



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 02:39 PM BST

PDB ID : 5O5U
Title : X-ray structure of human glutamate carboxypeptidase II (GCP II) in complex with a urea based inhibitor PSMA 1027
Authors : Novakova, Z.; Barinka, C.; Motlova, L.
Deposited on : 2017-06-02
Resolution : 1.53 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
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

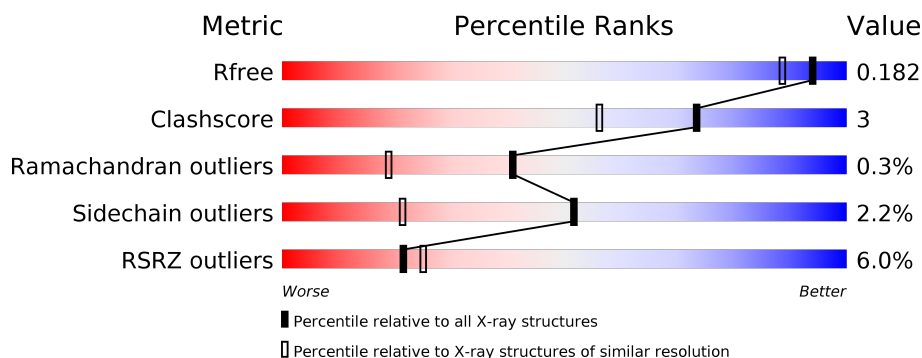
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.53 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.



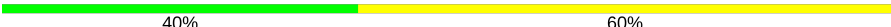
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2556 (1.56-1.52)
Clashscore	141614	2634 (1.56-1.52)
Ramachandran outliers	138981	2580 (1.56-1.52)
Sidechain outliers	138945	2577 (1.56-1.52)
RSRZ outliers	127900	2524 (1.56-1.52)

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	707	<div> <div>6%</div> <div> <div></div> <div>90%</div> <div>7% ..</div> </div> </div>
2	B	3	<div> <div>67%</div> <div>33%</div> </div>
2	D	3	<div> <div>33%</div> <div>67%</div> </div>
2	F	3	<div> <div>100%</div> </div>
3	C	2	<div> <div>50%</div> <div>50%</div> </div>
3	E	2	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
4	G	5	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BMA	B	3	-	-	-	X
2	BMA	D	3	-	-	-	X
3	NAG	C	2	-	-	-	X
3	NAG	E	2	-	-	-	X

2 Entry composition [i](#)

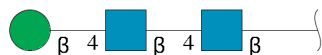
There are 10 unique types of molecules in this entry. The entry contains 6859 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glutamate carboxypeptidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	696	Total	C	N	O	S	0	56	0
			5918	3789	998	1109	22			

- Molecule 2 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
2	B	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	D	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	F	3	Total	C	N	O	0	0	0
			39	22	2	15			

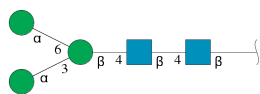
- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

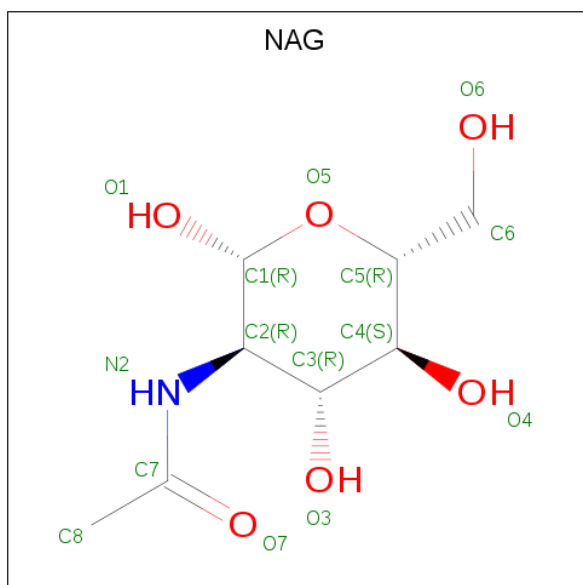
- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyran

ose-(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
4	G	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Zn	0	0
			2	2		

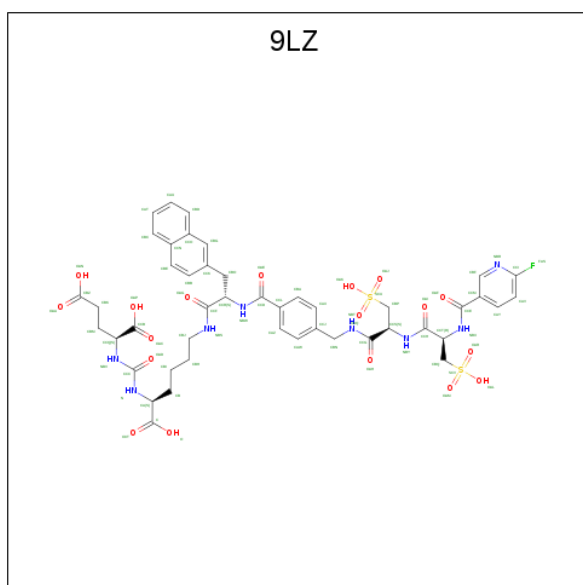
- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Cl 1 1	0	0

- Molecule 9 is (2 {S})-2-[[[(2 {S})-6-[[[(2 {S})-2-[[4-[[[(2 {S})-2-[(2 {R})-2-[(6-fluoranylpyridin-3-yl)carbonylamino]-3-sulfo-propanoyl]amino]-3-sulfo-propanoyl]amino]methyl]phenyl]carbonylamino]-3-naphthalen-2-yl-propanoyl]amino]-1-oxidanyl-1-oxidanylidene-hexan-2-yl]carbonylamino]pentanedioic acid (three-letter code: 9LZ) (formula: C₄₅H₅₁FN₈O₁₈S₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
9	A	1	Total	C	F	N	O	S	0	0
			74	45	1	8	18	2		

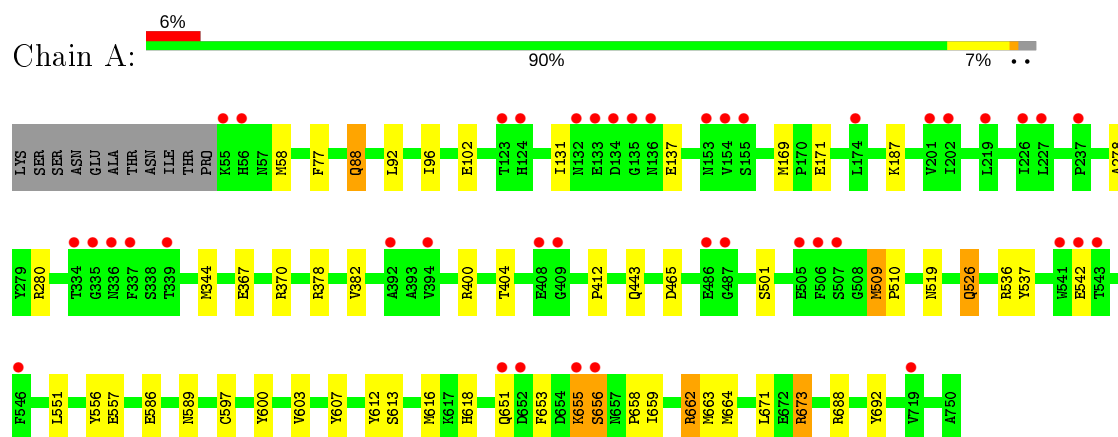
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	615	Total O 615 615	0	0

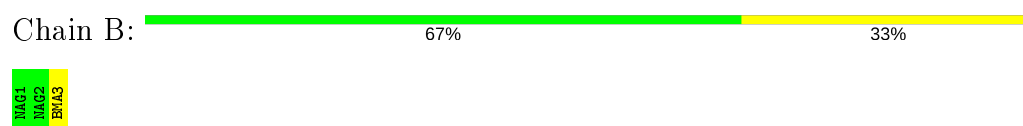
3 Residue-property plots [i](#)

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: Glutamate carboxypeptidase 2



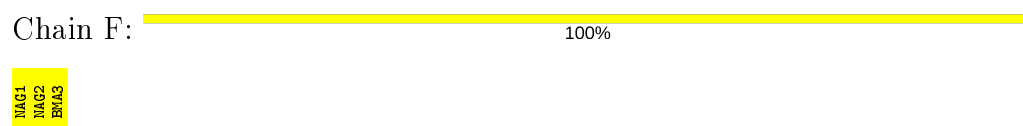
- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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

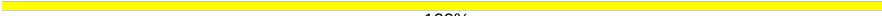


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  50% 50%

MAG1
MAG2

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

Chain E:  100%

MAG1
MAG2

- Molecule 4: 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:  40% 60%

MAG1
MAG2
BMA3
MAN4
MAN5

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	101.79Å 130.41Å 159.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.57 – 1.53 29.57 – 1.53	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.57-1.53) 99.0 (29.57-1.53)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 1.53Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.157 , 0.171 0.171 , 0.182	Depositor DCC
R_{free} test set	3103 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å ²)	21.5	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6859	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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: ZN, BMA, NAG, CL, CA, 9LZ, 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	0.76	1/6154 (0.0%)	0.87	13/8330 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	557	GLU	CD-OE2	-5.96	1.19	1.25

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	673	ARG	NE-CZ-NH1	8.59	124.60	120.30
1	A	370	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	A	673	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	A	465	ASP	CB-CG-OD1	6.69	124.32	118.30
1	A	662[A]	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	A	662[B]	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	A	688[A]	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	A	688[B]	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	A	662[A]	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	A	662[B]	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	A	77	PHE	CB-CG-CD1	5.35	124.55	120.80
1	A	536	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	378	ARG	NE-CZ-NH1	5.05	122.83	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5918	0	5759	39	0
2	B	39	0	34	0	0
2	D	39	0	34	0	0
2	F	39	0	34	0	0
3	C	28	0	25	1	0
3	E	28	0	25	0	0
4	G	61	0	52	0	0
5	A	14	0	13	0	0
6	A	2	0	0	0	0
7	A	1	0	0	0	0
8	A	1	0	0	0	0
9	A	74	0	0	0	0
10	A	615	0	0	7	1
All	All	6859	0	5976	40	1

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 (40) 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:659[B]:ILE:HG22	1:A:663[B]:MET:CE	2.02	0.90
1:A:659[B]:ILE:HG22	1:A:663[B]:MET:HE3	1.54	0.85
1:A:412:PRO:HA	1:A:589[A]:ASN:HD21	1.40	0.85
1:A:88:GLN:HE21	1:A:88:GLN:H	1.28	0.82
1:A:663[A]:MET:HE3	10:A:1422:HOH:O	1.80	0.81
1:A:597[B]:CYS:SG	1:A:671:LEU:HD22	2.26	0.76
1:A:603[B]:VAL:HG13	1:A:607:TYR:CE2	2.22	0.75
1:A:663[B]:MET:SD	10:A:1422:HOH:O	2.45	0.73
1:A:597[B]:CYS:SG	1:A:671:LEU:CD2	2.77	0.72
1:A:659[B]:ILE:CG2	1:A:663[B]:MET:CE	2.68	0.71
1:A:653[A]:PHE:CE1	1:A:655[A]:LYS:NZ	2.57	0.65
1:A:400:ARG:O	1:A:404[B]:THR:HG23	1.99	0.63
1:A:131:ILE:HD11	1:A:171[B]:GLU:HG3	1.87	0.57
1:A:659[B]:ILE:HG22	1:A:663[B]:MET:HE2	1.81	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:653[A]:PHE:O	1:A:655[A]:LYS:HD3	2.05	0.56
1:A:612:TYR:CZ	1:A:616:MET:HG3	2.44	0.53
1:A:659[B]:ILE:CG2	1:A:663[B]:MET:HE3	2.32	0.51
1:A:58:MET:CE	1:A:586:GLU:HG2	2.41	0.50
1:A:659[B]:ILE:CG2	1:A:663[B]:MET:HE2	2.38	0.50
1:A:412:PRO:HA	1:A:589[A]:ASN:ND2	2.20	0.49
1:A:613[B]:SER:OG	10:A:901:HOH:O	2.18	0.48
1:A:664[B]:MET:HE1	10:A:1144:HOH:O	2.14	0.47
1:A:443[B]:GLN:NE2	10:A:909:HOH:O	2.46	0.47
1:A:526[A]:GLN:NE2	1:A:692:TYR:O	2.48	0.47
1:A:656[B]:SER:O	1:A:658[B]:PRO:HD3	2.15	0.46
1:A:169:MET:HA	1:A:344:MET:O	2.16	0.46
1:A:92:LEU:O	1:A:96[B]:ILE:HG12	2.15	0.46
1:A:509:MET:HG3	1:A:510:PRO:HD2	1.98	0.45
1:A:659[B]:ILE:O	1:A:663[B]:MET:HG3	2.17	0.45
1:A:278:ALA:HB3	1:A:280[B]:ARG:CZ	2.49	0.43
1:A:131:ILE:HG22	1:A:137:GLU:HG2	2.00	0.43
1:A:526[A]:GLN:HE21	1:A:526[A]:GLN:HB3	1.53	0.42
1:A:367:GLU:OE1	1:A:662[B]:ARG:NH1	2.53	0.42
1:A:551:LEU:HD22	1:A:556:TYR:HB2	2.02	0.42
1:A:659[B]:ILE:HA	1:A:659[B]:ILE:HD13	1.79	0.41
1:A:662[B]:ARG:HD3	1:A:662[B]:ARG:HH11	1.75	0.41
1:A:597[B]:CYS:SG	1:A:671:LEU:HD23	2.59	0.41
1:A:618:HIS:HE1	10:A:1111:HOH:O	2.04	0.40
1:A:278:ALA:HB3	1:A:280[B]:ARG:NH1	2.35	0.40
10:A:1026:HOH:O	3:C:1:NAG:H83	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1207:HOH:O	10:A:1435:HOH:O[2_565]	2.18	0.02

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	750/707 (106%)	731 (98%)	16 (2%)	3 (0%)	34 13

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	656[A]	SER
1	A	656[B]	SER
1	A	382	VAL

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	649/603 (108%)	632 (97%)	17 (3%)	46 16

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	GLN
1	A	102[A]	GLU
1	A	102[B]	GLU
1	A	187	LYS
1	A	501	SER
1	A	509	MET
1	A	519	ASN
1	A	526[A]	GLN
1	A	526[B]	GLN
1	A	537	TYR
1	A	542	GLU
1	A	600	TYR
1	A	651[A]	GLN
1	A	651[B]	GLN
1	A	655[A]	LYS
1	A	655[B]	LYS

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Mol	Chain	Res	Type
1	A	673	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	GLN
1	A	136	ASN
1	A	216	ASN
1	A	303	GLN
1	A	345	HIS
1	A	618	HIS

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 ⓘ

18 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	B	1	1,2	14,14,15	0.41	0	17,19,21	0.72	0
2	NAG	B	2	2	14,14,15	0.51	0	17,19,21	0.87	0
2	BMA	B	3	2	11,11,12	0.86	0	15,15,17	1.48	3 (20%)
3	NAG	C	1	1,3	14,14,15	0.98	0	17,19,21	1.92	5 (29%)
3	NAG	C	2	3	14,14,15	0.58	0	17,19,21	0.98	0
2	NAG	D	1	1,2	14,14,15	0.71	0	17,19,21	1.01	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	D	2	2	14,14,15	0.47	0	17,19,21	1.05	1 (5%)
2	BMA	D	3	2	11,11,12	0.53	0	15,15,17	0.85	0
3	NAG	E	1	1,3	14,14,15	0.64	0	17,19,21	1.82	3 (17%)
3	NAG	E	2	3	14,14,15	0.51	0	17,19,21	1.92	1 (5%)
2	NAG	F	1	1,2	14,14,15	0.98	1 (7%)	17,19,21	1.21	1 (5%)
2	NAG	F	2	2	14,14,15	0.49	0	17,19,21	1.29	1 (5%)
2	BMA	F	3	2	11,11,12	0.68	0	15,15,17	1.10	1 (6%)
4	NAG	G	1	1,4	14,14,15	0.59	0	17,19,21	1.53	2 (11%)
4	NAG	G	2	4	14,14,15	0.66	0	17,19,21	1.39	4 (23%)
4	BMA	G	3	4	11,11,12	0.63	0	15,15,17	1.17	2 (13%)
4	MAN	G	4	4	11,11,12	0.62	0	15,15,17	1.04	0
4	MAN	G	5	4	11,11,12	0.56	0	15,15,17	0.86	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
2	NAG	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	BMA	B	3	2	-	0/2/19/22	0/1/1/1
3	NAG	C	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1
3	NAG	E	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	4/6/23/26	0/1/1/1
2	BMA	F	3	2	-	1/2/19/22	0/1/1/1
4	NAG	G	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	3/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
4	MAN	G	4	4	-	0/2/19/22	0/1/1/1
4	MAN	G	5	4	-	2/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1	NAG	O7-C7	2.80	1.29	1.23

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2	NAG	C1-O5-C5	6.64	121.19	112.19
3	C	1	NAG	C1-C2-N2	-4.44	102.89	110.49
3	E	1	NAG	C1-O5-C5	4.15	117.82	112.19
4	G	1	NAG	O5-C1-C2	-3.69	105.45	111.29
2	F	2	NAG	C8-C7-N2	3.47	121.98	116.10
2	F	1	NAG	C2-N2-C7	3.40	127.75	122.90
3	E	1	NAG	C8-C7-N2	3.37	121.80	116.10
4	G	1	NAG	O5-C5-C6	3.27	112.33	107.20
3	C	1	NAG	O5-C5-C6	3.15	112.15	107.20
3	C	1	NAG	C8-C7-N2	3.15	121.44	116.10
2	B	3	BMA	C3-C4-C5	2.99	115.58	110.24
2	F	3	BMA	C3-C4-C5	2.98	115.55	110.24
3	E	1	NAG	O5-C5-C6	2.83	111.64	107.20
4	G	3	BMA	O3-C3-C2	-2.70	104.82	109.99
2	B	3	BMA	C1-O5-C5	2.63	115.76	112.19
4	G	2	NAG	C8-C7-N2	2.53	120.38	116.10
4	G	3	BMA	O6-C6-C5	-2.47	102.81	111.29
2	D	1	NAG	C3-C4-C5	2.37	114.46	110.24
3	C	1	NAG	O6-C6-C5	2.20	118.86	111.29
4	G	2	NAG	C4-C3-C2	-2.18	107.82	111.02
3	C	1	NAG	O7-C7-N2	-2.18	117.94	121.95
4	G	2	NAG	O4-C4-C5	-2.17	103.91	109.30
2	D	2	NAG	O4-C4-C3	-2.15	105.39	110.35
2	B	3	BMA	O5-C5-C4	2.07	115.85	110.83
2	D	1	NAG	O4-C4-C3	-2.06	105.58	110.35
2	D	1	NAG	O5-C5-C6	2.05	110.42	107.20
4	G	2	NAG	O3-C3-C2	-2.01	105.30	109.47

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1	NAG	O5-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
3	E	1	NAG	C8-C7-N2-C2

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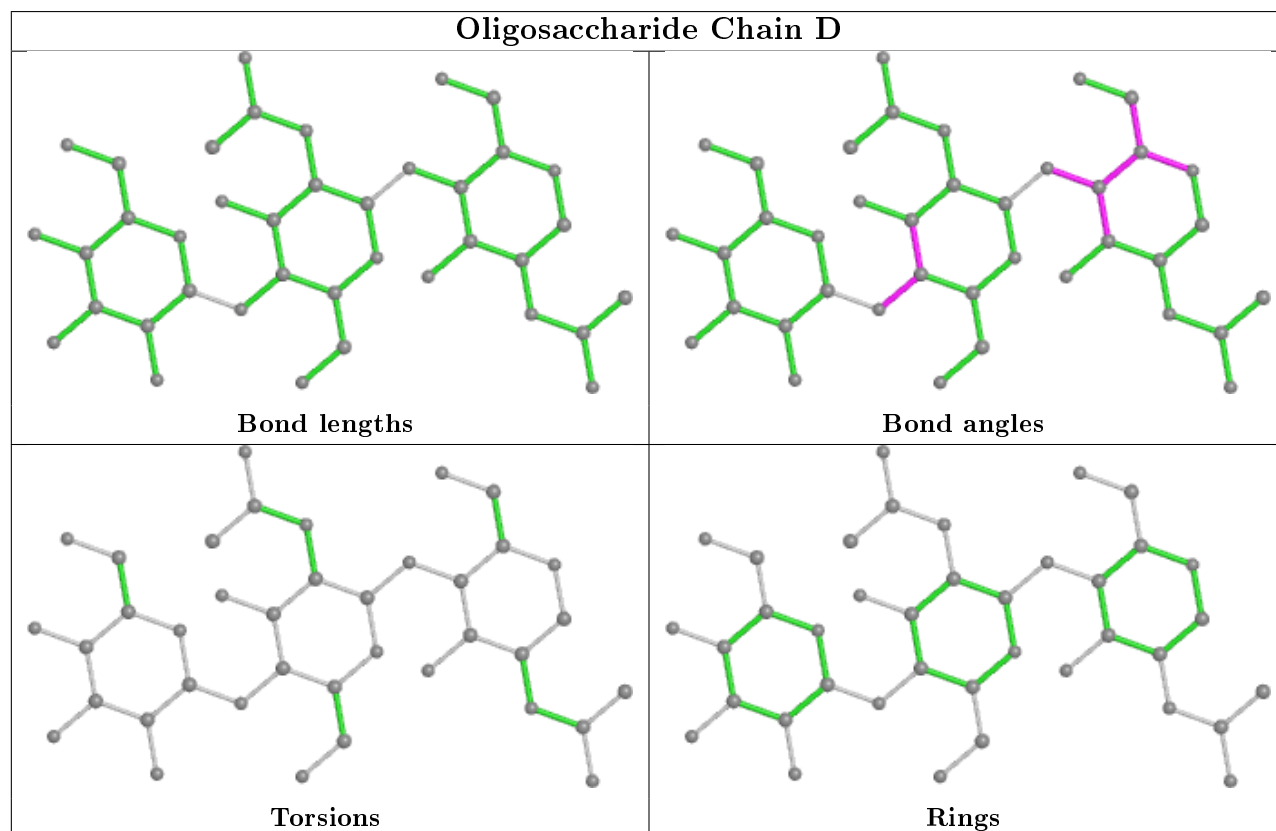
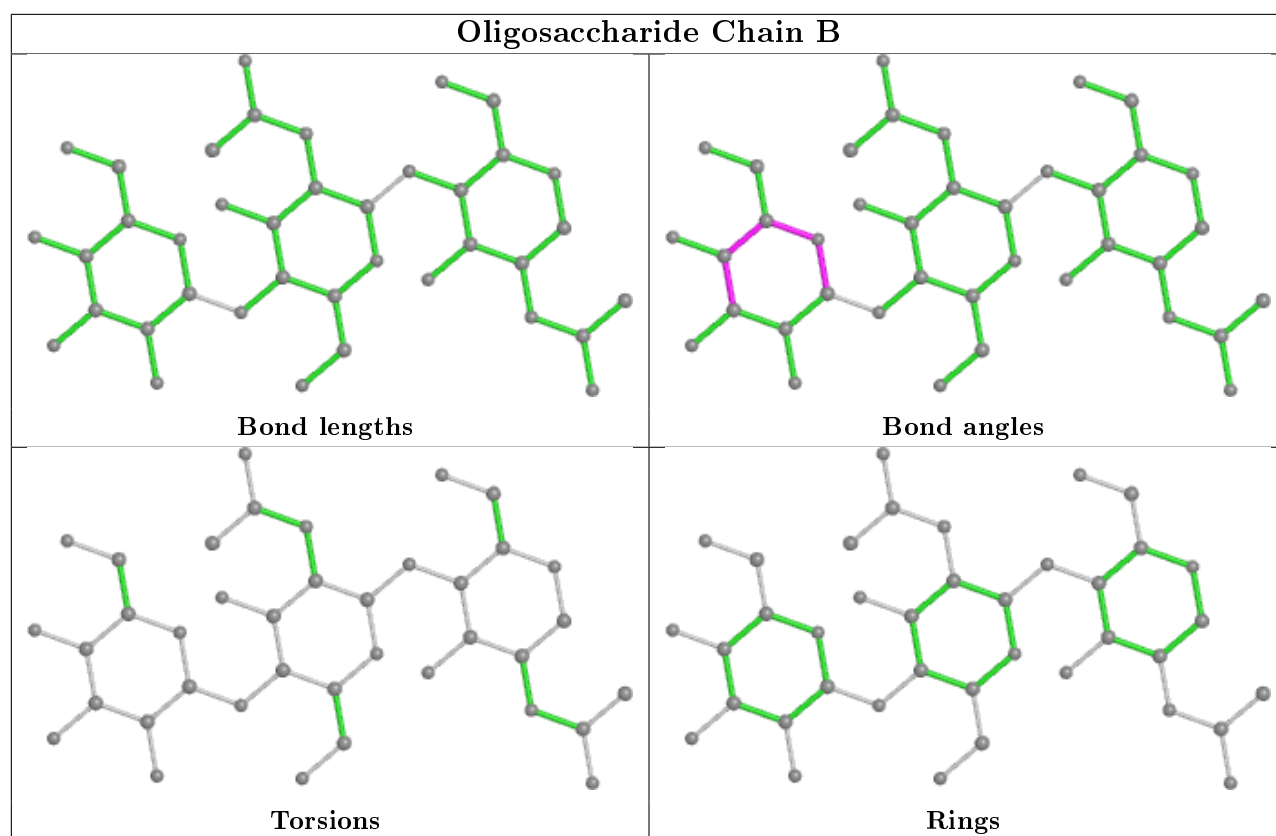
Mol	Chain	Res	Type	Atoms
3	E	1	NAG	O7-C7-N2-C2
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
4	G	2	NAG	C8-C7-N2-C2
4	G	2	NAG	O7-C7-N2-C2
3	E	1	NAG	C4-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
4	G	5	MAN	C4-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
4	G	5	MAN	O5-C5-C6-O6
2	F	3	BMA	C4-C5-C6-O6

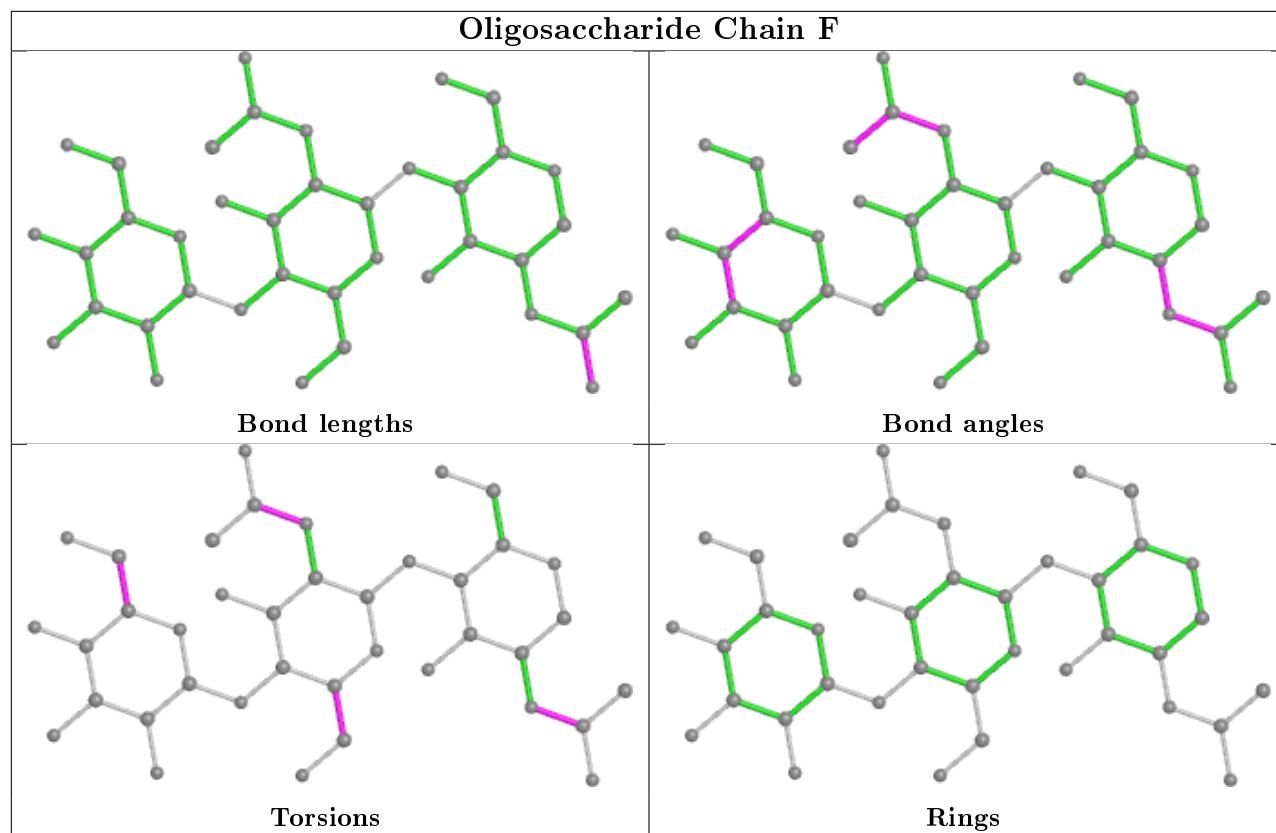
There are no ring outliers.

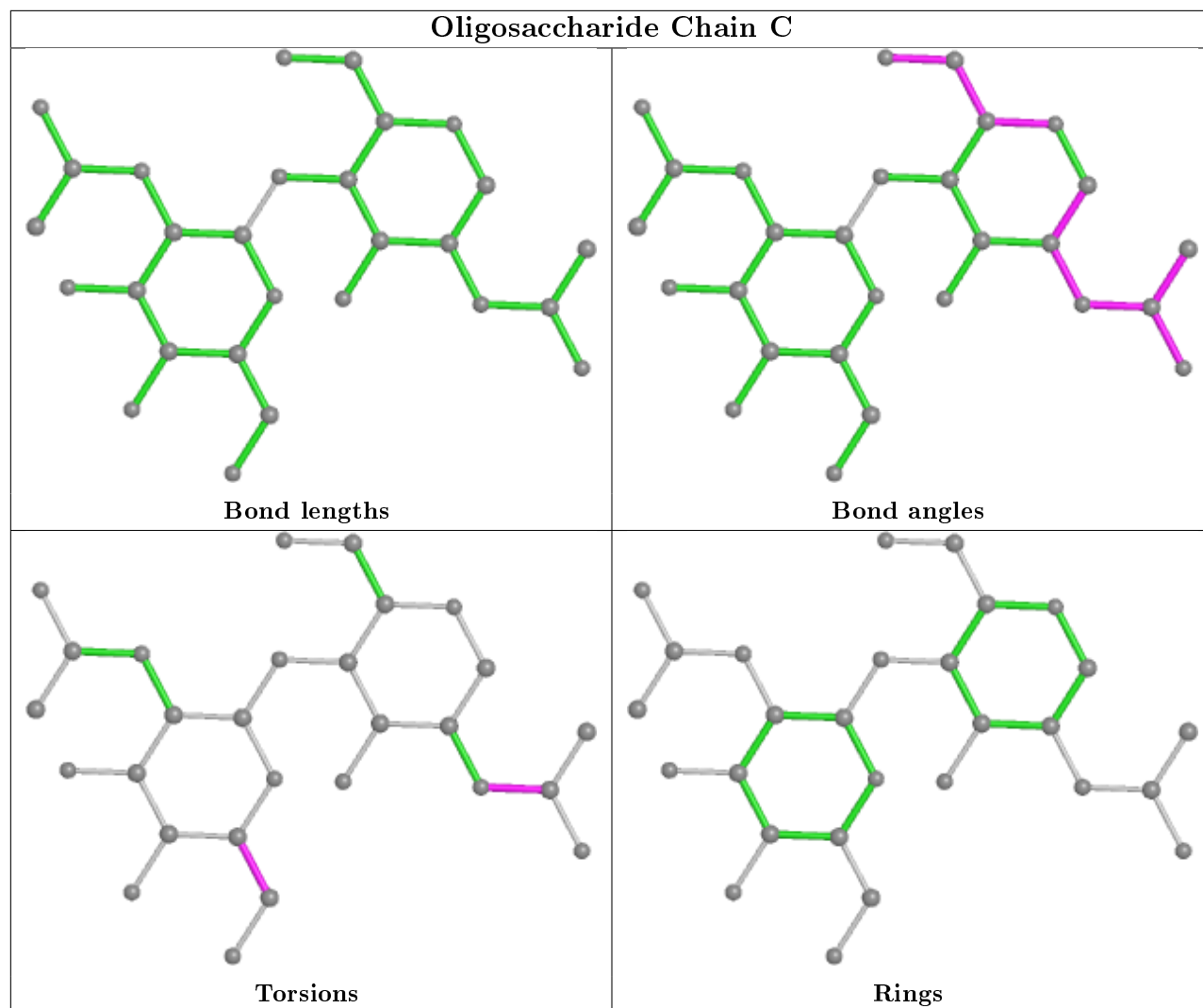
1 monomer is involved in 1 short contact:

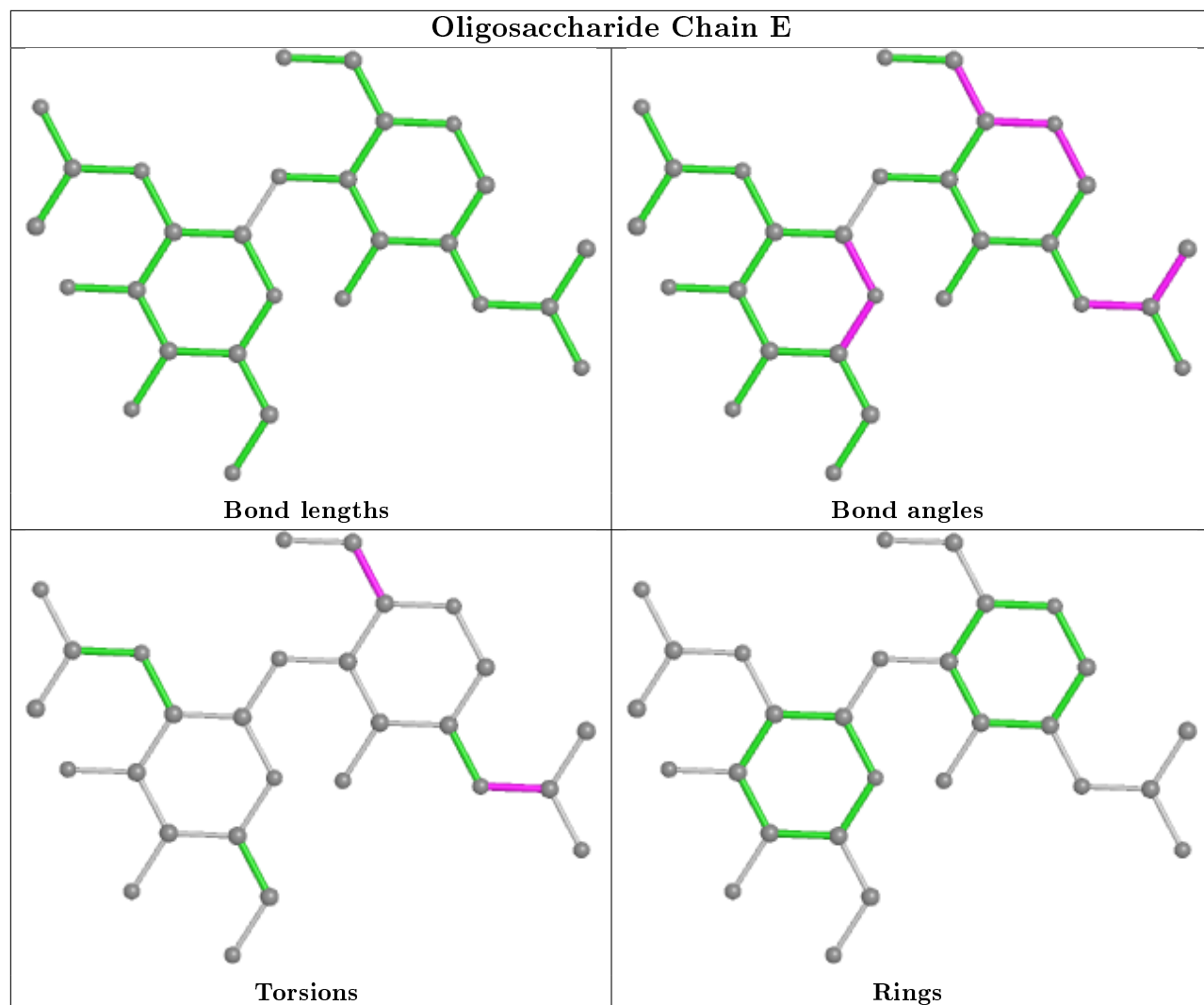
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	NAG	1	0

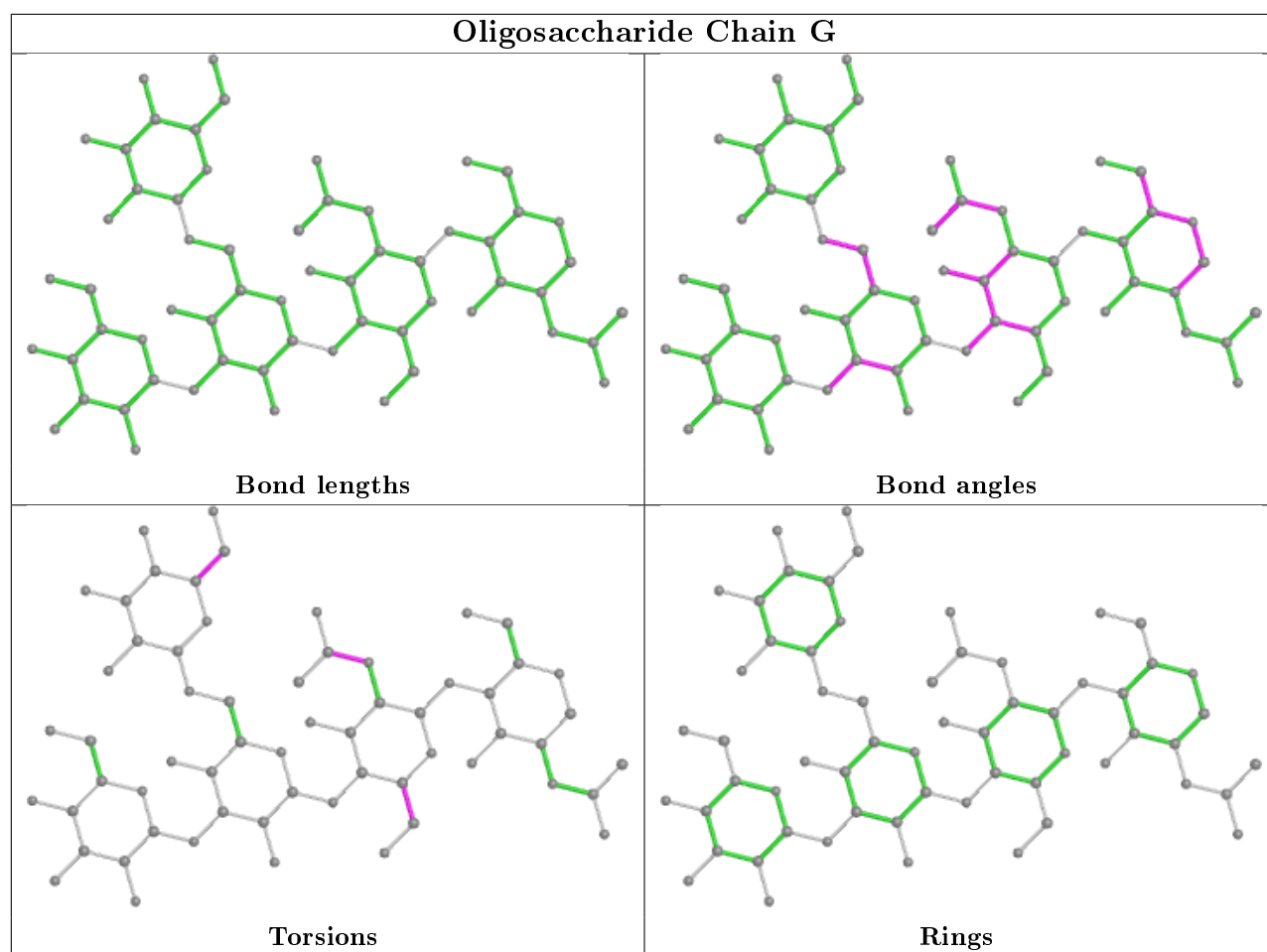
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	$\# Z > 2$
5	NAG	A	811	1	14,14,15	0.86	0	17,19,21	1.26	2 (11%)
9	9LZ	A	824	6	68,77,77	2.14	16 (23%)	88,107,107	3.90	30 (34%)

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
5	NAG	A	811	1	-	0/6/23/26	0/1/1/1
9	9LZ	A	824	6	-	13/70/80/80	0/4/4/4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	824	9LZ	CBN-NBT	-9.23	1.28	1.46
9	A	824	9LZ	CBO-CCR	-6.85	1.37	1.54
9	A	824	9LZ	CBP-CCS	-5.39	1.48	1.53
9	A	824	9LZ	CCI-NBR	5.34	1.36	1.30
9	A	824	9LZ	CBP-SCU	-3.61	1.64	1.77
9	A	824	9LZ	CCF-NBS	3.11	1.40	1.33
9	A	824	9LZ	CCR-CCF	3.08	1.60	1.52
9	A	824	9LZ	CBM-CCQ	2.56	1.56	1.53
9	A	824	9LZ	CA-N	2.44	1.49	1.46
9	A	824	9LZ	CBQ-CCT	2.37	1.56	1.53
9	A	824	9LZ	CBQ-SCV	-2.34	1.68	1.77
9	A	824	9LZ	OAG-CCF	2.22	1.27	1.23
9	A	824	9LZ	CAV-CCI	2.21	1.39	1.37
9	A	824	9LZ	CBO-CCK	-2.20	1.46	1.51
9	A	824	9LZ	CB-CA	2.15	1.56	1.53
9	A	824	9LZ	CCQ-NBV	-2.09	1.43	1.46

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	824	9LZ	CBF-NBR-CCI	19.90	122.24	115.75
9	A	824	9LZ	CAV-CCI-NBR	-12.99	119.71	126.83
9	A	824	9LZ	OAQ-SCU-CBP	10.88	119.87	106.94
9	A	824	9LZ	FAS-CCI-NBR	8.73	120.62	114.95
9	A	824	9LZ	CBO-CCR-CCF	-8.26	88.83	110.25
9	A	824	9LZ	CBO-CCR-NBW	8.03	127.72	110.79
9	A	824	9LZ	CCS-NBY-CCH	7.51	137.77	121.67
9	A	824	9LZ	CCJ-CBN-NBT	6.78	127.57	113.05
9	A	824	9LZ	OAG-CCF-NBS	-5.55	111.07	122.99
9	A	824	9LZ	OAK-SCU-CBP	-5.51	96.95	105.74
9	A	824	9LZ	CCH-CCT-NBX	5.32	125.65	111.16
9	A	824	9LZ	CCF-CCR-NBW	-4.60	98.64	111.16
9	A	824	9LZ	CBJ-NBS-CCF	4.22	130.12	122.59
9	A	824	9LZ	CCT-CCH-NBY	-4.20	107.50	116.70
9	A	824	9LZ	OAR-SCV-CBQ	4.02	111.72	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	824	9LZ	CAY-CAV-CCI	3.79	119.18	116.35
9	A	824	9LZ	CCR-CCF-NBS	3.34	123.28	116.54
9	A	824	9LZ	CBO-CCK-CBG	-3.27	113.37	120.57
9	A	824	9LZ	CCM-CCE-NBX	3.26	123.31	117.06
9	A	824	9LZ	OAI-CCH-NBY	2.98	128.45	122.93
9	A	824	9LZ	CBN-CCJ-CAX	-2.92	114.85	120.91
9	A	824	9LZ	OAJ-SCU-CBP	-2.92	103.47	106.94
9	A	824	9LZ	OAL-SCV-CBQ	2.71	110.05	105.74
9	A	824	9LZ	CBN-CCJ-CAW	2.67	126.46	120.91
9	A	824	9LZ	OAF-CCE-CCM	-2.47	116.53	120.94
9	A	824	9LZ	CCM-CBF-NBR	-2.47	120.23	123.67
9	A	824	9LZ	OAG-CCF-CCR	2.46	125.62	120.45
5	A	811	NAG	O5-C1-C2	-2.27	107.70	111.29
9	A	824	9LZ	OAD-CCC-NBV	-2.20	118.61	122.62
9	A	824	9LZ	CCR-NBW-CCD	-2.10	116.45	121.60
5	A	811	NAG	C1-O5-C5	2.09	115.02	112.19
9	A	824	9LZ	CCK-CBO-CCR	2.02	118.97	113.39

There are no chirality outliers.

All (13) torsion outliers are listed below:

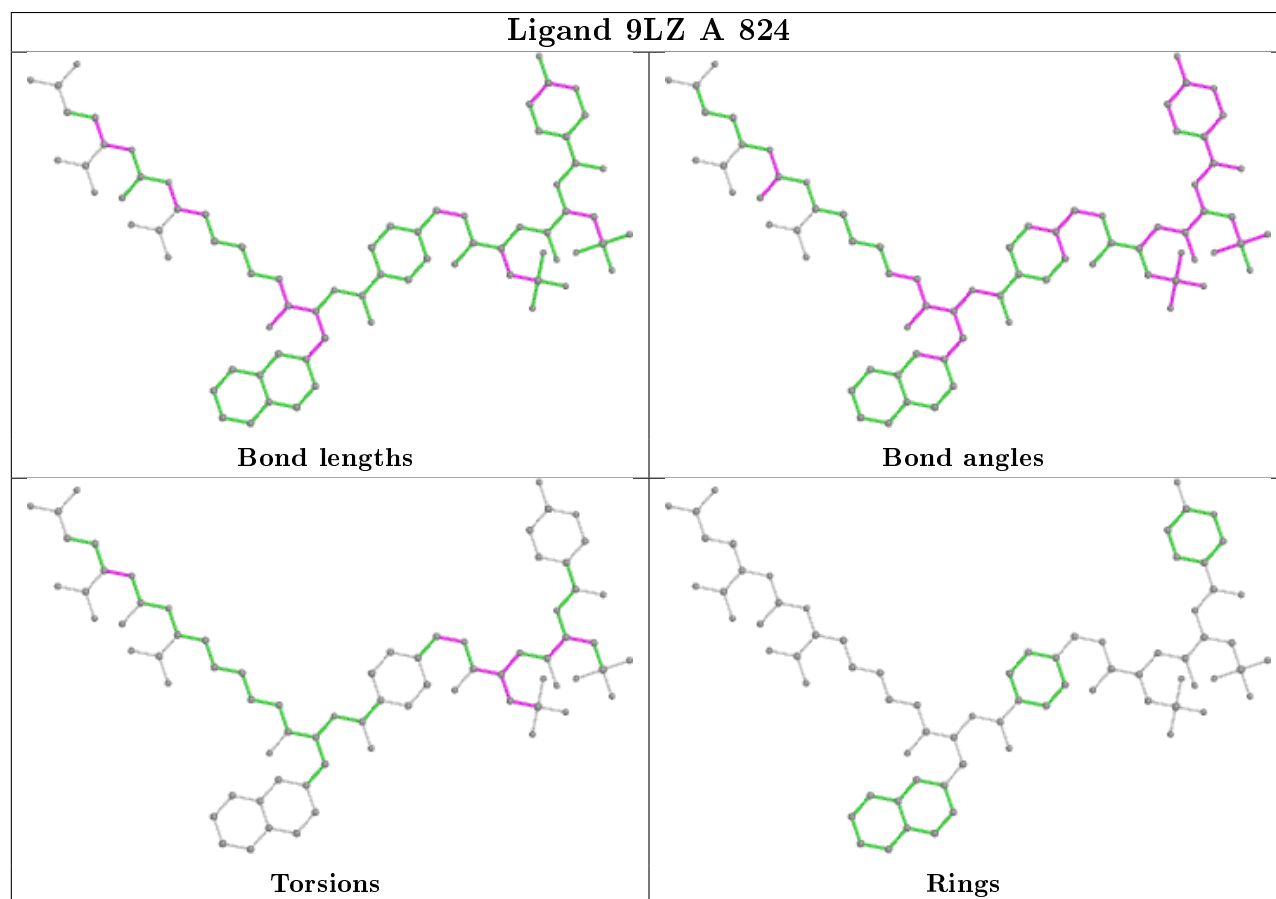
Mol	Chain	Res	Type	Atoms
9	A	824	9LZ	CCS-CBP-SCU-OAQ
9	A	824	9LZ	CCS-CBP-SCU-OAK
9	A	824	9LZ	CCS-CBP-SCU-OAJ
9	A	824	9LZ	SCV-CBQ-CCT-NBX
9	A	824	9LZ	CBP-CCS-NBY-CCH
9	A	824	9LZ	CCJ-CBN-NBT-CCG
9	A	824	9LZ	CCB-CCQ-NBV-CCC
9	A	824	9LZ	OAI-CCH-CCT-NBX
9	A	824	9LZ	SCU-CBP-CCS-NBY
9	A	824	9LZ	NBY-CCH-CCT-NBX
9	A	824	9LZ	OAH-CCG-CCS-NBY
9	A	824	9LZ	NBT-CCG-CCS-NBY
9	A	824	9LZ	SCV-CBQ-CCT-CCH

There are no ring outliers.

No monomer is involved in short contacts.

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

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	696/707 (98%)	0.14	42 (6%)	21 25	22, 31, 49, 74	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	55	LYS	5.3
1	A	542	GLU	4.5
1	A	155[A]	SER	4.5
1	A	656[A]	SER	4.3
1	A	652	ASP	4.2
1	A	506	PHE	4.1
1	A	153	ASN	4.1
1	A	507	SER	3.9
1	A	336	ASN	3.8
1	A	651[A]	GLN	3.8
1	A	134	ASP	3.7
1	A	719	VAL	3.5
1	A	337	PHE	3.5
1	A	56	HIS	3.3
1	A	541	TRP	3.3
1	A	136	ASN	3.1
1	A	334	THR	3.1
1	A	154	VAL	3.1
1	A	335	GLY	3.0
1	A	226	ILE	3.0
1	A	543	THR	3.0
1	A	237	PRO	2.9
1	A	339[A]	THR	2.9
1	A	202	ILE	2.8
1	A	135	GLY	2.7
1	A	505[A]	GLU	2.7
1	A	123	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	655[A]	LYS	2.5
1	A	227	LEU	2.5
1	A	133	GLU	2.4
1	A	546	PHE	2.4
1	A	174[A]	LEU	2.3
1	A	219	LEU	2.3
1	A	394	VAL	2.2
1	A	408	GLU	2.2
1	A	201	VAL	2.2
1	A	132	ASN	2.1
1	A	409	GLY	2.1
1	A	486	GLU	2.1
1	A	392	ALA	2.1
1	A	487	GLY	2.0
1	A	124	HIS	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.

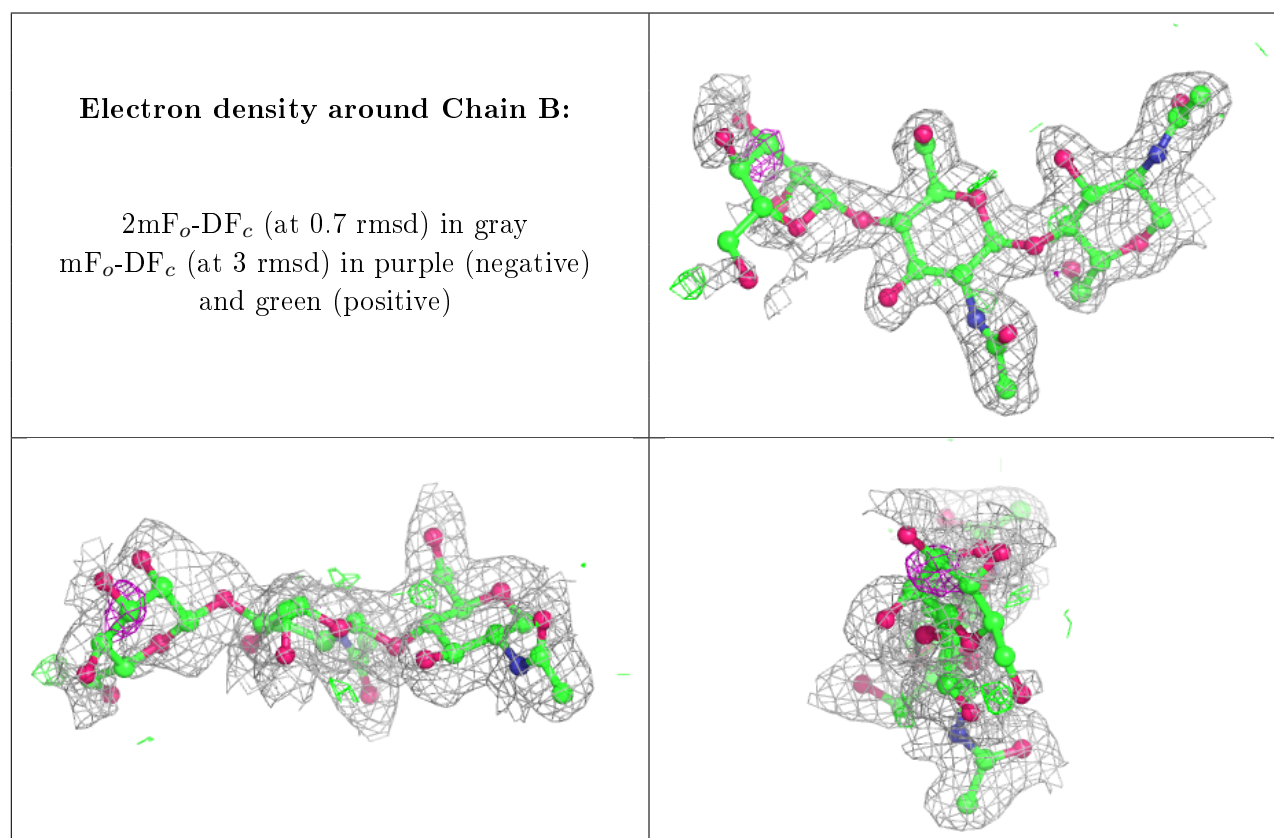
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BMA	B	3	11/12	0.35	0.47	79,90,92,93	0
3	NAG	E	2	14/15	0.57	0.54	99,107,110,112	0
3	NAG	C	2	14/15	0.58	0.42	73,74,78,78	0
2	BMA	F	3	11/12	0.61	0.35	68,76,82,85	0
3	NAG	E	1	14/15	0.64	0.25	68,77,82,93	0
2	BMA	D	3	11/12	0.69	0.46	92,95,99,101	0
2	NAG	B	2	14/15	0.71	0.24	47,53,62,71	0
2	NAG	D	2	14/15	0.75	0.31	58,63,72,84	0
4	MAN	G	5	11/12	0.76	0.33	59,63,67,71	0
3	NAG	C	1	14/15	0.77	0.28	49,57,67,67	0
2	NAG	D	1	14/15	0.82	0.17	44,47,52,53	0
2	NAG	F	2	14/15	0.86	0.20	43,50,60,63	0
4	NAG	G	2	14/15	0.87	0.19	42,45,55,55	0

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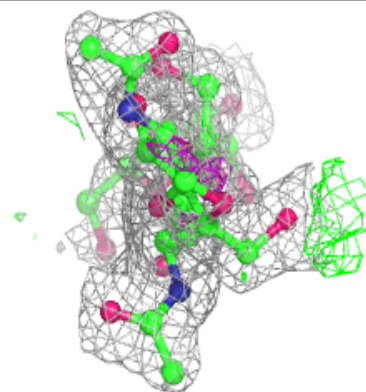
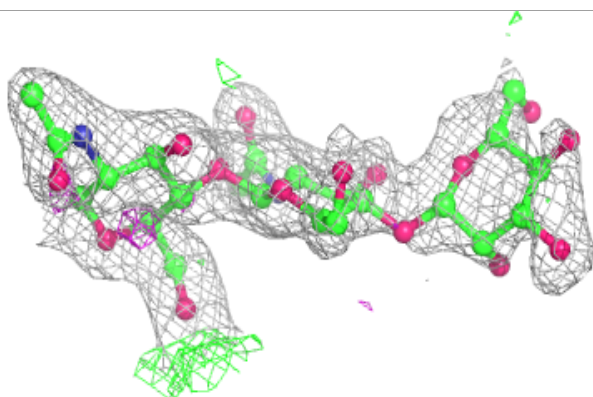
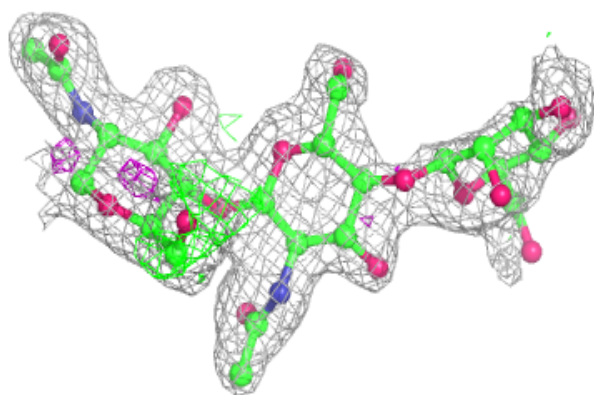
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	G	1	14/15	0.87	0.10	29,35,41,51	0
4	MAN	G	4	11/12	0.90	0.19	50,53,56,58	0
2	NAG	B	1	14/15	0.92	0.11	38,44,51,55	0
2	NAG	F	1	14/15	0.92	0.13	34,37,43,46	0
4	BMA	G	3	11/12	0.93	0.18	43,45,48,51	0

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.

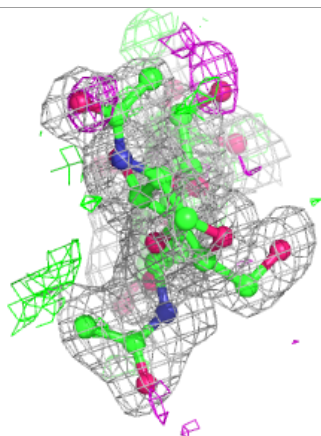
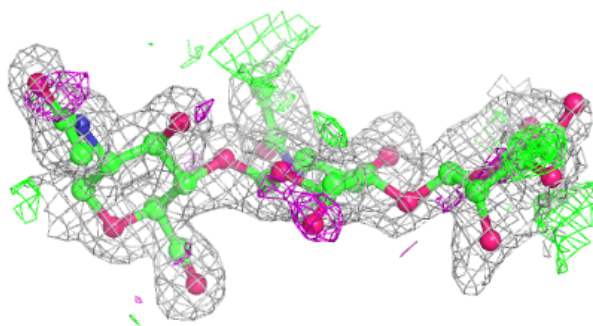
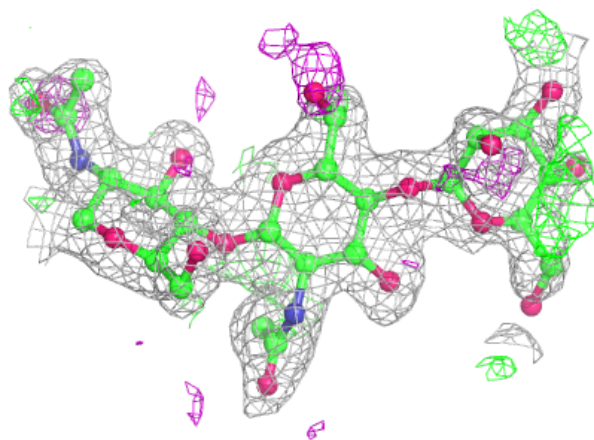


Electron density around Chain D:

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

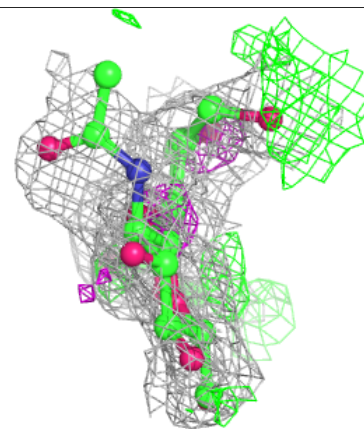
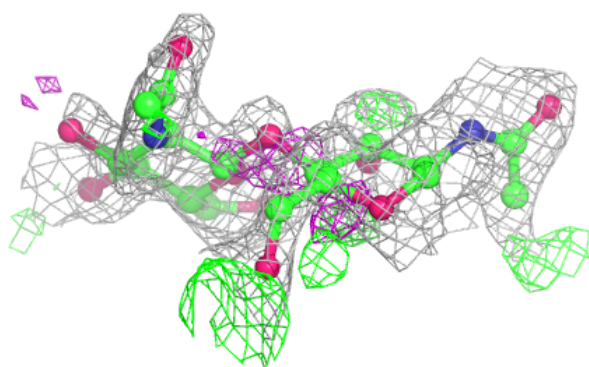
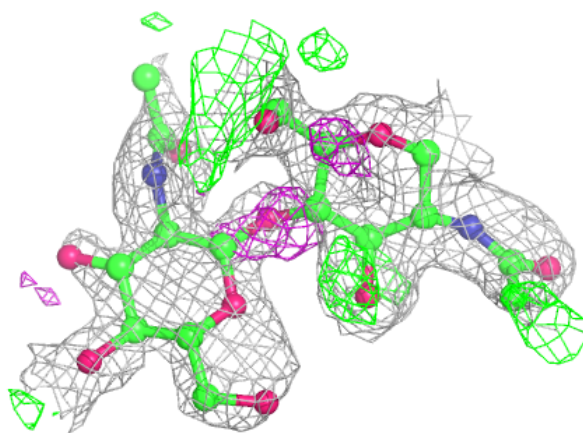
**Electron density around Chain F:**

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



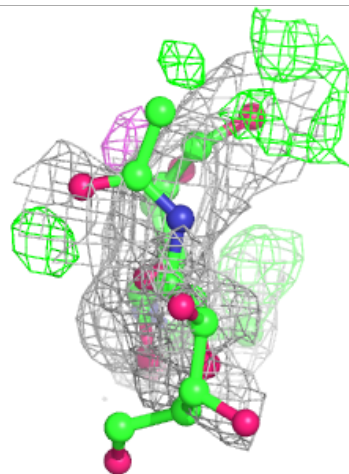
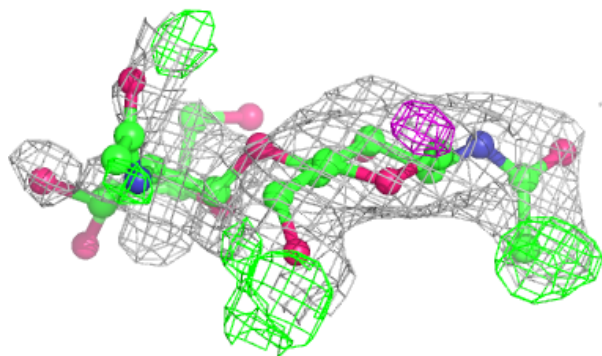
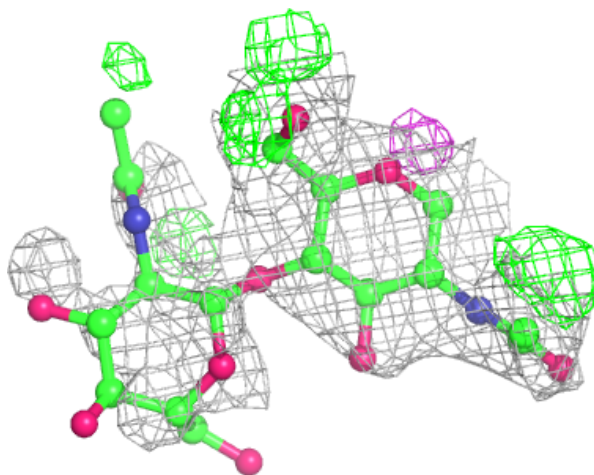
Electron density around Chain C:

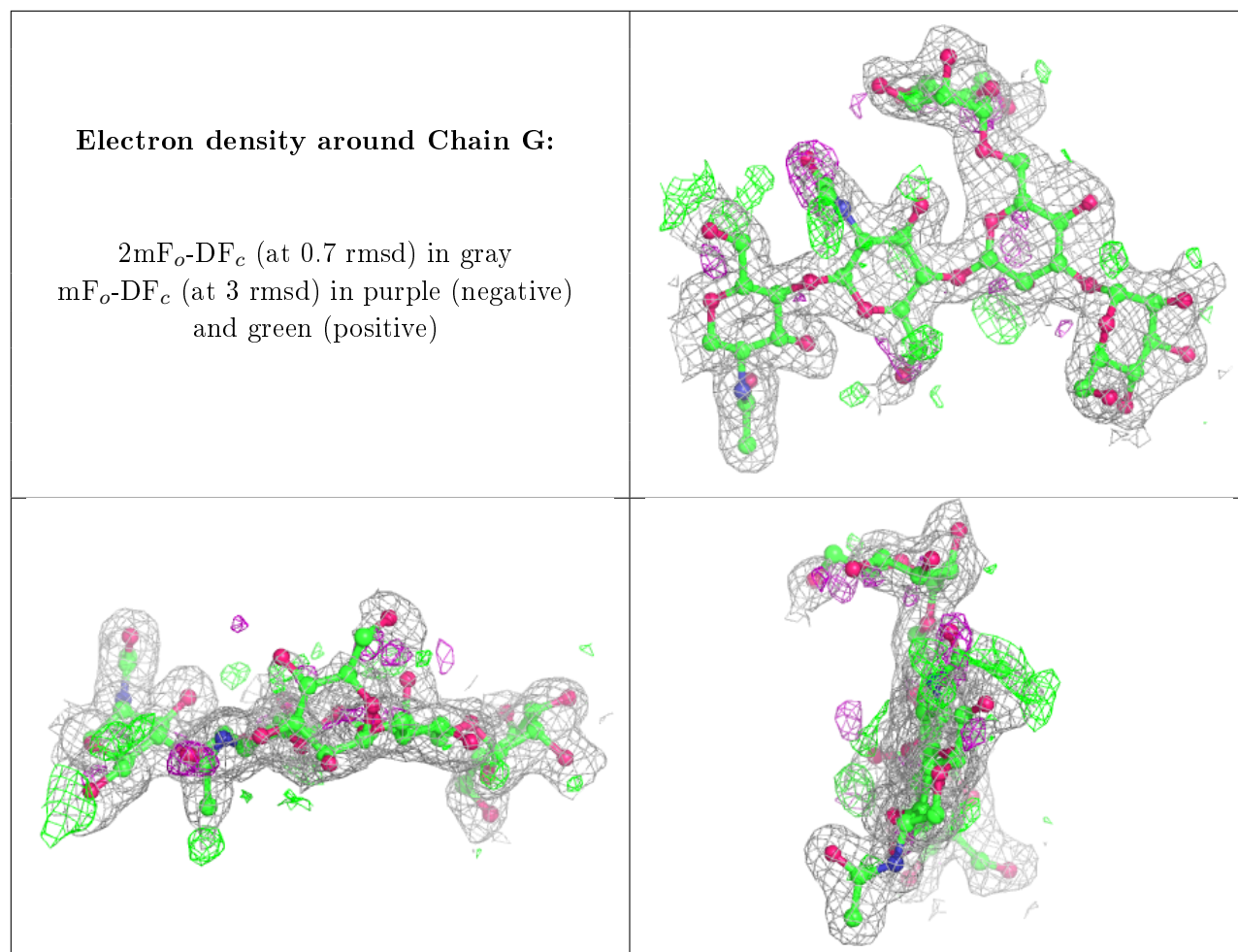
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain 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](#)

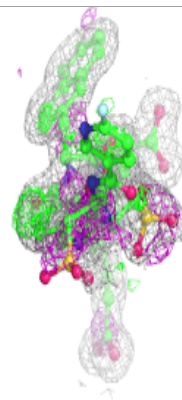
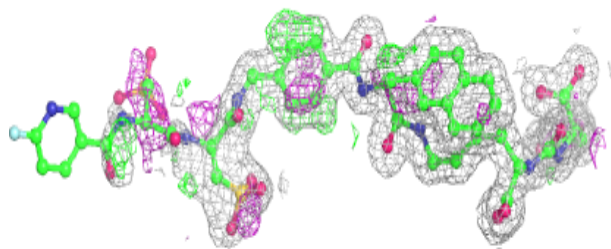
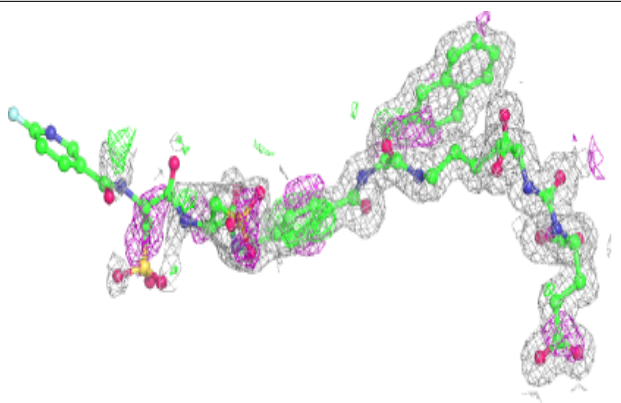
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	A	811	14/15	0.84	0.21	37,54,67,69	0
9	9LZ	A	824	74/74	0.91	0.15	23,27,130,141	0
8	CL	A	823	1/1	1.00	0.08	27,27,27,27	0
7	CA	A	822	1/1	1.00	0.06	22,22,22,22	0
6	ZN	A	821	1/1	1.00	0.05	24,24,24,24	0
6	ZN	A	820	1/1	1.00	0.05	24,24,24,24	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.

Electron density around 9LZ A 824:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.