



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 05:18 AM BST

PDB ID : 2XXL  
Title : Crystal structure of drosophila Grass clip serine protease of Toll pathway  
Authors : Kellenberger, C.; Leone, P.; Coquet, L.; Jouenne, T.; Reichhart, J.M.; Roussel, A.  
Deposited on : 2010-11-10  
Resolution : 1.80 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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.

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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 : 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

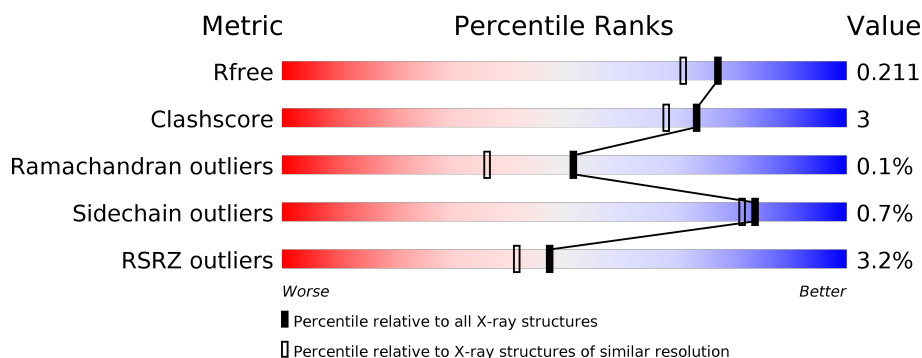
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	408	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>7%</div> <div>13%</div> </div> </div>
1	B	408	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>8%</div> <div>13%</div> </div> </div>
2	C	4	<div> <div></div> <div>100%</div> </div>
2	D	4	<div> <div></div> <div>100%</div> </div>
2	E	4	<div> <div></div> <div> <div>75%</div> <div>25%</div> </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	E	4	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6434 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 GRAM-POSITIVE SPECIFIC SERINE PROTEASE, ISO-FORM B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	354	Total	C	N	O	S	0	0	0
			2746	1713	483	527	23			
1	B	354	Total	C	N	O	S	0	0	0
			2746	1713	483	527	23			

There are 62 discrepancies between the modelled and reference sequences:

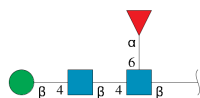
Chain	Residue	Modelled	Actual	Comment	Reference
A	378	LEU	-	expression tag	UNP Q9VB68
A	379	GLU	-	expression tag	UNP Q9VB68
A	380	SER	-	expression tag	UNP Q9VB68
A	381	ARG	-	expression tag	UNP Q9VB68
A	382	GLY	-	expression tag	UNP Q9VB68
A	383	PRO	-	expression tag	UNP Q9VB68
A	384	PHE	-	expression tag	UNP Q9VB68
A	385	GLU	-	expression tag	UNP Q9VB68
A	386	GLY	-	expression tag	UNP Q9VB68
A	387	LYS	-	expression tag	UNP Q9VB68
A	388	PRO	-	expression tag	UNP Q9VB68
A	389	ILE	-	expression tag	UNP Q9VB68
A	390	PRO	-	expression tag	UNP Q9VB68
A	391	ASN	-	expression tag	UNP Q9VB68
A	392	PRO	-	expression tag	UNP Q9VB68
A	393	LEU	-	expression tag	UNP Q9VB68
A	394	LEU	-	expression tag	UNP Q9VB68
A	395	GLY	-	expression tag	UNP Q9VB68
A	396	LEU	-	expression tag	UNP Q9VB68
A	397	ASP	-	expression tag	UNP Q9VB68
A	398	SER	-	expression tag	UNP Q9VB68
A	399	THR	-	expression tag	UNP Q9VB68
A	400	ARG	-	expression tag	UNP Q9VB68
A	401	THR	-	expression tag	UNP Q9VB68

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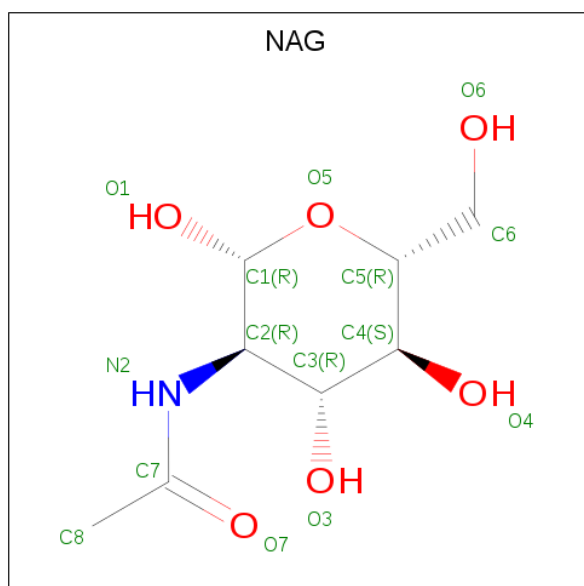
Chain	Residue	Modelled	Actual	Comment	Reference
A	402	GLY	-	expression tag	UNP Q9VB68
A	403	HIS	-	expression tag	UNP Q9VB68
A	404	HIS	-	expression tag	UNP Q9VB68
A	405	HIS	-	expression tag	UNP Q9VB68
A	406	HIS	-	expression tag	UNP Q9VB68
A	407	HIS	-	expression tag	UNP Q9VB68
A	408	HIS	-	expression tag	UNP Q9VB68
B	378	LEU	-	expression tag	UNP Q9VB68
B	379	GLU	-	expression tag	UNP Q9VB68
B	380	SER	-	expression tag	UNP Q9VB68
B	381	ARG	-	expression tag	UNP Q9VB68
B	382	GLY	-	expression tag	UNP Q9VB68
B	383	PRO	-	expression tag	UNP Q9VB68
B	384	PHE	-	expression tag	UNP Q9VB68
B	385	GLU	-	expression tag	UNP Q9VB68
B	386	GLY	-	expression tag	UNP Q9VB68
B	387	LYS	-	expression tag	UNP Q9VB68
B	388	PRO	-	expression tag	UNP Q9VB68
B	389	ILE	-	expression tag	UNP Q9VB68
B	390	PRO	-	expression tag	UNP Q9VB68
B	391	ASN	-	expression tag	UNP Q9VB68
B	392	PRO	-	expression tag	UNP Q9VB68
B	393	LEU	-	expression tag	UNP Q9VB68
B	394	LEU	-	expression tag	UNP Q9VB68
B	395	GLY	-	expression tag	UNP Q9VB68
B	396	LEU	-	expression tag	UNP Q9VB68
B	397	ASP	-	expression tag	UNP Q9VB68
B	398	SER	-	expression tag	UNP Q9VB68
B	399	THR	-	expression tag	UNP Q9VB68
B	400	ARG	-	expression tag	UNP Q9VB68
B	401	THR	-	expression tag	UNP Q9VB68
B	402	GLY	-	expression tag	UNP Q9VB68
B	403	HIS	-	expression tag	UNP Q9VB68
B	404	HIS	-	expression tag	UNP Q9VB68
B	405	HIS	-	expression tag	UNP Q9VB68
B	406	HIS	-	expression tag	UNP Q9VB68
B	407	HIS	-	expression tag	UNP Q9VB68
B	408	HIS	-	expression tag	UNP Q9VB68

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	4	Total	C	N	O	0	0	0
			49	28	2	19			
2	D	4	Total	C	N	O	0	0	0
			49	28	2	19			
2	E	4	Total	C	N	O	0	0	0
			49	28	2	19			

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



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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		

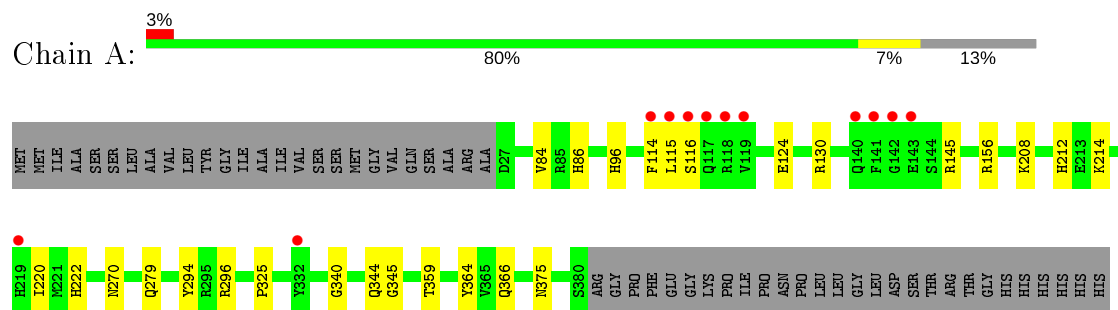
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	386	Total 386	O 386	0	0
5	B	393	Total 393	O 393	0	0

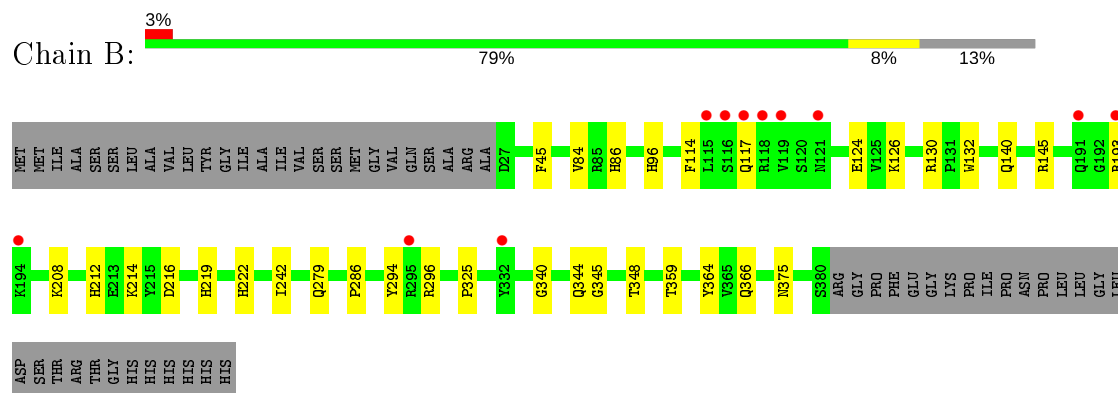
### 3 Residue-property plots [i](#)

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

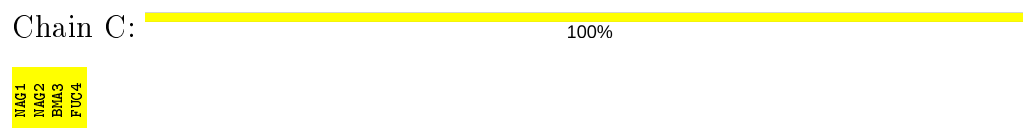
- Molecule 1: GRAM-POSITIVE SPECIFIC SERINE PROTEASE, ISOFORM B



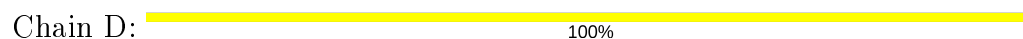
- Molecule 1: GRAM-POSITIVE SPECIFIC SERINE PROTEASE, ISOFORM B



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



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

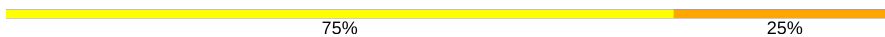




NAG1  
NAG2  
BMA3  
FUC4

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

Chain E:



NAG1  
NAG2  
BMA3  
FUC4

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.26Å 92.04Å 113.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.36 – 1.80 27.36 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (27.36-1.80) 100.0 (27.36-1.80)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.04 (at 1.80Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, $R_{free}$	0.177 , 0.203 0.182 , 0.211	Depositor DCC
$R_{free}$ test set	3839 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.8	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 50.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.56$ , $\langle L^2 \rangle = 0.40$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6434	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.40 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.5041e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, BMA, NAG, 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	0.49	0/2803	0.63	0/3790
1	B	0.49	0/2803	0.62	0/3790
All	All	0.49	0/5606	0.62	0/7580

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	2746	0	2659	17	0
1	B	2746	0	2659	20	0
2	C	49	0	43	0	0
2	D	49	0	43	0	0
2	E	49	0	43	1	0
3	A	14	0	13	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	386	0	0	2	0
5	B	393	0	0	2	0
All	All	6434	0	5460	37	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 (37) 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:130:ARG:HE	1:A:279:GLN:HE22	1.09	0.96
1:B:130:ARG:HE	1:B:279:GLN:HE22	1.09	0.95
1:B:212:HIS:HD2	1:B:214:LYS:H	1.31	0.76
1:A:212:HIS:HD2	1:A:214:LYS:H	1.32	0.76
1:A:115:LEU:HB2	1:A:116:SER:HA	1.77	0.67
1:B:130:ARG:NE	1:B:279:GLN:HE22	1.88	0.67
1:A:130:ARG:NE	1:A:279:GLN:HE22	1.88	0.66
1:B:212:HIS:CD2	1:B:214:LYS:H	2.17	0.62
1:A:212:HIS:CD2	1:A:214:LYS:H	2.17	0.61
1:B:348:THR:HG21	2:E:4:FUC:H62	1.84	0.57
1:A:96:HIS:HD1	1:A:366:GLN:NE2	2.05	0.55
1:B:130:ARG:HE	1:B:279:GLN:NE2	1.92	0.54
1:B:96:HIS:HD1	1:B:366:GLN:NE2	2.05	0.54
1:A:296:ARG:NH2	1:A:344:GLN:HE22	2.05	0.54
1:B:84:VAL:O	1:B:86:HIS:HD2	1.91	0.54
1:A:130:ARG:HE	1:A:279:GLN:NE2	1.92	0.54
1:A:84:VAL:O	1:A:86:HIS:HD2	1.92	0.53
1:B:296:ARG:NH2	1:B:344:GLN:HE22	2.05	0.53
1:A:124:GLU:HG2	5:A:2136:HOH:O	2.09	0.53
1:B:212:HIS:HE1	5:B:2237:HOH:O	1.96	0.48
1:B:124:GLU:HG2	5:B:2139:HOH:O	2.13	0.48
1:A:114:PHE:CZ	1:A:325:PRO:HB3	2.50	0.47
1:A:145:ARG:NH2	1:A:270:ASN:O	2.49	0.46
1:A:294:TYR:OH	1:A:345:GLY:HA3	2.15	0.46
1:B:294:TYR:OH	1:B:345:GLY:HA3	2.16	0.46
1:A:222:HIS:HD2	1:A:364:TYR:OH	2.01	0.44
1:B:216:ASP:OD2	1:B:219:HIS:HD2	2.00	0.44
1:B:208:LYS:NZ	1:B:375:ASN:HD22	2.16	0.44
1:A:212:HIS:HE1	5:A:2232:HOH:O	2.01	0.44
1:B:114:PHE:CZ	1:B:325:PRO:HB3	2.53	0.43
1:A:208:LYS:NZ	1:A:375:ASN:HD22	2.16	0.43
1:B:222:HIS:HD2	1:B:364:TYR:OH	2.02	0.43
1:B:140:GLN:NE2	1:B:145:ARG:HD3	2.34	0.42
1:B:117:GLN:NE2	1:B:126:LYS:H	2.16	0.42
1:B:340:GLY:HA2	1:B:359:THR:O	2.20	0.41
1:A:340:GLY:HA2	1:A:359:THR:O	2.20	0.41
1:B:132:TRP:CG	1:B:242:ILE:HB	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	352/408 (86%)	340 (97%)	11 (3%)	1 (0%)	41	27
1	B	352/408 (86%)	341 (97%)	11 (3%)	0	100	100
All	All	704/816 (86%)	681 (97%)	22 (3%)	1 (0%)	51	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	220	ILE

### 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	301/344 (88%)	300 (100%)	1 (0%)	92	91
1	B	301/344 (88%)	298 (99%)	3 (1%)	76	71
All	All	602/688 (88%)	598 (99%)	4 (1%)	84	81

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

Mol	Chain	Res	Type
1	A	156	ARG
1	B	45	PHE

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Mol	Chain	Res	Type
1	B	193	ARG
1	B	286	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	86	HIS
1	A	166	HIS
1	A	212	HIS
1	A	219	HIS
1	A	222	HIS
1	A	256	GLN
1	A	279	GLN
1	A	302	GLN
1	A	344	GLN
1	A	366	GLN
1	A	375	ASN
1	B	59	GLN
1	B	86	HIS
1	B	117	GLN
1	B	140	GLN
1	B	166	HIS
1	B	190	GLN
1	B	212	HIS
1	B	219	HIS
1	B	222	HIS
1	B	256	GLN
1	B	279	GLN
1	B	302	GLN
1	B	344	GLN
1	B	366	GLN
1	B	375	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

12 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	1.50	3 (21%)	17,19,21	1.94	5 (29%)
2	NAG	C	2	2	14,14,15	1.03	1 (7%)	17,19,21	1.29	3 (17%)
2	BMA	C	3	2	11,11,12	1.51	3 (27%)	15,15,17	1.65	3 (20%)
2	FUC	C	4	2	10,10,11	1.43	1 (10%)	14,14,16	0.96	1 (7%)
2	NAG	D	1	1,2	14,14,15	1.56	3 (21%)	17,19,21	2.10	7 (41%)
2	NAG	D	2	2	14,14,15	1.13	1 (7%)	17,19,21	1.32	3 (17%)
2	BMA	D	3	2	11,11,12	1.61	3 (27%)	15,15,17	1.75	3 (20%)
2	FUC	D	4	2	10,10,11	1.34	2 (20%)	14,14,16	1.00	1 (7%)
2	NAG	E	1	1,2	14,14,15	1.71	3 (21%)	17,19,21	1.70	2 (11%)
2	NAG	E	2	2	14,14,15	1.32	3 (21%)	17,19,21	1.35	3 (17%)
2	BMA	E	3	2	11,11,12	1.55	2 (18%)	15,15,17	1.54	3 (20%)
2	FUC	E	4	2	10,10,11	1.68	2 (20%)	14,14,16	1.84	4 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	1/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	FUC	C	4	2	-	-	0/1/1/1
2	NAG	D	1	1,2	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	2	2	-	1/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1
2	FUC	D	4	2	-	-	0/1/1/1
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	BMA	E	3	2	-	1/2/19/22	0/1/1/1
2	FUC	E	4	2	-	-	0/1/1/1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	NAG	C1-C2	4.29	1.58	1.52
2	D	1	NAG	C1-C2	2.98	1.56	1.52
2	C	1	NAG	C1-C2	2.96	1.56	1.52
2	E	3	BMA	C2-C3	2.79	1.56	1.52
2	D	2	NAG	C3-C2	2.71	1.58	1.52
2	D	3	BMA	O5-C5	2.66	1.48	1.43
2	E	2	NAG	C1-C2	2.58	1.56	1.52
2	E	4	FUC	C1-C2	2.50	1.57	1.52
2	C	2	NAG	C3-C2	2.47	1.57	1.52
2	E	3	BMA	C4-C3	2.42	1.58	1.52
2	D	1	NAG	C4-C5	2.41	1.58	1.53
2	E	1	NAG	C3-C2	2.37	1.57	1.52
2	C	3	BMA	O5-C5	2.34	1.48	1.43
2	E	1	NAG	C4-C5	2.24	1.57	1.53
2	C	4	FUC	C6-C5	2.24	1.56	1.51
2	C	3	BMA	C1-C2	2.21	1.57	1.52
2	D	3	BMA	C2-C3	2.20	1.55	1.52
2	C	3	BMA	C2-C3	2.12	1.55	1.52
2	D	3	BMA	O5-C1	2.12	1.47	1.43
2	C	1	NAG	O5-C1	2.12	1.47	1.43
2	E	2	NAG	C4-C3	2.10	1.57	1.52
2	C	1	NAG	C4-C3	2.08	1.57	1.52
2	D	4	FUC	C6-C5	2.06	1.56	1.51
2	E	2	NAG	C4-C5	2.04	1.57	1.53
2	D	1	NAG	O5-C1	2.02	1.46	1.43
2	E	4	FUC	C2-C3	2.01	1.55	1.52
2	D	4	FUC	O5-C5	2.01	1.47	1.43

All (38) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	NAG	C4-C3-C2	4.67	117.87	111.02
2	C	3	BMA	O5-C5-C6	3.74	113.06	107.20
2	E	3	BMA	C1-O5-C5	3.73	117.24	112.19
2	D	3	BMA	O5-C5-C6	3.65	112.92	107.20
2	E	4	FUC	C2-C3-C4	3.55	117.04	110.89
2	D	1	NAG	C1-C2-N2	3.41	116.32	110.49
2	C	1	NAG	C4-C3-C2	-3.40	106.04	111.02
2	D	1	NAG	C8-C7-N2	-3.29	110.53	116.10
2	D	1	NAG	C4-C3-C2	-3.29	106.20	111.02
2	E	2	NAG	O5-C1-C2	-3.00	106.56	111.29
2	C	1	NAG	C8-C7-N2	-2.99	111.05	116.10
2	E	3	BMA	C1-C2-C3	-2.92	106.08	109.67
2	D	3	BMA	C1-O5-C5	-2.81	108.38	112.19
2	E	4	FUC	O2-C2-C3	-2.63	104.86	110.14
2	E	4	FUC	O5-C5-C4	2.57	114.14	109.52
2	C	2	NAG	O5-C5-C6	2.56	111.22	107.20
2	C	3	BMA	C1-O5-C5	-2.56	108.73	112.19
2	E	1	NAG	C1-O5-C5	2.55	115.65	112.19
2	E	4	FUC	C1-C2-C3	2.53	112.78	109.67
2	C	2	NAG	O3-C3-C4	-2.48	104.61	110.35
2	C	1	NAG	O5-C5-C6	2.39	110.95	107.20
2	C	1	NAG	C1-C2-N2	2.21	114.27	110.49
2	D	1	NAG	O5-C5-C6	2.20	110.66	107.20
2	C	4	FUC	C1-C2-C3	-2.17	106.99	109.67
2	D	1	NAG	O3-C3-C4	-2.16	105.35	110.35
2	E	3	BMA	O3-C3-C4	2.16	115.34	110.35
2	C	2	NAG	O6-C6-C5	2.10	118.50	111.29
2	D	2	NAG	C4-C3-C2	2.10	114.09	111.02
2	E	2	NAG	O5-C5-C6	2.09	110.49	107.20
2	C	3	BMA	O3-C3-C2	2.08	113.98	109.99
2	D	2	NAG	O5-C5-C6	2.06	110.43	107.20
2	D	2	NAG	O3-C3-C4	-2.05	105.60	110.35
2	D	1	NAG	O4-C4-C3	-2.05	105.61	110.35
2	D	4	FUC	C1-C2-C3	-2.04	107.16	109.67
2	C	1	NAG	O6-C6-C5	-2.03	104.33	111.29
2	E	2	NAG	C1-O5-C5	-2.02	109.46	112.19
2	D	1	NAG	O5-C5-C4	-2.02	105.92	110.83
2	D	3	BMA	C1-C2-C3	-2.00	107.21	109.67

There are no chirality outliers.

All (6) torsion outliers are listed below:

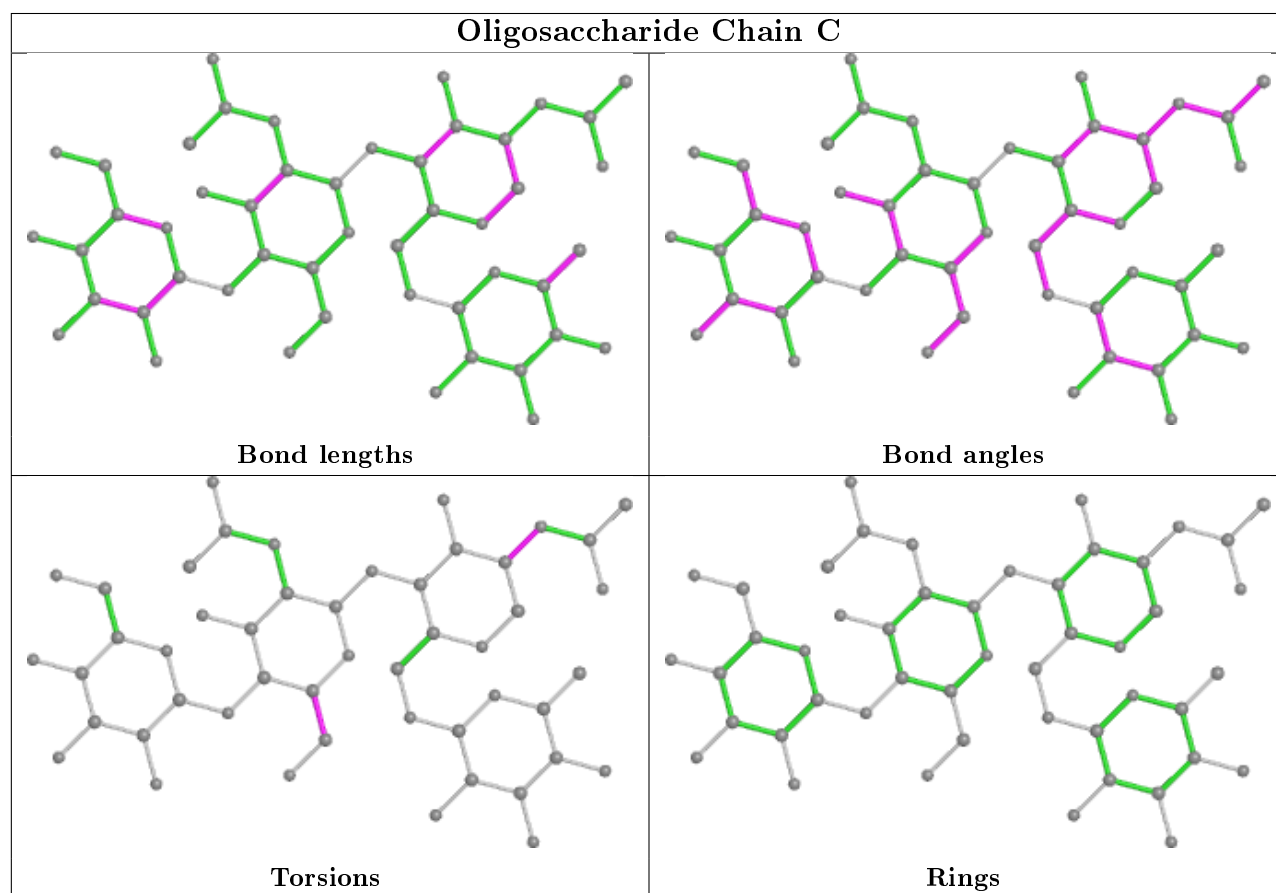
Mol	Chain	Res	Type	Atoms
2	D	2	NAG	C4-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	E	3	BMA	C4-C5-C6-O6
2	D	1	NAG	C1-C2-N2-C7
2	C	1	NAG	C1-C2-N2-C7
2	C	1	NAG	C3-C2-N2-C7

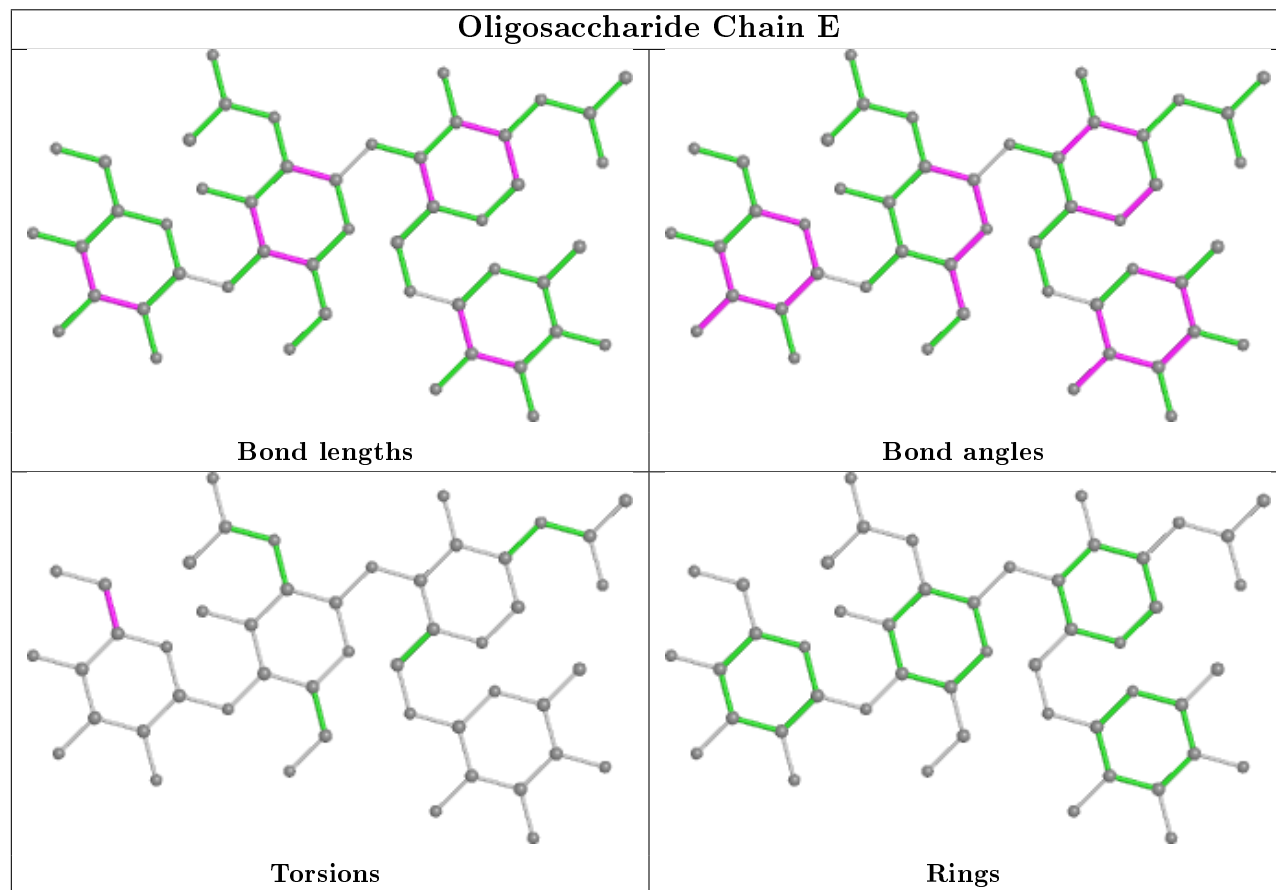
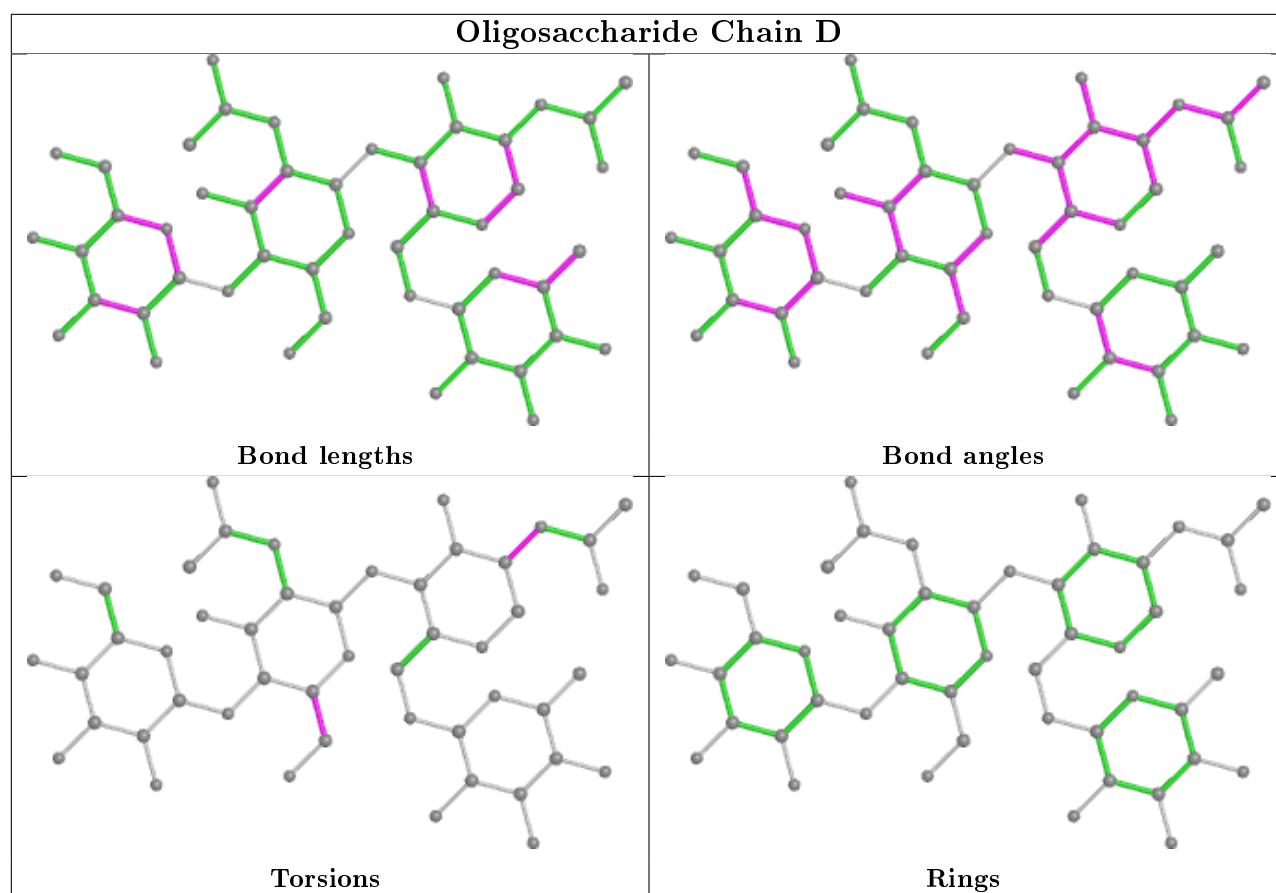
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	4	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

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	$\# Z  > 2$
3	NAG	A	1385	1	14,14,15	1.46	2 (14%)	17,19,21	1.46	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1385	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1385	NAG	C1-C2	2.99	1.56	1.52
3	A	1385	NAG	C3-C2	2.48	1.57	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1385	NAG	C4-C3-C2	3.93	116.78	111.02
3	A	1385	NAG	C1-C2-N2	2.49	114.74	110.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	354/408 (86%)	-0.14	12 (3%) 45 39	8, 15, 42, 79	0
1	B	354/408 (86%)	-0.23	11 (3%) 49 43	7, 14, 36, 81	0
All	All	708/816 (86%)	-0.18	23 (3%) 47 41	7, 15, 40, 81	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	141	PHE	8.8
1	B	118	ARG	8.2
1	A	118	ARG	5.9
1	B	116	SER	5.9
1	A	116	SER	5.3
1	A	119	VAL	5.2
1	A	115	LEU	5.0
1	B	117	GLN	4.9
1	A	143	GLU	3.5
1	A	142	GLY	3.1
1	A	140	GLN	2.9
1	B	332	TYR	2.8
1	B	119	VAL	2.8
1	A	117	GLN	2.7
1	B	115	LEU	2.6
1	B	194	LYS	2.6
1	B	295	ARG	2.5
1	B	193	ARG	2.4
1	A	219	HIS	2.2
1	B	121	ASN	2.2
1	A	114	PHE	2.1
1	B	191	GLN	2.1
1	A	332	TYR	2.0

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

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

## 6.3 Carbohydrates ⓘ

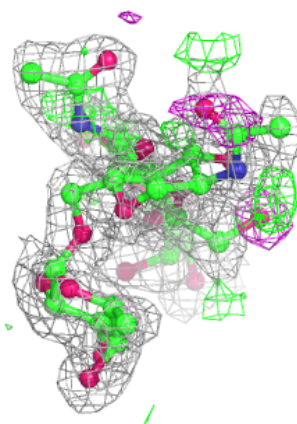
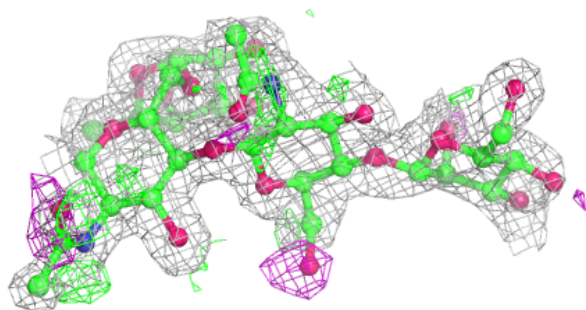
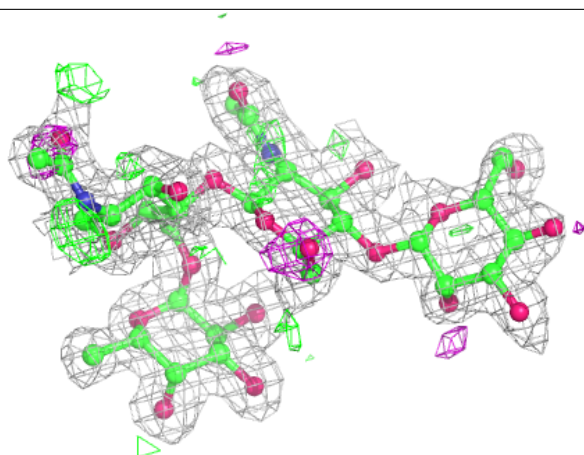
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	FUC	E	4	10/11	0.54	0.65	50,51,53,53	0
2	BMA	E	3	11/12	0.58	0.26	49,51,53,53	0
2	NAG	E	2	14/15	0.67	0.34	42,46,49,49	0
2	BMA	D	3	11/12	0.72	0.26	36,39,41,43	0
2	NAG	E	1	14/15	0.74	0.21	32,35,39,43	0
2	NAG	D	2	14/15	0.83	0.16	22,26,30,31	0
2	NAG	C	2	14/15	0.84	0.16	23,28,32,34	0
2	BMA	C	3	11/12	0.84	0.24	36,39,42,43	0
2	NAG	C	1	14/15	0.92	0.10	11,15,18,21	0
2	NAG	D	1	14/15	0.93	0.10	11,14,18,20	0
2	FUC	C	4	10/11	0.93	0.13	19,20,21,22	0
2	FUC	D	4	10/11	0.95	0.11	21,22,23,24	0

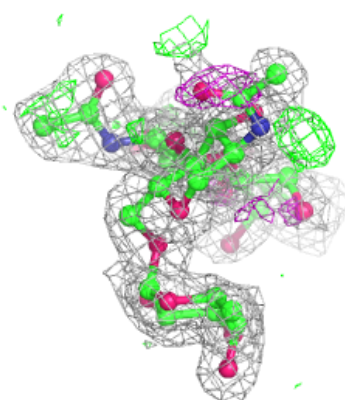
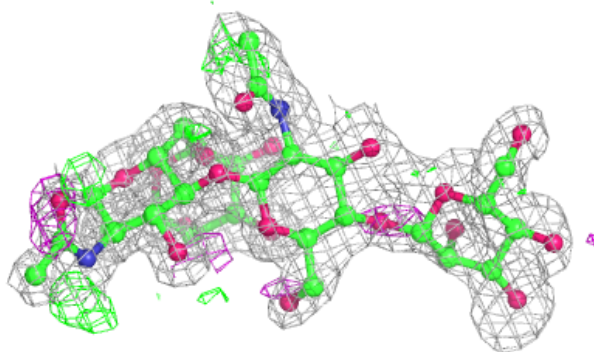
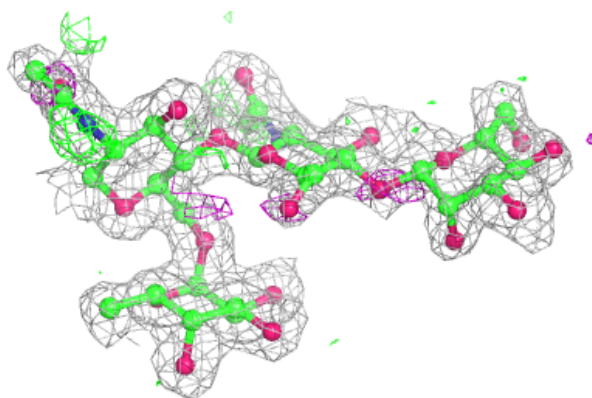
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around Chain C:**

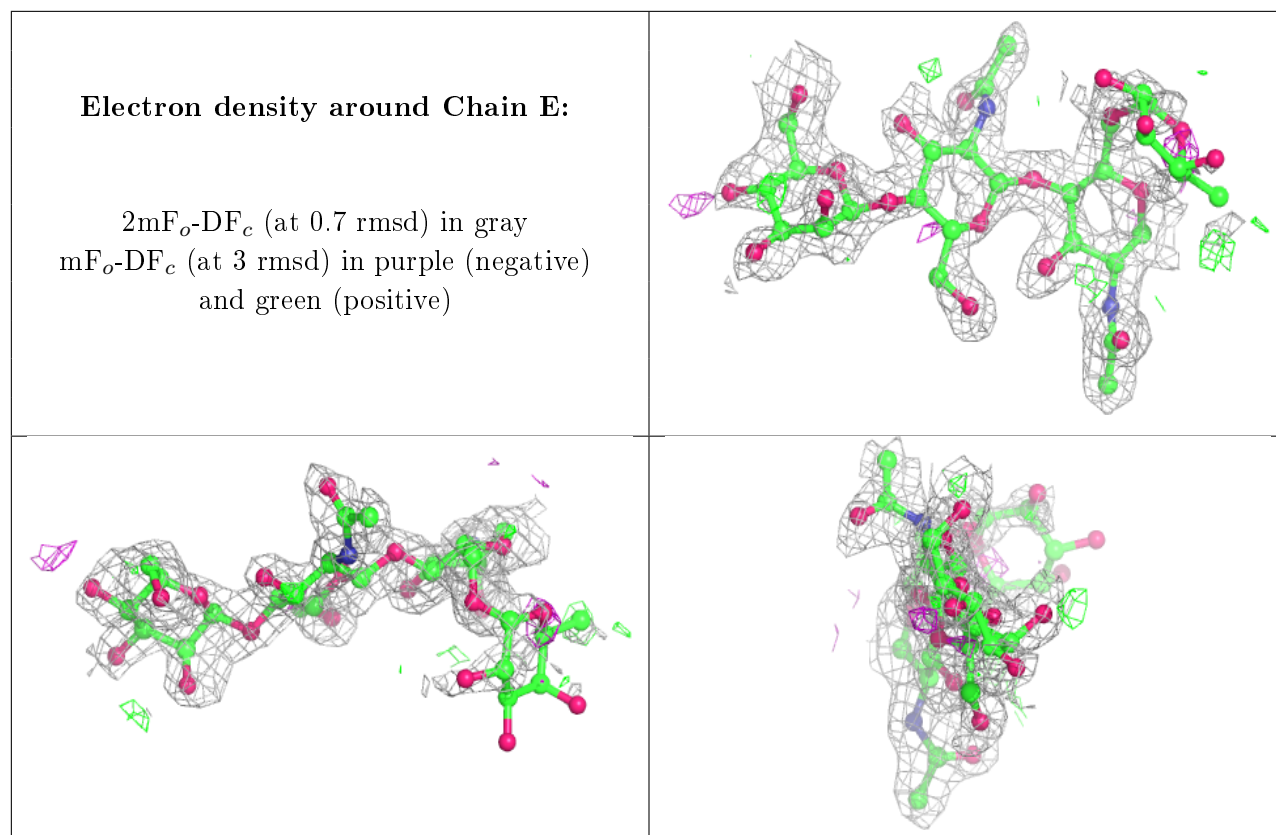
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around Chain D:**

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







## 6.4 Ligands [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
3	NAG	A	1385	14/15	0.64	0.28	66,70,73,73	0
4	CA	A	1386	1/1	0.99	0.03	10,10,10,10	0
4	CA	B	1389	1/1	1.00	0.04	10,10,10,10	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.