



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:51 AM UTC

PDB ID : 9GRB / pdb\_00009grb  
Title : Crystal structure of mouse Carboxylesterase 2b (Ces2b)  
Authors : Rammer, L.; Eisner, H.; Sagmeister, T.; Oberer, M.  
Deposited on : 2024-09-11  
Resolution : 2.55 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](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

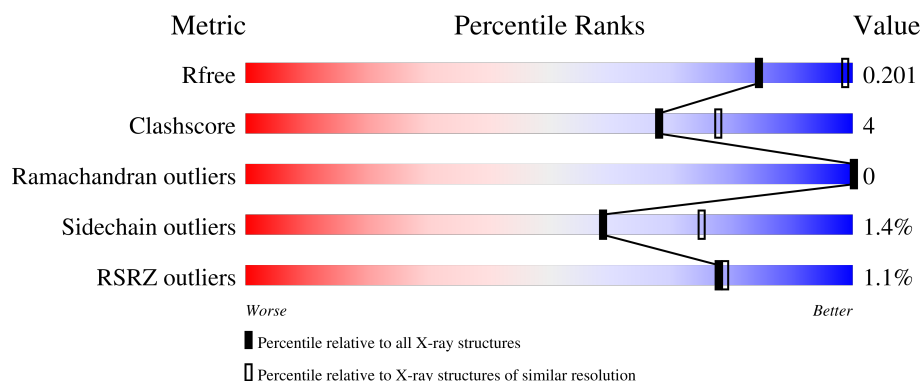
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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))
$R_{free}$	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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  $\geq 3$ , 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	523	<div> <div>%</div> <div>91% 7% .</div> </div>
1	B	523	<div> <div>%</div> <div>92% 6% ..</div> </div>
1	C	523	<div> <div>2%</div> <div>91% 8% .</div> </div>
1	D	523	<div> <div>%</div> <div>92% 6% ..</div> </div>
2	E	2	<div> <div>50% 50%</div> </div>

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Mol	Chain	Length	Quality of chain
2	G	2	

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	G	2	X	-	-	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16874 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 Carboxylic ester hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	520	Total	C	N	O	S	0	0	0
			4065	2597	690	753	25			
1	A	521	Total	C	N	O	S	0	0	0
			4071	2604	691	750	26			
1	B	516	Total	C	N	O	S	0	0	0
			4030	2577	685	743	25			
1	C	520	Total	C	N	O	S	0	1	0
			4075	2607	693	749	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	G	2	Total	C	N	O	0	0	0
			24	14	1	9			
2	E	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

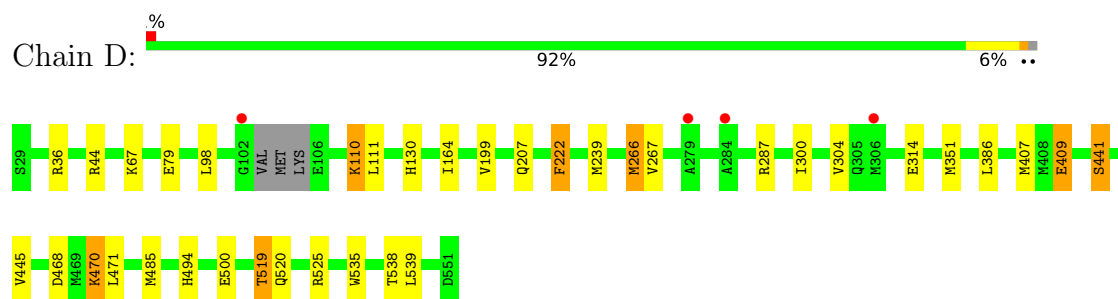
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	137	Total	O	0	0
			137	137		
4	A	175	Total	O	0	0
			175	175		
4	B	134	Total	O	0	0
			134	134		
4	C	125	Total	O	0	0
			125	125		

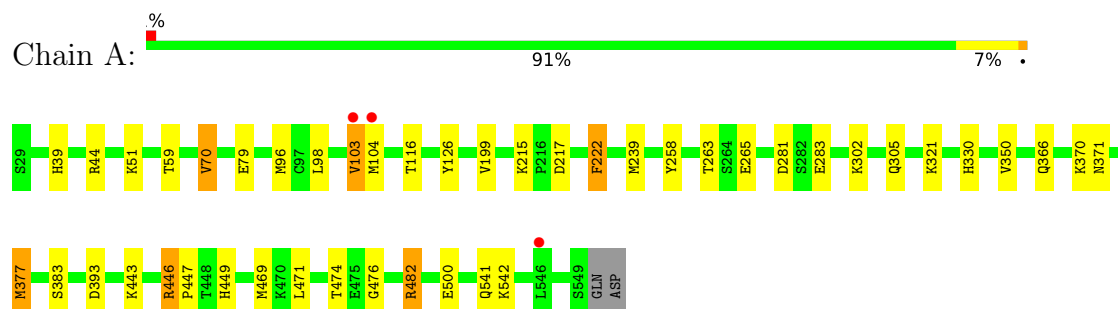
### 3 Residue-property plots [i](#)

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.

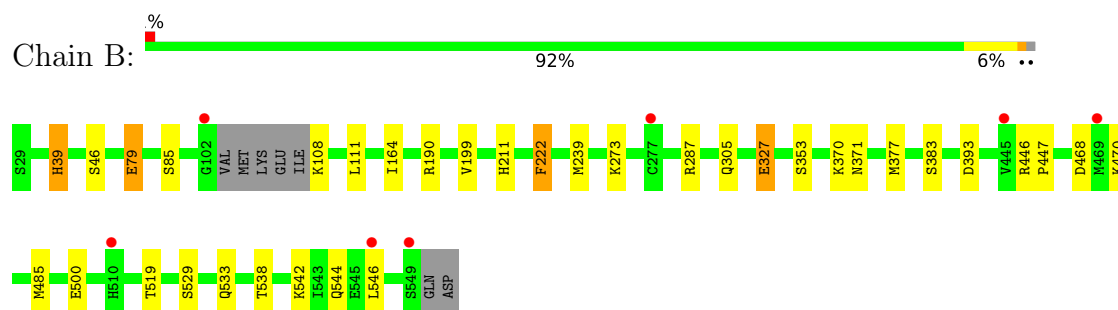
- Molecule 1: Carboxylic ester hydrolase



- Molecule 1: Carboxylic ester hydrolase

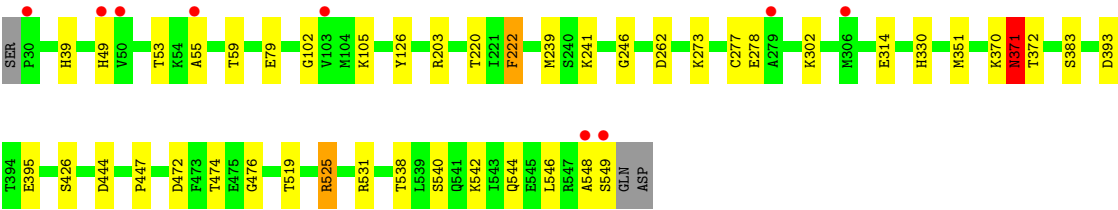


- Molecule 1: Carboxylic ester hydrolase

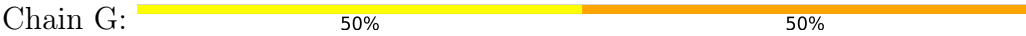


- Molecule 1: Carboxylic ester hydrolase





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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	180.75Å 109.80Å 135.44Å 90.00° 92.89° 90.00°	Depositor
Resolution (Å)	46.91 – 2.55 46.91 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.3 (46.91-2.55) 99.3 (46.91-2.55)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.59 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.105)	Depositor
R, $R_{free}$	0.171 , 0.205 (Not available) , 0.201	Depositor DCC
$R_{free}$ test set	4466 reflections (5.21%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.1	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 57.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.003 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	16874	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, NAG

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	0.63	0/4179	1.13	6/5678 (0.1%)
1	B	0.60	0/4137	1.12	10/5621 (0.2%)
1	C	0.61	2/4184 (0.0%)	1.61	16/5684 (0.3%)
1	D	0.60	0/4172	1.10	7/5667 (0.1%)
All	All	0.61	2/16672 (0.0%)	1.26	39/22650 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	3
1	D	0	2
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	372	THR	N-CA	6.92	1.54	1.46
1	C	371	ASN	C-O	-5.95	1.17	1.24

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	371	ASN	O-C-N	-85.47	34.04	122.07
1	C	371	ASN	CA-C-O	17.58	139.28	120.82
1	D	409	GLU	CB-CA-C	-9.02	95.82	110.79
1	A	541	GLN	CB-CA-C	8.48	124.88	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	39	HIS	CA-CB-CG	-8.46	105.34	113.80
1	D	110	LYS	CB-CG-CD	7.28	128.05	111.30
1	C	371	ASN	CA-C-N	-7.13	111.17	120.44
1	C	371	ASN	C-N-CA	-7.13	111.17	120.44
1	C	222	PHE	CA-CB-CG	6.89	120.69	113.80
1	D	525	ARG	N-CA-CB	-6.82	98.83	111.52
1	D	222	PHE	CA-CB-CG	6.76	120.56	113.80
1	C	372	THR	N-CA-C	6.72	118.26	111.07
1	B	222	PHE	CA-CB-CG	6.67	120.47	113.80
1	A	222	PHE	CA-CB-CG	6.30	120.10	113.80
1	C	542	LYS	CB-CA-C	6.29	122.75	110.67
1	D	500	GLU	CB-CG-CD	6.13	123.01	112.60
1	D	519	THR	CA-CB-OG1	-6.10	100.45	109.60
1	B	519	THR	CA-CB-OG1	-6.07	100.50	109.60
1	C	49[A]	HIS	CA-C-N	-5.82	114.07	122.45
1	C	49[A]	HIS	C-N-CA	-5.82	114.07	122.45
1	C	49[B]	HIS	CA-C-N	-5.82	114.07	122.45
1	C	49[B]	HIS	C-N-CA	-5.82	114.07	122.45
1	C	447	PRO	CA-C-N	5.81	128.87	120.38
1	C	447	PRO	C-N-CA	5.81	128.87	120.38
1	B	468	ASP	CA-CB-CG	5.77	118.37	112.60
1	B	542	LYS	CB-CA-C	5.74	121.69	110.67
1	B	377	MET	CB-CG-SD	5.69	129.77	112.70
1	B	305	GLN	CB-CA-C	5.66	119.73	109.83
1	D	525	ARG	CB-CA-C	-5.63	97.94	109.94
1	A	482	ARG	NE-CZ-NH2	5.47	124.12	119.20
1	C	472	ASP	CA-CB-CG	5.34	117.94	112.60
1	A	500	GLU	CB-CG-CD	5.33	121.66	112.60
1	B	108	LYS	CA-CB-CG	5.31	124.72	114.10
1	A	446	ARG	NE-CZ-NH1	-5.30	116.20	121.50
1	A	70	VAL	N-CA-CB	-5.28	103.59	112.47
1	C	525	ARG	CG-CD-NE	-5.14	100.69	112.00
1	B	79	GLU	CB-CA-C	5.11	118.90	109.71
1	B	39	HIS	CB-CA-C	5.10	120.07	110.63
1	C	372	THR	CA-CB-OG1	-5.02	102.08	109.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	482	ARG	Sidechain
1	C	203	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	371	ASN	Mainchain
1	C	525	ARG	Sidechain
1	D	287	ARG	Sidechain
1	D	36	ARG	Sidechain

## 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	4071	0	4003	36	1
1	B	4030	0	3954	27	0
1	C	4075	0	4005	33	0
1	D	4065	0	3983	28	1
2	E	24	0	22	6	0
2	G	24	0	22	6	0
3	C	14	0	13	1	0
4	A	175	0	0	13	0
4	B	134	0	0	4	0
4	C	125	0	0	15	0
4	D	137	0	0	15	0
All	All	16874	0	16002	115	1

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 4.

All (115) 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:371:ASN:HD21	2:G:1:NAG:C1	1.29	1.43
1:A:371:ASN:ND2	2:E:1:NAG:C1	1.89	1.35
1:A:371:ASN:HD21	2:E:1:NAG:C1	1.41	1.33
1:B:371:ASN:ND2	2:G:1:NAG:C1	2.01	1.20
1:B:287:ARG:HD2	4:B:702:HOH:O	1.46	1.10
1:C:102:GLY:HA3	4:C:714:HOH:O	1.46	1.10
1:C:519:THR:HG23	4:C:754:HOH:O	1.64	0.96
1:A:39:HIS:HB3	4:A:839:HOH:O	1.65	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:538:THR:OG1	1:C:393:ASP:OD2	1.85	0.93
1:C:239:MET:HE1	1:C:314:GLU:HG2	1.54	0.90
1:C:239:MET:HE1	1:C:314:GLU:CG	2.02	0.90
1:C:241:LYS:HB3	4:C:806:HOH:O	1.71	0.89
1:B:393:ASP:OD2	1:C:538:THR:OG1	1.89	0.88
1:C:102:GLY:CA	4:C:714:HOH:O	2.08	0.83
1:A:305:GLN:O	4:A:701:HOH:O	1.99	0.80
1:B:371:ASN:ND2	2:G:1:NAG:C2	2.45	0.79
1:D:445:VAL:HG23	4:D:671:HOH:O	1.85	0.76
1:A:258:TYR:OH	1:A:377:MET:HG3	1.85	0.76
1:D:519:THR:CG2	4:D:680:HOH:O	2.33	0.76
1:A:474:THR:CG2	4:A:813:HOH:O	2.35	0.75
1:B:371:ASN:HD21	2:G:1:NAG:C2	1.98	0.74
1:A:449:HIS:HE1	4:A:707:HOH:O	1.70	0.74
1:D:519:THR:HG22	4:D:680:HOH:O	1.88	0.74
1:A:103:VAL:HG21	4:A:840:HOH:O	1.87	0.74
1:A:474:THR:HG23	4:A:813:HOH:O	1.87	0.74
1:D:351:MET:HE1	4:D:733:HOH:O	1.88	0.72
1:D:44:ARG:HD3	4:D:658:HOH:O	1.88	0.71
1:A:366:GLN:HG3	4:A:753:HOH:O	1.90	0.71
1:B:164:ILE:HD12	1:B:485:MET:HE1	1.75	0.69
1:C:262:ASP:HB2	4:C:702:HOH:O	1.93	0.68
1:A:371:ASN:ND2	2:E:1:NAG:C2	2.58	0.67
1:C:426:SER:OG	4:C:701:HOH:O	2.14	0.66
1:C:330:HIS:HE1	4:C:790:HOH:O	1.79	0.65
1:D:535:TRP:CZ3	1:D:539:LEU:HD22	2.31	0.64
1:B:370:LYS:HE3	1:B:383:SER:OG	1.98	0.63
1:C:548:ALA:O	1:C:549:SER:HB2	2.00	0.61
1:C:351:MET:HG2	4:C:799:HOH:O	1.99	0.61
1:B:164:ILE:CD1	1:B:485:MET:HE1	2.30	0.61
1:B:371:ASN:ND2	2:G:1:NAG:H2	2.15	0.61
1:C:426:SER:CB	4:C:701:HOH:O	2.48	0.60
1:C:239:MET:CE	1:C:314:GLU:HG2	2.31	0.59
1:D:519:THR:HG21	4:D:680:HOH:O	2.00	0.59
1:B:327:GLU:HA	1:B:327:GLU:OE1	2.02	0.59
1:C:220:THR:CG2	4:C:750:HOH:O	2.50	0.59
1:D:470:LYS:HD2	4:D:653:HOH:O	2.02	0.59
1:D:207:GLN:HG2	4:C:788:HOH:O	2.03	0.57
1:D:266:MET:HE3	1:D:266:MET:HA	1.87	0.56
1:D:445:VAL:CG2	4:D:671:HOH:O	2.50	0.56
1:D:67:LYS:NZ	1:C:79:GLU:OE2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:ILE:HB	1:B:485:MET:CE	2.36	0.54
1:B:529:SER:HB2	4:B:695:HOH:O	2.06	0.54
1:C:370:LYS:HE3	1:C:383:SER:HB3	1.90	0.54
1:A:98:LEU:HA	1:A:116:THR:HG22	1.89	0.53
1:C:330:HIS:CE1	4:C:790:HOH:O	2.57	0.52
1:D:314:GLU:HG3	1:C:39:HIS:CE1	2.43	0.52
1:C:474:THR:HG22	1:C:476:GLY:H	1.74	0.52
1:A:330:HIS:CE1	4:A:786:HOH:O	2.63	0.52
1:C:426:SER:HB3	4:C:701:HOH:O	2.06	0.52
1:A:474:THR:HG22	1:A:476:GLY:H	1.75	0.52
1:A:44:ARG:HD3	4:A:710:HOH:O	2.10	0.51
1:A:79:GLU:CD	1:B:79:GLU:HG3	2.36	0.51
1:D:386:LEU:HB3	1:D:407:MET:HE2	1.93	0.51
1:A:258:TYR:OH	1:A:377:MET:CG	2.58	0.51
1:C:53:THR:HG22	1:C:55:ALA:HB3	1.92	0.51
1:D:164:ILE:HD12	1:D:485:MET:HE1	1.93	0.50
1:A:263:THR:OG1	1:A:265:GLU:OE1	2.21	0.50
1:B:211:HIS:CE1	4:B:609:HOH:O	2.64	0.50
1:D:494:HIS:CE1	4:D:682:HOH:O	2.65	0.49
1:D:300:ILE:O	1:D:304:VAL:HG12	2.12	0.49
1:C:273:LYS:HA	1:C:278:GLU:HG2	1.93	0.49
1:B:164:ILE:HB	1:B:485:MET:HE1	1.94	0.49
1:B:533:GLN:NE2	1:C:395:GLU:HG3	2.28	0.48
1:A:283:GLU:OE1	1:B:85:SER:HB3	2.13	0.48
1:B:199:VAL:HG11	1:B:239:MET:HE2	1.95	0.48
1:B:446:ARG:HB2	1:B:447:PRO:HD2	1.97	0.47
1:A:446:ARG:HB2	1:A:447:PRO:HD2	1.96	0.47
1:A:44:ARG:NE	4:A:710:HOH:O	2.45	0.47
1:D:494:HIS:HE1	4:D:682:HOH:O	1.97	0.47
1:C:544:GLN:C	1:C:546:LEU:H	2.23	0.47
1:B:353:SER:HA	2:G:2:FUC:H62	1.97	0.47
1:A:371:ASN:HD22	2:E:1:NAG:H83	1.80	0.47
1:A:199:VAL:HG11	1:A:239:MET:HE2	1.96	0.47
1:D:79:GLU:HG3	1:C:79:GLU:CD	2.40	0.46
1:B:544:GLN:HA	1:B:544:GLN:OE1	2.16	0.46
1:D:199:VAL:HG11	1:D:239:MET:HE2	1.97	0.46
1:A:104:MET:HE3	1:A:350:VAL:O	2.15	0.45
1:C:540:SER:HB2	4:C:786:HOH:O	2.14	0.45
1:A:39:HIS:NE2	1:B:190:ARG:HG3	2.31	0.45
1:C:277:CYS:O	1:C:278:GLU:C	2.59	0.45
1:C:531:ARG:HG2	4:C:793:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:LYS:HE2	1:D:468:ASP:HA	1.98	0.44
1:D:520:GLN:HG3	4:D:696:HOH:O	2.16	0.44
1:A:474:THR:HG21	4:A:842:HOH:O	2.18	0.44
1:A:96:MET:HG3	1:A:116:THR:HG23	2.00	0.43
1:A:371:ASN:ND2	2:E:1:NAG:O5	2.45	0.43
1:A:370:LYS:HA	1:A:383:SER:OG	2.18	0.43
1:A:51:LYS:HG2	4:A:833:HOH:O	2.17	0.43
1:B:39:HIS:CE1	4:B:609:HOH:O	2.70	0.43
1:A:283:GLU:OE1	1:B:85:SER:CB	2.67	0.43
1:D:409:GLU:HG3	4:D:637:HOH:O	2.17	0.43
1:A:321:LYS:HE2	1:A:321:LYS:HB3	1.78	0.43
1:A:215:LYS:HG2	1:A:217:ASP:OD1	2.18	0.43
1:B:164:ILE:HG21	1:B:485:MET:HE2	2.01	0.43
2:E:1:NAG:H83	2:E:1:NAG:H2	1.87	0.43
1:D:267:VAL:HG23	4:D:662:HOH:O	2.20	0.42
1:D:441:SER:HB2	1:D:471:LEU:HD22	2.01	0.42
1:D:130:HIS:HB2	4:D:669:HOH:O	2.19	0.42
1:A:469:MET:HB3	1:A:471:LEU:HD13	2.01	0.42
1:C:59:THR:HG22	1:C:126:TYR:CD2	2.56	0.41
1:C:371:ASN:OD1	3:C:601:NAG:H2	2.21	0.41
1:D:409:GLU:CG	4:D:637:HOH:O	2.68	0.41
1:A:443:LYS:HB3	4:A:703:HOH:O	2.20	0.41
1:D:98:LEU:HD23	1:D:98:LEU:HA	1.96	0.41
1:A:59:THR:HG22	1:A:126:TYR:CD2	2.56	0.41
1:C:220:THR:HG22	1:C:246:GLY:HA3	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:538:THR:OG1	1:A:393:ASP:OD2[3_546]	2.11	0.09

## 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	519/523 (99%)	500 (96%)	19 (4%)	0	100	100
1	B	512/523 (98%)	490 (96%)	22 (4%)	0	100	100
1	C	519/523 (99%)	495 (95%)	24 (5%)	0	100	100
1	D	516/523 (99%)	497 (96%)	19 (4%)	0	100	100
All	All	2066/2092 (99%)	1982 (96%)	84 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	440/442 (100%)	433 (98%)	7 (2%)	55	73
1	B	435/442 (98%)	427 (98%)	8 (2%)	51	70
1	C	440/442 (100%)	436 (99%)	4 (1%)	70	82
1	D	439/442 (99%)	434 (99%)	5 (1%)	65	79
All	All	1754/1768 (99%)	1730 (99%)	24 (1%)	59	75

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	111	LEU
1	D	222	PHE
1	D	266	MET
1	D	441	SER
1	D	470	LYS
1	A	70	VAL
1	A	103	VAL
1	A	222	PHE
1	A	281	ASP
1	A	302	LYS

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Mol	Chain	Res	Type
1	A	377	MET
1	A	542	LYS
1	B	46	SER
1	B	111	LEU
1	B	222	PHE
1	B	273	LYS
1	B	327	GLU
1	B	470	LYS
1	B	500	GLU
1	B	546	LEU
1	C	105	LYS
1	C	222	PHE
1	C	302	LYS
1	C	444	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	49	HIS
1	D	207	GLN
1	D	355	GLN
1	D	494	HIS
1	A	371	ASN
1	A	419	GLN
1	A	520	GLN
1	A	533	GLN
1	B	207	GLN
1	B	366	GLN
1	B	371	ASN
1	B	375	GLN
1	B	494	HIS
1	C	100	ASN
1	C	301	ASN
1	C	371	ASN
1	C	494	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



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

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

## 5.5 Carbohydrates ⓘ

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	E	1	2	14,14,15	0.42	0	17,19,21	0.99	1 (5%)
2	FUC	E	2	2	10,10,11	0.32	0	14,14,16	0.45	0
2	NAG	G	1	2	14,14,15	0.48	0	17,19,21	1.20	2 (11%)
2	FUC	G	2	2	10,10,11	0.44	0	14,14,16	0.49	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	2	-	3/6/23/26	0/1/1/1
2	FUC	E	2	2	-	-	0/1/1/1
2	NAG	G	1	2	-	1/6/23/26	0/1/1/1
2	FUC	G	2	2	1/1/4/5	-	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1	NAG	O5-C1-C2	-3.24	106.28	111.29
2	E	1	NAG	O5-C1-C2	-2.96	106.72	111.29
2	G	1	NAG	C1-C2-N2	2.64	114.59	110.43

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	G	2	FUC	C1

All (4) torsion outliers are listed below:

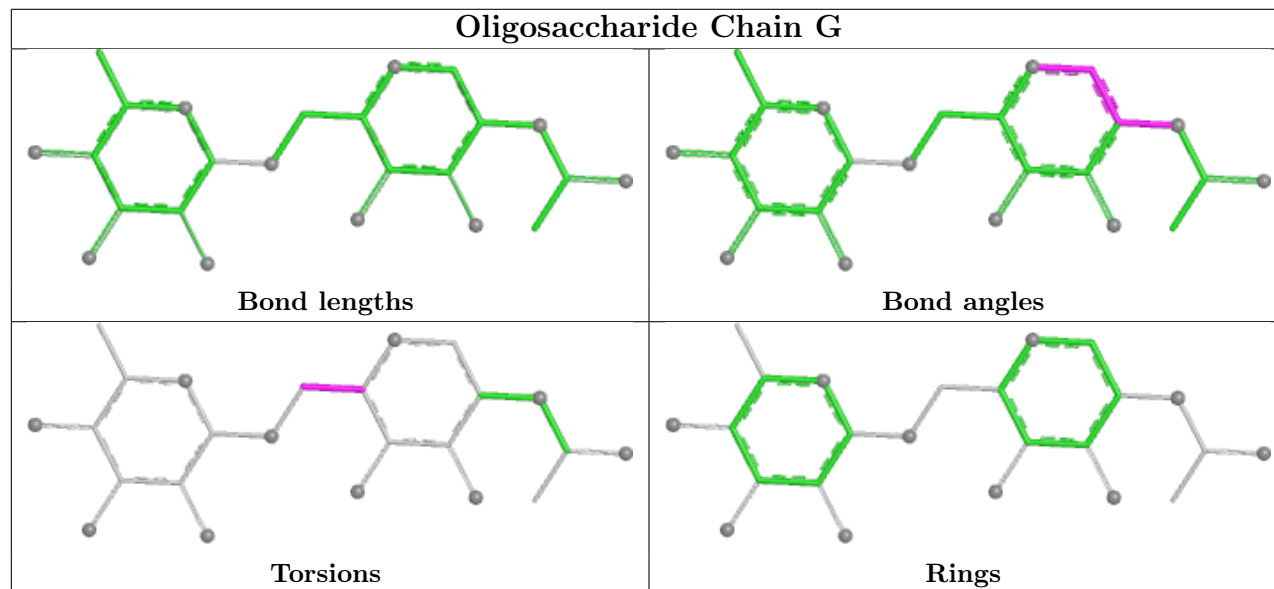
Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	G	1	NAG	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6

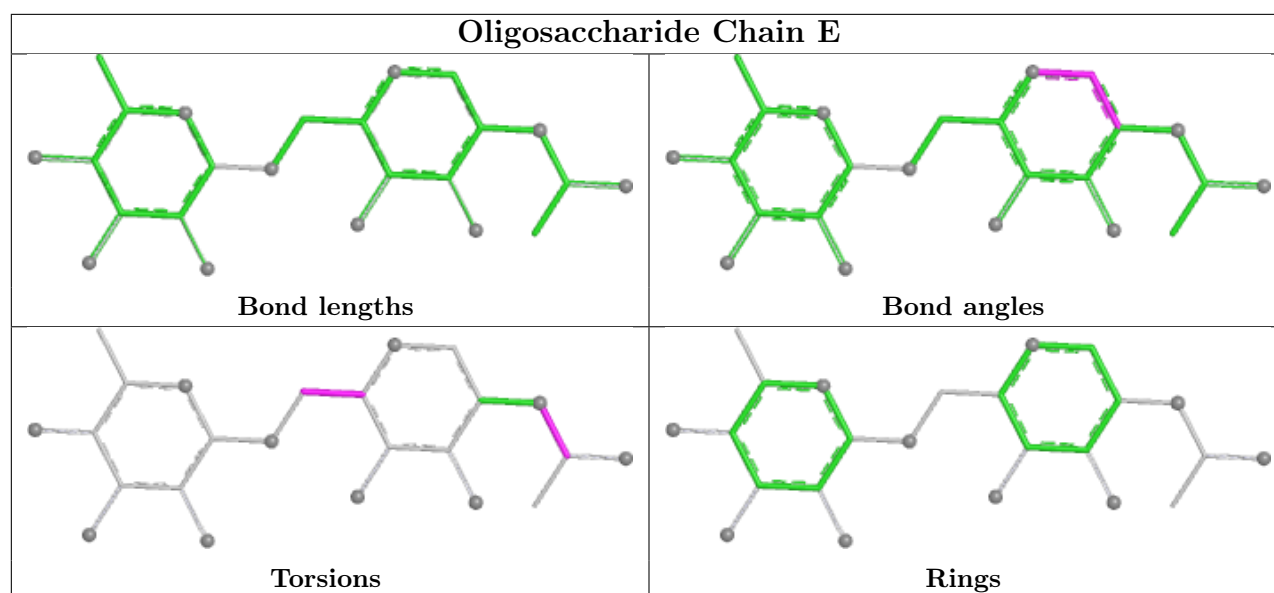
There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	NAG	6	0
2	G	1	NAG	5	0
2	G	2	FUC	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.





## 5.6 Ligand geometry [i](#)

1 ligand is 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	C	601	-	14,14,15	0.44	0	17,19,21	0.91	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	C	601	-	-	2/6/23/26	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( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	C	601	NAG	C1-C2-N2	2.82	114.88	110.43

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	601	NAG	C8-C7-N2-C2
3	C	601	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	601	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	521/523 (99%)	-0.36	3 (0%) 85 88	35, 55, 104, 167	0
1	B	516/523 (98%)	-0.24	7 (1%) 73 74	42, 61, 116, 171	0
1	C	520/523 (99%)	-0.22	9 (1%) 69 69	43, 65, 119, 172	1 (0%)
1	D	520/523 (99%)	-0.24	4 (0%) 82 84	44, 68, 114, 169	0
All	All	2077/2092 (99%)	-0.26	23 (1%) 78 79	35, 62, 115, 172	1 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	49[A]	HIS	4.6
1	D	279	ALA	3.9
1	C	30	PRO	3.4
1	C	549	SER	3.2
1	B	469	MET	2.9
1	A	103	VAL	2.9
1	A	546	LEU	2.8
1	D	102	GLY	2.7
1	C	548	ALA	2.6
1	B	549	SER	2.5
1	B	546	LEU	2.5
1	B	445	VAL	2.5
1	C	50	VAL	2.4
1	D	306	MET	2.4
1	C	103	VAL	2.3
1	B	102	GLY	2.3
1	C	55	ALA	2.3
1	D	284	ALA	2.2
1	B	510	HIS	2.2
1	C	279	ALA	2.2
1	C	306	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	104	MET	2.1
1	B	277	CYS	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](#)

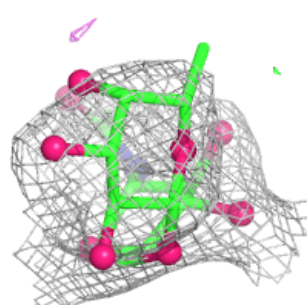
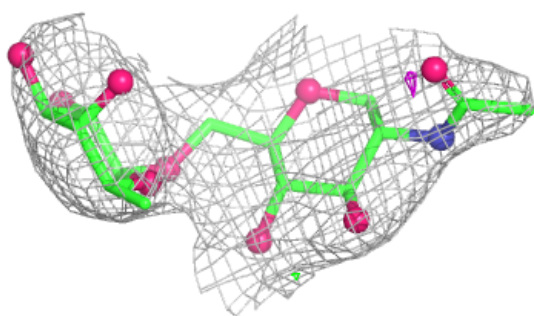
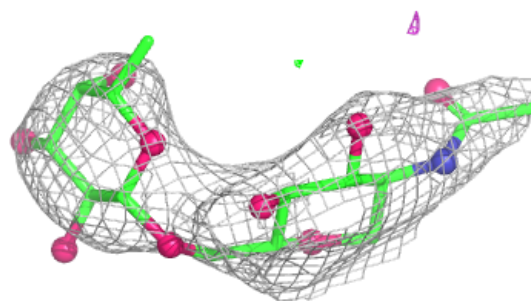
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	G	1	14/15	-	-	85,122,138,163	0
2	FUC	G	2	10/11	-	-	123,139,147,160	0
2	FUC	E	2	10/11	0.75	0.12	117,169,175,177	0
2	NAG	E	1	14/15	0.84	0.11	122,139,170,187	0

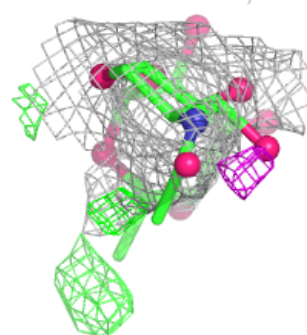
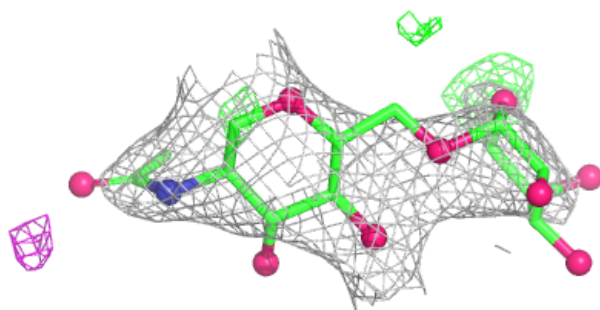
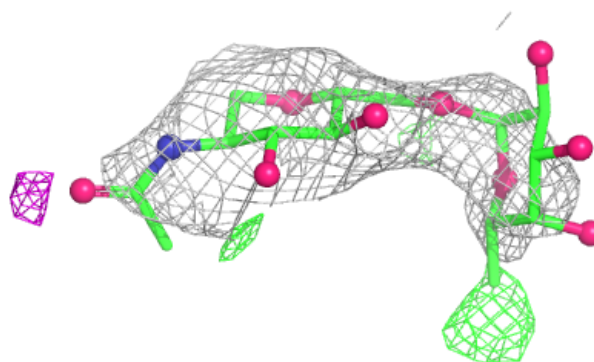
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around Chain G:**

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

**Electron density around Chain 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	NAG	C	601	14/15	0.73	0.15	121,136,155,155	0

## 6.5 Other polymers

There are no such residues in this entry.