



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 04:50 AM EDT

PDB ID : 3BXM
Title : Structure of an inactive mutant of human glutamate carboxypeptidase II [GCPII(E424A)] in complex with N-acetyl-Asp-Glu (NAAG)
Authors : Lubkowski, J.; Barinka, C.
Deposited on : 2008-01-14
Resolution : 1.71 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 : 2.23.2
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) : 2.23.2

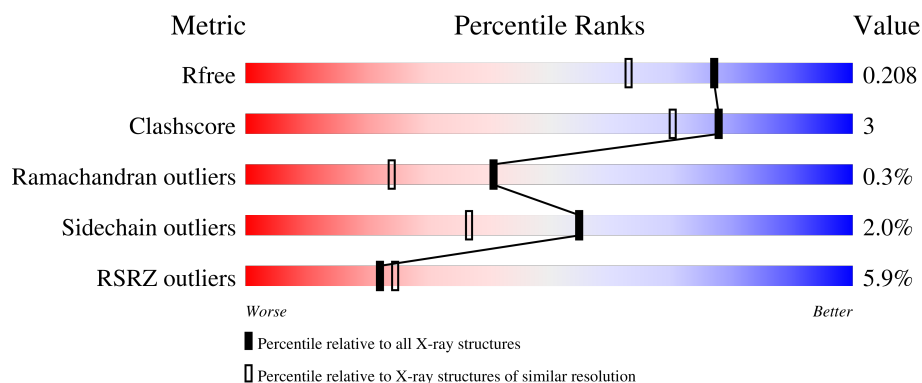
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.71 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.



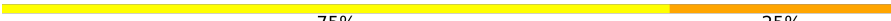
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5722 (1.74-1.70)
Clashscore	141614	6152 (1.74-1.70)
Ramachandran outliers	138981	6051 (1.74-1.70)
Sidechain outliers	138945	6051 (1.74-1.70)
RSRZ outliers	127900	5629 (1.74-1.70)

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

Mol	Chain	Length	Quality of chain
1	A	709	<div> <div>6%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div>..</div> </div> </div>
2	I	3	<div> <div>100%</div> </div>
3	B	2	<div> <div>50%</div> <div>50%</div> </div>
3	C	2	<div> <div>50%</div> <div>50%</div> </div>
3	D	2	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
4	E	4	 75% 25%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 6350 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	694	Total	C	N	O	S	0	25	0
			5653	3639	946	1046	22			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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 a protein called N-Acetyl-Aspartyl-Glutamate (NAAG).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	3	Total	C	N	O	0	0	0
			21	11	2	8			

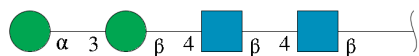
- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

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

e-(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 CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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

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

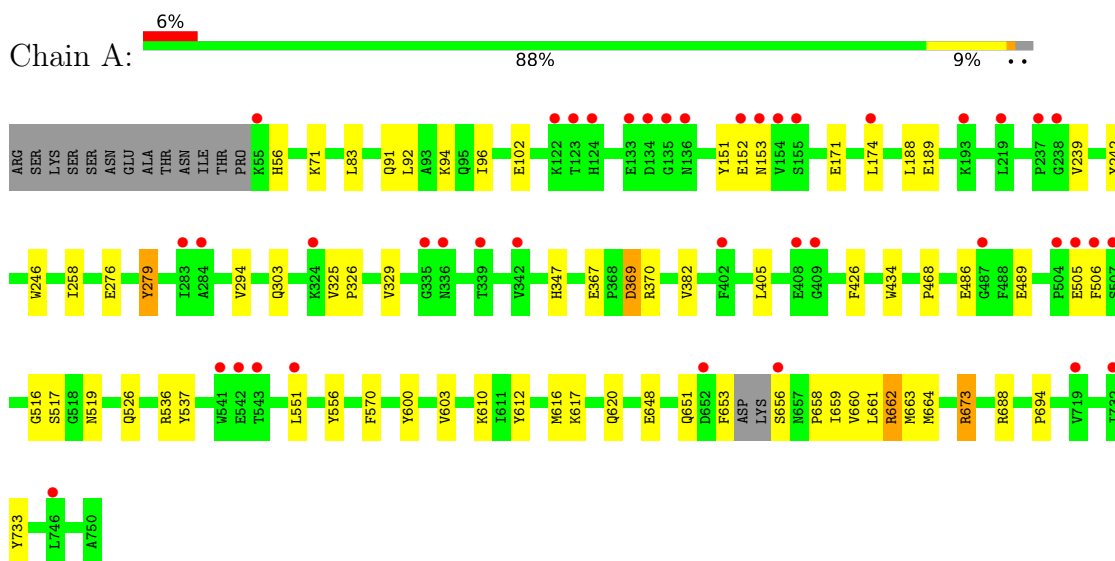
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	492	Total	O	0	0
			492	492		
9	I	4	Total	O	0	0
			4	4		

3 Residue-property plots

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: N-Acetyl-Aspartyl-Glutamate (NAAG)



There are no outlier residues recorded for this chain.

- Molecule 3: 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

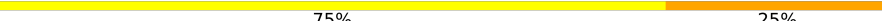


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  100%

MAG1
MAG2

- 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:  75% 25%

MAG1
MAG2
BMA3
MAN4

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	102.06Å 129.80Å 159.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 1.71 19.98 – 1.71	Depositor EDS
% Data completeness (in resolution range)	98.6 (15.00-1.71) 98.5 (19.98-1.71)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.184 , 0.213 0.184 , 0.208	Depositor DCC
R_{free} test set	1376 reflections (1.21%)	wwPDB-VP
Wilson B-factor (Å ²)	25.0	Xtriage
Anisotropy	0.509	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 58.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6350	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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: CL, ZN, NAG, CA, BMA, MAN, ACE

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	1.05	5/5883 (0.1%)	0.93	6/7971 (0.1%)
2	I	1.54	0/18	0.87	0/22
All	All	1.05	5/5901 (0.1%)	0.93	6/7993 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	733	TYR	CD1-CE1	6.55	1.49	1.39
1	A	434	TRP	CE3-CZ3	6.49	1.49	1.38
1	A	426	PHE	CE2-CZ	5.76	1.48	1.37
1	A	102	GLU	CG-CD	5.64	1.60	1.51
1	A	83	LEU	CG-CD2	5.12	1.70	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	536	ARG	NE-CZ-NH1	-7.18	116.71	120.30
1	A	369	ASP	CB-CG-OD1	6.59	124.23	118.30
1	A	370	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	A	370	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	A	536	ARG	NE-CZ-NH2	5.94	123.27	120.30
1	A	673	ARG	NE-CZ-NH1	5.56	123.08	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	5653	0	5507	32	1
2	I	21	0	13	0	0
3	B	28	0	25	1	0
3	C	28	0	25	1	0
3	D	28	0	25	0	0
4	E	50	0	43	0	1
5	A	42	0	39	1	0
6	A	2	0	0	0	0
7	A	1	0	0	0	0
8	A	1	0	0	0	0
9	A	492	0	0	10	0
9	I	4	0	0	0	0
All	All	6350	0	5677	34	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 (34) 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:660[A]:VAL:O	1:A:664[A]:MET:HG2	1.30	1.28
1:A:151:TYR:O	1:A:153:ASN:N	1.96	0.96
9:A:2014:HOH:O	3:B:2:NAG:H81	1.89	0.73
1:A:620:GLN:NE2	9:A:2200:HOH:O	2.02	0.72
1:A:610:LYS:HE2	9:A:1948:HOH:O	1.91	0.70
1:A:610:LYS:CE	9:A:1948:HOH:O	2.46	0.62
1:A:617:LYS:NZ	9:A:2132:HOH:O	2.38	0.55
1:A:325:VAL:HB	1:A:326:PRO:HD2	1.89	0.54
1:A:347:HIS:HE1	9:A:2078:HOH:O	1.90	0.53
1:A:653:PHE:HZ	1:A:661[A]:LEU:HD13	1.74	0.52
1:A:92:LEU:O	1:A:96[B]:ILE:HG12	2.10	0.51
1:A:246:TRP:CD1	5:A:1760:NAG:H83	2.45	0.51
1:A:688[B]:ARG:NH2	9:A:1836:HOH:O	2.26	0.51
1:A:367:GLU:OE1	1:A:662[A]:ARG:NH1	2.43	0.50
1:A:517:SER:HB2	1:A:694:PRO:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:656[B]:SER:O	1:A:658[B]:PRO:HD3	2.12	0.49
1:A:188:LEU:CD2	1:A:329:VAL:HG11	2.43	0.49
1:A:612:TYR:CZ	1:A:616:MET:HG3	2.48	0.49
1:A:369:ASP:OD2	1:A:662[B]:ARG:NH2	2.35	0.48
1:A:258:ILE:HD13	1:A:294:VAL:HB	1.94	0.48
1:A:648:GLU:O	1:A:651[B]:GLN:HG2	2.13	0.47
1:A:551:LEU:HD22	1:A:556:TYR:HB2	1.95	0.47
9:A:2098:HOH:O	3:C:2:NAG:H83	2.15	0.46
1:A:91:GLN:HE22	1:A:94:LYS:NZ	2.14	0.44
1:A:242:TYR:OH	9:A:2159:HOH:O	1.95	0.44
1:A:347:HIS:CE1	9:A:2078:HOH:O	2.69	0.44
1:A:489:GLU:H	1:A:489:GLU:CD	2.21	0.44
1:A:56:HIS:CD2	1:A:405[A]:LEU:HD22	2.54	0.43
1:A:71:LYS:HG3	1:A:570:PHE:CE2	2.55	0.42
1:A:505:GLU:HB2	1:A:506:PHE:CE1	2.55	0.41
1:A:516:GLY:O	1:A:526[B]:GLN:NE2	2.53	0.41
1:A:468:PRO:CG	1:A:603:VAL:HG21	2.51	0.40
1:A:659[B]:ILE:O	1:A:663[B]:MET:HG3	2.21	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)
1:A:276:GLU:OE1	4:E:3:BMA:O2[2_565]	2.10	0.10

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	714/709 (101%)	691 (97%)	21 (3%)	2 (0%)	41	24
2	I	1/3 (33%)	1 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	715/712 (100%)	692 (97%)	21 (3%)	2 (0%)	41 24

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	152	GLU
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	615/604 (102%)	601 (98%)	14 (2%)	50 31
2	I	2/2 (100%)	2 (100%)	0	100 100
All	All	617/606 (102%)	603 (98%)	14 (2%)	55 31

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	171	GLU
1	A	174	LEU
1	A	189	GLU
1	A	239	VAL
1	A	279[A]	TYR
1	A	279[B]	TYR
1	A	303	GLN
1	A	486	GLU
1	A	519	ASN
1	A	537	TYR
1	A	600	TYR
1	A	662[A]	ARG
1	A	662[B]	ARG
1	A	673	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	136	ASN
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 ⓘ

10 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	$\# Z > 2$
3	NAG	B	1	3,1	14,14,15	0.60	0	17,19,21	1.62	5 (29%)
3	NAG	B	2	3	14,14,15	0.64	0	17,19,21	1.53	2 (11%)
3	NAG	C	1	3,1	14,14,15	0.78	0	17,19,21	0.86	1 (5%)
3	NAG	C	2	3	14,14,15	0.36	0	17,19,21	1.78	6 (35%)
3	NAG	D	1	3,1	14,14,15	0.97	1 (7%)	17,19,21	1.53	2 (11%)
3	NAG	D	2	3	14,14,15	0.40	0	17,19,21	1.45	3 (17%)
4	NAG	E	1	4,1	14,14,15	1.07	1 (7%)	17,19,21	1.93	4 (23%)
4	NAG	E	2	4	14,14,15	0.61	0	17,19,21	1.40	2 (11%)
4	BMA	E	3	4	11,11,12	1.02	1 (9%)	15,15,17	1.23	2 (13%)
4	MAN	E	4	4	11,11,12	0.58	0	15,15,17	1.11	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
3	NAG	B	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	B	2	3	-	2/6/23/26	0/1/1/1
3	NAG	C	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	NAG	D	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
4	NAG	E	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	4/6/23/26	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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1	NAG	C1-C2	3.09	1.56	1.52
3	D	1	NAG	O7-C7	2.47	1.28	1.23
4	E	3	BMA	O5-C1	-2.41	1.39	1.43

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1	NAG	O5-C1-C2	-4.74	103.80	111.29
3	D	1	NAG	O5-C1-C2	-4.52	104.15	111.29
3	B	2	NAG	C1-O5-C5	4.41	118.16	112.19
3	C	2	NAG	C8-C7-N2	3.62	122.23	116.10
3	B	2	NAG	C2-N2-C7	3.58	128.00	122.90
3	D	1	NAG	O5-C5-C4	-3.10	103.29	110.83
3	D	2	NAG	C8-C7-N2	3.04	121.25	116.10
4	E	2	NAG	C3-C4-C5	-2.94	104.99	110.24
3	D	2	NAG	C1-O5-C5	2.94	116.17	112.19
4	E	1	NAG	O4-C4-C5	-2.89	102.12	109.30
3	B	1	NAG	C2-N2-C7	-2.80	118.92	122.90
4	E	1	NAG	C6-C5-C4	-2.77	106.52	113.00
3	C	2	NAG	O7-C7-C8	-2.77	116.92	122.06
3	B	1	NAG	C4-C3-C2	2.64	114.89	111.02
3	B	1	NAG	O5-C1-C2	-2.63	107.14	111.29
4	E	1	NAG	C1-O5-C5	2.62	115.74	112.19
4	E	3	BMA	O3-C3-C2	-2.57	105.07	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	4	MAN	O5-C5-C6	2.57	111.23	107.20
3	B	1	NAG	O3-C3-C4	-2.48	104.63	110.35
4	E	3	BMA	O5-C1-C2	-2.47	106.97	110.77
3	C	2	NAG	O5-C5-C6	2.29	110.80	107.20
3	C	2	NAG	C2-N2-C7	2.28	126.15	122.90
3	C	2	NAG	C4-C3-C2	-2.26	107.70	111.02
4	E	2	NAG	O4-C4-C5	-2.19	103.85	109.30
3	C	2	NAG	O4-C4-C5	2.08	114.47	109.30
3	D	2	NAG	O5-C1-C2	-2.04	108.06	111.29
3	B	1	NAG	O5-C5-C6	2.02	110.37	107.20
3	C	1	NAG	O5-C1-C2	-2.00	108.13	111.29

There are no chirality outliers.

All (12) torsion outliers are listed below:

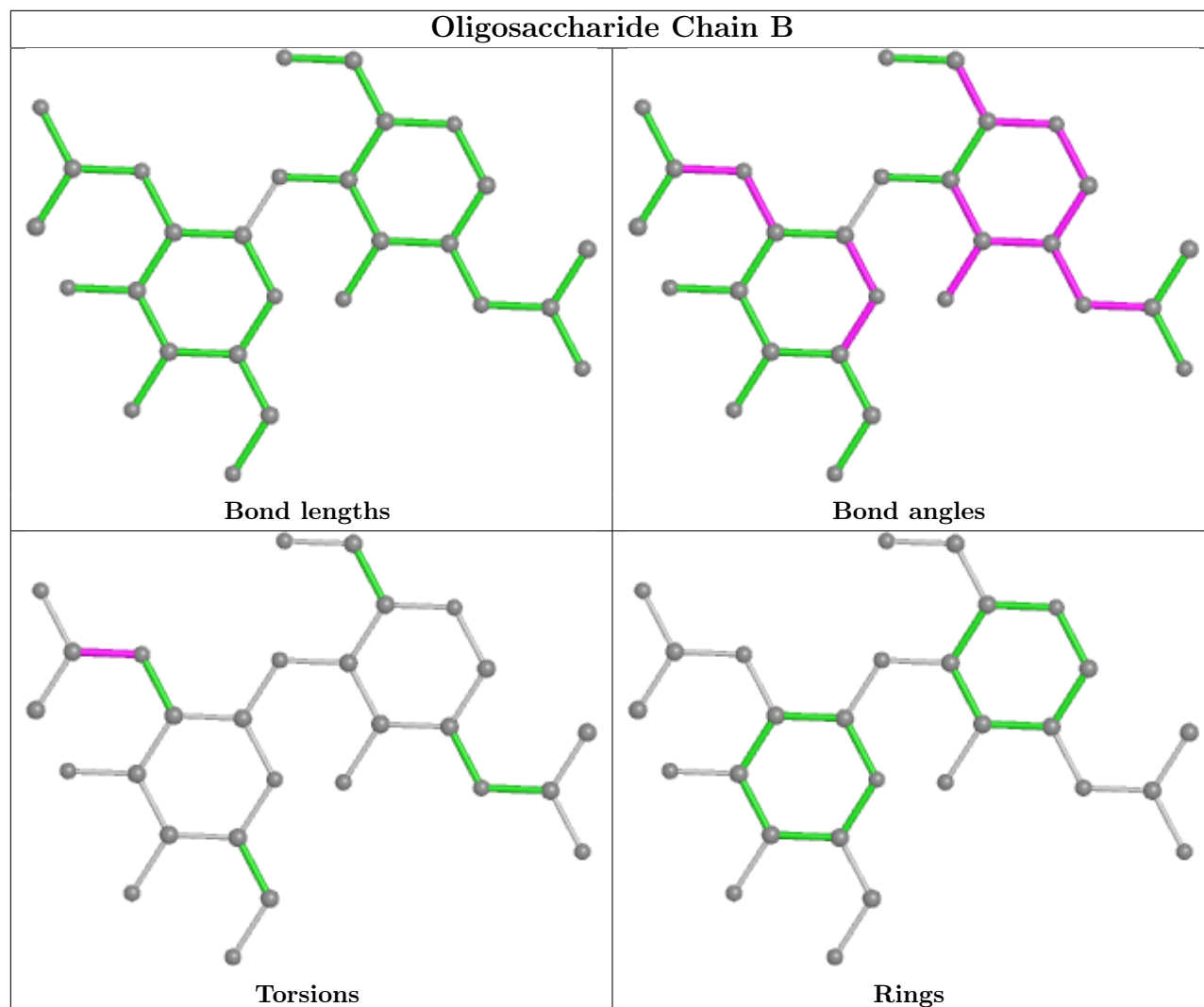
Mol	Chain	Res	Type	Atoms
3	B	2	NAG	C8-C7-N2-C2
3	B	2	NAG	O7-C7-N2-C2
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
3	D	2	NAG	C8-C7-N2-C2
3	D	2	NAG	O7-C7-N2-C2
4	E	2	NAG	C8-C7-N2-C2
4	E	2	NAG	O7-C7-N2-C2
4	E	2	NAG	O5-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6

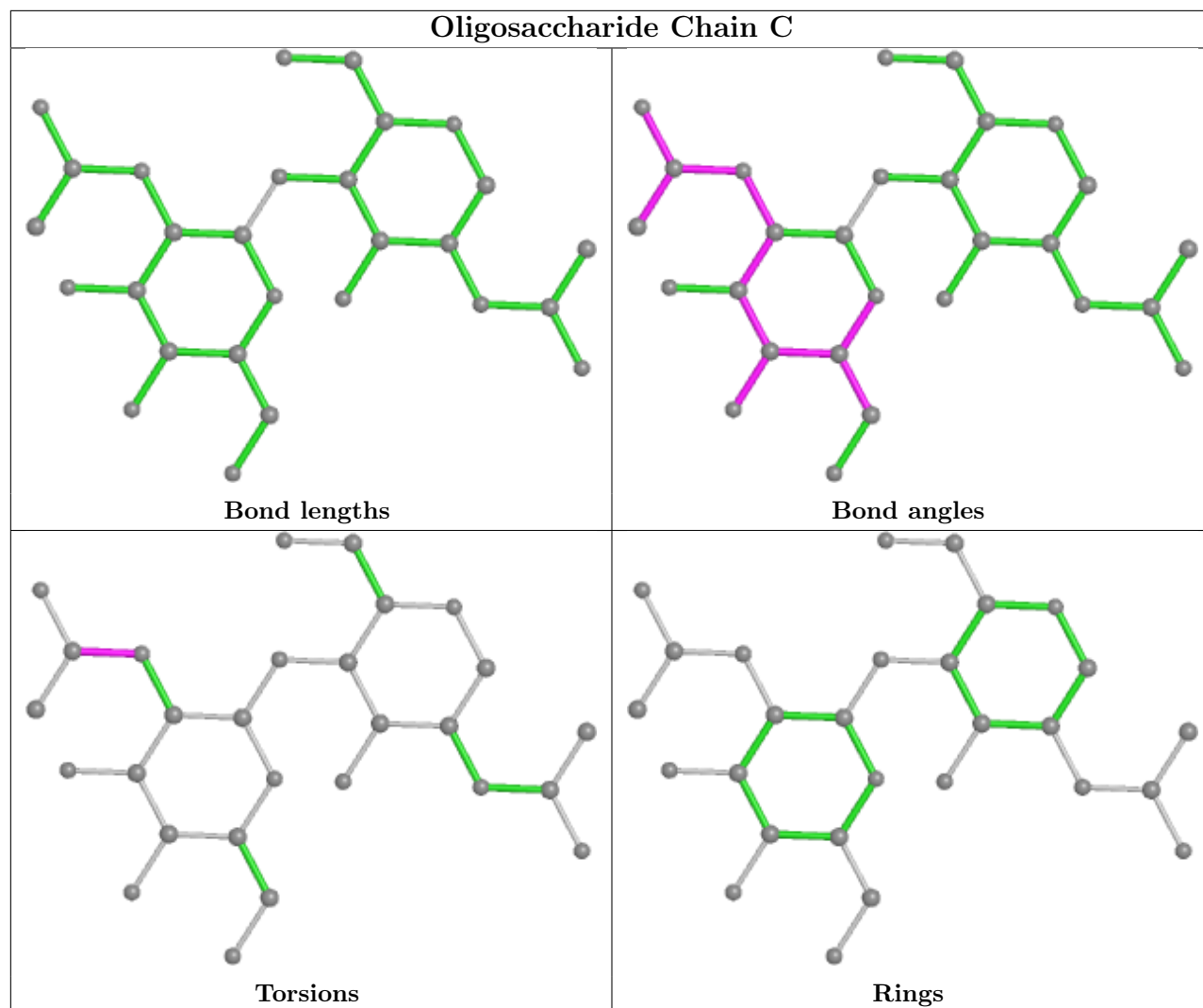
There are no ring outliers.

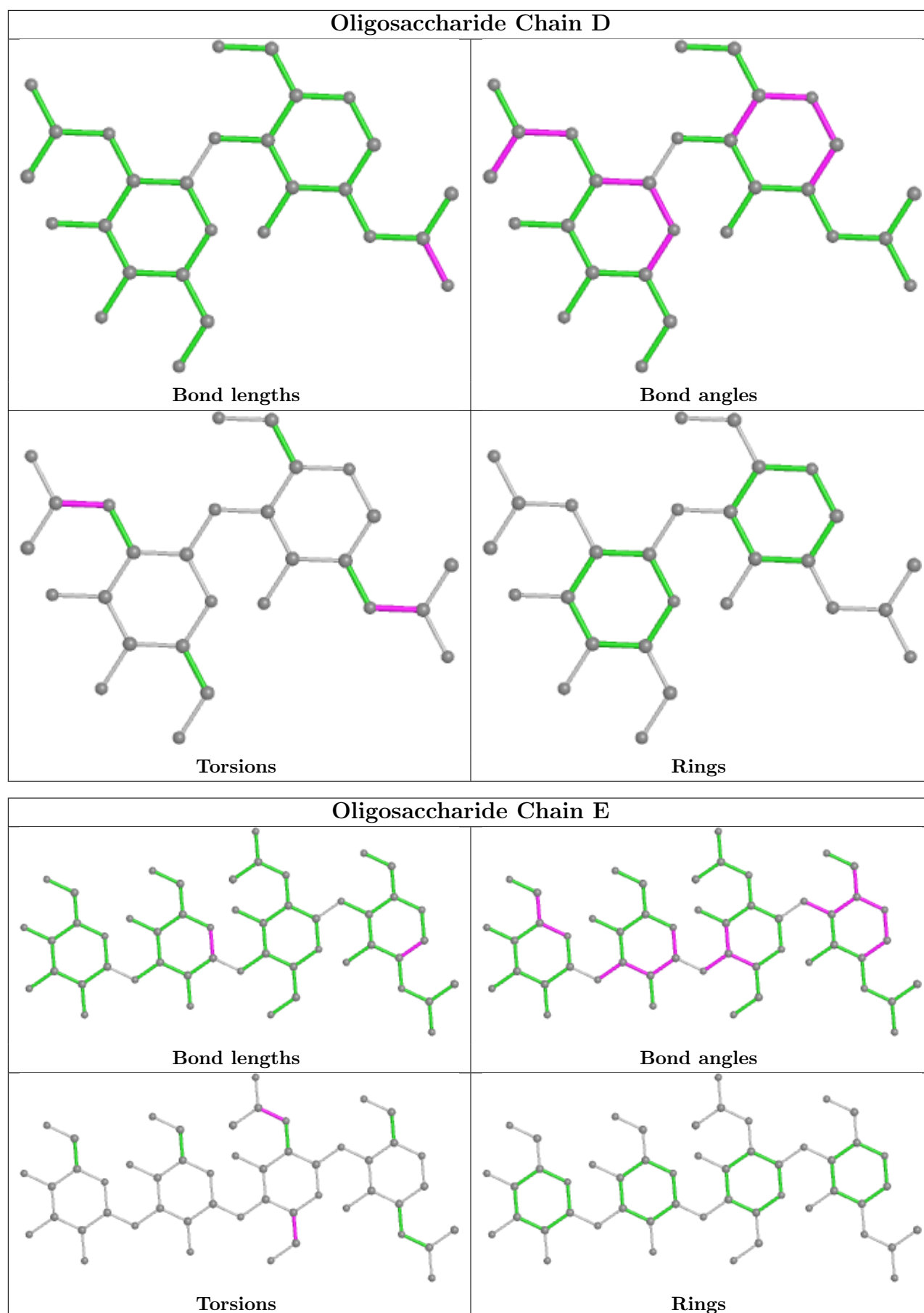
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2	NAG	1	0
3	B	2	NAG	1	0
4	E	3	BMA	0	1

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 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	1760	1	14,14,15	0.64	0	17,19,21	1.51	3 (17%)
5	NAG	A	1759	1	14,14,15	0.45	0	17,19,21	1.79	1 (5%)
5	NAG	A	1757	1	14,14,15	0.69	0	17,19,21	1.95	5 (29%)

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	1760	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1759	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1757	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1759	NAG	C1-O5-C5	6.53	121.04	112.19
5	A	1757	NAG	C1-O5-C5	5.35	119.45	112.19
5	A	1760	NAG	C1-O5-C5	3.45	116.87	112.19
5	A	1757	NAG	O5-C5-C6	3.21	112.23	107.20
5	A	1757	NAG	C3-C4-C5	2.68	115.03	110.24
5	A	1760	NAG	C2-N2-C7	-2.37	119.52	122.90
5	A	1757	NAG	C2-N2-C7	-2.25	119.70	122.90
5	A	1760	NAG	C8-C7-N2	2.15	119.73	116.10
5	A	1757	NAG	C8-C7-N2	2.13	119.71	116.10

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1759	NAG	O5-C5-C6-O6
5	A	1757	NAG	C8-C7-N2-C2
5	A	1757	NAG	O7-C7-N2-C2
5	A	1759	NAG	C4-C5-C6-O6
5	A	1757	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1760	NAG	1	0

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	694/709 (97%)	0.18	41 (5%) 22 24	17, 27, 46, 62	0
2	I	2/3 (66%)	-0.67	0 100 100	26, 26, 26, 27	0
All	All	696/712 (97%)	0.17	41 (5%) 22 24	17, 27, 46, 62	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	55	LYS	6.2
1	A	153	ASN	6.0
1	A	541	TRP	6.0
1	A	506	PHE	5.3
1	A	155	SER	4.9
1	A	719	VAL	4.9
1	A	542	GLU	4.9
1	A	335	GLY	4.1
1	A	134	ASP	3.7
1	A	336	ASN	3.6
1	A	507	SER	3.6
1	A	133	GLU	3.4
1	A	487	GLY	3.3
1	A	543	THR	3.2
1	A	237	PRO	3.1
1	A	652	ASP	3.0
1	A	656[A]	SER	3.0
1	A	136	ASN	3.0
1	A	402	PHE	2.9
1	A	154	VAL	2.9
1	A	324	LYS	2.9
1	A	123	THR	2.9
1	A	505	GLU	2.9
1	A	284	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	152	GLU	2.8
1	A	193	LYS	2.8
1	A	135	GLY	2.7
1	A	409	GLY	2.5
1	A	219	LEU	2.4
1	A	283	ILE	2.4
1	A	339	THR	2.4
1	A	746	LEU	2.3
1	A	174	LEU	2.3
1	A	551	LEU	2.3
1	A	124	HIS	2.3
1	A	122	LYS	2.2
1	A	732	ILE	2.1
1	A	504	PRO	2.1
1	A	408	GLU	2.1
1	A	238	GLY	2.1
1	A	342	VAL	2.0

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

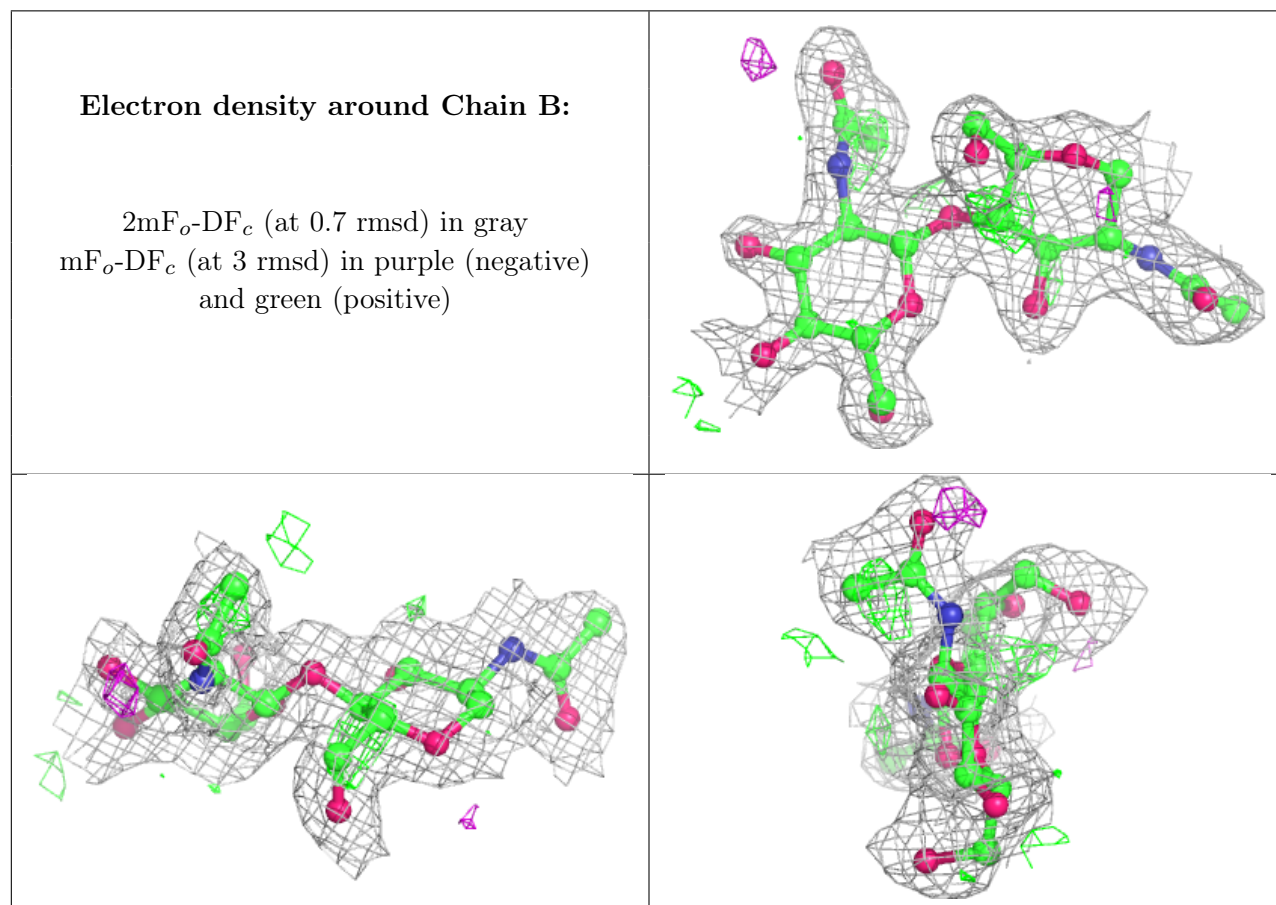
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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

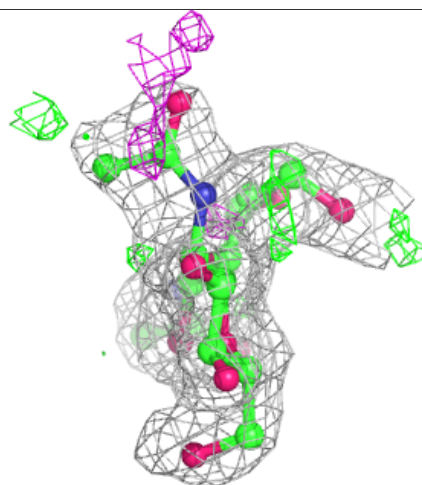
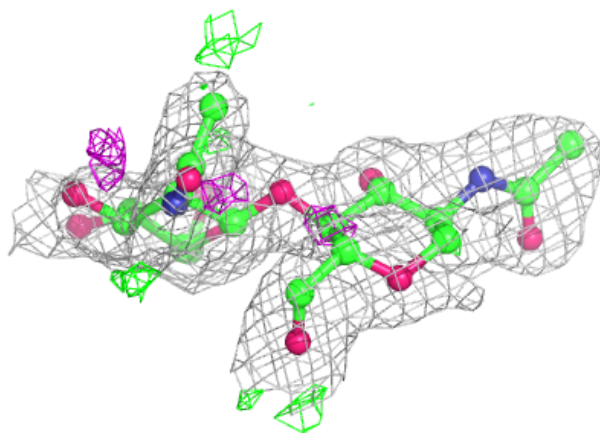
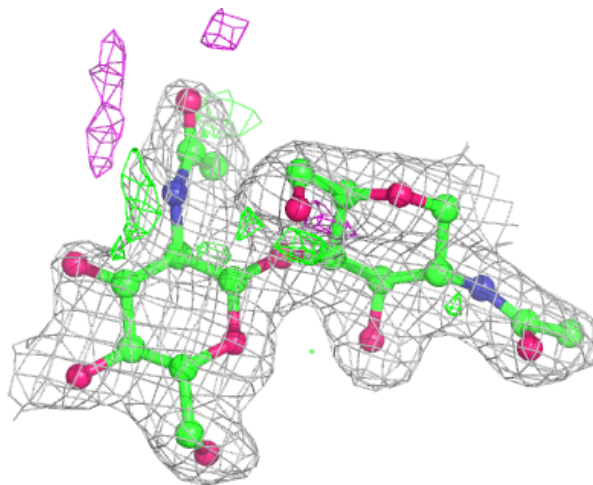
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	B	2	14/15	0.68	0.32	42,51,55,57	0
3	NAG	C	2	14/15	0.73	0.31	55,59,64,64	0
3	NAG	C	1	14/15	0.85	0.16	40,44,48,52	0
4	NAG	E	1	14/15	0.87	0.13	24,30,38,48	0
4	MAN	E	4	11/12	0.87	0.18	47,49,53,56	0
4	NAG	E	2	14/15	0.89	0.28	38,41,49,53	0
3	NAG	D	2	14/15	0.90	0.23	34,41,50,50	0
3	NAG	D	1	14/15	0.91	0.17	30,32,39,43	0
4	BMA	E	3	11/12	0.92	0.18	40,42,46,46	0
3	NAG	B	1	14/15	0.92	0.10	34,40,45,46	0

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



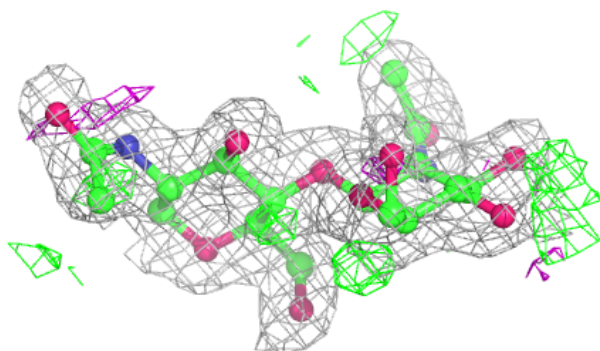
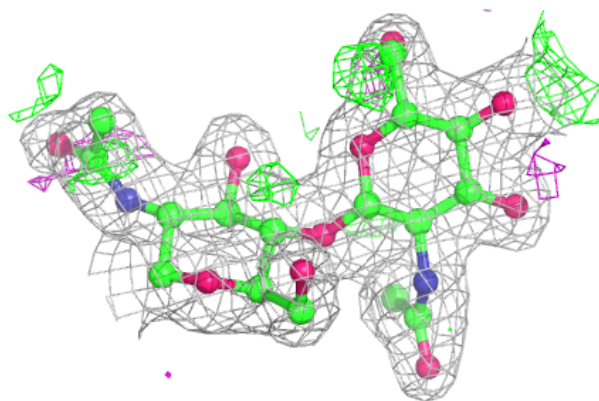
Electron density around Chain C:

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

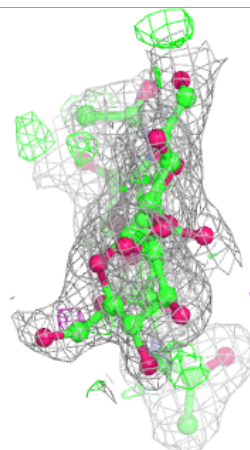
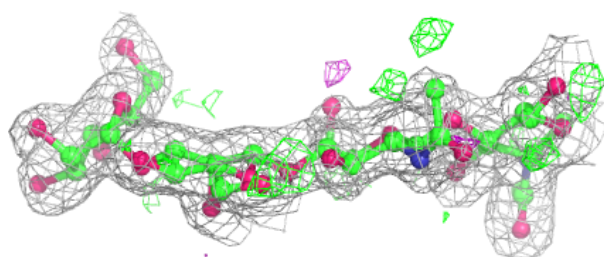
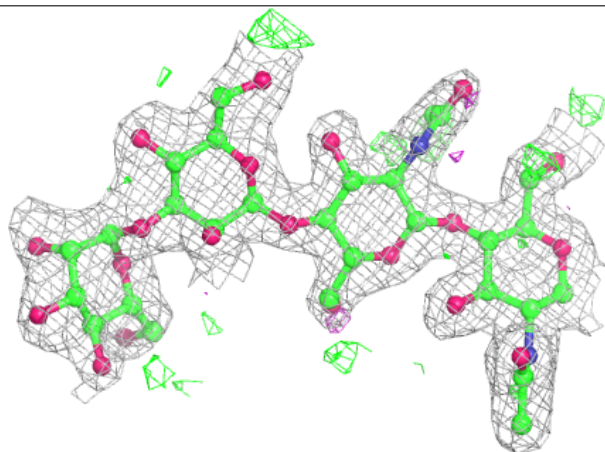


Electron density around Chain D:

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

**Electron density around Chain E:**

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



6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	NAG	A	1757	14/15	0.66	0.33	50,58,63,66	0
5	NAG	A	1760	14/15	0.80	0.17	30,43,46,49	0
5	NAG	A	1759	14/15	0.83	0.35	63,68,71,72	0
6	ZN	A	1751	1/1	1.00	0.03	21,21,21,21	0
6	ZN	A	1752	1/1	1.00	0.04	21,21,21,21	0
7	CA	A	1753	1/1	1.00	0.07	18,18,18,18	0
8	CL	A	1754	1/1	1.00	0.05	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.