



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 03:26 AM BST

PDB ID : 6HZZ
Title : Structure of human D-glucuronyl C5 epimerase
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Deposited on : 2018-10-24
Resolution : 2.52 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

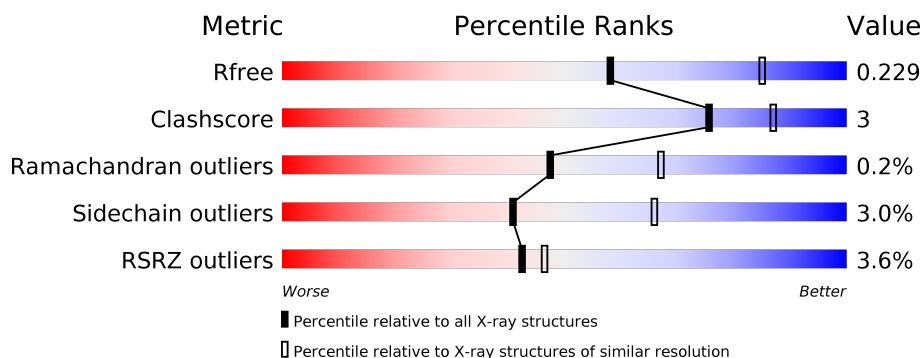
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 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.



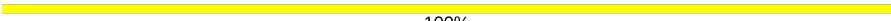
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	527	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 6% 89% 7% </div> </div>
1	B	527	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 6%, orange 1%, yellow 1%, green 92%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 6% 87% 9% </div> </div>
2	C	4	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 25%, green 75%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 25% 75% </div> </div>
3	D	5	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 80%, orange 20%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 80% 20% </div> </div>
3	G	5	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 100%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 100% </div> </div>
4	E	2	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 50%, yellow 50%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 50% 50% </div> </div>

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Mol	Chain	Length	Quality of chain
5	F	3	 100%

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 8991 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.

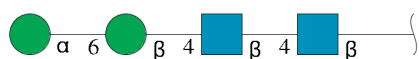
- Molecule 1 is a protein called D-glucuronyl C5-epimerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	511	Total	C	N	O	S	0	4	0
			4153	2677	699	763	14			
1	B	516	Total	C	N	O	S	0	6	0
			4197	2704	703	776	14			

There are 14 discrepancies between the modelled and reference sequences:

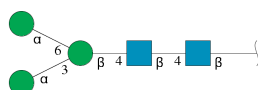
Chain	Residue	Modelled	Actual	Comment	Reference
A	91	ASP	-	expression tag	UNP O94923
A	92	TYR	-	expression tag	UNP O94923
A	93	LYS	-	expression tag	UNP O94923
A	94	ASP	-	expression tag	UNP O94923
A	95	ASP	-	expression tag	UNP O94923
A	96	ASP	-	expression tag	UNP O94923
A	97	ASP	-	expression tag	UNP O94923
B	91	ASP	-	expression tag	UNP O94923
B	92	TYR	-	expression tag	UNP O94923
B	93	LYS	-	expression tag	UNP O94923
B	94	ASP	-	expression tag	UNP O94923
B	95	ASP	-	expression tag	UNP O94923
B	96	ASP	-	expression tag	UNP O94923
B	97	ASP	-	expression tag	UNP O94923

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



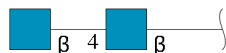
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



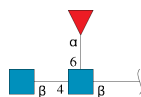
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	G	5	Total	C	N	O	0	0	0
			61	34	2	25			

- 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	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



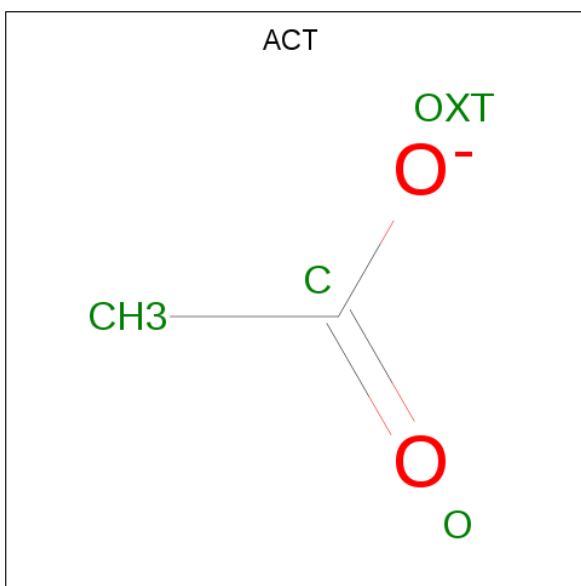
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	F	3	Total	C	N	O	0	0	0
			37	22	2	13			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	1	Total	Cl	0	0
			1	1		
10	A	1	Total	Cl	0	0
			1	1		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	201	Total	O	0	0
			201	201		

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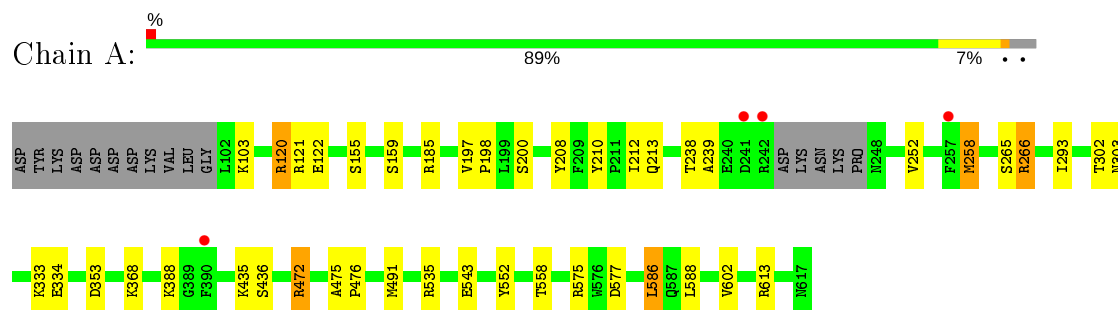
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	B	171	Total	O	0	0
			171	171		

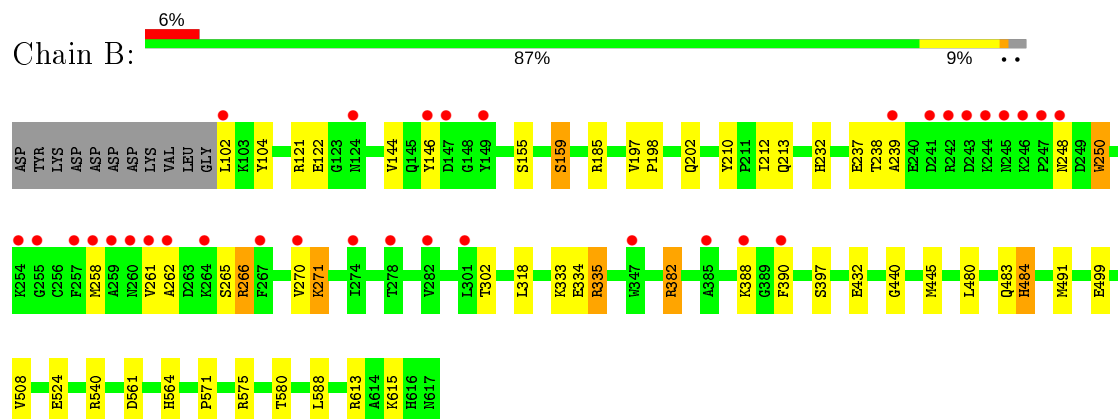
3 Residue-property plots [i](#)

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: D-glucuronyl C5-epimerase



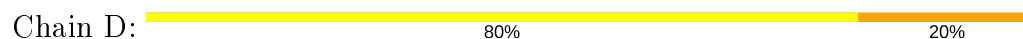
- Molecule 1: D-glucuronyl C5-epimerase



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



- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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 E: 50% 50%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	99.82Å 99.82Å 262.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.83 – 2.52 43.83 – 2.52	Depositor EDS
% Data completeness (in resolution range)	99.5 (43.83-2.52) 99.5 (43.83-2.52)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.176 , 0.226 0.180 , 0.229	Depositor DCC
R_{free} test set	2489 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	46.2	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 31.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.057 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8991	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, CL, CA, FUC, ACT, MAN, SO4

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	0.71	1/4275 (0.0%)	0.80	0/5784
1	B	0.67	2/4327 (0.0%)	0.77	0/5858
All	All	0.69	3/8602 (0.0%)	0.79	0/11642

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	6
All	All	0	9

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	543	GLU	CD-OE1	6.27	1.32	1.25
1	B	524	GLU	CD-OE2	6.22	1.32	1.25
1	B	382	ARG	CZ-NH1	5.26	1.39	1.33

There are no bond angle outliers.

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	120	ARG	Sidechain
1	A	472	ARG	Sidechain
1	A	613	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	121	ARG	Sidechain
1	B	248	ASN	Peptide
1	B	266	ARG	Sidechain
1	B	335	ARG	Sidechain
1	B	540	ARG	Sidechain
1	B	575	ARG	Sidechain

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	4153	0	4093	31	0
1	B	4197	0	4127	25	0
2	C	50	0	43	0	0
3	D	61	0	52	1	0
3	G	61	0	52	0	0
4	E	28	0	25	0	0
5	F	37	0	32	0	0
6	A	14	0	13	1	0
7	A	4	0	3	0	0
8	A	5	0	0	0	0
8	B	5	0	0	0	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
11	A	201	0	0	0	0
11	B	171	0	0	1	0
All	All	8991	0	8440	52	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 (52) 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:200:SER:HB2	1:A:213[B]:GLN:NE2	1.81	0.95
1:A:200:SER:HB2	1:A:213[B]:GLN:HE22	1.32	0.93
1:A:200:SER:CB	1:A:213[B]:GLN:HE22	1.99	0.75
1:A:120:ARG:NH1	1:B:122:GLU:OE1	2.24	0.71
1:A:252:VAL:HG22	1:A:258:MET:CE	2.25	0.66
1:A:200:SER:HB2	1:A:213[B]:GLN:CD	2.16	0.65
1:A:252:VAL:HG22	1:A:258:MET:HE2	1.79	0.65
1:A:200:SER:CB	1:A:213[B]:GLN:NE2	2.61	0.56
1:A:208:TYR:CE1	1:A:210:TYR:HB2	2.41	0.55
1:A:575:ARG:HG3	1:A:577:ASP:OD1	2.09	0.53
1:A:302:THR:HG22	1:A:388:LYS:H	1.75	0.51
1:B:159:SER:HB3	1:B:580:THR:HG21	1.93	0.51
1:B:588:LEU:C	1:B:588:LEU:HD23	2.32	0.51
1:B:318:LEU:O	1:B:335:ARG:HD2	2.12	0.50
1:A:303:ASN:OD1	6:A:1005:NAG:N2	2.44	0.50
1:B:440:GLY:O	1:B:484:HIS:NE2	2.37	0.50
1:A:588:LEU:C	1:A:588:LEU:HD23	2.32	0.50
1:A:122:GLU:OE2	1:B:104:TYR:HE2	1.94	0.50
1:B:237:GLU:HG2	1:B:250:TRP:HH2	1.77	0.49
1:A:185:ARG:NH1	1:A:213[A]:GLN:OE1	2.45	0.49
1:A:238:THR:O	1:A:239:ALA:HB3	2.12	0.49
1:A:491:MET:HE2	1:B:491:MET:HB2	1.95	0.49
1:B:185:ARG:NH1	1:B:213:GLN:OE1	2.45	0.49
1:A:200:SER:HB2	1:A:213[B]:GLN:OE1	2.14	0.48
1:B:302:THR:HG22	1:B:388:LYS:H	1.78	0.48
1:B:238:THR:O	1:B:239:ALA:HB3	2.15	0.47
1:A:303:ASN:C	1:A:303:ASN:OD1	2.54	0.46
1:B:250:TRP:CH2	1:B:271:LYS:HD2	2.51	0.46
1:B:564:HIS:HB3	1:B:571:PRO:HA	1.99	0.45
1:B:613[B]:ARG:NH1	11:B:1109:HOH:O	2.49	0.45
1:A:586:LEU:HB3	1:A:602:VAL:CG2	2.47	0.44
1:A:210:TYR:CZ	1:A:212:ILE:HD12	2.53	0.44
1:A:266:ARG:NH1	3:D:1:NAG:O7	2.50	0.43
1:B:261:VAL:HG12	1:B:262:ALA:O	2.18	0.43
1:A:197:VAL:HB	1:A:198:PRO:HD2	2.01	0.42
1:B:197:VAL:HB	1:B:198:PRO:HD2	2.01	0.42
1:A:120:ARG:NH1	1:B:122:GLU:CD	2.73	0.42
1:B:210:TYR:CZ	1:B:212:ILE:HD12	2.55	0.42
1:B:144:VAL:HG13	1:B:146:TYR:HE1	1.84	0.41
1:B:445:MET:HE1	1:B:499:GLU:OE2	2.20	0.41
1:A:586:LEU:HB3	1:A:602:VAL:HG22	2.03	0.41
1:B:508:VAL:HG22	1:B:561:ASP:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:TYR:O	1:A:558:THR:HA	2.21	0.41
1:A:266:ARG:HG2	1:A:266:ARG:NH1	2.36	0.41
1:B:159:SER:HB3	1:B:580:THR:CG2	2.50	0.40
1:B:270:VAL:CG1	1:B:390:PHE:HB3	2.51	0.40
1:A:293:ILE:HD13	1:A:353:ASP:HA	2.02	0.40
1:B:232:HIS:O	1:B:397:SER:HA	2.22	0.40
1:A:266:ARG:HH11	1:A:266:ARG:HG2	1.87	0.40
1:A:475:ALA:N	1:A:476:PRO:CD	2.84	0.40
1:B:480:LEU:H	1:B:483[B]:GLN:HE21	1.69	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	511/527 (97%)	490 (96%)	20 (4%)	1 (0%)	47	67
1	B	520/527 (99%)	500 (96%)	19 (4%)	1 (0%)	47	67
All	All	1031/1054 (98%)	990 (96%)	39 (4%)	2 (0%)	47	67

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	334	GLU
1	B	334	GLU

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	448/459 (98%)	435 (97%)	13 (3%)	42	67
1	B	453/459 (99%)	438 (97%)	15 (3%)	38	62
All	All	901/918 (98%)	873 (97%)	28 (3%)	41	65

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	LYS
1	A	121	ARG
1	A	155	SER
1	A	159	SER
1	A	258	MET
1	A	265	SER
1	A	266	ARG
1	A	333	LYS
1	A	368	LYS
1	A	435	LYS
1	A	436	SER
1	A	535	ARG
1	A	586	LEU
1	B	102	LEU
1	B	155	SER
1	B	159	SER
1	B	202	GLN
1	B	250	TRP
1	B	258	MET
1	B	265	SER
1	B	266	ARG
1	B	271	LYS
1	B	333	LYS
1	B	382	ARG
1	B	432[A]	GLU
1	B	432[B]	GLU
1	B	484	HIS
1	B	615	LYS

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

Mol	Chain	Res	Type
1	A	248	ASN
1	A	328	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

19 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAG	C	1	1,2	14,14,15	0.44	0	17,19,21	0.85	0
2	NAG	C	2	2	14,14,15	0.53	0	17,19,21	1.53	1 (5%)
2	BMA	C	3	2	11,11,12	0.66	0	15,15,17	1.15	1 (6%)
2	MAN	C	4	2	11,11,12	0.71	0	15,15,17	2.79	5 (33%)
3	NAG	D	1	1,3	14,14,15	0.30	0	17,19,21	1.59	3 (17%)
3	NAG	D	2	3	14,14,15	0.30	0	17,19,21	0.91	1 (5%)
3	BMA	D	3	3	11,11,12	0.51	0	15,15,17	1.11	1 (6%)
3	MAN	D	4	3	11,11,12	0.44	0	15,15,17	1.35	2 (13%)
3	MAN	D	5	3	11,11,12	0.67	0	15,15,17	1.03	1 (6%)
4	NAG	E	1	1,4	14,14,15	0.52	0	17,19,21	0.84	0
4	NAG	E	2	4	14,14,15	0.35	0	17,19,21	1.20	2 (11%)
5	NAG	F	1	1,5	14,14,15	1.00	1 (7%)	17,19,21	1.16	2 (11%)
5	NAG	F	2	5	14,14,15	0.54	0	17,19,21	1.28	3 (17%)
5	FUC	F	3	5	9,9,11	2.60	5 (55%)	10,12,16	2.41	4 (40%)
3	NAG	G	1	1,3	14,14,15	0.45	0	17,19,21	1.27	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	G	2	3	14,14,15	0.56	0	17,19,21	1.92	2 (11%)
3	BMA	G	3	3	11,11,12	0.59	0	15,15,17	1.82	5 (33%)
3	MAN	G	4	3	11,11,12	0.94	0	15,15,17	2.64	4 (26%)
3	MAN	G	5	3	11,11,12	0.49	0	15,15,17	1.35	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	BMA	C	3	2	-	2/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	BMA	D	3	3	-	2/2/19/22	0/1/1/1
3	MAN	D	4	3	-	0/2/19/22	0/1/1/1
3	MAN	D	5	3	-	2/2/19/22	0/1/1/1
4	NAG	E	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
5	NAG	F	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	F	2	5	-	0/6/23/26	0/1/1/1
5	FUC	F	3	5	-	-	0/1/1/1
3	NAG	G	1	1,3	-	2/6/23/26	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
3	MAN	G	4	3	-	2/2/19/22	0/1/1/1
3	MAN	G	5	3	-	2/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	3	FUC	O5-C5	3.86	1.47	1.43
5	F	3	FUC	C1-C2	3.55	1.60	1.52
5	F	3	FUC	C4-C5	3.28	1.57	1.51
5	F	1	NAG	O5-C1	3.03	1.48	1.43
5	F	3	FUC	O5-C1	2.59	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	3	FUC	O2-C2	2.22	1.48	1.43

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	4	MAN	C1-O5-C5	8.19	123.28	112.19
3	G	4	MAN	C1-C2-C3	6.72	117.93	109.67
3	G	2	NAG	C1-O5-C5	6.64	121.18	112.19
3	G	4	MAN	C1-O5-C5	5.48	119.62	112.19
5	F	3	FUC	O2-C2-C1	5.20	119.78	109.15
3	G	5	MAN	C1-O5-C5	4.33	118.06	112.19
2	C	2	NAG	C1-O5-C5	4.24	117.93	112.19
2	C	4	MAN	C1-C2-C3	4.12	114.72	109.67
3	G	4	MAN	O5-C5-C6	3.93	113.37	107.20
3	D	1	NAG	C1-O5-C5	3.86	117.42	112.19
3	G	3	BMA	C2-C3-C4	-3.71	104.48	110.89
2	C	4	MAN	O5-C1-C2	3.40	116.01	110.77
3	D	4	MAN	C1-C2-C3	3.22	113.63	109.67
3	G	3	BMA	O5-C5-C6	3.20	112.21	107.20
3	D	5	MAN	C1-C2-C3	3.07	113.44	109.67
3	G	3	BMA	O3-C3-C2	3.05	115.83	109.99
4	E	2	NAG	C4-C3-C2	3.03	115.46	111.02
2	C	4	MAN	O5-C5-C6	2.87	111.70	107.20
2	C	4	MAN	C3-C4-C5	-2.83	105.19	110.24
3	G	2	NAG	O5-C5-C4	2.83	117.72	110.83
3	D	1	NAG	O5-C1-C2	-2.81	106.85	111.29
3	D	1	NAG	C6-C5-C4	-2.79	106.48	113.00
3	G	4	MAN	O5-C1-C2	2.74	115.00	110.77
3	D	3	BMA	C3-C4-C5	2.71	115.06	110.24
5	F	3	FUC	C4-C3-C2	-2.68	106.95	110.27
3	D	4	MAN	C1-O5-C5	2.63	115.76	112.19
5	F	2	NAG	C1-O5-C5	2.44	115.50	112.19
3	G	1	NAG	C1-O5-C5	2.42	115.47	112.19
3	G	3	BMA	C3-C4-C5	-2.42	105.93	110.24
3	D	2	NAG	C1-C2-N2	2.42	114.61	110.49
5	F	1	NAG	C2-N2-C7	2.39	126.31	122.90
5	F	3	FUC	C3-C4-C5	2.36	115.02	111.23
2	C	3	BMA	O5-C5-C6	2.25	110.73	107.20
5	F	2	NAG	O5-C5-C6	2.23	110.70	107.20
5	F	3	FUC	O3-C3-C4	2.20	115.41	109.94
5	F	2	NAG	C2-N2-C7	2.19	126.02	122.90
4	E	2	NAG	C1-C2-N2	-2.16	106.80	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1	NAG	O5-C5-C6	2.12	110.52	107.20
3	G	3	BMA	O5-C1-C2	-2.02	107.65	110.77
5	F	1	NAG	C6-C5-C4	2.02	117.73	113.00
3	G	1	NAG	C6-C5-C4	-2.01	108.30	113.00

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	3	BMA	O5-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
3	G	3	BMA	C4-C5-C6-O6
2	C	3	BMA	O5-C5-C6-O6
3	D	3	BMA	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
3	G	5	MAN	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
3	G	5	MAN	C4-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
2	C	3	BMA	C4-C5-C6-O6
3	D	5	MAN	C4-C5-C6-O6
3	D	3	BMA	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
5	F	1	NAG	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
5	F	1	NAG	C4-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	G	4	MAN	O5-C5-C6-O6
3	D	5	MAN	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	G	4	MAN	C4-C5-C6-O6

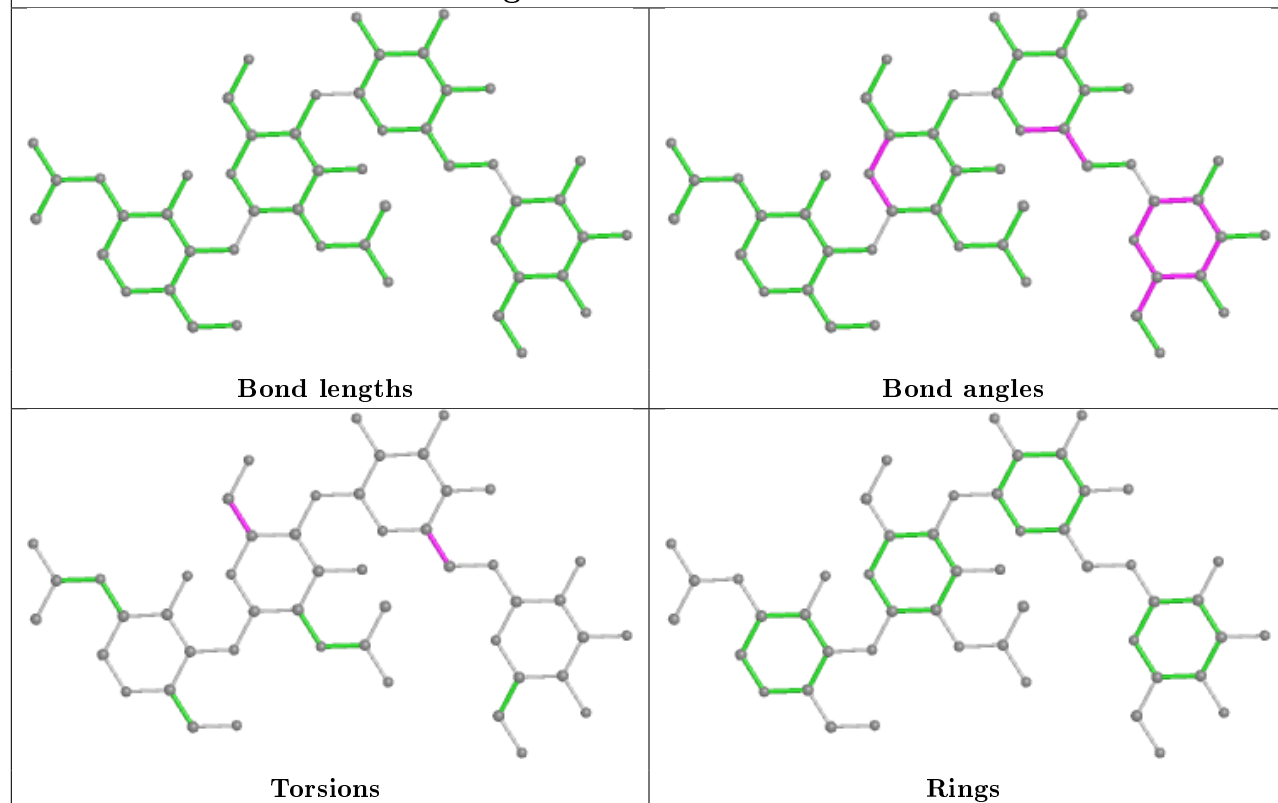
There are no ring outliers.

1 monomer is involved in 1 short contact:

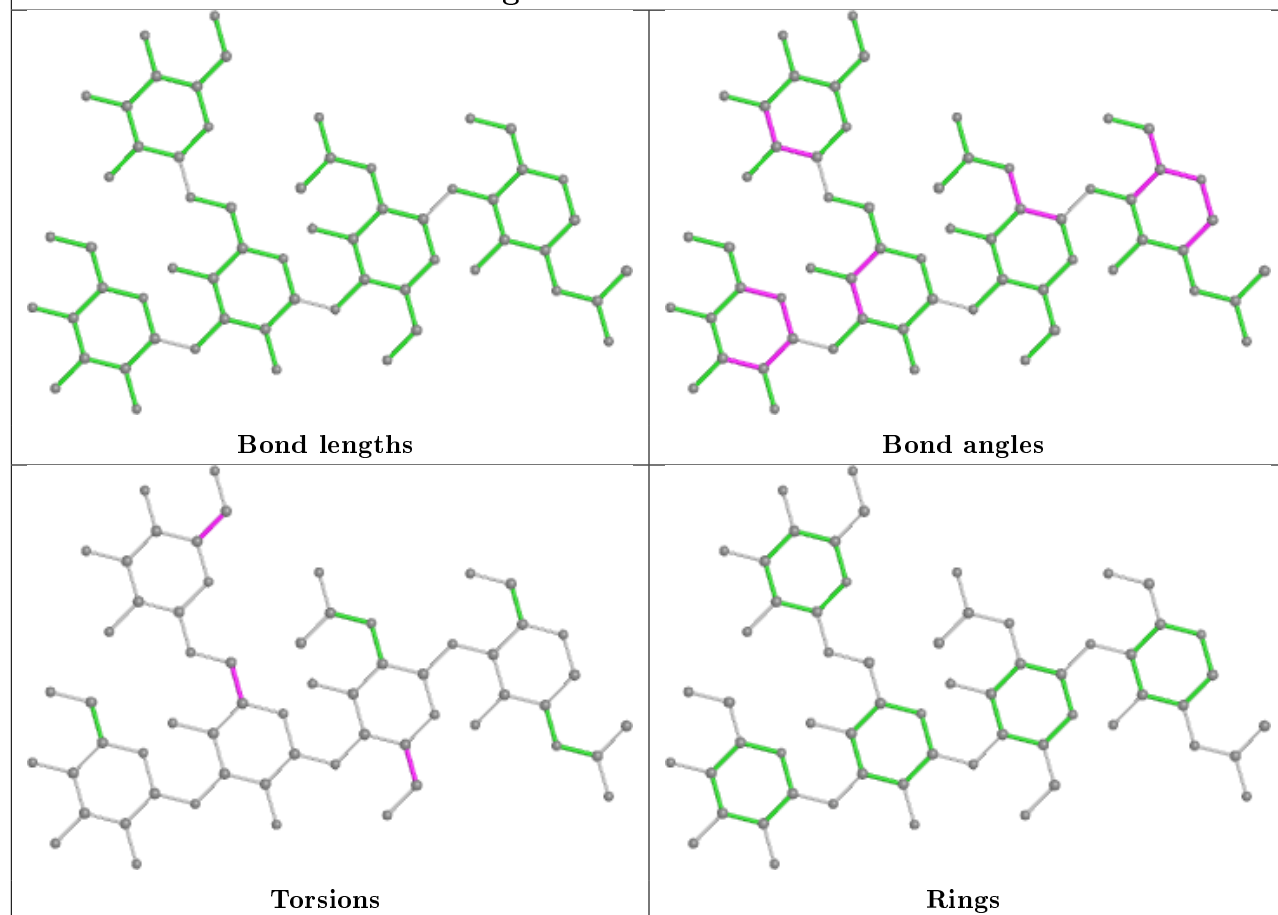
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1	NAG	1	0

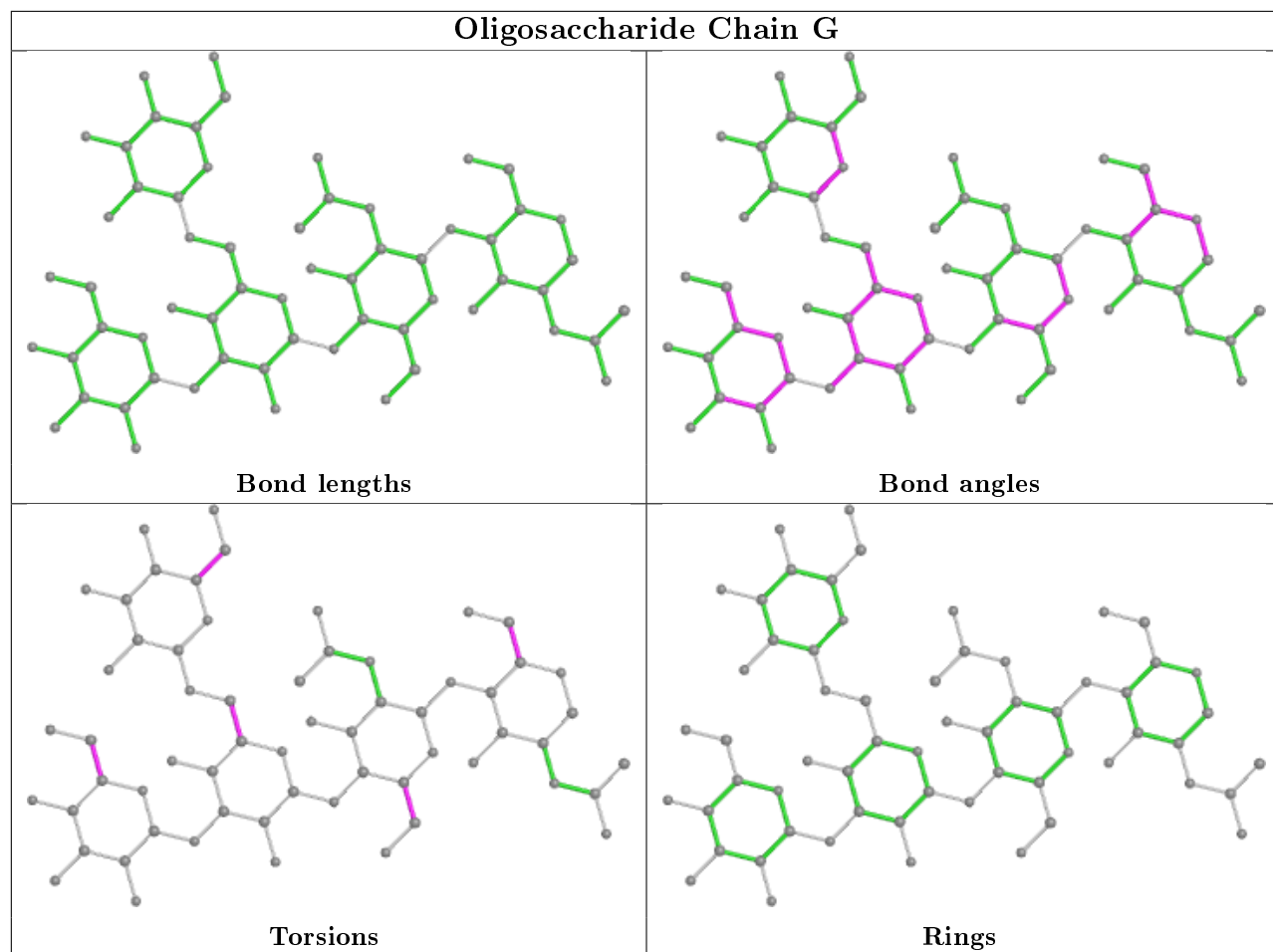
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

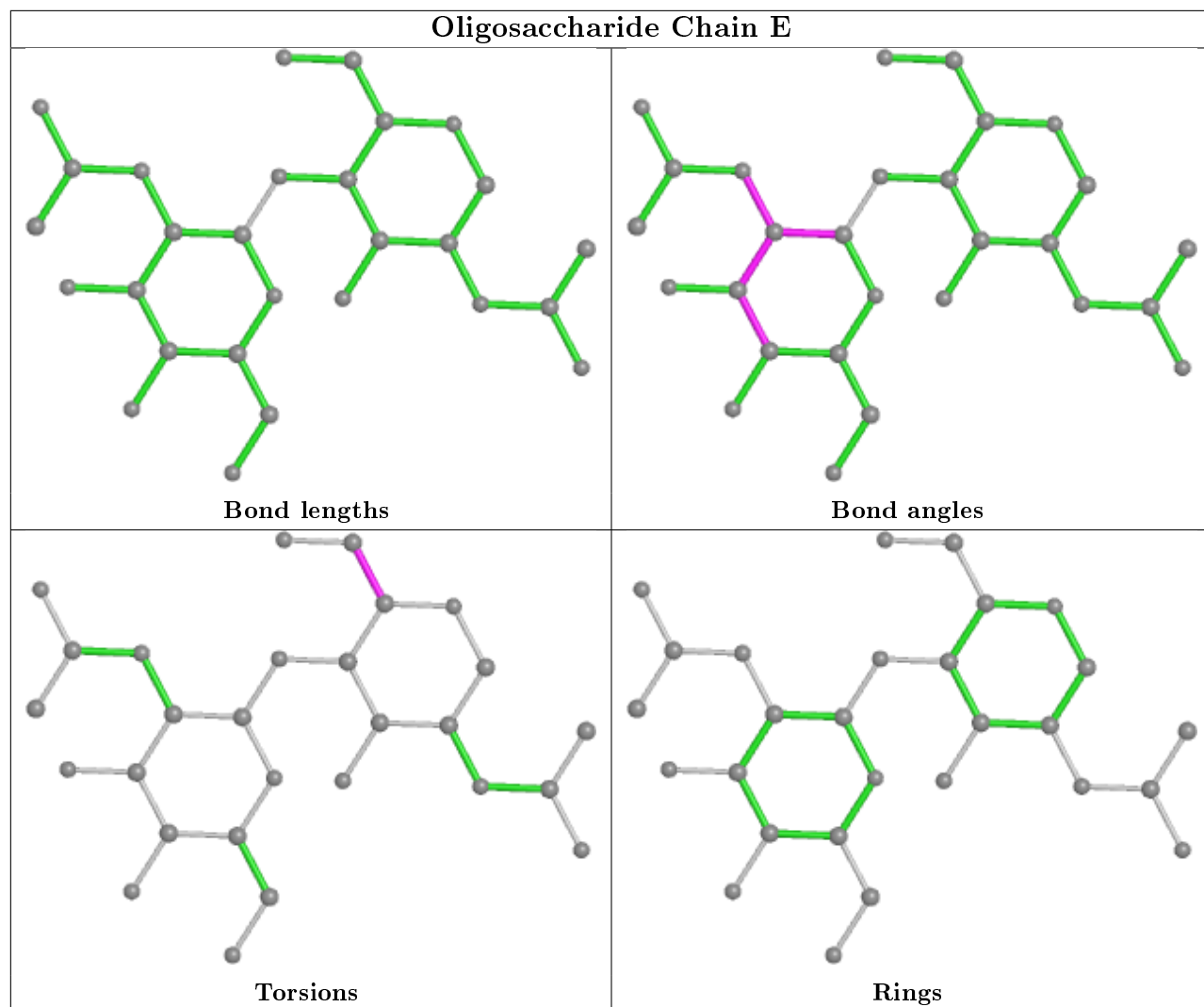
Oligosaccharide Chain C

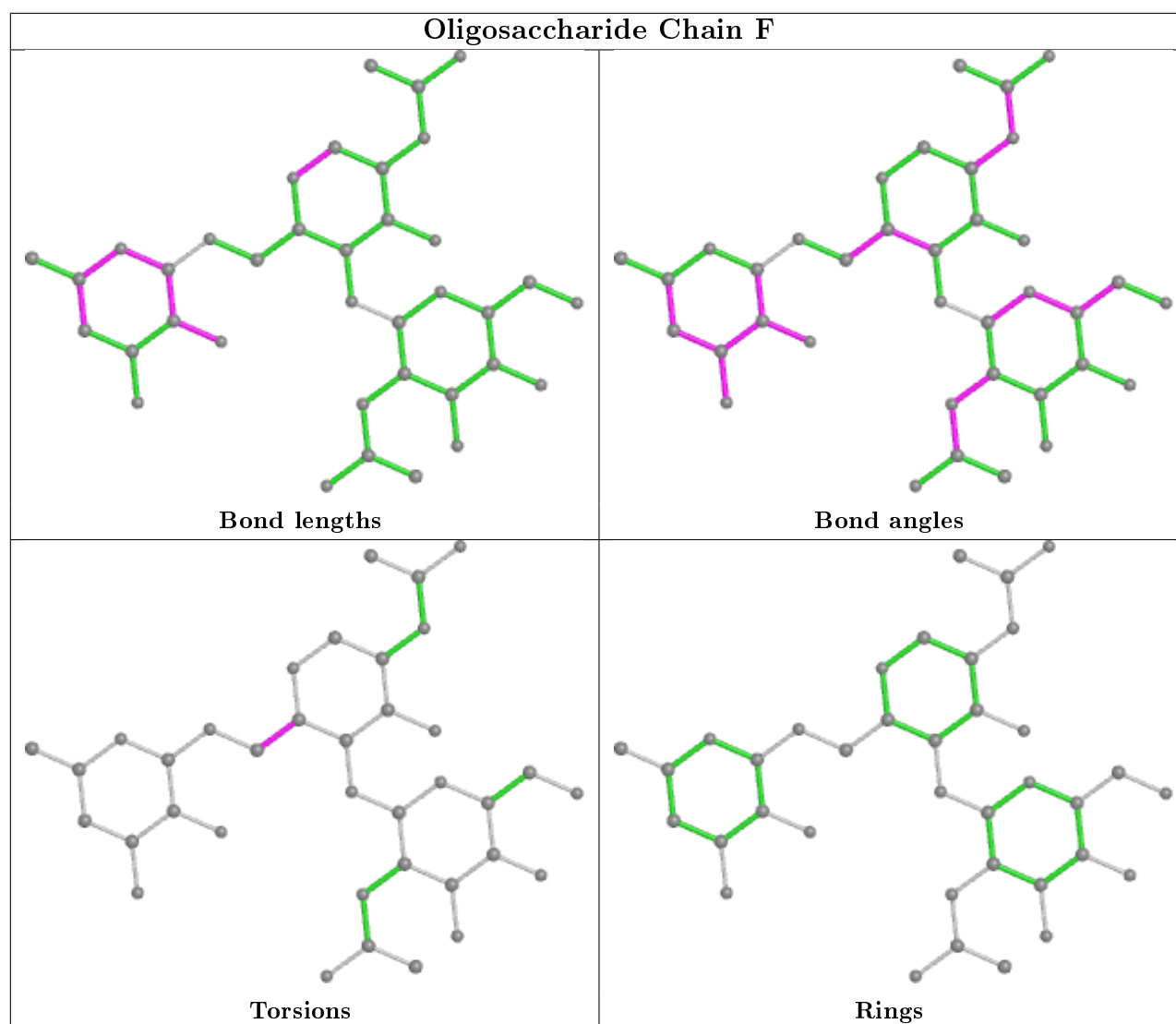


Oligosaccharide Chain D









5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\# Z > 2$
8	SO4	A	1012	-	4,4,4	0.46	0	6,6,6	0.40	0
6	NAG	A	1005	1	14,14,15	0.98	1 (7%)	17,19,21	1.81	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	ACT	A	1011	-	1,3,3	1.57	0	0,3,3	0.00	-
8	SO4	B	1011	-	4,4,4	0.52	0	6,6,6	0.41	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	1005	1	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1005	NAG	C1-C2	2.66	1.56	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1005	NAG	C1-O5-C5	5.79	120.04	112.19
6	A	1005	NAG	C2-N2-C7	2.34	126.23	122.90
6	A	1005	NAG	O5-C5-C6	2.28	110.78	107.20

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1005	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
6	A	1005	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	511/527 (96%)	-0.29	4 (0%) 86 88	27, 43, 85, 130	0
1	B	516/527 (97%)	0.04	33 (6%) 19 20	28, 49, 113, 173	0
All	All	1027/1054 (97%)	-0.12	37 (3%) 42 46	27, 45, 102, 173	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	102	LEU	7.0
1	B	262	ALA	6.3
1	B	257	PHE	5.6
1	B	247	PRO	4.4
1	B	245	ASN	4.1
1	B	390	PHE	3.6
1	B	388	LYS	3.6
1	B	242	ARG	3.5
1	B	274	ILE	3.5
1	B	244	LYS	3.3
1	B	254	LYS	3.3
1	B	149	TYR	3.3
1	A	257	PHE	3.2
1	B	246	LYS	3.1
1	B	267	PHE	3.1
1	B	147	ASP	3.0
1	B	301	LEU	2.9
1	B	282	VAL	2.8
1	B	248	ASN	2.8
1	B	258	MET	2.8
1	B	264	LYS	2.8
1	B	259	ALA	2.6
1	B	243	ASP	2.6
1	B	260	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	146	TYR	2.5
1	B	241	ASP	2.5
1	B	278	THR	2.5
1	A	242	ARG	2.4
1	B	239	ALA	2.4
1	B	255	GLY	2.3
1	B	385	ALA	2.3
1	A	390	PHE	2.3
1	B	270	VAL	2.2
1	A	241	ASP	2.2
1	B	347	TRP	2.2
1	B	124	ASN	2.2
1	B	261	VAL	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, 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.

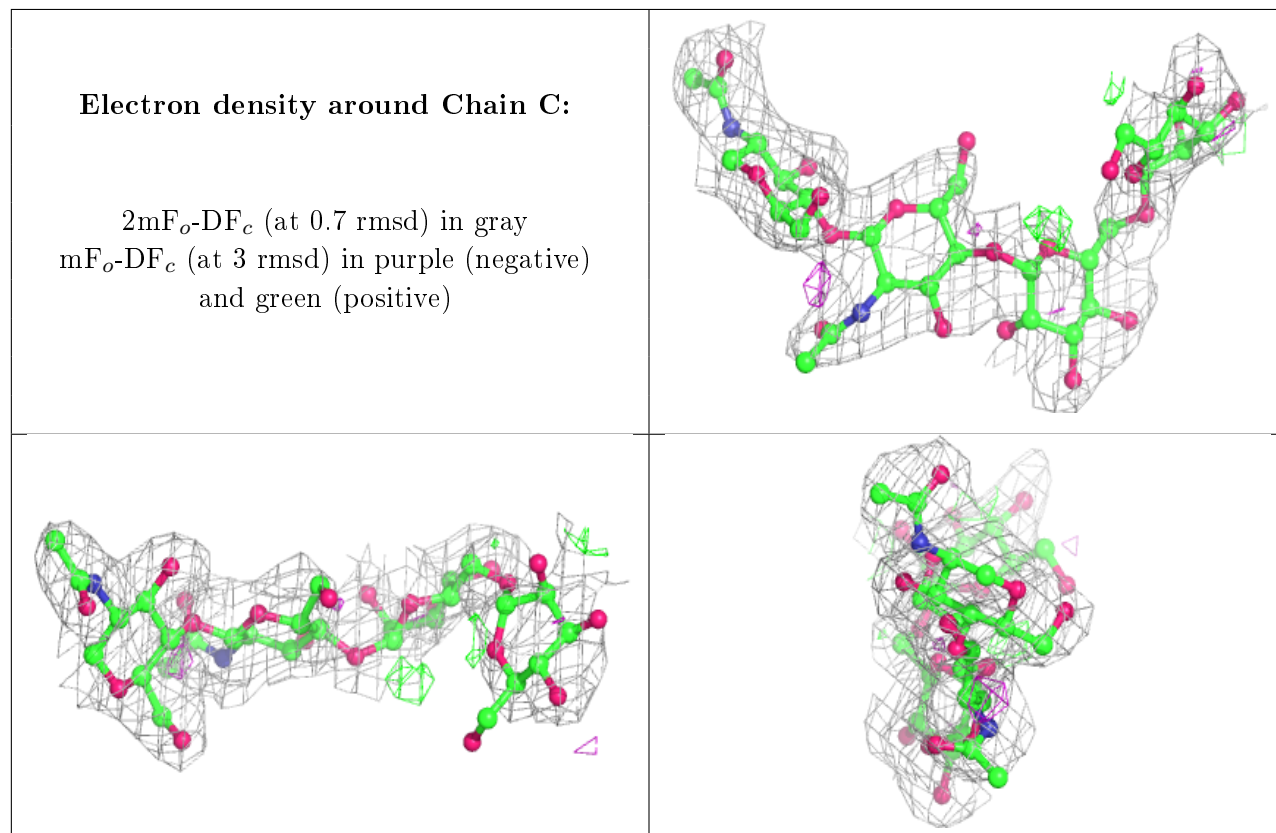
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BMA	C	3	11/12	0.40	0.25	124,142,152,153	0
3	MAN	G	4	11/12	0.72	0.32	105,130,139,139	0
3	MAN	D	5	11/12	0.73	0.14	90,120,127,129	0
3	MAN	G	5	11/12	0.74	0.21	128,135,142,150	0
2	MAN	C	4	11/12	0.76	0.38	118,133,143,157	0
3	BMA	D	3	11/12	0.82	0.16	123,126,131,135	0
3	BMA	G	3	11/12	0.82	0.19	104,118,131,134	0
5	NAG	F	2	14/15	0.82	0.31	108,128,138,140	0
3	MAN	D	4	11/12	0.84	0.28	108,132,136,138	0
5	FUC	F	3	9/11	0.84	0.41	62,68,72,80	0
2	NAG	C	2	14/15	0.85	0.22	79,98,119,136	0
4	NAG	E	2	14/15	0.89	0.16	81,91,95,95	0
5	NAG	F	1	14/15	0.91	0.21	75,87,118,119	0
4	NAG	E	1	14/15	0.94	0.13	41,54,72,73	0
3	NAG	D	2	14/15	0.94	0.17	73,80,91,109	0

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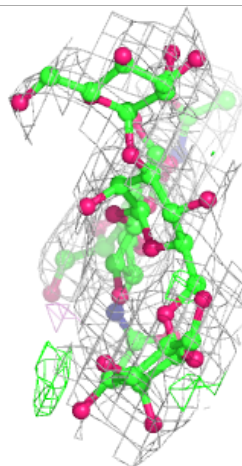
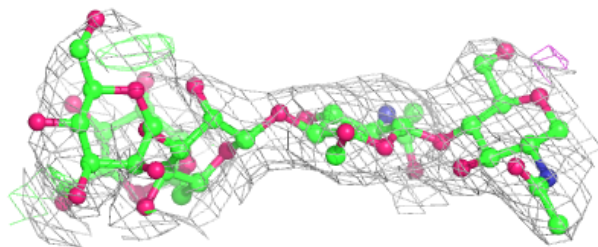
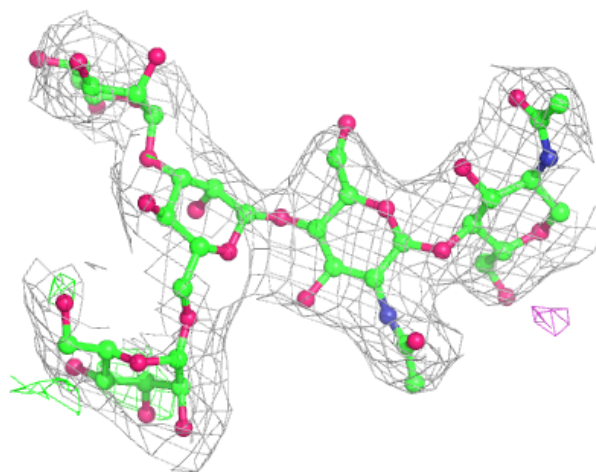
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	G	2	14/15	0.95	0.19	82,97,102,105	0
3	NAG	D	1	14/15	0.95	0.13	53,62,72,78	0
2	NAG	C	1	14/15	0.96	0.11	40,51,61,77	0
3	NAG	G	1	14/15	0.96	0.13	67,76,82,88	0

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.



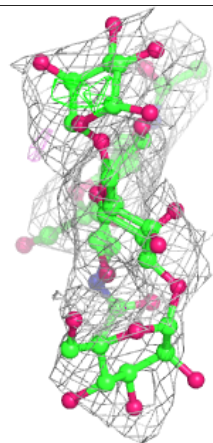
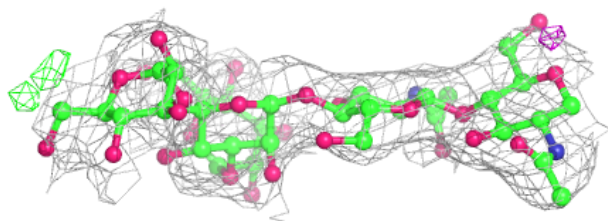
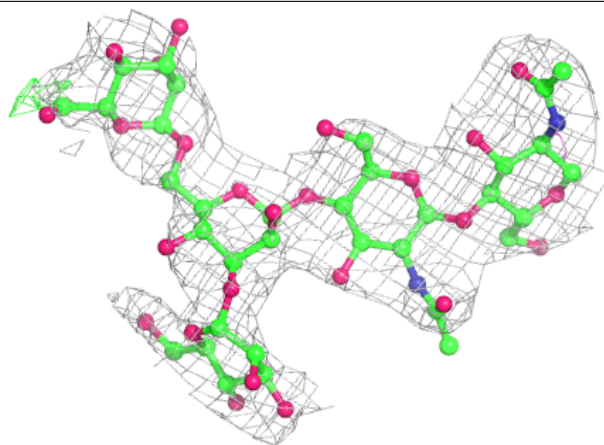
Electron density around Chain D:

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



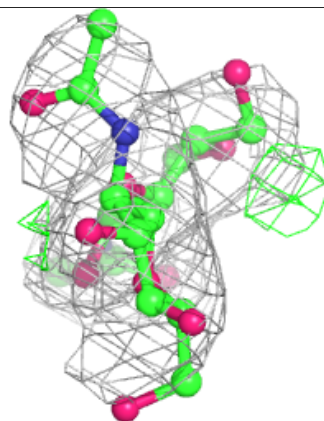
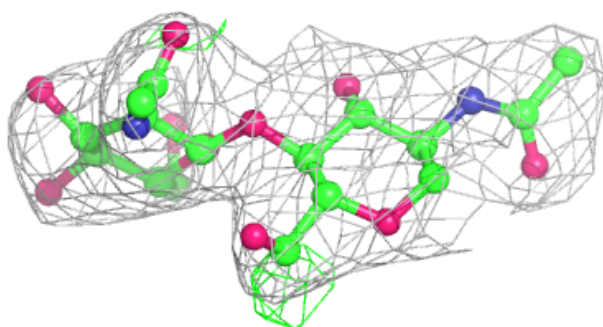
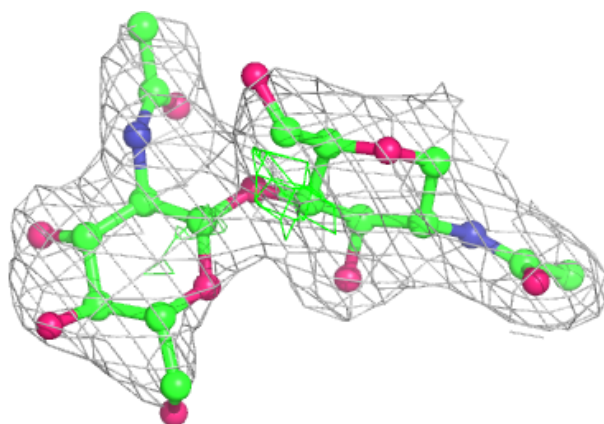
Electron density around Chain G:

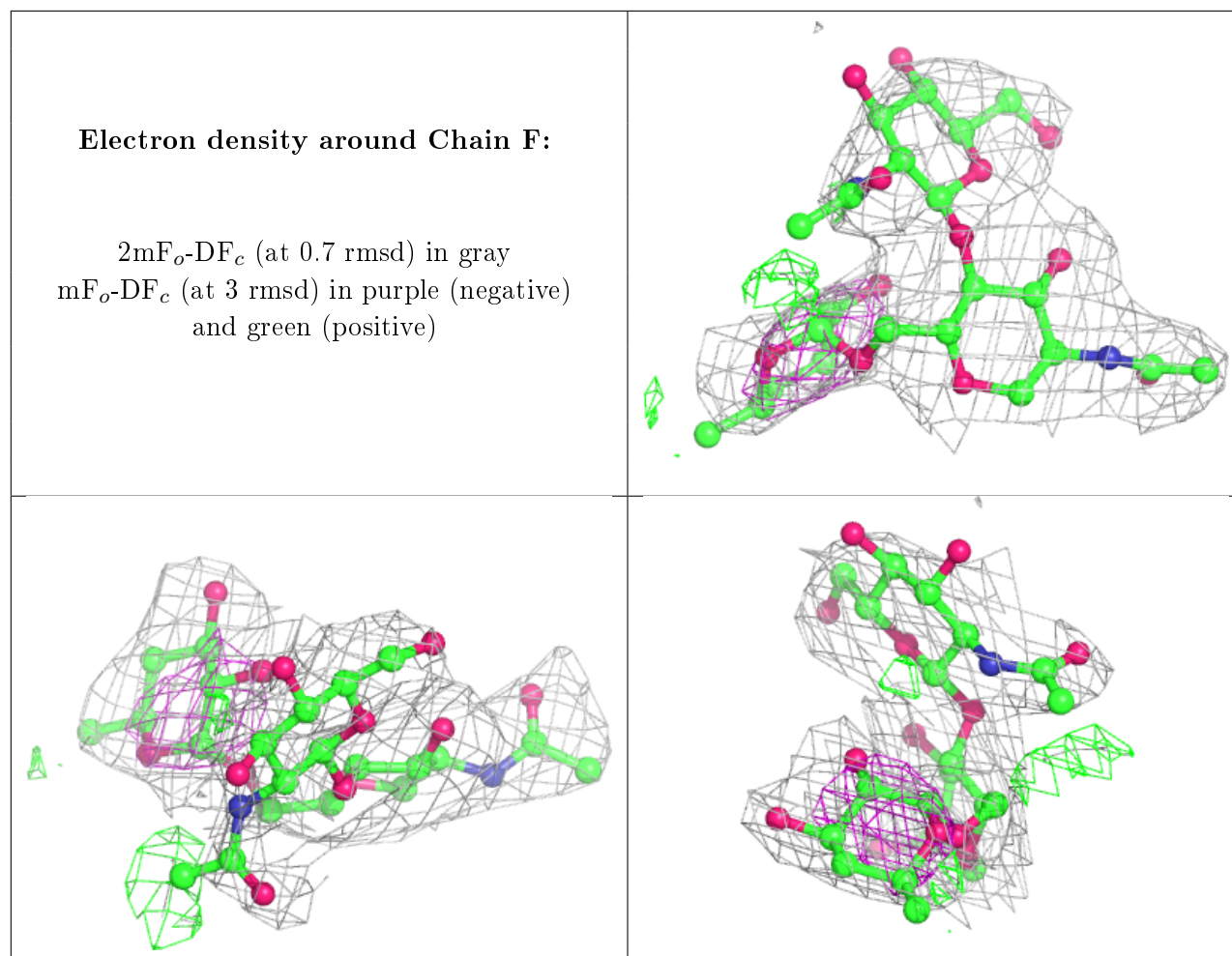
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain E:

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





6.4 Ligands [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(\AA^2)	Q<0.9
6	NAG	A	1005	14/15	0.81	0.24	97,107,113,114	0
7	ACT	A	1011	4/4	0.90	0.20	53,57,61,68	0
9	CA	B	1012	1/1	0.94	0.06	67,67,67,67	1
10	CL	B	1013	1/1	0.94	0.14	68,68,68,68	0
10	CL	A	1014	1/1	0.96	0.13	71,71,71,71	0
8	SO4	B	1011	5/5	0.96	0.13	61,67,71,71	0
8	SO4	A	1012	5/5	0.97	0.11	59,60,64,65	0
9	CA	A	1013	1/1	0.97	0.04	70,70,70,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.