



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 08:59 AM BST

PDB ID : 4WGK  
Title : Crystal structure of human neutral ceramidase with Zn-bound phosphate  
Authors : Airola, M.V.; Pulkoski-Gross, M.J.; Obeid, L.M.; Hannun, Y.A.  
Deposited on : 2014-09-18  
Resolution : 2.58 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

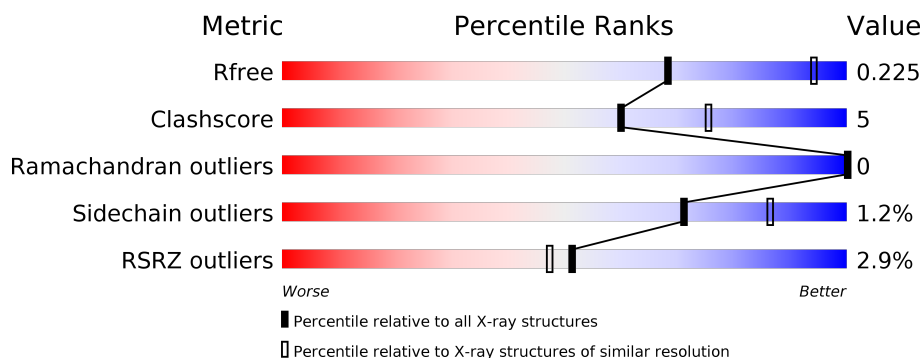
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.58 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	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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	688	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>11%</div> <div></div> </div> </div>
1	B	688	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div></div> </div> </div>
2	C	2	<div> <div>100%</div> </div>
2	E	2	<div> <div>100%</div> </div>
3	D	3	<div> <div>33%</div> <div>67%</div> </div>

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 11142 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 Neutral ceramidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	670	Total	C	N	O	S	0	1	0
			5197	3284	904	985	24			
1	B	672	Total	C	N	O	S	0	0	0
			5211	3292	906	989	24			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	781	HIS	-	expression tag	UNP Q9NR71
A	782	HIS	-	expression tag	UNP Q9NR71
A	783	HIS	-	expression tag	UNP Q9NR71
A	784	HIS	-	expression tag	UNP Q9NR71
A	785	HIS	-	expression tag	UNP Q9NR71
A	786	HIS	-	expression tag	UNP Q9NR71
B	781	HIS	-	expression tag	UNP Q9NR71
B	782	HIS	-	expression tag	UNP Q9NR71
B	783	HIS	-	expression tag	UNP Q9NR71
B	784	HIS	-	expression tag	UNP Q9NR71
B	785	HIS	-	expression tag	UNP Q9NR71
B	786	HIS	-	expression tag	UNP Q9NR71

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



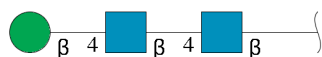
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

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

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



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

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

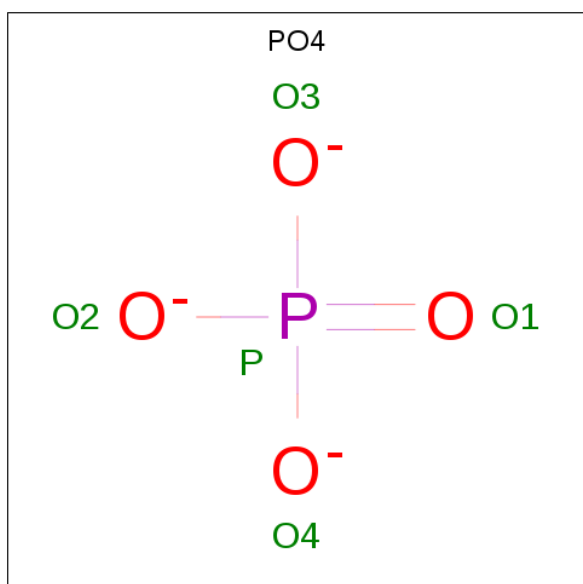
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Ca	0	0
			1	1		
5	A	1	Total	Ca	0	0
			1	1		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



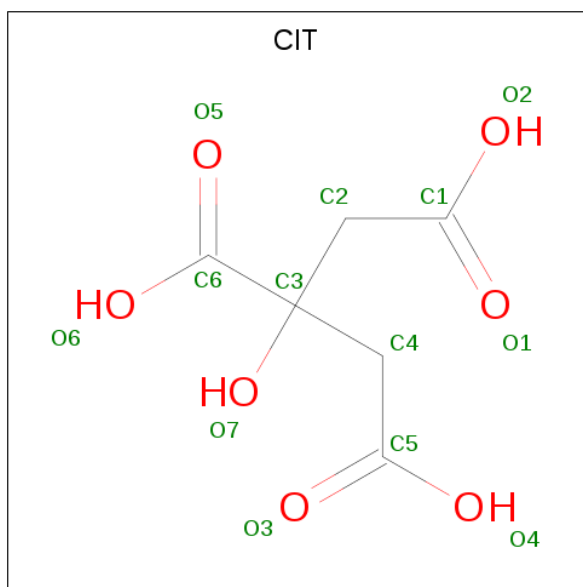
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O P 5 4 1	0	0
7	B	1	Total O P 5 4 1	0	0

- Molecule 8 is CITRIC ACID (three-letter code: CIT) (formula:  $C_6H_8O_7$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 13 6 7	0	0
8	A	1	Total C O 13 6 7	0	0
8	B	1	Total C O 13 6 7	0	0
8	B	1	Total C O 13 6 7	0	0

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula:  $Cl$ ).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Cl 1 1	0	0

- Molecule 10 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



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

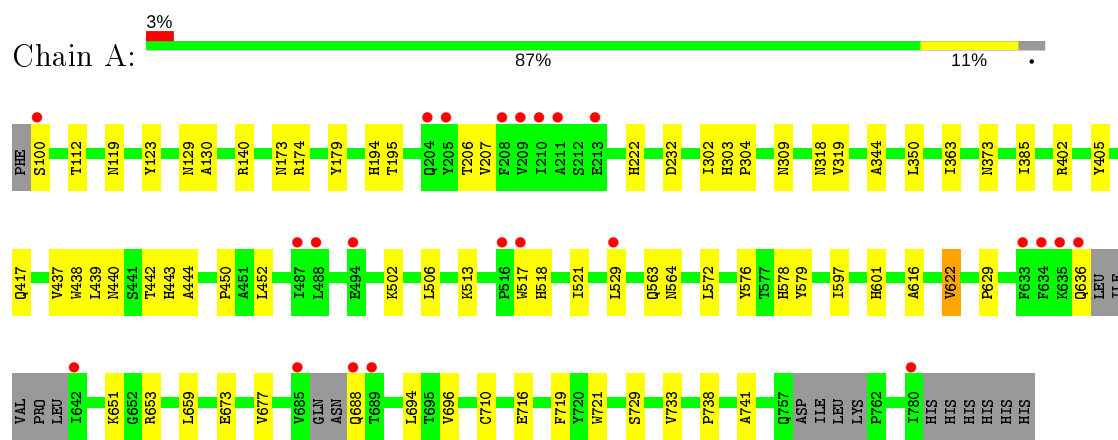
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	251	Total	O	0	0
			251	251		
11	B	243	Total	O	0	0
			243	243		

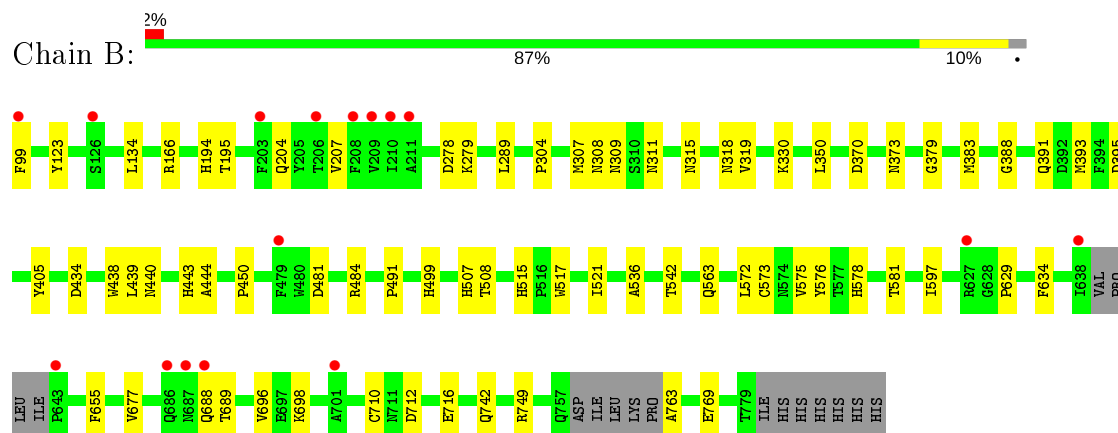
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

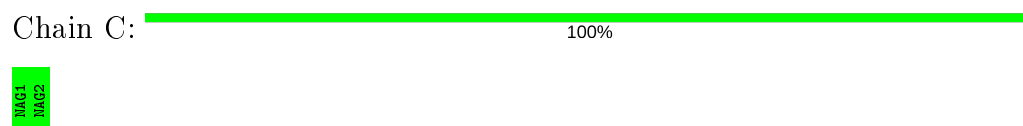
#### • Molecule 1: Neutral ceramidase



#### • Molecule 1: Neutral ceramidase




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





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



Chain E:  100%

MAG1  
MAG2

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

Chain D:  33%  67%

MAG1  
MAG2  
BOL3

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.48Å 156.63Å 80.33Å 90.00° 108.04° 90.00°	Depositor
Resolution (Å)	68.65 – 2.58 68.65 – 2.58	Depositor EDS
% Data completeness (in resolution range)	91.6 (68.65-2.58) 86.8 (68.65-2.58)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.77 (at 2.58Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.178 , 0.223 0.182 , 0.225	Depositor DCC
$R_{free}$ test set	1999 reflections (4.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.3	Xtriage
Anisotropy	0.552	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 48.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11142	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.02% 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, PO4, EDO, CIT, CA

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	0.22	0/5325	0.41	0/7232
1	B	0.22	0/5336	0.41	0/7247
All	All	0.22	0/10661	0.41	0/14479

There are no bond length outliers.

There are no bond angle outliers.

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	5197	0	5063	47	0
1	B	5211	0	5073	45	0
2	C	28	0	25	0	0
2	E	28	0	25	1	0
3	D	39	0	34	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	28	0	26	1	0
6	B	42	0	39	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	5	0	0	0	0
7	B	5	0	0	0	0
8	A	26	0	10	1	0
8	B	26	0	10	2	0
9	B	1	0	0	0	0
10	B	8	0	12	0	0
11	A	251	0	0	19	0
11	B	243	0	0	16	0
All	All	11142	0	10317	97	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 5.

All (97) 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:417:GLN:NE2	11:A:904:HOH:O	2.01	0.92
1:A:373:ASN:ND2	11:A:905:HOH:O	2.06	0.89
1:A:518:HIS:O	11:A:901:HOH:O	1.89	0.89
1:B:330:LYS:NZ	11:B:906:HOH:O	2.07	0.88
1:A:636:GLN:O	11:A:902:HOH:O	1.93	0.84
1:A:173:ASN:ND2	11:A:909:HOH:O	2.12	0.82
1:A:673:GLU:OE1	11:A:903:HOH:O	1.96	0.82
1:A:100:SER:N	11:A:910:HOH:O	2.13	0.81
1:B:395:ASP:OD2	11:B:902:HOH:O	2.00	0.80
1:B:508:THR:O	11:B:903:HOH:O	2.02	0.78
1:B:712:ASP:OD1	11:B:905:HOH:O	2.05	0.74
1:A:302:ILE:O	11:A:906:HOH:O	2.06	0.74
1:B:370:ASP:OD1	11:B:904:HOH:O	2.04	0.73
1:B:434:ASP:OD1	11:B:907:HOH:O	2.09	0.71
1:A:502:LYS:O	11:A:907:HOH:O	2.10	0.69
1:A:363:ILE:HD11	1:A:385:ILE:HD12	1.75	0.68
1:A:579:TYR:O	11:A:908:HOH:O	2.11	0.68
1:B:388:GLY:O	11:B:908:HOH:O	2.11	0.67
6:B:803:NAG:O4	11:B:901:HOH:O	1.81	0.65
1:A:651:LYS:O	11:A:911:HOH:O	2.15	0.64
1:B:688:GLN:O	1:B:689:THR:OG1	2.13	0.63
1:A:207:VAL:HG23	1:A:517:TRP:HB3	1.82	0.62
1:A:721:TRP:NE1	1:A:729:SER:OG	2.33	0.61
1:B:166:ARG:HD2	1:B:204:GLN:HB3	1.82	0.61
1:B:207:VAL:HG23	1:B:517:TRP:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:806:NAG:O7	11:B:909:HOH:O	2.16	0.60
1:B:373:ASN:ND2	11:B:914:HOH:O	2.22	0.60
1:B:440:ASN:HB2	1:B:443:HIS:HB3	1.82	0.60
8:A:811:CIT:O4	8:A:811:CIT:O7	2.17	0.59
1:A:513:LYS:NZ	11:A:921:HOH:O	2.28	0.58
1:B:749:ARG:NH2	1:B:769:GLU:OE1	2.36	0.58
1:A:440:ASN:HB2	1:A:443:HIS:HB3	1.86	0.57
1:A:440:ASN:HB2	1:A:443:HIS:H	1.69	0.57
1:B:194:HIS:HB2	1:B:572:LEU:HD13	1.87	0.56
1:B:536:ALA:O	11:B:910:HOH:O	2.17	0.56
2:E:1:NAG:O3	2:E:2:NAG:O7	2.20	0.56
1:B:481:ASP:OD1	1:B:484:ARG:NH2	2.39	0.55
1:B:438:TRP:CE3	1:B:444:ALA:HB2	2.42	0.54
1:A:112:THR:O	1:A:222[A]:HIS:ND1	2.40	0.54
1:A:440:ASN:HB3	1:A:442:THR:H	1.71	0.54
1:A:174:ARG:NH1	11:A:938:HOH:O	2.40	0.53
1:A:688:GLN:NE2	11:A:943:HOH:O	2.41	0.53
1:B:311:ASN:HB2	1:B:393:MET:HE2	1.90	0.53
1:A:179:TYR:OH	1:A:232:ASP:OD1	2.16	0.53
1:A:438:TRP:CE3	1:A:444:ALA:HB2	2.44	0.52
1:A:437:VAL:HG21	1:A:601:HIS:HB3	1.91	0.52
1:A:402:ARG:NH1	11:A:914:HOH:O	2.21	0.52
1:A:130:ALA:O	11:A:912:HOH:O	2.19	0.52
1:A:194:HIS:HB2	1:A:572:LEU:HD13	1.92	0.51
1:B:763:ALA:N	11:B:933:HOH:O	2.44	0.51
1:B:395:ASP:OD1	11:B:912:HOH:O	2.20	0.50
1:B:439:LEU:HD12	1:B:443:HIS:CD2	2.47	0.50
1:A:450:PRO:HA	1:A:597:ILE:O	2.13	0.49
1:A:738:PRO:HG2	1:A:741:ALA:HB2	1.94	0.49
1:B:307:MET:HA	1:B:393:MET:HE3	1.96	0.48
1:B:450:PRO:HA	1:B:597:ILE:O	2.13	0.48
1:B:542:THR:HG21	1:B:581:THR:HG22	1.96	0.47
1:B:278:ASP:HA	8:B:810:CIT:O7	2.15	0.47
1:A:119:ASN:HA	1:A:129:ASN:HA	1.97	0.47
1:A:564:ASN:ND2	11:A:948:HOH:O	2.43	0.46
1:A:576:TYR:CZ	1:A:578:HIS:HA	2.50	0.46
1:B:391:GLN:HG2	11:B:902:HOH:O	2.14	0.46
1:A:696:VAL:HB	1:A:710:CYS:HB2	1.98	0.46
1:B:279:LYS:HB2	8:B:810:CIT:H22	1.96	0.46
1:B:696:VAL:HB	1:B:710:CYS:HB2	1.97	0.46
1:A:694:LEU:HD22	1:A:733:VAL:HG13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:805:NAG:O6	11:A:913:HOH:O	2.20	0.46
1:A:123:TYR:CG	1:A:309:ASN:HB3	2.52	0.45
1:B:308:ASN:HB2	11:B:1004:HOH:O	2.16	0.45
1:B:576:TYR:CZ	1:B:578:HIS:HA	2.51	0.45
1:B:99:PHE:CZ	1:B:289:LEU:HD21	2.51	0.45
1:A:439:LEU:HD12	1:A:443:HIS:CD2	2.51	0.44
1:B:573:CYS:O	1:B:575:VAL:N	2.44	0.44
1:A:140:ARG:HD2	1:A:344:ALA:HB2	2.00	0.44
1:B:311:ASN:HB2	1:B:393:MET:CE	2.48	0.44
1:A:741:ALA:O	11:A:915:HOH:O	2.21	0.44
1:B:195:THR:HA	1:B:304:PRO:HB2	2.00	0.43
1:B:491:PRO:HG3	1:B:507:HIS:CD2	2.54	0.43
1:B:499:HIS:HE1	1:B:597:ILE:O	2.00	0.43
1:A:452:LEU:HD12	1:A:506:LEU:HD12	2.01	0.43
1:B:515:HIS:CE1	1:B:634:PHE:HB3	2.54	0.43
1:A:195:THR:HA	1:A:304:PRO:HB2	2.00	0.42
1:A:694:LEU:HD23	1:A:719:PHE:HB2	2.01	0.42
1:B:521:ILE:HD12	1:B:629:PRO:HG2	2.01	0.42
1:A:439:LEU:HB2	1:A:443:HIS:HD2	1.85	0.42
1:A:206:THR:HB	1:A:517:TRP:HA	2.01	0.42
1:A:318:ASN:OD1	1:A:319:VAL:N	2.53	0.42
1:B:318:ASN:OD1	1:B:319:VAL:N	2.52	0.42
1:B:655:PHE:HA	1:B:677:VAL:HG22	2.02	0.41
1:B:134:LEU:HB3	1:B:315:ASN:HB3	2.03	0.41
1:A:521:ILE:HD12	1:A:629:PRO:HG2	2.02	0.41
1:A:616:ALA:HB1	1:A:622:VAL:HA	2.02	0.41
1:A:440:ASN:HB2	1:A:443:HIS:N	2.35	0.41
1:B:698:LYS:HE3	1:B:742:GLN:HG3	2.03	0.41
1:B:379:GLY:HA3	1:B:383:MET:HG3	2.03	0.41
1:B:563:GLN:NE2	11:B:952:HOH:O	2.54	0.40
1:B:123:TYR:CG	1:B:309:ASN:HB3	2.57	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	663/688 (96%)	651 (98%)	12 (2%)	0	100	100
1	B	666/688 (97%)	653 (98%)	13 (2%)	0	100	100
All	All	1329/1376 (97%)	1304 (98%)	25 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	563/580 (97%)	553 (98%)	10 (2%)	59	78
1	B	564/580 (97%)	561 (100%)	3 (0%)	88	96
All	All	1127/1160 (97%)	1114 (99%)	13 (1%)	71	86

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	303	HIS
1	A	350	LEU
1	A	405	TYR
1	A	529	LEU
1	A	563	GLN
1	A	622	VAL
1	A	653	ARG
1	A	659	LEU
1	A	677	VAL
1	A	716	GLU
1	B	350	LEU
1	B	405	TYR
1	B	716	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	HIS
1	A	443	HIS
1	A	688	GLN
1	B	443	HIS
1	B	563	GLN

### 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 ⓘ

7 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	0.33	0	17,19,21	0.60	0
2	NAG	C	2	2	14,14,15	0.31	0	17,19,21	0.39	0
3	NAG	D	1	1,3	14,14,15	0.30	0	17,19,21	0.38	0
3	NAG	D	2	3	14,14,15	0.60	1 (7%)	17,19,21	0.61	0
3	BMA	D	3	3	11,11,12	1.49	2 (18%)	15,15,17	1.81	4 (26%)
2	NAG	E	1	1,2	14,14,15	0.27	0	17,19,21	0.63	0
2	NAG	E	2	2	14,14,15	0.26	0	17,19,21	0.44	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
2	NAG	C	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	BMA	D	3	3	-	2/2/19/22	0/1/1/1
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3	BMA	C1-C2	3.62	1.60	1.52
3	D	3	BMA	C2-C3	3.01	1.56	1.52
3	D	2	NAG	O5-C1	-2.09	1.40	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3	BMA	C1-C2-C3	4.41	115.08	109.67
3	D	3	BMA	O5-C1-C2	2.78	115.06	110.77
3	D	3	BMA	O5-C5-C4	-2.34	105.13	110.83
3	D	3	BMA	C2-C3-C4	2.17	114.65	110.89

There are no chirality outliers.

All (12) torsion outliers are listed below:

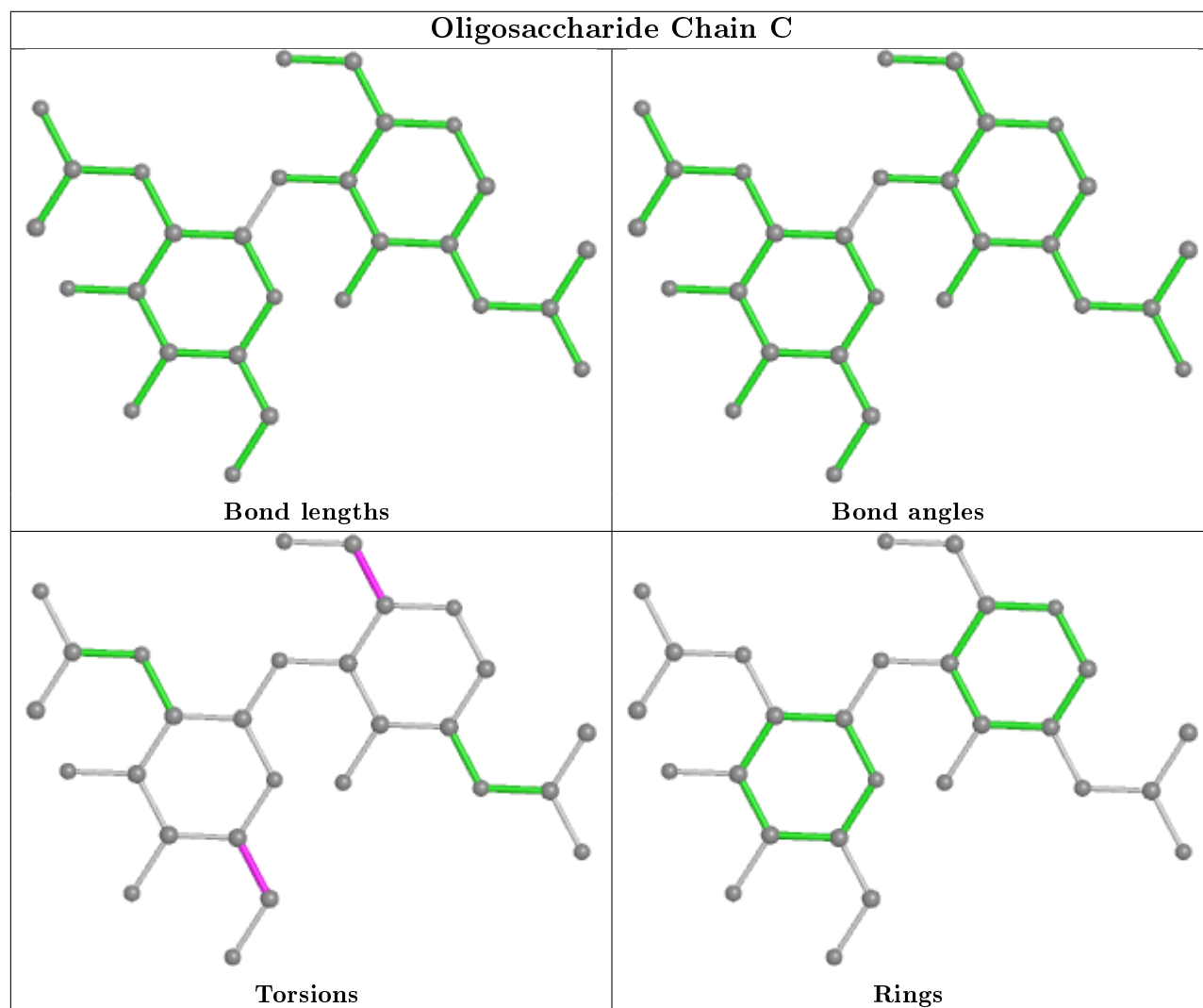
Mol	Chain	Res	Type	Atoms
2	C	1	NAG	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	D	3	BMA	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
3	D	3	BMA	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6

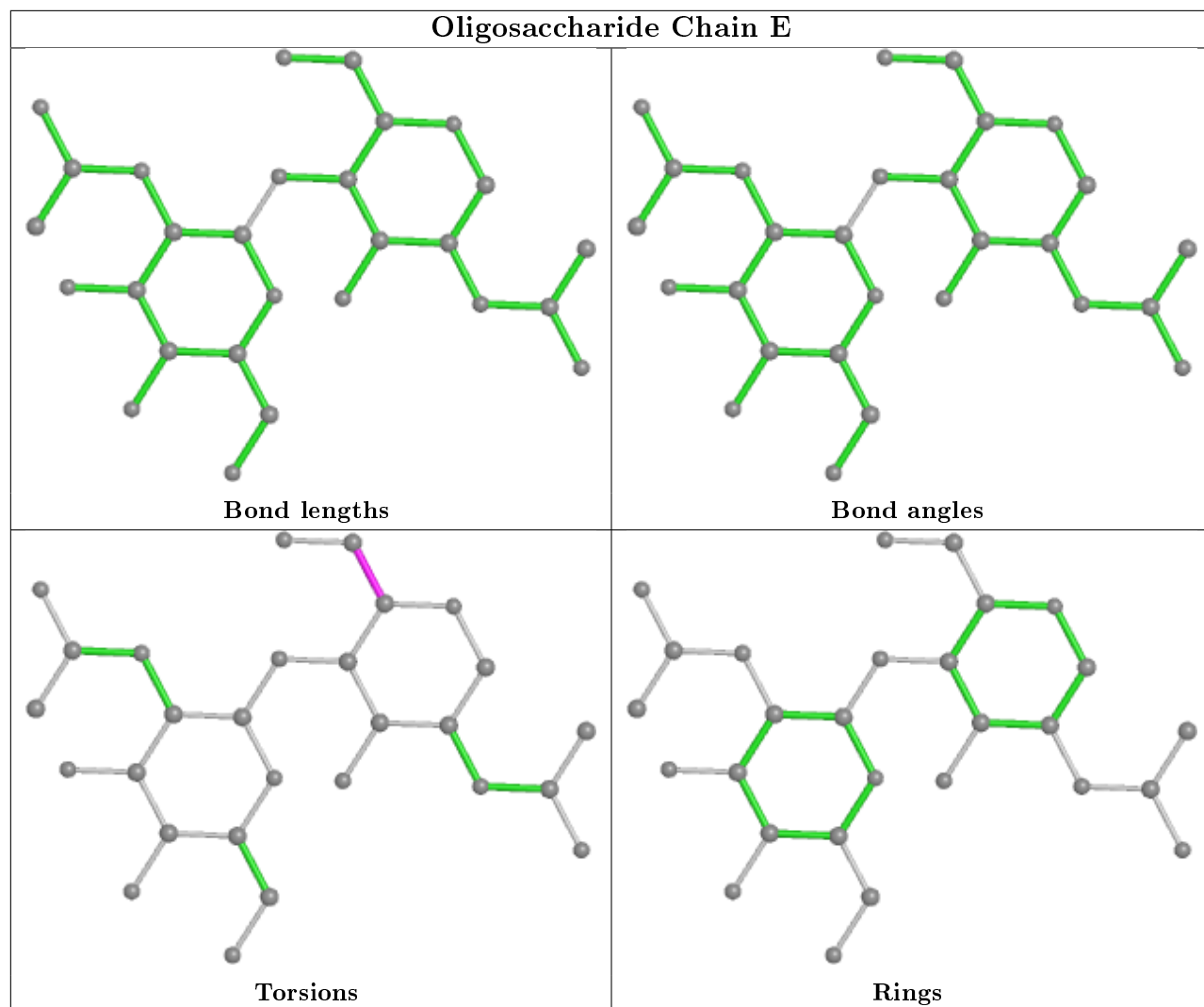
There are no ring outliers.

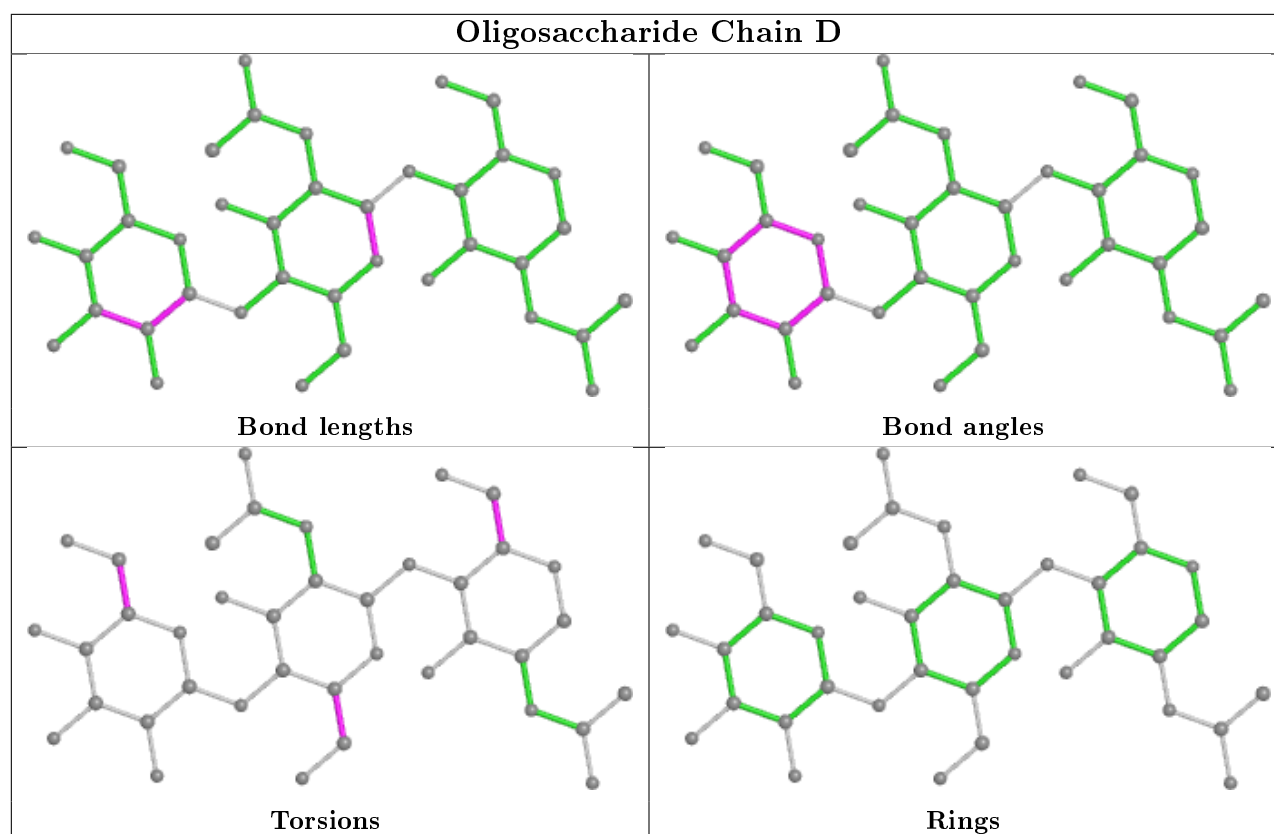
2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	NAG	1	0
2	E	1	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 18 ligands modelled in this entry, 5 are monoatomic - leaving 13 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	$\# Z  > 2$
6	NAG	B	807	1	14,14,15	0.25	0	17,19,21	0.43	0
8	CIT	B	810	-	3,12,12	1.19	0	3,17,17	2.20	1 (33%)
10	EDO	B	813	-	3,3,3	0.44	0	2,2,2	0.39	0
7	PO4	B	808	4	4,4,4	0.92	0	6,6,6	0.39	0
6	NAG	B	806	1	14,14,15	0.27	0	17,19,21	0.41	0
6	NAG	A	806	1	14,14,15	0.27	0	17,19,21	0.44	0
8	CIT	B	811	-	3,12,12	1.33	0	3,17,17	2.37	1 (33%)
8	CIT	A	811	-	3,12,12	1.31	0	3,17,17	1.48	1 (33%)
10	EDO	B	812	-	3,3,3	0.45	0	2,2,2	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	B	803	1	14,14,15	0.23	0	17,19,21	0.40	0
6	NAG	A	805	1	14,14,15	0.29	0	17,19,21	0.38	0
7	PO4	A	810	4	4,4,4	0.91	0	6,6,6	0.43	0
8	CIT	A	812	-	3,12,12	1.24	0	3,17,17	1.42	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
6	NAG	B	807	1	-	2/6/23/26	0/1/1/1
10	EDO	B	813	-	-	0/1/1/1	-
6	NAG	B	806	1	-	2/6/23/26	0/1/1/1
6	NAG	A	806	1	-	2/6/23/26	0/1/1/1
8	CIT	B	811	-	-	5/6/16/16	-
8	CIT	A	811	-	-	3/6/16/16	-
10	EDO	B	812	-	-	0/1/1/1	-
6	NAG	B	803	1	-	2/6/23/26	0/1/1/1
6	NAG	A	805	1	-	2/6/23/26	0/1/1/1
8	CIT	B	810	-	-	6/6/16/16	-
8	CIT	A	812	-	-	4/6/16/16	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	811	CIT	C3-C4-C5	-3.86	108.81	114.98
8	B	810	CIT	C3-C4-C5	-3.15	109.93	114.98
8	A	811	CIT	C3-C4-C5	-2.50	110.98	114.98

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	810	CIT	C1-C2-C3-O7
8	B	810	CIT	C1-C2-C3-C4
8	B	810	CIT	C1-C2-C3-C6
8	B	811	CIT	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
8	B	811	CIT	O7-C3-C4-C5
8	B	811	CIT	C6-C3-C4-C5
8	A	811	CIT	C2-C3-C4-C5
8	A	811	CIT	O7-C3-C4-C5
8	A	811	CIT	C6-C3-C4-C5
8	A	812	CIT	C1-C2-C3-O7
8	A	812	CIT	C1-C2-C3-C4
8	A	812	CIT	C1-C2-C3-C6
6	B	806	NAG	O5-C5-C6-O6
6	A	806	NAG	O5-C5-C6-O6
6	B	807	NAG	O5-C5-C6-O6
6	B	806	NAG	C4-C5-C6-O6
6	A	805	NAG	C4-C5-C6-O6
6	B	803	NAG	C4-C5-C6-O6
6	A	806	NAG	C4-C5-C6-O6
6	B	807	NAG	C4-C5-C6-O6
6	B	803	NAG	O5-C5-C6-O6
8	B	810	CIT	C2-C3-C4-C5
6	A	805	NAG	O5-C5-C6-O6
8	B	810	CIT	O7-C3-C4-C5
8	B	810	CIT	C6-C3-C4-C5
8	B	811	CIT	C1-C2-C3-C6
8	A	812	CIT	O7-C3-C4-C5
8	B	811	CIT	C1-C2-C3-O7

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	810	CIT	2	0
6	B	806	NAG	1	0
8	A	811	CIT	1	0
6	B	803	NAG	1	0
6	A	805	NAG	1	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 ⓘ

### 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	670/688 (97%)	0.22	23 (3%) 45 41	13, 26, 63, 90	0
1	B	672/688 (97%)	0.20	16 (2%) 59 55	13, 26, 62, 88	0
All	All	1342/1376 (97%)	0.21	39 (2%) 51 47	13, 26, 62, 90	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	209	VAL	3.7
1	A	642	ILE	3.5
1	A	688	GLN	3.5
1	B	686	GLN	3.5
1	A	685	VAL	3.4
1	B	687	ASN	3.4
1	A	633	PHE	3.1
1	B	210	ILE	3.0
1	B	211	ALA	3.0
1	A	209	VAL	2.9
1	A	487	ILE	2.9
1	B	688	GLN	2.9
1	A	635	LYS	2.9
1	A	689	THR	2.9
1	A	205	TYR	2.9
1	B	99	PHE	2.7
1	A	100	SER	2.7
1	B	126	SER	2.6
1	A	213	GLU	2.6
1	A	208	PHE	2.5
1	B	208	PHE	2.5
1	A	636	GLN	2.4
1	B	627	ARG	2.4
1	B	638	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	204	GLN	2.3
1	A	516	PRO	2.2
1	B	479	PHE	2.2
1	A	488	LEU	2.2
1	A	211	ALA	2.2
1	A	210	ILE	2.2
1	B	203	PHE	2.1
1	B	206	THR	2.1
1	B	643	PRO	2.1
1	A	529	LEU	2.1
1	A	634	PHE	2.1
1	A	494	GLU	2.1
1	A	517	TRP	2.1
1	B	701	ALA	2.0
1	A	780	ILE	2.0

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

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

## 6.3 Carbohydrates ⓘ

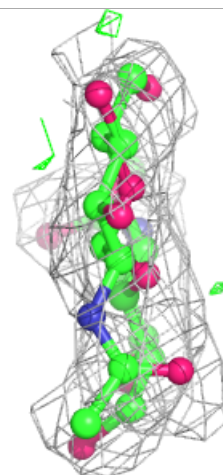
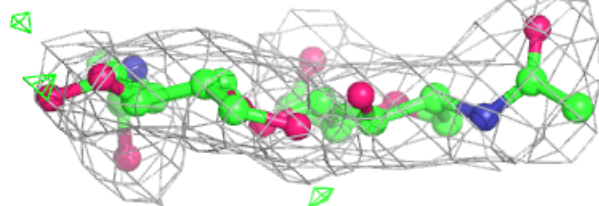
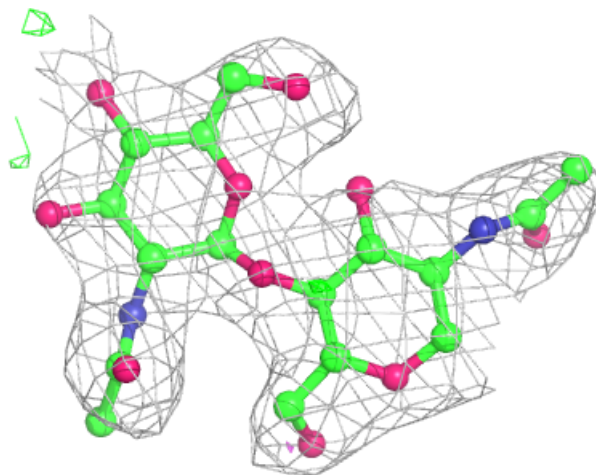
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<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
3	BMA	D	3	11/12	0.73	0.22	75,80,104,104	0
3	NAG	D	2	14/15	0.78	0.21	39,55,68,77	0
2	NAG	E	2	14/15	0.85	0.22	37,58,61,65	0
2	NAG	C	2	14/15	0.91	0.26	41,47,51,53	0
2	NAG	C	1	14/15	0.94	0.15	31,42,46,48	0
3	NAG	D	1	14/15	0.94	0.15	21,31,35,41	0
2	NAG	E	1	14/15	0.95	0.18	30,35,44,49	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.

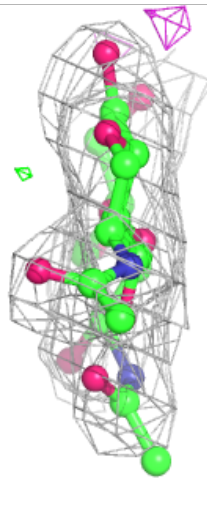
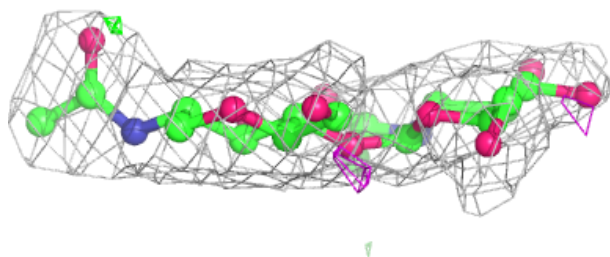
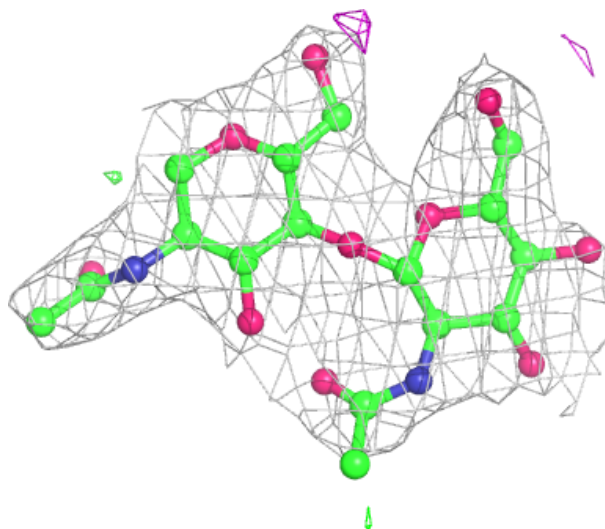
**Electron density around Chain C:**

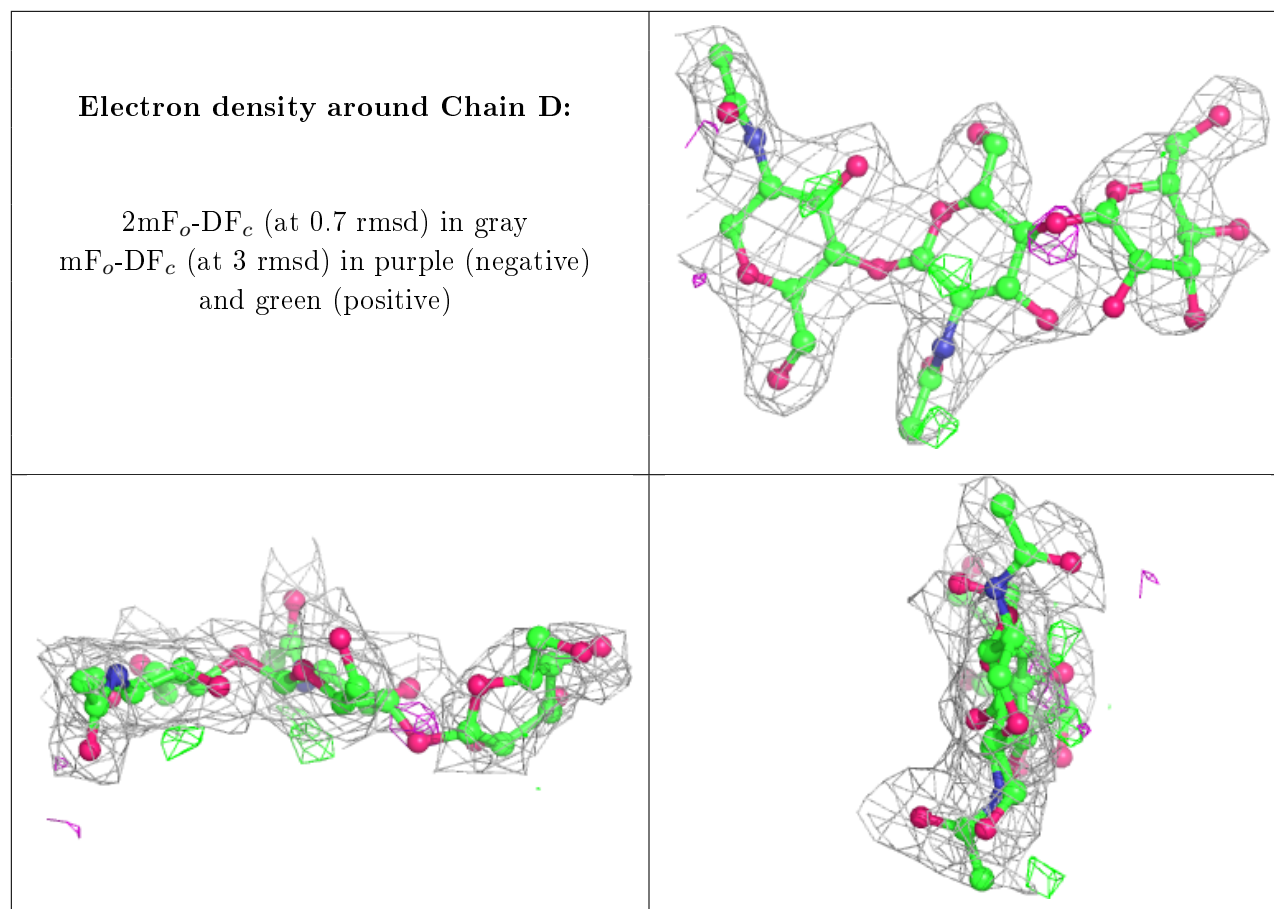
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain E:**

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





## 6.4 Ligands ⓘ

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
6	NAG	A	805	14/15	0.76	0.25	50,59,68,70	0
8	CIT	B	811	13/13	0.77	0.33	73,81,90,91	0
6	NAG	B	807	14/15	0.80	0.30	62,68,70,70	0
6	NAG	B	806	14/15	0.82	0.24	47,62,65,68	0
6	NAG	A	806	14/15	0.83	0.21	51,59,62,62	0
8	CIT	A	812	13/13	0.84	0.33	59,72,79,82	0
8	CIT	A	811	13/13	0.87	0.28	43,59,66,67	0
10	EDO	B	812	4/4	0.90	0.23	27,30,37,42	0
5	CA	B	802	1/1	0.91	0.07	74,74,74,74	0
8	CIT	B	810	13/13	0.92	0.17	25,34,38,41	0
5	CA	A	802	1/1	0.93	0.10	68,68,68,68	0
6	NAG	B	803	14/15	0.94	0.14	14,24,37,38	0
9	CL	B	809	1/1	0.94	0.11	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
10	EDO	B	813	4/4	0.95	0.21	36,38,43,46	0
7	PO4	B	808	5/5	0.96	0.17	25,35,37,37	0
4	ZN	B	801	1/1	0.99	0.13	28,28,28,28	0
7	PO4	A	810	5/5	0.99	0.15	35,35,39,42	0
4	ZN	A	801	1/1	1.00	0.09	21,21,21,21	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.