



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 01:42 AM BST

PDB ID : 2OR4  
Title : A high resolution crystal structure of human glutamate carboxypeptidase II  
in complex with quisqualic acid  
Authors : Barinka, C.; Lubkowski, J.  
Deposited on : 2007-02-01  
Resolution : 1.62 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

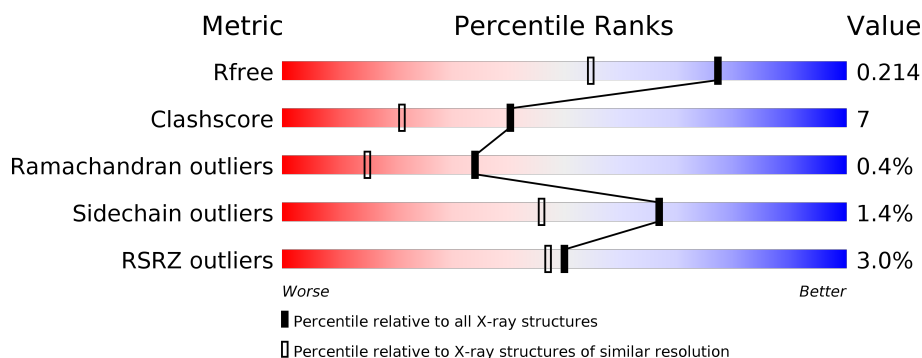
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.62 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	4693 (1.64-1.60)
Clashscore	141614	5002 (1.64-1.60)
Ramachandran outliers	138981	4888 (1.64-1.60)
Sidechain outliers	138945	4887 (1.64-1.60)
RSRZ outliers	127900	4609 (1.64-1.60)

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	709	
2	B	2	
2	C	2	
2	D	2	
3	E	4	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MAN	E	4	X	-	-	-

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 6771 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	689	Total	C	N	O	S	0	48	0
			5704	3671	951	1061	21			

There are 2 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

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



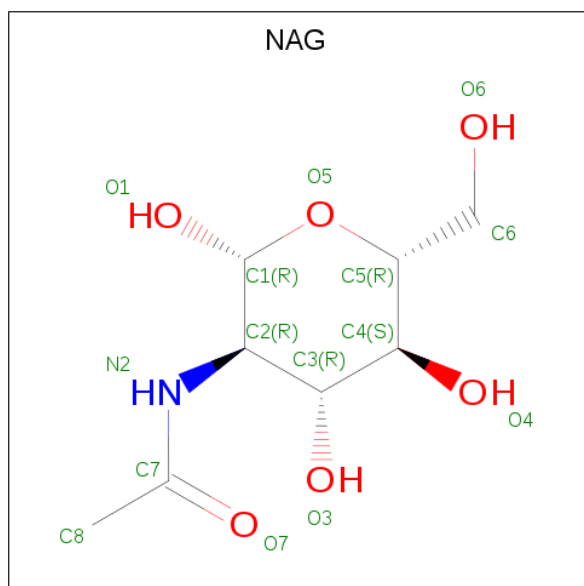
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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.



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

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

- 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		

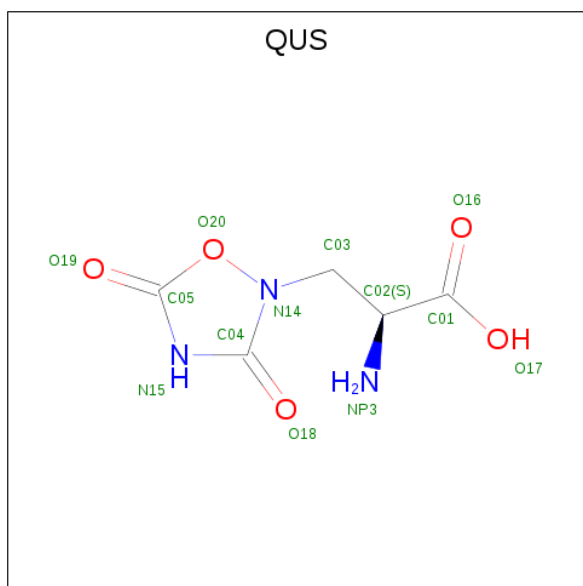
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- 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 (S)-2-AMINO-3-(3,5-DIOXO-[1,2,4]OXADIAZOLIDIN-2-YL)-PROPIONIC ACID (three-letter code: QUS) (formula: C<sub>5</sub>H<sub>7</sub>N<sub>3</sub>O<sub>5</sub>).



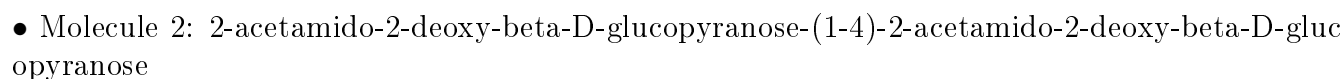
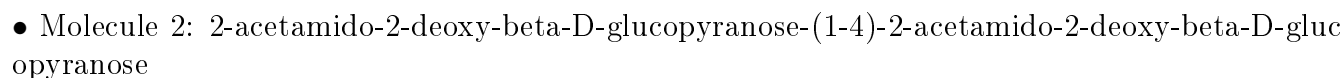
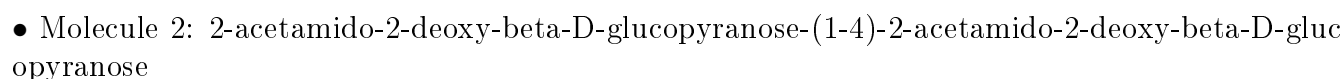
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C N O 13 5 3 5	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	874	Total O 874 874	0	0



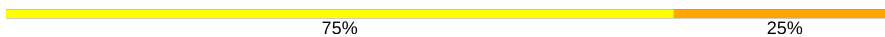
- Molecule 1: Glutamate carboxypeptidase 2



NAG1  
NAG2

- 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:



NAG1  
NAG2  
BMA3  
MAN4

## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.01Å 130.44Å 159.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.62 49.24 – 1.62	Depositor EDS
% Data completeness (in resolution range)	96.6 (30.00-1.62) 96.6 (49.24-1.62)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.62 (at 1.62Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.184 , 0.219 0.181 , 0.214	Depositor DCC
$R_{free}$ test set	6521 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.8	Xtriage
Anisotropy	0.583	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 59.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6771	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, BMA, NAG, CL, CA, QUS, 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	1.01	2/6029 (0.0%)	0.96	16/8161 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	733	TYR	CD1-CE1	5.22	1.47	1.39
1	A	733	TYR	CG-CD2	5.20	1.46	1.39

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	370	ARG	NE-CZ-NH1	10.09	125.34	120.30
1	A	370	ARG	NE-CZ-NH2	-7.53	116.54	120.30
1	A	369	ASP	CB-CG-OD1	6.75	124.38	118.30
1	A	210	ARG	NE-CZ-NH1	-6.70	116.95	120.30
1	A	688	ARG	NE-CZ-NH1	-6.62	116.99	120.30
1	A	662[A]	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	A	662[B]	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	A	746	LEU	CB-CG-CD1	-6.01	100.78	111.00
1	A	174[A]	LEU	CA-CB-CG	5.85	128.75	115.30
1	A	174[B]	LEU	CA-CB-CG	5.85	128.75	115.30
1	A	668	LEU	CB-CG-CD2	5.55	120.44	111.00
1	A	255	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	A	662[A]	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	A	662[B]	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	A	668	LEU	CB-CG-CD1	-5.37	101.87	111.00
1	A	688	ARG	NE-CZ-NH2	5.21	122.90	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	5704	0	5573	78	0
2	B	28	0	25	2	0
2	C	28	0	25	2	0
2	D	28	0	25	0	0
3	E	50	0	43	1	0
4	A	42	0	39	2	0
5	A	2	0	0	0	0
6	A	1	0	0	0	0
7	A	1	0	0	0	0
8	A	13	0	6	0	0
9	A	874	0	0	35	2
All	All	6771	0	5736	84	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 7.

All (84) 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	1.47	1.13
1:A:486:GLU:HG2	9:A:2052:HOH:O	1.47	1.12
1:A:189:GLU:HG2	9:A:2341:HOH:O	1.56	1.05
1:A:258[B]:ILE:CD1	1:A:290:PRO:HG3	2.01	0.91
1:A:652[A]:ASP:OD2	9:A:2545:HOH:O	1.90	0.89
1:A:655[A]:LYS:HG2	9:A:2604:HOH:O	1.75	0.84
1:A:655[B]:LYS:O	9:A:2604:HOH:O	1.99	0.81
1:A:400:ARG:O	1:A:404[B]:THR:HG23	1.80	0.80
1:A:733:TYR:HE2	9:A:2161:HOH:O	1.65	0.77
1:A:260:ASN:ND2	9:A:2477:HOH:O	2.17	0.76
9:A:2285:HOH:O	2:C:2:NAG:H81	1.88	0.74
1:A:258[B]:ILE:HD13	1:A:290:PRO:HG3	1.68	0.72
1:A:641:GLU:HG3	9:A:2318:HOH:O	1.91	0.70
9:A:2051:HOH:O	2:B:2:NAG:H81	1.94	0.67
1:A:613[B]:SER:OG	9:A:2054:HOH:O	2.13	0.66
1:A:546:PHE:O	9:A:2602:HOH:O	2.15	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90[B]:PHE:CE2	1:A:94:LYS:NZ	2.67	0.63
1:A:90[B]:PHE:HE2	1:A:94:LYS:HZ3	1.46	0.62
1:A:654[B]:ASP:OD2	1:A:655[B]:LYS:N	2.34	0.61
1:A:652[B]:ASP:OD2	9:A:2545:HOH:O	2.16	0.60
1:A:645:LYS:HD2	9:A:2332:HOH:O	2.02	0.59
4:A:1760:NAG:H3	9:A:2426:HOH:O	2.03	0.58
1:A:88[A]:GLN:NE2	9:A:2535:HOH:O	2.36	0.58
1:A:207:LYS:NZ	9:A:2308:HOH:O	2.31	0.57
1:A:258[B]:ILE:HD11	1:A:290:PRO:HG3	1.86	0.57
1:A:369:ASP:OD1	1:A:662[B]:ARG:NH2	2.38	0.56
1:A:656[B]:SER:HA	9:A:2606:HOH:O	2.07	0.55
1:A:287:VAL:CG1	9:A:2311:HOH:O	2.54	0.54
1:A:258[A]:ILE:HD13	1:A:294:VAL:HB	1.90	0.54
1:A:617:LYS:NZ	9:A:2220:HOH:O	2.39	0.54
1:A:90[B]:PHE:CE2	1:A:94:LYS:CE	2.92	0.52
1:A:652[B]:ASP:CG	9:A:2545:HOH:O	2.47	0.52
1:A:517:SER:HB3	1:A:699:LYS:HG3	1.92	0.52
1:A:90[B]:PHE:CE2	1:A:94:LYS:HE2	2.45	0.51
1:A:620:GLN:NE2	9:A:2147:HOH:O	2.42	0.51
1:A:276[D]:GLU:HB2	9:A:1971:HOH:O	2.12	0.50
1:A:653[B]:PHE:CD1	1:A:654[B]:ASP:N	2.80	0.49
1:A:406:LYS:HA	1:A:410:TRP:O	2.12	0.49
1:A:239[A]:VAL:HG22	1:A:247:ASN:ND2	2.27	0.49
1:A:169:MET:HA	1:A:344:MET:O	2.13	0.49
1:A:551:LEU:HD22	1:A:556:TYR:HB2	1.94	0.49
1:A:287:VAL:HG13	9:A:2311:HOH:O	2.14	0.48
1:A:246:TRP:CD1	4:A:1760:NAG:H83	2.48	0.48
1:A:651:GLN:HB2	9:A:2545:HOH:O	2.15	0.47
1:A:174[A]:LEU:HG	1:A:202:ILE:HG22	1.97	0.47
1:A:70:ILE:HG21	1:A:573:HIS:HB3	1.97	0.47
1:A:662[B]:ARG:HD2	9:A:2542:HOH:O	2.15	0.47
1:A:185:PHE:O	1:A:189:GLU:HG3	2.16	0.46
1:A:148:PRO:HG2	1:A:151:TYR:CD2	2.51	0.46
1:A:687:TYR:CZ	1:A:694:PRO:HG2	2.51	0.46
1:A:164:PHE:CD2	1:A:259:LEU:HG	2.51	0.46
1:A:218[B]:GLN:CD	1:A:291:SER:OG	2.54	0.46
1:A:733:TYR:CE2	9:A:2161:HOH:O	2.51	0.46
9:A:2171:HOH:O	2:C:2:NAG:H83	2.15	0.45
1:A:412:PRO:HA	1:A:589[C]:ASN:OD1	2.16	0.45
1:A:612:TYR:CZ	1:A:616:MET:HG3	2.51	0.45
1:A:169:MET:HE1	9:A:2461:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:721:PRO:HD2	9:A:1986:HOH:O	2.16	0.44
1:A:177:VAL:HG12	1:A:188:LEU:CD1	2.48	0.44
1:A:350:ASN:C	1:A:351[B]:GLU:HG2	2.37	0.44
1:A:90[B]:PHE:HE2	1:A:94:LYS:NZ	2.10	0.44
1:A:268:LEU:HD21	1:A:283[B]:ILE:HD13	2.00	0.44
1:A:258[A]:ILE:HD12	1:A:294:VAL:HG21	1.99	0.43
1:A:413:ARG:H	1:A:589[B]:ASN:HD22	1.66	0.43
1:A:654[B]:ASP:CG	1:A:655[B]:LYS:H	2.15	0.43
9:A:2361:HOH:O	3:E:2:NAG:H62	2.17	0.43
1:A:303:GLN:OE1	1:A:325:VAL:HG13	2.19	0.42
1:A:295:HIS:HB2	1:A:346:ILE:HD11	2.02	0.42
1:A:653[A]:PHE:HZ	1:A:661[A]:LEU:HD13	1.84	0.42
1:A:653[A]:PHE:CZ	1:A:661[A]:LEU:HA	2.55	0.42
1:A:618:HIS:HE1	9:A:1947:HOH:O	2.03	0.42
1:A:242:TYR:OH	9:A:2495:HOH:O	2.11	0.41
1:A:242:TYR:CG	1:A:243:PRO:HA	2.56	0.41
1:A:227:LEU:O	1:A:296:PRO:HA	2.20	0.41
1:A:444:GLU:HA	1:A:444:GLU:OE1	2.21	0.41
9:A:2051:HOH:O	2:B:2:NAG:C8	2.61	0.41
1:A:133:GLU:HB2	9:A:2126:HOH:O	2.21	0.41
1:A:177:VAL:HG12	1:A:188:LEU:HD11	2.02	0.41
1:A:506:PHE:HB2	1:A:509:MET:CG	2.51	0.40
1:A:177:VAL:CG2	1:A:201[B]:VAL:HG13	2.51	0.40
1:A:263:GLY:HA2	1:A:522:GLU:OE1	2.21	0.40
1:A:198:GLY:O	1:A:223:LYS:HE2	2.22	0.40

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)
9:A:2174:HOH:O	9:A:2313:HOH:O[2_565]	2.07	0.13
9:A:2176:HOH:O	9:A:2325:HOH:O[2_565]	2.15	0.05

## 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	731/709 (103%)	708 (97%)	19 (3%)	4 (0%)	29	11

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	654[A]	ASP
1	A	654[B]	ASP
1	A	382	VAL
1	A	335	GLY

### 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	634/605 (105%)	625 (99%)	9 (1%)	67	46

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	303	GLN
1	A	489	GLU
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	91	GLN

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Mol	Chain	Res	Type
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	$\# Z  > 2$
2	NAG	B	1	1,2	14,14,15	0.68	0	17,19,21	1.49	5 (29%)
2	NAG	B	2	2	14,14,15	0.62	0	17,19,21	1.03	1 (5%)
2	NAG	C	1	1,2	14,14,15	0.81	0	17,19,21	1.16	1 (5%)
2	NAG	C	2	2	14,14,15	0.43	0	17,19,21	1.27	1 (5%)
2	NAG	D	1	1,2	14,14,15	1.04	1 (7%)	17,19,21	1.72	2 (11%)
2	NAG	D	2	2	14,14,15	0.54	0	17,19,21	1.17	3 (17%)
3	NAG	E	1	1,3	14,14,15	0.90	1 (7%)	17,19,21	1.27	3 (17%)
3	NAG	E	2	3	14,14,15	0.74	1 (7%)	17,19,21	1.73	5 (29%)
3	BMA	E	3	1,3	11,11,12	0.93	1 (9%)	15,15,17	1.54	2 (13%)
3	MAN	E	4	3	11,11,12	0.61	0	15,15,17	3.91	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	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	BMA	E	3	1,3	-	0/2/19/22	0/1/1/1
3	MAN	E	4	3	1/1/4/5	0/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	3	BMA	O5-C1	-2.46	1.39	1.43
2	D	1	NAG	O7-C7	2.40	1.28	1.23
3	E	1	NAG	C1-C2	2.28	1.55	1.52
3	E	2	NAG	O5-C1	-2.18	1.40	1.43

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	4	MAN	C1-O5-C5	-11.28	96.91	112.19
3	E	4	MAN	C1-C2-C3	-8.72	98.95	109.67
2	D	1	NAG	O5-C1-C2	-4.91	103.54	111.29
3	E	3	BMA	O3-C3-C4	-4.68	99.54	110.35
3	E	4	MAN	O5-C5-C6	3.83	113.21	107.20
2	C	1	NAG	O5-C1-C2	-3.77	105.34	111.29
2	D	1	NAG	O5-C5-C4	-3.36	102.65	110.83
3	E	2	NAG	C8-C7-N2	3.33	121.74	116.10
3	E	2	NAG	O7-C7-C8	-3.19	116.13	122.06
3	E	2	NAG	C3-C4-C5	-3.18	104.57	110.24
2	B	1	NAG	O5-C1-C2	-3.10	106.39	111.29
3	E	1	NAG	O5-C1-C2	-2.71	107.01	111.29
2	D	2	NAG	C1-O5-C5	2.44	115.50	112.19
2	B	1	NAG	C2-N2-C7	-2.44	119.43	122.90
2	B	2	NAG	C1-O5-C5	2.39	115.43	112.19
3	E	3	BMA	O5-C1-C2	-2.38	107.10	110.77
3	E	2	NAG	O5-C5-C6	2.33	110.85	107.20
2	D	2	NAG	C8-C7-N2	2.29	119.98	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2	NAG	C2-N2-C7	2.28	126.15	122.90
2	B	1	NAG	O4-C4-C3	-2.28	105.08	110.35
2	B	1	NAG	O3-C3-C4	-2.27	105.09	110.35
2	C	2	NAG	O7-C7-C8	-2.22	117.93	122.06
3	E	1	NAG	C6-C5-C4	-2.20	107.86	113.00
2	B	1	NAG	O5-C5-C6	2.19	110.64	107.20
2	D	2	NAG	O7-C7-C8	-2.18	118.02	122.06
3	E	1	NAG	O4-C4-C5	-2.15	103.95	109.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	E	4	MAN	C1

All (10) torsion outliers are listed below:

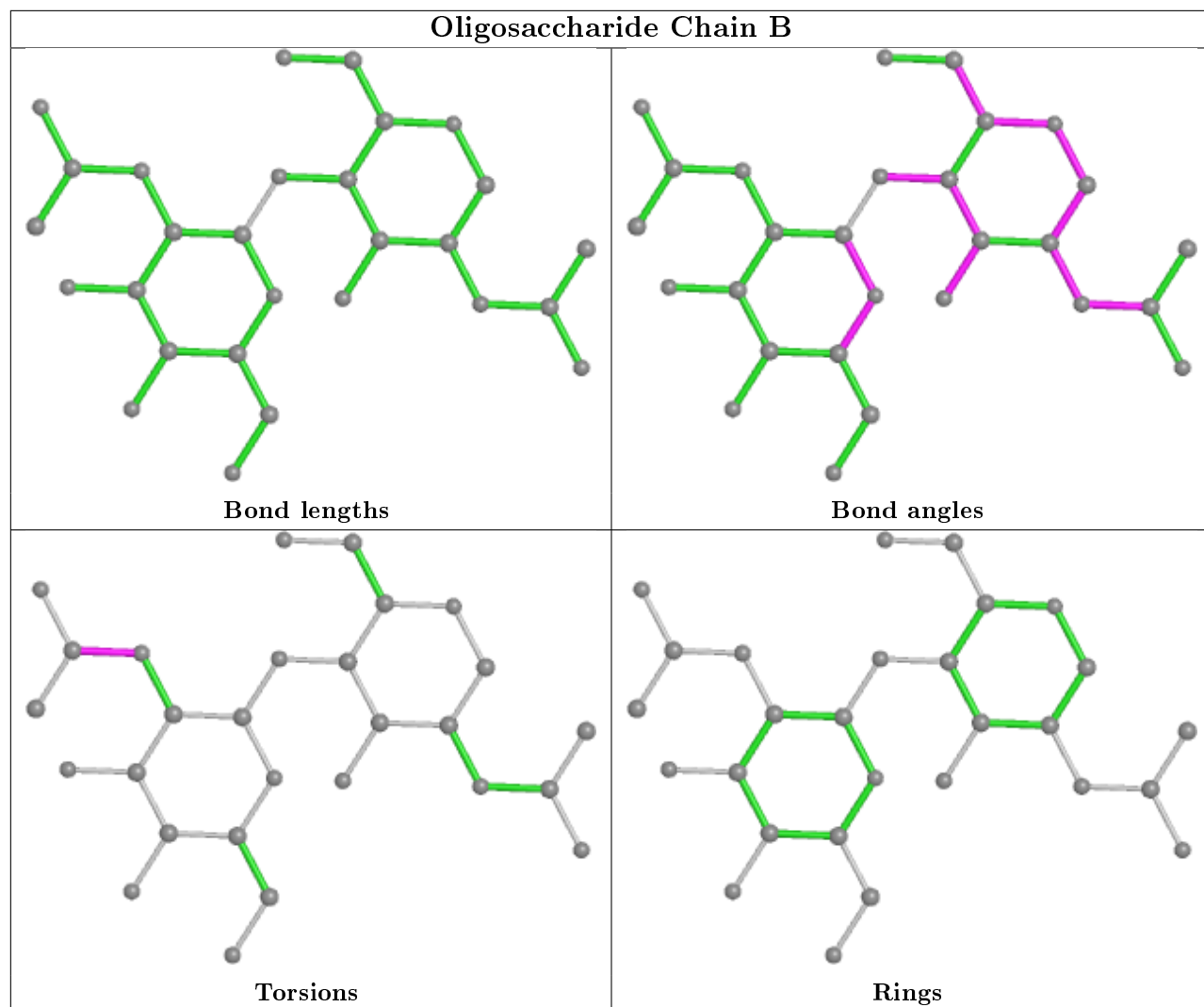
Mol	Chain	Res	Type	Atoms
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2

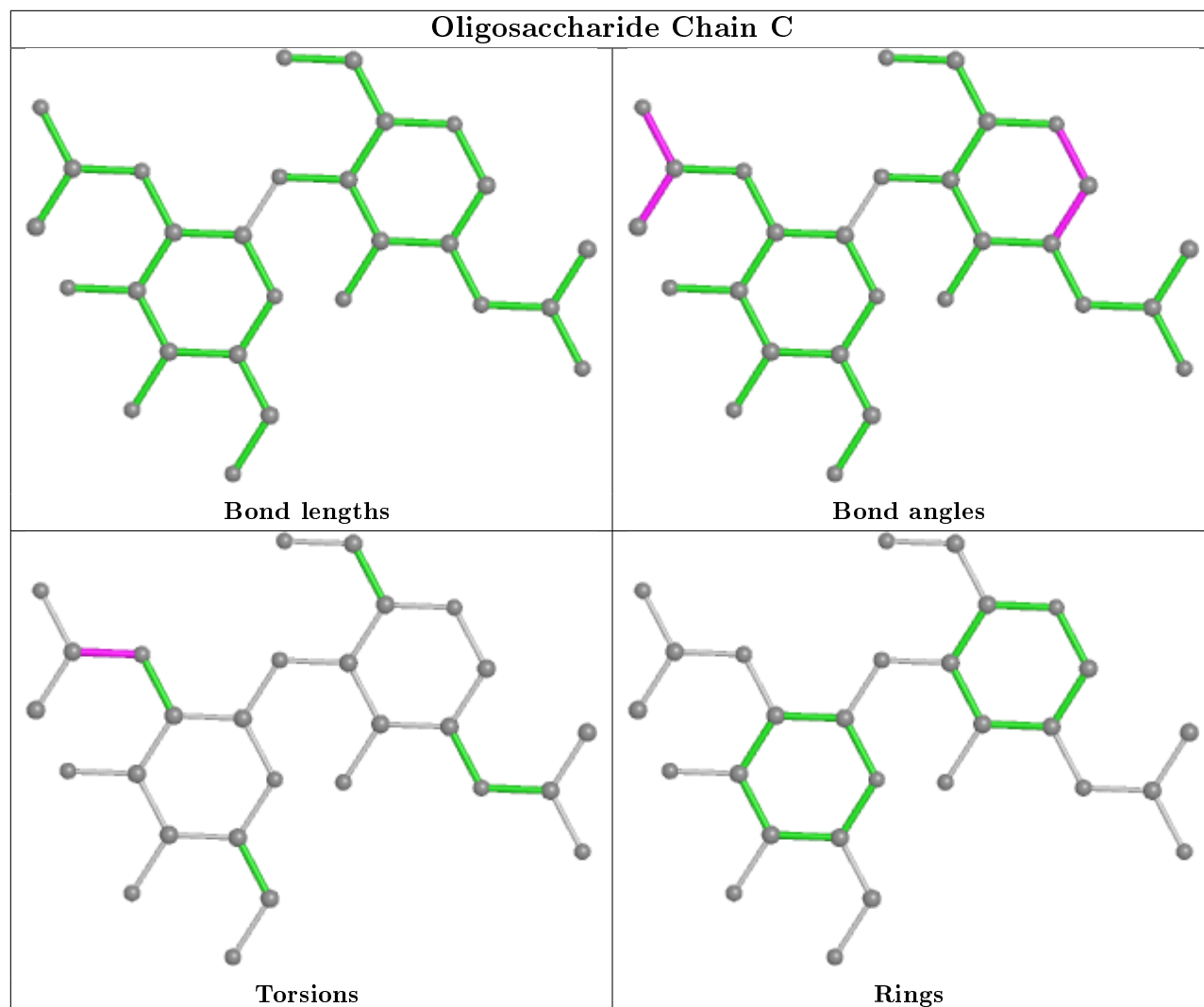
There are no ring outliers.

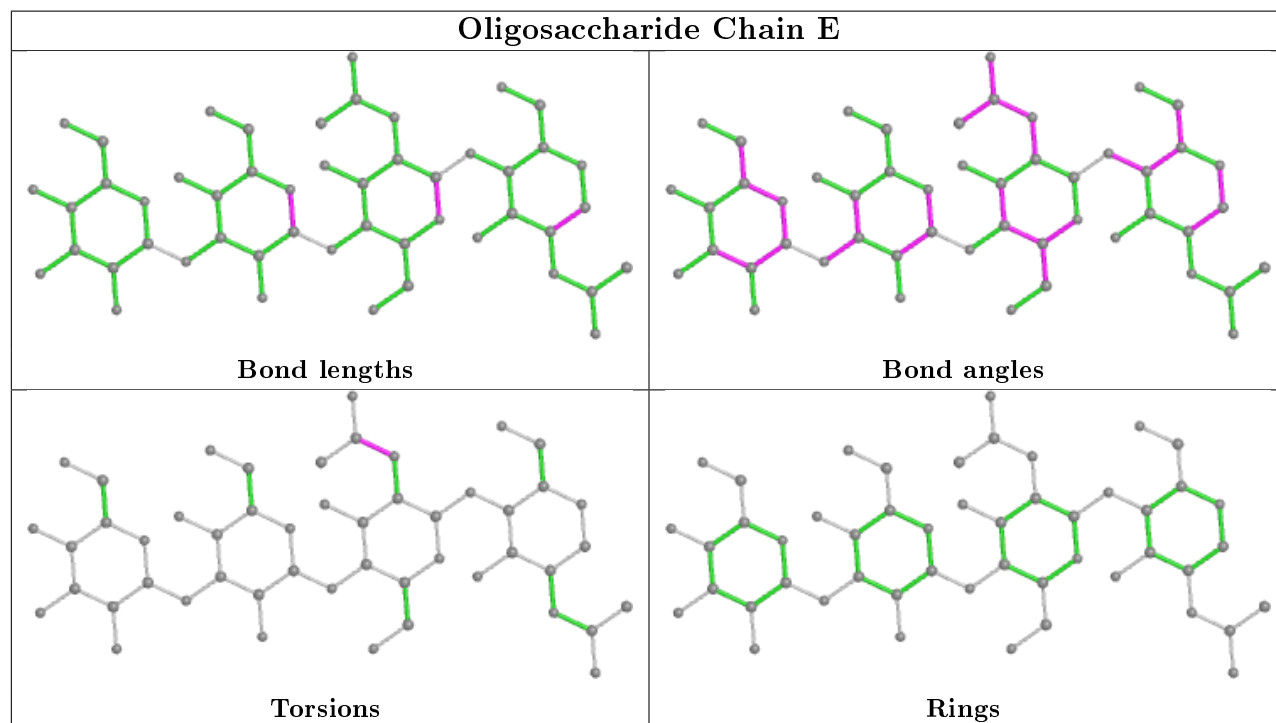
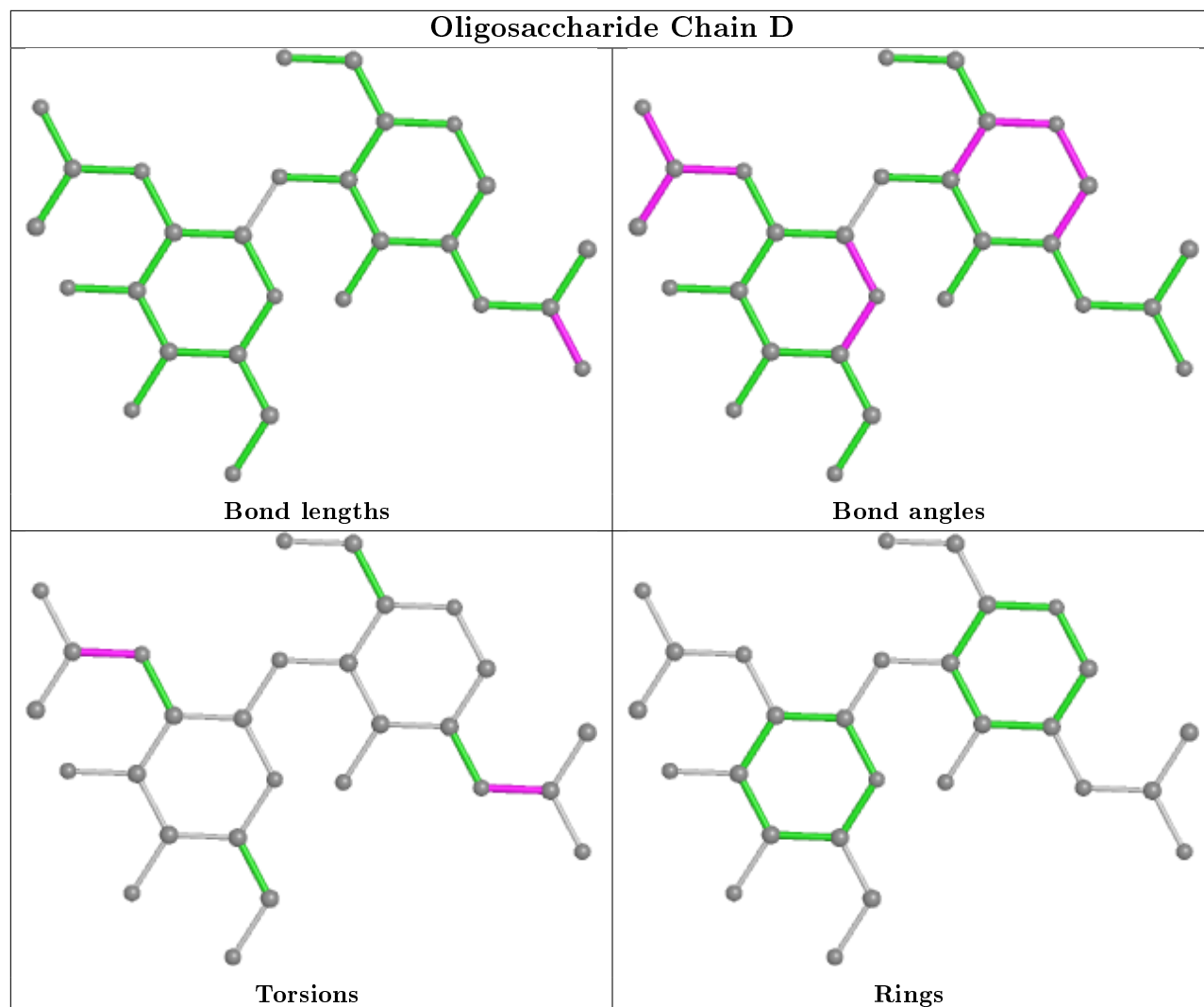
3 monomers are involved in 5 short contacts:

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

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







## 5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	1757	1	14,14,15	0.62	0	17,19,21	2.38	6 (35%)
8	QUS	A	1801	-	4,13,13	1.48	1 (25%)	0,18,18	0.00	-
4	NAG	A	1759	1	14,14,15	0.43	0	17,19,21	1.72	2 (11%)
4	NAG	A	1760	1	14,14,15	0.50	0	17,19,21	1.61	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1757	1	-	4/6/23/26	0/1/1/1
8	QUS	A	1801	-	-	1/2/8/8	0/1/1/1
4	NAG	A	1759	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1760	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1801	QUS	C02-NP3	-2.25	1.42	1.47

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1757	NAG	C1-O5-C5	7.42	122.25	112.19
4	A	1759	NAG	C1-O5-C5	5.66	119.86	112.19
4	A	1760	NAG	C1-O5-C5	4.86	118.77	112.19
4	A	1757	NAG	C3-C4-C5	2.69	115.04	110.24
4	A	1757	NAG	O5-C5-C6	2.61	111.30	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1759	NAG	C4-C3-C2	-2.47	107.40	111.02
4	A	1757	NAG	O5-C5-C4	2.46	116.81	110.83
4	A	1757	NAG	C1-C2-N2	-2.25	106.65	110.49
4	A	1757	NAG	O5-C1-C2	2.12	114.64	111.29
4	A	1760	NAG	C2-N2-C7	-2.10	119.92	122.90

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1757	NAG	C4-C5-C6-O6
4	A	1757	NAG	O5-C5-C6-O6
4	A	1760	NAG	C4-C5-C6-O6
4	A	1759	NAG	O5-C5-C6-O6
4	A	1760	NAG	O5-C5-C6-O6
4	A	1757	NAG	C8-C7-N2-C2
4	A	1757	NAG	O7-C7-N2-C2
4	A	1759	NAG	C4-C5-C6-O6
8	A	1801	QUS	NP3-C02-C03-N14

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1760	NAG	2	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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	689/709 (97%)	0.02	21 (3%)	50 47	13, 23, 41, 55	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	506	PHE	6.0
1	A	284	ALA	4.7
1	A	287	VAL	4.5
1	A	507	SER	4.4
1	A	505	GLU	3.9
1	A	283[A]	ILE	3.8
1	A	655[A]	LYS	3.2
1	A	285	GLU	3.2
1	A	288	GLY	3.1
1	A	487	GLY	3.1
1	A	336	ASN	3.0
1	A	55	LYS	3.0
1	A	544	ASN	2.9
1	A	719	VAL	2.9
1	A	134	ASP	2.6
1	A	335	GLY	2.5
1	A	334	THR	2.3
1	A	135	GLY	2.2
1	A	656[A]	SER	2.2
1	A	652[A]	ASP	2.1
1	A	536[A]	ARG	2.1

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

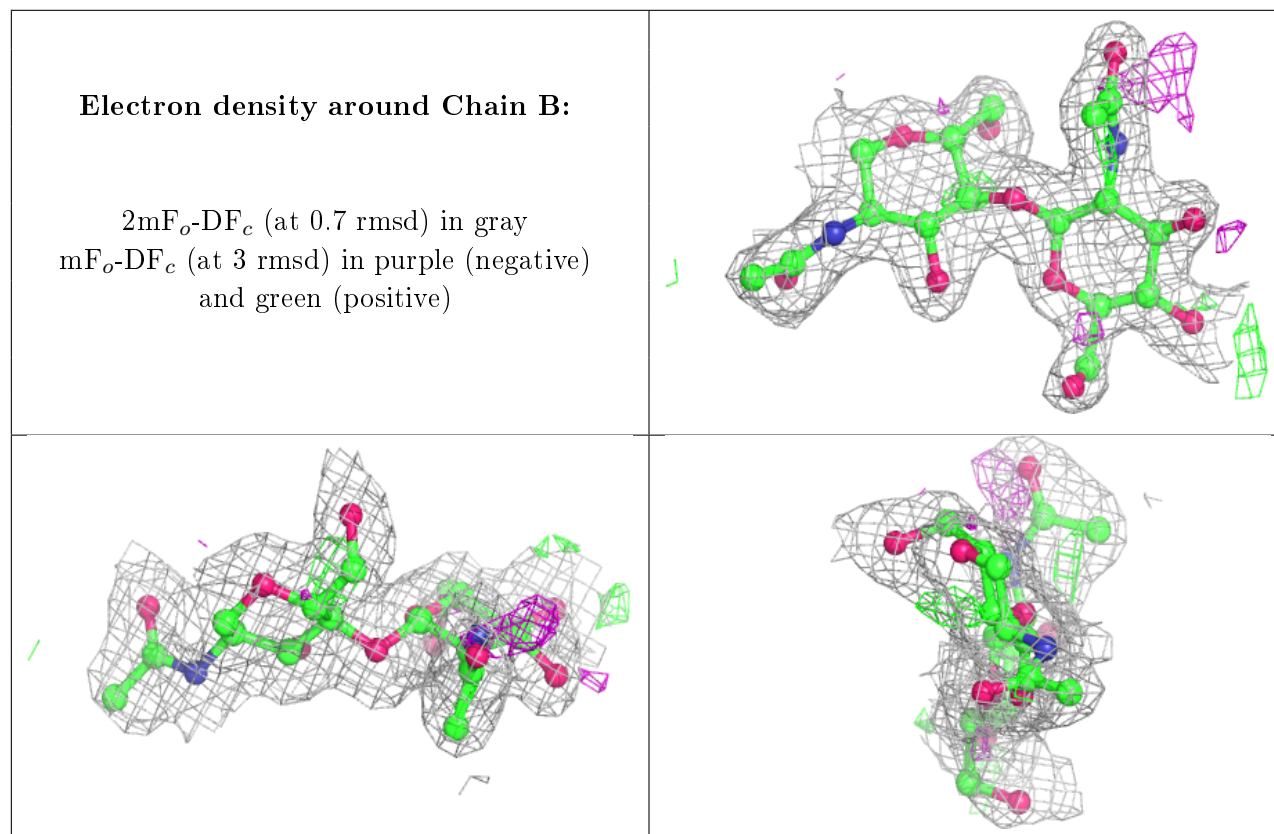
There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

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.

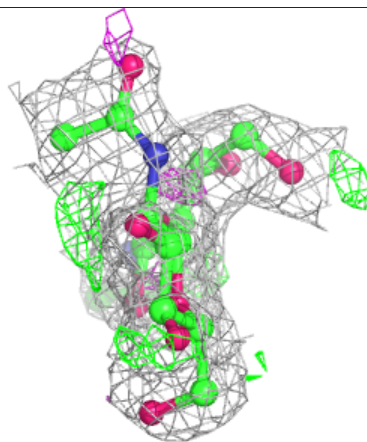
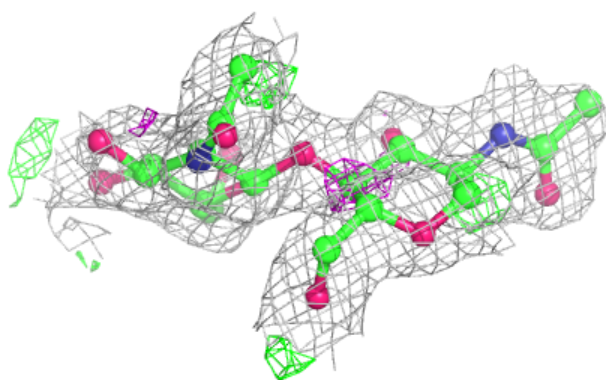
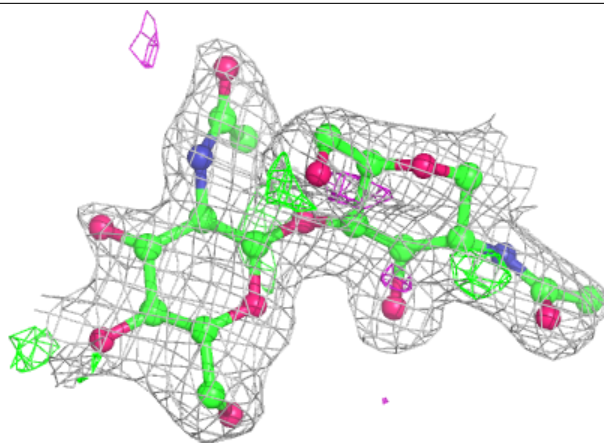
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	B	2	14/15	0.70	0.29	40,45,51,52	0
2	NAG	C	2	14/15	0.76	0.26	50,55,59,60	0
2	NAG	D	2	14/15	0.84	0.12	29,36,41,45	0
2	NAG	C	1	14/15	0.85	0.17	36,39,44,46	0
2	NAG	D	1	14/15	0.89	0.09	25,28,33,39	0
3	MAN	E	4	11/12	0.89	0.11	43,45,49,51	0
3	BMA	E	3	11/12	0.90	0.09	34,38,41,42	0
3	NAG	E	2	14/15	0.91	0.13	32,36,42,46	0
2	NAG	B	1	14/15	0.91	0.12	31,36,42,44	0
3	NAG	E	1	14/15	0.94	0.07	20,23,29,39	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.

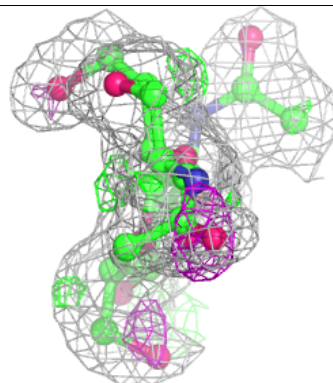
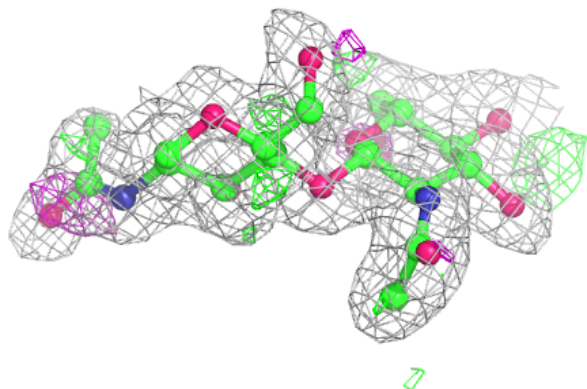
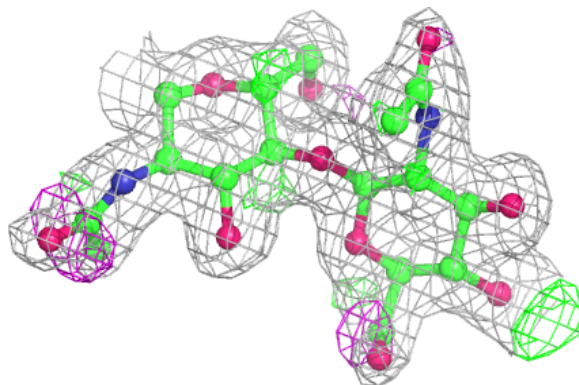


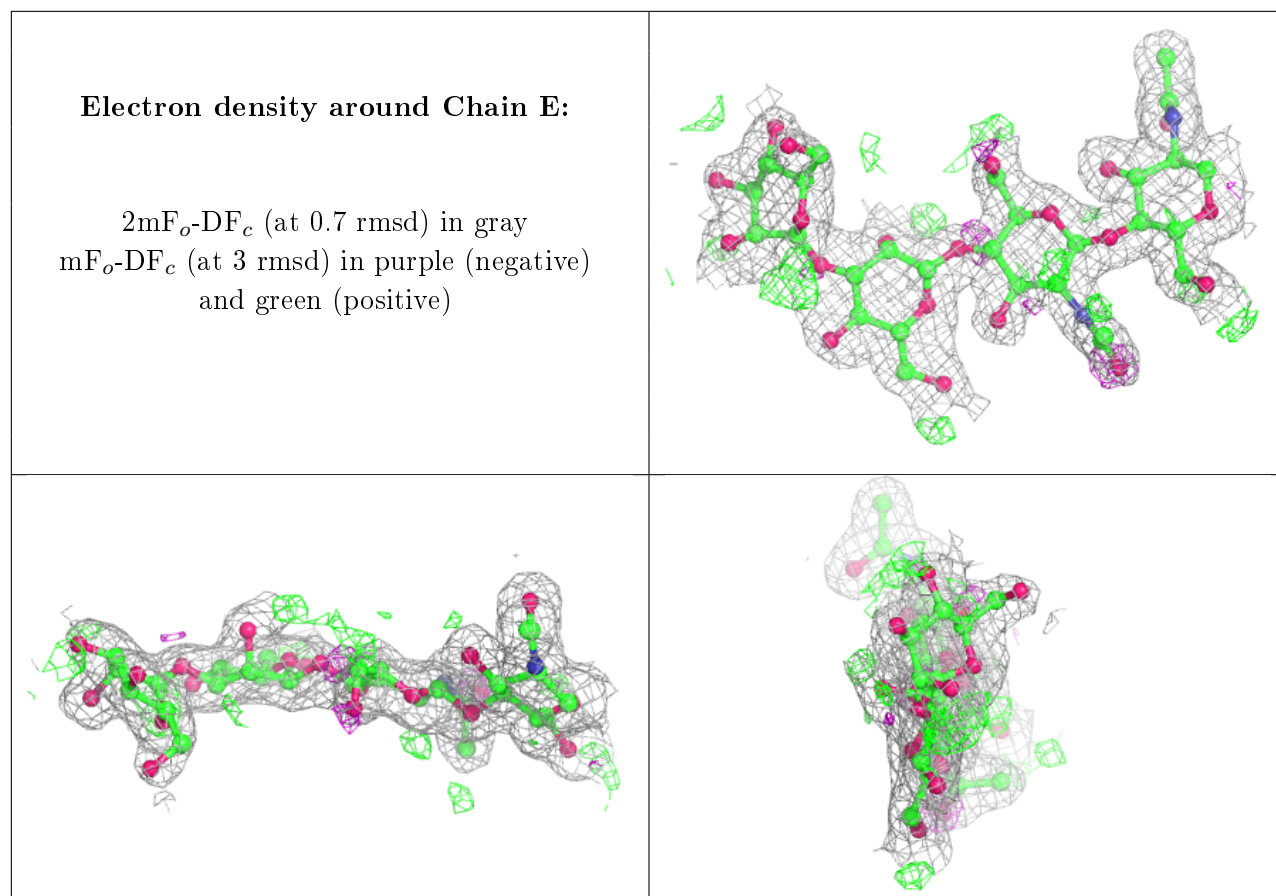
**Electron density around Chain C:**

$2mF_o-DF_c$  (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, 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
4	NAG	A	1757	14/15	0.61	0.26	45,51,56,56	0
4	NAG	A	1759	14/15	0.80	0.17	58,63,66,67	0
4	NAG	A	1760	14/15	0.81	0.15	28,48,56,56	0
8	QUS	A	1801	13/13	0.93	0.11	17,21,29,30	0
5	ZN	A	1751	1/1	1.00	0.05	20,20,20,20	0
5	ZN	A	1752	1/1	1.00	0.06	18,18,18,18	0
6	CA	A	1753	1/1	1.00	0.08	15,15,15,15	0
7	CL	A	1754	1/1	1.00	0.06	21,21,21,21	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.