



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 04:46 AM BST

PDB ID : 6I02
Title : Structure of human D-glucuronyl C5 epimerase in complex with product
Authors : Debarnot, C.; Monneau, Y.R.; Roig-Zamboni, V.; Le Narvor, C.; Goulet, A.;
Fadel, F.; Vives, R.R.; Bonnaffe, D.; Lortat-Jacob, H.; Bourne, Y.
Deposited on : 2018-10-24
Resolution : 2.45 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
buster-report : 1.1.7 (2018)
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

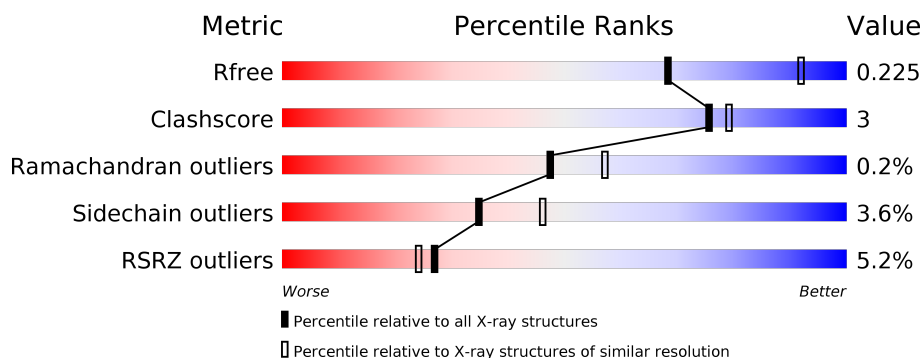
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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.



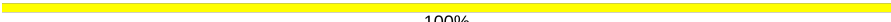

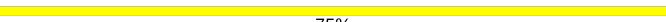
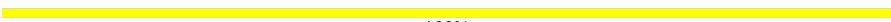
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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>2%</div> <div>87%</div> <div>9%</div> <div>••</div> </div>
1	B	527	<div> <div>9%</div> <div>89%</div> <div>8%</div> <div>••</div> </div>
2	C	8	<div> <div>75%</div> <div>25%</div> </div>
3	D	6	<div> <div>17%</div> <div>83%</div> </div>
4	E	3	<div> <div>100%</div> </div>
5	F	7	<div> <div>86%</div> <div>14%</div> </div>

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Mol	Chain	Length	Quality of chain
6	G	5	 100%
7	H	4	 25%  75%
8	I	2	 100%

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
3	NAG	D	5	-	-	-	X
6	BMA	G	3	-	-	-	X
6	MAN	G	5	-	-	-	X

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 9254 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.

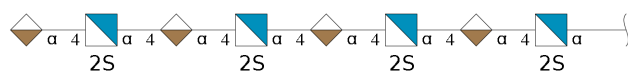
- Molecule 1 is a protein called D-glucuronyl C5-epimerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	511	Total	C	N	O	S	0	2	0
			4143	2672	698	759	14			
1	B	516	Total	C	N	O	S	0	3	0
			4180	2693	703	770	14			

There are 16 discrepancies between the modelled and reference sequences:

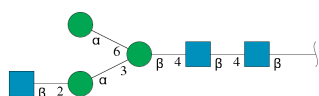
Chain	Residue	Modelled	Actual	Comment	Reference
A	91	ASP	-	expression tag	UNP O94923
A	92	TYR	-	expression tag	UNP O94923
A	93	LYS	-	expression tag	UNP O94923
A	94	ASP	-	expression tag	UNP O94923
A	95	ASP	-	expression tag	UNP O94923
A	96	ASP	-	expression tag	UNP O94923
A	97	ASP	-	expression tag	UNP O94923
A	578	PHE	TYR	engineered mutation	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
B	578	PHE	TYR	engineered mutation	UNP O94923

- Molecule 2 is an oligosaccharide called alpha-L-idopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	8	Total	C	N	O	S	0	0	0
			109	48	4	53	4			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-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	6	Total	C	N	O	0	0	0
			75	42	3	30			

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



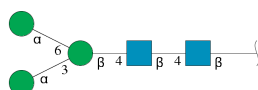
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is an oligosaccharide called alpha-L-idopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-alpha-L-idopyranuronic acid.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	7	Total	C	N	O	S	0	0	0
			94	42	3	46	3			

- Molecule 6 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
6	G	5	Total	C	N	O			
			61	34	2	25	0	0	0

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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
7	H	4	Total	C	N	O			
			50	28	2	20	0	0	0

- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

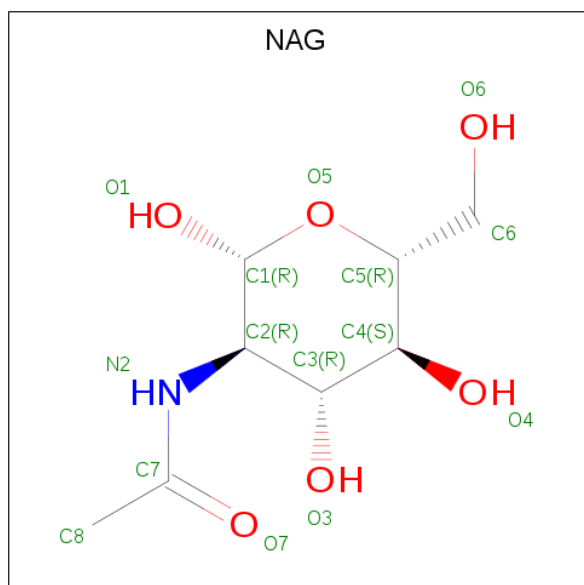


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	I	2	Total	C	N	O			
			28	16	2	10	0	0	0

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



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

- Molecule 11 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



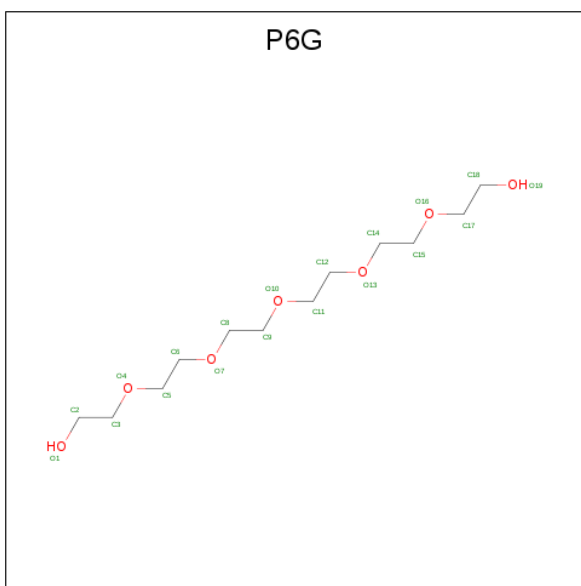
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			6	3	3		
11	A	1	Total	C	O	0	0
			6	3	3		
11	A	1	Total	C	O	0	0
			6	3	3		
11	A	1	Total	C	O	0	0
			6	3	3		
11	A	1	Total	C	O	0	0
			6	3	3		
11	A	1	Total	C	O	0	0
			6	3	3		
11	B	1	Total	C	O	0	0
			6	3	3		
11	B	1	Total	C	O	0	0
			6	3	3		
11	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 12 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 13 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: C₁₂H₂₆O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	A	1	Total	C	O	0	0
			19	12	7		

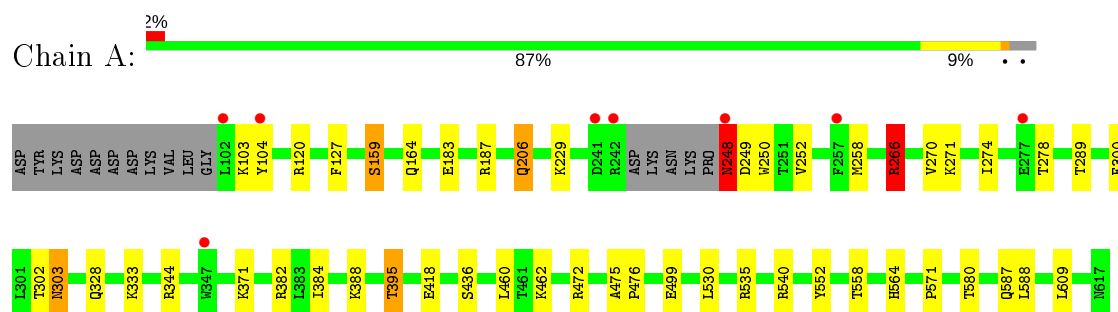
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	198	Total 198	O 198	0	0
14	B	164	Total 164	O 164	0	0

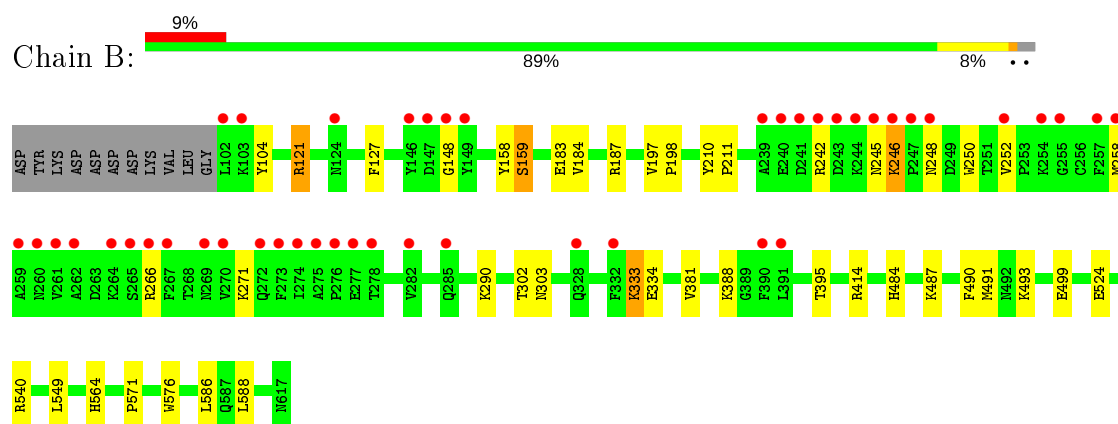
3 Residue-property plots [i](#)

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.

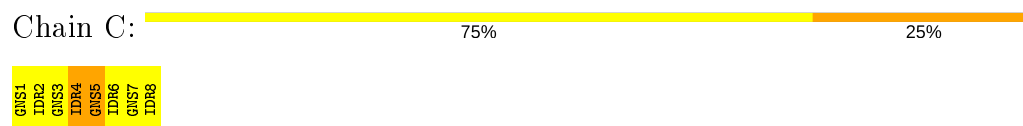
- Molecule 1: D-glucuronyl C5-epimerase



- Molecule 1: D-glucuronyl C5-epimerase



- Molecule 2: alpha-L-idopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose

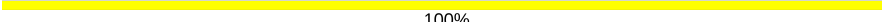


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  17% 83%

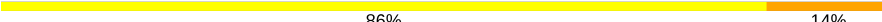
MAG1
MAG2
BMA3
MAN4
MAG5
MAN6

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

Chain E:  100%

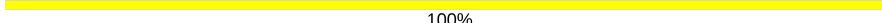
MAG1
MAG2
BMA3

- Molecule 5: alpha-L-idopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-alpha-L-idopyranuronic acid

Chain F:  86% 14%

IDR1
GMS2
IDR3
GMS4
IDR5
GMS6
IDR7

- Molecule 6: 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%

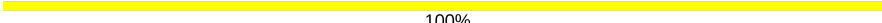
MAG1
MAG2
BMA3
MAN4
MAN5

- Molecule 7: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  25% 75%

MAG1
MAG2
BMA3
MAN4

- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	99.81Å 99.81Å 260.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.06 – 2.45 49.01 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.06-2.45) 99.9 (49.01-2.45)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.173 , 0.218 0.179 , 0.225	Depositor DCC
R_{free} test set	2671 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	47.1	Xtriage
Anisotropy	0.383	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 34.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.048 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9254	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 2.26% 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: GNS, BMA, NAG, GOL, CA, IDR, P6G, MES, MAN

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	0.67	0/4260	0.81	1/5764 (0.0%)
1	B	0.67	1/4301 (0.0%)	0.79	0/5822
All	All	0.67	1/8561 (0.0%)	0.80	1/11586 (0.0%)

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	5
1	B	0	7
All	All	0	12

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	524	GLU	CD-OE2	6.64	1.32	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	303	ASN	CB-CA-C	-5.47	99.46	110.40

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	248	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	A	266	ARG	Sidechain
1	A	472	ARG	Sidechain
1	A	535	ARG	Sidechain
1	A	540	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4143	0	4081	31	0
1	B	4180	0	4108	24	0
2	C	109	0	55	2	0
3	D	75	0	64	0	0
4	E	39	0	34	0	0
5	F	94	0	48	2	0
6	G	61	0	52	0	0
7	H	50	0	43	0	0
8	I	28	0	25	0	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
10	A	14	0	13	0	0
11	A	42	0	56	1	0
11	B	24	0	32	1	0
12	A	12	0	13	2	0
13	A	19	0	26	0	0
14	A	198	0	0	2	0
14	B	164	0	0	1	0
All	All	9254	0	8650	54	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.

The worst 5 of 54 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:248:ASN:N	1:A:248:ASN:HD22	1.62	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:VAL:HG22	1:A:258:MET:HE2	1.65	0.78
1:A:395:THR:HG22	14:A:1503:HOH:O	1.89	0.73
1:A:206:GLN:HE21	1:A:206:GLN:H	1.41	0.69
1:A:248:ASN:N	1:A:248:ASN:ND2	2.36	0.68

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	509/527 (97%)	494 (97%)	15 (3%)	0	100	100
1	B	517/527 (98%)	497 (96%)	18 (4%)	2 (0%)	34	41
All	All	1026/1054 (97%)	991 (97%)	33 (3%)	2 (0%)	47	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	246	LYS
1	B	248	ASN

5.3.2 Protein sidechains [i](#)

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	446/459 (97%)	423 (95%)	23 (5%)	23	30
1	B	450/459 (98%)	441 (98%)	9 (2%)	55	67
All	All	896/918 (98%)	864 (96%)	32 (4%)	35	46

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	333	LYS
1	A	436	SER
1	B	381	VAL
1	A	395	THR
1	A	460	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	206	GLN
1	A	510	ASN
1	B	202	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

35 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	GNS	C	1	2	15,16,16	5.20	1 (6%)	19,24,24	1.61	3 (15%)
2	IDR	C	2	2	9,12,13	0.54	0	12,17,19	1.22	2 (16%)
2	GNS	C	3	2	14,15,16	1.40	2 (14%)	17,22,24	1.34	1 (5%)
2	IDR	C	4	2	9,12,13	0.79	0	12,17,19	2.45	5 (41%)
2	GNS	C	5	2	14,15,16	4.86	1 (7%)	17,22,24	2.04	1 (5%)
2	IDR	C	6	2	9,12,13	0.26	0	12,17,19	1.68	2 (16%)
2	GNS	C	7	2	14,15,16	4.91	2 (14%)	17,22,24	2.11	5 (29%)
2	IDR	C	8	2	9,12,13	0.50	0	12,17,19	1.09	1 (8%)
3	NAG	D	1	1,3	14,14,15	0.62	0	17,19,21	1.19	2 (11%)
3	NAG	D	2	3	14,14,15	0.71	0	17,19,21	1.03	1 (5%)
3	BMA	D	3	3	11,11,12	0.89	0	15,15,17	1.07	0
3	MAN	D	4	3	11,11,12	1.17	2 (18%)	15,15,17	1.72	3 (20%)
3	NAG	D	5	3	14,14,15	0.78	0	17,19,21	1.59	2 (11%)
3	MAN	D	6	3	11,11,12	0.94	0	15,15,17	2.44	4 (26%)
4	NAG	E	1	1,4	14,14,15	1.06	0	17,19,21	1.84	4 (23%)
4	NAG	E	2	4	14,14,15	0.63	0	17,19,21	1.37	3 (17%)
4	BMA	E	3	4	11,11,12	0.73	0	15,15,17	1.76	5 (33%)
5	IDR	F	1	5	10,13,13	1.16	0	15,19,19	1.62	3 (20%)
5	GNS	F	2	5	14,15,16	5.29	2 (14%)	17,22,24	1.64	3 (17%)
5	IDR	F	3	5	9,12,13	1.07	0	12,17,19	2.61	5 (41%)
5	GNS	F	4	5	14,15,16	5.14	2 (14%)	17,22,24	1.48	2 (11%)
5	IDR	F	5	5	9,12,13	0.68	0	12,17,19	1.85	2 (16%)
5	GNS	F	6	5	14,15,16	5.36	1 (7%)	17,22,24	1.61	3 (17%)
5	IDR	F	7	5	9,12,13	0.34	0	12,17,19	0.72	0
6	NAG	G	1	1,6	14,14,15	0.48	0	17,19,21	1.50	4 (23%)
6	NAG	G	2	6	14,14,15	0.57	0	17,19,21	1.68	2 (11%)
6	BMA	G	3	6	11,11,12	0.62	0	15,15,17	1.80	5 (33%)
6	MAN	G	4	6	11,11,12	0.75	0	15,15,17	1.78	1 (6%)
6	MAN	G	5	6	11,11,12	0.72	0	15,15,17	1.87	4 (26%)
7	NAG	H	1	1,7	14,14,15	0.34	0	17,19,21	1.74	3 (17%)
7	NAG	H	2	7	14,14,15	0.51	0	17,19,21	1.00	0
7	BMA	H	3	7	11,11,12	0.69	0	15,15,17	1.85	4 (26%)
7	MAN	H	4	7	11,11,12	0.89	0	15,15,17	1.90	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	I	1	1,8	14,14,15	0.44	0	17,19,21	1.24	1 (5%)
8	NAG	I	2	8	14,14,15	0.48	0	17,19,21	1.13	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
2	GNS	C	1	2	-	0/7/27/27	0/1/1/1
2	IDR	C	2	2	-	0/0/21/24	0/1/1/1
2	GNS	C	3	2	-	3/7/24/27	0/1/1/1
2	IDR	C	4	2	-	0/0/21/24	0/1/1/1
2	GNS	C	5	2	-	3/7/24/27	0/1/1/1
2	IDR	C	6	2	-	0/0/21/24	0/1/1/1
2	GNS	C	7	2	-	0/7/24/27	0/1/1/1
2	IDR	C	8	2	-	0/0/21/24	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	NAG	D	5	3	-	4/6/23/26	0/1/1/1
3	MAN	D	6	3	-	0/2/19/22	0/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	BMA	E	3	4	-	1/2/19/22	0/1/1/1
5	IDR	F	1	5	-	0/0/24/24	0/1/1/1
5	GNS	F	2	5	-	1/7/24/27	0/1/1/1
5	IDR	F	3	5	-	0/0/21/24	0/1/1/1
5	GNS	F	4	5	-	3/7/24/27	0/1/1/1
5	IDR	F	5	5	-	0/0/21/24	0/1/1/1
5	GNS	F	6	5	-	2/7/24/27	0/1/1/1
5	IDR	F	7	5	-	0/0/21/24	0/1/1/1
6	NAG	G	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	G	2	6	-	0/6/23/26	0/1/1/1
6	BMA	G	3	6	-	2/2/19/22	0/1/1/1
6	MAN	G	4	6	-	2/2/19/22	1/1/1/1
6	MAN	G	5	6	-	2/2/19/22	0/1/1/1
7	NAG	H	1	1,7	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	H	2	7	-	2/6/23/26	0/1/1/1
7	BMA	H	3	7	-	2/2/19/22	0/1/1/1
7	MAN	H	4	7	-	0/2/19/22	0/1/1/1
8	NAG	I	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	I	2	8	-	0/6/23/26	0/1/1/1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	6	GNS	O2S-S1	19.93	1.64	1.42
2	C	1	GNS	O3S-S1	19.86	1.64	1.42
5	F	2	GNS	O3S-S1	19.39	1.64	1.42
5	F	4	GNS	O3S-S1	18.75	1.63	1.42
2	C	7	GNS	O3S-S1	18.08	1.62	1.42

The worst 5 of 91 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	5	GNS	O3S-S1-O2S	-7.23	103.08	120.16
6	G	4	MAN	C1-O5-C5	6.14	120.50	112.19
3	D	6	MAN	C1-C2-C3	5.91	116.93	109.67
3	D	6	MAN	C1-O5-C5	5.80	120.06	112.19
5	F	3	IDR	C1-C2-C3	5.75	116.73	109.67

There are no chirality outliers.

5 of 35 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	4	GNS	C2-N2-S1-O1S
5	F	4	GNS	C2-N2-S1-O3S
2	C	5	GNS	C2-N2-S1-O1S
2	C	5	GNS	C2-N2-S1-O2S
3	D	5	NAG	C1-C2-N2-C7

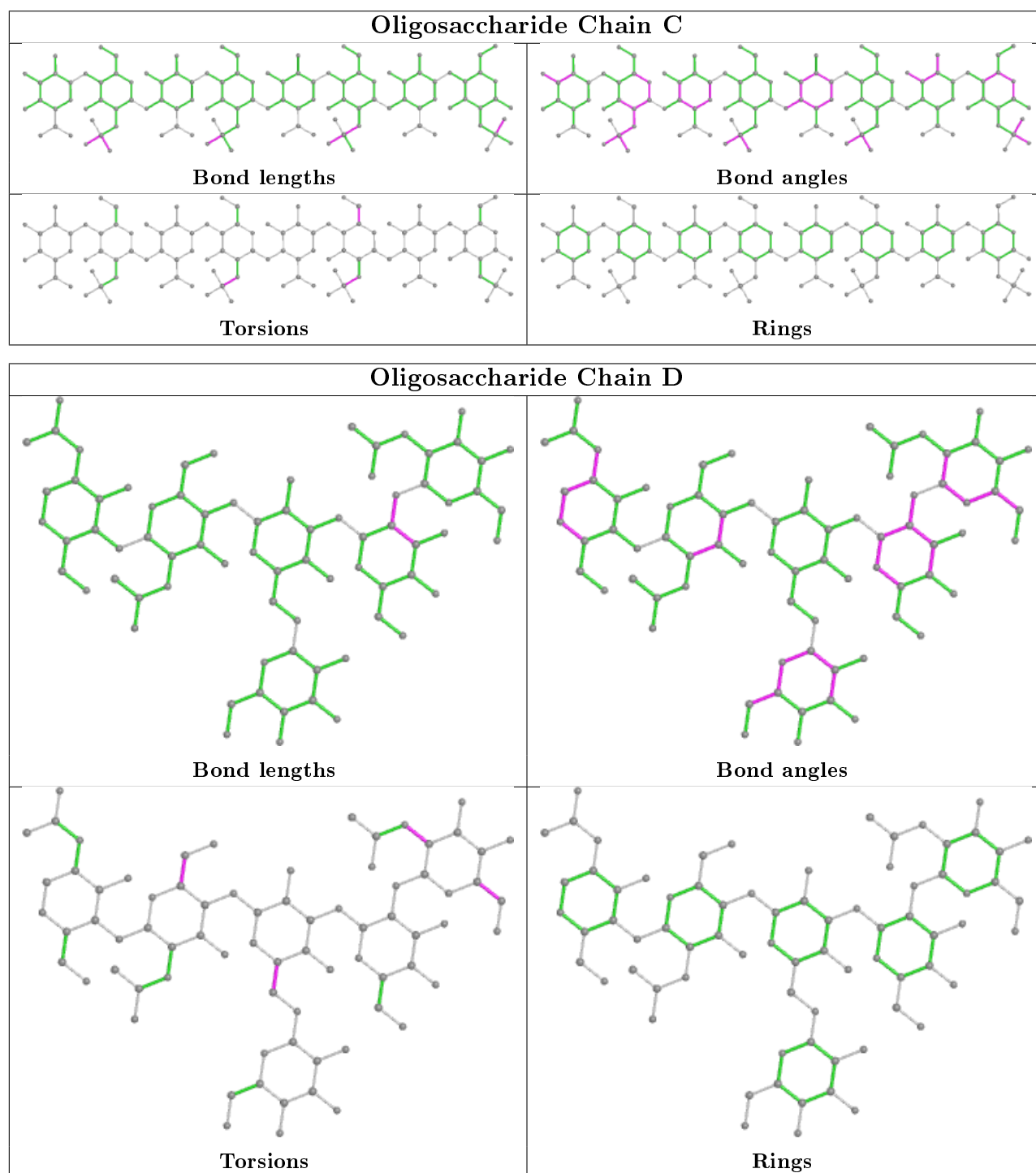
All (1) ring outliers are listed below:

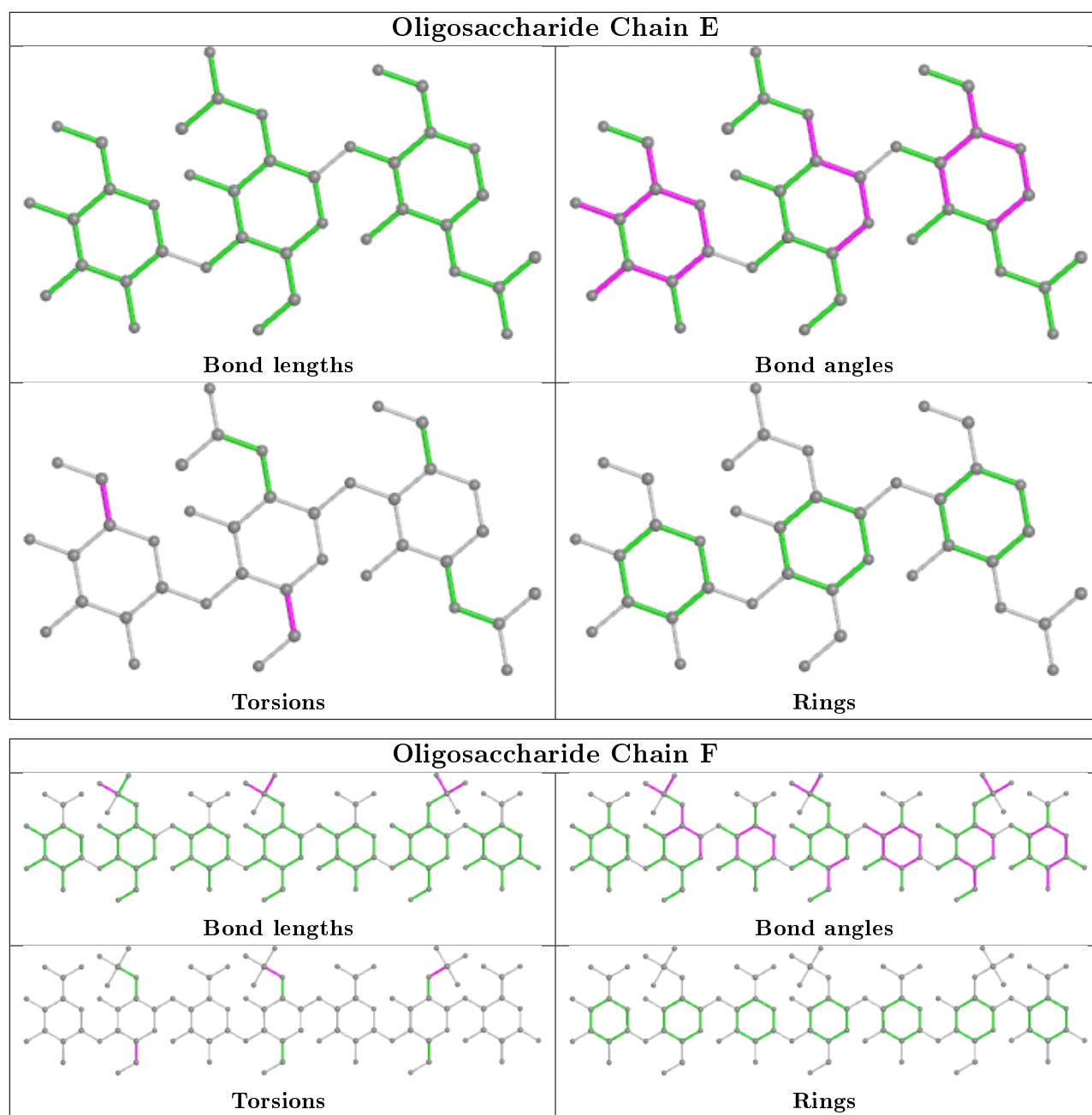
Mol	Chain	Res	Type	Atoms
6	G	4	MAN	C1-C2-C3-C4-C5-O5

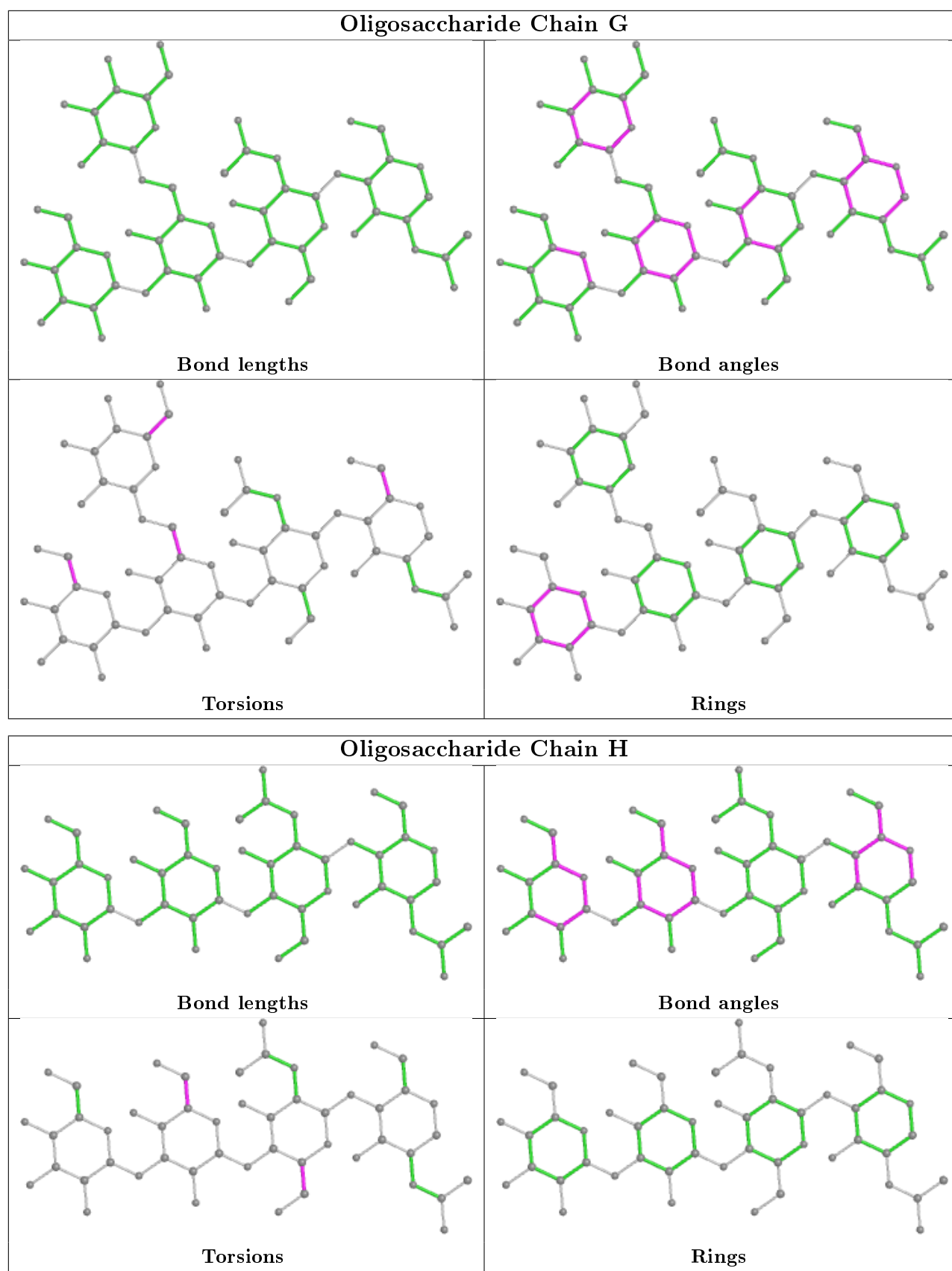
4 monomers are involved in 4 short contacts:

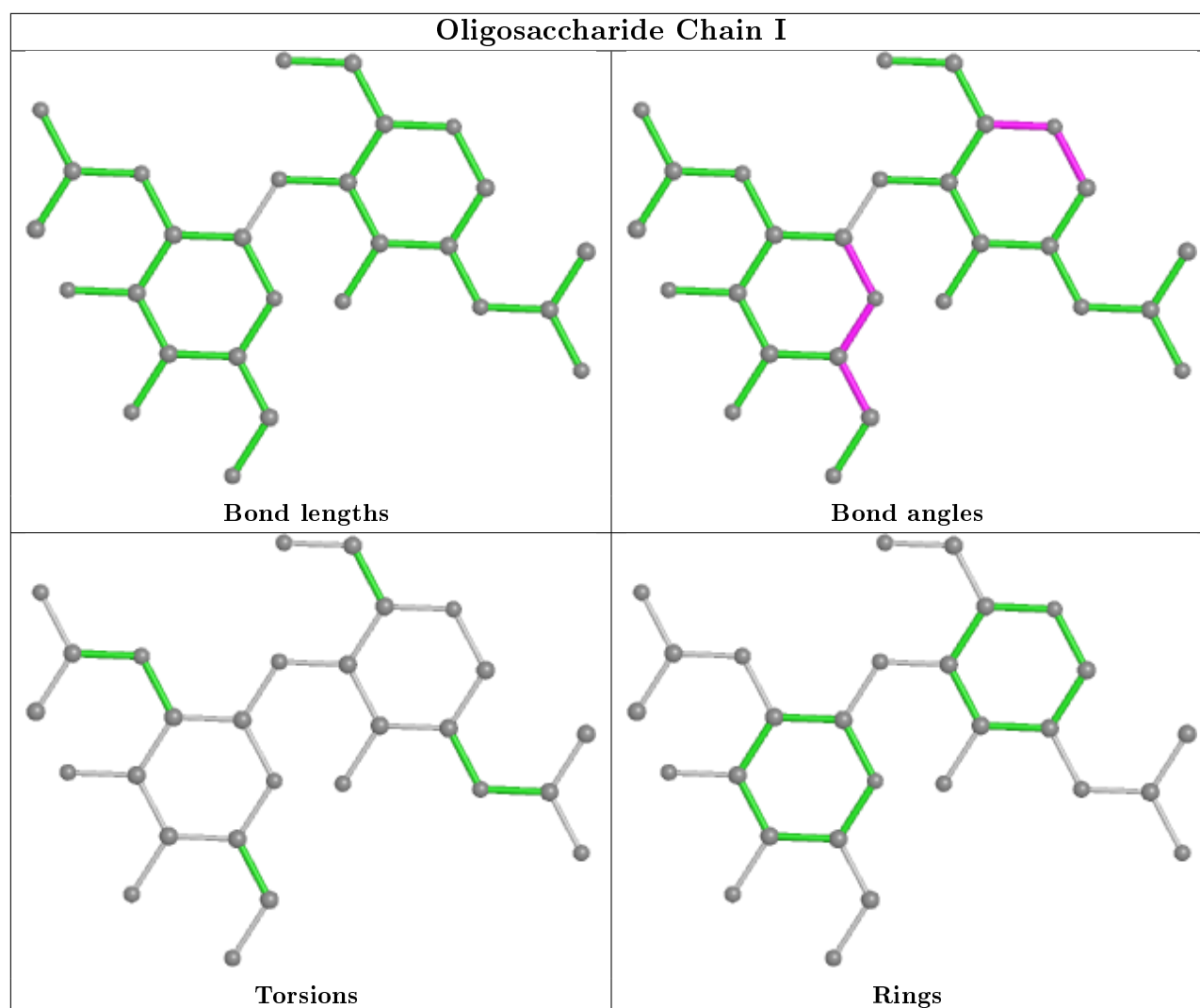
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	5	GNS	1	0
5	F	3	IDR	1	0
5	F	7	IDR	1	0
2	C	4	IDR	1	0

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 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 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	$\# Z > 2$
11	GOL	B	721	-	5,5,5	0.34	0	5,5,5	0.69	0
11	GOL	A	1422	-	5,5,5	0.34	0	5,5,5	0.66	0
10	NAG	A	1419	1	14,14,15	0.87	1 (7%)	17,19,21	1.75	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	GOL	A	1421	-	5,5,5	0.74	0	5,5,5	1.40	1 (20%)
11	GOL	A	1426	-	5,5,5	0.59	0	5,5,5	0.83	0
11	GOL	A	1425	-	5,5,5	0.32	0	5,5,5	0.49	0
11	GOL	B	720	-	5,5,5	0.94	0	5,5,5	1.44	1 (20%)
11	GOL	A	1420	-	5,5,5	0.68	0	5,5,5	1.01	0
11	GOL	B	723	-	5,5,5	0.36	0	5,5,5	0.71	0
11	GOL	A	1424	-	5,5,5	0.14	0	5,5,5	0.55	0
11	GOL	A	1423	-	5,5,5	0.27	0	5,5,5	0.61	0
13	P6G	A	1428	-	18,18,18	0.64	0	17,17,17	0.34	0
12	MES	A	1427	-	12,12,12	2.29	3 (25%)	14,16,16	1.29	1 (7%)
11	GOL	B	722	-	5,5,5	0.79	0	5,5,5	1.02	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
11	GOL	B	721	-	-	0/4/4/4	-
11	GOL	A	1422	-	-	2/4/4/4	-
10	NAG	A	1419	1	-	0/6/23/26	0/1/1/1
11	GOL	A	1421	-	-	0/4/4/4	-
11	GOL	A	1426	-	-	2/4/4/4	-
11	GOL	A	1425	-	-	2/4/4/4	-
11	GOL	B	720	-	-	2/4/4/4	-
11	GOL	A	1420	-	-	2/4/4/4	-
11	GOL	B	723	-	-	2/4/4/4	-
11	GOL	A	1424	-	-	0/4/4/4	-
11	GOL	A	1423	-	-	0/4/4/4	-
13	P6G	A	1428	-	-	7/16/16/16	-
12	MES	A	1427	-	-	3/6/14/14	0/1/1/1
11	GOL	B	722	-	-	3/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	1427	MES	C8-S	-7.17	1.67	1.77
10	A	1419	NAG	C1-C2	2.59	1.56	1.52
12	A	1427	MES	O1S-S	2.25	1.51	1.45
12	A	1427	MES	O2S-S	2.04	1.51	1.45

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1419	NAG	C1-O5-C5	3.94	117.53	112.19
12	A	1427	MES	O2S-S-C8	3.18	110.75	106.92
10	A	1419	NAG	O5-C5-C6	3.17	112.17	107.20
10	A	1419	NAG	C1-C2-N2	2.49	114.75	110.49
11	B	720	GOL	O2-C2-C1	2.39	119.66	109.12

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

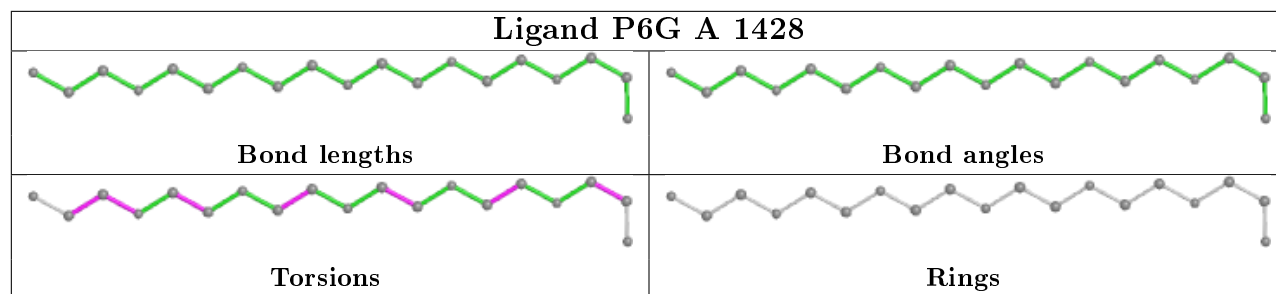
Mol	Chain	Res	Type	Atoms
11	A	1422	GOL	O1-C1-C2-C3
11	B	720	GOL	C1-C2-C3-O3
11	B	720	GOL	O2-C2-C3-O3
11	A	1420	GOL	O1-C1-C2-C3
11	B	723	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	1422	GOL	1	0
12	A	1427	MES	2	0
11	B	722	GOL	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.13	8 (1%) 72 69	30, 45, 79, 128	0
1	B	516/527 (97%)	0.26	45 (8%) 10 7	30, 50, 102, 155	0
All	All	1027/1054 (97%)	0.07	53 (5%) 27 24	30, 47, 93, 155	0

The worst 5 of 53 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	247	PRO	7.2
1	B	243	ASP	6.2
1	B	257	PHE	6.1
1	A	248	ASN	6.0
1	A	241	ASP	5.1

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
6	MAN	G	4	11/12	0.52	0.37	120,138,152,153	0
6	MAN	G	5	11/12	0.55	0.44	96,112,125,134	0
3	MAN	D	6	11/12	0.62	0.34	113,125,132,132	0
6	BMA	G	3	11/12	0.66	0.41	130,141,150,153	0
7	MAN	H	4	11/12	0.69	0.23	110,123,131,132	0

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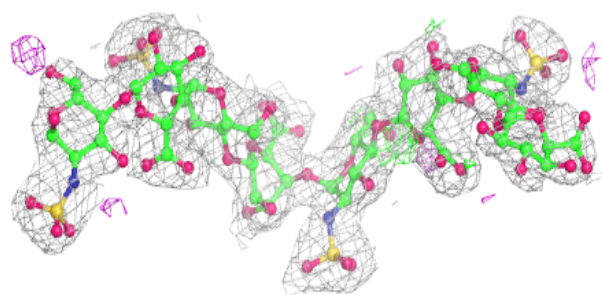
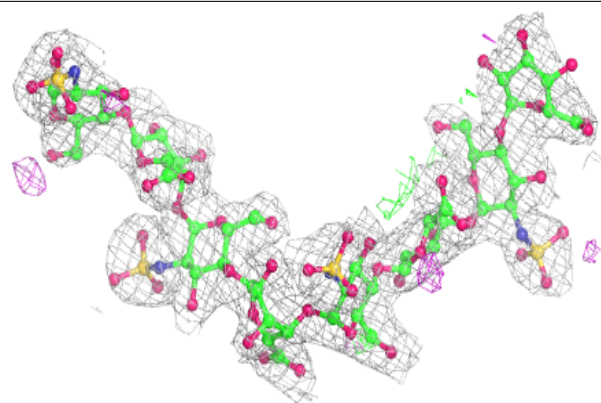
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	D	5	14/15	0.70	0.53	119,130,137,139	0
8	NAG	I	2	14/15	0.73	0.36	113,131,139,151	0
3	BMA	D	3	11/12	0.79	0.39	85,109,121,123	0
5	IDR	F	1	13/13	0.80	0.25	70,83,90,97	0
4	BMA	E	3	11/12	0.85	0.15	102,111,114,114	0
5	IDR	F	7	12/13	0.88	0.20	78,99,108,111	0
6	NAG	G	2	14/15	0.88	0.18	87,102,110,120	0
3	MAN	D	4	11/12	0.89	0.17	79,84,93,103	0
2	IDR	C	8	12/13	0.89	0.21	66,88,96,96	0
5	IDR	F	3	12/13	0.90	0.26	61,71,75,75	0
3	NAG	D	2	14/15	0.90	0.15	67,77,87,94	0
7	BMA	H	3	11/12	0.91	0.16	104,108,112,119	0
8	NAG	I	1	14/15	0.91	0.17	74,88,99,111	0
2	GNS	C	1	16/16	0.91	0.16	76,96,109,114	0
5	IDR	F	5	12/13	0.92	0.14	64,69,76,80	0
2	IDR	C	2	12/13	0.93	0.10	55,62,72,74	0
7	NAG	H	2	14/15	0.94	0.18	72,87,96,101	0
3	NAG	D	1	14/15	0.94	0.12	47,52,60,72	0
4	NAG	E	2	14/15	0.94	0.21	72,79,89,102	0
4	NAG	E	1	14/15	0.94	0.13	46,54,62,68	0
2	IDR	C	6	12/13	0.94	0.14	51,58,61,61	0
5	GNS	F	6	15/16	0.94	0.11	72,82,88,96	0
6	NAG	G	1	14/15	0.95	0.10	45,56,75,81	0
5	GNS	F	2	15/16	0.95	0.16	54,68,72,72	0
2	GNS	C	7	15/16	0.96	0.15	64,73,82,85	0
2	IDR	C	4	12/13	0.96	0.14	46,50,53,54	0
7	NAG	H	1	14/15	0.96	0.17	65,72,78,88	0
5	GNS	F	4	15/16	0.96	0.12	50,56,61,63	0
2	GNS	C	3	15/16	0.97	0.13	45,51,57,58	0
2	GNS	C	5	15/16	0.97	0.16	42,46,48,51	0

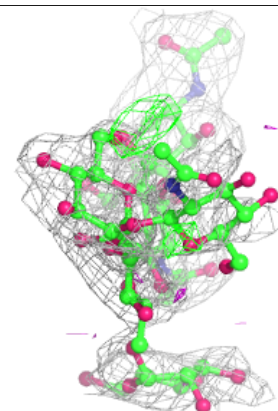
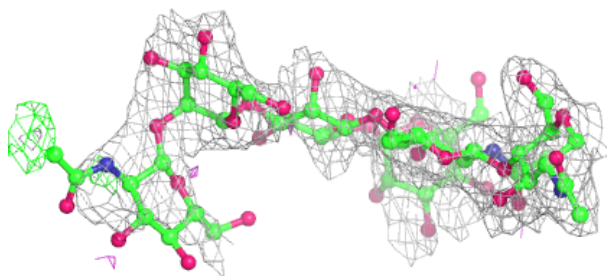
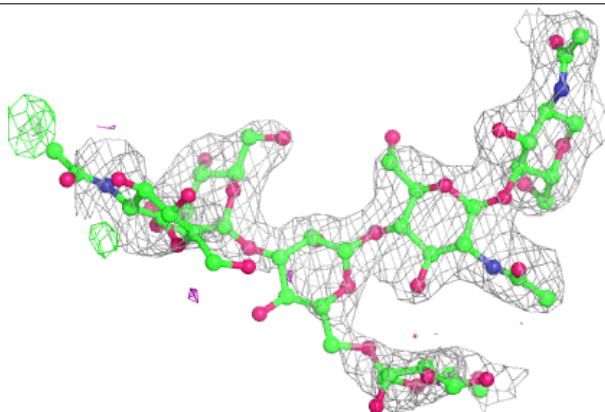
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

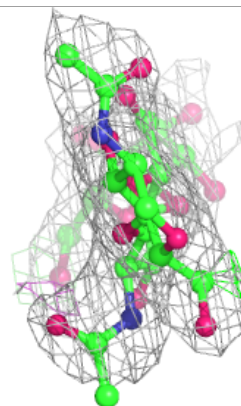
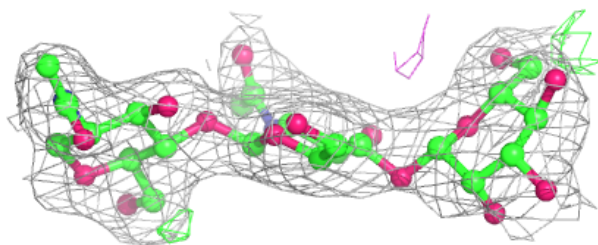
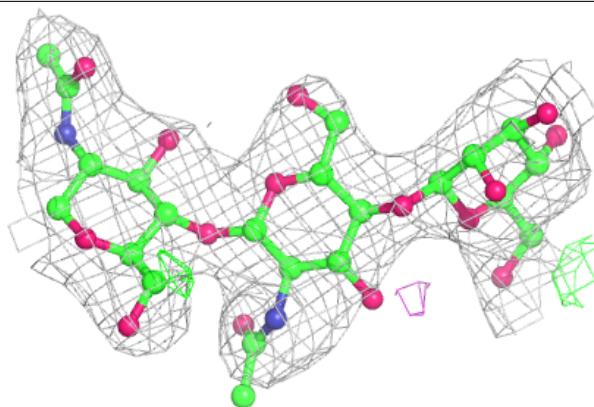
**Electron density around Chain D:**

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

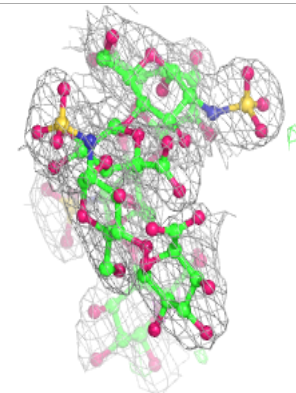
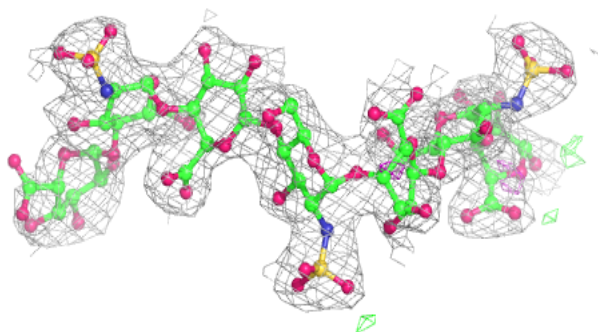
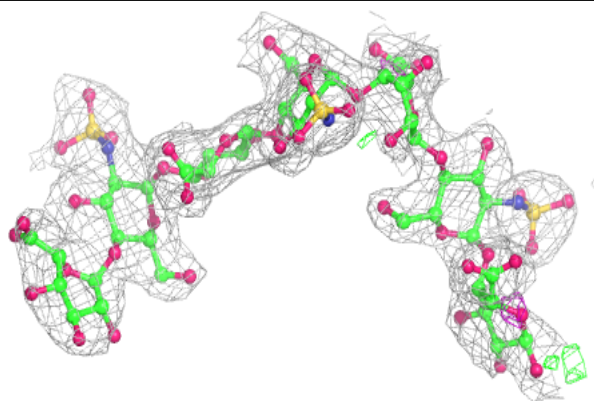


Electron density around Chain E:

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

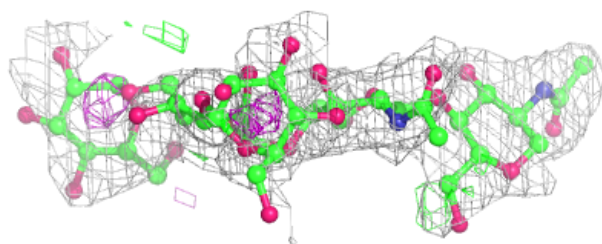
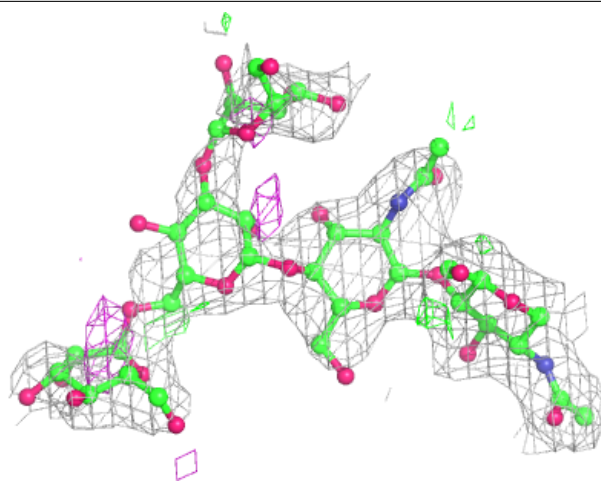
**Electron density around Chain F:**

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



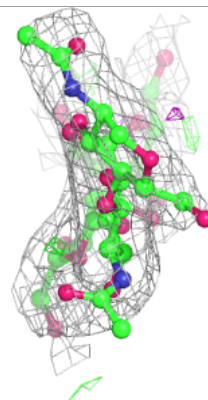
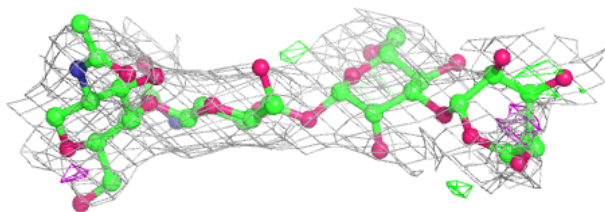
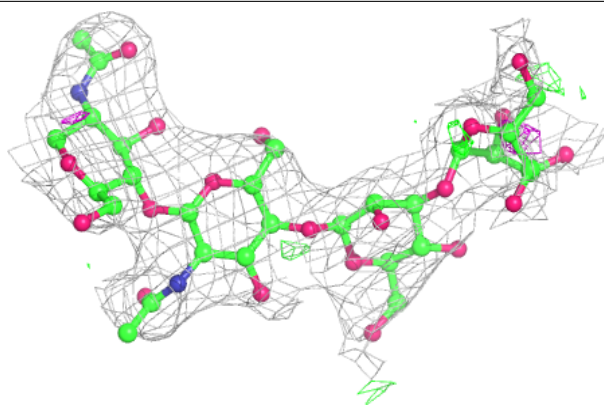
Electron density around Chain G:

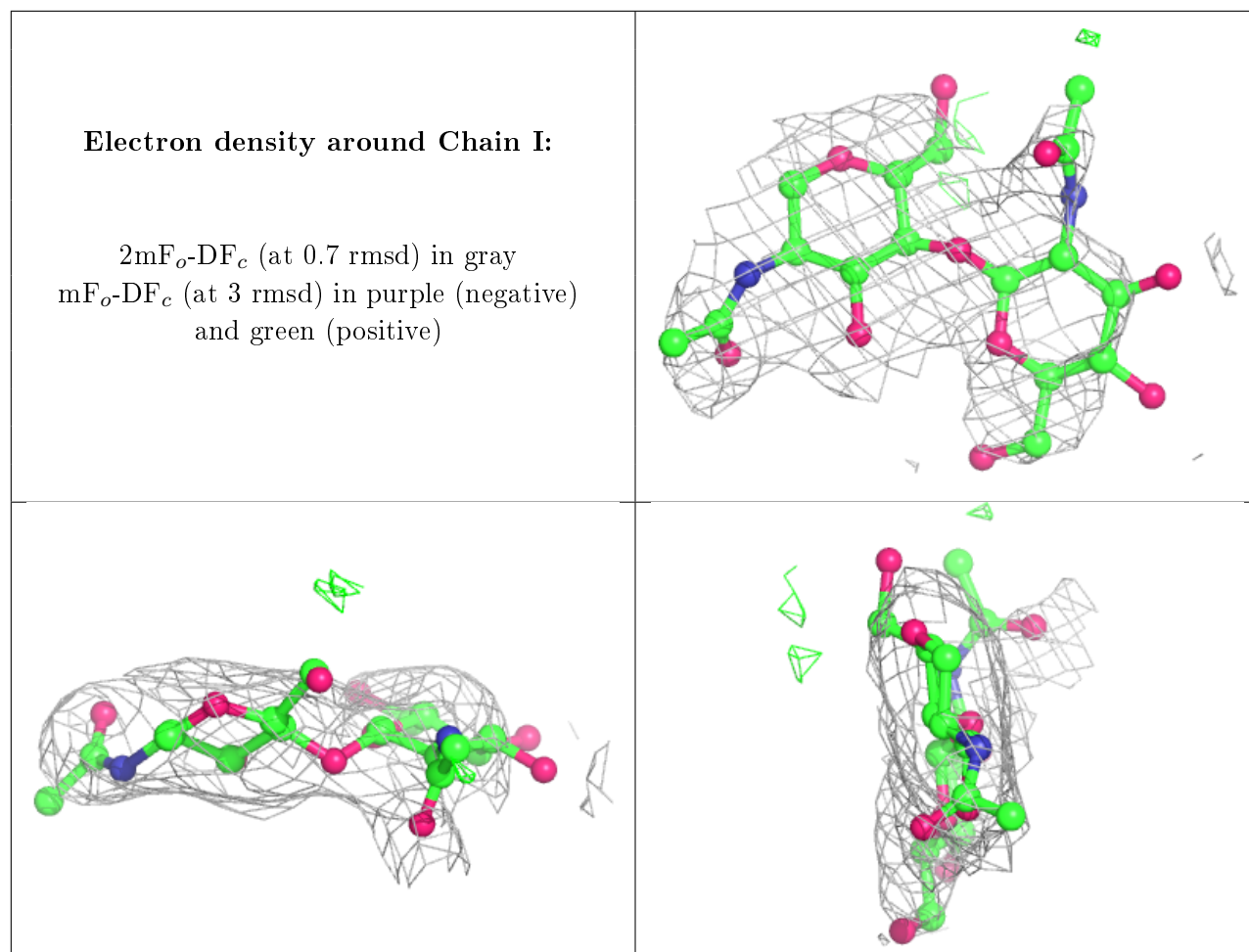
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain H:

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





6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

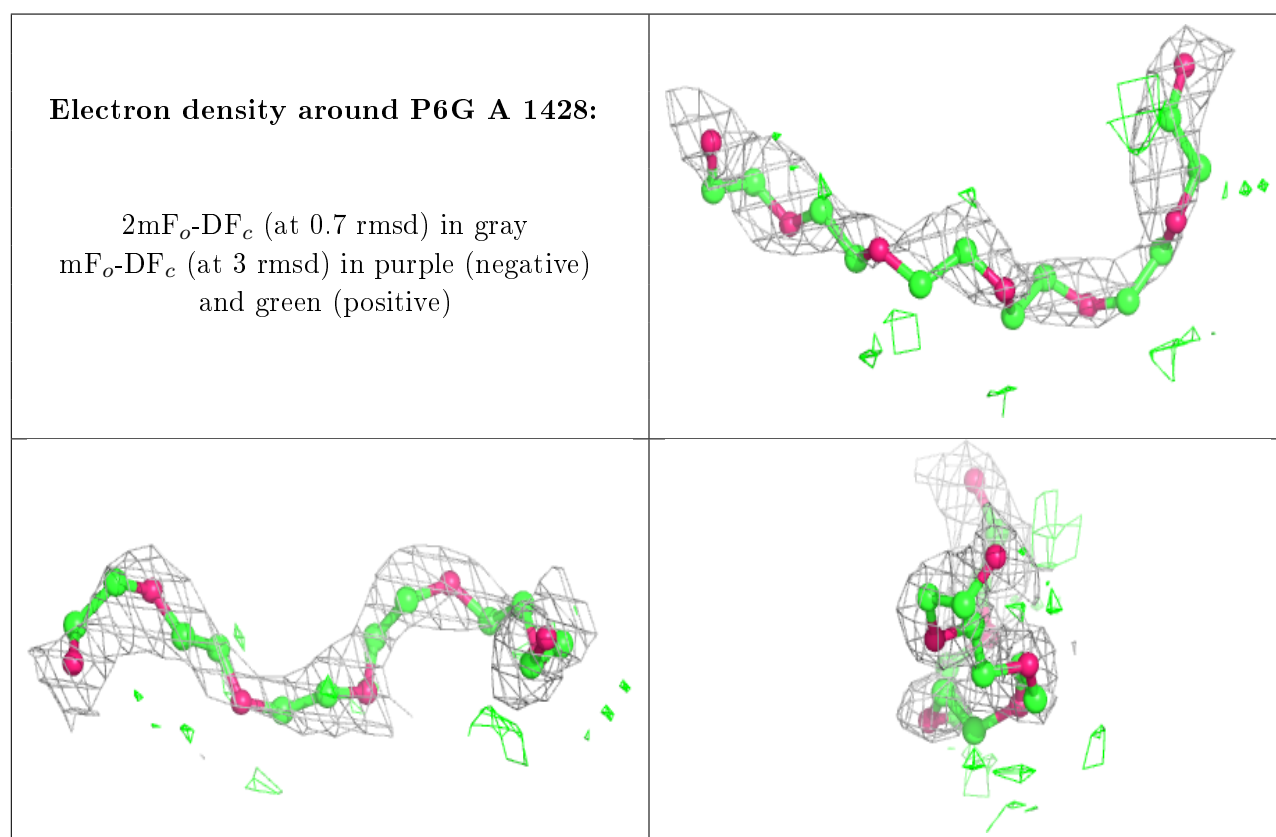
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
13	P6G	A	1428	19/19	0.71	0.32	77,107,119,119	0
11	GOL	A	1425	6/6	0.73	0.33	91,100,101,103	0
11	GOL	A	1426	6/6	0.75	0.27	56,66,78,81	0
12	MES	A	1427	12/12	0.78	0.24	68,90,107,109	0
10	NAG	A	1419	14/15	0.82	0.30	85,93,101,104	0
11	GOL	A	1420	6/6	0.85	0.21	41,52,58,67	0
11	GOL	B	722	6/6	0.87	0.24	54,63,64,65	0
11	GOL	A	1422	6/6	0.88	0.19	59,67,74,84	0
11	GOL	B	720	6/6	0.88	0.18	51,53,59,63	0
11	GOL	A	1424	6/6	0.89	0.34	70,75,78,90	0
11	GOL	A	1421	6/6	0.91	0.22	53,58,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
11	GOL	B	721	6/6	0.93	0.18	52,53,56,70	0
11	GOL	B	723	6/6	0.93	0.17	56,59,62,63	0
11	GOL	A	1423	6/6	0.94	0.29	54,63,71,83	0
9	CA	A	1409	1/1	0.97	0.04	74,74,74,74	0
9	CA	B	708	1/1	0.98	0.06	78,78,78,78	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.