



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:29 PM UTC

PDB ID : 2XXL / pdb_00002xxl
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 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

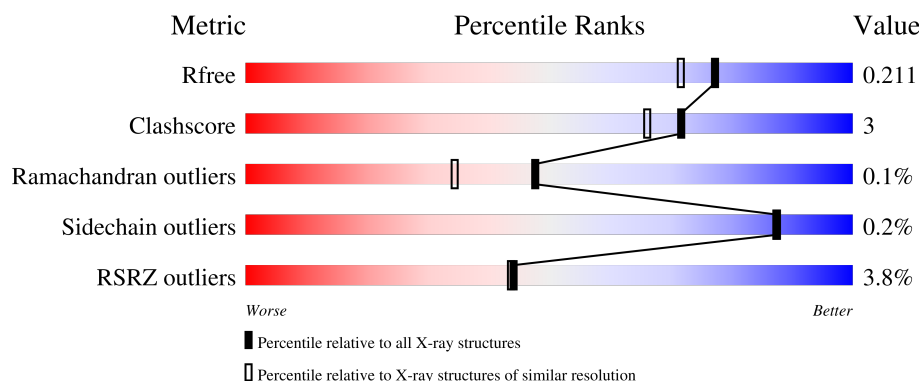
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

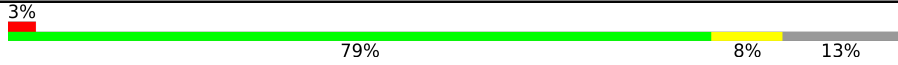
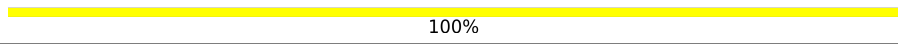
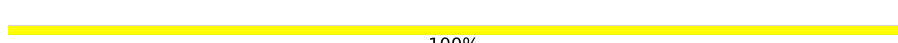
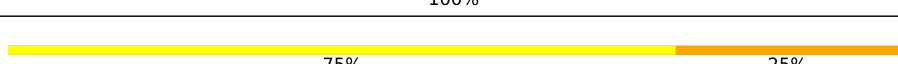
The reported resolution of this entry is 1.80 Å.

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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
1	B	408	
2	C	4	
2	D	4	
2	E	4	

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:

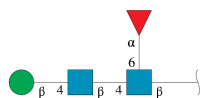
Chain	Residue	Modelled	Actual	Comment	Reference
A	378	LEU	-	expression tag	UNP Q9VB68
A	379	GLU	-	expression tag	UNP Q9VB68
A	380	SER	-	expression tag	UNP Q9VB68
A	381	ARG	-	expression tag	UNP Q9VB68
A	382	GLY	-	expression tag	UNP Q9VB68
A	383	PRO	-	expression tag	UNP Q9VB68
A	384	PHE	-	expression tag	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 (CCD ID: 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 (CCD ID: CA) (formula: Ca).

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

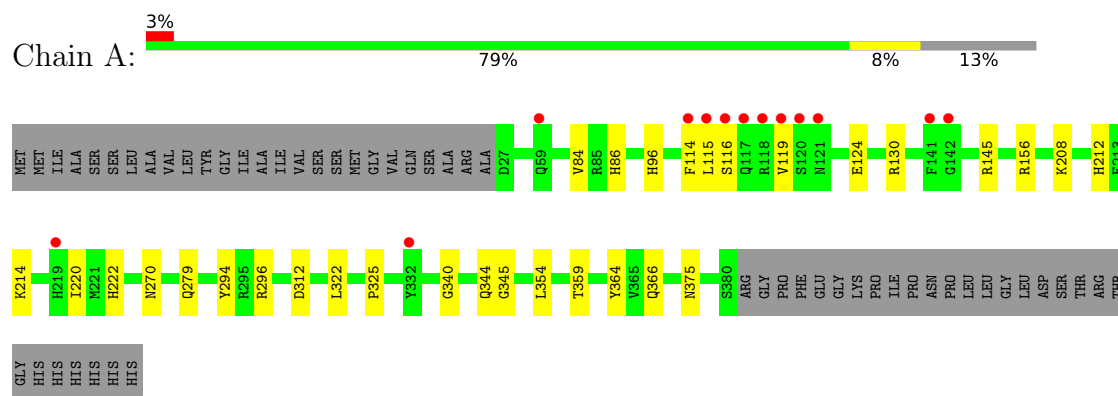
- Molecule 5 is water.

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

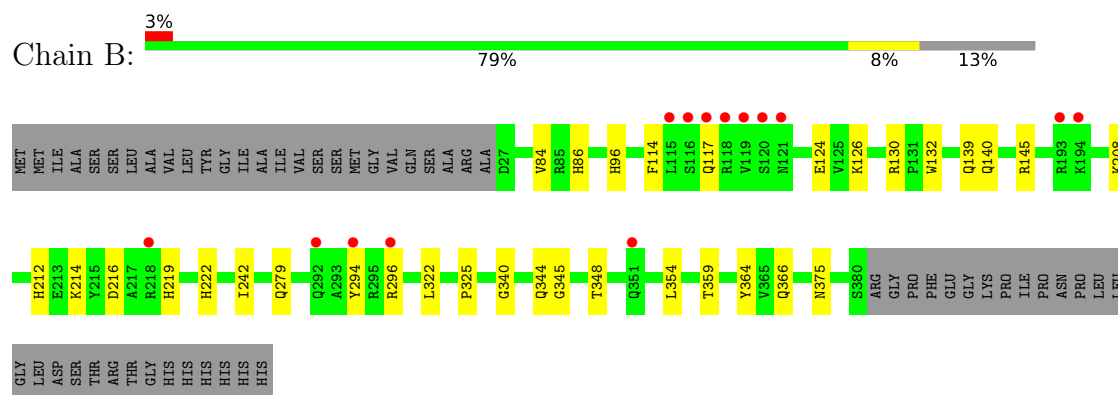
3 Residue-property plots [i](#)

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.

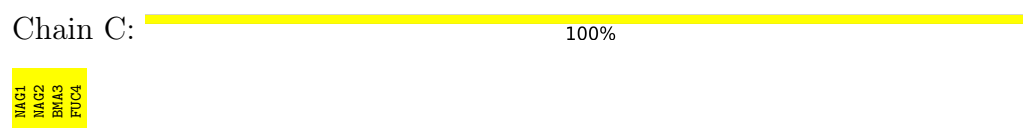
- Molecule 1: GRAM-POSITIVE SPECIFIC SERINE PROTEASE, ISOFORM B



- 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



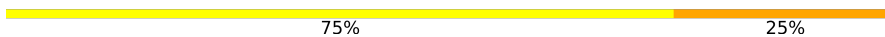
- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	13.8	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.56$, $\langle L^2 \rangle = 0.40$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, NAG, BMA, 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	0.78	0/2803	1.03	4/3790 (0.1%)
1	B	0.79	0/2803	1.01	3/3790 (0.1%)
All	All	0.78	0/5606	1.02	7/7580 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	312	ASP	CA-CB-CG	5.90	118.50	112.60
1	A	119	VAL	N-CA-C	5.84	116.82	108.93
1	B	354	LEU	N-CA-C	-5.84	103.42	110.13
1	A	322	LEU	N-CA-C	-5.17	100.10	108.52
1	B	322	LEU	N-CA-C	-5.10	100.20	108.52
1	B	139	GLN	N-CA-C	-5.04	102.40	109.96
1	A	354	LEU	N-CA-C	-5.04	103.80	110.40

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	2746	0	2659	17	0
1	B	2746	0	2659	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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:96:HIS:HD1	1:B:366:GLN:NE2	2.05	0.54
1:B:130:ARG:HE	1:B:279:GLN:NE2	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:HIS:HD2	1:A:364:TYR:OH	2.01	0.44
1:B:208:LYS:NZ	1:B:375:ASN:HD22	2.16	0.44
1:B:216:ASP:OD2	1:B:219:HIS:HD2	2.00	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 ⓘ

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	352/408 (86%)	340 (97%)	11 (3%)	1 (0%)	36	25
1	B	352/408 (86%)	341 (97%)	11 (3%)	0	100	100
All	All	704/816 (86%)	681 (97%)	22 (3%)	1 (0%)	48	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	220	ILE

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	301/344 (88%)	300 (100%)	1 (0%)	86	86
1	B	301/344 (88%)	301 (100%)	0	100	100
All	All	602/688 (88%)	601 (100%)	1 (0%)	87	87

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	156	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	86	HIS
1	A	95	GLN
1	A	140	GLN
1	A	166	HIS
1	A	212	HIS
1	A	219	HIS
1	A	222	HIS
1	A	236	GLN
1	A	279	GLN
1	A	281	ASN
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	95	GLN
1	B	140	GLN
1	B	190	GLN
1	B	212	HIS

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Mol	Chain	Res	Type
1	B	219	HIS
1	B	222	HIS
1	B	279	GLN
1	B	302	GLN
1	B	327	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	2,1	14,14,15	1.53	3 (21%)	17,19,21	1.92	4 (23%)
2	NAG	C	2	2	14,14,15	1.03	1 (7%)	17,19,21	1.21	2 (11%)
2	BMA	C	3	2	11,11,12	1.49	3 (27%)	15,15,17	1.46	2 (13%)
2	FUC	C	4	2	10,10,11	1.43	2 (20%)	14,14,16	0.88	0
2	NAG	D	1	2,1	14,14,15	1.59	2 (14%)	17,19,21	2.11	6 (35%)
2	NAG	D	2	2	14,14,15	1.13	1 (7%)	17,19,21	1.28	2 (11%)
2	BMA	D	3	2	11,11,12	1.59	3 (27%)	15,15,17	1.57	2 (13%)
2	FUC	D	4	2	10,10,11	1.33	2 (20%)	14,14,16	0.92	0
2	NAG	E	1	2,1	14,14,15	1.79	3 (21%)	17,19,21	1.71	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	E	2	2	14,14,15	1.36	3 (21%)	17,19,21	1.31	2 (11%)
2	BMA	E	3	2	11,11,12	1.53	2 (18%)	15,15,17	1.45	3 (20%)
2	FUC	E	4	2	10,10,11	1.66	2 (20%)	14,14,16	1.75	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	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	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	2,1	-	1/6/23/26	0/1/1/1
2	NAG	D	2	2	-	3/6/23/26	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	2,1	-	1/6/23/26	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	4.70	1.58	1.52
2	D	1	NAG	C1-C2	3.26	1.56	1.52
2	C	1	NAG	C1-C2	3.24	1.56	1.52
2	E	2	NAG	C1-C2	2.83	1.56	1.52
2	D	3	BMA	O5-C5	2.78	1.48	1.43
2	D	2	NAG	C3-C2	2.74	1.58	1.52
2	E	3	BMA	C2-C3	2.70	1.56	1.52
2	C	2	NAG	C3-C2	2.50	1.57	1.52
2	C	3	BMA	O5-C5	2.44	1.48	1.43
2	E	1	NAG	C3-C2	2.40	1.57	1.52
2	D	1	NAG	C4-C5	2.39	1.58	1.53
2	E	4	FUC	C1-C2	2.38	1.57	1.52
2	E	3	BMA	C4-C3	2.37	1.58	1.52
2	C	4	FUC	C6-C5	2.23	1.56	1.51
2	E	1	NAG	C4-C5	2.22	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4	FUC	O5-C5	2.15	1.47	1.43
2	D	3	BMA	C2-C3	2.13	1.55	1.52
2	C	4	FUC	O5-C5	2.12	1.47	1.43
2	E	4	FUC	O5-C5	2.12	1.47	1.43
2	C	3	BMA	C1-C2	2.11	1.57	1.52
2	C	3	BMA	C2-C3	2.06	1.55	1.52
2	D	4	FUC	C6-C5	2.06	1.56	1.51
2	E	2	NAG	C4-C3	2.06	1.57	1.52
2	C	1	NAG	C4-C3	2.04	1.57	1.52
2	C	1	NAG	O5-C1	2.02	1.47	1.43
2	D	3	BMA	O5-C1	2.02	1.47	1.43
2	E	2	NAG	C4-C5	2.02	1.57	1.53

All (30) 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	E	3	BMA	C1-O5-C5	3.77	117.24	112.19
2	D	1	NAG	C1-C2-N2	3.74	116.32	110.43
2	E	4	FUC	C2-C3-C4	3.51	117.04	110.86
2	C	1	NAG	C4-C3-C2	-3.40	106.04	111.02
2	D	1	NAG	C8-C7-N2	-3.37	110.53	116.12
2	D	1	NAG	C4-C3-C2	-3.29	106.20	111.02
2	E	2	NAG	O5-C1-C2	-3.06	106.56	111.29
2	C	1	NAG	C8-C7-N2	-3.06	111.05	116.12
2	D	3	BMA	C1-O5-C5	-2.84	108.38	112.19
2	C	3	BMA	O5-C5-C6	2.78	113.06	107.66
2	D	3	BMA	O5-C5-C6	2.70	112.92	107.66
2	E	1	NAG	C1-O5-C5	2.59	115.65	112.19
2	C	3	BMA	C1-O5-C5	-2.58	108.73	112.19
2	E	4	FUC	O2-C2-C3	-2.55	104.86	110.15
2	E	4	FUC	O5-C5-C4	2.55	114.14	109.55
2	E	3	BMA	C1-C2-C3	-2.45	106.08	109.64
2	C	2	NAG	O3-C3-C4	-2.45	104.61	110.38
2	C	1	NAG	C1-C2-N2	2.43	114.27	110.43
2	E	4	FUC	C1-C2-C3	2.15	112.78	109.64
2	E	1	NAG	C1-C2-N2	2.14	113.80	110.43
2	D	1	NAG	O3-C3-C4	-2.13	105.35	110.38
2	E	3	BMA	O3-C3-C4	2.11	115.34	110.38
2	C	2	NAG	O6-C6-C5	2.10	118.50	111.33
2	D	2	NAG	C4-C3-C2	2.10	114.09	111.02
2	C	1	NAG	O6-C6-C5	-2.06	104.33	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	NAG	C1-O5-C5	-2.04	109.46	112.19
2	D	2	NAG	O3-C3-C4	-2.03	105.60	110.38
2	D	1	NAG	O4-C4-C3	-2.02	105.61	110.38
2	D	1	NAG	O5-C5-C4	-2.02	105.92	110.83

There are no chirality outliers.

All (10) torsion outliers are listed below:

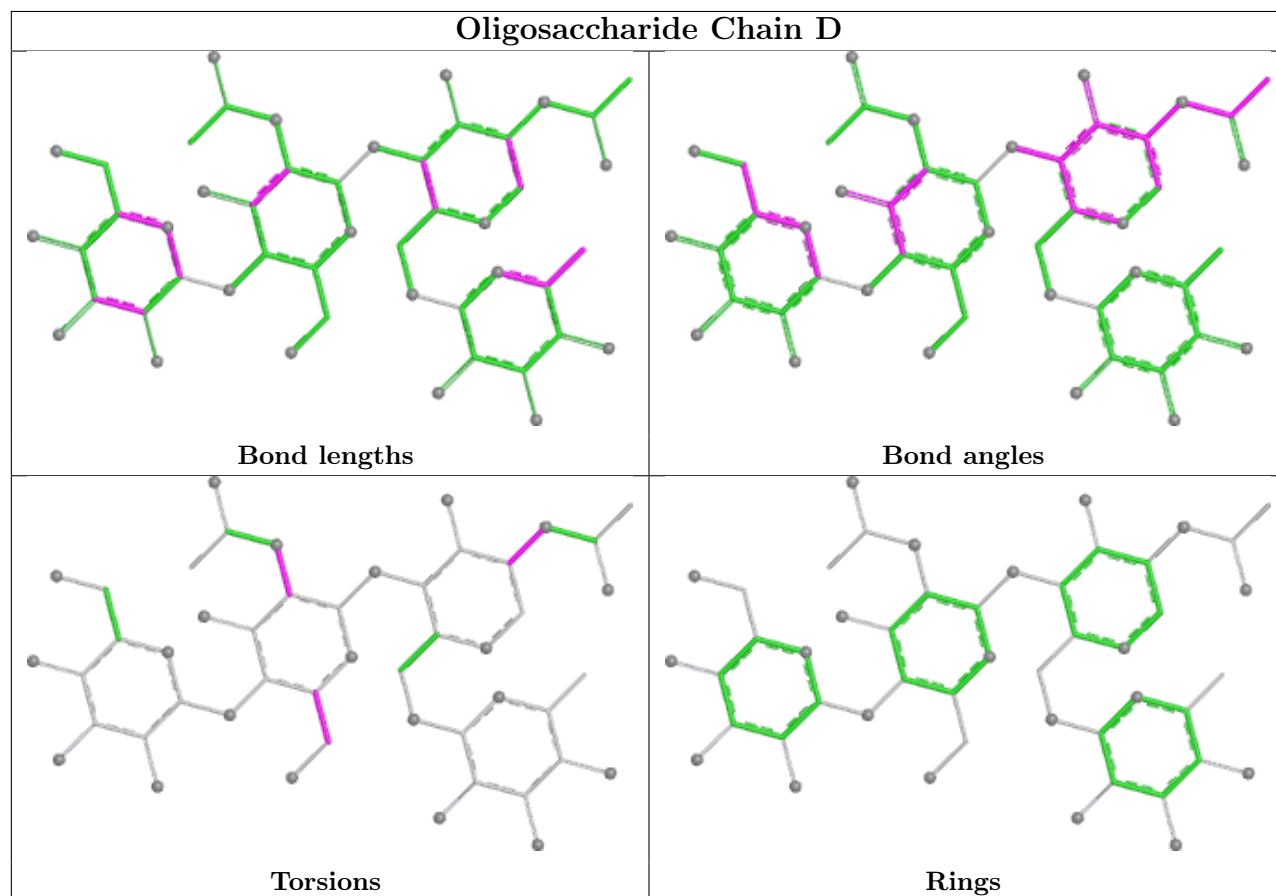
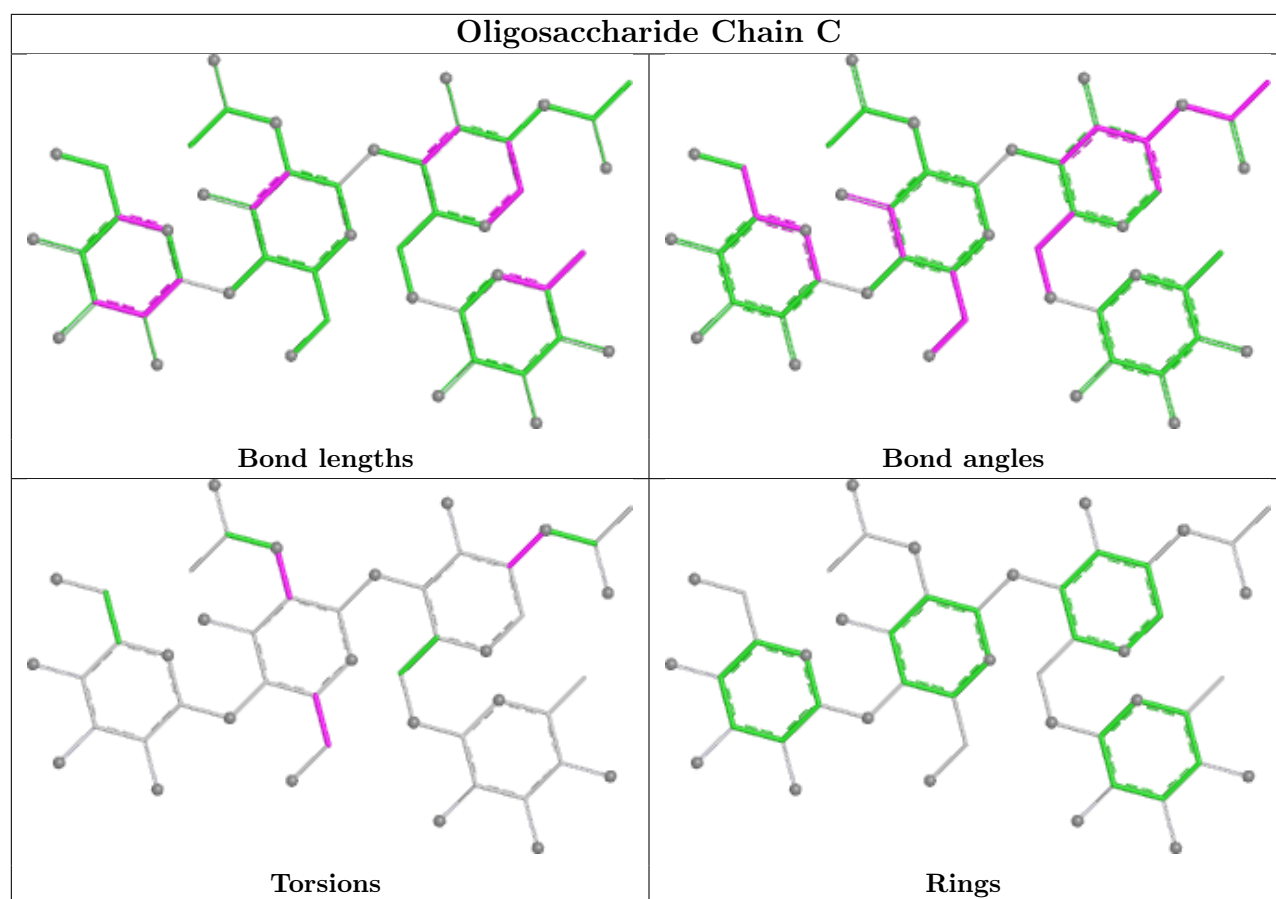
Mol	Chain	Res	Type	Atoms
2	D	2	NAG	C4-C5-C6-O6
2	C	1	NAG	C1-C2-N2-C7
2	D	1	NAG	C1-C2-N2-C7
2	C	2	NAG	C4-C5-C6-O6
2	E	3	BMA	C4-C5-C6-O6
2	C	2	NAG	C1-C2-N2-C7
2	D	2	NAG	C1-C2-N2-C7
2	C	1	NAG	C3-C2-N2-C7
2	E	1	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6

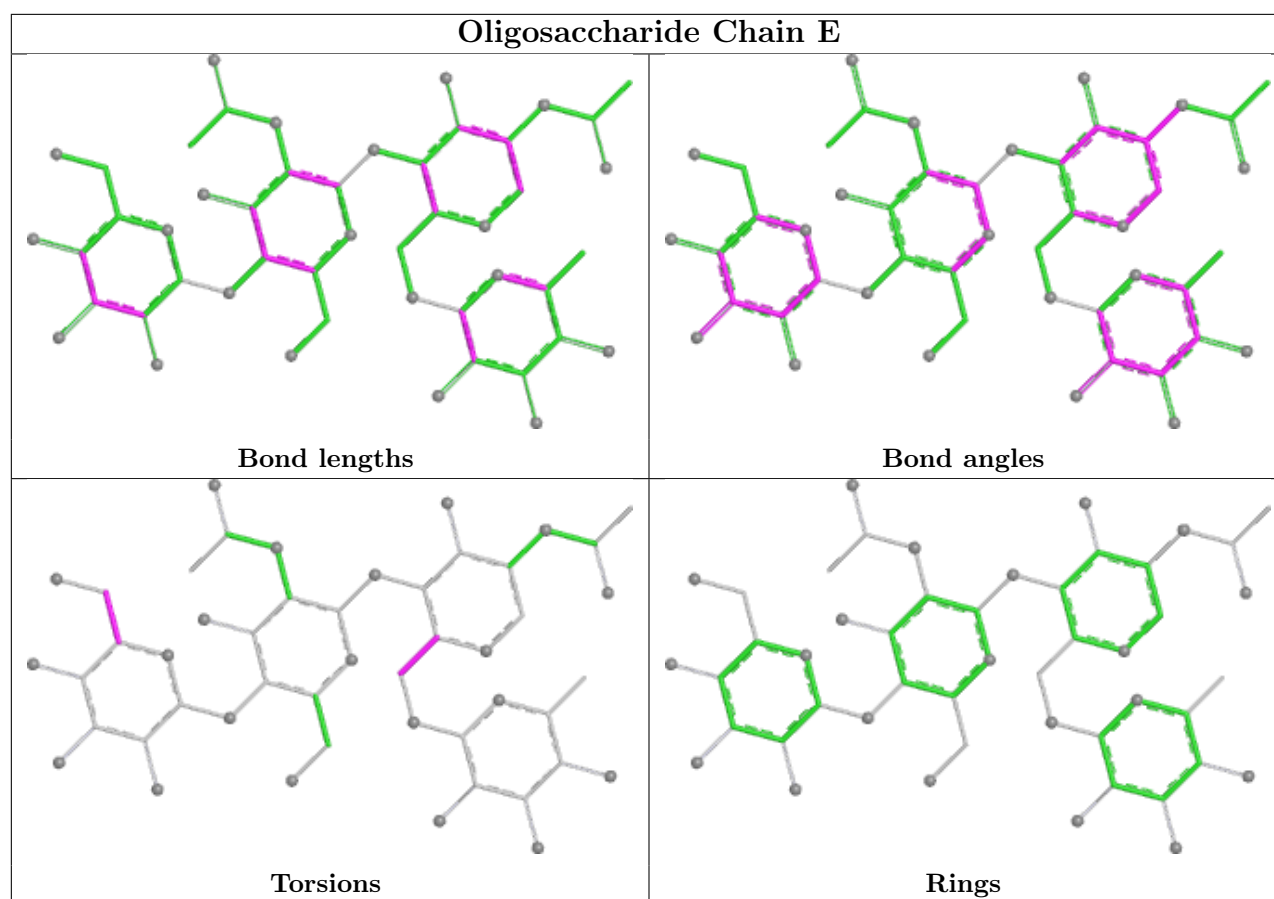
There are no ring outliers.

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 [i](#)

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	1.51	2 (14%)	17,19,21	1.49	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	3.28	1.56	1.52
3	A	1385	NAG	C3-C2	2.51	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	2.73	114.74	110.43

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 [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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	354/408 (86%)	-0.23	13 (3%) 45 45	8, 15, 42, 79	0
1	B	354/408 (86%)	-0.32	14 (3%) 42 41	7, 14, 36, 81	0
All	All	708/816 (86%)	-0.27	27 (3%) 44 44	7, 15, 40, 81	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	115	LEU	5.4
1	A	141	PHE	5.3
1	A	116	SER	5.1
1	B	119	VAL	4.5
1	B	117	GLN	4.3
1	A	118	ARG	3.4
1	B	121	ASN	3.3
1	A	119	VAL	3.3
1	B	218	ARG	3.3
1	B	193	ARG	3.1
1	B	116	SER	3.1
1	B	296	ARG	2.8
1	A	114	PHE	2.8
1	A	142	GLY	2.8
1	A	219	HIS	2.7
1	B	118	ARG	2.6
1	B	294	TYR	2.6
1	A	117	GLN	2.4
1	B	120	SER	2.4
1	B	115	LEU	2.2
1	A	121	ASN	2.1
1	A	120	SER	2.1
1	A	332	TYR	2.1
1	B	351	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	194	LYS	2.0
1	A	59	GLN	2.0
1	B	292	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

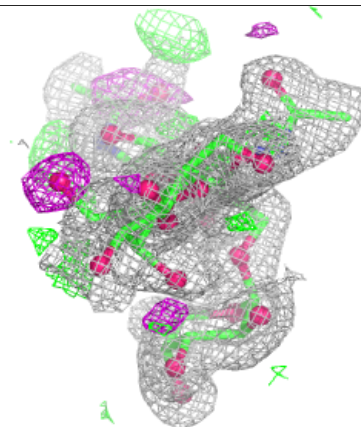
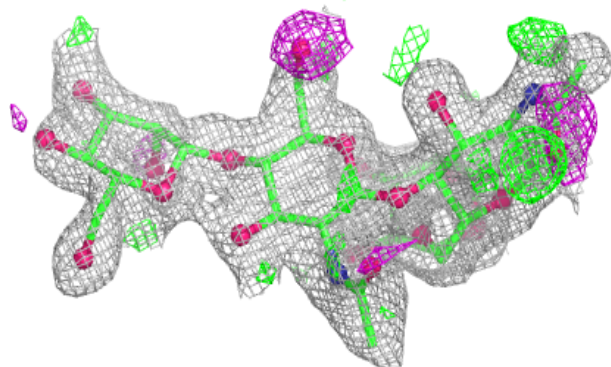
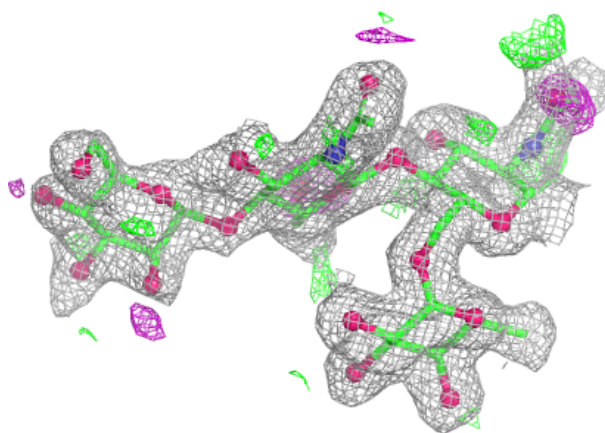
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FUC	E	4	10/11	0.26	0.22	50,51,53,53	0
2	BMA	E	3	11/12	0.67	0.17	49,51,53,53	0
2	NAG	E	2	14/15	0.67	0.15	42,46,49,49	0
2	BMA	D	3	11/12	0.73	0.14	36,39,41,43	0
2	BMA	C	3	11/12	0.76	0.13	36,39,42,43	0
2	NAG	C	2	14/15	0.82	0.14	23,28,32,34	0
2	NAG	E	1	14/15	0.84	0.11	32,35,39,43	0
2	NAG	D	2	14/15	0.85	0.13	22,26,30,31	0
2	NAG	C	1	14/15	0.91	0.08	11,15,18,21	0
2	NAG	D	1	14/15	0.92	0.08	11,14,18,20	0
2	FUC	C	4	10/11	0.93	0.08	19,20,21,22	0
2	FUC	D	4	10/11	0.93	0.08	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.

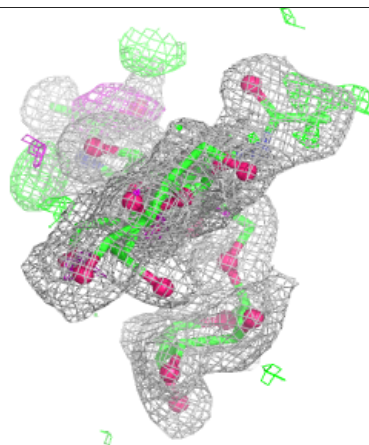
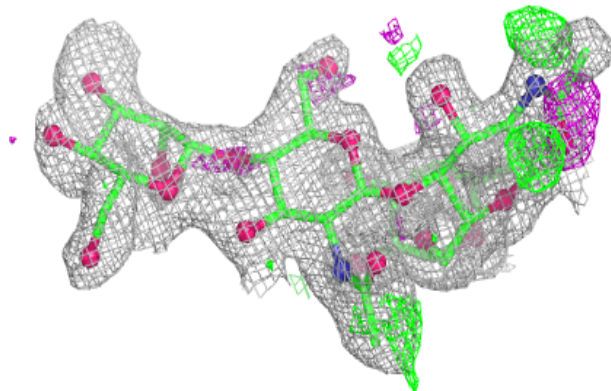
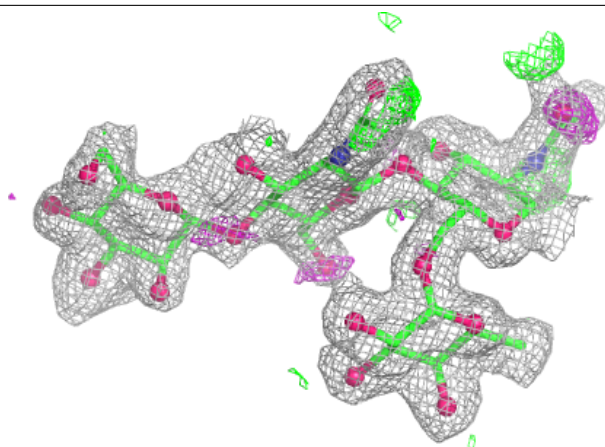
Electron density around Chain C:

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

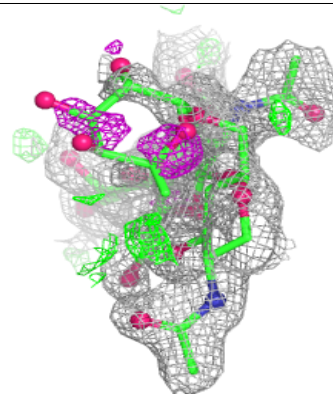
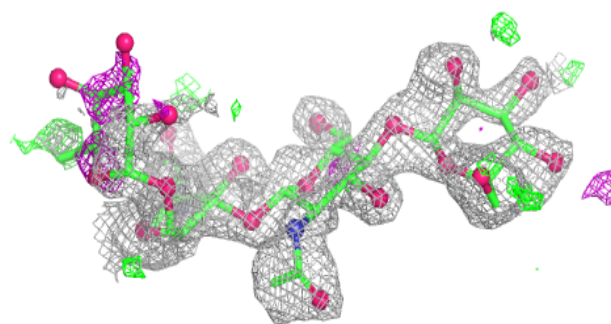
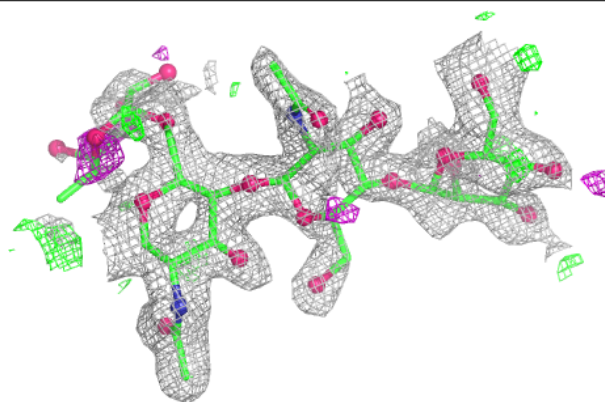


Electron density around Chain D:

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

**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 [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	A	1385	14/15	0.54	0.22	66,70,73,73	0
4	CA	A	1386	1/1	1.00	0.02	10,10,10,10	0
4	CA	B	1389	1/1	1.00	0.02	10,10,10,10	0

6.5 Other polymers [i](#)

There are no such residues in this entry.