	Type
1	B	179	ASN
1	B	228	ASN
1	B	386	GLN
1	B	416	GLN
1	B	422	GLN

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 ⓘ

8 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	0.48	0	17,19,21	0.99	1 (5%)
2	FUC	C	2	2	10,10,11	0.67	0	14,14,16	0.89	0
3	NAG	D	1	1,3	14,14,15	0.49	0	17,19,21	0.85	0
3	NAG	D	2	3	14,14,15	0.51	0	17,19,21	0.80	0
3	BMA	D	3	3	11,11,12	0.44	0	15,15,17	0.80	1 (6%)
3	NAG	E	1	1,3	14,14,15	0.55	0	17,19,21	1.17	3 (17%)
3	NAG	E	2	3	14,14,15	0.54	0	17,19,21	1.11	1 (5%)
3	BMA	E	3	3	11,11,12	0.53	0	15,15,17	0.89	1 (6%)

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	FUC	C	2	2	-	-	0/1/1/1
3	NAG	D	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	BMA	D	3	3	-	2/2/19/22	0/1/1/1
3	NAG	E	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	BMA	E	3	3	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2	NAG	C4-C3-C2	3.00	115.41	111.02
2	C	1	NAG	C1-O5-C5	2.80	115.98	112.19
3	E	1	NAG	O5-C1-C2	-2.49	107.36	111.29
3	E	1	NAG	C2-N2-C7	2.35	126.25	122.90
3	E	1	NAG	C1-O5-C5	2.29	115.29	112.19
3	D	3	BMA	C1-O5-C5	2.23	115.22	112.19
3	E	3	BMA	O5-C5-C6	2.09	110.48	107.20

There are no chirality outliers.

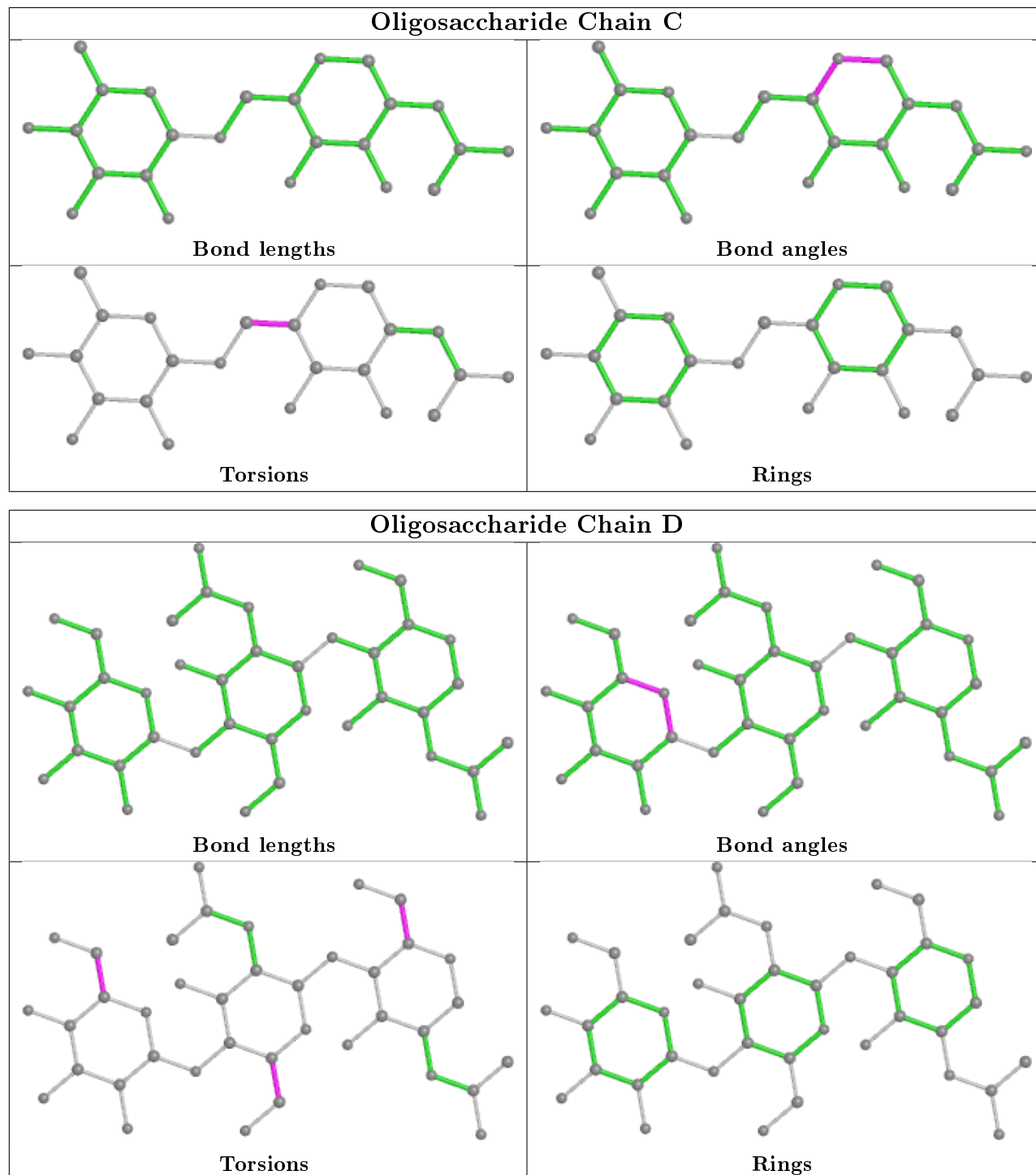
All (14) torsion outliers are listed below:

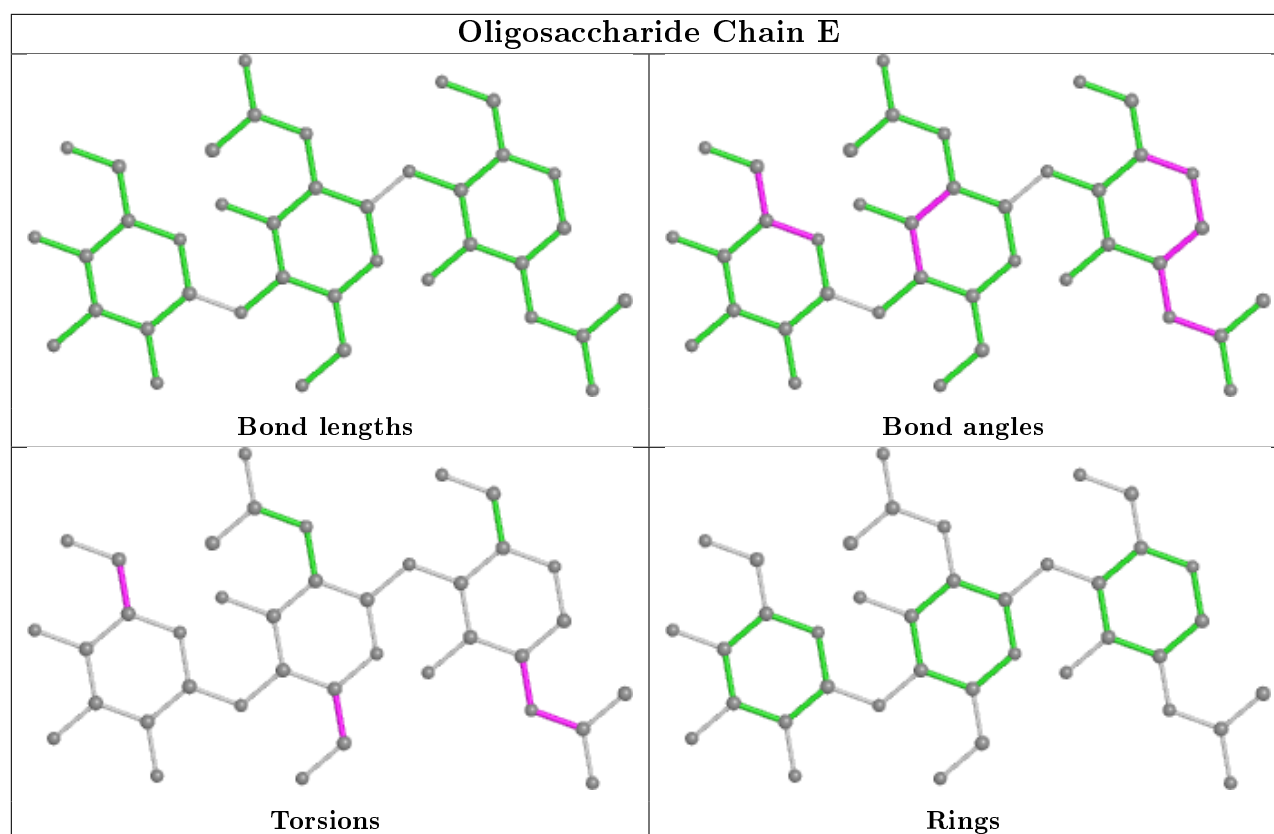
Mol	Chain	Res	Type	Atoms
3	E	1	NAG	C3-C2-N2-C7
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	E	3	BMA	O5-C5-C6-O6
3	D	3	BMA	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	D	3	BMA	C4-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
3	E	3	BMA	C4-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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





5.6 Ligand geometry [i](#)

10 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	$\# Z > 2$
6	ACY	A	841	-	1,3,3	1.13	0	0,3,3	0.00	-
5	SO4	B	821	-	4,4,4	0.13	0	6,6,6	0.10	0
5	SO4	A	823	-	4,4,4	0.15	0	6,6,6	0.29	0
6	ACY	B	842	-	1,3,3	1.61	0	0,3,3	0.00	-
4	NAG	A	715	1	14,14,15	0.55	0	17,19,21	1.01	1 (5%)
4	NAG	B	639	1	14,14,15	0.62	0	17,19,21	1.37	3 (17%)
7	GAL	B	803	-	12,12,12	0.63	0	17,17,17	1.00	1 (5%)
4	NAG	B	715	1	14,14,15	0.51	0	17,19,21	0.76	0
5	SO4	A	822	-	4,4,4	0.15	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	ACY	B	843	-	1,3,3	1.53	0	0,3,3	0.00	-

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	GAL	B	803	-	-	0/2/22/22	0/1/1/1
4	NAG	B	715	1	-	2/6/23/26	0/1/1/1
4	NAG	A	715	1	-	0/6/23/26	0/1/1/1
4	NAG	B	639	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	639	NAG	C4-C3-C2	2.65	114.90	111.02
4	A	715	NAG	C1-O5-C5	2.40	115.44	112.19
4	B	639	NAG	C2-N2-C7	2.40	126.31	122.90
4	B	639	NAG	O5-C5-C6	2.38	110.94	107.20
7	B	803	GAL	C4-C3-C2	2.13	114.55	110.82

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	639	NAG	O5-C5-C6-O6
4	B	639	NAG	C4-C5-C6-O6
4	B	715	NAG	C4-C5-C6-O6
4	B	715	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	803	GAL	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	390/398 (97%)	0.28	32 (8%) 11 15	30, 35, 42, 51	0
1	B	391/398 (98%)	0.42	39 (9%) 7 10	30, 35, 42, 55	0
All	All	781/796 (98%)	0.35	71 (9%) 9 12	30, 35, 42, 55	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	421	MET	5.5
1	B	102	SER	5.4
1	B	149	PHE	5.2
1	A	211	PHE	4.9
1	A	102	SER	4.7
1	A	91	ILE	4.0
1	A	133	ILE	3.9
1	B	103	GLU	3.6
1	B	286	LEU	3.5
1	A	45	LEU	3.5
1	B	178	GLU	3.5
1	B	422	GLN	3.4
1	A	90	CYS	3.4
1	A	287	TRP	3.2
1	A	57	GLN	3.1
1	A	288	ALA	3.0
1	A	285	ALA	3.0
1	B	150	GLY	3.0
1	A	286	LEU	2.9
1	A	268	LEU	2.9
1	B	104	GLY	2.9
1	B	133	ILE	2.9
1	B	99	GLN	2.8
1	B	396	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	294	LEU	2.8
1	B	379	ASN	2.8
1	B	175	ASP	2.7
1	B	154	ILE	2.7
1	A	166	LEU	2.7
1	B	119	GLN	2.6
1	A	420	THR	2.6
1	A	295	PHE	2.6
1	B	173	TYR	2.6
1	A	289	ILE	2.6
1	B	352	ALA	2.5
1	A	177	LEU	2.5
1	B	395	GLY	2.4
1	A	44	TRP	2.4
1	B	398	GLU	2.4
1	A	58	GLU	2.4
1	A	175	ASP	2.4
1	A	178	GLU	2.4
1	B	151	TYR	2.3
1	B	167	LEU	2.3
1	B	177	LEU	2.3
1	B	383	PHE	2.3
1	B	33	ASP	2.3
1	B	179	ASN	2.2
1	A	89	LEU	2.2
1	A	284	MET	2.2
1	A	396	PHE	2.2
1	B	251	GLU	2.2
1	A	167	LEU	2.2
1	B	285	ALA	2.1
1	B	209	TRP	2.1
1	B	139	ASN	2.1
1	B	221	GLN	2.1
1	A	132	GLY	2.1
1	B	399	TRP	2.1
1	B	111	GLN	2.1
1	B	404	ARG	2.1
1	A	352	ALA	2.1
1	A	414	LEU	2.1
1	B	268	LEU	2.1
1	A	149	PHE	2.1
1	B	114	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	282	THR	2.0
1	A	201	SER	2.0
1	B	161	ASP	2.0
1	B	105	ARG	2.0
1	B	212	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

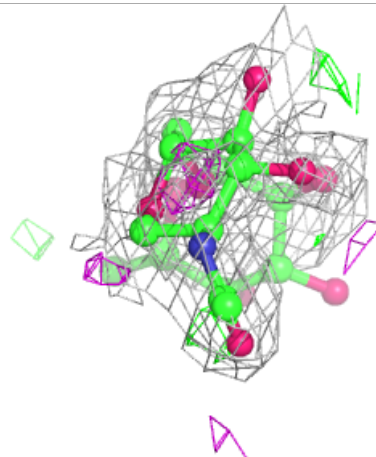
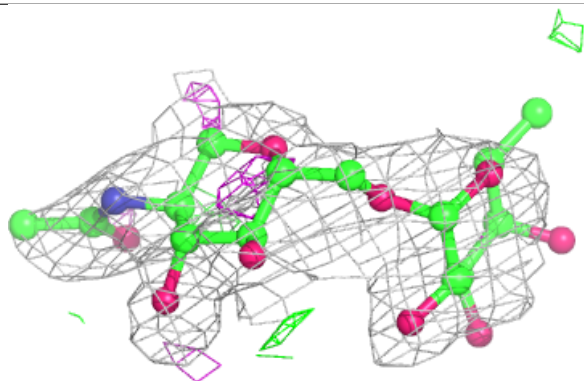
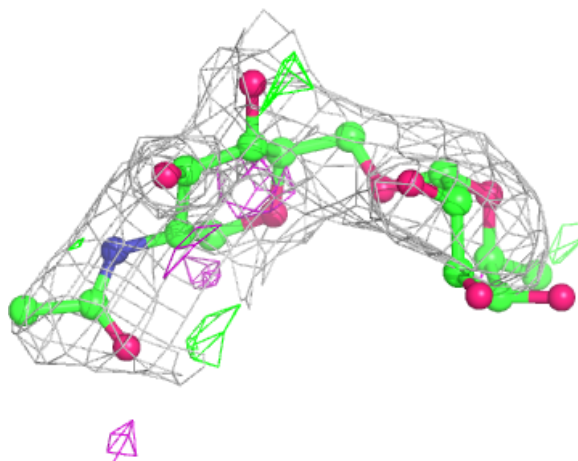
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BMA	E	3	11/12	0.43	0.34	72,74,74,75	0
2	NAG	C	1	14/15	0.75	0.31	58,62,67,71	0
3	BMA	D	3	11/12	0.79	0.30	64,66,67,67	0
2	FUC	C	2	10/11	0.80	0.49	73,75,75,76	0
3	NAG	E	1	14/15	0.85	0.20	52,57,60,62	0
3	NAG	E	2	14/15	0.87	0.27	63,65,67,70	0
3	NAG	D	2	14/15	0.93	0.18	55,58,59,62	0
3	NAG	D	1	14/15	0.94	0.14	45,46,49,52	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.

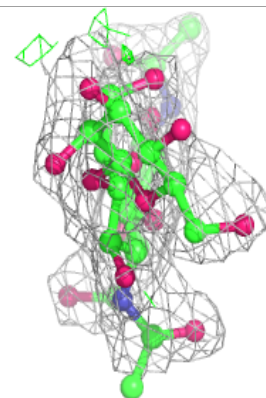
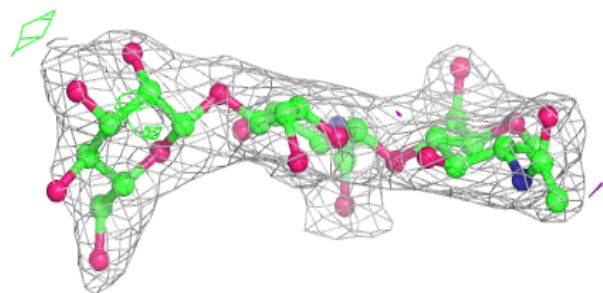
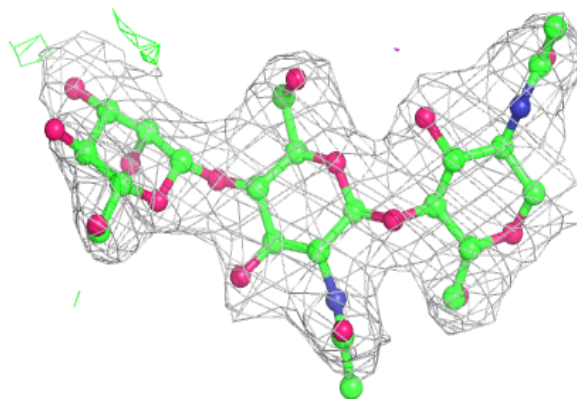
Electron density around Chain C:

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

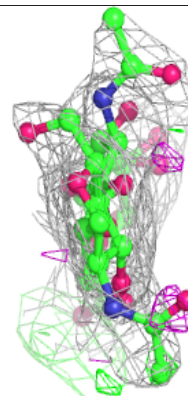
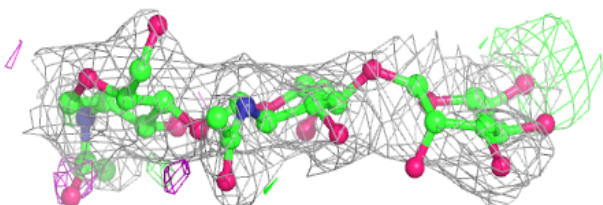
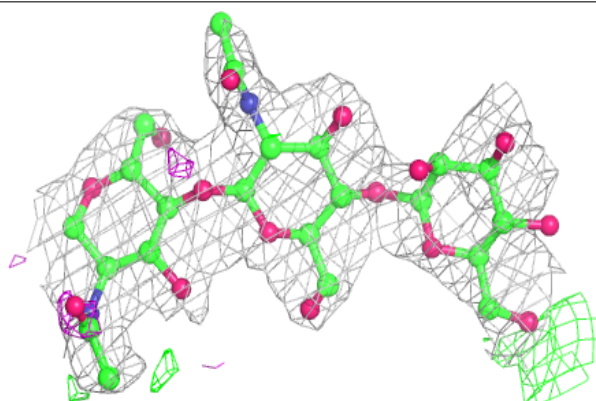


Electron density around Chain D:

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

**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)



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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	B	639	14/15	0.70	0.37	56,61,61,61	0
4	NAG	B	715	14/15	0.70	0.40	58,62,64,65	0
7	GAL	B	803	12/12	0.71	0.20	68,68,69,69	0
6	ACY	A	841	4/4	0.73	0.20	67,67,67,67	0
6	ACY	B	842	4/4	0.87	0.18	66,66,66,66	0
5	SO4	A	822	5/5	0.88	0.41	92,92,92,93	0
4	NAG	A	715	14/15	0.91	0.24	53,57,58,58	0
6	ACY	B	843	4/4	0.93	0.15	70,70,70,70	0
5	SO4	A	823	5/5	0.98	0.10	49,49,50,50	0
5	SO4	B	821	5/5	0.98	0.18	60,60,61,61	0

6.5 Other polymers

There are no such residues in this entry.