



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 12:30 PM BST

PDB ID : 4MCS  
Title : A high resolution structure of human glutamate carboxypeptidase II (GCPII)  
His475Tyr variant in complex with glutamic acid  
Authors : Ptacek, J.; Barinka, C.; Sacha, P.; Navratil, M.  
Deposited on : 2013-08-21  
Resolution : 1.83 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](mailto: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.

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

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

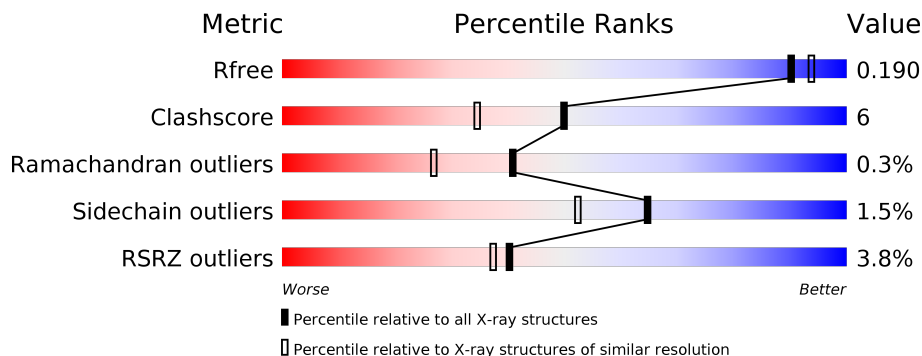
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.83 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	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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  $\geq 3$ , 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	757	 3% 80% 11% 9%
2	B	2	 50% 50%
2	C	2	 100%
2	D	2	 50% 50%
3	E	4	 100%

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 6485 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
			Total	C	N	O	S			
1	A	691	5702	3667	951	1063	21	0	45	0

There are 51 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP Q04609
A	-5	LYS	-	expression tag	UNP Q04609
A	-4	LEU	-	expression tag	UNP Q04609
A	-3	CYS	-	expression tag	UNP Q04609
A	-2	ILE	-	expression tag	UNP Q04609
A	-1	LEU	-	expression tag	UNP Q04609
A	0	LEU	-	expression tag	UNP Q04609
A	1	ALA	-	expression tag	UNP Q04609
A	2	VAL	-	expression tag	UNP Q04609
A	3	VAL	-	expression tag	UNP Q04609
A	4	ALA	-	expression tag	UNP Q04609
A	5	PHE	-	expression tag	UNP Q04609
A	6	VAL	-	expression tag	UNP Q04609
A	7	GLY	-	expression tag	UNP Q04609
A	8	LEU	-	expression tag	UNP Q04609
A	9	SER	-	expression tag	UNP Q04609
A	10	LEU	-	expression tag	UNP Q04609
A	11	GLY	-	expression tag	UNP Q04609
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	475	TYR	HIS	engineered mutation	UNP Q04609

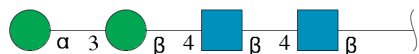
- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

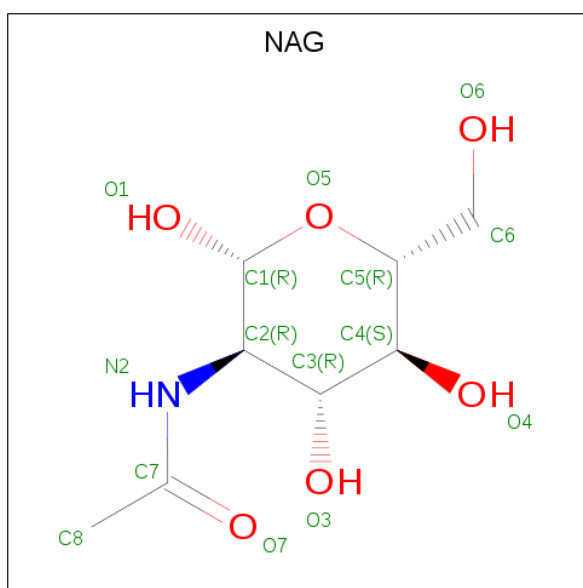
- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

pyranose.



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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

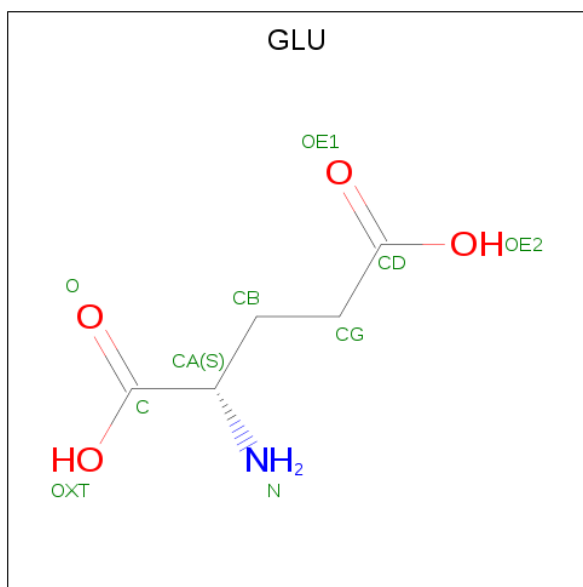
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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

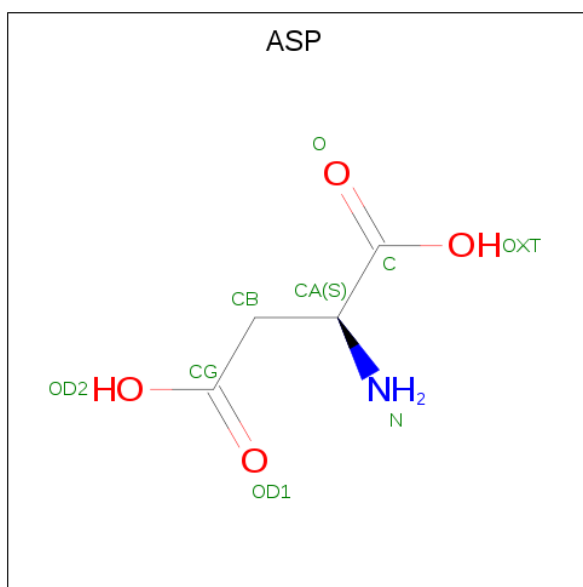
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Cl 1 1	0	0

- Molecule 8 is GLUTAMIC ACID (three-letter code: GLU) (formula: C<sub>5</sub>H<sub>9</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C N O 10 5 1 4	0	0

- Molecule 9 is ASPARTIC ACID (three-letter code: ASP) (formula: C<sub>4</sub>H<sub>7</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
9	A	1	9	4	1	4	0	0

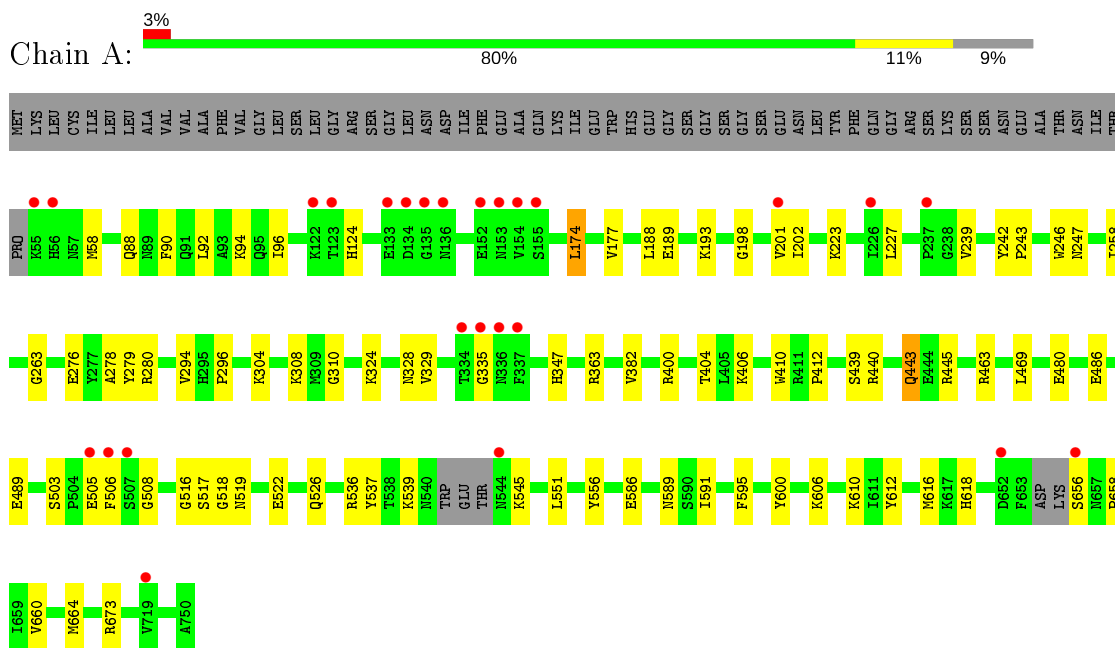
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	A	584	584	584	0	0

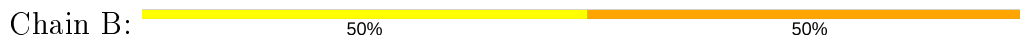
### 3 Residue-property plots [i](#)

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

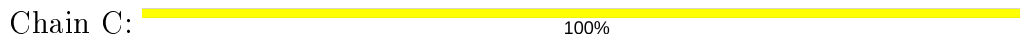


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1  
MAG2


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



MAG1  
MAG2


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



Chain D:  50% 50%

MAG1  
MAG2

- Molecule 3: 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%

MAG1  
MAG2  
BOA3  
MAT4

## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.55Å 130.40Å 158.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.53 – 1.83 28.53 – 1.83	Depositor EDS
% Data completeness (in resolution range)	93.0 (28.53-1.83) 93.0 (28.53-1.83)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.51 (at 1.83Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.159 , 0.191 0.158 , 0.190	Depositor DCC
$R_{free}$ test set	1736 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.3	Xtrriage
Anisotropy	0.048	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 58.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6485	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, BMA, NAG, CL, CA, 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	0.91	0/5994	0.77	4/8114 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	440	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	A	445	ARG	NE-CZ-NH1	-5.56	117.52	120.30
1	A	174[A]	LEU	CA-CB-CG	5.09	127.00	115.30
1	A	174[B]	LEU	CA-CB-CG	5.09	127.00	115.30

There are no chirality outliers.

There are no planarity outliers.

### 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	5702	0	5586	64	2
2	B	28	0	25	1	0
2	C	28	0	25	0	0
2	D	28	0	25	2	0
3	E	50	0	43	0	0
4	A	42	0	39	1	0
5	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	1	0	0	0	0
7	A	1	0	0	0	0
8	A	10	0	5	0	0
9	A	9	0	3	1	0
10	A	584	0	0	25	3
All	All	6485	0	5751	68	3

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 6.

All (68) 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	1.42	1.16
1:A:412:PRO:HA	1:A:589[B]:ASN:HD21	1.29	0.94
1:A:658[A]:PRO:HB3	10:A:1261:HOH:O	1.69	0.90
1:A:400:ARG:O	1:A:404[B]:THR:HG23	1.80	0.82
1:A:363[B]:ARG:NH2	10:A:1461:HOH:O	2.11	0.79
1:A:508:GLY:O	10:A:1463:HOH:O	2.01	0.79
1:A:463:ARG:HH21	1:A:545:LYS:HE3	1.55	0.71
1:A:276[B]:GLU:OE1	10:A:1187:HOH:O	2.11	0.69
1:A:363[B]:ARG:HD2	10:A:1460:HOH:O	1.93	0.68
1:A:480:GLU:HG3	10:A:1468:HOH:O	1.96	0.66
1:A:463:ARG:NH2	1:A:545:LYS:HG3	2.11	0.65
1:A:505:GLU:HG3	1:A:606[A]:LYS:HD2	1.80	0.63
1:A:612:TYR:CZ	1:A:616:MET:HG3	2.35	0.62
1:A:58:MET:CE	1:A:586[A]:GLU:HG2	2.30	0.61
10:A:1155:HOH:O	2:B:2:NAG:H81	2.01	0.60
9:A:819:ASP:N	10:A:1435:HOH:O	2.35	0.59
10:A:1117:HOH:O	2:D:2:NAG:C8	2.51	0.58
1:A:58:MET:HE1	1:A:586[A]:GLU:HG2	1.86	0.58
1:A:506:PHE:CE1	1:A:606[B]:LYS:NZ	2.74	0.56
1:A:88:GLN:HG2	10:A:1114:HOH:O	2.06	0.56
10:A:1117:HOH:O	2:D:2:NAG:H83	2.06	0.54
1:A:526[A]:GLN:NE2	10:A:1441:HOH:O	2.34	0.54
1:A:586[B]:GLU:HG2	10:A:1180:HOH:O	2.09	0.52
1:A:439:SER:O	1:A:443[A]:GLN:HB2	2.10	0.52
1:A:443[B]:GLN:HG3	1:A:443[B]:GLN:O	2.05	0.52
1:A:88:GLN:CG	10:A:1114:HOH:O	2.58	0.52
1:A:443[B]:GLN:NE2	10:A:935:HOH:O	2.44	0.51
1:A:188:LEU:HD21	1:A:329:VAL:HG11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239[A]:VAL:HG22	1:A:247:ASN:ND2	2.27	0.49
1:A:618:HIS:HE1	10:A:1046:HOH:O	1.94	0.49
1:A:412:PRO:HA	1:A:589[B]:ASN:ND2	2.11	0.49
1:A:90:PHE:CZ	1:A:94:LYS:HD2	2.48	0.49
1:A:610:LYS:NZ	10:A:1466:HOH:O	2.46	0.48
1:A:198:GLY:O	1:A:223:LYS:HE2	2.14	0.48
1:A:591[A]:ILE:HD12	10:A:1459:HOH:O	2.14	0.47
1:A:347:HIS:HE1	10:A:1245:HOH:O	1.97	0.47
1:A:124:HIS:CD2	1:A:347:HIS:CG	3.03	0.47
1:A:276[B]:GLU:HB2	10:A:1071:HOH:O	2.15	0.45
1:A:242:TYR:CG	1:A:243:PRO:HA	2.52	0.45
1:A:517:SER:OG	1:A:518:GLY:N	2.49	0.44
1:A:658[B]:PRO:HA	10:A:1261:HOH:O	2.17	0.44
1:A:278:ALA:HB3	1:A:280[A]:ARG:NH1	2.34	0.43
1:A:486:GLU:OE1	10:A:1157:HOH:O	2.20	0.43
1:A:516:GLY:O	1:A:526[B]:GLN:NE2	2.48	0.43
1:A:188:LEU:CD2	1:A:329:VAL:HG11	2.48	0.43
1:A:258:ILE:HD13	1:A:294:VAL:HB	2.01	0.43
1:A:177:VAL:CG1	1:A:201[B]:VAL:HG22	2.49	0.43
1:A:503:SER:HB3	1:A:506:PHE:O	2.17	0.43
1:A:188:LEU:HD21	1:A:329:VAL:CG1	2.48	0.43
1:A:310:GLY:O	1:A:328:ASN:HB3	2.19	0.43
1:A:304:LYS:HE3	10:A:1144:HOH:O	2.19	0.42
1:A:406:LYS:HA	1:A:410:TRP:O	2.19	0.42
1:A:58:MET:HE2	1:A:586[A]:GLU:HG2	2.00	0.42
1:A:469:LEU:O	1:A:595:PHE:HA	2.20	0.42
1:A:92:LEU:O	1:A:96:ILE:HG12	2.19	0.42
1:A:308:LYS:HB2	10:A:1243:HOH:O	2.20	0.42
1:A:489:GLU:CD	1:A:489:GLU:H	2.23	0.41
1:A:324:LYS:HD2	1:A:324:LYS:HA	1.88	0.41
1:A:258:ILE:HD12	1:A:294:VAL:HG21	2.02	0.41
1:A:246:TRP:CD1	4:A:807:NAG:H83	2.55	0.41
1:A:174[A]:LEU:HG	1:A:202:ILE:HG22	2.03	0.41
1:A:227:LEU:O	1:A:296:PRO:HA	2.20	0.41
1:A:551:LEU:HD22	1:A:556:TYR:HB2	2.03	0.41
1:A:263:GLY:HA2	1:A:522:GLU:OE1	2.21	0.41
1:A:58:MET:HE1	1:A:586[A]:GLU:CG	2.50	0.41
1:A:243:PRO:HD3	10:A:1443:HOH:O	2.21	0.40

All (3) 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:656[B]:SER:O	10:A:1261:HOH:O[4_566]	1.92	0.28
10:A:1122:HOH:O	10:A:1445:HOH:O[2_565]	1.93	0.27
1:A:656[B]:SER:OG	10:A:1261:HOH:O[4_566]	2.01	0.19

### 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	726/757 (96%)	708 (98%)	16 (2%)	2 (0%)	41 27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	335	GLY
1	A	382	VAL

#### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	630/643 (98%)	618 (98%)	12 (2%)	57 42

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	189[A]	GLU
1	A	189[B]	GLU

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Mol	Chain	Res	Type
1	A	193	LYS
1	A	443[A]	GLN
1	A	443[B]	GLN
1	A	519	ASN
1	A	536[A]	ARG
1	A	536[B]	ARG
1	A	537	TYR
1	A	539	LYS
1	A	600	TYR
1	A	673	ARG

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

Mol	Chain	Res	Type
1	A	124	HIS
1	A	303	GLN
1	A	618	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

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	$\# Z  > 2$
2	NAG	B	1	1,2	14,14,15	0.53	0	17,19,21	1.34	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	B	2	2	14,14,15	0.68	0	17,19,21	1.08	1 (5%)
2	NAG	C	1	1,2	14,14,15	0.53	0	17,19,21	1.19	2 (11%)
2	NAG	C	2	2	14,14,15	0.53	0	17,19,21	1.25	1 (5%)
2	NAG	D	1	1,2	14,14,15	0.81	1 (7%)	17,19,21	0.79	0
2	NAG	D	2	2	14,14,15	0.53	0	17,19,21	1.22	2 (11%)
3	NAG	E	1	1,3	14,14,15	0.59	0	17,19,21	1.49	3 (17%)
3	NAG	E	2	3	14,14,15	0.66	0	17,19,21	1.74	6 (35%)
3	BMA	E	3	3	11,11,12	0.47	0	15,15,17	1.34	2 (13%)
3	MAN	E	4	3	11,11,12	0.69	0	15,15,17	1.69	3 (20%)

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	-	2/6/23/26	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
2	NAG	D	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
3	MAN	E	4	3	-	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)
2	D	1	NAG	O7-C7	2.16	1.28	1.23

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	4	MAN	O5-C5-C6	5.06	115.13	107.20
3	E	2	NAG	C3-C4-C5	-3.52	103.96	110.24
3	E	1	NAG	C1-O5-C5	3.37	116.75	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	3	BMA	O3-C3-C2	-3.04	104.17	109.99
3	E	2	NAG	C2-N2-C7	-2.78	118.95	122.90
2	D	2	NAG	C8-C7-N2	2.73	120.72	116.10
2	C	1	NAG	C1-O5-C5	2.73	115.89	112.19
3	E	1	NAG	O6-C6-C5	-2.72	101.95	111.29
2	B	1	NAG	O5-C5-C6	2.67	111.39	107.20
3	E	2	NAG	C8-C7-N2	2.64	120.58	116.10
2	B	1	NAG	O5-C1-C2	-2.60	107.18	111.29
3	E	4	MAN	O3-C3-C2	2.60	114.96	109.99
2	C	2	NAG	O4-C4-C5	2.60	115.74	109.30
3	E	3	BMA	C1-C2-C3	2.58	112.83	109.67
3	E	1	NAG	C6-C5-C4	-2.54	107.06	113.00
2	D	2	NAG	C1-O5-C5	2.50	115.58	112.19
2	B	2	NAG	C2-N2-C7	2.34	126.23	122.90
3	E	4	MAN	C3-C4-C5	-2.22	106.27	110.24
3	E	2	NAG	C4-C3-C2	-2.14	107.88	111.02
2	B	1	NAG	O4-C4-C3	-2.12	105.45	110.35
2	C	1	NAG	C4-C3-C2	2.10	114.10	111.02
3	E	2	NAG	O7-C7-C8	-2.06	118.23	122.06
3	E	2	NAG	C1-C2-N2	2.03	113.96	110.49

There are no chirality outliers.

All (12) torsion outliers are listed below:

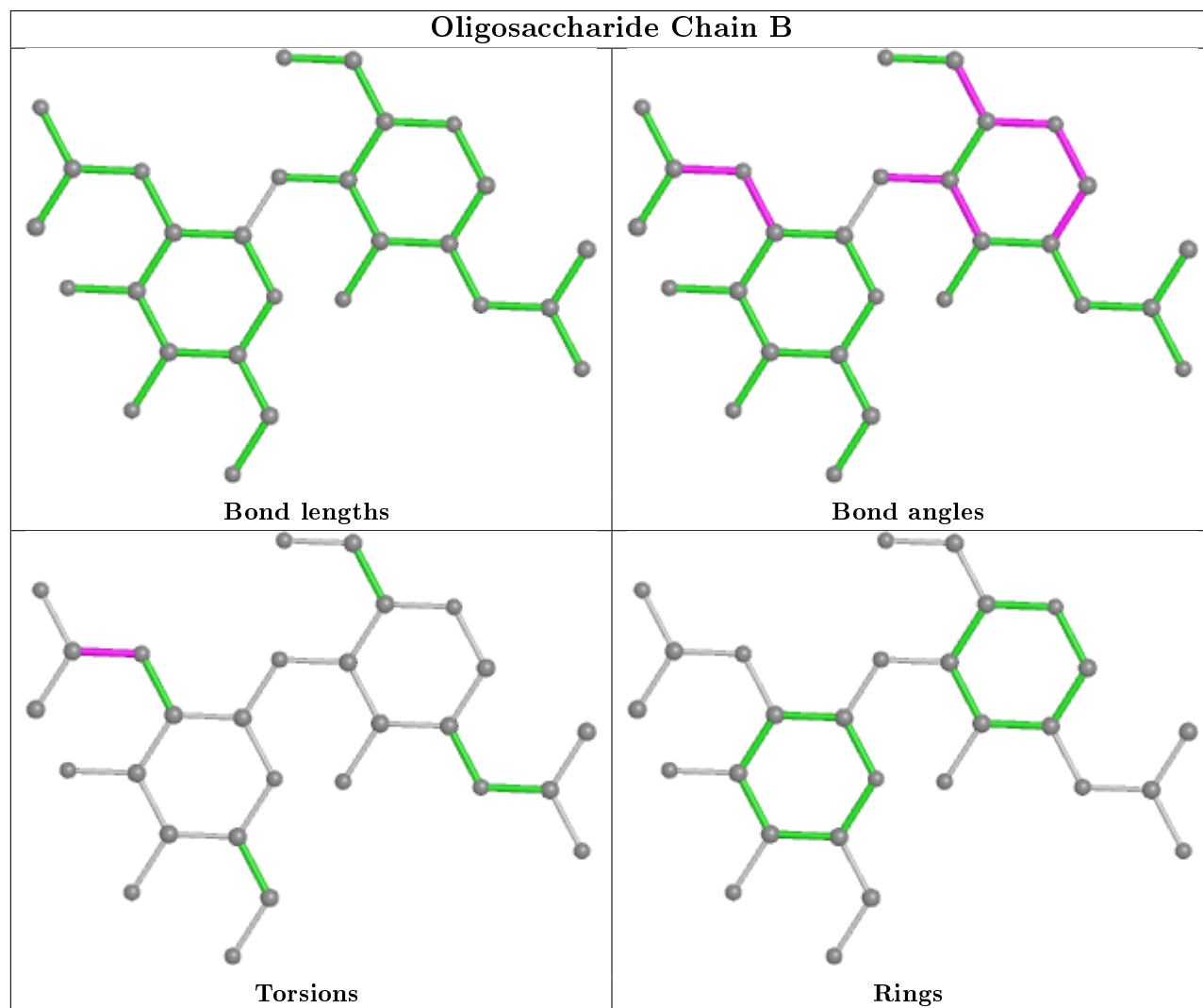
Mol	Chain	Res	Type	Atoms
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
2	C	2	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6

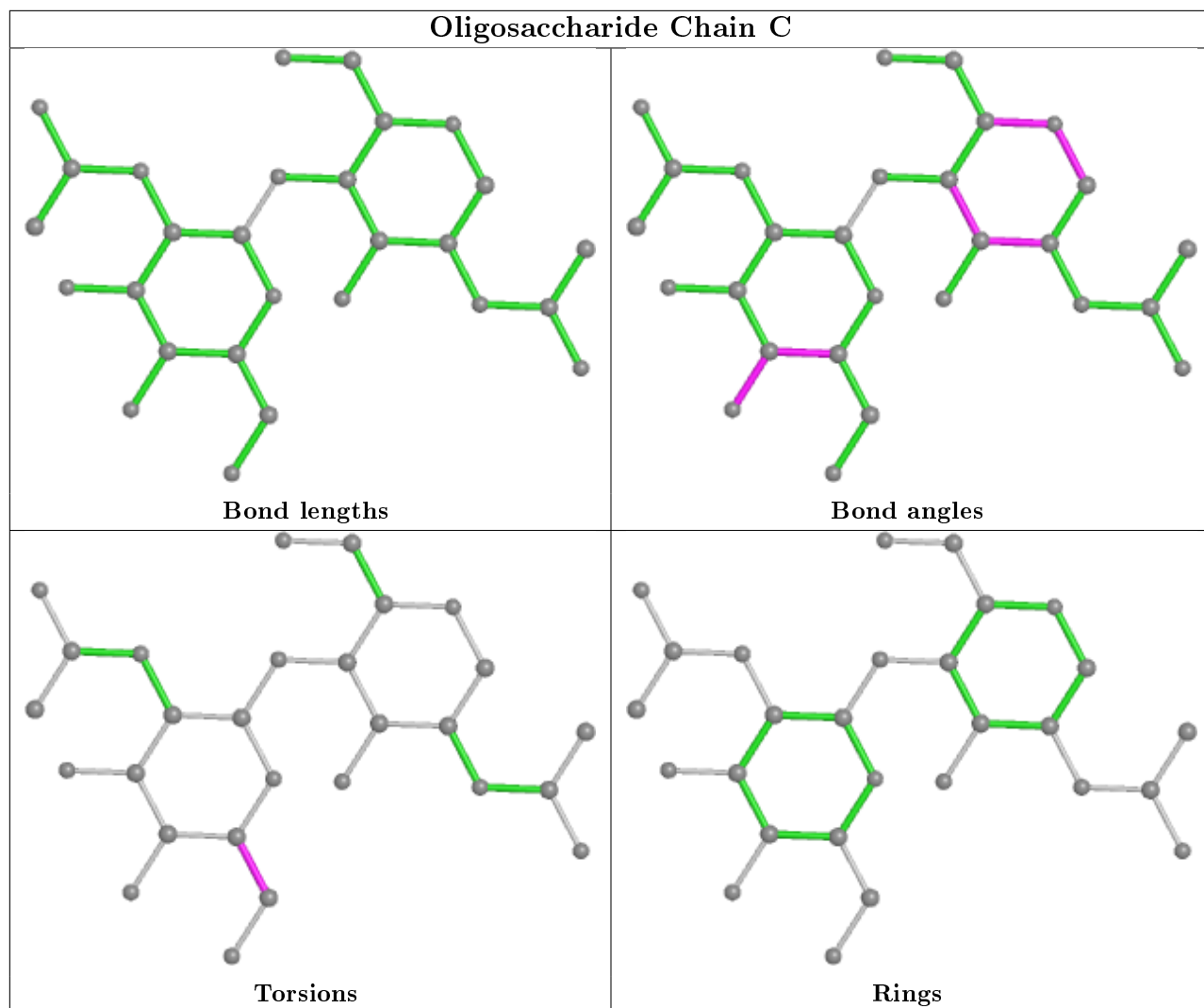
There are no ring outliers.

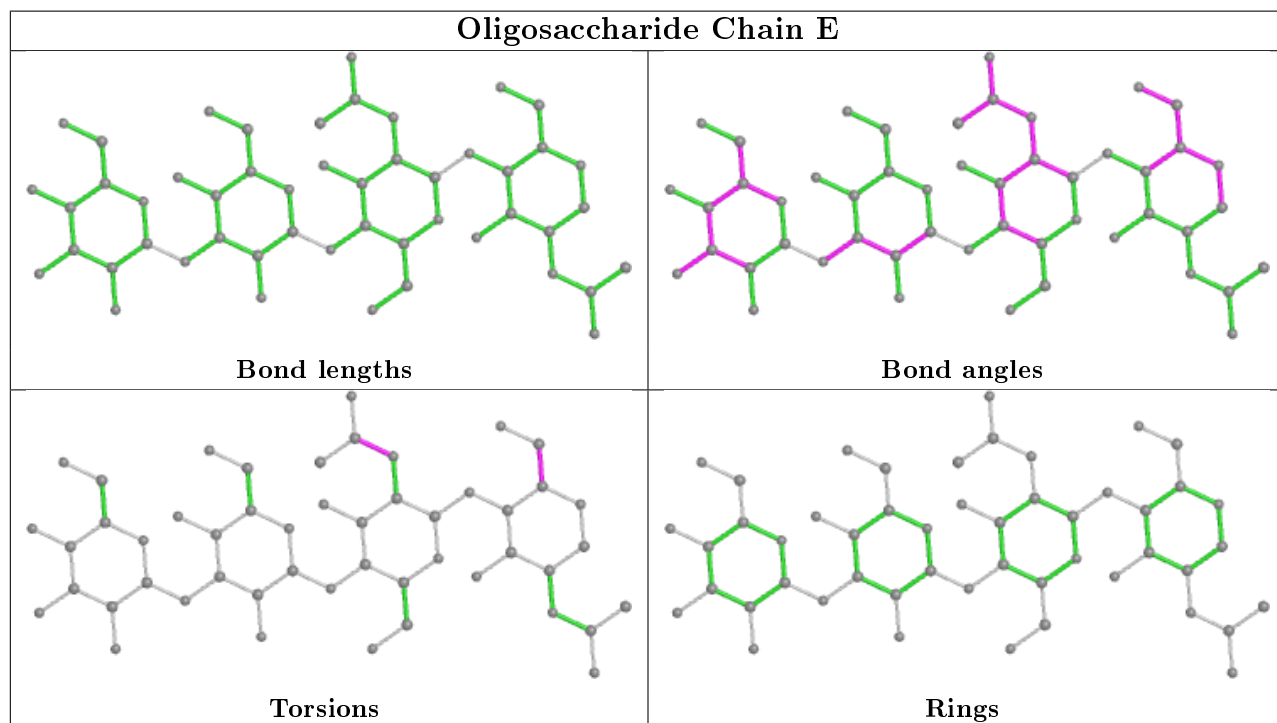
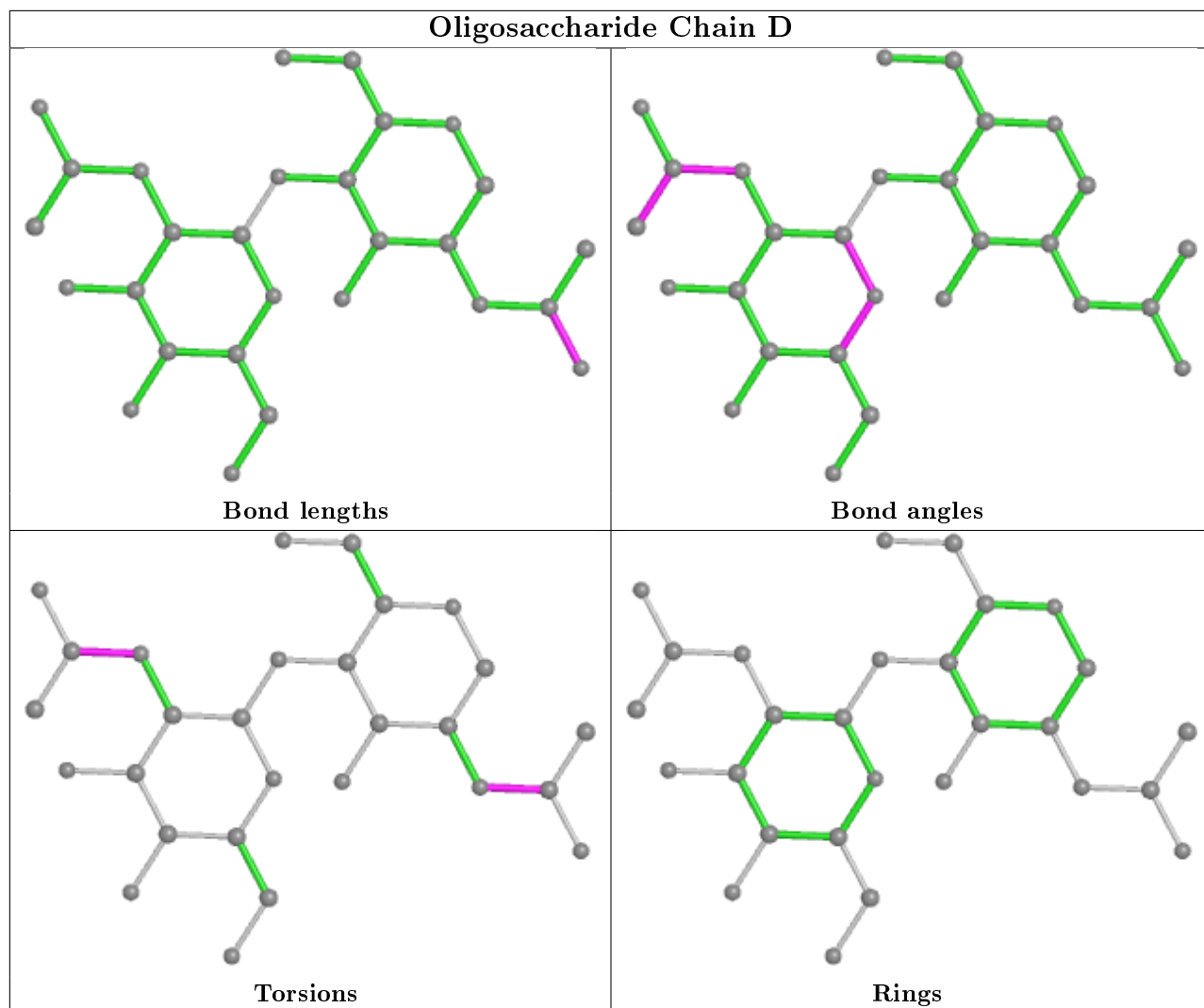
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	NAG	2	0
2	B	2	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 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
4	NAG	A	807	1	14,14,15	0.76	0	17,19,21	1.71	5 (29%)
4	NAG	A	806	1	14,14,15	0.53	0	17,19,21	1.31	2 (11%)
4	NAG	A	803	1	14,14,15	0.61	0	17,19,21	2.14	3 (17%)

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
4	NAG	A	807	1	-	0/6/23/26	0/1/1/1
4	NAG	A	806	1	-	0/6/23/26	0/1/1/1
4	NAG	A	803	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	803	NAG	C1-O5-C5	5.77	120.02	112.19
4	A	807	NAG	C1-O5-C5	4.08	117.72	112.19
4	A	803	NAG	C4-C3-C2	-4.04	105.09	111.02
4	A	806	NAG	O5-C5-C6	3.79	113.14	107.20
4	A	803	NAG	C2-N2-C7	-3.75	117.56	122.90
4	A	807	NAG	O3-C3-C4	-2.79	103.89	110.35
4	A	807	NAG	O7-C7-C8	-2.48	117.45	122.06
4	A	807	NAG	O5-C5-C6	2.42	111.00	107.20
4	A	806	NAG	C3-C4-C5	-2.07	106.55	110.24
4	A	807	NAG	O5-C1-C2	-2.02	108.10	111.29

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	803	NAG	C8-C7-N2-C2
4	A	803	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	807	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	691/757 (91%)	-0.30	26 (3%) <span style="border: 1px solid red; padding: 2px;">40</span> <span style="border: 1px solid red; padding: 2px;">37</span>	15, 28, 49, 70	2 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	55	LYS	4.1
1	A	544	ASN	3.9
1	A	506	PHE	3.4
1	A	155	SER	3.3
1	A	335	GLY	3.1
1	A	719	VAL	3.1
1	A	656[A]	SER	3.1
1	A	153	ASN	3.0
1	A	505	GLU	2.9
1	A	56	HIS	2.8
1	A	134	ASP	2.8
1	A	136	ASN	2.8
1	A	135	GLY	2.8
1	A	123	THR	2.8
1	A	226	ILE	2.6
1	A	201[A]	VAL	2.4
1	A	237	PRO	2.4
1	A	133	GLU	2.3
1	A	336	ASN	2.2
1	A	122	LYS	2.2
1	A	152	GLU	2.1
1	A	334	THR	2.1
1	A	652	ASP	2.1
1	A	337	PHE	2.1
1	A	507	SER	2.1
1	A	154	VAL	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, 95<sup>th</sup> 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.

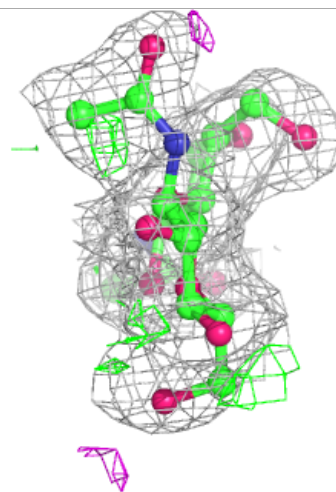
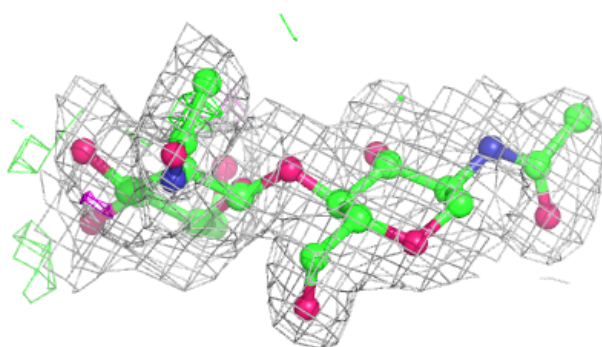
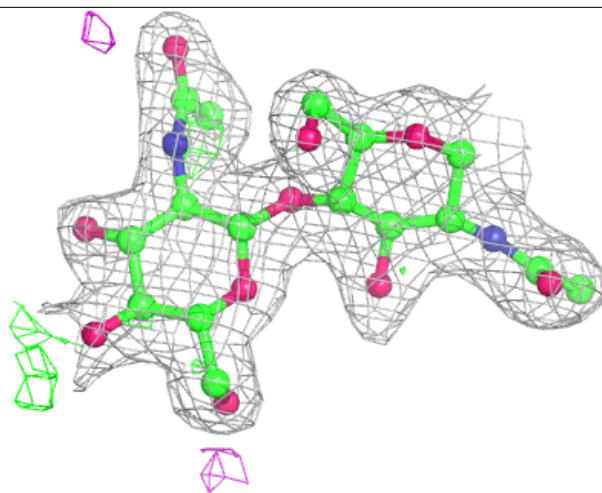
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	B	2	14/15	0.79	0.24	43,54,58,60	0
2	NAG	C	2	14/15	0.79	0.32	53,58,63,64	0
3	BMA	E	3	11/12	0.83	0.19	51,58,61,64	0
2	NAG	D	2	14/15	0.91	0.21	42,50,53,56	0
3	NAG	E	2	14/15	0.91	0.20	43,50,54,57	0
3	MAN	E	4	11/12	0.92	0.17	63,64,66,66	0
3	NAG	E	1	14/15	0.94	0.08	21,29,40,45	0
2	NAG	D	1	14/15	0.94	0.09	31,35,40,41	0
2	NAG	C	1	14/15	0.95	0.13	45,51,57,68	0
2	NAG	B	1	14/15	0.96	0.08	35,42,45,48	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.



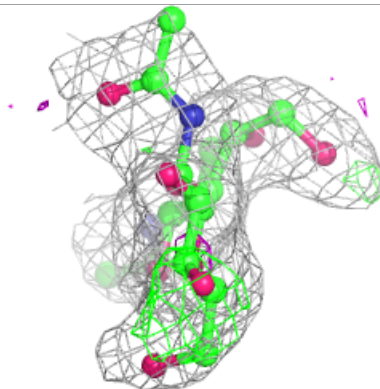
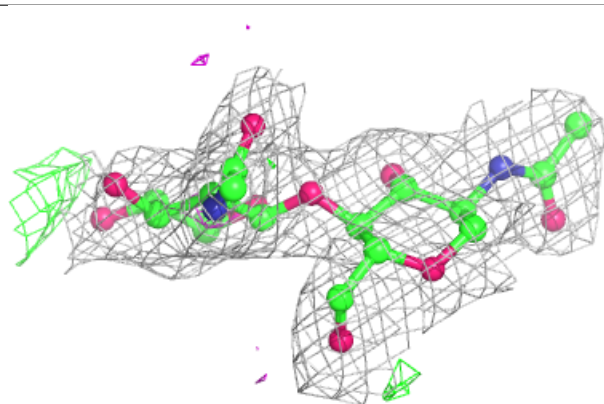
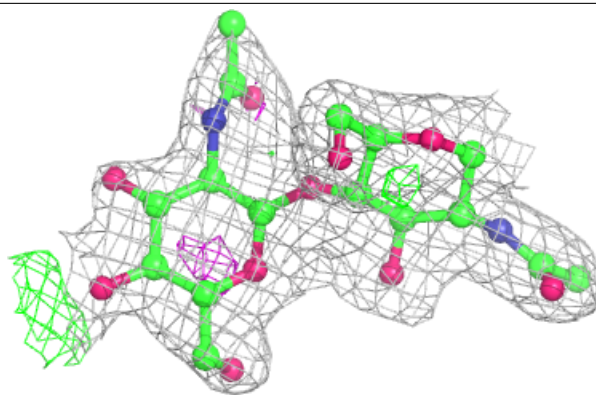
**Electron density around Chain B:**

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



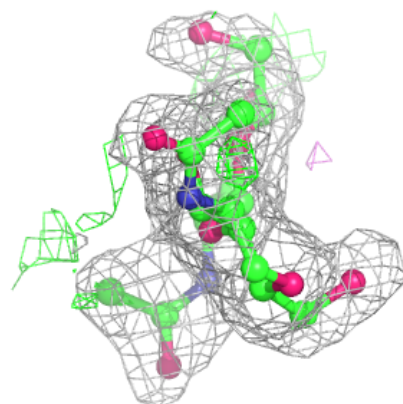
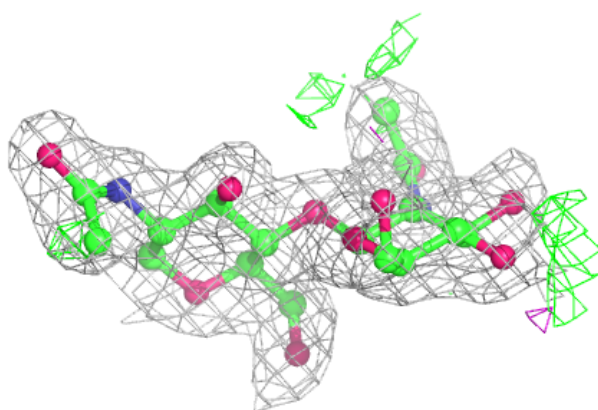
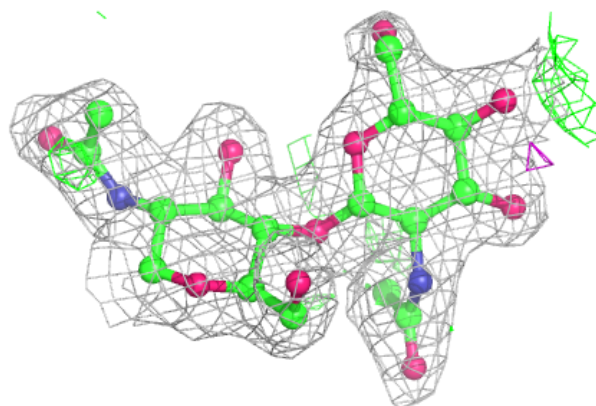
**Electron density around Chain C:**

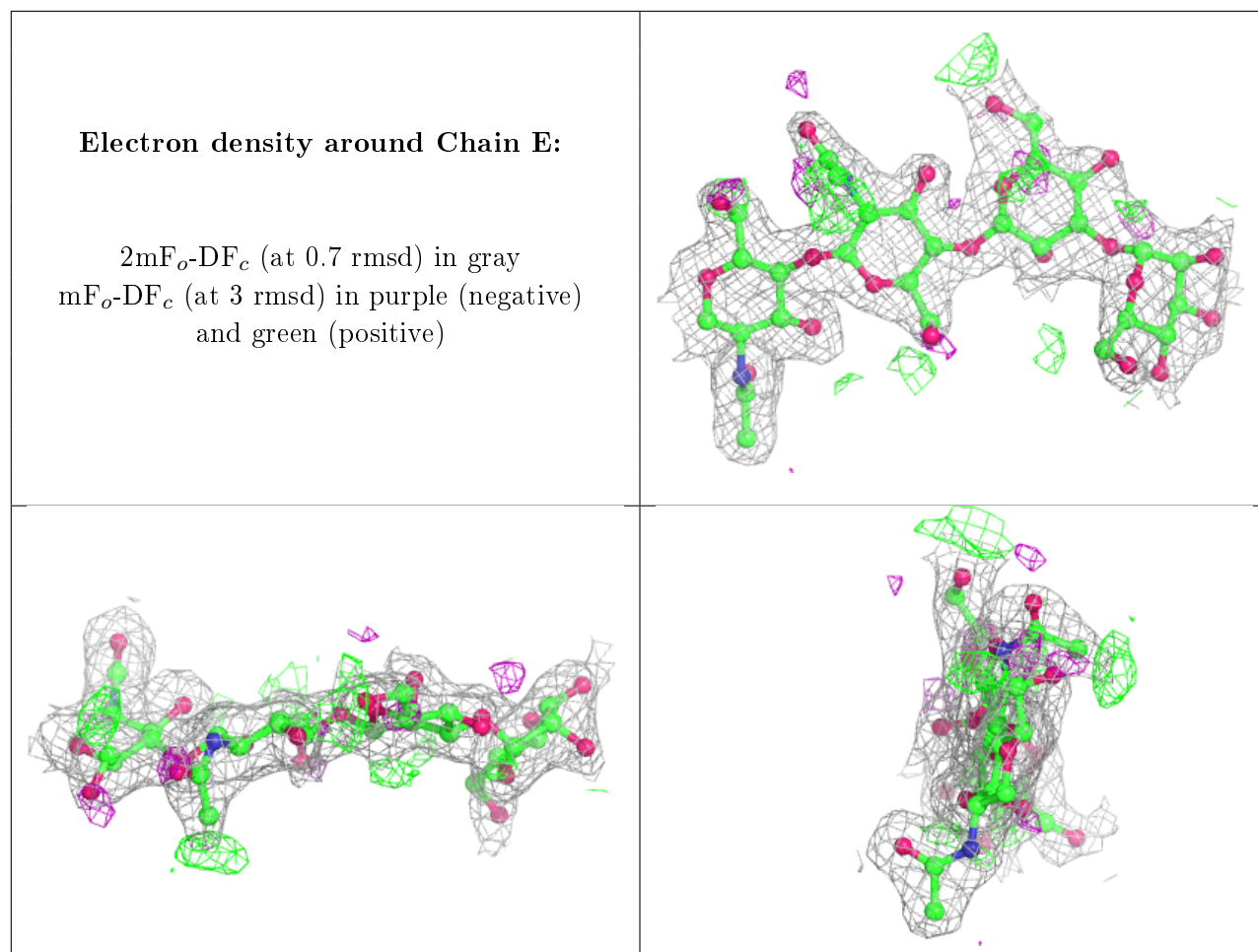
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain 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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	NAG	A	803	14/15	0.80	0.25	53,57,64,67	0
4	NAG	A	807	14/15	0.91	0.14	33,48,53,56	0
4	NAG	A	806	14/15	0.91	0.24	72,78,81,81	0
9	ASP	A	819	9/9	0.92	0.13	37,41,43,46	0
8	GLU	A	818	10/10	0.98	0.09	20,21,22,22	0
7	CL	A	817	1/1	1.00	0.08	23,23,23,23	0
5	ZN	A	815	1/1	1.00	0.06	20,20,20,20	0
5	ZN	A	814	1/1	1.00	0.07	23,23,23,23	0
6	CA	A	816	1/1	1.00	0.06	18,18,18,18	0

## 6.5 Other polymers

There are no such residues in this entry.