



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 06:01 PM BST

PDB ID : 5F09
Title : Structure of inactive GCPII mutant in complex with beta-citryl glutamate
Authors : Tykvar, J.; Navratil, M.; Pachl, P.; Konvalinka, J.
Deposited on : 2015-11-27
Resolution : 1.85 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

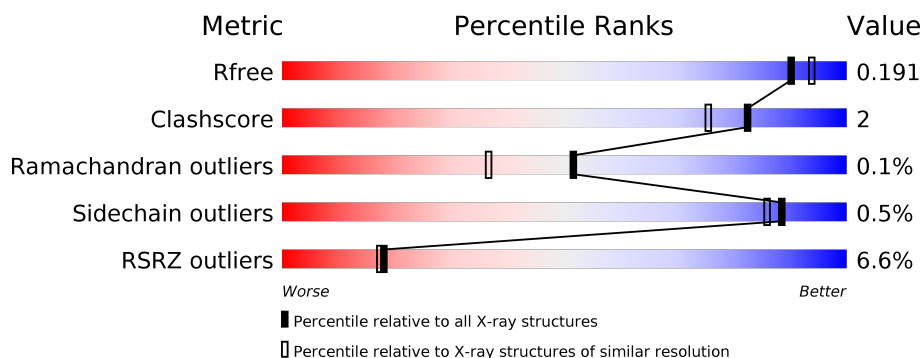
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	739	<div> <div>6%</div> <div> <div></div> <div>87%</div> <div>6%</div> <div>6%</div> </div> </div>
2	B	2	<div> <div>100%</div> </div>
2	C	2	<div> <div>100%</div> </div>
3	D	3	<div> <div>33%</div> <div>67%</div> </div>
4	E	4	<div> <div>100%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	C	2	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 6402 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	23	0
			5617	3612	940	1047	18			

There are 33 discrepancies between the modelled and reference sequences:

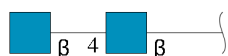
Chain	Residue	Modelled	Actual	Comment	Reference
A	12	ARG	-	expression tag	UNP Q04609
A	13	SER	-	expression tag	UNP Q04609
A	14	GLY	-	expression tag	UNP Q04609
A	15	LEU	-	expression tag	UNP Q04609
A	16	ASN	-	expression tag	UNP Q04609
A	17	ASP	-	expression tag	UNP Q04609
A	18	ILE	-	expression tag	UNP Q04609
A	19	PHE	-	expression tag	UNP Q04609
A	20	GLU	-	expression tag	UNP Q04609
A	21	ALA	-	expression tag	UNP Q04609
A	22	GLN	-	expression tag	UNP Q04609
A	23	LYS	-	expression tag	UNP Q04609
A	24	ILE	-	expression tag	UNP Q04609
A	25	GLU	-	expression tag	UNP Q04609
A	26	TRP	-	expression tag	UNP Q04609
A	27	HIS	-	expression tag	UNP Q04609
A	28	GLU	-	expression tag	UNP Q04609
A	29	GLY	-	expression tag	UNP Q04609
A	30	SER	-	expression tag	UNP Q04609
A	31	GLY	-	expression tag	UNP Q04609
A	32	SER	-	expression tag	UNP Q04609
A	33	GLY	-	expression tag	UNP Q04609
A	34	SER	-	expression tag	UNP Q04609
A	35	GLU	-	expression tag	UNP Q04609
A	36	ASN	-	expression tag	UNP Q04609
A	37	LEU	-	expression tag	UNP Q04609
A	38	TYR	-	expression tag	UNP Q04609

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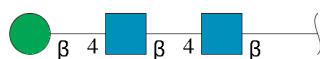
Chain	Residue	Modelled	Actual	Comment	Reference
A	39	PHE	-	expression tag	UNP Q04609
A	40	GLN	-	expression tag	UNP Q04609
A	41	GLY	-	expression tag	UNP Q04609
A	42	ARG	-	expression tag	UNP Q04609
A	43	SER	-	expression tag	UNP Q04609
A	424	ALA	GLU	engineered mutation	UNP Q04609

- Molecule 2 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
2	B	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 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.



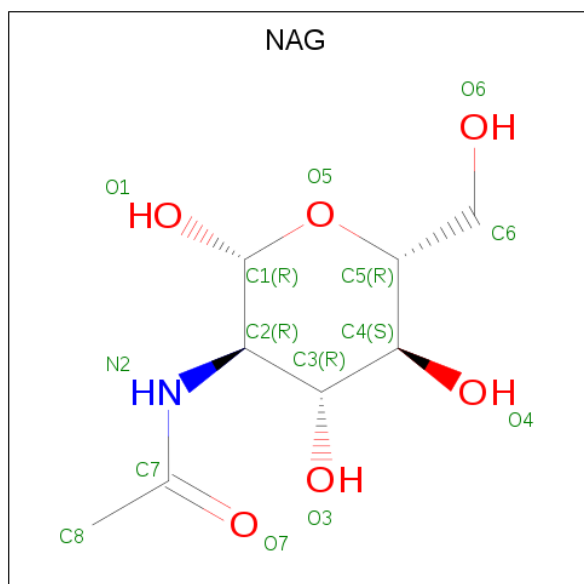
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 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
4	E	4	Total	C	N	O	0	0	0
			50	28	2	20			

- 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		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
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		

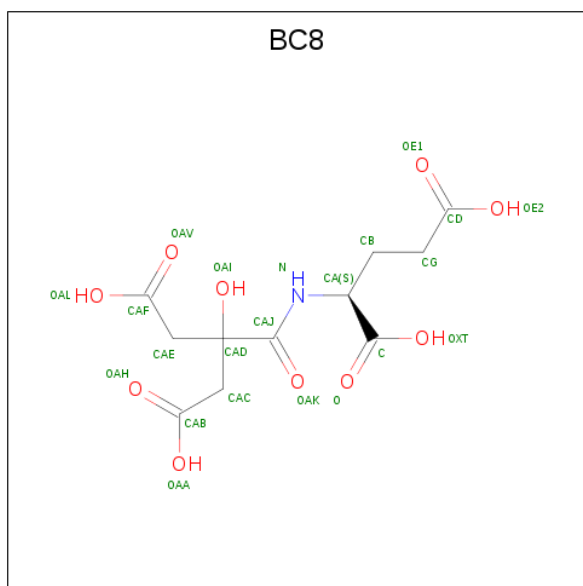
- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

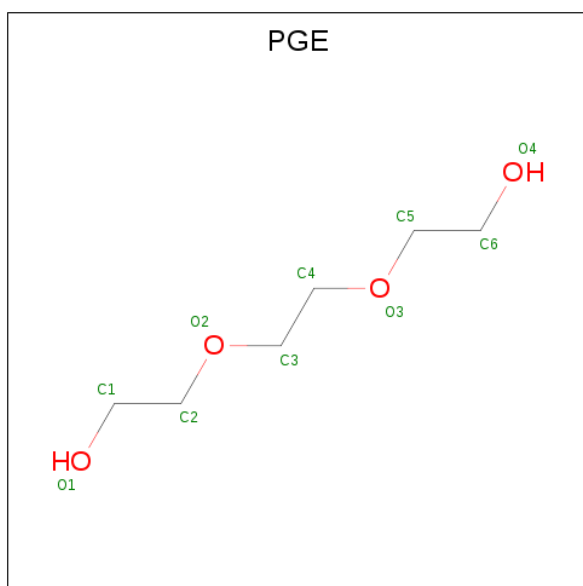
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Ca	0	0
			1	1		

- Molecule 9 is beta-citryl-L-glutamic acid (three-letter code: BC8) (formula: $C_{11}H_{15}NO_{10}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	1
			22	11	1	10		

- Molecule 10 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			10	6	4		

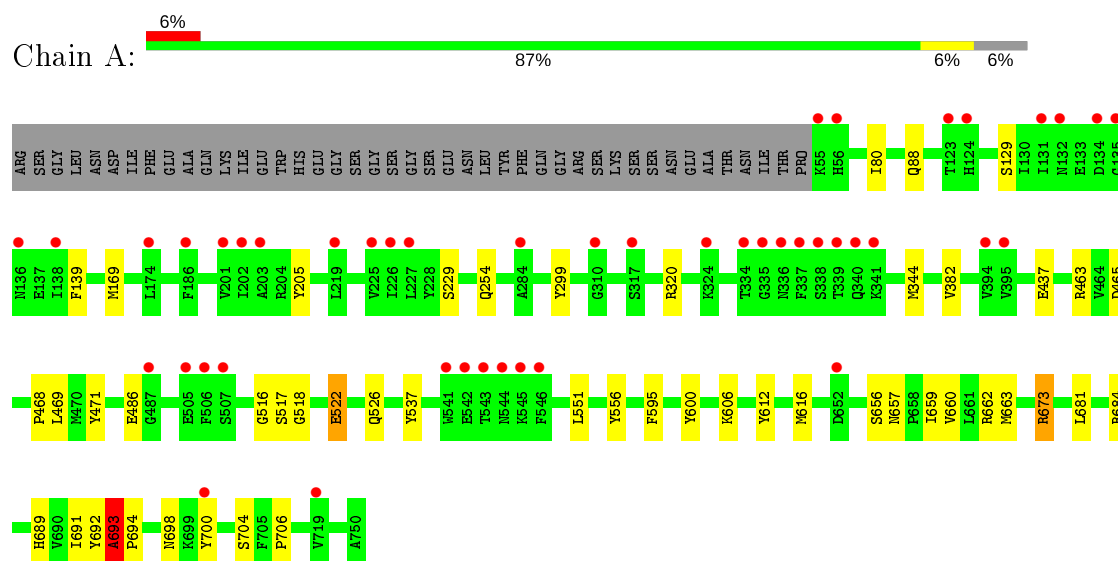
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	561	Total	O	0	32
			562	562		

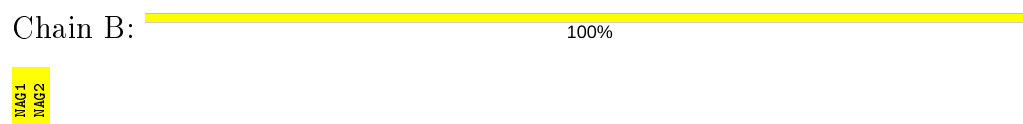
3 Residue-property plots [i](#)

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.

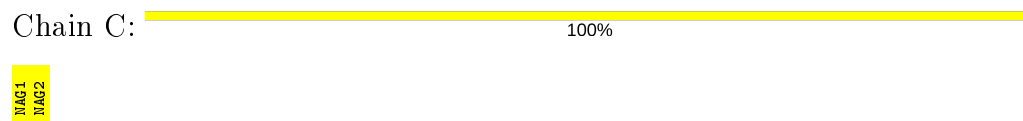
• Molecule 1: Glutamate carboxypeptidase 2



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



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



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





- Molecule 4: 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 E:

100%



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	100.90Å 130.92Å 159.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.85 29.40 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.0 (30.00-1.85) 99.1 (29.40-1.85)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.155 , 0.181 0.167 , 0.191	Depositor DCC
R_{free} test set	4444 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	30.1	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6402	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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, PGE, NAG, CL, CA, BMA, BC8, 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	0.77	4/5830 (0.1%)	0.86	10/7915 (0.1%)

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	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	522	GLU	CD-OE2	-6.01	1.19	1.25
1	A	437	GLU	CD-OE2	-5.94	1.19	1.25
1	A	656	SER	CA-C	5.40	1.67	1.52
1	A	486	GLU	CD-OE1	5.08	1.31	1.25

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	662	ARG	NE-CZ-NH2	14.83	127.72	120.30
1	A	662	ARG	NE-CZ-NH1	-14.06	113.27	120.30
1	A	673	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	A	463	ARG	NE-CZ-NH1	-6.82	116.89	120.30
1	A	465	ASP	CB-CG-OD1	5.97	123.67	118.30
1	A	693[A]	ALA	C-N-CD	5.62	140.21	128.40
1	A	693[B]	ALA	C-N-CD	5.62	140.21	128.40
1	A	463	ARG	NE-CZ-NH2	5.50	123.05	120.30
1	A	320	ARG	NE-CZ-NH1	5.22	122.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	662	ARG	CD-NE-CZ	5.12	130.77	123.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	693[A]	ALA	Mainchain

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	5617	0	5397	26	0
2	B	28	0	25	0	0
2	C	28	0	25	0	0
3	D	39	0	34	0	0
4	E	50	0	43	0	0
5	A	42	0	39	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	22	0	0	3	0
10	A	10	0	14	0	2
11	A	562	0	0	3	0
All	All	6402	0	5577	28	2

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 2.

All (28) 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:704[A]:SER:OG	11:A:901[A]:HOH:O	1.94	0.84
1:A:657:ASN:ND2	1:A:660:VAL:HG23	2.02	0.75
1:A:659:ILE:O	1:A:663[B]:MET:HG3	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517[A]:SER:OG	1:A:518:GLY:N	2.22	0.68
1:A:516:GLY:O	1:A:526[A]:GLN:NE2	2.32	0.63
1:A:657:ASN:HD22	1:A:660:VAL:HG23	1.65	0.61
1:A:684:ARG:NH2	1:A:694[B]:PRO:O	2.36	0.53
1:A:517[A]:SER:OG	1:A:522:GLU:OE2	2.20	0.53
1:A:612:TYR:CZ	1:A:616:MET:HG3	2.46	0.51
1:A:657:ASN:HD22	1:A:660:VAL:CG2	2.24	0.51
1:A:205:TYR:CE2	1:A:254:GLN:HB3	2.51	0.45
1:A:691:ILE:O	1:A:704[A]:SER:HA	2.17	0.45
1:A:689:HIS:HB3	1:A:692[A]:TYR:O	2.17	0.45
1:A:606:LYS:NZ	11:A:913:HOH:O	2.51	0.43
1:A:681:LEU:HD11	1:A:693[B]:ALA:HB3	1.99	0.42
1:A:698[A]:ASN:OD1	1:A:700[A]:TYR:HB2	2.18	0.42
9:A:819[A]:BC8:CAJ	11:A:902:HOH:O	2.67	0.42
1:A:518:GLY:O	9:A:819[A]:BC8:CAC	2.67	0.42
1:A:80:ILE:HD12	1:A:88:GLN:HG2	2.02	0.42
1:A:129:SER:HA	1:A:139:PHE:O	2.20	0.42
1:A:469:LEU:O	1:A:595:PHE:HA	2.20	0.42
1:A:693[A]:ALA:HB3	1:A:706:PRO:HG3	2.02	0.42
1:A:229:SER:O	1:A:299:TYR:HB3	2.21	0.41
1:A:551:LEU:HD22	1:A:556:TYR:HB2	2.02	0.41
1:A:468:PRO:HA	1:A:471:TYR:CE1	2.56	0.41
1:A:517[A]:SER:HB2	1:A:694[A]:PRO:HG3	2.03	0.41
9:A:819[A]:BC8:OAV	9:A:819[A]:BC8:CAB	2.69	0.41
1:A:169:MET:HA	1:A:344:MET:O	2.22	0.41

All (2) 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:820:PGE:O1	10:A:820:PGE:O1[2_555]	1.05	1.15
10:A:820:PGE:C1	10:A:820:PGE:O1[2_555]	2.08	0.12

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	717/739 (97%)	698 (97%)	18 (2%)	1 (0%)	51	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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	595/628 (95%)	592 (100%)	3 (0%)	88	86

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	537	TYR
1	A	600	TYR
1	A	673	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

11 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	0.48	0	17,19,21	1.18	1 (5%)
2	NAG	B	2	2	14,14,15	0.55	0	17,19,21	1.55	2 (11%)
2	NAG	C	1	1,2	14,14,15	0.62	0	17,19,21	1.25	3 (17%)
2	NAG	C	2	2	14,14,15	0.55	0	17,19,21	1.70	4 (23%)
3	NAG	D	1	1,3	14,14,15	0.99	1 (7%)	17,19,21	0.81	1 (5%)
3	NAG	D	2	3	14,14,15	0.56	0	17,19,21	1.00	0
3	BMA	D	3	3	11,11,12	0.87	0	15,15,17	2.36	4 (26%)
4	NAG	E	1	1,4	14,14,15	0.63	0	17,19,21	1.25	3 (17%)
4	NAG	E	2	4	14,14,15	0.69	0	17,19,21	1.70	5 (29%)
4	BMA	E	3	4	11,11,12	0.58	0	15,15,17	1.26	1 (6%)
4	MAN	E	4	4	11,11,12	0.65	0	15,15,17	1.44	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	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	1/6/23/26	0/1/1/1
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
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
4	NAG	E	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
4	MAN	E	4	4	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1	NAG	O5-C1	-2.53	1.39	1.43

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3	BMA	C1-O5-C5	6.06	120.41	112.19
2	C	2	NAG	C1-O5-C5	5.04	119.02	112.19
4	E	2	NAG	C1-O5-C5	4.16	117.83	112.19
4	E	4	MAN	O5-C5-C6	4.09	113.61	107.20
3	D	3	BMA	C1-C2-C3	4.08	114.67	109.67
3	D	3	BMA	C3-C4-C5	3.84	117.08	110.24
4	E	3	BMA	O3-C3-C2	-3.10	104.06	109.99
2	B	1	NAG	O5-C1-C2	-2.96	106.62	111.29
2	B	2	NAG	O5-C1-C2	-2.93	106.66	111.29
2	C	2	NAG	C4-C3-C2	-2.70	107.06	111.02
4	E	2	NAG	C2-N2-C7	-2.66	119.12	122.90
4	E	2	NAG	O3-C3-C2	-2.64	104.01	109.47
4	E	1	NAG	C6-C5-C4	-2.49	107.18	113.00
2	B	2	NAG	C2-N2-C7	2.34	126.23	122.90
2	C	1	NAG	O5-C1-C2	-2.32	107.62	111.29
4	E	2	NAG	O3-C3-C4	2.30	115.66	110.35
3	D	3	BMA	C2-C3-C4	2.26	114.80	110.89
4	E	1	NAG	O5-C1-C2	-2.23	107.76	111.29
4	E	1	NAG	C1-O5-C5	2.17	115.14	112.19
2	C	2	NAG	O4-C4-C5	2.14	114.60	109.30
3	D	1	NAG	C4-C3-C2	-2.10	107.94	111.02
4	E	2	NAG	C8-C7-N2	-2.09	112.55	116.10
2	C	1	NAG	C1-C2-N2	2.07	114.02	110.49
2	C	1	NAG	O3-C3-C2	-2.01	105.30	109.47
2	C	2	NAG	C6-C5-C4	-2.01	108.29	113.00

There are no chirality outliers.

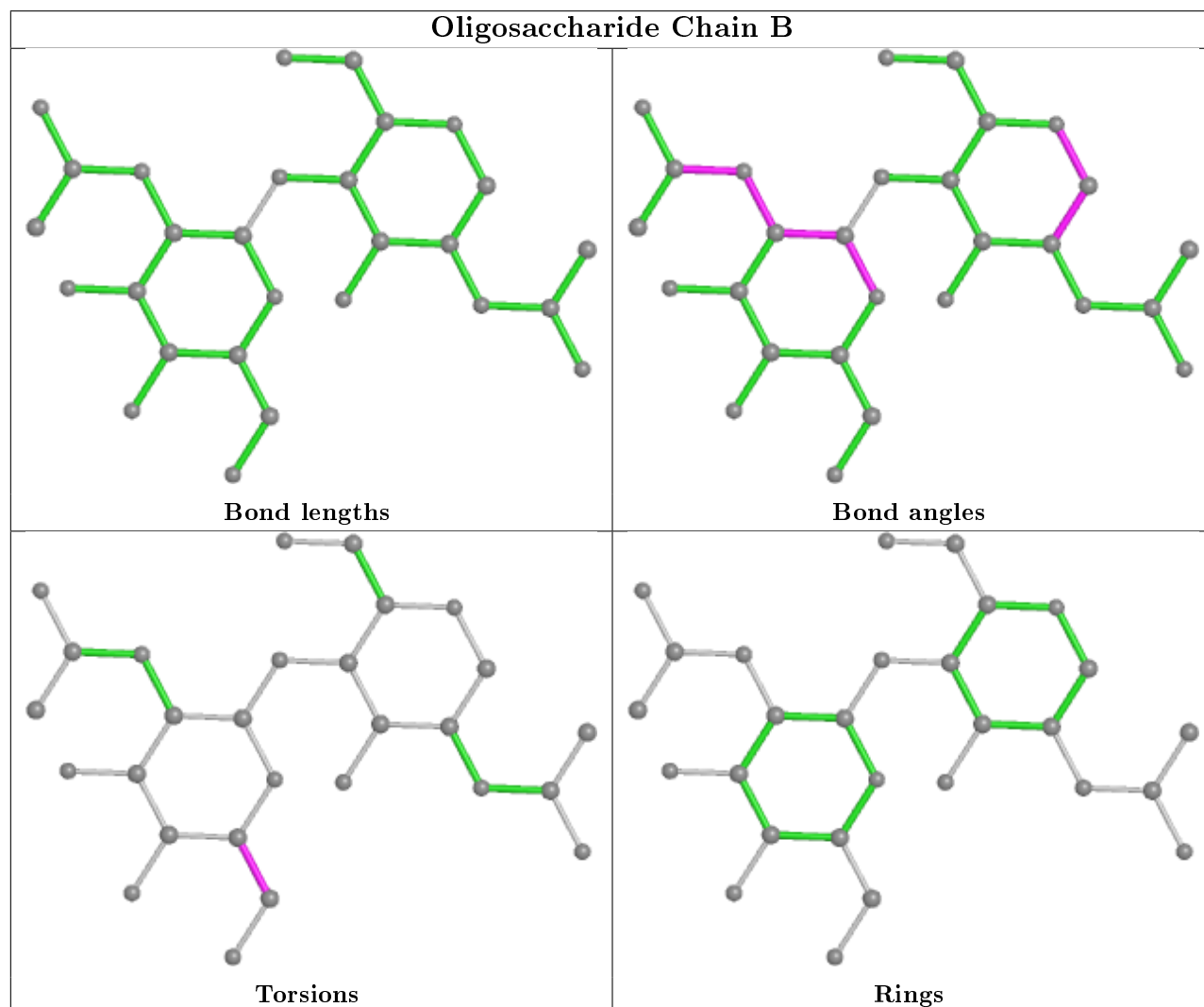
All (4) torsion outliers are listed below:

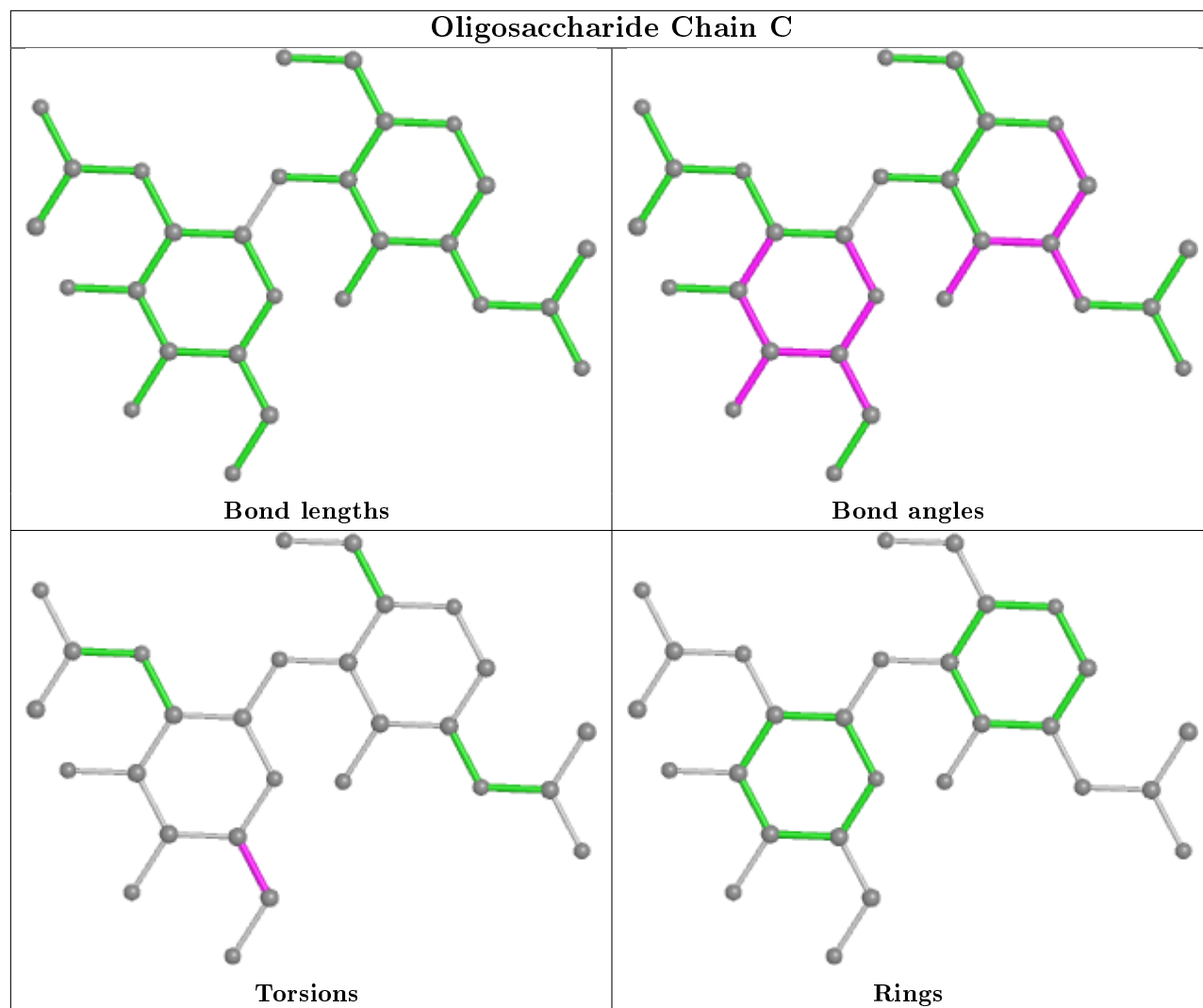
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6

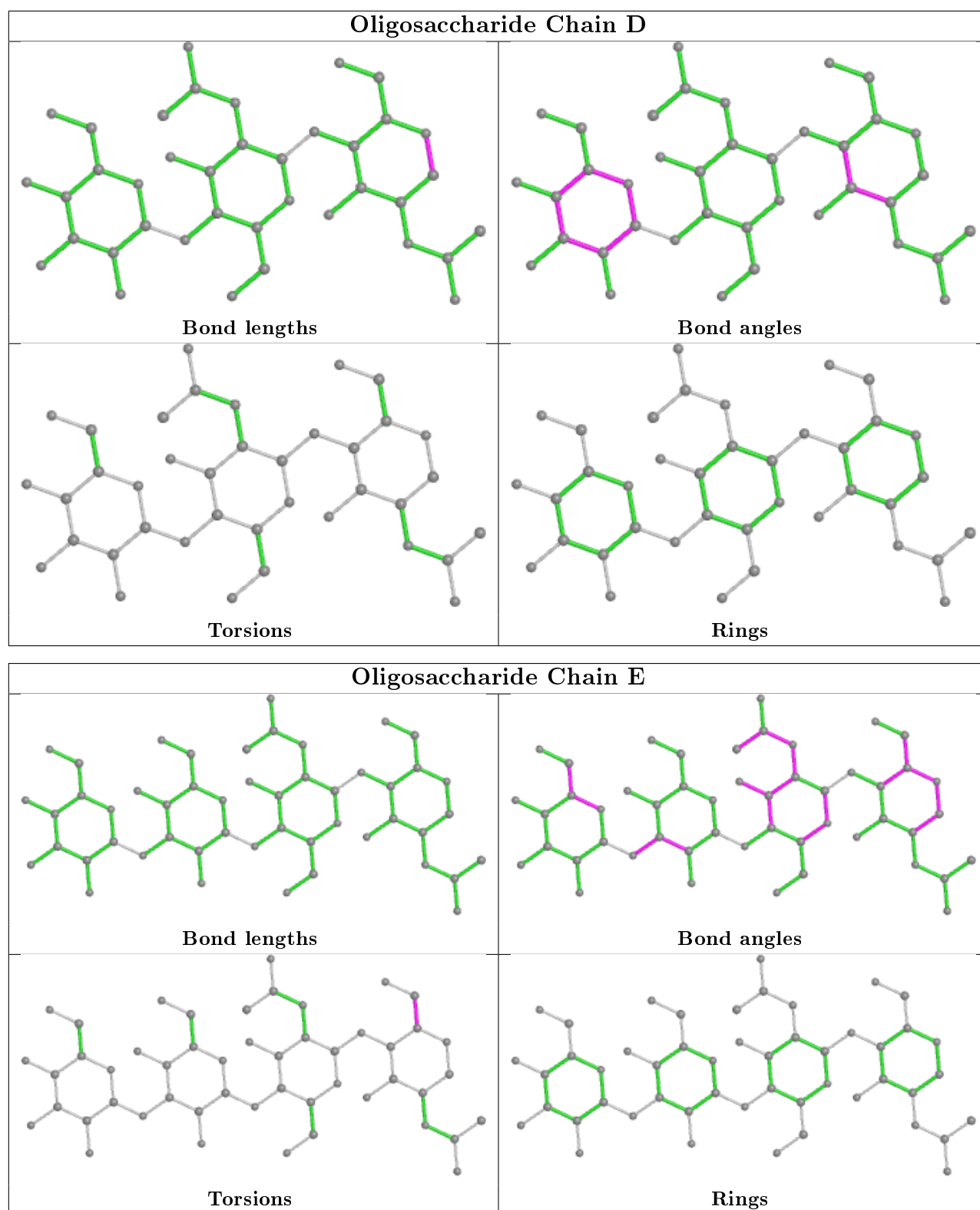
There are no ring outliers.

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 oligosaccharide.







5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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$
10	PGE	A	820	-	9,9,9	0.68	0	8,8,8	0.60	0
5	NAG	A	803	1	14,14,15	0.80	1 (7%)	17,19,21	1.81	3 (17%)
9	BC8	A	819[A]	6	6,21,21	1.00	0	15,29,29	2.52	6 (40%)
5	NAG	A	807	1	14,14,15	1.18	1 (7%)	17,19,21	2.09	3 (17%)
5	NAG	A	806	1	14,14,15	0.61	0	17,19,21	2.17	1 (5%)

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
10	PGE	A	820	-	-	3/7/7/7	-
5	NAG	A	803	1	-	0/6/23/26	0/1/1/1
9	BC8	A	819[A]	6	-	6/19/29/29	-
5	NAG	A	807	1	-	2/6/23/26	0/1/1/1
5	NAG	A	806	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	807	NAG	O5-C1	-3.25	1.38	1.43
5	A	803	NAG	O5-C5	2.11	1.47	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	806	NAG	C1-O5-C5	8.34	123.49	112.19
5	A	807	NAG	C1-O5-C5	6.38	120.83	112.19
9	A	819[A]	BC8	CAD-CAE-CAF	5.91	124.45	114.98
5	A	803	NAG	C1-O5-C5	4.90	118.83	112.19
9	A	819[A]	BC8	CAE-CAD-CAJ	-4.65	100.18	109.94
9	A	819[A]	BC8	CAC-CAD-CAJ	3.32	116.91	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	807	NAG	C3-C4-C5	3.31	116.14	110.24
9	A	819[A]	BC8	CB-CA-N	3.11	114.72	110.19
5	A	807	NAG	O5-C5-C4	3.03	118.21	110.83
5	A	803	NAG	O5-C1-C2	-2.68	107.05	111.29
5	A	803	NAG	O5-C5-C6	2.47	111.08	107.20
9	A	819[A]	BC8	CAD-CAJ-N	2.39	120.03	116.77
9	A	819[A]	BC8	OAI-CAD-CAE	2.38	114.93	109.41

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	819[A]	BC8	CAC-CAD-CAJ-OAK
9	A	819[A]	BC8	CAC-CAD-CAJ-N
9	A	819[A]	BC8	OAI-CAD-CAJ-OAK
9	A	819[A]	BC8	OAI-CAD-CAJ-N
10	A	820	PGE	C1-C2-O2-C3
5	A	806	NAG	C4-C5-C6-O6
5	A	807	NAG	O5-C5-C6-O6
5	A	806	NAG	O5-C5-C6-O6
9	A	819[A]	BC8	CB-CA-N-CAJ
5	A	807	NAG	C4-C5-C6-O6
10	A	820	PGE	C3-C4-O3-C5
10	A	820	PGE	O2-C3-C4-O3
9	A	819[A]	BC8	CAB-CAC-CAD-CAE

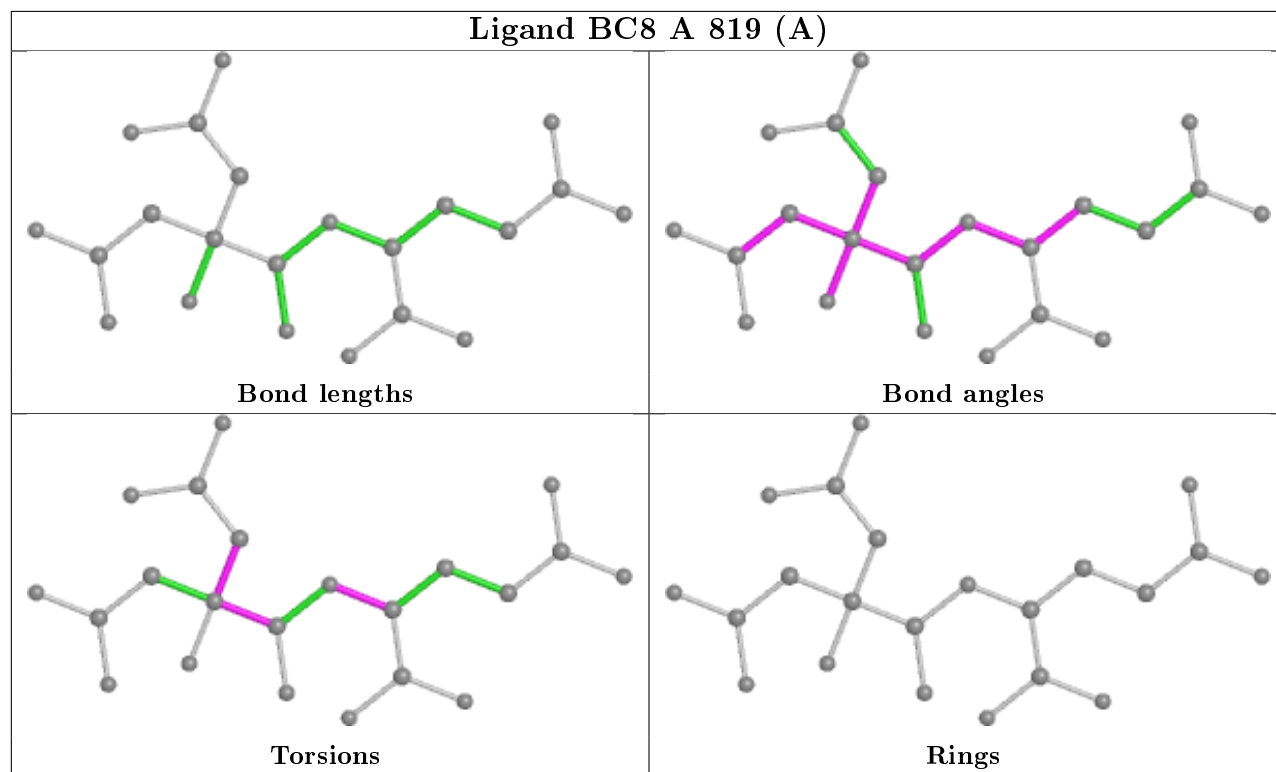
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	820	PGE	0	2
9	A	819[A]	BC8	3	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 ⓘ

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	696/739 (94%)	0.12	46 (6%) 18 17	20, 36, 81, 110	3 (0%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	334	THR	5.6
1	A	335	GLY	5.5
1	A	541	TRP	5.5
1	A	135	GLY	5.2
1	A	337	PHE	5.1
1	A	546	PHE	5.1
1	A	202	ILE	4.6
1	A	700[A]	TYR	4.4
1	A	219	LEU	4.3
1	A	543	THR	4.3
1	A	138	ILE	4.2
1	A	544	ASN	4.1
1	A	136	ASN	3.8
1	A	226	ILE	3.8
1	A	336	ASN	3.6
1	A	227	LEU	3.4
1	A	719	VAL	3.3
1	A	201	VAL	3.3
1	A	338	SER	3.3
1	A	506	PHE	3.3
1	A	55	LYS	3.2
1	A	134	ASP	3.2
1	A	225	VAL	3.0
1	A	340	GLN	3.0
1	A	339	THR	2.9
1	A	132	ASN	2.9
1	A	310	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	545	LYS	2.8
1	A	341	LYS	2.8
1	A	124	HIS	2.7
1	A	317	SER	2.7
1	A	131	ILE	2.6
1	A	652	ASP	2.6
1	A	394	VAL	2.6
1	A	186	PHE	2.5
1	A	324	LYS	2.5
1	A	56	HIS	2.4
1	A	487	GLY	2.4
1	A	174	LEU	2.3
1	A	505	GLU	2.3
1	A	507	SER	2.3
1	A	123	THR	2.3
1	A	395	VAL	2.1
1	A	542	GLU	2.1
1	A	284	ALA	2.1
1	A	203	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

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

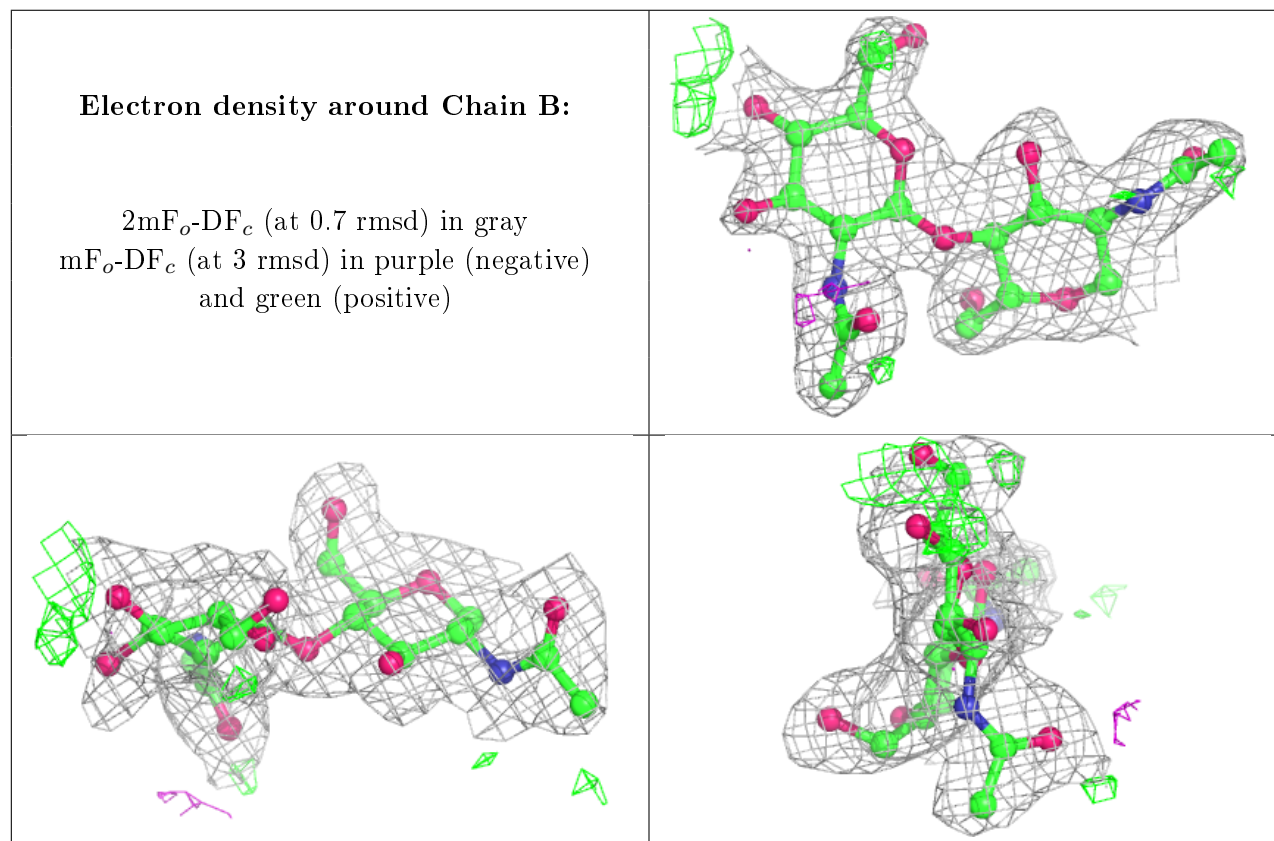
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	B	2	14/15	0.75	0.26	53,62,69,71	0
3	BMA	D	3	11/12	0.77	0.31	77,82,87,88	0
2	NAG	C	2	14/15	0.79	0.41	84,90,98,103	0
4	BMA	E	3	11/12	0.82	0.18	58,66,69,72	0
2	NAG	C	1	14/15	0.83	0.23	67,72,78,82	0
4	NAG	E	2	14/15	0.85	0.20	48,56,61,62	0
3	NAG	D	1	14/15	0.92	0.10	41,43,48,49	0
4	NAG	E	1	14/15	0.93	0.09	28,35,45,48	0
4	MAN	E	4	11/12	0.93	0.16	72,74,75,79	0

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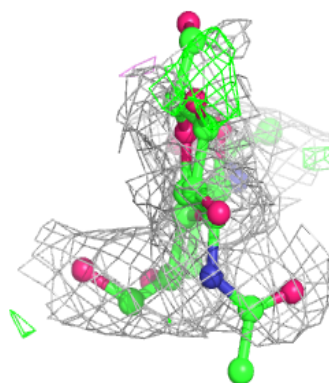
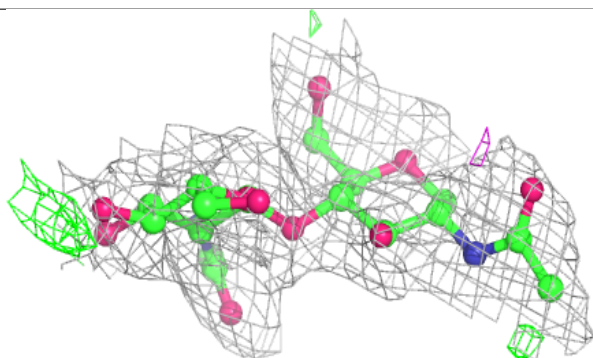
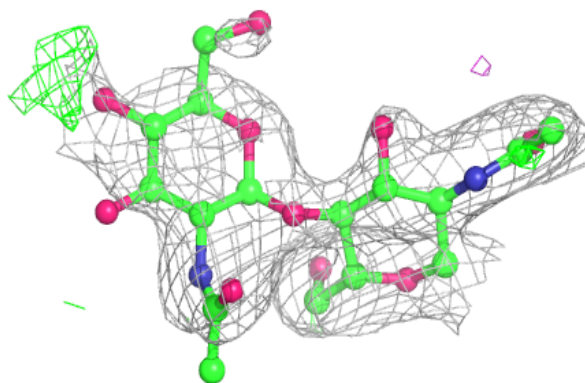
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	D	2	14/15	0.94	0.21	53,59,62,70	0
2	NAG	B	1	14/15	0.96	0.11	45,51,55,56	0

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

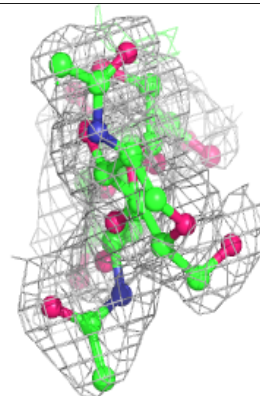
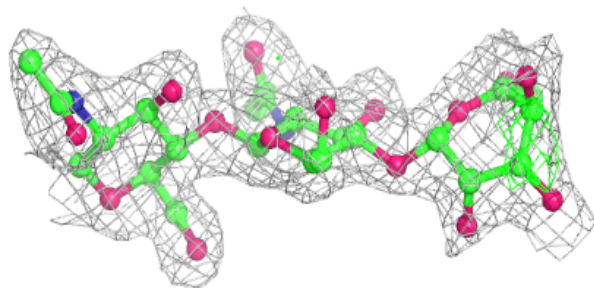
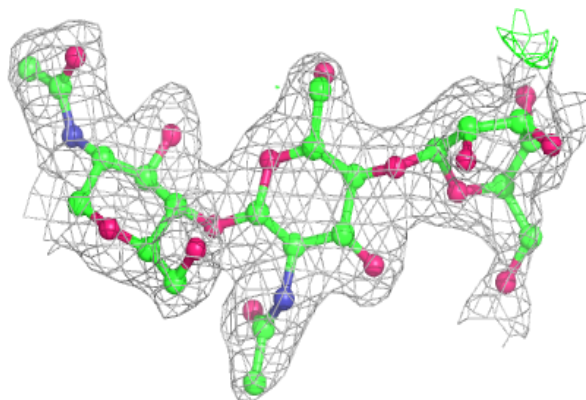


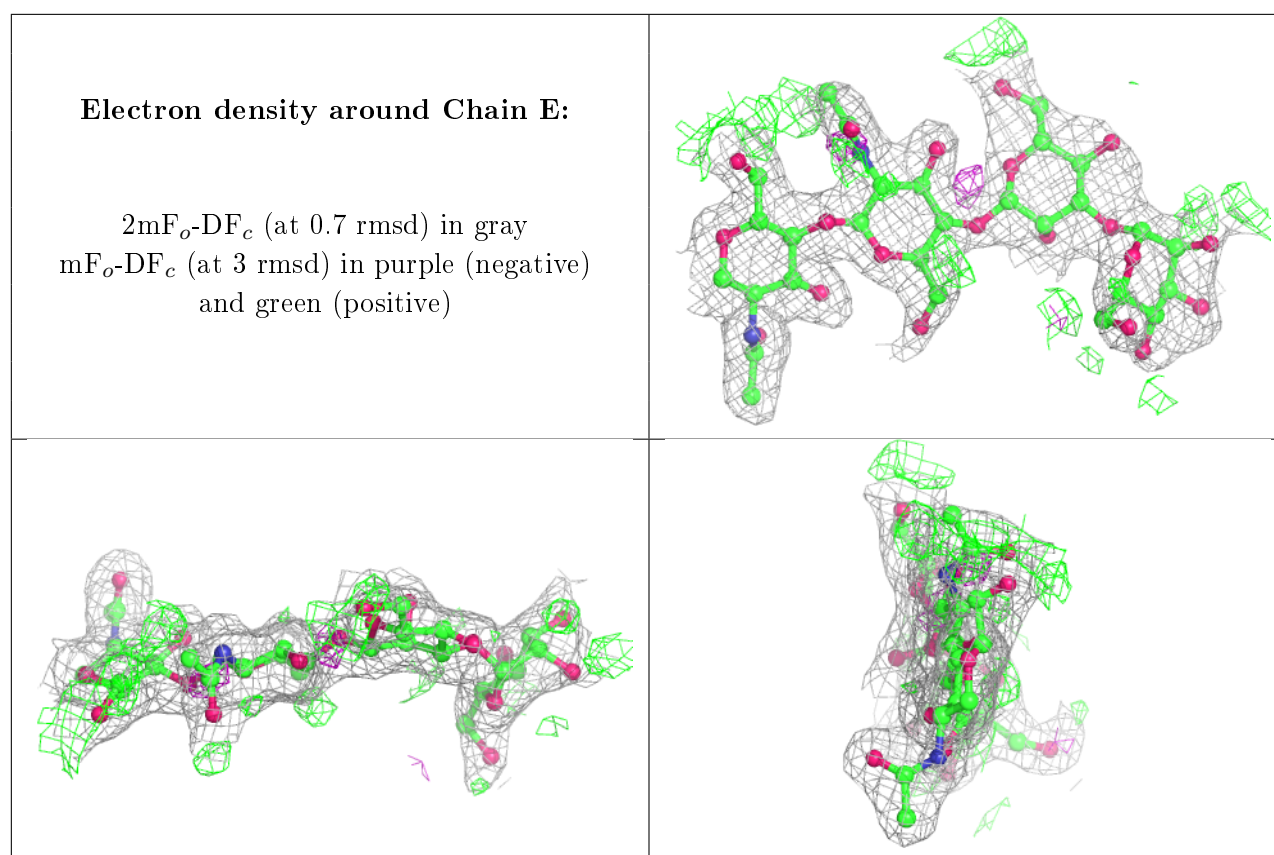
Electron density around Chain C:

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

**Electron density around Chain D:**

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





6.4 Ligands ⓘ

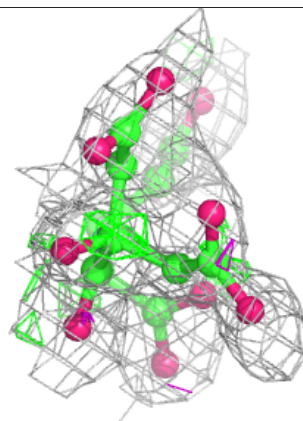
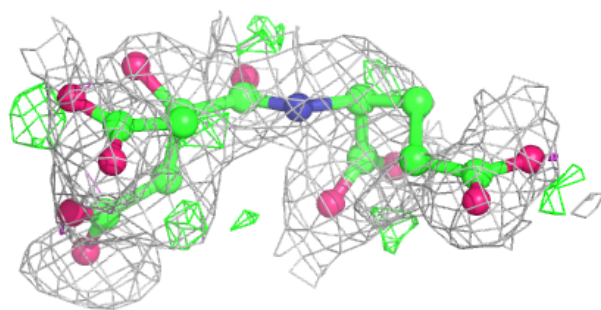
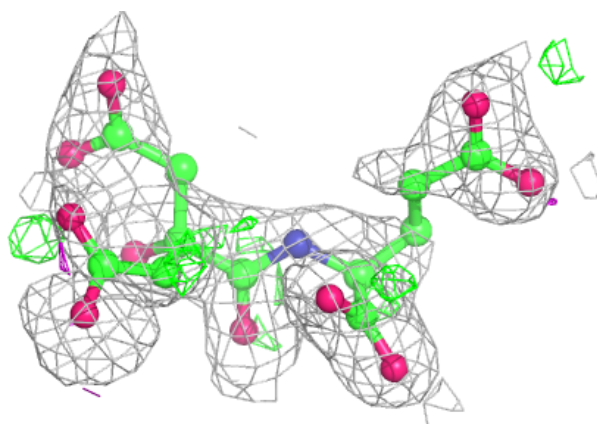
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	PGE	A	820	10/10	0.73	0.29	41,44,51,70	0
5	NAG	A	803	14/15	0.74	0.32	66,72,80,82	0
5	NAG	A	806	14/15	0.83	0.23	104,109,111,112	0
9	BC8	A	819[A]	22/22	0.88	0.19	25,37,48,50	22
5	NAG	A	807	14/15	0.91	0.21	43,54,63,64	0
6	ZN	A	815	1/1	1.00	0.08	27,27,27,27	0
8	CA	A	818	1/1	1.00	0.08	22,22,22,22	0
6	ZN	A	816	1/1	1.00	0.09	26,26,26,26	0
7	CL	A	817	1/1	1.00	0.08	29,29,29,29	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 BC8 A 819 (A):

$2mF_o - DF_c$ (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.