



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 10:00 AM BST

PDB ID : 3K36  
Title : Crystal Structure of B/Perth Neuraminidase  
Authors : Oakley, A.J.; McKimm-Breschkin, J.L.  
Deposited on : 2009-10-02  
Resolution : 2.20 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.

---

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

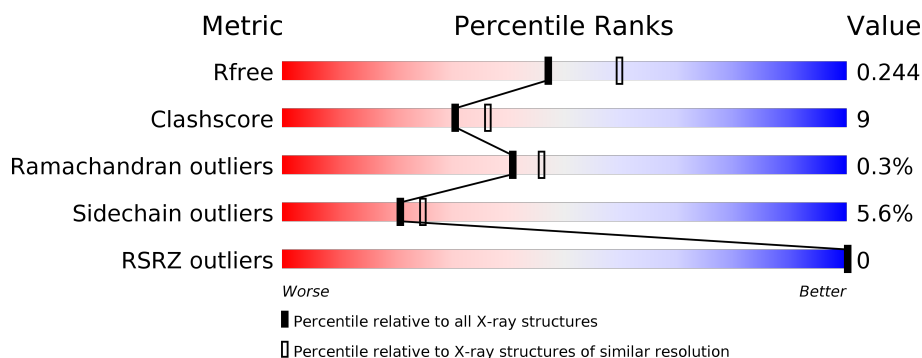
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	397	<div> <div>79%</div> <div>16%</div> <div>••</div> </div>
1	B	397	<div> <div>81%</div> <div>15%</div> <div>••</div> </div>
2	C	6	<div> <div>33%</div> <div>33%</div> <div>33%</div> </div>
2	D	6	<div> <div>33%</div> <div>33%</div> <div>33%</div> </div>

## 2 Entry composition [i](#)

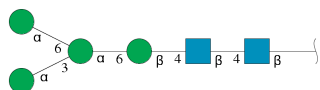
There are 7 unique types of molecules in this entry. The entry contains 6578 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Neuraminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	8	0
			3043	1912	523	579	29			
1	B	389	Total	C	N	O	S	0	5	0
			3031	1904	522	576	29			

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



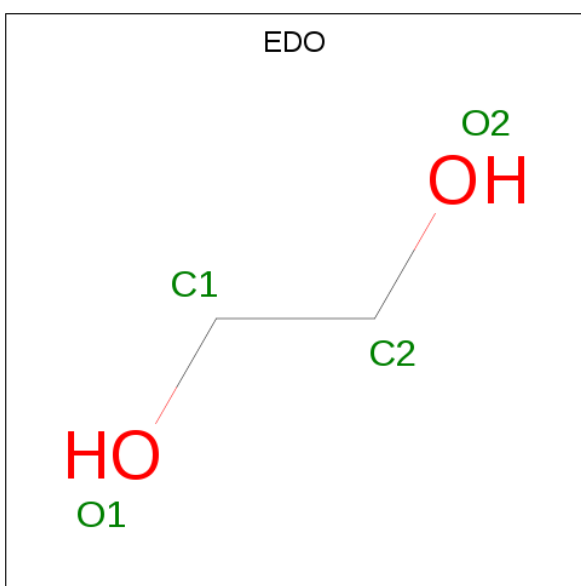
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	6	Total	C	N	O	0	0	0
			72	40	2	30			
2	D	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

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

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

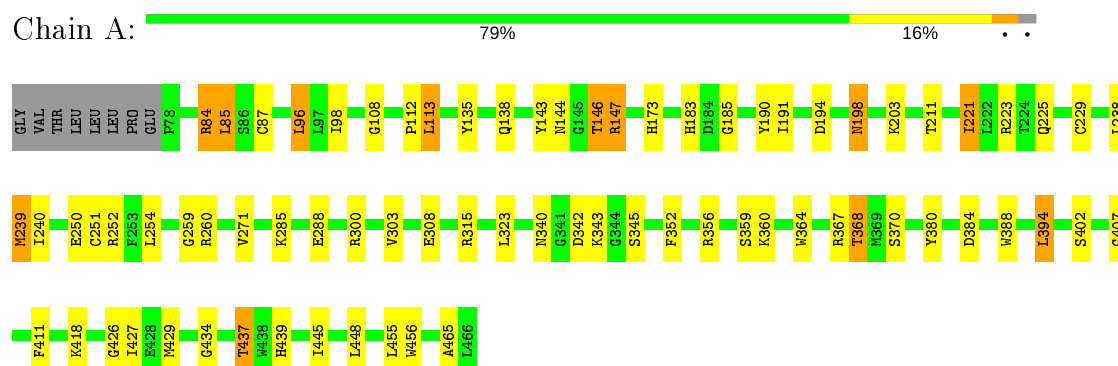
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	166	Total	O	0	0
			166	166		
7	B	150	Total	O	0	0
			150	150		

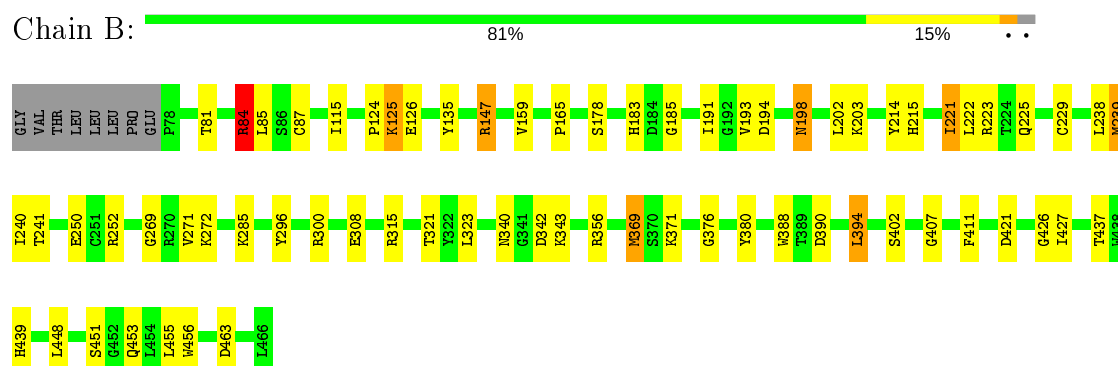
### 3 Residue-property plots [i](#)

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.

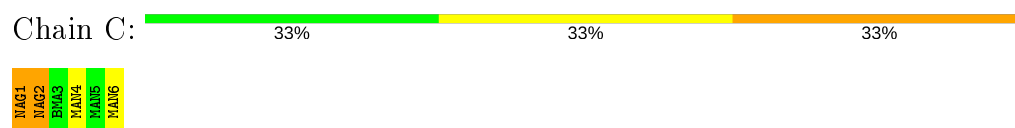
#### • Molecule 1: Neuraminidase



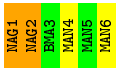
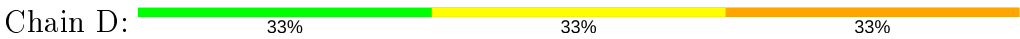
#### • Molecule 1: Neuraminidase



#### • Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



#### • Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.64Å 87.64Å 197.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	98.53 – 2.20 26.70 – 2.20	Depositor EDS
% Data completeness (in resolution range)	91.3 (98.53-2.20) 91.4 (26.70-2.20)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.43 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.182 , 0.239 0.188 , 0.244	Depositor DCC
$R_{free}$ test set	1726 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.9	Xtriage
Anisotropy	0.347	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 28.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.479 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6578	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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: GOL, BMA, NAG, CA, EDO, SO4, 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	0.68	0/3140	0.76	0/4240
1	B	0.68	0/3119	0.77	2/4211 (0.0%)
All	All	0.68	0/6259	0.77	2/8451 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	463	ASP	CB-CG-OD2	6.37	124.03	118.30
1	B	84	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	340	ASN	Peptide
1	B	340	ASN	Peptide

## 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	3043	0	2960	63	0
1	B	3031	0	2942	51	0
2	C	72	0	61	3	0
2	D	72	0	61	3	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	4	0	6	0	0
4	B	4	0	6	0	0
5	A	6	0	8	2	0
5	B	18	0	24	5	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	166	0	0	18	0
7	B	150	0	0	8	0
All	All	6578	0	6068	113	0

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 9.

All (113) 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:194:ASP:HB2	1:A:203:LYS:NZ	1.86	0.91
1:B:448:LEU:HD23	7:B:574:HOH:O	1.72	0.87
1:A:407:GLY:HA2	7:A:597:HOH:O	1.81	0.81
1:B:407:GLY:HA2	7:B:555:HOH:O	1.79	0.81
1:A:194:ASP:HB2	1:A:203:LYS:HZ1	1.43	0.81
1:A:183:HIS:HD2	1:A:185:GLY:H	1.30	0.80
1:B:225:GLN:HE21	1:B:239:MET:H	1.30	0.79
1:B:198:ASN:HD22	1:B:198:ASN:H	1.31	0.78
1:A:225:GLN:HE21	1:A:239:MET:H	1.30	0.78
5:B:471:GOL:H12	7:B:535:HOH:O	1.84	0.77
1:B:183:HIS:HD2	1:B:185:GLY:H	1.35	0.74
1:A:87:CYS:HB2	7:A:589:HOH:O	1.89	0.72
1:A:368:THR:CG2	1:A:370:SER:O	2.37	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:GLY:O	7:A:571:HOH:O	2.08	0.72
1:B:85:LEU:HD22	2:D:2:NAG:O6	1.91	0.71
1:B:183:HIS:CD2	1:B:185:GLY:H	2.10	0.69
1:B:221:ILE:O	1:B:223:ARG:HD3	1.93	0.68
1:A:221:ILE:O	1:A:223:ARG:HD3	1.92	0.68
1:A:250:GLU:HG2	1:A:271:VAL:HG12	1.76	0.67
1:A:198:ASN:HD22	1:A:198:ASN:H	1.41	0.67
1:A:211[A]:THR:HG23	1:A:259:GLY:O	1.94	0.66
1:A:96:LEU:HD11	1:A:98:ILE:HD11	1.78	0.66
1:A:211[A]:THR:HG21	1:A:259:GLY:HA3	1.79	0.64
1:B:315:ARG:HB2	1:B:388:TRP:CD1	2.32	0.64
1:A:146:THR:HG22	7:A:65:HOH:O	1.98	0.63
1:B:250[A]:GLU:HG3	1:B:271:VAL:CG1	2.28	0.63
1:B:240:ILE:HG23	7:B:500:HOH:O	1.97	0.63
1:A:143:TYR:O	1:A:146:THR:HB	1.98	0.63
1:A:437:THR:HG23	7:A:557:HOH:O	1.99	0.62
1:A:368:THR:HG23	1:A:370:SER:O	1.99	0.62
1:A:271:VAL:HG13	7:A:539:HOH:O	2.01	0.61
5:A:469:GOL:H32	7:A:547:HOH:O	2.00	0.60
1:A:271:VAL:HG12	1:A:271:VAL:O	2.01	0.59
1:B:271:VAL:HG13	7:B:532:HOH:O	2.01	0.59
5:A:469:GOL:C3	7:A:547:HOH:O	2.51	0.59
1:A:250:GLU:OE1	7:A:558:HOH:O	2.17	0.58
1:A:147:ARG:HH11	1:A:434:GLY:HA2	1.68	0.58
1:B:269:GLY:O	1:B:271:VAL:HG23	2.04	0.58
1:A:343:LYS:HE2	1:B:437:THR:HG21	1.86	0.57
1:A:198:ASN:HD22	1:A:198:ASN:N	2.03	0.57
1:A:411:PHE:CZ	1:A:426:GLY:HA3	2.39	0.57
1:A:437:THR:HG21	1:B:343:LYS:CE	2.36	0.55
1:B:250[A]:GLU:HG3	1:B:271:VAL:HG12	1.89	0.55
1:A:194:ASP:HB2	1:A:203:LYS:HZ2	1.66	0.55
1:B:194:ASP:OD1	1:B:203:LYS:NZ	2.38	0.55
1:B:215:HIS:HB2	5:B:469:GOL:H12	1.90	0.54
1:B:427:ILE:CG2	7:B:555:HOH:O	2.55	0.53
1:A:85:LEU:HD22	2:C:2:NAG:H61	1.90	0.53
1:B:369:MET:HB2	1:B:376:GLY:HA3	1.93	0.51
1:B:124:PRO:C	5:B:470:GOL:H12	2.30	0.51
1:B:87:CYS:HB2	7:B:574:HOH:O	2.10	0.51
1:A:465:ALA:HB3	1:B:371:LYS:HE3	1.93	0.50
1:B:271:VAL:HG12	1:B:271:VAL:O	2.12	0.50
1:A:345:SER:HB3	7:A:582:HOH:O	2.10	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:LYS:CE	1:B:437:THR:HG21	2.42	0.50
1:B:411:PHE:CZ	1:B:426:GLY:HA3	2.47	0.50
1:A:380:TYR:HB3	1:A:394:LEU:HB3	1.94	0.50
1:A:183:HIS:CD2	1:A:185:GLY:H	2.21	0.49
1:A:240:ILE:O	1:A:251:CYS:HB2	2.12	0.49
1:B:191:ILE:HD13	1:B:238:LEU:HD22	1.94	0.49
1:A:144:ASN:ND2	7:A:607:HOH:O	2.37	0.48
1:A:448:LEU:HD23	7:A:589:HOH:O	2.13	0.48
1:B:81[B]:THR:HG23	1:B:185:GLY:CA	2.44	0.48
1:B:321:THR:HB	1:B:394:LEU:HD22	1.94	0.48
1:B:115:ILE:C	1:B:115:ILE:HD12	2.34	0.47
1:B:300:ARG:HG3	1:B:323:LEU:HB2	1.96	0.47
1:A:356:ARG:HD2	2:C:1:NAG:H81	1.97	0.47
1:B:81[B]:THR:HG23	1:B:185:GLY:HA2	1.95	0.47
1:A:211[A]:THR:OG1	1:A:260:ARG:CZ	2.62	0.47
1:B:285:LYS:HG2	1:B:308:GLU:OE2	2.15	0.47
1:A:288:GLU:HA	1:A:303:VAL:O	2.15	0.46
1:A:315:ARG:HB2	1:A:388:TRP:CD1	2.51	0.46
1:A:198:ASN:ND2	1:A:198:ASN:H	2.11	0.46
1:A:225:GLN:NE2	1:A:238:LEU:HD12	2.30	0.46
1:B:84:ARG:HD3	1:B:421:ASP:OD1	2.16	0.45
1:A:85:LEU:HD22	2:C:2:NAG:C6	2.47	0.45
1:A:285:LYS:HE2	1:A:285:LYS:HB3	1.62	0.45
1:B:198:ASN:ND2	1:B:198:ASN:H	2.06	0.45
1:A:191:ILE:HD13	1:A:238:LEU:HD22	1.98	0.45
1:A:173:HIS:CE1	1:A:190:TYR:CE1	3.05	0.45
1:B:124:PRO:O	5:B:470:GOL:H12	2.18	0.44
1:A:225:GLN:NE2	1:A:239:MET:H	2.08	0.43
1:A:285:LYS:HG2	1:A:308:GLU:OE2	2.18	0.43
1:A:427:ILE:CG2	7:A:597:HOH:O	2.65	0.43
1:A:429:MET:HG2	7:A:597:HOH:O	2.17	0.43
1:B:125:LYS:HG3	1:B:126:GLU:HB2	1.99	0.43
1:B:147:ARG:HG3	1:B:439:HIS:CD2	2.54	0.43
1:B:159:VAL:HG11	1:B:165:PRO:HA	2.01	0.43
1:A:112:PRO:HD2	1:A:138:GLN:O	2.20	0.42
1:A:360:LYS:HG3	1:A:384:ASP:OD1	2.19	0.42
1:A:352:PHE:HA	1:A:364:TRP:O	2.19	0.42
1:B:202:LEU:HD13	1:B:240:ILE:HG21	2.02	0.42
1:A:271:VAL:CG1	1:A:271:VAL:O	2.65	0.42
1:B:272:LYS:HE2	1:B:296:TYR:CZ	2.54	0.42
1:B:178:SER:HB3	1:B:193:VAL:HB	2.01	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:LEU:HG	7:A:532:HOH:O	2.20	0.41
1:A:84:ARG:NH2	1:A:418:LYS:O	2.53	0.41
1:A:445:ILE:N	1:A:445:ILE:HD12	2.35	0.41
1:A:323:LEU:HD23	1:A:367:ARG:HD3	2.02	0.41
1:B:427:ILE:HG22	7:B:555:HOH:O	2.16	0.41
1:B:85:LEU:HD22	2:D:2:NAG:C6	2.50	0.41
7:A:599:HOH:O	1:B:343:LYS:HD3	2.20	0.41
1:B:356:ARG:HD2	2:D:1:NAG:H81	2.02	0.41
1:A:113:LEU:HA	1:A:113:LEU:HD12	1.85	0.41
1:B:380:TYR:HB3	1:B:394:LEU:HB3	2.03	0.41
1:A:343:LYS:HG3	7:A:569:HOH:O	2.21	0.41
1:B:390:ASP:C	1:B:390:ASP:OD1	2.58	0.40
1:B:193:VAL:HG11	1:B:222:LEU:O	2.21	0.40
1:B:315:ARG:HB2	1:B:388:TRP:CG	2.57	0.40
1:A:146:THR:CG2	1:A:439:HIS:H	2.33	0.40
1:B:214:TYR:CD1	5:B:469:GOL:H32	2.56	0.40
1:A:271:VAL:HG11	7:A:549:HOH:O	2.20	0.40
1:A:300:ARG:HG3	1:A:323:LEU:HB2	2.03	0.40

There are no symmetry-related clashes.

## 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	395/397 (100%)	376 (95%)	18 (5%)	1 (0%)	41	46
1	B	392/397 (99%)	373 (95%)	18 (5%)	1 (0%)	41	46
All	All	787/794 (99%)	749 (95%)	36 (5%)	2 (0%)	41	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	221	ILE
1	B	221	ILE

### 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	330/329 (100%)	311 (94%)	19 (6%)	20	23
1	B	327/329 (99%)	310 (95%)	17 (5%)	23	28
All	All	657/658 (100%)	621 (94%)	36 (6%)	21	26

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	ARG
1	A	85	LEU
1	A	96	LEU
1	A	113	LEU
1	A	135	TYR
1	A	146	THR
1	A	147	ARG
1	A	198	ASN
1	A	229	CYS
1	A	239	MET
1	A	252	ARG
1	A	342	ASP
1	A	359	SER
1	A	368	THR
1	A	394	LEU
1	A	402	SER
1	A	437	THR
1	A	455	LEU
1	A	456	TRP
1	B	84	ARG
1	B	125	LYS
1	B	135	TYR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	147	ARG
1	B	198	ASN
1	B	229	CYS
1	B	239	MET
1	B	241	THR
1	B	252	ARG
1	B	342	ASP
1	B	369	MET
1	B	394	LEU
1	B	402	SER
1	B	451	SER
1	B	453	GLN
1	B	455	LEU
1	B	456	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	183	HIS
1	A	198	ASN
1	A	225	GLN
1	A	431	HIS
1	A	439	HIS
1	B	183	HIS
1	B	198	ASN
1	B	225	GLN
1	B	439	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](#)

12 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	C	1	1,2	14,14,15	0.55	0	17,19,21	1.11	1 (5%)
2	NAG	C	2	2	14,14,15	0.66	0	17,19,21	1.21	2 (11%)
2	BMA	C	3	2	11,11,12	0.64	0	15,15,17	0.73	0
2	MAN	C	4	2	11,11,12	0.53	0	15,15,17	2.27	4 (26%)
2	MAN	C	5	2	11,11,12	0.60	0	15,15,17	0.70	0
2	MAN	C	6	2	11,11,12	0.85	0	15,15,17	2.27	3 (20%)
2	NAG	D	1	1,2	14,14,15	0.61	0	17,19,21	1.39	1 (5%)
2	NAG	D	2	2	14,14,15	0.62	0	17,19,21	1.18	2 (11%)
2	BMA	D	3	2	11,11,12	0.66	0	15,15,17	0.90	0
2	MAN	D	4	2	11,11,12	0.51	0	15,15,17	1.43	2 (13%)
2	MAN	D	5	2	11,11,12	0.58	0	15,15,17	0.68	0
2	MAN	D	6	2	11,11,12	0.48	0	15,15,17	1.60	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	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	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	1/2/19/22	0/1/1/1
2	MAN	C	5	2	-	2/2/19/22	0/1/1/1
2	MAN	C	6	2	-	0/2/19/22	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1
2	MAN	D	4	2	-	0/2/19/22	0/1/1/1
2	MAN	D	5	2	-	0/2/19/22	0/1/1/1
2	MAN	D	6	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	6	MAN	C1-C2-C3	6.83	118.06	109.67
2	D	6	MAN	C1-O5-C5	5.63	119.81	112.19
2	C	4	MAN	O5-C5-C6	5.05	115.13	107.20
2	C	4	MAN	C1-O5-C5	4.95	118.90	112.19
2	D	1	NAG	C1-O5-C5	4.42	118.18	112.19
2	C	6	MAN	C1-O5-C5	3.81	117.36	112.19
2	D	4	MAN	C1-O5-C5	3.49	116.92	112.19
2	C	4	MAN	O5-C1-C2	3.28	115.84	110.77
2	D	2	NAG	C3-C4-C5	2.99	115.56	110.24
2	C	1	NAG	C1-O5-C5	2.95	116.19	112.19
2	C	2	NAG	C3-C4-C5	2.71	115.07	110.24
2	D	4	MAN	C1-C2-C3	2.68	112.96	109.67
2	D	2	NAG	C4-C3-C2	2.67	114.93	111.02
2	C	6	MAN	C2-C3-C4	2.62	115.42	110.89
2	C	2	NAG	C4-C3-C2	2.40	114.54	111.02
2	C	4	MAN	C1-C2-C3	2.25	112.44	109.67

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	NAG	O5-C5-C6-O6
2	C	5	MAN	O5-C5-C6-O6
2	C	5	MAN	C4-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	C	4	MAN	O5-C5-C6-O6

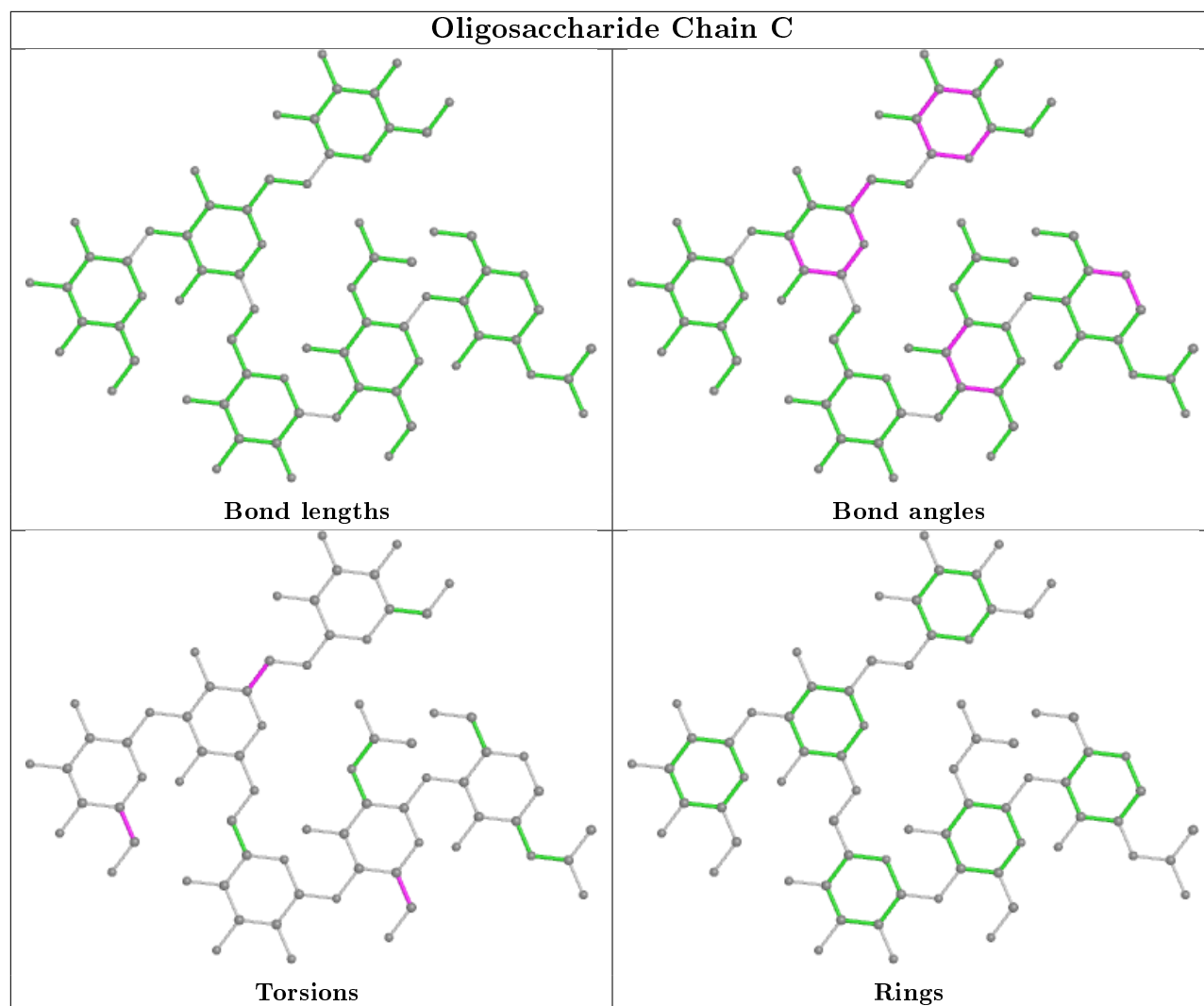
There are no ring outliers.

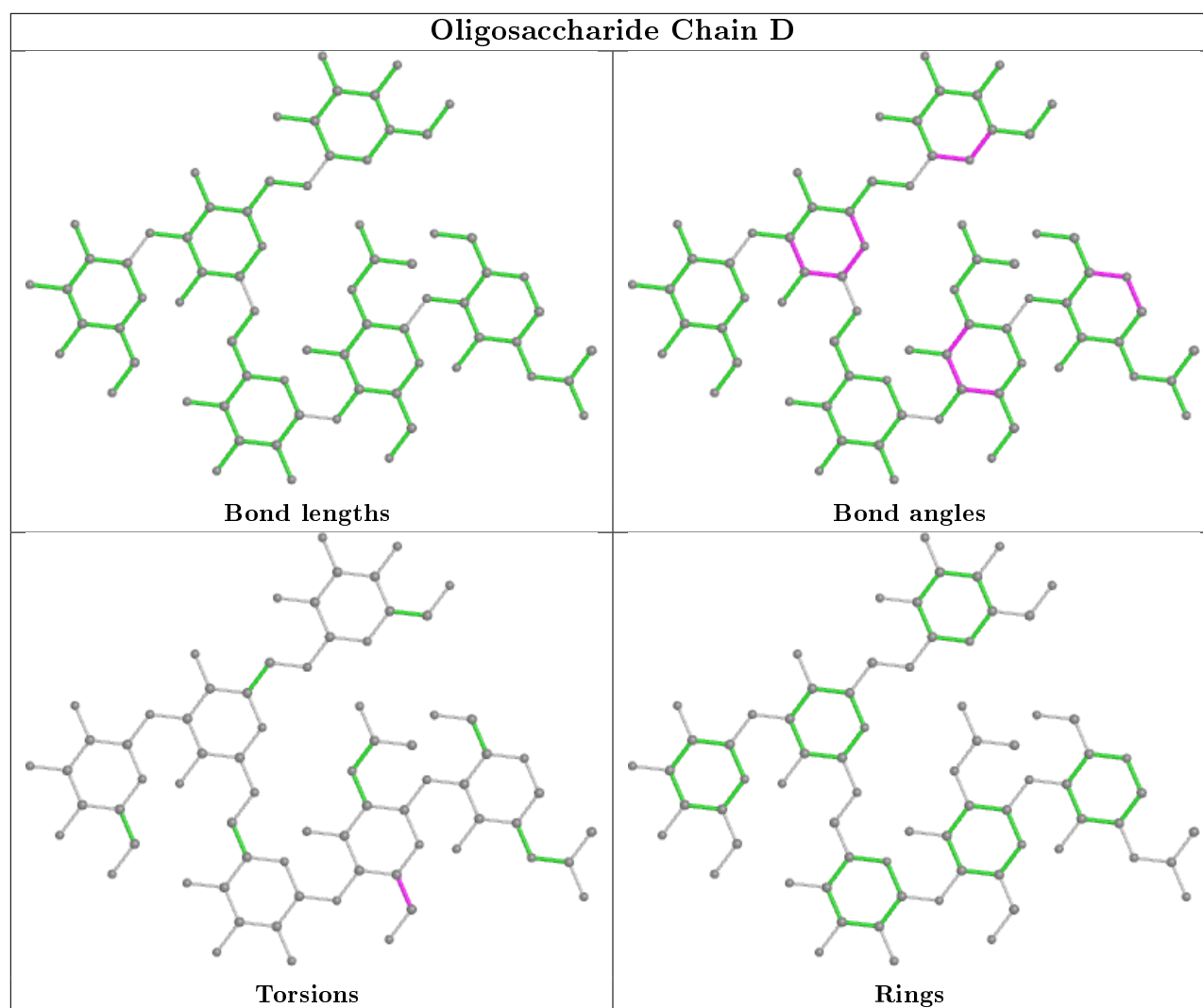
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	1	0
2	C	1	NAG	1	0
2	D	2	NAG	2	0
2	C	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 [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	EDO	B	468	-	3,3,3	0.54	0	2,2,2	0.14	0
4	EDO	A	468	-	3,3,3	0.45	0	2,2,2	0.02	0
5	GOL	B	471	-	5,5,5	0.35	0	5,5,5	0.17	0
3	SO4	B	467	-	4,4,4	0.21	0	6,6,6	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GOL	B	470	-	5,5,5	0.36	0	5,5,5	0.80	0
5	GOL	A	469	-	5,5,5	0.36	0	5,5,5	0.58	0
5	GOL	B	469	-	5,5,5	0.42	0	5,5,5	0.49	0
3	SO4	A	467	-	4,4,4	0.27	0	6,6,6	0.13	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	468	-	-	0/1/1/1	-
4	EDO	A	468	-	-	1/1/1/1	-
5	GOL	B	471	-	-	0/4/4/4	-
5	GOL	B	470	-	-	2/4/4/4	-
5	GOL	A	469	-	-	2/4/4/4	-
5	GOL	B	469	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	470	GOL	C1-C2-C3-O3
5	A	469	GOL	O1-C1-C2-C3
5	B	470	GOL	O2-C2-C3-O3
5	A	469	GOL	O1-C1-C2-O2
4	A	468	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	471	GOL	1	0
5	B	470	GOL	2	0
5	A	469	GOL	2	0
5	B	469	GOL	2	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	389/397 (97%)	-0.59	0 100 100	12, 19, 29, 40	1 (0%)
1	B	389/397 (97%)	-0.60	0 100 100	12, 19, 29, 36	5 (1%)
All	All	778/794 (97%)	-0.60	0 100 100	12, 19, 29, 40	6 (0%)

There are no RSRZ outliers to report.

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

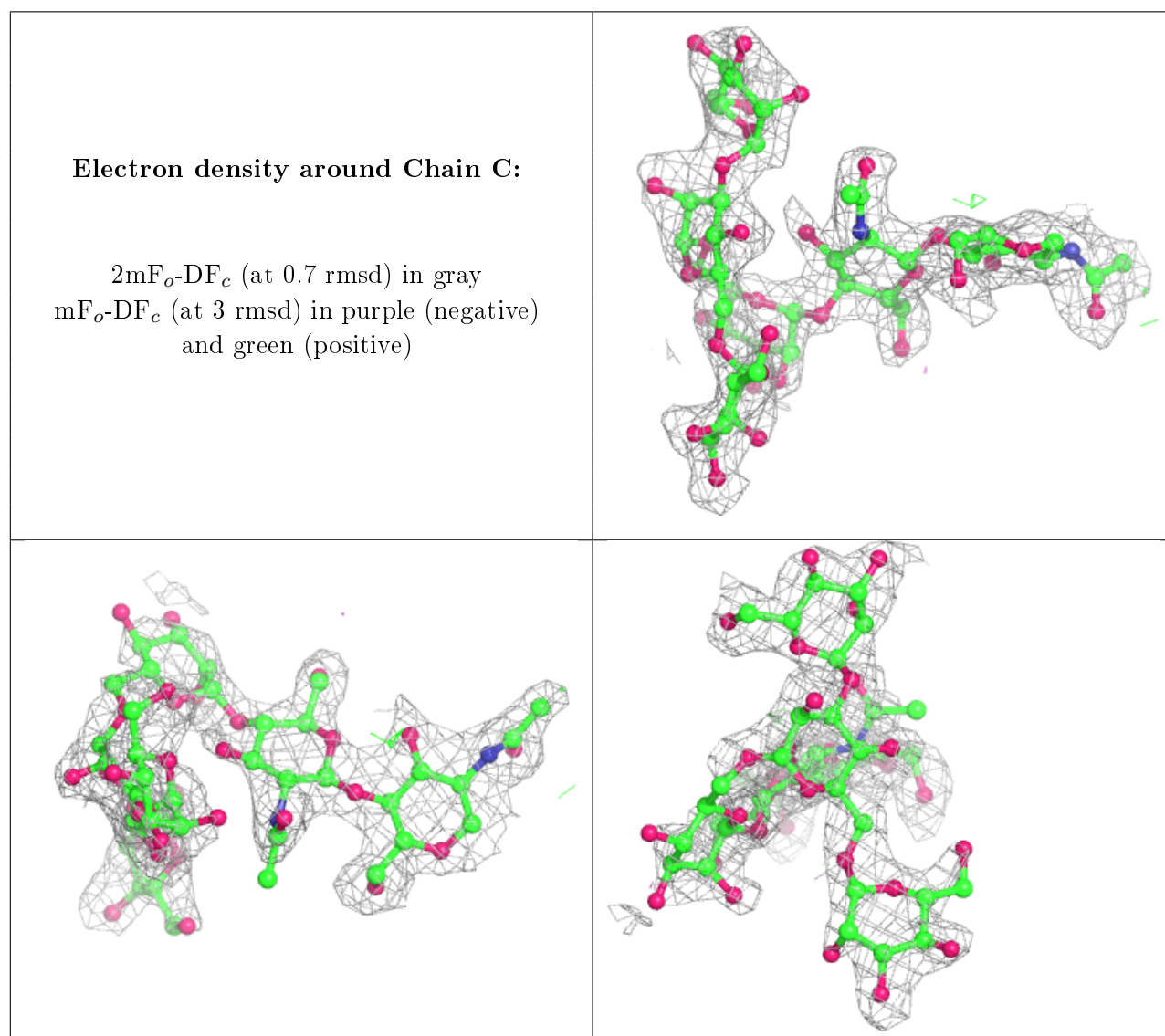
There are no non-standard protein/DNA/RNA residues in this entry.

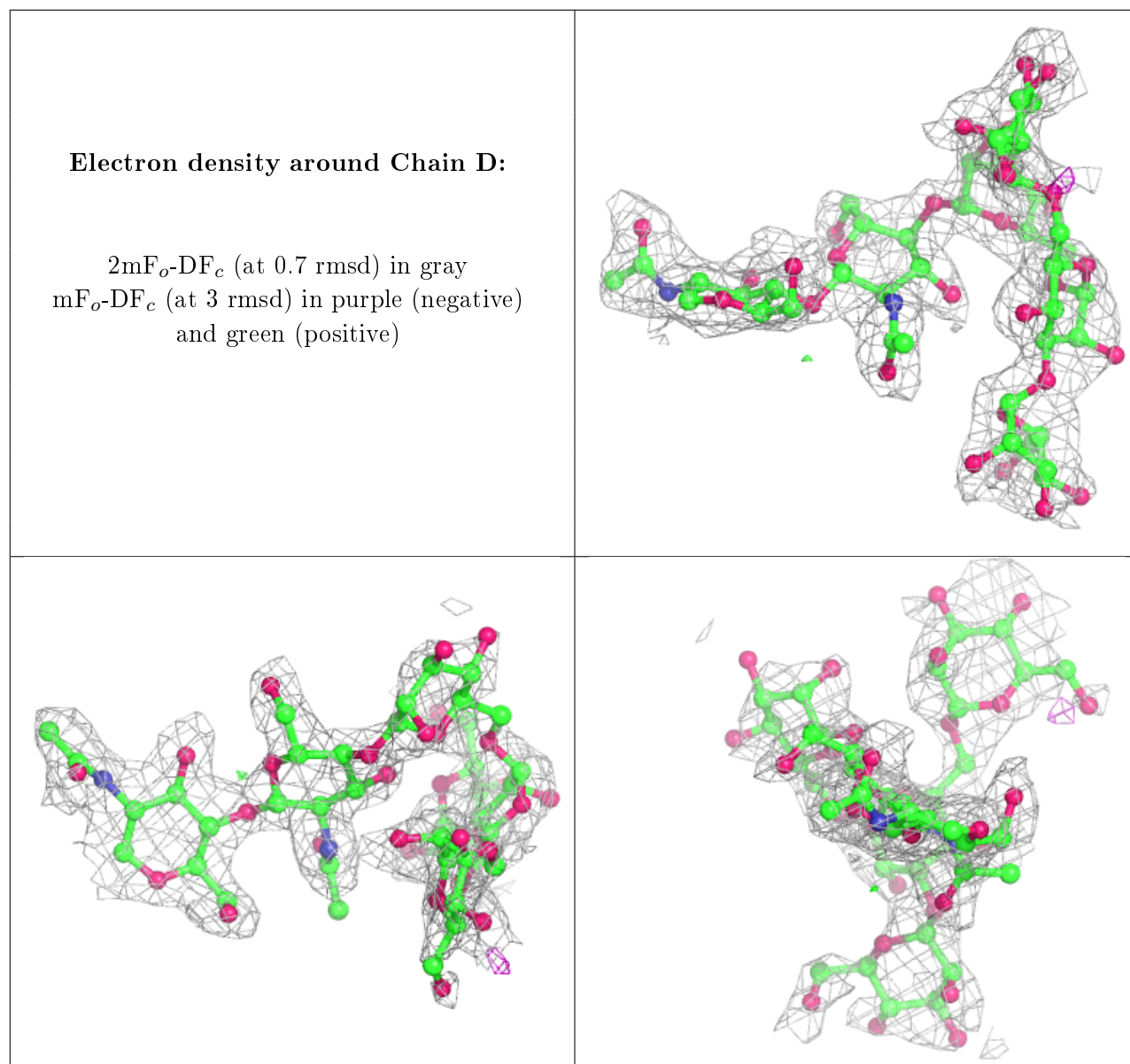
### 6.3 Carbohydrates [i](#)

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(Å <sup>2</sup> )	Q<0.9
2	MAN	D	5	11/12	0.63	0.21	73,73,74,74	0
2	BMA	C	3	11/12	0.72	0.27	61,63,64,64	0
2	MAN	D	6	11/12	0.74	0.20	74,74,75,76	0
2	MAN	C	6	11/12	0.78	0.22	67,67,68,68	0
2	MAN	C	5	11/12	0.79	0.18	69,69,70,70	0
2	MAN	C	4	11/12	0.80	0.14	64,65,66,67	0
2	BMA	D	3	11/12	0.81	0.25	64,66,69,70	0
2	NAG	C	2	14/15	0.83	0.22	49,52,54,58	0
2	MAN	D	4	11/12	0.84	0.15	70,71,73,74	0
2	NAG	D	2	14/15	0.86	0.22	51,54,57,61	0
2	NAG	D	1	14/15	0.90	0.13	35,38,42,46	0
2	NAG	C	1	14/15	0.90	0.13	36,39,43,46	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.





## 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(Å <sup>2</sup> )	Q<0.9
5	GOL	B	469	6/6	0.86	0.15	37,39,39,40	0
5	GOL	A	469	6/6	0.88	0.12	27,30,32,33	0
5	GOL	B	470	6/6	0.88	0.25	23,31,34,38	0
4	EDO	B	468	4/4	0.93	0.15	29,30,30,31	0
5	GOL	B	471	6/6	0.94	0.08	26,28,29,31	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	CA	A	470	1/1	0.96	0.12	40,40,40,40	0
6	CA	B	472	1/1	0.96	0.15	36,36,36,36	0
4	EDO	A	468	4/4	0.98	0.08	13,18,19,22	0
3	SO4	B	467	5/5	0.98	0.07	23,27,29,30	0
3	SO4	A	467	5/5	0.98	0.09	37,38,40,41	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.