



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 25, 2024 – 07:14 PM EST

PDB ID : 5OAR  
Title : Crystal structure of native beta-N-acetylhexosaminidase isolated from *Aspergillus oryzae*  
Authors : Skerlova, J.; Rezacova, P.; Brynda, J.; Pachl, P.; Otwinowski, Z.; Vanek, O.  
Deposited on : 2017-06-23  
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](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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

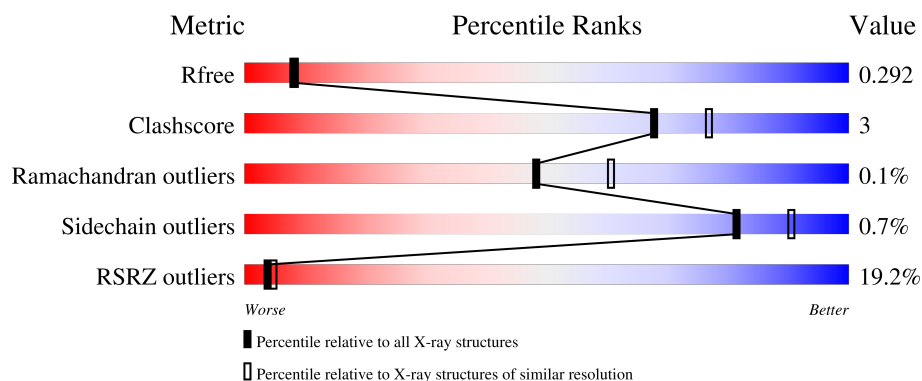
# 1 Overall quality at a glance

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.



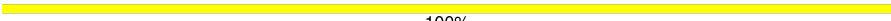
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (2.30-2.30)

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 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	78	<div> <div>10%</div> <div>86%</div> <div>6%</div> <div>8%</div> </div>
1	C	78	<div> <div>26%</div> <div>87%</div> <div>6%</div> <div>6%</div> </div>
2	B	499	<div> <div>14%</div> <div>93%</div> <div>7%</div> </div>
2	D	499	<div> <div>24%</div> <div>87%</div> <div>12%</div> </div>
3	E	3	<div> <div>33%</div> <div>67%</div> </div>
3	G	3	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
4	F	2	 100%

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 9552 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.

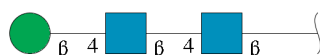
- Molecule 1 is a protein called Beta-hexosaminidase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	72	Total	C	N	O	0	0	0
			542	345	92	105			
1	C	73	Total	C	N	O	0	0	0
			549	350	93	106			

- Molecule 2 is a protein called Beta-hexosaminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	497	Total	C	N	O	S	0	0	0
			4007	2542	680	769	16			
2	D	498	Total	C	N	O	S	0	0	0
			4017	2547	682	772	16			

- 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.



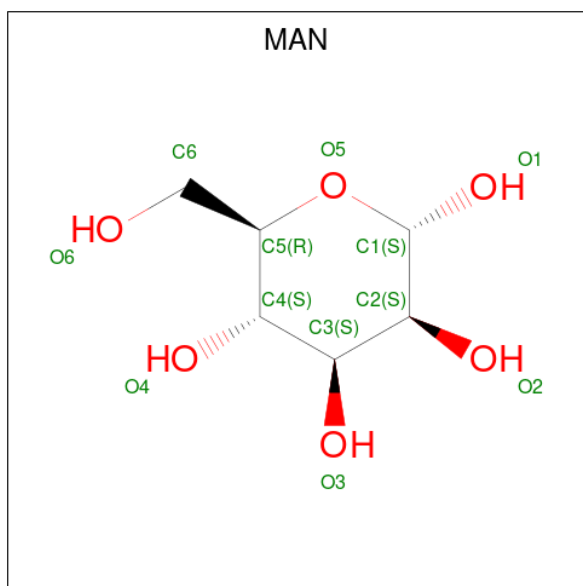
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	G	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 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
4	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



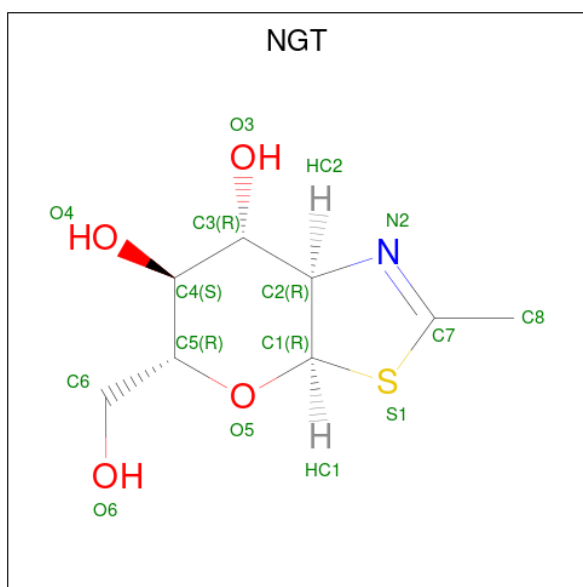
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	C	1	Total	C	O	0	0
			11	6	5		
5	C	1	Total	C	O	0	0
			11	6	5		
5	C	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 7 is 3AR,5R,6S,7R,7AR-5-HYDROXYMETHYL-2-METHYL-5,6,7,7A-TETRAHYDRO-3AH-PYRANO[3,2-D]THIAZOLE-6,7-DIOL (three-letter code: NGT) (formula: C<sub>8</sub>H<sub>13</sub>NO<sub>4</sub>S).



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

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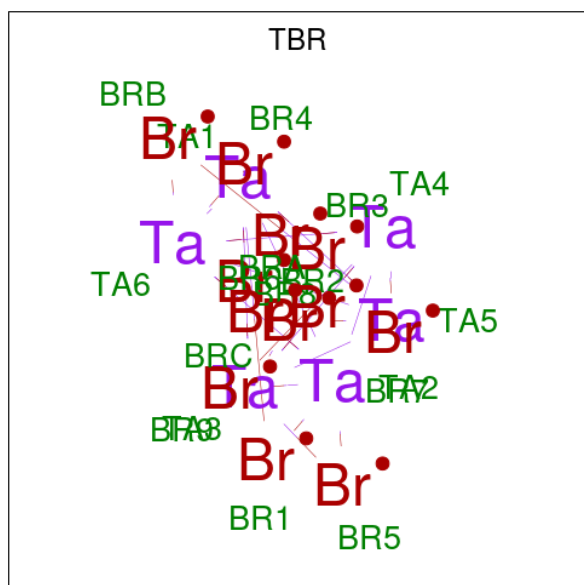
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	D	1	Total	C	N	O	S	0	0
			14	8	1	4	1		

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	7	Total	Cl	0	0
			7	7		
8	D	4	Total	Cl	0	1
			5	5		

- Molecule 9 is HEXATANTALUM DODECABROMIDE (three-letter code: TBR) (formula: Br<sub>12</sub>Ta<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	D	1	Total	Br	Ta	0	0
			18	12	6		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	14	Total	O	0	0
			14	14		
10	B	96	Total	O	0	2
			98	98		

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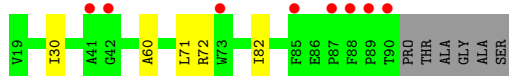
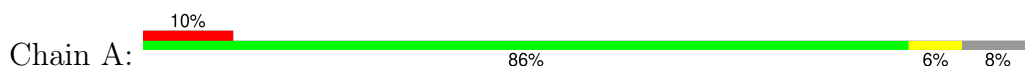
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	C	10	Total	O	0	0
			10	10		
10	D	57	Total	O	0	0
			57	57		



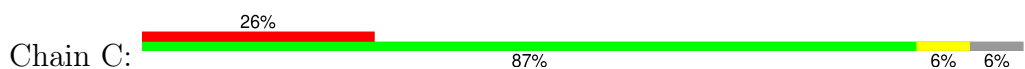
### 3 Residue-property plots

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

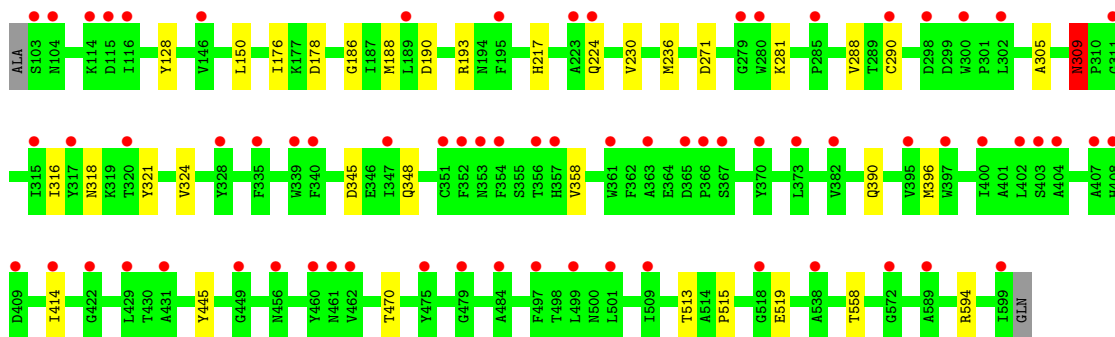
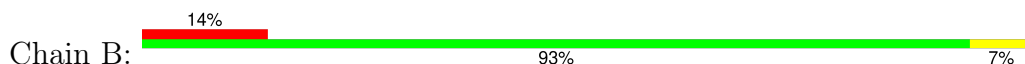
- Molecule 1: Beta-hexosaminidase



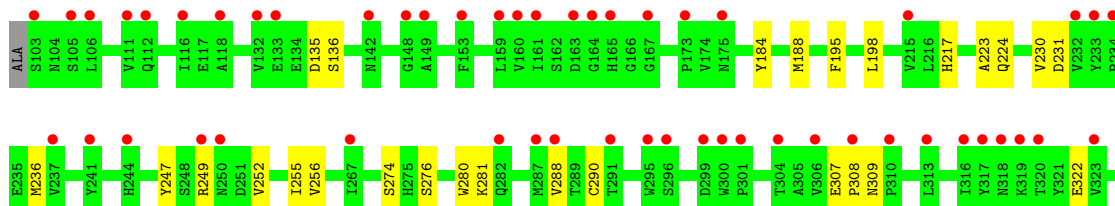
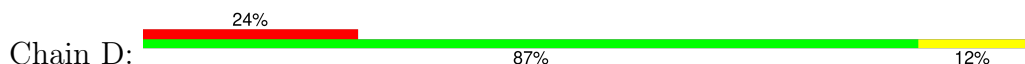
- Molecule 1: Beta-hexosaminidase

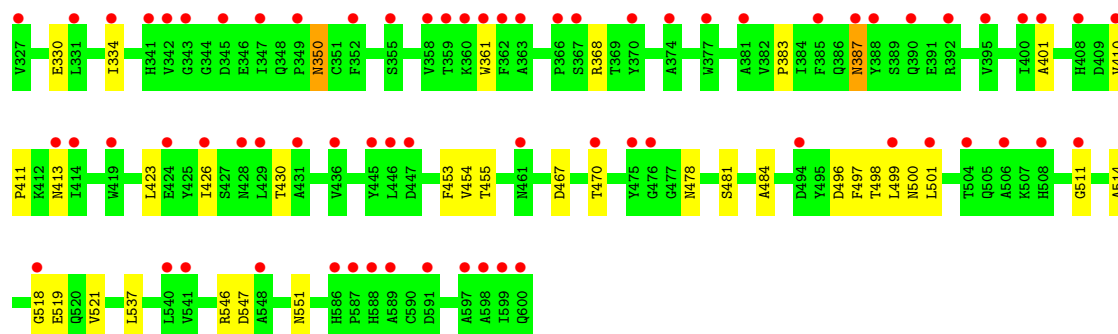


- Molecule 2: Beta-hexosaminidase



- Molecule 2: Beta-hexosaminidase





- 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: 33% 67%



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

Chain G: 100%



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

Chain F: 100%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.75Å 105.75Å 285.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.37 – 2.30 23.37 – 2.30	Depositor EDS
% Data completeness (in resolution range)	72.8 (23.37-2.30) 81.2 (23.37-2.30)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.56 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.189 , 0.241 0.271 , 0.292	Depositor DCC
$R_{free}$ test set	3697 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.4	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 34.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	9552	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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: CL, NGT, MAN, TBR, NAG, BMA

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	0.64	0/559	0.68	0/770
1	C	0.58	0/567	0.68	0/782
2	B	0.61	0/4126	0.68	0/5645
2	D	0.55	0/4136	0.62	0/5657
All	All	0.59	0/9388	0.66	0/12854

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	542	0	518	4	0
1	C	549	0	525	3	0
2	B	4007	0	3745	21	0
2	D	4017	0	3754	40	0
3	E	39	0	34	0	0
3	G	39	0	34	0	0
4	F	28	0	25	0	0
5	A	33	0	30	0	0
5	C	33	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	14	0	13	0	0
6	D	14	0	13	0	0
7	B	14	0	13	0	0
7	D	14	0	13	1	0
8	B	7	0	0	0	0
8	D	5	0	0	1	0
9	D	18	0	0	1	0
10	A	14	0	0	0	0
10	B	98	0	0	0	0
10	C	10	0	0	0	0
10	D	57	0	0	3	0
All	All	9552	0	8747	63	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (63) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:224:GLN:HA	2:B:309:ASN:OD1	1.87	0.74
2:D:454:VAL:HG13	10:D:841:HOH:O	1.94	0.68
1:C:38:LYS:NZ	2:D:136:SER:O	2.32	0.62
2:B:190:ASP:OD2	2:B:193:ARG:HG2	2.02	0.60
2:D:188:MET:HA	2:D:217:HIS:O	2.02	0.58
1:A:60:ALA:CB	2:B:150:LEU:HD22	2.34	0.58
2:B:316:ILE:HG12	2:B:358:VAL:HG22	1.86	0.56
1:A:30:ILE:HG13	2:B:176:ILE:HG12	1.88	0.55
2:D:308:PRO:O	2:D:309:ASN:HB3	2.06	0.55
2:B:230:VAL:HG21	2:B:236:MET:HE1	1.88	0.54
2:D:426:ILE:O	2:D:430:THR:HG22	2.08	0.54
2:D:223:ALA:C	2:D:309:ASN:OD1	2.47	0.53
2:B:281:LYS:HB3	2:B:288:VAL:HG21	1.90	0.53
2:B:396:MET:HE2	2:B:414:ILE:HD13	1.90	0.52
2:D:467:ASP:OD2	2:D:470:THR:OG1	2.26	0.52
2:D:514:ALA:HB2	2:D:537:LEU:HD22	1.90	0.52
2:B:390:GLN:H	2:B:390:GLN:CD	2.13	0.52
2:D:411:PRO:C	2:D:413:ASN:H	2.13	0.52
2:D:401:ALA:HB2	2:D:410:VAL:HG21	1.93	0.50
2:D:252:VAL:O	2:D:256:VAL:HG23	2.12	0.49
2:D:281:LYS:HB3	2:D:288:VAL:HG21	1.95	0.49
2:B:193:ARG:NH1	2:B:519:GLU:OE2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:478:ASN:HB2	2:D:481:SER:O	2.13	0.48
2:B:128:TYR:CE1	2:B:178:ASP:HB3	2.49	0.47
2:B:186:GLY:O	2:B:513:THR:HA	2.15	0.47
2:D:195:PHE:CE1	2:D:247:TYR:CZ	3.03	0.47
2:D:547:ASP:OD1	2:D:551:ASN:N	2.48	0.47
2:D:230:VAL:HG21	2:D:236:MET:CE	2.44	0.46
2:B:188:MET:HG3	2:B:217:HIS:CG	2.51	0.46
2:D:198:LEU:HD22	2:D:255:ILE:HD11	1.97	0.46
2:D:499:LEU:HD23	2:D:500:ASN:N	2.30	0.46
2:D:322:GLU:HB2	9:D:705:TBR:BRA	2.71	0.46
2:D:361:TRP:CH2	2:D:368:ARG:HD3	2.52	0.45
2:D:184:TYR:O	2:D:511:GLY:HA3	2.16	0.45
2:D:453:PHE:CE2	2:D:519:GLU:HG2	2.51	0.45
2:D:276:SER:HB3	2:D:280:TRP:CD1	2.52	0.45
2:D:307:GLU:OE2	7:D:706:NGT:HC4	2.17	0.45
2:D:518:GLY:HA2	2:D:521:VAL:HB	1.99	0.45
2:D:383:PRO:O	2:D:387:ASN:HB2	2.16	0.45
2:D:135:ASP:OD1	2:D:135:ASP:N	2.46	0.44
2:B:321:TYR:HA	2:B:324:VAL:HG22	1.98	0.44
1:C:71:LEU:O	1:C:72:ARG:C	2.56	0.44
2:D:274:SER:N	10:D:805:HOH:O	2.49	0.44
2:D:276:SER:HA	10:D:831:HOH:O	2.18	0.44
2:B:305:ALA:HA	2:B:348:GLN:HG3	1.99	0.44
2:B:445:TYR:CE1	2:B:515:PRO:HG2	2.53	0.43
1:A:71:LEU:O	1:A:72:ARG:C	2.56	0.43
2:D:423:LEU:HD21	2:D:497:PHE:HA	2.00	0.43
2:D:231:ASP:N	2:D:330:GLU:OE2	2.39	0.43
2:D:481:SER:HB3	2:D:484:ALA:HB2	2.00	0.42
2:D:230:VAL:HG21	2:D:236:MET:HE3	1.99	0.42
2:D:498:THR:HA	2:D:501:LEU:HD12	2.01	0.42
2:D:350:ASN:OD1	2:D:350:ASN:N	2.52	0.42
2:D:368:ARG:NH1	8:D:709[A]:CL:CL	2.90	0.42
1:A:82:ILE:HD13	2:B:594:ARG:HG2	2.01	0.41
2:D:249:ARG:CZ	2:D:334:ILE:HG22	2.50	0.41
2:B:230:VAL:HB	2:B:236:MET:HE3	2.03	0.41
2:B:271:ASP:OD2	2:B:345:ASP:OD1	2.39	0.41
1:C:74:VAL:O	1:C:75:PRO:C	2.59	0.41
2:D:224:GLN:N	2:D:309:ASN:OD1	2.54	0.41
2:B:558:THR:HG23	2:D:455:THR:HG21	2.03	0.40
2:D:496:ASP:CG	2:D:546:ARG:HH21	2.25	0.40
2:B:188:MET:HA	2:B:217:HIS:O	2.22	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	70/78 (90%)	67 (96%)	3 (4%)	0	100	100
1	C	71/78 (91%)	68 (96%)	3 (4%)	0	100	100
2	B	495/499 (99%)	478 (97%)	16 (3%)	1 (0%)	44	55
2	D	496/499 (99%)	472 (95%)	24 (5%)	0	100	100
All	All	1132/1154 (98%)	1085 (96%)	46 (4%)	1 (0%)	48	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	309	ASN

### 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	57/60 (95%)	57 (100%)	0	100	100
1	C	58/60 (97%)	58 (100%)	0	100	100
2	B	436/437 (100%)	432 (99%)	4 (1%)	75	87
2	D	437/437 (100%)	434 (99%)	3 (1%)	81	90
All	All	988/994 (99%)	981 (99%)	7 (1%)	81	90

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	290	CYS
2	B	309	ASN
2	B	318	ASN
2	B	470	THR
2	D	290	CYS
2	D	350	ASN
2	D	387	ASN

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

Mol	Chain	Res	Type
2	D	318	ASN
2	D	387	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
6	NAG	B	706	2	14,14,15	0.60	0	17,19,21	1.46	2 (11%)
5	MAN	A	101	1	11,11,12	0.81	0	15,15,17	1.17	1 (6%)
3	NAG	G	2	3	14,14,15	0.51	0	17,19,21	0.96	1 (5%)
6	NAG	D	704	2	14,14,15	0.54	0	17,19,21	1.25	2 (11%)
5	MAN	C	103	1	11,11,12	0.83	0	15,15,17	1.06	1 (6%)
5	MAN	A	102	1	11,11,12	0.67	0	15,15,17	0.91	0
5	MAN	A	103	1	11,11,12	0.66	0	15,15,17	1.29	2 (13%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	E	1	2,3	14,14,15	0.39	0	17,19,21	1.41	2 (11%)
5	MAN	C	101	1	11,11,12	0.77	0	15,15,17	0.91	0
3	NAG	G	1	2,3	14,14,15	0.42	0	17,19,21	1.83	5 (29%)
3	NAG	E	2	3	14,14,15	0.47	0	17,19,21	1.81	3 (17%)
5	MAN	C	102	1	11,11,12	0.55	0	15,15,17	1.10	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
6	NAG	B	706	2	-	2/6/23/26	0/1/1/1
5	MAN	A	101	1	-	0/2/19/22	0/1/1/1
3	NAG	G	2	3	-	1/6/23/26	0/1/1/1
6	NAG	D	704	2	-	2/6/23/26	0/1/1/1
5	MAN	C	103	1	-	0/2/19/22	0/1/1/1
5	MAN	A	102	1	-	0/2/19/22	0/1/1/1
5	MAN	A	103	1	-	2/2/19/22	0/1/1/1
3	NAG	E	1	2,3	-	0/6/23/26	0/1/1/1
5	MAN	C	101	1	-	0/2/19/22	0/1/1/1
3	NAG	G	1	2,3	-	4/6/23/26	0/1/1/1
3	NAG	E	2	3	-	4/6/23/26	0/1/1/1
5	MAN	C	102	1	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2	NAG	C1-O5-C5	5.08	118.99	112.19
5	A	103	MAN	C1-O5-C5	3.94	117.46	112.19
3	E	1	NAG	C1-O5-C5	3.83	117.33	112.19
3	G	1	NAG	C8-C7-N2	3.74	122.32	116.12
5	C	102	MAN	C1-O5-C5	3.49	116.87	112.19
3	G	1	NAG	C1-O5-C5	3.43	116.78	112.19
6	D	704	NAG	C1-O5-C5	3.31	116.62	112.19
3	G	1	NAG	O5-C1-C2	-2.91	106.79	111.29
5	A	101	MAN	C1-C2-C3	2.84	113.78	109.64
5	C	103	MAN	C1-C2-C3	2.82	113.75	109.64
6	B	706	NAG	C4-C3-C2	-2.77	106.97	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	706	NAG	C1-O5-C5	2.72	115.84	112.19
3	E	2	NAG	C8-C7-N2	2.61	120.44	116.12
3	E	1	NAG	O4-C4-C3	-2.53	104.40	110.38
3	G	1	NAG	C1-C2-N2	2.44	114.27	110.43
5	A	103	MAN	C1-C2-C3	2.37	113.09	109.64
3	G	1	NAG	O7-C7-C8	-2.19	118.16	122.05
6	D	704	NAG	O5-C1-C2	-2.13	108.00	111.29
3	G	2	NAG	O5-C1-C2	-2.11	108.02	111.29
3	E	2	NAG	O5-C5-C4	2.05	115.82	110.83

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	706	NAG	C3-C2-N2-C7
5	A	103	MAN	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
5	A	103	MAN	C4-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
3	G	1	NAG	C8-C7-N2-C2
3	G	1	NAG	O7-C7-N2-C2
3	G	1	NAG	C4-C5-C6-O6
6	B	706	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
6	D	704	NAG	C1-C2-N2-C7
6	D	704	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 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
3	NAG	E	1	2,3	14,14,15	0.39	0	17,19,21	1.41	2 (11%)
3	NAG	E	2	3	14,14,15	0.47	0	17,19,21	1.81	3 (17%)
3	BMA	E	3	3	11,11,12	0.56	0	15,15,17	0.81	0
4	NAG	F	1	4,2	14,14,15	0.52	0	17,19,21	1.62	4 (23%)
4	NAG	F	2	4	14,14,15	0.49	0	17,19,21	2.21	6 (35%)
3	NAG	G	1	2,3	14,14,15	0.42	0	17,19,21	1.83	5 (29%)
3	NAG	G	2	3	14,14,15	0.51	0	17,19,21	0.96	1 (5%)
3	BMA	G	3	3	11,11,12	0.61	0	15,15,17	1.22	2 (13%)

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	E	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	4/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
4	NAG	F	1	4,2	-	4/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
3	NAG	G	1	2,3	-	4/6/23/26	0/1/1/1
3	NAG	G	2	3	-	1/6/23/26	0/1/1/1
3	BMA	G	3	3	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	2	NAG	C1-O5-C5	5.11	119.04	112.19
3	E	2	NAG	C1-O5-C5	5.08	118.99	112.19
3	E	1	NAG	C1-O5-C5	3.83	117.33	112.19
3	G	1	NAG	C8-C7-N2	3.74	122.32	116.12
4	F	1	NAG	C8-C7-N2	3.49	121.90	116.12
4	F	1	NAG	O5-C1-C2	-3.47	105.92	111.29
3	G	1	NAG	C1-O5-C5	3.43	116.78	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	2	NAG	C8-C7-N2	3.35	121.67	116.12
4	F	2	NAG	C4-C3-C2	-3.25	106.26	111.02
4	F	2	NAG	O7-C7-C8	-3.02	116.67	122.05
3	G	1	NAG	O5-C1-C2	-2.91	106.79	111.29
4	F	1	NAG	C3-C4-C5	2.86	115.42	110.23
3	G	3	BMA	C3-C4-C5	2.72	115.17	110.23
3	E	2	NAG	C8-C7-N2	2.61	120.44	116.12
4	F	1	NAG	O7-C7-C8	-2.56	117.49	122.05
3	E	1	NAG	O4-C4-C3	-2.53	104.40	110.38
4	F	2	NAG	O5-C5-C4	2.49	116.89	110.83
3	G	1	NAG	C1-C2-N2	2.44	114.27	110.43
3	G	3	BMA	C1-C2-C3	2.36	113.08	109.64
4	F	2	NAG	C1-C2-N2	2.35	114.13	110.43
3	G	1	NAG	O7-C7-C8	-2.19	118.16	122.05
3	G	2	NAG	O5-C1-C2	-2.11	108.02	111.29
3	E	2	NAG	O5-C5-C4	2.05	115.82	110.83

There are no chirality outliers.

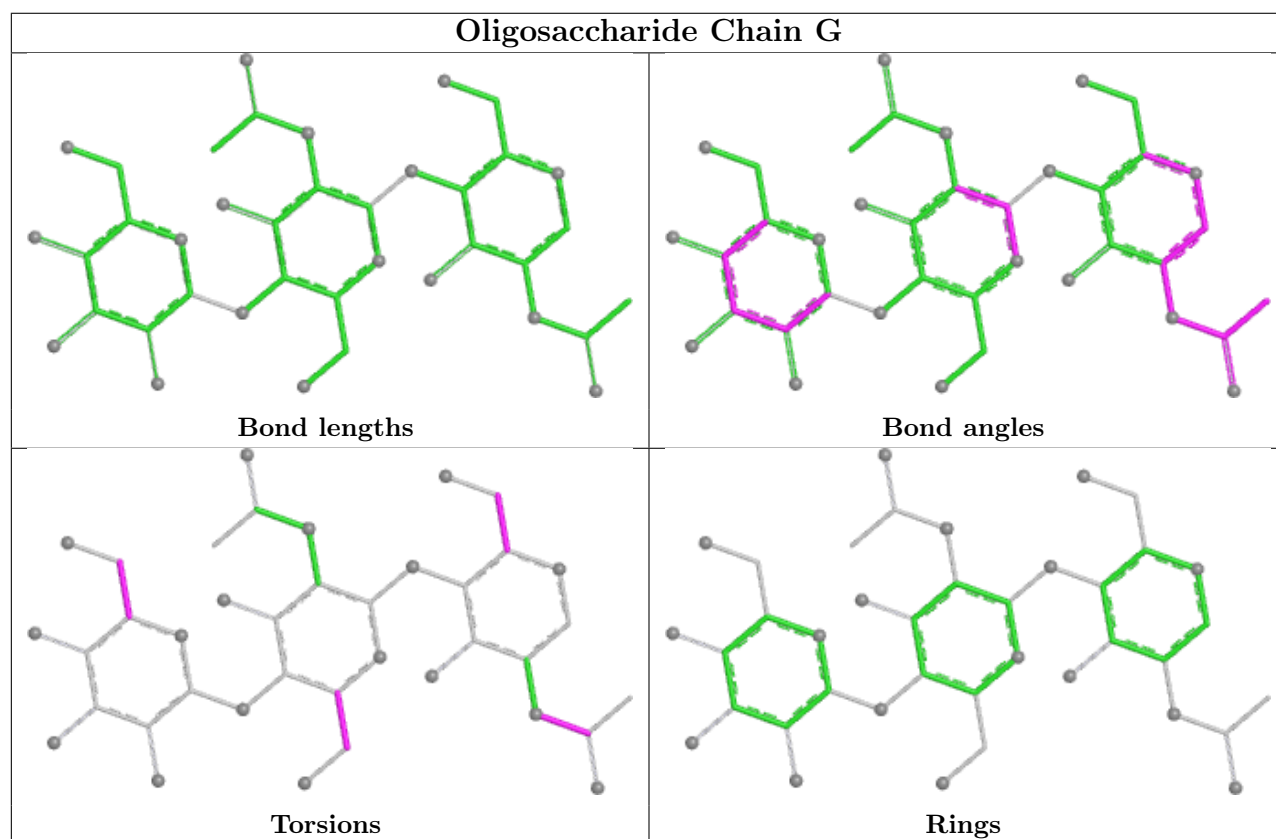
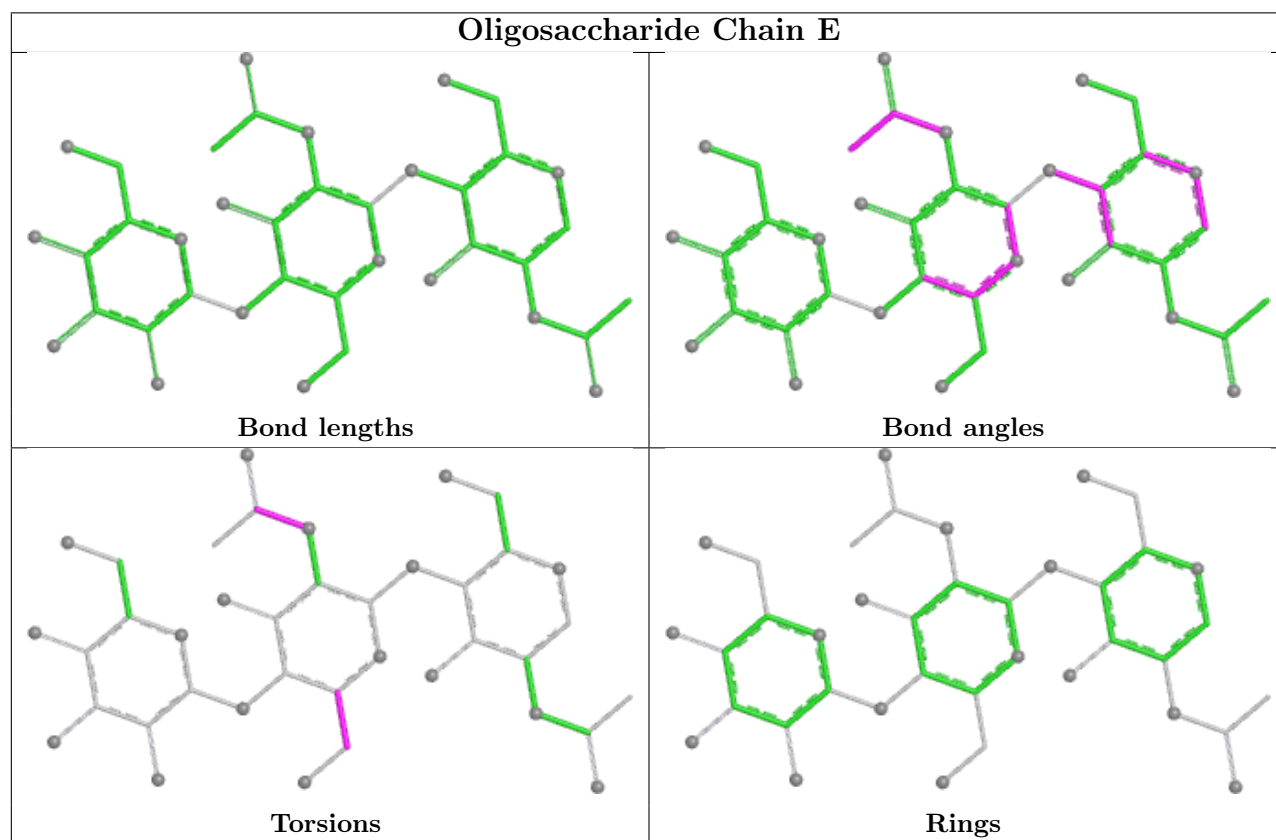
All (17) torsion outliers are listed below:

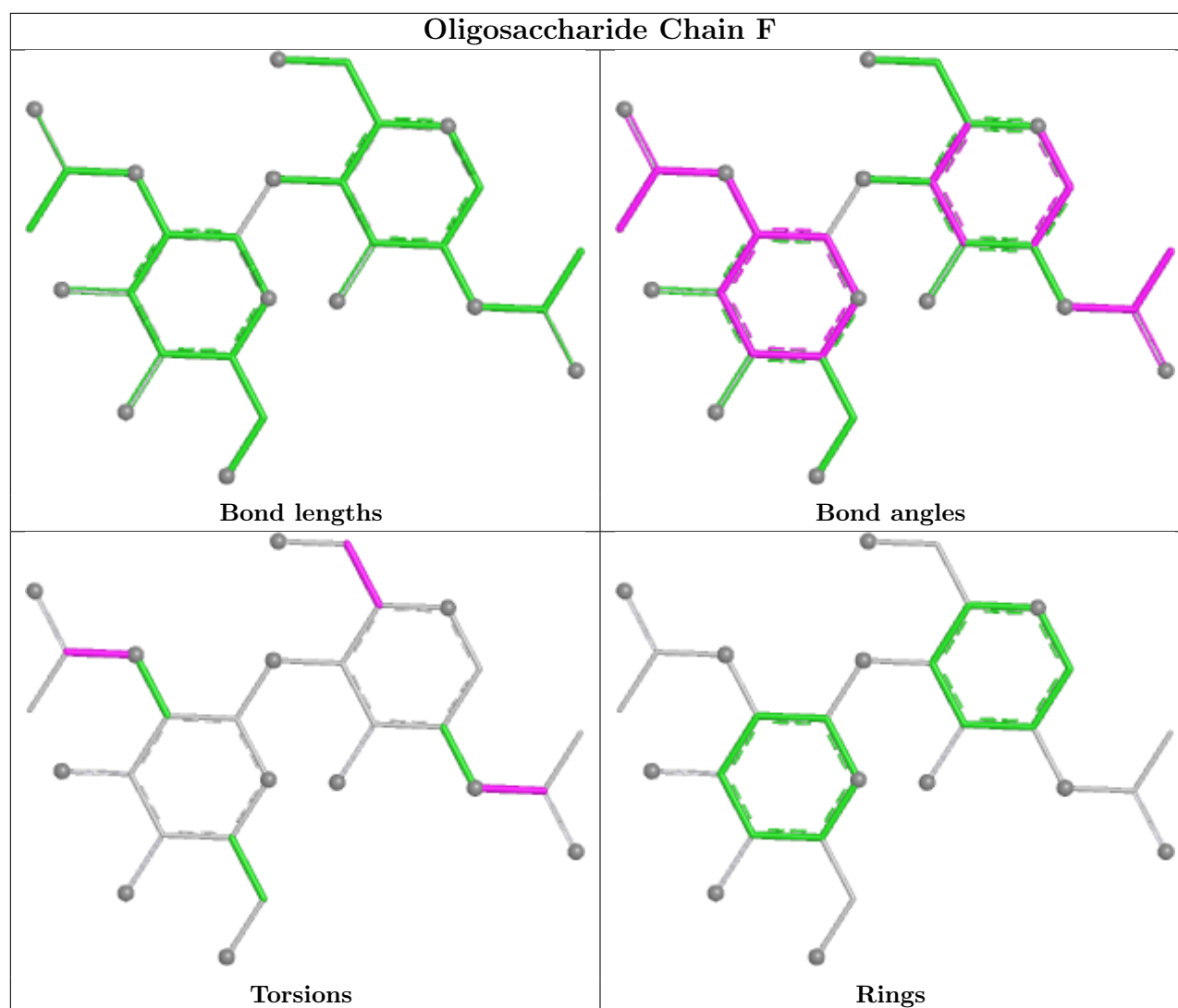
Mol	Chain	Res	Type	Atoms
4	F	1	NAG	C4-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	G	3	BMA	O5-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
3	G	1	NAG	C8-C7-N2-C2
3	G	1	NAG	O7-C7-N2-C2
4	F	1	NAG	C8-C7-N2-C2
4	F	1	NAG	O7-C7-N2-C2
4	F	2	NAG	C8-C7-N2-C2
4	F	2	NAG	O7-C7-N2-C2
3	G	1	NAG	C4-C5-C6-O6
3	G	3	BMA	C4-C5-C6-O6
3	G	2	NAG	O5-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](#)

Of 23 ligands modelled in this entry, 12 are monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
6	NAG	B	706	2	14,14,15	0.60	0	17,19,21	1.46	2 (11%)
5	MAN	A	101	1	11,11,12	0.81	0	15,15,17	1.17	1 (6%)
7	NGT	B	707	-	13,15,15	3.53	1 (7%)	14,22,22	1.45	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	MAN	C	103	1	11,11,12	0.83	0	15,15,17	1.06	1 (6%)
5	MAN	A	102	1	11,11,12	0.67	0	15,15,17	0.91	0
5	MAN	A	103	1	11,11,12	0.66	0	15,15,17	1.29	2 (13%)
9	TBR	D	705	-	0,36,36	-	-	-	-	-
5	MAN	C	101	1	11,11,12	0.77	0	15,15,17	0.91	0
6	NAG	D	704	2	14,14,15	0.54	0	17,19,21	1.25	2 (11%)
5	MAN	C	102	1	11,11,12	0.55	0	15,15,17	1.10	1 (6%)
7	NGT	D	706	-	13,15,15	3.78	1 (7%)	14,22,22	1.46	3 (21%)

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
6	NAG	B	706	2	-	2/6/23/26	0/1/1/1
5	MAN	A	101	1	-	0/2/19/22	0/1/1/1
7	NGT	B	707	-	-	0/2/30/30	0/2/2/2
5	MAN	C	103	1	-	0/2/19/22	0/1/1/1
5	MAN	A	102	1	-	0/2/19/22	0/1/1/1
5	MAN	A	103	1	-	2/2/19/22	0/1/1/1
5	MAN	C	101	1	-	0/2/19/22	0/1/1/1
6	NAG	D	704	2	-	2/6/23/26	0/1/1/1
5	MAN	C	102	1	-	0/2/19/22	0/1/1/1
7	NGT	D	706	-	-	2/2/30/30	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	706	NGT	C7-S1	-13.45	1.65	1.77
7	B	707	NGT	C7-S1	-12.58	1.66	1.77

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	103	MAN	C1-O5-C5	3.94	117.46	112.19
5	C	102	MAN	C1-O5-C5	3.49	116.87	112.19
7	D	706	NGT	C3-C2-N2	-3.36	105.86	110.56
6	D	704	NAG	C1-O5-C5	3.31	116.62	112.19
7	B	707	NGT	C8-C7-S1	2.93	123.37	118.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	101	MAN	C1-C2-C3	2.84	113.78	109.64
5	C	103	MAN	C1-C2-C3	2.82	113.75	109.64
6	B	706	NAG	C4-C3-C2	-2.77	106.97	111.02
6	B	706	NAG	C1-O5-C5	2.72	115.84	112.19
7	D	706	NGT	C8-C7-S1	2.70	123.03	118.96
7	B	707	NGT	C3-C2-N2	-2.47	107.11	110.56
7	D	706	NGT	C1-O5-C5	2.46	116.98	112.56
7	B	707	NGT	C1-O5-C5	2.42	116.91	112.56
5	A	103	MAN	C1-C2-C3	2.37	113.09	109.64
6	D	704	NAG	O5-C1-C2	-2.13	108.00	111.29

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	706	NAG	C3-C2-N2-C7
5	A	103	MAN	O5-C5-C6-O6
5	A	103	MAN	C4-C5-C6-O6
6	B	706	NAG	O5-C5-C6-O6
7	D	706	NGT	C4-C5-C6-O6
7	D	706	NGT	O5-C5-C6-O6
6	D	704	NAG	C1-C2-N2-C7
6	D	704	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	705	TBR	1	0
7	D	706	NGT	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 ⓘ

**Warning:** The R factor obtained from EDS is 0.2789, which does not match the depositor's R factor of 0.1886. Please interpret the results in this section carefully.

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	72/78 (92%)	1.10	8 (11%) 12 13	34, 45, 75, 87	0
1	C	73/78 (93%)	1.66	20 (27%) 2 2	43, 60, 84, 93	0
2	B	497/499 (99%)	1.13	70 (14%) 7 8	29, 44, 67, 90	0
2	D	498/499 (99%)	1.52	121 (24%) 2 2	36, 61, 90, 117	0
All	All	1140/1154 (98%)	1.33	219 (19%) 4 5	29, 52, 84, 117	0

All (219) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	359	THR	5.1
1	A	41	ALA	3.9
2	B	347	ILE	3.9
1	A	89	PRO	3.7
1	C	26	ALA	3.6
2	D	148	GLY	3.6
2	D	347	ILE	3.6
2	D	363	ALA	3.5
2	D	318	ASN	3.4
2	B	354	PHE	3.4
2	D	370	TYR	3.4
2	D	410	VAL	3.4
2	D	385	PHE	3.4
2	D	149	ALA	3.4
2	B	429	LEU	3.3
2	D	429	LEU	3.3
2	D	600	GLN	3.3
1	C	91	PRO	3.3
2	B	373	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
2	D	548	ALA	3.3
2	D	381	ALA	3.3
2	D	426	ILE	3.2
2	D	320	THR	3.2
2	D	313	LEU	3.2
2	D	401	ALA	3.2
2	B	285	PRO	3.1
2	D	334	ILE	3.1
2	D	132	VAL	3.1
2	D	249	ARG	3.1
2	B	366	PRO	3.1
2	D	250	ASN	3.0
1	C	88	PHE	3.0
2	D	317	TYR	3.0
1	A	90	THR	3.0
2	D	316	ILE	3.0
2	D	599	ILE	3.0
2	B	103	SER	3.0
2	B	317	TYR	3.0
2	D	103	SER	3.0
2	D	232	VAL	3.0
2	B	431	ALA	3.0
2	D	112	GLN	3.0
2	D	308	PRO	3.0
2	B	414	ILE	2.9
2	B	461	ASN	2.9
2	D	355	SER	2.9
2	D	367	SER	2.9
2	B	475	TYR	2.9
2	B	339	TRP	2.9
2	D	501	LEU	2.9
2	B	290	CYS	2.8
2	D	504	THR	2.8
2	D	414	ILE	2.8
2	D	233	TYR	2.8
1	C	37	PRO	2.8
2	D	164	GLY	2.8
2	B	315	ILE	2.8
2	D	295	TRP	2.8
2	D	342	VAL	2.8
2	D	288	VAL	2.8
2	D	388	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	40	ILE	2.7
1	C	82	ILE	2.7
2	D	111	VAL	2.7
1	C	32	TRP	2.7
2	D	476	GLY	2.7
2	D	511	GLY	2.7
2	B	302	LEU	2.7
2	D	446	LEU	2.7
2	D	310	PRO	2.7
2	B	352	PHE	2.7
2	B	538	ALA	2.7
2	D	377	TRP	2.7
2	D	400	ILE	2.7
2	D	160	VAL	2.7
2	D	327	VAL	2.7
2	B	114	LYS	2.7
2	D	291	THR	2.6
2	D	428	ASN	2.6
2	B	340	PHE	2.6
2	D	358	VAL	2.6
2	B	449	GLY	2.6
2	D	133	GLU	2.6
2	B	104	ASN	2.6
2	B	280	TRP	2.6
2	B	509	ILE	2.6
1	C	51	ASP	2.6
2	B	518	GLY	2.6
2	D	597	ALA	2.6
2	B	279	GLY	2.5
2	D	106	LEU	2.5
2	D	499	LEU	2.5
2	D	175	ASN	2.5
2	D	161	ILE	2.5
2	B	300	TRP	2.5
2	B	361	TRP	2.5
1	A	88	PHE	2.5
2	D	362	PHE	2.5
2	D	589	ALA	2.5
2	D	360	LYS	2.5
2	D	387	ASN	2.5
2	B	460	TYR	2.5
2	D	447	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	33	GLY	2.5
1	C	19	VAL	2.5
2	D	142	ASN	2.5
2	D	173	PRO	2.5
2	D	587	PRO	2.5
2	B	395	VAL	2.4
2	D	436	VAL	2.4
2	D	304	THR	2.4
2	D	118	ALA	2.4
2	D	343	GLY	2.4
2	D	586	HIS	2.4
2	B	224	GLN	2.4
2	D	159	LEU	2.4
2	D	331	LEU	2.4
2	B	353	ASN	2.4
2	D	419	TRP	2.4
2	D	287	MET	2.4
2	D	349	PRO	2.4
2	B	311	GLY	2.4
2	B	422	GLY	2.4
2	D	598	ALA	2.4
1	C	89	PRO	2.3
2	B	367	SER	2.3
2	B	409	ASP	2.3
2	B	599	ILE	2.3
2	D	296	SER	2.3
2	D	345	ASP	2.3
2	D	390	GLN	2.3
2	D	301	PRO	2.3
2	D	366	PRO	2.3
1	A	73	TRP	2.3
2	D	300	TRP	2.3
1	C	83	SER	2.3
1	C	76	ALA	2.3
2	B	407	ALA	2.3
2	B	462	VAL	2.3
2	D	237	VAL	2.3
2	D	541	VAL	2.3
2	B	298	ASP	2.3
2	D	341	HIS	2.3
2	B	456	ASN	2.3
2	B	404	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	589	ALA	2.3
2	B	382	VAL	2.3
2	D	319	LYS	2.2
2	B	499	LEU	2.2
2	D	413	ASN	2.2
2	B	356	THR	2.2
2	B	351	CYS	2.2
1	A	42	GLY	2.2
2	B	402	LEU	2.2
2	D	234	PRO	2.2
1	A	85	PHE	2.2
2	B	408	HIS	2.2
2	D	165	HIS	2.2
2	D	215	VAL	2.2
2	D	244	HIS	2.2
2	D	395	VAL	2.2
2	D	116	ILE	2.2
2	B	479	GLY	2.2
2	B	370	TYR	2.2
1	A	87	PRO	2.2
2	B	497	PHE	2.2
2	D	105	SER	2.2
2	D	494	ASP	2.2
2	B	572	GLY	2.2
2	D	267	ILE	2.2
2	B	397	TRP	2.2
2	D	540	LEU	2.2
2	D	506	ALA	2.2
2	B	195	PHE	2.2
2	B	365	ASP	2.2
2	D	167	GLY	2.1
2	D	361	TRP	2.1
2	B	189	LEU	2.1
2	D	408	HIS	2.1
2	B	223	ALA	2.1
2	B	363	ALA	2.1
2	D	241	TYR	2.1
2	D	323	VAL	2.1
2	D	591	ASP	2.1
2	D	518	GLY	2.1
2	D	588	HIS	2.1
2	D	461	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	87	PRO	2.1
1	C	90	THR	2.1
2	B	320	THR	2.1
2	D	475	TYR	2.1
2	D	153	PHE	2.1
1	C	47	ARG	2.1
2	D	392	ARG	2.1
2	B	116	ILE	2.1
2	B	400	ILE	2.1
2	D	508	HIS	2.1
2	B	146	VAL	2.1
2	B	328	TYR	2.1
2	D	306	VAL	2.1
2	B	335	PHE	2.1
2	B	115	ASP	2.1
2	D	163	ASP	2.1
1	C	31	SER	2.1
1	C	36	GLY	2.1
2	D	374	ALA	2.1
2	D	431	ALA	2.1
2	D	424	GLU	2.0
2	D	299	ASP	2.0
2	D	282	GLN	2.0
2	B	501	LEU	2.0
1	C	48	THR	2.0
2	B	484	ALA	2.0
2	D	470	THR	2.0
2	D	352	PHE	2.0
2	D	445	TYR	2.0
2	B	357	HIS	2.0
1	C	35	SER	2.0
2	B	403	SER	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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(Å <sup>2</sup> )	Q<0.9
6	NAG	B	706	14/15	0.58	0.18	69,77,86,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MAN	A	103	11/12	0.58	0.15	76,84,86,88	0
3	NAG	E	2	14/15	0.62	0.22	67,85,94,99	0
5	MAN	C	103	11/12	0.63	0.15	56,69,75,77	0
3	NAG	G	2	14/15	0.65	0.22	79,98,106,106	0
6	NAG	D	704	14/15	0.68	0.16	71,97,104,109	0
3	NAG	G	1	14/15	0.70	0.17	68,75,90,98	0
5	MAN	C	101	11/12	0.75	0.15	46,50,62,71	0
3	NAG	E	1	14/15	0.78	0.14	56,66,69,76	0
5	MAN	A	101	11/12	0.80	0.12	50,55,61,61	0
5	MAN	A	102	11/12	0.80	0.12	55,58,60,60	0
5	MAN	C	102	11/12	0.83	0.11	46,50,56,60	0

### 6.3 Carbohydrates

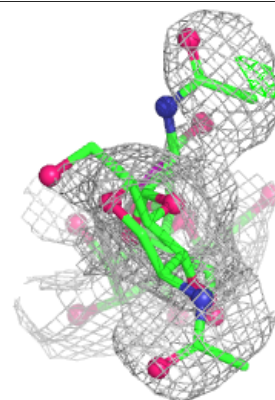
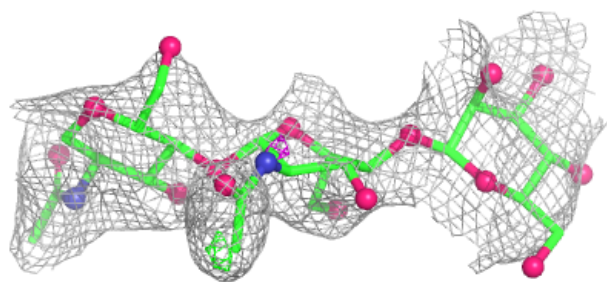
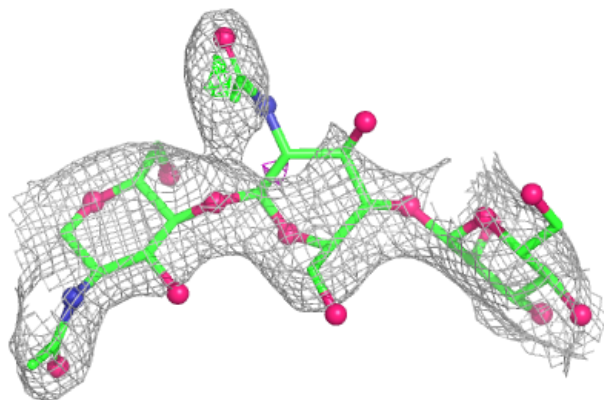
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
4	NAG	F	2	14/15	0.27	0.23	87,108,114,117	0
3	BMA	G	3	11/12	0.45	0.19	96,110,118,119	0
4	NAG	F	1	14/15	0.60	0.16	67,75,86,99	0
3	BMA	E	3	11/12	0.62	0.15	88,97,101,102	0
3	NAG	E	2	14/15	0.62	0.22	67,85,94,99	0
3	NAG	G	2	14/15	0.65	0.22	79,98,106,106	0
3	NAG	G	1	14/15	0.70	0.17	68,75,90,98	0
3	NAG	E	1	14/15	0.78	0.14	56,66,69,76	0

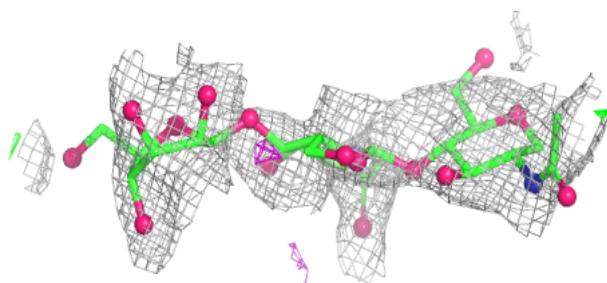
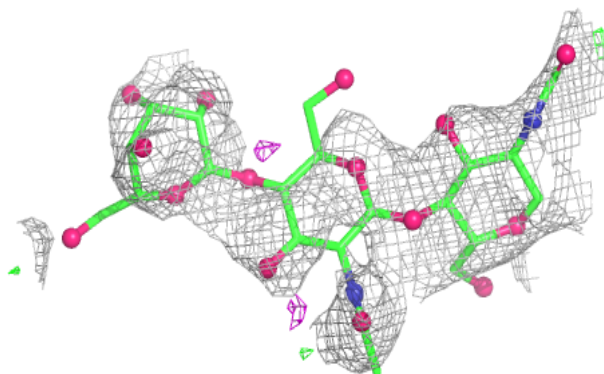
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around Chain E:**

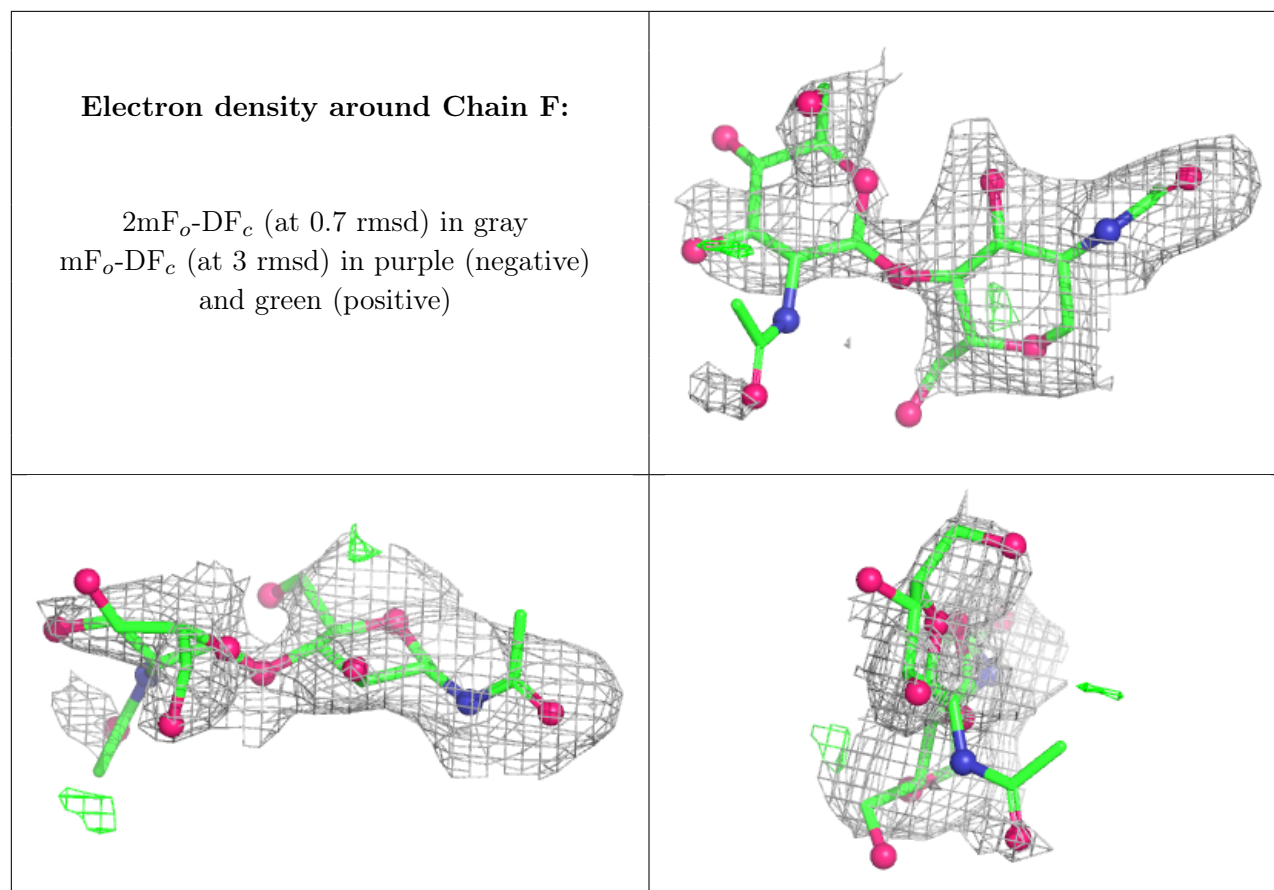
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around Chain G:**

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







## 6.4 Ligands [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(Å <sup>2</sup> )	Q<0.9
5	MAN	A	103	11/12	0.58	0.15	76,84,86,88	0
6	NAG	B	706	14/15	0.58	0.18	69,77,86,89	0
5	MAN	C	103	11/12	0.63	0.15	56,69,75,77	0
8	CL	B	708	1/1	0.63	0.12	69,69,69,69	0
6	NAG	D	704	14/15	0.68	0.16	71,97,104,109	0
5	MAN	C	101	11/12	0.75	0.15	46,50,62,71	0
8	CL	D	710	1/1	0.75	0.12	50,50,50,50	0
8	CL	B	710	1/1	0.77	0.16	59,59,59,59	0
8	CL	D	707	1/1	0.79	0.11	37,37,37,37	1
5	MAN	A	101	11/12	0.80	0.12	50,55,61,61	0
7	NGT	B	707	14/14	0.80	0.22	55,61,66,68	14
5	MAN	A	102	11/12	0.80	0.12	55,58,60,60	0
8	CL	B	711	1/1	0.83	0.16	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MAN	C	102	11/12	0.83	0.11	46,50,56,60	0
7	NGT	D	706	14/14	0.83	0.22	62,74,78,78	14
8	CL	B	709	1/1	0.86	0.08	42,42,42,42	0
8	CL	B	713	1/1	0.86	0.18	76,76,76,76	0
8	CL	D	709[A]	1/1	0.87	0.22	52,52,52,52	1
8	CL	D	709[B]	1/1	0.87	0.22	54,54,54,54	1
8	CL	B	714	1/1	0.87	0.13	54,54,54,54	0
8	CL	B	712	1/1	0.88	0.18	62,62,62,62	0
9	TBR	D	705	18/18	0.91	0.12	64,74,79,80	18
8	CL	D	708	1/1	0.94	0.15	52,52,52,52	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.